Supplementary Information

Asymmetric Büchner reaction and arene cyclopropanation via copper-catalyzed controllable cyclization of diynes

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1. General Information

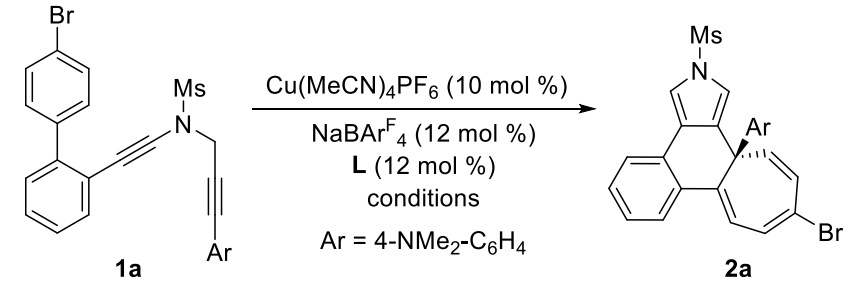
Ethyl acetate (ACS grade), hexanes (ACS grade), anhydrous 1,2-dichloroethane (ACS grade) and toluene (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

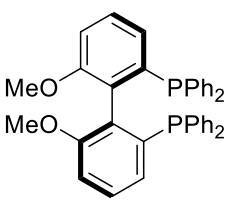
^{1}H NMR spectra and ^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer or a Bruker AV-500 or a Bruker AV-600 spectrometer in chloroform-d_3. For ^{1}H NMR spectra, chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. For ^{13}C NMR spectra, chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or unresolved, coupling constant(s) in Hz, integration).

Enantiomeric excesses (ee) were determined by an UltiMate 3000 chiral HPLC. The chiral columns used for the determination of enantiomeric excesses by chiral HPLC were Chiralpak columns (IA, IB, IC, IE, IG, AD-H). The particle size is 5 μm and dimensions is 4.6 mm I.D * 250 mm L.

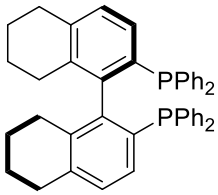
2. More Reaction Conditions, Scope and Mechanism Studies

Table S1. Optimization of reaction conditions for asymmetric Büchner reaction of *N*-propargyl ynamide **1a**.[a]

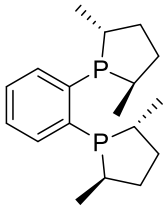




L13



L14



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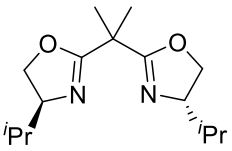

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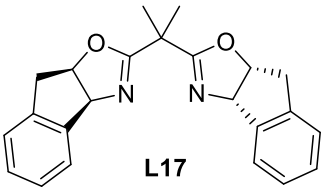

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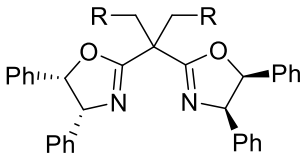
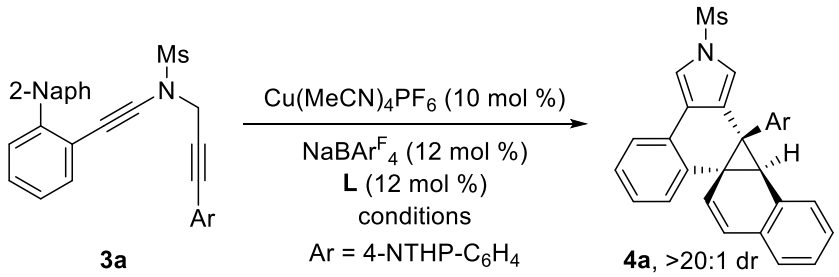


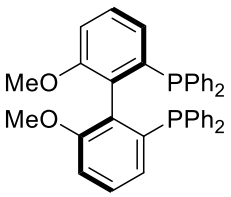
L18, R = 4-F-C_6H_4
L19, R = 2-Me-C_6H_4
L20, R = 3,5-F_2-C_6H_3
L21, R = 2-F-C_6H_4
L22, R = C_6Me_5

entry	L	conditions	yield (%)[b]	ee (%)[c]
1	**L12**	DCM, 35 °C, 0.5 h	66	15
2	**L13**	DCM, 35 °C, 0.5 h	93	18
3	**L14**	DCM, 35 °C, 3 h	91	29
4	**L15**	DCM, 35 °C, 1 h	27	17
5	**L16**	DCM, 35 °C, 0.5 h	72	<5
6	**L17**	DCM, 35 °C, 0.5 h	54	<5
7	**L18**	DCM, 35 °C, 0.5 h	57	22
8	**L19**	DCM, 35 °C, 1 h	69	29
9	**L20**	DCM, 35 °C, 0.5 h	78	12
10	**L21**	DCM, 35 °C, 0.5 h	81	41
11	**L22**	DCM, 35 °C, 0.5 h	90	63
12	**L12**	$CHCl_3$, 35 °C, 0.5 h	75	43
13	**L12**	PhCl, 35 °C, 0.5 h	71	72
14	**L12**	$PhCF_3$, 35 °C, 0.5 h	62	75
15	**L12**	*o*-xylene, 35 °C, 0.5 h	69	78

[a]Reaction conditions: **2a** (0.05 mmol), $Cu(MeCN)_4PF_6$ (0.005 mmol), **L** (0.006 mmol), $NaBAr^F_4$ (0.006 mmol), DCM (1 mL), 35 °C, in Schlenk tubes. [b]Measured by ^1H NMR using diethyl phthalate as internal standard. [c]Determined by HPLC analysis.

Table S2. Optimization of reaction conditions for asymmetric arene cyclopropanation reaction of *N*-propargyl ynamide **3a**.[a]





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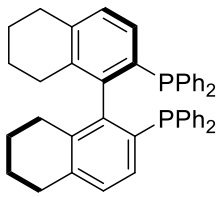

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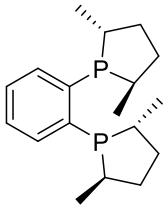

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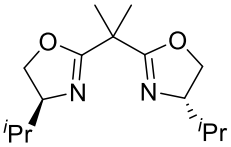

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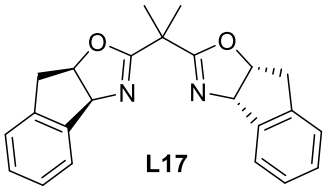

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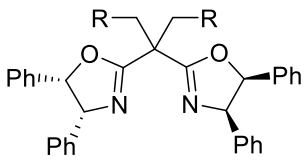


L18, R = 4-F-C_6H_4
L19, R = 2-Me-C_6H_4
L20, R = 3,5-F_2-C_6H_3
L23, R = 4-Me-C_6H_4
L24, R = 3,5-$(O^nPr)_2$-C_6H_3

entry	L	conditions	yield (%)[b]	ee (%)[c]
1	**L8**	DCM, 35 °C, 0.5 h	78	90
2	**L13**	DCM, 35 °C, 0.5 h	57	20
3	**L14**	DCM, 35 °C, 0.5 h	69	68
4	**L15**	DCM, 35 °C, 0.5 h	54	<5
5	**L16**	DCM, 35 °C, 0.5 h	51	<5
6	**L17**	DCM, 35 °C, 0.5 h	39	38
7	**L18**	DCM, 35 °C, 0.5 h	48	92
8	**L19**	DCM, 35 °C, 0.5 h	69	89
9	**L20**	DCM, 35 °C, 0.5 h	79	91
10	**L23**	DCM, 35 °C, 0.5 h	72	91
11	**L24**	DCM, 35 °C, 0.5 h	84	91
12	**L12**	DCE, 35 °C, 0.5 h	51	82
13	**L12**	$CHCl_3$, 35 °C, 0.5 h	79	91
14	**L12**	PhCl, 35 °C, 0.5 h	54	78
15	**L12**	*o*-xylene, 35 °C, 0.5 h	81	92

[a]Reaction conditions: **4a** (0.05 mmol), $Cu(MeCN)_4PF_6$ (0.005 mmol), **L** (0.006 mmol), $NaBAr^F_4$ (0.006 mmol), DCM (1 mL), 35 °C, in Schlenk tubes. [b]Measured by ^1H NMR using diethyl phthalate as internal standard. [c]Determined by HPLC analysis.

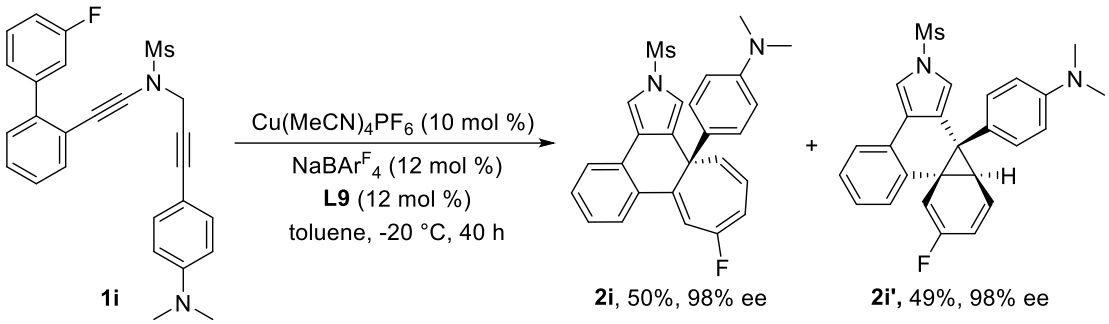


Fig. S1. The use of diyne **1i** possessing a *meta*-fluoro-substituent at the biaryl moiety led to the desired Büchner reaction product **2i** (50%, 98% ee) and arene cyclopropanation product **2i′** (49%, 98% ee), respectively.

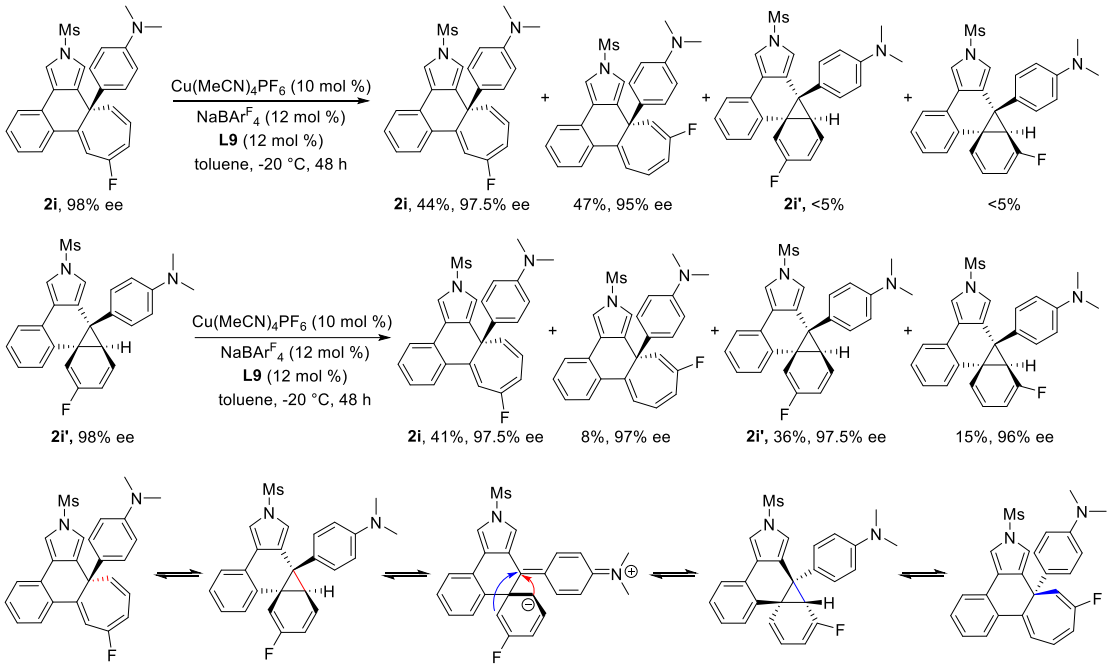


Fig. S2. Control experiments showed that the conversion of seven-membered Büchner cyclization product **2i** into arene cyclopropanation product **2i′** was very slowly (<5%, 48 h) under the standard reaction conditions, while the conversion of **2i′** into **2i** was relatively fast (41%, 48 h) under the standard conditions, and the enantioselectivity was almost maintained during this process. In particular, the formation of the corresponding regioisomers of **2i** and **2i′** could be observed in this *meta*-fluoro-substituted diyne substrate probably due to the above process.

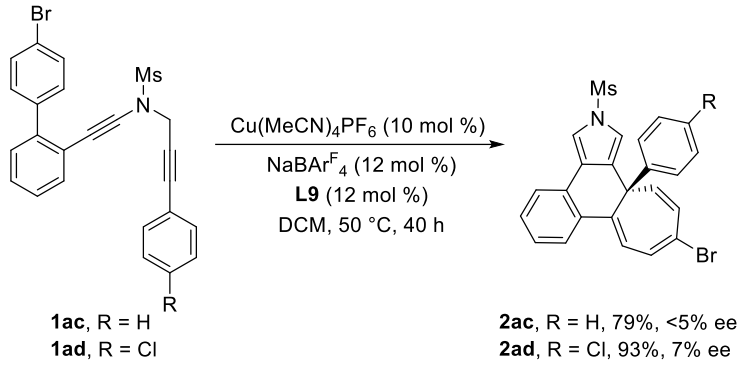


Fig. S3. Our attempts to extend the reaction to diynes with non-electron-rich groups **1ac** and **1ad** only led to low enantioselectivities (<10% ee).

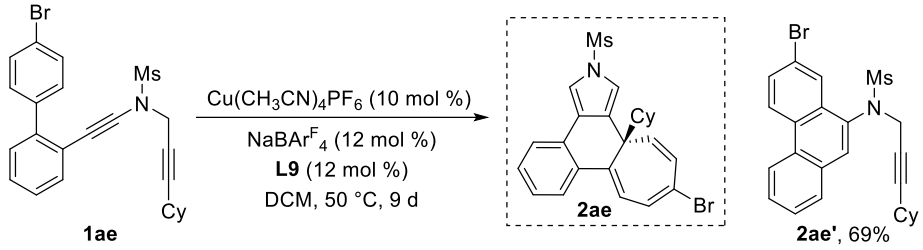


Fig. S4. Our attempts to extend the reaction to Cy-substituted diyne **1ae** failed to obtain the corresponding Büchner product, and instead a hydroarylation product was isolated in 69% yield.

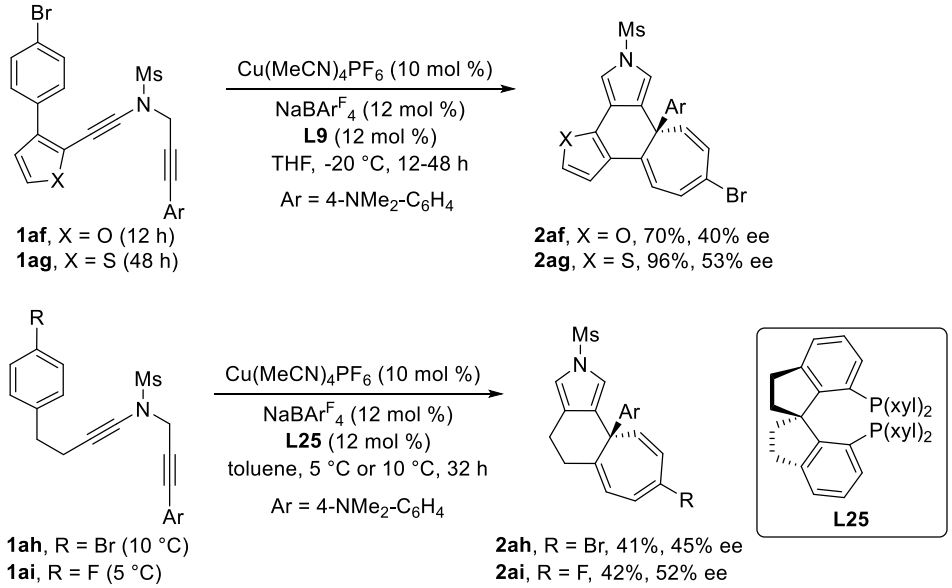


Fig. S5. The reaction proceeded smoothly with the heteroatomic diynes **1af**–**1ag** and the alkyl-linked aryl diynes **1ah**–**1ai**, but only gave the desired cycloheptatrienes **2af**–**2ai** with moderate enantioselectivities (40–53% ees) under the optimized conditions.

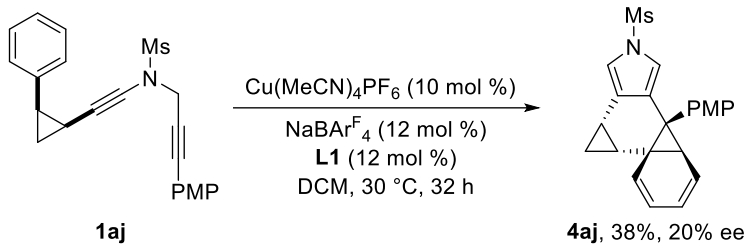


Fig. S6. Attempts to extend the reaction to the cyclopropyl-linked aryl diyne **1aj** only led to the formation of the corresponding cyclopropane **4aj** in 38% yield with 20% ee.

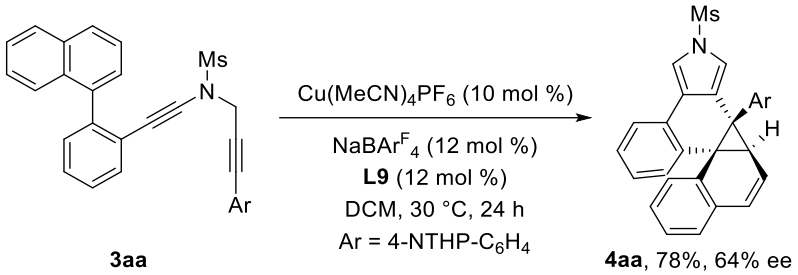


Fig. S7. Our attempts to extend the reaction to the 1-naphthyl diyne **3aa** only led to the corresponding cyclopropane product **4aa** with moderate enantioselectivity (64% ee).

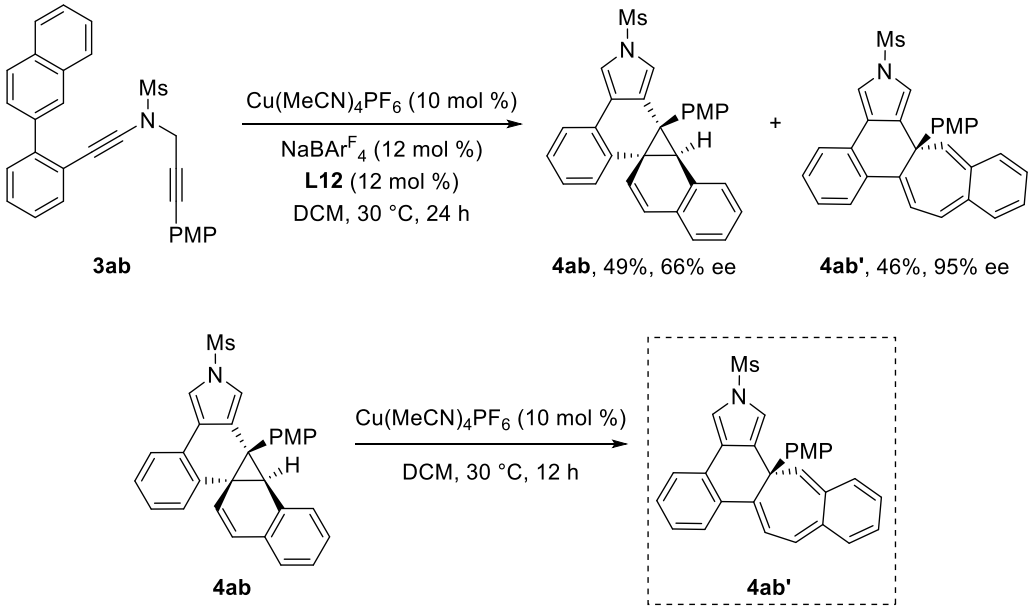


Fig. S8. The reaction of PMP-substituted 2-naphthyl diyne **3ab** only led to a mixture of cyclopropanation product **4ab** (49%, 66% ee) and Büchner product **4ab′** (46%, 95% ee). Of note, **4ab** could not be further converted into **4ab′**.

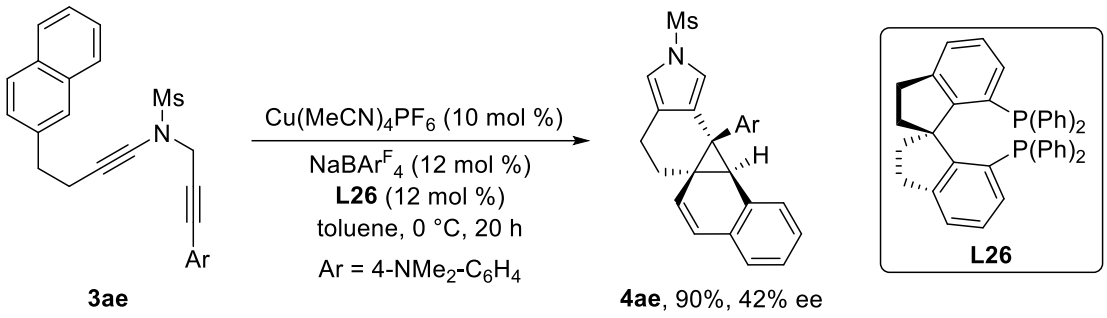
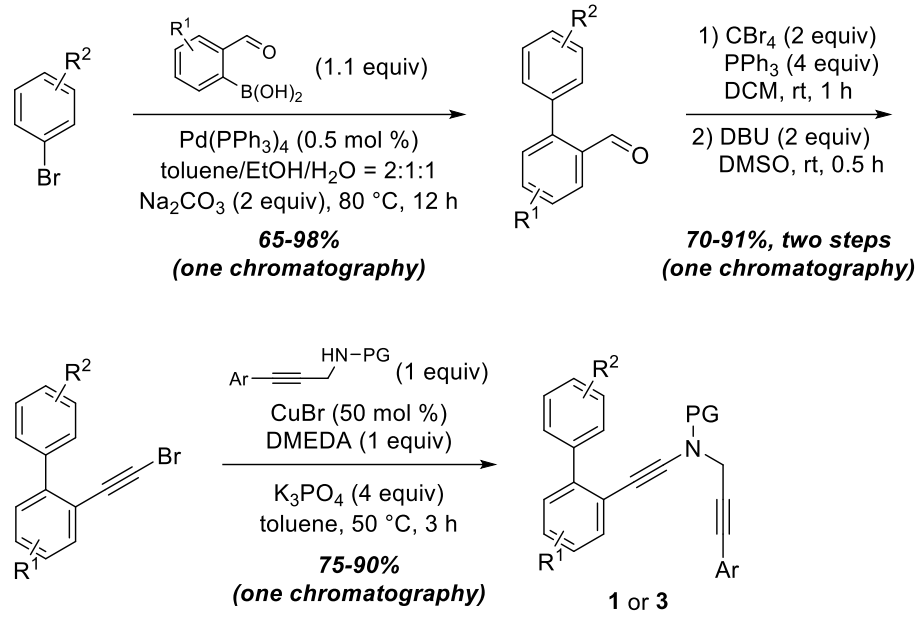


Fig. S9. The use of the alkyl-linked naphthyl-diyne **3ae** only led to the desired benzonorcaradiene **4ae** (90%) with 42% ee under the optimized reaction conditions.

3. Preparation of Starting Materials

3.1. General Procedure S1 for Synthesis of *N*-propargyl Ynamides 1 and 3[1]



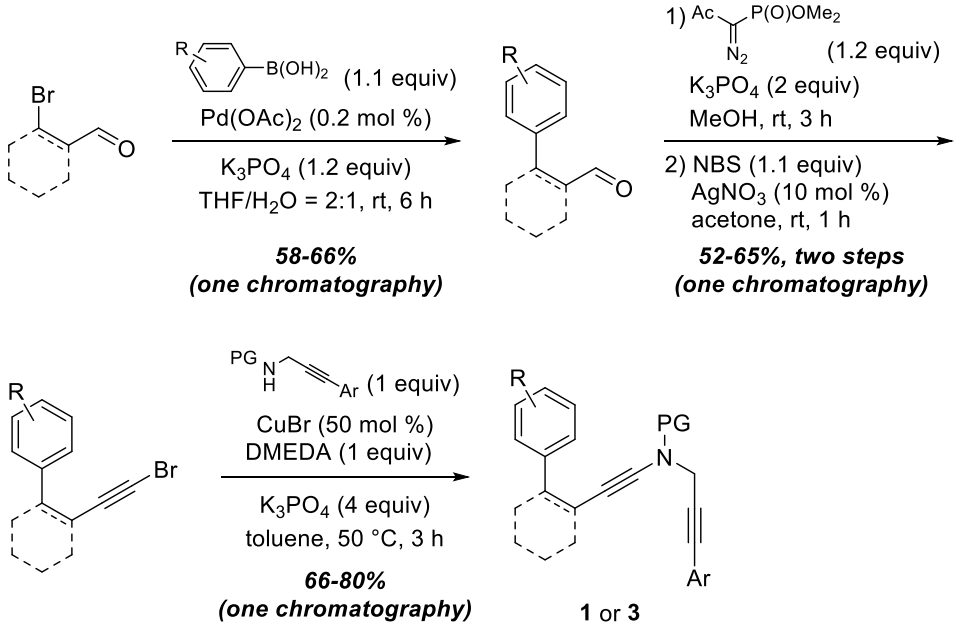
To a solution of substituted bromobenzene (10 mmol) in toluene (40 mL), EtOH (20 mL) and H_2O (20 mL) were added substituted 2-formylbenzeneboronic acid (11 mmol), Na_2CO_3 (20 mmol, 2.12 g) and $Pd(PPh_3)_4$ (0.05 mmol, 57.8 mg) at room temperature. The reaction mixture was stirred at 80 °C for 12 h. Upon completion (monitored by TLC), the reaction was filtered, extracted with ethyl acetate for three times, dried over $MgSO_4$ and filtered. The filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (eluent: PE/EtOAc) to afford the desired biaryl aldehyde (65–98% yield).

Corey-Fuchs reaction was applied in the next step as follows: To a solution of PPh_3 (26 mmol, 6.82 g) in DCM (20 mL) was added CBr_4 (13 mmol, 3.98 g) carefully at 0 °C, and the reaction was stirred at this temperature for 0.5 h. Then the solution of the above biaryl aldehyde (6.5 mmol) in DCM (10 mL) was added slowly at 0 °C. The reaction was warmed to room temperature and stirred for additional 0.5 h. Upon completion (monitored by TLC), the reaction mixture was diluted with petroleum ether (150 mL), filtered through a Celite pad, and washed with petroleum ether for three times. The filtrate was concentrated under reduced pressure and directly used in the next step

without further purification. To a solution of dibromide derivative (6.5 mmol) in DCM (20 mL) was added DBU (13 mmol, 2 mL) and the reaction was stirred at room temperature for 30 min. Upon completion (monitored by TLC), the reaction mixture was diluted with water, extracted with ethyl acetate for three times, dried over $MgSO_4$, and filtered. The filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (eluent: PE) to afford the alkynyl bromide (70%–91% yield, two steps).

To a solution of the above alkynyl bromide (1 mmol) in toluene (5 mL) were added copper bromide (0.5 mmol, 72.0 mg), DMEDA (1 mmol, 100.0 mg), K_3PO_4 (4 mmol, 0.85 g), and protected propargylamide derivative (1 mmol)[1]. The reaction was stirred at 50 °C for 3 h. Upon completion (monitored by TLC), the solution was filtered and concentrated under reduced pressure. The residue was purified by chromatography on silica gel (eluent: PE/EtOAc) to give the desired ynamide **1** or **3** (75–90% yield).

3.2. General Procedure S2 for Synthesis of *N*-propargyl Ynamides 1ab, 1ac, 1ah-1aj, 3z and 3ae



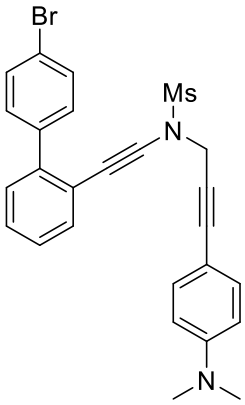
To a solution of 2-bromo-1-cyclohexene-1-carboxaldehyde (10 mmol) in THF (20 mL) and H_2O (10 mL) were added boronic acid derivative (11 mmol), K_3PO_4 (12 mmol, 2.54 g), and $Pd(OAc)_2$ (0.2 mmol, 4.5 mg) at room temperature and the reaction mixture

was stirred at room temperature for 6 h. Upon completion (monitored by TLC), the reaction was diluted with water (40 mL), extracted with ethyl acetate for three times, dried over $MgSO_4$ and filtered. The filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (eluent: PE/EtOAc) to afford the desired aldehyde (58–66% yield).

To a solution of above product (6 mmol) in MeOH (20 mL) were added K_3PO_4 (7.3 mmol, 1.69 g) and Ohira-Bestmann reagent (7 mmol, 1.4 mL). The mixture was stirred at room temperature for 3 h. Upon completion (monitored by TLC), the reaction was filtered through a Celite pad, extracted with EtOAc for three times, dried over $MgSO_4$ and filtered. The resulting mixture was concentrated under reduced pressure to give crude alkyne without further purification. To a solution of the above alkyne in acetone (20 mL) were added NBS (6.6 mmol, 2.33 g) and $AgNO_3$ (0.3 mmol, 0.11 g) at 0 ºC and stirred at room temperature for 1 h. Upon completion (monitored by TLC), the reaction mixture was filtered through a Celite pad and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: PE) to afford the desired alkynyl bromide (52–65% yield, 2 steps).

To a solution of the above alkynyl bromide (1 mmol) in toluene (5 mL) were added copper bromide (0.5 mmol, 72.0 mg), DMEDA (1 mmol, 100.0 mg), K_3PO_4 (4 mmol, 0.85 g), and protected propargylamide derivative (1 mmol).[1] The reaction was stirred at 50 °C for 3 h. Upon completion (monitored by TLC), the solution was then filtered and concentrated under reduced pressure. The residue was purified by chromatography on silica gel (eluent: PE/EtOAc) to give the desired ynamide **1** or **3** (66–80% yield).

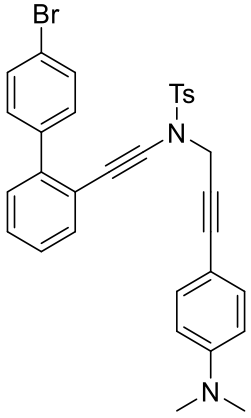
_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1a)



1a

Compound **1a** was prepared in 80% yield (406.0 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.5 Hz, 1H), 7.50 – 7.44 (m, 4H), 7.36 – 7.24 (m, 5H), 6.60 (d, *J* = 9.0 Hz, 2H), 4.46 (s, 2H), 2.97 (s, 3H), 2.95 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.5, 142.1, 139.3, 132.9, 132.7, 131.1, 130.9, 129.0, 128.2, 127.3, 121.5, 120.6, 111.6, 107.9, 88.2, 84.7, 79.2, 70.6, 43.1, 40.0, 38.5; IR (neat): 3055, 2927, 2214, 1606, 1539, 1521, 1361, 1266, 1160, 945; HRESIMS Calcd for $[C_{26}H_{23}BrN_2NaO_2S]^+$ (M + Na^+) 529.0556, found 529.0537.

***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1b)**

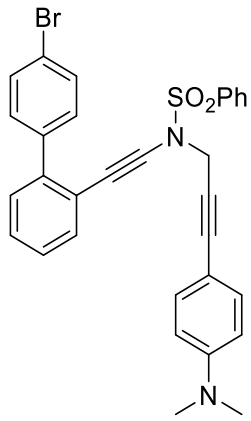


1b

Compound **1b** was prepared in 78% yield (455.2 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.49 – 7.38 (m, 4H), 7.35 – 7.21 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.54 (d, *J* = 8.8 Hz, 2H), 4.45 (s, 2H), 2.94 (s, 6H),

2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 144.6, 141.8, 139.3, 134.5, 133.2, 132.8, 131.1, 130.9, 129.5, 129.1, 128.0, 127.9, 127.3, 121.6, 121.0, 111.5, 108.6, 87.5, 85.2, 78.9, 70.4, 43.1, 40.1, 21.6; IR (neat): 3090, 3053, 2221, 1601, 1549, 1516, 1456, 1371, 1191, 1042; HRESIMS Calcd for $[C_{32}H_{27}BrN_2NaO_2S]^+$ (M + Na^+) 605.0869, found 605.0852.

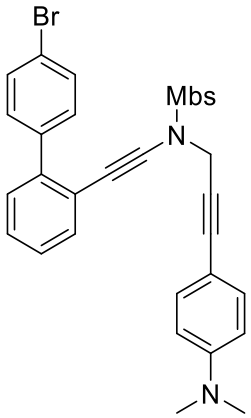
***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)benzenesulfonamide (1c)**



1c

Compound **1c** was prepared in 85% yield (484.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.5 Hz, 2H), 7.58 – 7.53 (m, 1H), 7.51 (d, *J* = 7.5 Hz, 1H), 7.46 – 7.34 (m, 6H), 7.35 – 7.24 (m, 3H), 7.04 (d, *J* = 9.0 Hz, 2H), 6.54 (d, *J* = 9.0 Hz, 2H), 4.49 (s, 2H), 2.94 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.3, 141.8, 139.3, 137.3, 133.5, 133.2, 132.8, 131.1, 130.9, 129.2, 128.8, 128.1, 127.9, 127.3, 121.6, 120.8, 111.5, 108.4, 87.6, 84.9, 78.8, 70.5, 43.1, 40.1; IR (neat): 3062, 2921, 2230, 1608, 1522, 1447, 1366, 1264, 1171, 1003; HRESIMS Calcd for $[C_{31}H_{25}BrN_2NaO_2S]^+$ (M + Na^+) 591.0712, found 591.0694.

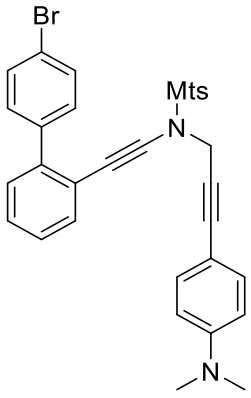
***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-4-methoxybenzenesulfonamide (1d)**



1d

Compound **1d** was prepared in 81% yield (485.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.9 Hz, 2H), 7.55 – 7.40 (m, 5H), 7.37 – 7.19 (m, 3H), 7.04 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 6.54 (d, *J* = 9.2 Hz, 2H), 4.44 (s, 2H), 3.78 (s, 3H), 2.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 150.3, 141.7, 139.4, 133.1, 132.8, 131.1, 130.9, 130.2, 129.1, 128.9, 128.0, 127.3, 121.5, 121.0, 114.0, 111.5, 108.6, 87.5, 85.4, 79.0, 70.4, 55.6, 43.0, 40.1; IR (neat): 3053, 2925, 2807, 2230, 1607, 1578, 1475, 1312, 1227, 1129, 1030; HRESIMS Calcd for $[C_{32}H_{27}BrN_2NaO_3S]^+$ (M + Na^+) 621.0818, found 621.0805.

***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-2,4,6-trimethylbenzenesulfonamide (1e)**

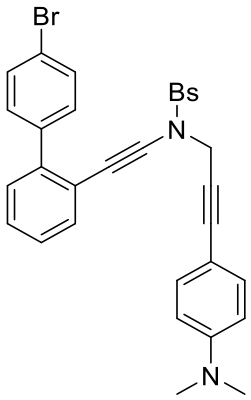


1e

Compound **1e** was prepared in 75% yield (458.7 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.36 (m, 5H), 7.29 – 7.21

(m, 3H), 7.17 (d, *J* = 8.8 Hz, 2H), 6.93 (s, 2H), 6.57 (d, *J* = 9.2 Hz, 2H), 4.47 (s, 2H), 2.94 (s, 6H), 2.61 (s, 6H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 143.6, 141.8, 140.9, 139.2, 133.0, 132.9, 132.0, 131.8, 130.9, 130.8, 129.0, 128.0, 127.2, 121.5, 121.1, 111.6, 108.7, 87.0, 85.2, 79.4, 71.5, 41.5, 40.1, 23.1 21.0; IR (neat): 2982, 2857, 2219, 1609, 1519, 1441, 1342, 1187, 1036, 911; HRESIMS Calcd for $[C_{34}H_{31}BrN_2NaO_2S]^+$ (M + Na^+) 633.1182, found 633.1177.

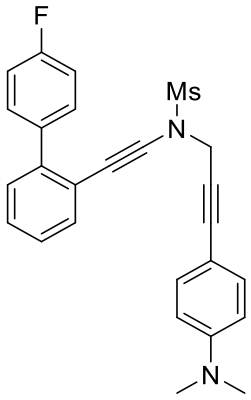
4-bromo-*N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)benzenesulfonamide (1f)



1f

Compound **1f** was prepared in 81% yield (525.2 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.8Hz, 2H), 7.54 – 7.48 (m, 3H), 7.47 – 7.42 (m, 4H), 7.37 – 7.25 (m, 3H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.57 (d, *J* = 8.8 Hz, 2H), 4.48 (s, 2H), 2.95 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 141.9, 139.3, 136.5, 133.0, 132.8, 132.1, 131.2, 130.9, 129.4, 129.2 128.9, 128.2, 127.3, 121.7 120.7, 111.7 108.2 88.0, 84.7 78.5, 70.6, 43.3 40.1; IR (neat): 3059, 2858, 2231, 1606, 1518, 1475, 1373, 1174, 1069, 944; HRESIMS Calcd for $[C_{31}H_{24}Br_2N_2NaO_2S]^+$ (M + Na^+) 668.9817, found 668.9801.

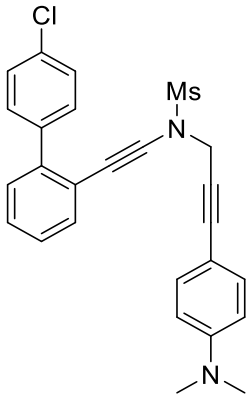
***N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-*N*-((4'-fluoro-[1,1'-biphenyl]-2-yl)ethynyl)methanesulfonamide (1g)**



1g

Compound **1g** was prepared in 77% yield (343.8 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.44 (m, 3H), 7.36 – 7.21 (m, 5H), 7.08 – 6.98 (m, 2H), 6.57 (d, *J* = 9.2 Hz, 2H), 4.44 (s, 2H), 2.98 (s, 3H), 2.91 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1 (d, *J* = 245 Hz), 150.4, 142.2, 136.3 (d, *J* = 3.0 Hz), 132.8, 132.6, 130.8 (d, *J* = 8.0 Hz), 129.1, 128.1, 127.0, 120.6, 114.8 (d, *J* = 21.0 Hz), 111.5, 107.8, 88.1, 84.4, 79.1, 70.7, 43.0, 39.9, 38.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.9 (s). IR (neat): 3042, 2927, 2233, 1608, 1480, 1360, 1265, 1191, 1031, 967; HRESIMS Calcd for $[C_{26}H_{23}FN_2NaO_2S]^+$ (M + Na^+) 469.1356, found 469.1343.

***N*-((4'-chloro-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1h)**

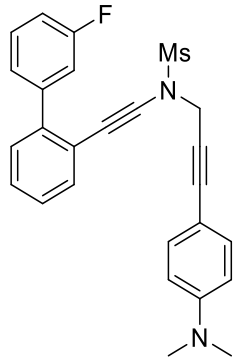


1h

Compound **1h** was prepared in 89% yield (412.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 3H),

7.42 – 7.13 (m, 7H), 6.60 (d, *J* = 8.4 Hz, 2H), 4.46 (s, 2H), 2.98 (s, 3H), 2.95 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 142.1, 138.9, 133.4, 132.9, 132.7, 130.6, 129.1, 128.2, 128.1, 127.3, 120.7, 111.7, 108.0, 88.2, 84.7, 79.2, 70.7, 43.2, 40.0, 38.5; IR (neat): 2926, 2854, 2234, 1608, 1523, 1444, 1323, 1191, 1089, 964; HRESIMS Calcd for $[C_{26}H_{23}ClN_2NaO_2S]^+$ (M + Na^+) 485.1061, found 485.1040.

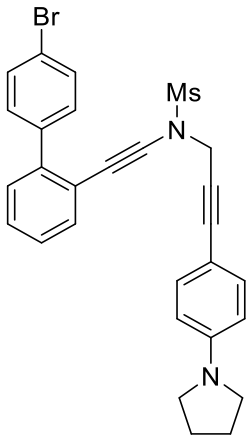
_N_-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-_N_-((3'-fluoro-[1,1'-biphenyl]-2-yl)ethynyl)methanesulfonamide (1i)



1i

Compound **1i** was prepared in 75% yield (334.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.51 (m, 1H), 7.43 – 7.37 (m, 1H), 7.36 – 7.33 (m, 2H), 7.32 – 7.26 (m, 3H), 7.25 – 7.21 (m, 2H), 7.02 – 6.95 (m, 1H), 6.58 (d, *J* = 8.8 Hz, 2H), 4.46 (s, 2H), 3.01 (s, 3H), 2.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4 (d, *J* = 244.0 Hz), 150.4, 142.6 (d, *J* = 8.0 Hz), 142.0 (d, *J* = 2.0 Hz), 132.9, 132.7, 129.5 (d, *J* = 8.0 Hz), 129.2, 128.2, 127.5, 125.1 (d, *J* = 3.0 Hz), 120.8, 116.0 (d, *J* = 21.0 Hz), 114.2 (d, *J* = 21.0 Hz), 111.6, 108.0, 88.1, 84.7, 79.1, 70.5, 43.2, 40.0, 38.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.9 – -116.3 (m); IR (neat): 3014, 2236, 1607, 1524, 1446, 1362, 1261, 1160, 1035, 966; HRESIMS Calcd for $[C_{26}H_{23}FKN_2O_2S]^+$ (M + K^+) 485.1096, found 485.1094.

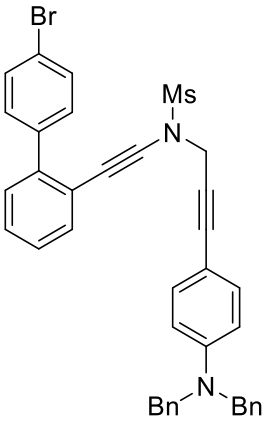
_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (1j)



1j

Compound **1j** was prepared in 80% yield (421.4 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.5 Hz, 1H), 7.51 – 7.40 (m, 4H), 7.38 – 7.26 (m, 5H), 6.45 (d, *J* = 8.5 Hz, 2H), 4.47 (s, 2H), 3.34 – 3.16 (m, 4H), 2.98 (s, 3H), 2.06 – 1.91 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.0, 142.1, 139.4, 133.0, 132.7, 131.1, 130.9, 129.1, 128.2, 127.3, 121.6, 120.7, 111.3, 107.0, 88.5, 84.8, 79.0, 70.6, 47.4, 43.3, 38.5, 25.4; IR (neat): 3053, 2923, 2231, 1622, 1516, 1488, 1394, 1263, 1165, 1031; HRESIMS Calcd for $[C_{28}H_{25}BrN_2NaO_2S]^+$ (M + Na^+) 555.0712, found 555.0697.

***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dibenzylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1k)**

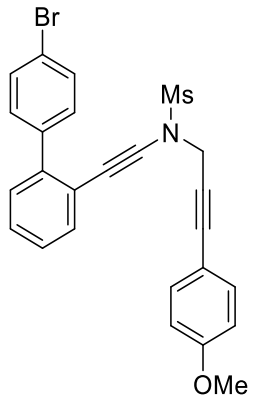


1k

Compound **1k** was prepared in 76% yield (500.2 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.0 Hz,

1H), 7.50 – 7.40 (m, 4H), 7.35 – 7.28 (m, 6H), 7.28 – 7.21 (m, 2H), 7.22 – 7.14 (m, 7H), 6.63 (d, *J* = 8.8 Hz, 2H), 4.65 (s, 4H), 4.43 (s, 2H), 2.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 142.1, 139.3, 137.6, 133.1, 132.8, 131.1, 130.9, 129.1, 128.7, 128.3, 127.3, 127.1, 126.4, 121.6, 120.6, 112.0, 108.7, 87.9, 84.6, 79.3, 70.6, 54.1, 43.1, 38.5; IR (neat): 3053, 2850, 2231, 1646, 1506, 1472, 1338, 1263, 1127, 1002; HRESIMS Calcd for $[C_{38}H_{31}BrN_2NaO_2S]^+$ (M + Na^+) 681.1182, found 681.1159.

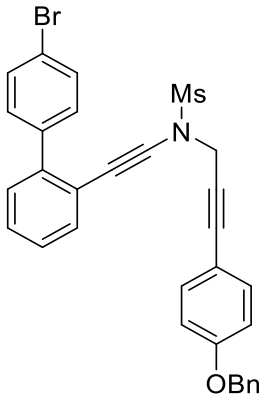
_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1l)



1l

Compound **1l** was prepared in 78% yield (385.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.52 – 7.43 (m, 4H), 7.38 – 7.26 (m, 5H), 6.84 (d, *J* = 8.8 Hz, 2H), 4.46 (s, 2H), 3.78 (s, 3H), 2.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 142.1, 139.3, 133.2, 132.7, 131.0, 130.8, 129.0, 128.3, 127.3, 121.5, 120.5, 114.0, 113.5, 86.8, 84.4, 80.1, 70.7, 55.2, 42.8, 38.4; IR (neat): 3048, 2931, 2230, 1647, 1506, 1472, 1362, 1254, 1092, 960; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_3S]^+$ (M + Na^+) 516.0239, found 516.0220.

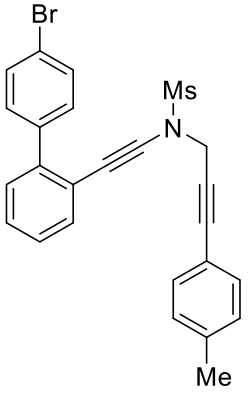
_N_-(3-(4-(benzyloxy)phenyl)prop-2-yn-1-yl)-_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)methanesulfonamide (1m)



1m

Compound **1m** was prepared in 80% yield (456.4 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.5 Hz, 1H), 7.49 – 7.44 (m, 4H), 7.42 – 7.28 (m, 10H), 6.91 (d, *J* = 9.0 Hz, 2H), 5.05 (s, 2H), 4.45 (s, 2H), 2.97 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.3, 142.2, 139.3, 136.3, 133.3, 132.7, 131.1, 130.9, 129.1, 128.6, 128.3, 128.1, 127.4, 121.6, 120.6, 115.0, 113.8, 86.9, 84.5, 80.2, 70.8, 70.0, 42.8, 38.5; IR (neat): 3033, 2929, 2234, 1603, 1505, 1455, 1367, 1252, 1165, 1003; HRESIMS Calcd for $[C_{31}H_{24}BrKNO_3S]^+$ (M + K^+) 608.0292, found 608.0276.

***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(*p*-tolyl)prop-2-yn-1-yl)methanesulfonamide (1n)**

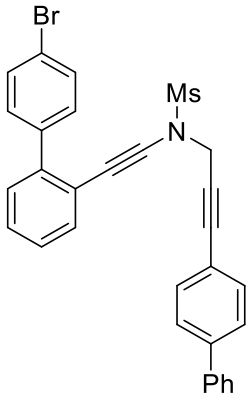


1n

Compound **1n** was prepared in 90% yield (430.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.50 – 7.42 (m, 4H), 7.38 – 7.26 (m, 5H), 7.12 (d, *J* = 8.0 Hz, 2H), 4.46 (s, 2H),

2.98 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 139.3(1), 139.2(9), 132.7, 131.6, 131.1, 130.9, 129.2, 129.1, 128.3, 127.4, 121.6, 120.5, 118.4, 87.0, 84.4, 80.8, 70.8, 42.7, 38.4, 21.4; IR (neat): 3058, 2977, 2236, 1608, 1508, 1410, 1361, 1265, 1166, 1014; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_2S]^+$ (M + Na^+) 500.0290, found 500.0278.

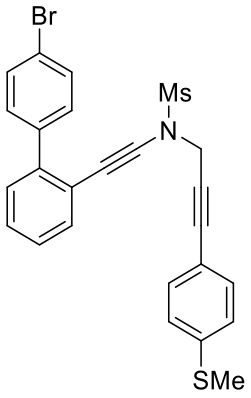
***N*-(3-([1,1'-biphenyl]-4-yl)prop-2-yn-1-yl)-*N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)methanesulfonamide (1o)**



1o

Compound **1o** was prepared in 82% yield (443.2 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.52 (m, 5H), 7.51 – 7.40 (m, 8H), 7.39 – 7.27 (m, 4H), 4.50 (s, 2H), 3.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 141.8, 140.0, 139.3, 132.7, 132.2, 131.1, 130.9, 129.1, 128.9, 128.4, 127.8, 127.4, 127.1, 127.0, 121.6, 120.5, 120.3, 86.8, 84.3, 82.1, 70.9, 42.7, 38.5; IR (neat): 3059, 2928, 2234, 1599, 1519, 1487, 1361, 1265, 1129, 1003; HRESIMS Calcd for $[C_{24}H_{18}BrKNO_2S]^+$ (M + K^+) 501.9873, found 501.9850

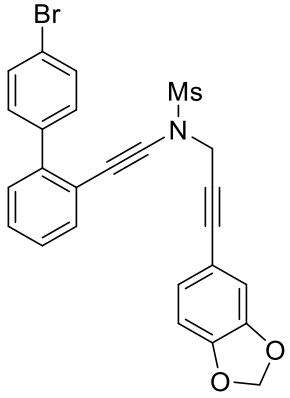
***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(methylthio)phenyl)prop-2-yn-1-yl)methanesulfonamide (1p)**



1p

Compound **1p** was prepared in 88% yield (449.2 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.50 – 7.42 (m, 4H), 7.38 – 7.24 (m, 5H), 7.15 (d, *J* = 8.4 Hz, 2H), 4.46 (s, 2H), 2.97 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.0, 140.5, 139.2, 132.6, 131.9, 131.0, 130.8, 129.0, 128.3, 127.3, 125.6, 121.5, 120.4, 117.4, 86.6, 84.3, 81.4, 70.8, 42.6, 38.4, 15.0; IR (neat): 3066, 2918, 2242, 1590, 1455, 1361, 1268, 1185, 1045, 943; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_2S_2]^+$ (M + Na^+) 532.0011, found 532.0002.

***N*-(3-(benzo[d][1,3]dioxol-5-yl)prop-2-yn-1-yl)-*N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)methanesulfonamide (1q)**

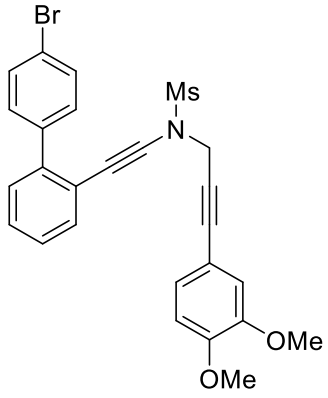


1q

Compound **1q** was prepared in 83% yield (421.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.51 – 7.43 (m, 4H), 7.38 – 7.27 (m, 3H), 6.91 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.80 (d, *J* = 1.2 Hz, 1H), 6.75 (d, *J* = 8.0 Hz, 1H), 5.96 (s, 2H), 4.45 (s, 2H), 2.97 (s, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$) δ 148.5, 147.5, 142.1, 139.3, 132.7, 131.1, 130.9, 129.1, 128.3, 127.4, 126.6, 121.6, 120.5, 114.6, 111.6, 108.5, 101.4, 86.8, 84.3, 79.8, 70.8, 42.7, 38.4; IR (neat): 3059, 2926, 2231, 1602, 1502, 1442, 1363, 1249, 1168, 1031; HRESIMS Calcd for $[C_{25}H_{18}BrNNaO_4S]^+$ (M + Na^+) 530.0032, found 530.0016.

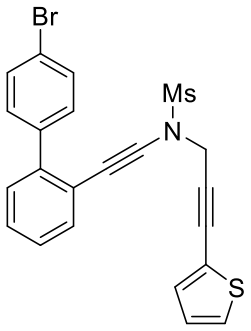
_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-(3,4-dimethoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1r)



1r

Compound **1r** was prepared in 89% yield (451.1 mg) according to the general procedure S1 as a pale yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.6 Hz, 1H), 7.50 – 7.42 (m, 4H), 7.38 – 7.28 (m, 3H), 7.01 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.90 (d, *J* = 1.6 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 4.48 (s, 2H), 3.88 (s, 3H), 3.84 (s, 3H), 2.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 148.6, 142.1, 139.2, 132.6, 131.0, 130.8, 129.0, 128.3, 127.3, 125.2, 121.5, 120.5, 114.2, 113.6, 111.0, 87.0, 84.4, 80.0, 70.8, 55.8, 42.7, 38.4; IR (neat): 3059, 2933, 2232, 1599, 1474, 1324, 1210, 1137, 1026, 964; HRESIMS Calcd for $[C_{26}H_{22}BrNNaO_4S]^+$ (M + Na^+) 546.0345, found 546.0304.

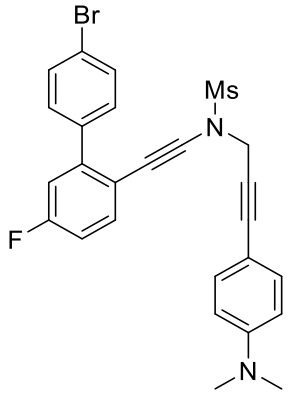
_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-(thiophen-2-yl)prop-2-yn-1-yl)methanesulfonamide (1s)



1s

Compound **1s** was prepared in 91% yield (428.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.5 Hz, 1H), 7.51 – 7.42 (m, 4H), 7.37 – 7.26 (m, 4H), 7.25 – 7.19 (m, 1H), 6.97 (dd, *J* = 5.0, 4.0 Hz, 1H), 4.48 (s, 2H), 2.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.2, 139.3, 133.1, 132.7, 131.1, 130.9, 129.1, 128.4, 128.1, 127.4, 127.1, 121.6, 121.2, 120.4, 85.5, 84.2, 80.2, 71.0, 42.8, 38.4; IR (neat): 3107, 3022, 2229, 1587, 1424, 1362, 1265, 1129, 1031, 963; HRESIMS Calcd for $[C_{22}H_{16}BrNNaO_2S_2]^+$ (M + Na^+) 491.9698, found 491.9683.

***N*-((4'-bromo-5-fluoro-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1t)**

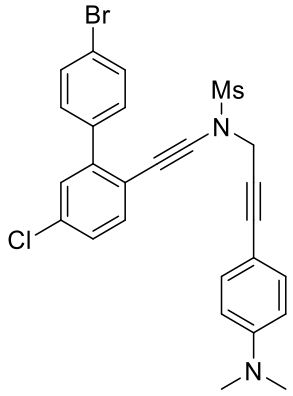


1t

Compound **1t** was prepared in 83% yield (425.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.39 (m, 5H), 7.32 – 7.19 (m, 2H), 7.10 – 6.93 (m, 2H), 6.61 (d, *J* = 8.4 Hz, 2H), 4.46 (s, 2H), 2.98 (s, 3H), 2.96 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2 (d, *J* = 249.0 Hz), 150.5, 144.5 (d, *J* = 8.0 Hz), 138.2, 134.8 (d, *J* = 9.0 Hz), 132.9, 131.3, 130.7, 122.2, 116.7 (d, *J* = 3.0 Hz), 116.1 (d, *J* = 23.0 Hz), 114.6 (d, *J* = 22.0 Hz), 111.7, 107.9, 88.2, 84.2, 79.2, 69.6, 43.1,

40.0, 38.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.4 – -113.8 (m); IR (neat): 3043, 2811, 2238, 1607, 1521, 1416, 1362, 1259, 1163, 1009; HRESIMS Calcd for $[C_{24}H_{17}BrFNNaO_2S]^+$ (M + Na^+) 547.0462, found 547.0444.

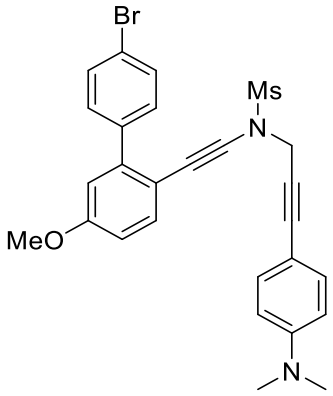
***N*-((4'-bromo-5-chloro-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1u)**



1u

Compound **1u** was prepared in 92% yield (499.0 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, CDCl3) δ 7.52 – 7.40 (m, 5H), 7.32 (d, *J* = 2.0 Hz, 1H), 7.30 – 7.21 (m, 3H), 6.60 (d, *J* = 8.8 Hz, 2H), 4.46 (s, 2H), 2.98 (s, 3H), 2.96 (s, 6H); ^{13}C NMR (100 MHz, CDCl3) δ 150.5, 143.5, 138.0, 133.9, 133.8, 132.9, 131.3, 130.7, 129.0, 127.5, 122.1, 119.2, 111.6, 107.8, 88.3, 85.5, 79.1, 69.8, 43.1, 40.0, 38.6; IR (neat): 2924, 2808, 2239, 1608, 1520, 1475, 1368, 1265, 1107, 1008; HRESIMS Calcd for $[C_{26}H_{22}BrClN_2NaO_2S]^+$ (M + Na^+) 563.0166, found 563.0159.

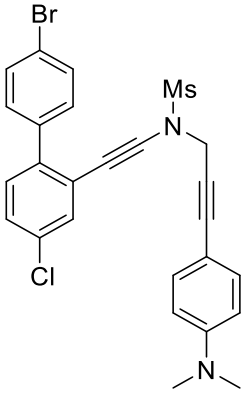
***N*-((4'-bromo-5-methoxy-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1v)**



1v

Compound **1v** was prepared in 80% yield (430.0 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.36 (m, 5H), 7.26 (d, *J* = 8.8 Hz, 2H), 6.89 – 6.76 (m, 2H), 6.60 (d, *J* = 8.8 Hz, 2H), 4.45 (s, 2H), 3.81 (s, 3H), 2.95 (s, 6H), 2.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 150.5, 144.2, 139.3, 134.8, 132.9, 131.0, 130.8, 121.6, 114.7, 113.1, 112.6, 111.7, 108.0, 88.0, 83.0, 79.3, 70.2, 55.3, 43.2, 40.0, 38.3; IR (neat): 3009, 2837, 2213, 1607, 1557, 1446, 1361, 1266, 1159, 1033 ; HRESIMS Calcd for $[C_{27}H_{25}BrKN_2O_3S]^+$ ($M + K^+$) 575.0401, found 575.0389.

***N*-((4'-bromo-4-chloro-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1w)**

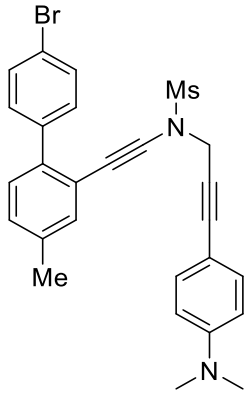


1w

Compound **1w** was prepared in 78% yield (422.7 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.33 (m, 5H), 7.34 – 7.18 (m, 4H), 6.60 (d, *J* = 8.8 Hz, 2H), 4.47 (s, 2H), 2.99 (s, 3H), 2.96 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 140.3, 138.2, 133.2, 132.9, 132.0, 131.2, 130.7,

130.2, 128.3, 122.4, 121.9, 111.7, 107.8, 88.4, 85.8, 79.0, 69.8, 43.1, 40.0, 38.7; IR (neat): 3048, 2927, 2237, 1607, 1522, 1445, 1357, 1227, 1166, 963; HRESIMS Calcd for $[C_{26}H_{22}BrClN_2NaO_2S]^+$ (M + Na^+) 563.0166, found 563.0150.

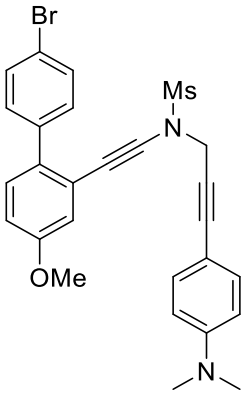
***N*-((4'-bromo-4-methyl-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1x)**



1x

Compound **1x** was prepared in 77% yield (401.5 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.40 (m, 4H), 7.36 (s, 1H), 7.27 (d, *J* = 9.2 Hz, 2H), 7.23 – 7.21 (m, 1H), 7.15 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.60 (d, *J* = 9.2 Hz, 2H), 4.46 (s, 2H), 2.99 (s, 3H), 2.95 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 139.3, 139.2, 137.2, 133.2, 132.9, 131.0, 130.8, 129.2, 128.9, 121.3, 120.3, 111.6, 107.9, 88.2, 84.3, 79.2, 70.8, 43.1, 40.0, 38.4, 20.8; IR (neat): 3023, 2860, 2236, 1608, 1525, 1446, 1362, 1266, 1161, 1037; HRESIMS Calcd for $[C_{27}H_{25}BrN_2NaO_2S]^+$ (M + Na^+) 543.0712, found 543.0452.

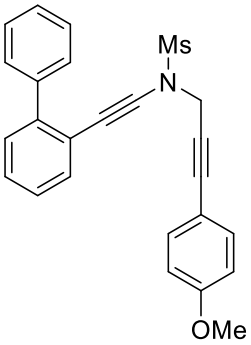
***N*-((4'-bromo-4-methoxy-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1y)**



1y

Compound **1y** was prepared in 95% yield (510.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.42 (m, 4H), 7.30 – 7.17 (m, 3H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.90 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.59 (d, *J* = 8.8 Hz, 2H), 4.47 (s, 2H), 3.79 (s, 3H), 2.99 (s, 3H), 2.95 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 150.5, 139.1, 134.8, 132.9, 131.0, 130.8, 130.2, 121.5, 121.0, 116.8, 115.1, 111.6, 107.9, 88.2, 84.4, 79.2, 70.8, 55.4, 43.1, 40.0, 38.5; IR (neat): 3050, 2989, 2245, 1609, 1525, 1429, 1303, 1225, 1168, 1013; HRESIMS Calcd for $[C_{27}H_{25}BrN_2NaO_3S]^+$ (M + Na^+) 559.0661, found 559.0649.

_N_-([1,1'-biphenyl]-2-ylethynyl)-_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)methanesulfonamide (1z)

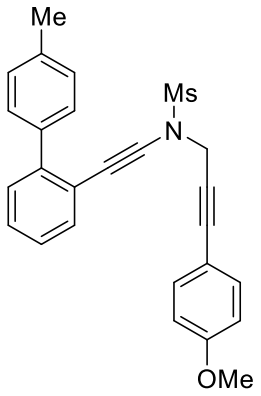


1z

Compound **1z** was prepared in 93% yield (386.4 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 6.8 Hz, 2H), 7.56 – 7.50 (m, 1H), 7.39 – 7.25 (m, 8H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.43 (s, 2H), 3.76 (s, 3H), 2.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 143.5, 140.4, 133.2, 132.5, 129.3,

129.1, 128.2, 127.9, 127.2, 127.0, 120.6, 113.9, 113.6, 86.7, 84.0, 80.2, 71.0, 55.2, 42.8, 38.4; IR (neat): 3050, 2916, 2244, 1609, 1525, 1416, 1303, 1225, 1168, 1013; HRESIMS Calcd for $[C_{25}H_{21}KNO_3S]^+$ (M + K^+) 454.0874, found 454.0885.

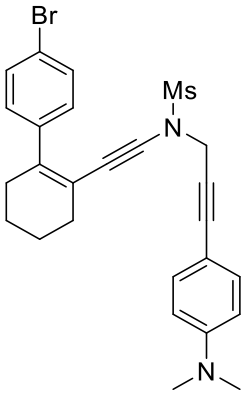
_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-_N_-((4'-methyl-[1,1'-biphenyl]-2-yl)ethynyl)methanesulfonamide (1aa)



1aa

Compound **1aa** was prepared in 86% yield (369.4 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.48 (m, 3H), 7.39 – 7.29 (m, 4H), 7.28 – 7.23 (m, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.45 (s, 2H), 3.77 (s, 3H), 2.95 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 143.4, 137.5, 137.0, 133.3, 132.6, 129.2, 129.0, 128.6, 128.2, 126.7, 120.5, 114.0, 113.6, 86.7, 83.9, 80.2, 71.2, 55.2, 42.8, 38.3, 21.0; IR (neat): 3022, 2839, 2234, 1606, 1509, 1481, 1363, 1250, 1128, 963; HRESIMS Calcd for $[C_{26}H_{23}NNaO_3S]^+$ (M + Na^+) 452.1291, found 452.1279.

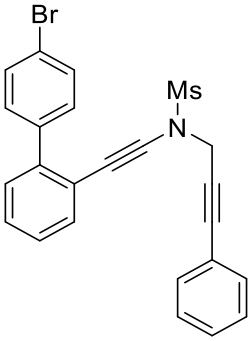
_N_-((4'-bromo-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1ab)



1ab

Compound **1ab** was prepared in 80% yield (383.6 mg) according to the general procedure S2 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.30 (m, 4H), 7.30 – 7.21 (m, 2H), 6.62 (d, *J* = 8.8 Hz, 2H), 4.39 (s, 2H), 2.98 (s, 6H), 2.89 (s, 3H), 2.44 – 2.25 (m, 4H), 1.83 – 1.64 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 142.0, 141.6, 132.9, 130.9, 129.6, 120.6, 116.4, 111.7, 108.2, 87.9, 83.4, 79.4, 72.5, 43.2, 40.1, 38.0, 30.9, 30.6, 22.5, 22.2; IR (neat): 3045, 2860, 2213, 1604, 1521, 1446, 1373, 1226, 1133, 1053; HRESIMS Calcd for $[C_{26}H_{27}BrN_2NaO_2S]^+$ (M + Na^+) 533.0869, found 533.0861.

***N*-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-*N*-(3-phenylprop-2-yn-1-yl)methanesulfonamide (1ac)**

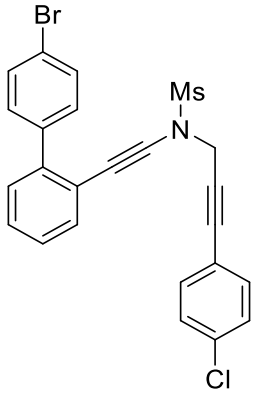


1ac

Compound **1ac** was prepared in 84% yield (390.0 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.52 (m, 1H), 7.49 – 7.43 (m, 4H), 7.41 – 7.26 (m, 8H), 4.47 (s, 2H), 2.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 139.3, 132.7, 131.7, 131.1, 130.8, 129.1, 129.0, 128.4, 128.3,

127.4, 121.6, 121.5, 120.5, 86.8, 84.3, 81.4, 70.8, 42.6, 38.5; IR (neat): 3059, 2928, 2234, 1599, 1519, 1487, 1361, 1265, 1129, 1003; IR (neat): 3060, 3022, 2235, 1597, 1490, 1410, 1363, 1264, 1166, 1038; HRESIMS Calcd for $[C_{24}H_{18}BrKNO_2S]^+$ (M + K^+) 501.9873, found 501.9892.

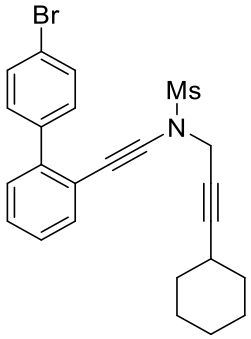
_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-(4-chlorophenyl)prop-2-yn-1-yl)methanesulfonamide (1ad)



1ad

Compound **1ad** was prepared in 89% yield (443.9 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.2 Hz, 1H), 7.55 – 7.47 (m, 4H), 7.42 – 7.36 (m, 3H), 7.35 – 7.28 (m, 4H), 4.52 (s, 2H), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 139.3, 135.1, 132.9, 132.7, 131.1, 130.8, 129.1, 128.8, 128.4, 127.4, 121.6, 120.4, 119.9, 85.6, 84.1, 82.5, 71.0, 42.5, 38.5; IR (neat): 3058, 2928, 2236, 1593, 1475, 1410, 1323, 1129, 1040, 920; HRESIMS Calcd for $[C_{24}H_{17}BrClNNaO_2S]^+$ (M + Na^+) 519.9744, found 519.9750.

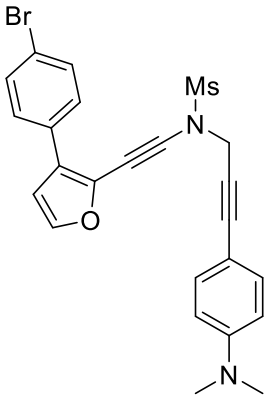
_N_-((4'-bromo-[1,1'-biphenyl]-2-yl)ethynyl)-_N_-(3-cyclohexylprop-2-yn-1-yl)methanesulfonamide (1ae)



1ae

Compound **1ae** was prepared in 87% yield (408.0 mg) according to the general procedure S2 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.52 (d, *J* = 9.5 Hz, 2H), 7.46 (d, *J* = 8.5 Hz, 2H), 7.35 – 7.30 (m, 2H), 7.30 – 7.25 (m, 1H), 4.22 (s, 2H), 2.95 (s, 3H), 2.44 – 2.19 (m, 1H), 1.78 – 1.68 (m, 2H), 1.68 – 1.56 (m, 2H), 1.53 – 1.42 (m, 1H), 1.40 – 1.29 (m, 2H), 1.30 – 1.19 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.7, 139.2, 132.5, 130.9, 130.7, 128.9, 128.1, 127.2, 121.4, 120.5, 91.8, 84.5, 72.3, 70.4, 42.2, 38.3, 32.2, 28.7, 25.5, 24.5. IR (neat): 2927, 2853, 2235, 1588, 1471, 1360, 1299, 1162, 1072, 967; HRESIMS Calcd for $[C_{24}H_{24}BrKNO_2S]^+$ (M + K^+) 508.0343, found 508.0347.

***N*-((3-(4-bromophenyl)furan-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1af)**

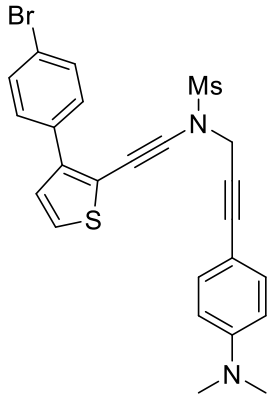


1af

Compound **1af** was prepared in 60% yield (298.4) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 2.0 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 9.2 Hz, 2H), 6.66 (d, *J* = 2.0 Hz,

1H), 6.62 (d, *J* = 8.8 Hz, 2H), 4.62 (s, 2H), 3.25 (s, 3H), 2.99 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 144.3, 133.1, 132.3, 131.8, 130.8, 130.4, 128.4, 121.5, 111.8, 110.4, 107.8, 88.9, 88.7, 79.1, 62.8, 43.6, 40.1, 39.3; IR (neat): 2924, 2853, 2215, 1608, 1522, 1490, 1362, 1166, 1111, 1034; HRESIMS Calcd for $[C_{24}H_{21}BrKN_2O_3S]^+$ (M + K^+) 535.0088, found 535.0083.

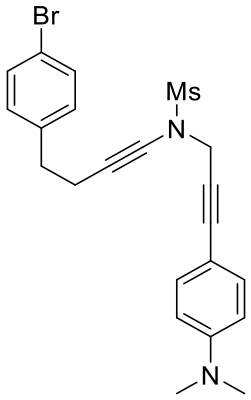
***N*-((3-(4-bromophenyl)thiophen-2-yl)ethynyl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1ag)**



1ag

Compound **1ag** was prepared in 81% yield (430.5 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.57 (m, 2H), 7.44 – 7.34 (m, 2H), 7.31 – 7.20 (m, 3H), 7.14 (d, *J* = 5.6 Hz, 1H), 6.62 (d, *J* = 8.8 Hz, 2H), 4.57 (s, 2H), 3.17 (s, 3H), 2.98 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 144.5, 134.1, 133.0, 131.5, 129.5, 127.6, 127.4, 121.7, 117.6, 111.8, 107.9, 88.5, 87.5, 79.2, 64.9, 43.5, 40.1, 39.0; IR (neat): 2925, 2214, 1608, 1523, 1486, 1444, 1362, 1190, 1063, 962; HRESIMS Calcd for $[C_{24}H_{21}BrKN_2O_2S_2]^+$ (M + K^+) 550.9859, found 550.9858.

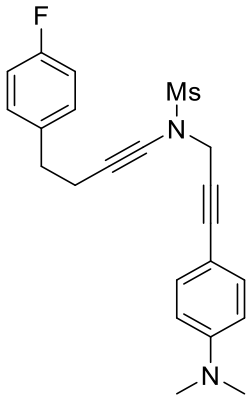
***N*-(4-(4-bromophenyl)but-1-yn-1-yl)-*N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)methanesulfonamide (1ah)**



1ah

Compound **1ah** was prepared in 90% yield (413.0 mg) according to the general procedure S2 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 6.60 (d, *J* = 9.2 Hz, 2H), 4.38 (s, 2H), 3.03 (s, 3H), 2.93 (s, 6H), 2.80 – 2.70 (m, 2H), 2.62 – 2.45 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 139.2, 132.7, 131.1, 130.2, 119.8, 111.5, 107.9, 87.8, 79.2, 73.7, 69.5, 42.9, 39.8, 37.7, 34.1, 20.2; IR (neat): 2925, 2861, 2211, 1608, 1522, 1487, 1359, 1226, 1164, 1070; HRESIMS Calcd for $[C_{22}H_{23}BrN_2NaO_2S]^+$ (M + Na^+) 481.0556, found 481.0554.

***N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-*N*-(4-(4-fluorophenyl)but-1-yn-1-yl)methanesulfonamide (1ai)**

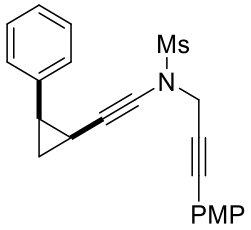


1ai

Compound **1ai** was prepared in 88% yield (350.4 mg) according to the general procedure S2 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.09 (m, 2H), 6.93 – 6.87 (m, 2H), 6.60 (d, *J* = 8.5 Hz, 2H), 4.38 (s, 2H),

3.04 (s, 3H), 2.93 (s, 6H), 2.77 (t, *J* = 6.5 Hz, 2H), 2.57 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.2 (d, *J* = 242.5 Hz), 150.3, 135.9 (d, *J* = 3.8 Hz), 132.7, 129.9 (d, *J* = 7.5 Hz), 114.7 (d, *J* = 21.3 Hz), 111.4, 107.9, 87.7, 79.2, 73.6, 69.6, 42.9, 39.7, 37.6, 33.9, 20.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.98; IR (neat): 2928, 2251, 2211, 1610, 1508, 1446, 1364, 1221, 1159, 1095 HRESIMS Calcd for $[C_{22}H_{23}FN_2NaO_2S]^+$ (M + Na^+) 421.1356, found 421.1343.

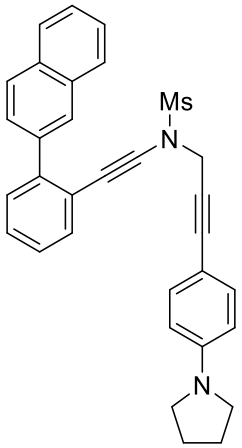
_N_-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-_N_-(((1_S_,2_R_)-2-phenylcyclopropyl)ethynyl)methanesulfonamide (1aj)



1aj

Compound **1aj** was prepared in 91% yield (345.3 mg) according to the general procedure S2 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.8 Hz, 2H), 7.26 – 7.19 (m, 2H), 7.17 – 7.04 (m, 3H), 6.84 (d, *J* = 8.8 Hz, 2H), 4.30 (d, *J* = 18.0 Hz, 1H), 4.15 (d, *J* = 18.0 Hz, 1H), 3.74 (s, 3H), 2.60 (s, 3H), 2.30 (dd, *J* = 15.2, 8.4 Hz, 1H), 1.89 – 1.78 (m, 1H), 1.40 – 1.29 (m, 1H), 1.20 (dd, *J* = 12.0, 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 137.5, 132.9, 128.2, 127.5, 125.8, 113.8, 113.5, 86.1, 80.2, 71.7, 71.3, 54.9, 42.4, 37.0, 23.7, 14.4, 8.9; IR (neat): 3011, 2932, 2246, 1606, 1509, 1458, 1359, 1259, 1162, 1032; HRESIMS Calcd for $[C_{22}H_{21}KNO_3S]^+$ (M + K^+) 418.0874, found 418.0868.

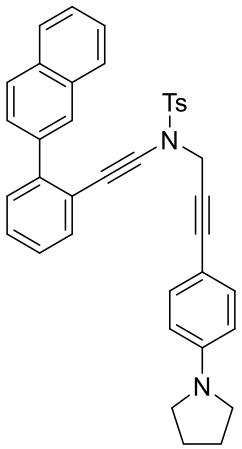
_N_-((2-(naphthalen-2-yl)phenyl)ethynyl)-_N_-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3a)



3a

Compound **3a** was prepared in 81% yield (408.8 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.94 – 7.86 (m, 1H), 7.85 – 7.73 (m, 3H), 7.58 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.50 – 7.41 (m, 3H), 7.40 – 7.34 (m, 1H), 7.33 – 7.25 (m, 1H), 7.17 (d, *J* = 8.8 Hz, 2H), 6.38 (d, *J* = 8.8 Hz, 2H), 4.40 (s, 2H), 3.30 – 3.18 (m, 4H), 2.77 (s, 3H), 2.04 – 1.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 143.3, 138.0, 133.1, 133.0, 132.8, 132.5, 129.6, 128.3, 128.2, 128.0, 127.5(1), 127.4(8), 127.4, 127.1, 126.0, 126.0, 121.0, 111.2, 107.1, 88.5, 84.5, 79.0, 71.0, 47.4, 43.2, 38.3, 25.3; ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.0, 132.8, 129.6, 128.3, 128.2, 128.0, 127.5, 127.5, 127.4, 127.1, 126.0, 126.1, 111.2, 47.4, 43.2, 38.3, 25.3; IR (neat): 3053, 2929, 2233, 1607, 1520, 1462, 1361, 1266, 1166, 1034; HRESIMS Calcd for $[C_{32}H_{28}KN_2O_2S]^+$ (M + K^+) 543.1503, found 543.1518.

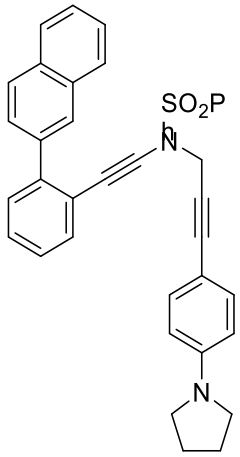
4-methyl-*N*-((2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)benzenesulfonamide (3b)



3b

Compound **3b** was prepared in 88% yield (511.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.94 – 7.82 (m, 1H), 7.82 – 7.76 (m, 3H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.42 (m, 3H), 7.37 – 7.31 (m, 1H), 7.31 – 7.25 (m, 1H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, 2H), 6.35 (d, *J* = 8.8 Hz, 2H), 4.39 (s, 2H), 3.27 – 3.19 (m, 4H), 2.21 (s, 3H), 2.01 – 1.91 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 144.3, 142.9, 138.1, 134.3, 133.2, 132.9(4), 132.9(1), 132.6, 129.7, 129.2, 128.3, 127.9, 127.8, 127.6, 127.5, 127.4, 127.0, 125.9(3), 125.8(8), 121.4, 111.0, 107.7, 87.9, 85.1, 78.6, 70.7, 47.4, 43.1, 25.4, 21.4; IR (neat): 3051, 2965, 2230, 1607, 1521, 1461, 1367, 1187, 1090, 814; HRESIMS Calcd for $[C_{38}H_{32}N_2NaO_2S]^+$ (M + Na^+) 603.2077, found 603.2072.

***N*-((2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)benzenesulfonamide (3c)**

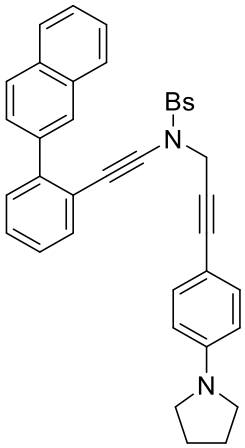


3c

Compound **3c** was prepared in 76% yield (430.7 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.94 – 7.85 (m, 1H), 7.83 – 7.69 (m, 3H), 7.60 (d, *J* = 7.2 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 1H), 7.50 – 7.40 (m, 3H), 7.39 – 7.23 (m, 3H), 7.14 – 6.86 (m, 4H), 6.35 (d, *J* = 8.4 Hz, 2H), 4.42 (s, 2H), 3.42 – 3.09 (m, 4H), 2.07 – 1.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 142.9, 138.1, 137.1, 133.2, 132.9, 132.6, 129.7, 128.5, 128.3, 127.9(4), 127.8(7), 127.8, 127.6, 127.5(4), 127.4(5), 127.0, 126.0, 125.9, 121.3, 111.1, 107.5, 88.0, 84.8, 78.5 70.8, 47.4,

43.2, 25.3; IR (neat): 3054, 2967, 2231, 1608, 1522, 1447, 1368, 1172, 1089, 920; HRESIMS Calcd for $[C_{37}H_{30}N_2NaO_2S]^+$ (M + Na^+) 589.1920, found 589.1913

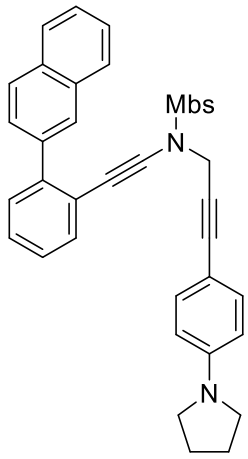
4-bromo-*N*-((2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)benzenesulfonamide (3d)



3d

Compound **3d** was prepared in 90% yield (581.0 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.92 – 7.85 (m, 1H), 7.84 – 7.76 (m, 2H), 7.73 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.50 – 7.41 (m, 3H), 7.39 – 7.31 (m, 3H), 7.31 – 7.24 (m, 1H), 7.09 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.36 (d, *J* = 8.7 Hz, 2H), 4.42 (s, 2H), 3.31 – 3.16 (m, 4H), 2.04 – 1.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 143.1, 138.1, 136.3, 133.1, 132.9(0), 132.8(7), 132.5, 131.8, 129.7, 129.2, 128.6, 128.3, 128.1, 127.9, 127.6, 127.5, 127.0, 126.1, 121.1, 111.2, 107.2, 88.3, 84.5, 78.3, 70.9, 47.4, 43.4, 25.3; IR (neat): 3054, 2970, 2232, 1607, 1540, 1456, 1373, 1263, 1123, 1037; HRESIMS Calcd for $[C_{37}H_{29}BrN_2NaO_2S]^+$ (M + Na^+) 667.1025, found 667.1023.

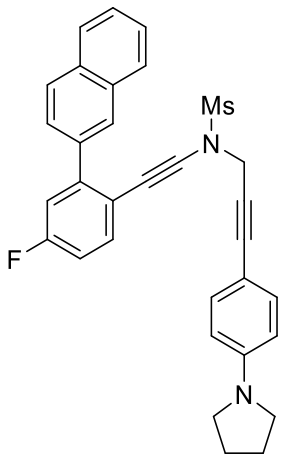
4-methoxy-*N*-((2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)benzenesulfonamide (3e)



3e

Compound **3e** was prepared in 79% yield (471.4 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.95 – 7.87 (m, 1H), 7.86 – 7.76 (m, 3H), 7.58 – 7.48 (m, 3H), 7.47 – 7.41 (m, 3H), 7.38 – 7.30 (m, 1H), 7.30 – 7.23 (m, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.48 (d, *J* = 8.8 Hz, 2H), 6.34 (d, *J* = 8.8 Hz, 2H), 4.39 (s, 2H), 3.61 (s, 3H), 3.31 – 3.11 (m, 4H), 2.04 – 1.85 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 147.7, 142.7, 138.2, 133.2, 132.9, 132.8, 132.6, 130.1, 129.6, 128.7, 128.3, 127.9, 127.8, 127.7, 127.6, 127.5, 127.0, 126.0, 125.9, 121.5, 113.7, 111.0, 107.7, 87.9, 85.3, 78.7, 70.8, 55.4, 47.4, 43.1, 25.4; IR (neat): 3054, 2967, 2230, 1608, 1521, 1441, 1367, 1263, 1164, 1090; HRESIMS Calcd for $[C_{38}H_{32}N_2NaO_3S]^+$ ($M + Na^+$) 619.2026, found 619.2028.

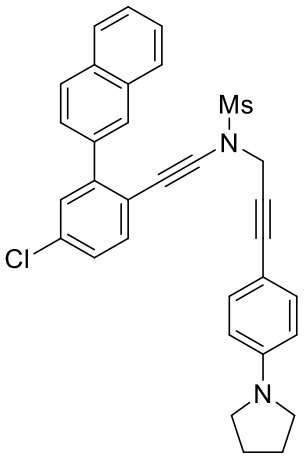
***N*-((4-fluoro-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3f)**



3f

Compound **3f** was prepared in 88% yield (459.9 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.94 – 7.86 (m, 1H), 7.84 – 7.70 (m, 3H), 7.62 – 7.52 (m, 1H), 7.49 – 7.40 (m, 2H), 7.27 – 7.12 (m, 3H), 7.07 – 6.94 (m, 1H), 6.38 (d, *J* = 8.8 Hz, 2H), 4.41 (s, 2H), 3.51 – 3.03 (m, 4H), 2.77 (s, 3H), 2.14 – 1.79 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2 (d, *J* = 248.0 Hz), 147.9, 145.8 (d, *J* = 8.0 Hz), 136.9 (d, *J* = 1.0 Hz), 134.8 (d, *J* = 9.0 Hz), 133.0(1), 132.9(9), 132.7, 128.4, 128.1, 127.6, 127.5, 127.1, 126.3, 126.2, 117.1 (d, *J* = 3.0 Hz), 116.6 (d, *J* = 23.0 Hz), 114.3 (d, *J* = 22.0 Hz), 111.3, 107.0, 88.5, 84.0, 78.9, 70.0, 47.4, 43.2, 38.4, 25.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.9 (s); IR (neat): 3052, 2968, 2235, 1607, 1521, 1462, 1362, 1265, 1118, 964; HRESIMS Calcd for $[C_{32}H_{27}FN_2NaO_2S]^+$ (M + Na^+) 545.1669, found 545.1663.

***N*-((4-chloro-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3g)**

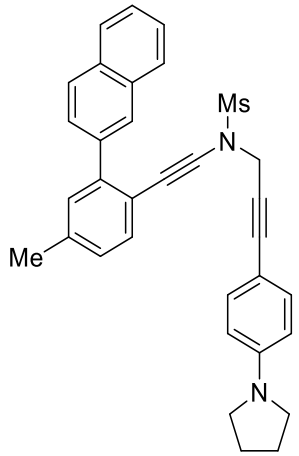


3g

Compound **3g** was prepared in 86% yield (463.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.95 – 7.85 (m, 1H), 7.85 – 7.76 (m, 2H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.54 – 7.40 (m, 4H), 7.27 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.38 (d, *J* = 8.8 Hz, 2H), 4.40 (s, 2H), 3.41 – 3.03 (m, 4H), 2.77 (s, 3H), 2.05 – 1.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 144.7, 136.6, 133.8(4), 133.8(0), 133.0, 132.9, 132.6, 129.5, 128.3, 128.0,

127.6, 127.5, 127.1, 127.0, 126.2(4), 126.1(5), 119.5, 111.2, 106.9, 88.6, 85.3, 78.8, 70.1, 47.3, 43.1, 38.4, 25.3; IR (neat): 3053, 2928, 2231, 1607, 1520, 1463, 1361, 1265, 1162, 1032; HRESIMS Calcd for $[C_{32}H_{28}ClN_2O_2S+]^+$ (M + H^+) 539.1555, found 539.1551.

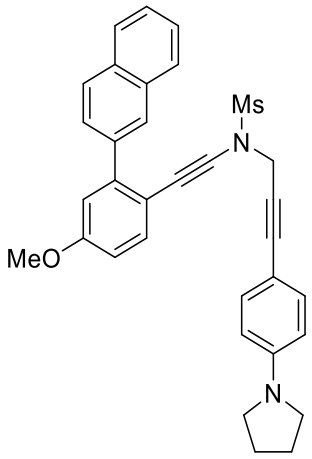
***N*-((4-methyl-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3h)**



3h

Compound **3h** was prepared in 78% yield (404.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.93 – 7.85 (m, 1H), 7.83 – 7.71 (m, 3H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.30 (s, 1H), 7.20 – 7.03 (m, 3H), 6.39 (d, *J* = 8.7 Hz, 2H), 4.41 (s, 2H), 3.39 – 3.08 (m, 4H), 2.76 (s, 3H), 2.41 (s, 3H), 2.06 – 1.91 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 143.5, 138.4, 138.2, 133.2, 133.1, 132.9, 132.5, 130.4, 128.3, 128.0, 127.9, 127.6, 127.5, 127.4, 126.0, 125.9, 118.0, 111.3, 107.2, 88.4, 83.8, 79.1, 70.9, 47.4, 43.3, 38.3, 25.4, 21.4; IR (neat): 2927, 2846, 2237, 1608, 1521, 1460, 1362, 1264, 1165, 1032; HRESIMS Calcd for $[C_{33}H_{31}N_2O_2S]^+$ (M + H^+ 519.2101, found 519.2111.

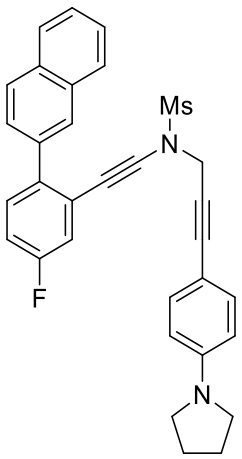
***N*-((4-methoxy-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3i)**



3i

Compound **3i** was prepared in 88% yield (470.5 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.93 – 7.84 (m, 1H), 7.83 – 7.60 (m, 3H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.49 – 7.32 (m, 2H), 7.17 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 2.7 Hz, 1H), 6.87 (dd, *J* = 8.8, 2.8 Hz, 1H), 6.40 (d, *J* = 8.8 Hz, 2H), 4.41 (s, 2H), 3.84 (s, 3H), 3.41 – 3.03 (m, 4H), 2.74 (s, 3H), 2.18 – 1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 147.9, 145.5, 138.0, 134.8, 133.1, 133.0, 132.5, 128.3, 128.0, 127.5(0), 127.4(6), 127.4, 126.1, 126.0, 115.1, 113.1, 113.0, 111.3, 107.2, 88.3, 82.9, 79.1, 70.6, 55.4, 47.4, 43.3, 38.2, 25.4; IR (neat): 3055, 2967, 2210, 1606, 1521, 1463, 1361, 1268, 1165, 1034; HRESIMS Calcd for $[C_{33}H_{31}N_2O_3S]^+$ (M + H^+) 535.2050, found 535.2029.

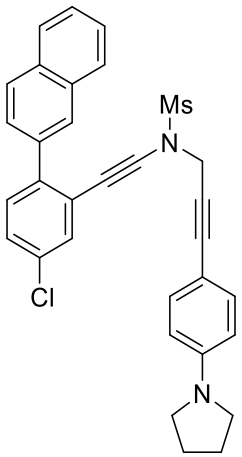
***N*-((5-fluoro-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3j)**



3j

Compound **3j** was prepared in 93% yield (486.0 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.93 – 7.85 (m, 1H), 7.85 – 7.76 (m, 2H), 7.71 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.50 – 7.36 (m, 3H), 7.27 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.17 (d, *J* = 8.8 Hz, 2H), 7.11 – 7.00 (m, 1H), 6.39 (d, *J* = 8.7 Hz, 2H), 4.39 (s, 2H), 3.34 – 3.11 (m, 4H), 2.77 (s, 3H), 2.05 – 1.80 (m, 4H); ^{13}C NMR (100 Hz, $CDCl_3$) δ 161.5 (d, *J* = 245.0 Hz), 148.0, 139.5 (d, *J* = 3.0 Hz), 137.1, 133.1, 133.0, 132.5, 131.2 (d, *J* = 8.0 Hz), 128.3, 128.0, 127.5(4), 127.4(9), 127.4, 126.1, 126.0, 122.8 (d, *J* = 10.0 Hz), 118.9 (d, *J* = 23.0 Hz), 115.4 (d, *J* = 21.0 Hz), 111.3, 107.0, 88.6, 85.4, 78.8, 70.3, 47.4, 43.2, 38.5, 25.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.5 (s); IR (neat): 3052, 2965, 2237, 1607, 1577, 1462, 1323, 1166, 1035, 967; HRESIMS Calcd for $[C_{32}H_{27}FKN_2O_2S]^+$ ($M + K^+$) 561.1409, found 561.1420.

***N*-((5-chloro-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3k)**

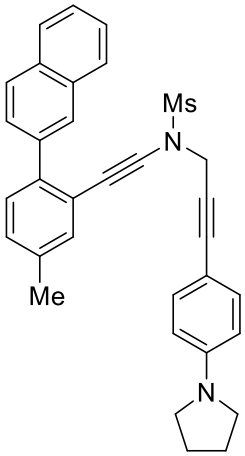


3k

Compound **3k** was prepared in 86% yield (463.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 1.4 Hz, 1H), 7.92 – 7.87 (m, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.83 – 7.78 (m, 1H), 7.72 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.56 (d, *J* = 2.4 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.34 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.18 (d, *J* = 8.8 Hz, 2H), 6.40 (d, *J* = 9.2 Hz, 2H), 4.41 (s, 2H), 3.35 – 3.19 (m, 4H), 2.80 (s, 3H), 2.06 – 1.89 (m, 4H); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 148.0, 141.6, 136.8, 133.1, 133.0, 132.9, 132.6, 132.1, 130.8, 128.3(3), 128.2(8), 128.0, 127.6, 127.5, 127.2, 126.2, 122.7, 111.3, 107.0, 88.7, 85.6, 78.8, 70.1, 47.4, 43.2, 38.6, 25.4; IR (neat): 3054, 2928, 2233, 1608, 1521, 1461, 1363, 1323, 1166, 1034; HRESIMS Calcd for $[C_{32}H_{27}ClN_2NaO_2S]^+$ (M + Na^+) 561.1374, found 561.1380.

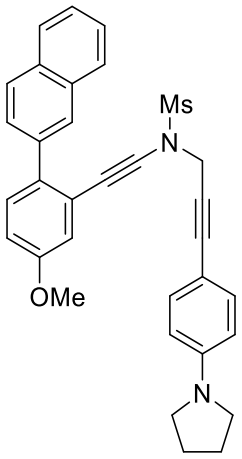
***N*-((5-methyl-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3l)**



3l

Compound **3l** was prepared in 90% yield (466.8 mg) according to the general procedure S1 as a pale yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.94 – 7.85 (m, 1H), 7.84 – 7.69 (m, 3H), 7.52 – 7.39 (m, 3H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.12 (m, 3H), 6.39 (d, *J* = 8.4 Hz, 2H), 4.41 (s, 2H), 3.33 – 3.13 (m, 4H), 2.80 (s, 3H), 2.36 (s, 3H), 2.11 – 1.85 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 140.5, 138.0, 137.9, 133.3, 133.2, 133.0, 132.4, 129.5, 129.2, 128.3, 127.9, 127.6, 127.5, 127.4, 126.0, 125.9, 120.7, 111.3, 107.2, 88.5, 84.2, 79.0, 71.2, 47.4, 43.3, 38.3, 25.4, 20.8; IR (neat): 3049, 2926, 2234, 1608, 1522, 1460, 1363, 1266, 1166, 1036; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_2S]^+$ (M + Na^+) 541.1920, found 541.1909.

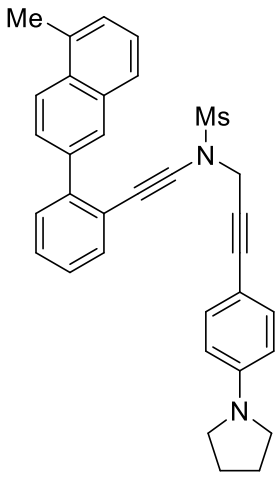
***N*-((5-methoxy-2-(naphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3m)**



3m

Compound **3m** was prepared in 82% yield (438.4 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.92 – 7.85 (m, 1H), 7.84 – 7.71 (m, 3H), 7.47 – 7.41 (m, 2H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.17 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 2.4 Hz, 1H), 6.95 (dd, *J* = 8.4, 2.8 Hz, 1H), 6.39 (d, *J* = 8.8 Hz, 2H), 4.42 (s, 2H), 3.82 (s, 3H), 3.33 – 3.13 (m, 4H), 2.79 (s, 3H), 2.06 – 1.86 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 148.0, 137.8, 136.1, 133.2, 133.0, 132.3, 130.8, 128.2, 127.8, 127.7, 127.5, 127.4, 126.0, 125.8, 121.8, 116.9, 115.2, 111.3, 107.1, 88.5, 84.3, 79.0, 71.1, 55.4, 47.4, 43.3, 38.4, 25.4; IR (neat): 3052, 2968, 2236, 1605, 1560, 1462, 1362, 1226, 1166, 1043; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ (M + Na^+) 557.1869, found 557.1839.

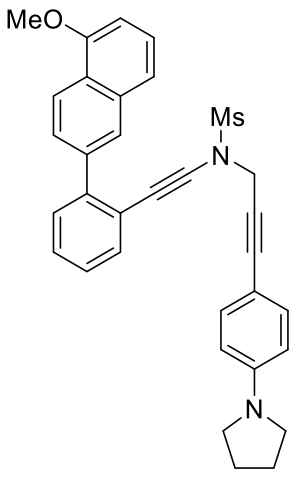
***N*-((2-(5-methylnaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3n)**



3n

Compound **3n** was prepared in 76% yield (394.2 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 1.6 Hz, 1H), 7.95 (d, *J* = 8.8 Hz, 1H), 7.86 – 7.78 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.59 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.48 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.40 – 7.26 (m, 4H), 7.17 (d, *J* = 8.8 Hz, 2H), 6.38 (d, *J* = 8.4 Hz, 2H), 4.41 (s, 2H), 3.29 – 3.06 (m, 4H), 2.78 (s, 3H), 2.62 (s, 3H), 2.04 – 1.77 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 143.3, 137.7, 133.9, 133.2, 133.0, 132.9, 131.6, 129.6, 128.6, 128.2, 127.3, 127.0, 126.8, 126.7, 125.8, 123.8, 121.0, 111.2, 107.1, 88.5, 84.5, 79.0, 70.9, 47.4, 43.3, 38.4, 25.4, 19.3; IR (neat): 3048, 2967, 2232, 1608, 1521, 1461, 1362, 1166, 1034, 919; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_2S]^+$ (M + Na^+) 541.1920, found 541.1904.

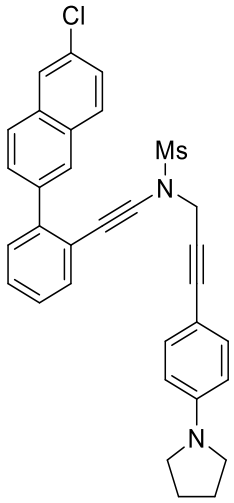
***N*-((2-(5-methoxynaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3o)**



3o

Compound **3o** was prepared in 89% yield (475.9 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.8 Hz, 1H), 8.04 (d, *J* = 1.2 Hz, 1H), 7.74 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.58 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.43 – 7.27 (m, 3H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 7.6 Hz, 1H), 6.38 (d, *J* = 8.8 Hz, 2H), 4.41 (s, 2H), 3.96 (s, 3H), 3.40 – 3.03 (m, 4H), 2.81 (s, 3H), 2.08 – 1.85 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 147.9, 143.3, 138.5, 134.2, 133.0, 132.8, 129.6, 128.2, 127.7, 127.0, 126.7, 126.1, 124.6, 121.8, 121.0, 120.6, 111.2, 107.1, 103.9, 88.5, 84.5, 79.0, 71.0, 55.4, 47.4, 43.3, 38.4, 25.4; IR (neat): 3054, 2965, 2231, 1606, 1522, 1450, 1362, 1246, 1127, 963; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ (M + Na^+) 557.1869, found 557.1904.

***N*-((2-(6-chloronaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3p)**

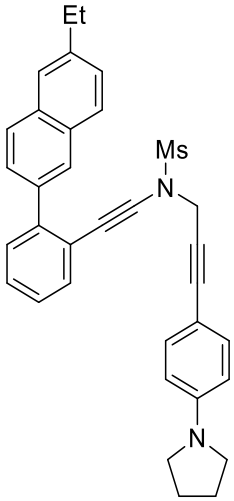


3p

Compound **3p** was prepared in 83% yield (447.5 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.86 – 7.75 (m, 2H), 7.77 – 7.68 (m, 2H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.29 (m, 3H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.41 (d, *J* = 8.8 Hz, 2H), 4.43 (s, 2H), 3.39 – 3.14 (m, 4H), 2.82 (s, 3H), 2.10 – 1.96 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 142.9, 138.3, 133.1, 133.0, 132.9(8), 131.6, 131.3, 129.9, 129.6, 128.6, 128.3,

127.9, 127.3, 126.9, 126.6, 126.2, 120.9, 111.3, 107.0, 88.5, 84.6, 79.0, 70.8, 47.4, 43.3, 38.4, 25.4; IR (neat): 3052, 2927, 2232, 1607, 1522, 1461, 1363, 1265, 1166, 964; HRESIMS Calcd for $[C_{32}H_{27}ClN_2NaO_2S]^+$ (M + Na^+) 561.1374, found 561.1347.

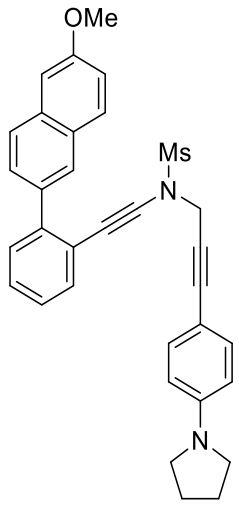
***N*-((2-(6-ethylnaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3q)**



3q

Compound **3q** was prepared in 82% yield (436.8 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.81 – 7.72 (m, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.35 – 7.28 (m, 2H), 7.18 (d, *J* = 8.8 Hz, 2H), 6.41 (d, *J* = 8.4 Hz, 2H), 4.43 (s, 2H), 3.43 – 3.21 (m, 4H), 2.90 – 2.60 (m, 5H), 2.12 – 1.90 (m, 4H), 1.32 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 143.5, 141.9, 137.1, 133.0, 132.8, 131.6, 129.6, 128.2(0), 128.1(5), 127.7, 127.5, 127.3, 127.0, 126.9, 125.1, 120.9, 111.2, 107.1, 88.5, 84.4, 79.0, 71.0, 47.3, 43.2, 38.3, 29.0, 25.3, 15.4; IR (neat): 2964, 2927, 2232, 1608, 1522, 1486, 1363, 1186, 1035, 963; HRESIMS Calcd for $[C_{34}H_{32}KN_2O_2S]^+$ (M + K^+) 571.1816, found 571.1798.

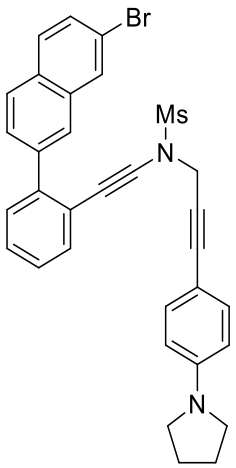
***N*-((2-(6-methoxynaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3r)**



3r

Compound **3r** was prepared in 94% yield (502.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.78 (d, *J* = 9.2 Hz, 1H), 7.76 – 7.69 (m, 2H), 7.57 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.46 (d, *J* = 7.2 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.32 – 7.27 (m, 1H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.13 – 7.05 (m, 2H), 6.37 (d, *J* = 8.8 Hz, 2H), 4.42 (s, 2H), 3.88 (s, 3H), 3.33 – 3.09 (m, 4H), 2.80 (s, 3H), 2.02 – 1.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 147.9, 143.5, 135.8, 133.7, 133.0, 132.8, 129.8, 129.5, 128.6, 128.2, 128.0, 127.8, 126.8, 126.3, 120.9, 118.8, 111.2, 107.1, 105.4, 88.4, 84.4, 79.0, 71.0, 55.2, 47.3, 43.2, 38.3, 25.3; IR (neat): 2963, 2848, 2232, 1603, 1522, 1462, 1362, 1264, 1186, 1032; HRESIMS Calcd for $[C_{33}H_{31}N_2O_3S]^+$ (M + H^+) 535.2050, found 535.2061.

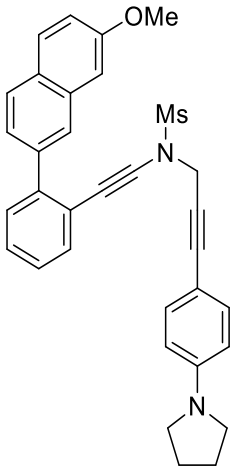
***N*-((2-(7-bromonaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3s)**



3s

Compound **3s** was prepared in 79% yield (461.0 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.93 (s, 1H), 7.84 – 7.73 (m, 2H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.5 Hz, 1H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.41 – 7.36 (m, 1H), 7.36 – 7.30 (m, 1H), 7.11 (d, *J* = 8.5 Hz, 2H), 6.38 (d, *J* = 8.5 Hz, 2H), 4.44 (s, 2H), 3.37 – 3.18 (m, 4H), 2.85 (s, 3H), 2.06 – 1.86 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.9, 142.8, 139.2, 134.3, 133.0, 132.8, 130.9, 130.2, 129.6, 129.3, 129.2, 128.3, 128.1, 127.4, 127.3, 127.0, 121.0, 120.0, 111.2, 107.0, 88.5, 84.7, 78.9, 70.8, 47.4, 43.2, 38.5, 25.4; IR (neat): 3053, 2928, 2232, 1602, 1525, 1461, 1362, 1248, 1165, 1034; HRESIMS Calcd for $[C_{32}H_{27}BrN_2NaO_2S]^+$ (M + Na^+) 605.0869, found 605.0856.

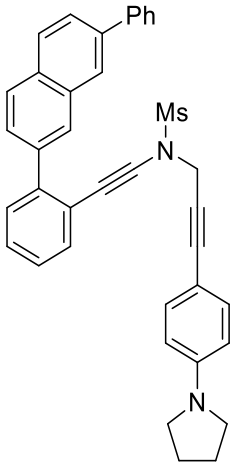
***N*-((2-(7-methoxynaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3t)**



3t

Compound **3t** was prepared in 80% yield (427.7 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.63 – 7.55 (m, 2H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.34 – 7.28 (m, 1H), 7.25 (d, *J* = 2.4 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.12 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.39 (d, *J* = 8.8 Hz, 2H), 4.42 (s, 2H), 3.85 (s, 3H), 3.35 – 3.08 (m, 4H), 2.81 (s, 3H), 2.08 – 1.85 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 147.9, 143.4, 138.5, 134.3, 133.0, 132.7, 129.6, 129.0, 128.1, 128.0, 127.3, 127.0, 125.3, 121.0, 119.0, 111.2, 107.1, 106.1, 88.5, 84.5, 79.1, 71.1, 55.2, 47.4, 43.3, 38.4, 25.4; IR (neat): 3051, 2965, 2209, 1608, 1459, 1366, 1213, 1124, 1030, 946; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ ($M + Na^+$) 557.1869, found 557.1891.

***N*-((2-(7-phenylnaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3u)**

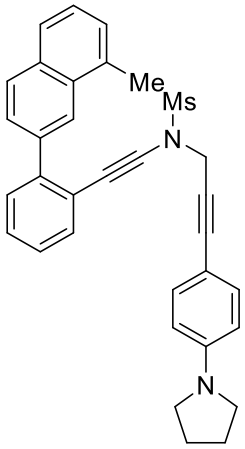


3u

Compound **3u** was prepared in 75% yield (435.6 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 8.11 (s, 1H), 7.89 – 7.82 (m, 2H), 7.80 – 7.69 (m, 4H), 7.60 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.47 – 7.42 (m, 3H), 7.41 – 7.30 (m, 3H), 7.11 (d, *J* = 8.8 Hz, 2H), 6.33 (d, *J* = 8.8 Hz, 2H), 4.41 (s, 2H), 3.22 – 3.09 (m, 4H), 2.83 (s, 3H), 1.96 – 1.86 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 143.3, 140.8, 138.6, 138.5, 133.4, 133.0, 132.7, 131.7, 129.6, 128.8, 128.3, 128.2, 128.1, 127.7, 127.3(1), 127.2(6), 127.2, 127.1, 126.1, 125.7, 121.0,

111.2, 107.0, 88.5, 84.6, 79.0, 70.9, 47.3, 43.3, 38.4, 25.3; IR (neat): 3056, 2967, 2232, 1607, 1522, 1460, 1363, 1265, 1166, 1034; HRESIMS Calcd for $[C_{38}H_{32}N_2NaO_2S]^+$ (M + Na^+) 603.2077, found 603.2054.

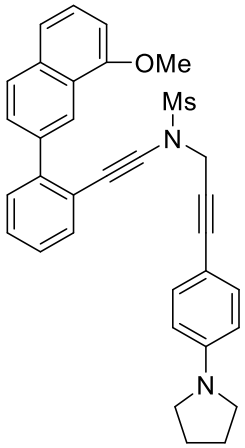
***N*-((2-(8-methylnaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3v)**



3v

Compound **3v** was prepared in 76% yield (394.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.87 – 7.73 (m, 2H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.44 – 7.27 (m, 4H), 7.13 (d, *J* = 8.8 Hz, 2H), 6.39 (d, *J* = 8.4 Hz, 2H), 4.39 (s, 2H), 3.38 – 3.12 (m, 4H), 2.76 (s, 3H), 2.71 (s, 3H), 2.06 – 1.86 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 144.1, 138.2, 134.6, 133.0, 132.8, 132.6, 132.4, 129.8, 128.2, 127.9, 127.3, 127.1, 126.8, 126.0, 125.7, 124.4, 121.2, 111.2, 107.2, 88.4, 84.5, 79.0, 70.9, 47.4, 43.3, 38.3, 25.4, 19.4; IR (neat): 3050, 2920, 2232, 1607, 1521, 1486, 1362, 1186, 1032, 961, 918; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_2S]^+$ (M + Na^+) 541.1920, found 541.1903.

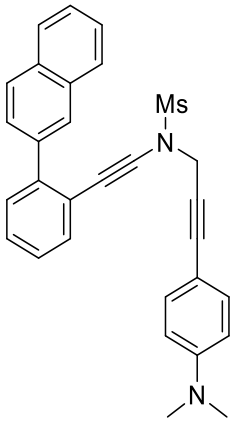
***N*-((2-(8-methoxynaphthalen-2-yl)phenyl)ethynyl)-*N*-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3w)**



3w

Compound **3w** was prepared in 88% yield (470.5 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.85 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 6.8 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.43 – 7.34 (m, 3H), 7.33 – 7.26 (m, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 6.80 (dd, *J* = 6.4, 1.6 Hz, 1H), 6.38 (d, *J* = 8.8 Hz, 2H), 4.43 (s, 2H), 3.97 (s, 3H), 3.38 – 3.00 (m, 4H), 2.86 (s, 3H), 2.16 – 1.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 147.9, 143.8, 137.5, 133.6, 133.0, 132.8, 129.8, 128.2, 128.1, 127.0, 126.1, 125.3, 122.2, 121.0, 119.9, 111.2, 107.2, 103.9, 88.3, 84.5, 79.0, 70.9, 55.4, 47.4, 43.2, 38.5, 25.4; IR (neat): 3053, 2968, 2229, 1607, 1544, 1460, 1363, 1272, 1165, 1068; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ (M + Na^+) 557.1869, found 557.1853.

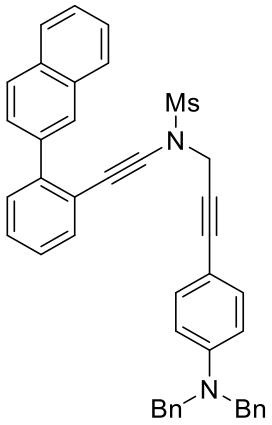
***N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-*N*-((2-(naphthalen-2-yl)phenyl)ethynyl)methanesulfonamide (3x)**



3x

Compound **3x** was prepared in 85% yield (406.8 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.81 – 7.73 (m, 1H), 7.73 – 7.62 (m, 3H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.39 – 7.29 (m, 3H), 7.28 – 7.23 (m, 1H), 7.22 – 7.16 (m, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.41 (d, *J* = 8.8 Hz, 2H), 4.29 (s, 2H), 2.79 (s, 6H), 2.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 143.3, 137.9, 133.1, 132.9, 132.8, 132.4, 129.6, 128.2, 128.1, 128.0, 127.6, 127.5, 127.4, 127.0, 126.1, 126.0, 120.9, 111.5, 108.0, 88.1, 84.4, 79.2, 70.9, 43.1, 39.9, 38.3; IR (neat): 3052, 2925, 2232, 1608, 1524, 1445, 1323, 1266, 1166, 1035; HRESIMS Calcd for $[C_{30}H_{26}KN_2O_2S]^+$ (M + K^+) 517.1347, found 517.1355.

***N*-(3-(4-(dibenzylamino)phenyl)prop-2-yn-1-yl)-*N*-((2-(naphthalen-2-yl)phenyl)ethynyl)methanesulfonamide (3y)**

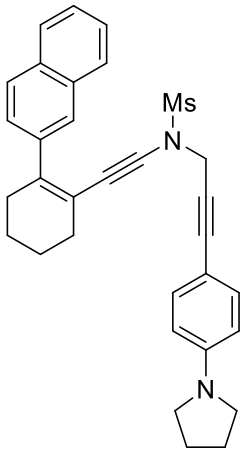


3y

Compound **3y** was prepared in 80% yield (555.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.91 – 7.81 (m, 1H), 7.80 – 7.68 (m, 3H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 6.8 Hz, 1H), 7.43 – 7.35 (m, 3H), 7.33 – 7.21 (m, 7H), 7.21 – 7.14 (m, 4H), 7.06 (d, *J* = 8.8 Hz, 2H), 6.57 (d, *J* = 9.2 Hz, 2H), 4.63 (s, 4H), 4.38 (s, 2H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 143.4, 138.1, 137.7, 133.1, 132.9, 132.5, 129.6, 128.7, 128.3, 128.2, 128.0, 127.5(4), 127.4(9), 127.4, 127.1(0), 127.0(8), 126.4, 126.0(4), 125.9(9), 121.0, 112.0, 108.8, 87.9, 84.4, 79.4, 71.0, 54.1, 43.1, 38.3; IR (neat): 3060, 2928, 2230, 1608,

1519, 1452, 1361, 1236, 1166, 1030; HRESIMS Calcd for $[C_{42}H_{34}N_2NaO_2S]^+$ (M + Na^+) 653.2233, found 653.2248.

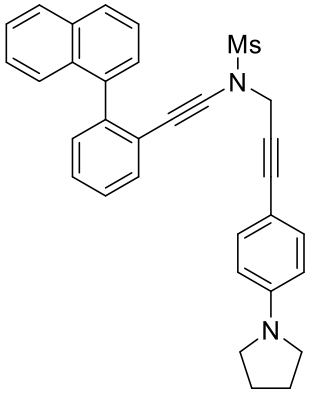
_N_-((2-(naphthalen-2-yl)cyclohex-1-en-1-yl)ethynyl)-_N_-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3z)



3z

Compound **3z** was prepared in 66% yield (335.7 mg) according to the general procedure S2 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.86 – 7.79 (m, 1H), 7.77 – 7.66 (m, 2H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.44 – 7.33 (m, 2H), 7.17 (d, *J* = 8.8 Hz, 2H), 6.40 (d, *J* = 8.8 Hz, 2H), 4.34 (s, 2H), 3.33 – 3.16 (m, 4H), 2.66 (s, 3H), 2.59 – 2.48 (m, 2H), 2.43 – 2.32 (m, 2H), 2.03 – 1.93 (m, 4H), 1.87 – 1.66 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 143.1, 140.2, 133.1, 133.0, 132.4, 128.2, 127.4, 127.1, 126.5, 126.3, 125.8, 125.6, 116.3, 111.3, 107.3, 88.2, 83.1, 79.1, 72.8, 47.4, 43.2, 37.8, 31.0, 30.9, 25.4, 22.7, 22.3; IR (neat): 3049, 2928, 2212, 1608, 1521, 1461, 1321, 1165, 1056, 962; HRESIMS Calcd for $[C_{32}H_{32}N_2NaO_2S]^+$ (M + Na^+) 531.2077, found 531.2079.

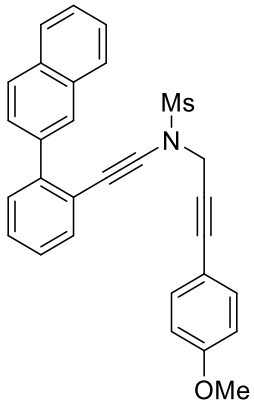
_N_-((2-(naphthalen-1-yl)phenyl)ethynyl)-_N_-(3-(4-(pyrrolidin-1-yl)phenyl)prop-2-yn-1-yl)methanesulfonamide (3aa)



3aa

Compound **3aa** was prepared in 90% yield (454.1 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.81 (m, 1H), 7.81 – 7.74 (m, 1H), 7.65 – 7.56 (m, 2H), 7.49 – 7.44 (m, 2H), 7.44 – 7.35 (m, 5H), 7.15 (d, *J* = 8.8 Hz, 2H), 6.45 (d, *J* = 8.8 Hz, 2H), 4.20 – 3.85 (m, 2H), 3.43 – 3.03 (m, 4H), 2.41 (s, 3H), 2.13 – 1.90 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 142.7, 138.8, 133.4, 133.1, 131.8, 131.7, 130.4, 128.0, 127.8, 127.4, 126.3, 126.0, 125.7, 125.4, 122.9, 111.2, 107.4, 88.0, 84.9, 78.7, 70.4, 47.5, 43.1, 37.8, 25.4; IR (neat): 3048, 2843, 2232, 1605, 1524, 1461, 1360, 1265, 1164, 1035; HRESIMS Calcd for $[C_{32}H_{28}N_2NaO_2S]^+$ (M + Na^+) 527.1764, found 527.1780.

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

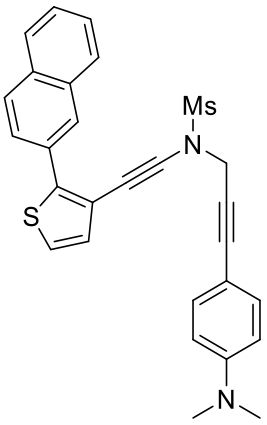


3ab

Compound **3ab** was prepared in 89% yield (395.7 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.92 –

7.83 (m, 1H), 7.83 – 7.68 (m, 3H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.48 – 7.38 (m, 3H), 7.38 – 7.32 (m, 1H), 7.32 – 7.24 (m, 1H), 7.18 (d, *J* = 8.8 Hz, 2H), 6.73 (d, *J* = 8.8 Hz, 2H), 4.38 (s, 2H), 3.72 (s, 3H), 2.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 143.3, 137.9, 133.2, 133.0, 132.7, 132.4, 129.6, 128.3, 128.2, 127.9, 127.4(2), 127.4(1), 127.3, 127.0, 126.0(1), 125.9(7), 120.8, 113.9, 113.5, 86.8, 84.2, 80.1, 71.1, 55.1, 42.7, 38.2; IR (neat): 3057, 2939, 2233, 1605, 1568, 1464, 1324, 1251, 1164, 1033; HRESIMS Calcd for $[C_{29}H_{23}NNaO_3S]^+$ (M + Na^+) 488.1291, found 488.1295.

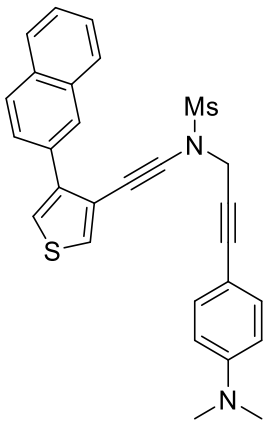
_N_-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-_N_-((2-(naphthalen-2-yl)thiophen-3-yl)ethynyl)methanesulfonamide (3ac)



3ac

Compound **3ac** was prepared in 90% yield (436.2 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.96 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.93 – 7.88 (m, 1H), 7.80 – 7.66 (m, 2H), 7.43 – 7.39 (m, 2H), 7.23 – 7.16 (m, 3H), 7.14 (d, *J* = 5.5 Hz, 1H), 6.48 (d, *J* = 9.0 Hz, 2H), 4.56 (s, 2H), 3.13 (s, 3H), 2.90 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.4, 145.9, 133.3, 132.9, 132.8, 132.0, 131.0, 128.4, 128.2, 127.5, 126.4(1), 126.3(6), 126.2, 125.8, 123.7, 116.9, 111.6, 107.9, 88.4, 83.6, 79.2, 67.3, 43.3, 40.0, 38.7; IR (neat): 3442, 2231, 1607, 1520, 1354, 1323, 1226, 1166, 1043, 965; HRESIMS Calcd for $[C_{28}H_{24}KN_2O_2S_2]^+$ (M + K^+) 523.0911, found 523.0907.

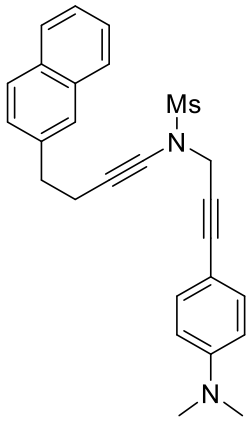
_N_-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-_N_-((4-(naphthalen-2-yl)thiophen-3-yl)ethynyl)methanesulfonamide (3ad)



3ad

Compound **3ad** was prepared in 85% yield (411.9 mg) according to the general procedure S1 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.92 – 7.85 (m, 1H), 7.80 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.79 – 7.72 (m, 2H), 7.58 (d, *J* = 3.5 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.36 (d, *J* = 3.5 Hz, 1H), 7.15 (d, *J* = 9.0 Hz, 2H), 6.49 (d, *J* = 9.0 Hz, 2H), 4.51 (s, 2H), 3.00 (s, 3H), 2.91 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.4, 143.4, 133.3, 132.9, 132.7, 132.6, 130.7, 128.2, 127.8, 127.5, 126.8, 126.4, 126.1, 125.9, 122.4, 120.6, 111.6, 108.0, 88.3, 83.1, 79.2, 66.6, 43.3, 40.0, 38.6; IR (neat): 2925, 2242, 2212, 1607, 1522, 1445, 1323, 1266, 1165, 1036; HRESIMS Calcd for $[C_{28}H_{24}KN_2O_2S_2]^+$ (M + K^+) 523.0911, found 523.0906.

***N*-(3-(4-(dimethylamino)phenyl)prop-2-yn-1-yl)-*N*-(4-(naphthalen-2-yl)but-1-yn-1-yl)methanesulfonamide (3ae)**

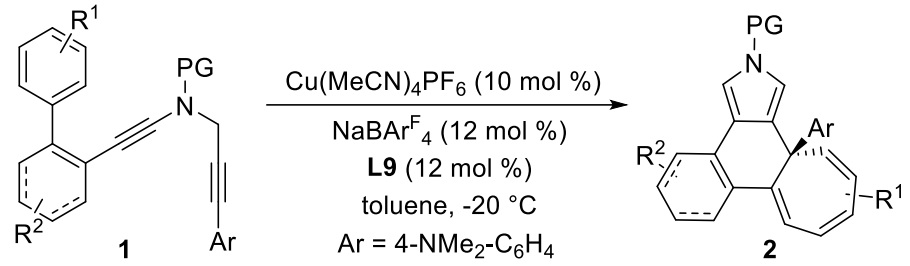


3ae

Compound **3ae** was prepared in 92% yield (396.1 mg) according to the general procedure S2 as a pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 – 7.71 (m, 1H), 7.71 – 7.67 (m, 2H), 7.65 (s, 1H), 7.41 – 7.31 (m, 3H), 7.26 (d, *J* = 9.0 Hz, 2H), 6.54 (d, *J* = 9.0 Hz, 2H), 4.37 (s, 2H), 2.99 – 2.93 (m, 2H), 2.91 (s, 3H), 2.87 (s, 6H), 2.71 – 2.61 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.3, 137.8, 133.3, 132.8, 131.9, 127.7, 127.4, 127.3, 127.0, 126.7, 125.7, 125.1, 111.5 108.0, 87.8, 79.3, 73.6, 69.9, 43.0, 39.8, 37.6, 35.0, 20.4; IR (neat): 2926, 2858, 2213, 1608, 1523, 1445, 1359, 1272, 1191, 1045; HRESIMS Calcd for $[C_{26}H_{27}N_2O_2S]^+$ ($M + H^+$) 431.1788, found 431.1787.

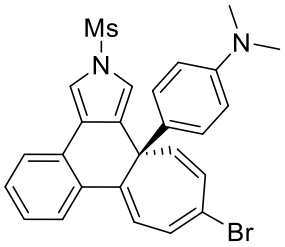
4. General Procedures for Copper-Catalyzed Controllable Cyclization of Diynes

4.1. General Procedure for Synthesis of Chiral Cycloheptatrienes 2



To an oven-dried Schlenk tube with a stir bar were sequentially added $Cu(MeCN)_4PF_6$ (0.01 mmol, 3.8 mg), **L9** (0.012 mmol, 8.8 mg) and $NaBAr^F_4$ (0.012 mmol, 10.6 mg, white crystal) under argon atmosphere. After injecting toluene (1 mL) into the Schlenk tube, the mixture was stirred at 25 °C for 2 h. Then the mixture reaction was cooled to -20 °C, and *N*-propargyl ynamide **1** (0.1 mmol) in toluene (1 mL) was added into the reaction mixture dropwise. The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was directly purified by column chromatography on silica gel (eluent: PE/EtOAc) to afford the desired chiral cycloheptatriene **2**.

(*S*)-4-(10-bromo-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2a)

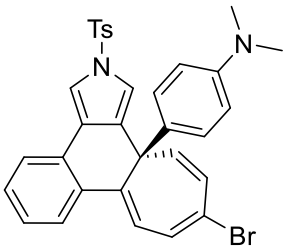


2a

Compound **2a** was prepared in 95% yield (48.2 mg) according to the general procedure. Pale yellow solid (mp 131–132 °C). $[\alpha]_D^{25}$ = -221.1° (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 40/60 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.54 min (minor), 7.87 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.61 (m, 1H), 7.61 – 7.52 (m, 1H), 7.39 (d, *J* = 2.0 Hz, 1H), 7.31 – 7.25 (m, 1H), 7.24 – 7.19 (m, 1H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 1H), 6.72 (d, *J* = 2.4 Hz,

1H), 6.61 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.54 (d, *J* = 9.2 Hz, 1H), 6.45 (d, *J* = 8.8 Hz, 2H), 4.78 (d, *J* = 9.2 Hz, 1H), 3.09 (s, 3H), 2.85 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 132.8, 132.0, 131.9, 131.4, 128.0, 127.6(4), 127.6(1), 127.3, 127.0, 123.4, 122.2, 121.8, 121.7, 118.9, 113.1, 111.5, 109.9, 42.8(2), 42.7(6), 40.5; IR (neat): 2923, 1609, 1518, 1473, 1398, 1364, 1172, 1054, 984; HRESIMS Calcd for $[C_{26}H_{23}BrN_2NaO_2S]^+$ (M + Na^+) 529.0556, found 529.0568.

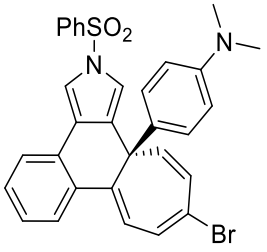
(*S*)-4-(10-bromo-2-tosylbenzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2b)



2b

Compound **2b** was prepared in 95% yield (55.4 mg) according to the general procedure. Pale yellow solid (mp 186–187 °C). $[\alpha]_D^{25}$ = -134.6º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.05 min (minor), 14.83 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.5 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.54 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.38 (d, *J* = 2.5 Hz, 1H), 7.24 – 7.13 (m, 4H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 2.0 Hz, 1H), 6.60 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.51 (d, *J* = 9.0 Hz, 1H), 6.43 (d, *J* = 9.0 Hz, 2H), 4.73 (d, *J* = 9.0 Hz, 1H), 2.85 (s, 6H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 144.9, 135.9, 133.0, 132.0, 131.8, 129.9, 127.9, 127.5(3), 127.4(7), 127.4(4), 127.3(8), 127.3, 126.6, 123.5, 122.3, 122.0, 121.7, 119.6, 113.4, 113.0, 111.6, 111.1, 43.1, 40.6, 21.6; IR (neat): 3131, 2922, 1611, 1516, 1445, 1373, 1283, 1172, 1091, 982; HRESIMS Calcd for $[C_{32}H_{27}BrN_2NaO_2S]^+$ (M + Na^+) 605.0869, found 605.0860.

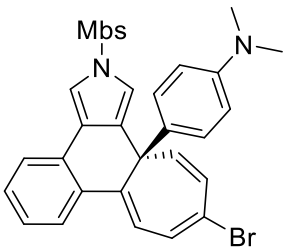
(*S*)-4-(10-bromo-2-(phenylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2c)



2c

Compound **2c** was prepared in 95% yield (54.1 mg) according to the general procedure. Pale yellow solid (mp 228–229 °C). $[\alpha]_D^{25}$ = -155.0º (c = 1.0, $CHCl_3$). 91% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.95 min (minor), 13.34 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.6 Hz, 2H), 7.63 – 7.49 (m, 3H), 7.45 – 7.37 (m, 3H), 7.23 – 7.15 (m, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 2.0 Hz, 1H), 6.60 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.51 (d, *J* = 9.2 Hz, 1H), 6.43 (d, *J* = 8.8 Hz, 2H), 4.72 (d, *J* = 9.2 Hz, 1H), 2.85 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 138.8, 133.7, 133.3, 132.0, 131.9, 131.7, 129.3, 128.0, 127.6, 127.4(3), 127.4(0), 127.2, 126.5, 123.5, 122.3, 122.1, 121.7, 119.7, 113.4, 112.7, 111.6, 110.9, 43.1, 40.6; IR (neat): 3129, 3027, 1610, 1516, 1477, 1372, 1216, 1173, 1054, 969; HRESIMS Calcd for $[C_{31}H_{25}BrN_2NaO_2S]^+$ (M + Na^+) 591.0712, found 591.0712.

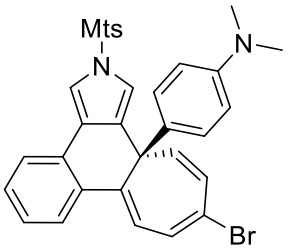
(*S*)-4-(10-bromo-2-((4-methoxyphenyl)sulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2d)



2d

Compound **2d** was prepared in 96% yield (57.6 mg) according to the general procedure. Pale yellow solid (mp 127–128 °C). $[\alpha]_D^{25}$ = -157.6º (c = 1.0, $CHCl_3$). 92% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 11.94 min (minor), 18.65 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 9.0 Hz, 2H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.55 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.25 – 7.14 (m, 2H), 6.96 – 6.84 (m, 4H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.74 (d, *J* = 2.0 Hz, 1H), 6.61 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.52 (d, *J* = 9.0 Hz, 1H), 6.44 (d, *J* = 8.5 Hz, 2H), 4.74 (d, *J* = 9.0 Hz, 1H), 3.81 (s, 3H), 2.86 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.7, 148.7, 132.9, 132.0, 131.8, 130.3, 129.0, 127.9, 127.6, 127.5, 127.4(4), 127.3(9), 127.3(7), 123.5, 122.3, 121.9, 121.7, 119.5, 114.5, 113.3, 111.6, 111.1, 55.6, 43.2, 40.6; IR (neat): 3132, 2924, 1610, 1517, 1459, 1370, 1264, 1165, 1053, 969; HRESIMS Calcd for $[C_{32}H_{27}BrN_2NaO_3S]^+$ (M + Na^+) 621.0818, found 621.0866.

(*S*)-4-(10-bromo-2-(mesitylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2e)

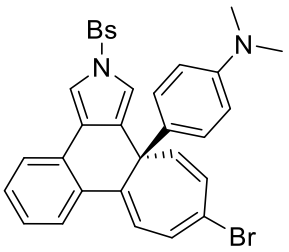


2e

Compound **2e** was prepared in 99% yield (60.5 mg) according to the general procedure. Pale yellow solid (mp 120–121 °C). $[\alpha]_D^{25}$ = -170.9º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.48 min (minor), 11.96 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.56 (m, 1H), 7.50 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.23 – 7.11 (m, 3H), 6.91 (s, 2H), 6.89 – 6.82 (m, 3H), 6.75 (d, *J* = 2.4 Hz, 1H), 6.63 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.53 (d, *J* = 9.2 Hz, 1H), 6.42 (d, *J* = 8.8 Hz, 2H), 4.87 (d, *J* = 9.2 Hz, 1H), 2.84 (s, 6H), 2.46 (s, 6H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 144.1, 140.2, 132.6, 132.3, 132.1, 131.6, 130.8, 127.9, 127.6, 127.4(8), 127.4(5), 127.2, 123.3, 122.5, 121.4, 120.7, 119.6,

115.7, 113.4, 112.4, 111.7, 43.7, 40.6, 22.6, 21.0; IR (neat): 2962, 2925, 1608, 1516, 1446, 1361, 1261, 1171, 1054, 812; HRESIMS Calcd for $[C_{34}H_{31}BrN_2NaO_2S]^+$ (M + Na^+) 633.1182, found 633.1174.

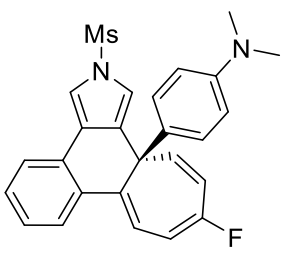
(*S*)-4-(10-bromo-2-((4-bromophenyl)sulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2f)



2f

Compound **2f** was prepared in 99% yield (64.2 mg) according to the general procedure. Pale yellow solid (mp 194–195 °C). $[\alpha]_D^{25}$ = -156.1º (c = 1.0, $CHCl_3$). 92% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.35 min (minor), 10.56 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.0 Hz, 1H), 7.56 – 7.46 (m, 5H), 7.36 (d, *J* = 2.0 Hz, 1H), 7.24 – 7.16 (m, 2H), 6.87 – 6.80 (m, 3H), 6.74 (d, *J* = 2.2 Hz, 1H), 6.61 (dd, *J* = 8.5, 1.0 Hz, 1H), 6.52 (d, *J* = 9.0 Hz, 1H), 6.42 (d, *J* = 9.0 Hz, 2H), 4.76 (d, *J* = 9.0 Hz, 1H), 2.86 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 137.6, 133.9, 132.6, 132.1, 131.9, 131.7, 128.9, 128.0, 127.7, 127.6, 127.5, 127.3, 127.0, 123.6, 122.6, 122.4, 121.8, 119.8, 113.4, 113.2, 111.5, 111.3, 43.2, 40.5; IR (neat): 3128, 2925, 1610, 1516, 1456, 1375, 1265, 1175, 1053, 813; HRESIMS Calcd for $[C_{31}H_{24}Br_2N_2NaO_2S]^+$ (M + Na^+) 668.9817, found 668.9850.

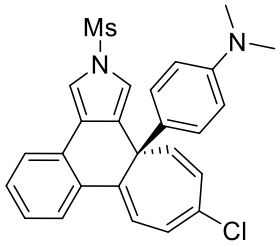
(*S*)-4-(10-fluoro-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2g)



2g

Compound **2g** was prepared in 86% yield (38.4 mg) according to the general procedure. Pale yellow solid (mp 147–148 °C). $[\alpha]_D^{25}$ = -92.7º (c = 1.0, $CHCl_3$). 97% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.17 min (minor), 8.63 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.61 (m, 1H), 7.61 – 7.49 (m, 1H), 7.38 (d, *J* = 2.0 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.24 – 7.16 (m, 1H), 7.08 (dd, *J* = 8.4, 5.6 Hz, 1H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.77 (d, *J* = 2.4 Hz, 1H), 6.42 (d, *J* = 8.8 Hz, 2H), 6.39 – 6.29 (m, 1H), 6.18 (ddd, *J* = 15.2, 8.4, 2.4 Hz, 1H), 5.28 (dd, *J* = 9.6, 5.6 Hz, 1H), 3.08 (s, 3H), 2.83 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0 (d, *J* = 246.0 Hz), 148.7, 133.3, 132.6, 131.8, 127.7, 127.6, 127.3(0), 127.2(6), 126.9, 123.4, 121.9, 120.0 (d, *J* = 11.0 Hz), 118.9, 118.2 (d, *J* = 13.0 Hz), 116.2 (d, *J* = 3.0 Hz), 116.0 (d, *J* = 31.0 Hz), 113.6 (d, *J* = 28.0 Hz), 113.0, 111.4, 44.5, 42.7, 40.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -104.7 – -105.4 (m); IR (neat): 2958, 2926, 1610, 1518, 1418, 1365, 1261, 1147, 1055, 984; HRESIMS Calcd for $[C_{26}H_{23}FKN_2O_2S]^+$ (M + K^+) 485.1096, found 485.1080.

(*S*)-4-(10-chloro-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2h)

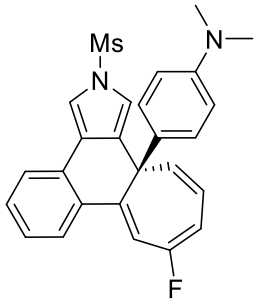


2h

Compound **2h** was prepared in 89% yield (41.2 mg) according to the general procedure. Pale yellow solid (mp 142–143 °C). $[\alpha]_D^{25}$ = -249.2º (c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.14 min (minor), 8.65 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 – 7.56 (m, 2H), 7.39 (d, *J* = 2.5 Hz, 1H), 7.29 – 7.24 (m, 2H), 6.97 – 6.89 (m, 3H), 6.72 (d, *J* = 2.0 Hz, 1H), 6.45 (d, *J* = 9.0 Hz, 2H), 6.42 – 6.35 (m, 2H), 4.80 (d, *J* = 9.0 Hz, 1H), 3.08 (s, 3H), 2.85 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 132.8, 132.7,

132.1, 131.4, 128.8, 127.9, 127.8, 127.7, 127.6, 127.0, 124.8, 123.4, 121.7, 121.6, 119.0, 113.2, 111.5, 108.1, 42.7, 42.4, 40.5; IR (neat): 3025, 2924, 1610, 1516, 1364, 1172, 1055, 984, 894; HRESIMS Calcd for $[C_{26}H_{23}ClN_2NaO_2S]^+$ (M + Na^+) 485.1061, found 485.1053.

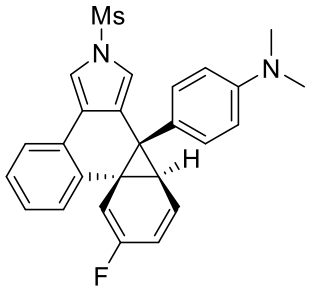
(*S*)-4-(9-fluoro-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2i)



2i

Compound **2i** was prepared in 50% yield (22.3 mg) according to the general procedure. Pale yellow solid (mp 195–196 °C). $[\alpha]_D^{25}$ = -135.7° (c = 1.0, $CHCl_3$). 98% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.21 min (minor), 10.99 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.32 (d, *J* = 2.4 Hz, 1H), 7.27 – 7.19 (m, 2H), 6.94 (d, *J* = 11.2 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.72 (d, *J* = 2.4 Hz, 1H), 6.39 – 6.33 (m, 3H), 6.12 – 6.03 (m, 1H), 5.04 (d, *J* = 9.2 Hz, 1H), 3.03 (s, 3H), 2.78 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0 (d, *J* = 241.0 Hz), 148.7, 133.5, 132.8, 130.8 (d, *J* = 2.0 Hz), 128.7, 127.8, 127.6 (d, *J* = 11.0 Hz), 127.4, 123.5, 123.3, 121.8, 121.6 (d, *J* = 13.0 Hz), 118.8, 115.7 113.1, 112.8, 112.4 (d, *J* = 8.0 Hz), 112.1, 111.5, 45.0, 42.8, 40.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.0 – -101.2 (m); IR (neat): 2927, 2852, 1608, 1517, 1445, 1363, 1222, 1172, 1051, 985; HRESIMS Calcd for $[C_{26}H_{23}FN_2NaO_2S]^+$ (M + Na^+) 469.1356, found 469.1350.

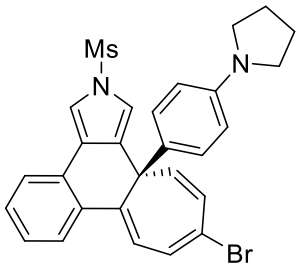
4-((3b*S*,3c*S*,7a*R*)-4-fluoro-2-(methylsulfonyl)-2*H*-benzo[*e*]benzo[1,3]cyclopropa[1,2-*g*]isoindol-3b(3c*H*)-yl)-*N*,*N*-dimethylaniline (2i′)



2i′

Compound **2i′** was prepared in 49% yield (21.9 mg) according to the general procedure. Pale yellow solid (mp 86–87 °C). $[\alpha]_D^{25}$ = -45.3º (c = 1.0, $CHCl_3$). 98% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.68 min (minor), 9.79 min (major)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 – 7.49 (m, 1H), 7.41 – 7.36 (m, 1H), 7.35 (d, *J* = 2.4 Hz, 1H), 7.25 – 7.19 (m, 2H), 6.97 (d, *J* = 8.4 Hz, 2H), 6.62 (d, *J* = 2.4 Hz, 1H), 6.48 (d, *J* = 8.4 Hz, 2H), 6.22 (d, *J* = 9.0 Hz, 1H), 5.97 – 5.86 (m, 1H), 5.62 – 5.46 (m, 1H), 3.05 (s, 3H), 3.01 (d, *J* = 10.8 Hz, 1H), 2.84 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.4 (d, *J* = 253.5 Hz), 149.0, 135.0, 130.6, 130.2, 129.4, 127.6, 127.2, 126.0 (d, *J* = 9.0 Hz), 125.9, 123.2, 121.4, 121.2 (d, *J* = 3.0 Hz), 119.0, 113.6, 111.6, 105.9 (d, *J* = 24.0 Hz), 67.9, 57.9, 42.8, 40.5, 28.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.4 (s); IR (neat): 2926, 1666, 1519, 1479, 1366, 1225, 1173, 1075, 983, 846; HRESIMS Calcd for $[C_{26}H_{23}FN_2NaO_2S]^+$ (M + Na^+) 469.1356, found 469.1358.

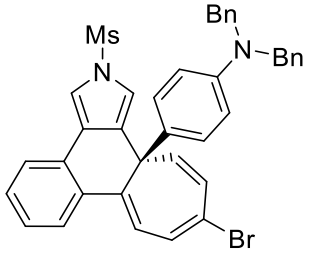
(*S*)-10-bromo-2-(methylsulfonyl)-12a-(4-(pyrrolidin-1-yl)phenyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2j)



2j

Compound **2j** was prepared in 94% yield (50.1 mg) according to the general procedure. Pale yellow solid (mp 156–157 °C). $[\alpha]_D^{25}$ = -247.4º (c = 1.0, $CHCl_3$). 92% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.66 min (minor), 9.63 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.55 (m, 2H), 7.39 (d, *J* = 2.4 Hz, 1H), 7.30 – 7.25 (m, 1H), 7.24 – 7.20 (m, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.72 (d, *J* = 2.4 Hz, 1H), 6.60 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.54 (d, *J* = 8.8 Hz, 1H), 6.28 (d, *J* = 8.8 Hz, 2H), 4.71 (d, *J* = 9.2 Hz, 1H), 3.22 – 3.13 (m, 4H), 3.08 (s, 3H), 1.99 – 1.85 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 132.9, 132.1, 131.9, 130.0, 127.9, 127.8, 127.7, 127.6, 127.2, 127.0, 123.4, 122.0, 121.9, 121.7, 118.9, 113.1, 110.5, 109.8, 108.3, 47.5, 42.8, 42.5, 25.4; IR (neat): 3020, 2926, 1611, 1516, 1462, 1367, 1246, 1172, 1055, 984; HRESIMS Calcd for $[C_{28}H_{25}BrKN_2O_2S]^+$ ($M + K^+$) 571.0452, found 571.0437.

(*S*)-*N*,*N*-dibenzyl-4-(10-bromo-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)aniline (2k)

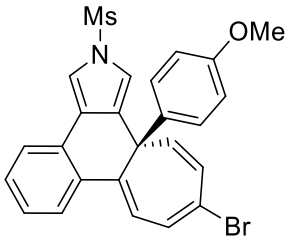


2k

Compound **2k** was prepared in 99% yield (65.3 mg) according to the general procedure. Pale yellow solid (mp 128–129 °C). $[\alpha]_D^{25}$ = -200.4º (c = 1.0, $CHCl_3$). 80% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.48 min (minor), 8.29 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.52 (m, 2H), 7.38 (d, *J* = 2.4 Hz, 1H), 7.31 – 7.23 (m, 6H), 7.22 – 7.16 (m, 6H), 6.89 – 6.80 (m, 3H), 6.75 (d, *J* = 2.0 Hz, 1H), 6.61 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.53 – 6.38 (m, 3H), 4.74 (d, *J* = 9.2 Hz, 1H), 4.51 (dd, *J* = 28 Hz, 16.8 Hz, 4H), 3.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 138.7, 132.5, 132.1, 131.9, 131.7, 128.4, 128.0, 127.8,

127.6, 127.2, 127.0, 126.8, 126.7, 123.4, 122.1, 121.8, 121.7, 119.0, 113.1, 111.8, 111.2, 109.8, 54.2, 42.7(3), 42.7(2); IR (neat): 3133, 2927, 1609, 1452, 1362, 1262, 1174, 1055, 983; HRESIMS Calcd for $[C_{38}H_{31}BrN_2NaO_2S]^+$ (M + Na^+) 681.1182, found 681.1175.

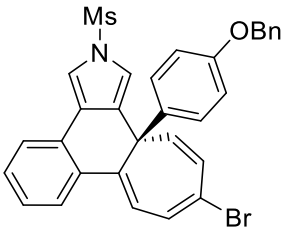
(*S*)-10-bromo-12a-(4-methoxyphenyl)-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2l)



2l

Compound **2l** was prepared in 99% yield (48.9 mg) according to the general procedure except in DCM at 20 °C for 33 h. Pale yellow solid (mp 222–223 °C). $[\alpha]_D^{25}$ = -248.3º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.96 min (minor), 9.17 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.2 Hz, 1H), 7.60 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.41 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.25 (m, 2H), 6.99 (d, *J* = 9.2 Hz, 2H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.70 (d, *J* = 2.4 Hz, 1H), 6.67 – 6.59 (m, 3H), 6.56 (d, *J* = 9.2 Hz, 1H), 4.90 (d, *J* = 9.2 Hz, 1H), 3.72 (s, 3H), 3.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 135.8, 132.4, 132.3, 131.6, 128.2, 127.8, 127.7, 127.6, 127.5, 127.1, 123.5, 122.6, 121.7, 119.0, 114.1, 113.2, 112.7, 112.2, 55.1, 43.6, 42.8; IR (neat): 3023, 2928, 1606, 1507, 1464, 1366, 1247, 1171, 1077, 984; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_3S]^+$ (M + Na^+) 516.0239, found 516.0233.

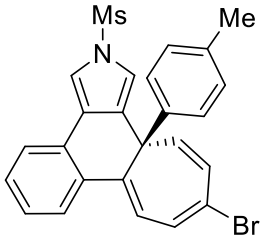
(*S*)-12a-(4-(benzyloxy)phenyl)-10-bromo-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2m)



2m

Compound **2m** was prepared in 86% yield (49.1 mg) according to the general procedure except in DCM at 20 °C for 32 h. Pale yellow solid (mp 150–151 °C). $[\alpha]_D^{25}$ = -211.5 (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.91 min (minor), 10.59 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.46 – 7.24 (m, 8H), 6.99 (d, *J* = 7.2 Hz, 2H), 6.90 (d, *J* = 7.6 Hz, 1H), 6.75 – 6.60 (m, 4H), 6.56 (d, *J* = 9.2 Hz, 1H), 4.94 (s, 2H), 4.91 (s, 1H), 3.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 137.0, 136.2, 132.3, 131.5, 128.5, 128.2, 127.9, 127.8, 127.7, 127.6, 127.5, 127.1, 123.5, 122.6, 121.6, 119.1, 114.8, 113.6, 113.2, 112.8, 69.9, 43.7, 42.8; IR (neat): 3023, 2928, 1606, 1507, 1463, 1366, 1247, 1172, 1055, 984; HRESIMS Calcd for $[C_{31}H_{24}BrNNaO_3S]^+$ (M + Na^+) 592.0552, found 592.0542.

(*S*)-10-bromo-2-(methylsulfonyl)-12a-(*p*-tolyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2n)

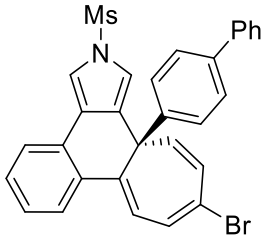


2n

Compound **2n** was prepared in 88% yield (42.1 mg) according to the general procedure except in DCM at 20 °C for 144 h. Pale yellow solid (mp 236–237 °C). $[\alpha]_D^{25}$ = -253.6º (c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.71 min (minor), 7.74 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 1H), 7.60 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.24 (m, 2H), 6.98 – 6.90 (m, 3H), 6.86 (d, *J* = 8.0 Hz, 2H),

6.71 (d, *J* = 2.0 Hz, 1H), 6.64 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.57 (d, *J* = 9.2 Hz, 1H), 5.00 (d, *J* = 9.2 Hz, 1H), 3.09 (s, 3H), 2.22 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 135.6, 132.3, 131.4, 128.3, 128.0, 127.7, 127.6, 127.5, 127.2, 126.5, 123.5, 122.8, 121.7, 121.5, 119.1, 116.6, 114.5, 113.2, 44.5, 42.8, 20.9; IR (neat): 3021, 2926, 1647, 1525, 1472, 1362, 1262, 1172, 1054, 983; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_2S]^+$ (M + Na^+) 500.0290, found 500.0274.

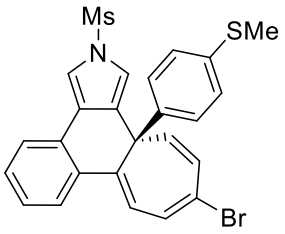
(*S*)-12a-([1,1'-biphenyl]-4-yl)-10-bromo-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2o)



2o

Compound **2o** was prepared in 94% yield (50.8 mg) according to the general procedure except in DCM at 20 °C for 242 h. Pale yellow solid (mp 127–128 °C). $[\alpha]_D^{25}$ = -162.6º (c = 1.0, $CHCl_3$). 89% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.74 min (minor), 10.65 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.61 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.42 (d, *J* = 2.0 Hz, 1H), 7.40 – 7.34 (m, 2H), 7.33 – 7.24 (m, 5H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 2.4 Hz, 1H), 6.68 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.61 (d, *J* = 9.2 Hz, 1H), 5.12 (d, *J* = 9.2 Hz, 1H), 3.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 140.5, 138.7, 132.6, 132.0, 131.2, 128.6, 128.4, 127.9, 127.8, 127.4, 127.2, 127.0, 126.9, 126.8, 125.9, 123.5, 123.1, 121.7, 121.4, 119.2, 118.9, 116.5, 113.3, 45.2, 42.8; IR (neat): 3027, 2926, 1600, 1485, 1404, 1338, 1264, 1173, 1055, 984; HRESIMS Calcd for $[C_{30}H_{22}BrNNaO_2S]^+$ (M + Na^+) 562.0447, found 562.0445.

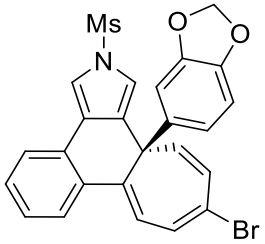
(*S*)-10-bromo-2-(methylsulfonyl)-12a-(4-(methylthio)phenyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2p)



2p

Compound **2p** was prepared in 85% yield (43.4 mg) according to the general procedure except in DCM at 20 °C for 69 h. Pale yellow solid (mp 149–150 °C). $[\alpha]_D^{25}$ = -184.9º (c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.86 min (minor), 11.53 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.41 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.25 (m, 2H), 7.03 – 6.91 (m, 5H), 6.70 (d, *J* = 2.4 Hz, 1H), 6.66 (d, *J* = 7.6 Hz, 1H), 6.58 (d, *J* = 9.6 Hz, 1H), 5.03 (d, *J* = 9.2 Hz, 1H), 3.10 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 135.7, 132.5, 132.0, 131.2, 128.4, 127.8, 127.5, 127.2, 127.1, 125.5, 123.5, 123.0, 121.6, 121.4, 119.1, 117.5, 115.2, 113.3, 44.7, 42.9, 15.6; IR (neat): 3020, 2925, 1592, 1524, 1438, 1367, 1262, 1173, 1055, 984; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_2S_2]^+$ (M + Na^+) 532.0011, found 532.0007.

(*S*)-12a-(benzo[*d*][1,3]dioxol-5-yl)-10-bromo-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2q)

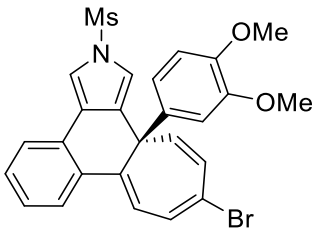


2q

Compound **2q** was prepared in 99% yield (50.3 mg) according to the general procedure except in DCM at 30 °C for 24 h. Pale yellow solid (mp 222–223 °C). $[\alpha]_D^{25}$ = -232.2º (c = 1.0, $CHCl_3$). 92% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.62 min (minor), 9.81 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 1H), 7.59 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.33 – 7.24 (m, 2H), 6.94 (d, *J* = 8.0 Hz, 1H), 6.75 (d, *J* = 2.0 Hz,

1H), 6.71 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.63 – 6.39 (m, 4H), 5.84 (dd, *J* = 3.6, 1.2 Hz, 2H), 4.99 (d, *J* = 9.2 Hz, 1H), 3.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.7, 145.7, 137.9, 132.4, 132.1, 131.2, 128.3, 127.7, 127.6, 127.5, 127.1, 123.5, 122.9, 121.6, 121.5, 119.6, 119.0, 116.6, 114.6, 113.3, 107.8, 106.9, 100.8, 45.6, 42.9; IR (neat): 3134, 2923, 1605, 1503, 1435, 1367, 1238, 1172, 1078, 984; HRESIMS Calcd for $[C_{25}H_{18}BrKNO_4S]^+$ (M + K^+) 545.9771, found 545.9749.

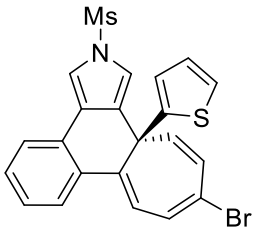
(*S*)-10-bromo-12a-(3,4-dimethoxyphenyl)-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2r)



2r

Compound **2r** was prepared in 99% yield (51.9 mg) according to the general procedure except at in DCM at 20 °C for 50 h. Pale yellow solid (mp 134–135 °C). $[\alpha]_D^{25}$ = -168.5º (c = 1.0, $CHCl_3$). 81% ee (determined by HPLC: Chiralpak IE Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.21 min (minor), 9.75 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.42 (s, 1H), 7.34 – 7.25 (m, 2H), 6.92 (d, *J* = 8.0 Hz, 1H), 6.72 (s, 1H), 6.67 (d, *J* = 8.8 Hz, 1H), 6.64 – 6.47 (m, 4H), 4.98 (d, *J* = 9.2 Hz, 1H), 3.79 (s, 3H), 3.77 (s, 3H), 3.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 147.1, 136.4, 132.4, 132.2, 131.3, 128.3, 127.7, 127.6, 127.1, 123.5, 122.8, 121.6, 121.4, 119.4, 118.9, 116.3, 114.1, 113.2, 110.4, 110.1, 55.9, 55.6, 44.4, 42.8; IR (neat): 3038, 2928, 1591, 1512, 1464, 1366, 1260, 1173, 1056, 985; HRESIMS Calcd for $[C_{26}H_{22}BrNNaO_4S]^+$ (M + Na^+) 546.0345, found 546.0322.

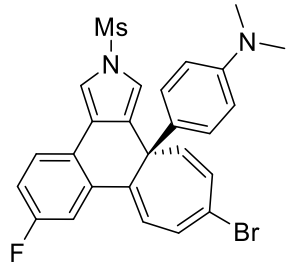
(*S*)-10-bromo-2-(methylsulfonyl)-12a-(thiophen-2-yl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2s)



2s

Compound **2s** was prepared in 95% yield (44.7 mg) according to the general procedure except in DCM at 30 °C for 11 h. Pale yellow solid (mp 198–199 °C). $[\alpha]_D^{25}$ = -216.5º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.98 min (minor), 9.46 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.43 (d, *J* = 2.0 Hz, 1H), 7.34 – 7.23 (m, 2H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.95 – 6.88 (m, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.74 – 6.66 (m, 1H), 6.66 – 6.59 (m, 1H), 6.53 (d, *J* = 9.2 Hz, 1H), 5.21 (d, *J* = 9.2 Hz, 1H), 3.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 132.8, 131.6, 130.5, 128.4, 128.2, 127.8, 127.3, 127.0, 125.2, 125.0, 123.5(4), 123.5(0), 122.6, 121.8, 121.5, 120.3, 119.2, 118.8, 113.4, 42.9, 42.3; IR (neat): 3132, 2927, 1592, 1525, 1431, 1367, 1262, 1174, 1055, 985; HRESIMS Calcd for $[C_{22}H_{16}BrNNaO_2S_2]^+$ (M + Na^+) 491.9698, found 491.9683.

(*S*)-4-(10-bromo-6-fluoro-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2t)

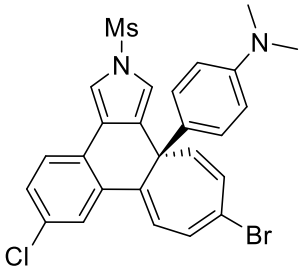


2t

Compound **2t** was prepared in 98% yield (51.5 mg) according to the general procedure. Pale yellow solid (mp 217–218 °C). $[\alpha]_D^{25}$ = -212.5º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.07 min (minor), 11.10 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55

(dd, *J* = 8.8, 6.0 Hz, 1H), 7.34 (d, *J* = 2.4 Hz, 1H), 7.30 (dd, *J* = 11.2, 2.8 Hz, 1H), 7.04 – 6.95 (m, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.76 (d, *J* = 8.4 Hz, 1H), 6.71 (d, *J* = 2.0 Hz, 1H), 6.60 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.55 (d, *J* = 9.2 Hz, 1H), 6.45 (d, *J* = 8.8 Hz, 2H), 4.72 (d, *J* = 8.8 Hz, 1H), 3.10 (s, 3H), 2.86 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2 (d, *J* = 244.0 Hz), 148.8, 134.3 (d, *J* = 7.0 Hz), 132.3, 131.8, 130.8, 127.7, 127.4, 125.1 (d, *J* = 8.0 Hz), 123.3 (d, *J* = 3.0 Hz), 122.6, 122.4, 121.0, 119.0, 115.5 (d, *J* = 23.0 Hz), 113.8 (d, *J* = 23.0 Hz), 112.7 (d, *J* = 1.0 Hz), 111.5, 108.8 (d, *J* = 3.0 Hz), 108.5, 42.8, 42.2, 40.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.5 – -113.8 (m); IR (neat): 3133, 2924, 1614, 1516, 1475, 1362, 1262, 1171, 1075, 985; HRESIMS Calcd for $[C_{26}H_{22}BrFN_2NaO_2S]^+$ (M + Na^+) 547.0462, found 547.0461.

(*S*)-4-(10-bromo-6-chloro-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2u)

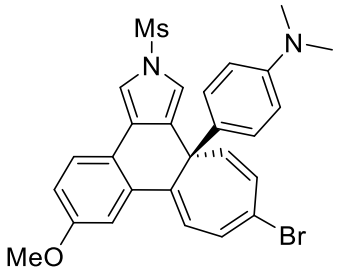


2u

Compound **2u** was prepared in 91% yield (49.3 mg) according to the general procedure. Pale yellow solid (mp 143–144 °C). $[\alpha]_D^{25}$ = -172.5º (c = 1.0, $CHCl_3$). 90% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.60 min (minor), 12.08 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 2.0 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.25 – 7.22 (m, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.76 (d, *J* = 8.4 Hz, 1H), 6.71 (d, *J* = 2.4 Hz, 1H), 6.58 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.54 (d, *J* = 8.9 Hz, 1H), 6.46 (d, *J* = 8.8 Hz, 2H), 4.61 (d, *J* = 8.8 Hz, 1H), 3.10 (s, 3H), 2.87 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 134.0, 133.2, 132.3, 131.8, 128.0, 127.9, 127.7, 127.2, 125.5, 124.7, 122.6, 122.4, 120.8, 119.1, 113.3, 111.6, 105.8, 42.9, 41.7, 40.5; IR (neat): 3135, 2925, 1611, 1517, 1464, 1367,

1262, 1126, 1045, 949; HRESIMS Calcd for $[C_{26}H_{22}BrClN_2NaO_2S]^+$ (M + Na^+) 563.0166, found 563.0148.

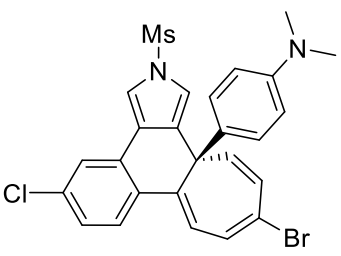
(*S*)-4-(10-bromo-6-methoxy-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2v)



2v

Compound **2v** was prepared in 97% yield (52.1 mg) according to the general procedure. Pale yellow solid (mp 153–154 °C). $[\alpha]_D^{25}$ = -219.9º (c = 1.0, $CHCl_3$). 90% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.01 min (minor), 21.20 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.4 Hz, 1H), 7.30 (d, *J* = 2.0 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 6.93 – 6.85 (m, 3H), 6.80 (d, *J* = 8.0 Hz, 1H), 6.69 (d, *J* = 2.0 Hz, 1H), 6.58 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.54 (d, *J* = 8.9 Hz, 1H), 6.46 (d, *J* = 8.9 Hz, 2H), 4.66 (d, *J* = 8.9 Hz, 1H), 3.85 (s, 3H), 3.08 (s, 3H), 2.86 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 148.7, 133.6, 132.4, 131.8, 131.1, 127.9, 127.2, 124.8, 122.2, 122.0, 121.7, 120.3, 118.9, 115.0, 112.0(4), 111.9(8), 111.5, 108.0, 106.9, 55.4, 42.7, 42.1, 40.5; IR (neat): 3133, 2925, 1612, 1517, 1479, 1366, 1260, 1170, 1075, 984; HRESIMS Calcd for $[C_{27}H_{25}BrN_2NaO_3S]^+$ (M + Na^+) 559.0661, found 559.0649.

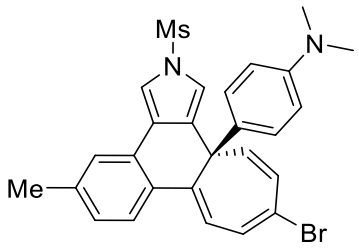
(*S*)-4-(10-bromo-5-chloro-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2w)



2w

Compound **2w** was prepared in 99% yield (53.6 mg) according to the general procedure. Pale yellow solid (mp 160–161 °C). $[\alpha]_D^{25}$ = -200.6º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.78 min (minor), 11.5 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.49 (m, 2H), 7.39 (d, *J* = 2.0 Hz, 1H), 7.19 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.73 (d, *J* = 2.4 Hz, 1H), 6.61 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.55 (d, *J* = 8.8 Hz, 1H), 6.45 (d, *J* = 8.8 Hz, 2H), 4.80 (d, *J* = 9.2 Hz, 1H), 3.11 (s, 3H), 2.86 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.8, 134.0, 132.7, 132.0, 131.2, 130.4, 129.1, 128.7, 127.6, 127.5, 123.2, 122.6, 121.8, 120.7, 119.1, 113.6, 111.5, 110.7, 42.9, 40.5; IR (neat): 3137, 2926, 1611, 1516, 1472, 1367, 1262, 1172, 1020, 984; HRESIMS Calcd for $[C_{26}H_{22}BrClN_2NaO_2S]^+$ (M + Na^+) 563.0166, found 563.0150.

(*S*)-4-(10-bromo-5-methyl-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2x)

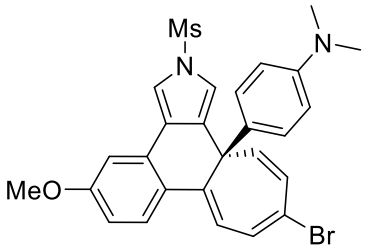


2x

Compound **2x** was prepared in 99% yield (51.6 mg) according to the general procedure. Pale yellow solid (mp 156–157 °C). $[\alpha]_D^{25}$ = -162.3º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.67 min (minor), 11.41 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.4 Hz, 1H), 7.40 (d, *J* = 11.6 Hz, 2H), 7.25 (d, *J* = 1.6 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.94 – 6.82 (m, 2H), 6.75 – 6.68 (m, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.54 (d, *J* = 9.6 Hz, 1H), 6.44 (d, *J* = 7.6 Hz, 2H), 4.96 (d, *J* = 9.2 Hz, 1H), 3.09 (s, 3H), 2.85 (s, 6H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 138.1, 133.3, 132.3, 132.0, 129.1, 128.8, 127.6, 127.5, 127.3, 127.1, 123.9, 122.2, 121.8, 120.7, 118.9, 117.2, 114.8, 113.0, 111.5, 44.1, 42.8, 40.5, 21.1; IR (neat): 3133, 2921, 1614, 1517, 1445, 1367,

1262, 1172, 1050, 983; HRESIMS Calcd for $[C_{27}H_{25}BrKN_2O_2S]^+$ (M + K^+) 559.0452, found 559.0444.

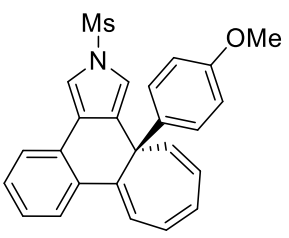
(*S*)-4-(10-bromo-5-methoxy-2-(methylsulfonyl)benzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2y)



2y

Compound **2y** was prepared in 98% yield (52.7mg) according to the general procedure. Pale yellow solid (mp 148–149 °C). $[\alpha]_D^{25}$ = -101.4º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 40/60 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.93 min (minor), 10.65 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 9.2 Hz, 1H), 7.38 (d, *J* = 2.4 Hz, 1H), 7.06 (d, *J* = 2.8 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.85 – 6.78 (m, 2H), 6.74 (d, *J* = 2.0 Hz, 1H), 6.68 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.55 (dd, *J* = 9.6, 0.4 Hz, 1H), 6.43 (d, *J* = 8.8 Hz, 2H), 5.12 (d, *J* = 9.6 Hz, 1H), 3.87 (s, 3H), 3.10 (s, 3H), 2.85 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 148.6, 133.6, 132.5(4), 132.4(9), 129.1, 128.7, 127.8, 127.0, 124.6, 122.1, 122.0, 121.8, 119.4, 118.9, 118.8, 114.9, 113.1, 111.5, 107.0, 55.4, 45.2, 42.7, 40.5; IR (neat): 3130, 2921, 1609, 1516, 1491, 1364, 1230, 1172, 1075, 985; HRESIMS Calcd for $[C_{27}H_{25}BrKN_2O_3S]^+$ (M + K^+) 575.0401, found 575.0389.

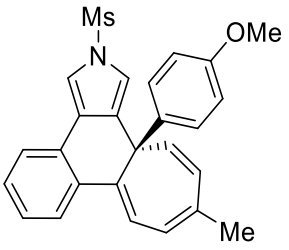
(*S*)-12a-(4-methoxyphenyl)-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2z)



2z

Compound **2z** was prepared in 98% yield (40.7 mg) according to the general procedure except in DCM at 30 °C for 10 h. Pale yellow solid (mp 144–145 °C). $[\alpha]_D^{25}$ = -201.9º (c = 1.0, $CHCl_3$). 91% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.50 min (minor), 11.28 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.54 (m, 2H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.31 – 7.24 (m, 2H), 7.05 – 6.92 (m, 3H), 6.71 (d, *J* = 2.0 Hz, 1H), 6.58 (d, *J* = 8.8 Hz, 2H), 6.46 – 6.38 (m, 1H), 6.37 – 6.23 (m, 2H), 4.70 (d, *J* = 8.8 Hz, 1H), 3.70 (s, 3H), 3.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 135.7, 133.0, 132.8, 128.9, 128.8, 128.0, 127.8, 127.6, 126.7, 124.9, 123.3, 122.1, 121.9, 118.9, 113.2, 112.3, 105.2, 104.1, 55.0, 42.7, 41.3; IR (neat): 3022, 2927, 1606, 1507, 1441, 1366, 1245, 1172, 1077, 949; HRESIMS Calcd for $[C_{25}H_{21}KNO_3S]^+$ ($M + K^+$) 454.0874, found 454.0885.

(*S*)-12a-(4-methoxyphenyl)-10-methyl-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2aa)

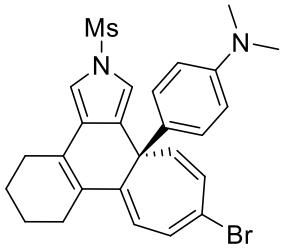


2aa

Compound **2aa** was prepared in 99% yield (42.5 mg) according to the general procedure except in DCM at 30 °C for 8 h. Pale white solid (mp 100–101 °C). $[\alpha]_D^{25}$ = -176.1º (c = 1.0, $CHCl_3$). 83% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.21 min (minor), 12.92 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.60 (m, 1H), 7.60 – 7.53 (m, 1H), 7.38 (d, *J* = 2.4 Hz, 1H), 7.25 – 7.19 (m, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 6.85 (d, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 2.4 Hz, 1H), 6.58 (d, *J* = 8.8 Hz, 2H), 6.16 (d, *J* = 8.8 Hz, 1H), 6.08 (d, *J* = 8.0 Hz, 1H), 4.57 (d, *J* = 8.8 Hz, 1H), 3.71 (s, 3H), 3.08 (s, 3 H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 136.9, 136.3, 133.2, 133.1, 128.6, 128.4, 127.5, 127.2,

126.5, 125.3, 123.3, 122.4, 122.1, 118.8, 113.1, 112.3, 101.7, 55.0, 42.7, 40.7, 22.6; IR (neat): 3018, 2923, 1606, 1507, 1464, 1366, 1246, 1172, 1077, 984; HRESIMS Calcd for $[C_{26}H_{23}NNaO_3S]^+$ (M + Na^+) 452.1291, found 452.1287.

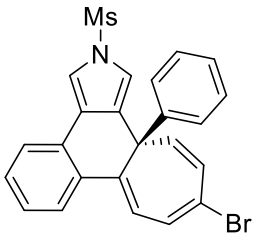
(*S*)-4-(10-bromo-2-(methylsulfonyl)-4,5,6,7-tetrahydrobenzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)-*N*,*N*-dimethylaniline (2ab)



2ab

Compound **2ab** was prepared in 85% yield (43.5 mg) according to the general procedure. Pale yellow solid (mp 138–139 °C). $[\alpha]_D^{25}$ = -482.8º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.16 min (minor), 9.21 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (d, *J* = 2.0 Hz, 1H), 6.91 (d, *J* = 9.2 Hz, 2H), 6.71 (d, *J* = 2.4 Hz, 1H), 6.68 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.51 (dd, *J* = 10.0, 0.8 Hz, 1H), 6.44 (d, *J* = 8.8 Hz, 2H), 6.35 (d, *J* = 8.0 Hz, 1H), 5.49 (d, *J* = 10.4 Hz, 1H), 3.05 (s, 3H), 2.85 (s, 6H), 2.63 – 2.54 (m, 1H), 2.54 – 2.39 (m, 2H), 2.37 – 2.23 (m, 1H), 1.91 – 1.82 (m, 1H), 1.83 – 1.71 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 137.6, 134.1, 133.5, 133.1, 128.6, 128.3, 128.2, 127.7, 126.3, 124.6, 121.8, 119.6, 118.1, 112.6, 111.5, 47.6, 42.6, 40.6, 27.1, 26.6, 23.2, 21.7. IR (neat): 3133, 2924, 1608, 1516, 1447, 1366, 1261, 1169, 1066, 983; HRESIMS Calcd for $[C_{26}H_{27}BrN_2NaO_2S]^+$ (M + Na^+) 533.0869, found 533.0861.

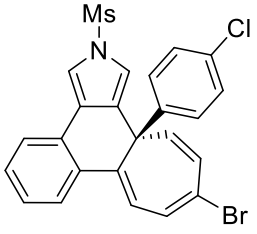
(*S*)-10-bromo-2-(methylsulfonyl)-12a-phenyl-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2ac)



2ac

Compound **2ac** was prepared in 79% yield (36.7 mg) according to the general procedure except in DCM at 50 °C for 40 h. Pale yellow solid (mp 152–153 °C). $[\alpha]_D^{25}$ = -3.2º (c = 1.0, $CHCl_3$). 2% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 5.97 min (minor), 6.81 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 1H), 7.60 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.33 – 7.25 (m, 2H), 7.15 – 7.04 (m, 5H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.71 (d, *J* = 2.4 Hz, 1H), 6.64 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.58 (d, *J* = 9.6 Hz, 1H), 5.06 (d, *J* = 9.2 Hz, 1H), 3.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 132.4, 132.1, 131.3, 128.3, 127.8, 127.7, 127.4, 127.3, 127.2, 126.6, 126.2, 123.5, 123.0, 121.7, 121.5, 119.2, 117.7, 115.5, 113.3, 45.1, 42.8; IR (neat): 3022, 2925, 1596, 1527, 1446, 1366, 1261, 1173, 1054, 984; HRESIMS Calcd for $[C_{24}H_{18}BrKNO_2S]^+$ (M + K^+) 501.9873, found 501.9850.

(*S*)-10-bromo-12a-(4-chlorophenyl)-2-(methylsulfonyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (2ad)

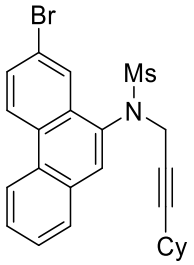


2ad

Compound **2ad** was prepared in 93% yield (46.4 mg) according to the general procedure except in DCM at 50 °C for 40 h. Pale yellow solid (mp 146–147 °C). $[\alpha]_D^{25}$ = -29.3º (c = 1.0, $CHCl_3$). 7% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 5.97 min (minor), 7.03 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.64 (m, 1H), 7.60 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.42 (d,

J = 2.4 Hz, 1H), 7.35 – 7.26 (m, 2H), 7.06 – 7.00 (m, 4H), 6.97 (d, *J* = 8.0 Hz, 1H), 6.72 – 6.64 (m, 2H), 6.59 (d, *J* = 9.6 Hz, 1H), 5.10 (d, *J* = 9.2 Hz, 1H), 3.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 132.8, 131.8, 131.7, 131.0, 128.6, 128.0, 127.9, 127.6, 127.5, 127.2, 123.6, 123.3, 121.6, 121.4, 119.4, 119.2, 116.8, 113.5, 45.2, 43.0; IR (neat): 2960, 2927, 1603, 1524, 1487, 1367, 1264, 1173, 1015, 949; HRESIMS Calcd for $[C_{24}H_{17}BrClKNO_2S]^+$ (M + K^+) 535.9483, found 535.9483

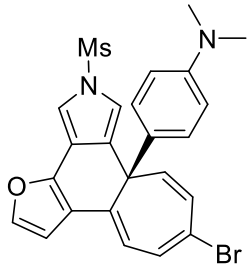
_N_-(7-bromophenanthren-9-yl)-_N_-(3-cyclohexylprop-2-yn-1-yl)methanesulfonamide (2ae′)



2ae′

Compound **2ae′** was prepared in 69% yield (32.6 mg) according to the general procedure in DCM at 50 °C for 9 d. Pale yellow solid (mp 191–192 °C). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (d, *J* = 8.0 Hz, 1H), 8.55 (d, *J* = 9.0 Hz, 1H), 8.43 (d, *J* = 2.0 Hz, 1H), 8.08 (s, 1H), 7.89 – 7.85 (m, 1H), 7.78 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.75 – 7.70 (m, 1H), 7.68 – 7.61 (m, 1H), 4.84 (dd, *J* = 18.0, 2.0 Hz, 1H), 4.19 (dd, *J* = 18.0, 2.0 Hz, 1H), 3.27 (s, 3H), 2.50 – 2.34 (m, 1H), 1.84 – 1.74 (m, 2H), 1.73 – 1.63 (m, 2H), 1.56 – 1.47 (m, 1H), 1.47 – 1.36 (m, 2H), 1.35 – 1.23 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.9, 132.2, 130.9, 130.7, 130.3, 130.2, 129.0, 128.8, 128.2, 127.4, 126.8, 124.7, 122.6, 122.0, 91.2, 74.6, 42.0, 39.7, 32.4, 29.0, 25.7, 24.7; IR (neat): 2929, 2853, 1593, 1483, 1346, 1265, 1155, 1071, 952, 775; HRESIMS Calcd for $[C_{24}H_{24}BrKNO_2S]^+$ (M + K^+) 508.0343, found 508.0342.

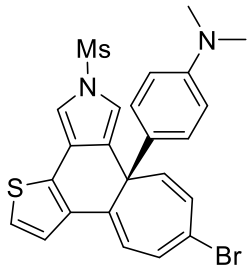
(_S_)-4-(6-bromo-10-(methylsulfonyl)cyclohepta[_e_]furo[3,2-g]isoindol-8a(10_H_)-yl)-_N_,_N_-dimethylaniline (2af)



2af

Compound **2af** was prepared in 70% yield (35.9 mg) according to the general procedure except in THF (12 h). Pale yellow solid (mp 221–222 °C). $[\alpha]_D^{25}$ = 130.3º (c = 1.0, $CHCl_3$). 40% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.60 min (major), 13.63 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 2.0 Hz, 1H), 7.16 (d, *J* = 2.4 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.80 (d, *J* = 2.0 Hz, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 2.0 Hz, 1H), 6.55 (d, *J* = 10.4 Hz, 1H), 6.49 – 6.41 (m, 3H), 5.53 (d, *J* = 10.4 Hz, 1H), 3.08 (s, 3H), 2.85 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 145.8, 142.9, 136.1, 132.5, 132.3, 131.8, 129.0, 127.6, 126.4, 122.1, 120.6, 119.2, 118.5, 115.1, 111.6, 110.2, 107.8, 48.6, 42.7, 40.5; IR (neat): 2923, 2853, 1609, 1516, 1365, 1320, 1170, 1144, 1073, 998; HRESIMS Calcd for $[C_{24}H_{21}BrKN_2O_3S]^+$ ($M + K^+$) 535.0088, found 535.0087.

(*S*)-4-(6-bromo-10-(methylsulfonyl)cyclohepta[*e*]thieno[3,2-*g*]isoindol-8a(10*H*)-yl)-*N*,*N*-dimethylaniline (2ag)

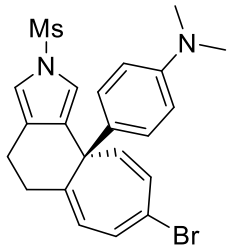


2ag

Compound **2ag** was prepared in 96% yield (49.1 mg) according to the general procedure in THF. Pale yellow solid (mp 211–212 °C). $[\alpha]_D^{25}$ = 273.4º (c = 1.0, $CHCl_3$). 53% ee (determined by HPLC: Chiralpak IG Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.07 min (major), 9.99 min (minor)). ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.26 (d, *J* = 5.6 Hz, 1H), 7.15 (d, *J* = 2.4 Hz, 1H), 7.13 (d, *J* = 5.6 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 2H), 6.77 (d, *J* = 2.0 Hz, 1H), 6.70 (s, 2H), 6.55 (d, *J* = 10.4 Hz, 1H), 6.43 (d, *J* = 8.8 Hz, 2H), 5.50 (d, *J* = 10.0 Hz, 1H), 3.06 (s, 3H), 2.83 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 135.3, 134.5, 132.6, 132.5, 131.3, 130.2, 128.7, 127.6, 126.4, 125.2, 123.4, 122.7, 119.8, 118.8, 118.7, 111.6, 111.5, 47.8, 42.7, 40.4; IR (neat): 2924, 2854, 1609, 1517, 1455, 1363, 1262, 1172, 1065, 948; HRESIMS Calcd for $[C_{24}H_{21}BrN_2NaO_2S_2]^+$ (M + Na^+) 535.0120, found 535.0117.

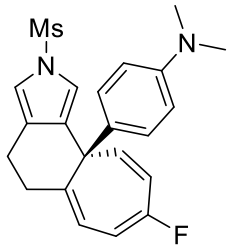
(*R*)-4-(8-bromo-2-(methylsulfonyl)-4,5-dihydrocyclohepta[*e*]isoindol-10a(2*H*)-yl)-*N*,*N*-dimethylaniline (2ah)



2ah

Compound **2ah** was prepared in 41% yield (18.9 mg) according to the general procedure employing **L25** as chiral ligand in 10 °C for 32 h. Pale yellow solid (mp 190–191 °C). $[\alpha]_D^{25}$ = -57.9º (c = 1.0, $CHCl_3$). 45% ee (determined by HPLC: Chiralpak IA Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.05 min (minor), 8.72 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (d, *J* = 8.8 Hz, 2H), 6.81 (s, 1H), 6.50 (s, 1H), 6.48 (d, *J* = 6.8 Hz, 2H), 6.40 (s, 1H), 6.38 (s, 1H), 6.14 (d, *J* = 8.0 Hz, 1H), 4.79 (d, *J* = 9.6 Hz, 1H), 3.00 (s, 3H), 2.87 (s, 6H), 2.83 – 2.73 (m, 1H), 2.73 – 2.62 (m, 2H), 2.50 – 2.38 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 135.5, 130.8, 130.0, 128.1, 127.6, 124.4, 124.0, 121.3, 120.7, 117.4, 114.8, 112.3, 111.4, 42.7, 42.5, 40.5, 33.5, 21.5; IR (neat): 3121, 2919, 1610, 1518, 1446, 1362, 1287, 1170, 1107, 1063; HRESIMS Calcd for $[C_{22}H_{23}BrN_2NaO_2S]^+$ (M + Na^+) 481.0556, found 481.0549.

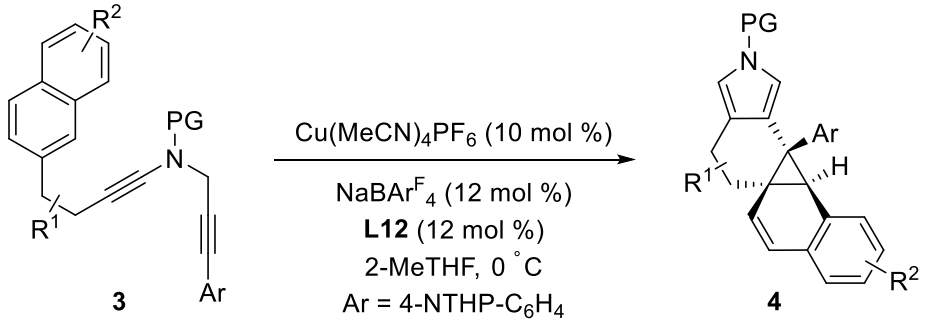
(*R*)-4-(8-fluoro-2-(methylsulfonyl)-4,5-dihydrocyclohepta[*e*]isoindol-10a(2*H*)-yl)-*N*,*N*-dimethylaniline (2ai)



2ai

Compound **2ai** was prepared in 42% yield (16.8 mg) according to the general procedure employing **L25** as chiral ligand at 5 °C for 32 h. Pale yellow solid (mp 210–211 °C). $[\alpha]_D^{25}$ = -9.4º (c = 1.0, $CHCl_3$). 52% ee (determined by HPLC: Chiralpak IA Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.36 min (minor), 9.11 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.99 (d, *J* = 9.0 Hz, 2H), 6.81 (s, 1H), 6.57 (d, *J* = 2.0 Hz, 1H), 6.47 (d, *J* = 9.0 Hz, 2H), 6.34 – 6.25 (m, 1H), 6.25 – 6.15 (m, 1H), 5.99 – 5.87 (m, 1H), 5.21 (dd, *J* = 10.0, 5.5 Hz, 1H), 3.01 (s, 3H), 2.86 (s, 6H), 2.83 – 2.70 (m, 3H), 2.50 – 2.29 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7 (d, *J* = 242.5 Hz), 148.7, 136.1, 131.1, 127.8 , 125.0(3), 124.9(7), 121.5 (d, *J* = 10.0 Hz), 120.4 (d, *J* = 12.5 Hz), 117.3, 116.7 (d, *J* = 32.5 Hz), 114.7, 111.6 (d, *J* = 26.3 Hz), 111.3, 44.6, 42.5, 40.4, 34.3, 22.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.05 – -107.29 (m); IR (neat): 2936, 2818, 1611, 1518, 1416, 1364, 1221, 1161, 1063, 1004; HRESIMS Calcd for $[C_{22}H_{23}FN_2NaO_2S]^+$ (M + Na^+) 421.1356, found 421.1346.

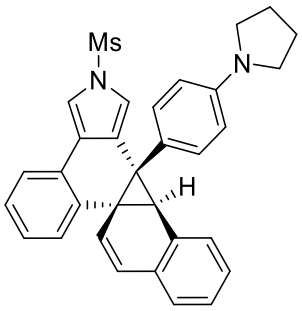
4.2. General Procedure for Synthesis of Chiral Tetracyclopropanes 4



To an oven-dried Schlenk tube with a stir bar were sequentially added $Cu(MeCN)_4PF_6$ (0.015 mmol, 5.7 mg), **L12** (0.018 mmol, 15.0 mg) and $NaBAr^F_4$ (0.0018 mmol, 16.2 mg, white crystal) under argon atmosphere. After injecting 2-MeTHF (1.5 mL) into the

Schlenk tube, the mixture was stirred at 25 °C for 2 h. Then the mixture reaction was cooled to 0 °C, and *N*-propargyl ynamide **3** (0.15 mmol) in 2-MeTHF (1.5 mL) was added into the reaction mixture dropwise. The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (eluent: PE/EtOAc) to afford the desired chiral benzonorcaradiene **4**.

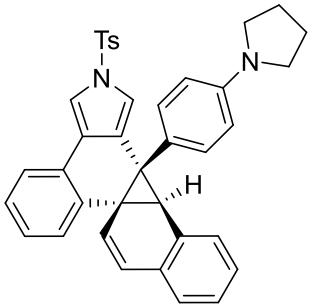
(3b*S*,3c*S*,9a*R*)-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4a)



4a

Compound **4a** was prepared in 95% yield (71.9 mg) according to the general procedure. Pale yellow solid (mp 266–267 °C). $[\alpha]_D^{25}$ = -514.5º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.78 min (major), 11.86 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 6.8 Hz, 1H), 7.45 (d, *J* = 2.0 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.30 – 7.19 (m, 3H), 7.13 – 7.03 (m, 1H), 6.91 (d, *J* = 7.2 Hz, 1H), 6.83 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.57 (d, *J* = 2.0 Hz, 1H), 6.55 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.39 – 6.29 (m, 2H), 6.21 (d, *J* = 10.0 Hz, 1H), 6.05 (dd, *J* = 8.3, 2.0 Hz, 1H), 3.22 – 3.10 (m, 4H), 3.07 (s, 3H), 2.62 (s, 1H), 1.98 – 1.81 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 137.9, 133.3, 132.1, 131.4, 131.3, 131.2, 129.9, 128.9, 127.5, 127.4(0), 127.3(7), 127.3, 126.1, 126.0, 125.9, 125.3, 124.0, 123.1, 121.6, 118.7, 113.7, 111.6, 109.6, 47.4, 42.7, 41.5, 37.3, 27.9, 25.4; IR (neat): 2928, 2855, 1608, 1521, 1461, 1362, 1246, 1165, 1056; HRESIMS Calcd for $[C_{32}H_{28}KN_2O_2S]^+$ (M + K^+) 543.1503, found 543.1518.

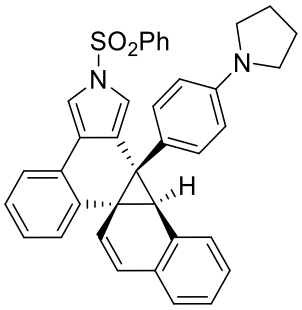
(3b*S*,3c*S*,9a*R*)-3b-(4-(pyrrolidin-1-yl)phenyl)-2-tosyl-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4b)



4b

Compound **4b** was prepared in 73% yield (63.6 mg) according to the general procedure. Pale yellow solid (mp 175–176 °C). $[\alpha]_D^{25}$ = -408.7º (c = 1.0, $CHCl_3$). 92% ee (determined by HPLC: Chiralpak IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.96 min (major), 12.24 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 6.8 Hz, 1H), 7.48 (d, *J* = 2.0 Hz, 1H), 7.36 – 7.21 (m, 5H), 7.21 – 7.14 (m, 2H), 7.11 – 7.03 (m, 1H), 6.88 (d, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 8.0 Hz, 1H), 6.62 (d, *J* = 2.4 Hz, 1H), 6.50 (d, *J* = 8.4 Hz, 1H), 6.34 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.30 (d, *J* = 10.0 Hz, 1H), 6.15 (d, *J* = 9.6 Hz, 1H), 6.03 (d, *J* = 8.0 Hz, 1H), 3.34 – 2.86 (m, 4H), 2.56 (s, 1H), 2.36 (s, 3H), 2.02 – 1.77 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 144.8, 137.8, 136.0, 133.3, 132.2, 131.4, 131.3, 131.1, 129.9, 128.9, 127.4, 127.2, 126.8, 126.0, 125.4, 124.1, 123.0, 121.9, 119.1, 113.9, 111.7, 109.5, 47.4, 41.4, 37.4, 28.0, 25.4, 21.6; IR (neat): 2963, 2926, 1613, 1526, 1461, 1332, 1261, 1147, 1066, 965; HRESIMS Calcd for $[C_{38}H_{32}N_2NaO_2S]^+$ (M + Na^+) 603.2077, found 603.2072.

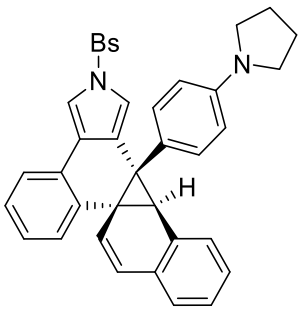
(3b*S*,3c*S*,9a*R*)-2-(phenylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4c)



4c

Compound **4c** was prepared in 98% yield (83.3 mg) according to the general procedure. Pale yellow solid (mp 186–187 °C). $[\alpha]_D^{25}$ = -486.1° (c = 1.0, $CHCl_3$). 90% ee (determined by HPLC: Chiralpak IE Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.96 min (minor), 12.03 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 6.8 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.50 (d, *J* = 2.0 Hz, 1H), 7.48 – 7.40 (m, 2H), 7.37 – 7.23 (m, 3H), 7.20 – 7.16 (m, 2H), 7.14 – 7.05 (m, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 1.6 Hz, 1H), 6.58 – 6.46 (m, 1H), 6.42 – 6.26 (m, 2H), 6.16 (d, *J* = 10.0 Hz, 1H), 6.09 – 5.89 (m, 1H), 3.29 – 3.06 (m, 4H), 2.56 (s, 1H), 2.00 – 1.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 139.0, 137.9, 133.7, 133.3, 132.1, 131.4, 131.3, 129.9, 129.3, 128.9, 127.3(9), 127.3(4), 127.2(9), 127.2(5), 126.8, 126.0(1), 126.0(0), 125.9, 125.3, 124.0, 123.1, 122.1, 119.2, 114.0, 111.7, 109.5, 47.4, 41.5, 37.4, 27.9, 25.4; IR (neat): 2965, 2849, 1613, 1526, 1448, 1333, 1261, 1148, 1044, 816; HRESIMS Calcd for $[C_{37}H_{30}N_2NaO_2S]^+$ ($M + Na^+$) 589.1920, found 589.1913.

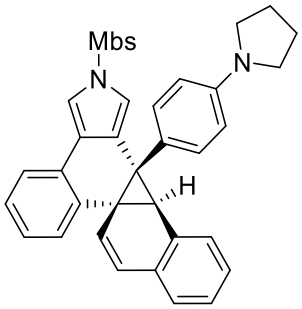
(3b*S*,3c*S*,9a*R*)-2-((4-bromophenyl)sulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4d)



4d

Compound **4d** was prepared in 96% yield (93.0 mg) according to the general procedure. Pale yellow solid (mp 175–176 °C). $[\alpha]_D^{25}$ = -427.8º (c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IG Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.38 min (minor), 15.47 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.50 (m, 5H), 7.47 (d, *J* = 1.6 Hz, 1H), 7.37 – 7.22 (m, 3H), 7.20 – 7.13 (m, 2H), 7.11 – 7.05 (m, 1H), 6.88 (d, *J* = 7.2 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.60 (d, *J* = 1.6 Hz, 1H), 6.50 (d, *J* = 8.0 Hz, 1H), 6.40 – 6.25 (m, 2H), 6.15 (d, *J* = 9.6 Hz, 1H), 6.03 (d, *J* = 7.2 Hz, 1H), 3.28 – 2.89 (m, 4H), 2.57 (s, 1H), 2.09 – 1.75 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 137.9, 137.8, 133.2, 132.6, 132.0, 131.8, 131.3, 129.9, 128.9, 128.2, 127.5, 127.4(0), 127.3(5), 127.3, 126.0(4), 126.0(1), 125.8, 125.1, 123.9, 123.1, 122.4, 119.0, 113.9, 111.7, 109.5, 47.4, 41.5, 37.4, 27.9, 25.3; IR (neat): 2966, 2918, 1613, 1527, 1478, 1376, 1261, 1183, 1045, 965; HRESIMS Calcd for $[C_{37}H_{29}BrN_2NaO_2S]^+$ (M + Na^+) 667.1025, found 667.1023.

(3b*S*,3c*S*,9a*R*)-2-((4-methoxyphenyl)sulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4e)

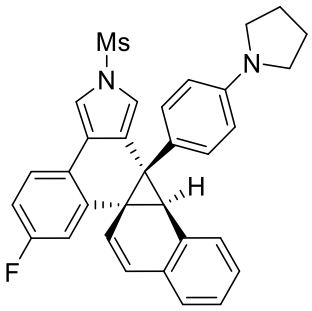


4e

Compound **4e** was prepared in 93% yield (85.3 mg) according to the general procedure. Pale yellow solid (mp 180–181 °C). $[\alpha]_D^{25}$ = -494.3º (c = 1.0, $CHCl_3$). 93% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.25 min (major), 11.33 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.8 Hz, 2H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.47 (s, 1H), 7.35 – 7.25 (m, 2H), 7.25 – 7.14 (m, 3H), 7.12 – 7.06 (m, 1H), 6.98 – 6.85 (m, 3H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.61 (s, 1H), 6.50 (d, *J* = 7.6 Hz, 1H), 6.40 – 6.24 (m, 2H), 6.15 (d, *J* = 10.0 Hz, 1H), 6.03

(d, *J* = 7.2 Hz, 1H), 3.79 (s, 3H), 3.34 – 2.95 (m, 4H), 2.56 (s, 1H), 2.06 – 1.74 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 146.0, 137.8, 133.3, 132.2, 131.4, 131.3, 130.9, 130.4, 129.9, 129.1, 128.9, 127.4, 127.2(3), 127.2(0), 126.0(0), 125.9(7), 125.5, 124.1, 123.0, 121.7, 119.0, 114.5, 113.8, 111.7, 109.5, 55.6, 47.4, 41.4, 37.4, 28.0, 25.4; IR (neat): 2964, 2926, 1613, 1577, 1461, 1372, 1263, 1165, 1044, 832; HRESIMS Calcd for $[C_{38}H_{32}N_2NaO_3S]^+$ (M + Na^+) 619.2026, found 619.2028.

(3b*S*,3c*S*,9a*R*)-11-fluoro-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4f)

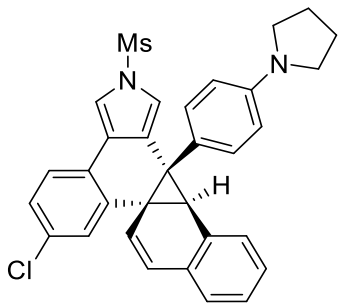


4f

Compound **4f** was prepared in 80% yield (62.7 mg) according to the general procedure. Pale yellow solid (mp 267–268 °C). $[\alpha]_D^{25}$ = -579.4º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.21 min (minor), 11.36 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.58 (m, 1H), 7.41 (d, *J* = 2.0 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.15 – 7.09 (m, 1H), 7.06 (dd, *J* = 10.0, 2.8 Hz, 1H), 7.01 – 6.88 (m, 2H), 6.82 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.58 (d, *J* = 1.6 Hz, 1H), 6.54 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.44 – 6.28 (m, 2H), 6.16 (d, *J* = 9.6 Hz, 1H), 6.06 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.26 – 3.13 (m, 4H), 3.12 (s, 3H), 2.64 (s, 1H), 1.94 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2 (d, *J* = 245.0 Hz), 146.1, 140.3 (d, *J* = 7.0 Hz), 133.2, 131.8, 131.3, 131.2, 130.8, 128.9, 127.9, 127.6, 127.4, 126.2, 125.0, 124.7 (d, *J* = 8.0 Hz), 123.6, 121.5 (d, *J* = 3.0 Hz), 120.9, 118.8, 116.6 (d, *J* = 22.6 Hz), 113.3(3) (d, *J* = 21.0 Hz), 113.3(0), 111.7, 109.7, 47.4, 42.7, 41.5, 37.3, 28.1, 25.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.0 (s); IR (neat):

2964, 2851, 1614, 1558, 1463, 1371, 1260, 1171, 1073, 980; HRESIMS Calcd for $[C_{32}H_{27}FN_2NaO_2S]^+$ (M + Na^+) 545.1669, found 545.1663.

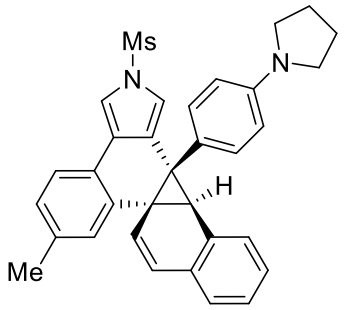
(3b*S*,3c*S*,9a*R*)-11-chloro-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4g)



4g

Compound **4g** was prepared in 87% yield (70.4 mg) according to the general procedure. Pale yellow solid (mp 239–240 °C). $[\alpha]_D^{25}$ = -537.8º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.19 min (minor), 11.38 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 2.0 Hz, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.32 (d, *J* = 2.0 Hz, 1H), 7.24 – 7.18 (m, 2H), 7.15 – 7.03 (m, 1H), 6.92 (d, *J* = 7.2 Hz, 1H), 6.81 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.58 (d, *J* = 2.0 Hz, 1H), 6.54 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.42 – 6.31 (m, 2H), 6.15 (d, *J* = 9.6 Hz, 1H), 6.11 – 6.00 (m, 1H), 3.29 – 3.12 (m, 4H), 3.11 (s, 3H), 2.62 (s, 1H), 2.01 – 1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 139.7, 133.2, 132.9, 131.7, 131.3, 131.1, 130.9, 129.9, 128.9, 127.9, 127.7, 127.4, 126.3, 126.2, 125.0, 124.4, 123.9, 123.6, 120.7, 118.8, 113.8, 111.7, 109.7, 47.4, 42.7, 41.4, 37.0, 28.0, 25.4; IR (neat): 2964, 2854, 1614, 1526, 1463, 1337, 1260, 1170, 1067, 983; HRESIMS Calcd for $[C_{32}H_{28}ClN_2O_2S+]^+$ (M + H^+) 539.1555, found 539.1551.

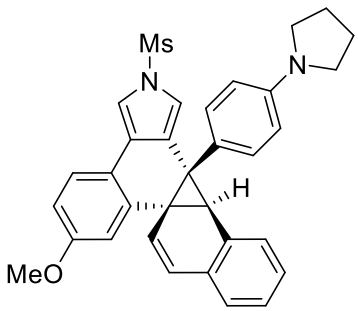
(3b*S*,3c*S*,9a*R*)-11-methyl-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4h)



4h

Compound **4h** was prepared in 85% yield (66.1 mg) according to the general procedure. Pale yellow solid (mp 277–278 °C). $[\alpha]_D^{25}$ = -511.9º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IA Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.05 min (major), 13.32 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 2.4 Hz, 1H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.23 – 7.18 (m, 1H), 7.15 (s, 1H), 7.13 – 7.04 (m, 2H), 6.92 (d, *J* = 7.2 Hz, 1H), 6.83 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.63 – 6.50 (m, 2H), 6.43 – 6.32 (m, 2H), 6.22 (d, *J* = 9.6 Hz, 1H), 6.05 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.25 – 3.12 (m, 4H), 3.10 (s, 3H), 2.61 (s, 1H), 2.36 (s, 3H), 2.00 – 1.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 137.9, 137.3, 133.3, 132.1, 131.4(3), 131.3(6), 131.2, 130.5, 128.9, 127.5, 127.3(3), 127.3(0), 127.0, 126.1, 126.0, 124.1, 123.1, 122.5, 121.8, 118.8, 113.3, 111.7, 109.7, 47.4, 42.7, 41.6, 37.3, 28.0, 25.4, 21.4; IR (neat): 2964, 2853, 1615, 1521, 1456, 1373, 1260, 1170, 1063; HRESIMS Calcd for $[C_{33}H_{31}N_2O_2S]^+$ ($M + H^+$) 519.2101, found 519.2111.

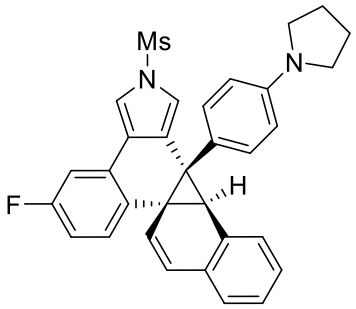
(3b*S*,3c*S*,9a*R*)-11-methoxy-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4i)



4i

Compound **4i** was prepared in 96% yield (78.0 mg) according to the general procedure. Pale yellow solid (mp 185–186 °C). $[\alpha]_D^{25}$ = -476.1º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 11.20 min (minor), 16.27 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.4 Hz, 1H), 7.43 – 7.29 (m, 2H), 7.22 – 7.19 (m, 1H), 7.14 – 7.01 (m, 1H), 6.91 (d, *J* = 7.2 Hz, 1H), 6.88 (d, *J* = 2.4 Hz, 1H), 6.86 – 6.77 (m, 2H), 6.62 – 6.47 (m, 2H), 6.45 – 6.31 (m, 2H), 6.21 (d, *J* = 10.0 Hz, 1H), 6.05 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.80 (s, 3H), 3.26 – 3.08 (m, 4H), 3.07 (s, 3H), 2.64 (s, 1H), 2.03 – 1.68 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 146.0, 139.6, 133.3, 132.1, 131.4, 131.3, 130.8, 128.9, 127.6, 127.5, 127.3, 126.1, 125.7, 124.4, 124.0, 121.6, 118.7, 118.1, 114.8, 112.5, 112.4, 111.6, 109.6, 55.3, 47.4, 42.6, 41.6, 37.5, 28.1, 25.4; IR (neat): 2963, 2837, 1612, 1569, 1463, 1321, 1261, 1170, 1042; HRESIMS Calcd for $[C_{33}H_{31}N_2O_3S]^+$ (M + H^+) 535.2050, found 535.2029.

(3b*S*,3c*S*,9a*R*)-12-fluoro-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4j)

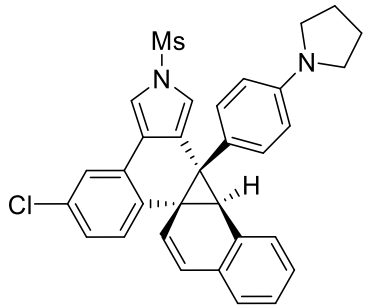


4j

Compound **4j** was prepared in 98% yield (76.8 mg) according to the general procedure. Pale yellow solid (mp 280–281 °C). $[\alpha]_D^{25}$ = -613.4º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 12.83 min (minor), 16.75 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 2.0 Hz, 1H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.32 – 7.26 (m, 2H), 7.22 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.15 – 7.07 (m, 1H), 7.01 – 6.95 (m, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.82 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.59 (d, *J* = 2.4 Hz, 1H), 6.54 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.40 –

6.25 (m, 2H), 6.18 (s, 1H), 6.05 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.25 – 3.13 (m, 4H), 3.12 (s, 3H), 2.58 (s, 1H), 2.00 – 1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3 (d, *J* = 243 Hz), 146.1, 133.8, 133.7, 133.3, 131.9, 131.6 (d, *J* = 9.0 Hz), 131.4, 131.2, 128.9, 127.6, 127.5, 127.4, 127.1 (d, *J* = 8.0 Hz), 126.1, 125.7, 123.7, 121.0 (d, *J* = 2.0 Hz), 118.9, 114.3 (d, *J* = 21.0 Hz), 114.2, 111.6, 109.6, 109.4 (d, *J* = 23.0 Hz), 47.4, 42.7, 41.3, 36.8, 27.7, 25.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.6 (s); IR (neat): 2965, 2852, 1613, 1557, 1462, 1370, 1259, 1143, 1067, 982; HRESIMS Calcd for $[C_{32}H_{27}FKN_2O_2S]^+$ (M + K^+) 561.1409, found 561.1420.

(3b*S*,3c*S*,9a*R)*-12-chloro-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4k)

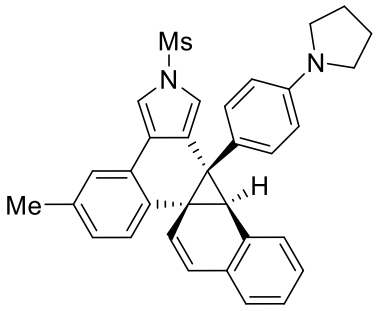


4k

Compound **4k** was prepared in 94% yield (76.0 mg) according to the general procedure. Pale yellow solid (mp 255–256 °C). $[\alpha]_D^{25}$ = -514.4º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 13.86 min (minor), 17.31 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 1.6 Hz, 1H), 7.45 (d, *J* = 2.4 Hz, 1H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.22 – 7.19 (m, 1H), 7.15 – 7.06 (m, 1H), 6.91 (d, *J* = 7.2 Hz, 1H), 6.80 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.58 (d, *J* = 2.4 Hz, 1H), 6.53 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.40 – 6.28 (m, 2H), 6.14 (d, *J* = 10.0 Hz, 1H), 6.05 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.23 – 3.11 (m, 4H), 3.09 (s, 3H), 2.59 (s, 1H), 1.97 – 1.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 136.3, 133.2, 132.0, 131.8, 131.4, 131.2, 131.0, 128.9, 127.7, 127.6, 127.4, 127.2, 127.1, 126.2, 125.4, 123.6, 122.9, 120.6, 118.9, 114.2, 111.6, 109.7, 47.4, 42.8, 41.4, 36.9,

27.9, 25.4; IR (neat): 2963, 2853, 1613, 1558, 1475, 1368, 1260, 1170, 1066, 982; HRESIMS Calcd for $[C_{32}H_{27}ClN_2NaO_2S]^+$ (M + Na^+) 561.1374, found 561.1380.

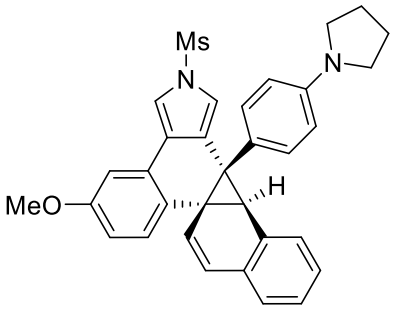
(3b*S*,3c*S*,9a*R*)-12-methyl-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4l)



4l

Compound **4l** was prepared in 94% yield (73.1 mg) according to the general procedure. Pale yellow solid (mp 256–257 °C). $[\alpha]_D^{25}$ = -498.2º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.18 min (minor), 11.58 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.41 (m, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.23 – 7.17 (m, 2H), 7.14 – 7.02 (m, 2H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.82 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.56 (d, *J* = 2.0 Hz, 1H), 6.54 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.42 – 6.28 (m, 2H), 6.20 (d, *J* = 9.6 Hz, 1H), 6.13 – 5.96 (m, 1H), 3.25 – 3.11 (m, 4H), 3.08 (s, 3H), 2.59 (s, 1H), 2.37 (s, 3H), 1.99 – 1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 135.6, 135.2, 133.3, 132.2, 131.4(1), 131.3(7), 129.8, 128.9, 128.4, 127.4, 127.3, 126.1, 126.0, 125.1, 124.1, 123.6, 121.8, 118.8, 113.6, 111.7, 109.6, 47.4, 42.6, 41.6, 37.2, 27.8, 25.4, 21.0; IR (neat): 2963, 2854, 1614, 1522, 1463, 1368, 1262, 1172, 1068, 982; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_2S]^+$ (M + Na^+) 541.1920, found 541.1909.

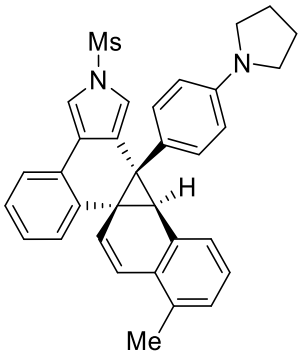
(3b*S*,3c*S*,9a*R*)-12-methoxy-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4m)



4m

Compound **4m** was prepared in 89% yield (71.4 mg) according to the general procedure. Pale yellow solid (mp 174–175 °C). $[\alpha]_D^{25}$ = -501.0º (c = 1.0, $CHCl_3$). 92% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 13.52 min (minor), 17.88 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 2.0 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.27 – 7.20 (m, 2H), 7.15 (d, *J* = 2.8 Hz, 1H), 7.12 – 7.05 (m, 1H), 6.93 – 6.79 (m, 3H), 6.57 (d, *J* = 2.4 Hz, 1H), 6.54 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.39 – 6.28 (m, 2H), 6.19 (d, *J* = 10.0 Hz, 1H), 6.05 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.84 (s, 3H), 3.24 – 3.13 (m, 4H), 3.09 (s, 3H), 2.57 (s, 1H), 2.01 – 1.81 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 146.0, 133.3, 132.2, 131.4(4), 131.4(1), 131.3, 131.0, 130.7, 128.9, 127.4, 127.3, 126.3, 126.2, 125.9, 124.1, 121.7, 118.8, 113.8(4), 113.8(1), 111.6, 109.6, 107.6, 55.4, 47.4, 42.7, 41.5, 36.9, 27.5, 25.4; IR (neat): 2965, 2928, 1613, 1521, 1463, 1367, 1263, 1171, 1067, 982; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ (M + Na^+) 557.1869, found 557.1839.

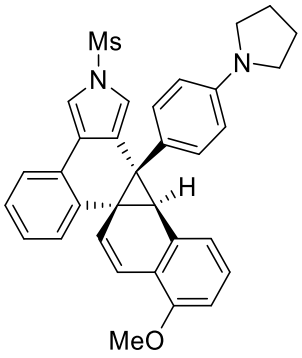
(3b*S*,3c*S*,9a*R*)-7-methyl-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4n)



4n

Compound **4n** was prepared in 95% yield (73.9 mg) according to the general procedure. Pale yellow solid (mp 264–265 °C). $[\alpha]_D^{25}$ = -563.1º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.90 min (minor), 11.90 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.57 (m, 1H), 7.46 (d, *J* = 2.0 Hz, 1H), 7.38 – 7.31 (m, 1H), 7.30 – 7.24 (m, 2H), 7.22 – 7.17 (m, 1H), 7.15 – 7.08 (m, 1H), 6.95 (d, *J* = 7.2 Hz, 1H), 6.83 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.65 – 6.45 (m, 3H), 6.37 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.25 (d, *J* = 10.0 Hz, 1H), 6.05 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.32 – 3.13 (m, 4H), 3.09 (s, 3H), 2.62 (s, 1H), 2.18 (s, 3H), 2.02 – 1.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 137.9, 133.9, 133.1, 132.1, 131.4, 131.3, 129.9, 129.6, 127.9, 127.4, 127.1, 127.0, 126.1, 126.0, 125.3, 124.3, 123.7, 123.1, 121.7, 118.7, 113.7, 111.7, 109.7, 47.5, 42.7, 41.9, 37.2, 27.6, 25.4, 19.0; IR (neat): 2928, 2853, 1613, 1525, 1464, 1370, 1274, 1173, 1068, 982; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_2S]^+$ ($M + Na^+$) 541.1920, found 541.1904.

(3b*S*,3c*S*,9a*R*)-7-methoxy-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4o)

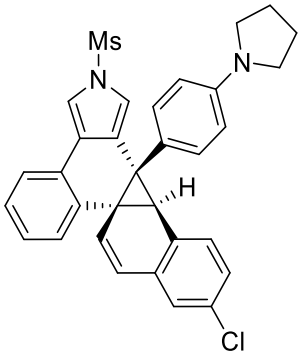


4o

Compound **4o** was prepared in 90% yield (72.2 mg) according to the general procedure. Pale yellow solid (mp 165–166 °C). $[\alpha]_D^{25}$ = -507.6º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 14.84 min (major), 18.18 min (minor)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.45 (d, *J* = 2.0 Hz, 1H), 7.34 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.29 – 7.25 (m, 2H), 7.19 – 7.14 (m, 1H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.82 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.78 (d, *J* = 10.0 Hz, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.60 (dd, *J* = 8.5, 2.0 Hz, 1H),

6.56 (d, *J* = 2.0 Hz, 1H), 6.37 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.21 (d, *J* = 10.5 Hz, 1H), 6.08 (dd, *J* = 8.4, 2.5 Hz, 1H), 3.70 (s, 3H), 3.26 – 3.11 (m, 4H), 3.07 (s, 3H), 2.58 (s, 1H), 1.98 – 1.87 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.1, 146.1, 138.0, 133.3, 133.1, 131.3, 131.2, 129.9, 127.8, 127.4, 126.0, 125.3, 125.0, 124.2, 123.0, 121.7(2), 121.6(9), 120.7, 118.7, 113.7, 111.8, 109.8, 108.2, 55.5, 47.4, 42.6, 41.5, 37.2, 27.6, 25.4; IR (neat): 2962, 2853, 1613, 1525, 1469, 1367, 1263, 1171, 1022, 982; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ (M + Na^+) 557.1869, found 557.1904.

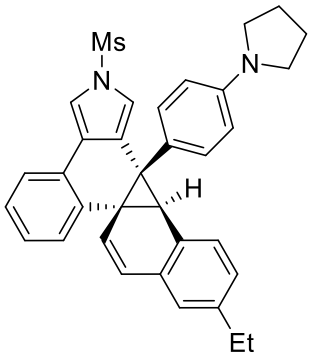
(3b*S*,3c*S*,9a*R*)-6-chloro-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4p)



4p

Compound **4p** was prepared in 88% yield 71.2 mg) according to the general procedure. Pale yellow solid (mp 254–255 °C). $[\alpha]_D^{25}$ = -556.5º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.48 min (minor), 12.77 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.2 Hz, 1H), 7.46 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.20 (m, 4H), 7.16 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.88 (d, *J* = 1.6 Hz, 1H), 6.79 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.58 (d, *J* = 2.0 Hz, 1H), 6.55 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.36 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.32 – 6.18 (m, 2H), 6.09 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.25 – 3.11 (m, 4H), 3.09 (s, 3H), 2.58 (s, 1H), 1.99 – 1.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 137.5, 133.2, 132.8, 131.4(4), 131.3(7), 130.7, 130.5, 130.0, 129.8, 127.5(0), 127.4(7), 127.3, 126.9, 126.4, 126.3, 125.3, 123.5, 123.1, 121.5, 118.8, 113.8, 111.7, 109.8, 47.4, 42.7, 41.0, 37.4, 28.2, 25.4; IR (neat): 2962, 2851, 1613, 1519, 1480, 1367, 1260, 1172, 1043, 983; HRESIMS Calcd for $[C_{32}H_{27}ClN_2NaO_2S]^+$ (M + Na^+) 561.1374, found 561.1347.

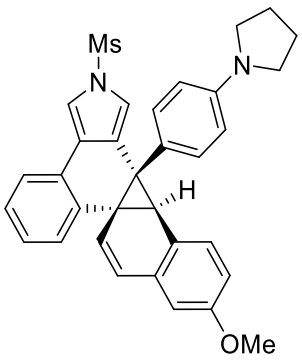
(3b*S*,3c*S*,9a*R*)-6-methoxy-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4q)



4q

Compound **4q** was prepared in 82% yield (65.5 mg) according to the general procedure. Pale yellow solid (mp 192–193 °C). $[\alpha]_D^{25}$ = -597.5° (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.64 min (minor), 11.73 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.57 (m, 1H), 7.45 (d, *J* = 2.4 Hz, 1H), 7.33 – 7.24 (m, 3H), 7.24 – 7.20 (m, 1H), 7.07 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.87 – 6.81 (m, 1H), 6.76 (d, *J* = 1.2 Hz, 1H), 6.62 – 6.49 (m, 2H), 6.42 – 6.35 (m, 1H), 6.33 (d, *J* = 10.0 Hz, 1H), 6.20 (d, *J* = 10.0 Hz, 1H), 6.12 – 6.02 (m, 1H), 3.24 – 3.11 (m, 4H), 3.09 (s, 3H), 2.62 – 2.48 (m, 3H), 2.00 – 1.83 (m, 4H), 1.19 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 142.0, 138.1, 133.3, 131.5, 131.4, 131.2, 129.9, 129.3, 128.8, 127.5, 127.4, 127.2, 126.8, 126.0, 125.9, 125.3, 124.2, 123.0, 121.7, 118.7, 113.7, 111.6, 109.7, 47.4, 42.7, 41.2, 37.2, 28.4, 27.9, 25.4, 15.6; IR (neat): 2964, 2853, 1613, 1522, 1479, 1367, 1261, 1173, 1043, 982; HRESIMS Calcd for $[C_{34}H_{32}KN_2O_2S]^+$ ($M + K^+$) 571.1816, found 571.1798.

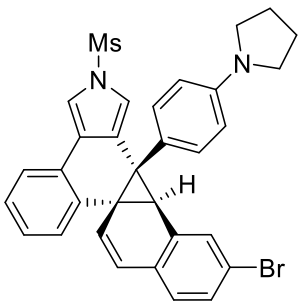
(3b*S*,3c*S*,9a*R*)-6-ethyl-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4r)



4r

Compound **4r** was prepared in 94% yield (80.2 mg) according to the general procedure. Pale yellow solid (mp 195–196 °C). $[\alpha]_D^{25}$ = -479.0º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.62 min (minor), 12.98 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.2 Hz, 1H), 7.44 (d, *J* = 2.0 Hz, 1H), 7.36 – 7.23 (m, 3H), 7.21 – 7.12 (m, 1H), 6.87 – 6.75 (m, 2H), 6.63 – 6.51 (m, 2H), 6.47 (d, *J* = 2.4 Hz, 1H), 6.37 (d, *J* = 7.2 Hz, 1H), 6.33 – 6.18 (m, 2H), 6.09 (d, *J* = 7.6 Hz, 1H), 3.73 (s, 3H), 3.34 – 3.10 (m, 4H), 3.07 (s, 3H), 2.58 (s, 1H), 1.99 – 1.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 146.0, 137.9, 133.3, 132.3, 131.5, 131.3, 129.8, 129.7, 127.3(8), 127.3(6), 126.7, 126.0, 125.2, 124.3, 123.1, 121.6, 118.6, 113.8, 113.7, 111.9, 111.7, 109.8, 55.2, 47.4, 42.6, 40.8, 37.1, 27.8, 25.3; IR (neat): 2964, 2853, 1613, 1522, 1479, 1367, 1261, 1173, 1043, 982; HRESIMS Calcd for $[C_{33}H_{31}N_2O_3S]^+$ (M + H^+) 535.2050, found 535.2061.

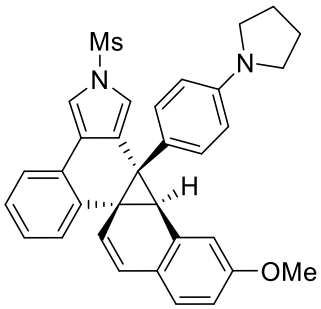
(3b*S*,3c*S*,9a*R*)-5-bromo-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4s)



4s

Compound **4s** was prepared in 93% yield (81.4 mg) according to the general procedure. Pale yellow solid (mp 206–207 °C). $[\alpha]_D^{25}$ = -738.8º (c = 1.0, $CHCl_3$). 85% ee (determined by HPLC: Chiralpak IE Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 17.59 min (minor), 21.79 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 6.8 Hz, 1H), 7.54 – 7.36 (m, 2H), 7.34 – 7.25 (m, 3H), 7.20 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.89 – 6.67 (m, 2H), 6.66 – 6.48 (m, 2H), 6.36 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.26 (dd, *J* = 19.2, 10.0 Hz, 2H), 6.17 – 6.02 (m, 1H), 3.30 – 3.13 (m, 4H), 3.10 (s, 3H), 2.56 (s, 1H), 2.04 – 1.80 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 137.4, 134.3, 133.2, 131.4, 131.3, 130.6, 130.3, 129.8, 129.0, 128.6, 127.5, 126.6, 126.5, 126.3, 125.3, 123.5, 123.1, 121.4, 120.8, 118.9, 113.8, 111.7, 109.8, 47.4, 42.7, 41.1, 37.5, 28.3, 25.4; IR (neat): 2964, 2851, 1614, 1525, 1478, 1369, 1261, 1173, 1043, 982; HRESIMS Calcd for $[C_{32}H_{27}BrN_2NaO_2S]^+$ (M + Na^+) 605.0869, found 605.0856.

(3b*S*,3c*S*,9a*R*)-5-methoxy-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4t)

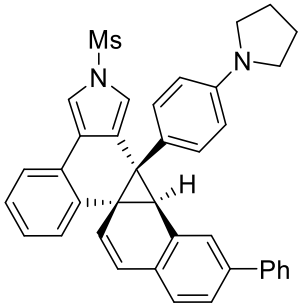


4t

Compound **4t** was prepared in 94% yield (75.4 mg) according to the general procedure. Pale yellow solid (mp 190–191 °C). $[\alpha]_D^{25}$ = -689.3º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.05 min (minor), 12.14 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.58 (m, 1H), 7.46 (d, *J* = 2.4 Hz, 1H), 7.35 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.29 – 7.23 (m, 2H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.83 (dd, *J* = 8.4, 3.6 Hz, 2H), 6.65 (dd, *J* = 8.4, 2.8 Hz, 1H), 6.62 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.58 (d, *J* = 2.4 Hz, 1H), 6.42 – 6.34 (m, 1H), 6.29 (d, *J* = 9.6 Hz, 1H), 6.14 – 5.98 (m, 2H), 3.80 (s, 3H), 3.26 – 3.12 (m, 4H), 3.08 (s, 3H),

2.57 (s, 1H), 1.97 – 1.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 146.0, 138.0, 133.6, 133.2, 131.3, 129.9, 128.4, 127.4, 126.7, 126.1, 125.3, 124.8, 124.1, 123.4, 123.1, 121.7, 118.6, 113.7, 112.1, 111.6, 109.7, 55.2, 47.4, 42.7, 41.7, 37.2, 28.2, 25.4; IR (neat): 2963, 2837, 1607, 1525, 1463, 1367, 1259, 1127, 1043, 982; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ (M + Na^+) 557.1869, found 557.1891.

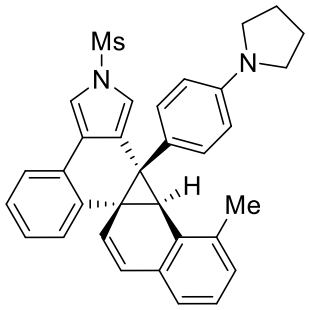
(3b*S*,3c*S*,9a*R*)-2-(methylsulfonyl)-5-phenyl-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4u)



4u

Compound **4u** was prepared in 92% yield (80.1 mg) according to the general procedure. Pale yellow solid (mp 180–181 °C). $[\alpha]_D^{25}$ = -941.6º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.72 min (minor), 21.82 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.56 (m, 4H), 7.47 (d, *J* = 2.0 Hz, 1H), 7.44 – 7.23 (m, 7H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 6.8 Hz, 1H), 6.66 – 6.50 (m, 2H), 6.38 (d, *J* = 9.6 Hz, 2H), 6.23 (d, *J* = 9.6 Hz, 1H), 6.04 (d, *J* = 8.0 Hz, 1H), 3.26 – 3.12 (m, 4H), 3.09 (s, 3H), 2.70 (s, 1H), 1.99 – 1.79 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 140.7, 140.1, 137.8, 133.3, 132.6, 131.4, 131.1, 130.5, 129.9, 128.7, 127.7, 127.4(4), 127.3(6), 127.2, 127.0, 126.9, 126.2, 125.3, 124.8, 123.9, 123.1, 121.6, 118.7, 113.8, 111.7, 109.8, 47.4, 42.7, 41.7, 37.5, 28.3, 25.4; IR (neat): 2963, 2853, 1613, 1526, 1462, 1370, 1261, 1173, 1068, 982; HRESIMS Calcd for $[C_{38}H_{32}N_2NaO_2S]^+$ (M + Na^+) 603.2077, found 603.2054.

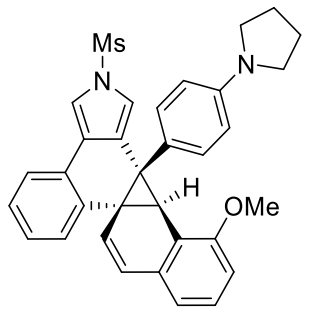
(3b*S*,3c*S*,9a*R*)-4-methyl-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4v)



4v

Compound **4v** was prepared in 88% yield (68.5 mg) according to the general procedure. Pale yellow solid (mp 154–155 °C). $[\alpha]_D^{25}$ = -577.4º (c = 1.0, $CHCl_3$). 89% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.07 min (minor), 7.74 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.58 (m, 1H), 7.46 (d, *J* = 2.4 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.24 (m, 2H), 7.08 (d, *J* = 7.2 Hz, 1H), 7.04 – 6.92 (m, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.2 Hz, 1H), 6.60 (d, *J* = 2.4 Hz, 1H), 6.48 (d, *J* = 8.0 Hz, 1H), 6.36 (d, *J* = 8.4 Hz, 1H), 6.33 (d, *J* = 10.0 Hz, 1H), 6.19 (d, *J* = 9.6 Hz, 1H), 6.07 (d, *J* = 8.4 Hz, 1H), 3.24 – 3.12 (m, 4H), 3.09 (s, 3H), 2.58 (s, 1H), 2.39 (s, 3H), 1.99 – 1.85 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 138.4, 136.1, 133.2, 131.5, 131.2, 131.0, 130.8, 129.9, 129.1, 128.0, 127.4, 126.1, 125.7, 125.5(3), 125.4(9), 125.3, 124.2, 123.1, 121.8, 118.6, 113.8, 111.5, 109.8, 47.4, 42.6, 38.9, 37.1, 27.1, 25.4, 19.7; IR (neat): 2963, 2852, 1614, 1524, 1462, 1369, 1262, 1173, 1046, 982; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_2S]^+$ ($M + Na^+$) 541.1920, found 541.1903.

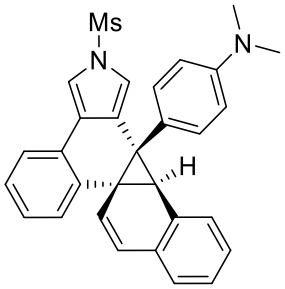
(3b*S*,3c*S*,9a*R*)-4-methoxy-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4w)



4w

Compound **4w** was prepared in 90% yield (72.2 mg) according to the general procedure. Pale yellow solid (mp 281–282 °C). $[\alpha]_D^{25}$ = -508.5º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak ADH Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 11.53 min (major), 19.18 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.58 (m, 1H), 7.46 (d, *J* = 2.4 Hz, 1H), 7.38 – 7.26 (m, 2H), 7.24 – 7.19 (m, 1H), 7.10 – 7.03 (m, 1H), 6.84 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 6.64 – 6.47 (m, 3H), 6.38 (d, *J* = 7.6 Hz, 1H), 6.33 (d, *J* = 10.0 Hz, 1H), 6.23 (d, *J* = 10.0 Hz, 1H), 6.10 (d, *J* = 8.4 Hz, 1H), 3.84 (s, 3H), 3.26 – 3.13 (m, 4H), 3.10 (s, 3H), 2.89 (s, 1H), 1.97 – 1.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 146.1, 138.4, 133.1, 132.4, 131.4, 129.9, 127.4, 127.3, 126.4(3), 126.3(7), 126.0, 125.4, 124.5, 123.0, 121.9, 120.7, 120.0, 118.8, 113.7, 111.5, 109.9, 109.3, 55.6, 47.4, 42.7, 36.7, 36.0, 27.1, 25.4; IR (neat): 2962, 2925, 1614, 1526, 1470, 1369, 1263, 1172, 1044, 982; HRESIMS Calcd for $[C_{33}H_{30}N_2NaO_3S]^+$ ($M + Na^+$) 557.1869, found 557.1853.

***N*,*N*-dimethyl-4-((3b*S*,3c*S*,9a*R*)-2-(methylsulfonyl)-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindol-3b(3c*H*)-yl)aniline (4x)**

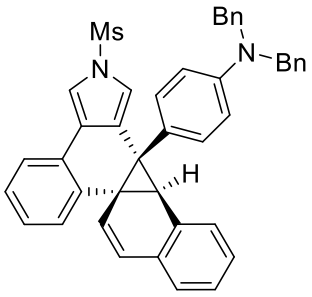


4x

Compound **4x** was prepared in 93% yield (66.8 mg) according to the general procedure. Pale yellow solid (mp 256–257 °C). $[\alpha]_D^{25}$ = -594.3º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IC Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 9.48 min (major), 11.43 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 2.0 Hz, 1H), 7.45 – 7.37 (m, 2H), 7.37 – 7.29 (m, 3H), 7.20 – 7.13 (m, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 10.0 Hz, 1H), 6.70 – 6.50 (m, 3H), 6.40 (d, *J* = 10. Hz, 1H), 6.32 – 6.08 (m, 2H), 3.15 (s, 3H), 2.89 (s, 6H), 2.70 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 137.8, 133.2, 132.0, 131.3, 131.0, 129.9,

128.9, 127.5, 127.4, 127.3, 126.1(2), 126.0(8), 125.9, 125.3, 125.1, 123.1, 121.6, 118.7, 113.8, 112.5, 110.5, 42.7, 41.4, 40.3, 37.2, 27.8; IR (neat): 2925, 2854, 1615, 1526, 1454, 1366, 1261, 1171, 1044, 983; HRESIMS Calcd for $[C_{30}H_{26}KN_2O_2S]^+$ (M + K^+) 517.1347, found 517.1355.

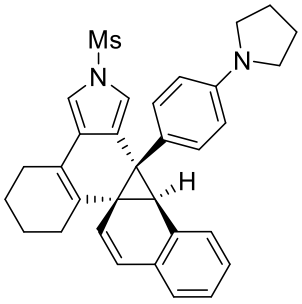
_N_,_N_-dibenzyl-4-((3b_S_,3c_S_,9a_R_)-2-(methylsulfonyl)-2_H_-benzo[_e_]naphtho[2',1':1,3]cyclopropa[1,2-_g_]isoindol-3b(3c_H_)-yl)aniline (4y)



4y

Compound **4y** was prepared in 81% yield (76.6 mg) according to the general procedure. Pale yellow solid (mp 146–147 °C). $[\alpha]_D^{25}$ = -400.7º (c = 1.0, $CHCl_3$). 90% ee (determined by HPLC: Chiralpak IA Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.98 min (major), 16.98 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.2 Hz, 1H), 7.45 (d, *J* = 2.0 Hz, 1H), 7.35 – 7.19 (m, 10H), 7.18 – 7.11 (m, 5H), 7.10 – 7.03 (m, 1H), 6.90 (d, *J* = 7.4 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 2.0 Hz, 1H), 6.54 (d, *J* = 6.4 Hz, 1H), 6.49 (d, *J* = 8.4 Hz, 1H), 6.32 (d, *J* = 10.0 Hz, 1H), 6.27 – 6.21 (m, 1H), 6.18 (d, *J* = 10.0 Hz, 1H), 4.46 (s, 4H), 3.07 (s, 3H), 2.60 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 138.6, 137.8, 133.4, 132.0, 131.4, 131.3, 130.8, 129.9, 128.9, 128.4, 127.5, 127.4, 127.2, 126.8, 126.7, 126.1(2), 126.0(8), 125.9, 125.4, 125.2, 123.1, 121.7, 118.8, 113.8, 112.8, 110.9, 53.9, 42.7, 41.4, 37.3, 27.8; IR (neat): 3027, 2927, 1612, 1563, 1454, 1366, 1261, 1171, 1044, 982; HRESIMS Calcd for $[C_{42}H_{34}N_2NaO_2S]^+$ (M + Na^+) 653.2233, found 653.2248.

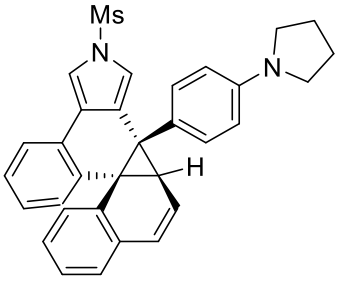
(3b*S*,3c*S*,9a*R*)-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c,10,11,12,13-hexahydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4z)



4z

Compound **4z** was prepared in 90% yield (68.7 mg) according to the general procedure. Pale yellow solid (mp 276–277 °C). $[\alpha]_D^{25}$ = -460.2º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.58 min (minor), 9.61 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.2 Hz, 1H), 7.27 – 7.18 (m, 1H), 7.15 – 7.01 (m, 1H), 6.94 (d, *J* = 2.4 Hz, 1H), 6.91 – 6.80 (m, 2H), 6.59 – 6.45 (m, 2H), 6.39 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.20 (d, *J* = 10.0 Hz, 1H), 6.10 (d, *J* = 10.0 Hz, 1H), 6.06 (dd, *J* = 8.4, 2.4 Hz, 1H), 3.25 – 3.13 (m, 4H), 3.07 (s, 3H), 2.57 – 2.47 (m, 1H), 2.46 (s, 1H), 2.42 – 2.27 (m, 3H), 2.00 – 1.89 (m, 4H), 1.88 – 1.73 (m, 3H), 1.70 – 1.61 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.9, 135.5, 133.5, 133.0, 131.4, 131.1, 130.8, 128.6, 127.2, 127.1, 126.4, 125.8, 125.7, 124.6, 124.4, 118.7, 118.3, 112.2, 111.5, 109.6, 47.4, 42.4, 40.3, 39.2, 28.6, 28.5, 25.4, 25.2, 23.4, 22.3; IR (neat): 2926, 2854, 1613, 1520, 1461, 1367, 1263, 1170, 1063, 980; HRESIMS Calcd for $[C_{32}H_{32}N_2NaO_2S]^+$ (M + Na^+) 531.2077, found 531.2079.

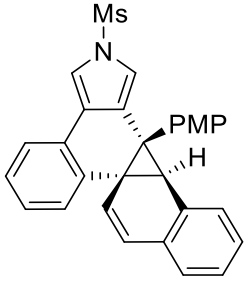
2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[1',2':1,3]cyclopropa[1,2-*g*]isoindole (4aa)



4aa

Compound **4aa** was prepared in 78% yield (39.4 mg) according to the general procedure. Pale yellow solid (mp 233–234 °C). $[\alpha]_D^{25}$ = 130.9º (c = 1.0, $CHCl_3$). 64% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.71 min (major), 8.15 min (minor)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.48 – 7.41 (m, 2H), 7.35 – 7.28 (m, 1H), 7.23 – 7.18 (m, 1H), 7.18 – 6.09 (m, 3H), 7.05 – 6.98 (m, 1H), 6.81 (d, *J* = 7.5 Hz, 1H), 6.55 (d, *J* = 2.5 Hz, 1H), 6.39 – 6.29 (m, 2H), 6.25 – 6.18 (m, 1H), 6.14 (d, *J* = 9.5 Hz, 1H), 6.03 (d, *J* = 7.5 Hz, 1H), 3.20 – 3.12 (m, 4H), 3.07 (s, 3H), 1.97 (d, *J* = 5.5 Hz, 1H), 1.95 – 1.83 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.0, 138.5, 133.6, 133.5, 132.7, 132.1, 131.2(2), 131.1(8), 130.9, 127.0, 126.6(9), 126.6(7), 126.0, 125.9(4), 125.9(0), 124.2, 123.3, 123.1, 121.8, 118.7, 113.6, 111.3, 109.8, 47.4, 42.7, 39.3, 38.0, 28.2, 25.4; IR (neat): 2963, 2854, 1612, 1521, 1487, 1367, 1263, 1128, 1058, 982; HRESIMS Calcd for $[C_{32}H_{28}KN_2O_2S]^+$ ($M + Na^+$) 543.1503, found 543.1502.

(3b*S*,3c*S*,9a*R*)-3b-(4-methoxyphenyl)-2-(methylsulfonyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (4ab)

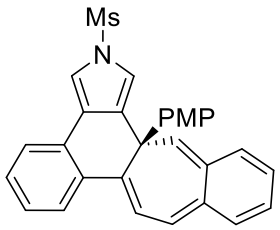


4ab

Compound **4ab** was prepared in 49% yield (39.4 mg) according to the general procedure. Pale yellow solid (mp 94–95 °C). $[\alpha]_D^{25}$ = -379.4º (c = 1.0, $CHCl_3$). 66% ee (determined by HPLC: Chiralpak IB Column, 40/60 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = (6.10 min (major), 7.57 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.2 Hz, 1H), 7.48 (d, *J* = 1.6 Hz, 1H), 7.40 – 7.20 (m, 5H), 7.14 – 7.07 (m, 1H), 7.02 – 6.86 (m, 2H), 6.74 – 6.61 (m, 2H), 6.54 (d, *J* = 1.6 Hz, 1H), 6.45 – 6.38 (m, 1H), 6.32 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 9.6 Hz, 1H), 3.67 (s, 3H), 3.10 (s, 3H), 2.66 (s,

1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 137.5, 133.8, 131.7(4), 131.6(6), 131.2, 130.4, 129.9, 129.3, 128.9, 127.7, 127.5, 127.3, 126.3, 125.8, 125.2, 123.1, 121.6, 118.7, 114.1, 113.9, 111.6, 54.9, 42.7, 41.3, 37.2, 27.8; IR (neat): 3132, 2926, 1609, 1514, 1463, 1361, 1246, 1175, 1044, 983; HRESIMS Calcd for $[C_{29}H_{23}NNaO_3S]^+$ (M + Na^+) 488.1291, found 488.1293.

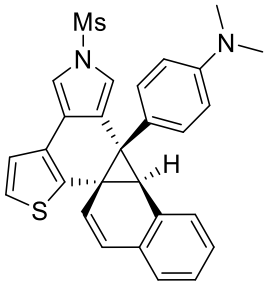
(*S*)-14a-(4-methoxyphenyl)-2-(methylsulfonyl)-2,14a-dihydrobenzo[*e*]benzo[4,5]cyclohepta[1,2-*g*]isoindole (4ab′)



4ab′

Compound **4ab′** was prepared in 46% yield (21.4 mg) according to the general procedure except at 30 °C in DCM for 24 h. Pale yellow solid (mp 131–132 °C). $[\alpha]_D^{25}$ = 182.6º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IG Column, 40/60 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 11.72 min (minor), 14.75 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.70 (m, 1H), 7.52 – 7.46 (m, 1H), 7.43 (d, *J* = 2.0 Hz, 1H), 7.26 – 7.18 (m, 5H), 7.17 – 7.10 (m, 2H), 7.07 – 6.98 (m, 3H), 6.54 (d, *J* = 11.6 Hz, 1H), 6.51 (d, *J* = 9.2 Hz, 2H), 6.01 (d, *J* = 11.6 Hz, 1H), 3.61 (s, 3H), 3.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 139.9, 139.1, 135.5, 135.2, 135.0, 134.4, 133.4, 132.1, 130.3, 128.4, 128.0, 127.8, 127.6(1), 127.5(9), 127.3, 127.0, 126.5, 123.6, 123.1, 117.7, 113.6, 112.9, 55.0, 48.8, 42.8; IR (neat): 2929, 2854, 1737, 1668, 1559, 1464, 1363, 1243, 1182, 984; HRESIMS Calcd for $[C_{29}H_{23}NNaO_3S]^+$ (M + Na^+) 488.1291, found 488.1294.

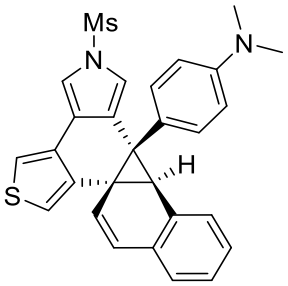
***N*,*N*-dimethyl-4-((6b*S*,12b*R*,12c*R*)-2-(methylsulfonyl)-2H-naphtho[2',1':2,3]cyclopropa[1,2-*e*]thieno[2,3-*g*]isoindol-12c(12b*H*)-yl)aniline (4ac)**



4ac

Compound **4ac** was prepared in 99% yield (48.0 mg) according to the general procedure. Pale yellow solid (mp 251–252 °C). $[\alpha]_D^{25}$ = -397.2º (c = 1.0, $CHCl_3$). 74% ee (determined by HPLC: Chiralpak IC Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.64 min (major), 10.67 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 5.2 Hz, 1H), 7.25 – 7.19 (m, 3H), 7.16 – 7.05 (m, 1H), 6.91 (d, *J* = 7.2 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 6.59 (d, *J* = 2.0 Hz, 1H), 6.59 – 6.48 (m, 2H), 6.31 (d, *J* = 10.0 Hz, 1H), 6.26 – 6.17 (m, 2H), 3.09 (s, 3H), 2.83 (s, 6H), 2.67 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 142.2, 133.3, 132.2, 131.4, 131.1, 130.7, 128.8, 128.3, 127.7, 127.6, 126.2, 124.7, 124.6, 124.4, 124.3, 122.9, 119.9, 119.3, 112.4, 112.3, 110.6, 42.6, 41.3, 40.3, 36.7, 29.4; IR (neat): 2925, 1613, 1523, 1486, 1365, 1264, 1171, 1056, 980, 945; HRESIMS Calcd for $[C_{28}H_{24}KN_2O_2S_2]^+$ (M + K^+) 523.0911, found 523.0905.

_N_,_N_-dimethyl-4-((6b_S_,12b_S_,12c_S_)-2-(methylsulfonyl)-2_H_-naphtho[2',1':2,3]cyclopropa[1,2-_e_]thieno[3,4-_g_]isoindol-12c(12b_H_)-yl)aniline (4ad)

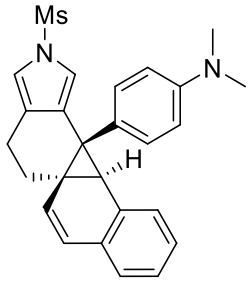


4ad

Compound **4ad** was prepared in 96% yield (46.5 mg) according to the general procedure. Pale yellow solid (mp 271–272 °C). $[\alpha]_D^{25}$ = -602.2º (c = 1.0, $CHCl_3$). 93%

ee (determined by HPLC: Chiralpak ADH Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 10.86 min (major), 17.04 min (minor)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.33 (m, 3H), 7.25 – 7.15 (m, 1H), 7.15 – 7.07 (m, 1H), 7.05 (d, *J* = 3.0 Hz, 1H), 6.89 (d, *J* = 7.0 Hz, 1H), 6.84 (d, *J* = 7.0 Hz, 1H), 6.57 (d, *J* = 2.0 Hz, 1H), 6.56 – 6.47 (m, 2H), 6.31 (d, *J* = 9.5 Hz, 1H), 6.23 (d, *J* = 9.5 Hz, 1H), 6.22 – 6.19 (m, 1H), 3.07 (s, 3H), 2.82 (s, 6H), 2.67 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.6, 141.1, 133.2, 132.0, 131.6, 131.5, 131.4, 128.9, 127.8, 127.6, 127.5, 127.4, 126.2, 125.1, 124.6, 121.7, 119.0, 118.9, 116.9, 113.4, 112.4, 110.7, 42.6, 42.5, 40.3, 36.5, 27.5; IR (neat): 2926, 1613, 1523, 1412, 1365, 1264, 1170, 1140, 1062, 981; HRESIMS Calcd for $[C_{28}H_{24}KN_2O_2S_2]^+$ ($M + K^+$) 523.0911, found 523.0908.

_N_,_N_-dimethyl-4-((5a_R_,11b_S_,11c_S_)-2-(methylsulfonyl)-4,5-dihydro-2_H_-naphtho[2',1':2,3]cyclopropa[1,2-_e_]isoindol-11c(11b_H_)-yl)aniline (4ae)

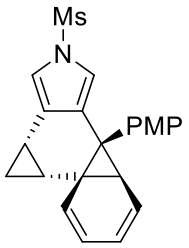


4ae

Compound **4ae** was prepared in 90% yield (38.8 mg) according to the general procedure except by employing **L26** as chiral ligand in toluene for 20 h. Pale yellow solid (mp 244–245 °C). $[\alpha]_D^{25}$ = -166.8º (c = 1.0, $CHCl_3$). 42% ee (determined by HPLC: Chiralpak IA Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 7.49 min (minor), 9.62 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.6 Hz, 1H), 7.21 – 7.11 (m, 1H), 7.10 – 6.96 (m, 1H), 6.94 – 6.69 (m, 3H), 6.67 – 6.27 (s, 2H), 6.25 (s, 2H), 6.12 (d, *J* = 10.0 Hz, 1H), 5.95 (d, *J* = 9.6 Hz, 1H), 3.04 (s, 1H), 2.99 (s, 3H), 2.82 (s, 6H), 2.73 – 2.63 (m, 1H), 2.54 – 2.41 (m, 1H), 2.35 – 2.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.5, 133.6, 132.6, 132.3, 129.0, 128.8, 127.1, 127.0, 126.2, 125.9, 124.6, 121.9, 117.6, 115.6, 42.4, 40.4, 35.7, 34.9, 27.2, 24.0, 17.7; IR (neat):

2919, 1613, 1526, 1488, 1455, 1361, 1262, 1166, 1063, 983; HRESIMS Calcd for $[C_{26}H_{26}N_2NaO_2S]^+$ (M + Na^+) 453.1607, found 453.1611.

(3b*S*,7a*R*,7b*S*,8a*R*)-3b-(4-methoxyphenyl)-2-(methylsulfonyl)-2,3b,3c,7b,8,8a-hexahydrobenzo[2,3]cyclopropa[1,2-*e*]cyclopropa[*g*]isoindole (4aj)

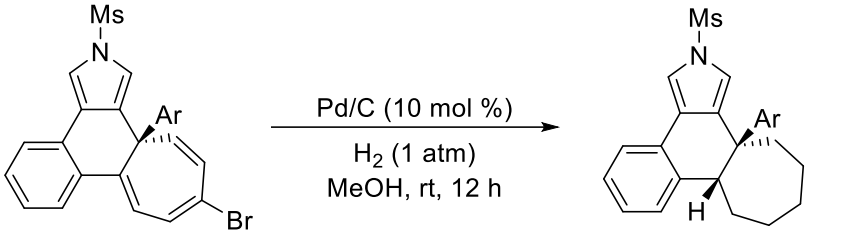


4aj

Compound **4aj** was prepared in 38% yield (14.4 mg) according to the general procedure except in DCM at 30 °C for 32 h. Pale solid (mp 152–153 °C). $[\alpha]_D^{25}$ = -7.4º (c = 1.0, $CHCl_3$). 20% ee (determined by HPLC: Chiralpak IA Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.29 min (minor), 8.84 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 2H), 6.61 (d, *J* = 2.4 Hz, 1H), 6.34 (d, *J* = 8.0 Hz, 1H), 6.26 – 6.20 (m, 1H), 6.00– 5.93 (m, 1H), 5.93 – 5.86 (m, 1H), 3.73 (s, 3H), 3.65 (d, *J* = 7.2 Hz, 1H), 3.04 (s, 3H), 2.10 (td, *J* = 8.4, 5.6 Hz, 1H), 2.02 (td, *J* = 8.0, 4.8 Hz, 1H), 1.38 (td, *J* = 8.4, 4.4 Hz, 1H), 0.82 (dd, *J* = 9.6, 4.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 132.8, 131.3, 130.7, 126.8, 126.2, 124.9, 124.8, 123.6, 118.6, 115.7, 112.5, 80.6, 79.9, 55.0, 42.5, 31.9, 20.8, 18.0, 9.8; IR (neat): 2926, 2853, 1607, 1510, 1411, 1362, 1245, 1169, 1067, 983; HRESIMS Calcd for $[C_{22}H_{21}NNaO_3S]^+$ (M + Na^+) 402.1134, found 402.1135.

5. Synthetic Utility Study

N,*N*-dimethyl-4-((7b*R*,12a*R*)-2-(methylsulfonyl)-7b,8,9,10,11,12-hexahydrobenzo[*e*]cyclohepta[*g*]isoindol-12a(2*H*)-yl)aniline (5a)

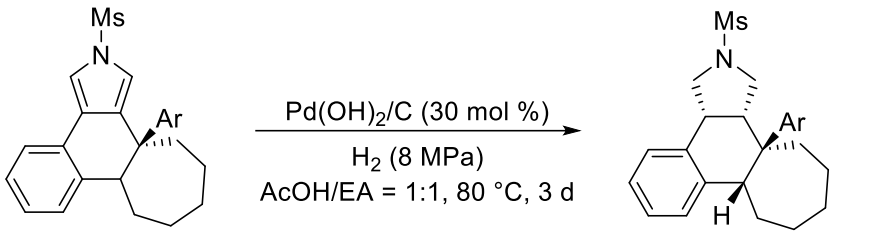


2a, 94% ee
Ar = 4-NMe_2-C_6H_4

5a, 98%, 94% ee, 12:1 dr

Compound **5a** was prepared according to the known procedure (0.25 mmol scale)[2] in 98% yield (106.5 mg) as a colourless solid (mp 241–243 °C). $[\alpha]_D^{25}$ = +21.6º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 12.00 min (major), 14.12 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.6 Hz, 1H), 7.35 – 7.29 (m, 2H), 7.24 – 7.19 (m, 1H), 7.16 – 7.08 (m, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 6.40 (d, *J* = 8.8 Hz, 2H), 3.20 – 3.17 (s, 1H), 3.16 (s, 3H), 2.78 (s, 6H), 2.70 – 2.58 (m, 1H), 2.43 – 2.33 (m, 1H), 2.28 – 2.15 (m, 2H), 2.10 – 2.01 (m, 1H), 1.86 – 1.79 (m, 1H), 1.69 – 1.63 (m, 2H), 1.52 – 1.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 140.4, 137.1, 132.1, 129.7, 128.6, 127.2, 126.2, 125.7, 125.0, 123.5, 114.7, 114.0, 111.8, 49.6, 45.3, 42.6, 40.4, 39.3, 28.5, 28.4, 26.0, 22.5; IR (neat): 3021, 2926, 1730, 1610, 1520, 1456, 1372, 1265, 1180, 1082; HRESIMS Calcd for $[C_{26}H_{30}N_2NaO_2S]^+$ (M + Na^+) 457.1920, found 457.1919.

N,*N*-dimethyl-4-((3a*R*,7b*R*,12a*S*,12b*S*)-2-(methylsulfonyl)-2,3,3a,7b,8,9,10,11,12,12b-decahydrobenzo[*e*]cyclohepta[*g*]isoindol-12a(1*H*)-yl)aniline (5b)

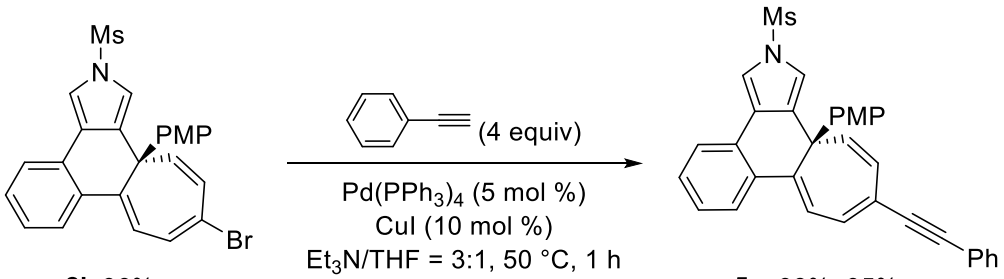


5a, 94% ee, 12:1 dr
Ar = 4-NMe_2-C_6H_4

5b, 50%, 94% ee, 12:1 dr

Compound **5b** was prepared according to the known procedure (0.15 mmol scale)[2] in 50% yield (32.7 mg) as a white solid (mp 158–159 °C). $[\alpha]_D^{25}$ = 3.4º (c = 1.0, $CHCl_3$). 94% ee (determined by HPLC: Chiralpak IE Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 34.56 min (major), 38.58 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.23 – 7.17 (m, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 9.2 Hz, 2H), 6.48 (d, *J* = 8.4 Hz, 2H), 3.67 – 3.59 (m, 2H), 3.57 – 3.51 (m, 1H), 3.46 – 3.41 (m, 1H), 3.08 – 3.00 (m, 1H), 2.83 (s, 6H), 2.74 – 2.64 (m, 2H), 2.56 – 2.46 (m, 1H), 2.47 – 2.38 (m, 1H), 2.36 (s, 3H), 1.87 – 1.48 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 134.4, 130.4, 127.8, 127.2, 125.7, 125.1, 111.9, 51.8, 49.9, 49.8, 47.6, 44.6, 43.0, 41.6, 40.4, 35.6, 29.4, 27.1, 26.6, 23.9; IR (neat): 2931, 2857, 1612, 1521, 1446, 1336, 1262, 1148, 1073, 950; HRESIMS Calcd for $[C_{26}H_{34}N_2NaO_2]^+$ (M + Na^+) 461.2233, found 461.2269.

(*S*)-12a-(4-methoxyphenyl)-2-(methylsulfonyl)-10-(phenylethynyl)-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (5c)



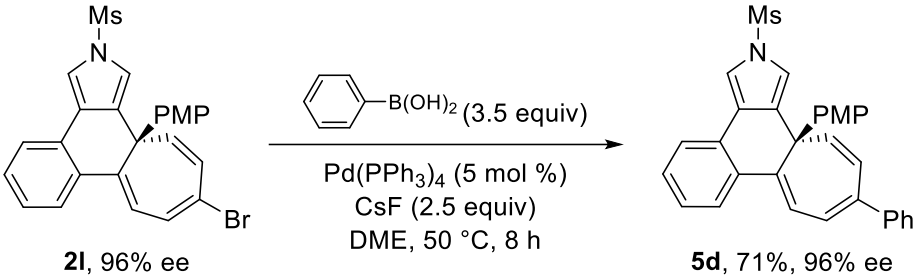
2l, 96% ee

5c, 98%, 95% ee

To an oven-dried 10 mL vial with a stir bar were added **2l** (0.15 mmol, 74.2 mg), THF (3 mL) and Et_3N (1 mL). Then phenylacetylene (0.6 mmol, 66 μL), $Pd(PPh_3)_4$ (0.0075 mmol, 8.6 mg) and CuI (0.015 mmol, 5.7 mg) were added sequentially and stirred at 50 °C for 1 h. Upon completion, the mixture was filtered, extracted with ethyl acetate

for three times, dried over $MgSO_4$ and concentrated. The residue was purified by chromatography on silica gel (eluent: PE/EtOAc) to afford **5c** in 98% yield (75.8 mg) as a pale yellow solid (mp 118–119 °C). $[\alpha]_D^{25}$ = -233.9º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 8.15 min (minor), 11.22 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.56 (m, 2H), 7.46 – 7.40 (m, 3H), 7.35 – 7.25 (m, 5H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.70 (d, *J* = 2.0 Hz, 1H), 6.65 – 6.58 (m, 3H), 6.55 (d, *J* = 8.0 Hz, 1H), 4.64 (d, *J* = 8.4 Hz, 1H), 3.70 (s, 3H), 3.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 135.3, 132.6(3), 132.5(8), 132.5, 131.5, 128.7, 128.2, 128.1, 128.0(3), 127.9(5), 127.9, 127.7, 126.9, 123.4, 122.3, 121.7, 119.0, 113.3, 112.7, 104.7, 101.8, 90.6, 90.1, 55.0, 42.8, 41.5; IR (neat): 3131, 2931, 1607, 1506, 1488, 1471, 1373, 1243, 1167, 1071, 981; HRESIMS Calcd for $[C_{33}H_{25}NNaO_3S]^+$ (M + Na^+) 538.1447, found 538.1485.

(*S*)-12a-(4-methoxyphenyl)-2-(methylsulfonyl)-10-phenyl-2,12a-dihydrobenzo[*e*]cyclohepta[*g*]isoindole (5d)

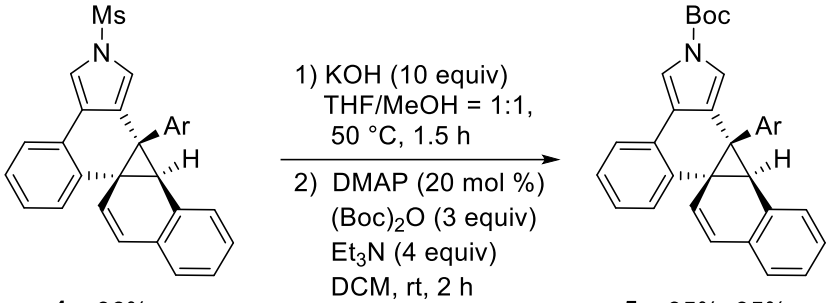


2l, 96% ee **5d**, 71%, 96% ee

To an oven-dried 10-mL Schlenk tube with a stir bar were added **2l** (0.15 mmol, 74.2 mg) and DME (3 mL). Then $PhB(OH)_2$ (0.53 mmol, 64.0 mg), $Pd(PPh_3)_4$ (0.0075 mmol, 8.7 mg) and CsF (0.38 mmol, 57.0 mg) were added sequentially and stirred at 50 °C for 8 h. Upon completion, the mixture was filtered, extracted with ethyl acetate for three times, dried over $MgSO_4$ and concentrated. The residue was purified by chromatography on silica gel (eluent: PE/EtOAc) to obtain **5d** in 71% yield (51.2 mg) as a pale yellow solid (mp 234–235 °C). $[\alpha]_D^{25}$ = -152.8º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 40/60 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.82 min (minor), 9.58 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d,

J = 20.4 Hz, 2H), 7.42 (s, 1H), 7.36 – 7.23 (m, 7H), 7.14 – 6.91 (m, 3H), 6.73 (s, 1H), 6.66 – 6.22 (m, 4H), 4.66 (d, *J* = 8.4 Hz, 1H), 3.65 (s, 3H), 3.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 141.3, 139.7, 135.5, 133.0, 132.7, 128.8, 128.4, 128.0, 127.7, 127.6, 127.5, 127.1, 126.7, 126.5, 124.4, 123.4, 122.9, 121.9, 118.9, 113.3, 112.5, 101.2, 99.8, 55.0, 42.8, 40.6; IR (neat): 3023, 2923, 1606, 1579, 1470, 1367, 1244, 1174, 1055, 949; HRESIMS Calcd for $[C_{31}H_{25}NNaO_3S]^+$ (M + Na^+) 514.1447, found 514.1469.

tert-butyl (3b*S*,3c*S*,9a*R*)-3b-(4-(pyrrolidin-1-yl)phenyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole-2-carboxylate (5e)

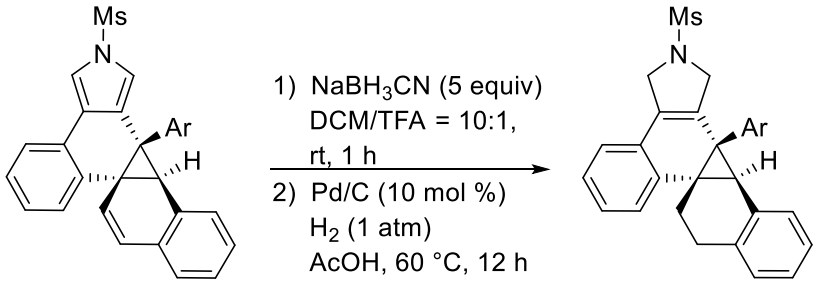


4a, 96% ee
Ar = 4-NTHP-C_6H_4

5e, 95%, 95% ee

Compound **5e** was prepared according to the known procedure (0.15 mmol scale)[3,4] in 95% yield (75.1 mg) as a pale yellow solid (mp 156–157 °C). $[\alpha]_D^{25}$ = -399.3º (c = 1.0, $CHCl_3$). 95% ee (determined by HPLC: Chiralpak IB Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.89 min (minor), 8.65 min (major)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.2 Hz, 1H), 7.58 (s, 1H), 7.37 – 7.28 (m, 2H), 7.27 – 7.15 (m, 3H), 7.13 – 7.05 (m, 1H), 6.91 (d, *J* = 7.2 Hz, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 6.71 (s, 1H), 6.56 (d, *J* = 7.8 Hz, 1H), 6.39 (d, *J* = 7.2 Hz, 1H), 6.34 (d, *J* = 9.6 Hz, 1H), 6.23 (d, *J* = 9.6 Hz, 1H), 6.07 (d, *J* = 8.4 Hz, 1H), 3.23 – 3.04 (m, 4H), 2.63 (s, 1H), 2.01 – 1.82 (m, 4H), 1.56 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.8, 146.0, 137.8, 133.3, 132.4, 131.4(3), 131.4(0), 129.9, 129.2, 128.9, 127.3, 127.2, 127.1, 126.8, 126.4, 126.3, 126.0, 125.9, 124.6, 122.9, 120.0, 118.3, 113.3, 111.6, 109.7, 83.7, 47.4, 41.7, 37.3, 28.0, 27.9, 25.4; IR (neat): 2975, 2931, 1808, 1738, 1614, 1521, 1479, 1394, 1274, 1157; HRESIMS Calcd for $[C_{36}H_{34}N_2NaO_2]^+$ (M + Na^+) 549.2512, found 549.2536.

(3b*S*,3c*S*,9a*R*)-2-(methylsulfonyl)-3b-(4-(pyrrolidin-1-yl)phenyl)-2,3,3b,3c,8,9-hexahydro-1*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (5f)

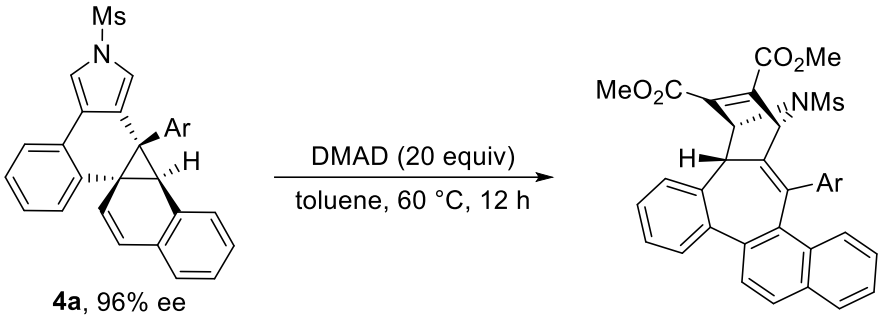


4a, 96% ee
Ar = 4-NTHP-C_6H_4

5f, 51%, 96% ee

Compound **5f** was prepared according to the known procedure (0.25 mmol scale)[2,5] in 51% yield (64.9 mg) as a white solid (mp 146–147 °C). $[\alpha]_D^{25}$ = -189.0º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IE Column, 30/70 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 15.05 min (minor), 18.79 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.25 (m, 3H), 7.21 – 7.13 (m, 1H), 7.12 – 7.05 (m, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.55 – 6.38 (m, 2H), 6.12 (d, *J* = 8.4 Hz, 1H), 4.73 – 4.49 (m, 2H), 4.34 – 4.16 (m, 1H), 3.73 – 3.60 (m, 1H), 3.25 – 3.11 (m, 4H), 2.91 – 2.81 (m, 1H), 2.80 (s, 3H), 2.59 – 2.46 (m, 1H), 2.21 – 2.11 (m, 1H), 2.02 – 1.93 (m, 4H), 1.92 (s, 1H), 1.78 – 1.65 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 139.0, 138.7, 135.5, 133.9, 131.0, 130.2, 129.1, 128.2, 127.5, 127.4, 126.0, 125.9, 125.5, 124.4, 123.5, 112.4, 110.9, 57.1, 54.7, 47.4, 41.1, 35.7, 34.6, 32.8, 27.4, 25.4, 23.8; IR (neat): 3058, 2919, 1612, 1525, 1488, 1378, 1266, 1154, 1053, 959; HRESIMS Calcd for $[C_{32}H_{32}N_2NaO_2S]^+$ (M + Na^+) 531.2077, found 531.2115.

dimethyl (12*R*,15*S*,15a*S*)-16-(methylsulfonyl)-11-(4-(pyrrolidin-1-yl)phenyl)-15,15a-dihydro-12*H*-12,15-epiminodibenzo[3,4:5,6]cyclohepta[1,2-*a*]naphthalene-13,14-dicarboxylate (5g)

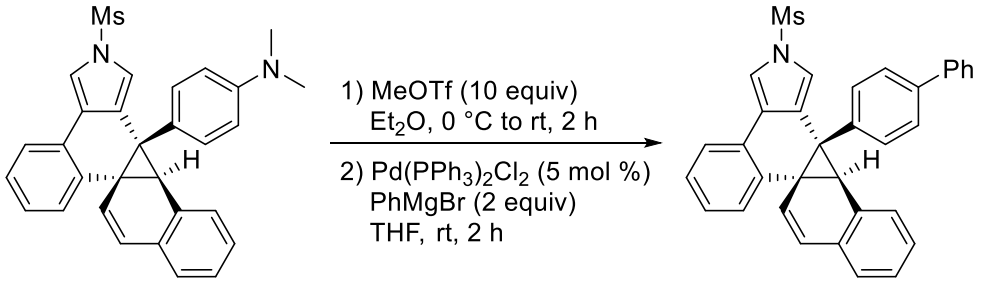


4a, 96% ee
Ar = 4-NTHP-C_6H_4

5g, 90%, 96% ee, 7:1 dr

Compound **5g** was prepared according to the known procedure (0.1 mmol scale)[6] in 90% yield (58.2 mg) as pale yellow solid (mp 141–142 °C). $[\alpha]_D^{25}$ = +172.2º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralpak IC Column, 50/50 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 18.30 min (major), 29.17 min (minor)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.8 Hz, 1H), 7.83 – 7.74 (m, 3H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.48 – 7.38 (m, 2H), 7.36 – 7.29 (m, 1H), 7.22 – 7.16 (m, 1H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.36 (d, *J* = 8.8 Hz, 2H), 5.82 (s, 1H), 5.76 (s, 1H), 4.04 (s, 3H), 3.73 (s, 3H), 3.24 (s, 1H), 3.22 – 3.13 (m, 4H), 2.89 (s, 3H), 1.99 – 1.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 162.2, 147.4, 146.8, 140.7, 139.7, 139.1, 136.9, 136.8, 135.3, 132.9, 132.4, 131.6, 129.8, 128.9, 128.2, 128.1, 128.0, 127.9(1), 127.8(7), 126.8, 125.7, 125.4, 123.7, 111.4, 67.2, 65.8, 53.0, 52.5, 47.4, 45.6, 40.8, 25.4; IR (neat): 2925, 2852, 1716, 1683, 1521, 1487, 1339, 1266, 1158, 1124, 1084, 1019, 766; HRESIMS Calcd for $[C_{38}H_{34}N_2NaO_6S]^+$ (M + Na^+) 669.2030, found 669.2093.

(3b*S*,3c*S*,9a*R*)-3b-([1,1'-biphenyl]-4-yl)-2-(methylsulfonyl)-3b,3c-dihydro-2*H*-benzo[*e*]naphtho[2',1':1,3]cyclopropa[1,2-*g*]isoindole (5h)



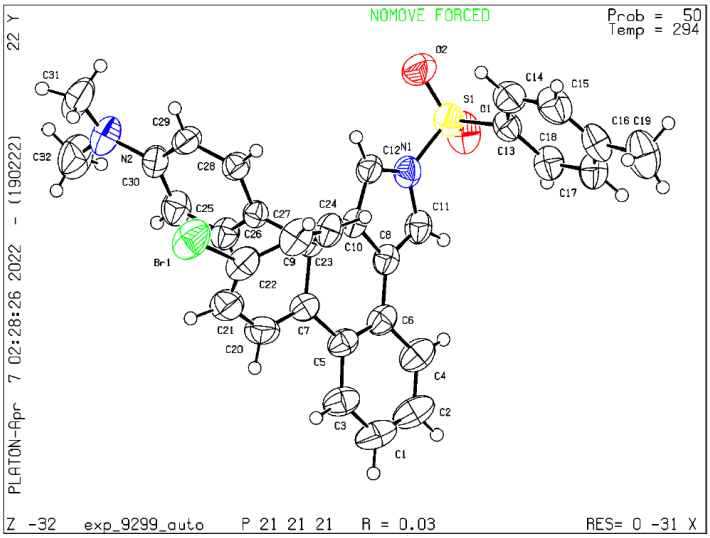
4x, 95% ee

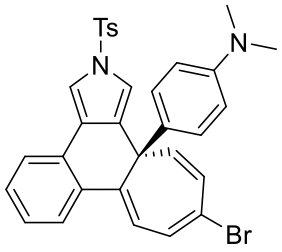
5h, 75%, 95% ee

Compound **5h** was prepared according to the known procedure (0.15 mmol scale)[5] in 75% yield (38.4 mg) as a white solid (mp 161–162 °C). $[\alpha]_D^{25}$ = +602.2º (c = 1.0,

$CHCl_3$). 95% ee (determined by HPLC: Chiralpak IE Column, 40/60 *i*-PrOH/hexane, 1.0 mL/min, 254 nm; TR = 6.04 min (minor), 7.06 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.65 (m, 1H), 7.53 – 7.48 (m, 3H), 7.45 – 7.34 (m, 5H), 7.34 – 7.25 (m, 4H), 7.17 – 7.02 (m, 3H), 6.90 (d, *J* = 7.2 Hz, 1H), 6.78 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.60 (d, *J* = 2.4 Hz, 1H), 6.39 – 6.20 (m, 2H), 3.14 (s, 3H), 2.73 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.6, 138.8, 137.5, 136.3, 133.2, 131.7, 131.1(3), 131.1(0), 130.0, 129.0, 128.6, 127.8, 127.7, 127.6, 127.5, 127.1, 126.9, 126.8, 126.4, 125.8, 125.4, 125.2, 123.2, 121.6, 118.8, 114.0, 42.8, 41.2, 37.1, 28.2. IR (neat): 3028, 2927, 1600, 1479, 1367, 1322, 1265, 1208, 1173, 1069; HRESIMS Calcd for $[C_{34}H_{25}NNaO_2S]^+$ ($M + Na^+$) 534.1498, found 534.1538.

6. Crystal Data





Bond precision:	C-C = 0.0042 A		Wavelength=1.54184
Cell:	a=11.5974(1)	b=11.6264(1)	c=20.4174(2)
	alpha=90	beta=90	gamma=90
Temperature:	294 K		

	Calculated	Reported
Volume	2753.00(4)	2753.00(4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C32 H27 Br N2 O2 S	C32 H27 Br N2 O2 S
Sum formula	C32 H27 Br N2 O2 S	C32 H27 Br N2 O2 S
Mr	583.52	583.52
Dx,g cm-3	1.408	1.408
Z	4	4
Mu (mm-1)	2.996	2.996
F000	1200.0	1200.0
F000'	1201.44	
h,k,lmax	14,14,25	14,14,25
Nref	5722[3226]	5603
Tmin,Tmax	0.942,0.942	0.841,1.000
Tmin'	0.942	

Correction method= # Reported T Limits: Tmin=0.841 Tmax=1.000
AbsCorr = MULTI-SCAN

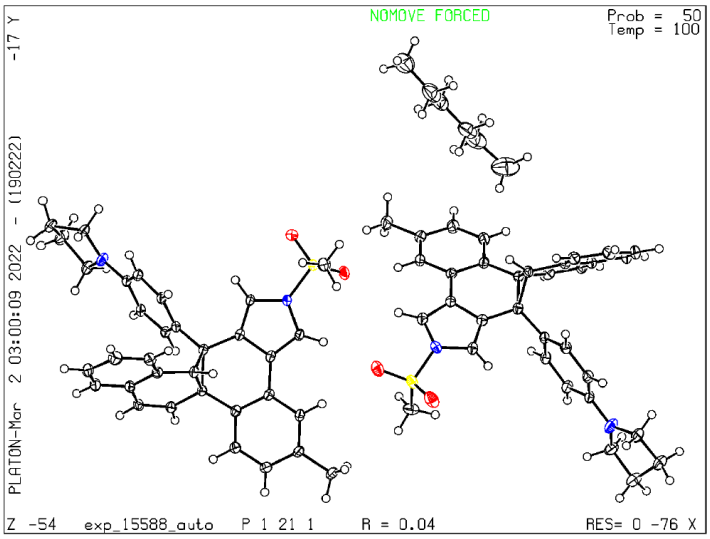
Data completeness= 1.74/0.98 Theta(max)= 75.395

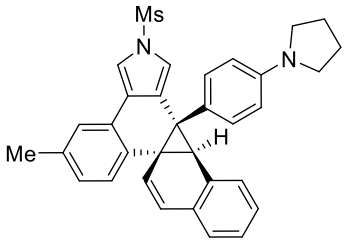
R(reflections)= 0.0293(5350) wR2(reflections)= 0.0834(5603)

S = 1.033 Npar= 346

Table S3. Crystal data and structure refinement for **2b**.

CCDC Number = 2301623.





Bond precision: C-C = 0.0038 A Wavelength=1.54184

Cell: a=15.6026(2) b=10.9134(1) c=17.5508(2)
alpha=90 beta=95.753(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2973.45(6)	2973.45(6)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	2(C33 H30 N2 O2 S), C6 H14	C33 H30 N2 O2 S, 0.5(C6 H14)
Sum formula	C72 H74 N4 O4 S2	C36 H37 N2 O2 S
Mr	1123.47	561.73
Dx,g cm-3	1.255	1.255
Z	2	4
Mu (mm-1)	1.236	1.236
F000	1196.0	1196.0
F000'	1200.42	
h,k,lmax	19,13,21	19,13,21
Nref	12141[6403]	8473
Tmin,Tmax	0.940,0.976	0.749,1.000
Tmin'	0.940	

Correction method= # Reported T Limits: Tmin=0.749 Tmax=1.000
AbsCorr = MULTI-SCAN

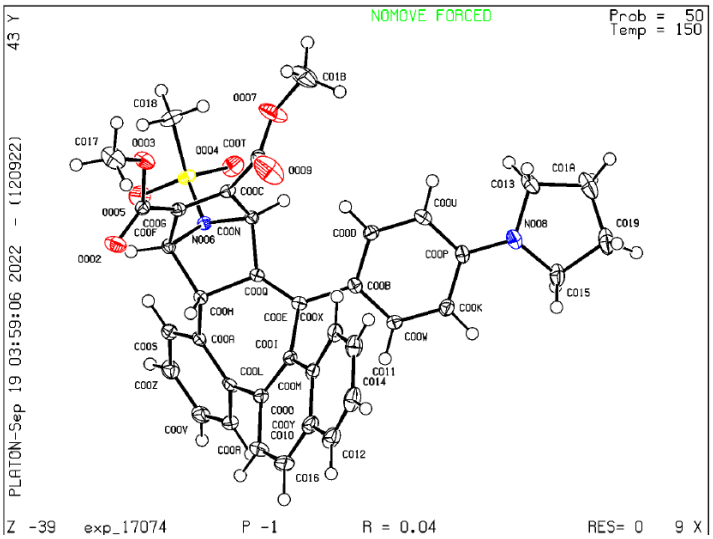
Data completeness= 1.32/0.70 Theta(max)= 74.408

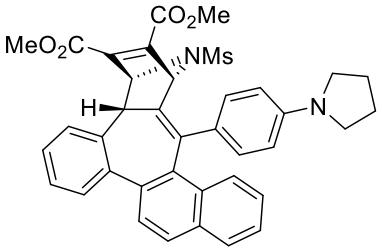
R(reflections)= 0.0359(8012) wR2(reflections)= 0.0900(8473)

S = 1.047 Npar= 745

Table S4. Crystal data and structure refinement for **4l**.

CCDC Number = 2301624.





Bond precision:	C-C = 0.0026 A		Wavelength=1.54184
Cell:	a=10.3211(6)	b=10.9346(5)	c=17.0233(8)
	alpha=92.326(4)	beta=95.527(4)	gamma=116.468(5)
Temperature:	150 K		

	Calculated	Reported
Volume	1704.30(17)	1704.29(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H34 N2 O6 S [+ solvent]	C38 H34 N2 O6 S
Sum formula	C38 H34 N2 O6 S [+ solvent]	C38 H34 N2 O6 S
Mr	646.73	646.73
Dx,g cm-3	1.260	1.260
Z	2	2
Mu (mm-1)	1.241	1.241
F000	680.0	680.0
F000'	682.67	
h,k,lmax	12,13,21	12,13,21
Nref	6936	6714
Tmin,Tmax	0.748,0.793	
Tmin'	0.679	

Correction method= Not given

Data completeness= 0.968 Theta(max)= 74.308

R(reflections)= 0.0415(5675) wR2(reflections)= 0.1087(6714)

S = 1.041 Npar= 428

Table S5. Crystal data and structure refinement for **5g.**

CCDC Number = 2301659.

7. Computational Studies

7.1. Computational Details

All density functional theory (DFT) calculations were performed using Gaussian 16 program[7]. Geometry optimizations of all structures were carried using B3LYP functional[8,9] with Grimme's dispersion corrections[10,11] and 6-31G(d) basis set [12] for C, H, N, O, S, and LANL2DZ pseudo-potential basis set[13] for Cu and Br. The solvation effects in toluene/2-MeTHF were calculated with a self-consistent reaction field (SCRF) using the PCM solvation model[14,15]. Frequency analysis was performed at the same level of theory as geometry optimization to confirm whether optimized stationary points were either local minimum or transition state, as well as to evaluate zero-point vibrational energies and thermal corrections for enthalpies and free energies at 298.15 K. For critical transition states, intrinsic reaction coordinates (IRC) analysis was also performed at the same level of theory as geometry optimization to verify the proposed process. Single-point energies were computed with PBE0 functional[16] with Grimme's dispersion corrections and 6-311++G(d,p) basis set[17] for C, H, N, O, S, and Stuttgart pseudo-potential basis set[18] for Cu and Br with the inclusion of solvent correction at the PCM (toluene/2-Me THF) level. The 3D diagrams of DFT-optimized structures were generated with CYLview2.0 software[19]. Independent gradient model (IGM) analysis was used to verify non-covalent interactions[20-22].

To correct the Gibbs free energies under 1 atm to the standard state in solution (1 mol/L), a correction of RTln(cs/cg) is added to energies of all species. cs stands for the standard molar concentration in solution (1 mol/L), cg stands for the standard molar concentration in gas phase (0.040876 mol/L), and R is the gas constant. For calculated intermediates at the standard state of 1 mol/L at 298.15 K, the correction value equaling to 1.89 kcal/mol was used.

To correct the entropy change in solution, we applied an empirical approach[23] because there is currently no widely accepted quantum mechanics-based approach to correct entropy in solution. For each component change in a reaction at 298 K and 1 atm, a correction of 4.3 kcal/mol is applied to the reaction free energy (i.e., a reaction

from m- to ncomponents has an additional free energy correction for (n-m) × 4.3 kcal/mol). This approach has been validated through a number of computational and experimental studies.

Conformational Search

For conformational search, we applied the Conformer-Rotamer Ensemble Sampling Tool (CREST, version 2.10.2)[24] using the xTB package (version 6.1)[25] in combination with DFT optimizations. The conformers generated by CREST were optimized with GFN2-xTB. The solvation effects in toluene were calculated with GBSA implicit solvation model. An energy window of 6.0 kcal/mol and a RMSD threshold of 0.25 Å was used for sampling. For conformational samplings of transition state structures, atoms in the forming/cleaving bonds were constrained by applying a force constant of 1.0 Hartree/Bohr^2.

7.2. Table of Energies

Table S6. Low-energy conformers for **CuL9-*S*-TS$_{B1}$** with relative enthalpies and Gibbs free energies stability (in kcal/mol) with respect to the most stable geometry.

Structure	$\Delta\Delta G^{\ddagger}_{Sol}$	$\Delta\Delta H^{\ddagger}_{Sol}$
CuL9-*S*-TS$_{B1}$	0.0	0.0
CuL9-*S*-TS$_{B1}$-S1	4.1	3.0
CuL9-*S*-TS$_{B1}$-S2	0.8	0.7
CuL9-*S*-TS$_{B1}$-S3	2.1	4.0

Table S7. Low-energy conformers for **CuL9-*R*-TS$_{B1}$** with relative enthalpies and Gibbs free energies stability (in kcal/mol) with respect to the most stable geometry.

Structure	$\Delta\Delta G^{\ddagger}_{Sol}$	$\Delta\Delta H^{\ddagger}_{Sol}$
CuL9-*R*-TS$_{B1}$	0.0	0.0
CuL9-*R*-TS$_{B1}$-S1	2.0	0.6
CuL9-*R*-TS$_{B1}$-S2	2.6	3.0
CuL9-*R*-TS$_{B1}$-S3	1.2	2.6

Table S8. Low-energy conformers for **CuL12-*S*-TS$_{B2}$** with relative enthalpies and Gibbs free energies stability (in kcal/mol) with respect to the most stable geometry.

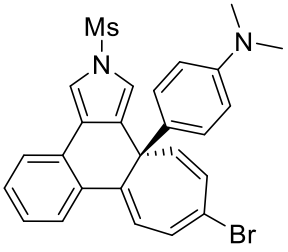
Structure	$\Delta\Delta G^{\ddagger}_{Sol}$	$\Delta\Delta H^{\ddagger}_{Sol}$
CuL12-*S*-TS$_{B2}$	0.0	0.0
CuL12-*S*-TS$_{B2}$-S1	3.0	1.8
CuL12-*S*-TS$_{B2}$-S2	3.7	2.8
CuL12-*S*-TS$_{B2}$-S3	3.9	3.0

Table S9. Low-energy conformers for **CuL12-*R*-TS$_{B2}$** with relative enthalpies and Gibbs free energies stability (in kcal/mol) with respect to the most stable geometry.

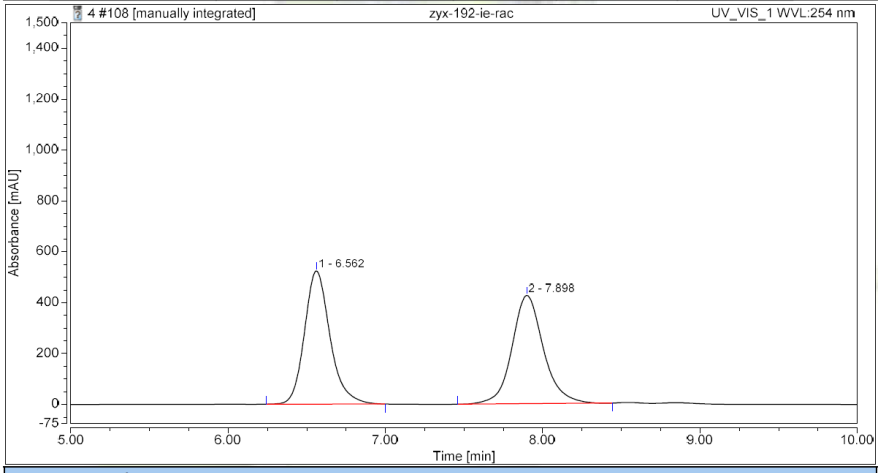
Structure	$\Delta\Delta G^{\ddagger}_{Sol}$	$\Delta\Delta H^{\ddagger}_{Sol}$
CuL12-*R*-TS$_{B2}$	0.0	0.0
CuL12-*R*-TS$_{B2}$-S1	3.5	2.2
CuL12-*R*-TS$_{B2}$-S2	1.6	-0.3
CuL12-*R*-TS$_{B2}$-S3	4.0	1.8

8. HPLC Chromatograms

2a: IE, *i*-PrOH/hexane = 40/60, v = 1.0 mL/min, λ = 254 nm



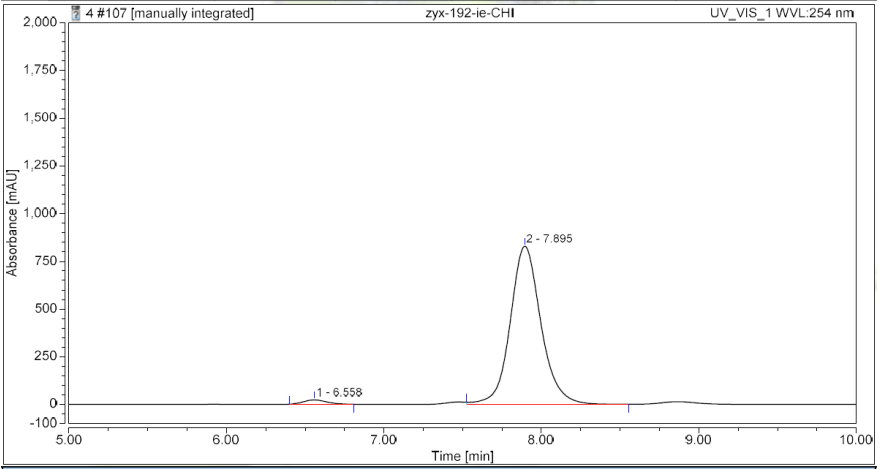
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		6.562	98.585	523.758	50.02	55.18	n.a.
300		7.898	98.515	425.378	49.98	44.82	n.a.
Total:			**197.100**	**949.136**	**100.00**	**100.00**	

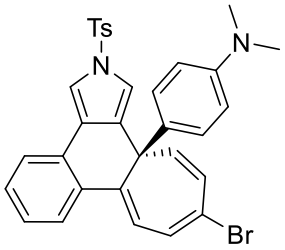
Chromatogram

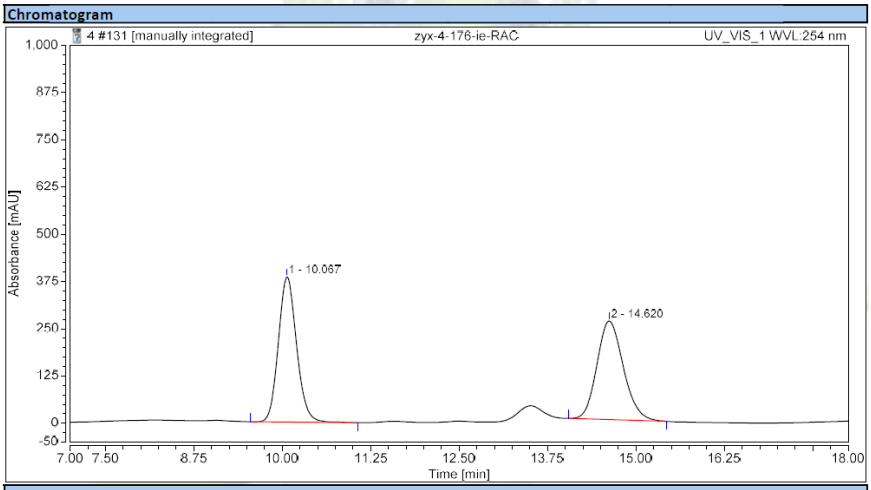


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		6.558	3.817	22.357	2.00	2.63	n.a.
300		7.895	186.793	828.501	98.00	97.37	n.a.
Total:			**190.611**	**850.858**	**100.00**	**100.00**	

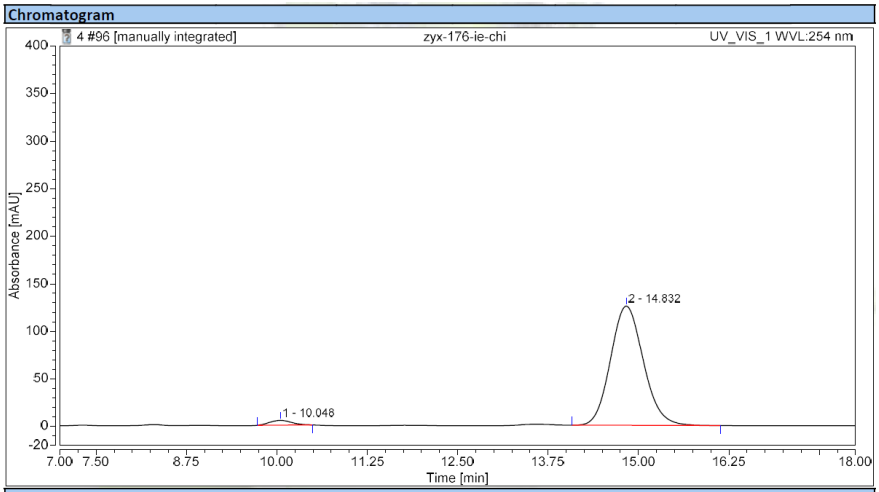
2b: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

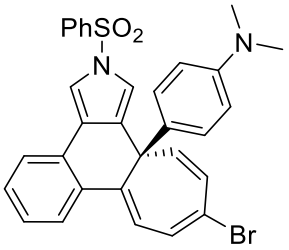
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		10.067	114.823	384.493	50.40	59.57	n.a.
300		14.620	113.009	260.997	49.60	40.43	n.a.
Total:			**227.832**	**645.490**	**100.00**	**100.00**	

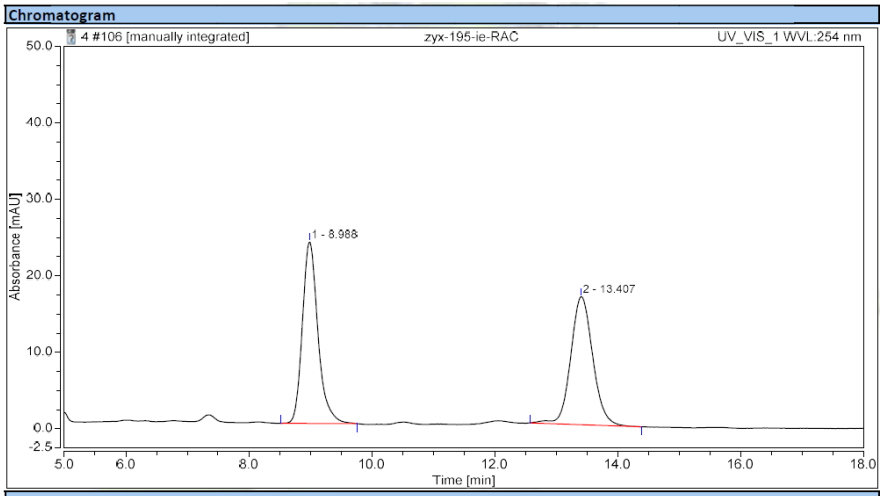


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		10.048	1.732	4.955	2.56	3.80	n.a.
300		14.832	66.035	125.452	97.44	96.20	n.a.
Total:			**67.768**	**130.407**	**100.00**	**100.00**	

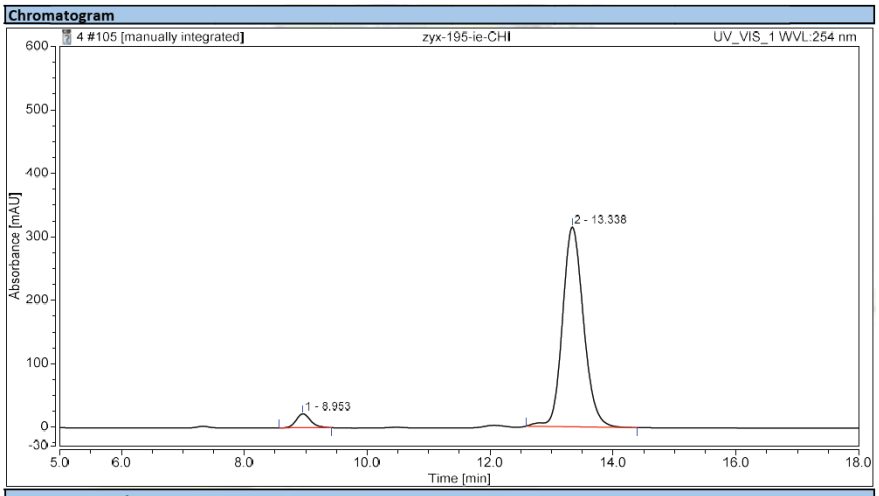
2c: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

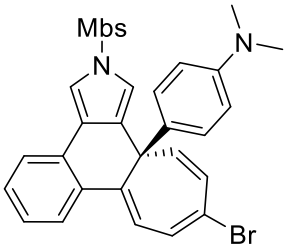
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		8.988	6.987	23.786	50.11	58.66	n.a.
300		13.407	6.955	16.762	49.89	41.34	n.a.
Total:			**13.942**	**40.549**	**100.00**	**100.00**	



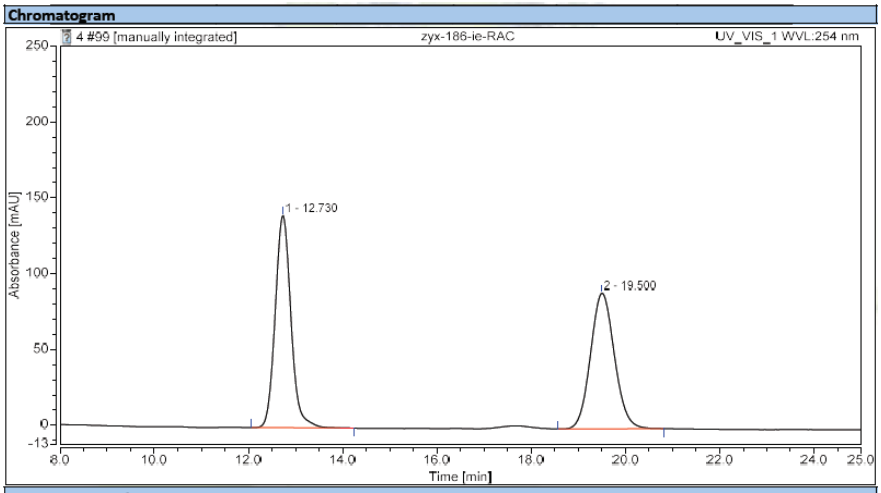
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		8.953	5.982	22.001	4.57	6.53	n.a.
300		13.338	124.820	315.058	95.43	93.47	n.a.
Total:			**130.802**	**337.059**	**100.00**	**100.00**	

2d: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



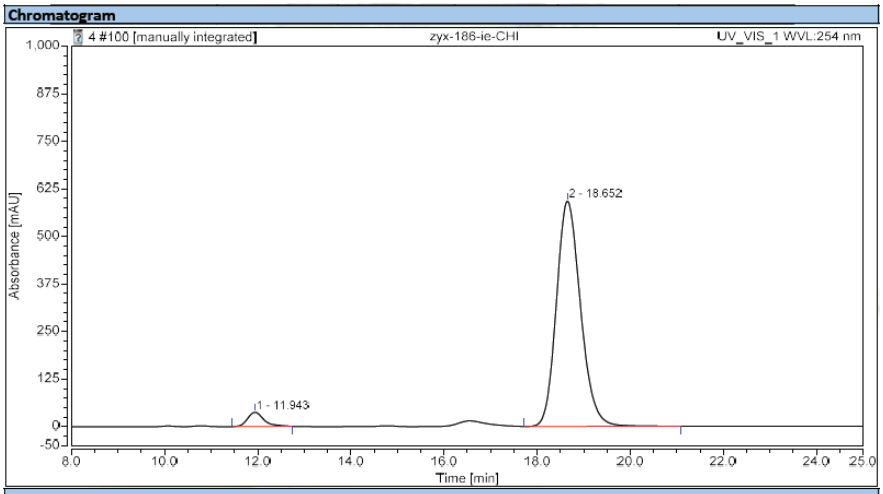
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		12.730	54.253	140.092	50.77	61.01	n.a.
300		19.500	52.605	89.531	49.23	38.99	n.a.
Total:			**106.858**	**229.623**	**100.00**	**100.00**	

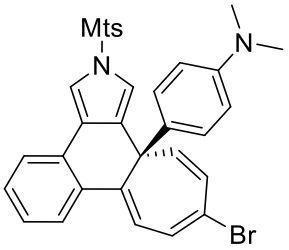
Chromatogram

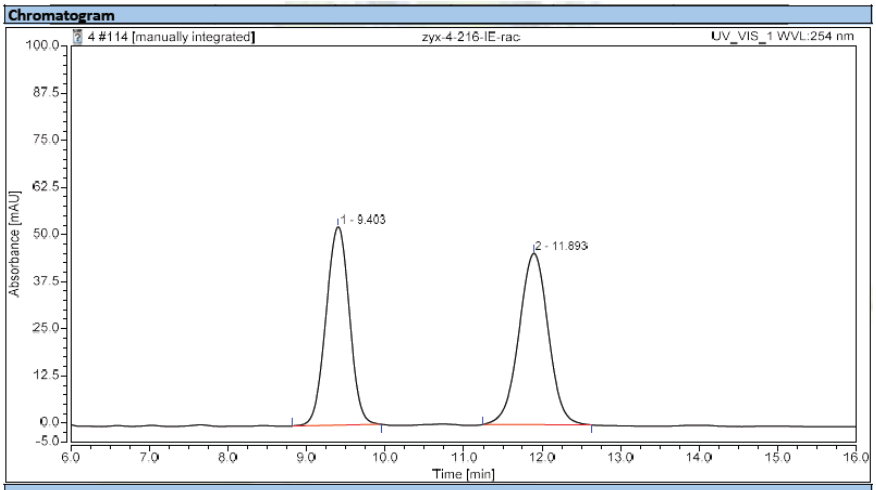


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		11.943	15.128	37.303	4.08	5.92	n.a.
300		18.652	355.772	592.606	95.92	94.08	n.a.
Total:			**370.901**	**629.908**	**100.00**	**100.00**	

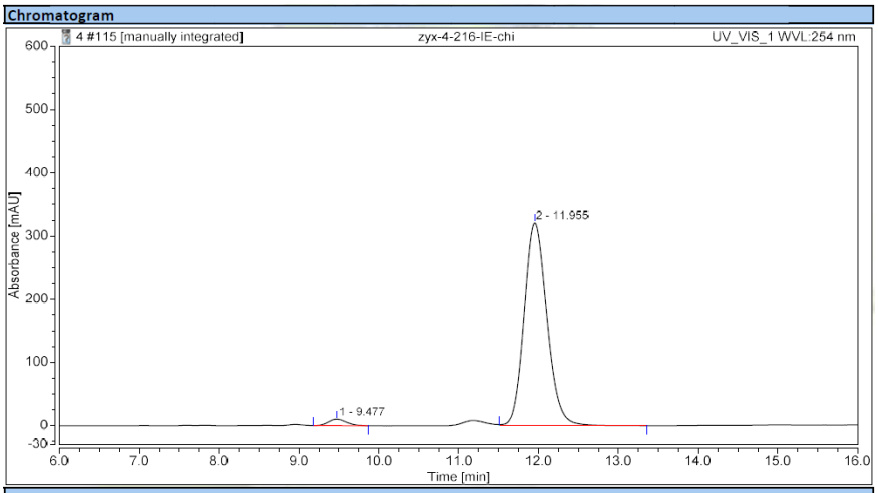
2e: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

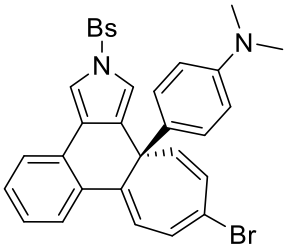
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		9.403	18.164	52.652	47.99	53.64	n.a.
300		11.893	19.684	45.508	52.01	46.36	n.a.
Total:			**37.848**	**98.160**	**100.00**	**100.00**	

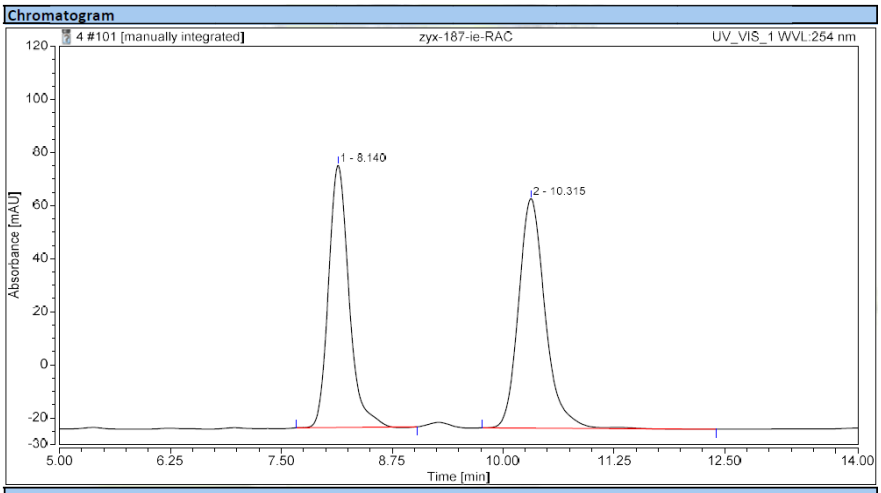


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		9.477	2.672	10.302	2.46	3.11	n.a.
300		11.955	106.044	321.067	97.54	96.89	n.a.
Total:			**108.716**	**331.369**	**100.00**	**100.00**	

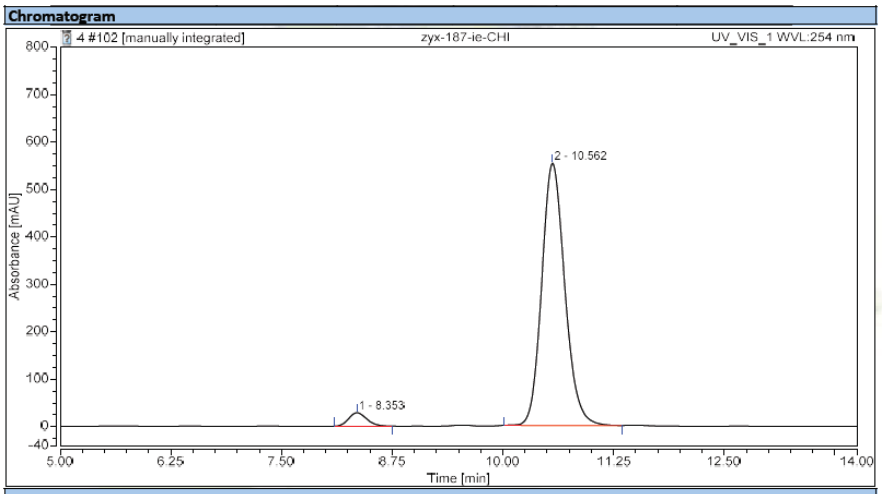
2f: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

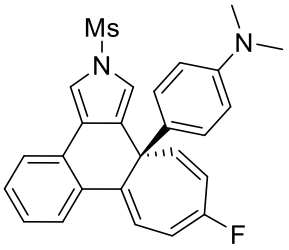
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		8.140	26.409	98.844	46.71	53.33	n.a.
300		10.315	30.128	86.490	53.29	46.67	n.a.
Total:			**56.537**	**185.335**	**100.00**	**100.00**	

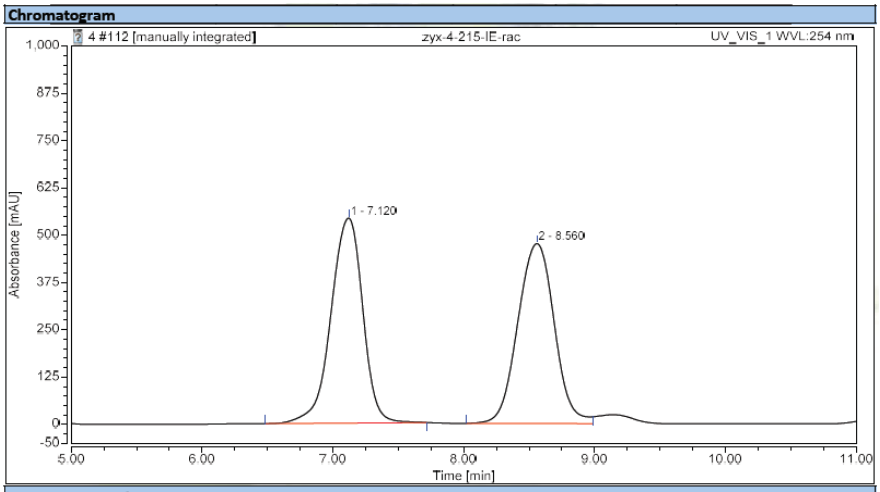


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		8.353	6.716	28.446	3.87	4.89	n.a.
300		10.562	167.031	552.915	96.13	95.11	n.a.
Total:			**173.747**	**581.360**	**100.00**	**100.00**	

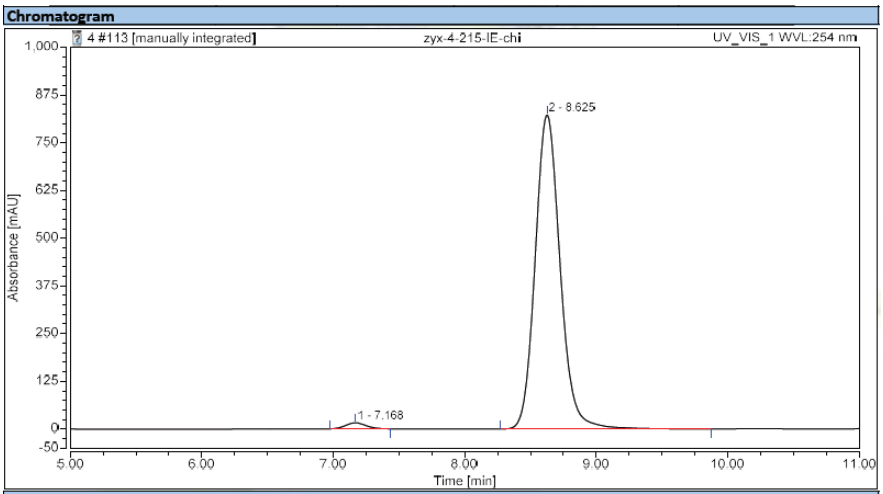
2g: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

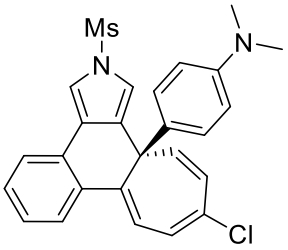
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.120	152.816	542.275	49.84	53.26	n.a.
300		8.560	153.806	475.926	50.16	46.74	n.a.
Total:			**306.622**	**1018.201**	**100.00**	**100.00**	

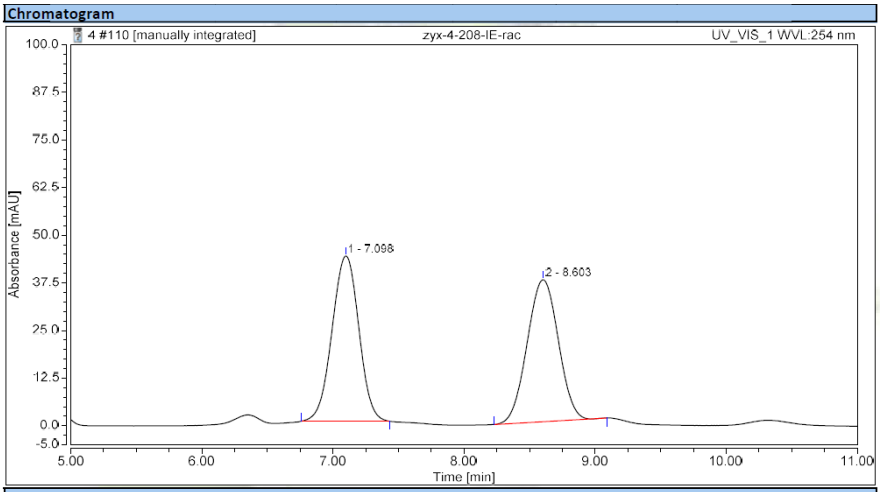


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.168	2.829	15.741	1.54	1.88	n.a.
300		8.625	180.684	823.545	98.46	98.12	n.a.
Total:			**183.512**	**839.287**	**100.00**	**100.00**	

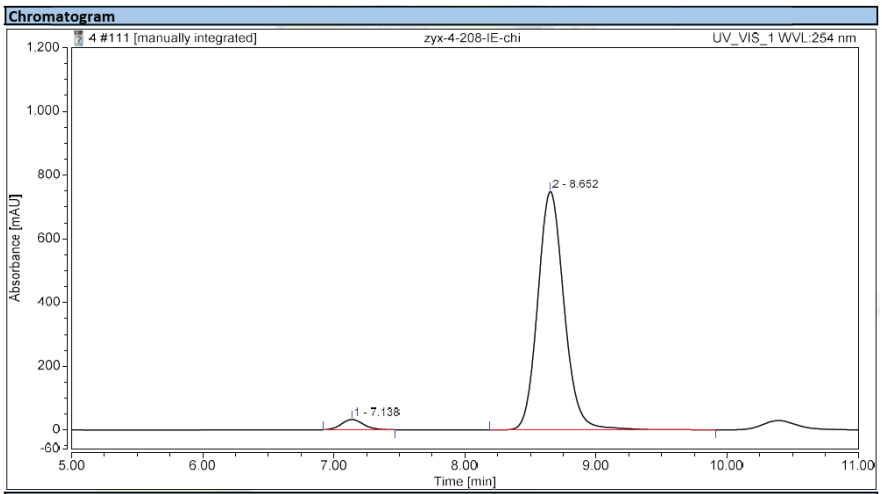
2h: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

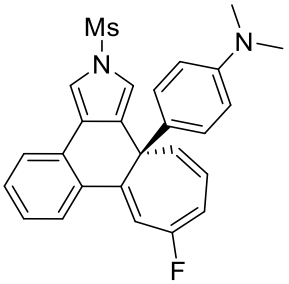
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.098	10.270	43.401	50.07	53.81	n.a.
300		8.603	10.242	37.253	49.93	46.19	n.a.
Total:			**20.513**	**80.654**	**100.00**	**100.00**	

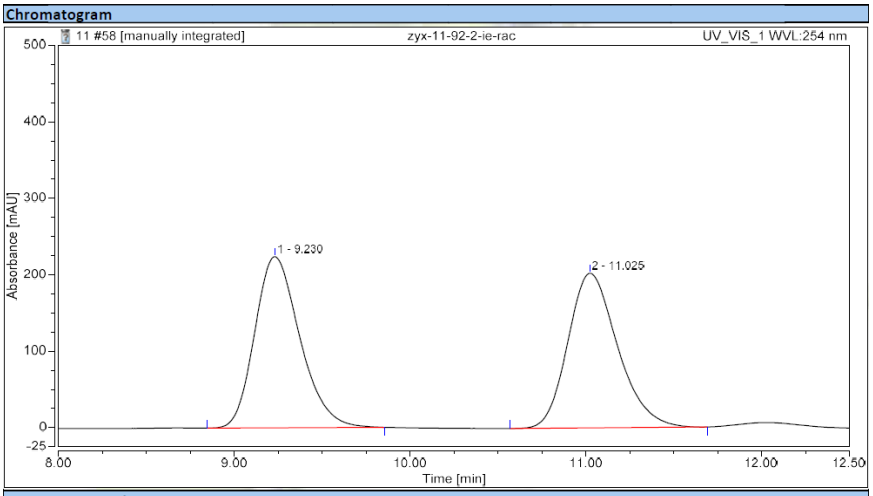


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.138	6.235	32.322	3.46	4.14	n.a.
300		8.652	174.210	748.892	96.54	95.86	n.a.
Total:			**180.446**	**781.214**	**100.00**	**100.00**	

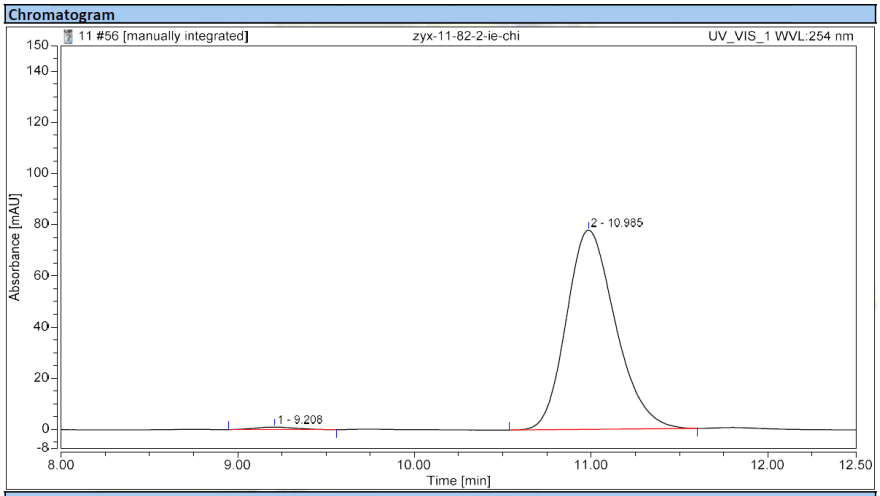
2i: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

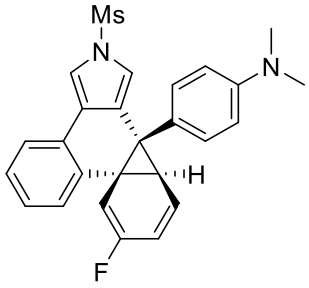
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.230	66.537	223.909	50.12	52.55	n.a.
2		11.025	66.215	202.179	49.88	47.45	n.a.
Total:			**132.751**	**426.088**	**100.00**	**100.00**	



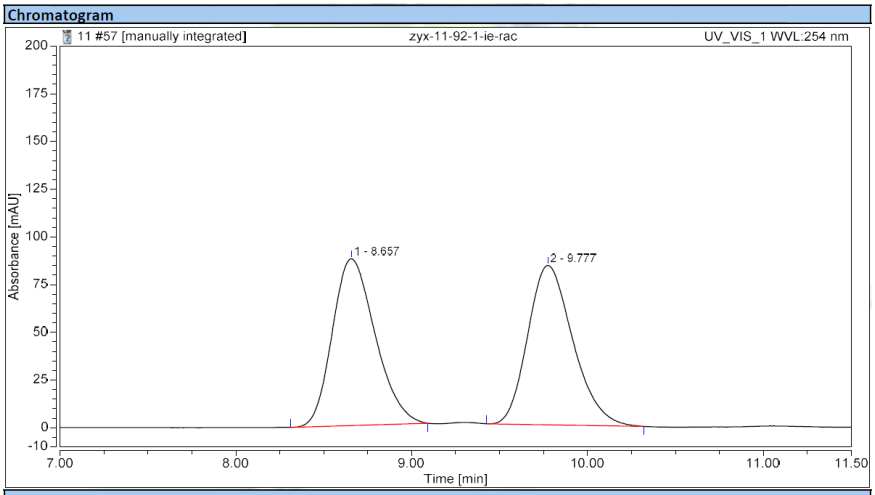
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.208	0.253	0.970	1.00	1.23	n.a.
2		10.985	25.062	77.899	99.00	98.77	n.a.
Total:			**25.315**	**78.869**	**100.00**	**100.00**	

2i′: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



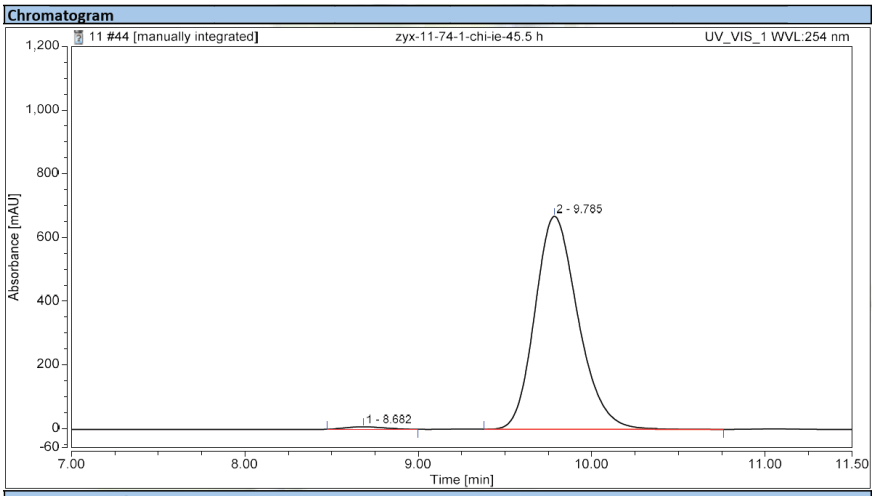
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.657	24.660	87.373	49.83	51.13	n.a.
2		9.777	24.827	83.496	50.17	48.87	n.a.
Total:			**49.487**	**170.869**	**100.00**	**100.00**	

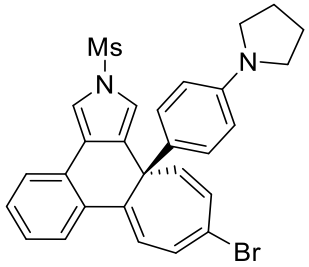
Chromatogram



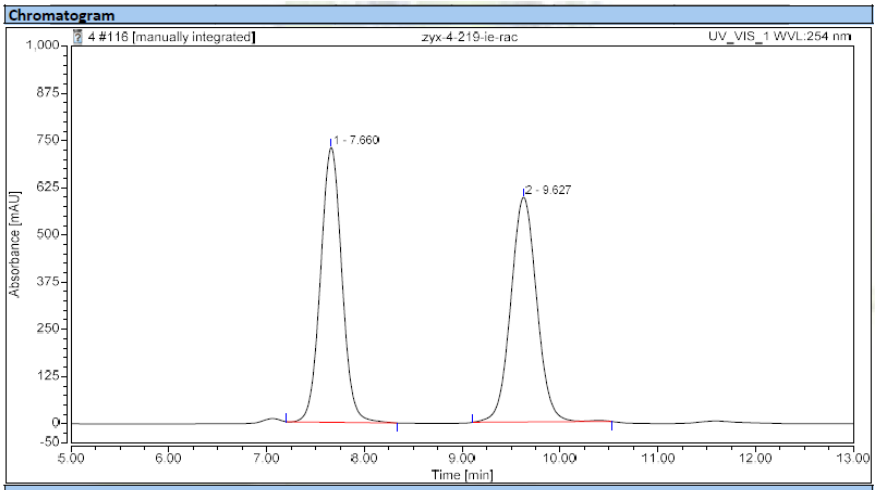
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.682	1.943	7.883	1.00	1.17	n.a.
2		9.785	192.505	668.388	99.00	98.83	n.a.
Total:			**194.448**	**676.271**	**100.00**	**100.00**	

2j: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



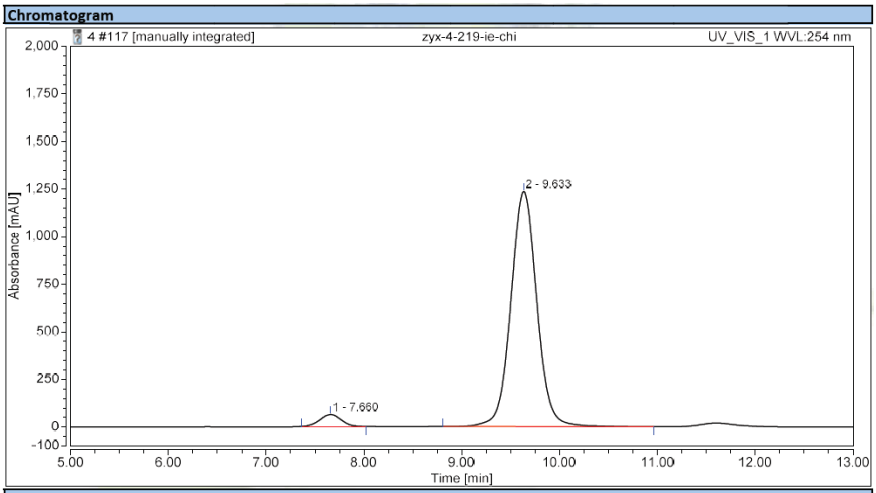
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.660	184.171	727.802	50.08	55.00	n.a.
300		9.627	183.616	595.468	49.92	45.00	n.a.
Total:			**367.787**	**1323.270**	**100.00**	**100.00**	

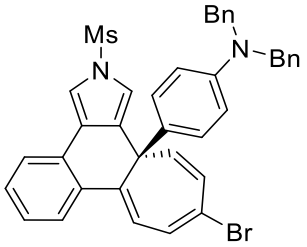
Chromatogram

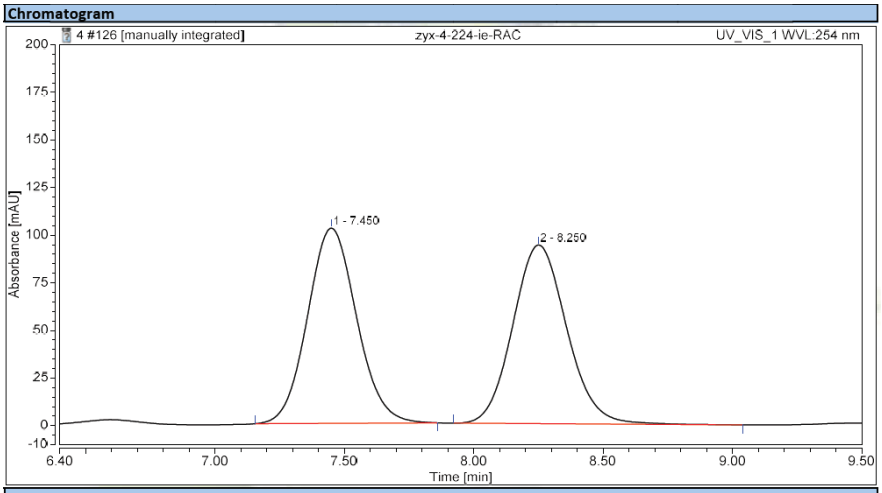


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.660	15.877	62.751	4.01	4.83	n.a.
300		9.633	380.362	1236.100	95.99	95.17	n.a.
Total:			**396.240**	**1298.851**	**100.00**	**100.00**	

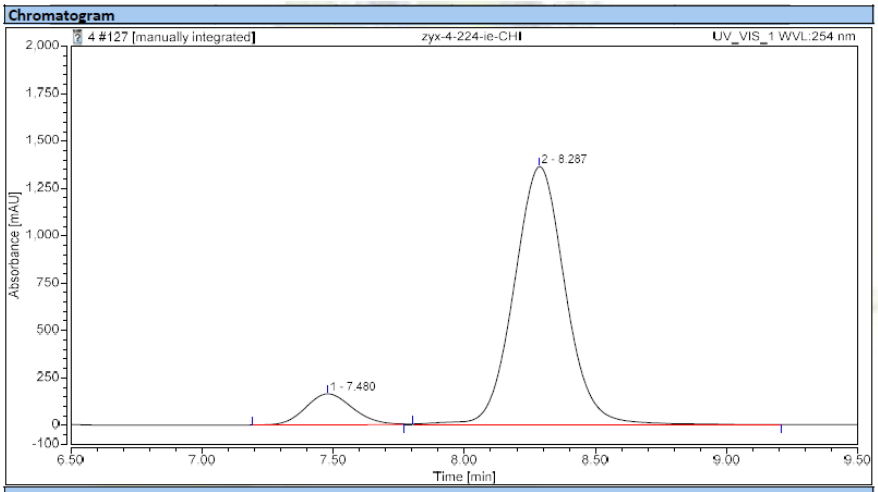
2k: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

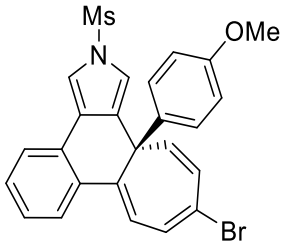
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.450	22.534	102.542	49.87	52.21	n.a.
300		8.250	22.656	93.872	50.13	47.79	n.a.
Total:			**45.190**	**196.415**	**100.00**	**100.00**	

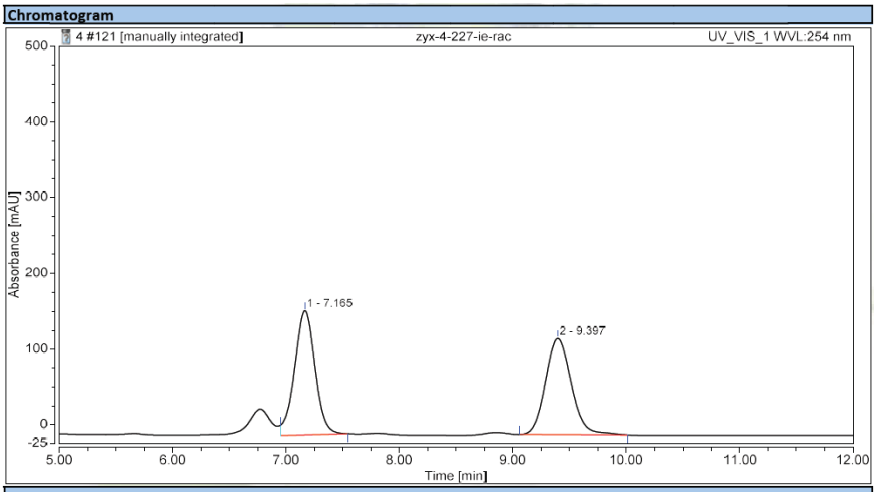


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.480	34.116	163.694	9.95	10.73	n.a.
300		8.287	308.803	1362.365	90.05	89.27	n.a.
Total:			**342.919**	**1526.059**	**100.00**	**100.00**	

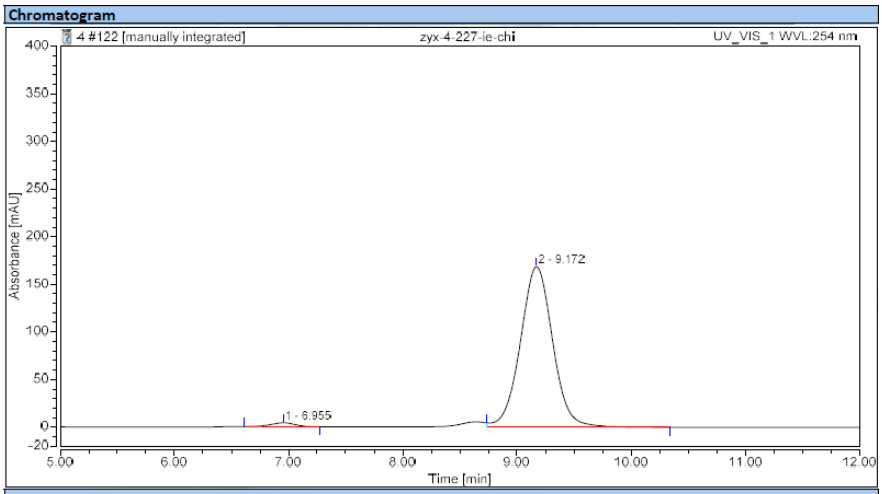
2l: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

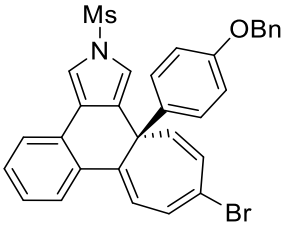
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.165	34.277	164.634	50.59	56.36	n.a.
300		9.397	33.483	127.501	49.41	43.64	n.a.
Total:			**67.760**	**292.135**	**100.00**	**100.00**	



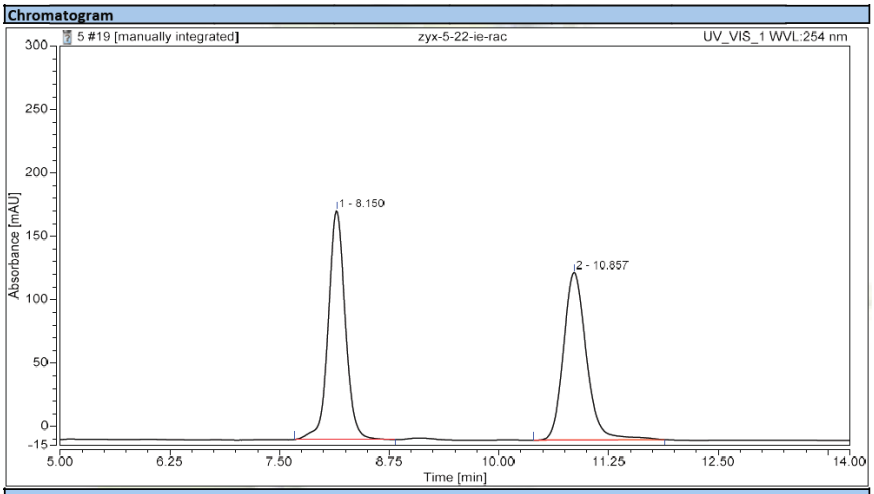
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		6.955	1.043	4.151	1.85	2.40	n.a.
300		9.172	55.380	168.690	98.15	97.60	n.a.
Total:			**56.423**	**172.841**	**100.00**	**100.00**	

2m: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



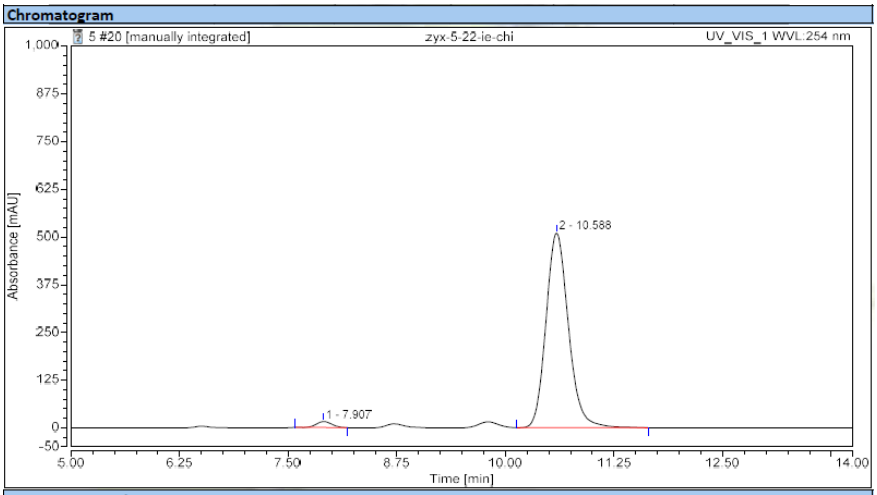
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.150	40.528	180.492	50.27	57.73	n.a.
2		10.857	40.099	132.158	49.73	42.27	n.a.
Total:			**80.627**	**312.649**	**100.00**	**100.00**	

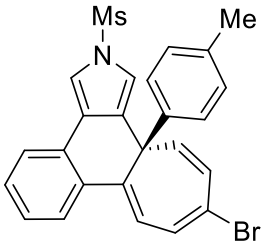
Chromatogram

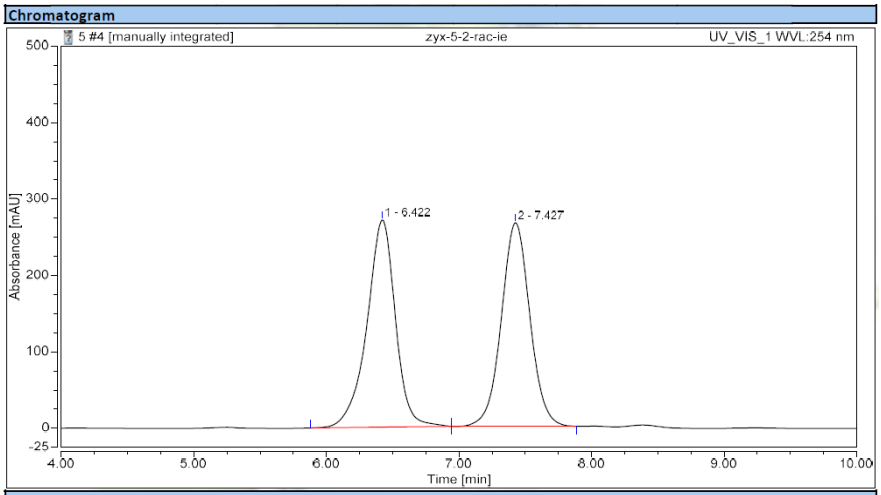


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.907	3.220	15.640	2.06	2.98	n.a.
2		10.588	152.833	509.912	97.94	97.02	n.a.
Total:			**156.053**	**525.552**	**100.00**	**100.00**	

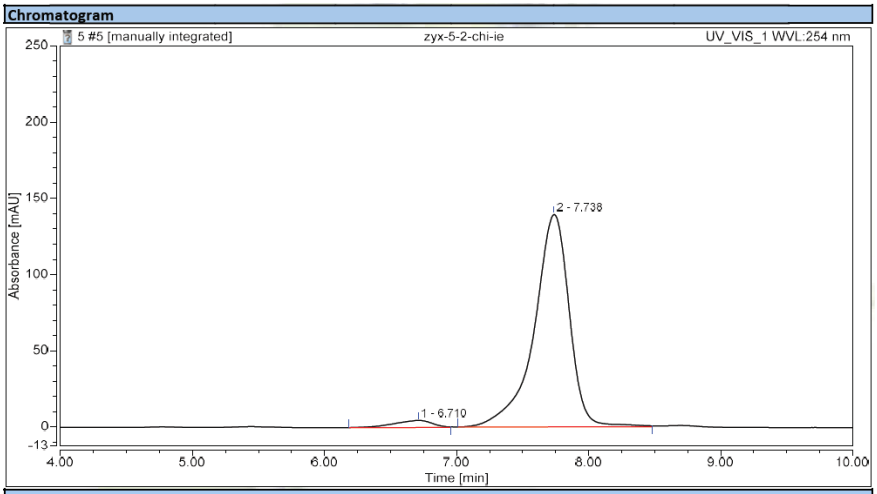
2n: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

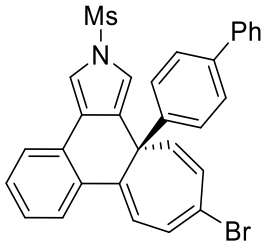
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.422	67.688	271.441	50.42	50.44	n.a.
2		7.427	66.559	266.678	49.58	49.56	n.a.
Total:			**134.248**	**538.119**	**100.00**	**100.00**	

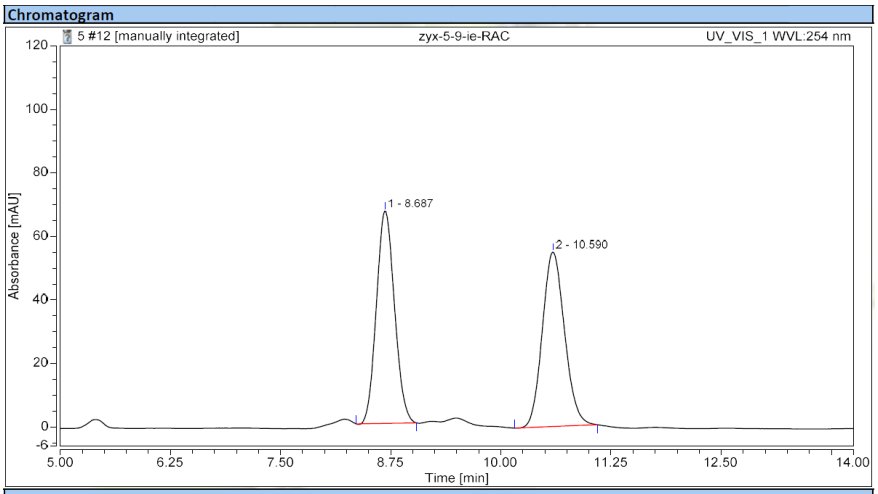


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.710	1.559	4.657	3.49	3.23	n.a.
2		7.738	43.088	139.405	96.51	96.77	n.a.
Total:			**44.648**	**144.062**	**100.00**	**100.00**	

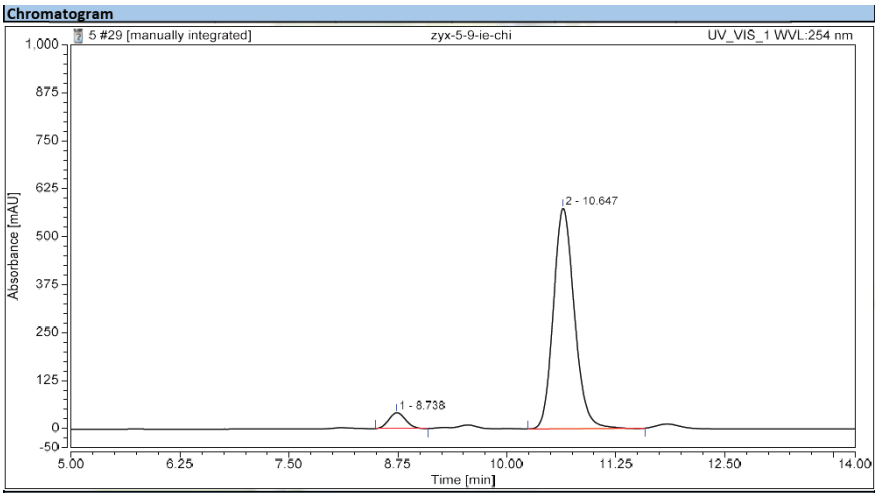
2o: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

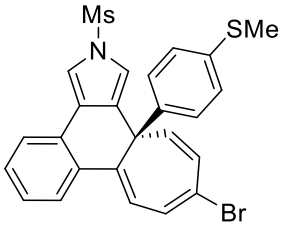
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.687	15.927	66.908	49.82	54.91	n.a.
2		10.590	16.043	54.949	50.18	45.09	n.a.
Total:			**31.970**	**121.857**	**100.00**	**100.00**	



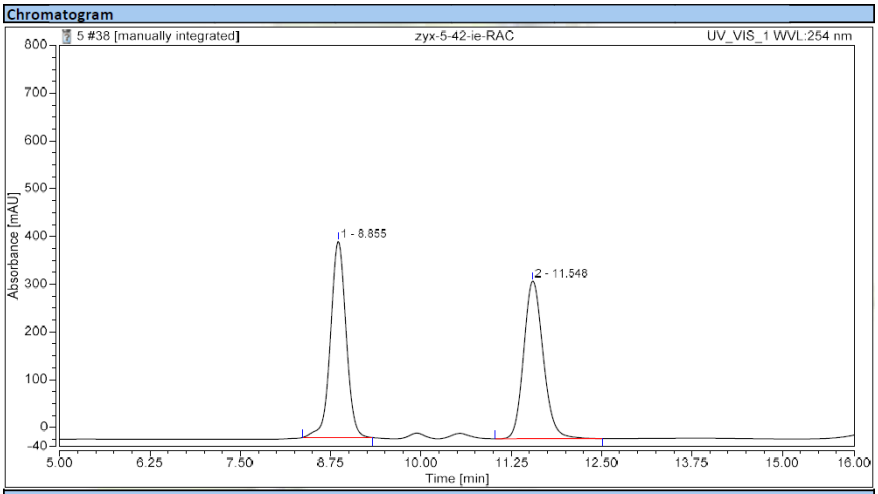
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.738	9.240	41.356	5.45	6.71	n.a.
2		10.647	160.403	574.734	94.55	93.29	n.a.
Total:			**169.643**	**616.090**	**100.00**	**100.00**	

2p: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



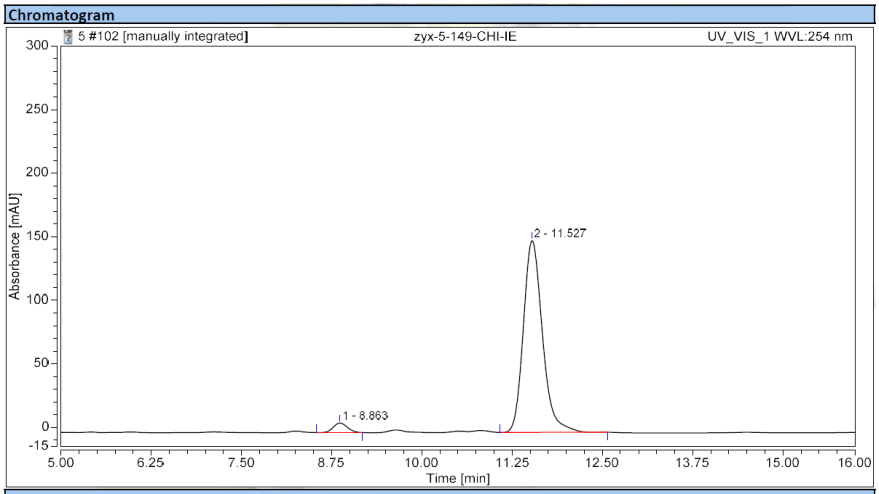
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.855	102.922	411.355	49.86	55.46	n.a.
2		11.548	103.517	330.415	50.14	44.54	n.a.
Total:			**206.439**	**741.770**	**100.00**	**100.00**	

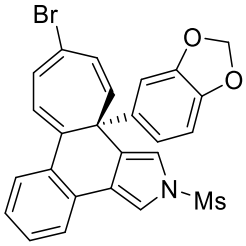
Chromatogram



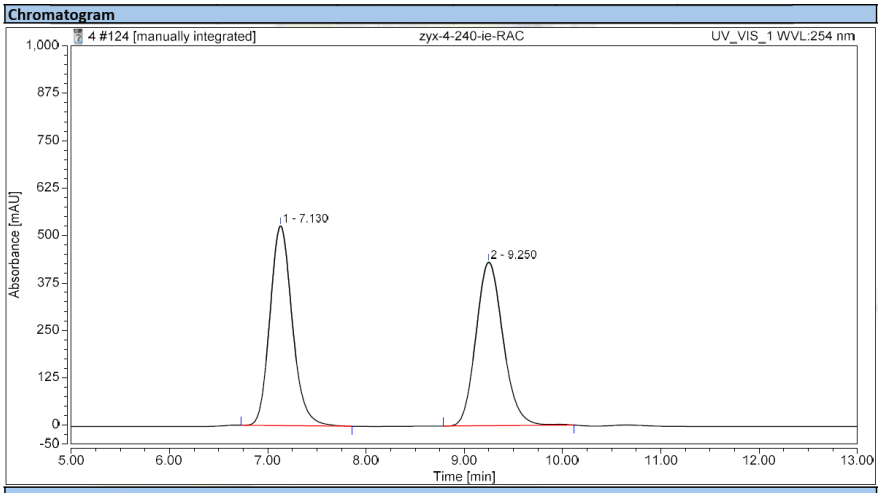
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.863	1.693	7.541	3.53	4.76	n.a.
2		11.527	46.237	150.980	96.47	95.24	n.a.
Total:			**47.929**	**158.522**	**100.00**	**100.00**	

2q: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



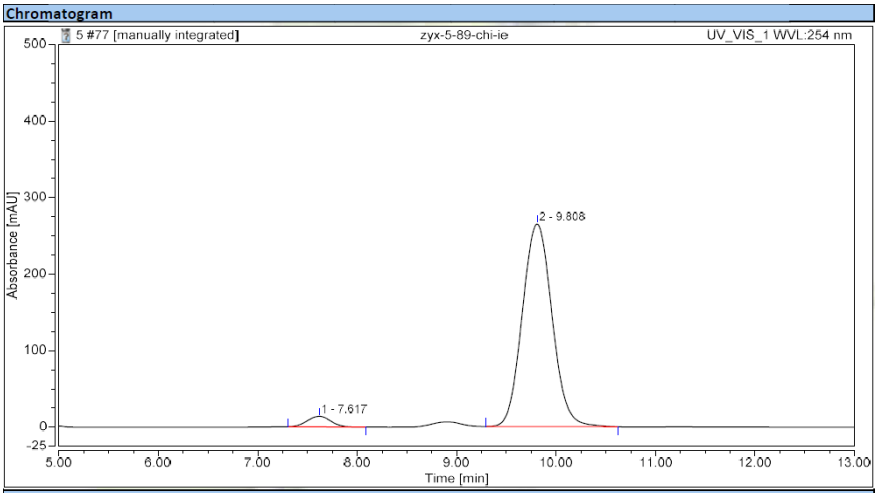
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		7.130	138.358	526.713	50.02	55.00	n.a.
300		9.250	138.251	431.009	49.98	45.00	n.a.
Total:			**276.609**	**957.722**	**100.00**	**100.00**	

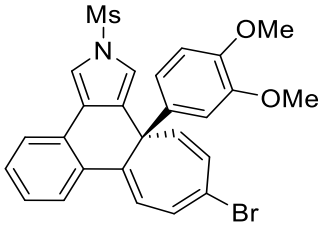
Chromatogram



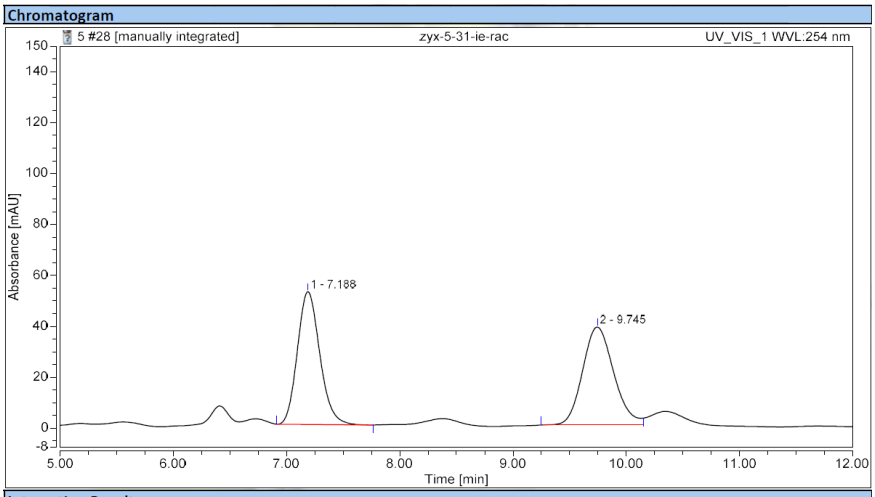
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.617	3.732	13.726	3.91	4.93	n.a.
2		9.808	91.696	264.625	96.09	95.07	n.a.
Total:			**95.428**	**278.351**	**100.00**	**100.00**	

2r: IE, *i*-PrOH/hexane = 50/50, v = 1.0 mL/min, λ = 254 nm



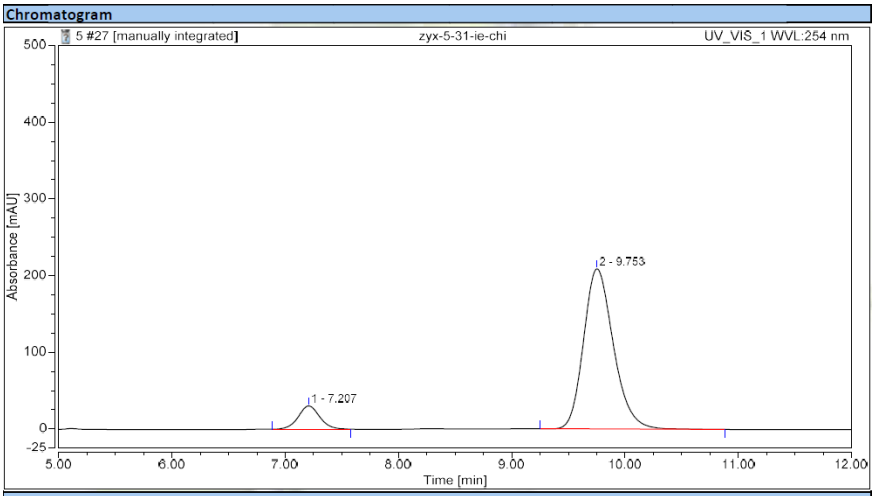
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.188	11.952	52.176	49.31	57.55	n.a.
2		9.745	12.285	38.480	50.69	42.45	n.a.
Total:			**24.237**	**90.657**	**100.00**	**100.00**	

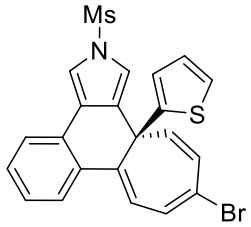
Chromatogram



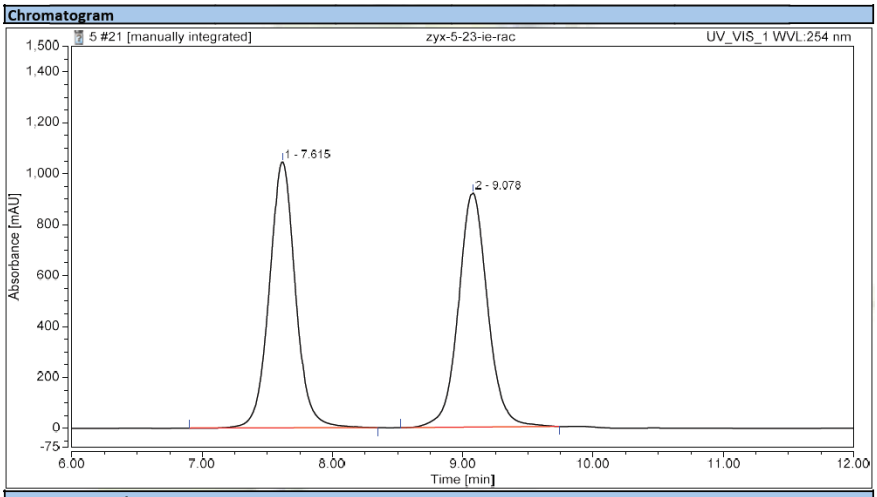
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.207	6.701	30.411	9.50	12.71	n.a.
2		9.753	63.870	208.926	90.50	87.29	n.a.
Total:			**70.572**	**239.337**	**100.00**	**100.00**	

2s: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



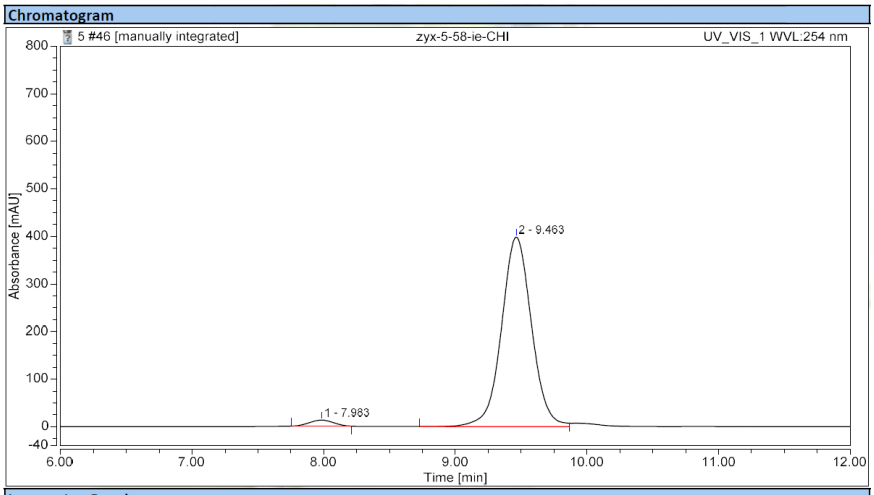
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.615	243.217	1045.052	50.38	53.20	n.a.
2		9.078	239.518	919.431	49.62	46.80	n.a.
Total:			**482.735**	**1964.484**	**100.00**	**100.00**	

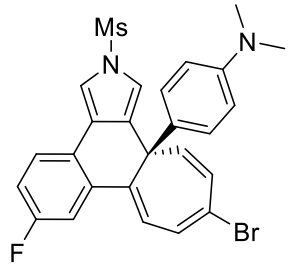
Chromatogram

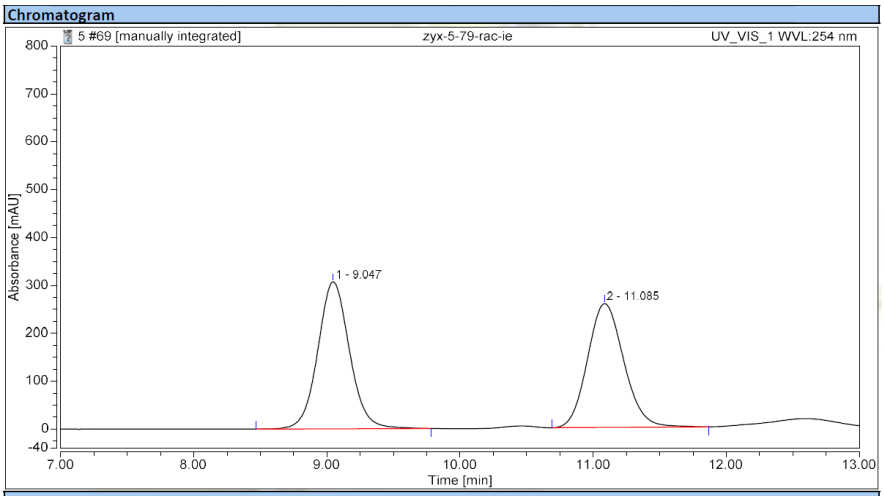


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.983	2.720	12.797	2.51	3.11	n.a.
2		9.463	105.508	398.704	97.49	96.89	n.a.
Total:			**108.229**	**411.500**	**100.00**	**100.00**	

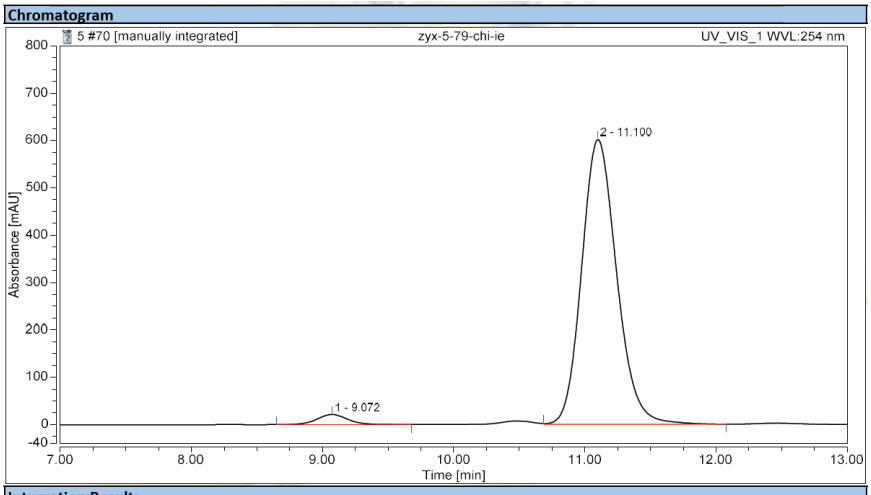
2t: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

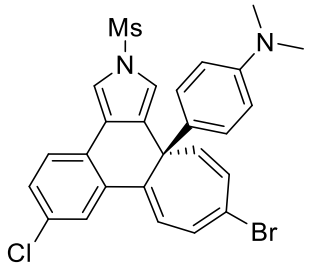
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.047	84.754	306.782	50.93	54.24	n.a.
2		11.085	81.652	258.785	49.07	45.76	n.a.
Total:			**166.407**	**565.567**	**100.00**	**100.00**	

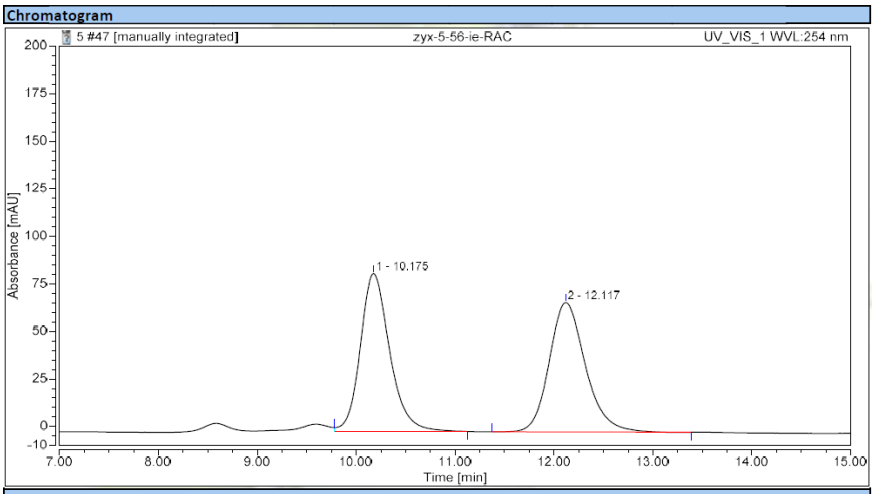


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.072	5.762	21.262	3.00	3.41	n.a.
2		11.100	186.141	601.829	97.00	96.59	n.a.
Total:			**191.903**	**623.091**	**100.00**	**100.00**	

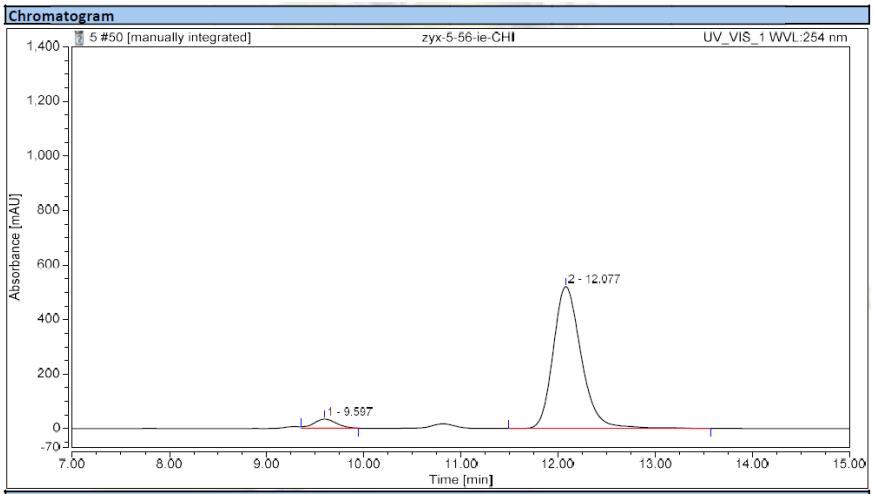
2u: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

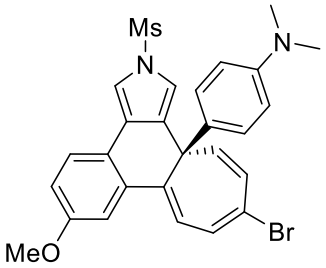
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.175	28.639	83.116	49.77	54.96	n.a.
2		12.117	28.904	68.123	50.23	45.04	n.a.
Total:			**57.543**	**151.238**	**100.00**	**100.00**	



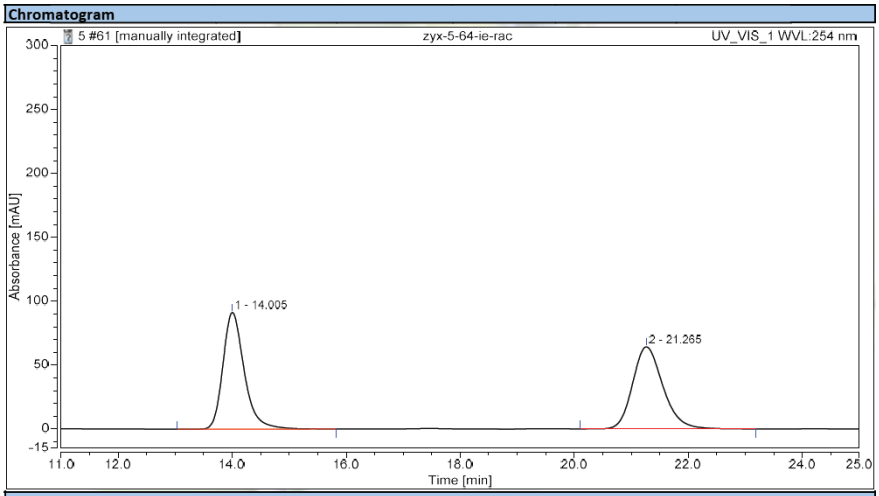
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.597	8.999	33.366	4.91	6.03	n.a.
2		12.077	174.159	520.299	95.09	93.97	n.a.
Total:			**183.159**	**553.665**	**100.00**	**100.00**	

2v: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



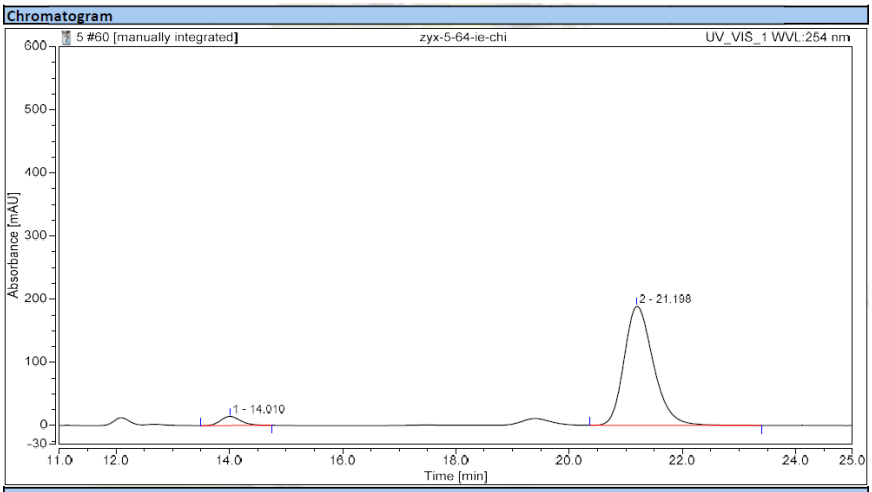
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.005	39.671	91.430	49.92	58.71	n.a.
2		21.265	39.804	64.299	50.08	41.29	n.a.
Total:			**79.475**	**155.729**	**100.00**	**100.00**	

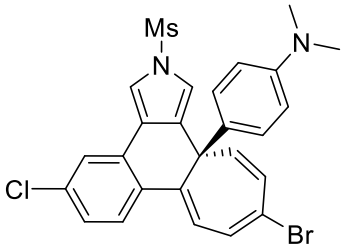
Chromatogram

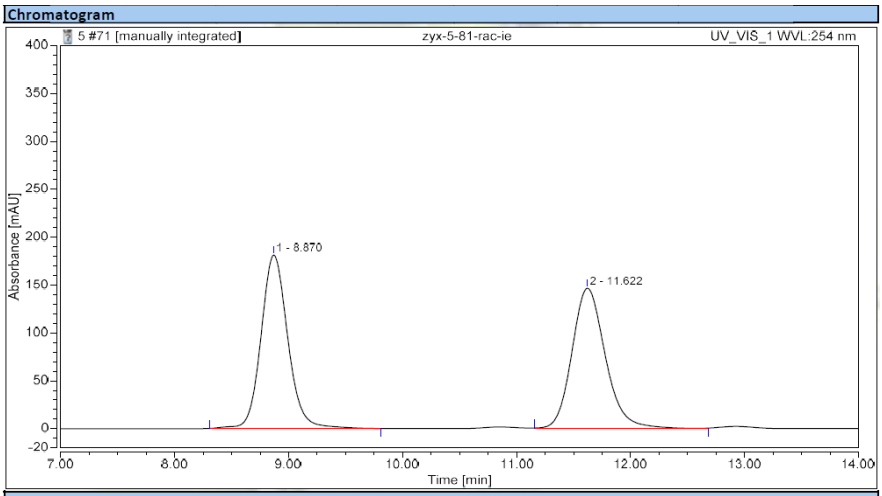


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.010	5.961	14.398	5.01	7.09	n.a.
2		21.198	112.913	188.593	94.99	92.91	n.a.
Total:			**118.875**	**202.991**	**100.00**	**100.00**	

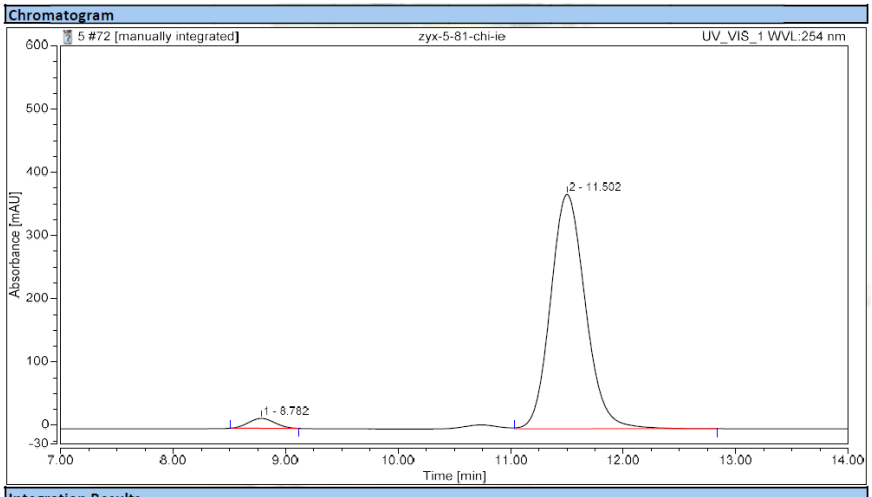
2w: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

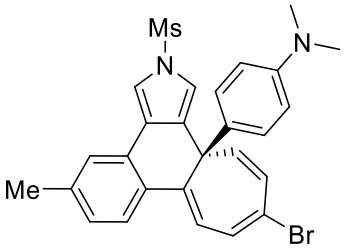
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.870	49.175	180.980	50.10	55.37	n.a.
2		11.622	48.985	145.863	49.90	44.63	n.a.
Total:			**98.160**	**326.843**	**100.00**	**100.00**	

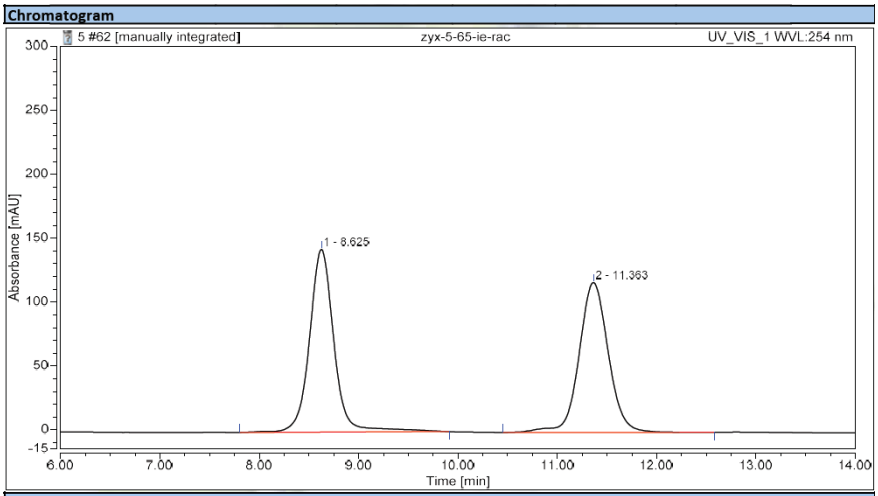


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.782	4.214	15.587	3.07	4.04	n.a.
2		11.502	133.044	370.680	96.93	95.96	n.a.
Total:			**137.258**	**386.266**	**100.00**	**100.00**	

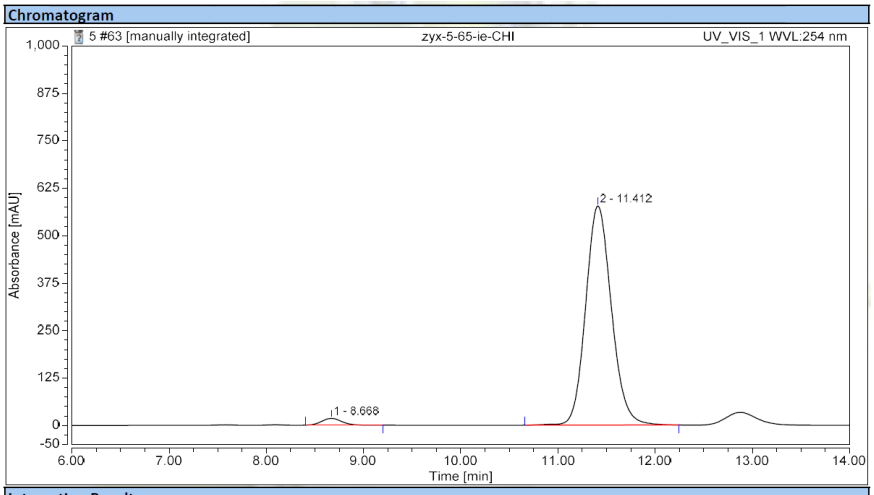
2x: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

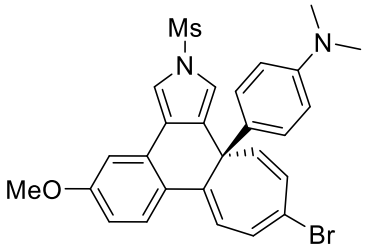
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.625	40.982	143.010	50.56	54.94	n.a.
2		11.363	40.079	117.300	49.44	45.06	n.a.
Total:			**81.060**	**260.310**	**100.00**	**100.00**	

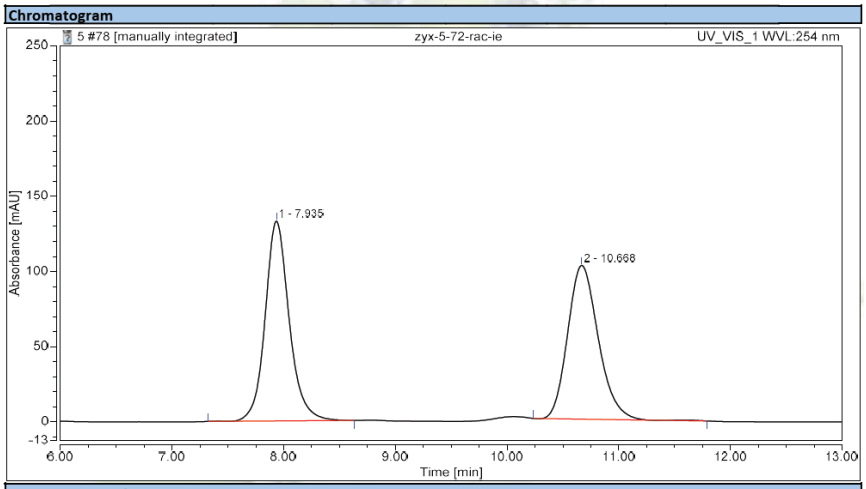


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.668	4.363	18.026	2.39	3.03	n.a.
2		11.412	177.883	577.750	97.61	96.97	n.a.
Total:			**182.246**	**595.776**	**100.00**	**100.00**	

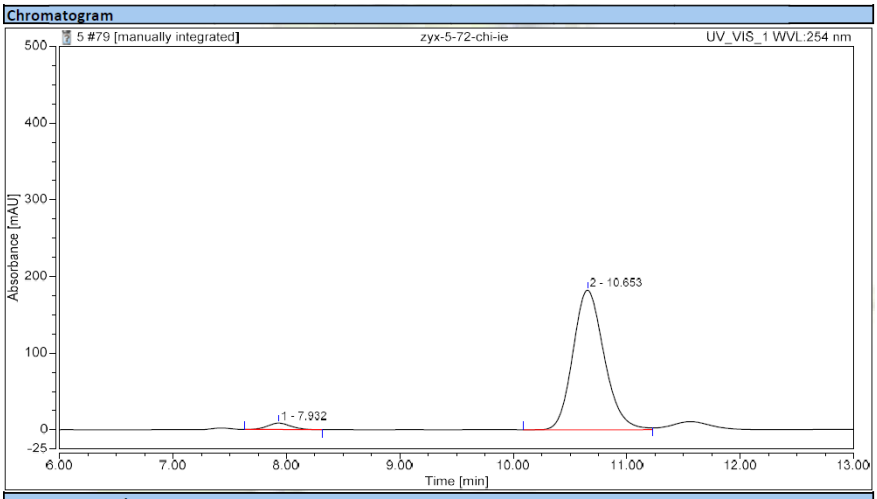
2y: IE, *i*-PrOH/hexane = 40/60, v = 1.0 mL/min, λ = 254 nm





Integration Results

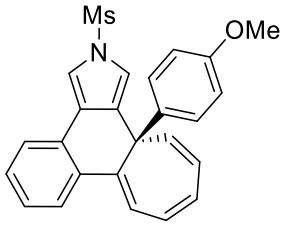
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.935	33.174	132.901	50.50	56.52	n.a.
2		10.668	32.515	102.219	49.50	43.48	n.a.
Total:			**65.689**	**235.120**	**100.00**	**100.00**	



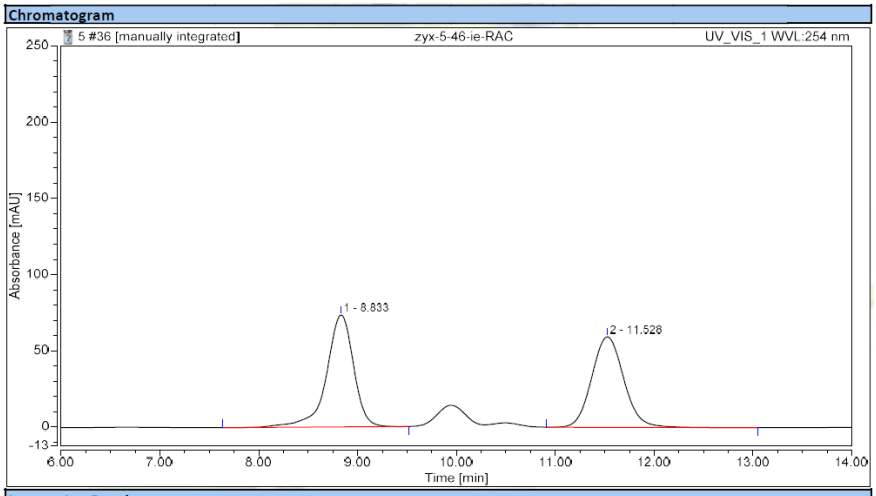
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.932	1.957	8.270	3.25	4.34	n.a.
2		10.653	58.300	182.096	96.75	95.66	n.a.
Total:			**60.257**	**190.366**	**100.00**	**100.00**	

2z: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



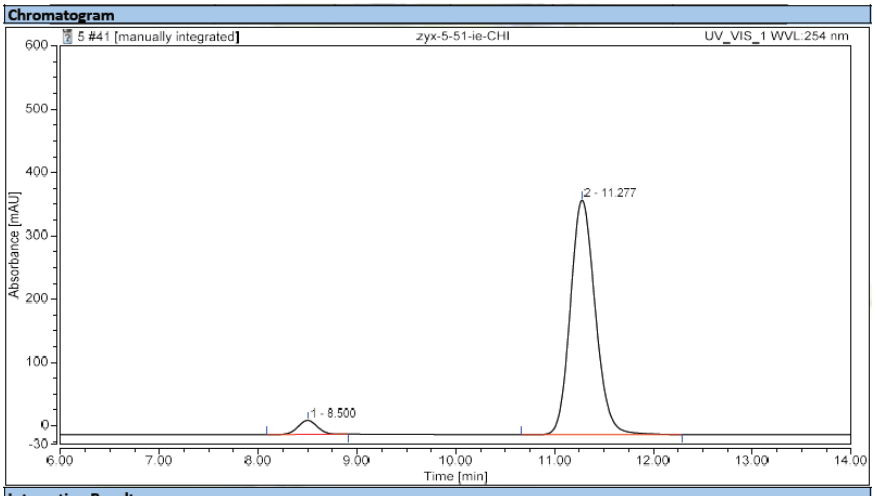
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.833	23.372	73.414	51.27	55.31	n.a.
2		11.528	22.214	59.328	48.73	44.69	n.a.
Total:			**45.586**	**132.742**	**100.00**	**100.00**	

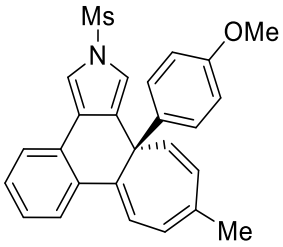
Chromatogram

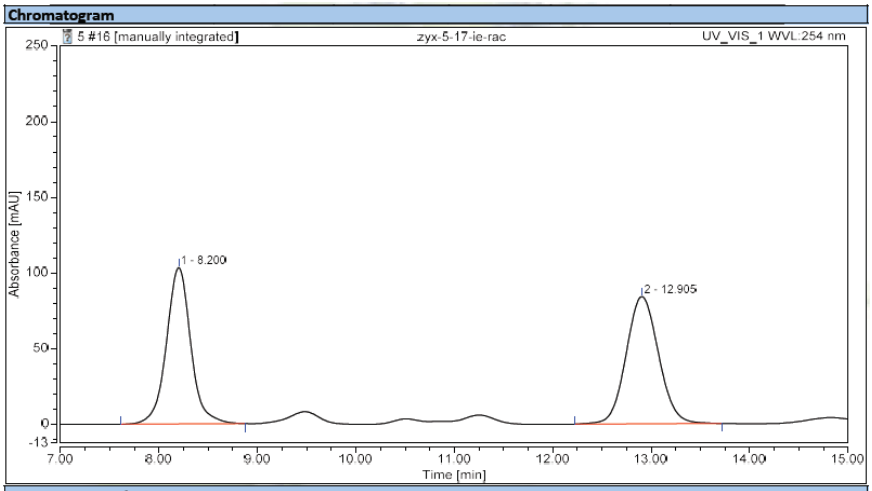


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.500	4.995	22.120	4.42	5.63	n.a.
2		11.277	108.107	370.871	95.58	94.37	n.a.
Total:			**113.103**	**392.992**	**100.00**	**100.00**	

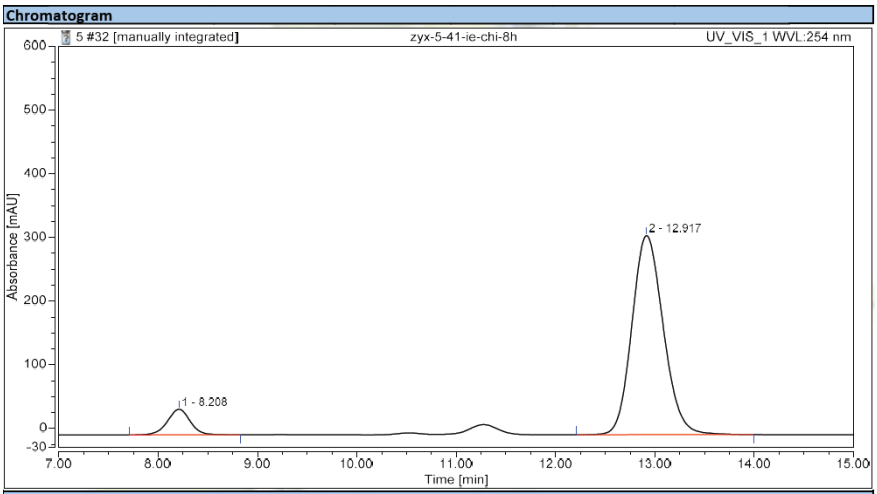
2aa: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

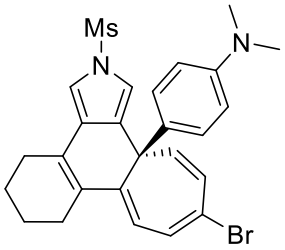
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.200	29.647	103.323	47.97	55.12	n.a.
2		12.905	32.156	84.130	52.03	44.88	n.a.
Total:			**61.803**	**187.453**	**100.00**	**100.00**	

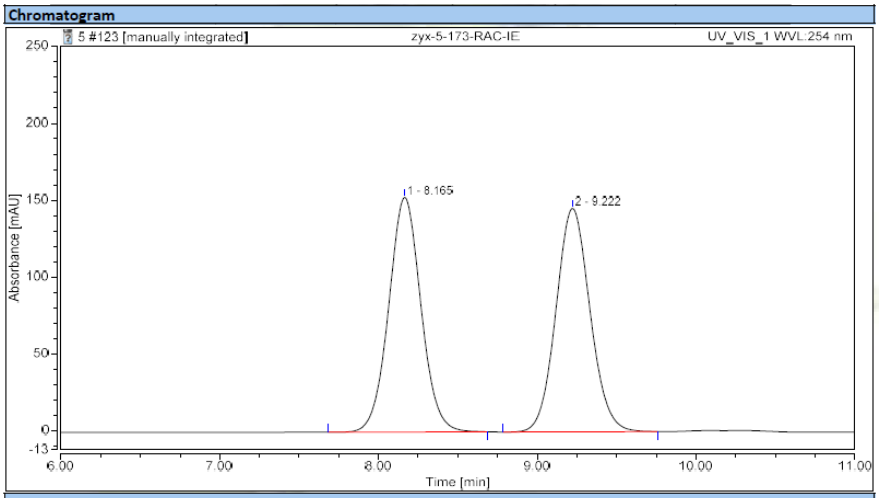


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.208	10.666	40.106	8.52	11.36	n.a.
2		12.917	114.476	312.874	91.48	88.64	n.a.
Total:			**125.142**	**352.980**	**100.00**	**100.00**	

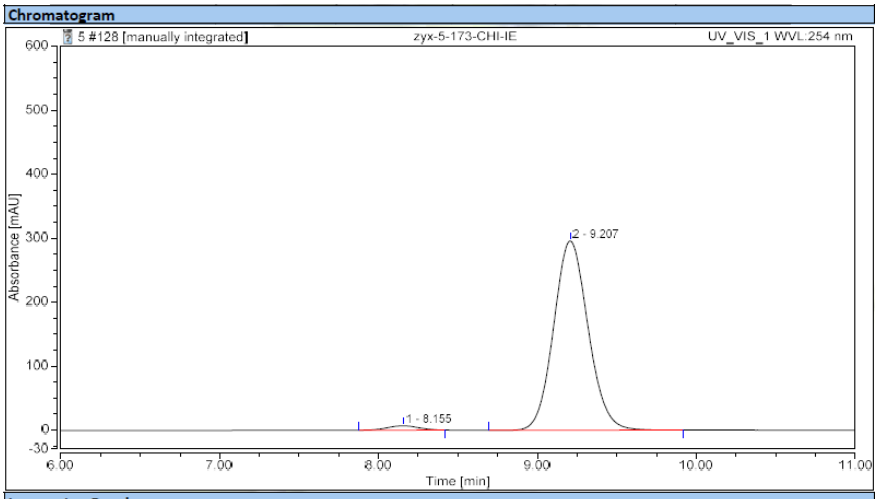
2ab: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

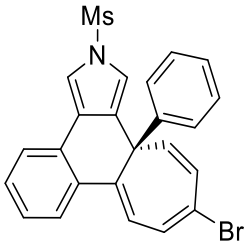
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.165	35.915	152.566	49.82	51.20	n.a.
2		9.222	36.179	145.386	50.18	48.80	n.a.
Total:			**72.095**	**297.952**	**100.00**	**100.00**	

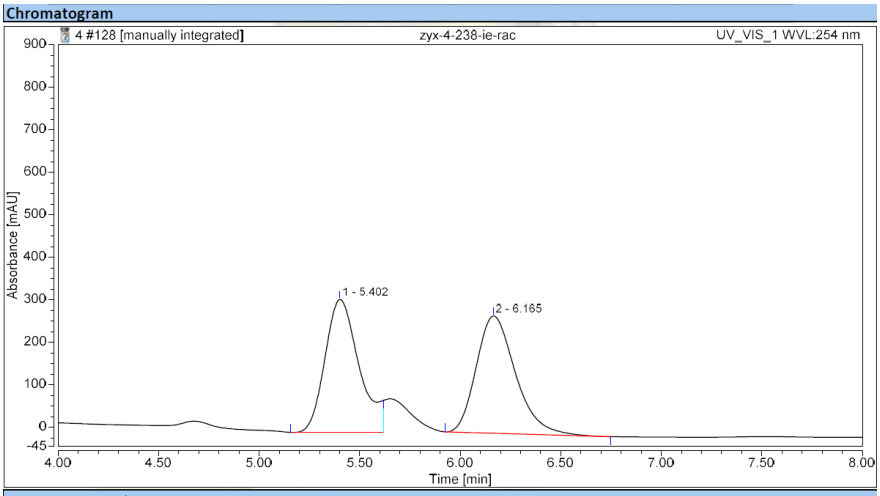


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.155	1.539	6.793	2.02	2.24	n.a.
2		9.207	74.620	296.200	97.98	97.76	n.a.
Total:			**76.159**	**302.994**	**100.00**	**100.00**	

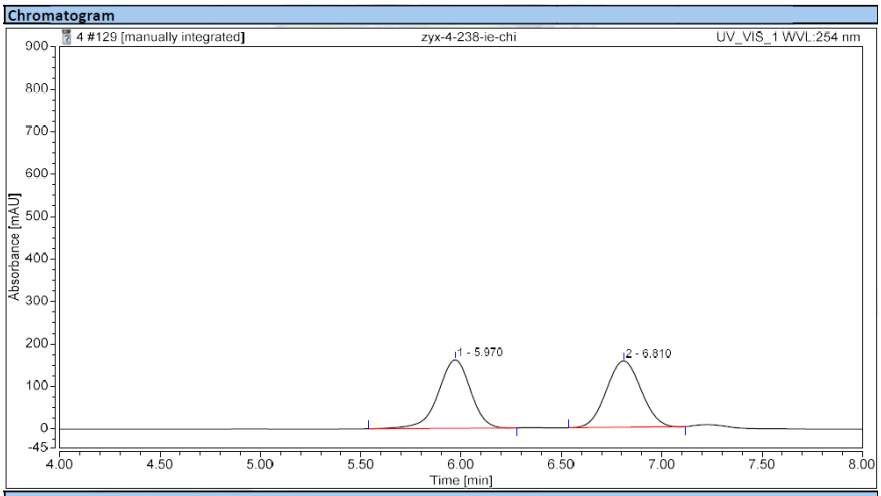
2ac: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Integration Results

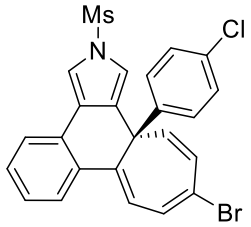
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		5.402	61.241	312.634	49.50	53.12	n.a.
300		6.165	62.490	275.888	50.50	46.88	n.a.
Total:			**123.731**	**588.522**	**100.00**	**100.00**	



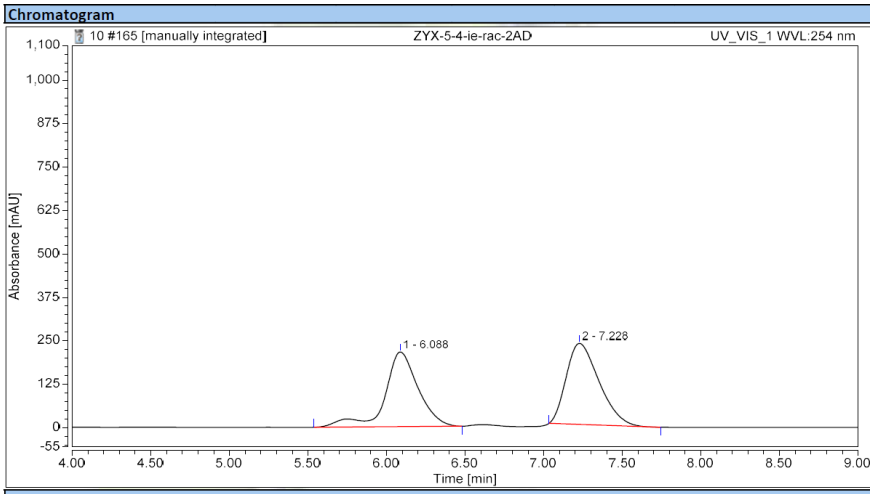
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		5.970	30.172	161.237	49.12	50.79	n.a.
300		6.810	31.252	156.219	50.88	49.21	n.a.
Total:			**61.424**	**317.456**	**100.00**	**100.00**	

2ad: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



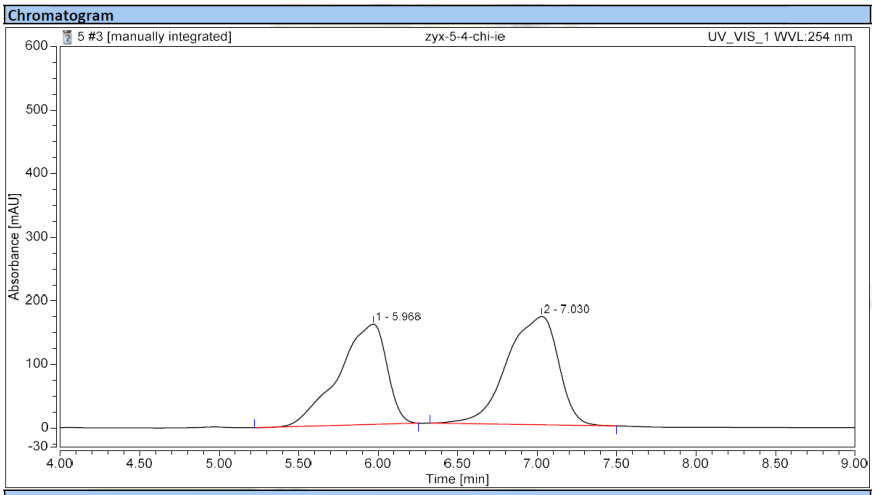
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.088	53.001	215.187	48.40	47.98	n.a.
2		7.228	56.515	233.310	51.60	52.02	n.a.
Total:			**109.516**	**448.496**	**100.00**	**100.00**	

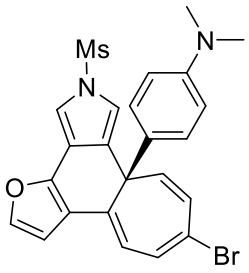
Chromatogram



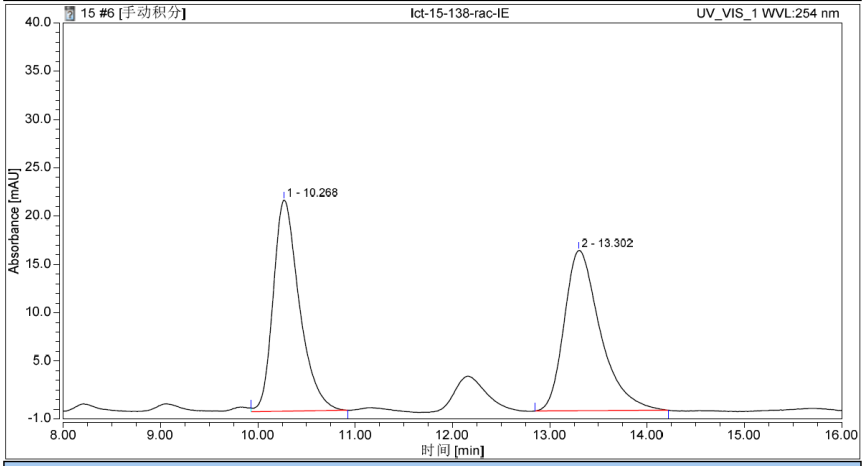
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.968	55.267	157.683	46.44	48.09	n.a.
2		7.030	63.747	170.185	53.56	51.91	n.a.
Total:			**119.014**	**327.867**	**100.00**	**100.00**	

2af: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



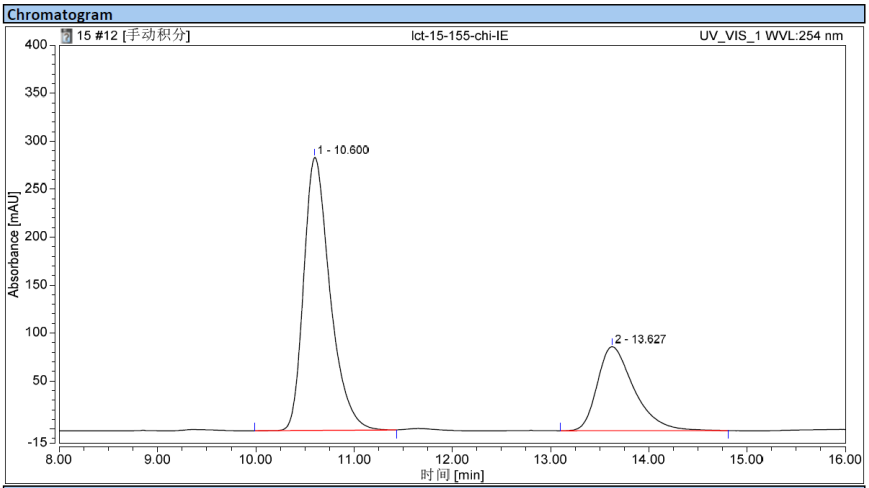
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.268	6.814	21.861	48.86	56.84	n.a.
2		13.302	7.132	16.600	51.14	43.16	n.a.
Total:			**13.946**	**38.461**	**100.00**	**100.00**	

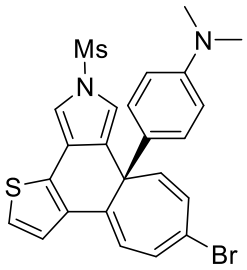
Chromatogram

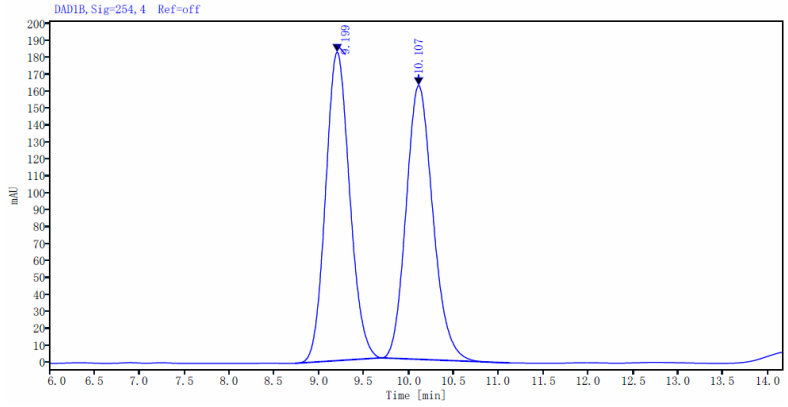


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.600	88.518	284.751	70.08	76.49	n.a.
2		13.627	37.788	87.509	29.92	23.51	n.a.
Total:			**126.306**	**372.261**	**100.00**	**100.00**	

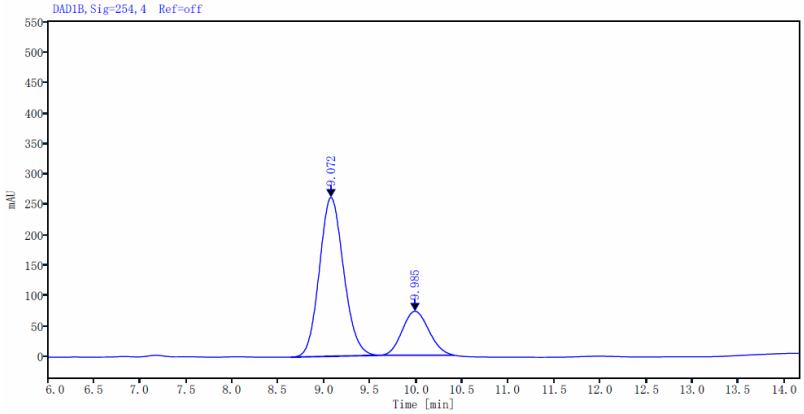
2ag: IG, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm





Signal: DAD1B, Sig=254, 4 Ref=off

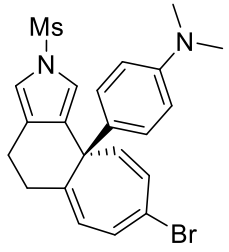
RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
9.19914	MM m	0.95776	3403.74389	182.44536	50.28081
10.10705	MM m	1.43665	3365.72520	161.96147	49.71919
		Totals:	6769.46910		

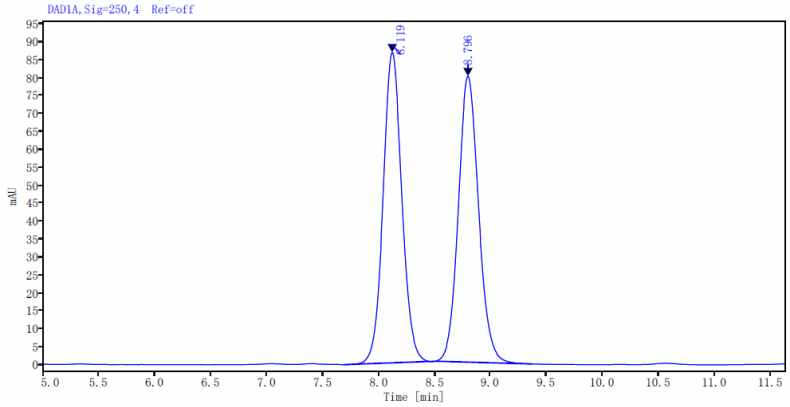


Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
9.07241	MM m	0.95768	4790.90021	261.58068	76.66412
9.98471	MM m	0.82087	1458.30785	72.45797	23.33588
		Totals:	6249.20806		

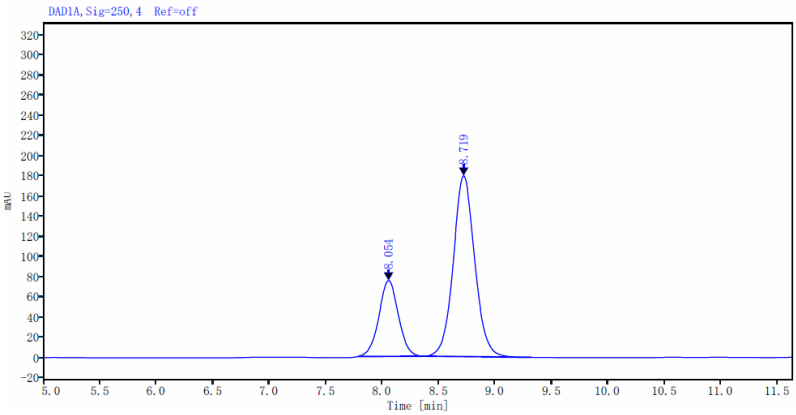
2ah: IA, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm





Signal: DAD1A, Sig=250, 4 Ref=off

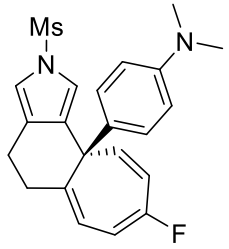
RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
8.11936	MM m	0.82076	1003.91123	86.54497	50.01778
8.79639	MM m	0.86180	1003.19758	79.70568	49.98222
		Totals:	2007.10881		

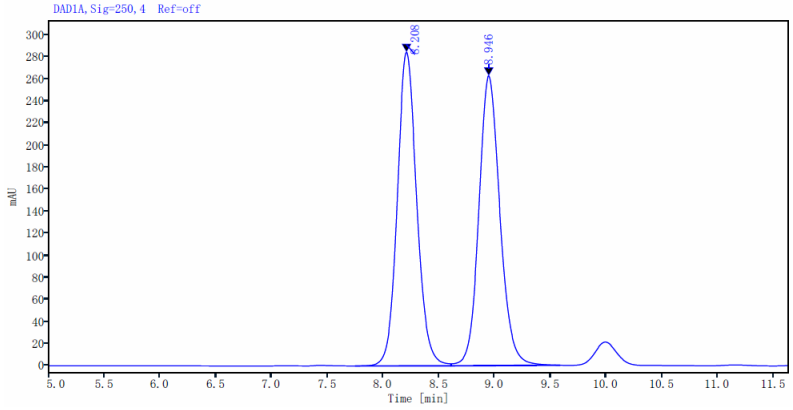


Signal: DAD1A, Sig=250, 4 Ref=off

RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
8.05378	MM m	0.59505	899.76919	75.03049	27.55930
8.71902	MM m	0.94387	2365.07872	179.07686	72.44070
		Totals:	3264.84791		

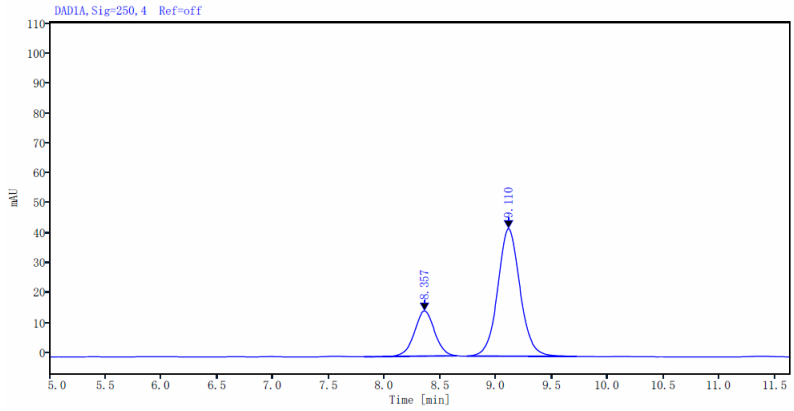
2ai: IA, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm





Signal: DAD1A, Sig=250, 4 Ref=off

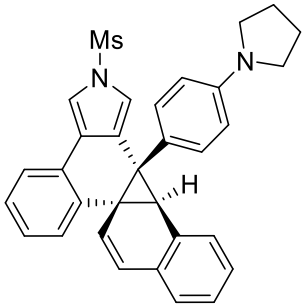
RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
8.20804	BV	0.86117	3451.06344	284.45718	49.96208
8.94551	MM m	0.97841	3456.30132	262.77674	50.03792
		Totals:	6907.36476		

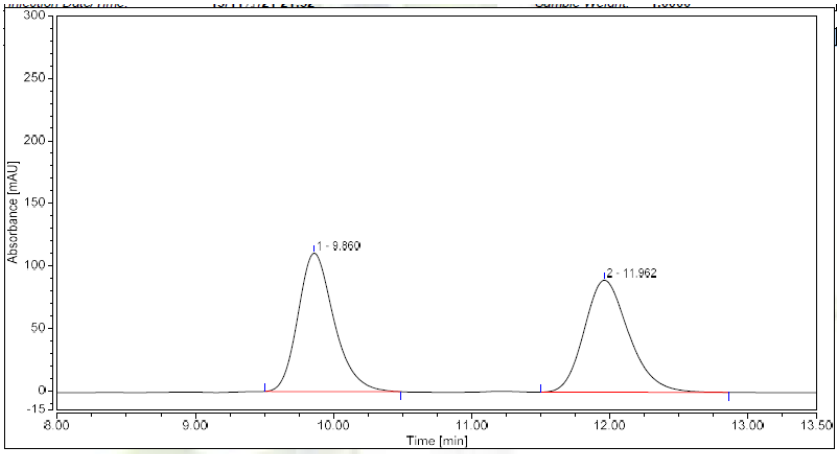


Signal: DAD1A, Sig=250, 4 Ref=off

RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
8.35653	MM m	0.82861	189.60513	15.12916	24.19183
9.10991	MM m	0.98491	594.15166	42.69410	75.80817
		Totals:	783.75679		

4a: IC, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm

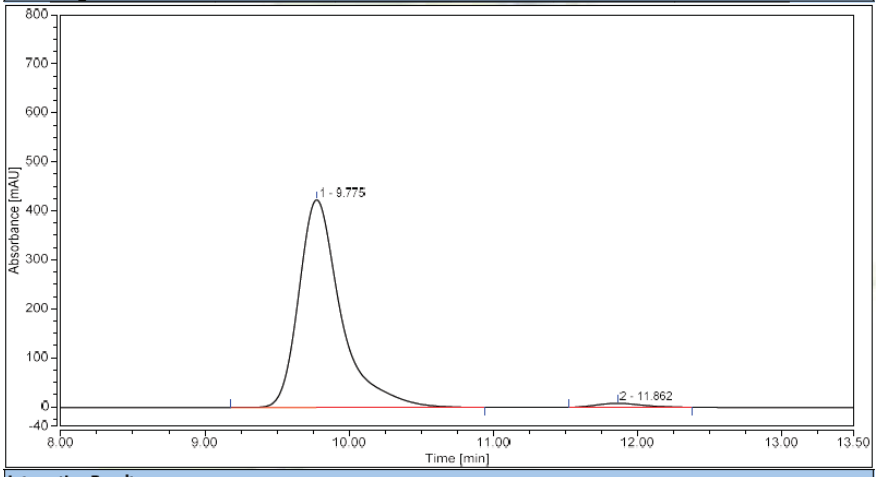




Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.860	33.493	110.665	49.99	55.28	n.a.
2		11.962	33.506	89.515	50.01	44.72	n.a.
Total:			**66.999**	**200.180**	**100.00**	**100.00**	

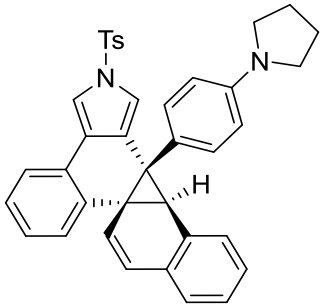
Chromatogram

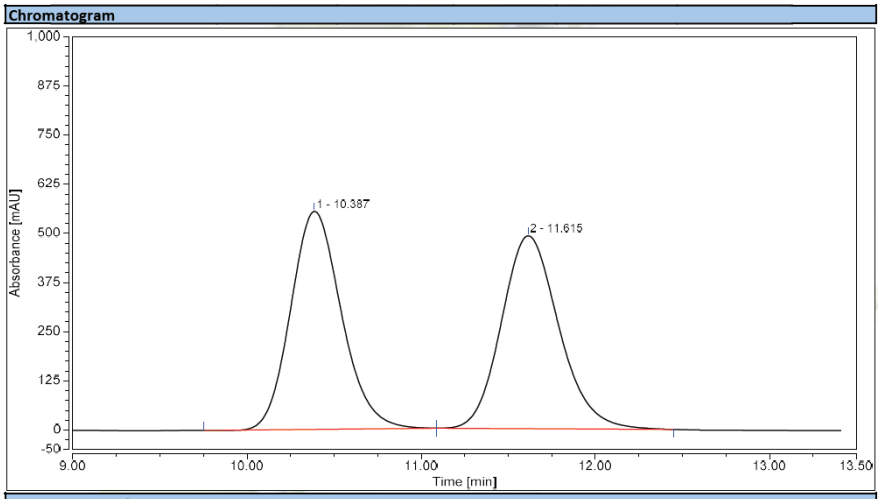


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.775	142.777	423.290	98.00	98.14	n.a.
2		11.862	2.908	8.010	2.00	1.86	n.a.
Total:			**145.685**	**431.300**	**100.00**	**100.00**	

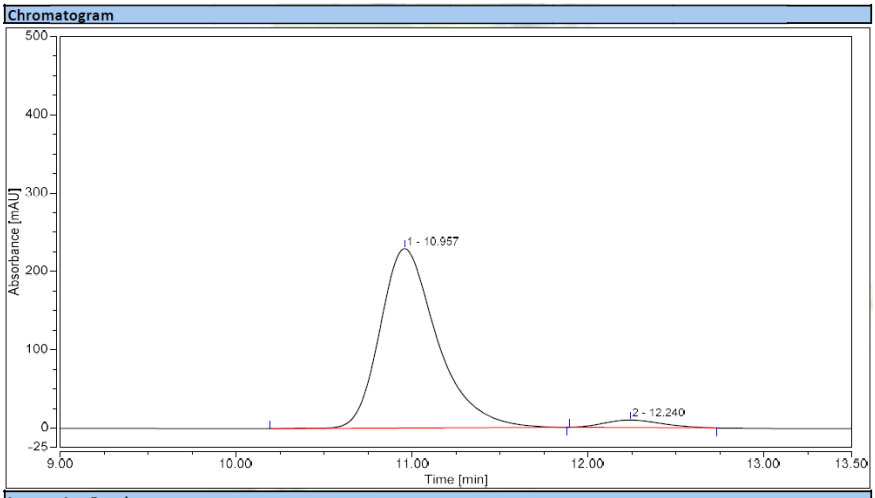
4b: IC, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm





Integration Results

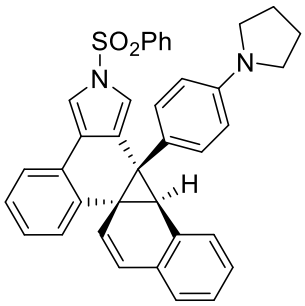
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.387	187.145	554.462	49.95	53.05	n.a.
2		11.615	187.492	490.679	50.05	46.95	n.a.
Total:			**374.637**	**1045.141**	**100.00**	**100.00**	



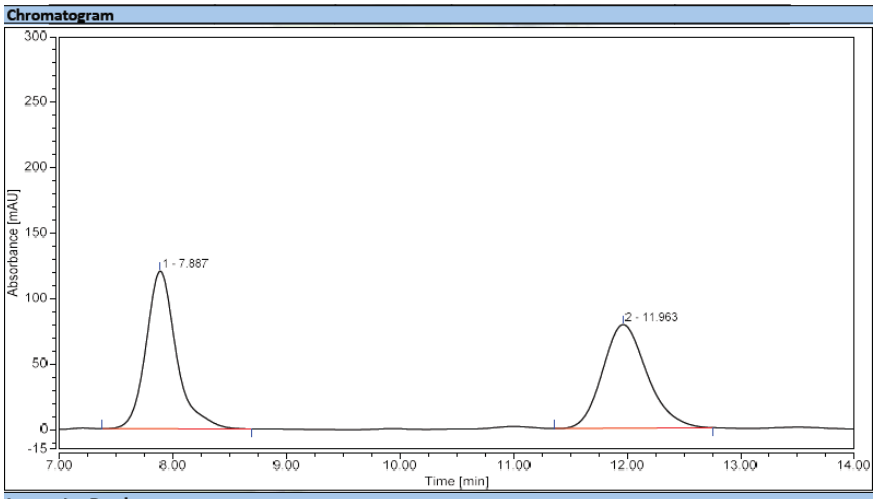
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.957	86.473	229.046	96.01	95.99	n.a.
2		12.240	3.595	9.560	3.99	4.01	n.a.
Total:			**90.068**	**238.606**	**100.00**	**100.00**	

4c: IE, *i*-PrOH/hexane = 50/50, v = 1.0 mL/min, λ = 254 nm



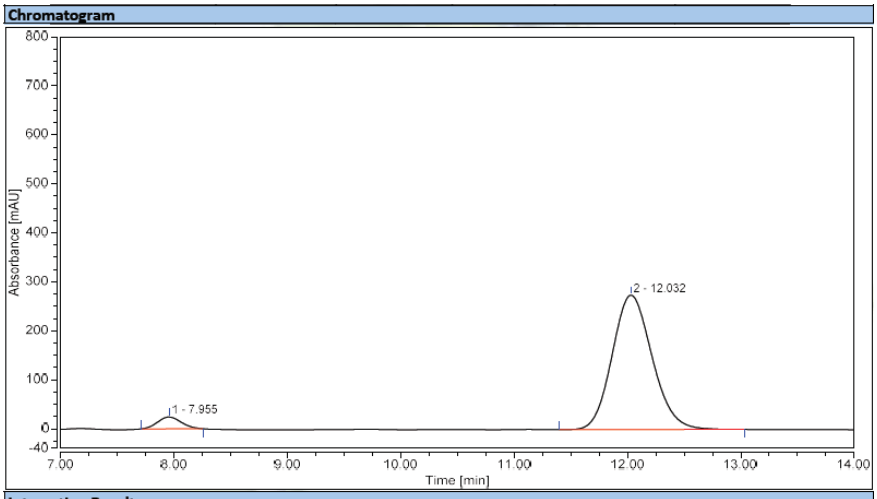
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.887	37.362	120.447	50.95	60.36	n.a.
2		11.963	35.963	79.084	49.05	39.64	n.a.
Total:			**73.325**	**199.531**	**100.00**	**100.00**	

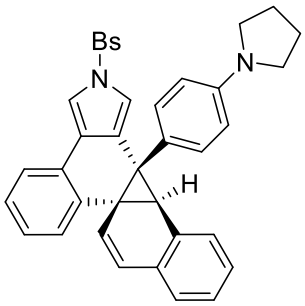
Chromatogram



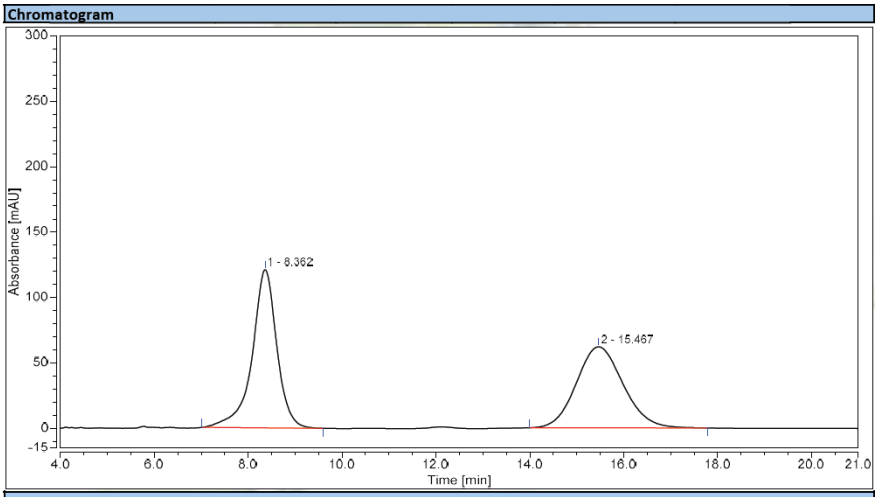
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.955	5.805	24.047	4.92	8.06	n.a.
2		12.032	112.126	274.127	95.08	91.94	n.a.
Total:			**117.931**	**298.174**	**100.00**	**100.00**	

4d: IG, *i*-PrOH/hexane = 50/50, v = 1.0 mL/min, λ = 254 nm



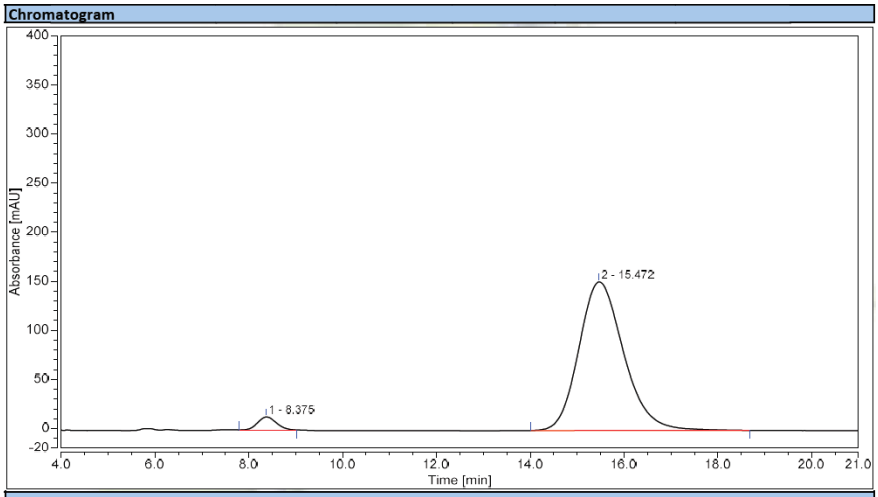
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.362	73.655	121.000	50.79	66.16	n.a.
2		15.467	71.353	61.886	49.21	33.84	n.a.
Total:			**145.008**	**182.886**	**100.00**	**100.00**	

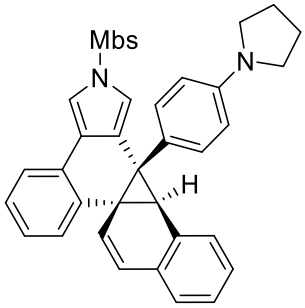
Chromatogram

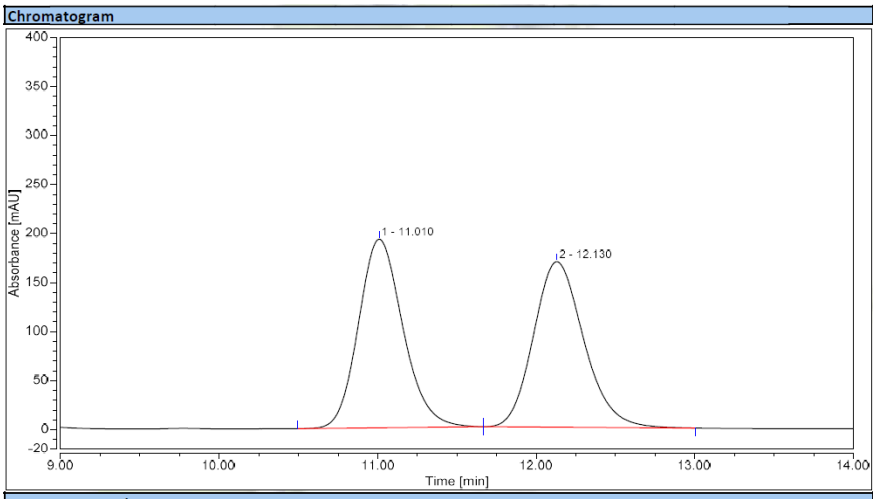


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.375	6.032	13.189	3.48	8.02	n.a.
2		15.472	167.167	151.321	96.52	91.98	n.a.
Total:			**173.199**	**164.510**	**100.00**	**100.00**	

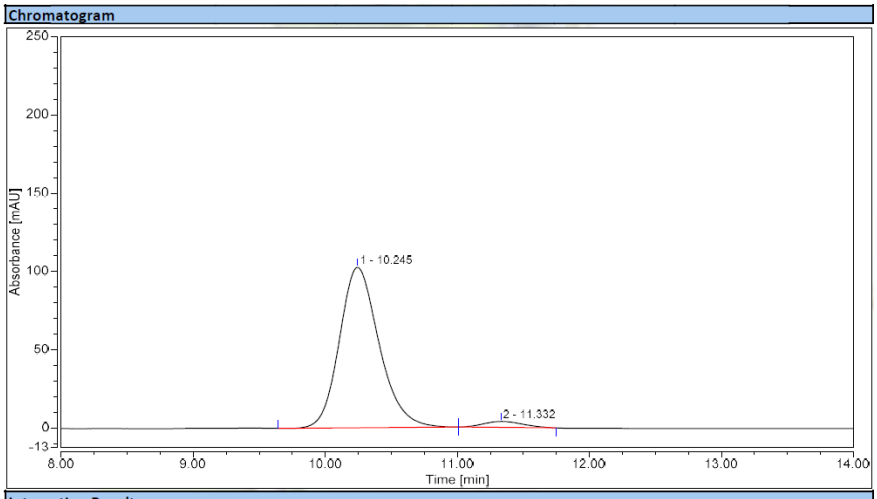
4e: IC, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

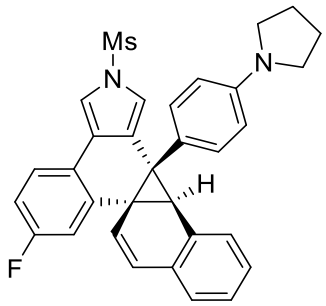
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.010	62.572	192.531	50.21	53.27	n.a.
2		12.130	62.049	168.862	49.79	46.73	n.a.
Total:			**124.621**	**361.393**	**100.00**	**100.00**	



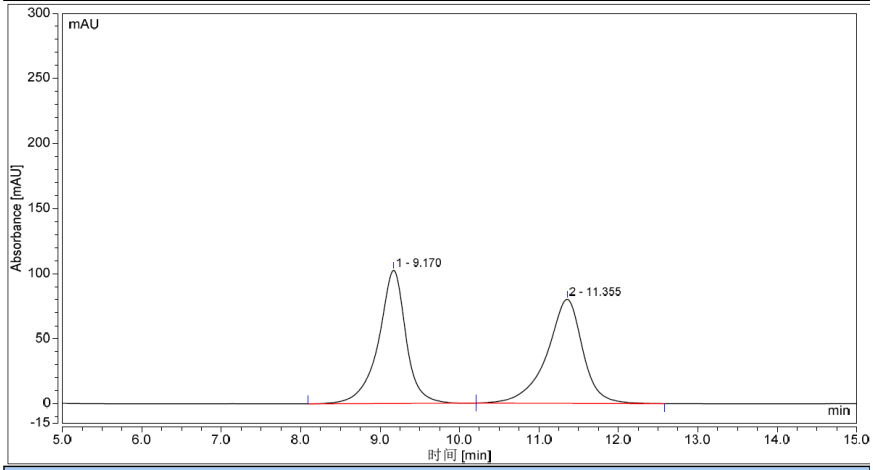
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.245	35.770	102.488	96.47	96.43	n.a.
2		11.332	1.309	3.796	3.53	3.57	n.a.
Total:			**37.079**	**106.284**	**100.00**	**100.00**	

4f: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



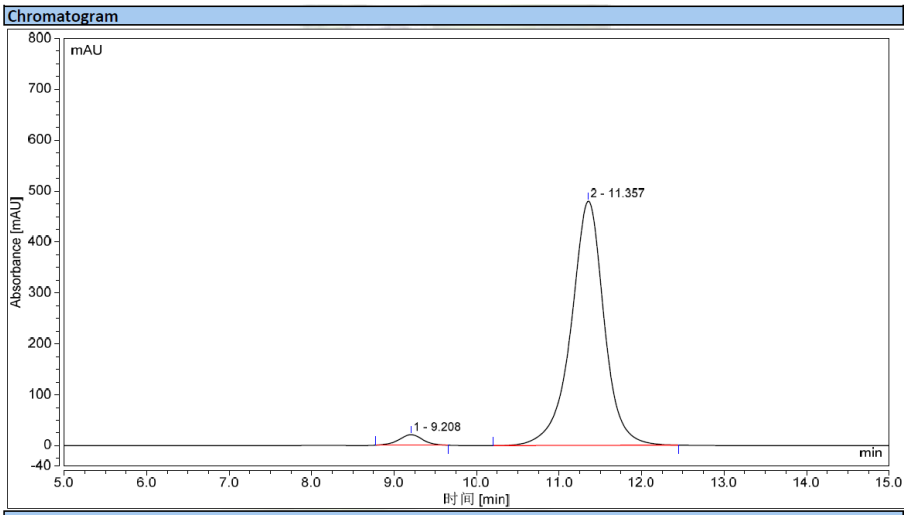
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.170	41.110	102.339	49.48	56.12	n.a.
2		11.355	41.967	80.013	50.52	43.88	n.a.
Total:			**83.076**	**182.353**	**100.00**	**100.00**	

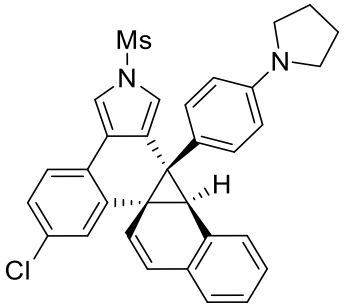
Chromatogram



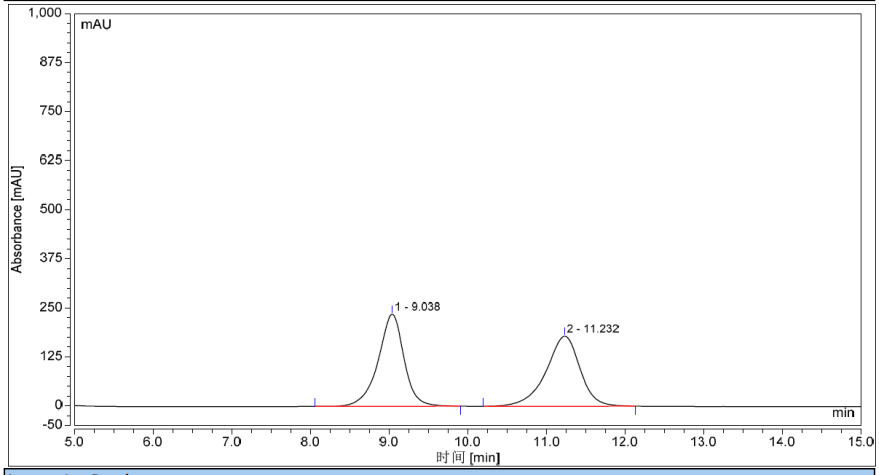
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.208	6.784	20.649	2.95	4.12	n.a.
2		11.357	222.800	480.130	97.05	95.88	n.a.
Total:			**229.584**	**500.779**	**100.00**	**100.00**	

4g: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



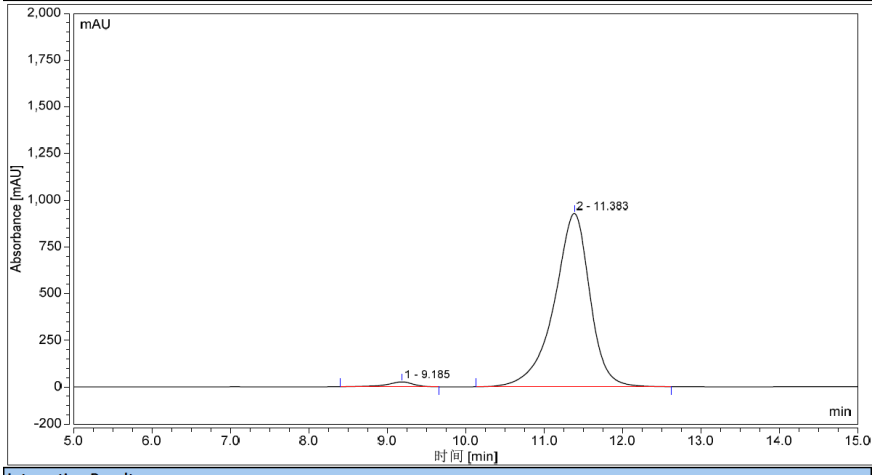
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.038	89.722	234.754	50.00	56.78	n.a.
2		11.232	89.715	178.682	50.00	43.22	n.a.
Total:			**179.437**	**413.437**	**100.00**	**100.00**	

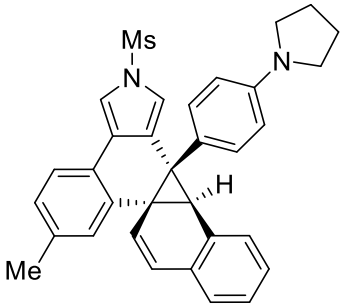
Chromatogram

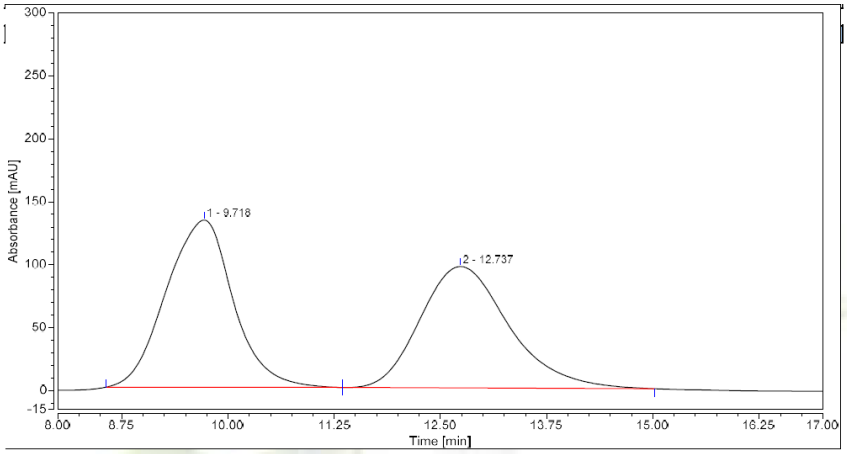


Integration Results

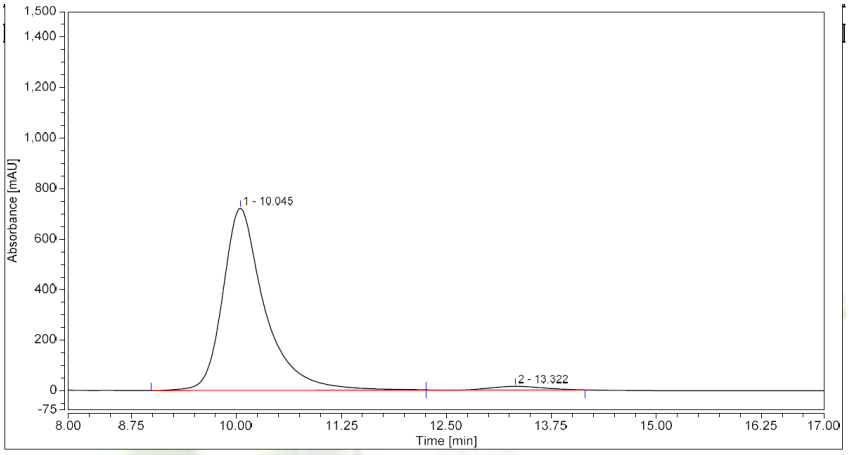
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.185	10.394	26.322	2.07	2.76	n.a.
2		11.383	490.585	927.678	97.93	97.24	n.a.
Total:			**500.979**	**954.000**	**100.00**	**100.00**	

4h: IA, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



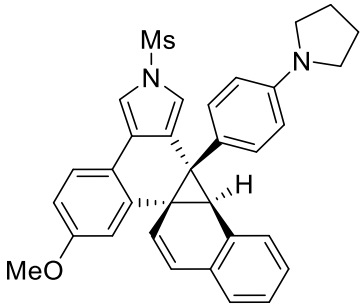


Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.718	121.795	132.792	51.07	57.94	n.a.
2		12.737	116.688	96.400	48.93	42.06	n.a.
Total:			**238.483**	**229.192**	**100.00**	**100.00**	

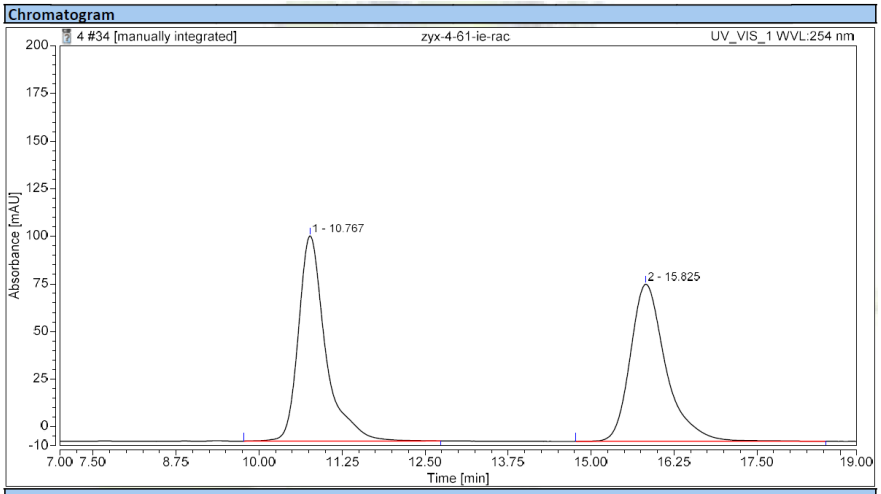


Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.045	418.185	720.268	97.52	98.03	n.a.
2		13.322	10.620	14.505	2.48	1.97	n.a.
Total:			**428.805**	**734.773**	**100.00**	**100.00**	

4i: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



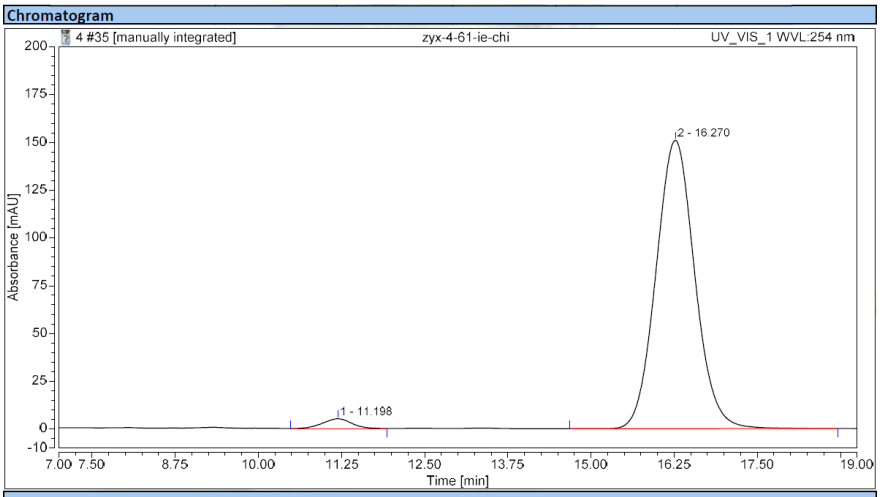
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		10.767	51.051	107.812	49.93	56.64	n.a.
300		15.825	51.191	82.548	50.07	43.36	n.a.
Total:			**102.242**	**190.360**	**100.00**	**100.00**	

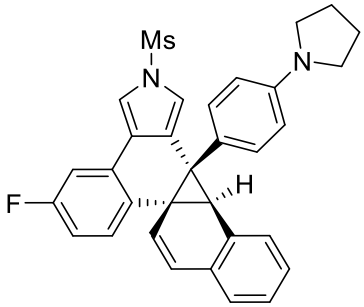
Chromatogram



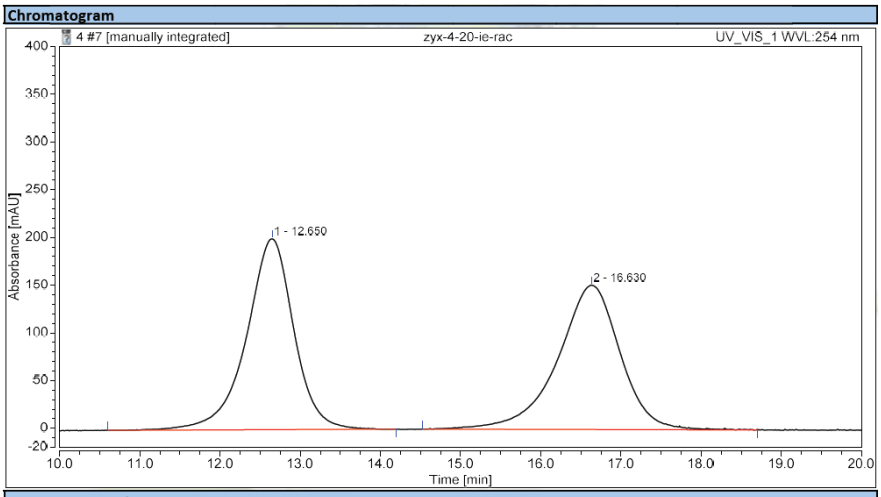
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		11.198	2.560	5.081	2.45	3.26	n.a.
300		16.270	101.757	150.967	97.55	96.74	n.a.
Total:			**104.317**	**156.048**	**100.00**	**100.00**	

4j: IE, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm



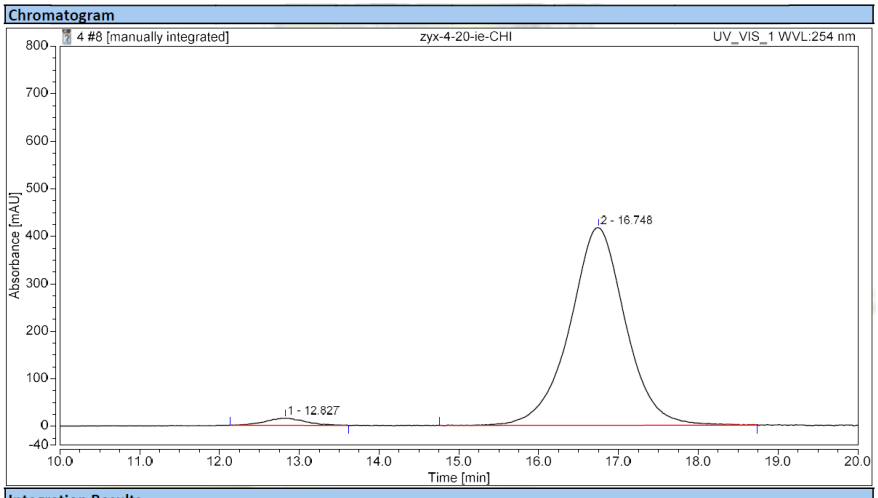
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		12.650	137.496	200.335	50.09	56.95	n.a.
300		16.630	137.027	151.425	49.91	43.05	n.a.
Total:			**274.523**	**351.760**	**100.00**	**100.00**	

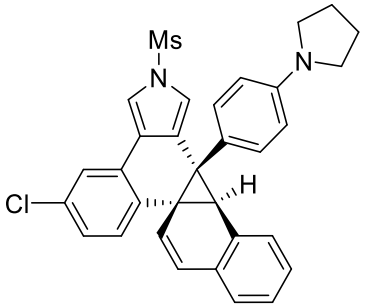
Chromatogram



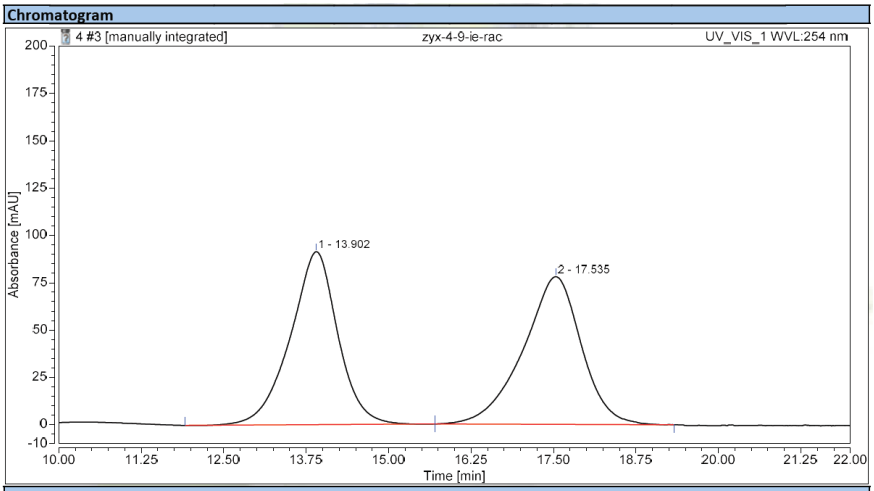
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		12.827	8.619	15.304	2.50	3.54	n.a.
300		16.748	336.642	416.465	97.50	96.46	n.a.
Total:			**345.261**	**431.770**	**100.00**	**100.00**	

4k: IE, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm



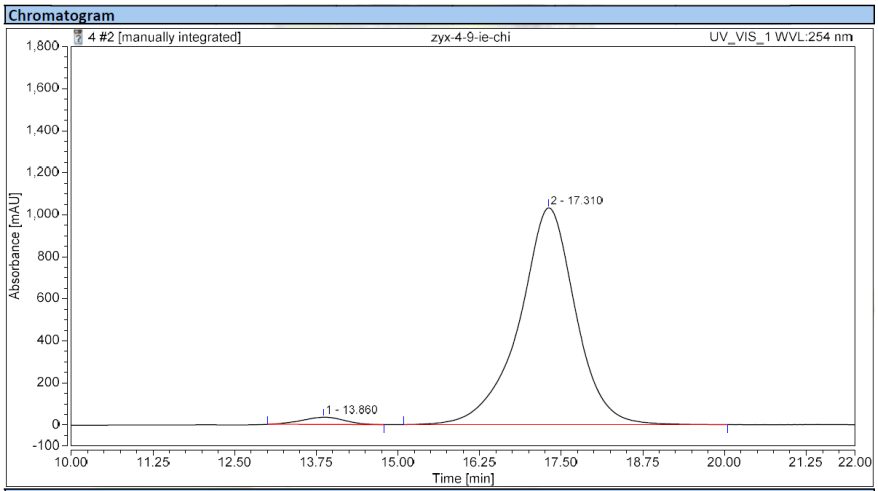
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		13.902	76.408	91.393	48.90	53.94	n.a.
300		17.535	79.849	78.039	51.10	46.06	n.a.
Total:			**156.256**	**169.433**	**100.00**	**100.00**	

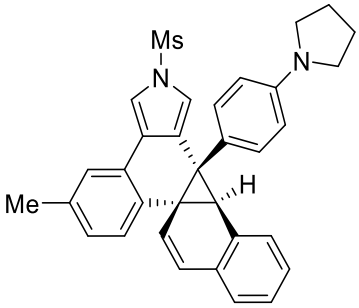
Chromatogram



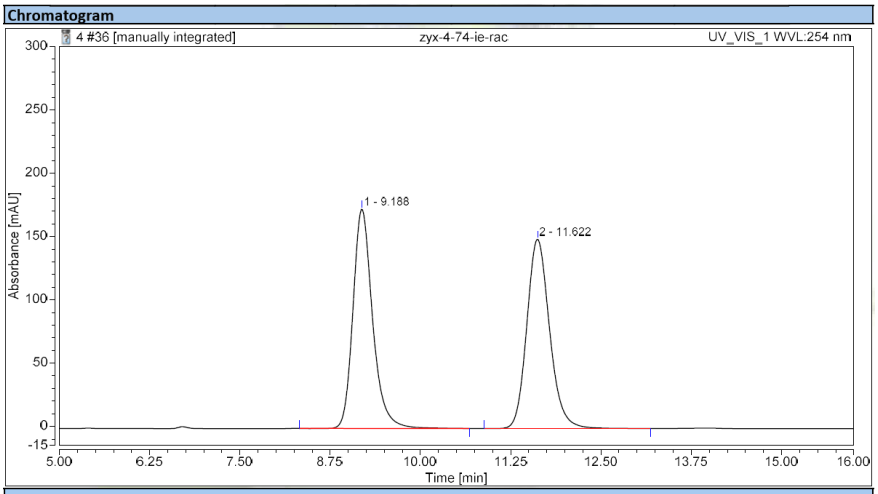
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		13.860	26.485	34.801	2.50	3.26	n.a.
300		17.310	1031.861	1031.401	97.50	96.74	n.a.
Total:			**1058.346**	**1066.202**	**100.00**	**100.00**	

4l: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



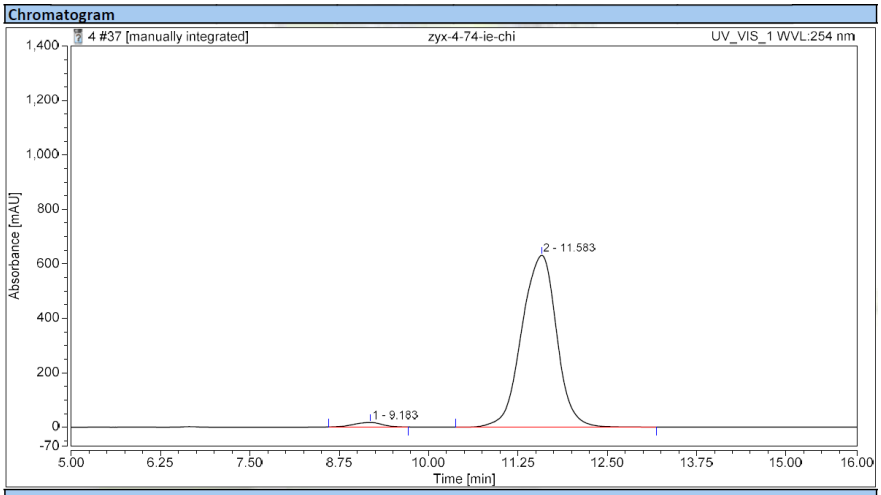
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		9.188	54.647	173.317	49.89	53.67	n.a.
300		11.622	54.888	149.606	50.11	46.33	n.a.
Total:			**109.535**	**322.923**	**100.00**	**100.00**	

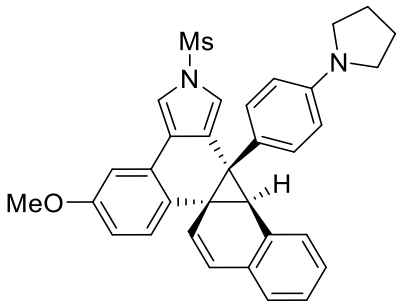
Chromatogram

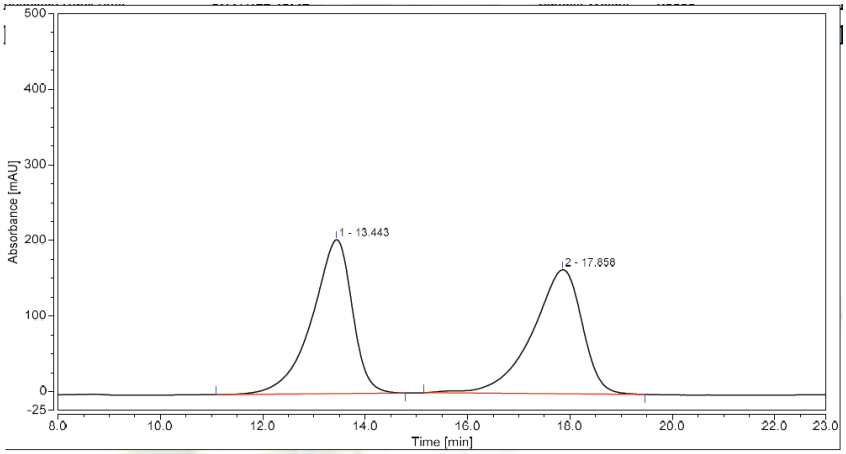


Integration Results

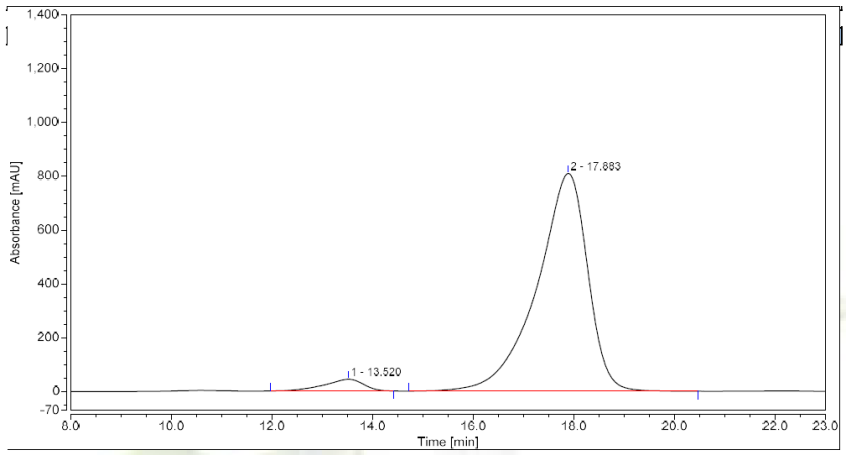
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		9.183	7.608	16.663	2.09	2.57	n.a.
300		11.583	357.204	631.445	97.91	97.43	n.a.
Total:			**364.812**	**648.108**	**100.00**	**100.00**	

4m: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



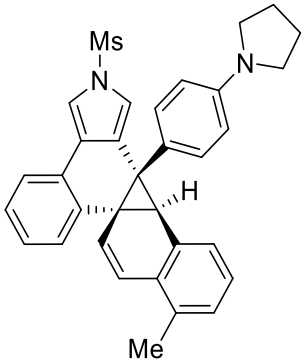


Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13.443	185.657	203.603	50.01	55.35	n.a.
2		17.858	185.607	164.253	49.99	44.65	n.a.
Total:			**371.264**	**367.856**	**100.00**	**100.00**	

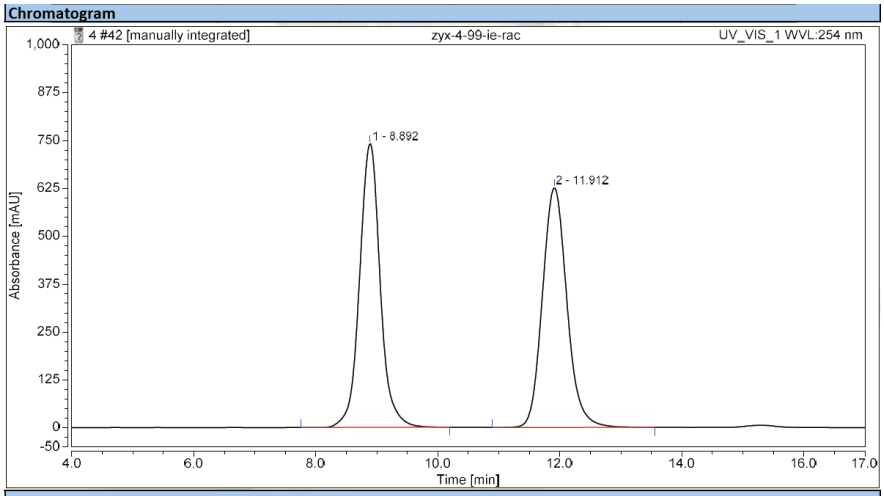


Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13.520	39.773	43.690	4.04	5.12	n.a.
2		17.883	944.894	809.319	95.96	94.88	n.a.
Total:			**984.667**	**853.009**	**100.00**	**100.00**	

4n: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



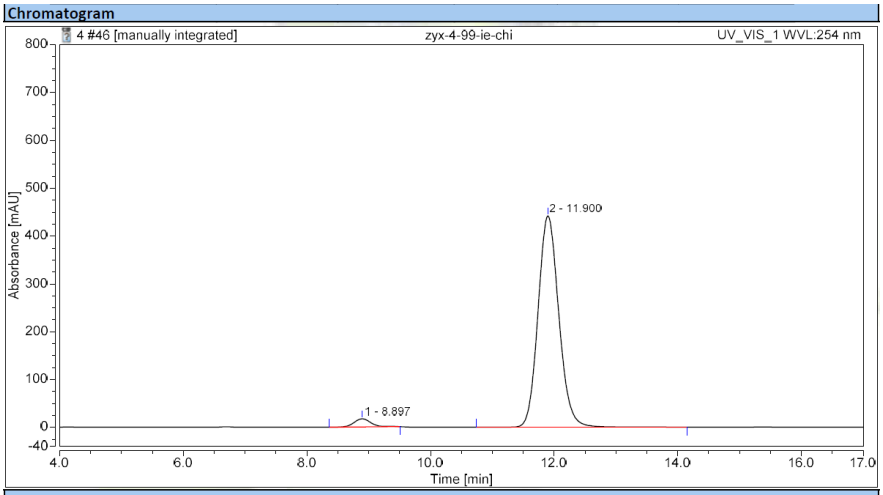
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		8.892	290.270	740.689	49.94	54.21	n.a.
300		11.912	290.978	625.617	50.06	45.79	n.a.
Total:			**581.247**	**1366.306**	**100.00**	**100.00**	

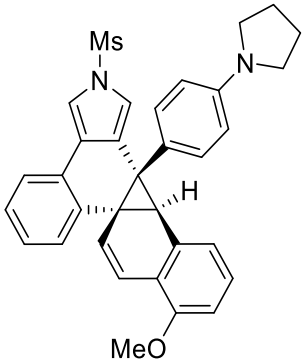
Chromatogram



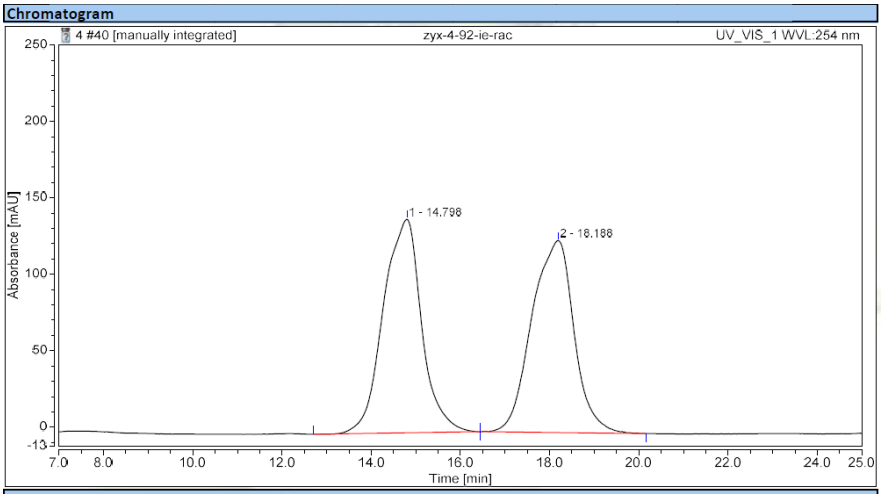
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		8.897	5.432	17.022	3.06	3.71	n.a.
300		11.900	172.048	442.145	96.94	96.29	n.a.
Total:			**177.480**	**459.167**	**100.00**	**100.00**	

4o: IE, *i*-PrOH/hexane = 15/85, v = 1.0 mL/min, λ = 254 nm



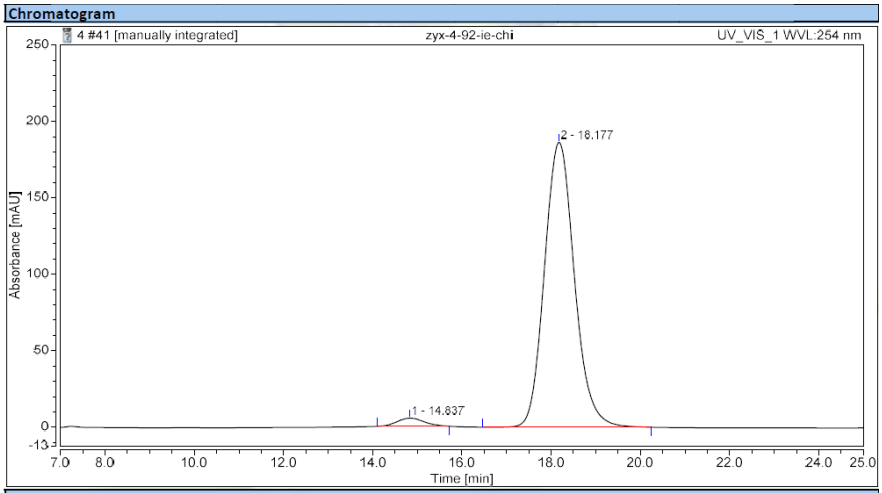
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		14.798	138.799	139.675	50.24	52.65	n.a.
300		18.188	137.488	125.621	49.76	47.35	n.a.
Total:			**276.287**	**265.296**	**100.00**	**100.00**	

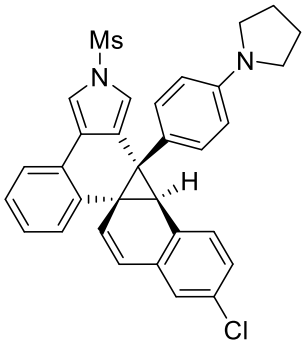
Chromatogram

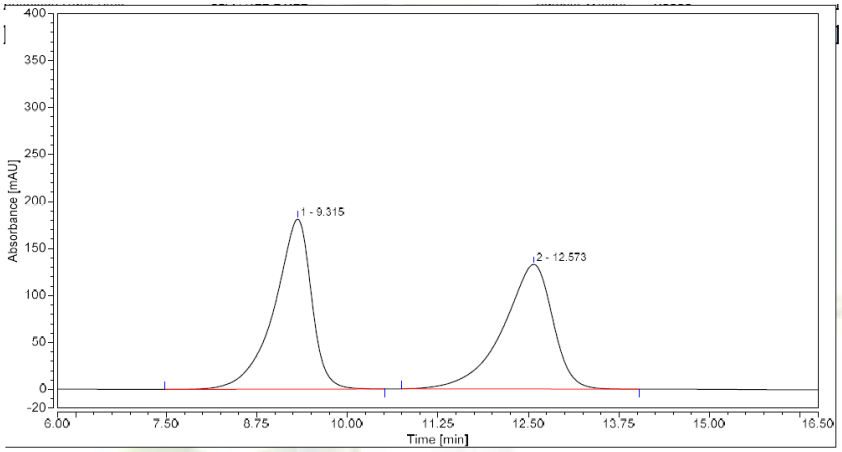


Integration Results

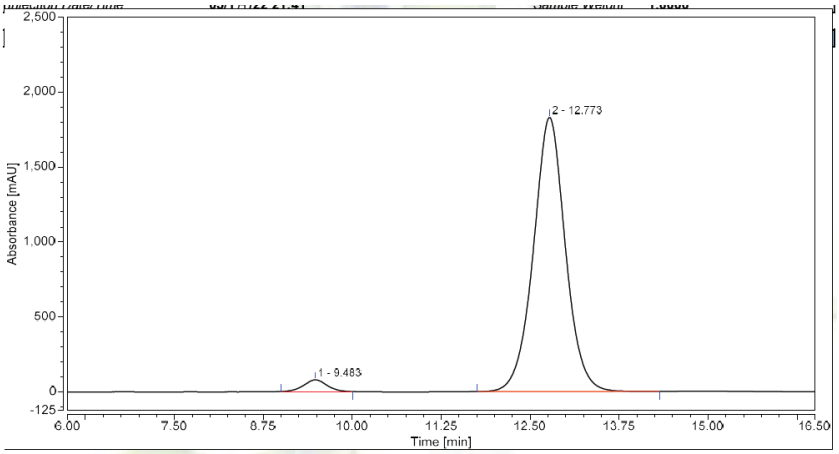
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		14.837	3.829	5.410	2.57	2.82	n.a.
300		18.177	144.979	186.464	97.43	97.18	n.a.
Total:			**148.809**	**191.874**	**100.00**	**100.00**	

4p: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



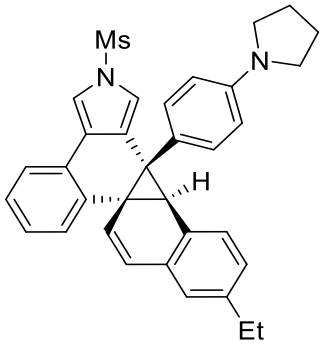


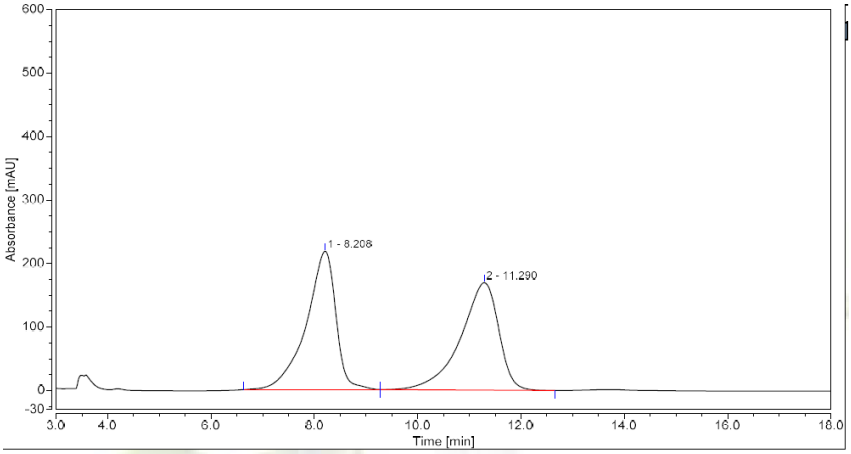
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.315	108.235	181.029	50.52	57.71	n.a.
2		12.573	106.018	132.669	49.48	42.29	n.a.
Total:			**214.253**	**313.699**	**100.00**	**100.00**	



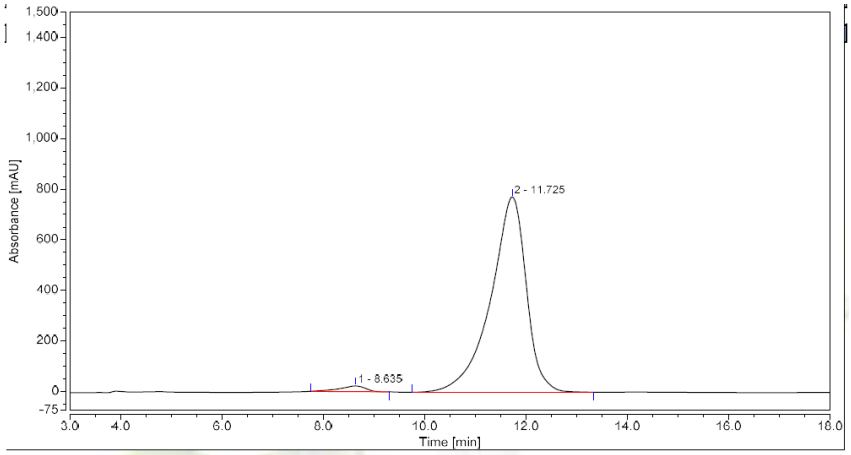
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.483	29.635	78.341	3.02	4.11	n.a.
2		12.773	952.621	1829.489	96.98	95.89	n.a.
Total:			**982.256**	**1907.830**	**100.00**	**100.00**	

4q: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



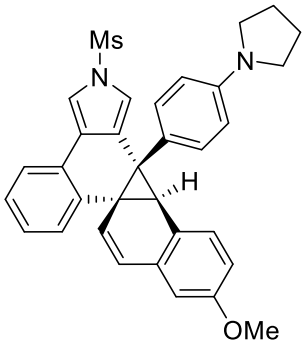


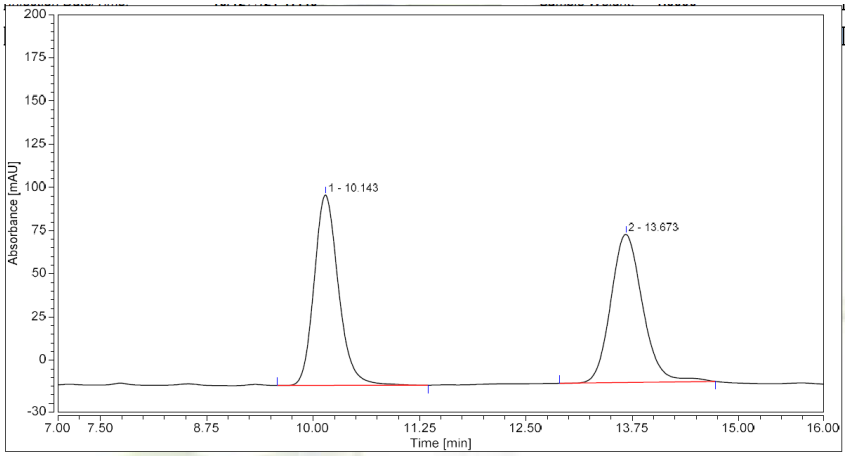
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.208	144.631	217.865	50.03	56.30	n.a.
2		11.290	144.479	169.131	49.97	43.70	n.a.
Total:			**289.110**	**386.996**	**100.00**	**100.00**	



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.635	13.221	22.037	2.06	2.78	n.a.
2		11.725	628.518	771.968	97.94	97.22	n.a.
Total:			**641.739**	**794.005**	**100.00**	**100.00**	

4r: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm

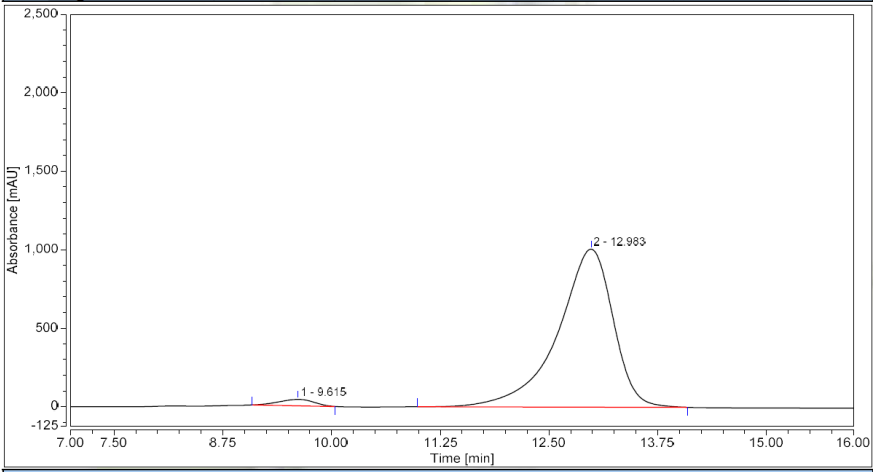




Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.143	36.413	110.090	49.46	56.22	n.a.
2		13.673	37.205	85.716	50.54	43.78	n.a.
Total:			**73.618**	**195.807**	**100.00**	**100.00**	

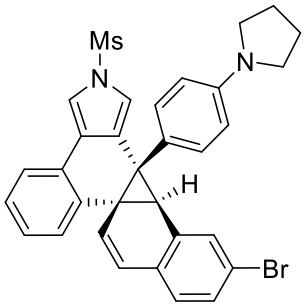
Chromatogram



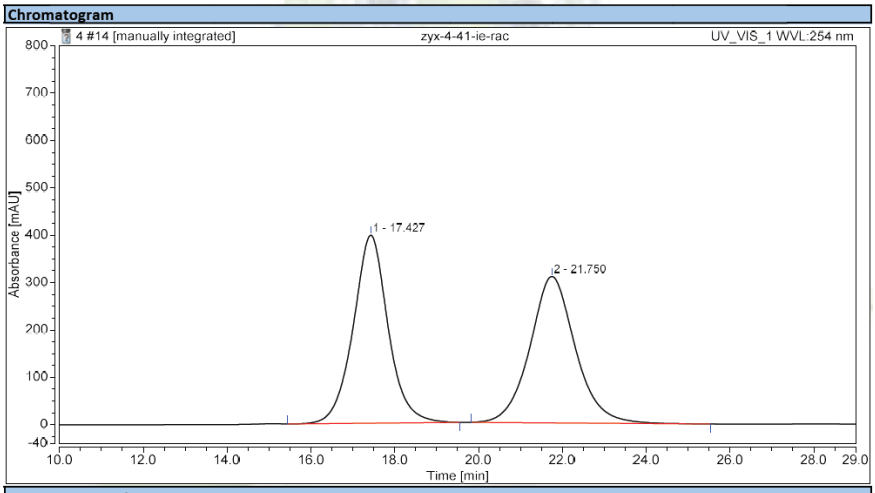
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.615	19.031	41.316	2.50	3.94	n.a.
2		12.983	742.926	1007.004	97.50	96.06	n.a.
Total:			**761.957**	**1048.320**	**100.00**	**100.00**	

4s: IE, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm



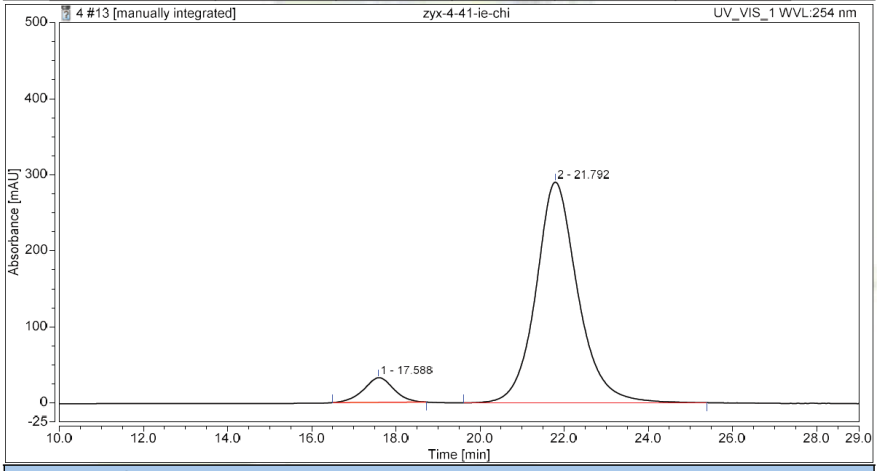
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		17.427	383.435	397.102	49.70	56.22	n.a.
300		21.750	388.136	309.256	50.30	43.78	n.a.
Total:			**771.571**	**706.358**	**100.00**	**100.00**	

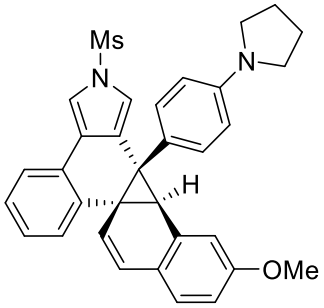
Chromatogram



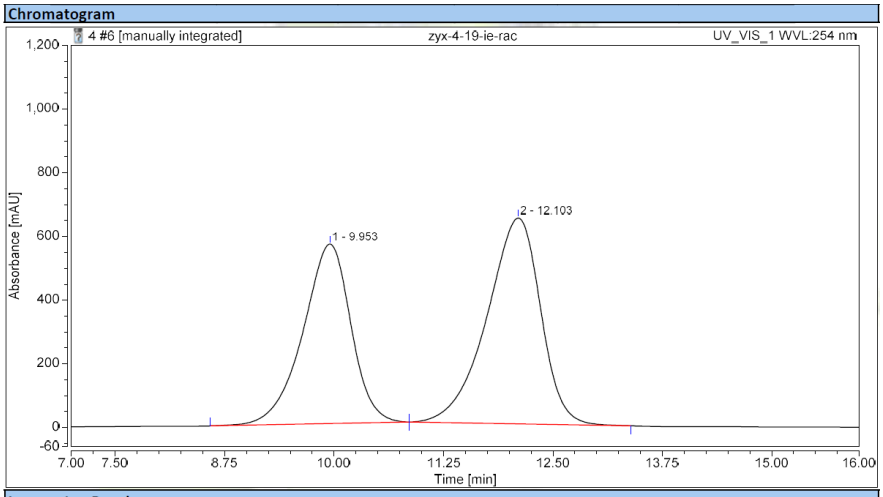
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		17.588	26.962	32.416	7.44	10.05	n.a.
300		21.792	335.253	290.231	92.56	89.95	n.a.
Total:			**362.215**	**322.648**	**100.00**	**100.00**	

4t: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



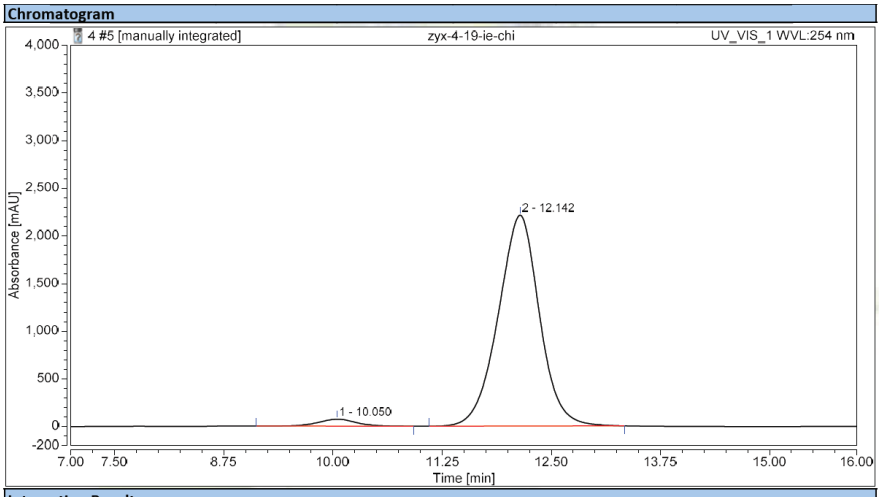
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		9.953	358.801	563.799	43.84	46.59	n.a.
300		12.103	459.639	646.254	56.16	53.41	n.a.
Total:			**818.439**	**1210.053**	**100.00**	**100.00**	

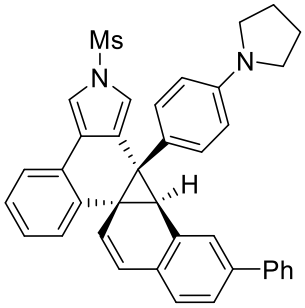
Chromatogram



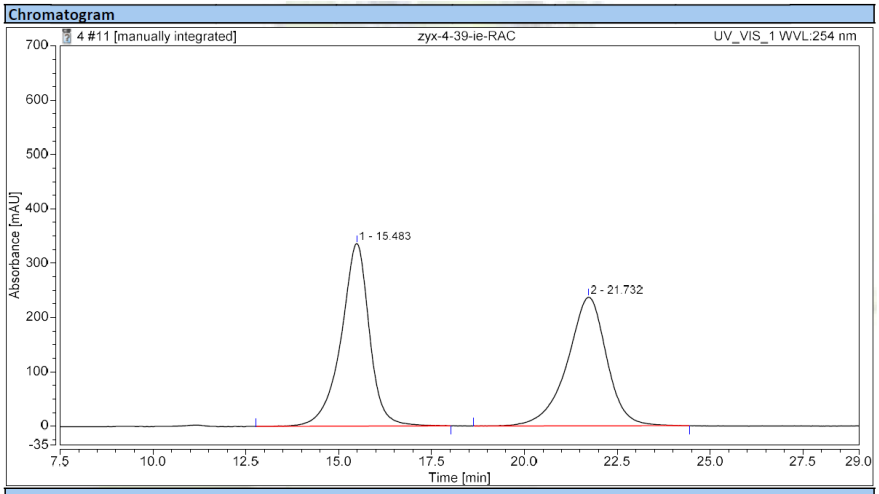
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		10.050	37.007	72.818	2.97	3.19	n.a.
300		12.142	1209.940	2212.802	97.03	96.81	n.a.
Total:			**1246.947**	**2285.620**	**100.00**	**100.00**	

4u: IE, *i*-PrOH/hexane = 15/85, v = 1.0 mL/min, λ = 254 nm



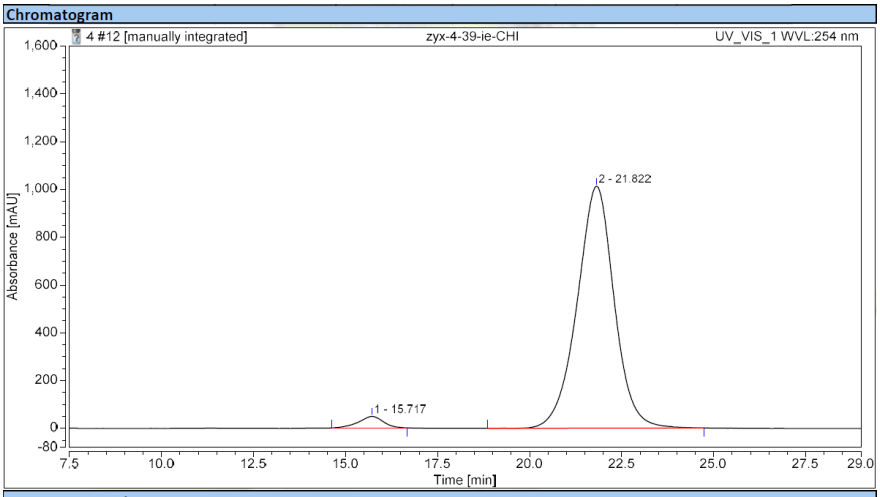
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		15.483	298.381	336.211	50.55	58.66	n.a.
300		21.732	291.897	236.915	49.45	41.34	n.a.
Total:			**590.277**	**573.126**	**100.00**	**100.00**	

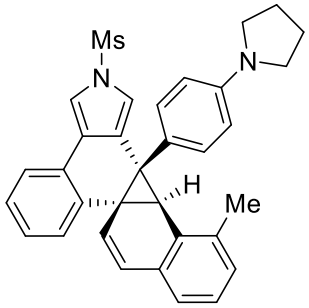
Chromatogram



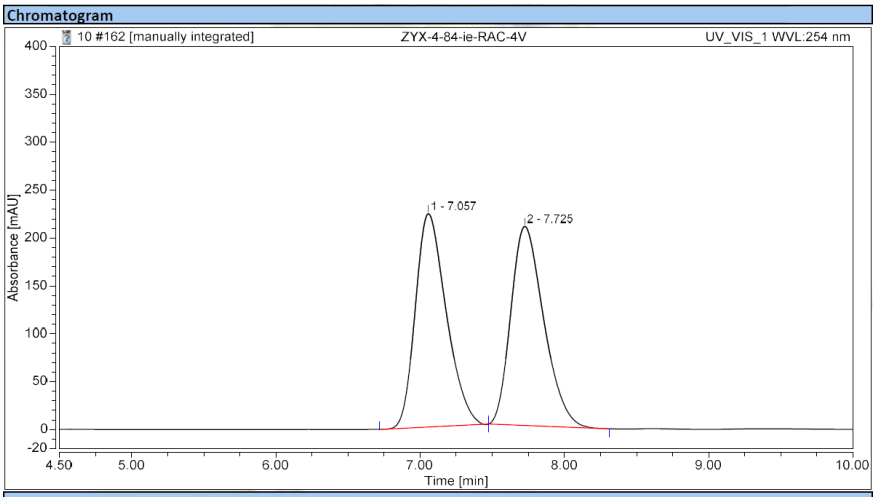
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		15.717	37.299	48.027	3.05	4.52	n.a.
300		21.822	1185.039	1013.470	96.95	95.48	n.a.
Total:			**1222.338**	**1061.497**	**100.00**	**100.00**	

4v: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



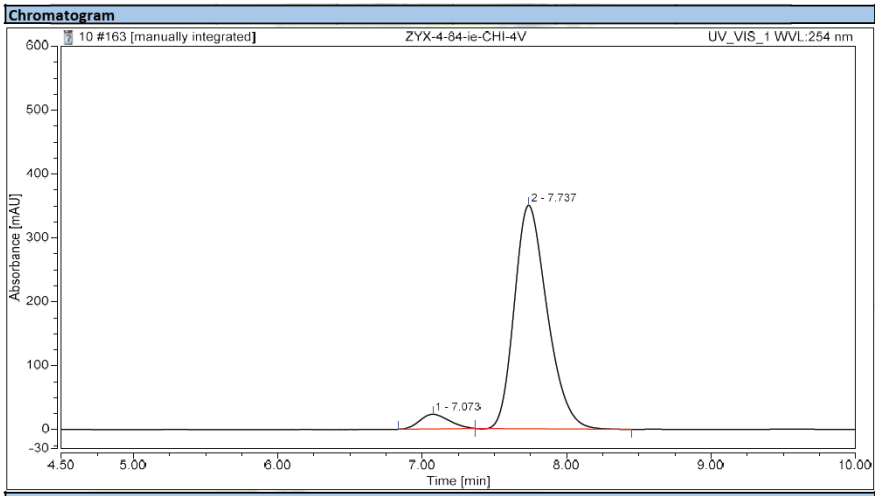
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.057	55.189	222.771	50.08	51.73	n.a.
2		7.725	55.013	207.874	49.92	48.27	n.a.
Total:			**110.201**	**430.645**	**100.00**	**100.00**	

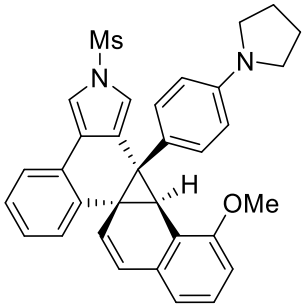
Chromatogram



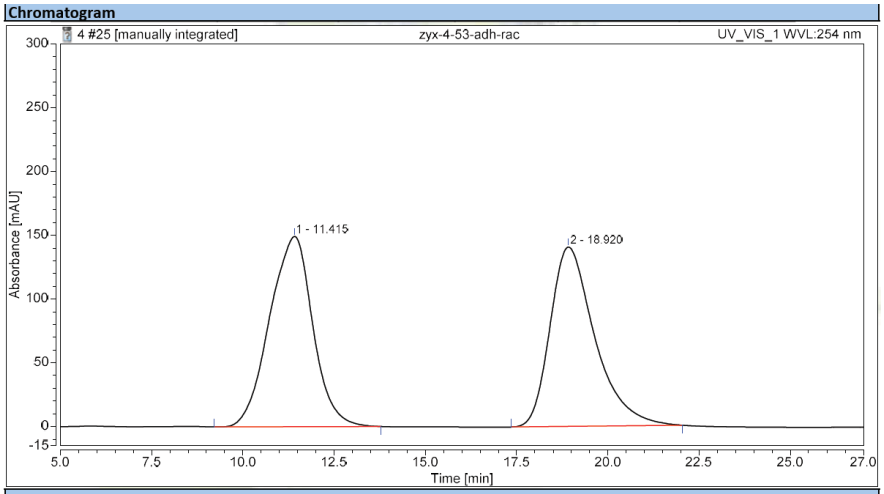
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.073	5.378	22.856	5.51	6.13	n.a.
2		7.737	92.267	349.829	94.49	93.87	n.a.
Total:			**97.645**	**372.685**	**100.00**	**100.00**	

4w: ADH, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



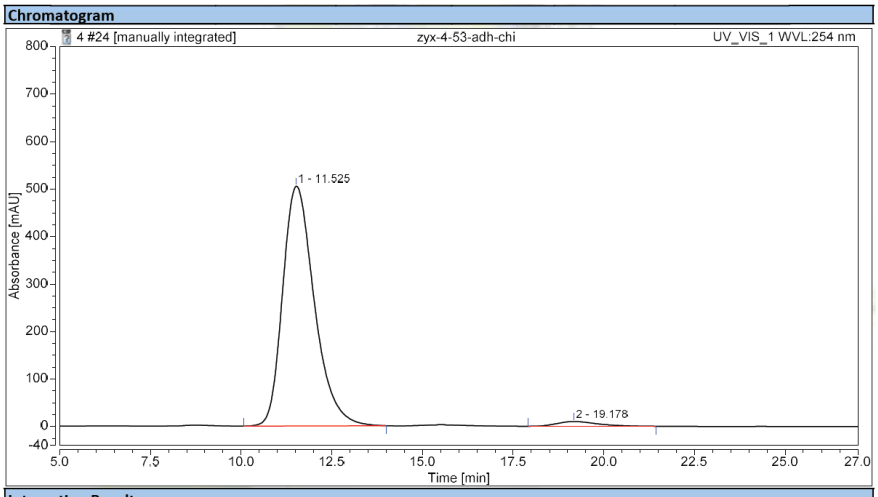
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		11.415	204.844	149.245	50.65	51.48	n.a.
300		18.920	199.561	140.669	49.35	48.52	n.a.
Total:			**404.405**	**289.914**	**100.00**	**100.00**	

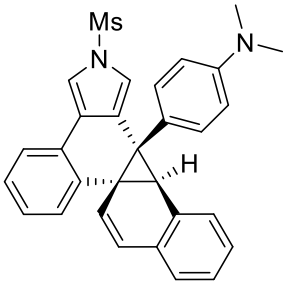
Chromatogram

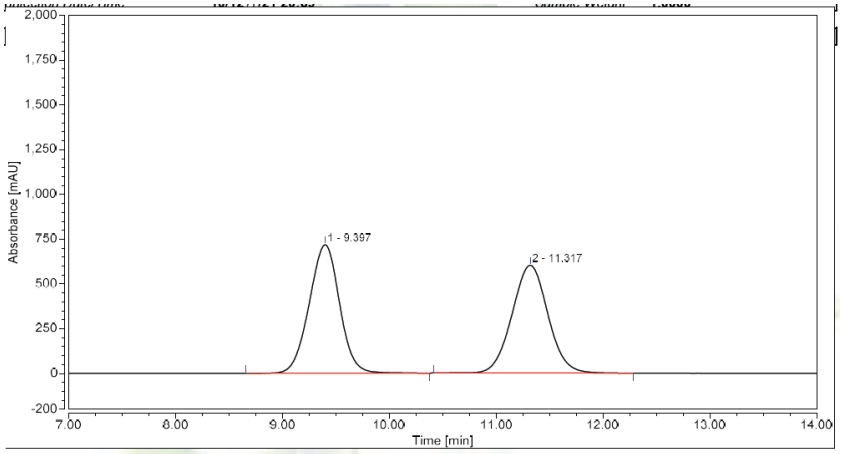


Integration Results

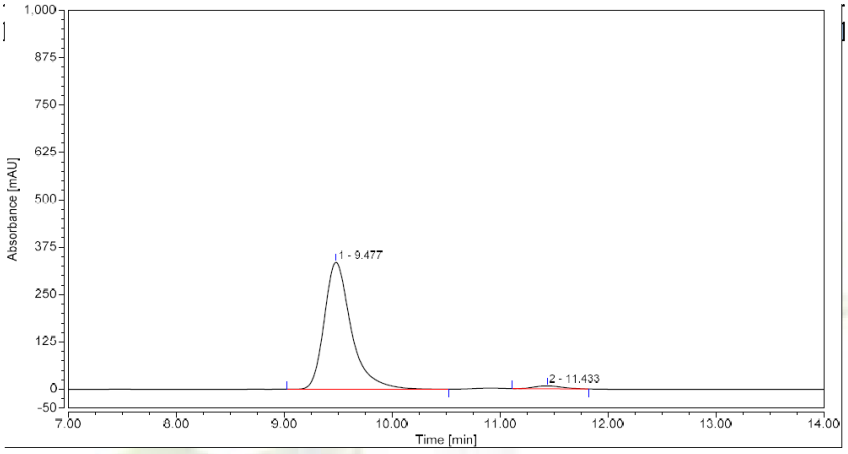
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
300		11.525	511.603	505.094	97.52	98.06	n.a.
300		19.178	12.993	9.972	2.48	1.94	n.a.
Total:			**524.596**	**515.066**	**100.00**	**100.00**	

4x: IC, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm



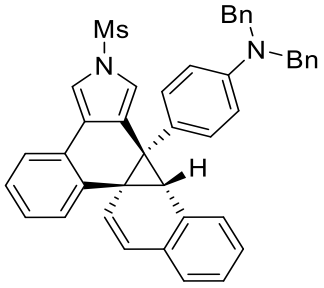


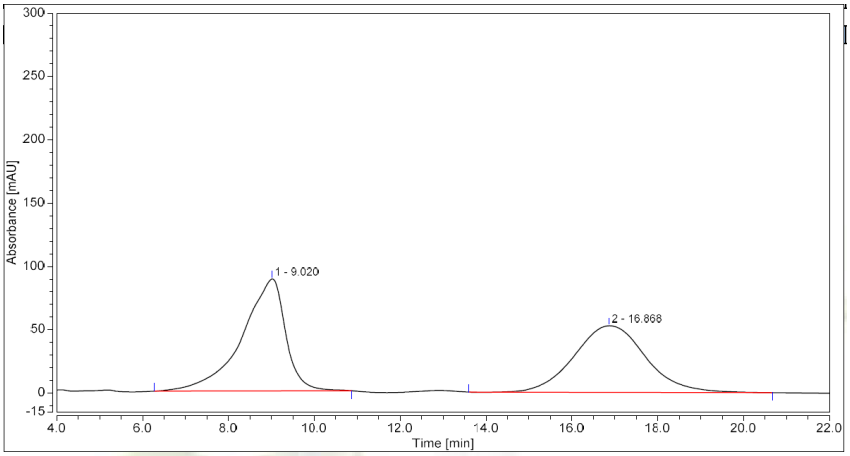
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.397	235.689	716.790	50.18	54.37	n.a.
2		11.317	234.036	601.651	49.82	45.63	n.a.
Total:			**469.724**	**1318.441**	**100.00**	**100.00**	



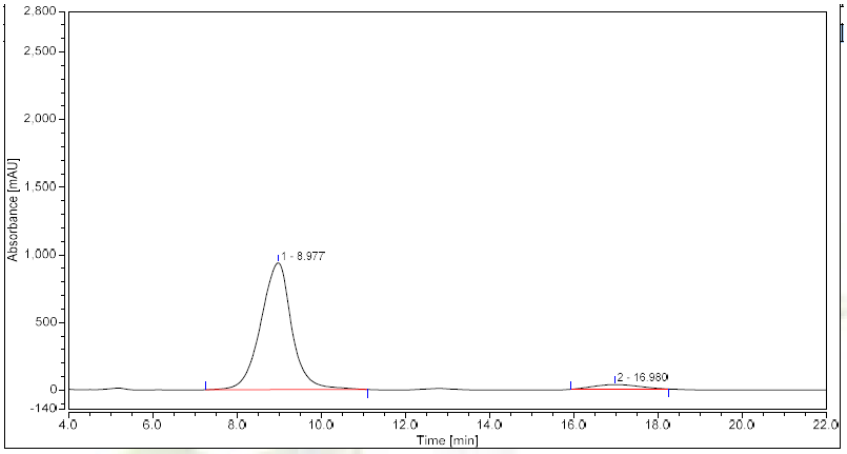
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.477	97.044	335.069	97.63	97.75	n.a.
2		11.433	2.354	7.718	2.37	2.25	n.a.
Total:			**99.398**	**342.787**	**100.00**	**100.00**	

4y: IA, *i*-PrOH/hexane = 50/50, v = 1.0 mL/min, λ = 254 nm



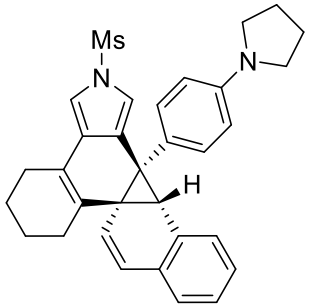


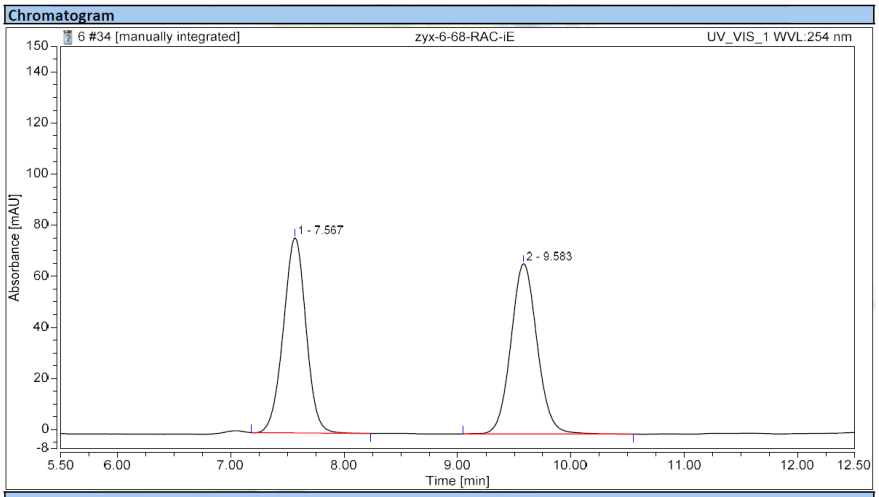
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.020	103.922	88.371	50.61	62.73	n.a.
2		16.868	101.421	52.506	49.39	37.27	n.a.
Total:			**205.343**	**140.877**	**100.00**	**100.00**	



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.977	798.424	938.167	94.96	96.56	n.a.
2		16.980	42.381	33.450	5.04	3.44	n.a.
Total:			**840.805**	**971.617**	**100.00**	**100.00**	

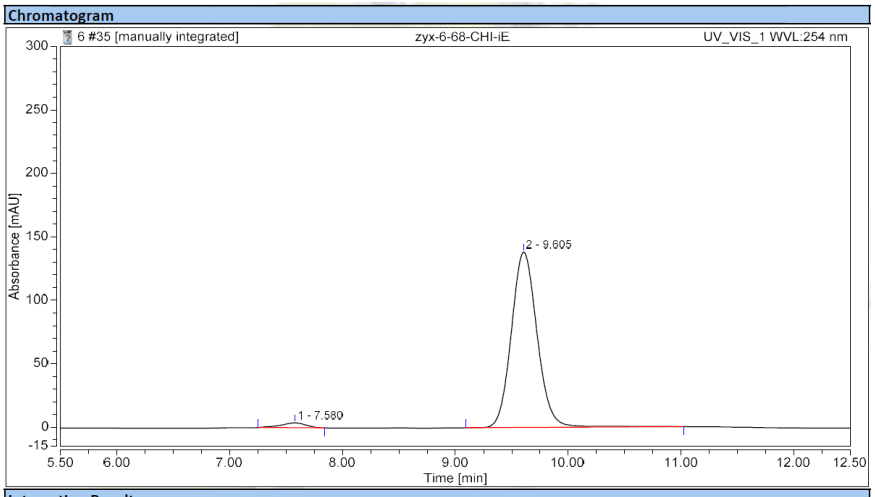
4z: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

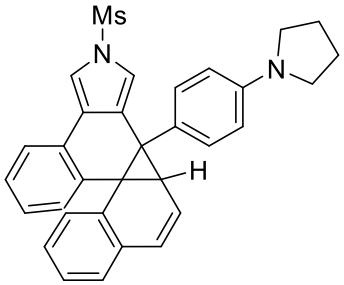
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.567	17.698	76.443	49.76	53.42	n.a.
2		9.583	17.870	66.656	50.24	46.58	n.a.
Total:			**35.567**	**143.099**	**100.00**	**100.00**	



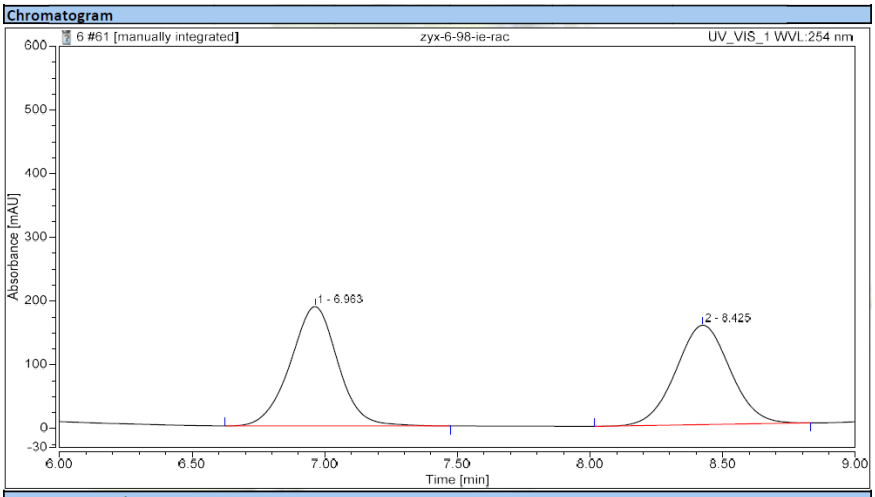
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.580	0.955	3.759	2.54	2.65	n.a.
2		9.605	36.642	138.197	97.46	97.35	n.a.
Total:			**37.597**	**141.956**	**100.00**	**100.00**	

4aa: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



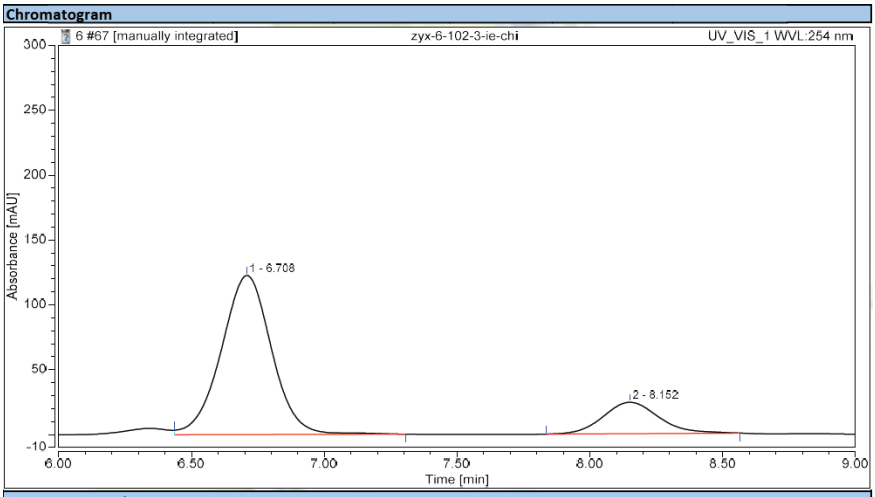
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.963	38.971	187.200	51.17	54.54	n.a.
2		8.425	37.187	156.012	48.83	45.46	n.a.
Total:			**76.158**	**343.212**	**100.00**	**100.00**	

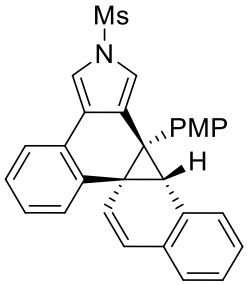
Chromatogram

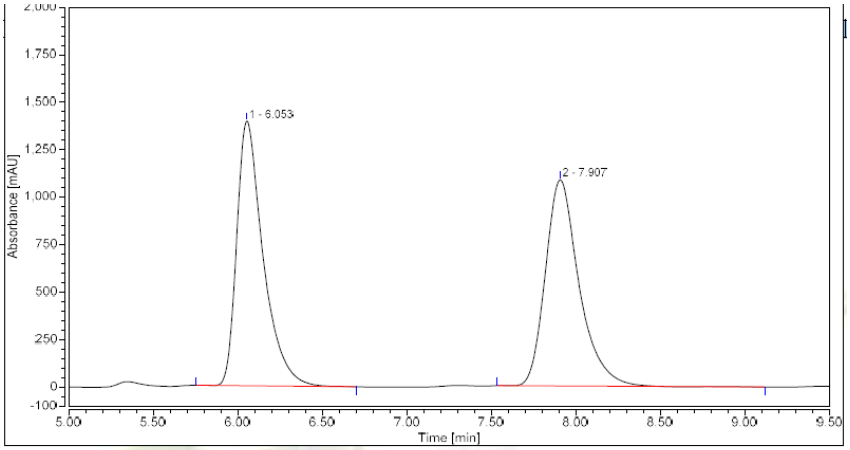


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.708	26.942	122.760	82.08	83.52	n.a.
2		8.152	5.883	24.218	17.92	16.48	n.a.
Total:			**32.824**	**146.977**	**100.00**	**100.00**	

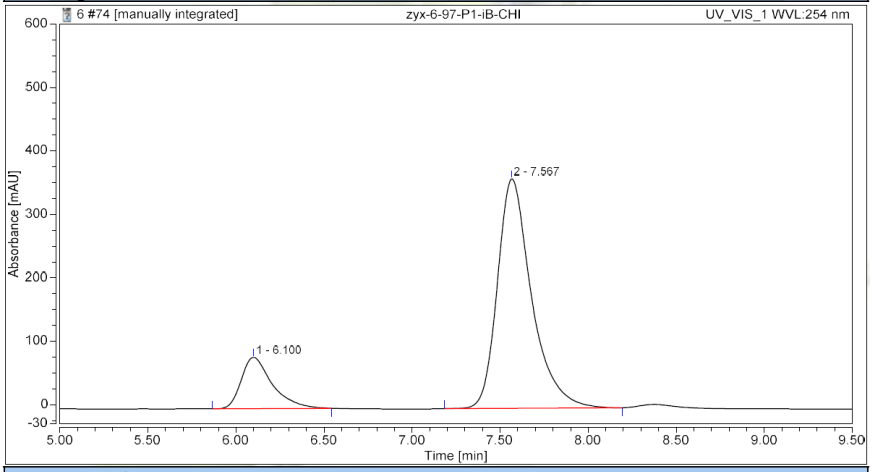
4ab: IB, *i*-PrOH/hexane = 40/60, v = 1.0 mL/min, λ = 254 nm





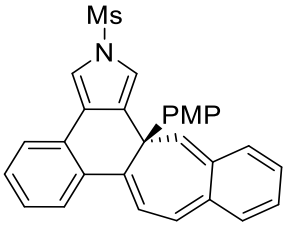
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.053	251.856	1394.074	50.09	56.22	n.a.
2		7.907	250.975	1085.591	49.91	43.78	n.a.
Total:			**502.832**	**2479.665**	**100.00**	**100.00**	

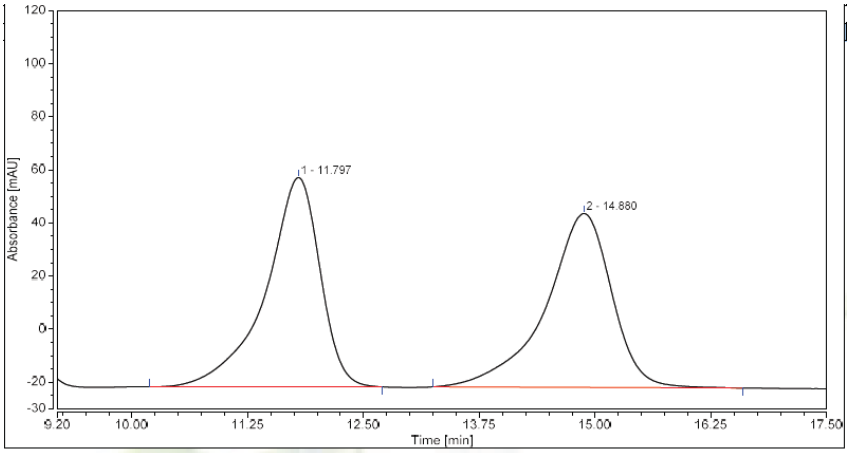
Chromatogram



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.100	16.466	80.875	16.86	18.28	n.a.
2		7.567	81.191	361.592	83.14	81.72	n.a.
Total:			**97.657**	**442.467**	**100.00**	**100.00**	

4ab′: IG, *i*-PrOH/hexane = 40/60, v = 1.0 mL/min, λ = 254 nm

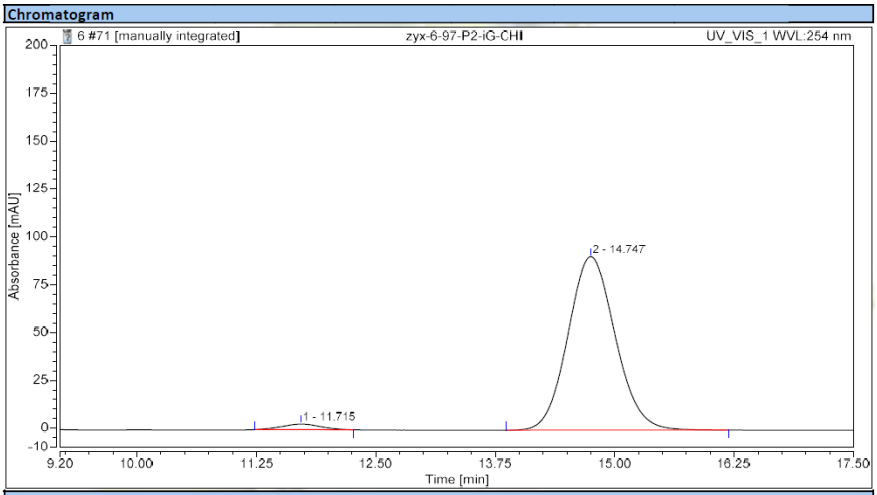




Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.797	53.506	78.826	49.74	54.62	n.a.
2		14.880	54.069	65.490	50.26	45.38	n.a.
Total:			**107.575**	**144.315**	**100.00**	**100.00**	

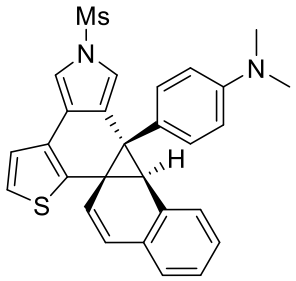
Chromatogram



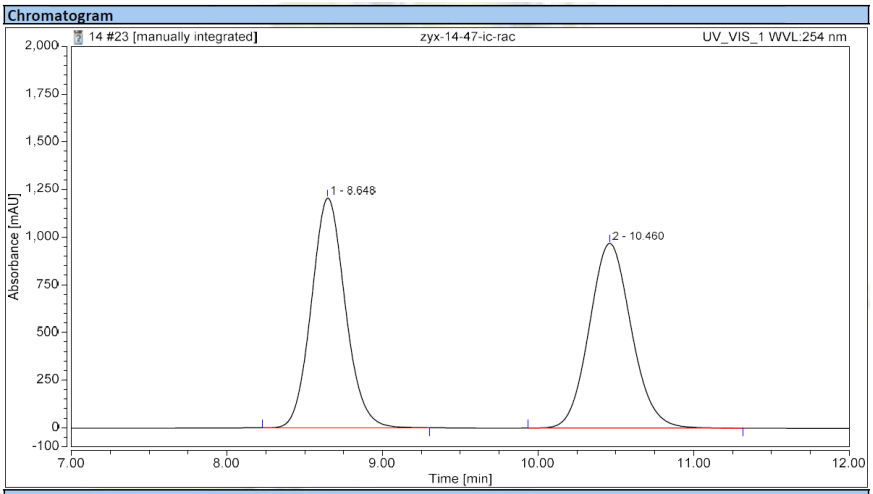
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.715	1.343	2.885	2.52	3.09	n.a.
2		14.747	51.922	90.629	97.48	96.91	n.a.
Total:			**53.265**	**93.514**	**100.00**	**100.00**	

4ac: IC, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



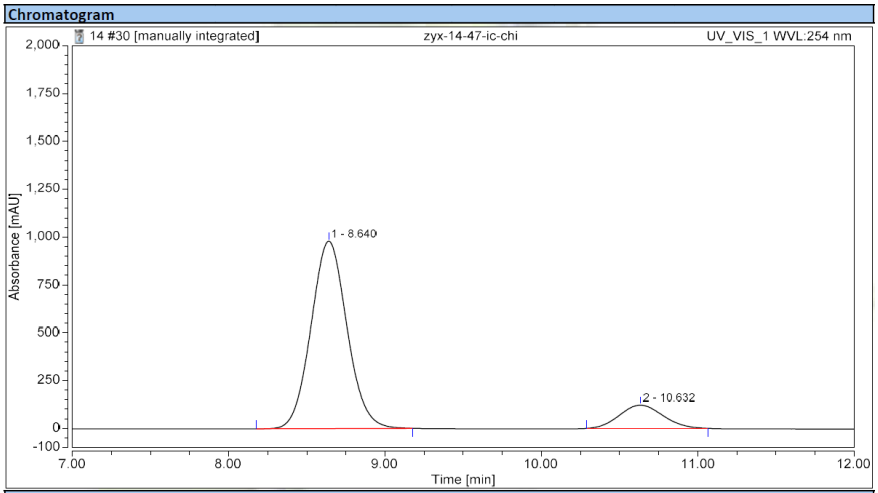
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.648	304.027	1205.184	50.08	55.43	n.a.
2		10.460	303.020	969.002	49.92	44.57	n.a.
Total:			**607.048**	**2174.186**	**100.00**	**100.00**	

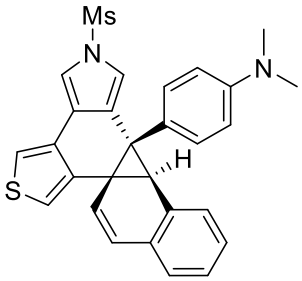
Chromatogram



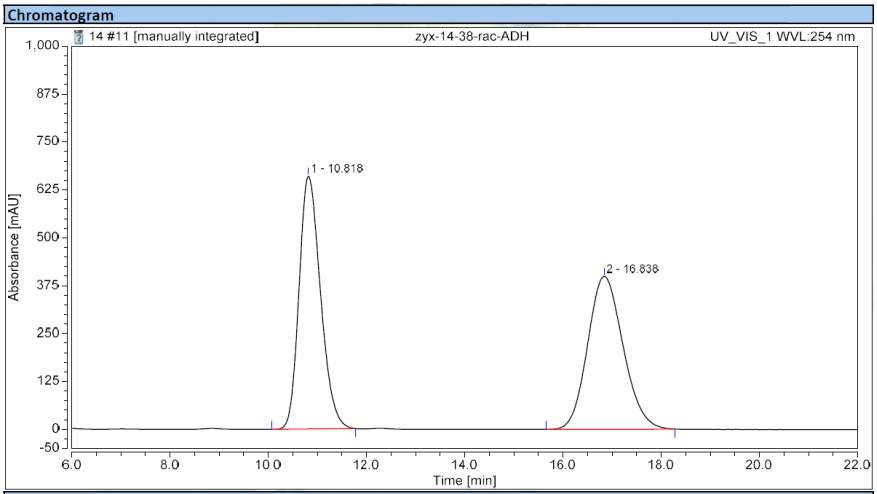
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.640	261.323	979.641	87.05	88.98	n.a.
2		10.632	38.884	121.322	12.95	11.02	n.a.
Total:			**300.207**	**1100.963**	**100.00**	**100.00**	

4ad: ADH, *i*-PrOH/hexane = 50/50, v = 1.0 mL/min, λ = 254 nm



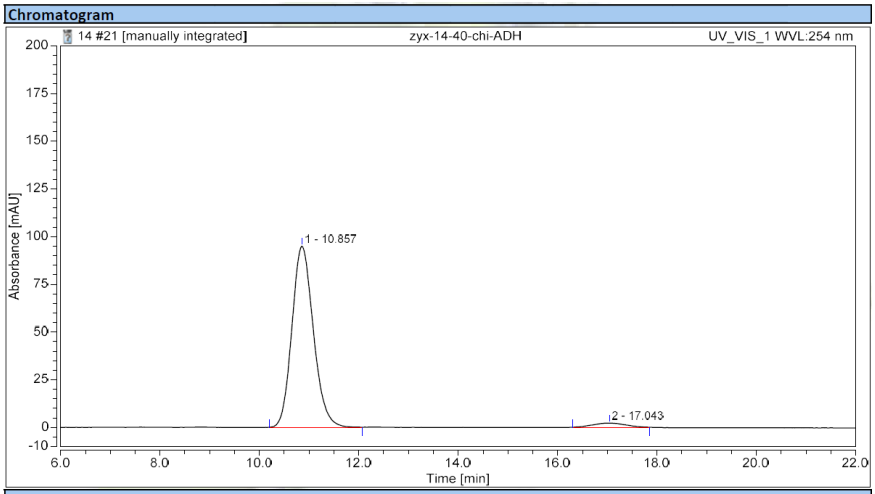
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.818	333.961	660.647	50.03	62.33	n.a.
2		16.838	333.570	399.277	49.97	37.67	n.a.
Total:			**667.532**	**1059.924**	**100.00**	**100.00**	

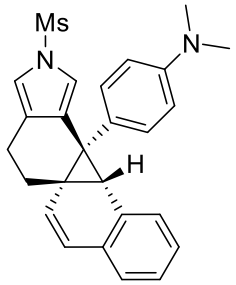
Chromatogram

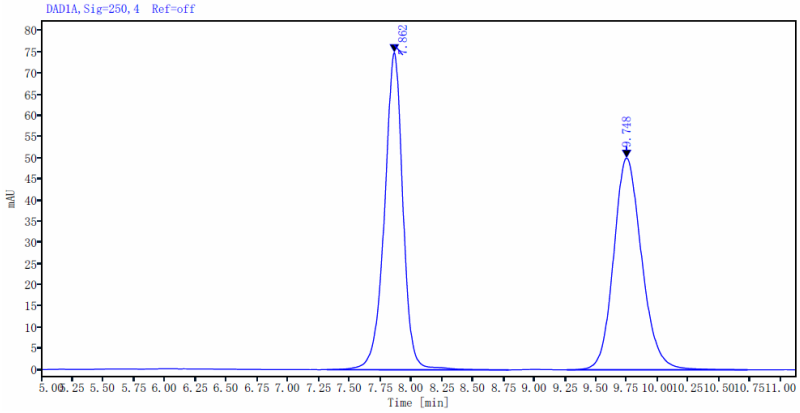


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.857	47.470	94.877	96.60	97.70	n.a.
2		17.043	1.671	2.232	3.40	2.30	n.a.
Total:			**49.141**	**97.109**	**100.00**	**100.00**	

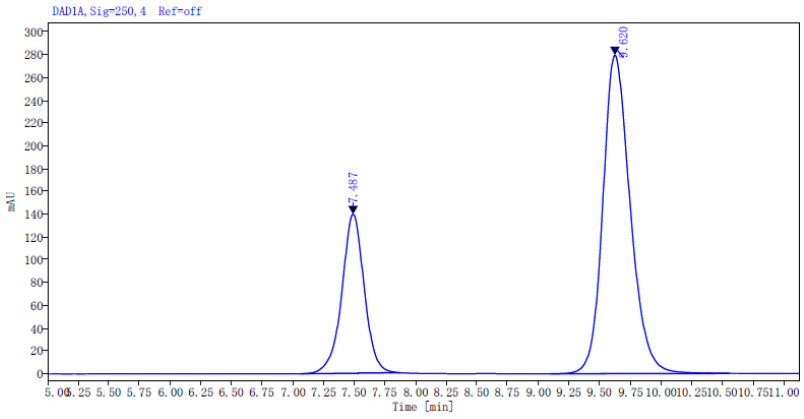
4ae: IA, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm





Signal: DAD1A, Sig=250, 4 Ref=off

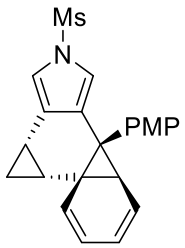
RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
7.86187	BB	1.47333	782.68547	74.91899	49.64307
9.74762	BB	1.46667	793.94045	49.99458	50.35693
		Totals:	1576.62592		

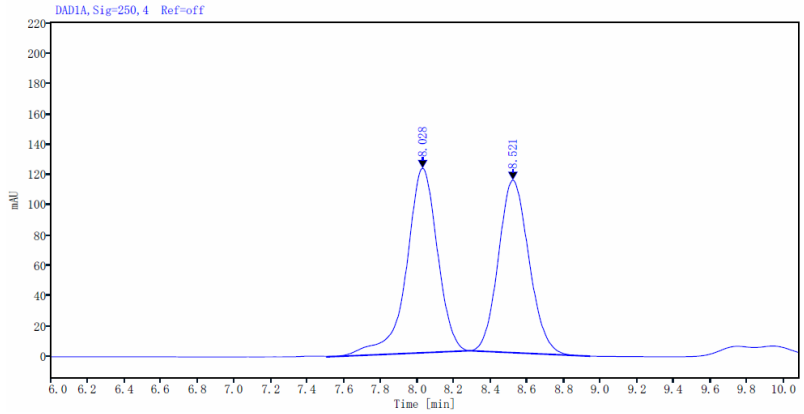


Signal: DAD1A, Sig=250, 4 Ref=off

RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
7.48679	MM m	0.81050	1774.41131	139.52239	28.99429
9.62042	BM m	1.45341	4345.45286	279.59271	71.00571
		Totals:	6119.86418		

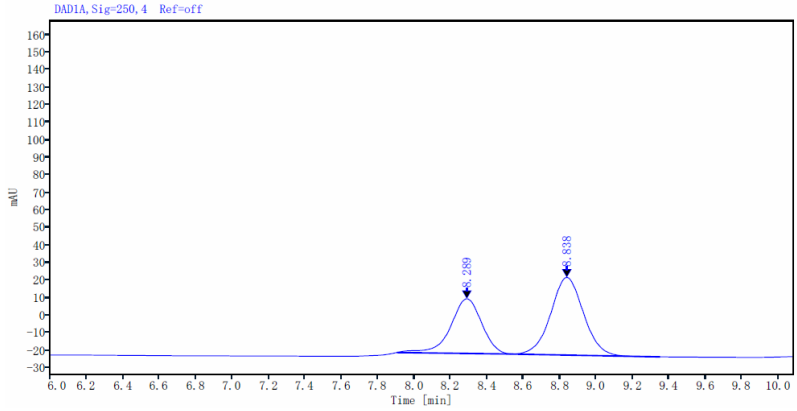
4aj: IA, *i*-PrOH/hexane = 10/90, v = 1.0 mL/min, λ = 254 nm





Signal: DAD1A, Sig=250, 4 Ref=off

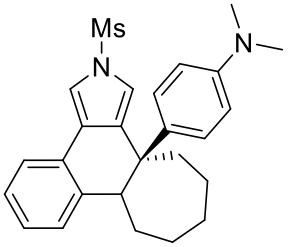
RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
8.02832	VM m	0.78065	1436.59326	121.96390	52.07792
8.52077	MM m	0.65814	1321.95245	114.08904	47.92208
		Totals:	2758.54571		

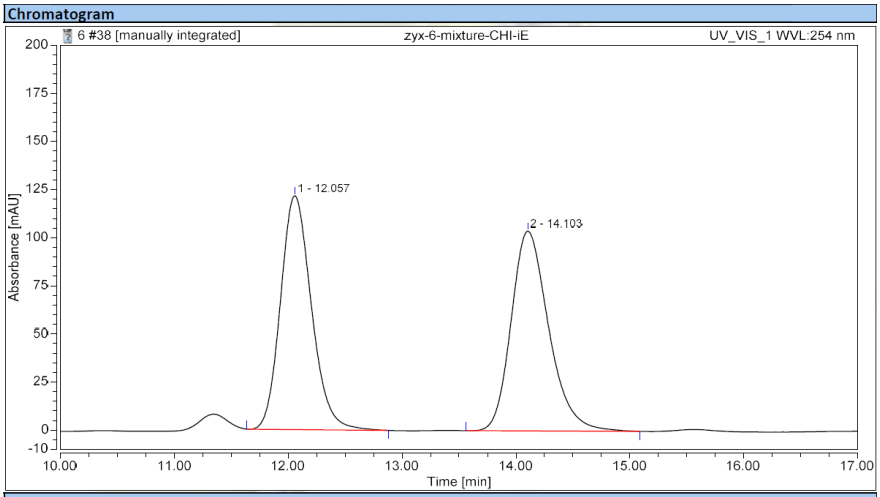


Signal: DAD1A, Sig=250, 4 Ref=off

RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
8.28884	MM m	0.62583	369.90344	31.19948	40.04620
8.83773	MM m	0.82076	553.78835	44.28689	59.95380
		Totals:	923.69179		

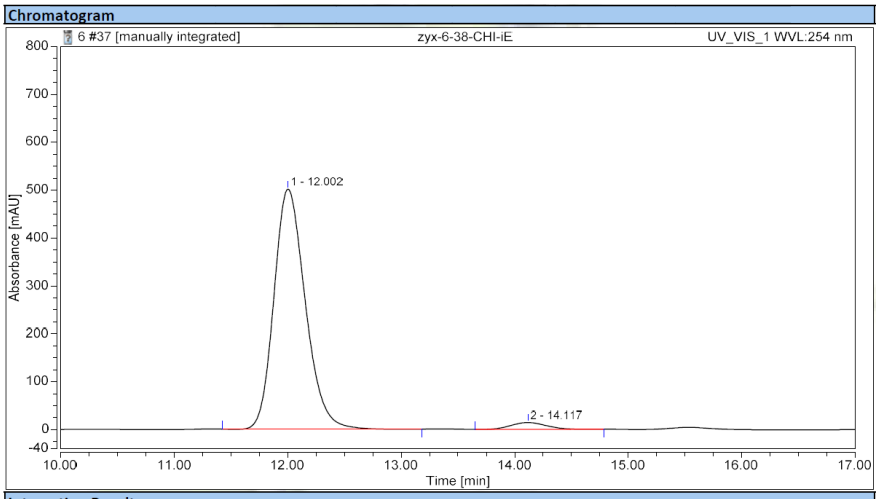
5a: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

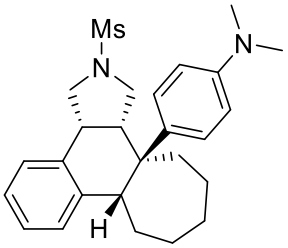
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12.057	38.202	121.481	49.11	53.94	n.a.
2		14.103	39.585	103.754	50.89	46.06	n.a.
Total:			**77.787**	**225.235**	**100.00**	**100.00**	

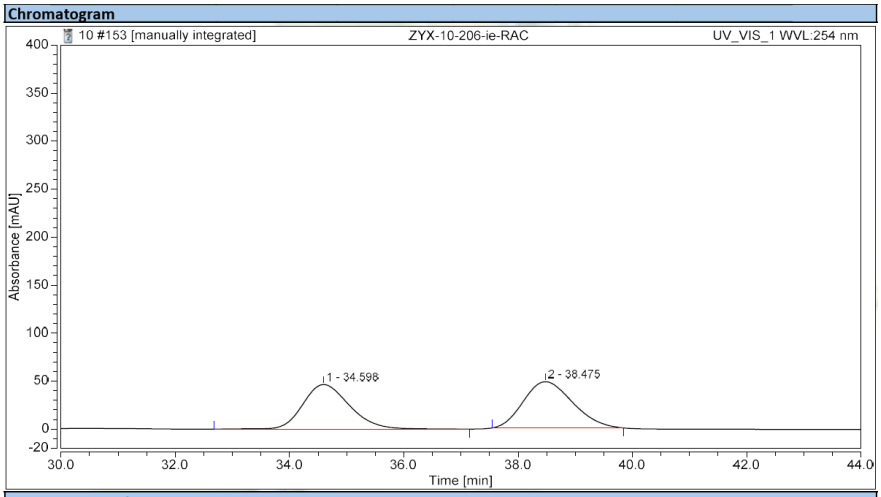


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12.002	160.238	501.426	96.96	97.27	n.a.
2		14.117	5.031	14.087	3.04	2.73	n.a.
Total:			**165.268**	**515.512**	**100.00**	**100.00**	

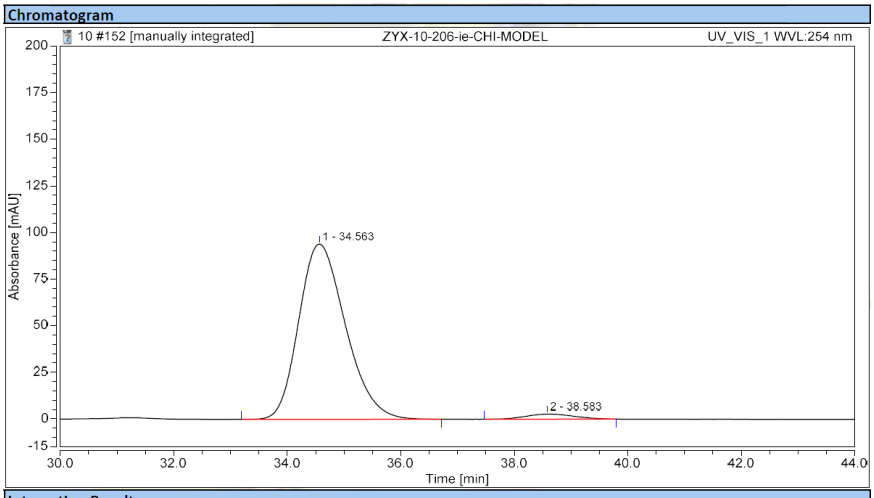
5b: IE, *i*-PrOH/hexane = 20/80, v = 1.0 mL/min, λ = 254 nm





Integration Results

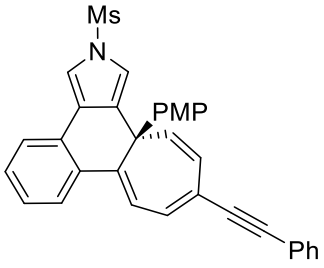
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		34.598	43.907	46.386	47.78	49.07	n.a.
2		38.475	47.991	48.141	52.22	50.93	n.a.
Total:			**91.898**	**94.527**	**100.00**	**100.00**	



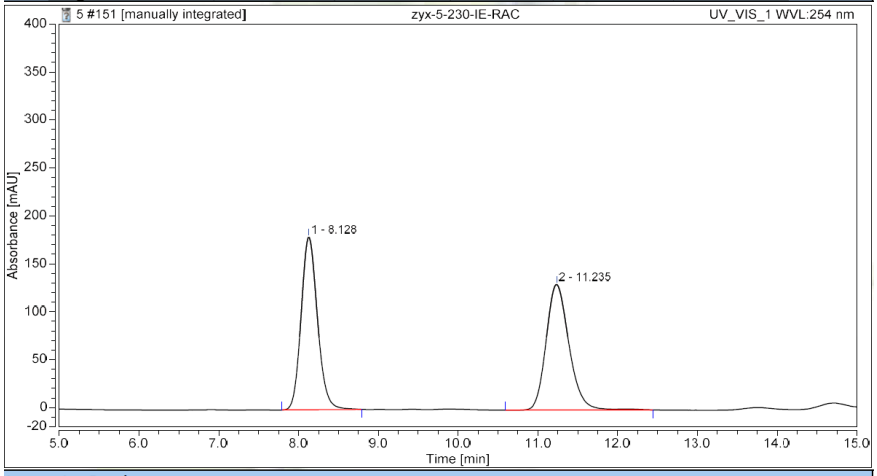
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		34.563	89.604	94.026	97.04	97.13	n.a.
2		38.583	2.730	2.776	2.96	2.87	n.a.
Total:			**92.334**	**96.802**	**100.00**	**100.00**	

5c: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



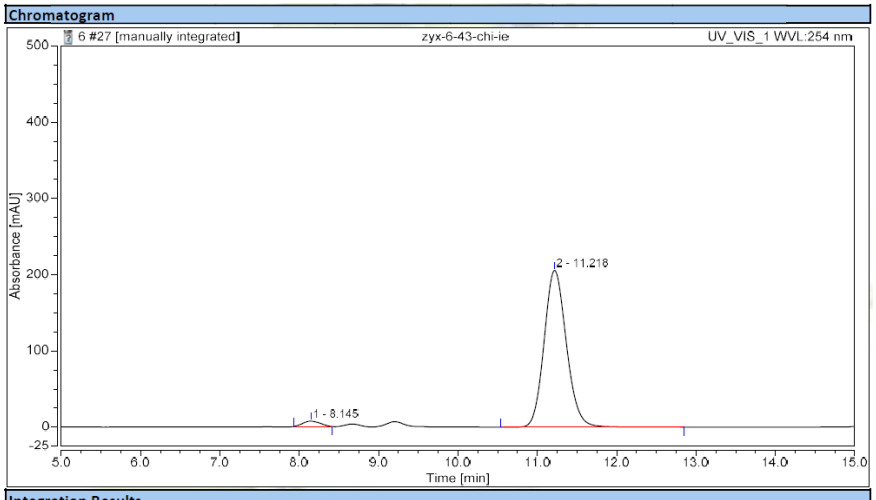
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.128	42.689	180.269	49.61	57.93	n.a.
2		11.235	43.365	130.918	50.39	42.07	n.a.
Total:			**86.054**	**311.187**	**100.00**	**100.00**	

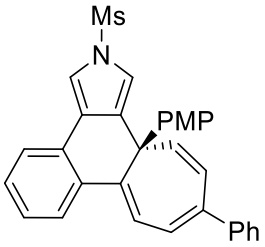
Chromatogram

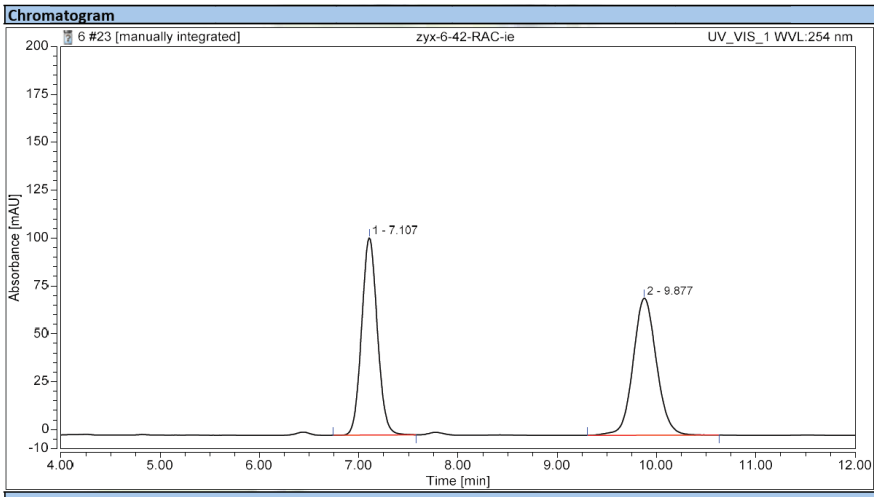


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.145	1.717	7.003	2.50	3.29	n.a.
2		11.218	66.952	205.918	97.50	96.71	n.a.
Total:			**68.669**	**212.922**	**100.00**	**100.00**	

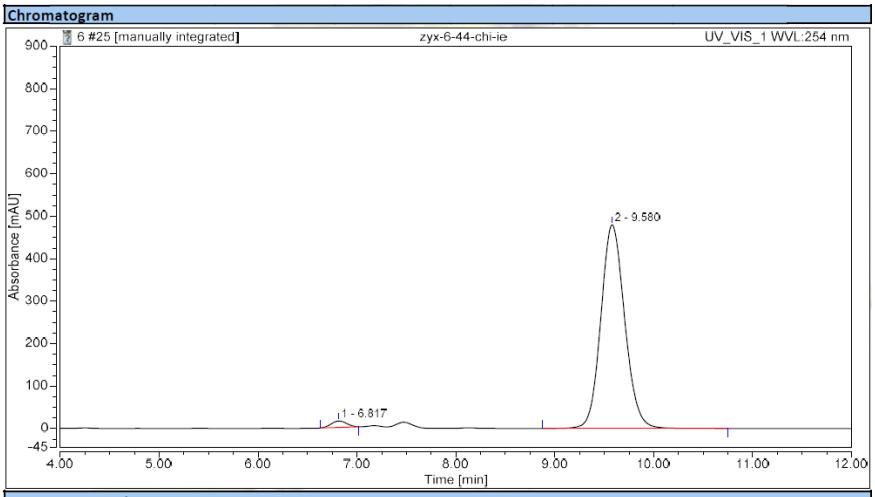
5d: IE, *i*-PrOH/hexane = 40/60, v = 1.0 mL/min, λ = 254 nm





Integration Results

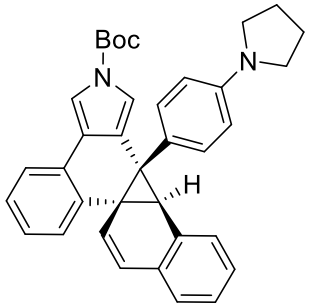
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.107	18.875	103.018	49.11	59.01	n.a.
2		9.877	19.556	71.570	50.89	40.99	n.a.
Total:			**38.431**	**174.588**	**100.00**	**100.00**	



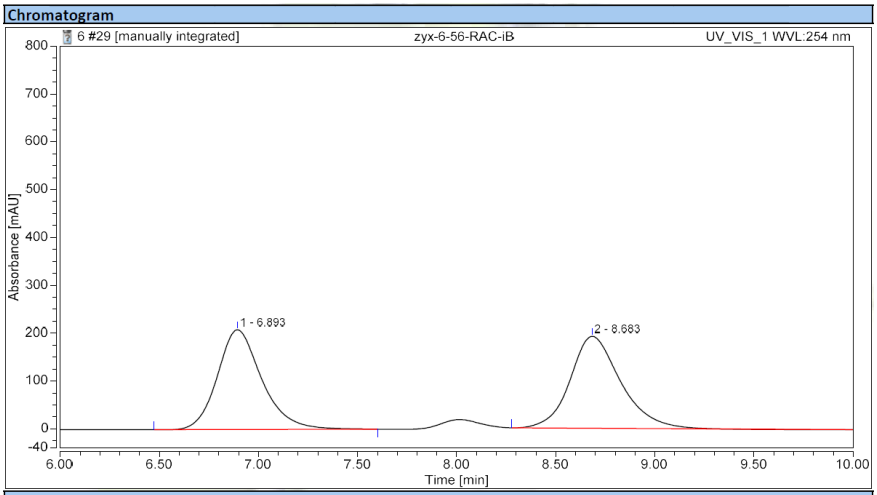
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.817	2.771	15.381	2.02	3.11	n.a.
2		9.580	134.299	479.791	97.98	96.89	n.a.
Total:			**137.071**	**495.172**	**100.00**	**100.00**	

5e: IB, *i*-PrOH/hexane = 20/0, v = 1.0 mL/min, λ = 254 nm



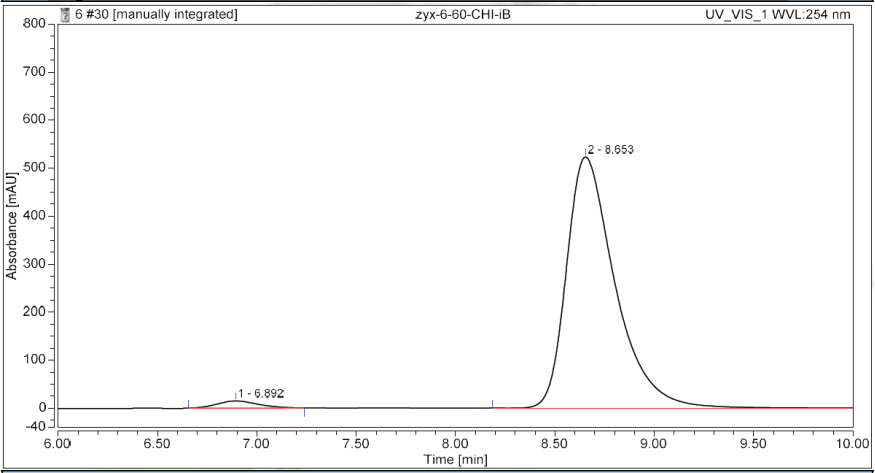
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.893	54.246	208.529	49.00	52.05	n.a.
2		8.683	56.449	192.139	51.00	47.95	n.a.
Total:			**110.696**	**400.668**	**100.00**	**100.00**	

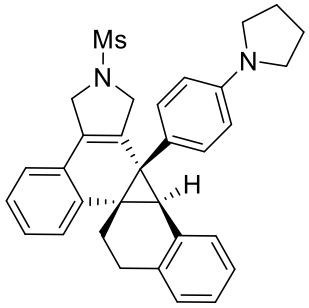
Chromatogram



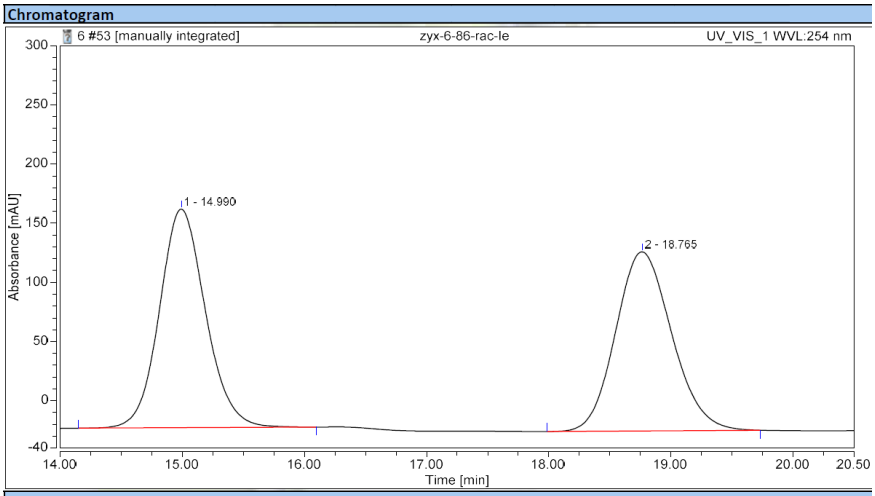
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.892	3.525	14.844	2.33	2.76	n.a.
2		8.653	147.959	523.004	97.67	97.24	n.a.
Total:			**151.484**	**537.848**	**100.00**	**100.00**	

5f: IE, *i*-PrOH/hexane = 30/70, v = 1.0 mL/min, λ = 254 nm



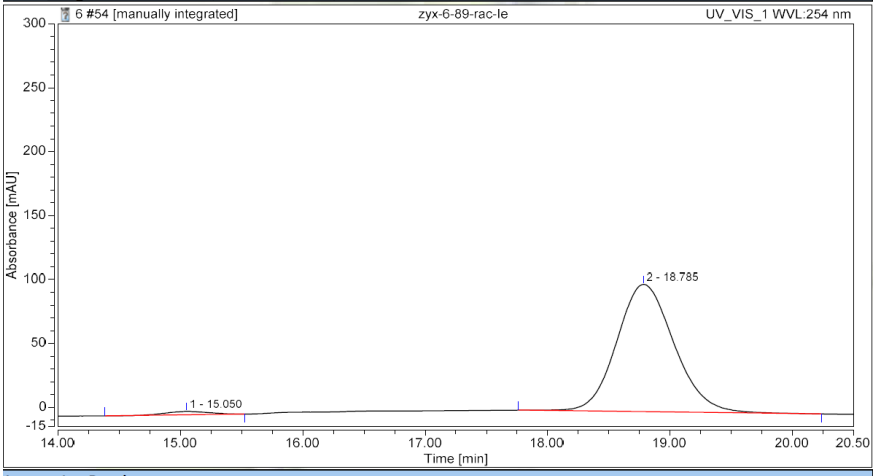
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.990	80.800	184.796	50.09	54.97	n.a.
2		18.765	80.509	151.353	49.91	45.03	n.a.
Total:			**161.309**	**336.149**	**100.00**	**100.00**	

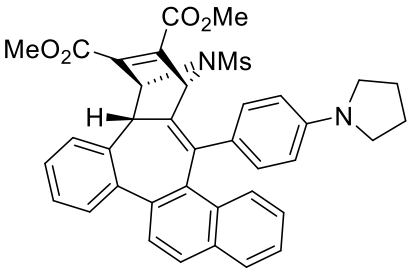
Chromatogram



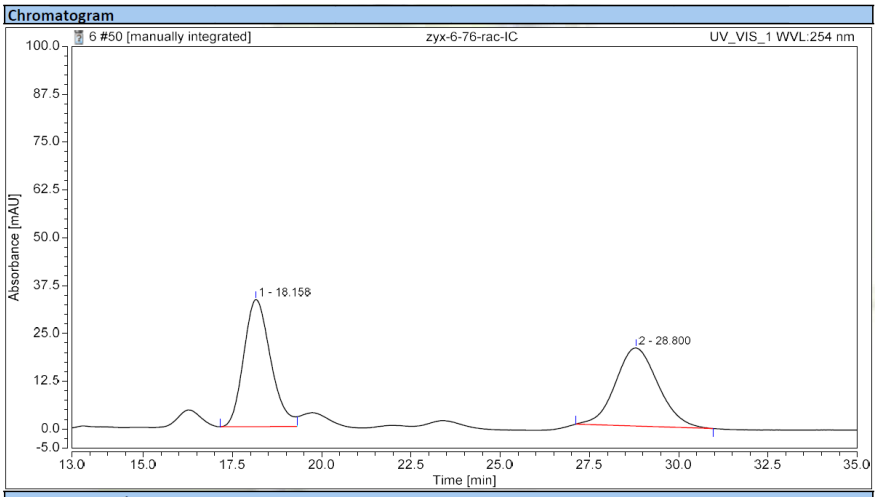
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.050	1.054	2.605	1.91	2.55	n.a.
2		18.785	54.097	99.507	98.09	97.45	n.a.
Total:			**55.151**	**102.112**	**100.00**	**100.00**	

5g: IC, *i*-PrOH/hexane = 50/50, v = 1.0 mL/min, λ = 254 nm



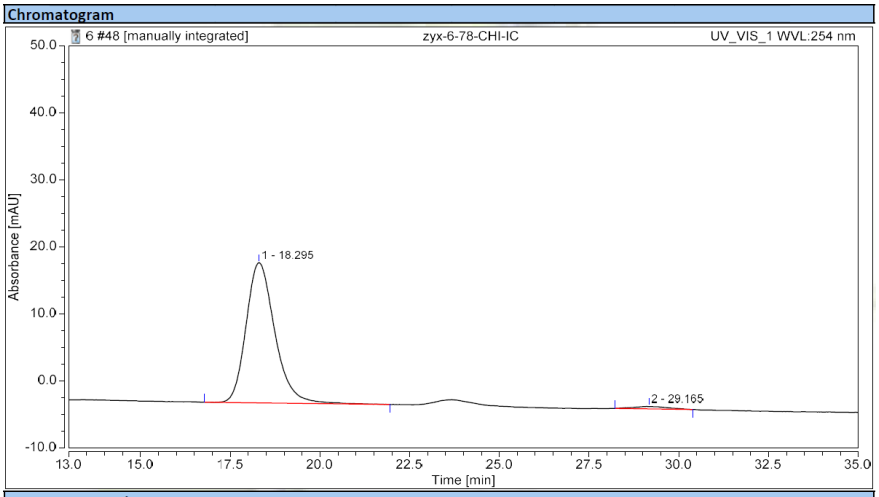
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18.158	29.146	33.202	50.77	61.93	n.a.
2		28.800	28.266	20.411	49.23	38.07	n.a.
Total:			**57.412**	**53.613**	**100.00**	**100.00**	

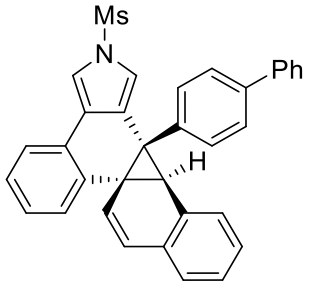
Chromatogram

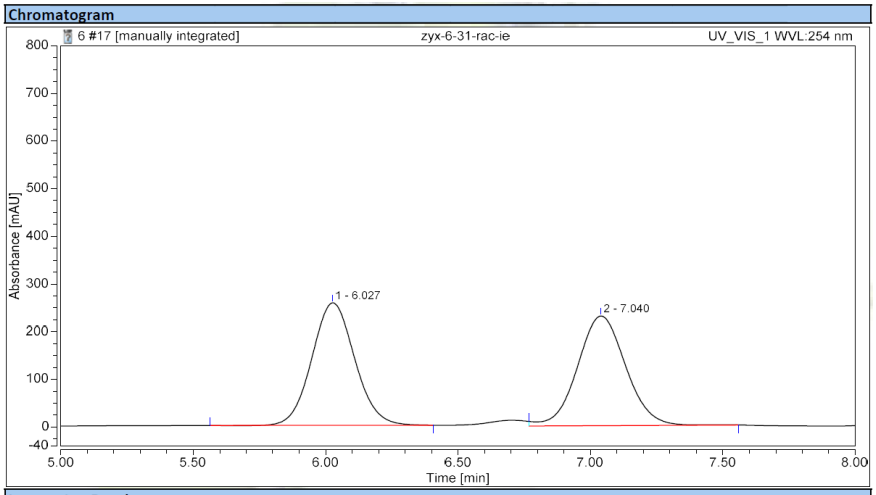


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18.295	19.420	20.913	98.03	98.30	n.a.
2		29.165	0.390	0.362	1.97	1.70	n.a.
Total:			**19.809**	**21.275**	**100.00**	**100.00**	

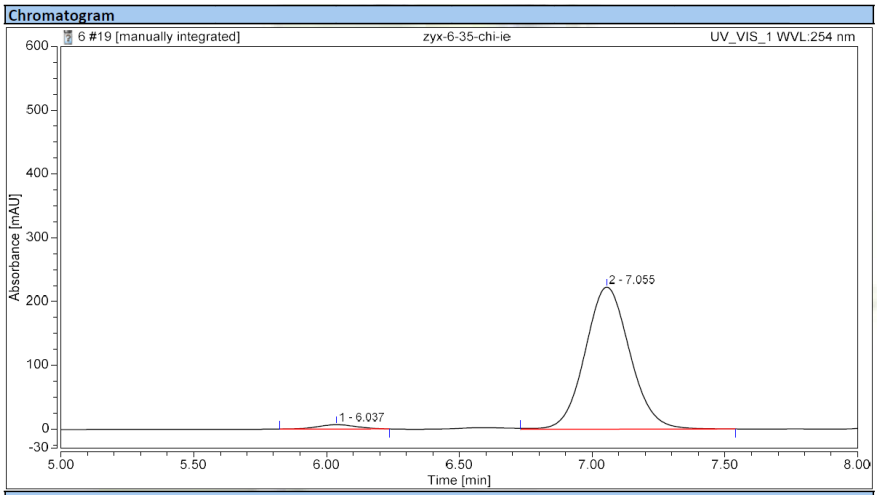
5h: IE, *i*-PrOH/hexane = 40/60, v = 1.0 mL/min, λ = 254 nm





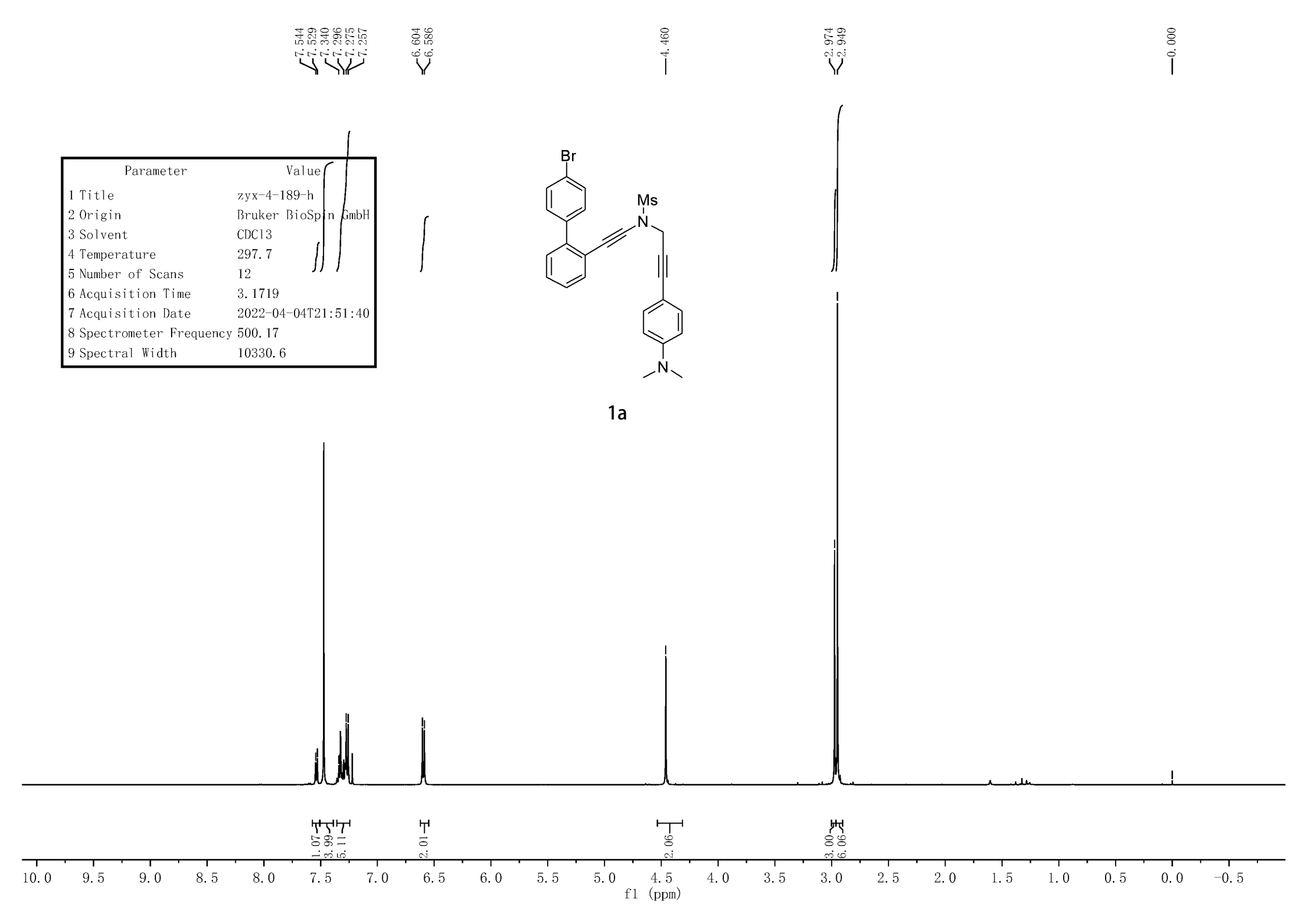
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.027	48.287	257.085	49.81	52.75	n.a.
2		7.040	48.661	230.242	50.19	47.25	n.a.
Total:			**96.948**	**487.327**	**100.00**	**100.00**	



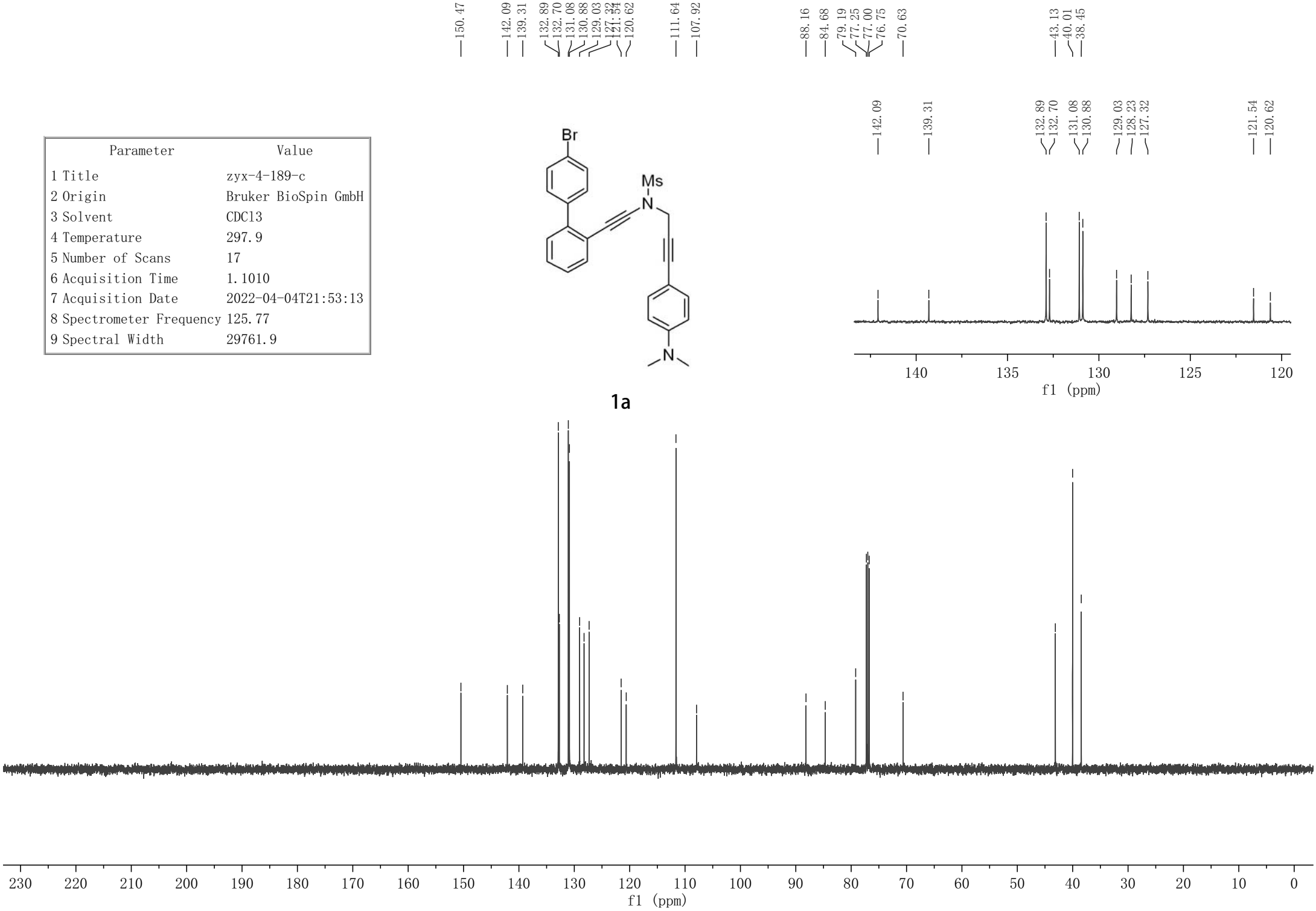
Integration Results

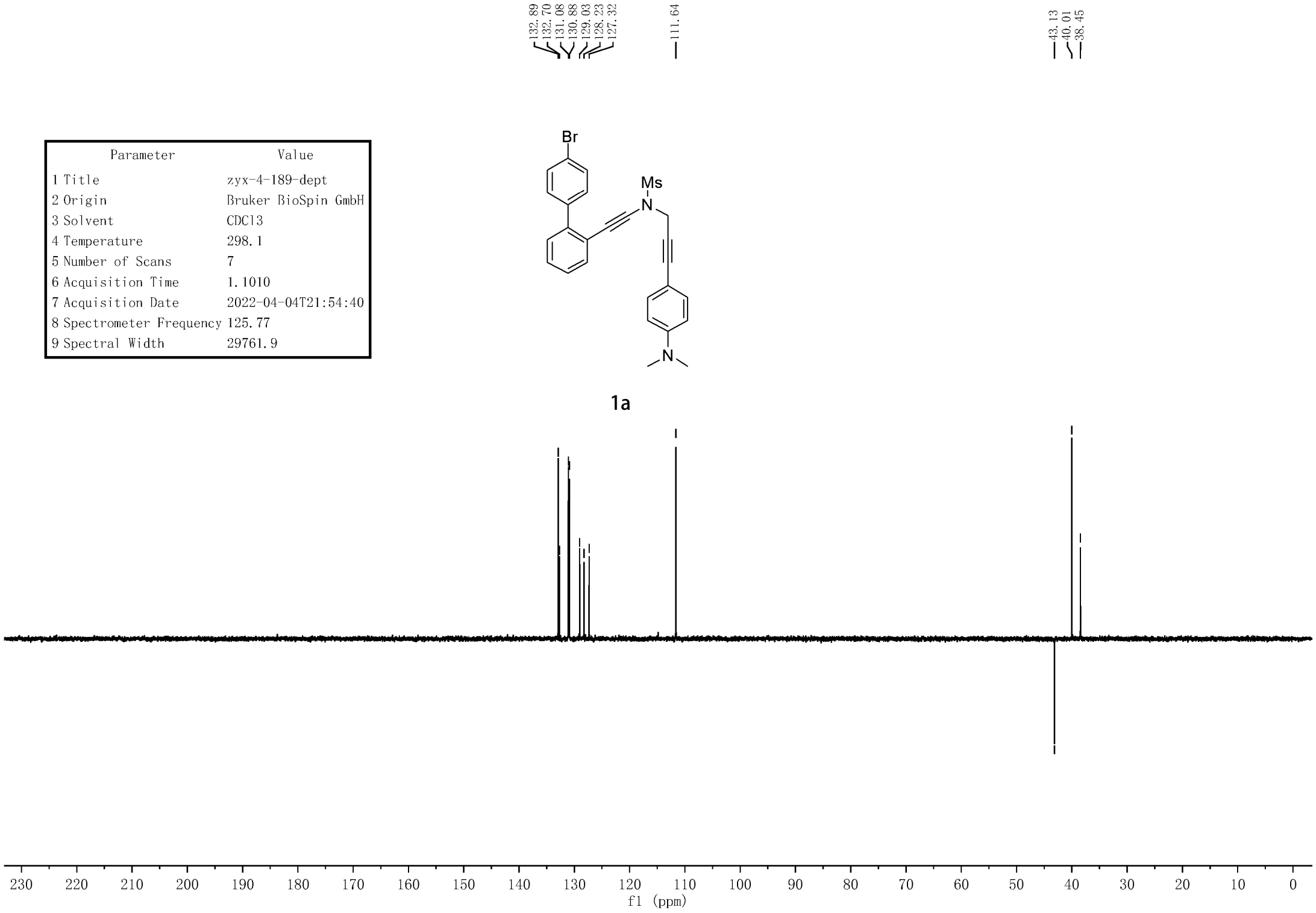
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.037	1.132	6.689	2.53	2.92	n.a.
2		7.055	43.540	222.663	97.47	97.08	n.a.
Total:			**44.672**	**229.352**	**100.00**	**100.00**	


7.544
7.529
7.340
7.296
7.275
7.257
6.604
6.586
4.460
2.974
2.949
0.000
Parameter Value
1 Title zyx-4-189-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.7
5 Number of Scans 12
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-04T21:51:40
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
Ms
N
N
1a
1.07
3.99
5.11
2.01
2.06
3.00
6.06
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)

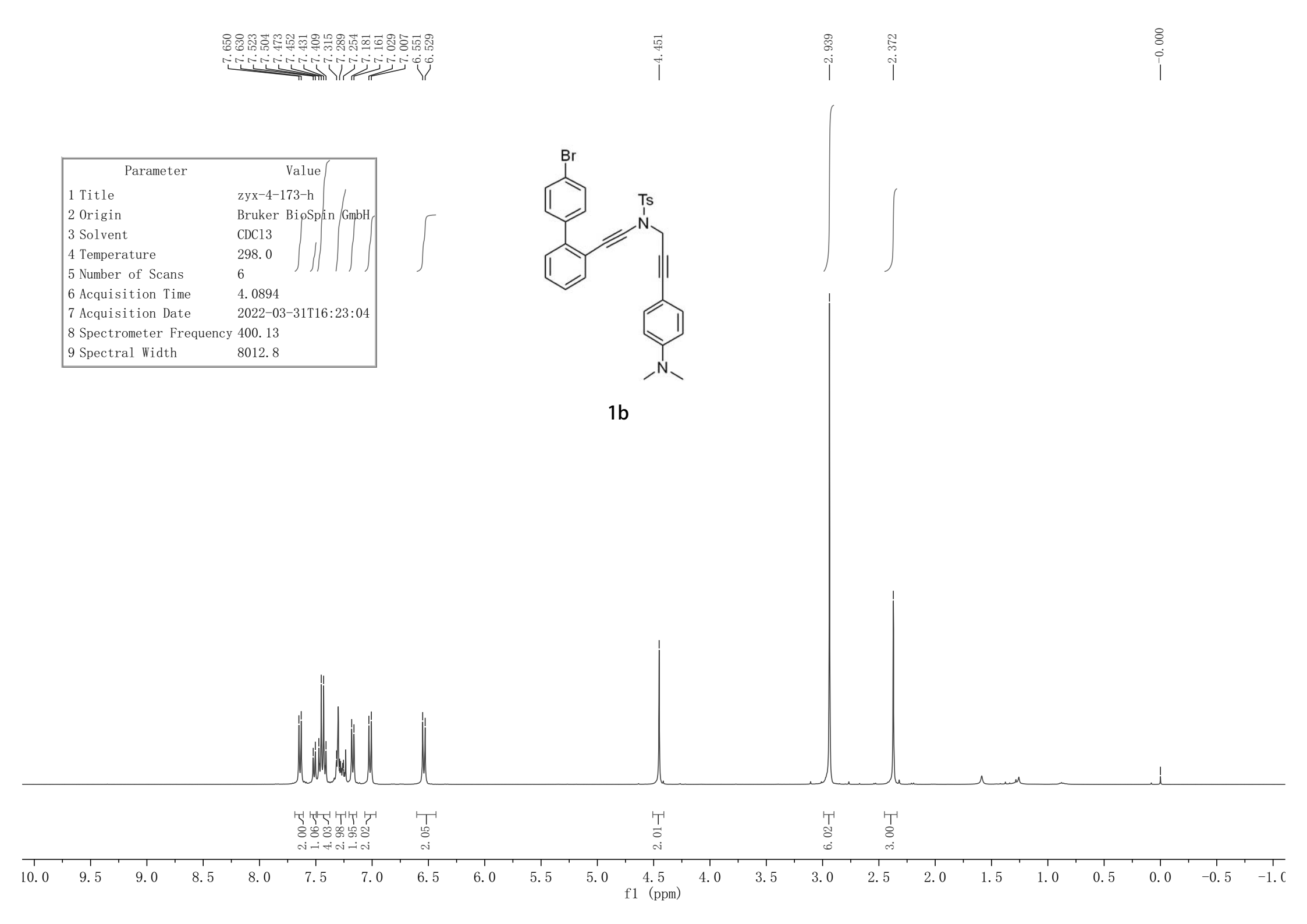
Parameter	Value
1 Title	zyx-4-189-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.9
5 Number of Scans	17
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-04T21:53:13
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

1a



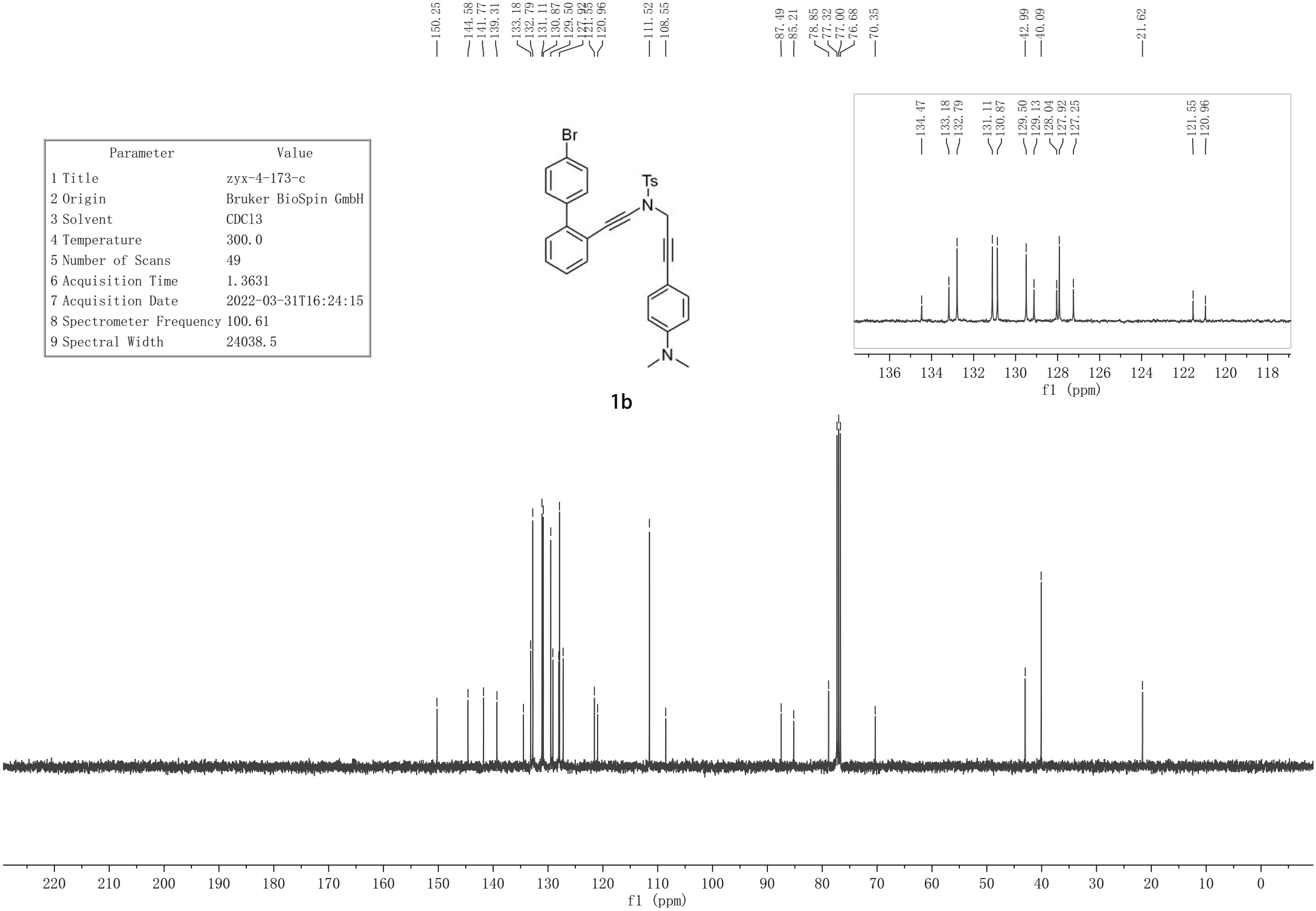


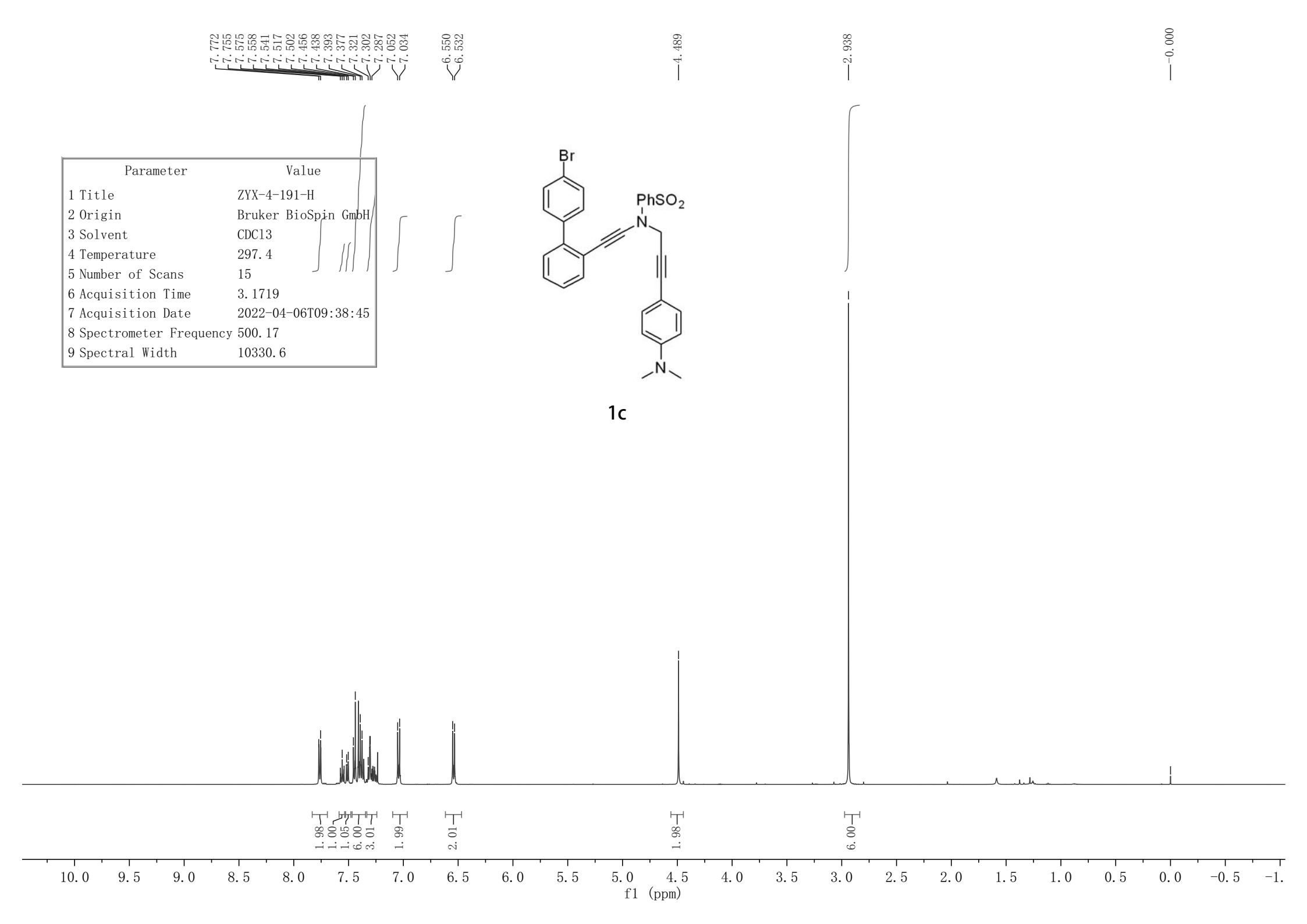
Parameter	Value
1 Title	zyx-4-189-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	7
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-04T21:54:40
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9


7.650
7.630
7.523
7.504
7.473
7.452
7.431
7.409
7.315
7.289
7.254
7.181
7.161
7.029
7.007
6.551
6.529
4.451
2.939
2.372
0.000
Parameter Value
1 Title zyx-4-173-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 6
6 Acquisition Time 4.0894
7 Acquisition Date 2022-03-31T16:23:04
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Br
Ts
N
N
1b
2.00
1.06
4.03
2.98
1.95
2.02
2.05
2.01
6.02
3.00
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
-1.0
f1 (ppm)

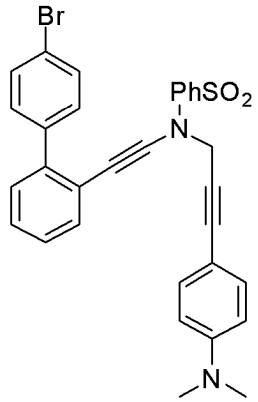
Parameter	Value
1 Title	zyx-4-173-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	49
6 Acquisition Time	1.3631
7 Acquisition Date	2022-03-31T16:24:15
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

1b

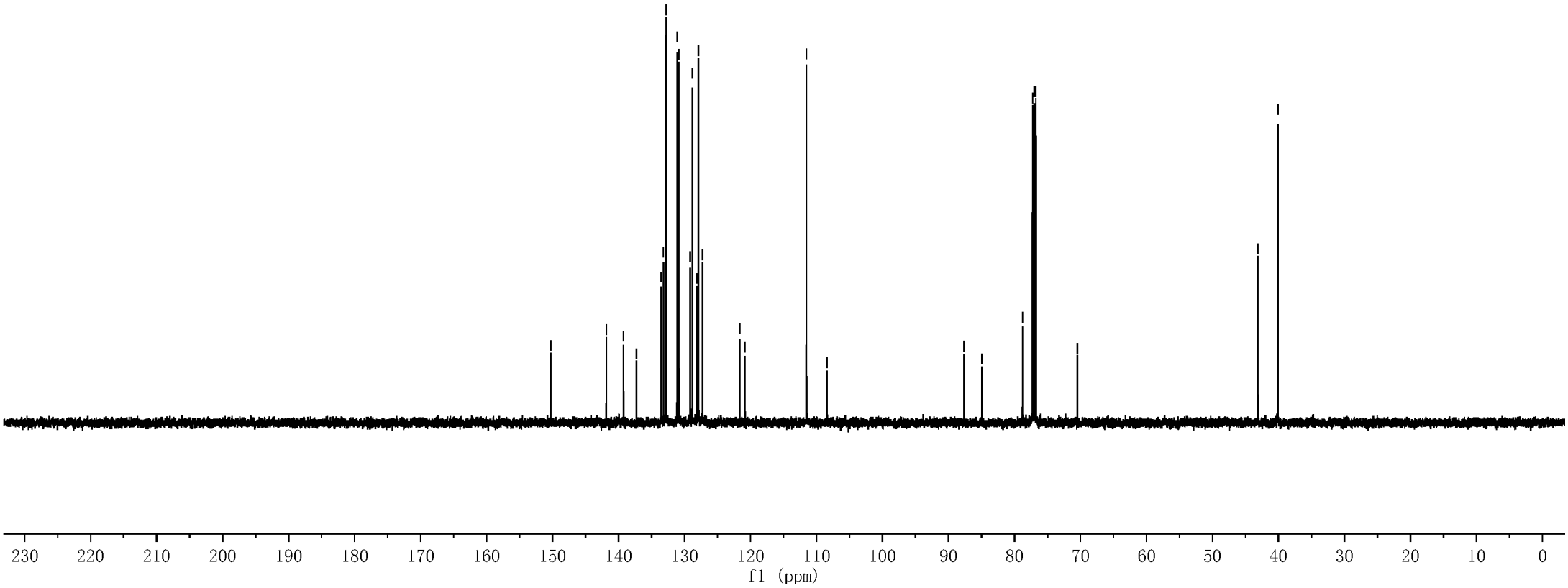


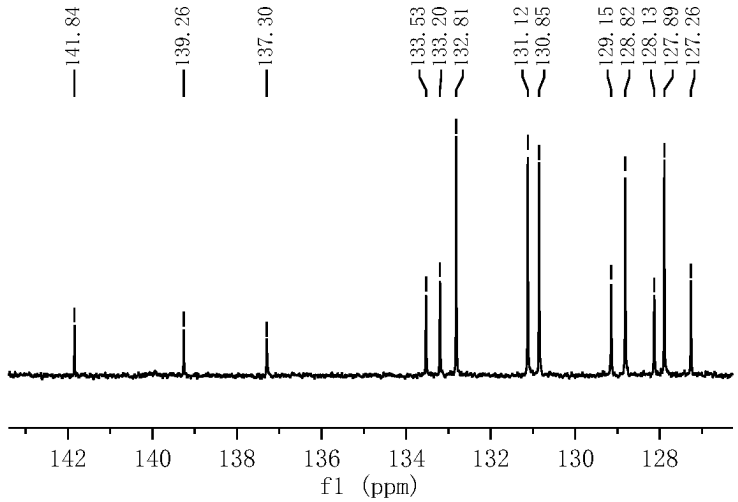

7.772
7.755
7.575
7.558
7.541
7.517
7.502
7.456
7.438
7.393
7.377
7.321
7.302
7.287
7.052
7.034
6.550
6.532
4.489
2.938
0.000
Parameter Value
1 Title ZYX-4-191-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.4
5 Number of Scans 15
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-06T09:38:45
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
PhSO2
N
N
1c
1.98
1.00
1.05
6.00
3.01
1.99
2.01
1.98
6.00
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
-1.
f1 (ppm)

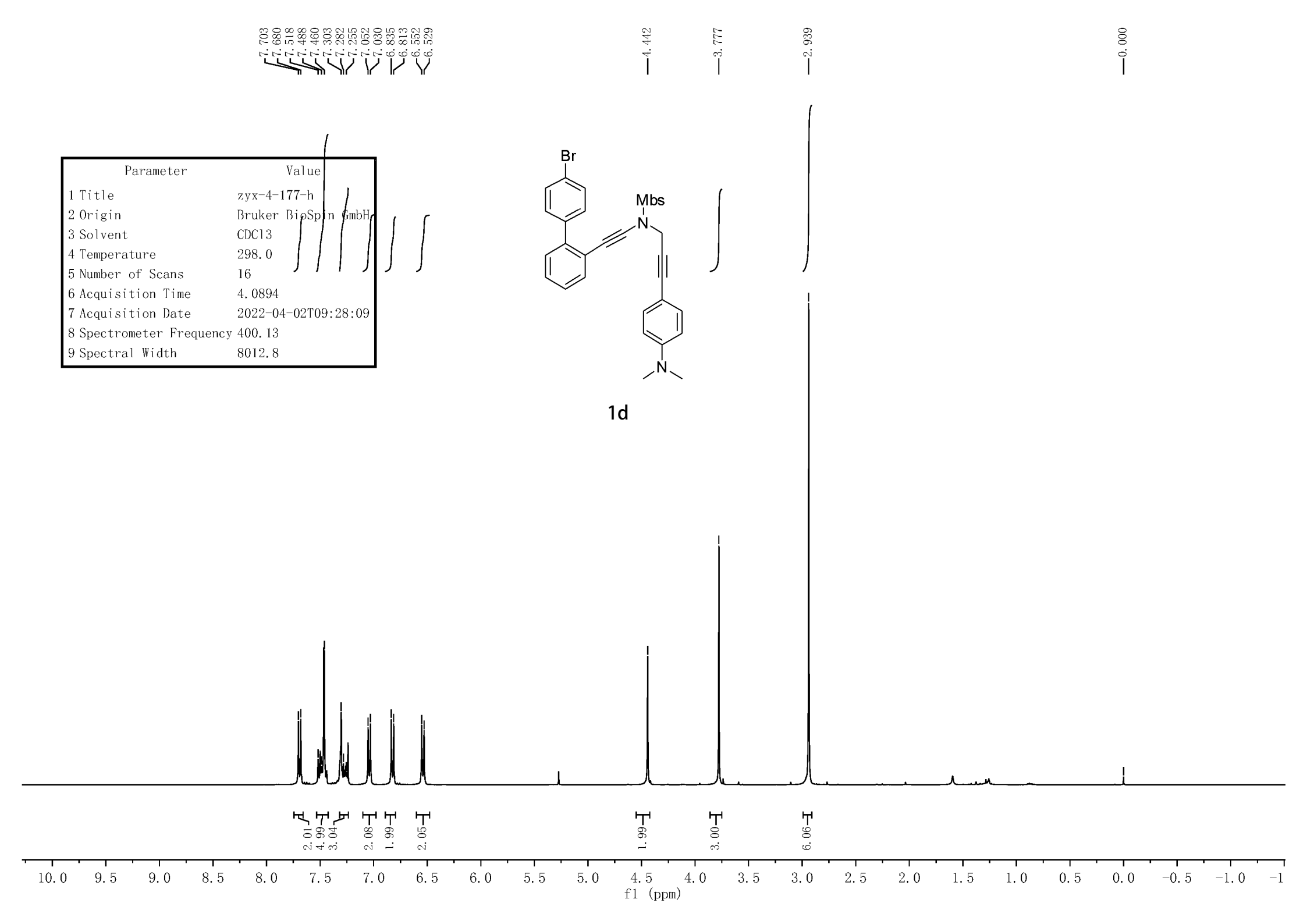
Parameter	Value
1 Title	ZYX-4-191-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	66
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-06T09:40:29
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9



1c

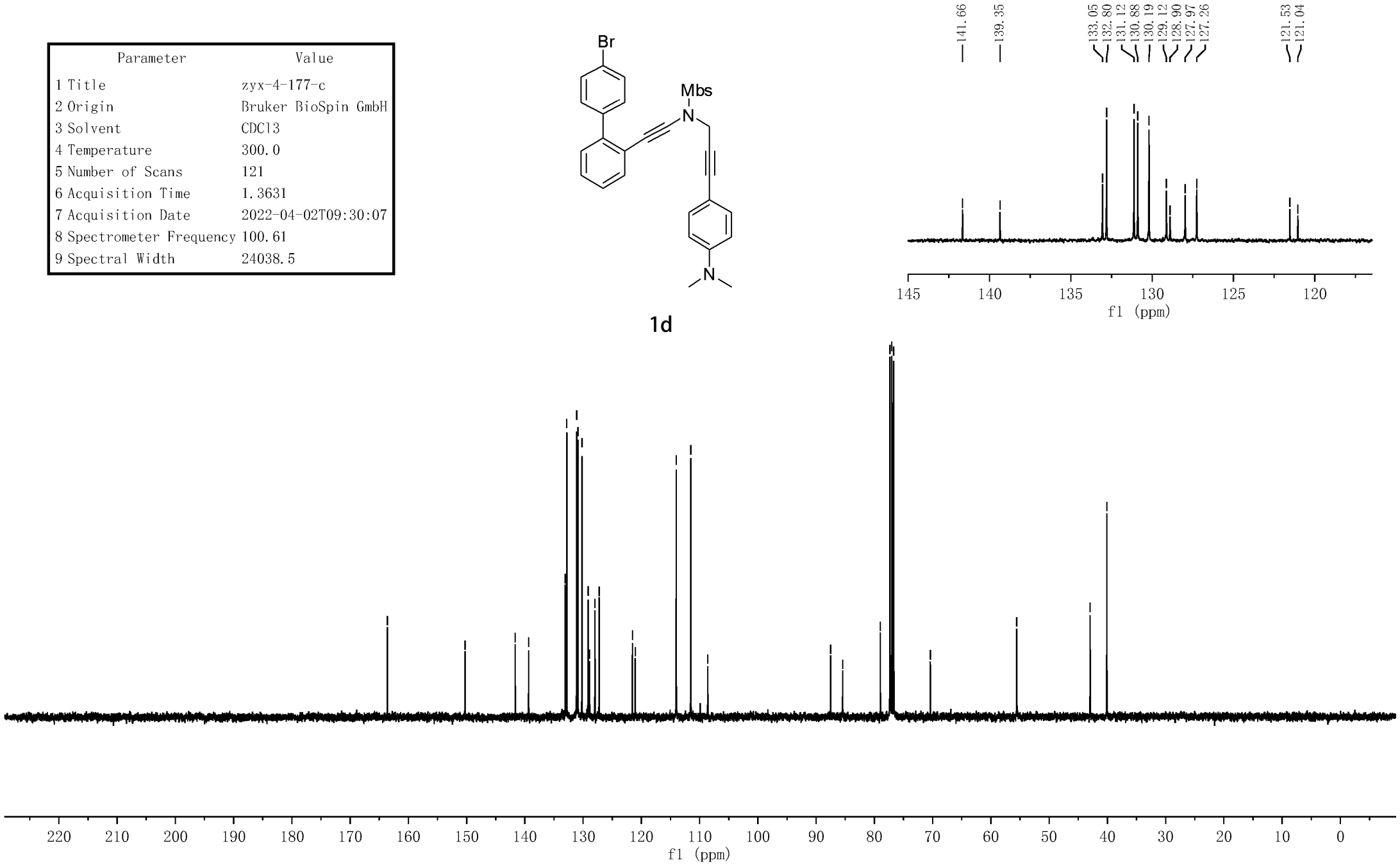


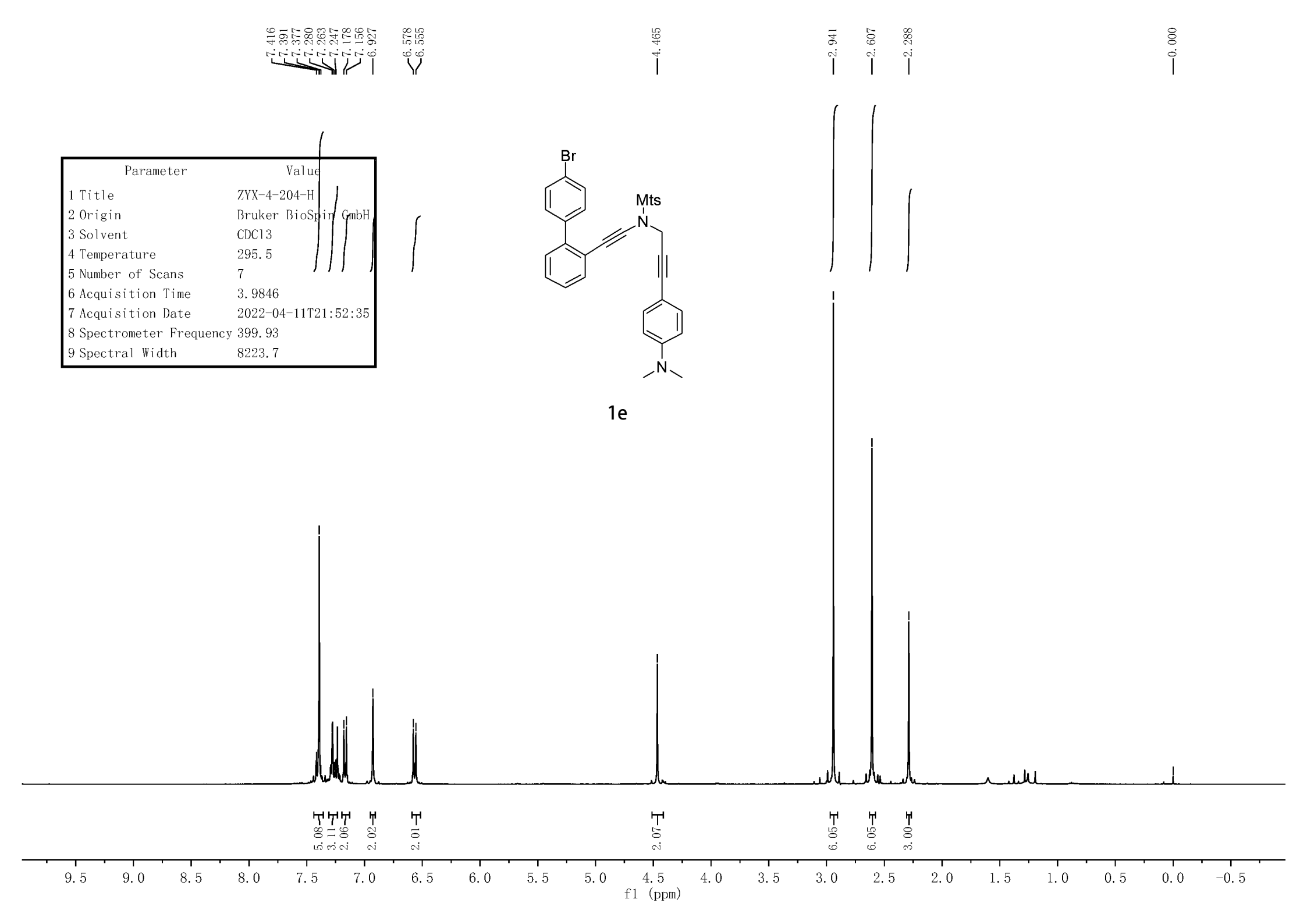



7.703
7.680
7.518
7.488
7.460
7.303
7.282
7.255
7.052
7.030
6.835
6.813
6.552
6.529
4.442
3.777
2.939
0.000
Parameter Value
1 Title zyx-4-177-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 16
6 Acquisition Time 4.0894
7 Acquisition Date 2022-04-02T09:28:09
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Br
Mbs
N
N
1d
2.01
4.99
3.04
2.08
1.99
2.05
1.99
3.00
6.06
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 -1.0 -1
f1 (ppm)

Parameter	Value
1 Title	zyx-4-177-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	121
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-02T09:30:07
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

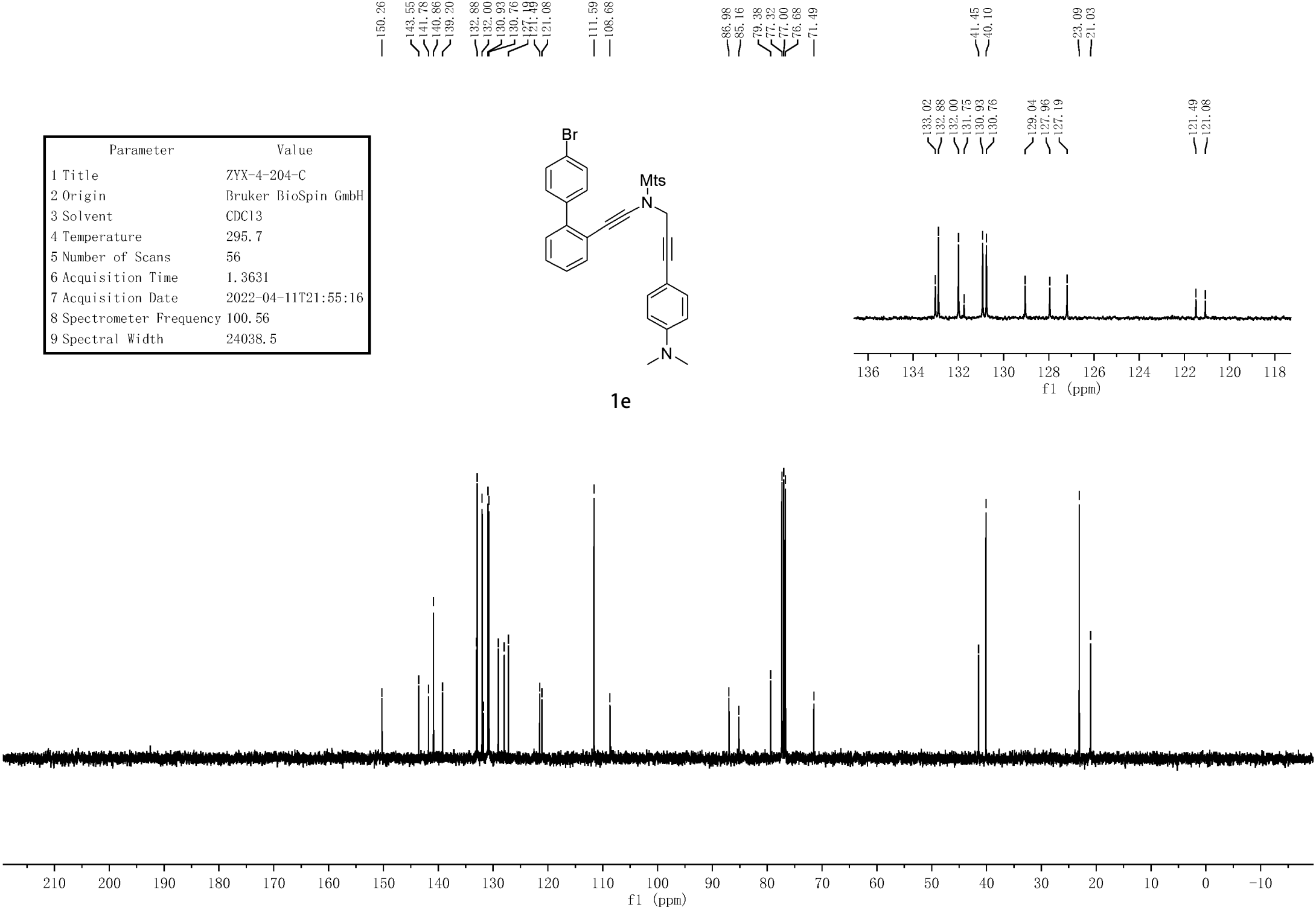
1d

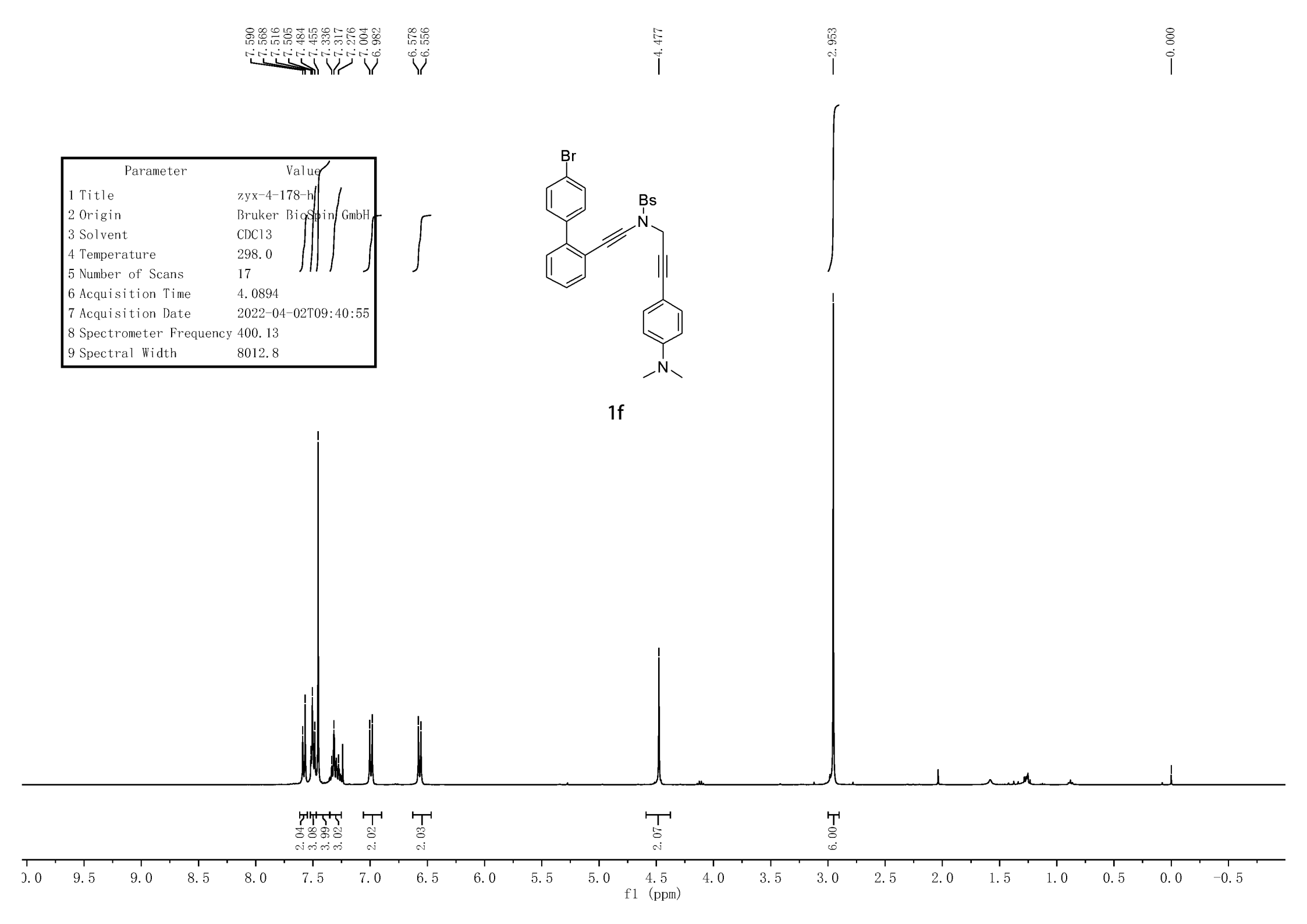



7.416
7.391
7.377
7.280
7.263
7.247
7.178
7.156
6.927
6.578
6.555
4.465
2.941
2.607
2.288
0.000
Parameter Value
1 Title ZYX-4-204-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.5
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-11T21:52:35
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Mts
N
N
1e
5.08
3.11
2.06
2.02
2.01
2.07
6.05
6.05
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)

Parameter	Value
1 Title	ZYX-4-204-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.7
5 Number of Scans	56
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-11T21:55:16
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

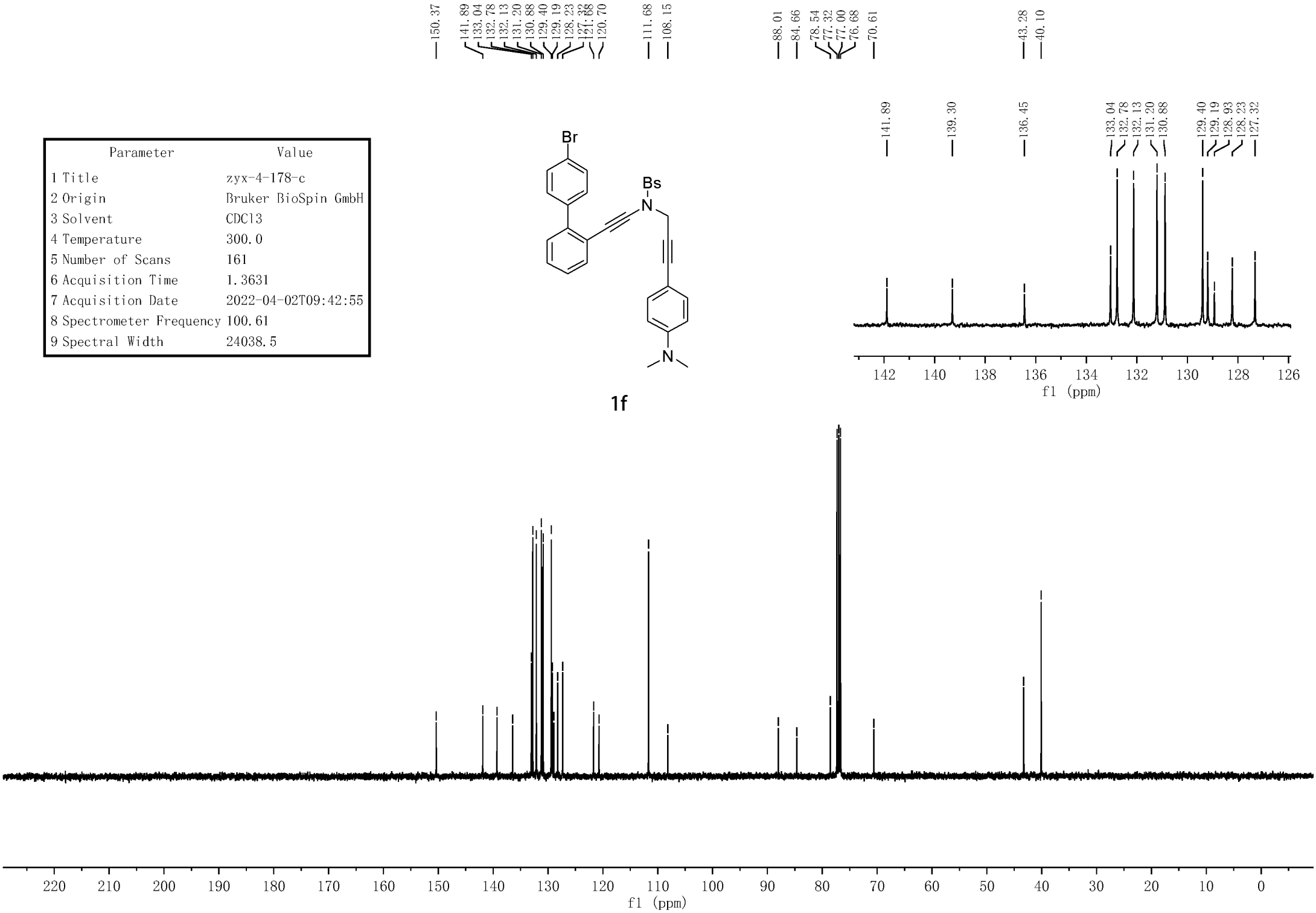
1e

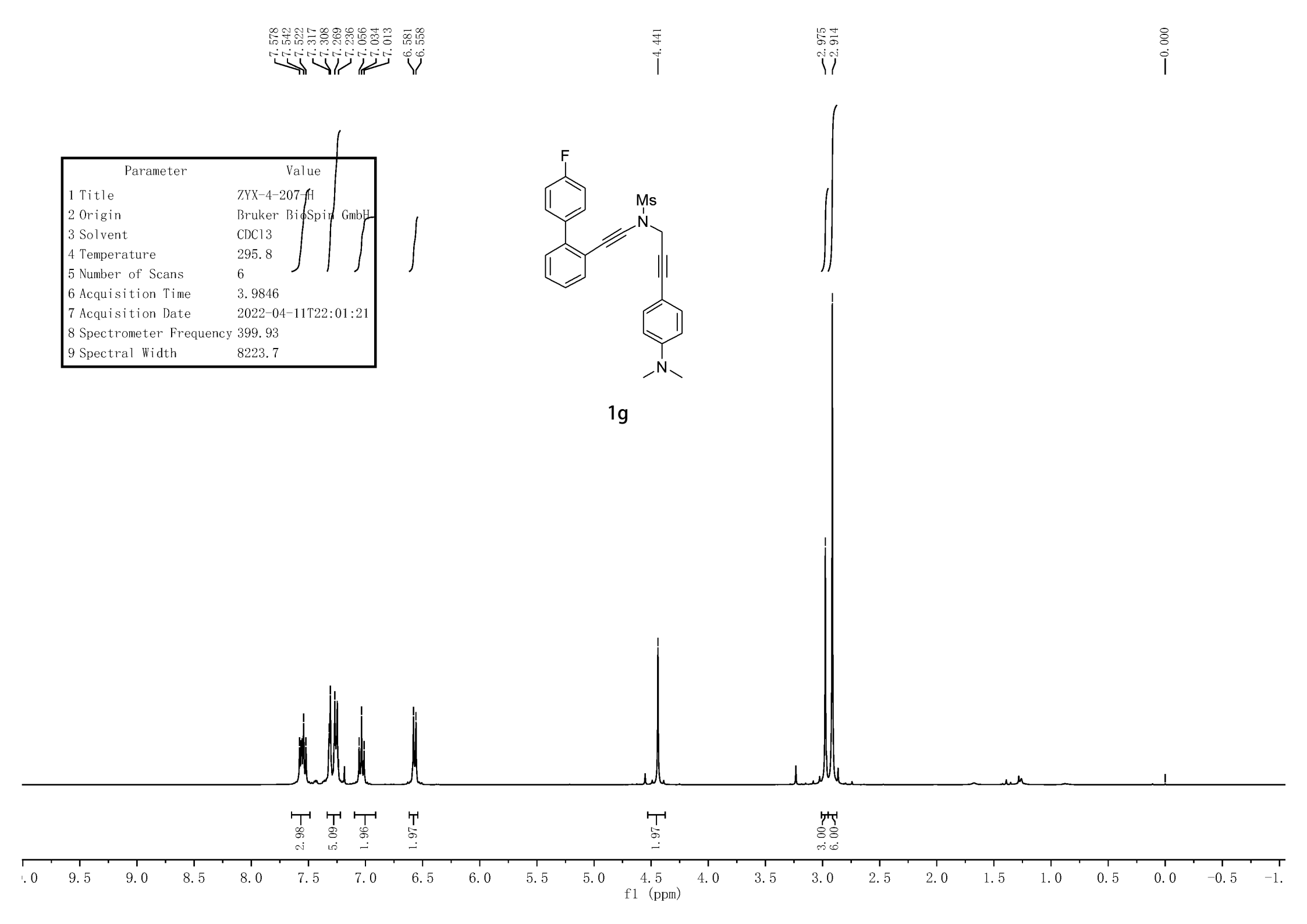



7.590
7.568
7.516
7.505
7.484
7.455
7.336
7.317
7.276
7.004
6.982
6.578
6.556
4.477
2.953
0.000
Parameter Value
1 Title zyx-4-178-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 17
6 Acquisition Time 4.0894
7 Acquisition Date 2022-04-02T09:40:55
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Br
Bs
N
N
1f
2.04
3.08
3.99
3.02
2.02
2.03
2.07
6.00
f1 (ppm)

Parameter	Value
1 Title	zyx-4-178-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	161
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-02T09:42:55
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

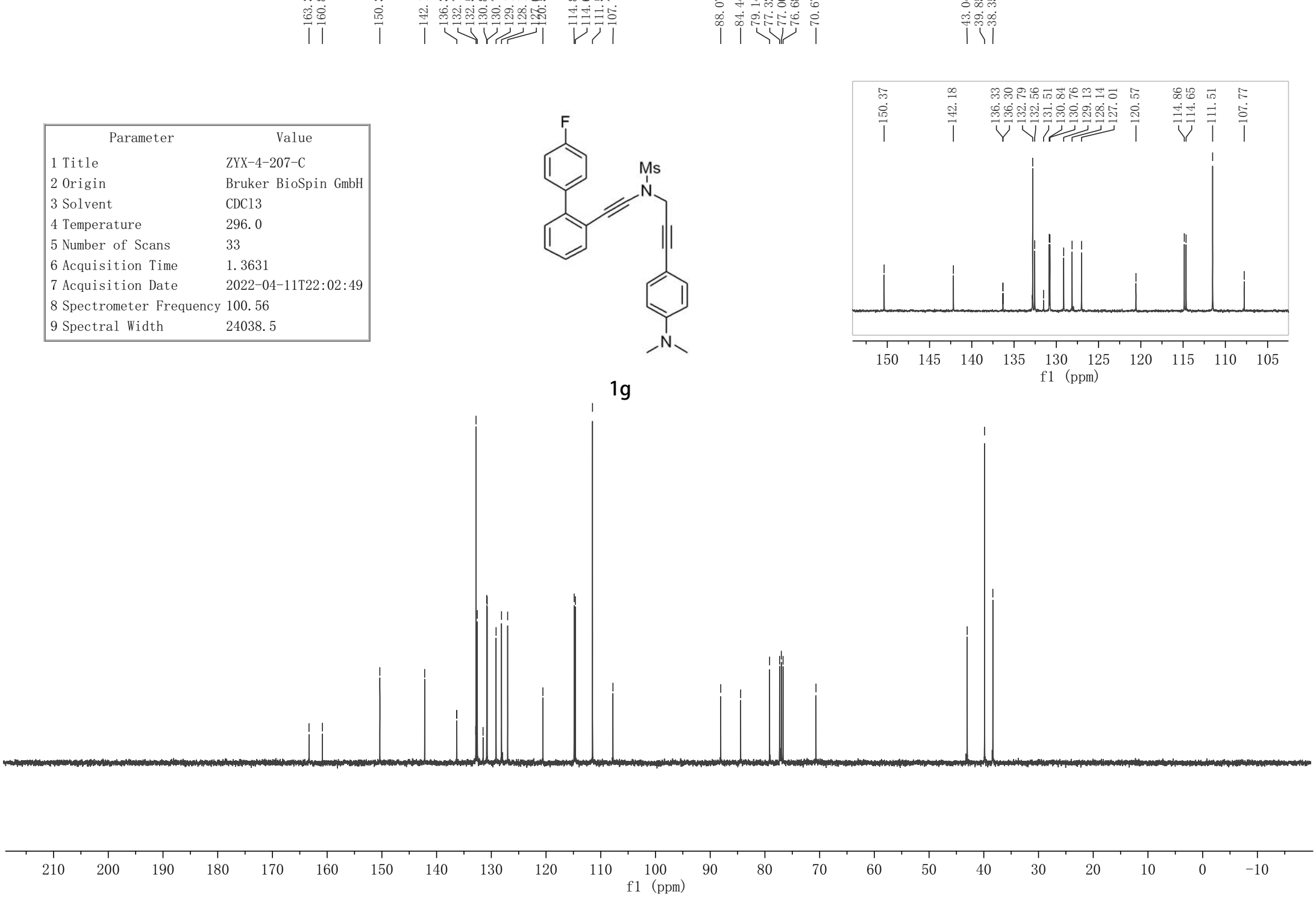
1f



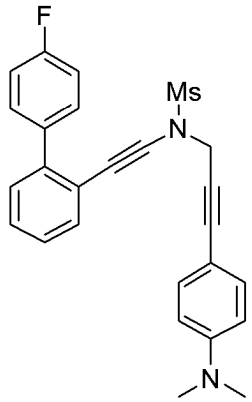

7.578
7.542
7.522
7.317
7.308
7.269
7.236
7.056
7.034
7.013
6.581
6.558
4.441
2.975
2.914
0.000
Parameter Value
1 Title ZYX-4-207-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.8
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-11T22:01:21
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
F
Ms
N
N
1g
2.98
5.09
1.96
1.97
1.97
3.00
6.00
f1 (ppm)

Parameter	Value
1 Title	ZYX-4-207-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.0
5 Number of Scans	33
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-11T22:02:49
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

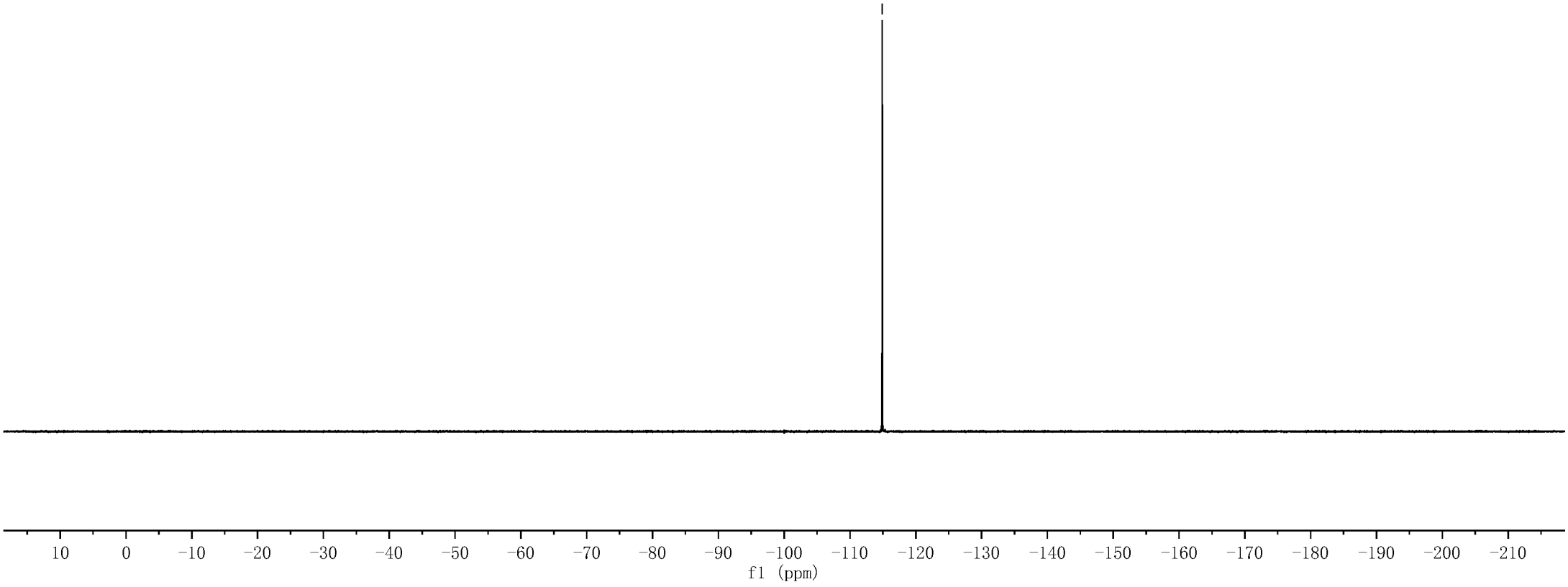
1g

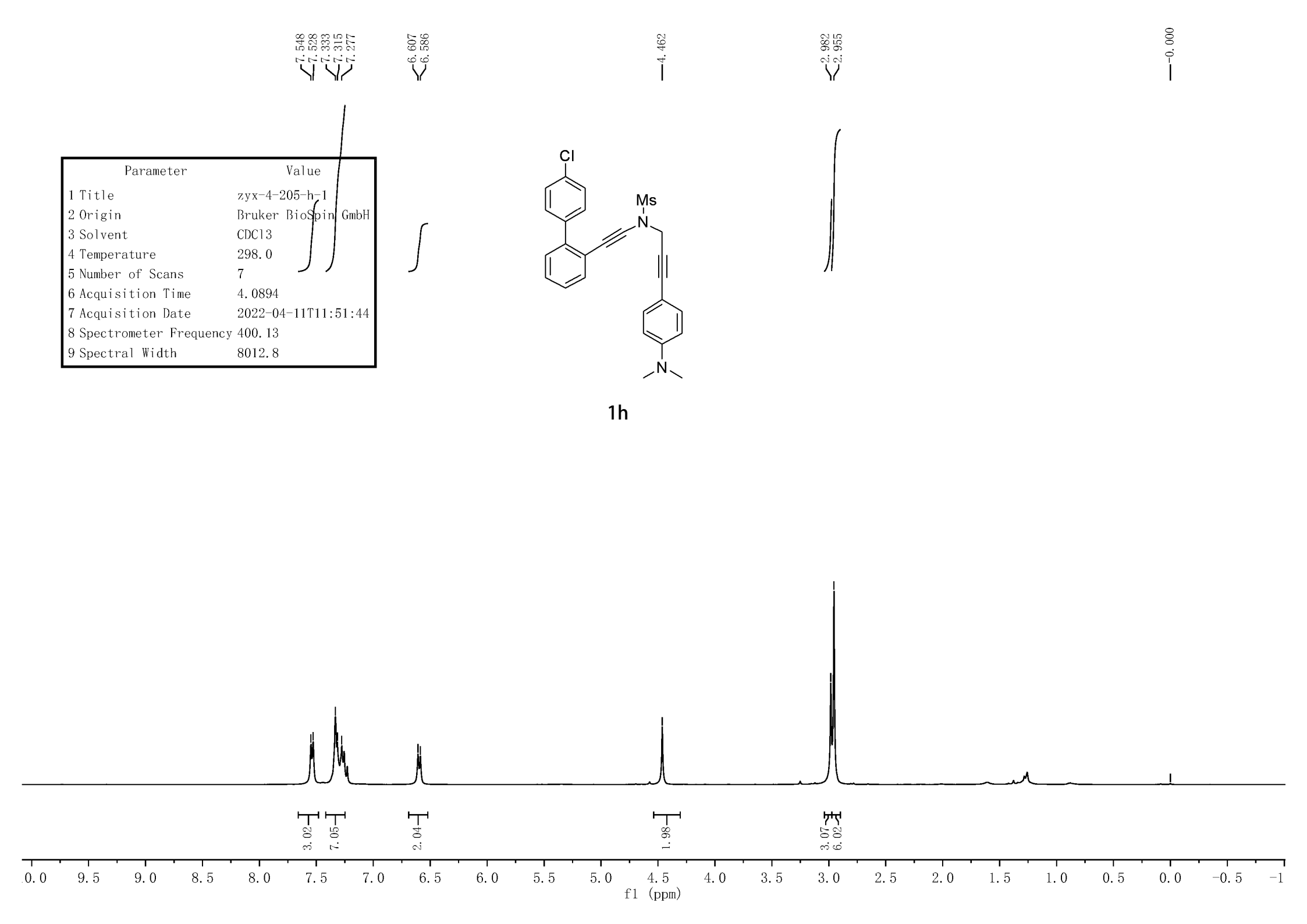


Parameter	Value
1 Title	ZYX-4-207-FF
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.2
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-08-30T09:26:27
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



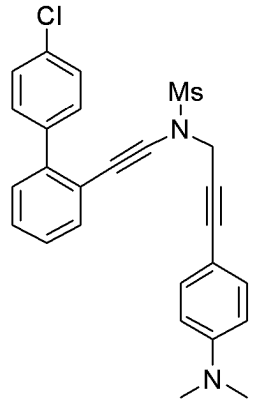
1g



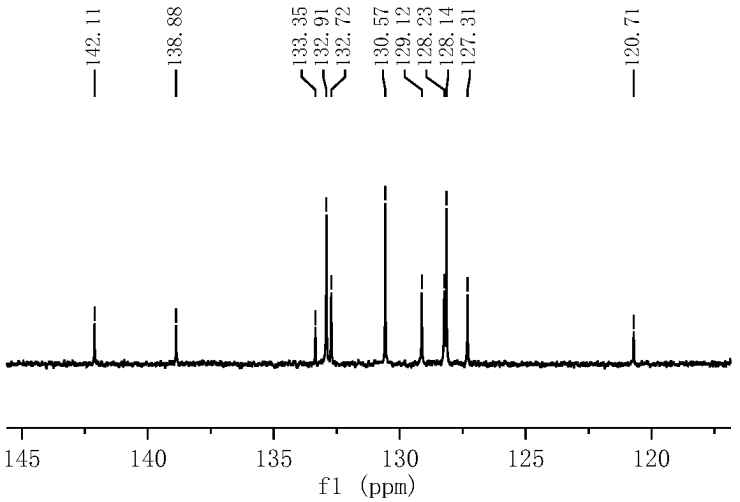

7.548
7.528
7.333
7.315
7.277
6.607
6.586
4.462
2.982
2.955
0.000
Parameter Value
1 Title zyx-4-205-h-1
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 7
6 Acquisition Time 4.0894
7 Acquisition Date 2022-04-11T11:51:44
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Cl
Ms
N
N
3.02
7.05
2.04
1.98
3.07
6.02
f1 (ppm)

1h

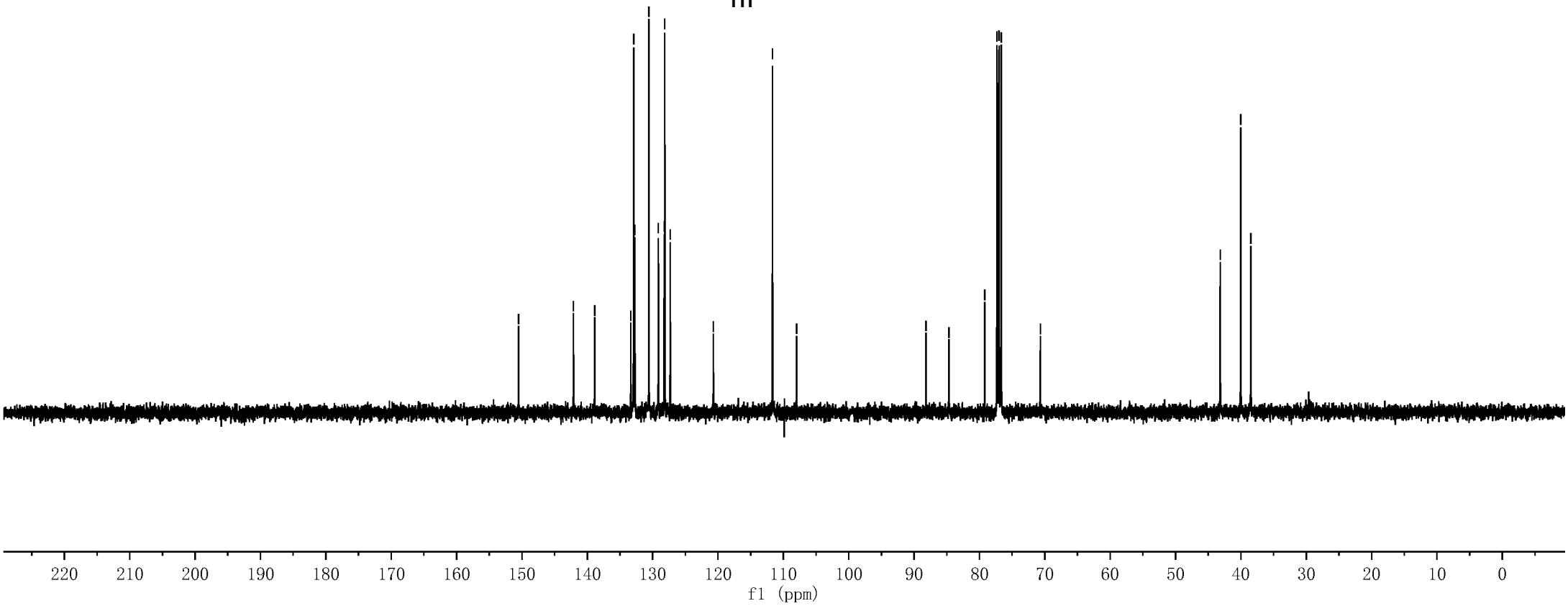
Parameter	Value
1 Title	zyx-4-205-c-1
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	44
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-11T11:52:57
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

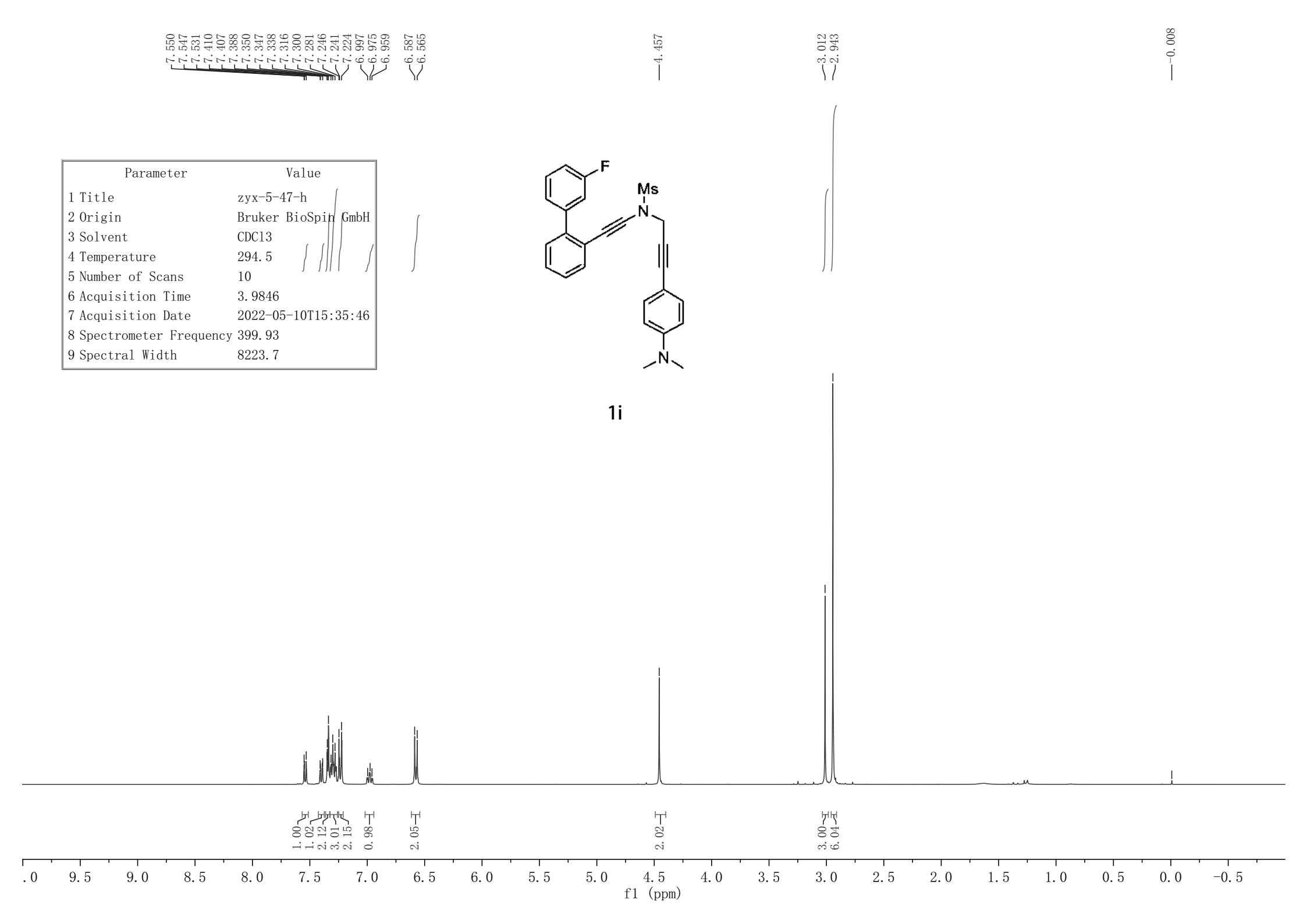


150.51
142.11
138.88
132.91
132.72
130.57
129.12
128.23
128.14
127.31
120.71
111.66
107.98
88.17
84.67
79.20
77.32
77.00
76.68
70.68
43.16
40.03
38.49



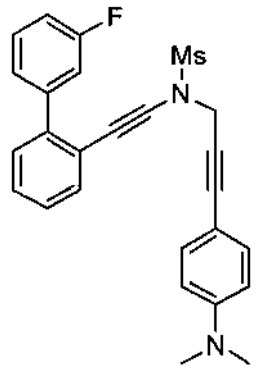
1h

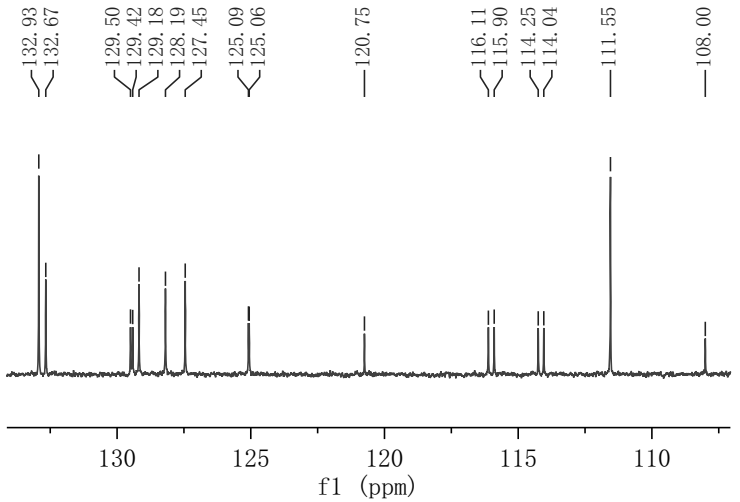



7.550
7.547
7.531
7.410
7.407
7.388
7.350
7.347
7.338
7.316
7.300
7.281
7.246
7.241
7.224
6.997
6.975
6.959
6.587
6.565
4.457
3.012
2.943
-0.008
Parameter Value
1 Title zyx-5-47-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 294.5
5 Number of Scans 10
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-10T15:35:46
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
F
Ms
N
N
1i
1.00
1.02
2.12
3.01
2.15
0.98
2.05
2.02
3.00
6.04
f1 (ppm)

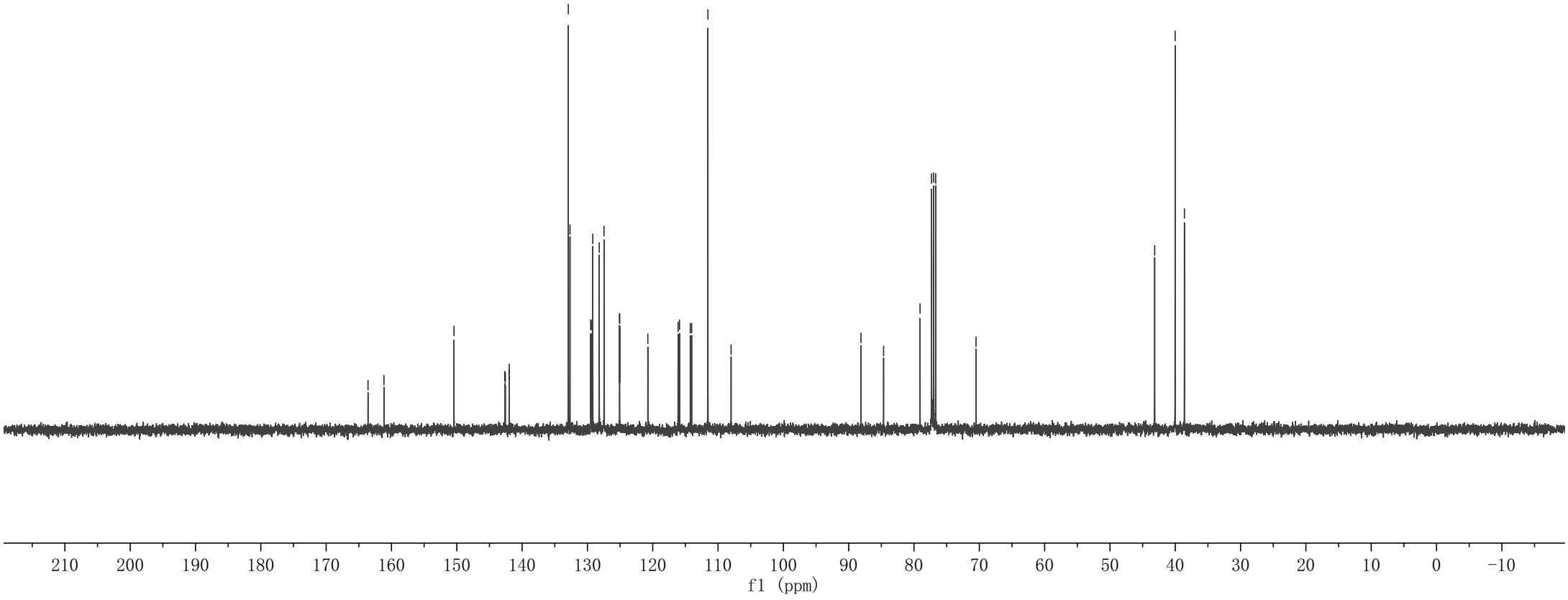
163.59
161.15
150.43
142.65
142.57
141.98
141.96
132.93
132.67
129.50
129.42
129.18
128.19
127.45
125.09
125.06
120.75
116.11
115.90
114.25
114.04
111.55
108.00
88.12
84.66
79.07
77.32
77.00
76.68
70.51
43.15
40.02
38.60

Parameter	Value
1 Title	zyx-5-47-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	294.8
5 Number of Scans	52
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-10T15:37:09
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

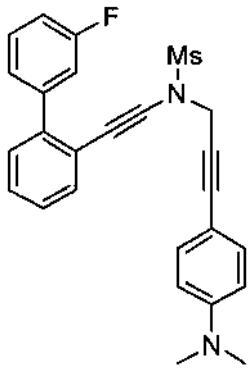




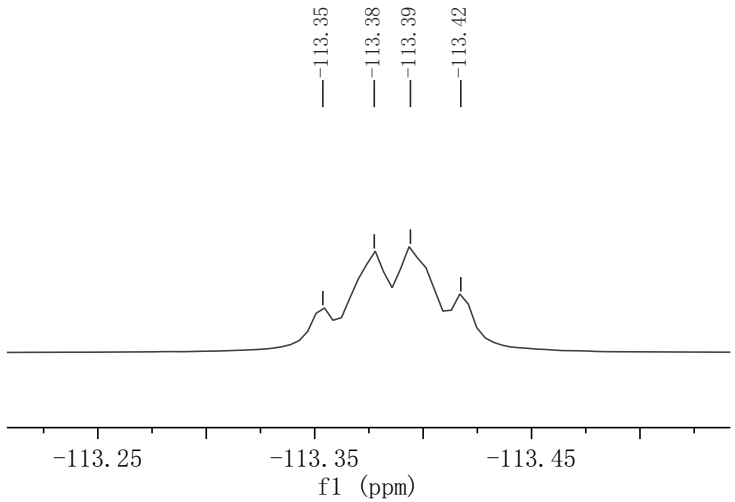
1i

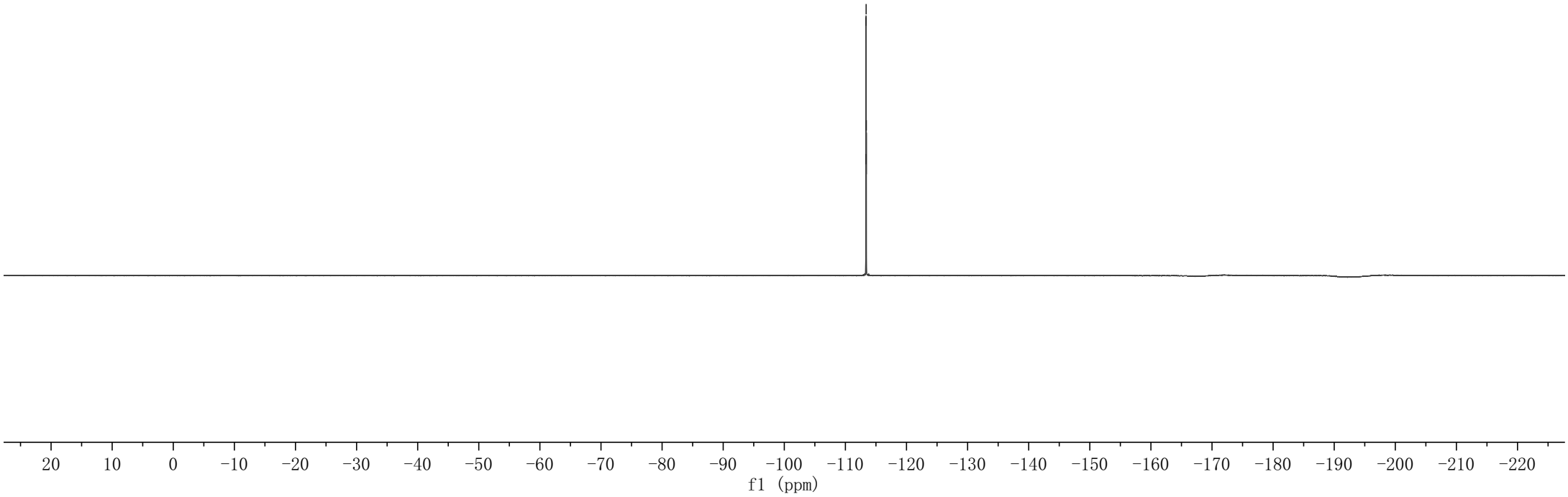


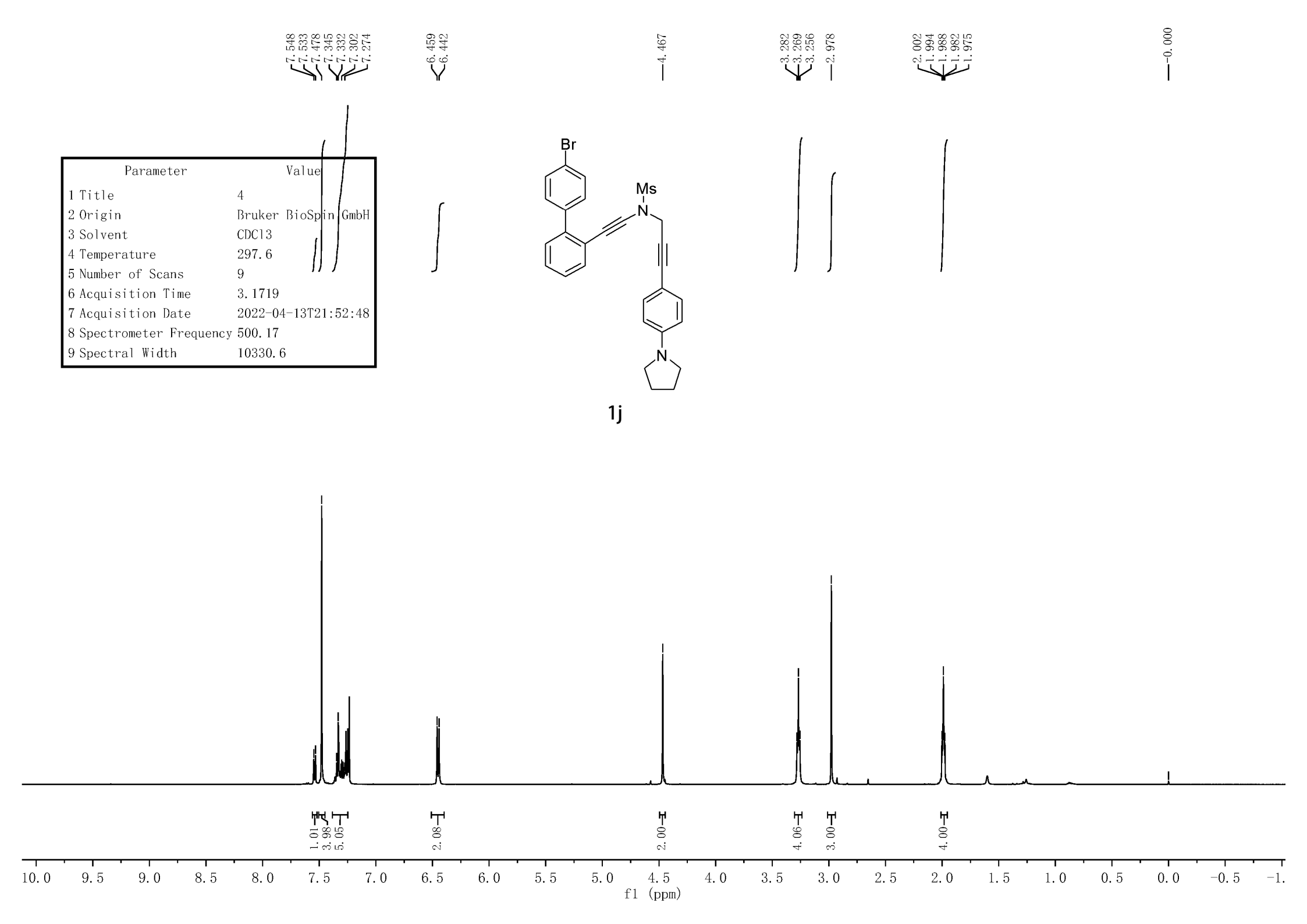
Parameter	Value
1 Title	zyx-11-74-s-f
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.5
5 Number of Scans	16
6 Acquisition Time	1.0000
7 Acquisition Date	2023-11-21T17:21:37
8 Spectrometer Frequency	376.28
9 Spectral Width	96153.0



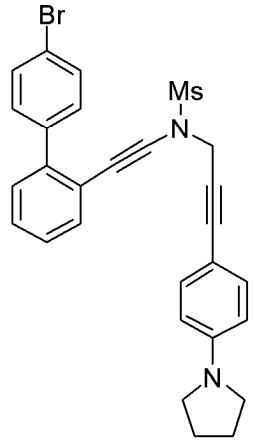
1i



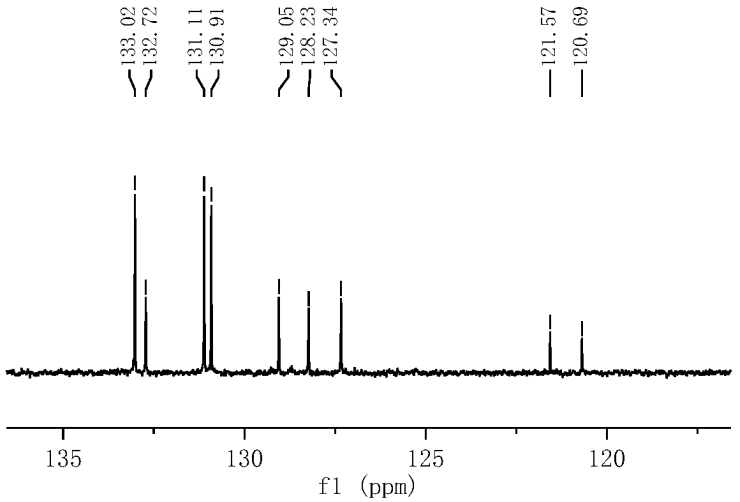


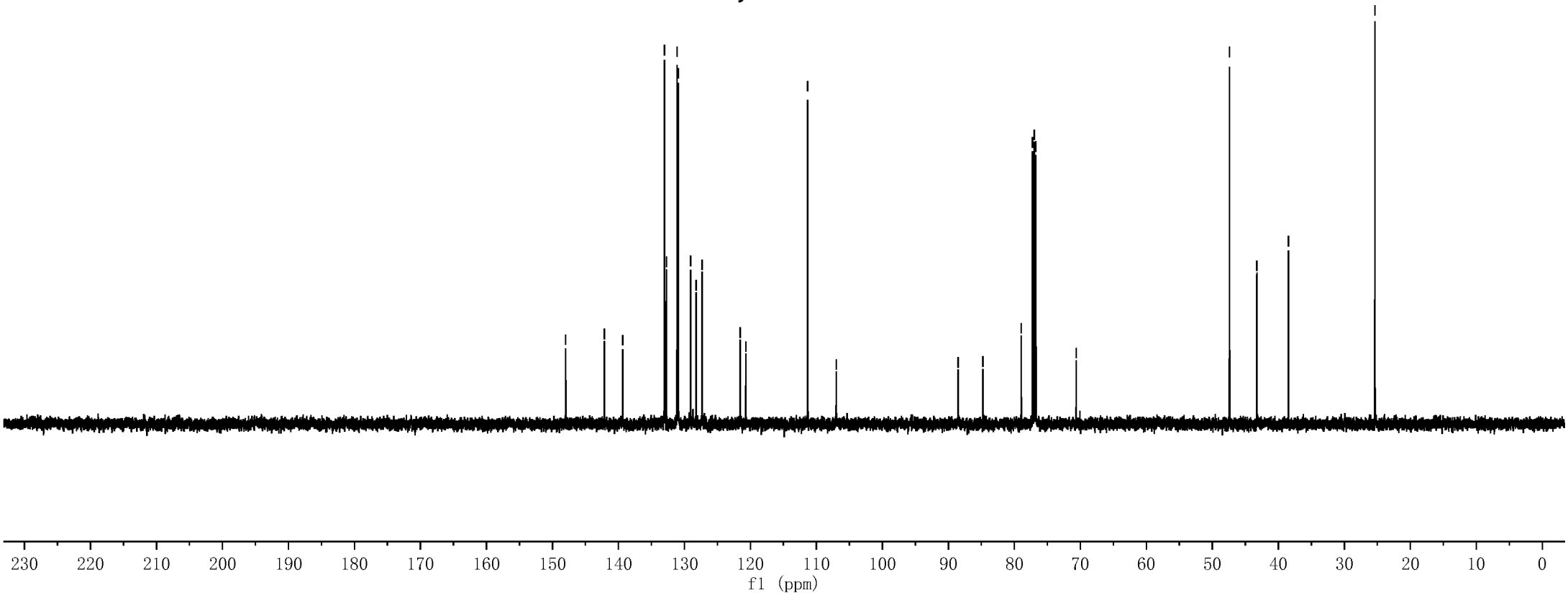

7.548
7.533
7.478
7.345
7.332
7.302
7.274
6.459
6.442
4.467
3.282
3.269
3.256
2.978
2.002
1.994
1.988
1.982
1.975
0.000
Parameter Value
1 Title 4
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.6
5 Number of Scans 9
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-13T21:52:48
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
Ms
N
N
1j
1.01
3.98
5.05
2.08
2.00
4.06
3.00
4.00
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
-1.
f1 (ppm)

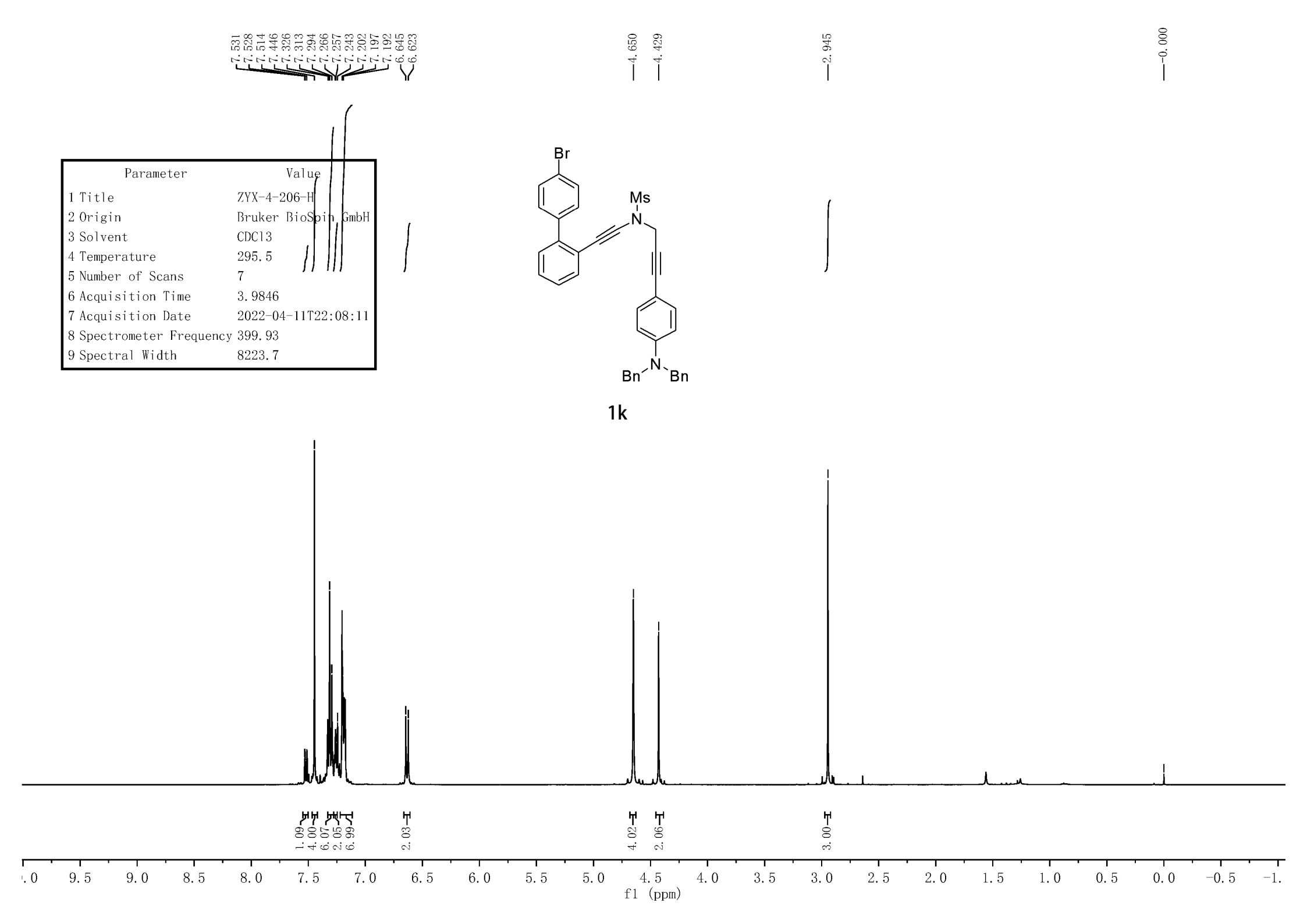
Parameter	Value
1 Title	zyx-4-213-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.7
5 Number of Scans	28
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-13T21:53:59
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9



1j

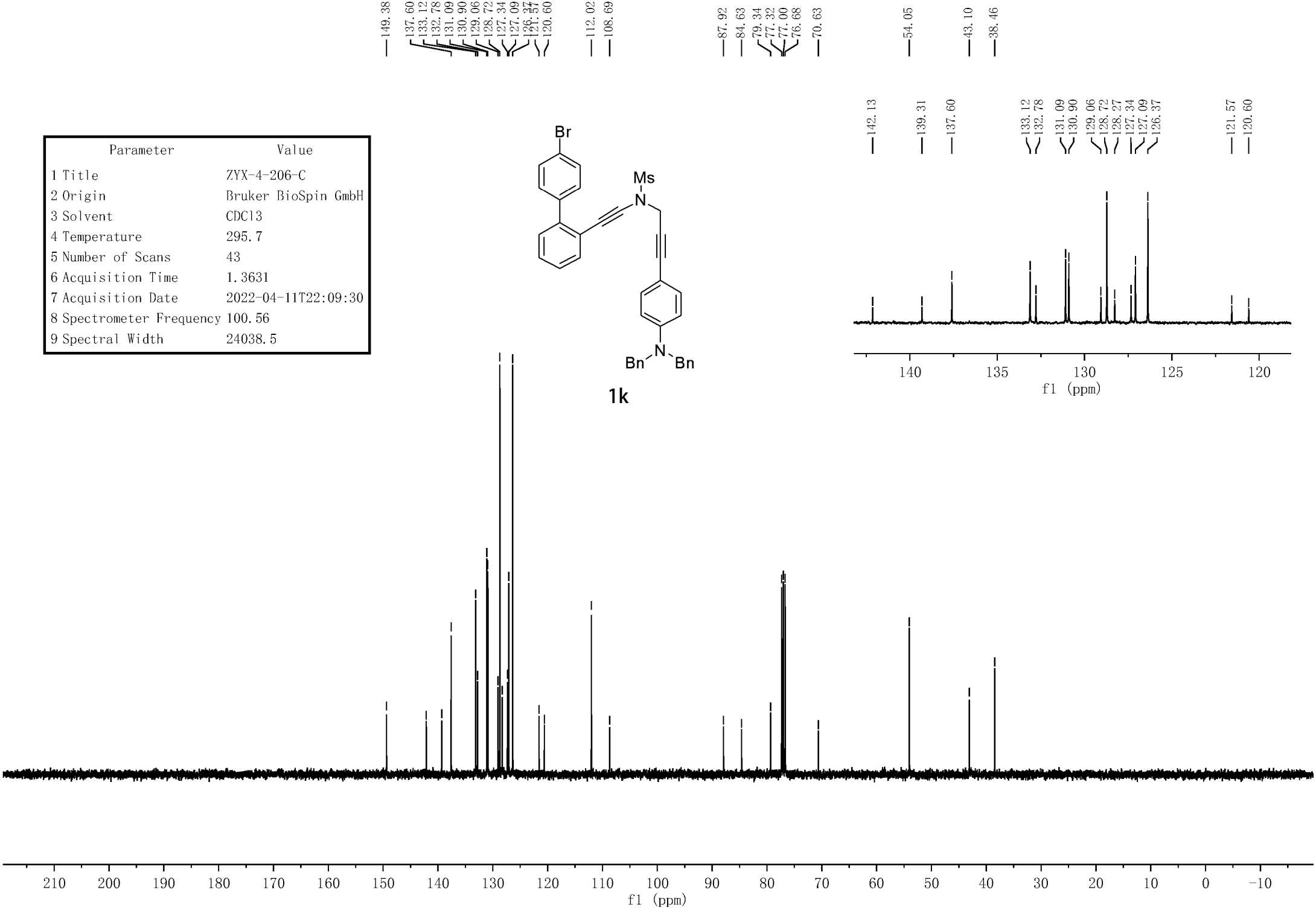


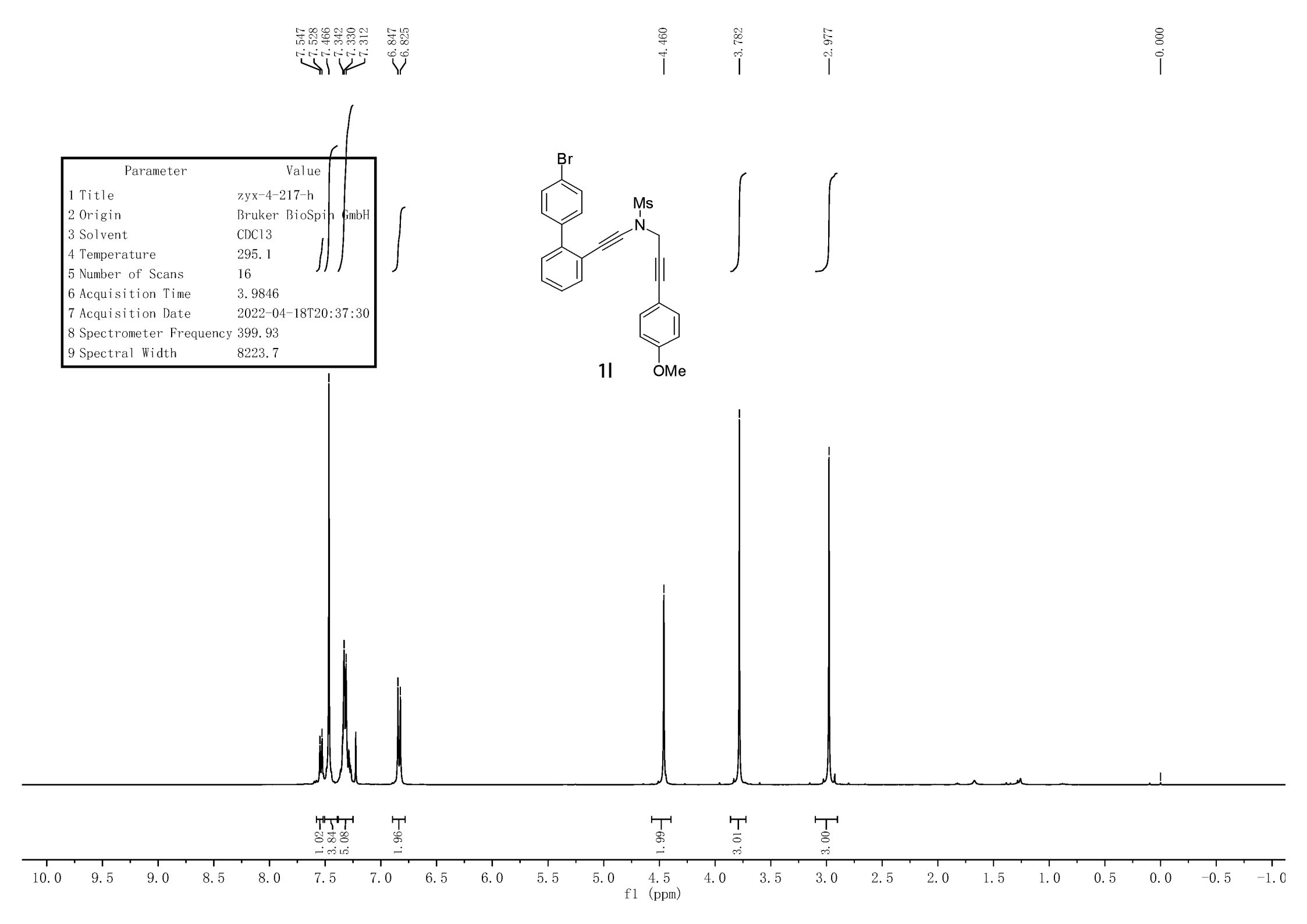



7.531
7.528
7.514
7.446
7.326
7.313
7.294
7.266
7.257
7.243
7.202
7.197
7.192
6.645
6.623
4.650
4.429
2.945
-0.000
Parameter Value
1 Title ZYX-4-206-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.5
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-11T22:08:11
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
N
Bn
Bn
1k
1.09
4.00
6.07
2.05
6.99
2.03
4.02
2.06
3.00
f1 (ppm)

Parameter	Value
1 Title	ZYX-4-206-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.7
5 Number of Scans	43
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-11T22:09:30
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

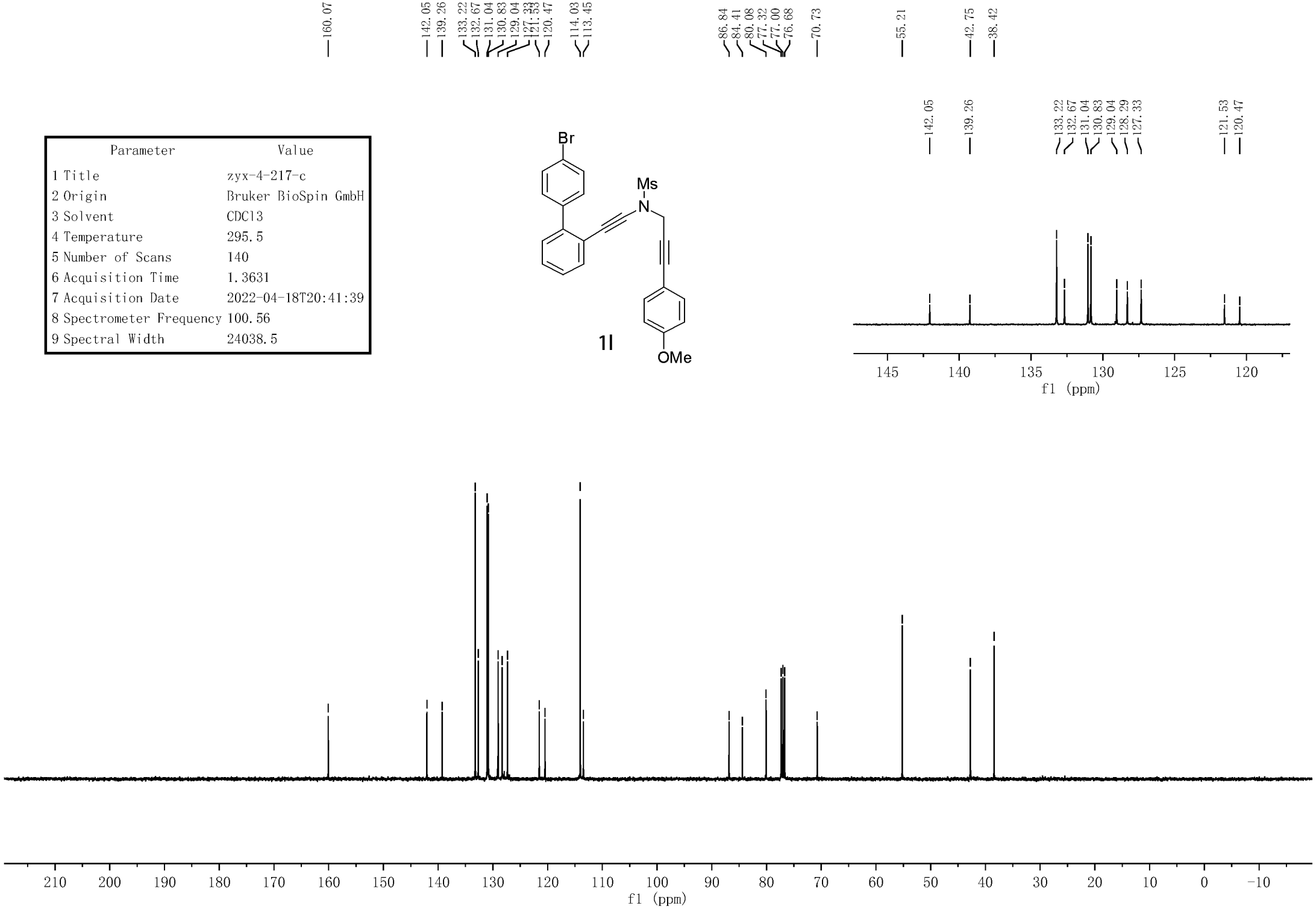
1k

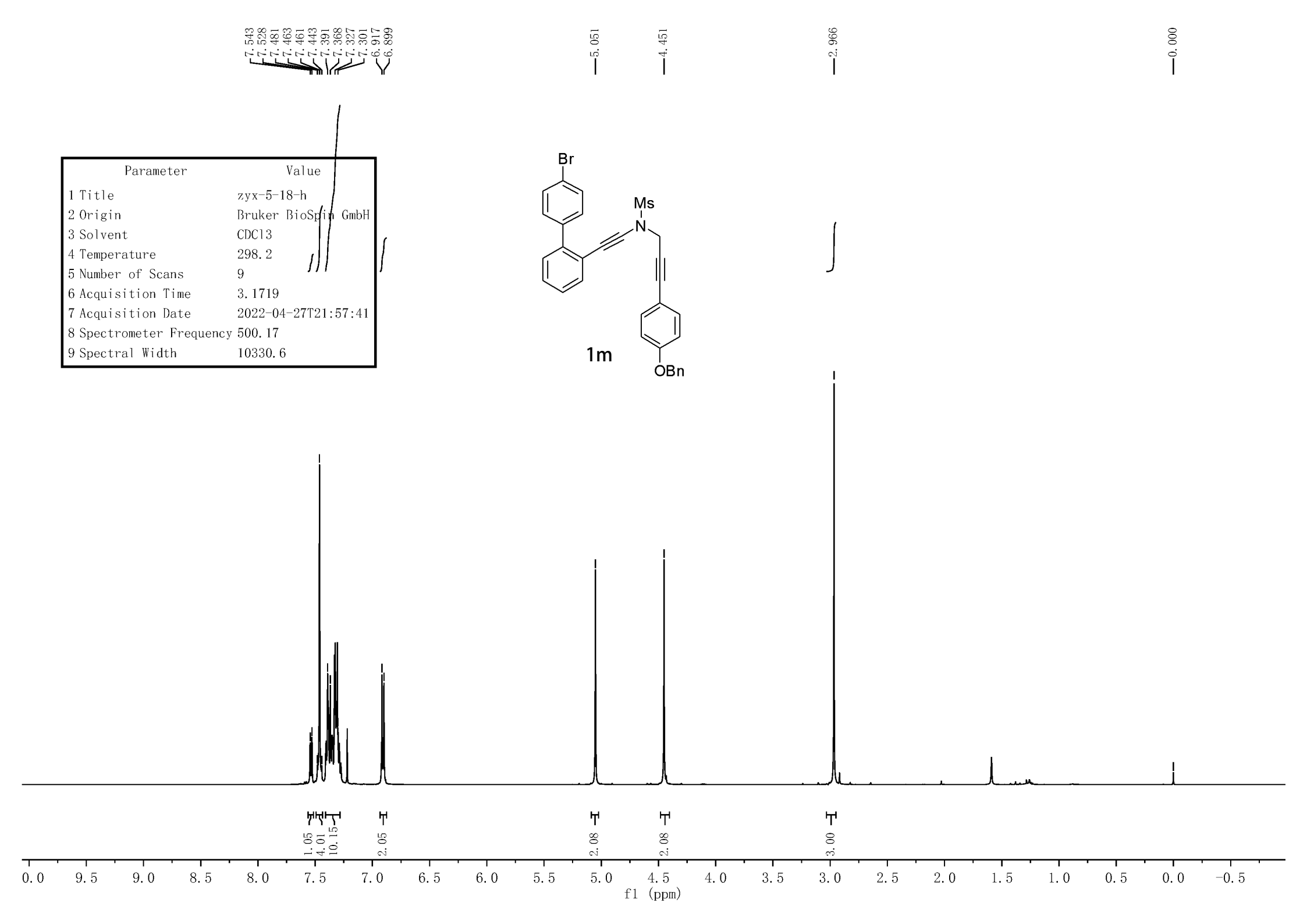



7.547
7.528
7.466
7.342
7.330
7.312
6.847
6.825
4.460
3.782
2.977
0.000
Parameter Value
1 Title zyx-4-217-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.1
5 Number of Scans 16
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-18T20:37:30
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
OMe
1l
1.02
3.84
5.08
1.96
1.99
3.01
3.00
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
-1.0
f1 (ppm)

Parameter	Value
1 Title	zyx-4-217-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	140
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-18T20:41:39
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

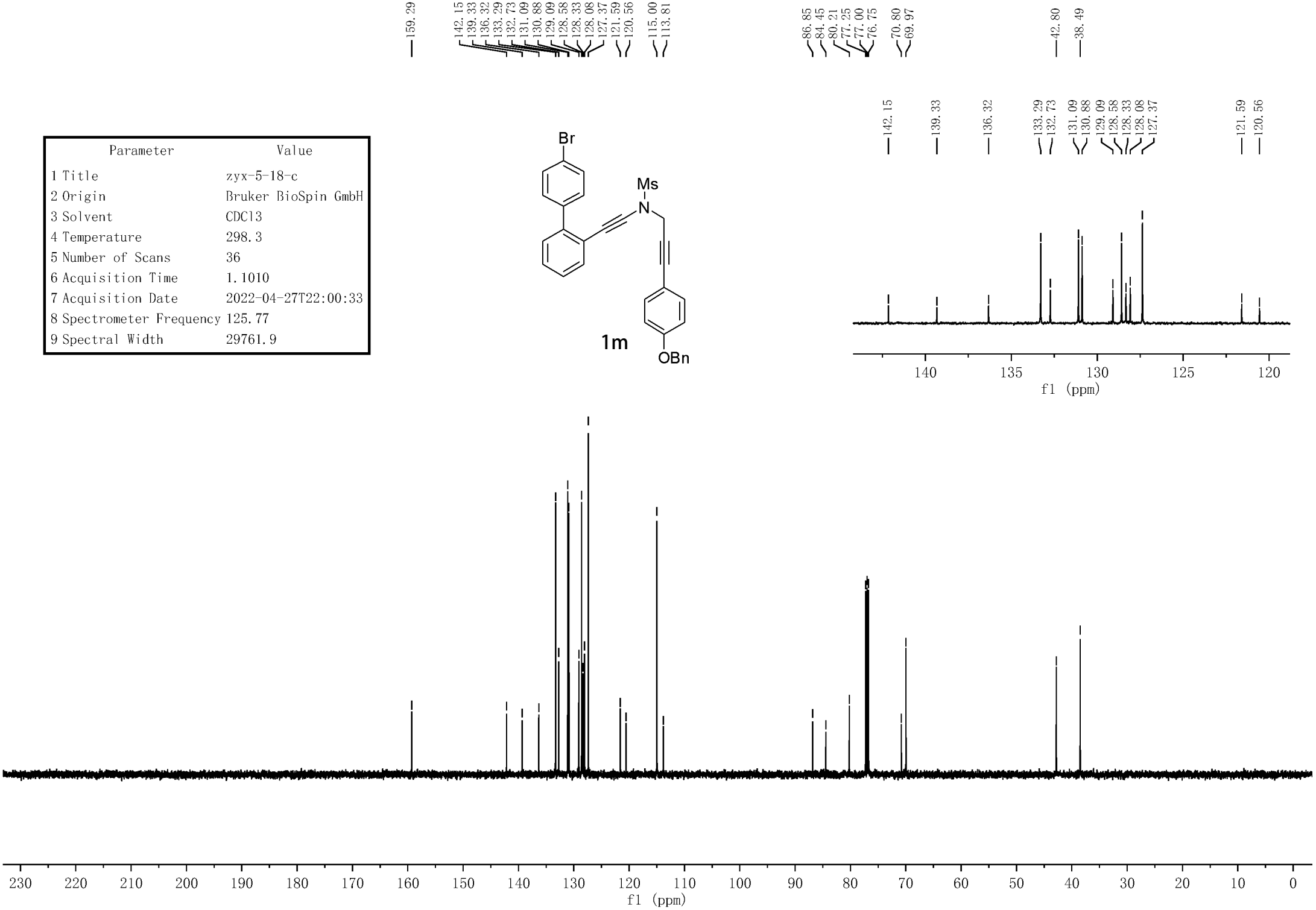
1l

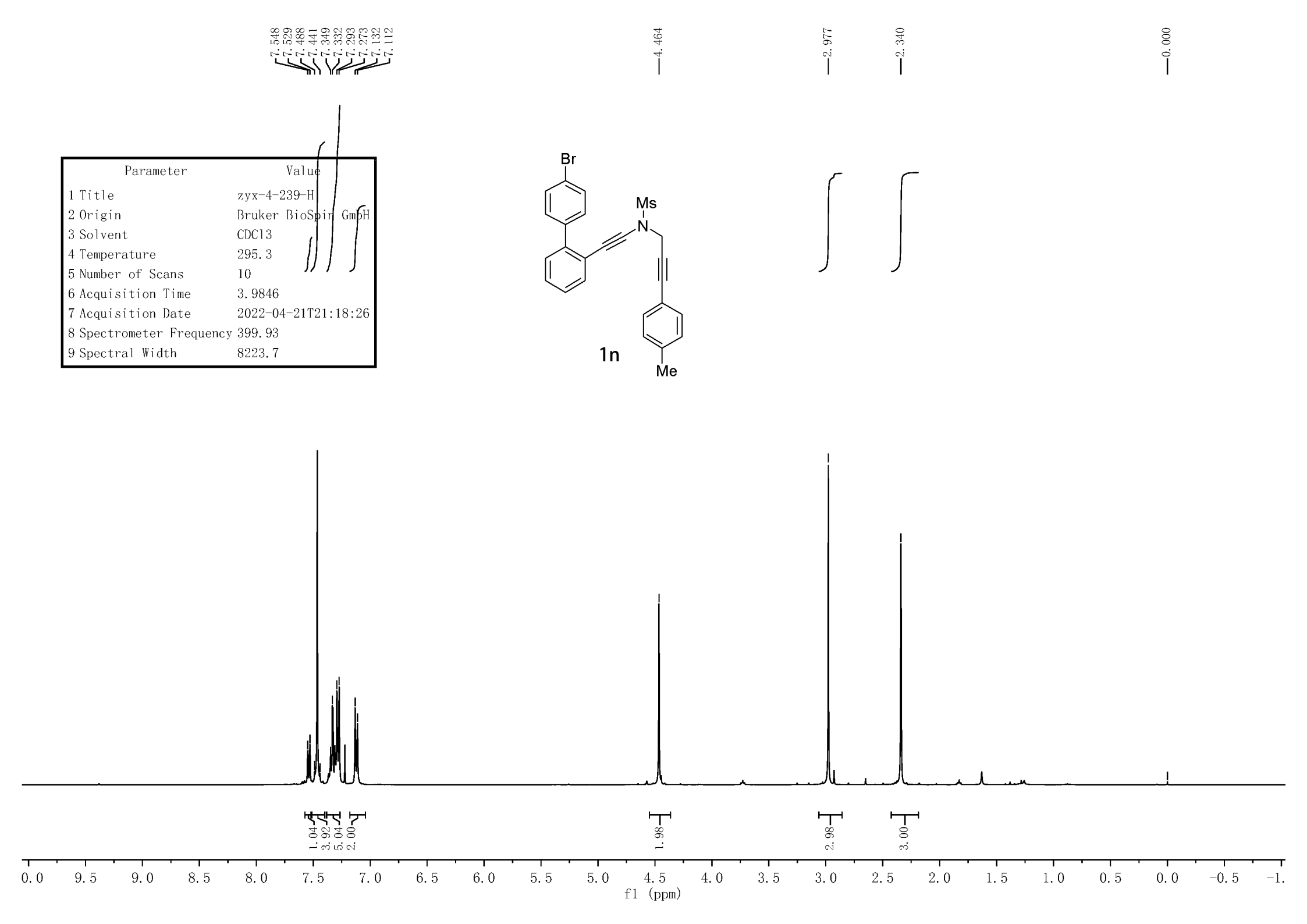



7.543
7.528
7.481
7.463
7.461
7.443
7.391
7.368
7.327
7.301
6.917
6.899
5.051
4.451
2.966
0.000
Parameter Value
1 Title zyx-5-18-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.2
5 Number of Scans 9
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-27T21:57:41
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
Ms
N
OBn
1m
1.05
4.01
10.15
2.05
2.08
2.08
3.00
0.0
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)

Parameter	Value
1 Title	zyx-5-18-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.3
5 Number of Scans	36
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-27T22:00:33
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

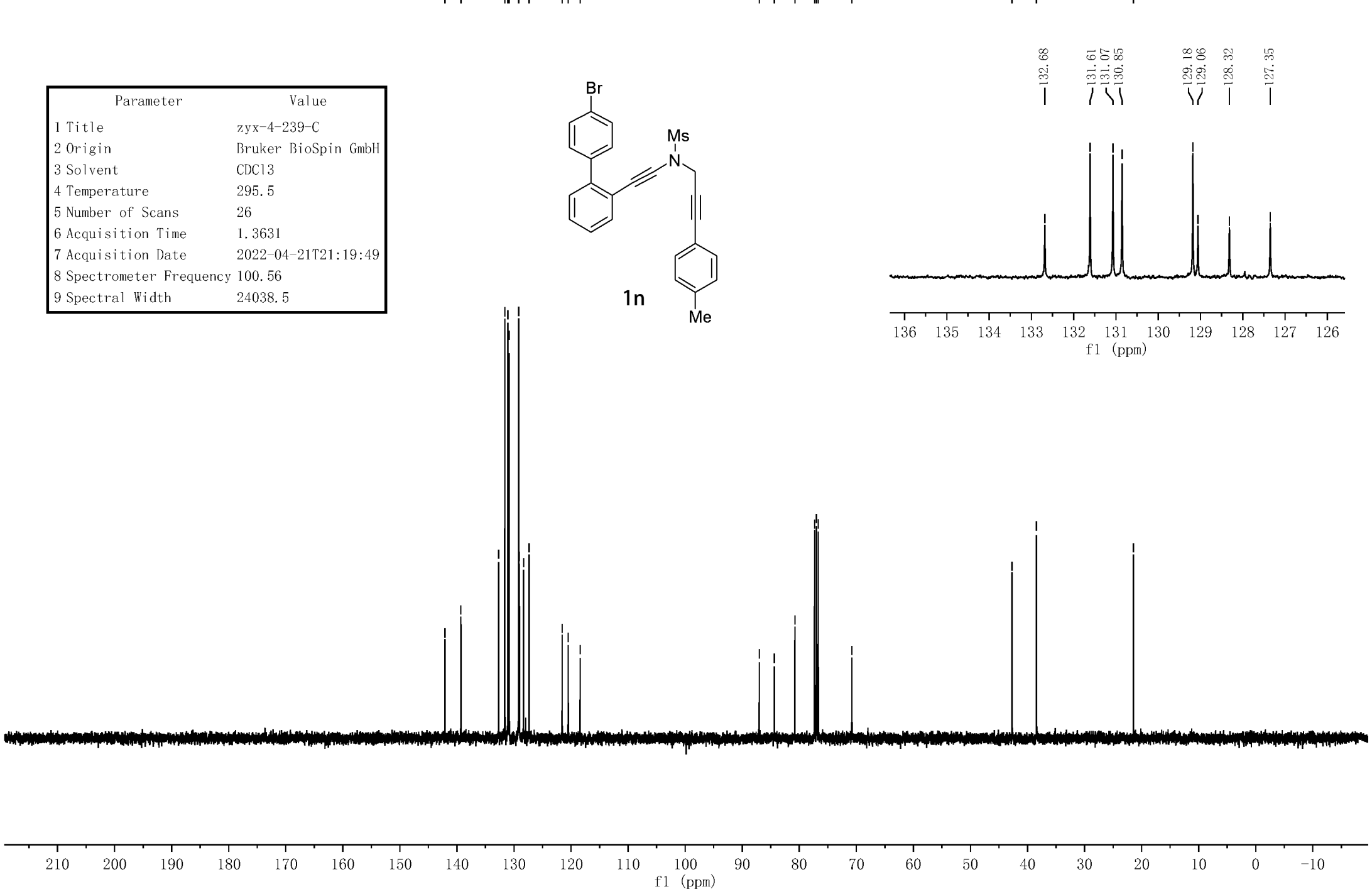
1m

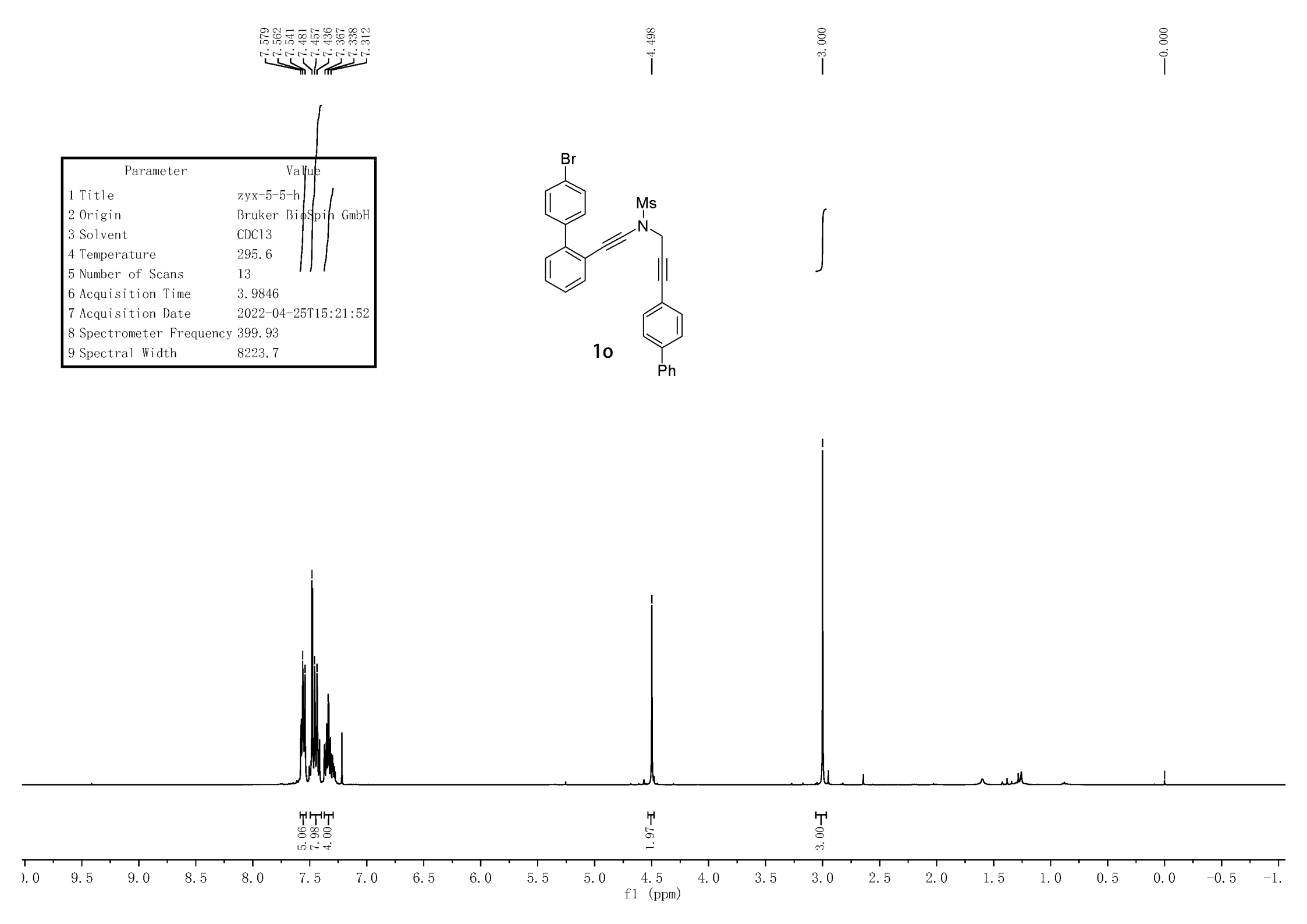



7.548
7.529
7.488
7.441
7.349
7.332
7.293
7.273
7.132
7.112
4.464
2.977
2.340
0.000
Parameter Value
1 Title zyx-4-239-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.3
5 Number of Scans 10
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-21T21:18:26
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
Me
1n
1.04
3.92
5.04
2.00
1.98
2.98
3.00
0.0
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
-1.
f1 (ppm)

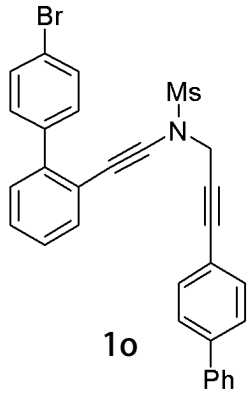
Parameter	Value
1 Title	zyx-4-239-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	26
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-21T21:19:49
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

1n

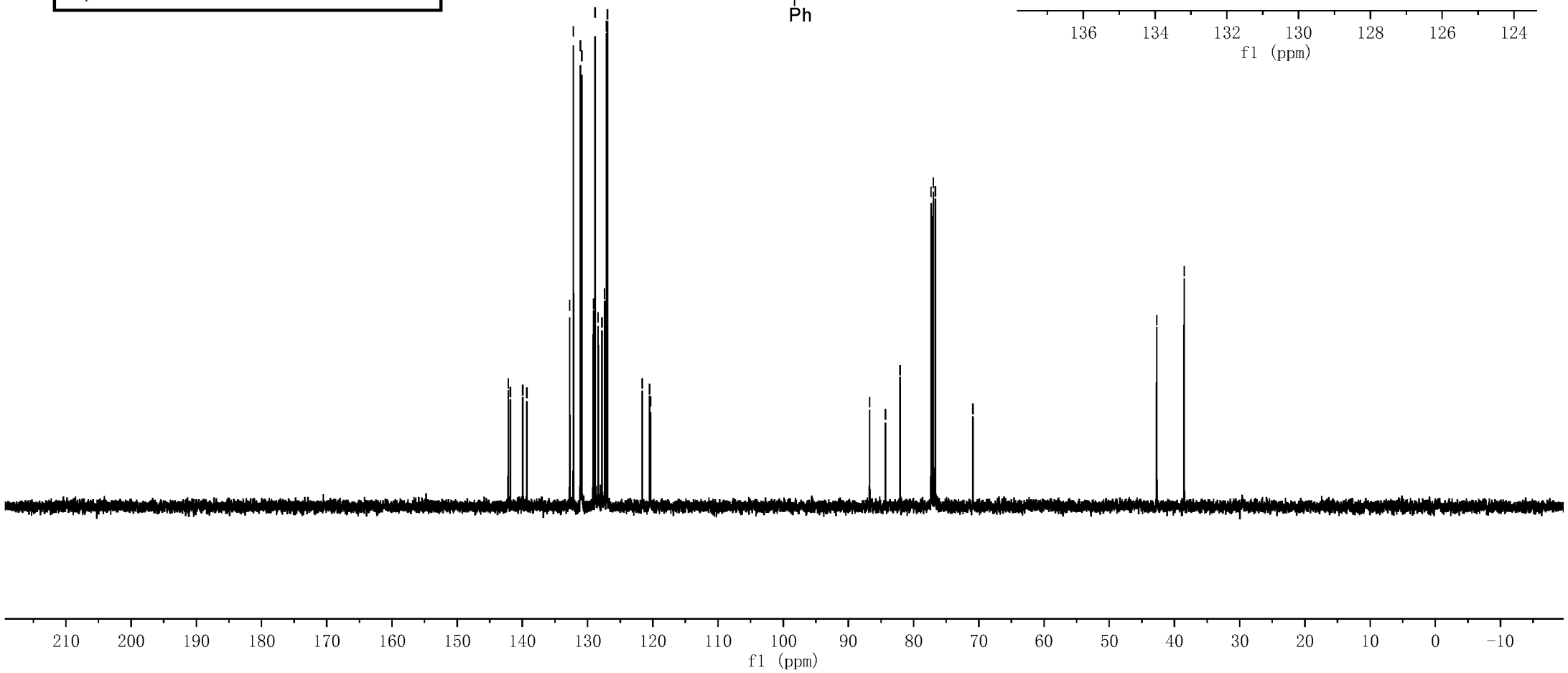


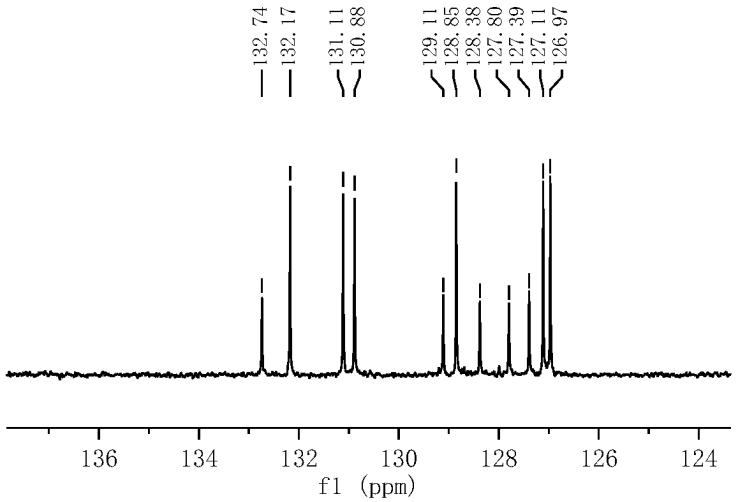

7.579
7.562
7.541
7.481
7.457
7.436
7.367
7.338
7.312
4.498
3.000
0.000
Parameter Value
1 Title zyx-5-5-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.6
5 Number of Scans 13
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-25T15:21:52
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
1o
Ph
5.06
7.98
4.00
1.97
3.00
f1 (ppm)

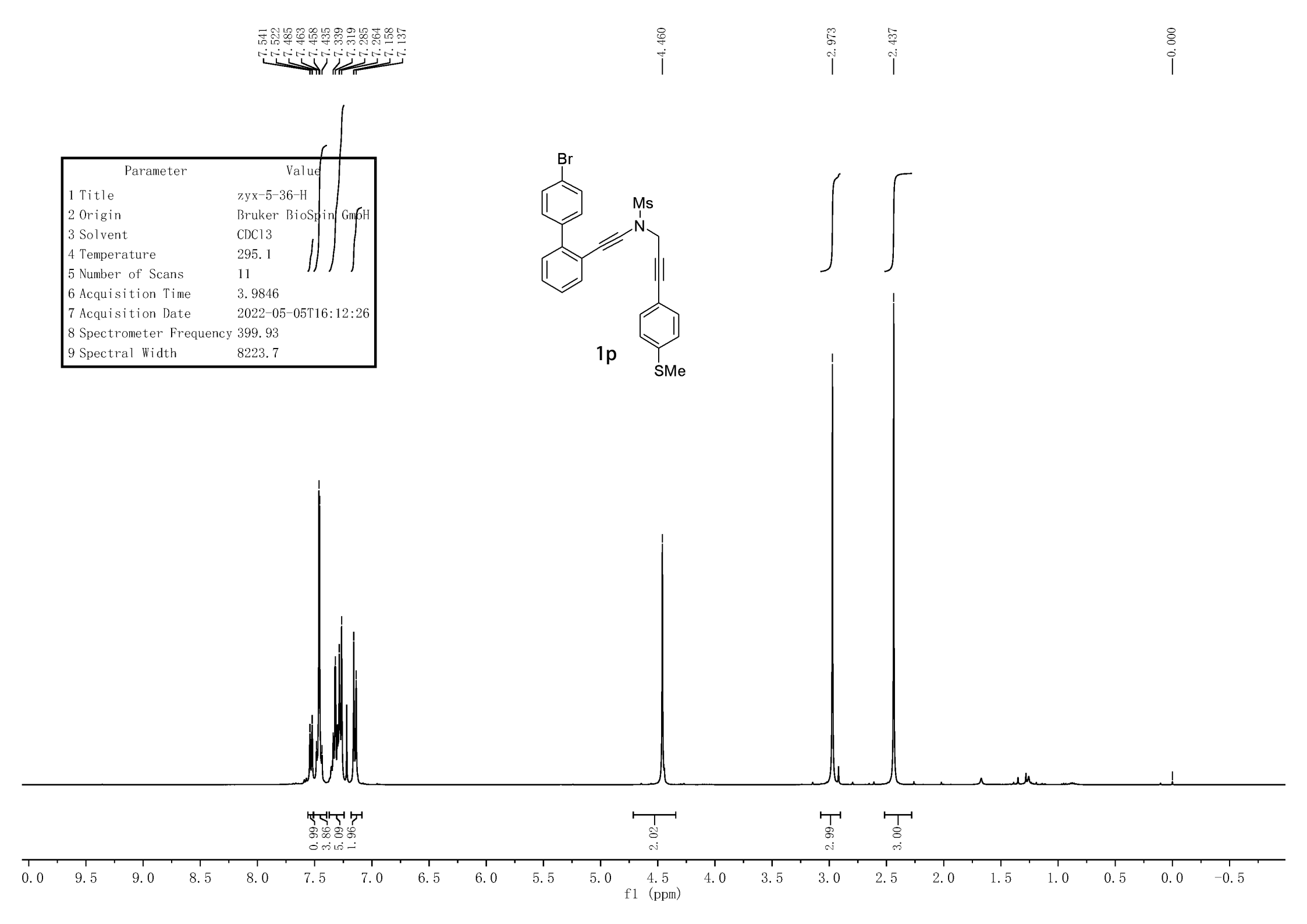
Parameter	Value
1 Title	zyx-5-5-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.9
5 Number of Scans	56
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-25T15:25:11
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



1o

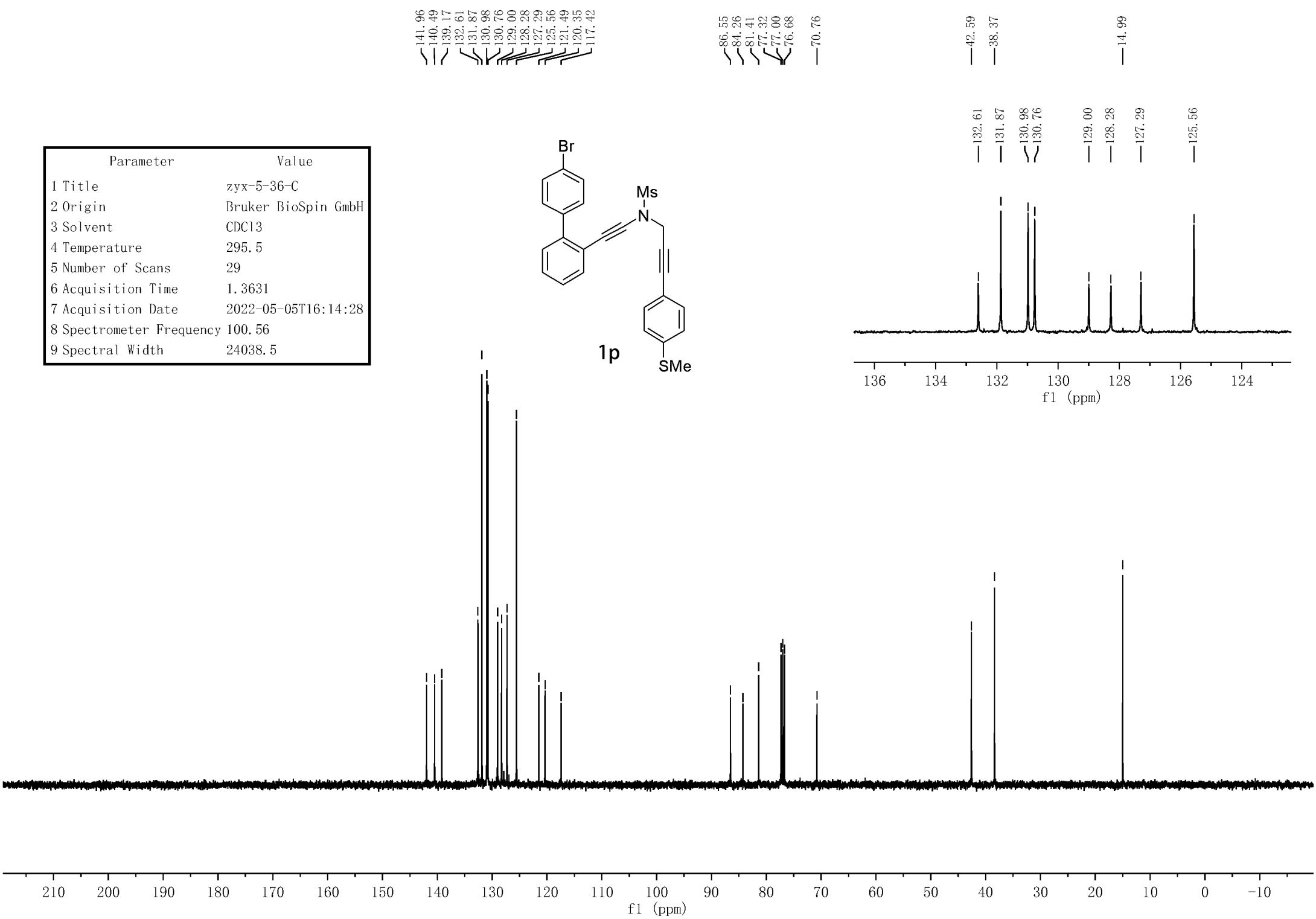


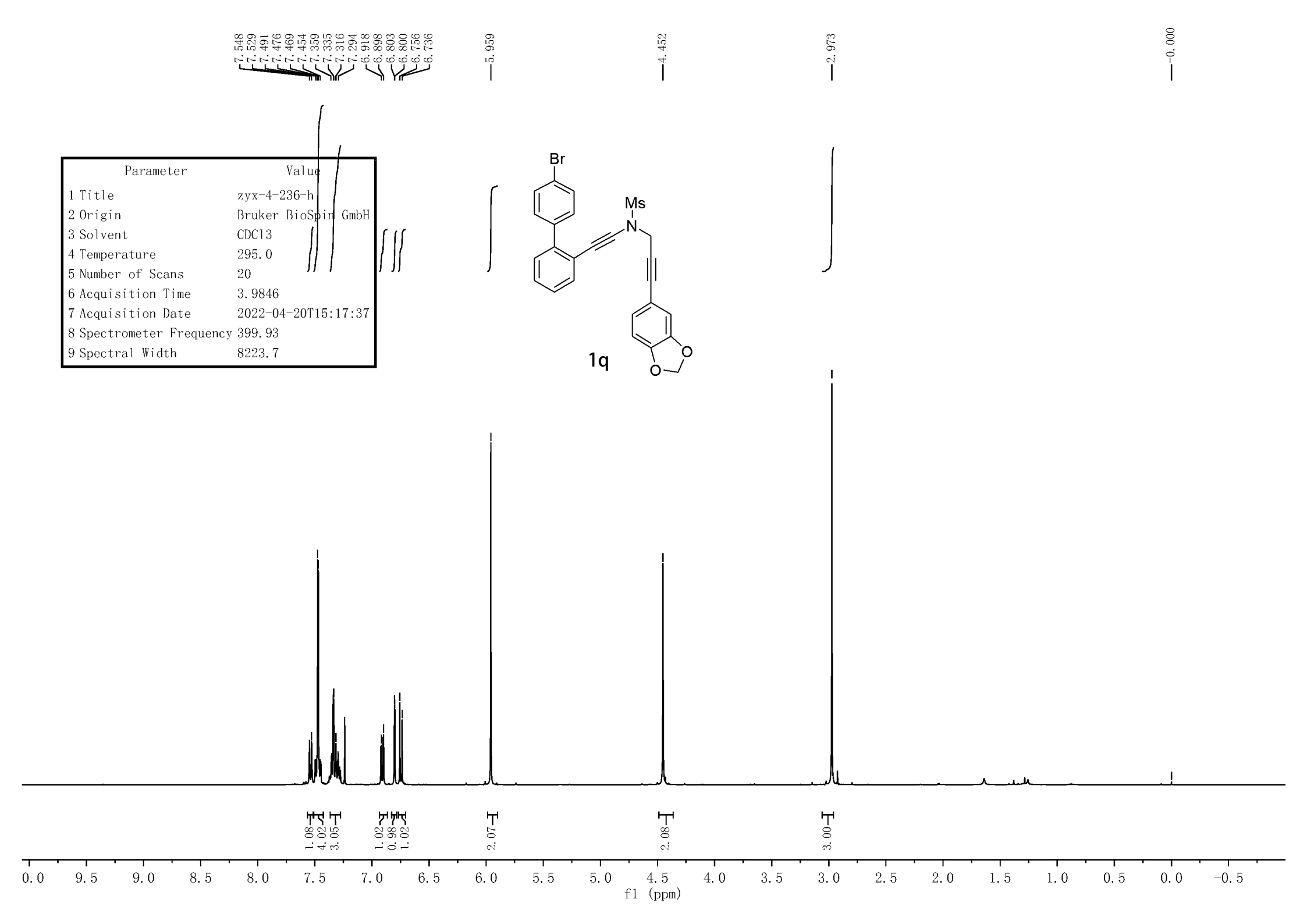



7.541
7.522
7.485
7.463
7.458
7.435
7.339
7.319
7.285
7.264
7.158
7.137
4.460
2.973
2.437
0.000
Parameter Value
1 Title zyx-5-36-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.1
5 Number of Scans 11
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-05T16:12:26
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
SMe
1p
0.99
3.86
5.09
1.96
2.02
2.99
3.00
0.0
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)

Parameter	Value
1 Title	zyx-5-36-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	29
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-05T16:14:28
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

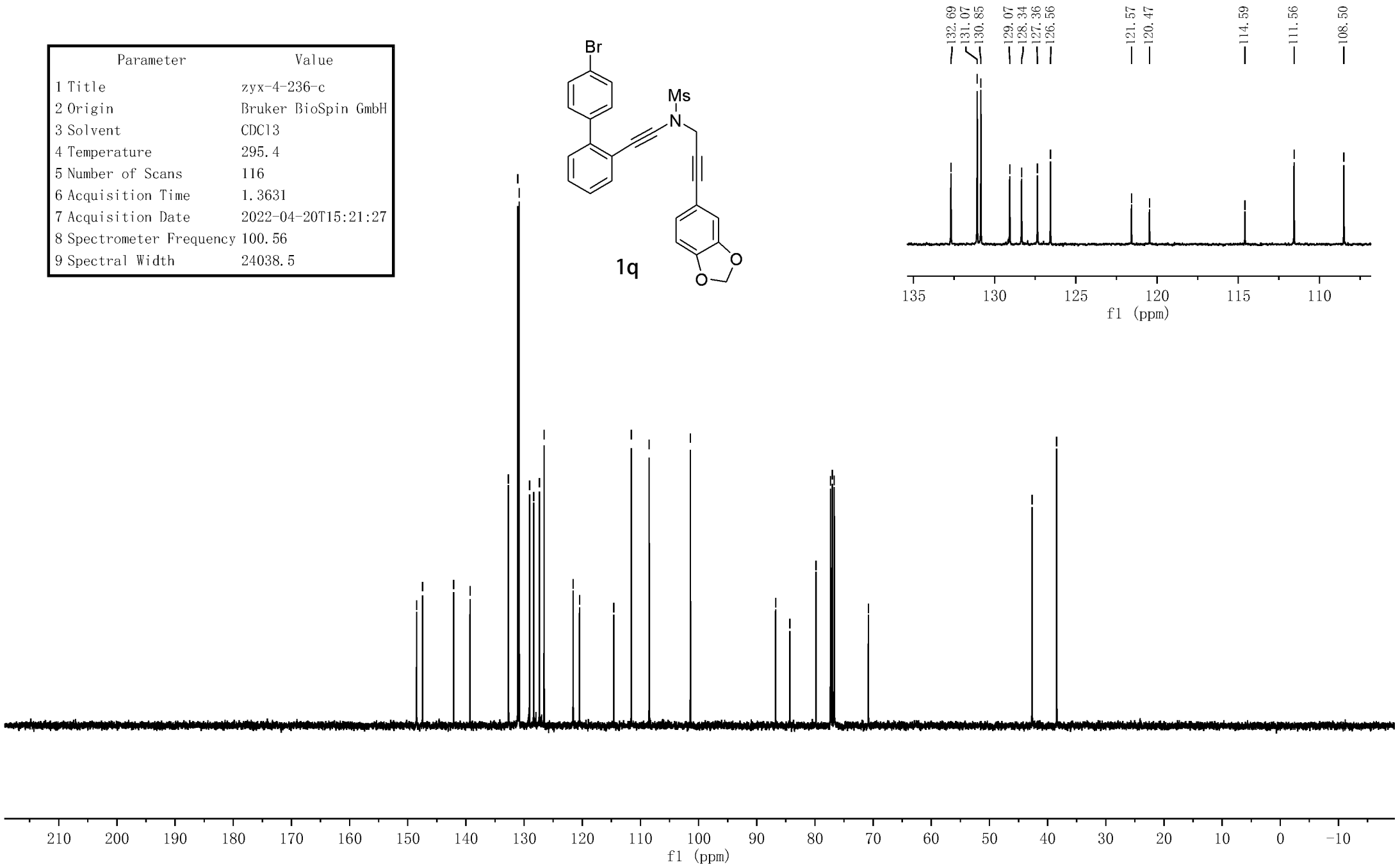
1p

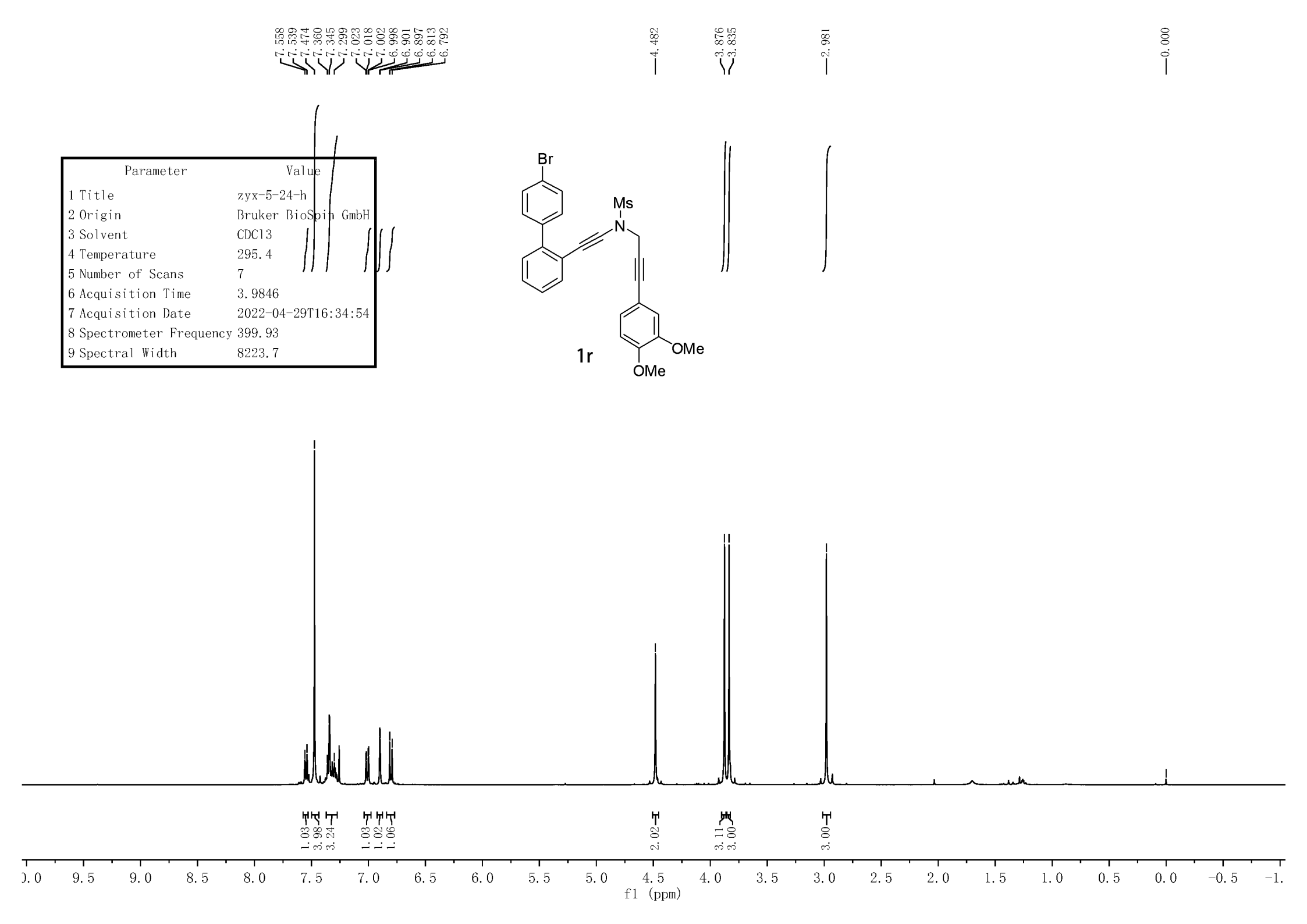



7.548
7.529
7.491
7.476
7.469
7.454
7.359
7.335
7.316
7.294
6.918
6.898
6.803
6.800
6.756
6.736
5.959
4.452
2.973
-0.000
Parameter Value
1 Title zyx-4-236-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.0
5 Number of Scans 20
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-20T15:17:37
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
O
O
1q
1.08
4.02
3.05
1.02
0.98
1.02
2.07
2.08
3.00
0.0
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)

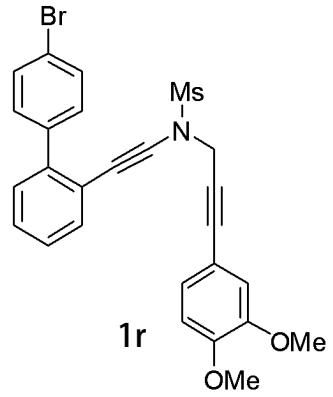
Parameter	Value
1 Title	zyx-4-236-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.4
5 Number of Scans	116
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-20T15:21:27
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

1q

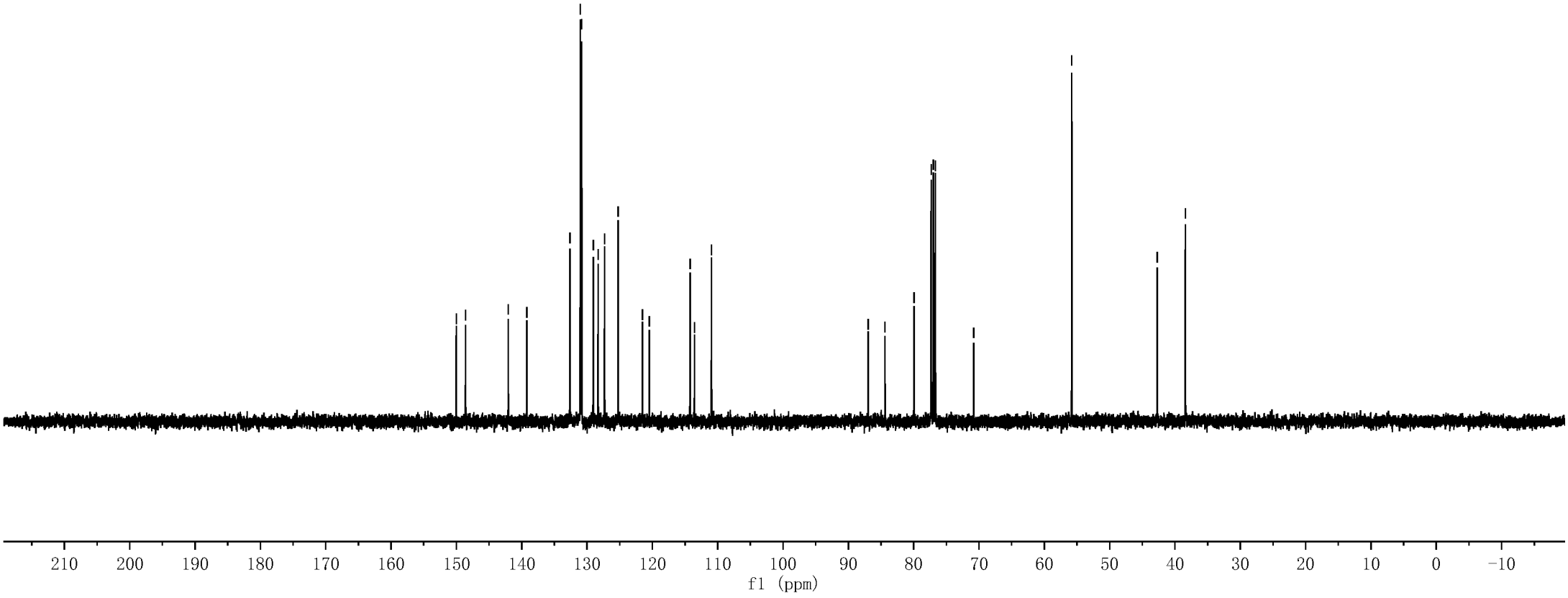


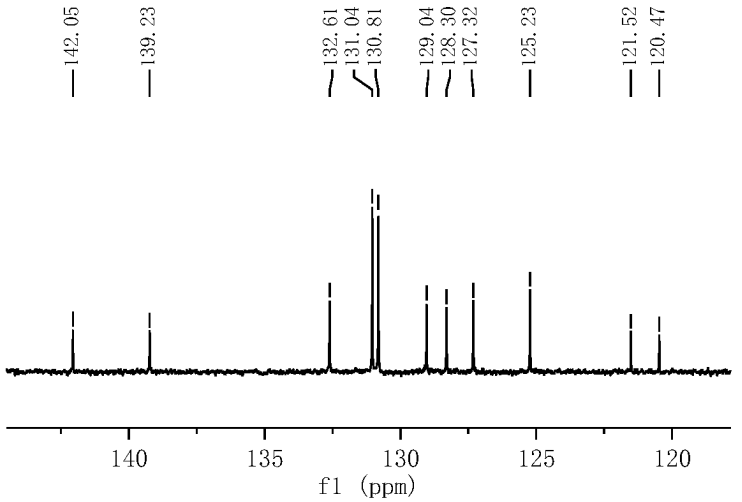

7.558
7.539
7.474
7.360
7.345
7.299
7.023
7.018
7.002
6.998
6.901
6.897
6.813
6.792
4.482
3.876
3.835
2.981
0.000
Parameter Value
1 Title zyx-5-24-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.4
5 Number of Scans 7
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-29T16:34:54
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
OMe
OMe
1r
1.03
3.98
3.24
1.03
1.02
1.06
2.02
3.11
3.00
3.00
f1 (ppm)

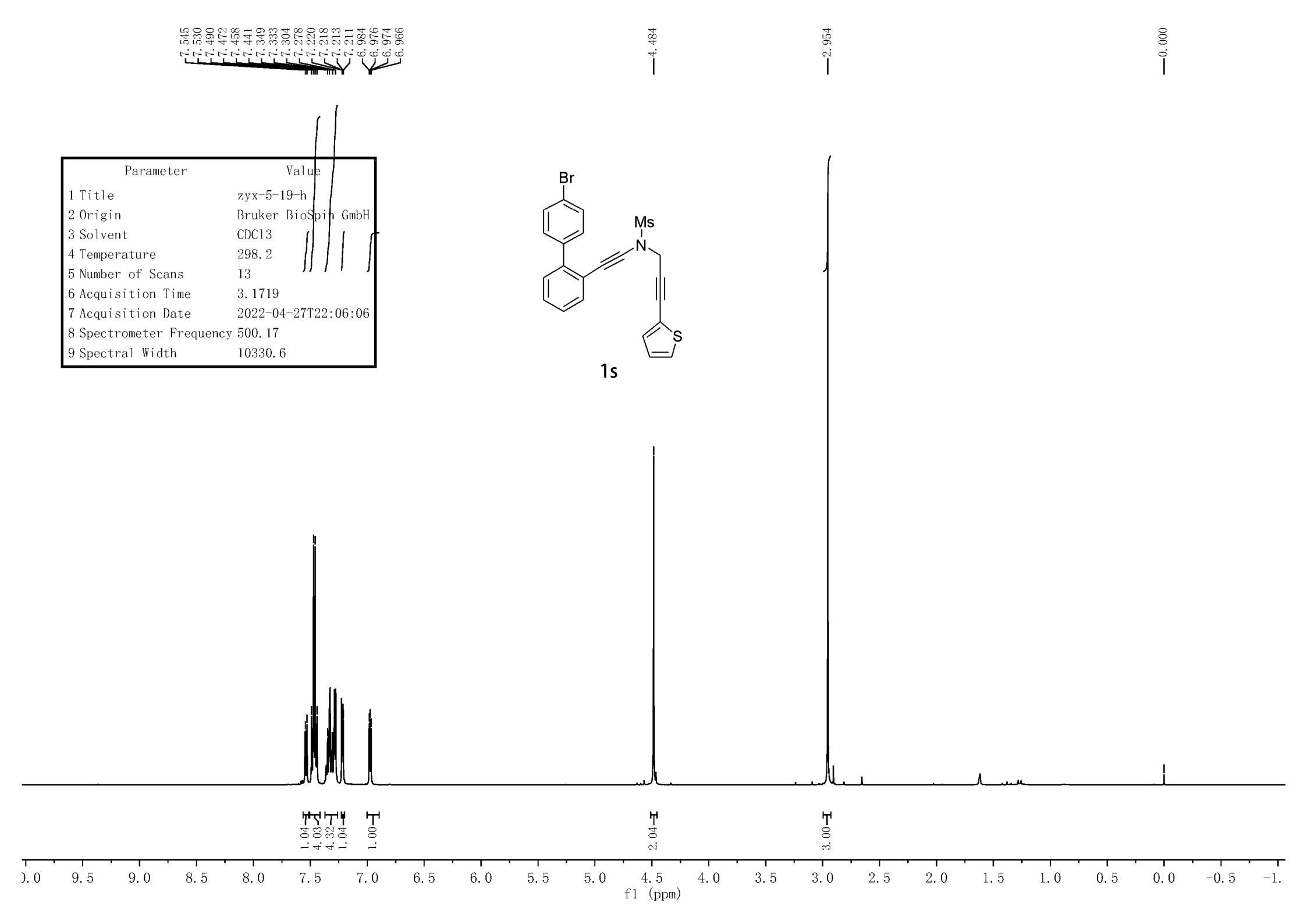
Parameter	Value
1 Title	zyx-5-24-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	29
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-29T16:37:30
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



1r

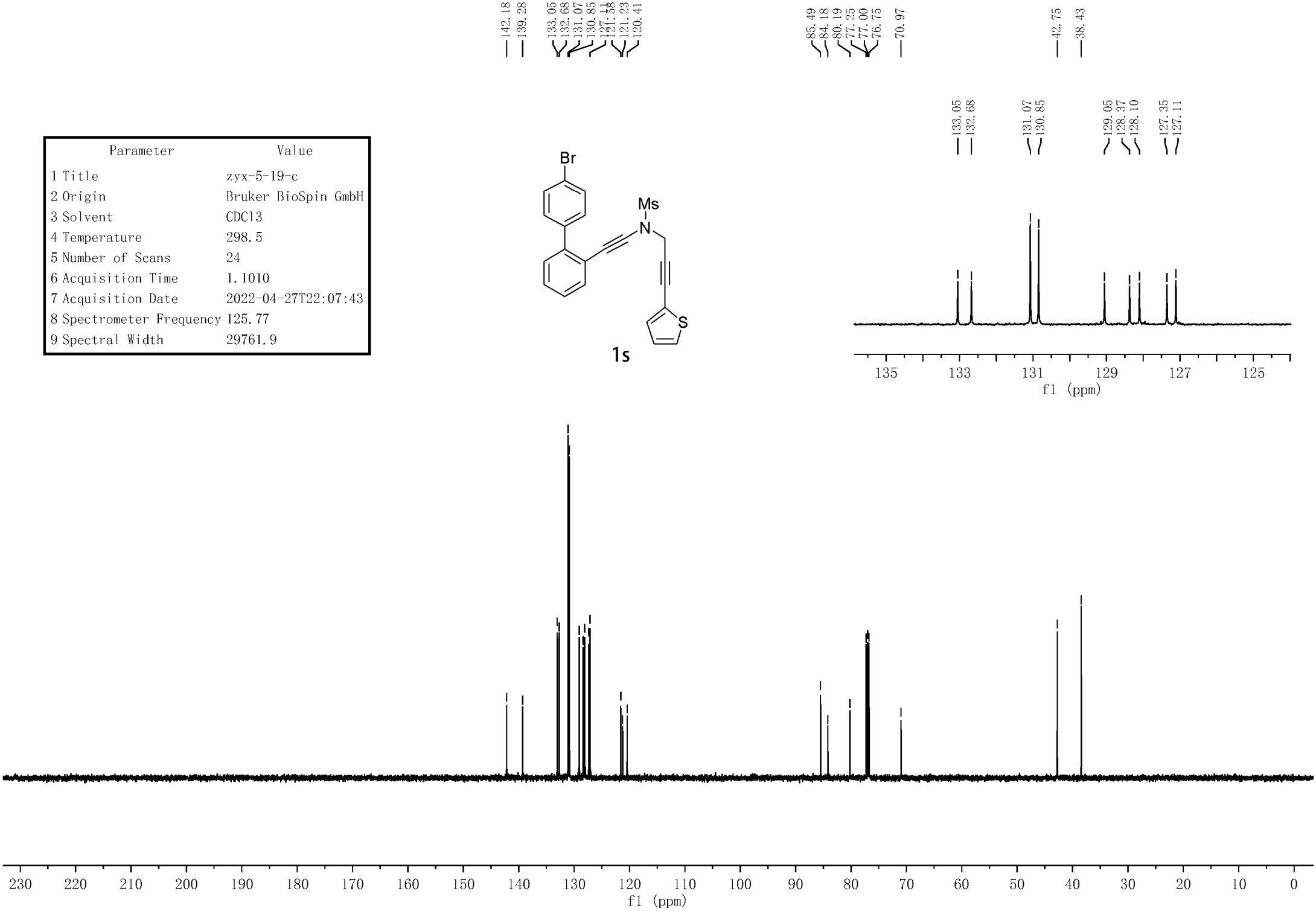


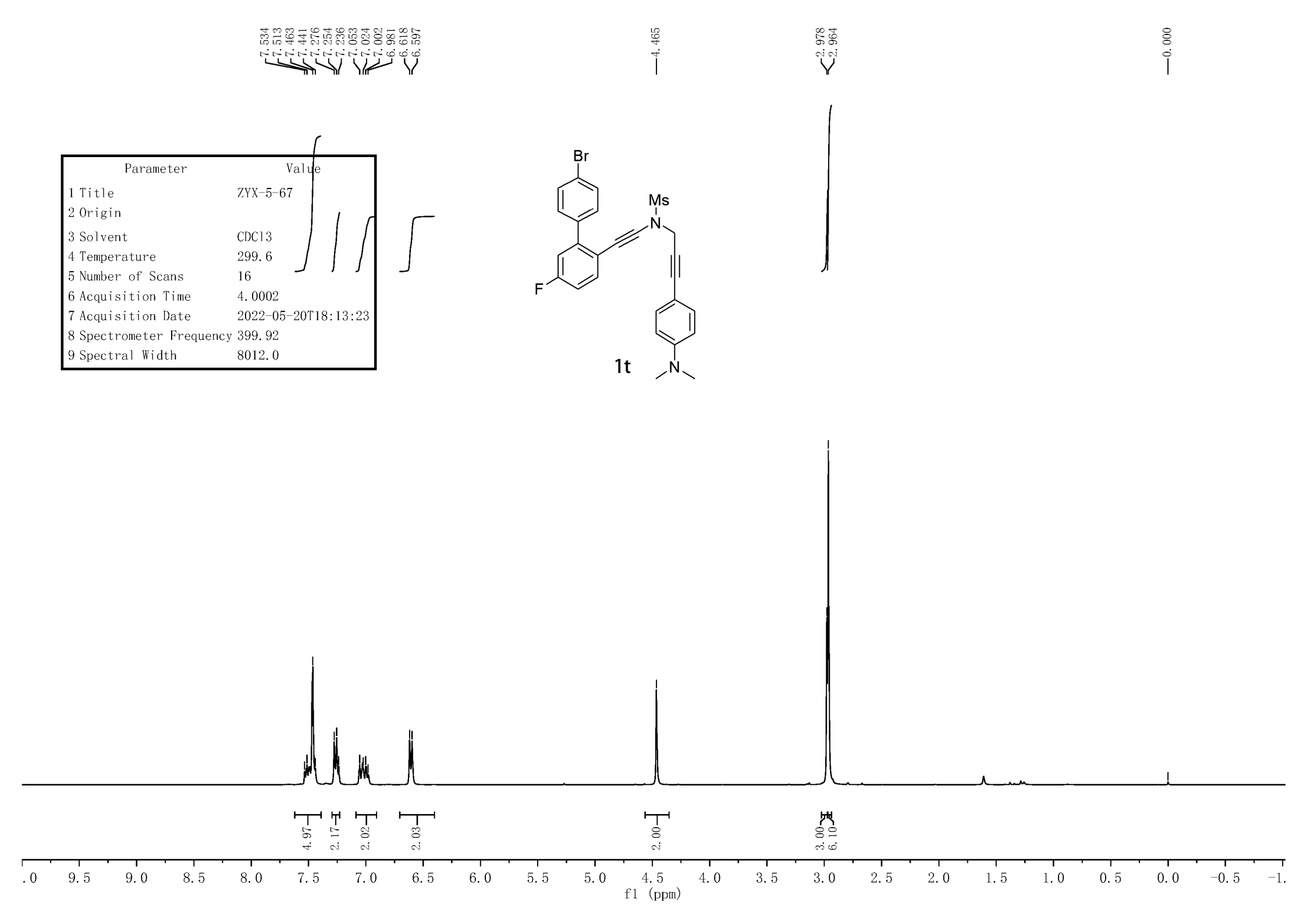


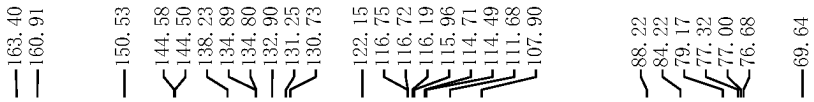

7.545
7.530
7.490
7.472
7.458
7.441
7.349
7.333
7.304
7.278
7.220
7.218
7.213
7.211
6.984
6.976
6.974
6.966
4.484
2.954
0.000
Parameter Value
1 Title zyx-5-19-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.2
5 Number of Scans 13
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-27T22:06:06
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
Ms
N
S
1s
1.04
4.03
4.32
1.04
1.00
2.04
3.00
f1 (ppm)

Parameter	Value
1 Title	zyx-5-19-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.5
5 Number of Scans	24
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-27T22:07:43
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

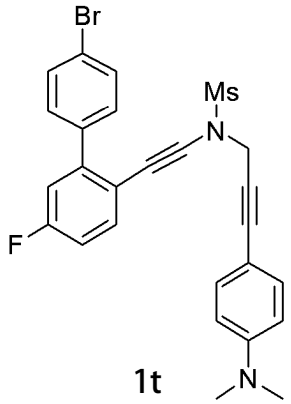
1s



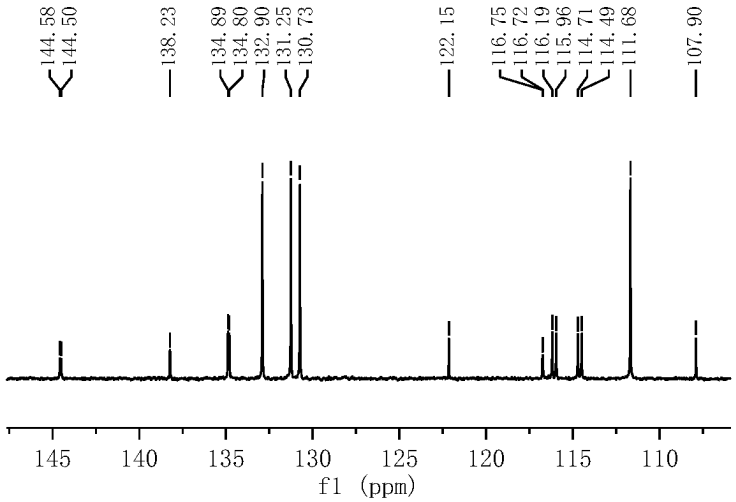

7.534
7.513
7.463
7.441
7.276
7.254
7.236
7.053
7.024
7.002
6.981
6.618
6.597
4.465
2.978
2.964
0.000
Parameter Value
1 Title ZYX-5-67
2 Origin
3 Solvent CDCl3
4 Temperature 299.6
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-05-20T18:13:23
8 Spectrometer Frequency 399.92
9 Spectral Width 8012.0
Br
Ms
N
F
1t
N
4.97
2.17
2.02
2.03
2.00
3.00
6.10
f1 (ppm)

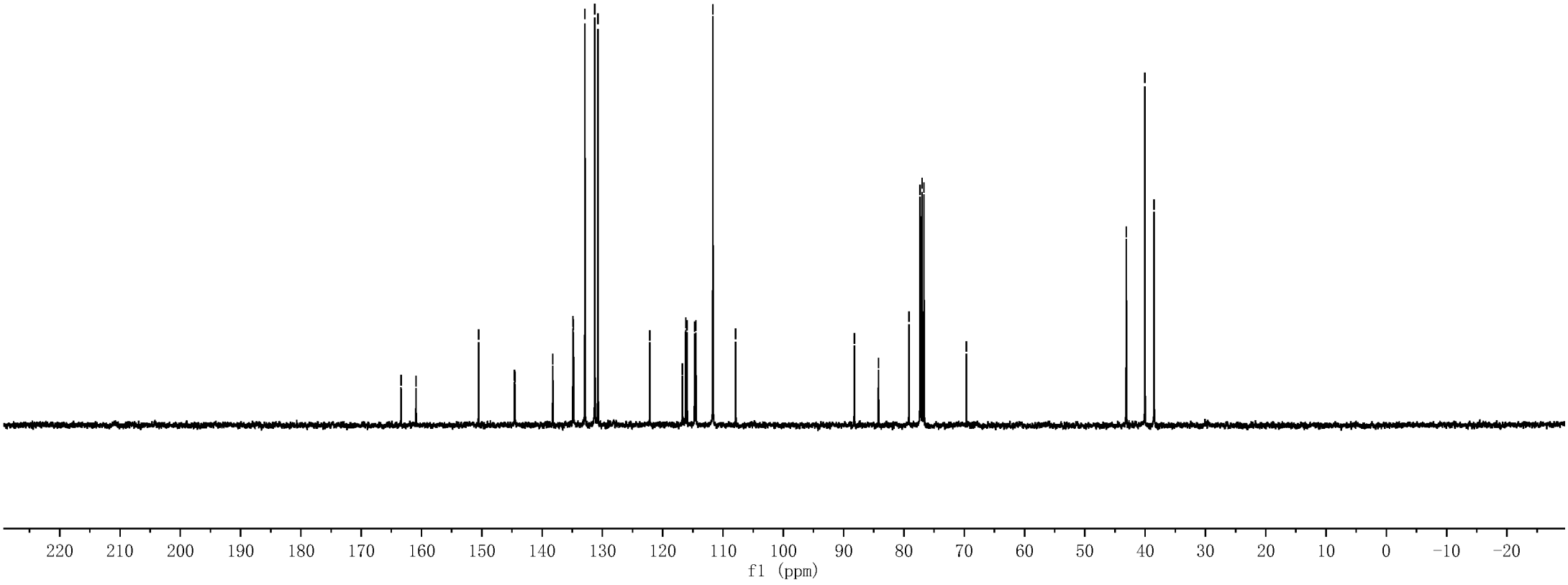


Parameter	Value
1 Title	ZYX-5-67
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.6
5 Number of Scans	300
6 Acquisition Time	1.0000
7 Acquisition Date	2022-05-20T18:23:38
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

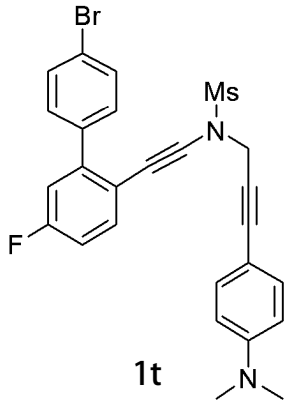


1t

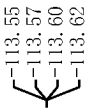


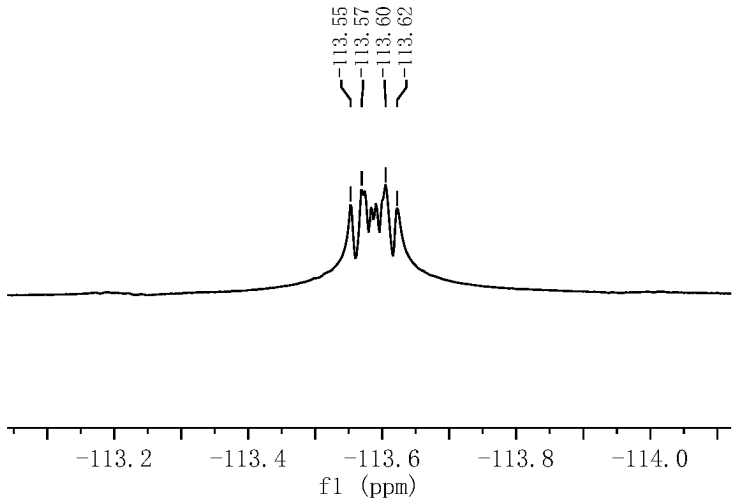


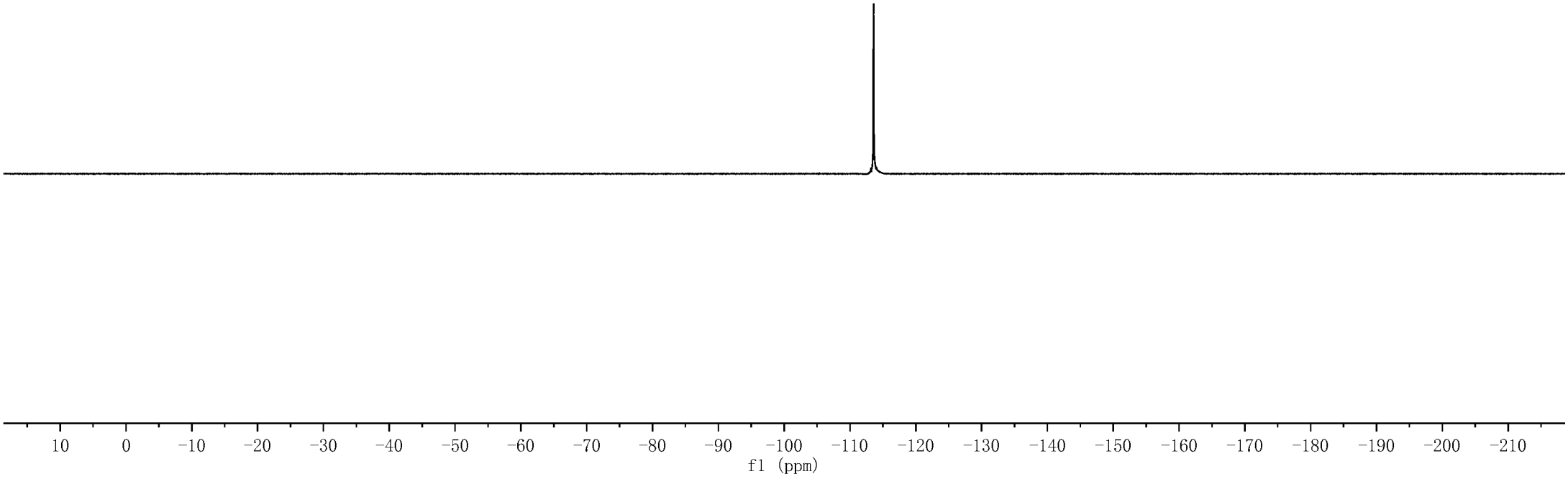
Parameter	Value
1 Title	ZYX-5-79-FF
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	49
6 Acquisition Time	0.7340
7 Acquisition Date	2022-05-28T11:04:14
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

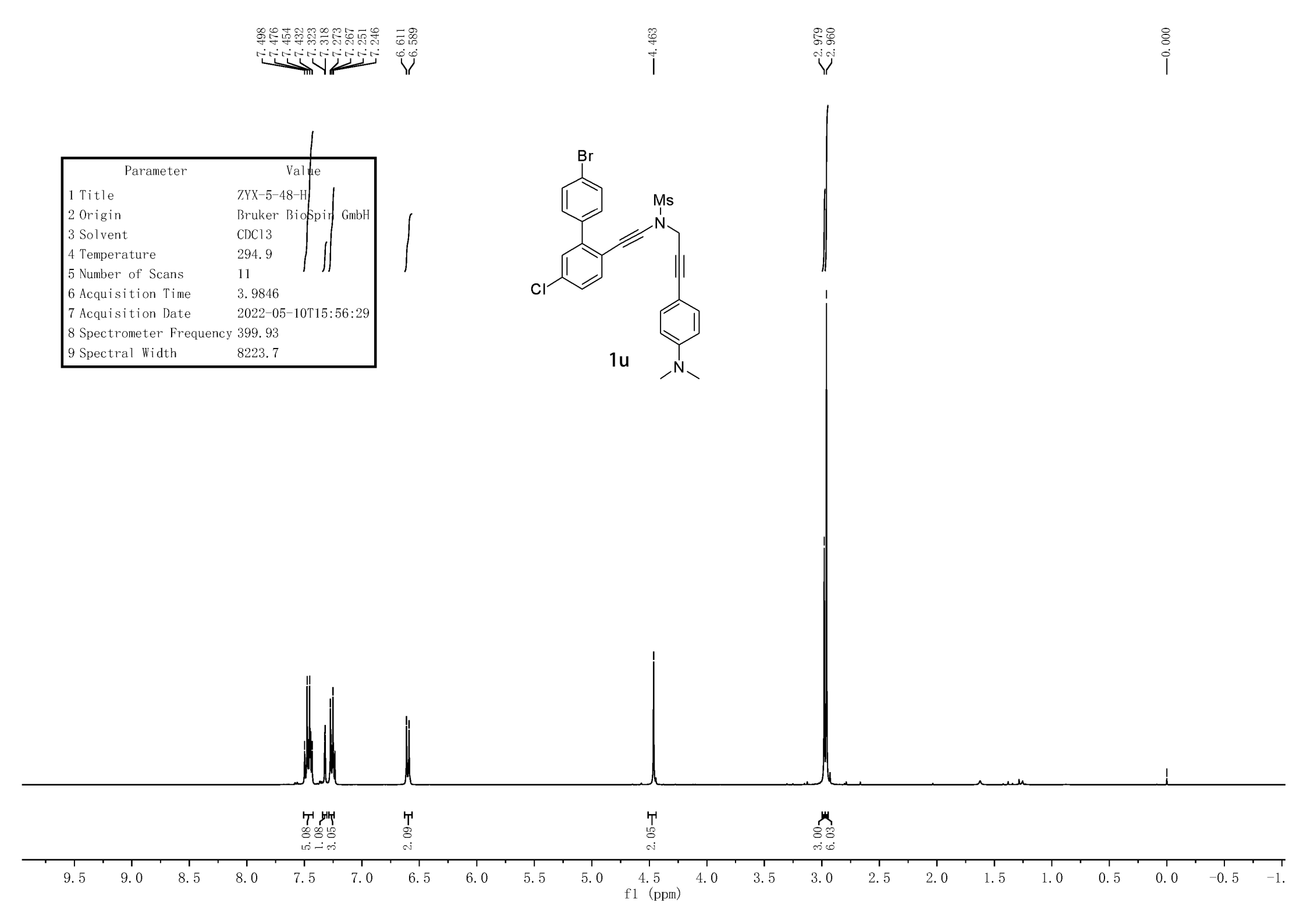


1t



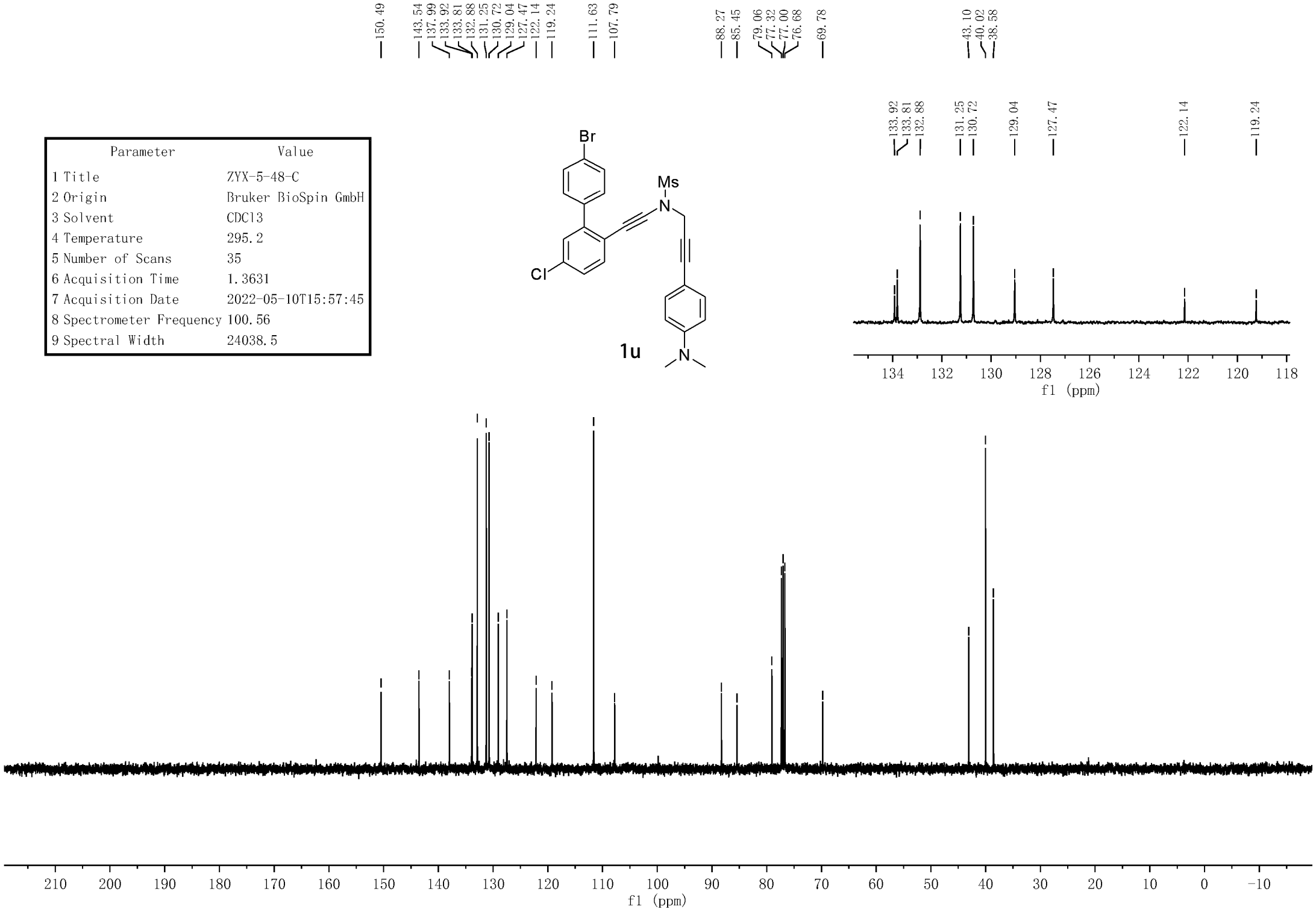


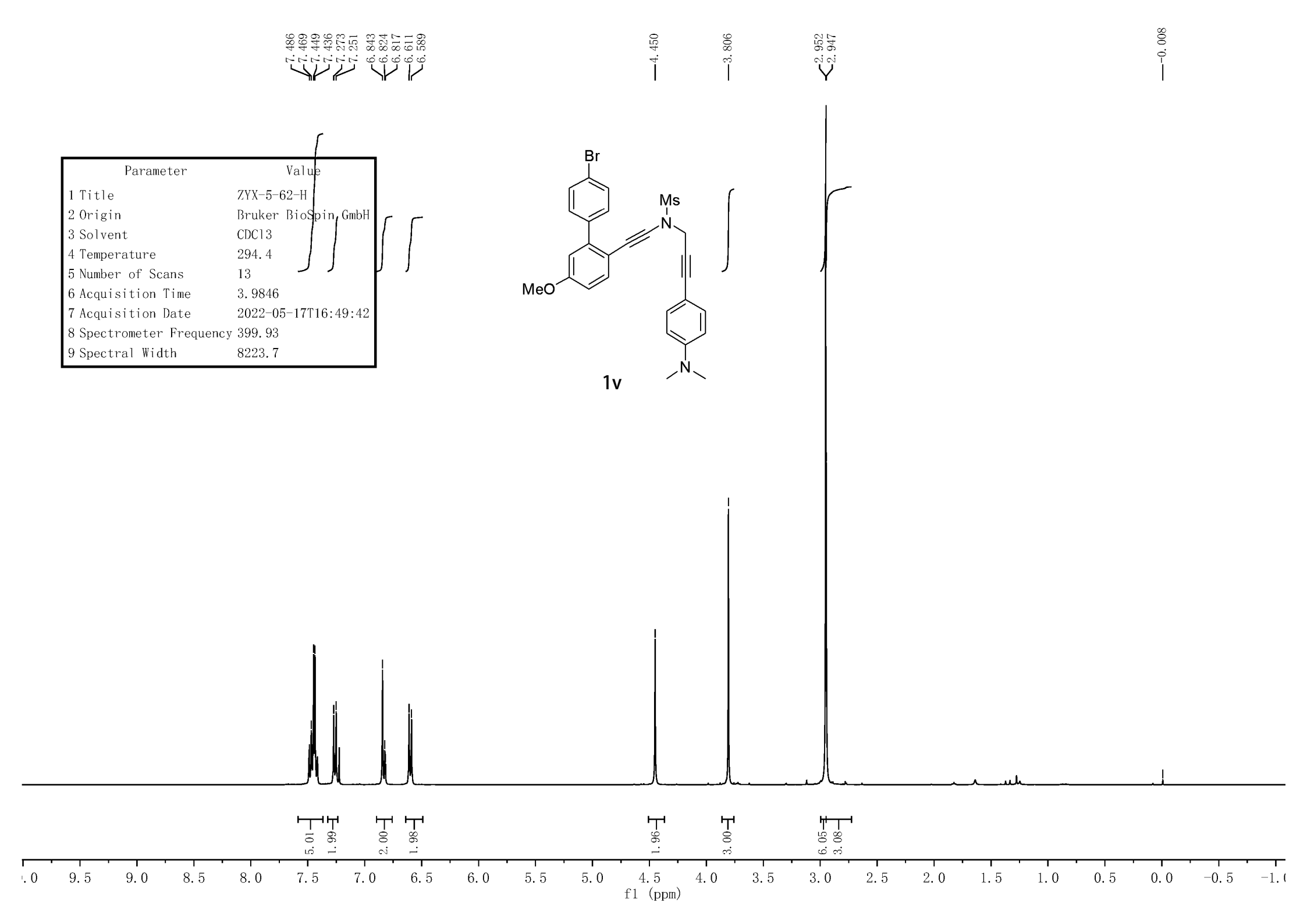



7.498
7.476
7.454
7.432
7.323
7.318
7.273
7.267
7.251
7.246
6.611
6.589
4.463
2.979
2.960
0.000
Parameter Value
1 Title ZYX-5-48-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 294.9
5 Number of Scans 11
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-10T15:56:29
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
Cl
N
1u
5.08
1.08
3.05
2.09
2.05
3.00
6.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

Parameter	Value
1 Title	ZYX-5-48-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.2
5 Number of Scans	35
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-10T15:57:45
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

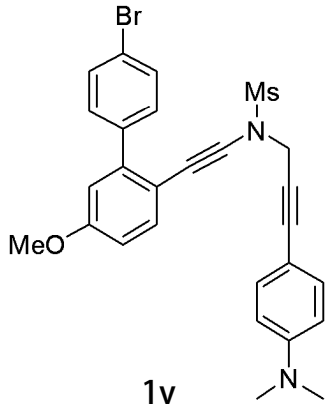
1u



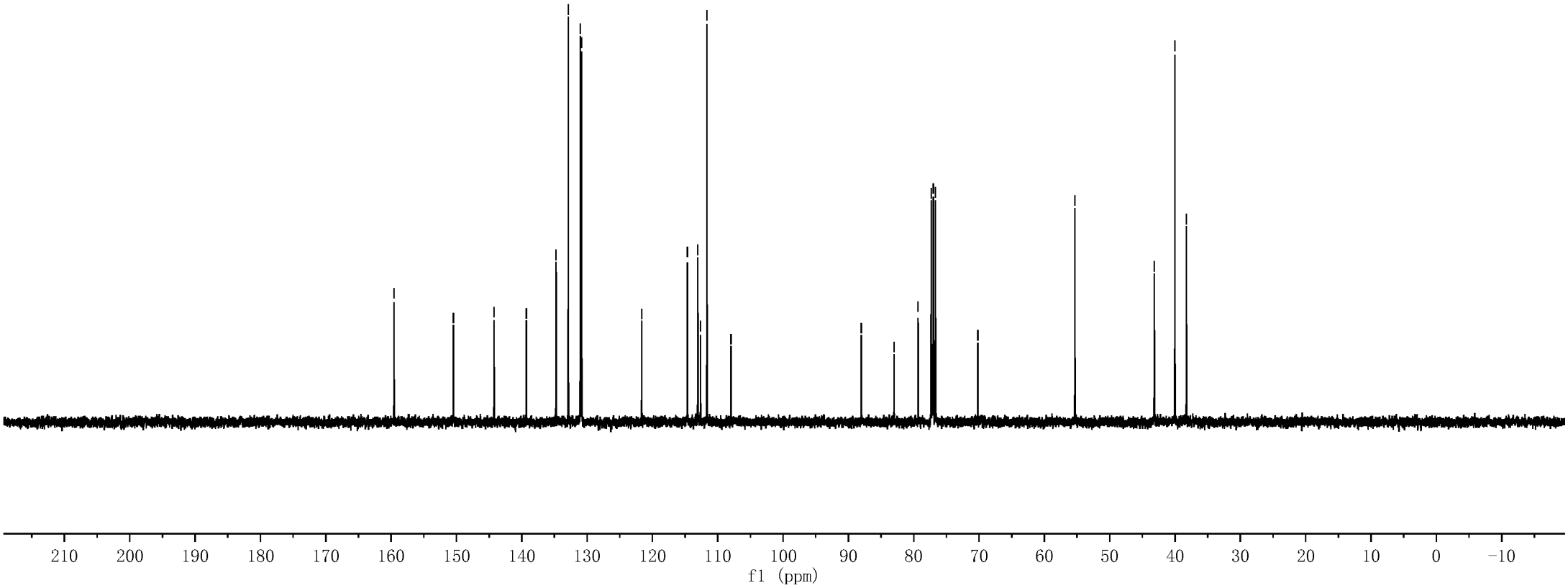

7.486
7.469
7.449
7.436
7.273
7.251
6.843
6.824
6.817
6.611
6.589
4.450
3.806
2.952
2.947
-0.008
Parameter Value
1 Title ZYX-5-62-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 294.4
5 Number of Scans 13
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-17T16:49:42
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
MeO
N
1v
5.01
1.99
2.00
1.98
1.96
3.00
6.05
3.08
f1 (ppm)

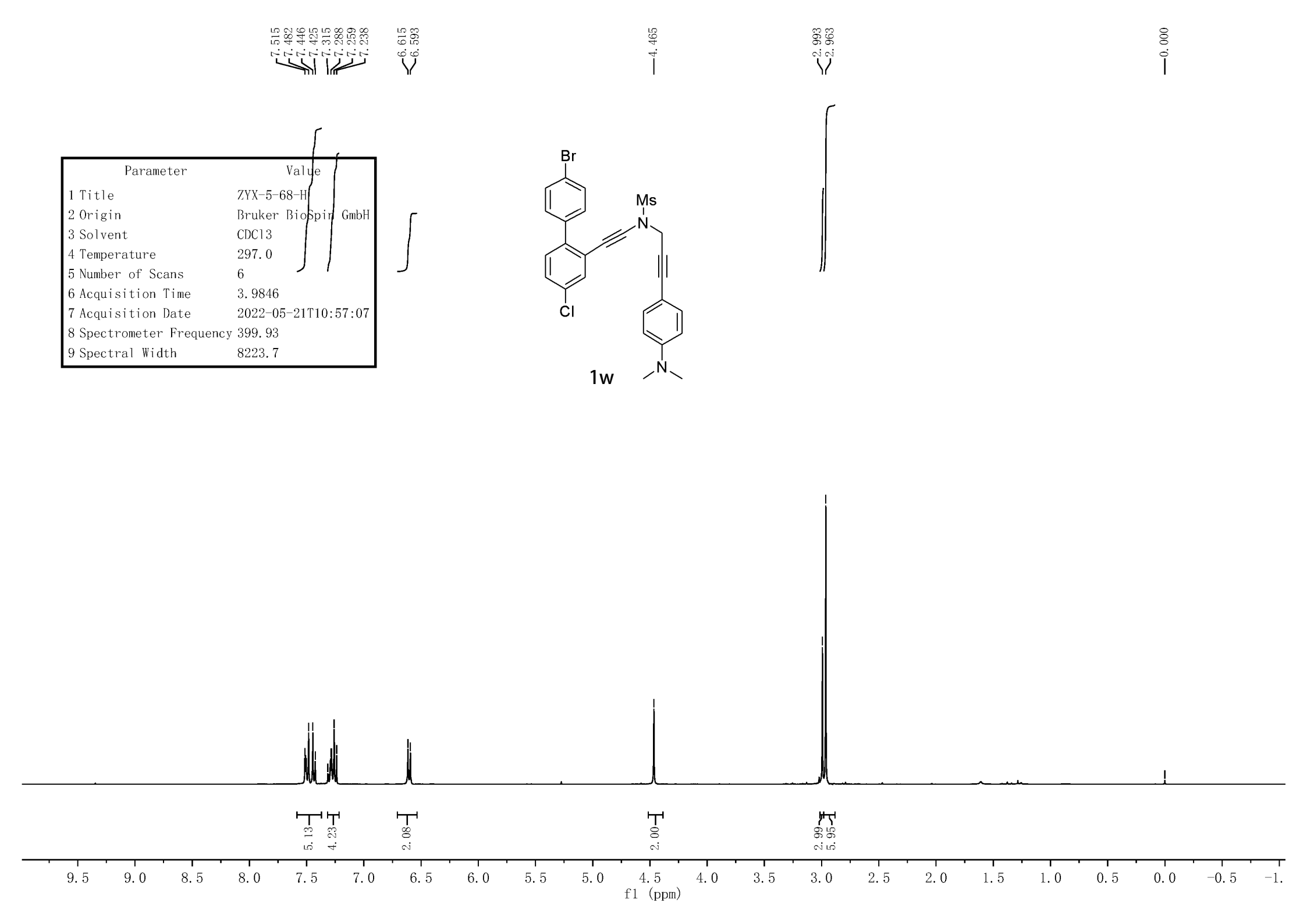
159.55
150.45
144.24
139.28
134.75
132.87
131.03
130.84
121.64
114.65
113.05
112.64
111.66
107.96
88.02
83.01
79.34
77.32
77.00
76.68
70.20
55.33
43.17
40.02
38.26

Parameter	Value
1 Title	ZYX-5-62-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.0
5 Number of Scans	48
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-17T16:51:50
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



1v

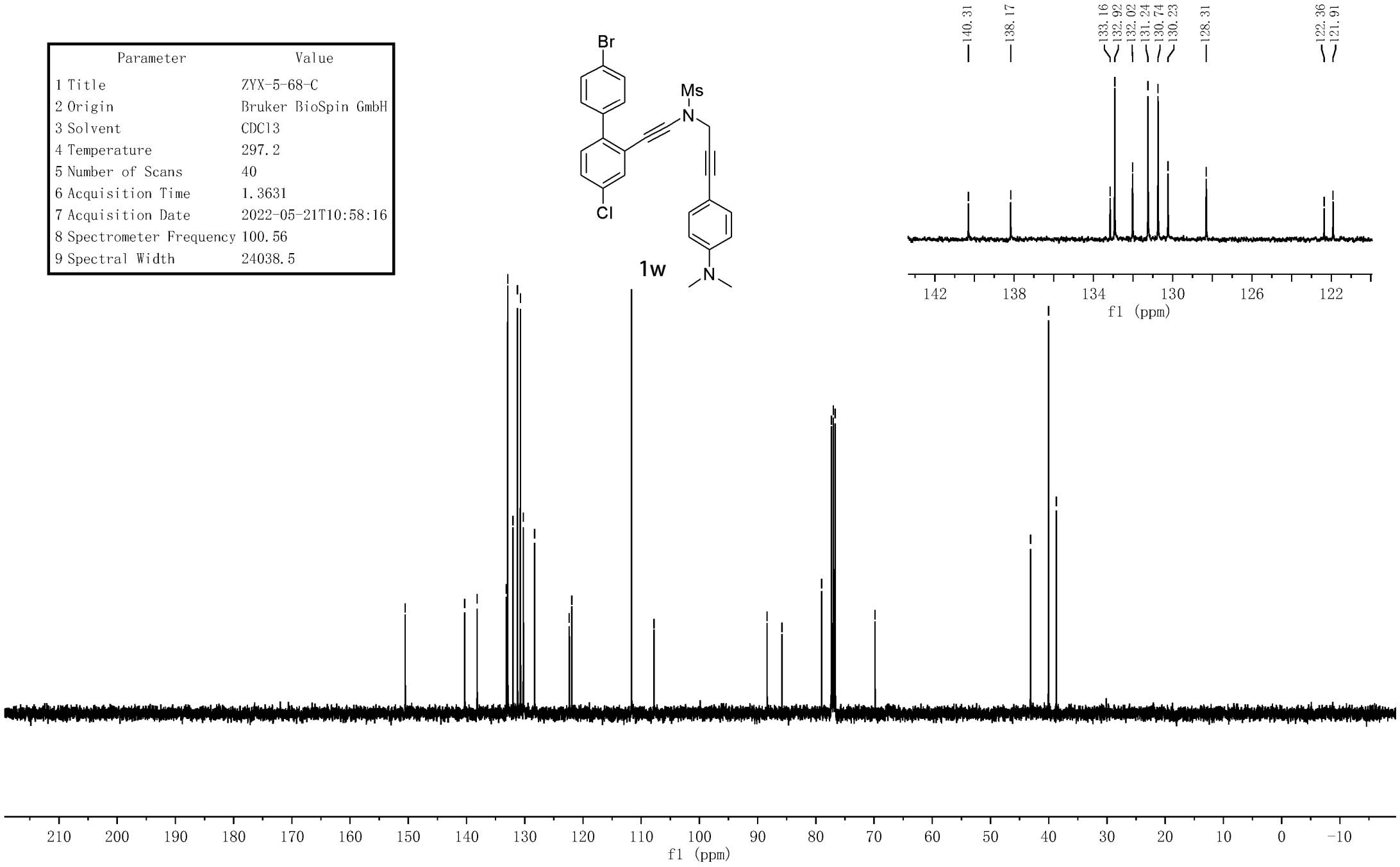




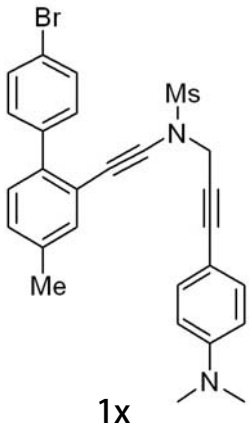
Parameter	Value
1 Title	ZYX-5-68-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	6
6 Acquisition Time	3.9846
7 Acquisition Date	2022-05-21T10:57:07
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

Parameter	Value
1 Title	ZYX-5-68-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.2
5 Number of Scans	40
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-21T10:58:16
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

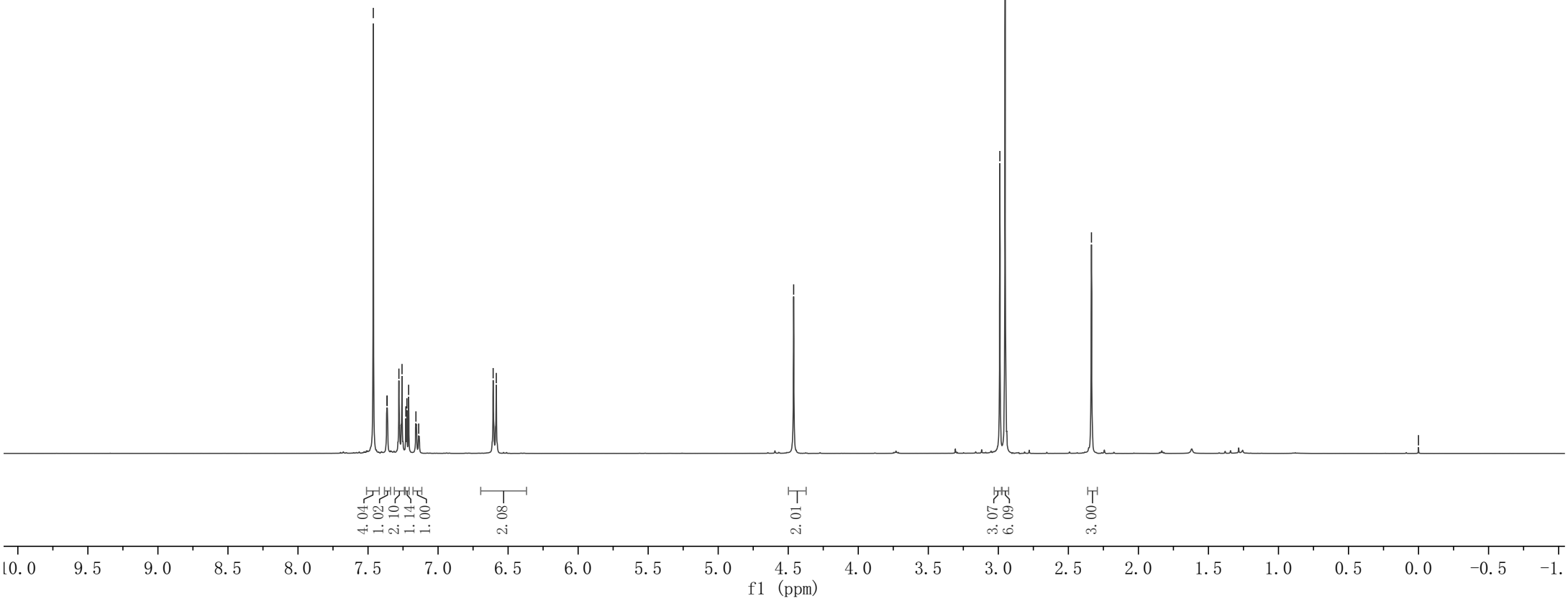
1w

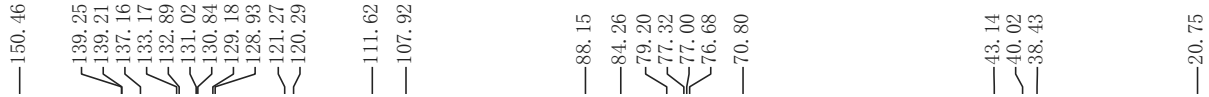


Parameter	Value
1 Title	ZYX-5-61-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	294.6
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2022-05-17T16:41:35
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

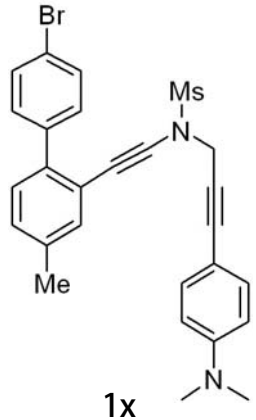


1x

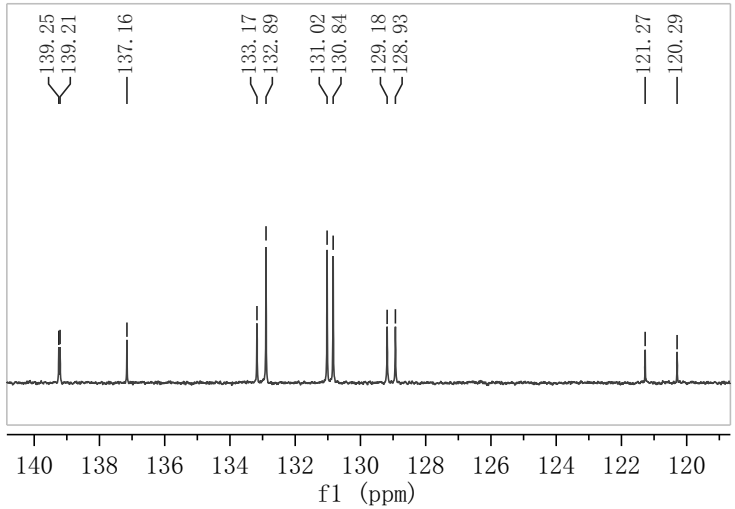


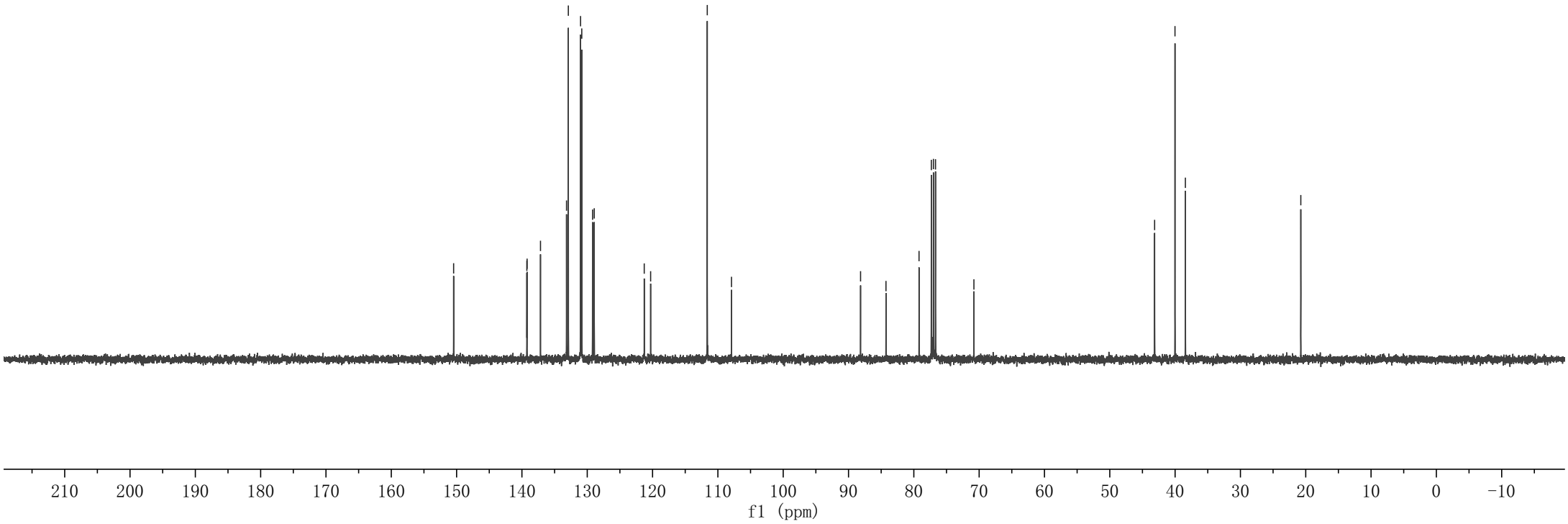


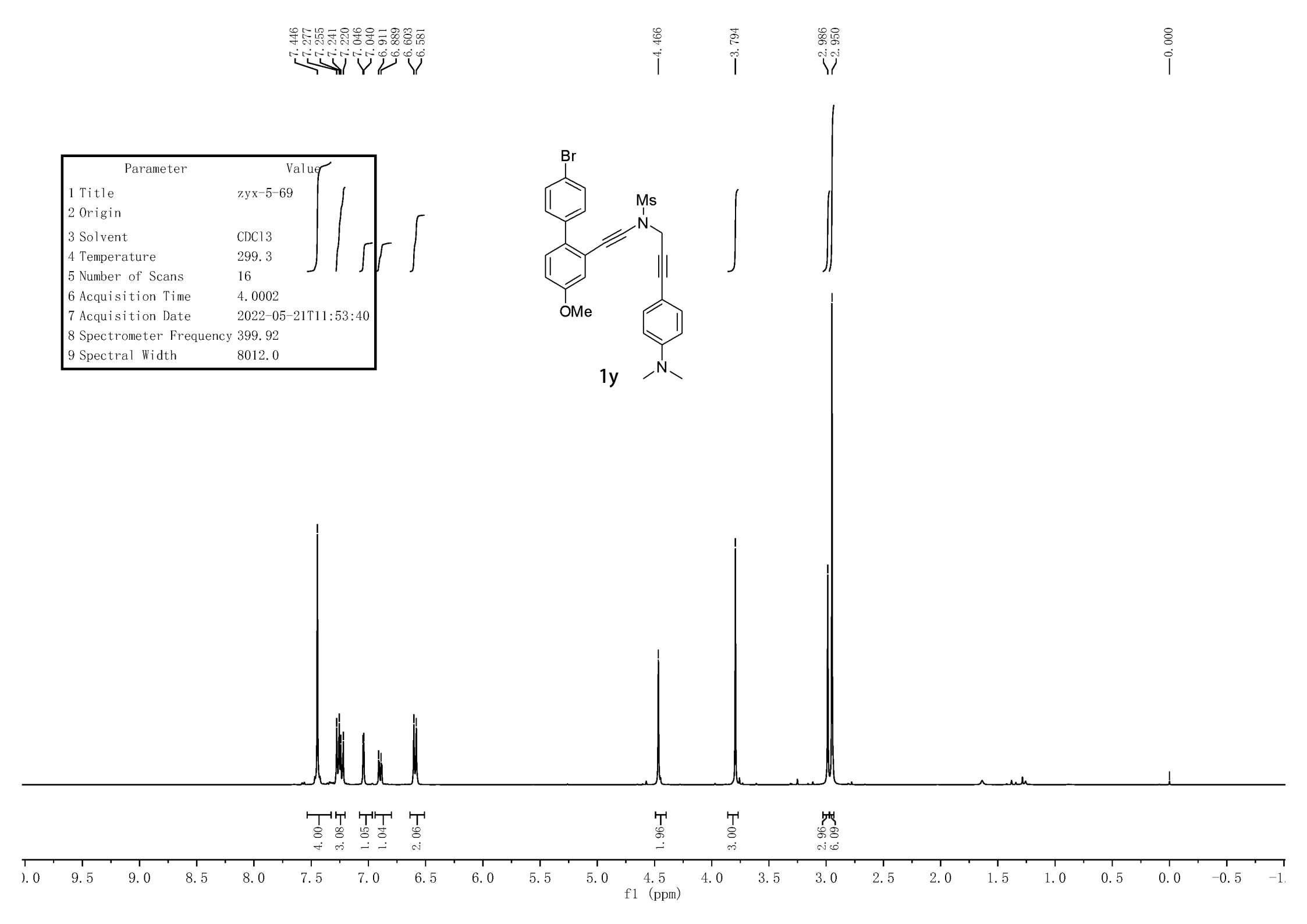
Parameter	Value
1 Title	ZYX-5-61-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	294.9
5 Number of Scans	53
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-17T16:43:12
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



1x

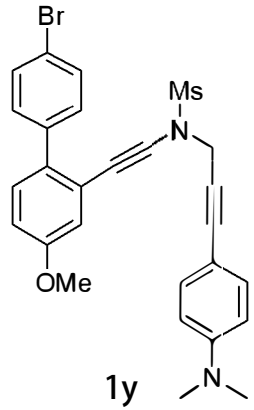




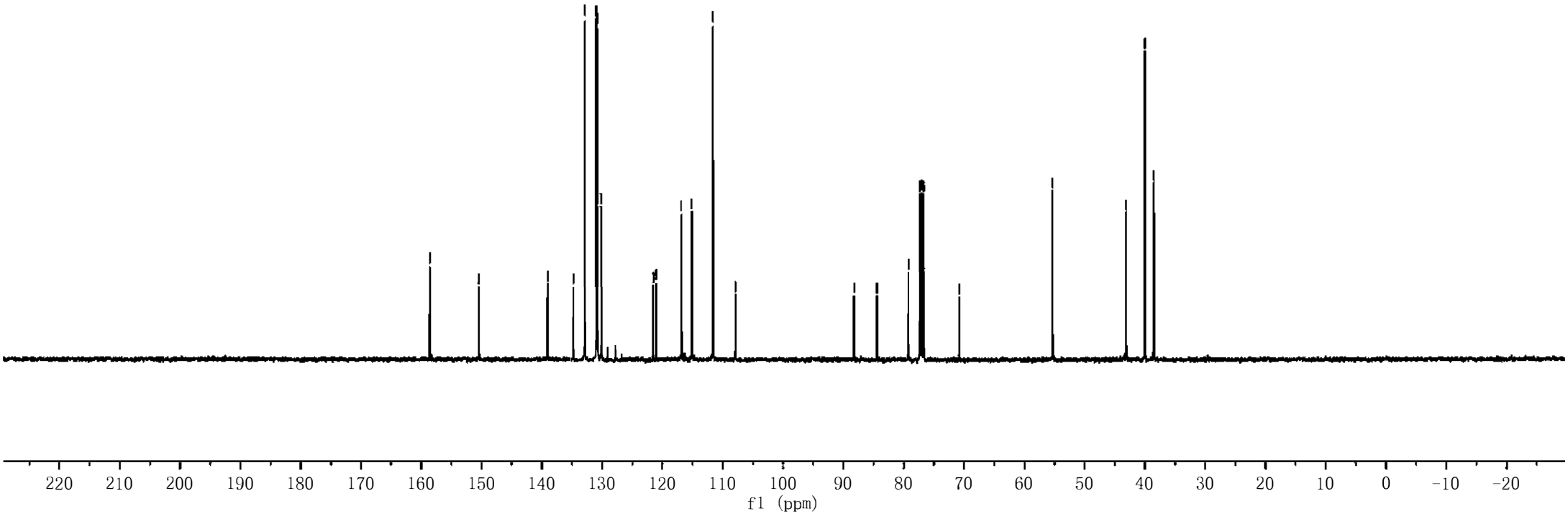

7.446
7.277
7.255
7.241
7.220
7.046
7.040
6.911
6.889
6.603
6.581
4.466
3.794
2.986
2.950
0.000
Parameter Value
1 Title zyx-5-69
2 Origin
3 Solvent CDCl3
4 Temperature 299.3
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-05-21T11:53:40
8 Spectrometer Frequency 399.92
9 Spectral Width 8012.0
Br
Ms
N
OMe
N
1y
4.00
3.08
1.05
1.04
2.06
1.96
3.00
2.96
6.09
f1 (ppm)

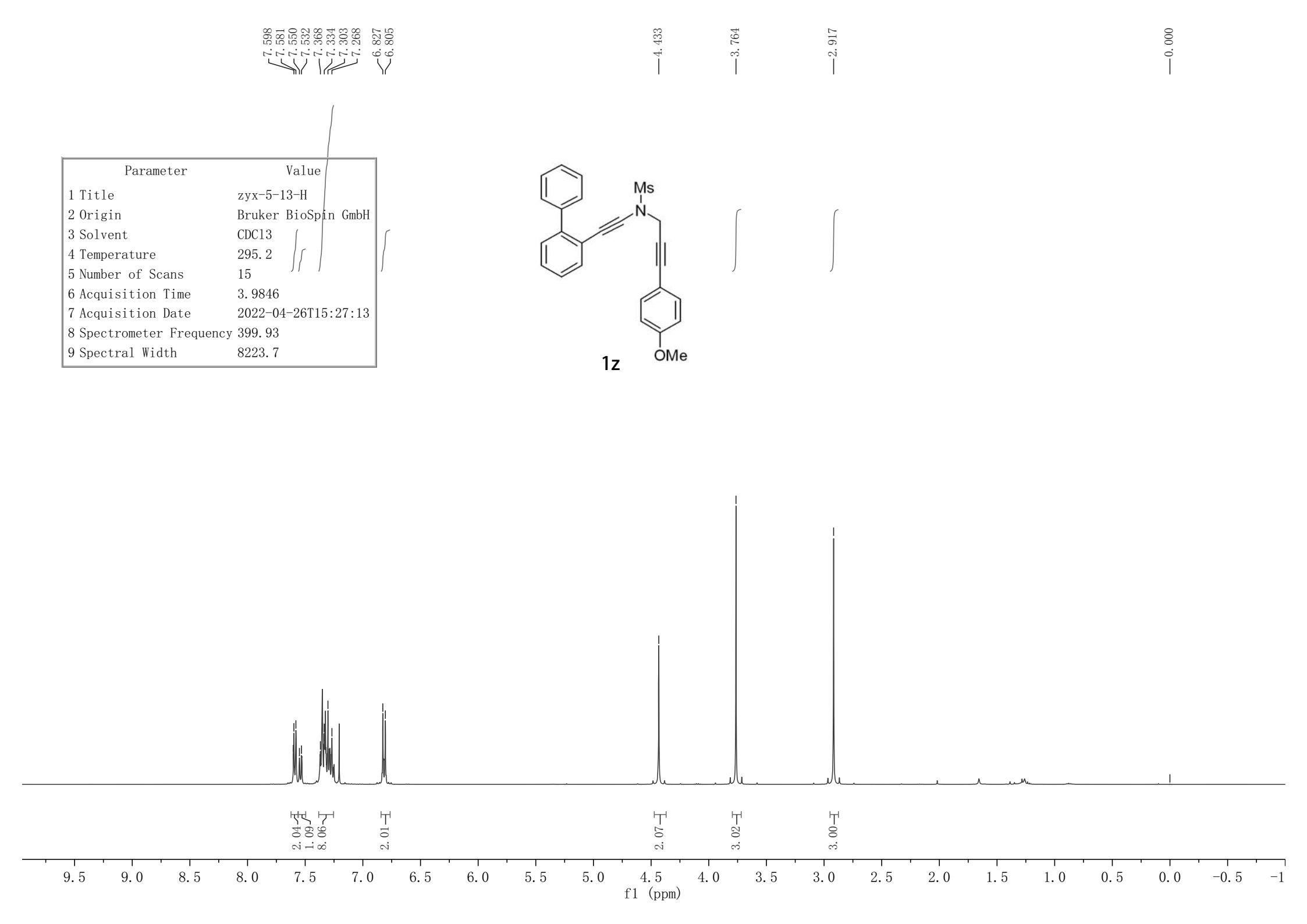
158.59
150.48
139.05
134.78
132.89
131.00
130.84
130.18
121.49
121.02
116.83
115.10
111.64
107.90
88.23
84.43
79.16
77.32
77.00
76.68
70.78
55.36
43.12
40.00
38.51

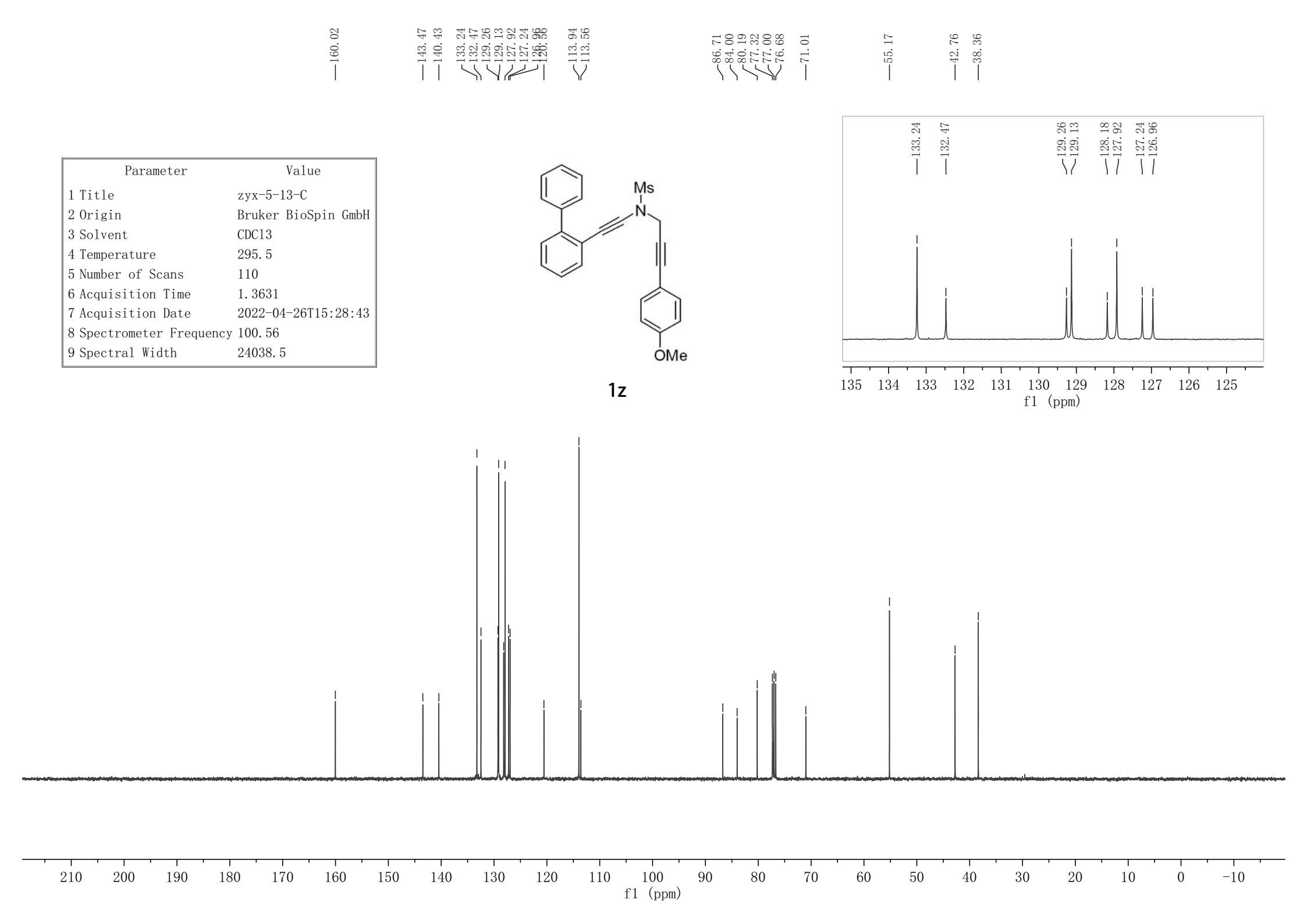
Parameter	Value
1 Title	zyx-5-69
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.1
5 Number of Scans	300
6 Acquisition Time	1.0000
7 Acquisition Date	2022-05-21T12:05:57
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

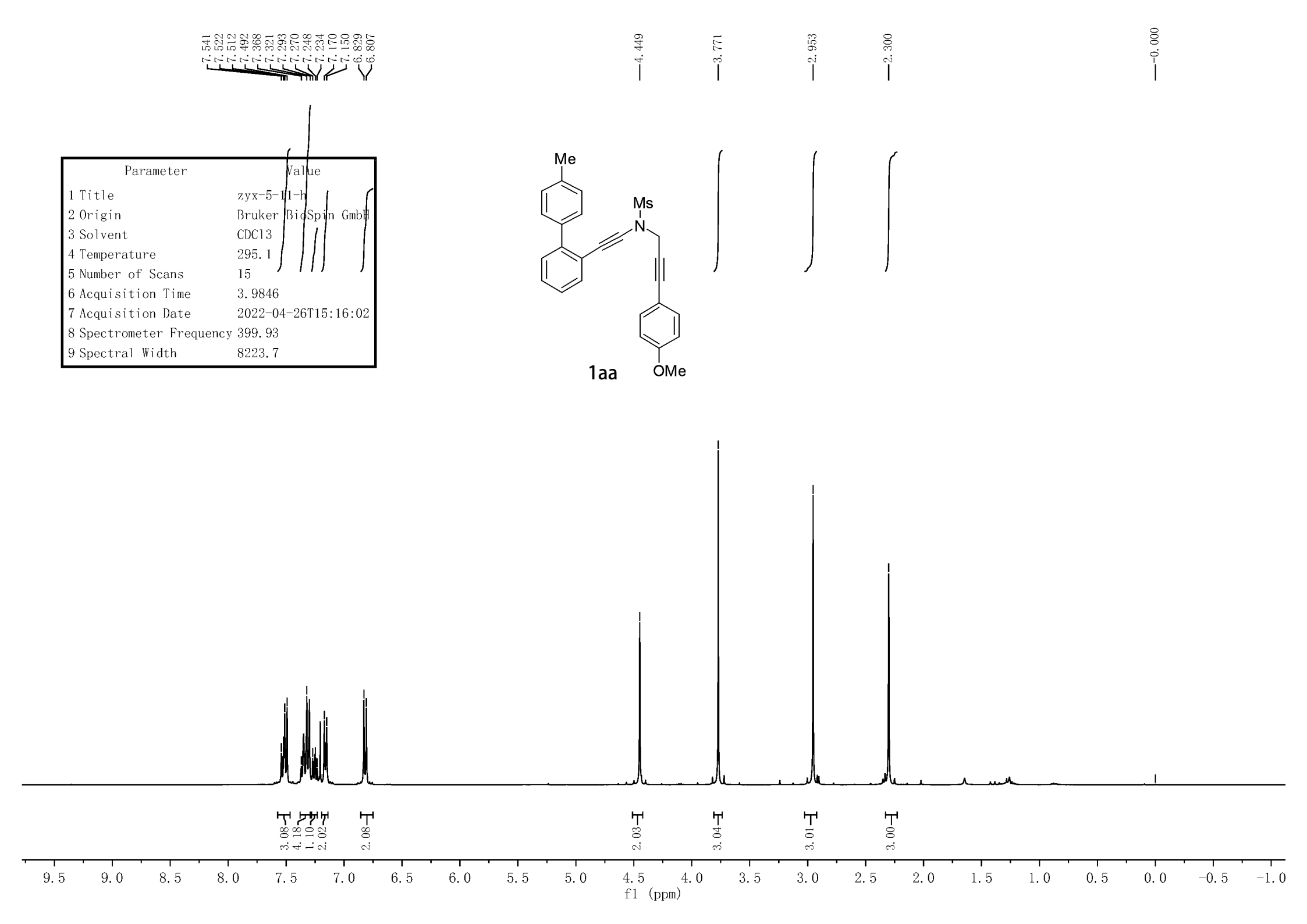


1y



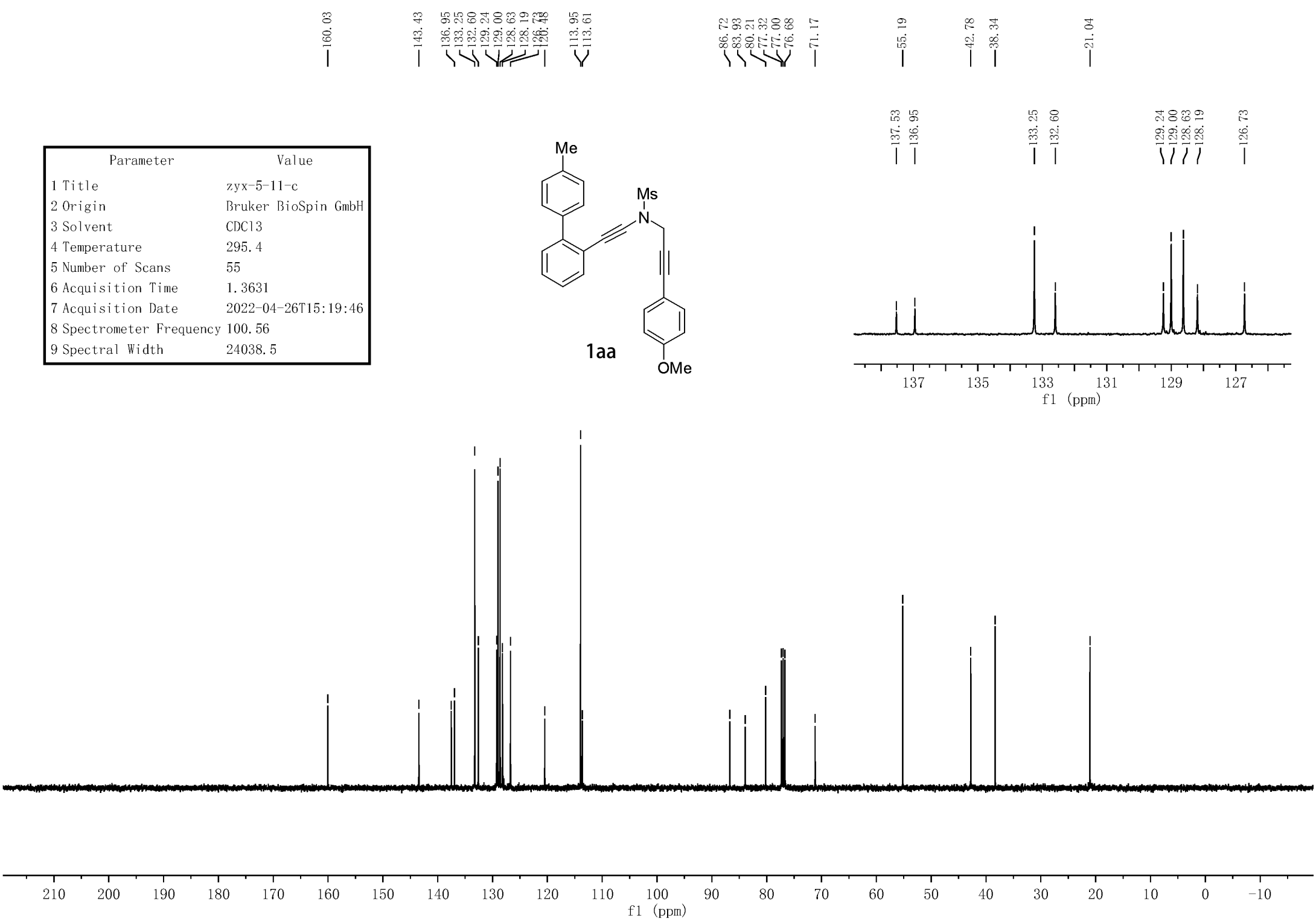

7.598
7.581
7.550
7.532
7.368
7.334
7.303
7.268
6.827
6.805
4.433
3.764
2.917
0.000
Parameter Value
1 Title zyx-5-13-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.2
5 Number of Scans 15
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-26T15:27:13
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
OMe
1z
2.04
1.09
8.06
2.01
2.07
3.02
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 -1
f1 (ppm)

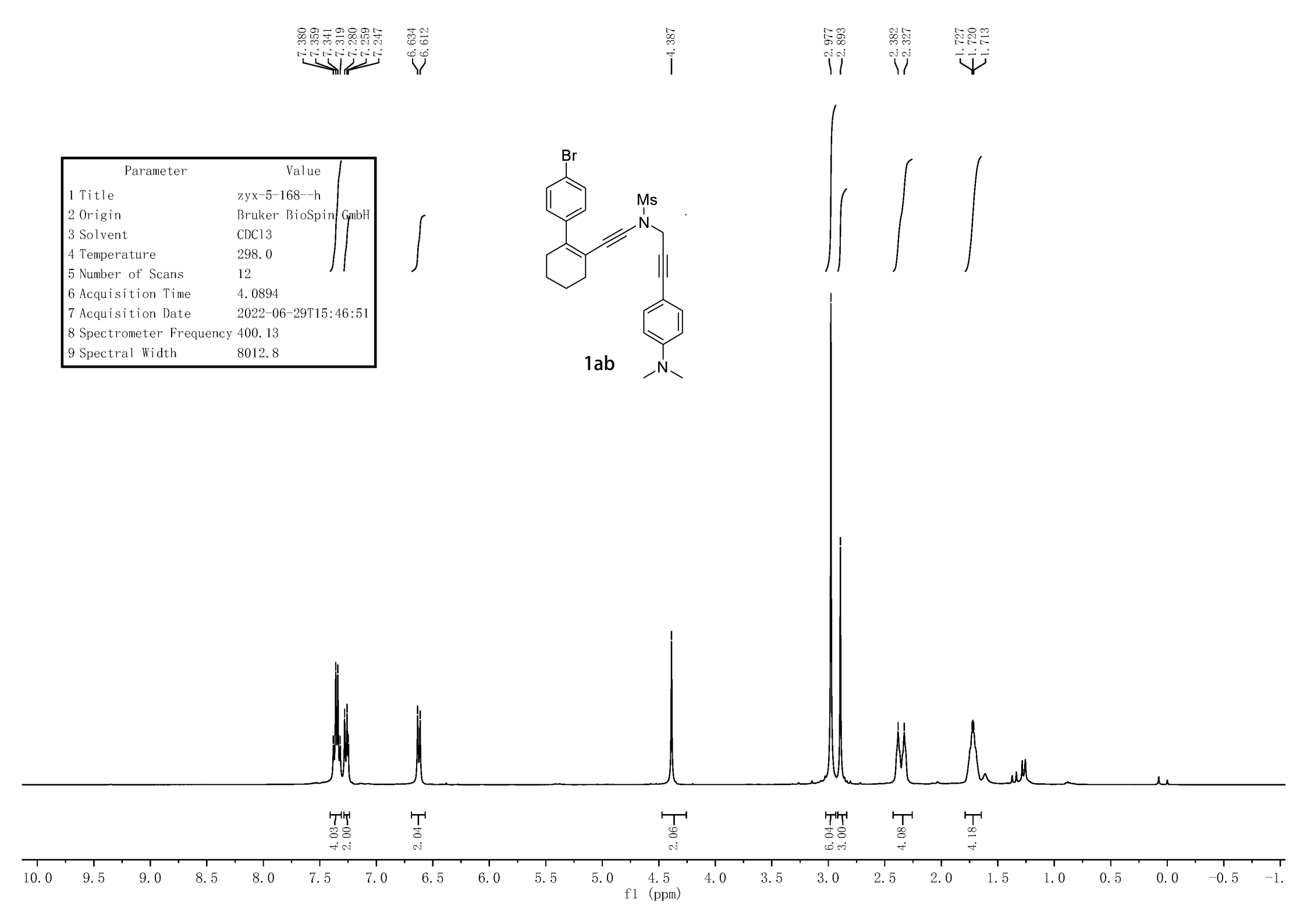

160.02
143.47
140.43
133.24
132.47
129.26
129.13
127.92
127.24
126.96
120.58
113.94
113.56
86.71
84.00
80.19
77.32
77.00
76.68
71.01
55.17
42.76
38.36
Parameter Value
1 Title zyx-5-13-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.5
5 Number of Scans 110
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-26T15:28:43
8 Spectrometer Frequency 100.56
9 Spectral Width 24038.5
Ms
N
OMe
1z
133.24
132.47
129.26
129.13
128.18
127.92
127.24
126.96
135 134 133 132 131 130 129 128 127 126 125
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)

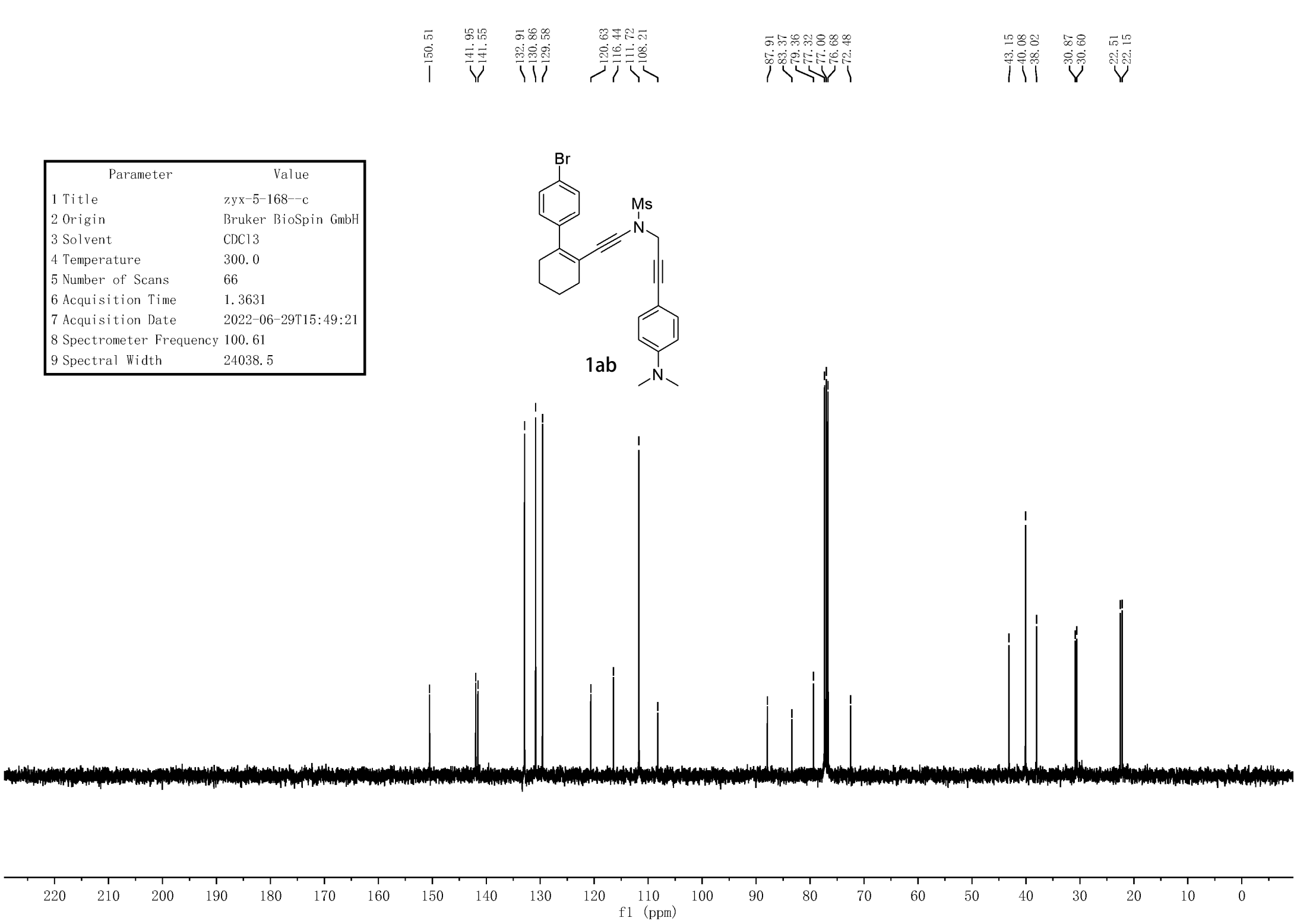

7.541
7.522
7.512
7.492
7.368
7.321
7.293
7.270
7.248
7.234
7.170
7.150
6.829
6.807
4.449
3.771
2.953
2.300
-0.000
Parameter Value
1 Title zyx-5-11-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.1
5 Number of Scans 15
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-26T15:16:02
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Me
Ms
N
OMe
1aa
3.08
4.18
1.10
2.02
2.08
2.03
3.04
3.01
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 -1.0
f1 (ppm)

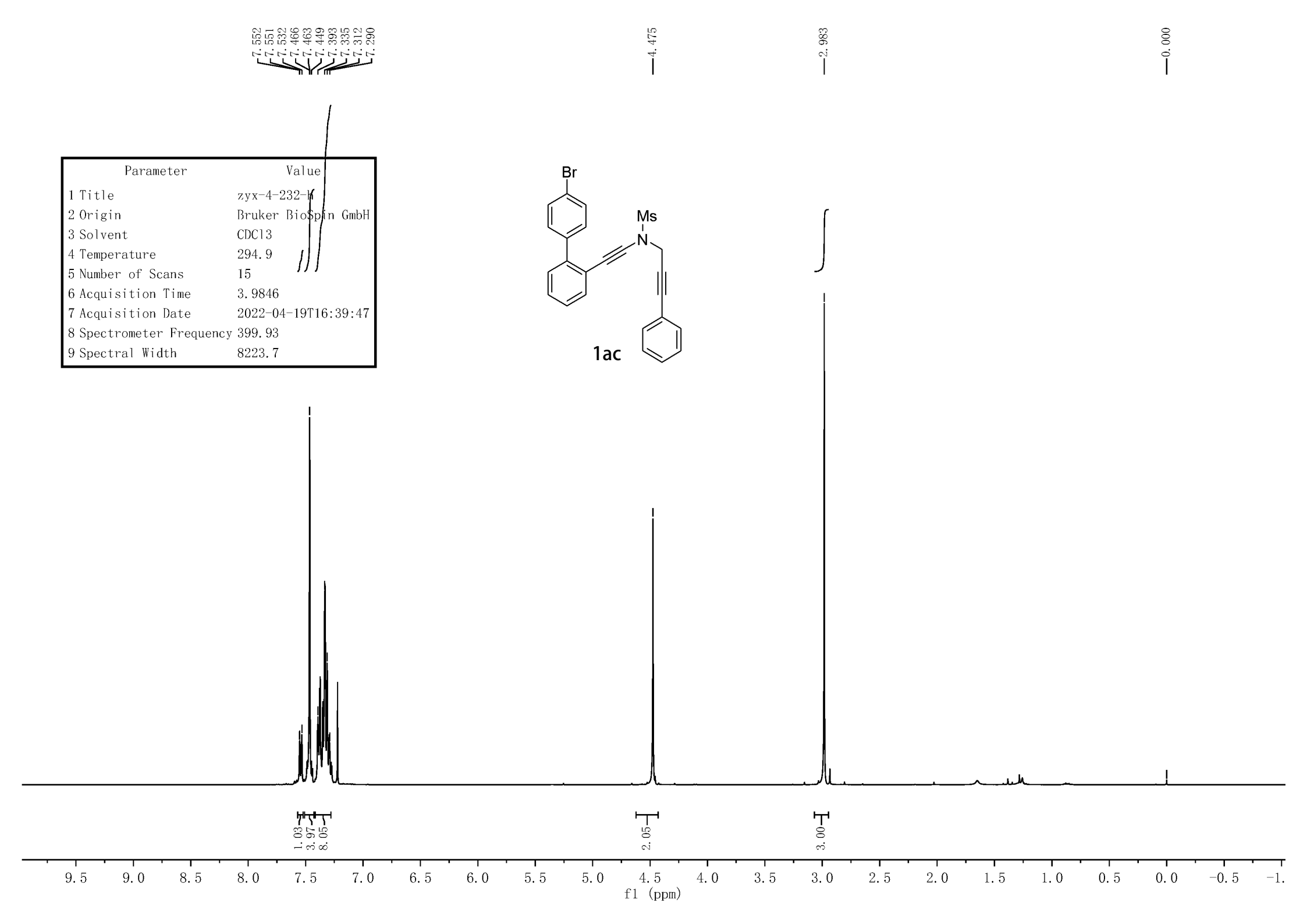
Parameter	Value
1 Title	zyx-5-11-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.4
5 Number of Scans	55
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-26T15:19:46
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

1aa



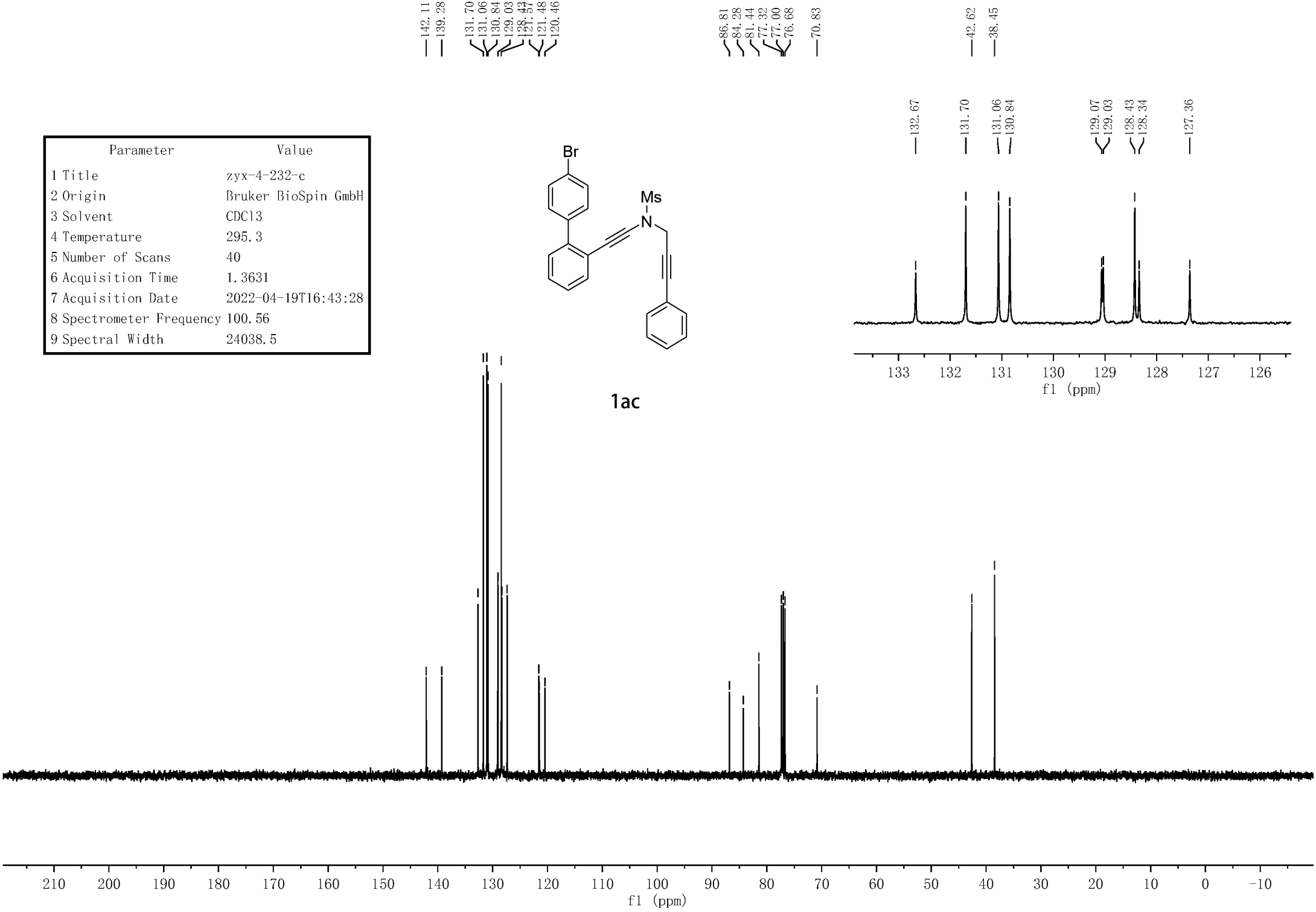

7.380
7.359
7.341
7.319
7.280
7.259
7.247
6.634
6.612
4.387
2.977
2.893
2.382
2.327
1.727
1.720
1.713
Parameter Value
1 Title zyx-5-168--h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 12
6 Acquisition Time 4.0894
7 Acquisition Date 2022-06-29T15:46:51
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Br
Ms
N
N
1ab
4.03
2.00
2.04
2.06
6.04
3.00
4.08
4.18
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 -1.
f1 (ppm)

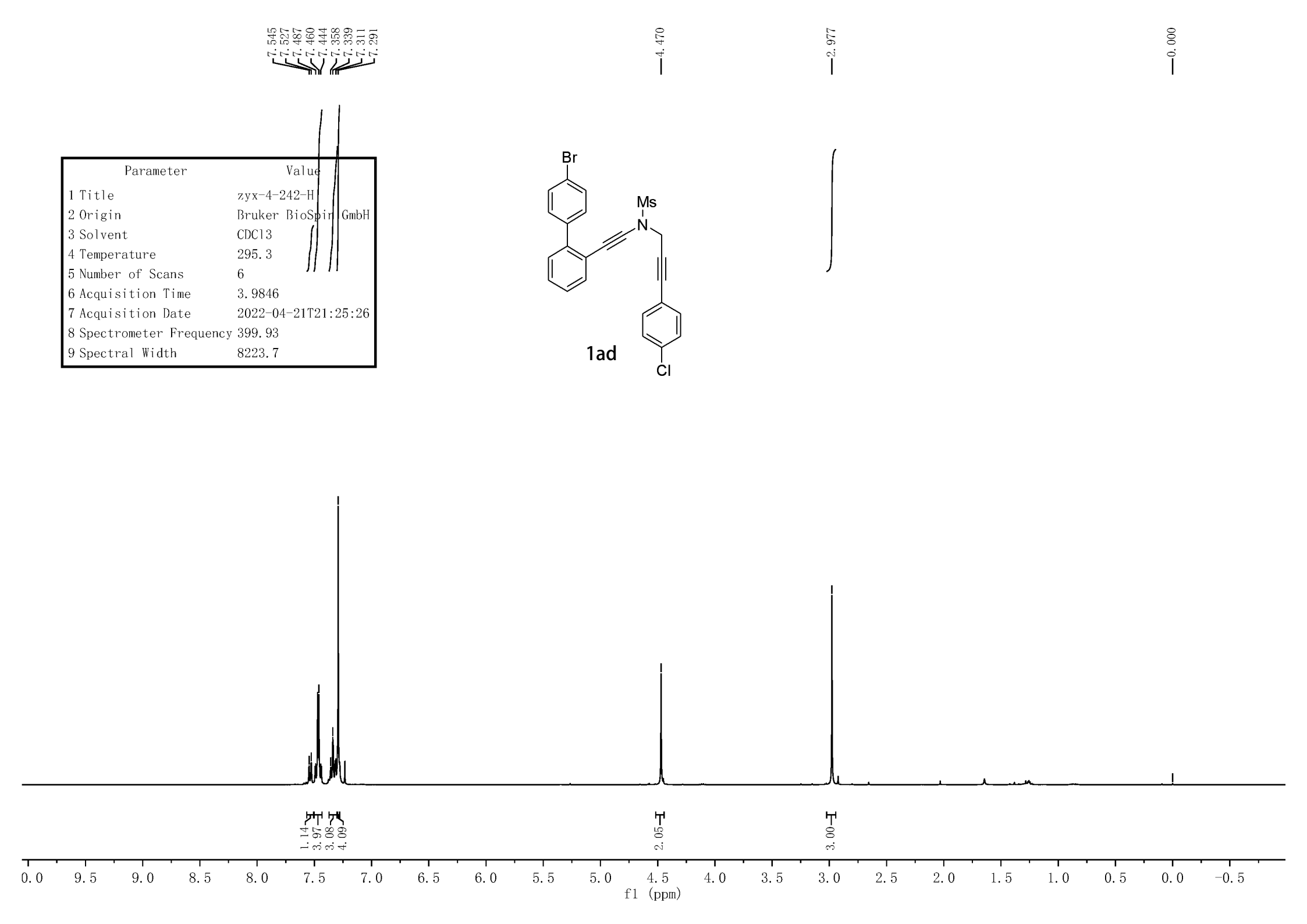

150.51
141.95
141.55
132.91
130.86
129.58
120.63
116.44
111.72
108.21
87.91
83.37
79.36
77.32
77.00
76.68
72.48
43.15
40.08
38.02
30.87
30.60
22.51
22.15
Br
Ms
N
N
1ab
Parameter Value
1 Title zyx-5-168--c
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 66
6 Acquisition Time 1.3631
7 Acquisition Date 2022-06-29T15:49:21
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.552
7.551
7.532
7.466
7.463
7.449
7.393
7.335
7.312
7.290
4.475
2.983
0.000
Parameter Value
1 Title zyx-4-232-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 294.9
5 Number of Scans 15
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-19T16:39:47
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
1ac
1.03
3.97
8.05
2.05
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 -1.
f1 (ppm)

Parameter	Value
1 Title	zyx-4-232-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.3
5 Number of Scans	40
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-19T16:43:28
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

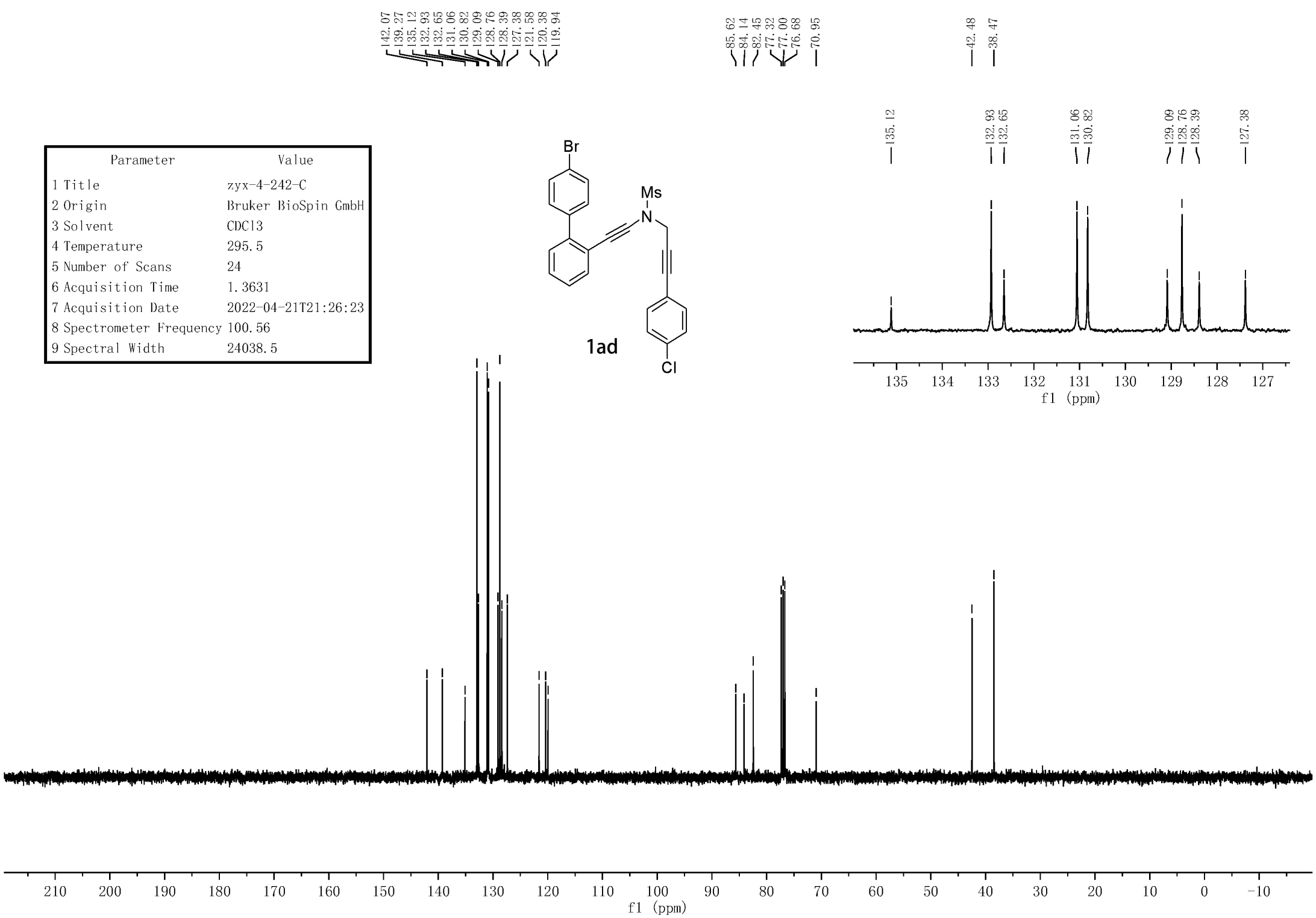
1ac

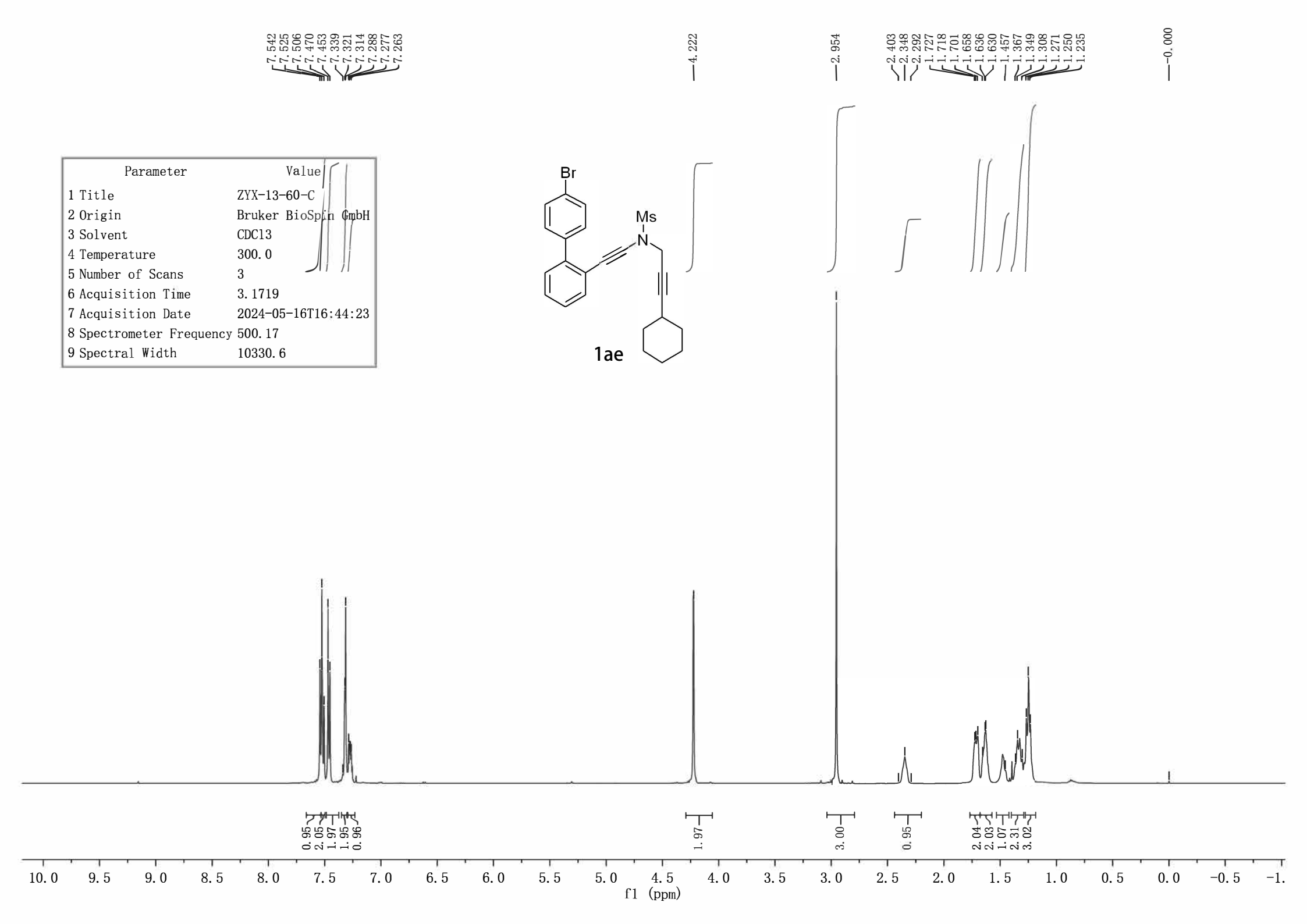



7.545
7.527
7.487
7.460
7.444
7.358
7.339
7.311
7.291
4.470
2.977
0.000
Parameter Value
1 Title zyx-4-242-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.3
5 Number of Scans 6
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-21T21:25:26
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Br
Ms
N
Cl
1ad
1.14
3.97
3.08
4.09
2.05
3.00
0.0
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)

Parameter	Value
1 Title	zyx-4-242-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	24
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-21T21:26:23
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

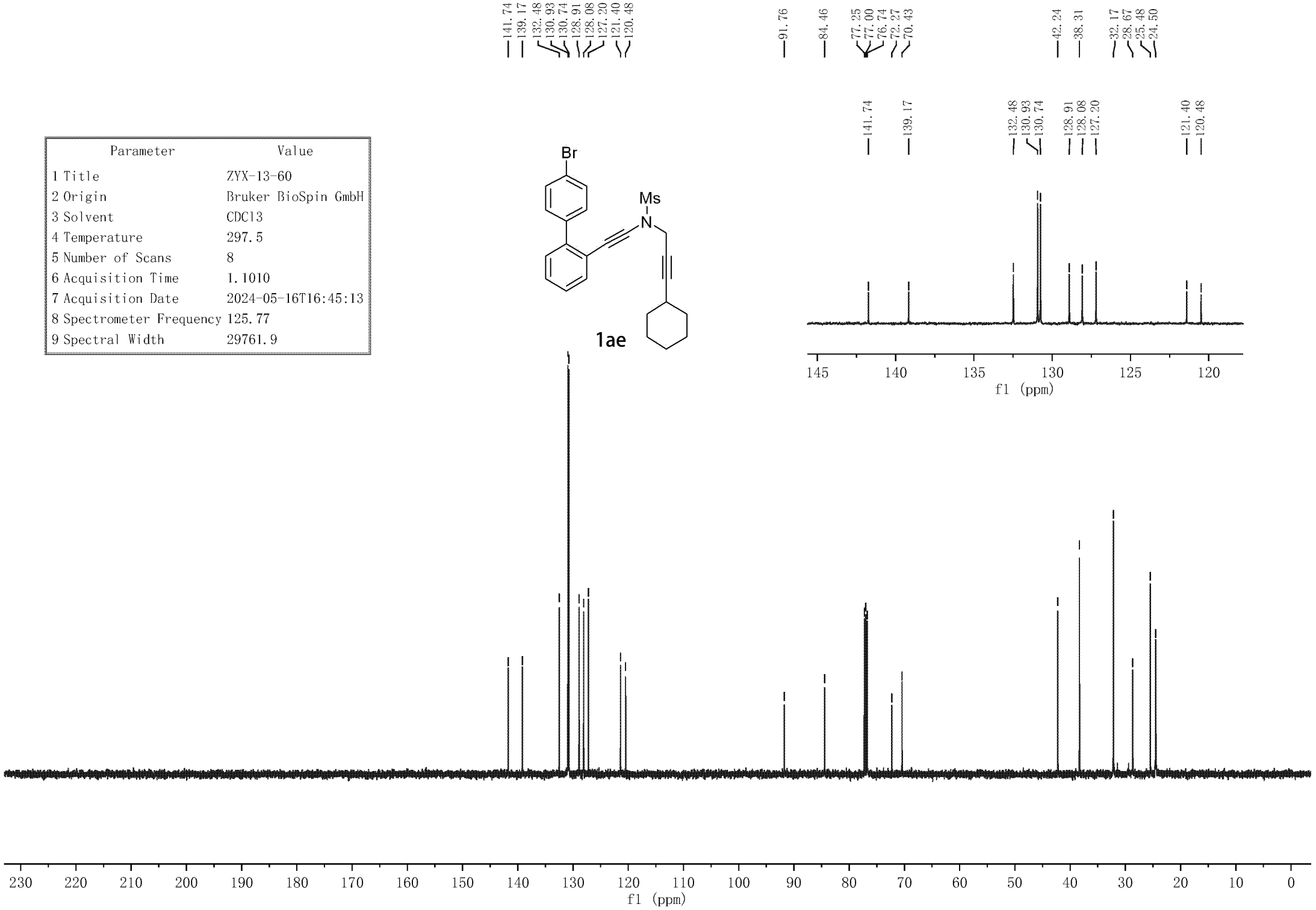
1ad

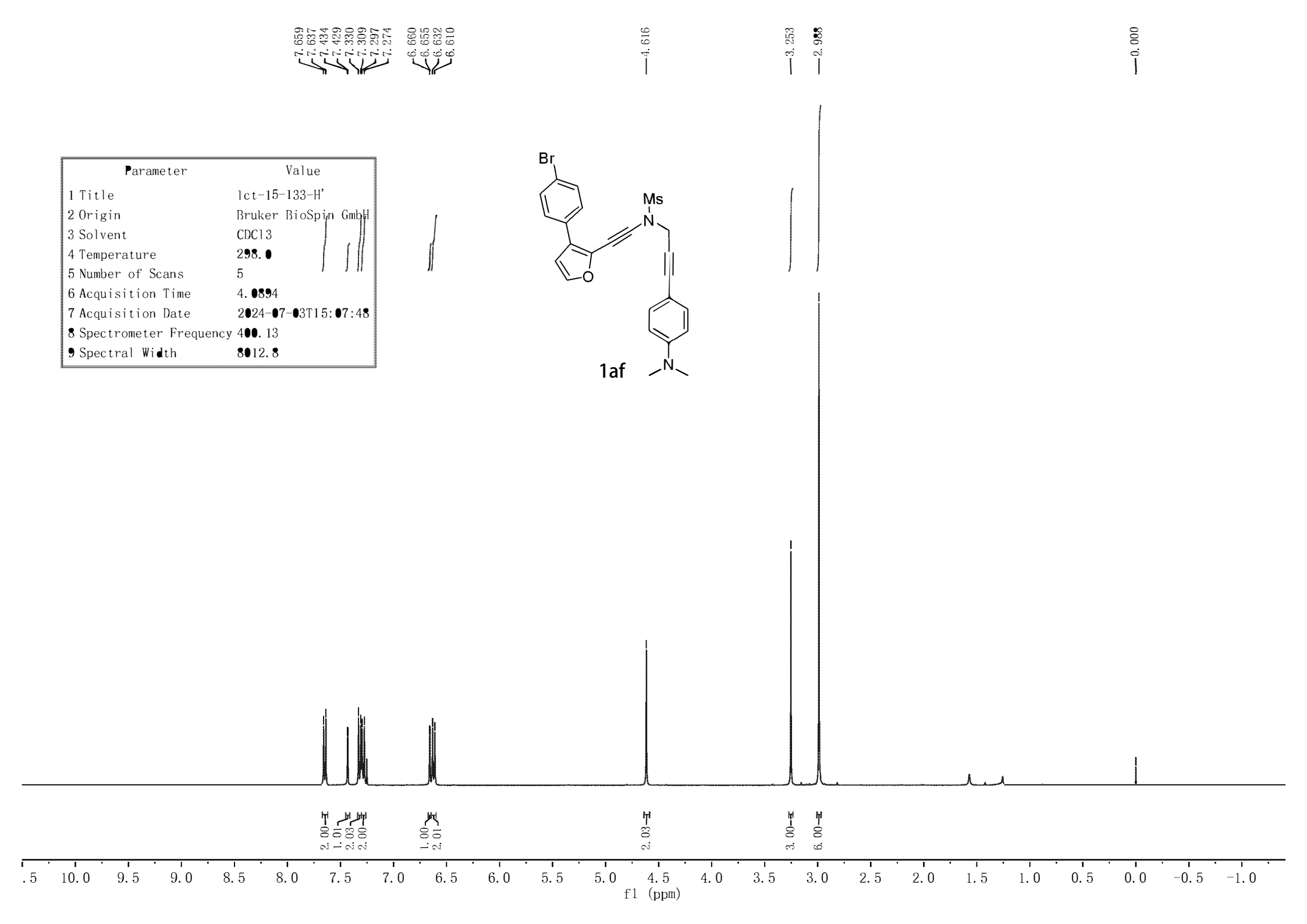


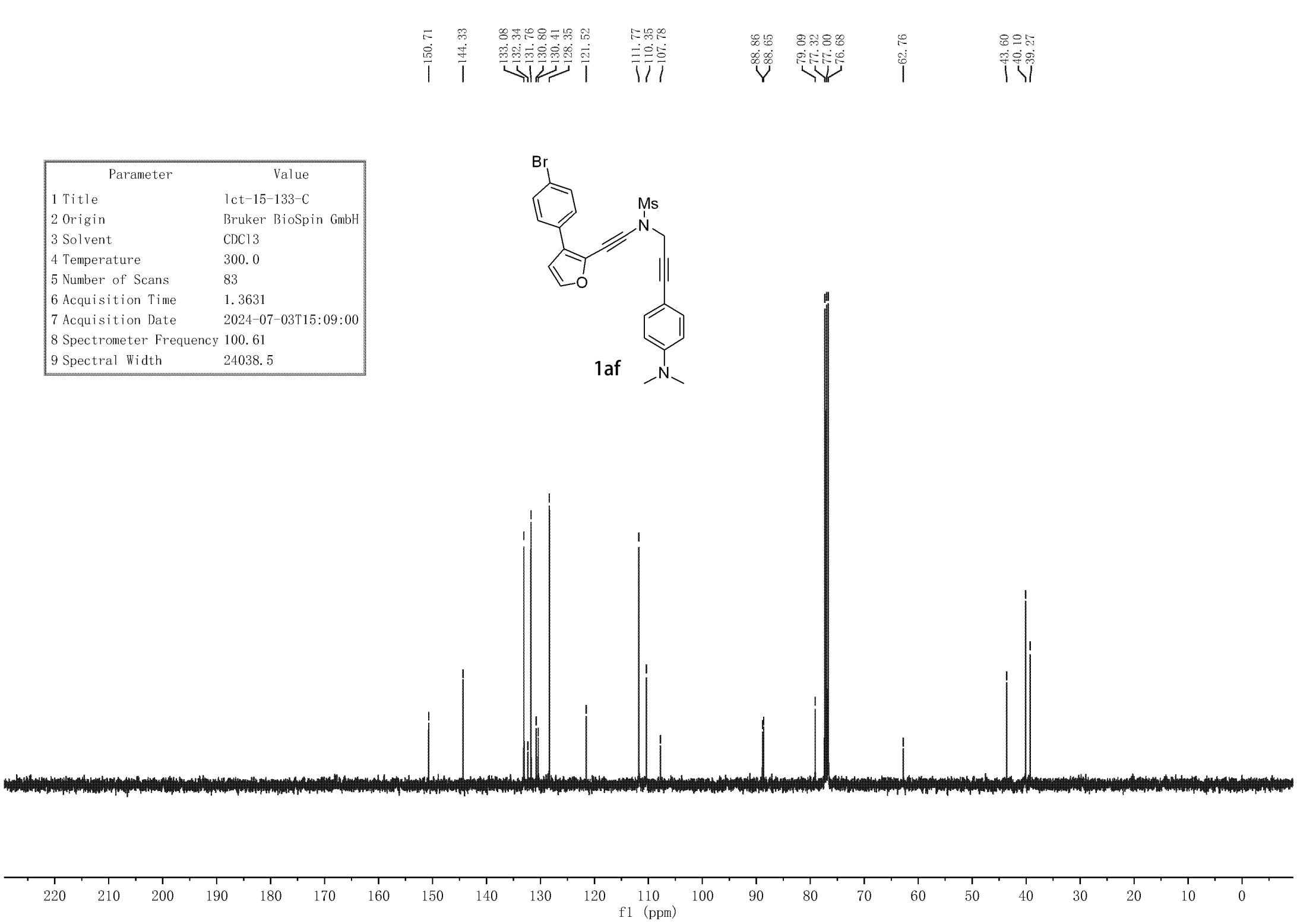

7.542
7.525
7.506
7.470
7.453
7.339
7.321
7.314
7.288
7.277
7.263
4.222
2.954
2.403
2.348
2.292
1.727
1.718
1.701
1.658
1.636
1.630
1.457
1.367
1.349
1.308
1.271
1.250
1.235
0.000
Parameter Value
1 Title ZYX-13-60-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 3
6 Acquisition Time 3.1719
7 Acquisition Date 2024-05-16T16:44:23
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
Ms
N
1ae
0.95
2.05
1.97
1.95
0.96
1.97
3.00
0.95
2.04
2.03
1.07
2.31
3.02
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
-1.
f1 (ppm)

Parameter	Value
1 Title	ZYX-13-60
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.5
5 Number of Scans	8
6 Acquisition Time	1.1010
7 Acquisition Date	2024-05-16T16:45:13
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

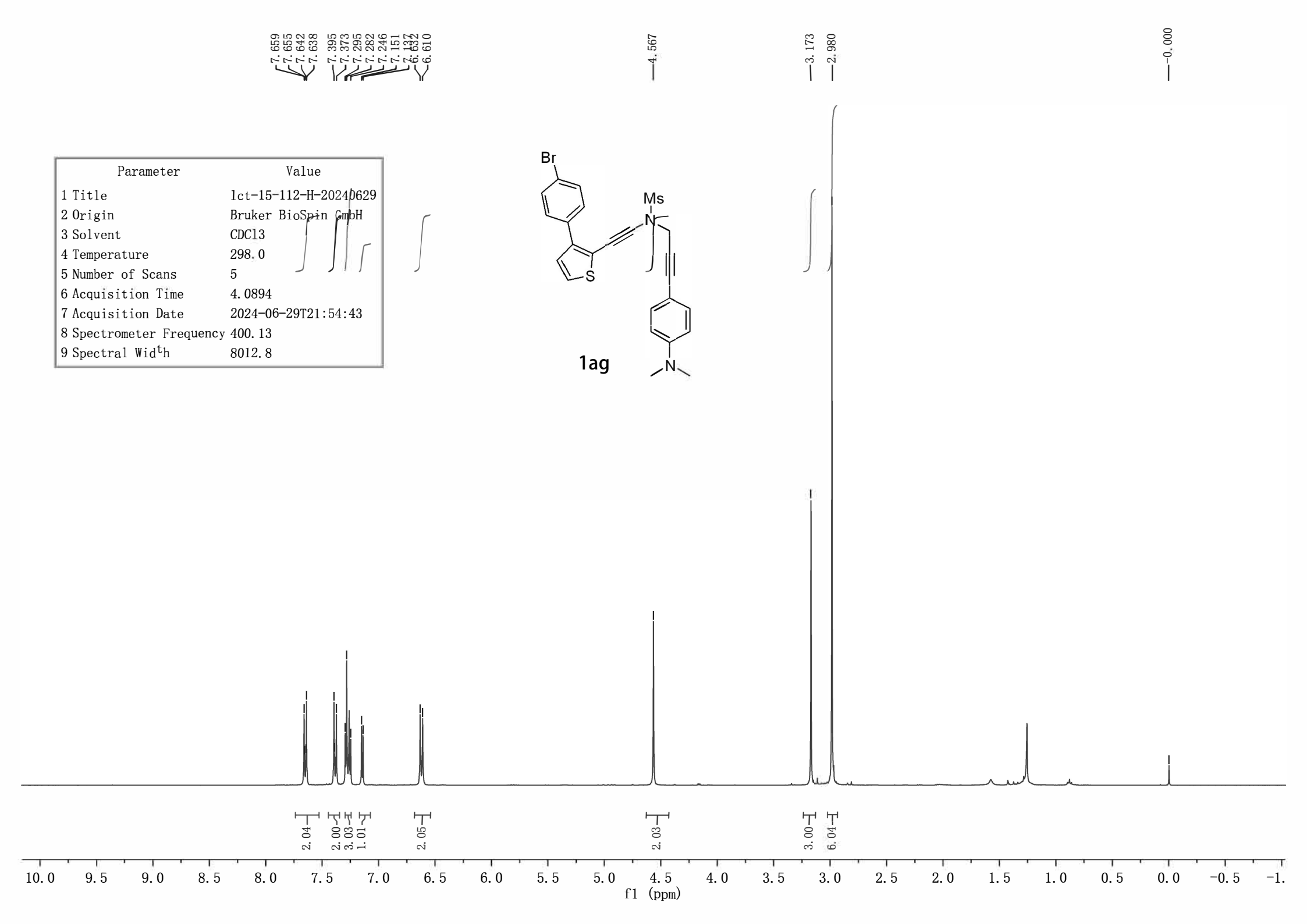
1ae

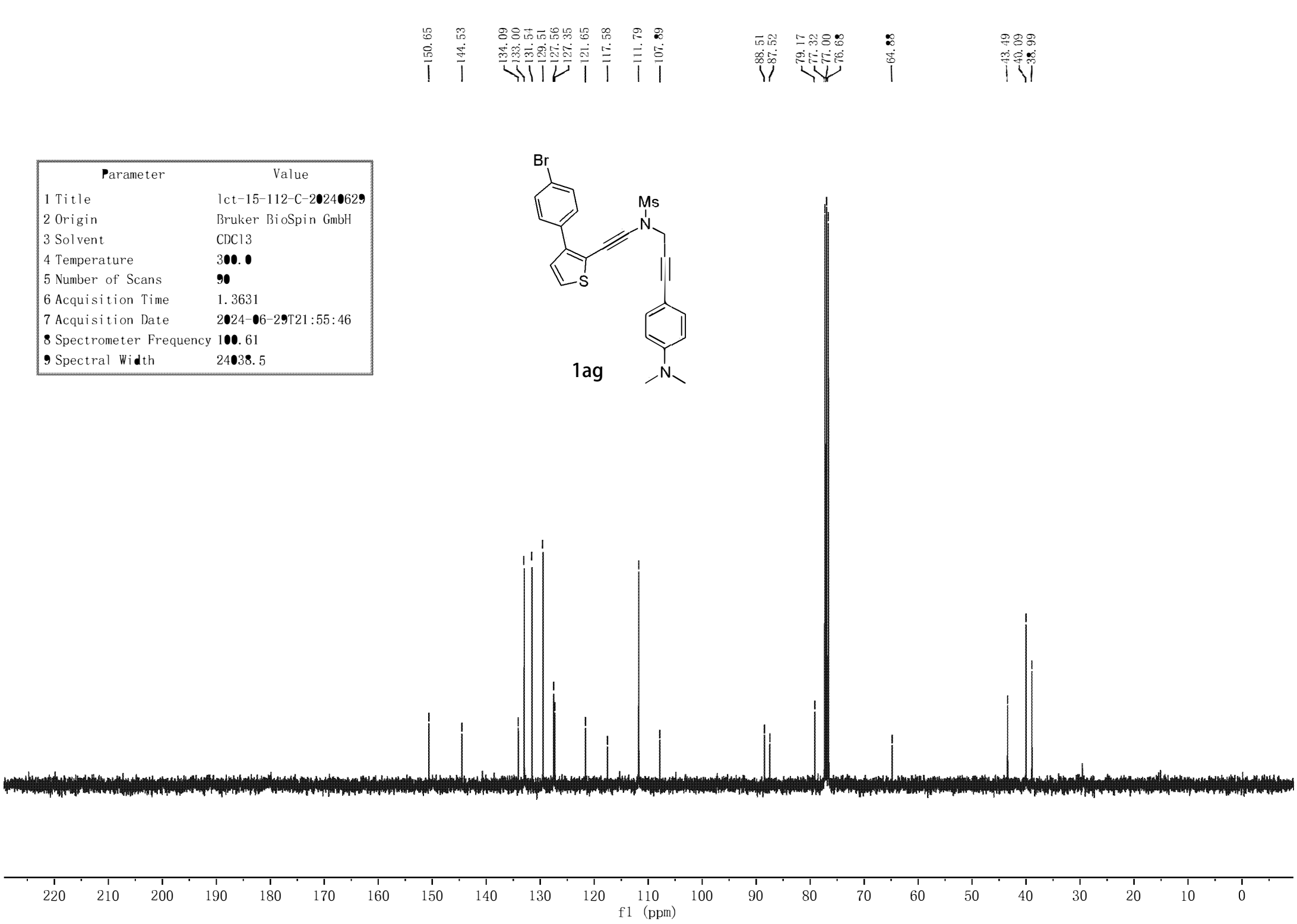



7.659
7.637
7.434
7.429
7.330
7.309
7.297
7.274
6.660
6.655
6.632
6.610
4.616
3.253
2.988
0.000
Parameter Value
1 Title lct-15-133-H'
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 5
6 Acquisition Time 4.0894
7 Acquisition Date 2024-07-03T15:07:48
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Br
Ms
N
O
N
1af
2.00
1.01
2.03
2.00
1.00
2.01
2.03
3.00
6.00
f1 (ppm)

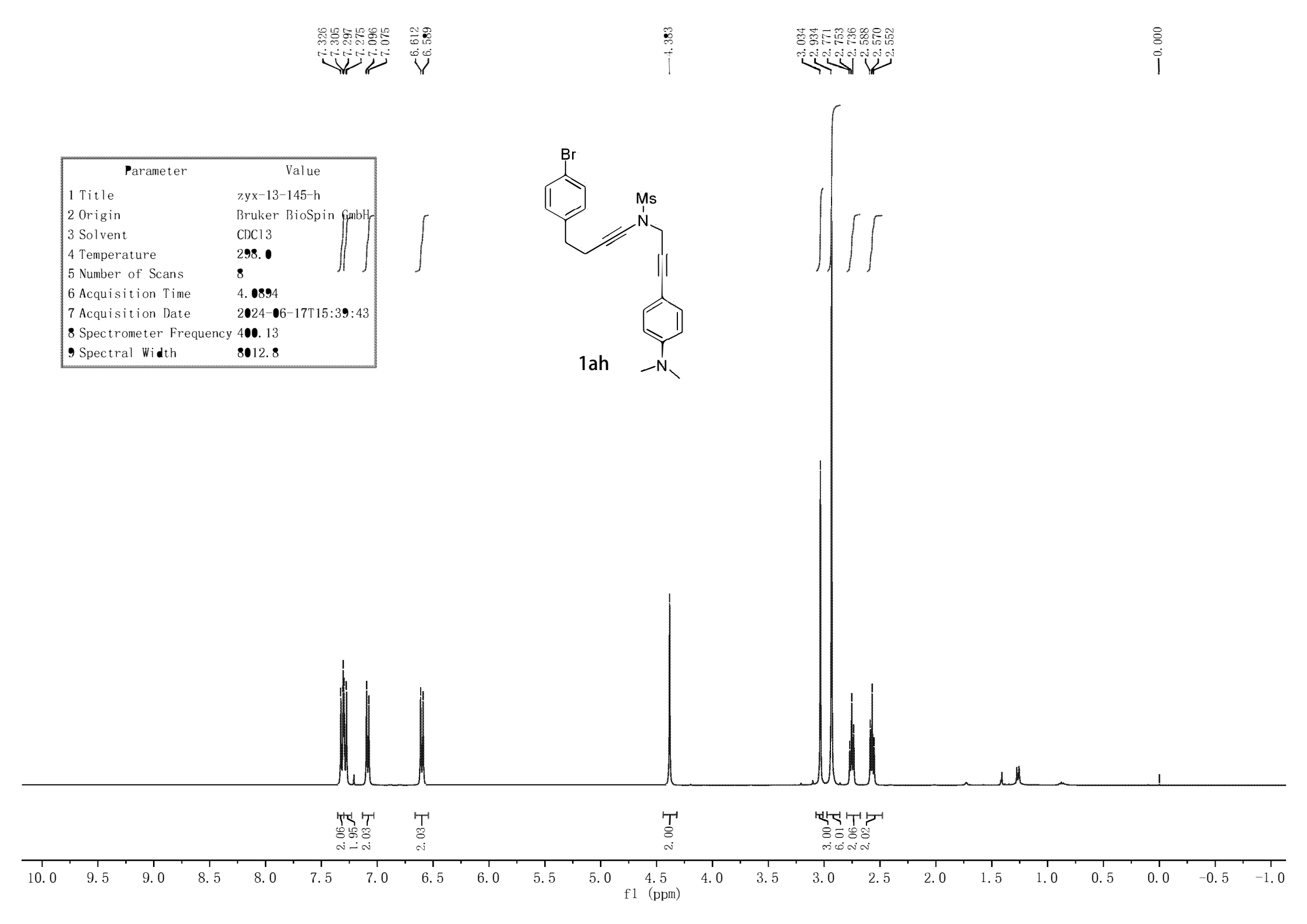


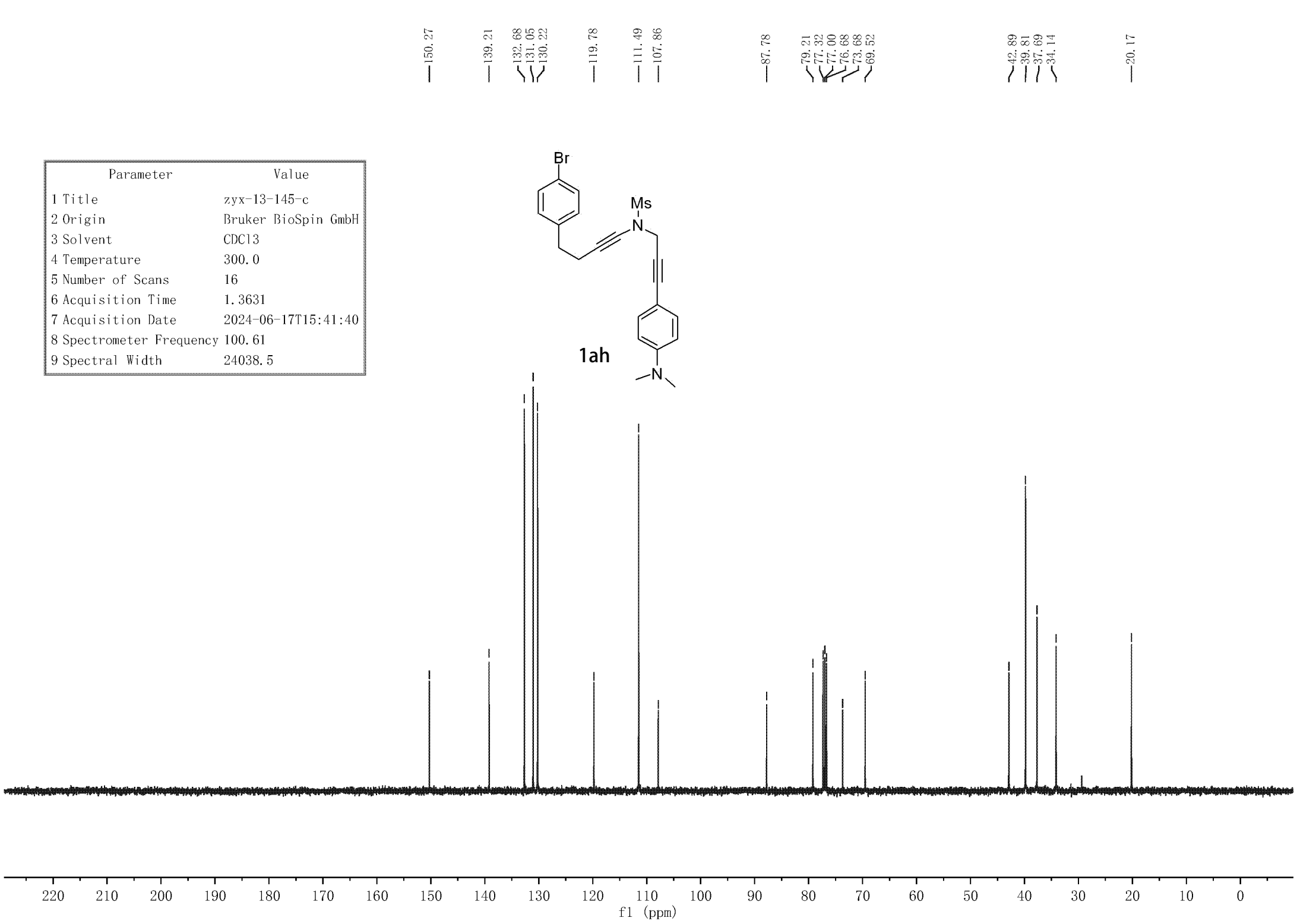
Parameter	Value
1 Title	lct-15-133-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	83
6 Acquisition Time	1.3631
7 Acquisition Date	2024-07-03T15:09:00
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5


7.659
7.655
7.642
7.638
7.395
7.373
7.295
7.282
7.246
7.151
7.137
6.632
6.610
4.567
3.173
2.980
0.000
Parameter Value
1 Title lct-15-112-H-20240629
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 2024-06-29T21:54:43
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Br
Ms
N
S
N
1ag
2.04
2.00
3.03
1.01
2.05
2.03
3.00
6.04
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
-1.
f1 (ppm)

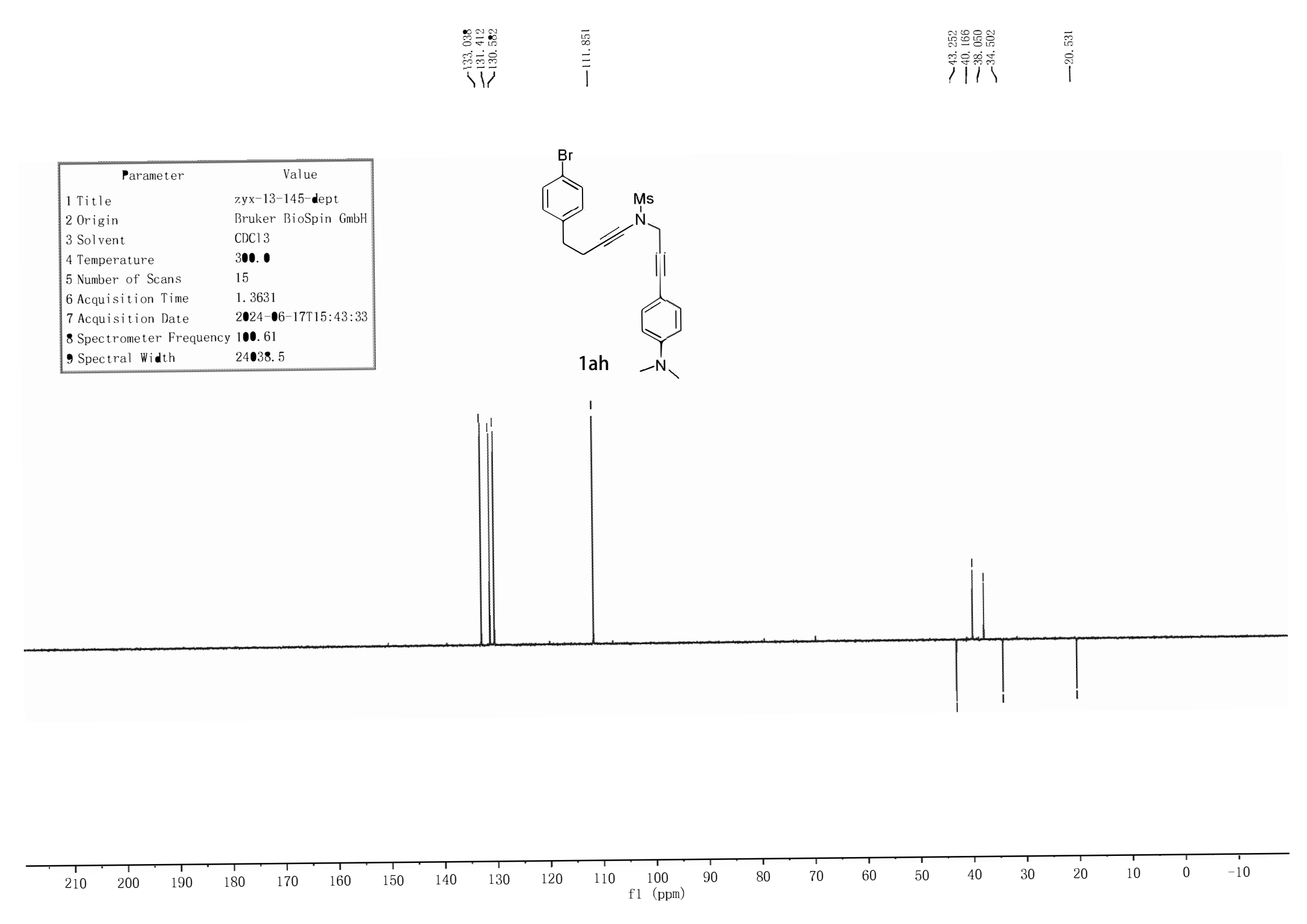


Parameter	Value
1 Title	lct-15-112-C-20240629
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	90
6 Acquisition Time	1.3631
7 Acquisition Date	2024-06-29T21:55:46
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5


7.326
7.305
7.297
7.275
7.096
7.075
6.612
6.589
4.383
3.034
2.934
2.771
2.753
2.736
2.588
2.570
2.552
0.000
Parameter Value
1 Title zyx-13-145-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2024-06-17T15:39:43
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Br
Ms
N
N
1ah
2.06
1.95
2.03
2.03
2.00
3.00
6.01
2.06
2.02
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 -1.0
f1 (ppm)

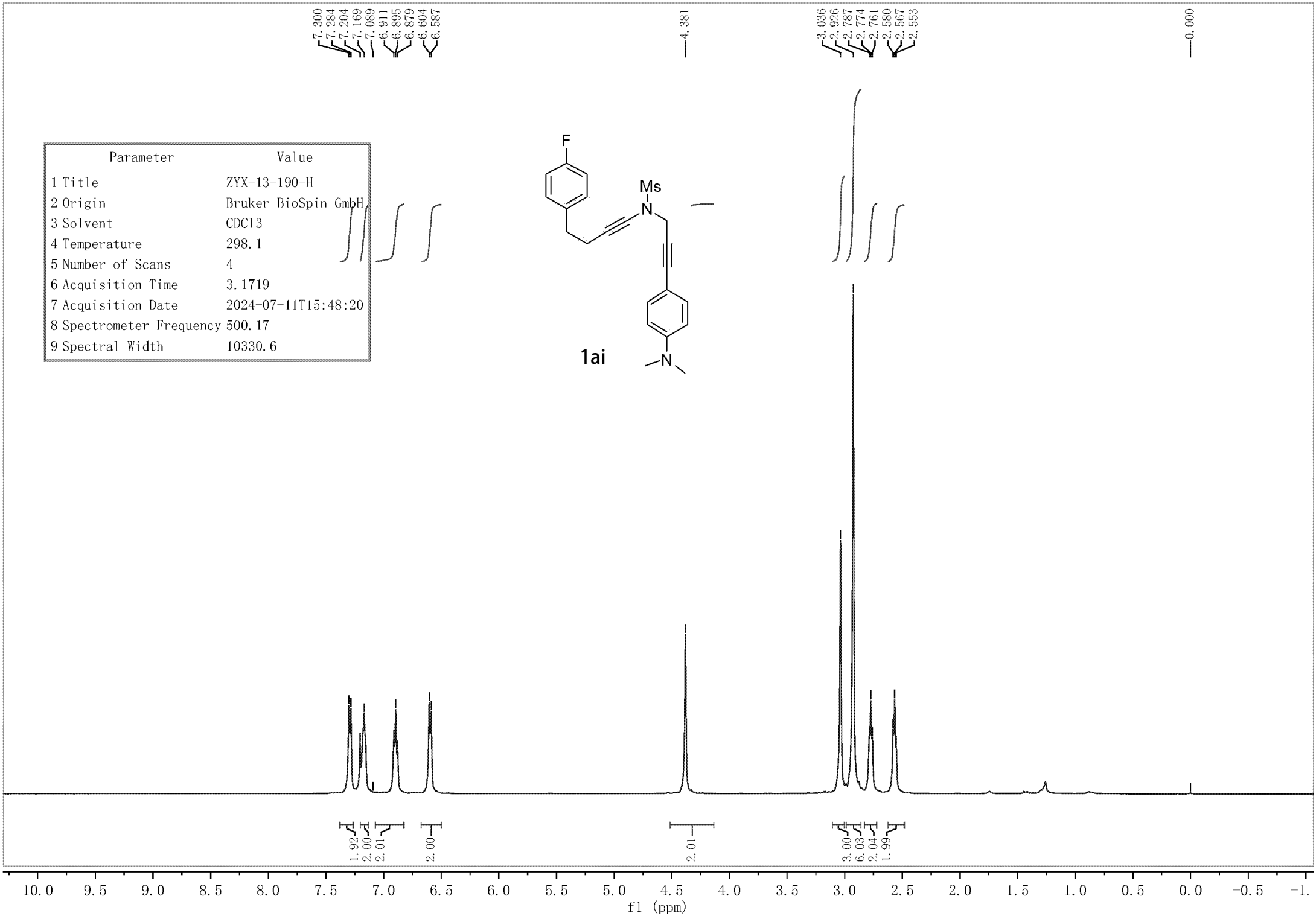


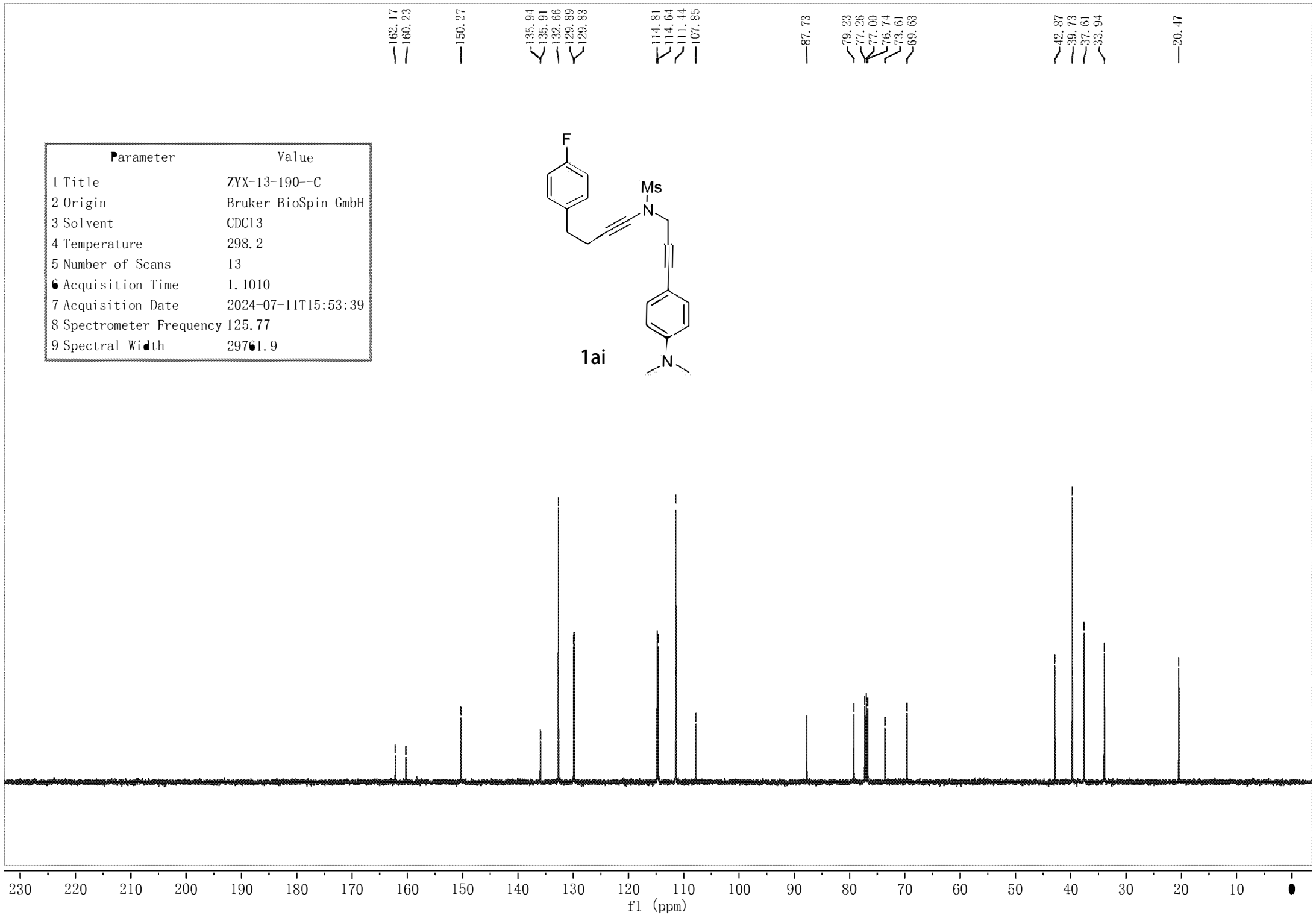
Parameter	Value
1 Title	zyx-13-145-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	16
6 Acquisition Time	1.3631
7 Acquisition Date	2024-06-17T15:41:40
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5


133.038
131.412
130.582
111.851
43.252
40.166
38.050
34.502
20.531
Parameter Value
1 Title zyx-13-145-dept
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 2024-06-17T15:43:33
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Br
Ms
N
1ah
N
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)

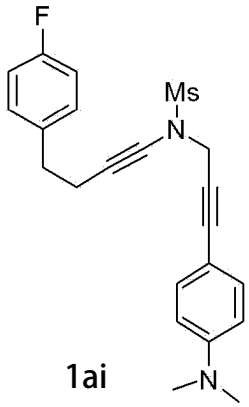
Parameter	Value
1 Title	ZYX-13-190-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	4
6 Acquisition Time	3.1719
7 Acquisition Date	2024-07-11T15:48:20
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6

1ai

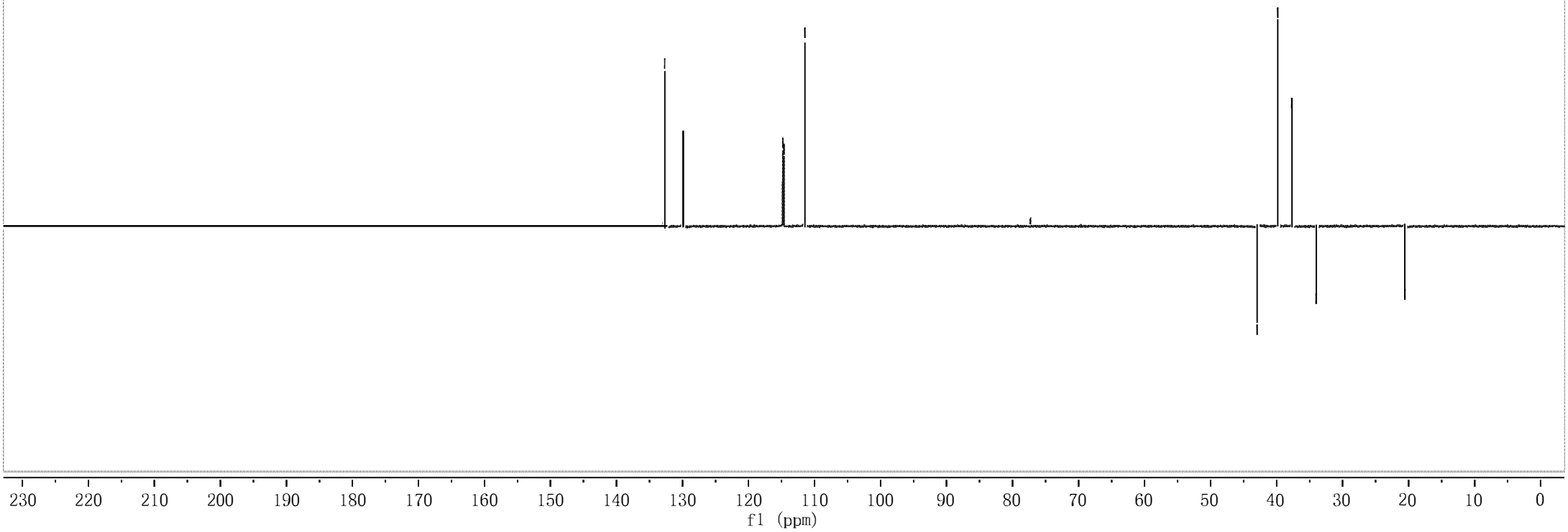



162.17
160.23
150.27
135.94
135.91
132.66
129.89
129.83
114.81
114.64
111.44
107.85
87.73
79.23
77.26
77.00
76.74
73.61
69.63
42.87
39.73
37.61
33.94
20.47
Parameter Value
1 Title ZYX-13-190--C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.2
5 Number of Scans 13
6 Acquisition Time 1.1010
7 Acquisition Date 2024-07-11T15:53:39
8 Spectrometer Frequency 125.77
9 Spectral Width 29761.9
F
Ms
N
N
1ai
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Parameter	Value
1 Title	ZYX-13-190-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.3
5 Number of Scans	12
6 Acquisition Time	1.1010
7 Acquisition Date	2024-07-11T15:55:19
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

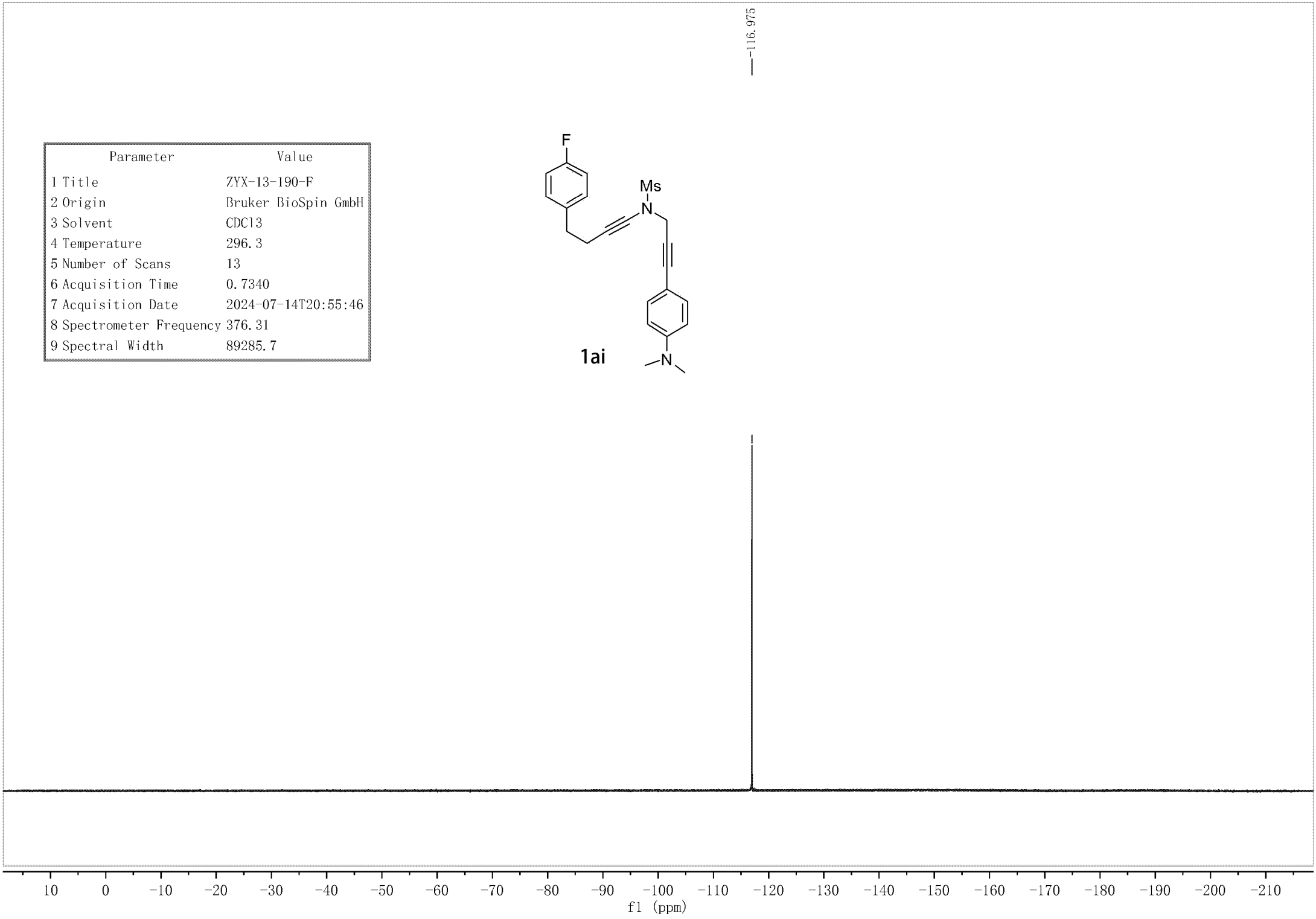


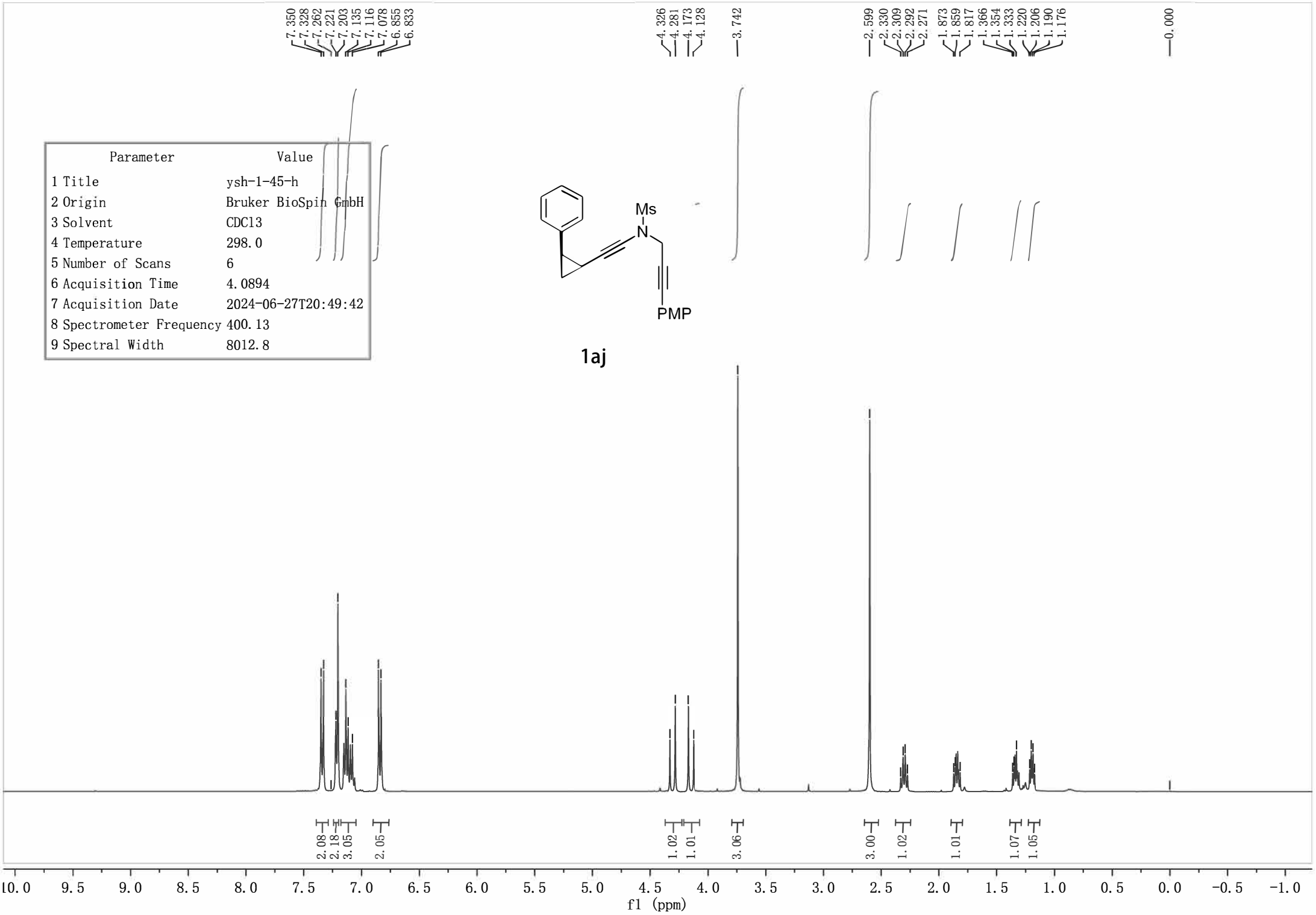
1ai

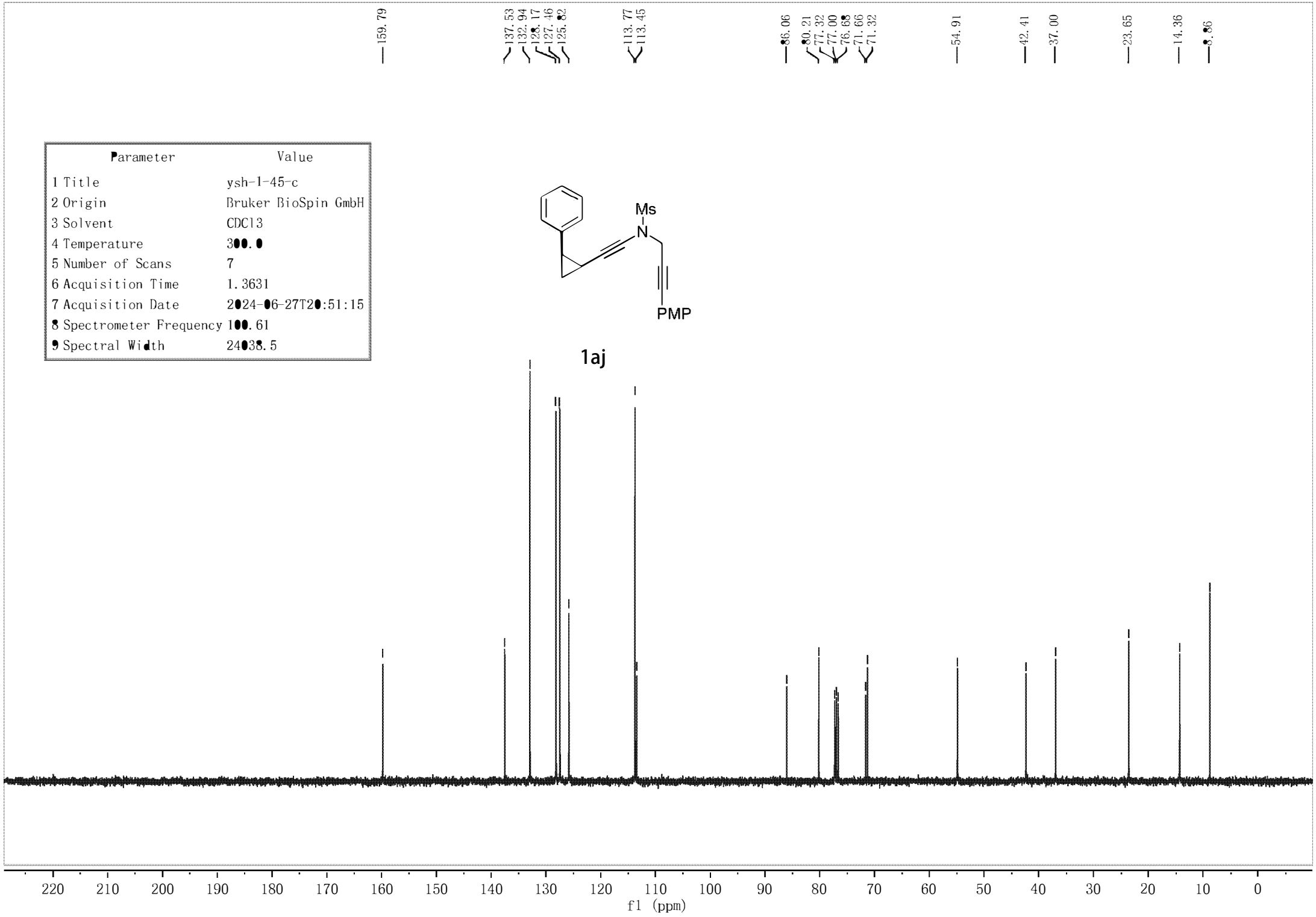


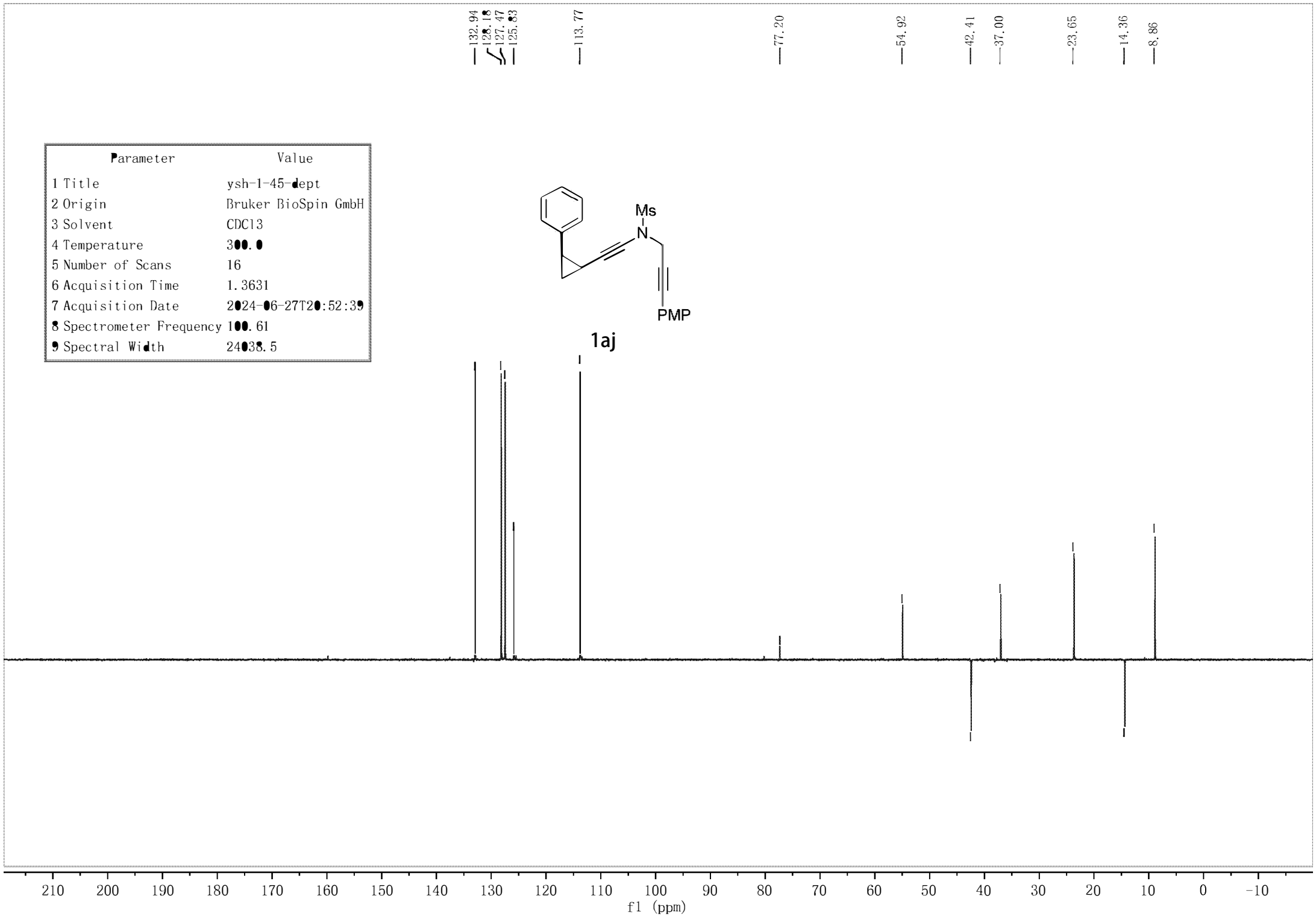
Parameter	Value
1 Title	ZYX-13-190-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.3
5 Number of Scans	13
6 Acquisition Time	0.7340
7 Acquisition Date	2024-07-14T20:55:46
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

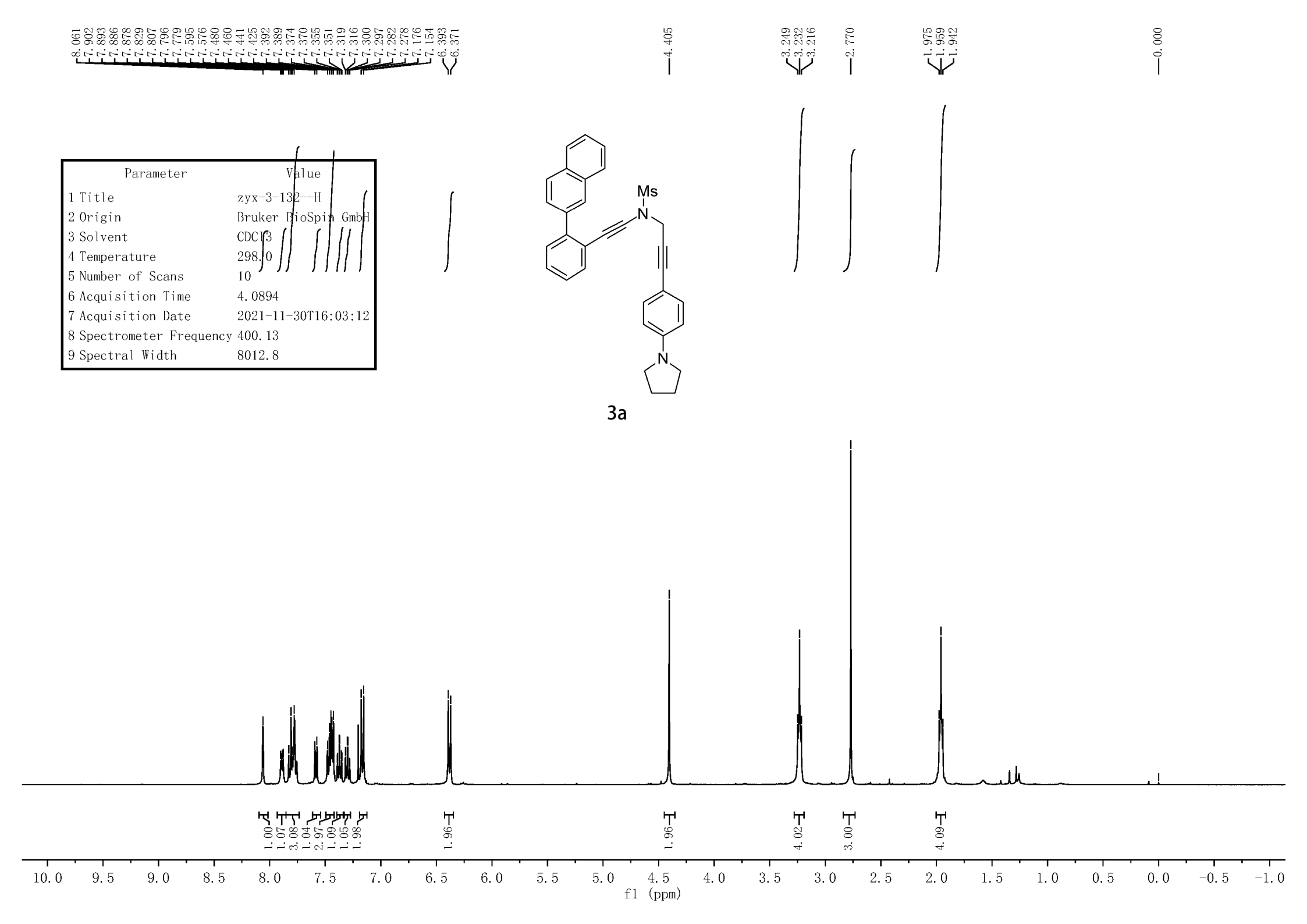
1ai




7.350
7.328
7.262
7.221
7.203
7.135
7.116
7.078
6.855
6.833
4.326
4.281
4.173
4.128
3.742
2.599
2.330
2.309
2.292
2.271
1.873
1.859
1.817
1.366
1.354
1.333
1.220
1.206
1.190
1.176
0.000
Parameter Value
1 Title ysh-1-45-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 6
6 Acquisition Time 4.0894
7 Acquisition Date 2024-06-27T20:49:42
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
PMP
1aj
2.08
2.18
3.05
2.05
1.02
1.01
3.06
3.00
1.02
1.01
1.07
1.05
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
-1.0
f1 (ppm)

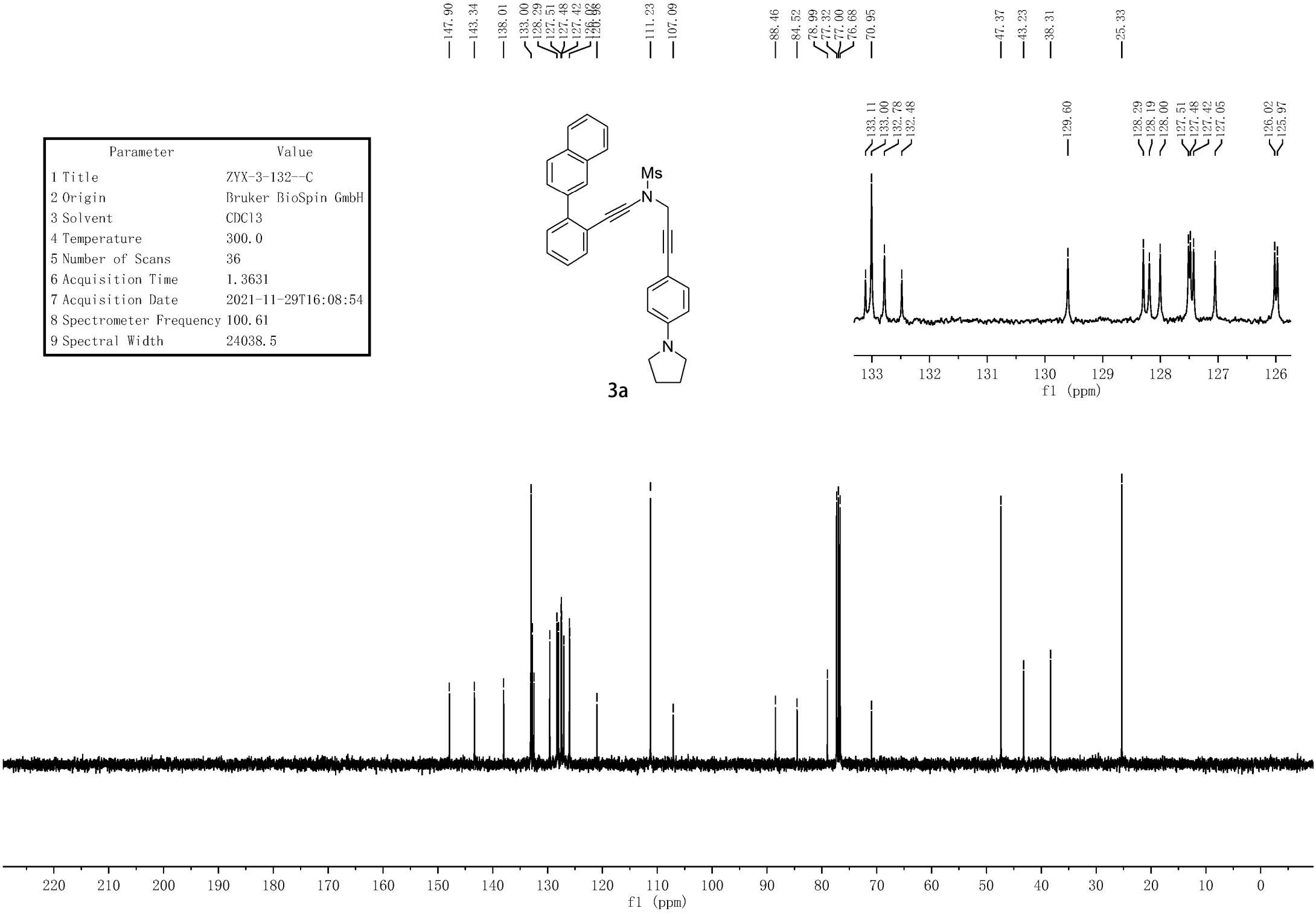

159.79
137.53
132.94
128.17
127.46
125.82
113.77
113.45
86.06
80.21
77.32
77.00
76.68
71.66
71.32
54.91
42.41
37.00
23.65
14.36
8.86
Parameter Value
1 Title ysh-1-45-c
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 7
6 Acquisition Time 1.3631
7 Acquisition Date 2024-06-27T20:51:15
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
PMP
1aj
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

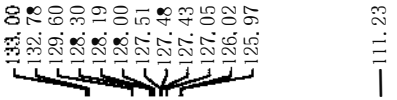

132.94
128.18
127.47
125.83
113.77
77.20
54.92
42.41
37.00
23.65
14.36
8.86
Parameter Value
1 Title ysh-1-45-dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 16
6 Acquisition Time 1.3631
7 Acquisition Date 2024-06-27T20:52:39
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
PMP
1aj
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)


8.061
7.902
7.893
7.886
7.878
7.829
7.807
7.796
7.779
7.595
7.576
7.480
7.460
7.441
7.425
7.392
7.389
7.374
7.370
7.355
7.351
7.319
7.316
7.300
7.297
7.282
7.278
7.176
7.154
6.393
6.371
4.405
3.249
3.232
3.216
2.770
1.975
1.959
1.942
0.000
Parameter Value
1 Title zyx-3-132--H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 10
6 Acquisition Time 4.0894
7 Acquisition Date 2021-11-30T16:03:12
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
3a
1.00
1.07
3.08
1.04
2.97
1.09
1.05
1.98
1.96
1.96
4.02
3.00
4.09
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
-1.0
f1 (ppm)

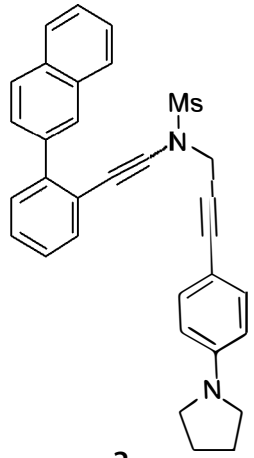
Parameter	Value
1 Title	ZYX-3-132--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	36
6 Acquisition Time	1.3631
7 Acquisition Date	2021-11-29T16:08:54
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

3a

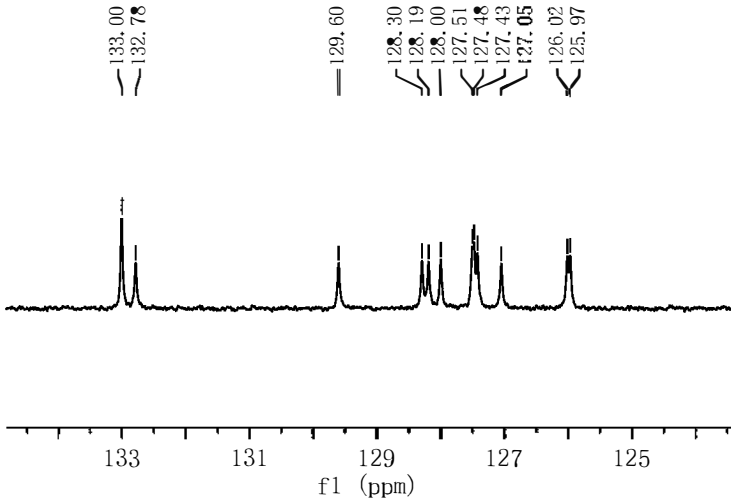


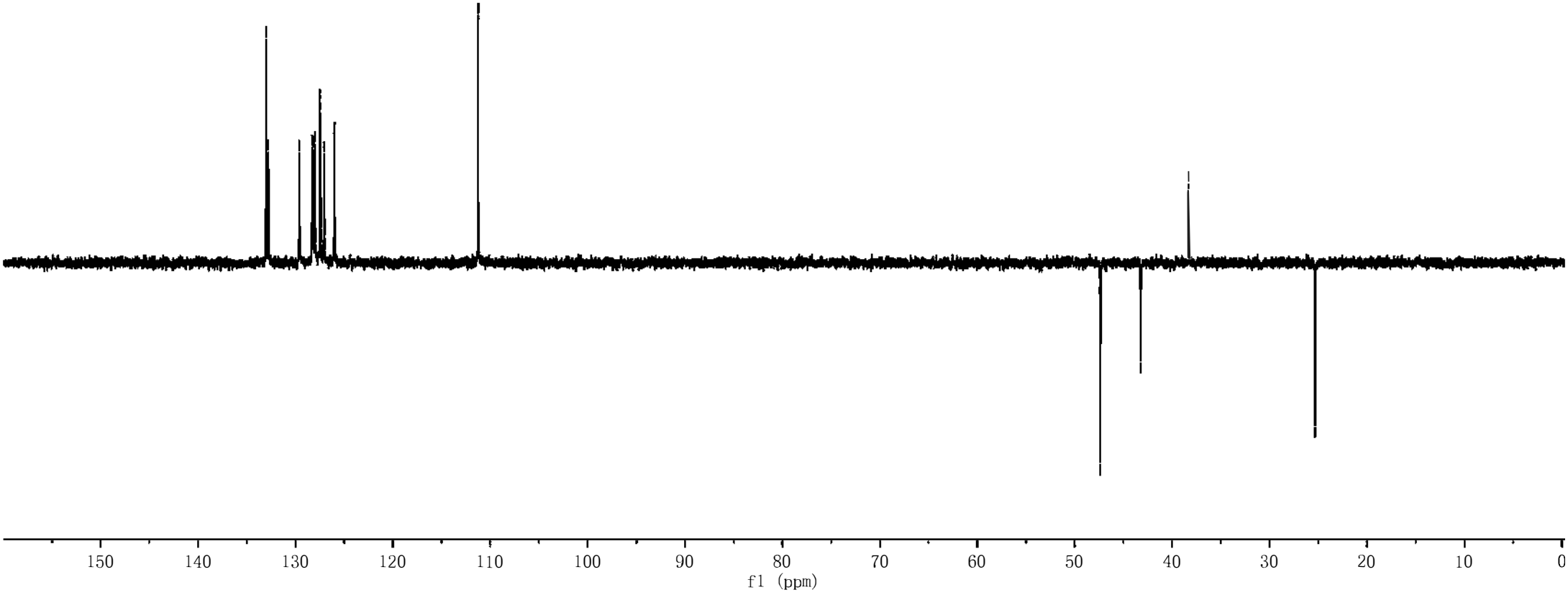


Parameter	Value
1 Title	ZYX-3-132--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	36
6 Acquisition Time	1.3631
7 Acquisition Date	2021-11-29T16:08:54
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

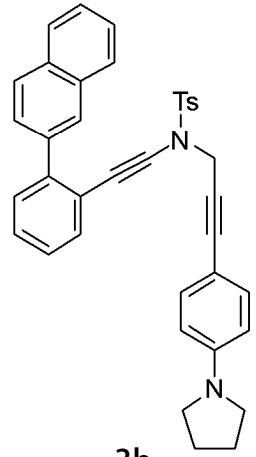


3a

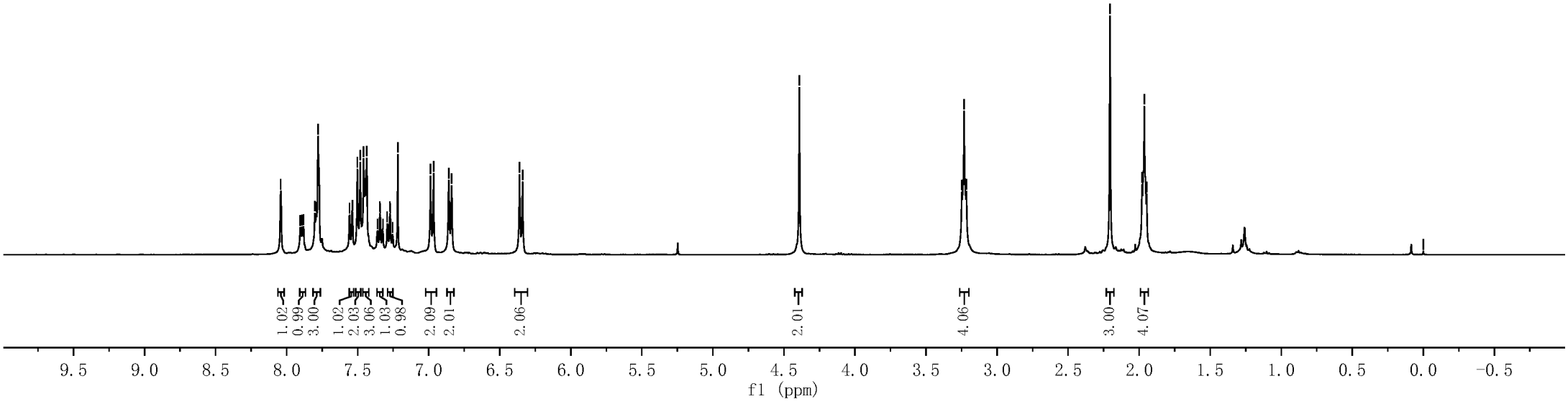




Parameter	Value
1 Title	ZYX-3--70--1H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	8
6 Acquisition Time	4.0894
7 Acquisition Date	2021-11-29T16:20:31
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

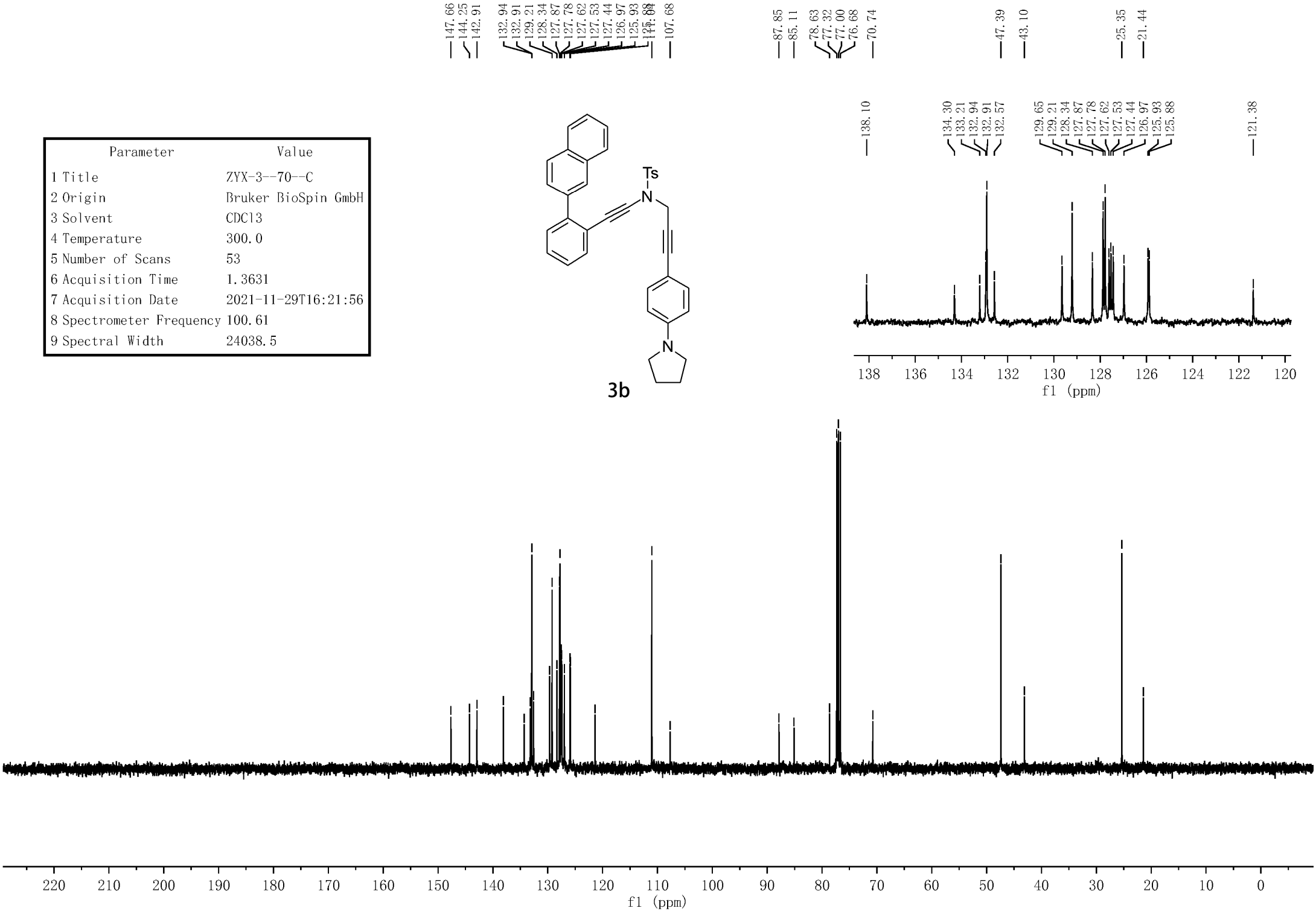


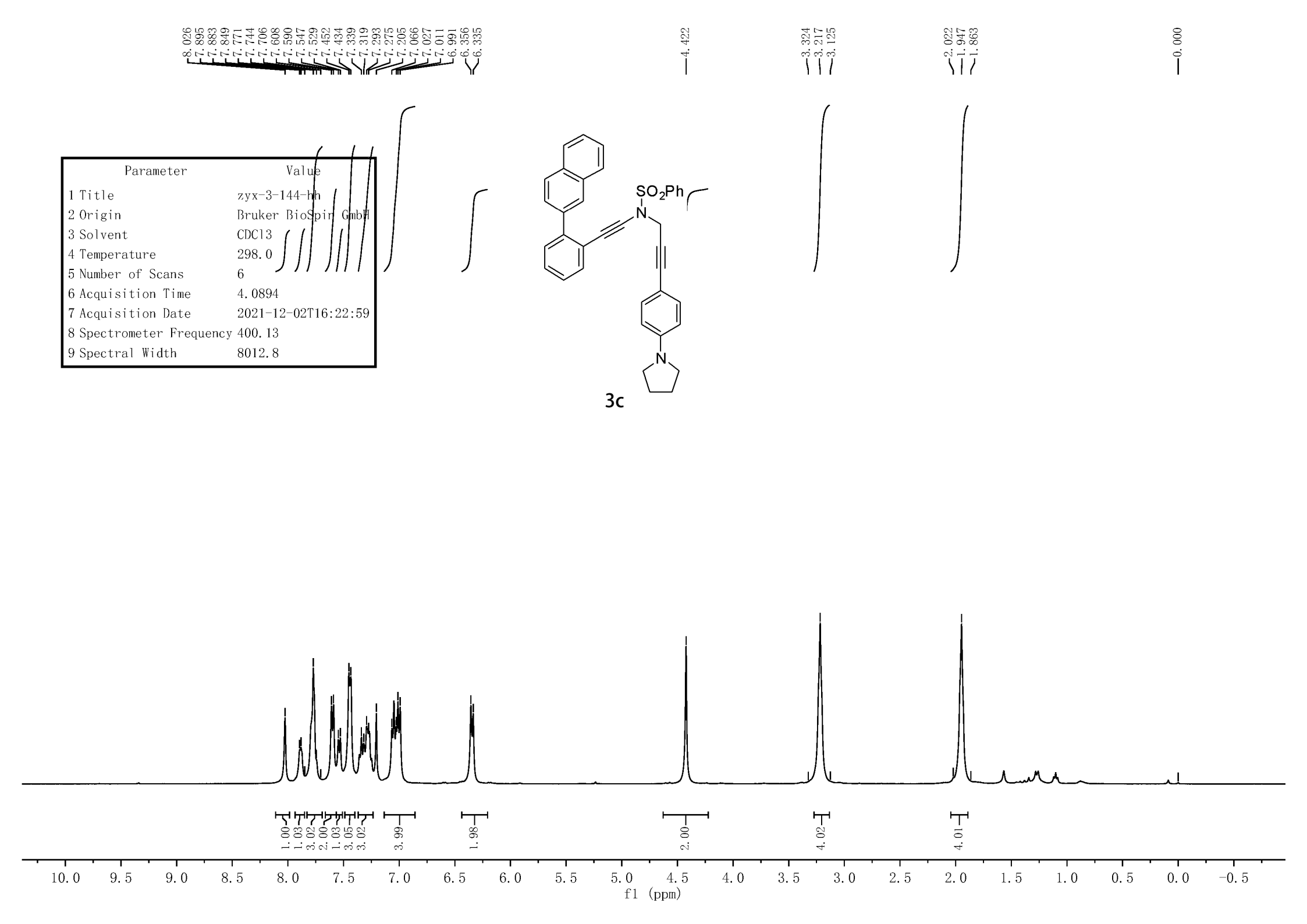
3b



Parameter	Value
1 Title	ZYX-3--70--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	53
6 Acquisition Time	1.3631
7 Acquisition Date	2021-11-29T16:21:56
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

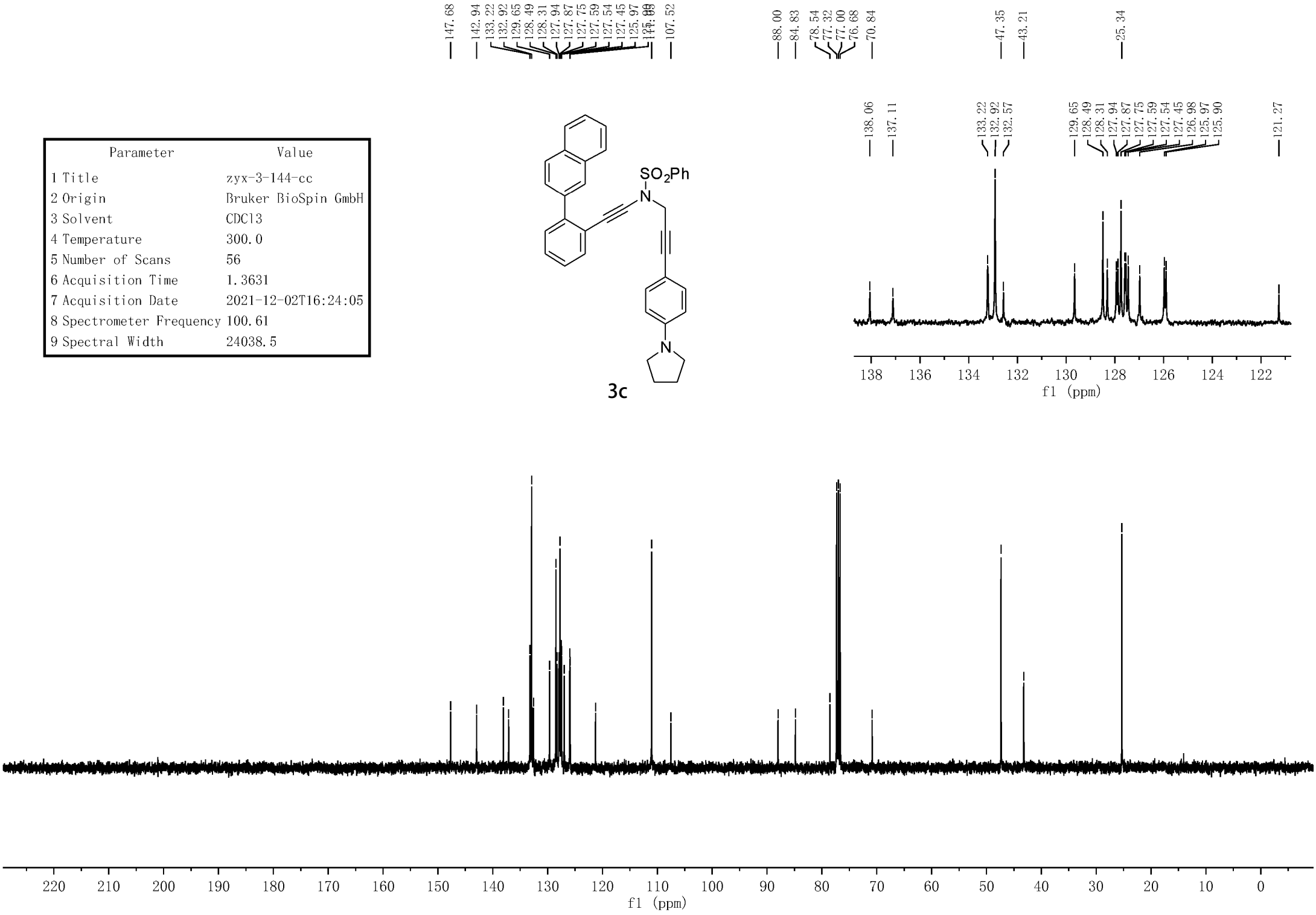
3b

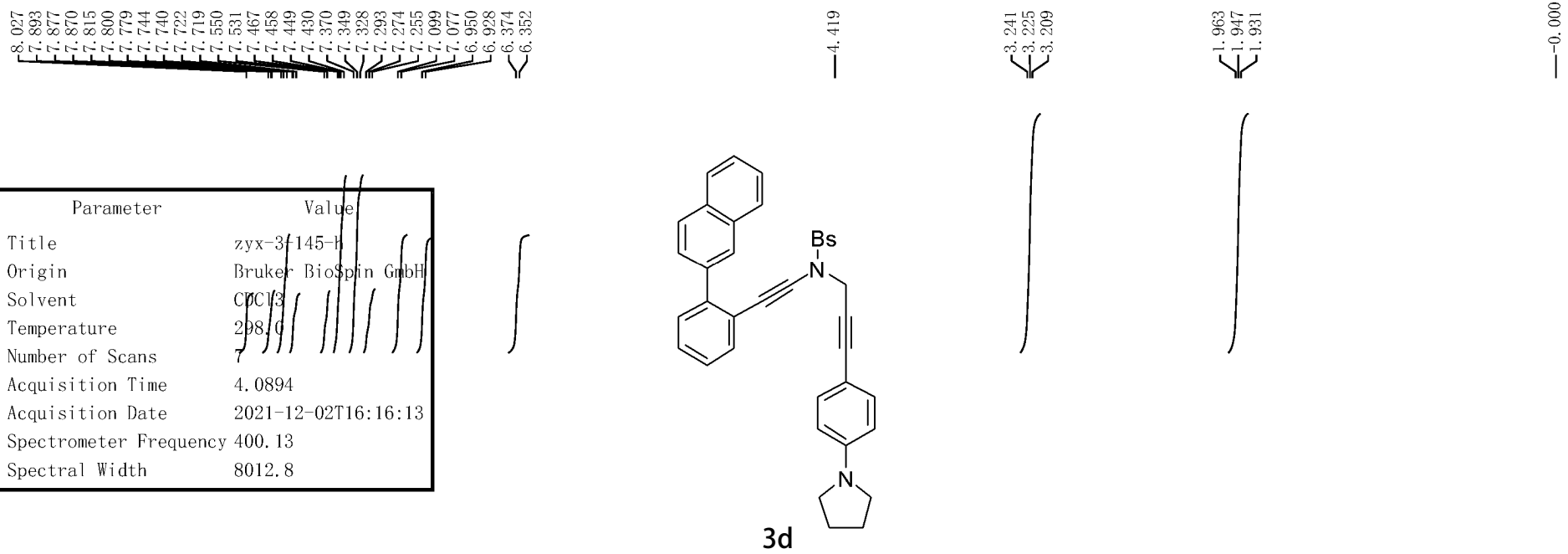


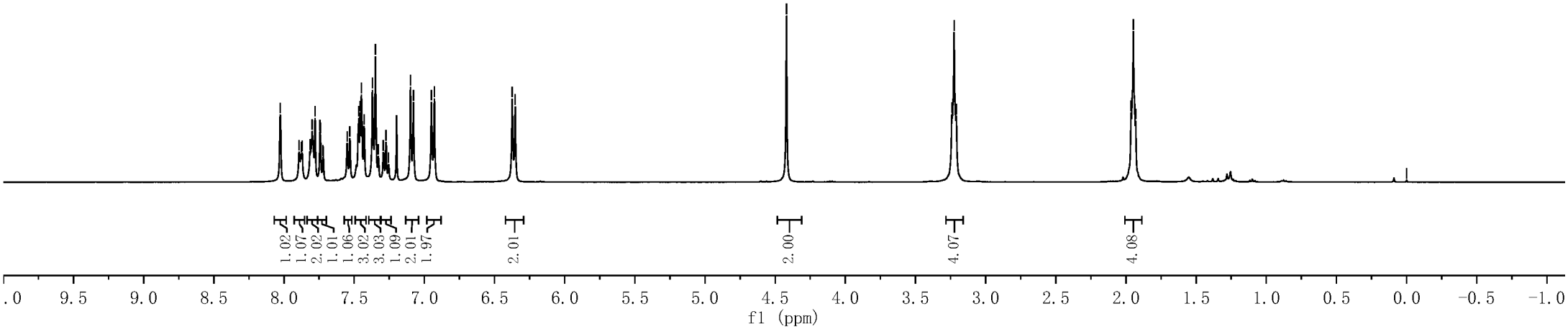

8.026
7.895
7.883
7.849
7.771
7.744
7.706
7.608
7.590
7.547
7.529
7.452
7.434
7.339
7.319
7.293
7.275
7.205
7.066
7.027
7.011
6.991
6.356
6.335
4.422
3.324
3.217
3.125
2.022
1.947
1.863
0.000
Parameter Value
1 Title zyx-3-144-hh
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 6
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-02T16:22:59
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
SO2Ph
N
N
3c
1.00
1.03
3.02
2.00
1.03
3.05
3.02
3.99
1.98
2.00
4.02
4.01
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)

Parameter	Value
1 Title	zyx-3-144-cc
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	56
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-02T16:24:05
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

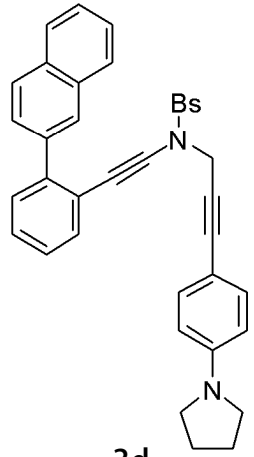
3c



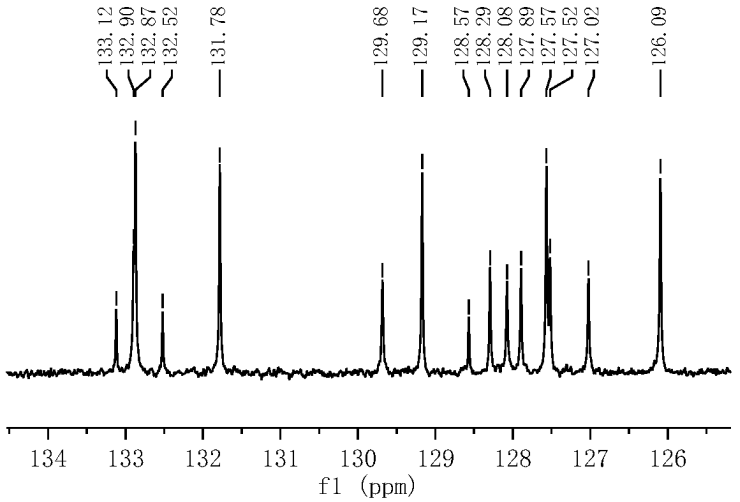

8.027
7.893
7.877
7.870
7.815
7.800
7.779
7.744
7.740
7.722
7.719
7.550
7.531
7.467
7.458
7.449
7.430
7.370
7.349
7.328
7.293
7.274
7.255
7.099
7.077
6.950
6.928
6.374
6.352
4.419
3.241
3.225
3.209
1.963
1.947
1.931
0.000
Parameter Value
1 Title zyx-3f145-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 7
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-02T16:16:13
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Bs
N
N
3d

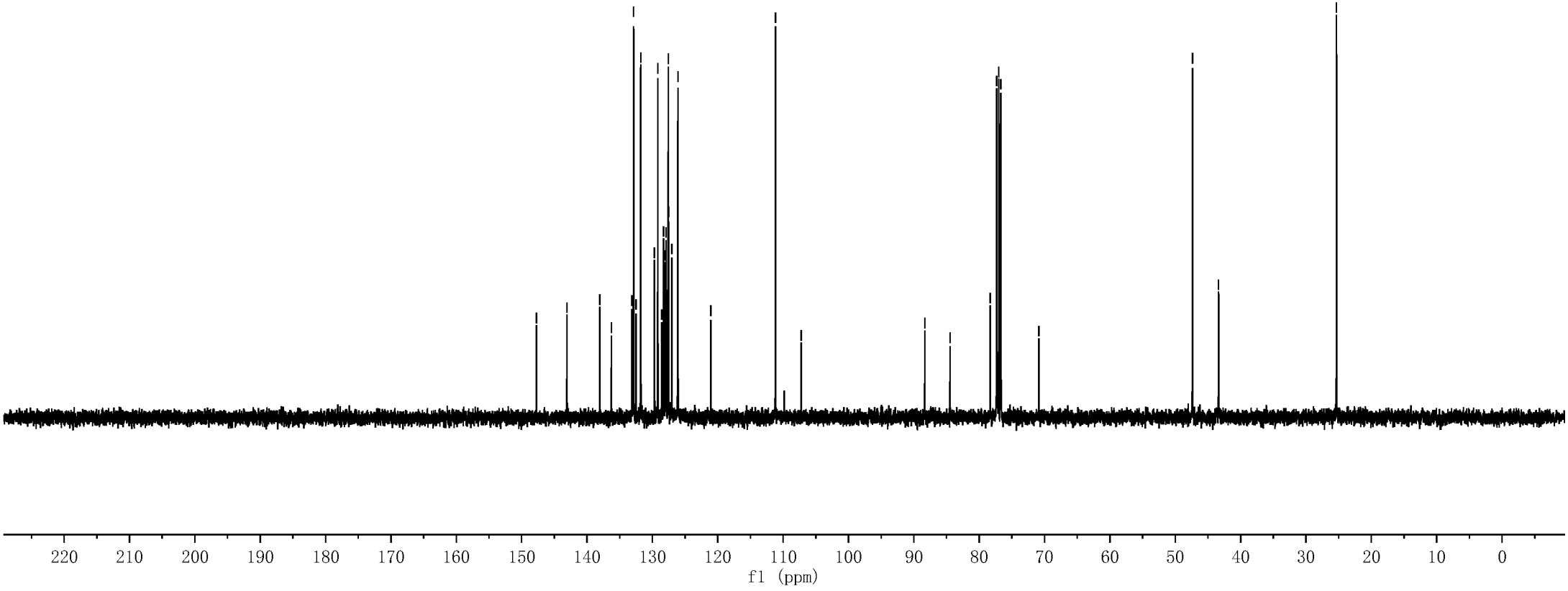

1.02
1.07
2.02
1.01
1.06
3.02
3.03
1.09
2.01
1.97
2.01
2.00
4.07
4.08
.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

Parameter	Value
1 Title	zyx-3-145-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	32
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-02T16:17:28
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

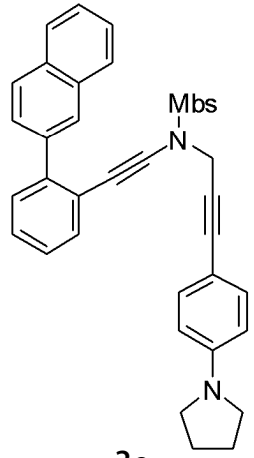


3d

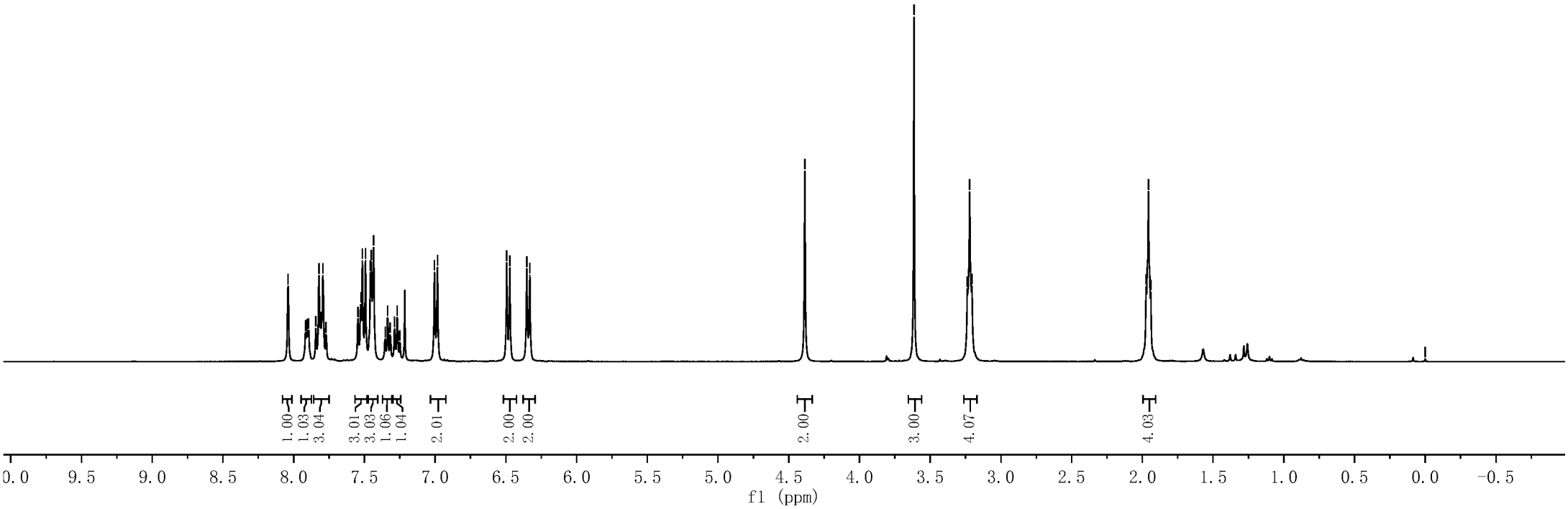




Parameter	Value
1 Title	zyx-3-146-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2021-12-02T16:29:42
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

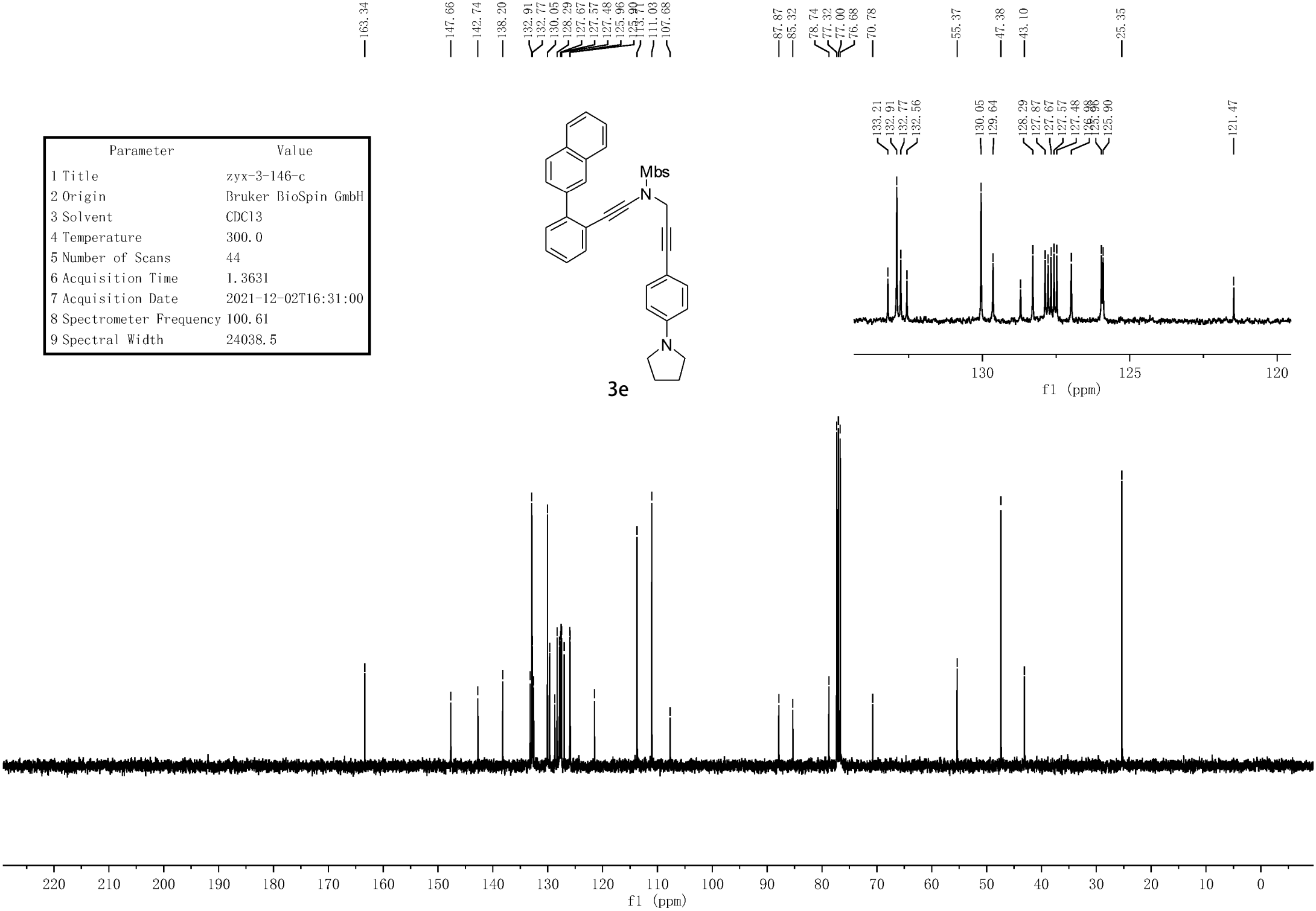


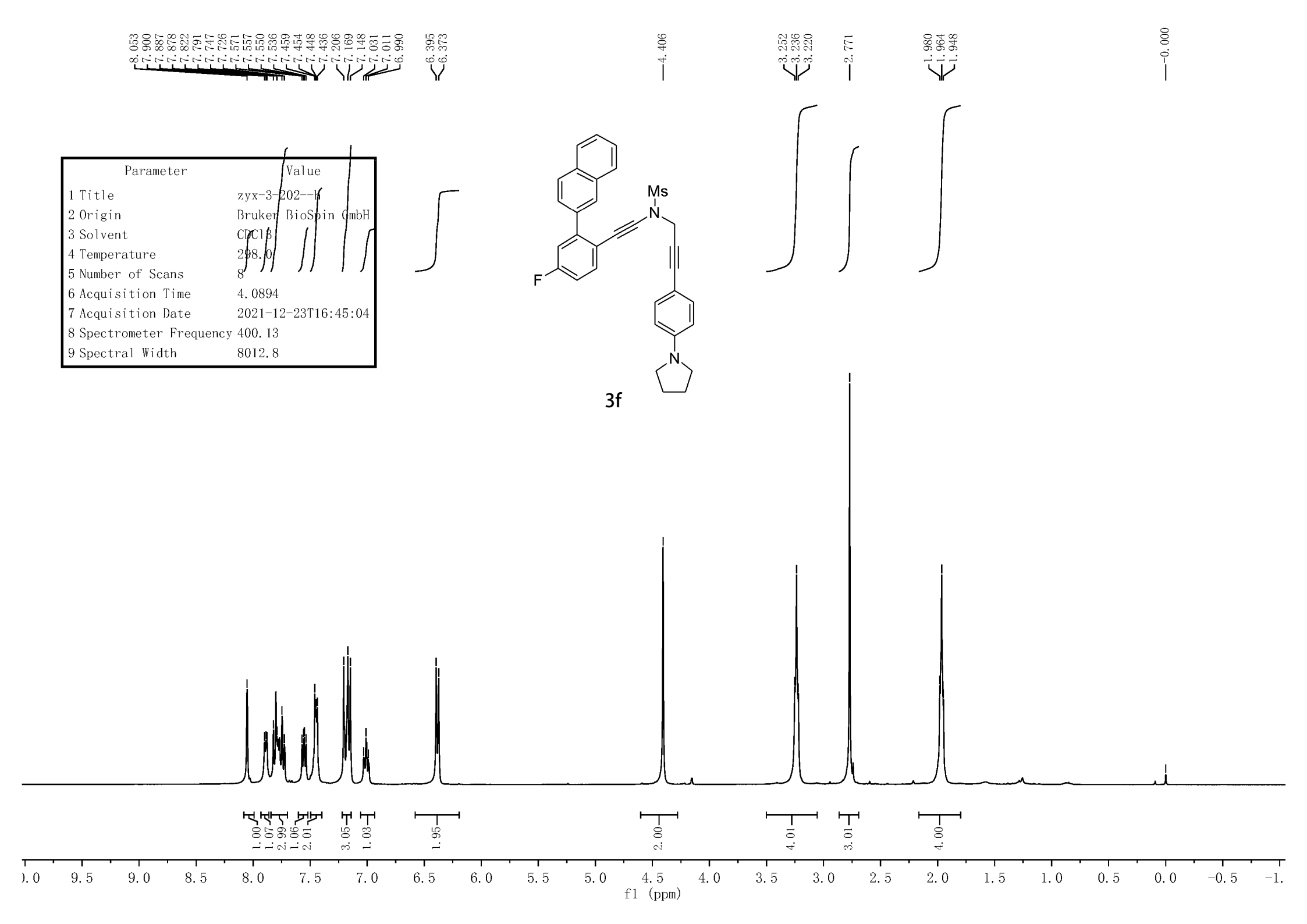
3e



Parameter	Value
1 Title	zyx-3-146-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	44
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-02T16:31:00
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

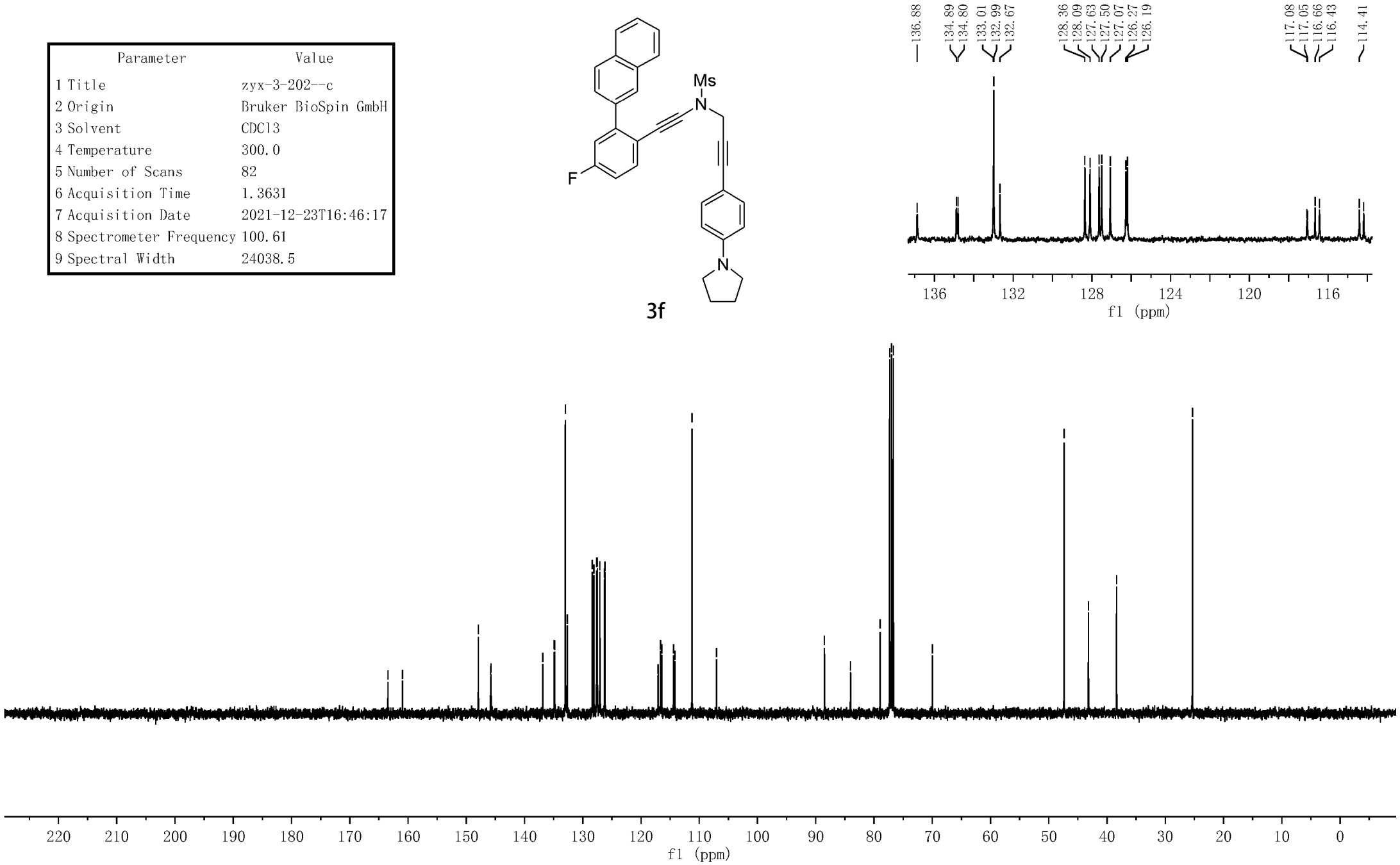
3e



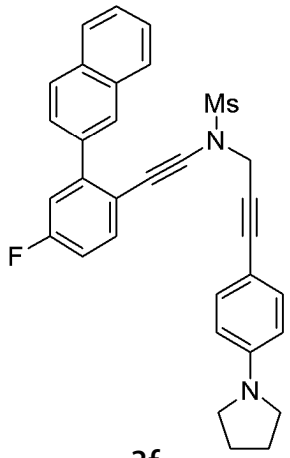

8.053
7.900
7.887
7.878
7.822
7.791
7.747
7.726
7.571
7.557
7.550
7.536
7.459
7.454
7.448
7.436
7.206
7.169
7.148
7.031
7.011
6.990
6.395
6.373
4.406
3.252
3.236
3.220
2.771
1.980
1.964
1.948
0.000
Parameter Value
1 Title zyx-3-202--h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-23T16:45:04
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
F
N
3f
1.00
1.07
2.99
1.06
2.01
3.05
1.03
1.95
2.00
4.01
3.01
4.00
f1 (ppm)

Parameter	Value
1 Title	zyx-3-202--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	82
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-23T16:46:17
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

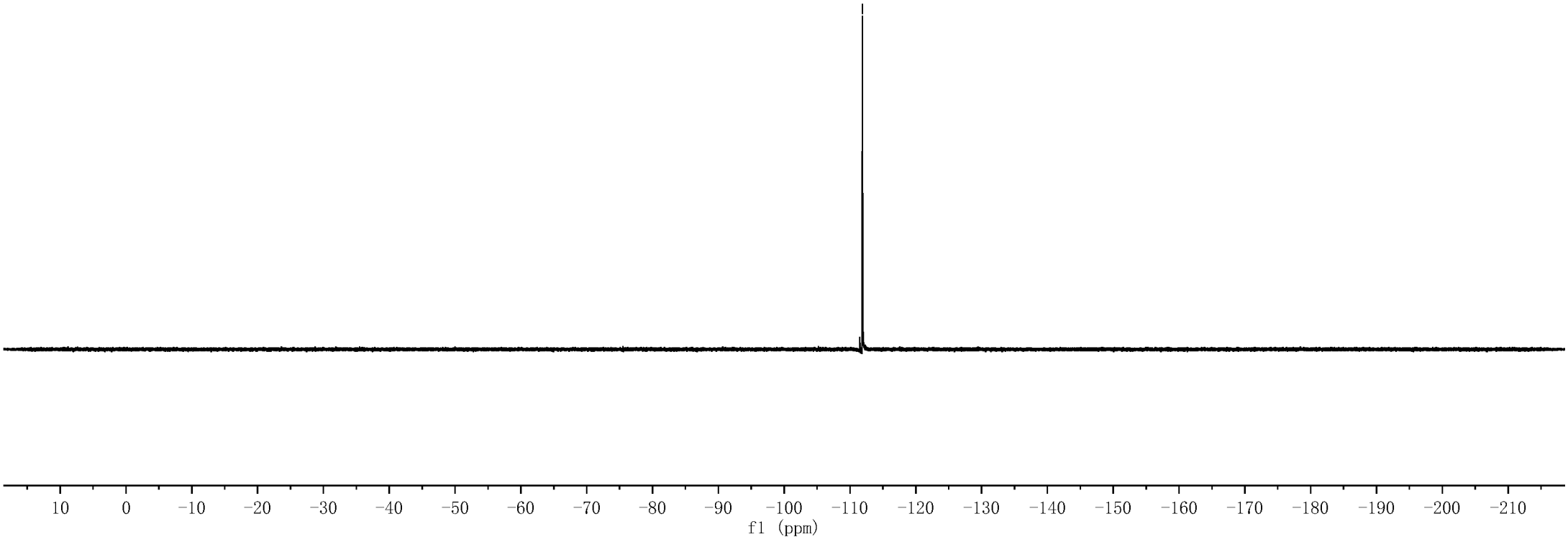
3f

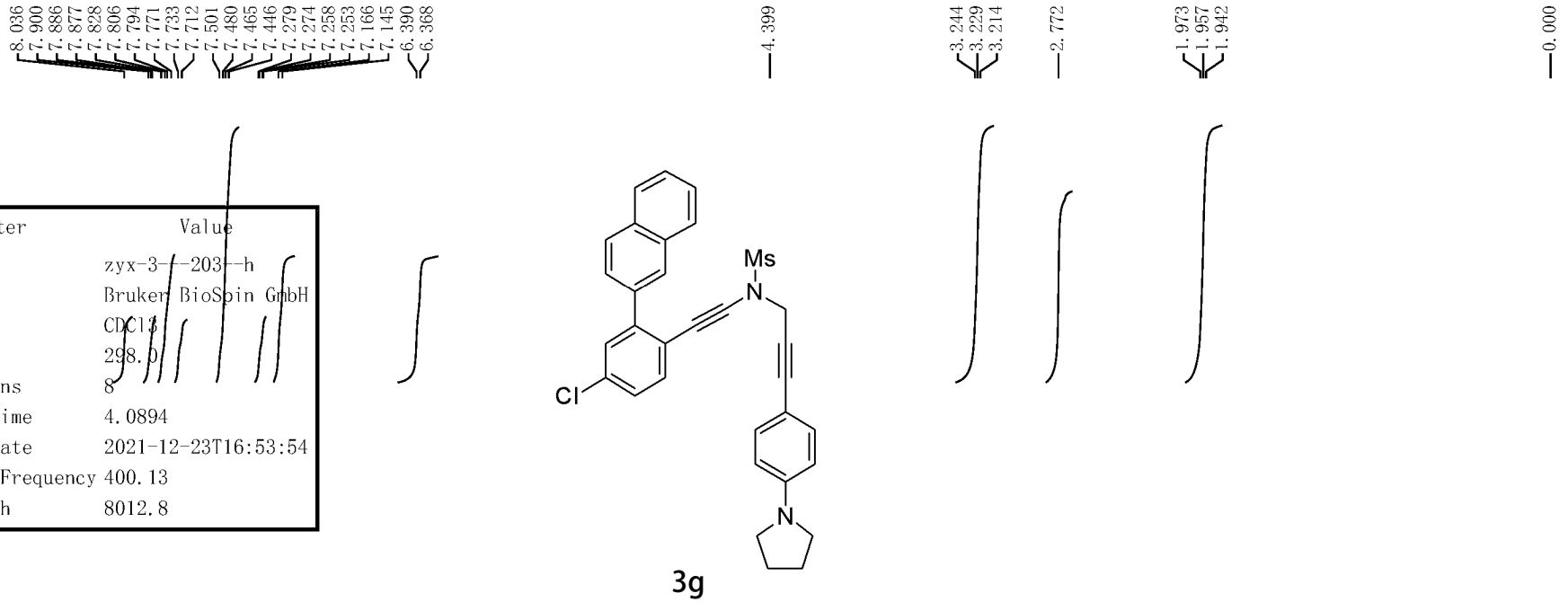


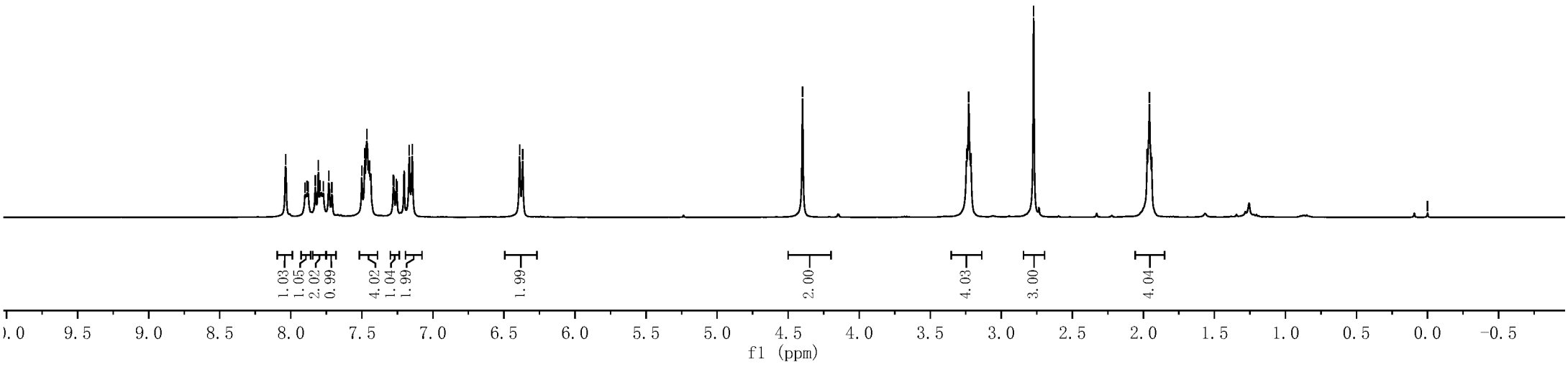
Parameter	Value
1 Title	ZYX-3-202-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-19T16:39:59
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



3f

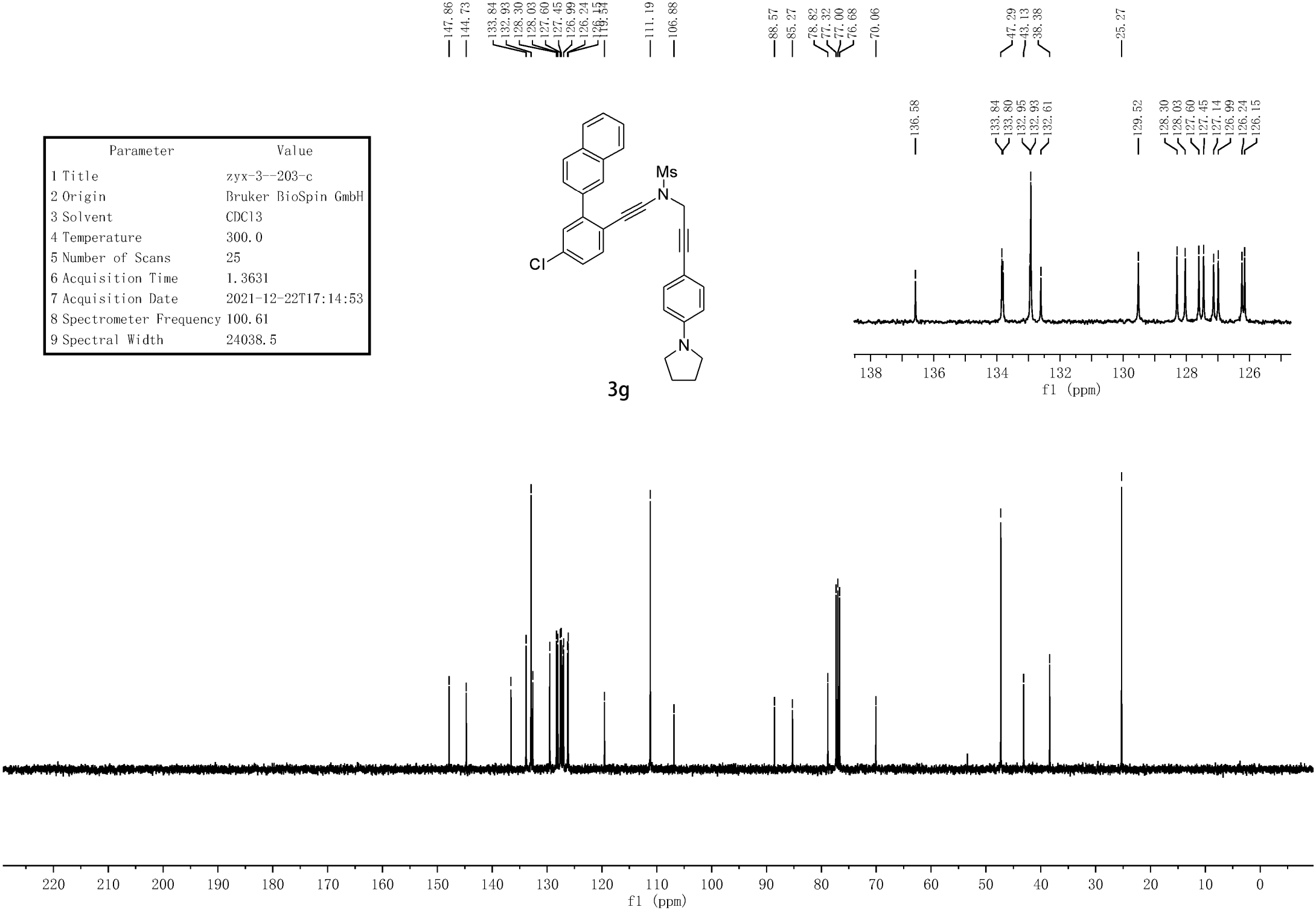


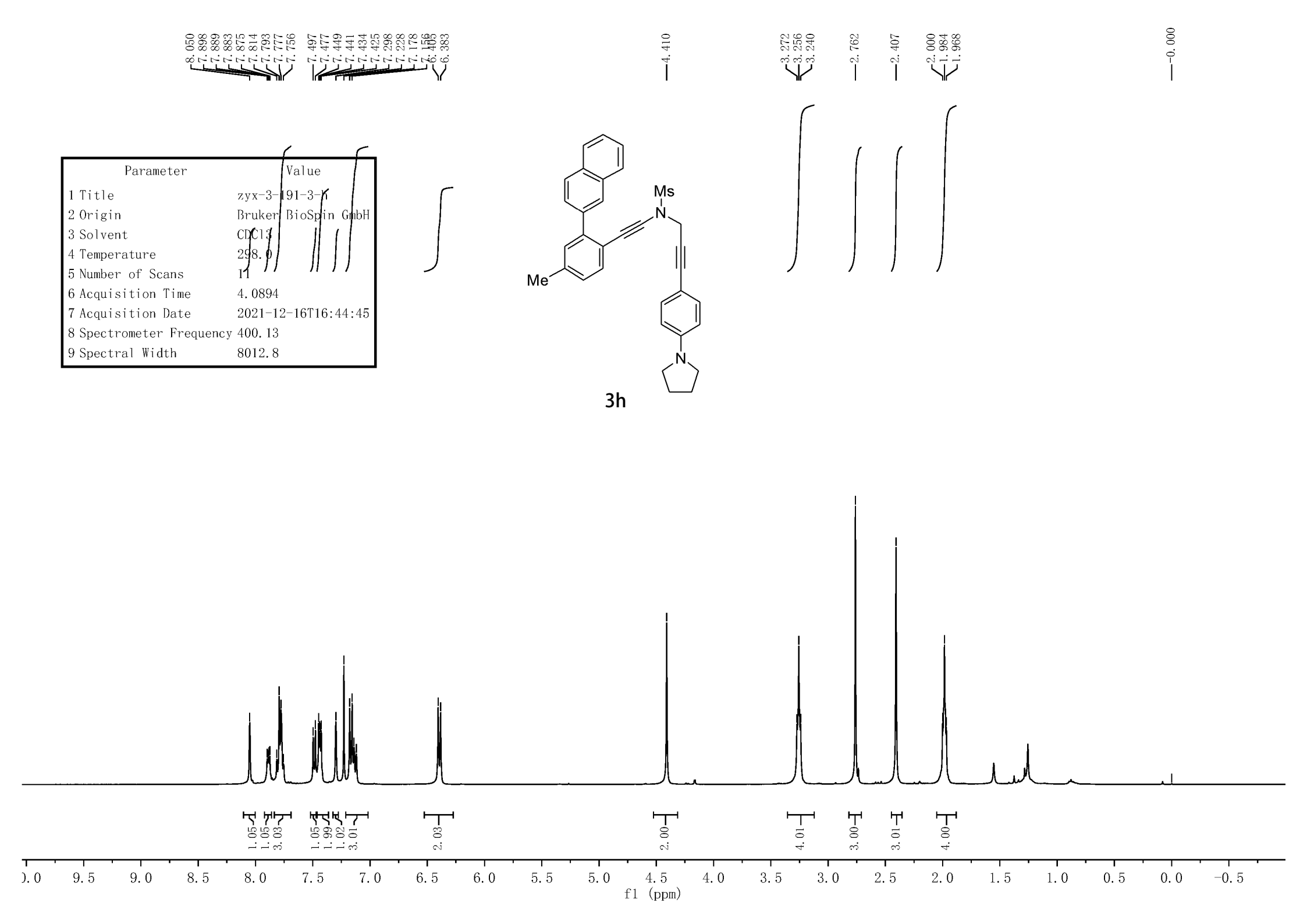

8.036
7.900
7.886
7.877
7.828
7.806
7.794
7.771
7.733
7.712
7.501
7.480
7.465
7.446
7.279
7.274
7.258
7.253
7.166
7.145
6.390
6.368
4.399
3.244
3.229
3.214
2.772
1.973
1.957
1.942
0.000
Parameter Value
1 Title zyx-3--203--h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-23T16:53:54
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
Cl
N
3g


1.03
1.05
2.02
0.99
4.02
1.04
1.99
1.99
2.00
4.03
3.00
4.04
f1 (ppm)

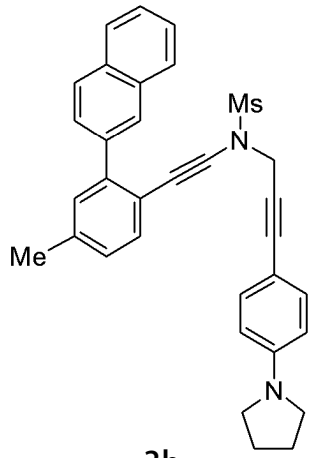
Parameter	Value
1 Title	zyx-3--203-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	25
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-22T17:14:53
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

3g

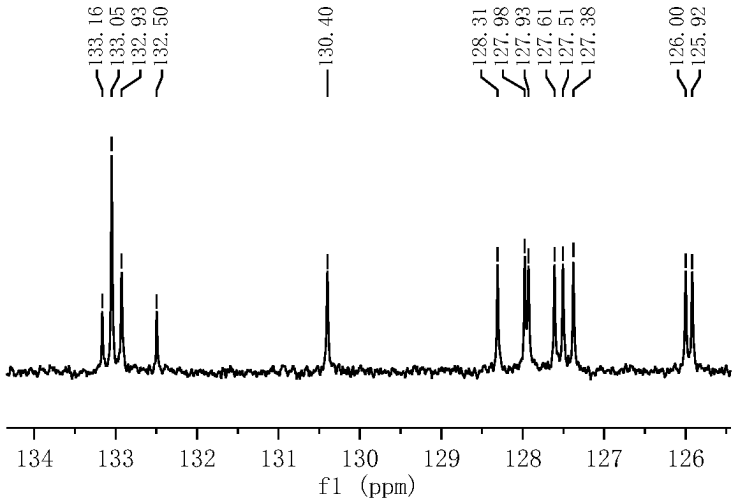


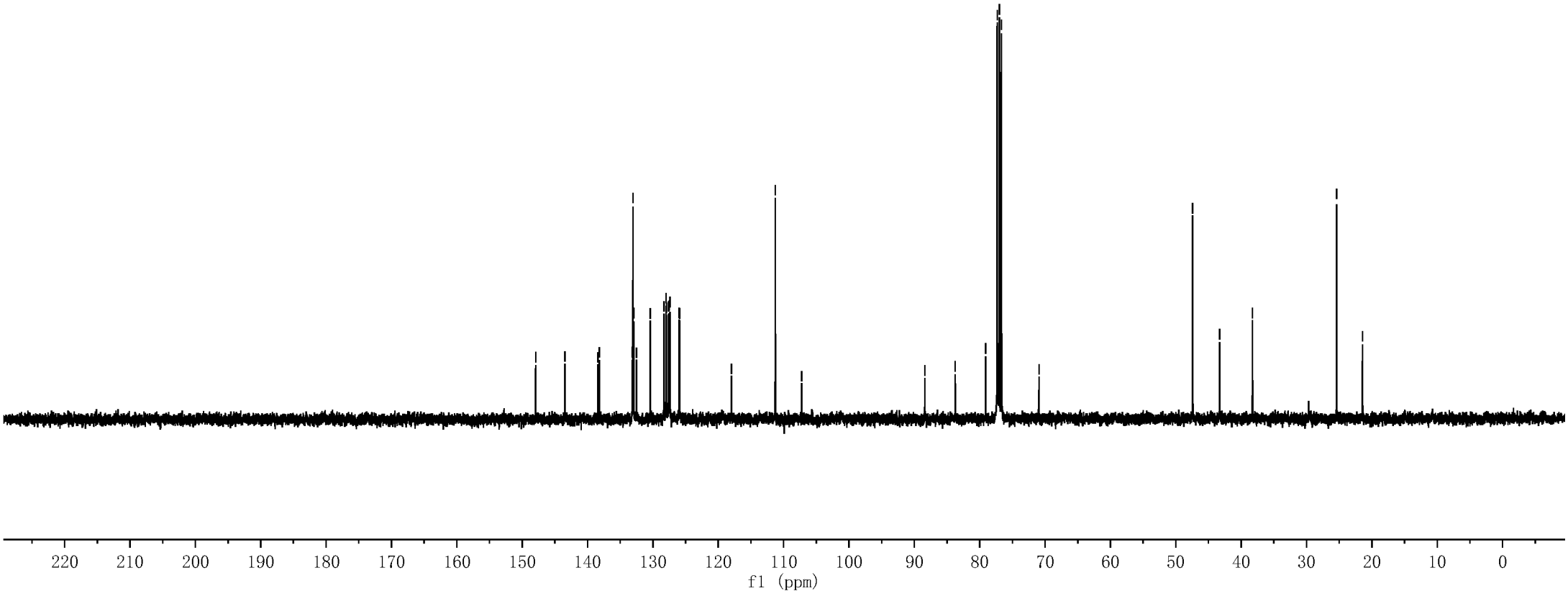

8.050
7.898
7.889
7.883
7.875
7.814
7.793
7.777
7.756
7.497
7.477
7.449
7.441
7.434
7.425
7.298
7.228
7.178
6.405
6.383
4.410
3.272
3.256
3.240
2.762
2.407
2.000
1.984
1.968
-0.000
Parameter Value
1 Title zyx-3-191-3-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 11
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-16T16:44:45
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
Me
N
3h
1.05
1.05
3.03
1.05
1.99
1.02
3.01
2.03
2.00
4.01
3.00
3.01
4.00
f1 (ppm)

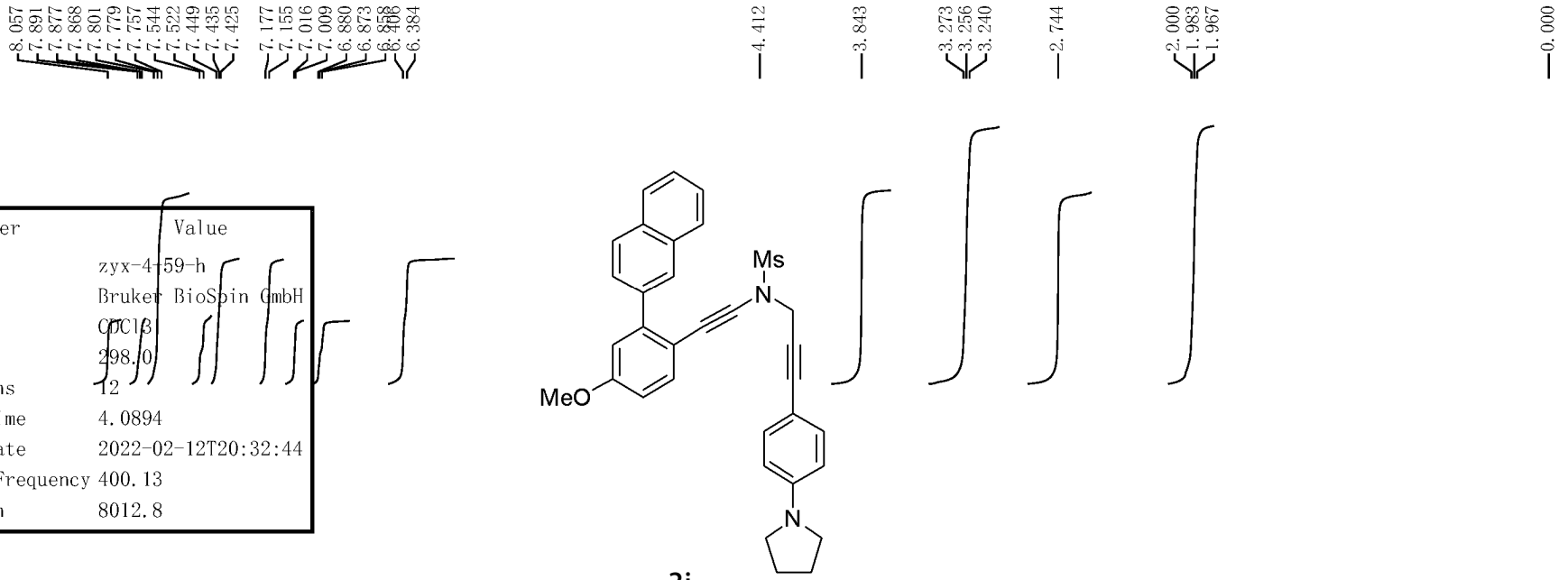
Parameter	Value
1 Title	zyx-3-191-3-cc
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	106
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-16T16:46:38
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



3h

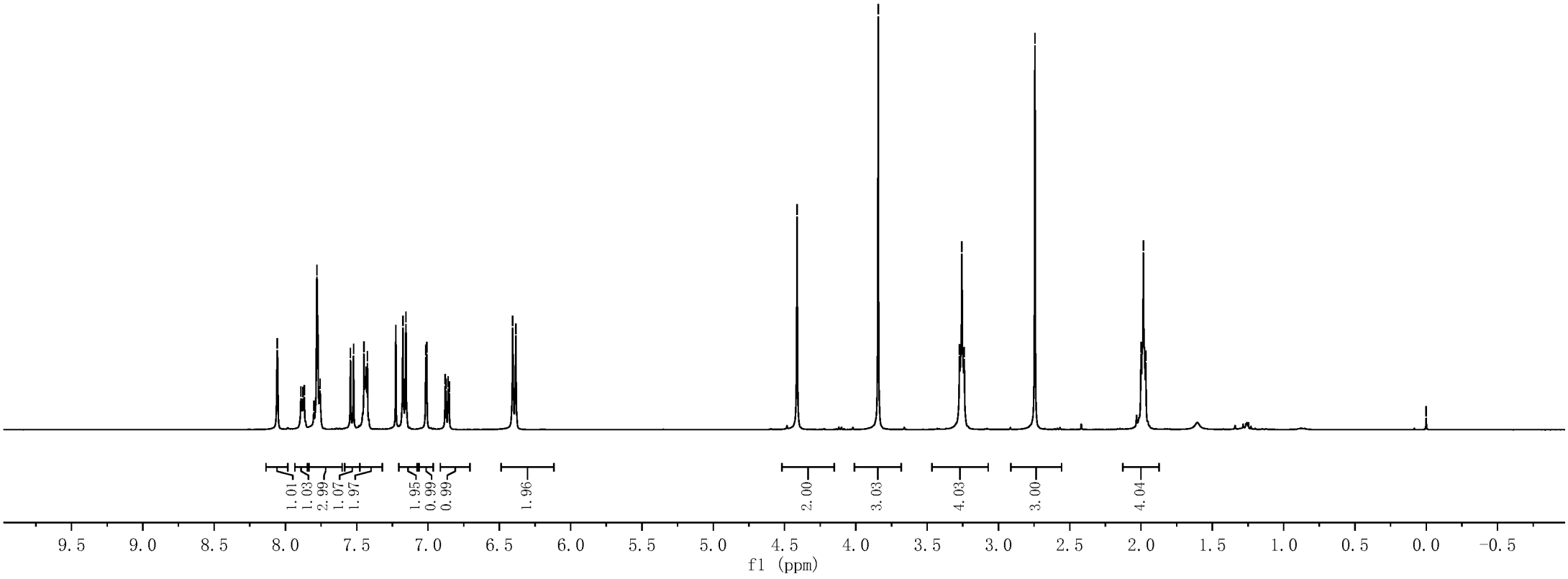




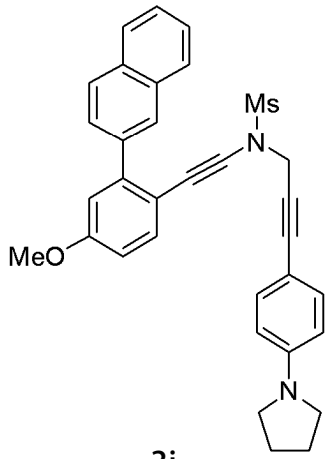


Parameter	Value
1 Title	zyx-4-59-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	12
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-12T20:32:44
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

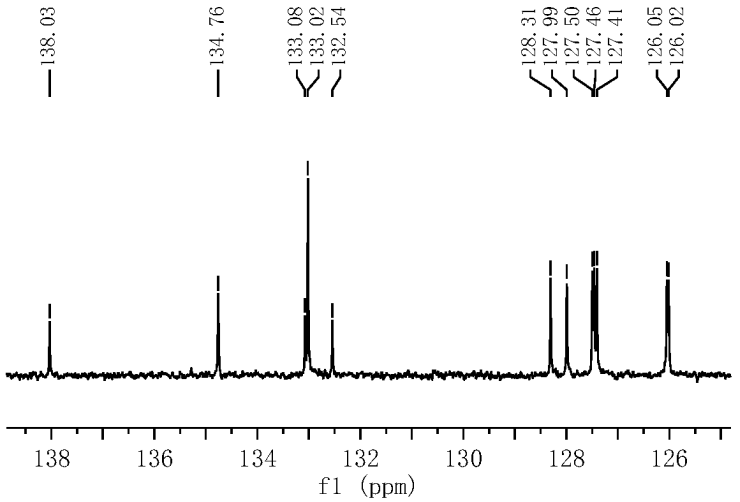
3i

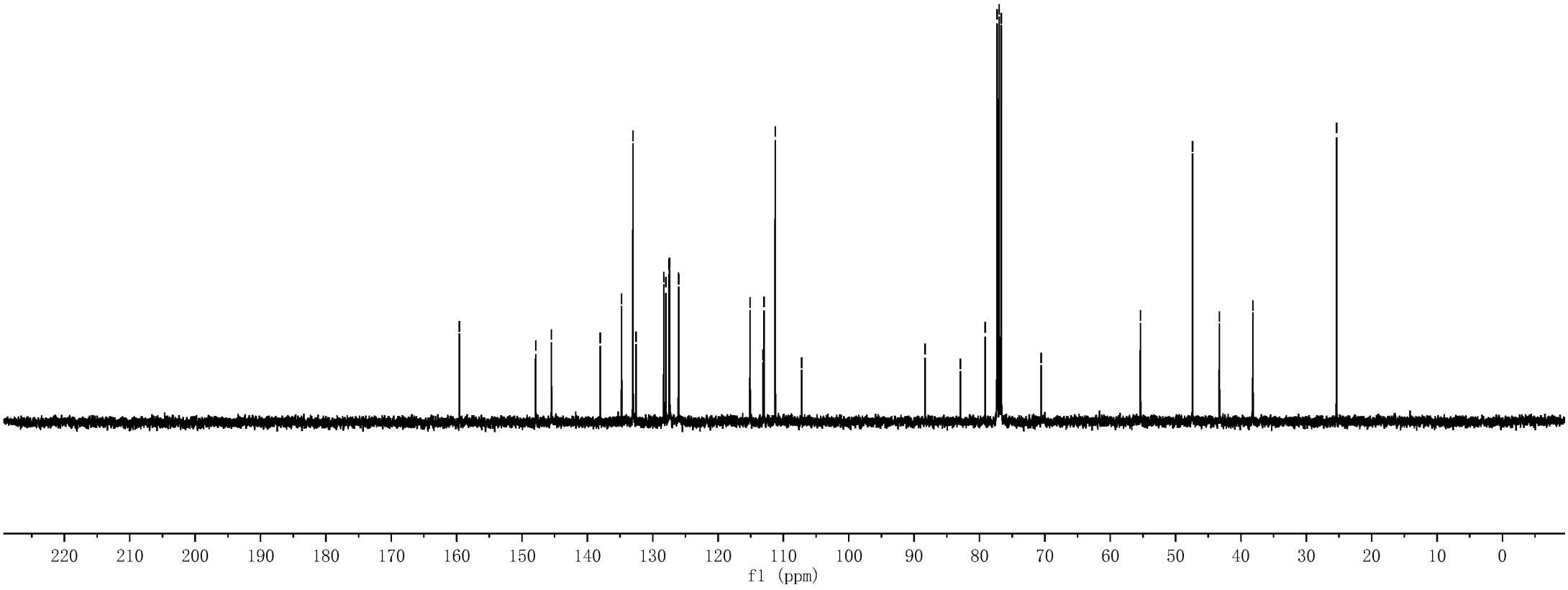


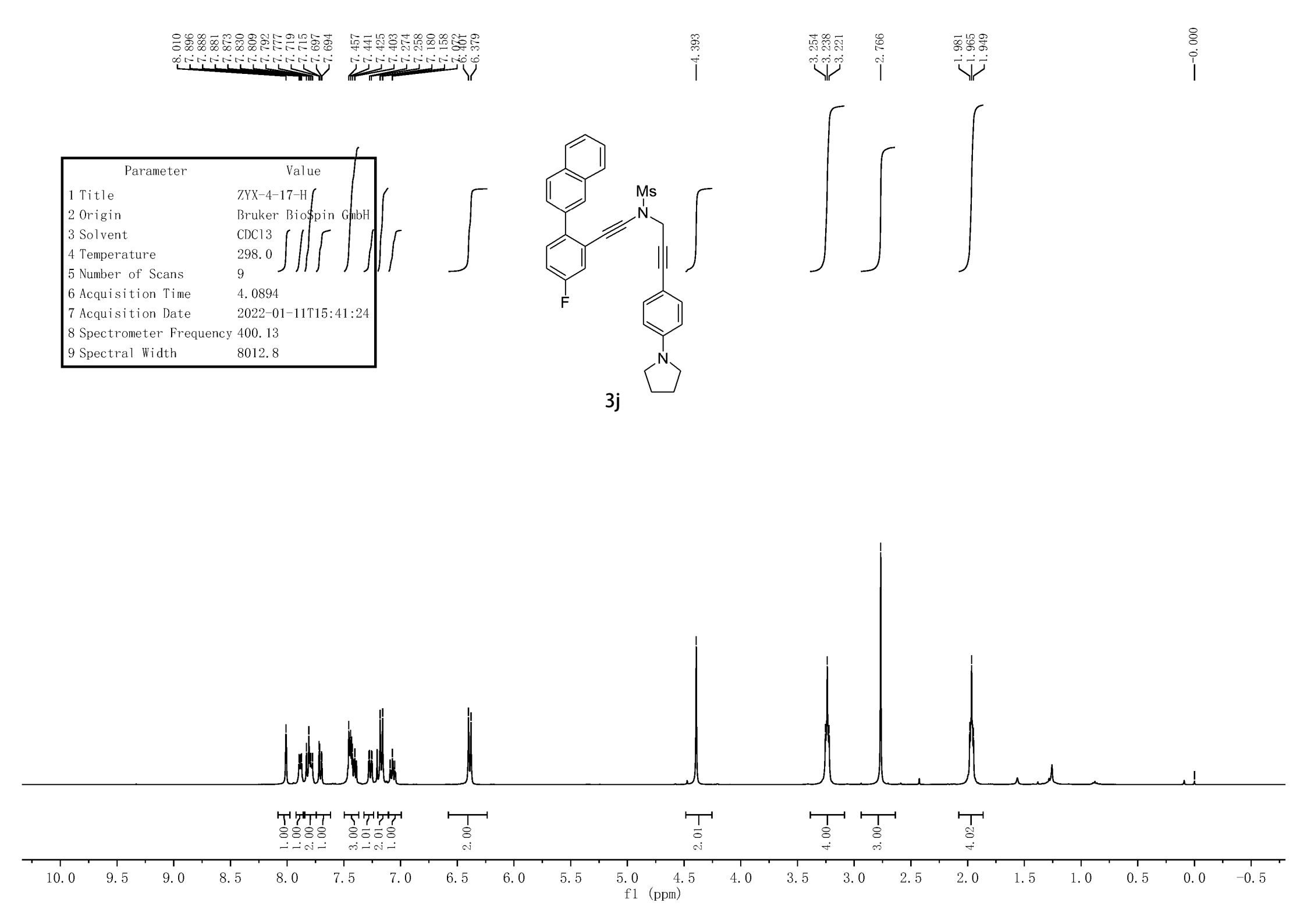
Parameter	Value
1 Title	zyx-4-59-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	54
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-12T20:34:41
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



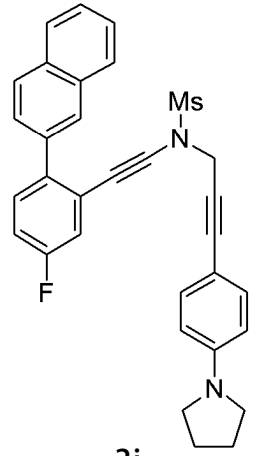
3i



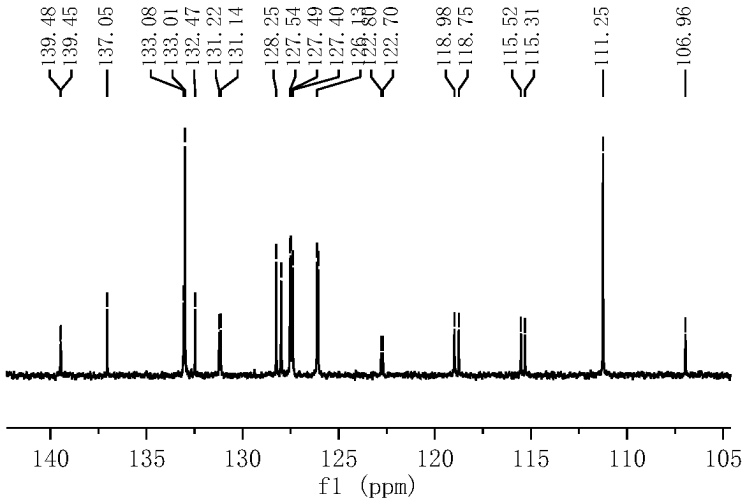


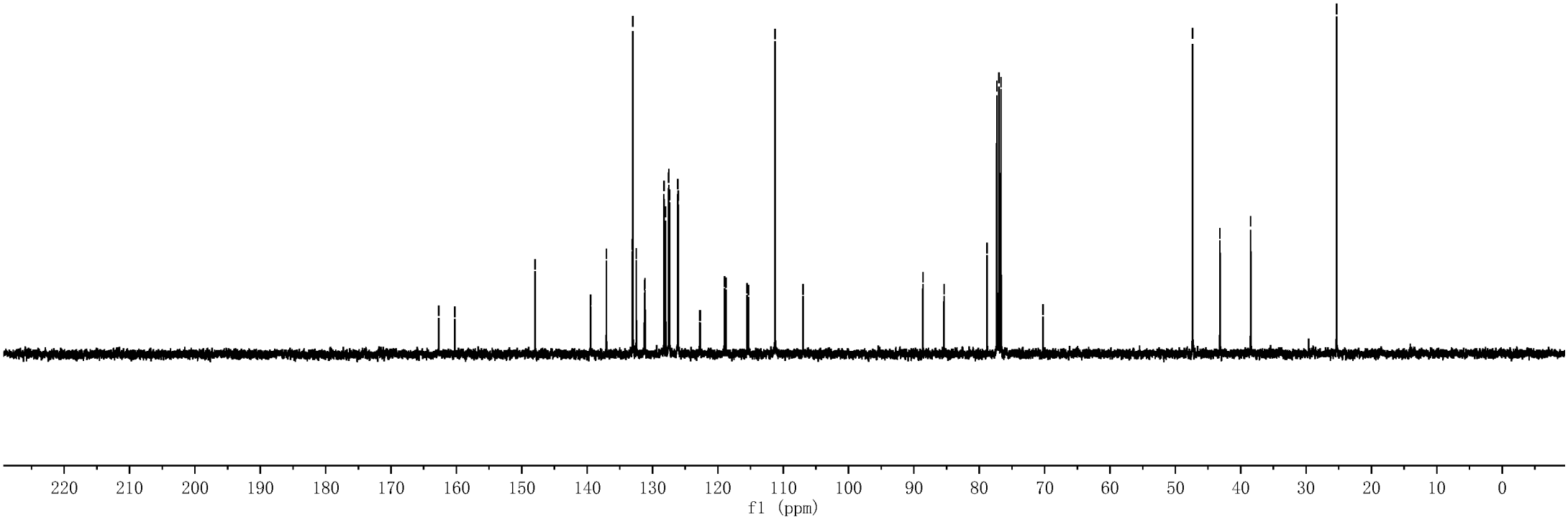

8.010
7.896
7.888
7.881
7.873
7.830
7.809
7.792
7.777
7.719
7.715
7.697
7.694
7.457
7.441
7.425
7.403
7.274
7.258
7.180
7.158
7.072
6.401
6.379
4.393
3.254
3.238
3.221
2.766
1.981
1.965
1.949
0.000
Parameter Value
1 Title ZYX-4-17-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 9
6 Acquisition Time 4.0894
7 Acquisition Date 2022-01-11T15:41:24
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
F
N
3j
1.00
1.00
2.00
1.00
3.00
1.01
2.01
1.00
2.00
2.01
4.00
3.00
4.02
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)

Parameter	Value
1 Title	ZYX-4-17-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	57
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-11T15:42:46
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



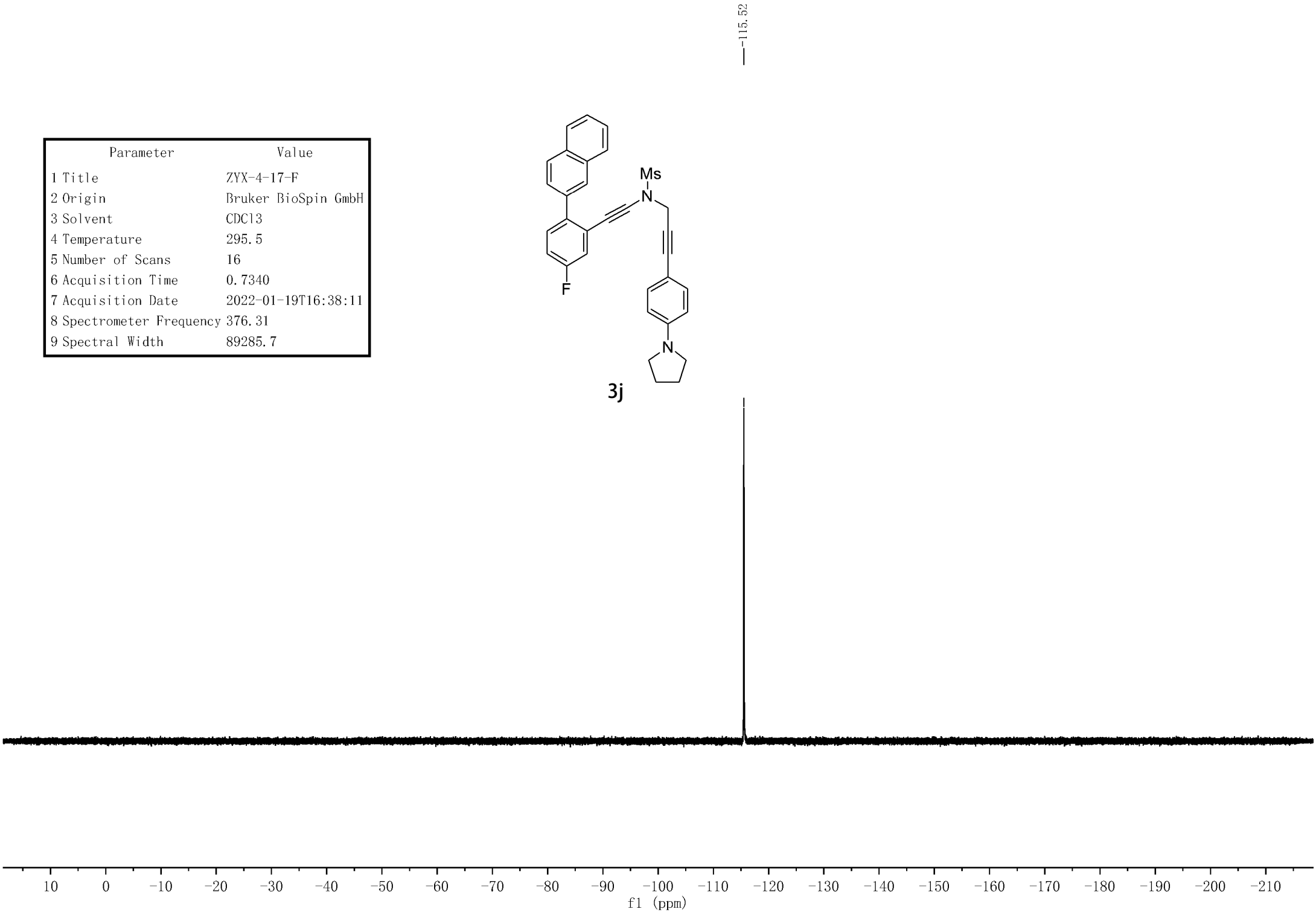
3j

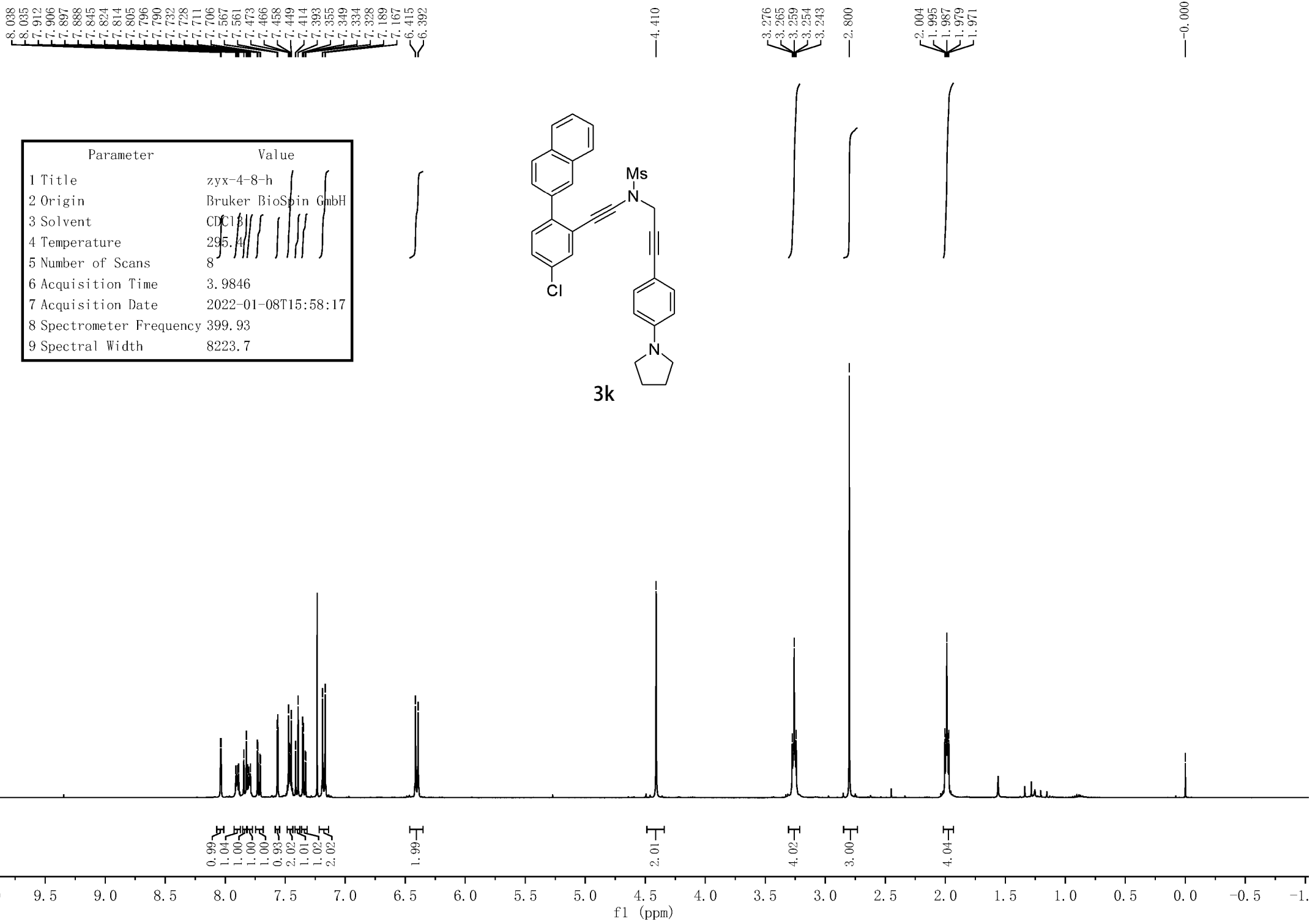




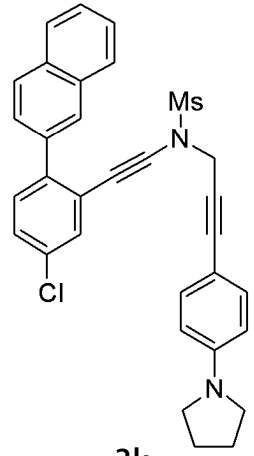
Parameter	Value
1 Title	ZYX-4-17-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-19T16:38:11
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

3j

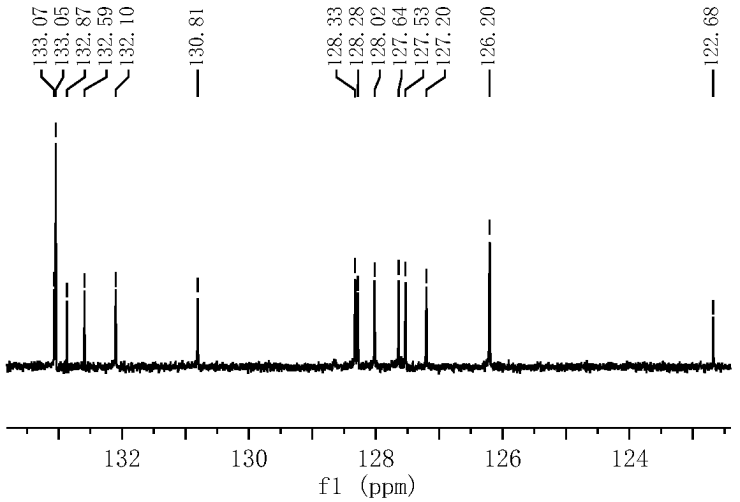


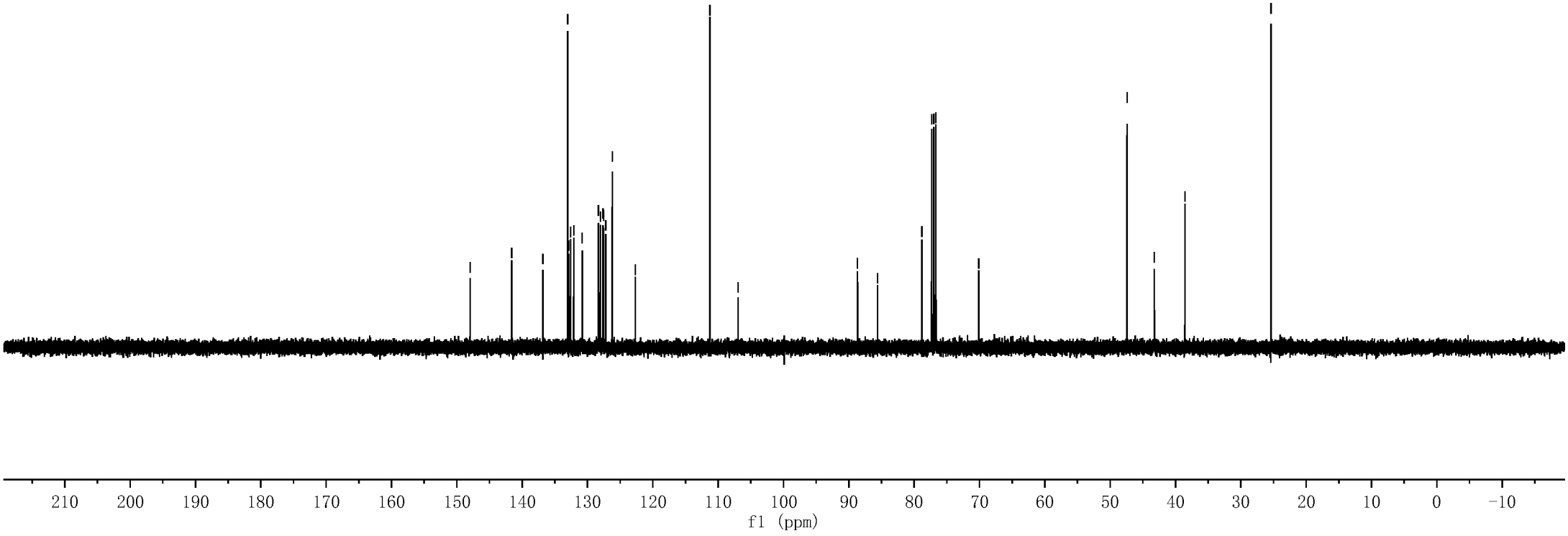

8.038
8.035
7.912
7.906
7.897
7.888
7.845
7.824
7.814
7.805
7.796
7.790
7.732
7.728
7.711
7.706
7.567
7.561
7.473
7.466
7.458
7.449
7.414
7.393
7.355
7.349
7.334
7.328
7.189
7.167
6.415
6.392
4.410
3.276
3.265
3.259
3.254
3.243
2.800
2.004
1.995
1.987
1.979
1.971
0.000
Parameter Value
1 Title zyx-4-8-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.4
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2022-01-08T15:58:17
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
Cl
N
3k
0.99
1.04
1.00
1.00
1.00
0.93
2.02
1.01
1.02
2.02
1.99
2.01
4.02
3.00
4.04
f1 (ppm)

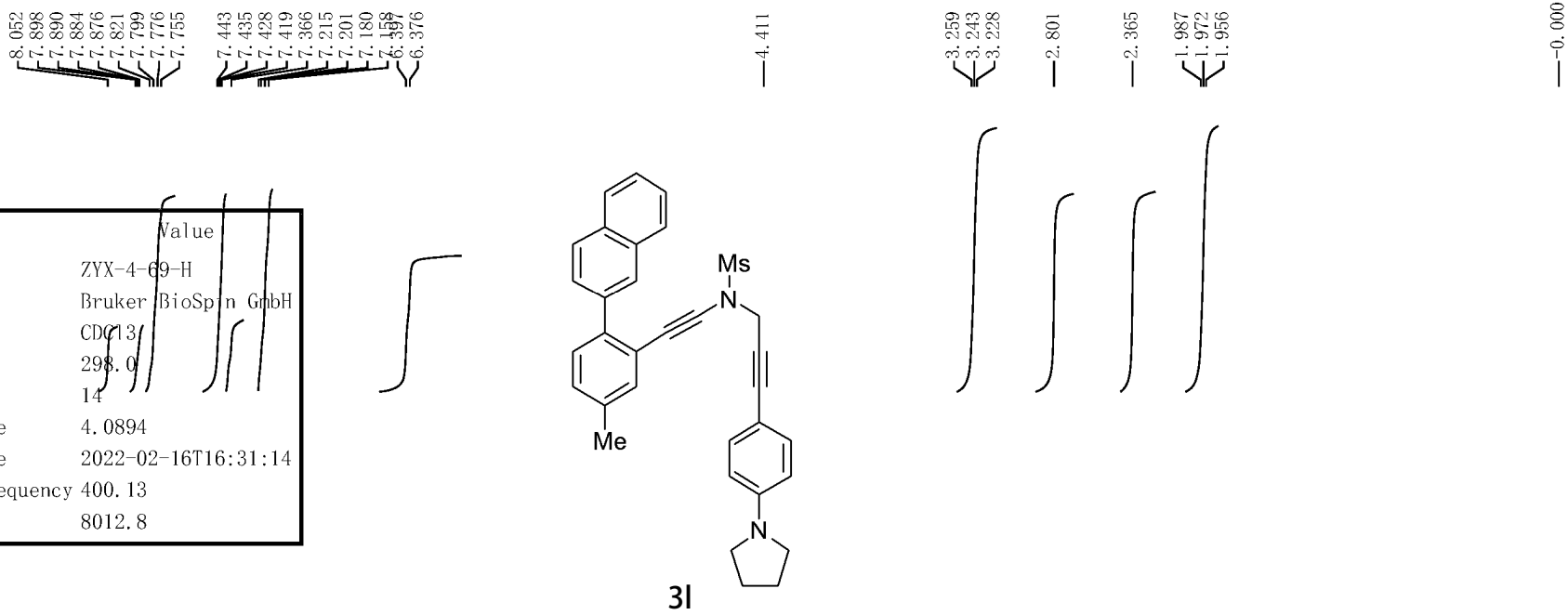
Parameter	Value
1 Title	zyx-4-8-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	85
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-08T15:59:45
8 Spectrometer Frequency	100.57
9 Spectral Width	24038.5



3k

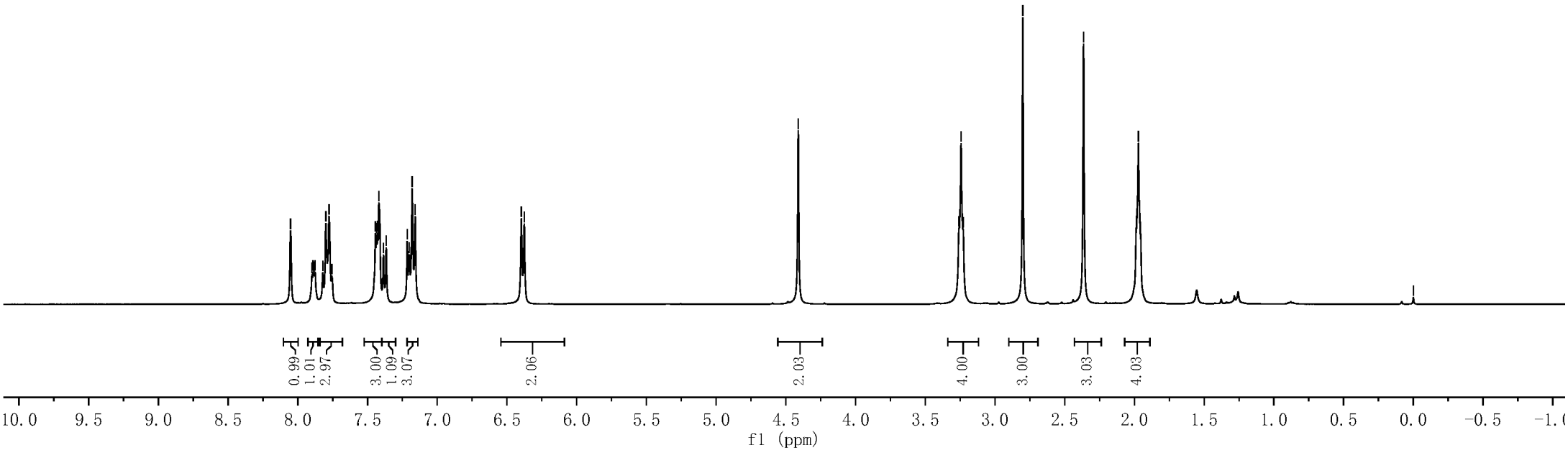






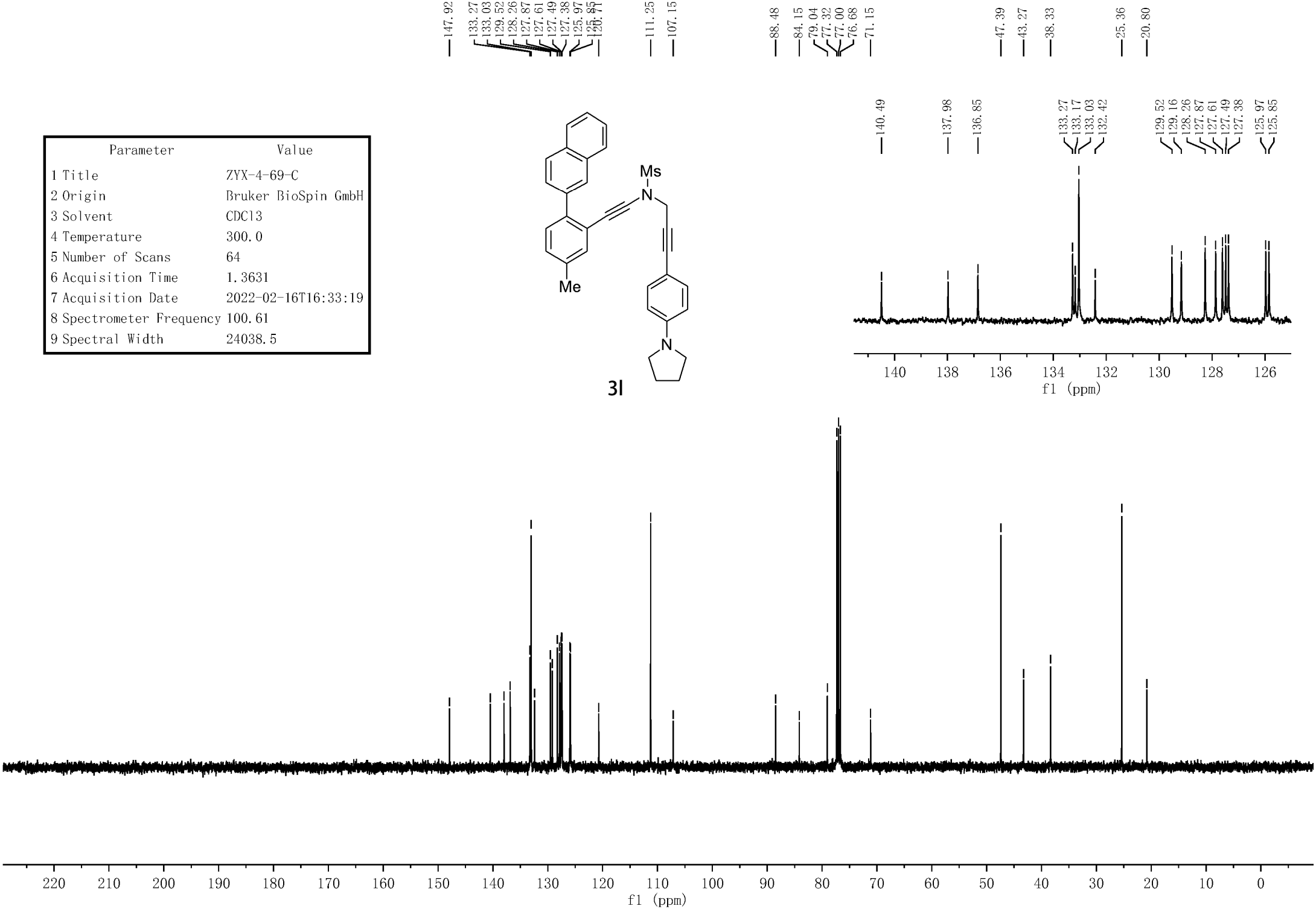
Parameter	Value
1 Title	ZYX-4-69-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	14
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-16T16:31:14
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

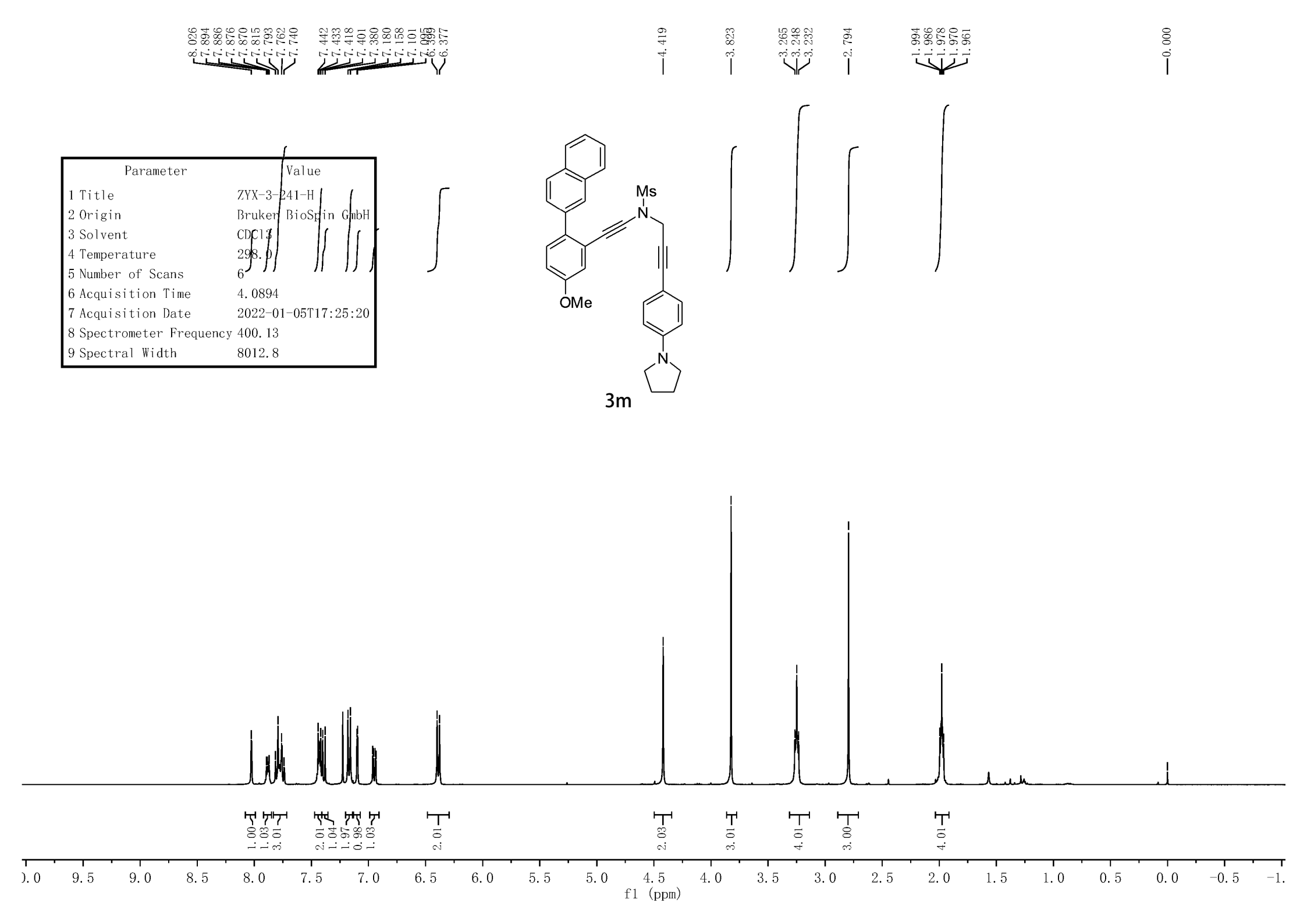
3l



Parameter	Value
1 Title	ZYX-4-69-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	64
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-16T16:33:19
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

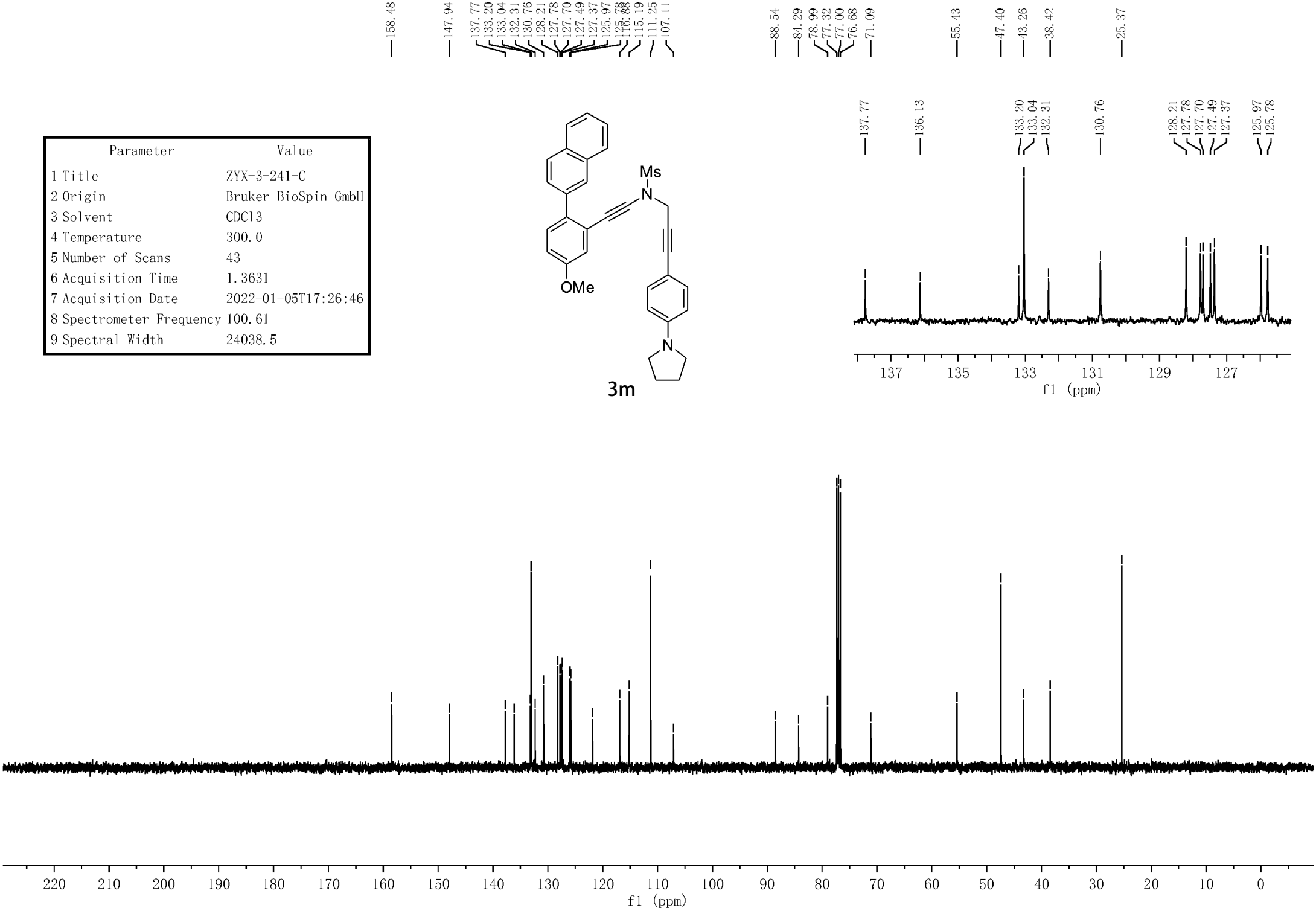
3l

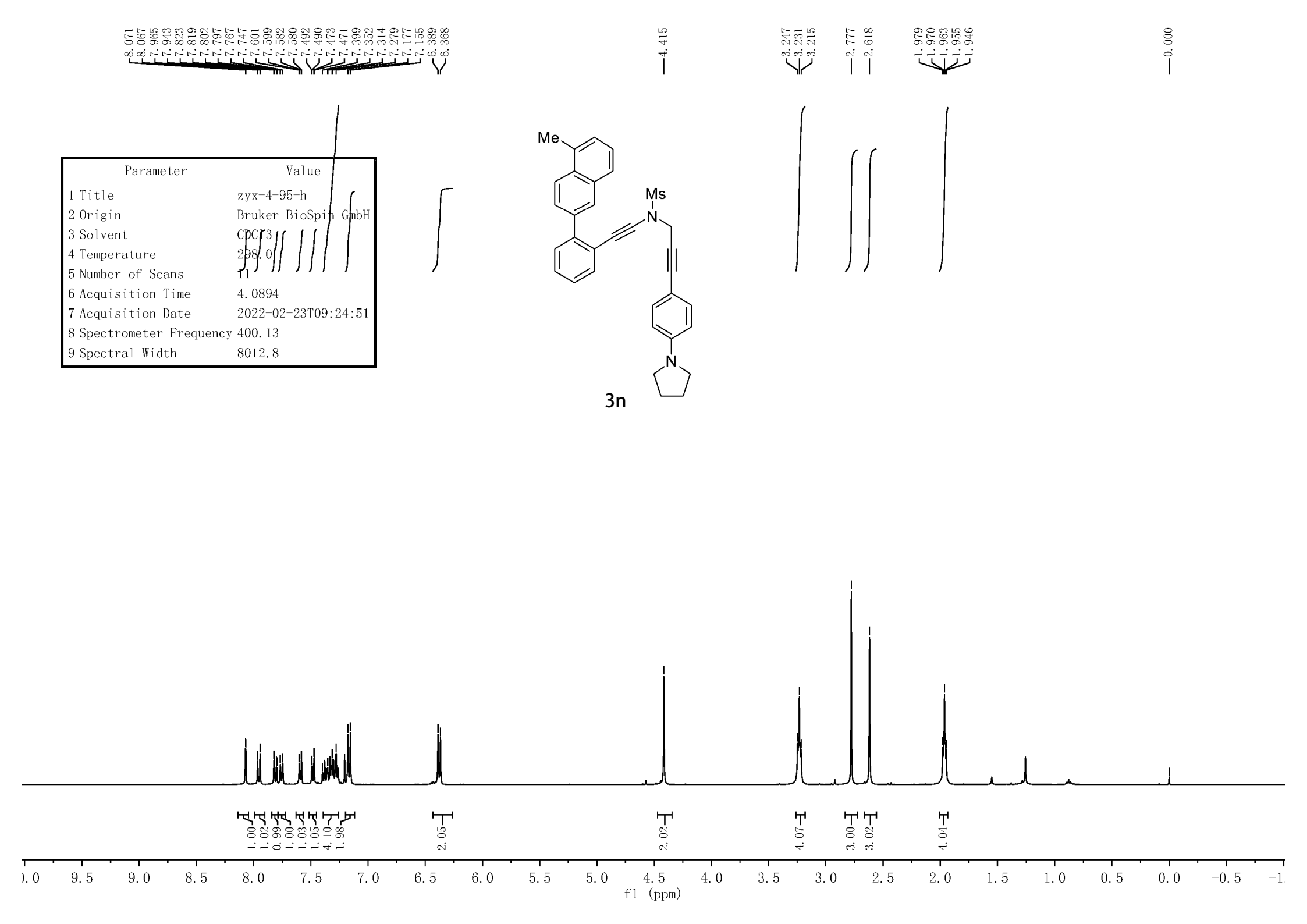



8.026
7.894
7.886
7.876
7.870
7.815
7.793
7.762
7.740
7.442
7.433
7.418
7.401
7.380
7.180
7.158
7.101
6.399
6.377
4.419
3.823
3.265
3.248
3.232
2.794
1.994
1.986
1.978
1.970
1.961
0.000
Parameter Value
1 Title ZYX-3-241-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 6
6 Acquisition Time 4.0894
7 Acquisition Date 2022-01-05T17:25:20
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
OMe
N
3m
1.00
1.03
3.01
2.01
1.04
1.97
0.98
1.03
2.01
2.03
3.01
4.01
3.00
4.01
f1 (ppm)

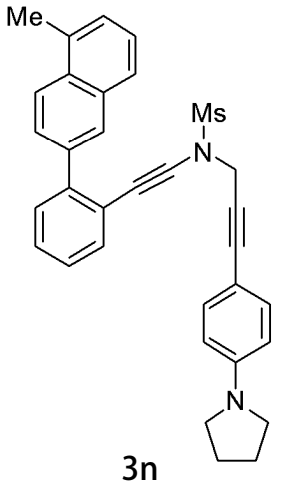
Parameter	Value
1 Title	ZYX-3-241-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	43
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-05T17:26:46
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

3m

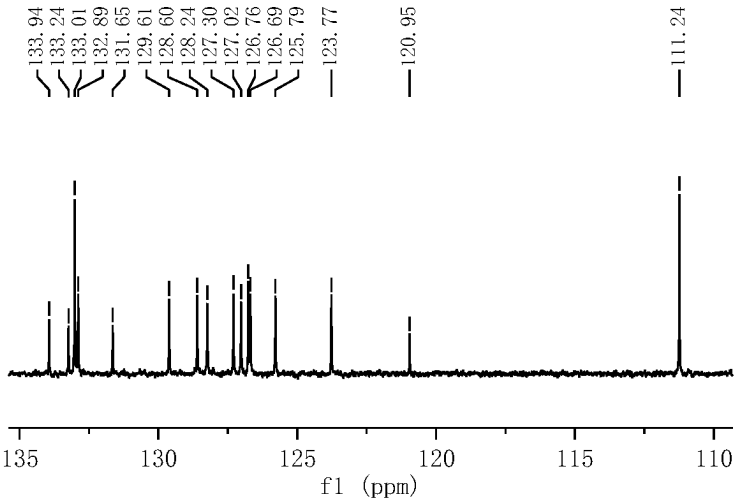


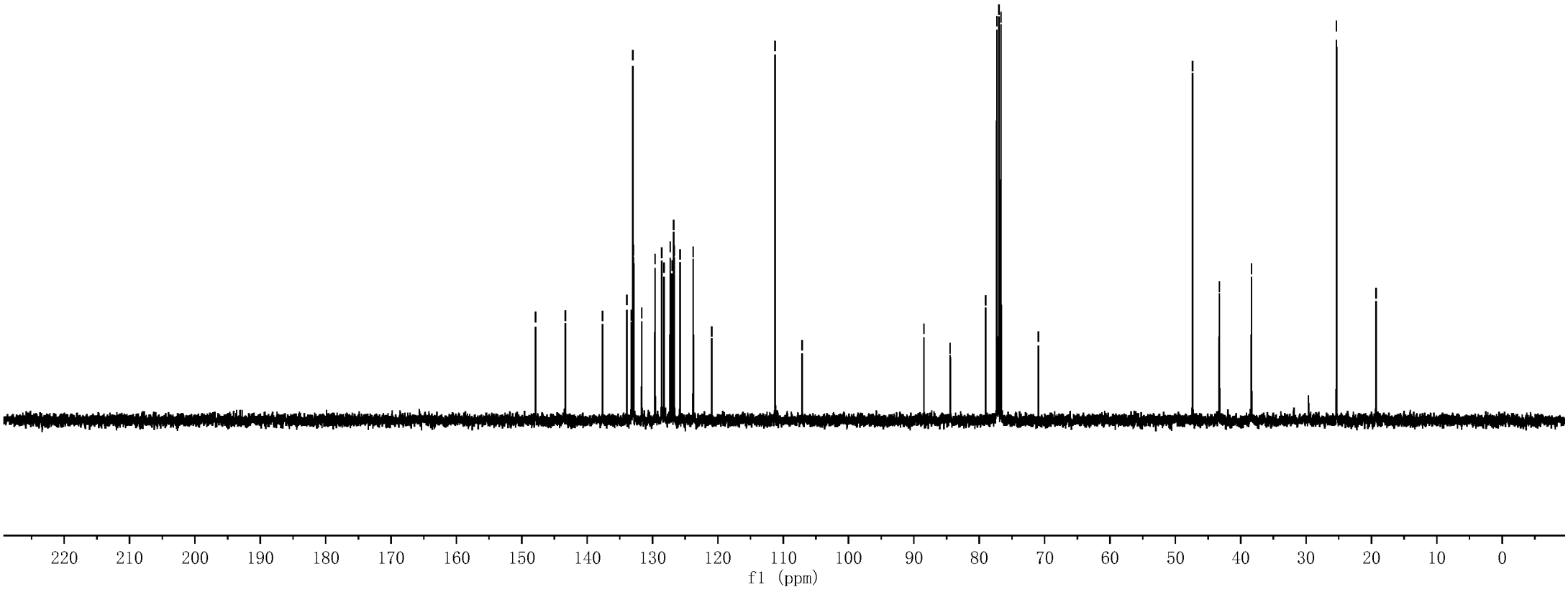

8.071
8.067
7.965
7.943
7.823
7.819
7.802
7.797
7.767
7.747
7.601
7.599
7.582
7.580
7.492
7.490
7.473
7.471
7.399
7.352
7.314
7.279
7.177
7.155
6.389
6.368
4.415
3.247
3.231
3.215
2.777
2.618
1.979
1.970
1.963
1.955
1.946
0.000
Parameter Value
1 Title zyx-4-95-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 11
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-23T09:24:51
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Me
Ms
N
N
3n
1.00
1.02
0.99
1.00
1.03
1.05
4.10
1.98
2.05
2.02
4.07
3.00
3.02
4.04
f1 (ppm)

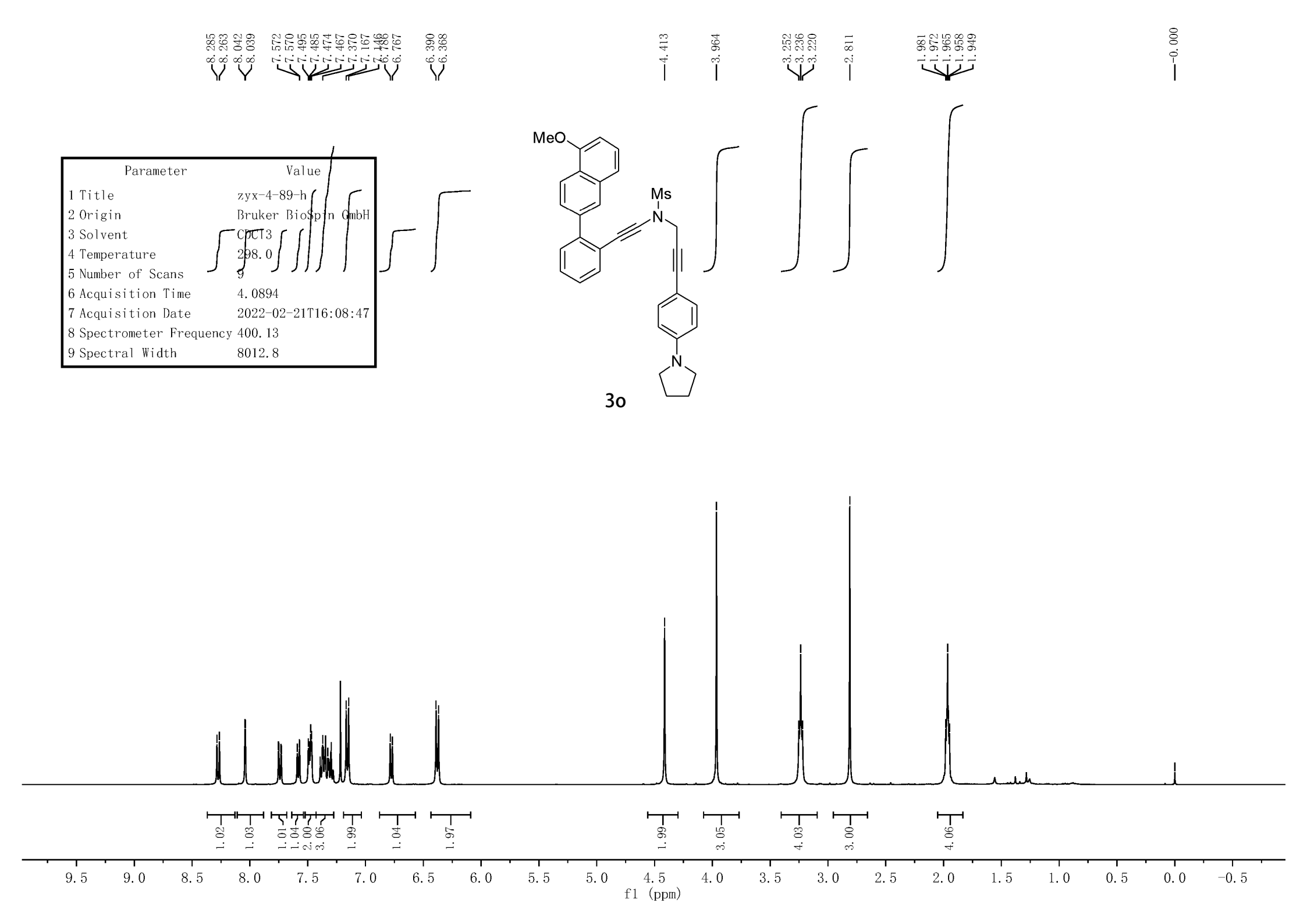
Parameter	Value
1 Title	zyx-4-95-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	45
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-23T09:26:44
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



3n

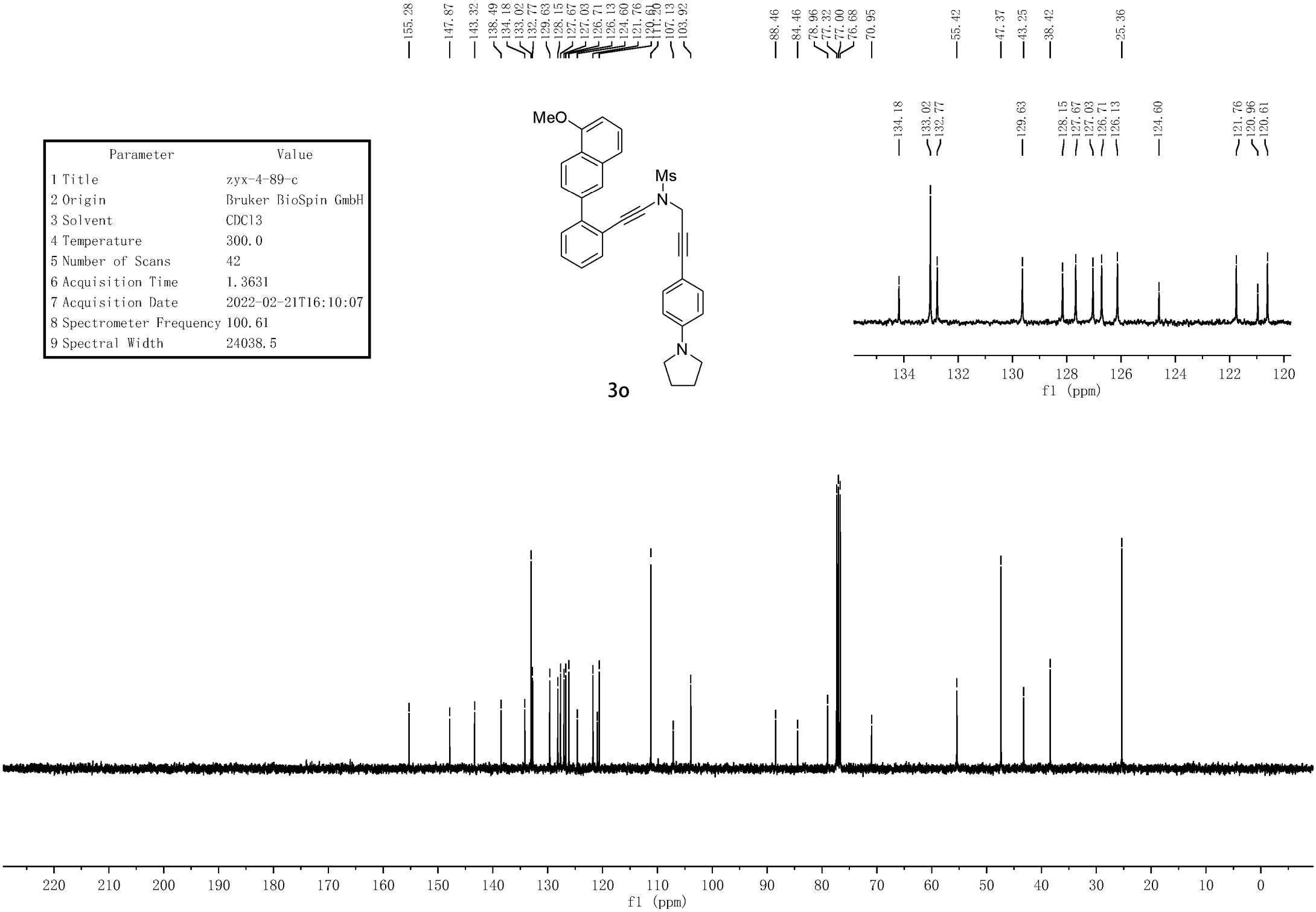


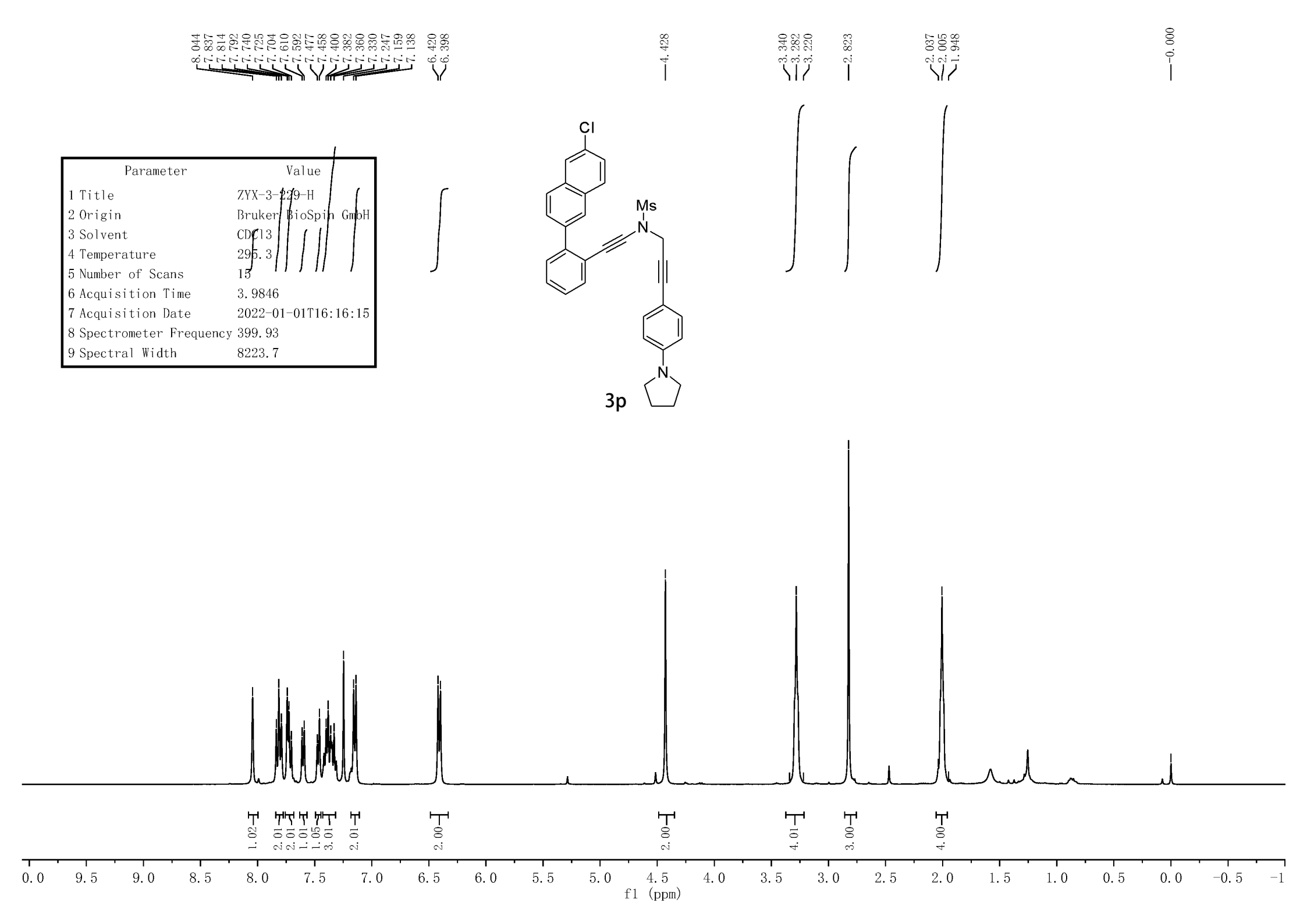


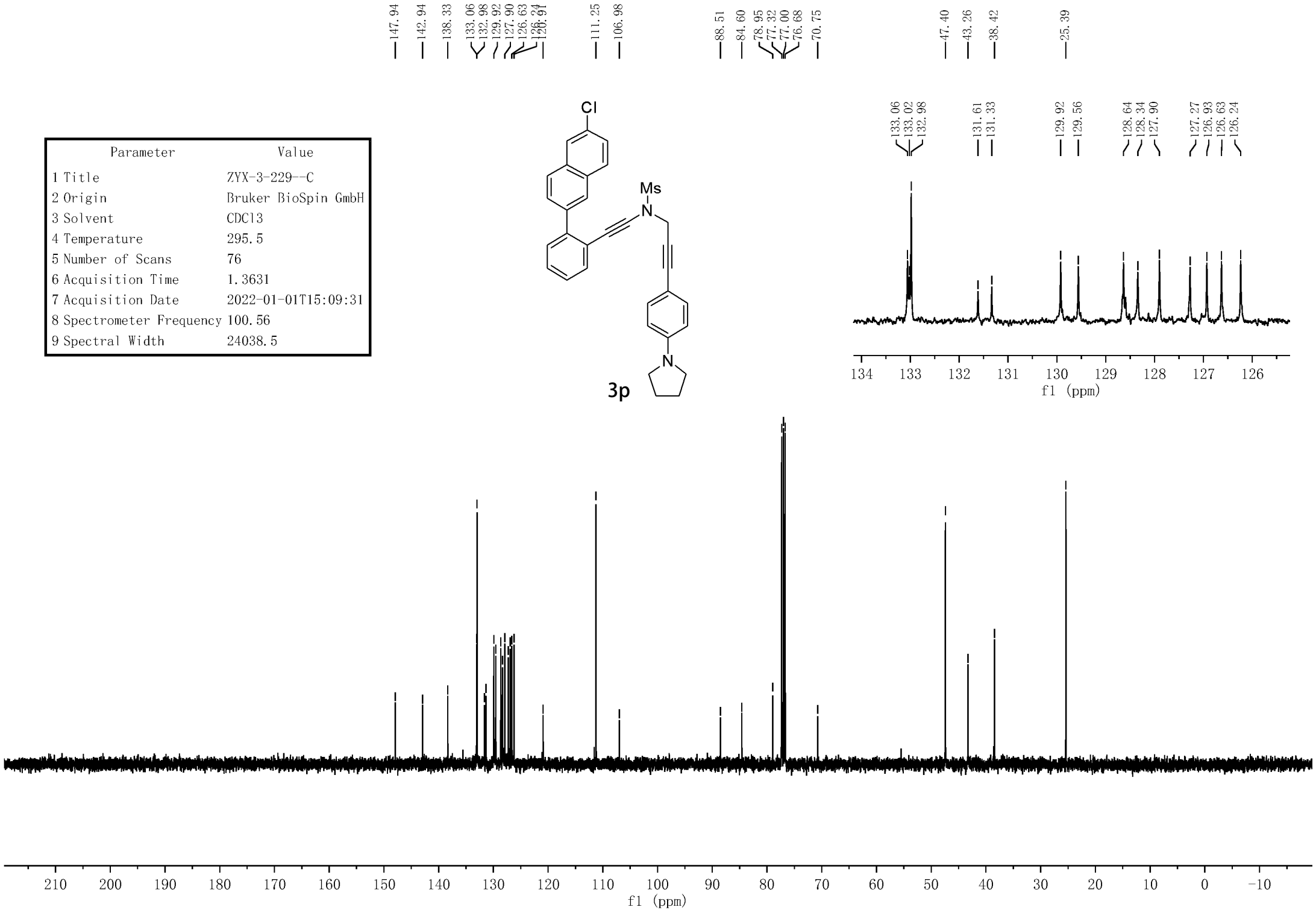

8.285
8.263
8.042
8.039
7.572
7.570
7.495
7.485
7.474
7.467
7.370
7.167
6.767
6.390
6.368
4.413
3.964
3.252
3.236
3.220
2.811
1.981
1.972
1.965
1.958
1.949
0.000
Parameter Value
1 Title zyx-4-89-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 9
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-21T16:08:47
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
MeO
Ms
N
N
3o
1.02
1.03
1.01
1.04
2.00
3.06
1.99
1.04
1.97
1.99
3.05
4.03
3.00
4.06
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)

Parameter	Value
1 Title	zyx-4-89-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	42
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-21T16:10:07
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

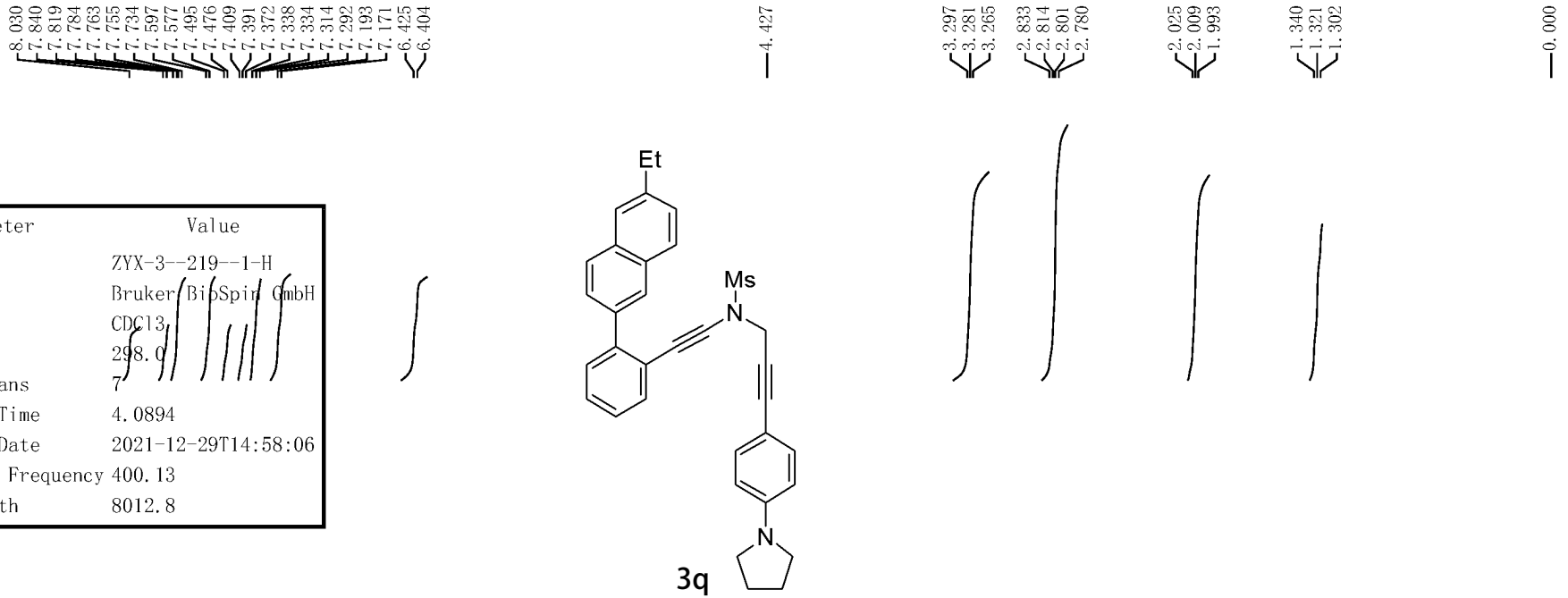
3o



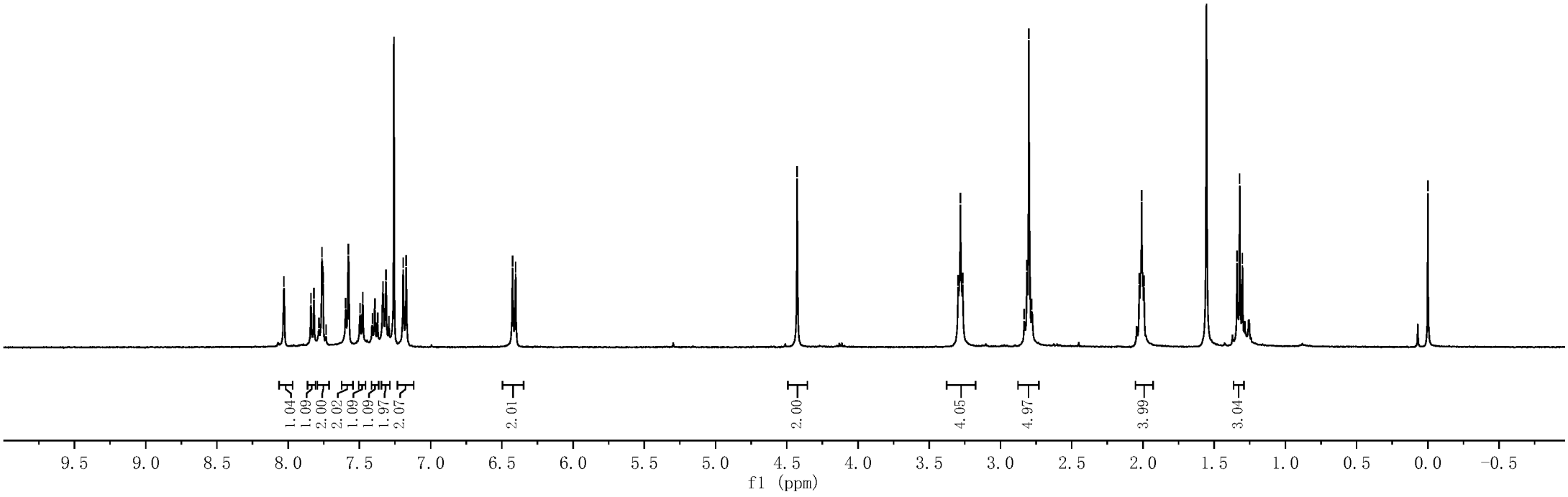

8.044
7.837
7.814
7.792
7.740
7.725
7.704
7.610
7.592
7.477
7.458
7.400
7.382
7.360
7.330
7.247
7.159
7.138
6.420
6.398
4.428
3.340
3.282
3.220
2.823
2.037
2.005
1.948
-0.000
Parameter Value
1 Title ZYX-3-229-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.3
5 Number of Scans 15
6 Acquisition Time 3.9846
7 Acquisition Date 2022-01-01T16:16:15
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Cl
Ms
N
N
3p
1.02
2.01
2.01
1.01
1.05
3.01
2.01
2.00
2.00
4.01
3.00
4.00
0.0
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
-1
f1 (ppm)



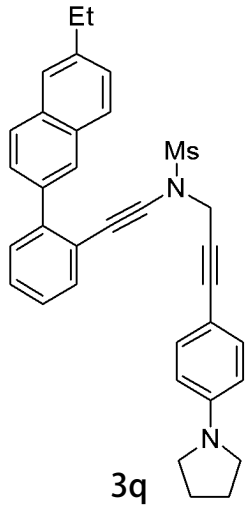
Parameter	Value
1 Title	ZYX-3-229--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	76
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-01T15:09:31
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



Parameter	Value
1 Title	ZYX-3--219--1-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	7
6 Acquisition Time	4.0894
7 Acquisition Date	2021-12-29T14:58:06
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

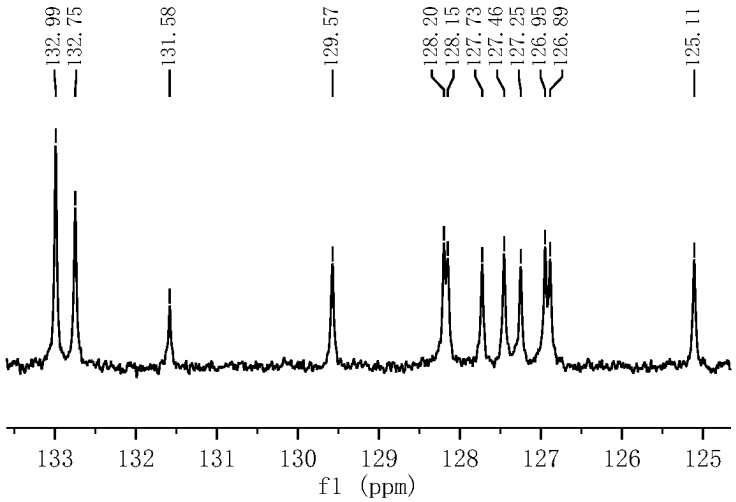


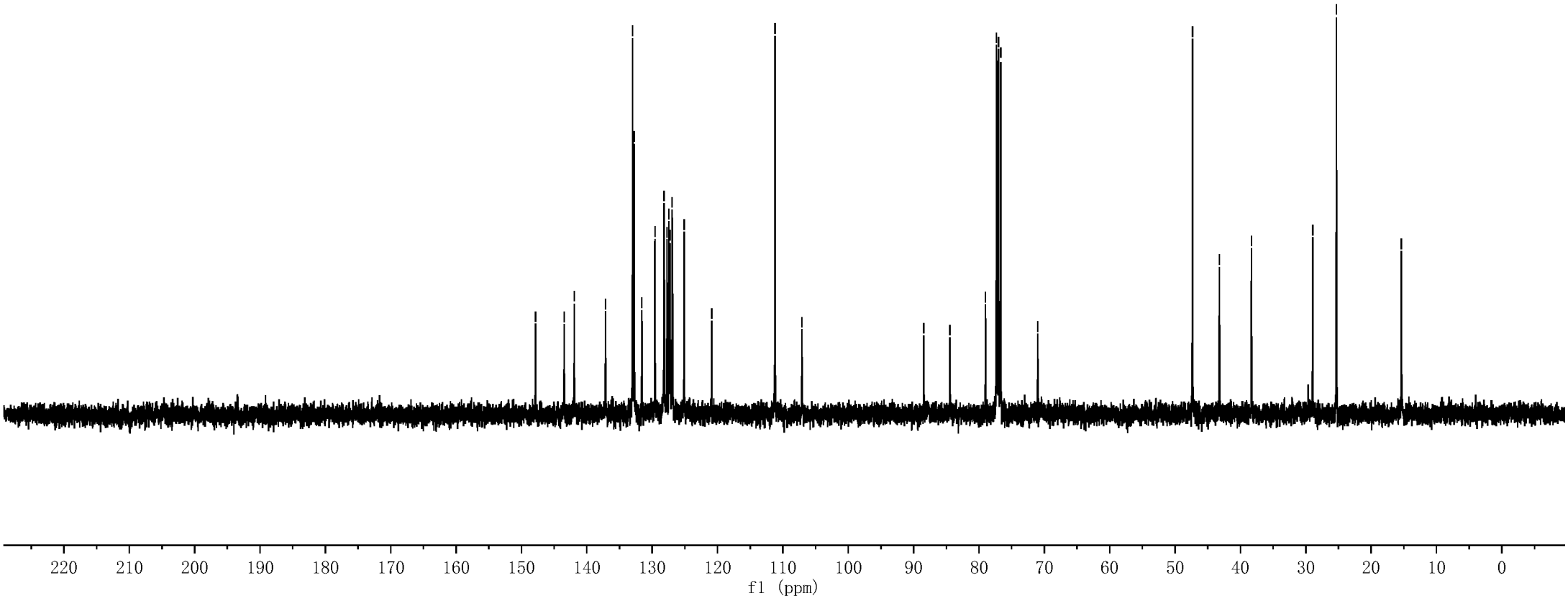
Parameter	Value
1 Title	ZYX-3--219-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	46
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-29T14:51:33
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

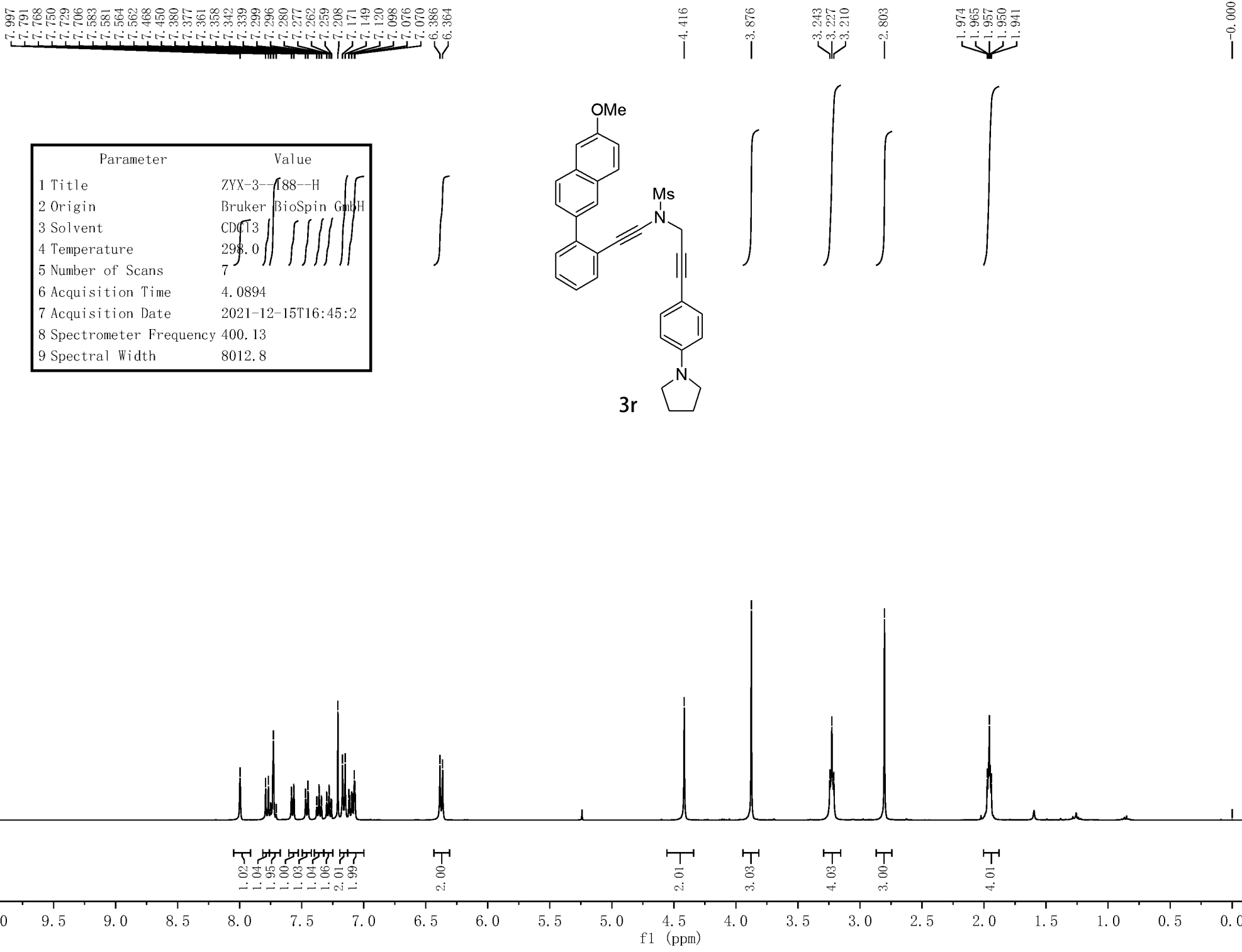


3q

147.86 143.46 141.91 137.14 132.99 132.75 131.58 129.57 128.20 128.15 127.73 127.46 127.25 126.95 126.89 125.11 120.90 111.20 107.09 88.45 84.44 79.00 77.32 77.00 76.68 71.01 47.33 43.22 38.31 28.95 25.31 15.37

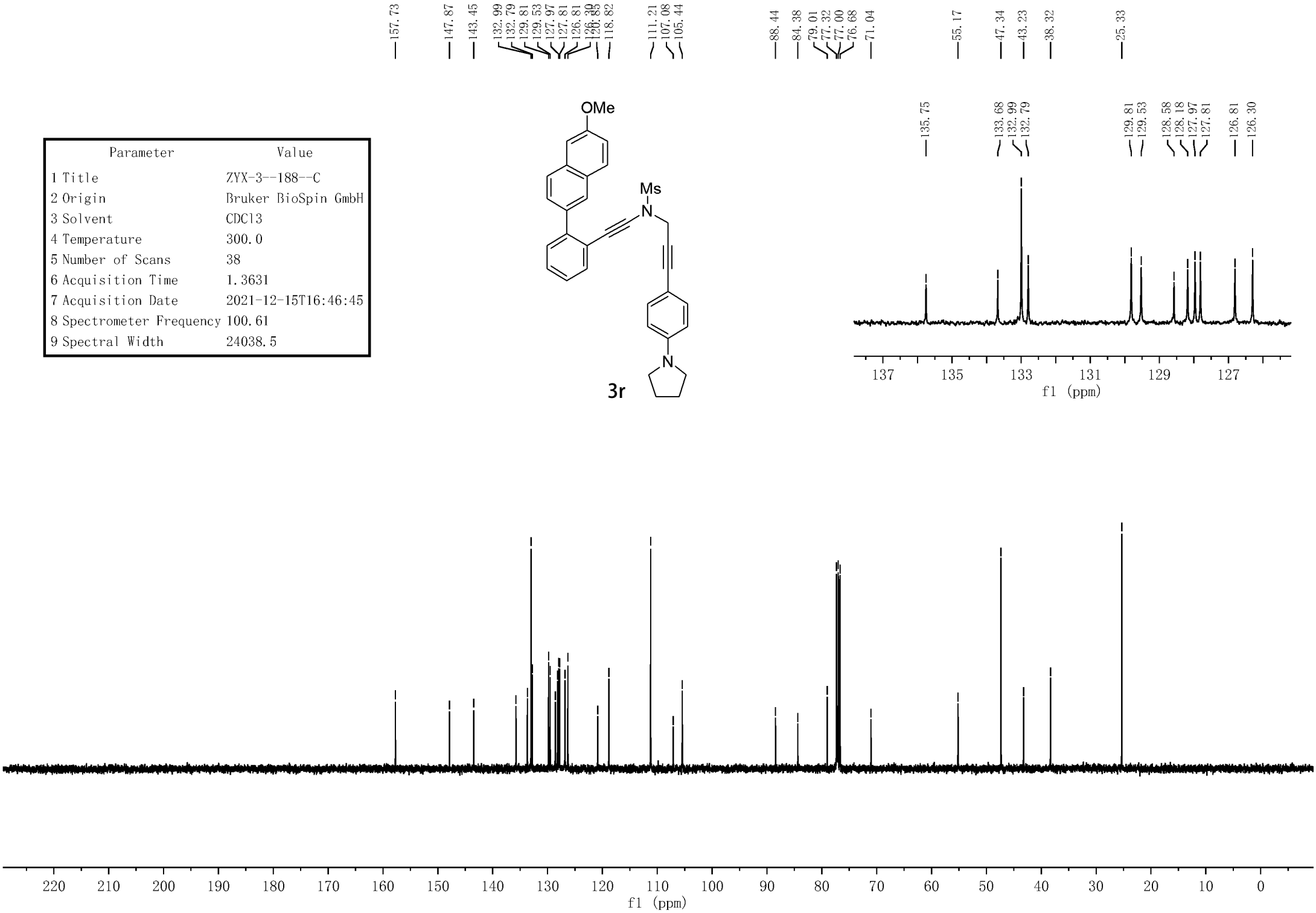


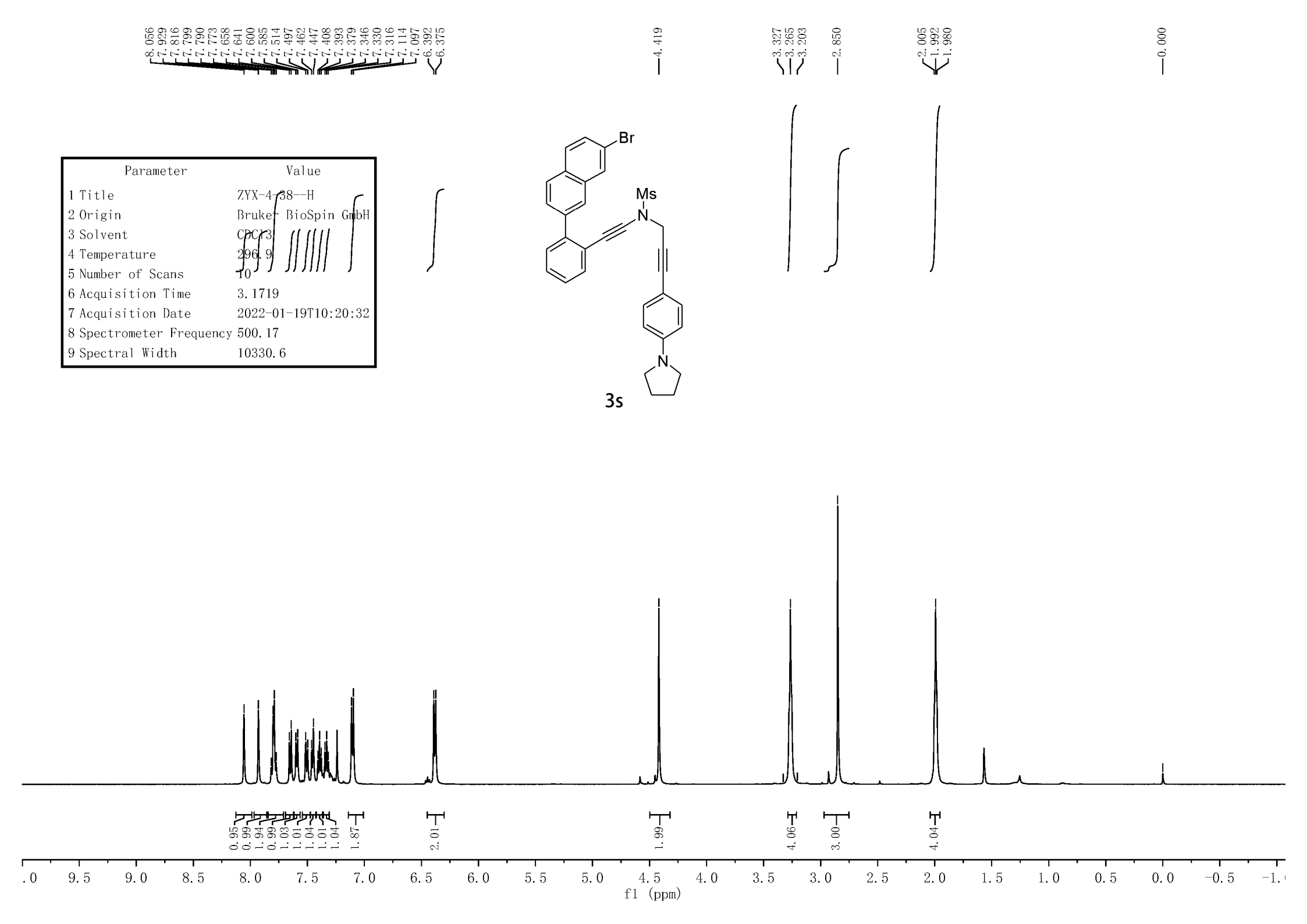



7.997
7.791
7.768
7.750
7.729
7.706
7.583
7.581
7.564
7.562
7.468
7.450
7.380
7.377
7.361
7.358
7.342
7.339
7.299
7.296
7.280
7.277
7.262
7.259
7.208
7.171
7.149
7.120
7.098
7.076
7.070
6.386
6.364
4.416
3.876
3.243
3.227
3.210
2.803
1.974
1.965
1.957
1.950
1.941
-0.000
Parameter
Value
1 Title
ZYX-3--188--H
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
298.0
5 Number of Scans
7
6 Acquisition Time
4.0894
7 Acquisition Date
2021-12-15T16:45:2
8 Spectrometer Frequency
400.13
9 Spectral Width
8012.8
OMe
Ms
N
N
3r
1.02
1.04
1.95
1.00
1.03
1.04
1.06
2.01
1.99
2.00
2.01
3.03
4.03
3.00
4.01
f1 (ppm)

Parameter	Value
1 Title	ZYX-3--188--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	38
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-15T16:46:45
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

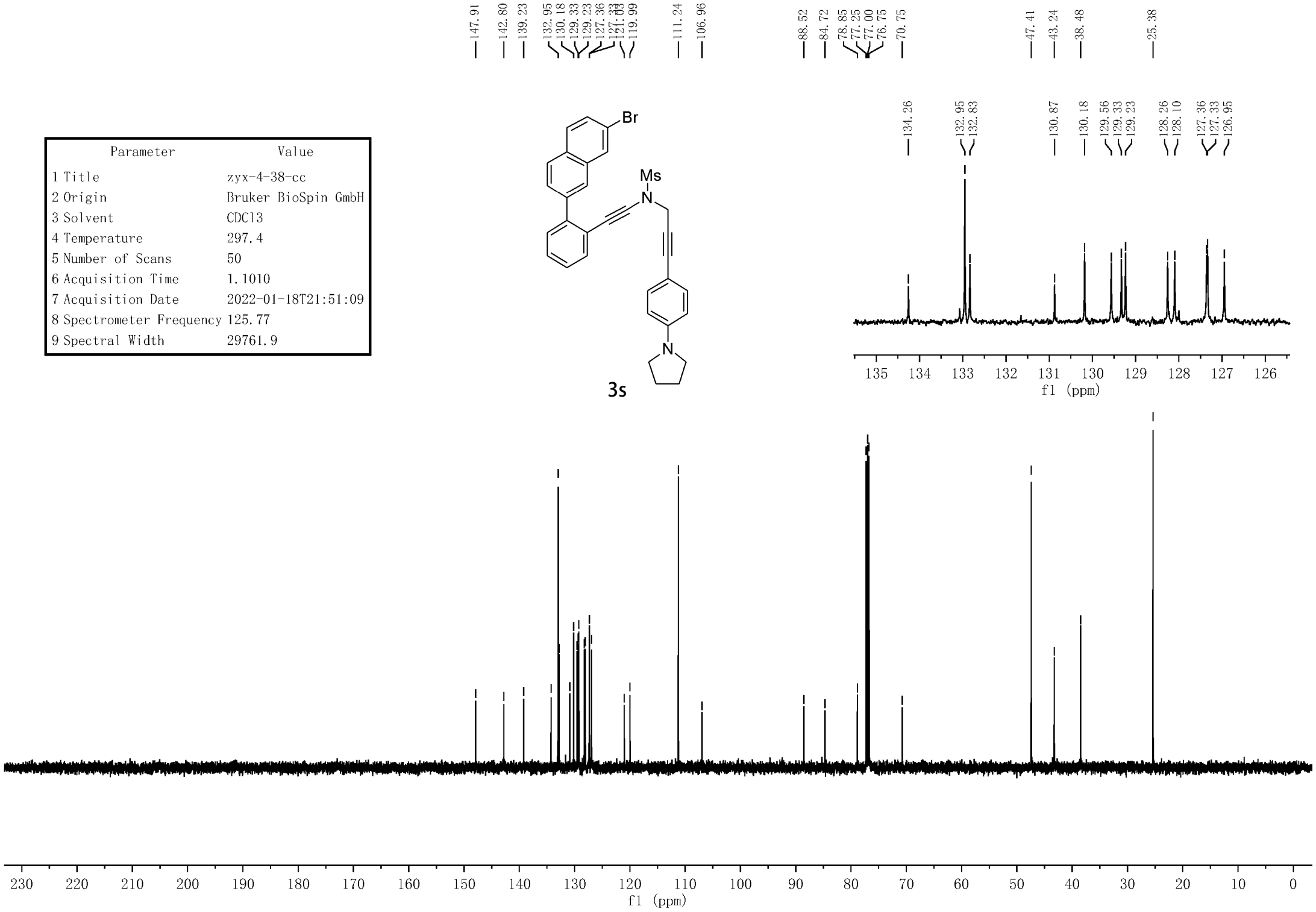
3r

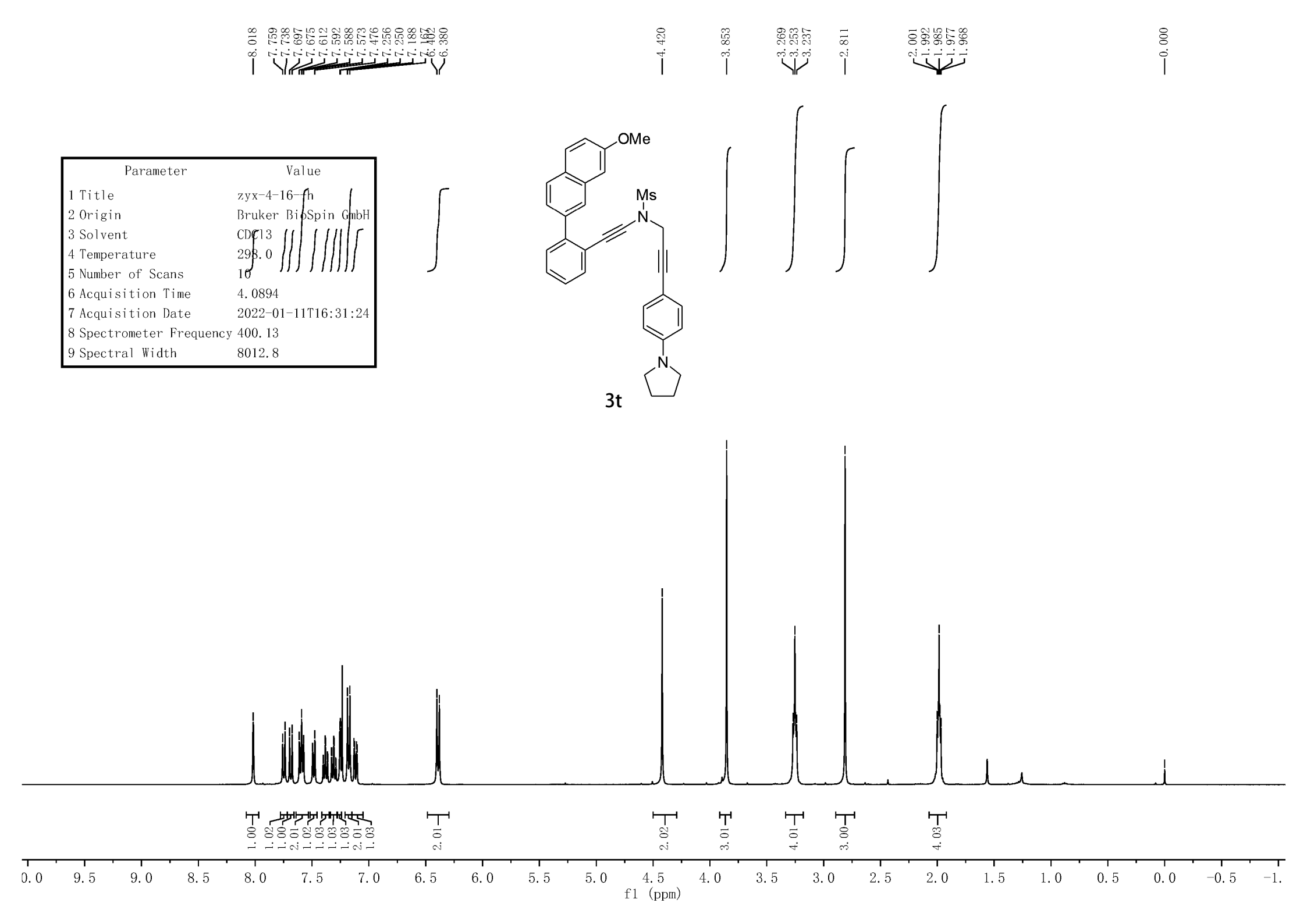



8.056
7.929
7.816
7.799
7.790
7.773
7.658
7.641
7.600
7.585
7.514
7.497
7.462
7.447
7.408
7.393
7.379
7.346
7.330
7.316
7.114
7.097
6.392
6.375
4.419
3.327
3.265
3.203
2.850
2.005
1.992
1.980
0.000
Parameter Value
1 Title ZYX-4-38--H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.9
5 Number of Scans 10
6 Acquisition Time 3.1719
7 Acquisition Date 2022-01-19T10:20:32
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
Ms
N
N
3s
0.95
0.99
1.94
0.99
1.03
1.01
1.04
1.01
1.04
1.87
2.01
1.99
4.06
3.00
4.04
f1 (ppm)

Parameter	Value
1 Title	zyx-4-38-cc
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.4
5 Number of Scans	50
6 Acquisition Time	1.1010
7 Acquisition Date	2022-01-18T21:51:09
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

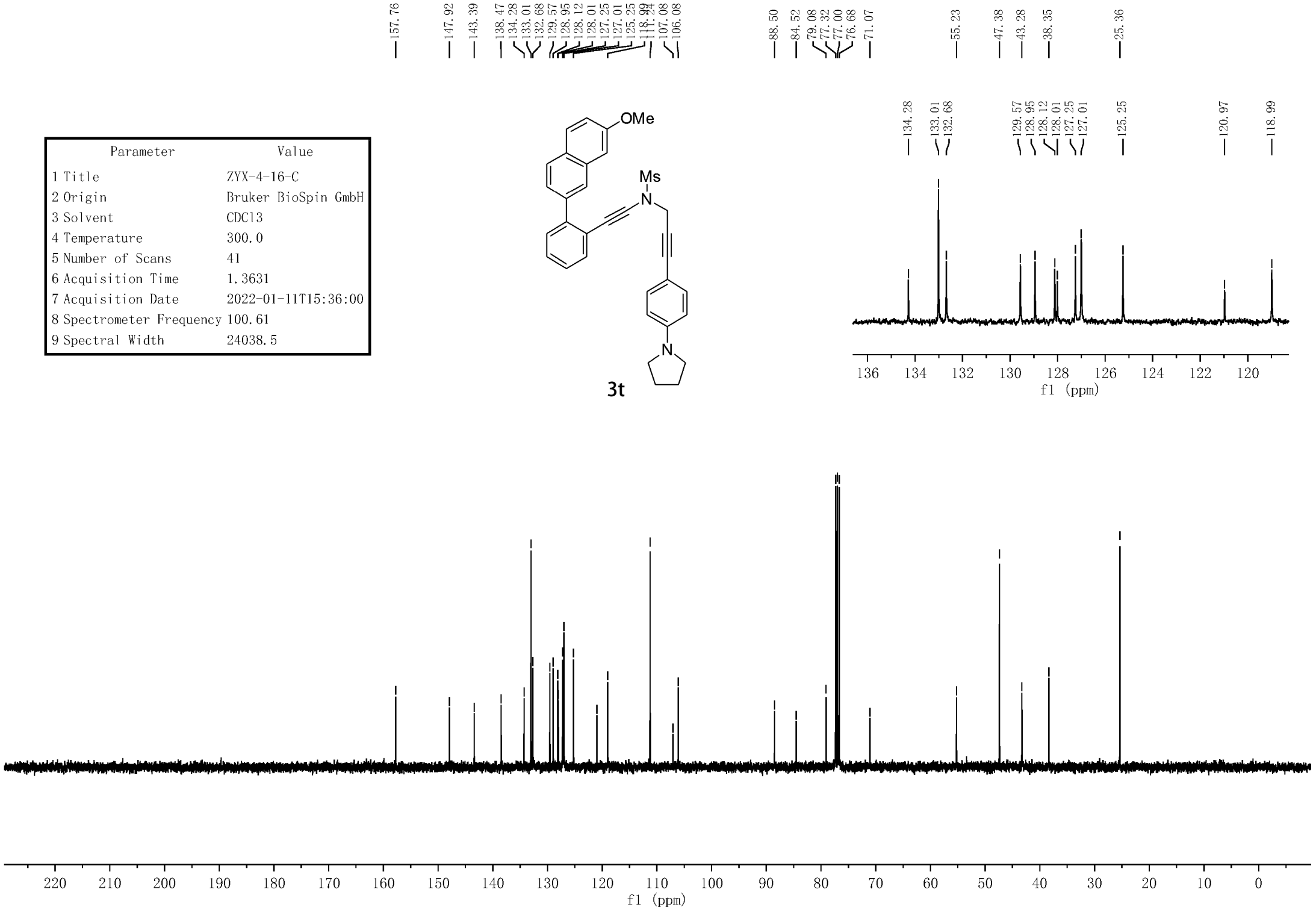
3s

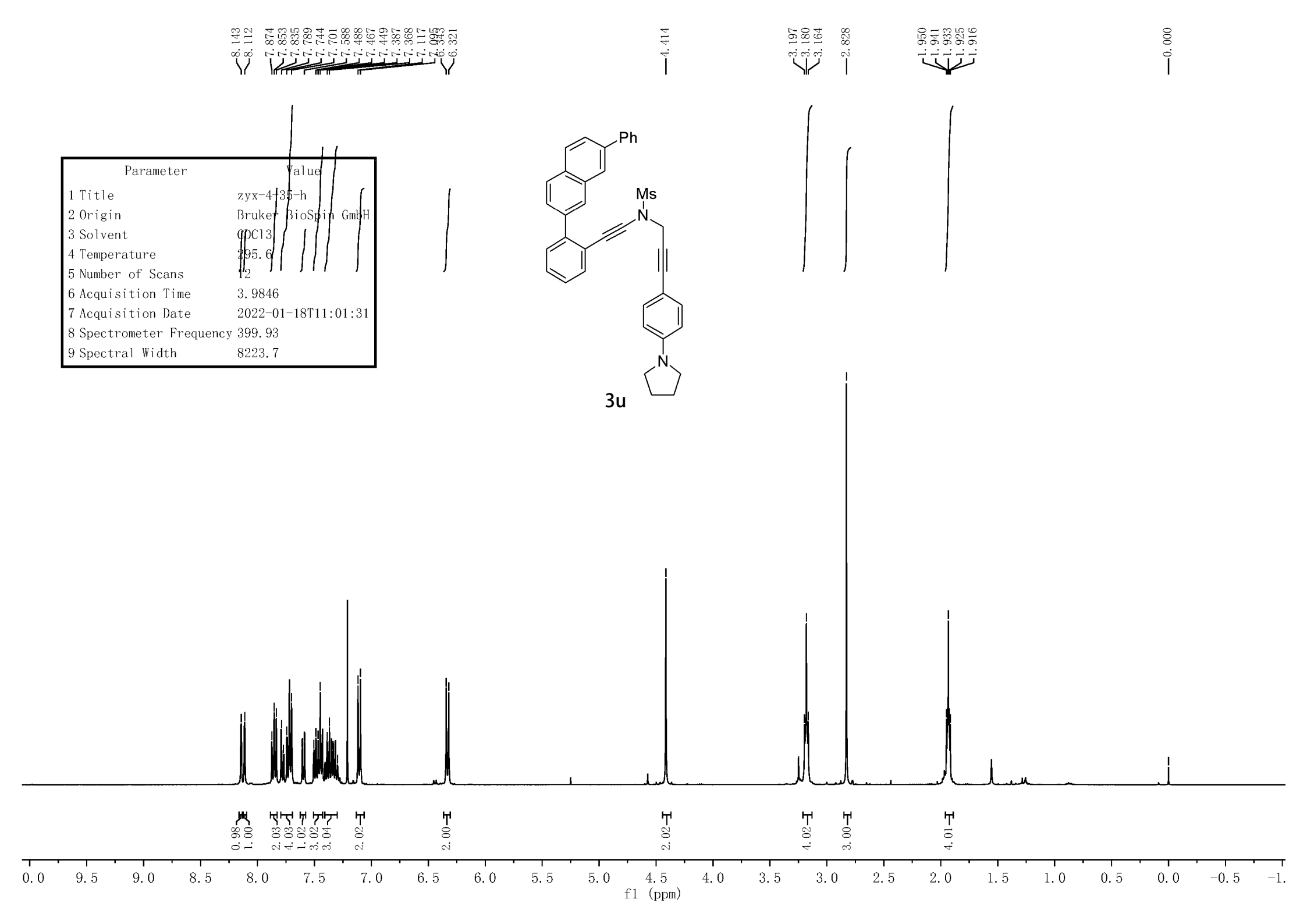



8.018
7.759
7.738
7.697
7.675
7.612
7.592
7.588
7.573
7.476
7.256
7.250
7.188
7.167
6.402
6.380
4.420
3.853
3.269
3.253
3.237
2.811
2.001
1.992
1.985
1.977
1.968
0.000
Parameter Value
1 Title zyx-4-16-fh
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 16
6 Acquisition Time 4.0894
7 Acquisition Date 2022-01-11T16:31:24
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
OMe
Ms
N
N
3t
1.00
1.02
1.00
2.01
1.02
1.03
1.03
1.03
2.01
1.03
2.01
2.02
3.01
4.01
3.00
4.03
f1 (ppm)

Parameter	Value
1 Title	ZYX-4-16-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	41
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-11T15:36:00
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

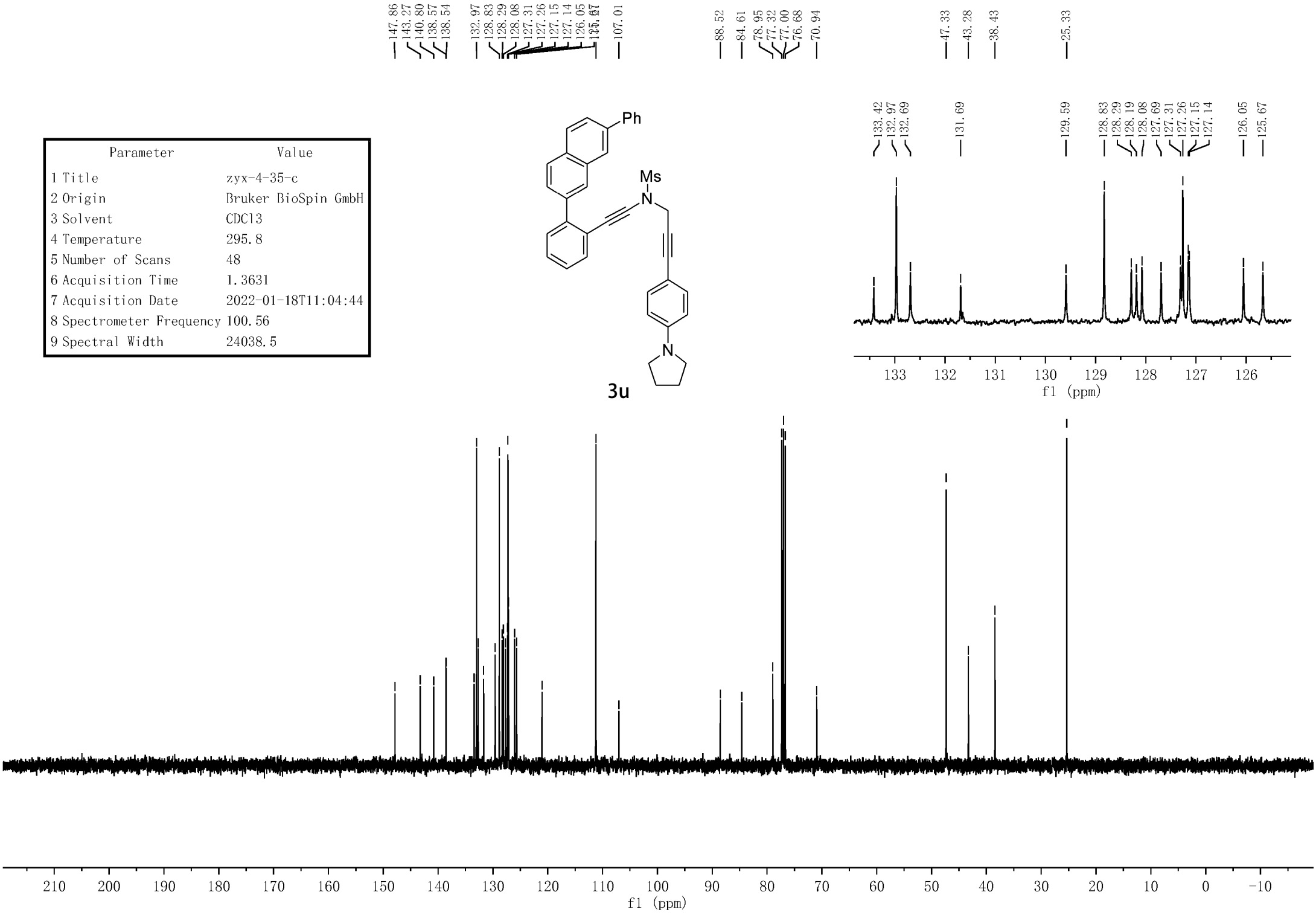
3t

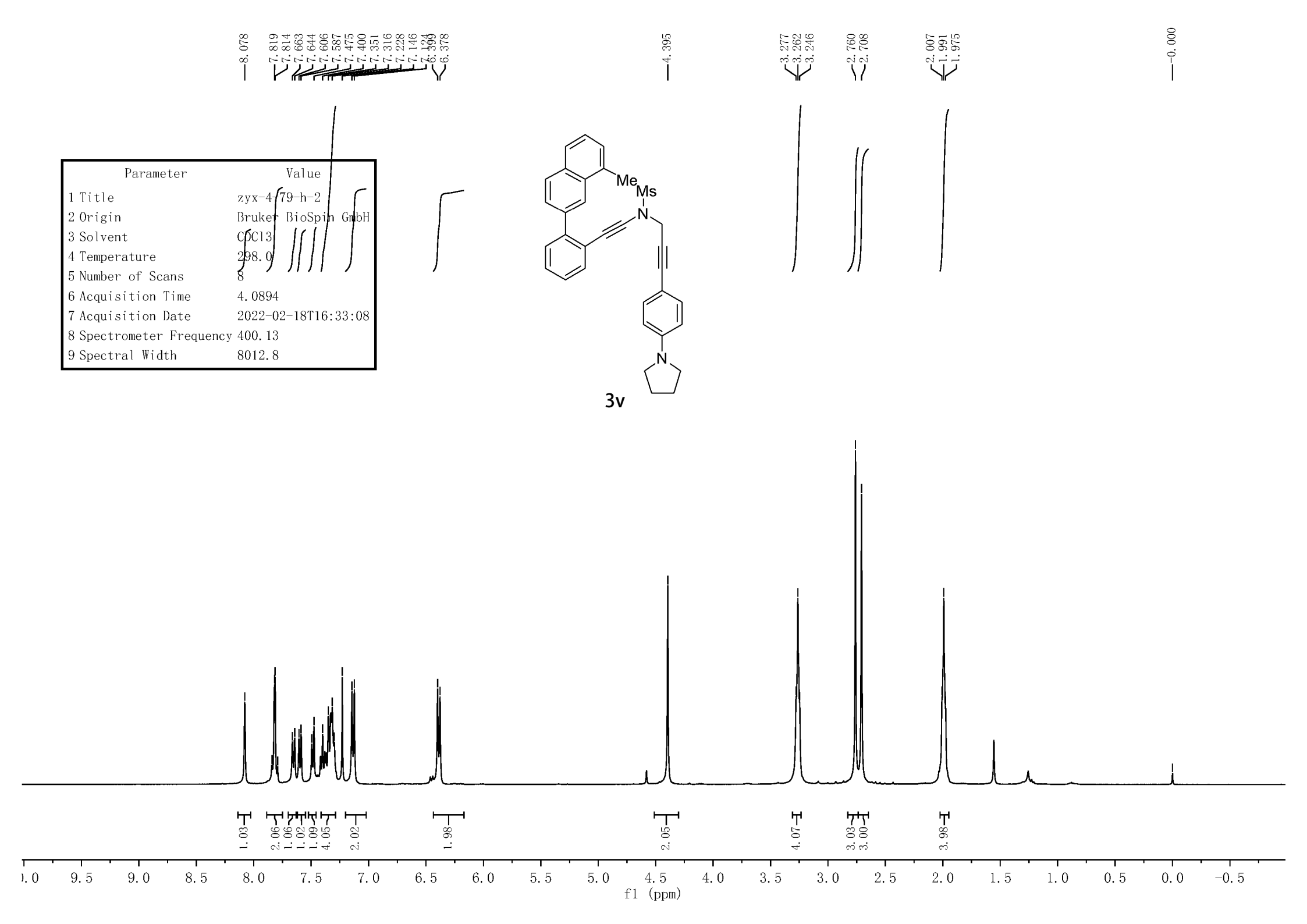



8.143
8.112
7.874
7.853
7.835
7.789
7.744
7.701
7.588
7.488
7.467
7.449
7.387
7.368
7.117
7.095
6.343
6.321
4.414
3.197
3.180
3.164
2.828
1.950
1.941
1.933
1.925
1.916
0.000
Parameter Value
1 Title zyx-4-35-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.6
5 Number of Scans 12
6 Acquisition Time 3.9846
7 Acquisition Date 2022-01-18T11:01:31
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ph
Ms
N
N
3u
0.98
1.00
2.03
4.03
1.02
3.02
3.04
2.02
2.00
2.02
4.02
3.00
4.01
0.0
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
-1.
f1 (ppm)

Parameter	Value
1 Title	zyx-4-35-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	48
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-18T11:04:44
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

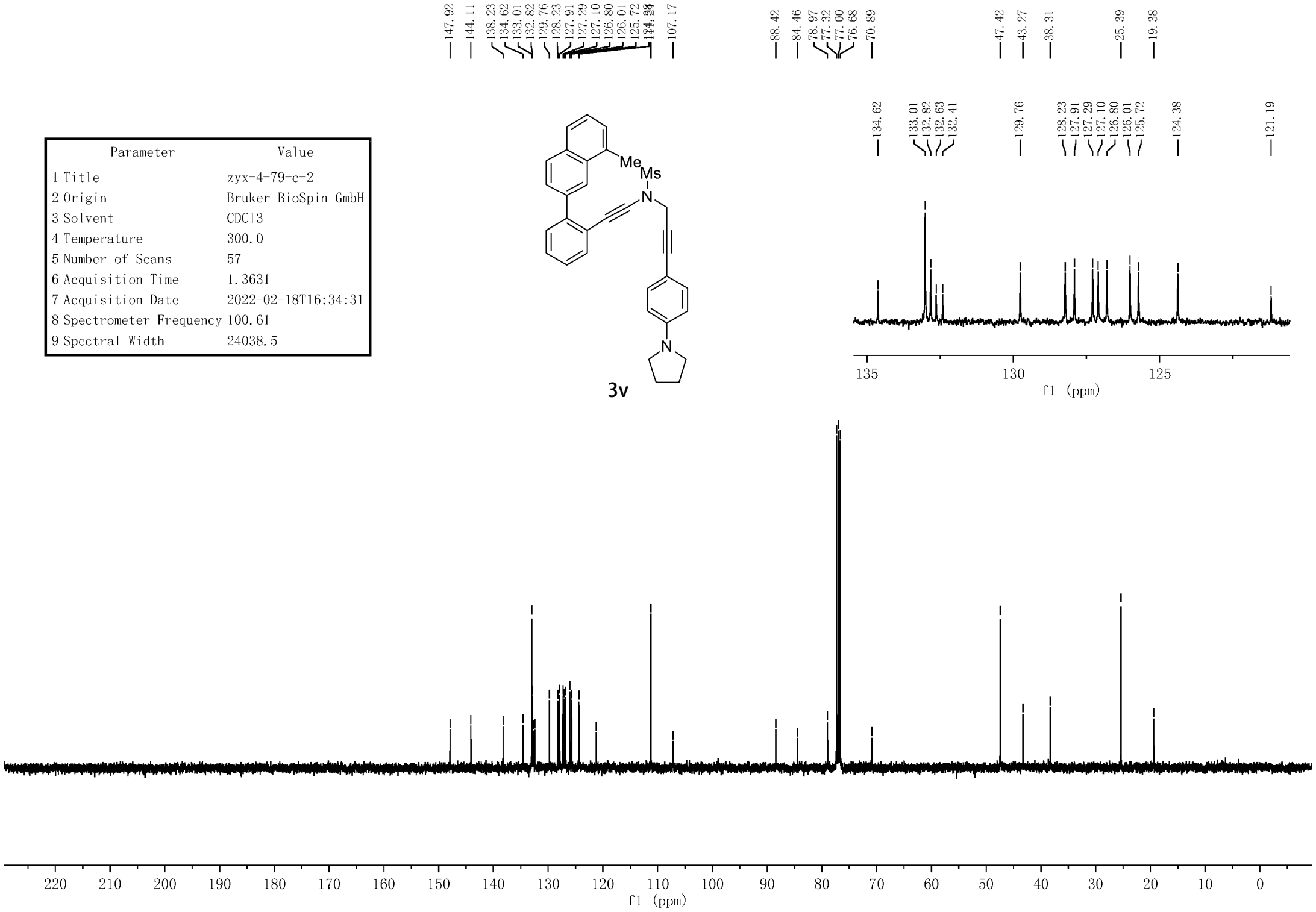
3u

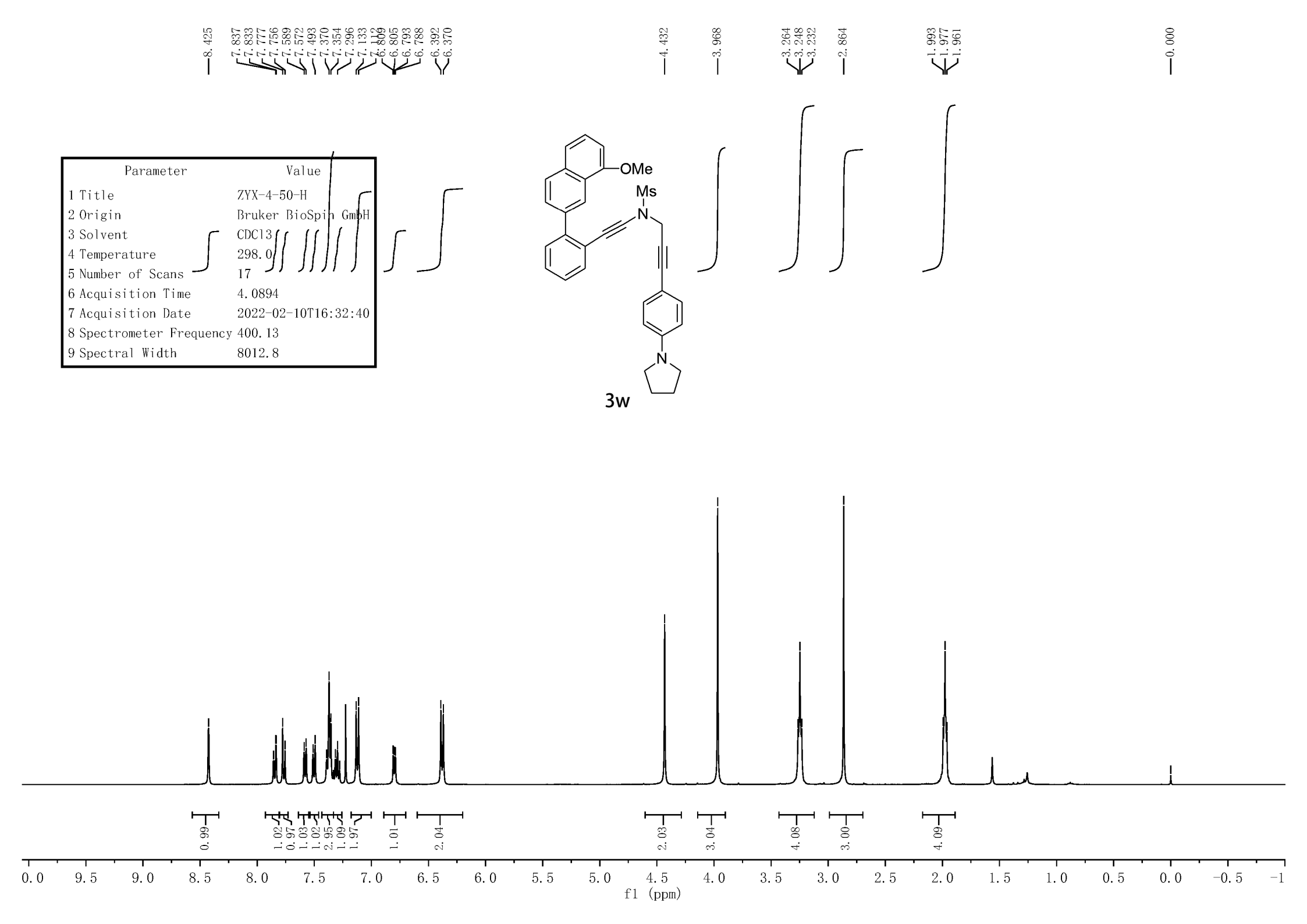


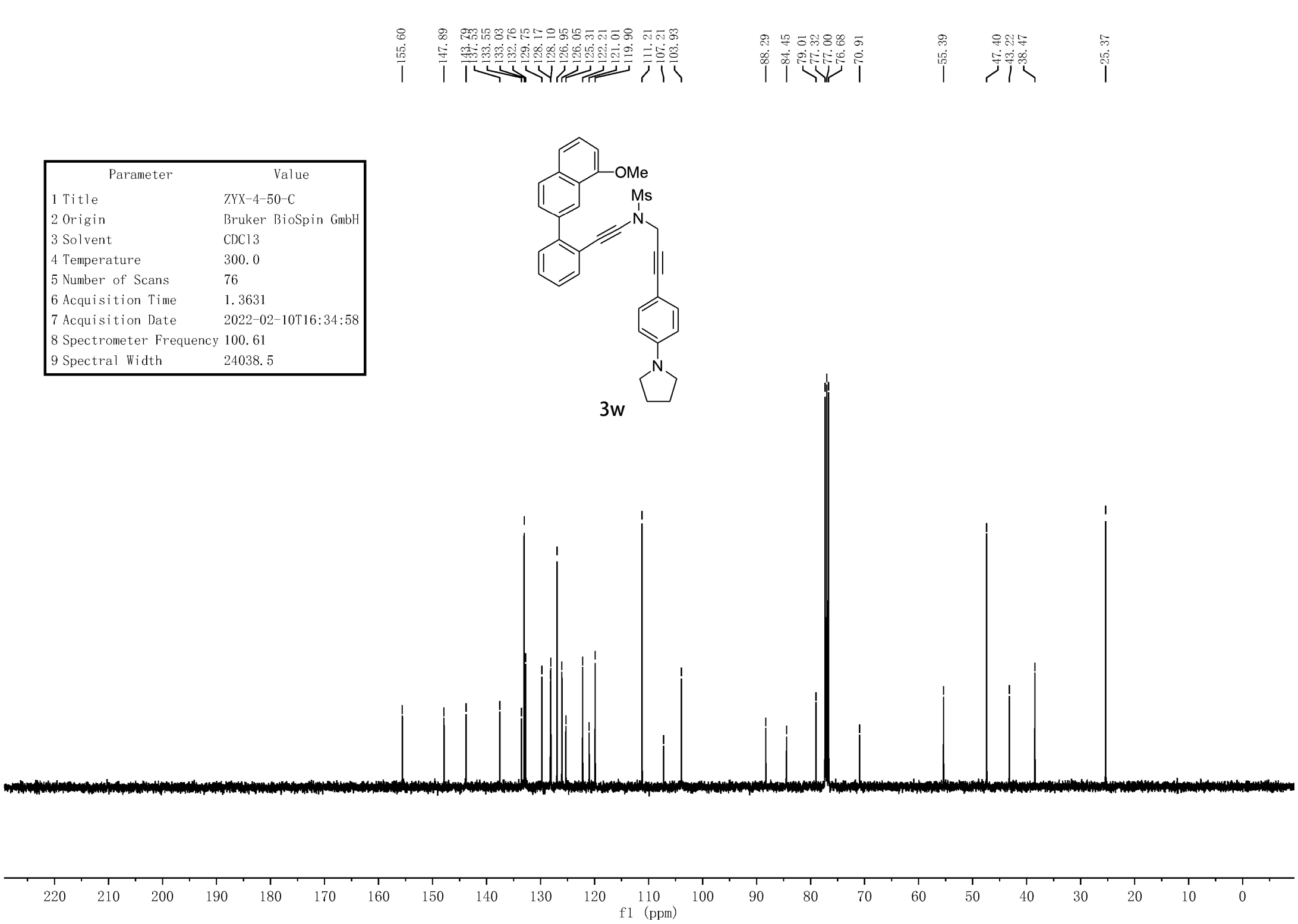

8.078
7.819
7.814
7.663
7.644
7.606
7.587
7.475
7.400
7.351
7.316
7.228
7.146
7.124
6.399
6.378
4.395
3.277
3.262
3.246
2.760
2.708
2.007
1.991
1.975
-0.000
Parameter Value
1 Title zyx-4-79-h-2
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-18T16:33:08
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Me
Ms
N
N
3v
1.03
2.06
1.06
1.02
1.09
4.05
2.02
1.98
2.05
4.07
3.03
3.00
3.98
f1 (ppm)

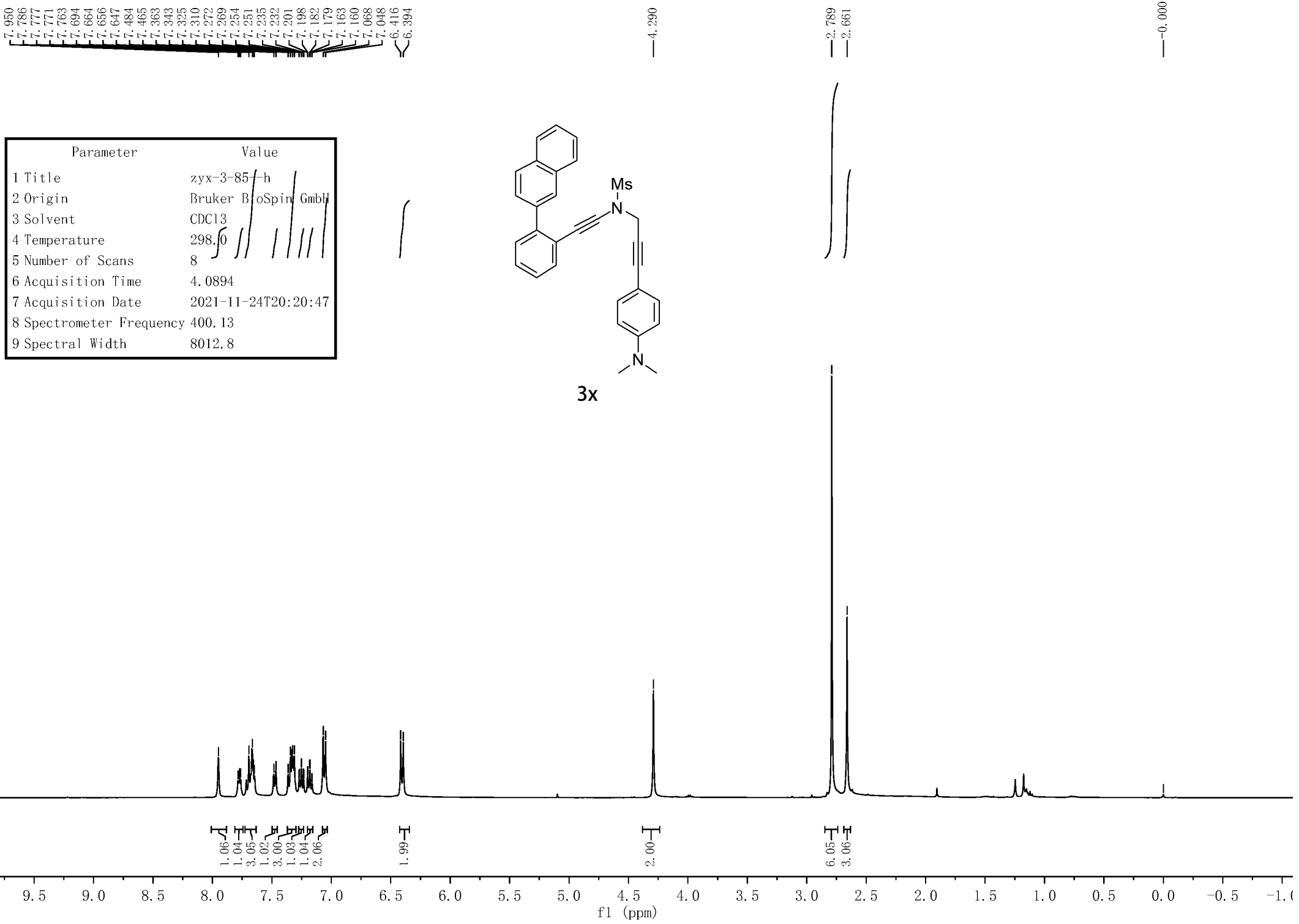
Parameter	Value
1 Title	zyx-4-79-c-2
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	57
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-18T16:34:31
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

3v



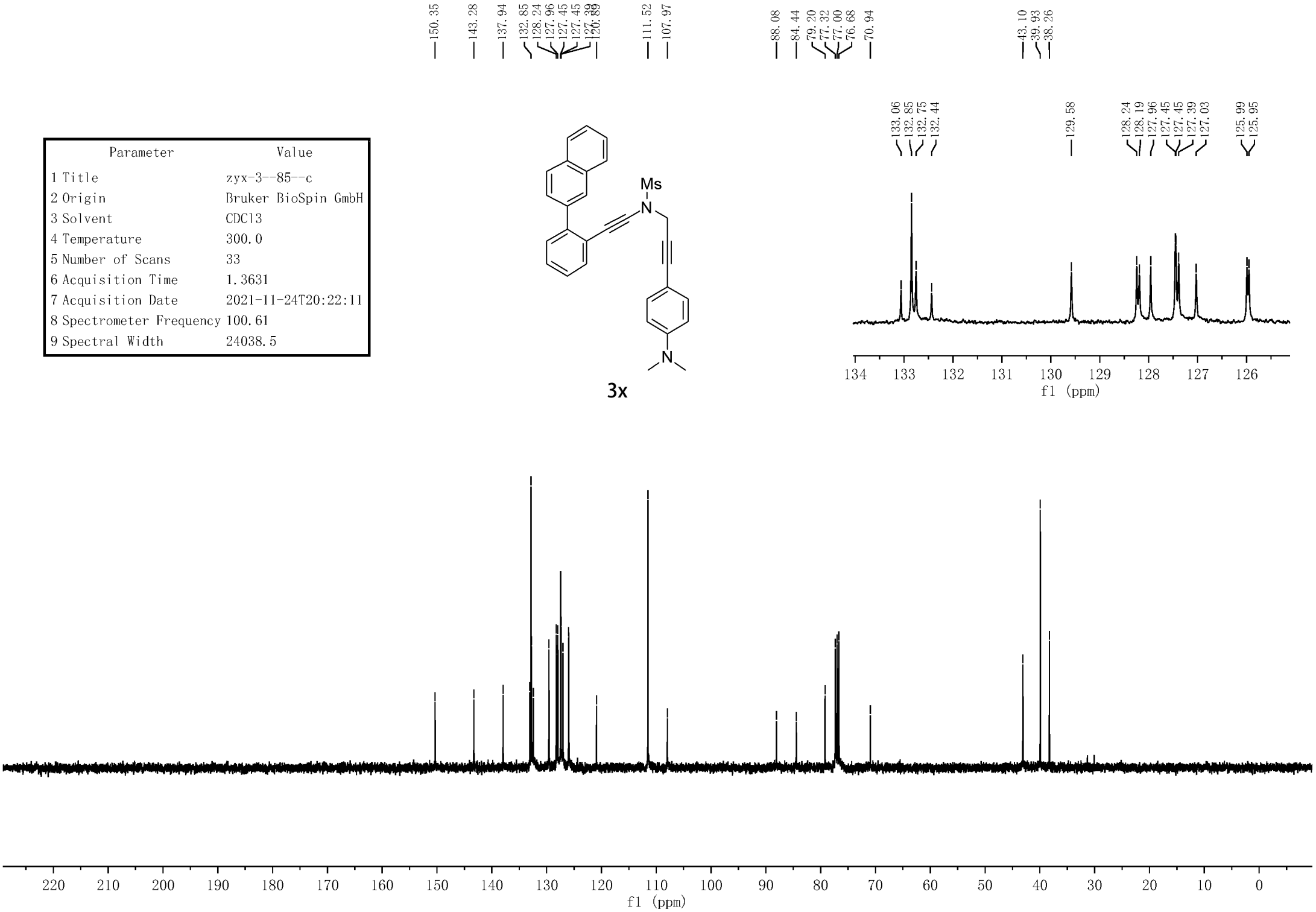

8.425
7.837
7.833
7.777
7.756
7.589
7.572
7.493
7.370
7.354
7.296
7.133
7.112
6.809
6.805
6.793
6.788
6.392
6.370
4.432
3.968
3.264
3.248
3.232
2.864
1.993
1.977
1.961
0.000
Parameter Value
1 Title ZYX-4-50-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 17
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-10T16:32:40
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
OMe
Ms
N
N
3w
0.99
1.02
0.97
1.03
1.02
2.95
1.09
1.97
1.01
2.04
2.03
3.04
4.08
3.00
4.09
f1 (ppm)

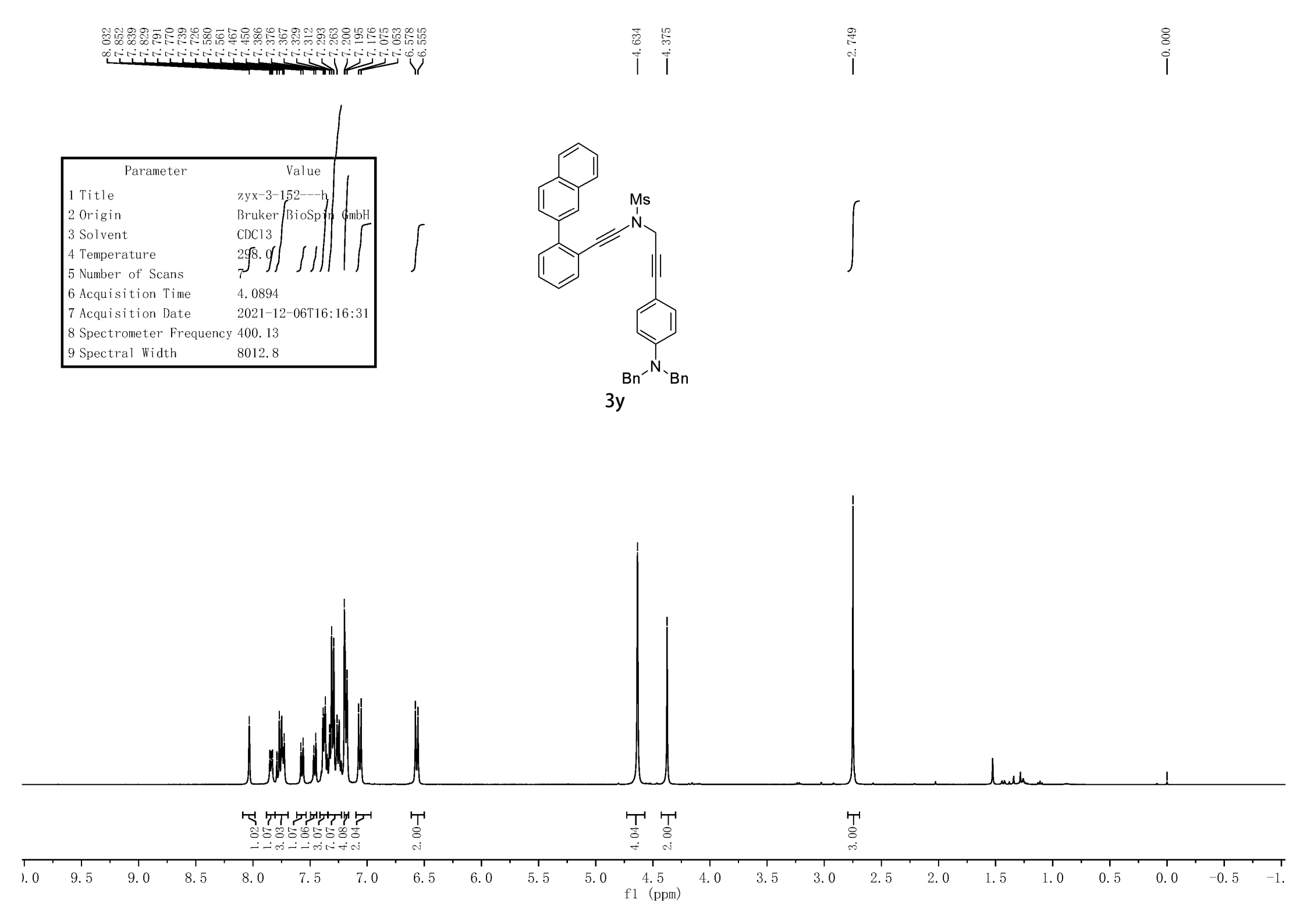

155.60
147.89
143.79
137.53
133.55
133.03
132.76
129.75
128.17
128.10
126.95
126.05
125.31
122.21
121.01
119.90
111.21
107.21
103.93
88.29
84.45
79.01
77.32
77.00
76.68
70.91
55.39
47.40
43.22
38.47
25.37
OMe
Ms
N
N
3w
Parameter
Value
1 Title
ZYX-4-50-C
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
300.0
5 Number of Scans
76
6 Acquisition Time
1.3631
7 Acquisition Date
2022-02-10T16:34:58
8 Spectrometer Frequency
100.61
9 Spectral Width
24038.5
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.950
7.786
7.777
7.771
7.763
7.694
7.664
7.656
7.647
7.484
7.465
7.363
7.343
7.325
7.310
7.272
7.269
7.254
7.251
7.235
7.232
7.201
7.198
7.182
7.179
7.163
7.160
7.068
7.048
6.416
6.394
4.290
2.789
2.661
0.000
Parameter Value
1 Title zyx-3-85-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2021-11-24T20:20:47
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
3x
1.06
1.04
3.05
1.02
3.00
1.03
1.04
2.06
1.99
2.00
6.05
3.06
f1 (ppm)

Parameter	Value
1 Title	zyx-3--85--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	33
6 Acquisition Time	1.3631
7 Acquisition Date	2021-11-24T20:22:11
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

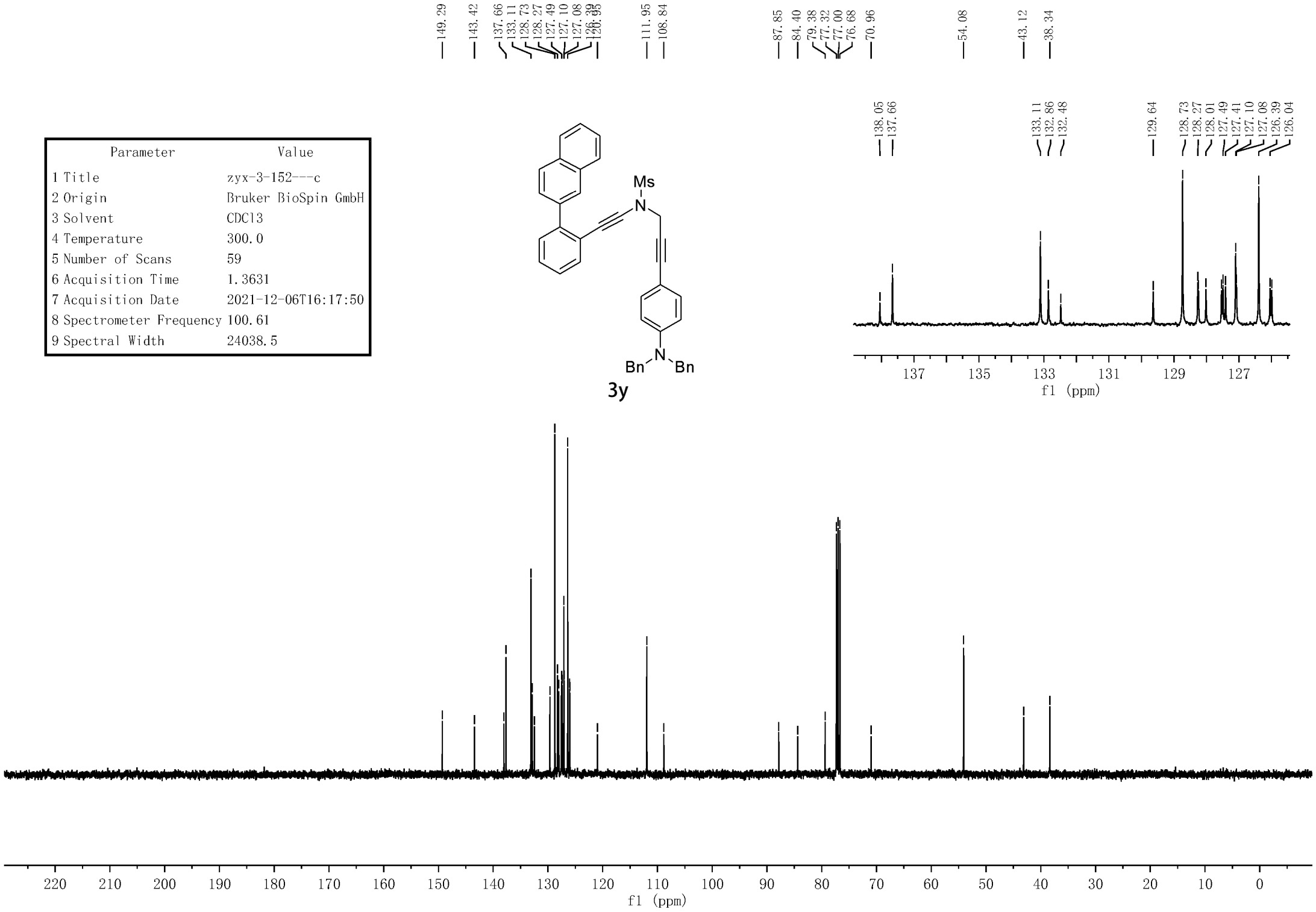
3x



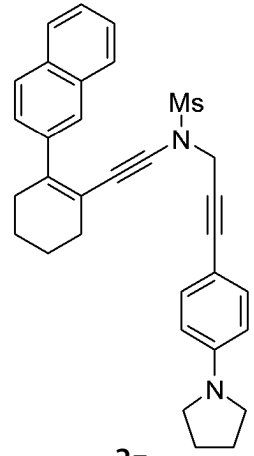

8.032
7.852
7.839
7.829
7.791
7.770
7.739
7.726
7.580
7.561
7.467
7.450
7.386
7.376
7.367
7.329
7.312
7.293
7.263
7.200
7.195
7.176
7.075
7.053
6.578
6.555
4.634
4.375
2.749
0.000
Parameter Value
1 Title zyx-3-152---h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 7
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-06T16:16:31
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
Bn
Bn
3y
1.02
1.07
3.03
1.07
1.06
3.07
7.07
4.08
2.04
2.00
4.04
2.00
3.00
f1 (ppm)

Parameter	Value
1 Title	zyx-3-152---c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	59
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-06T16:17:50
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

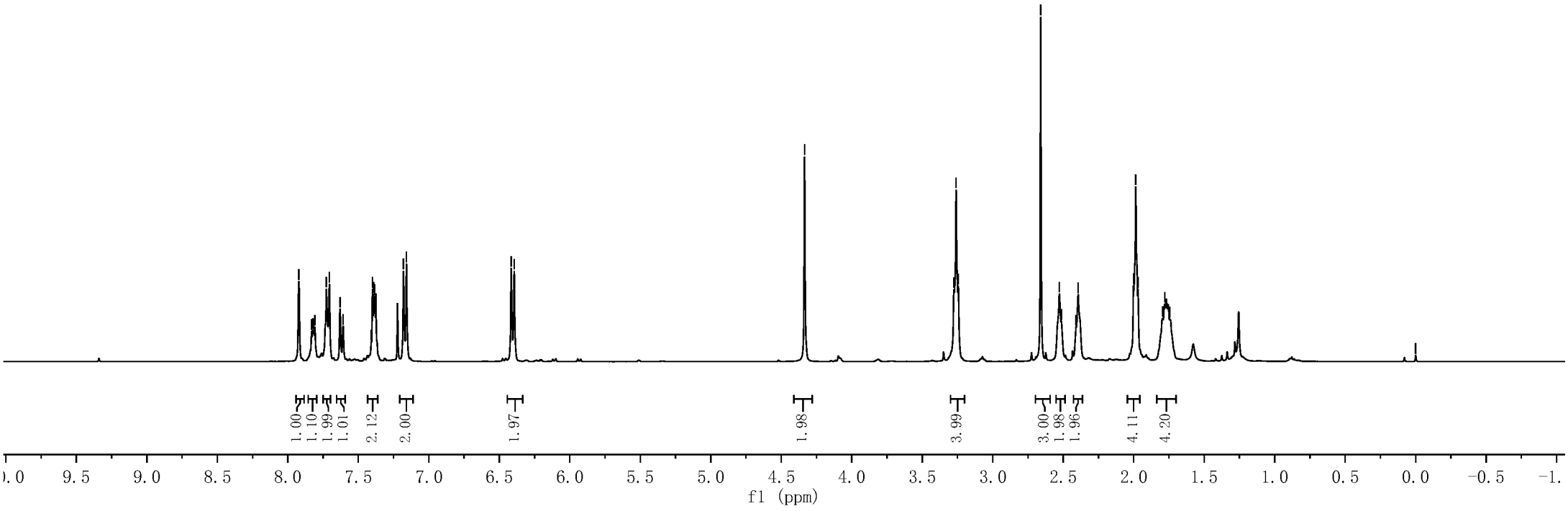
3y



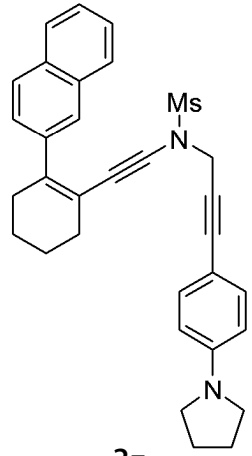
Parameter	Value
1 Title	zyx-6-66-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	104
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-15T15:29:49
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



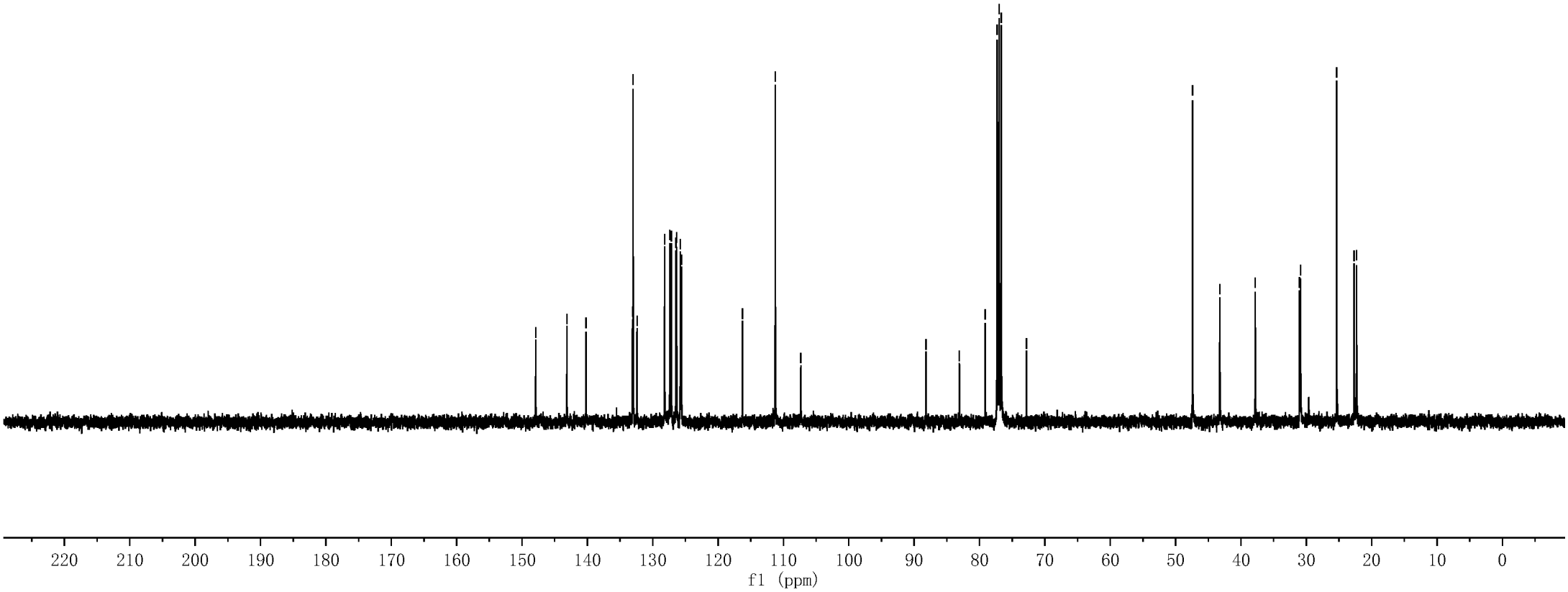
3z

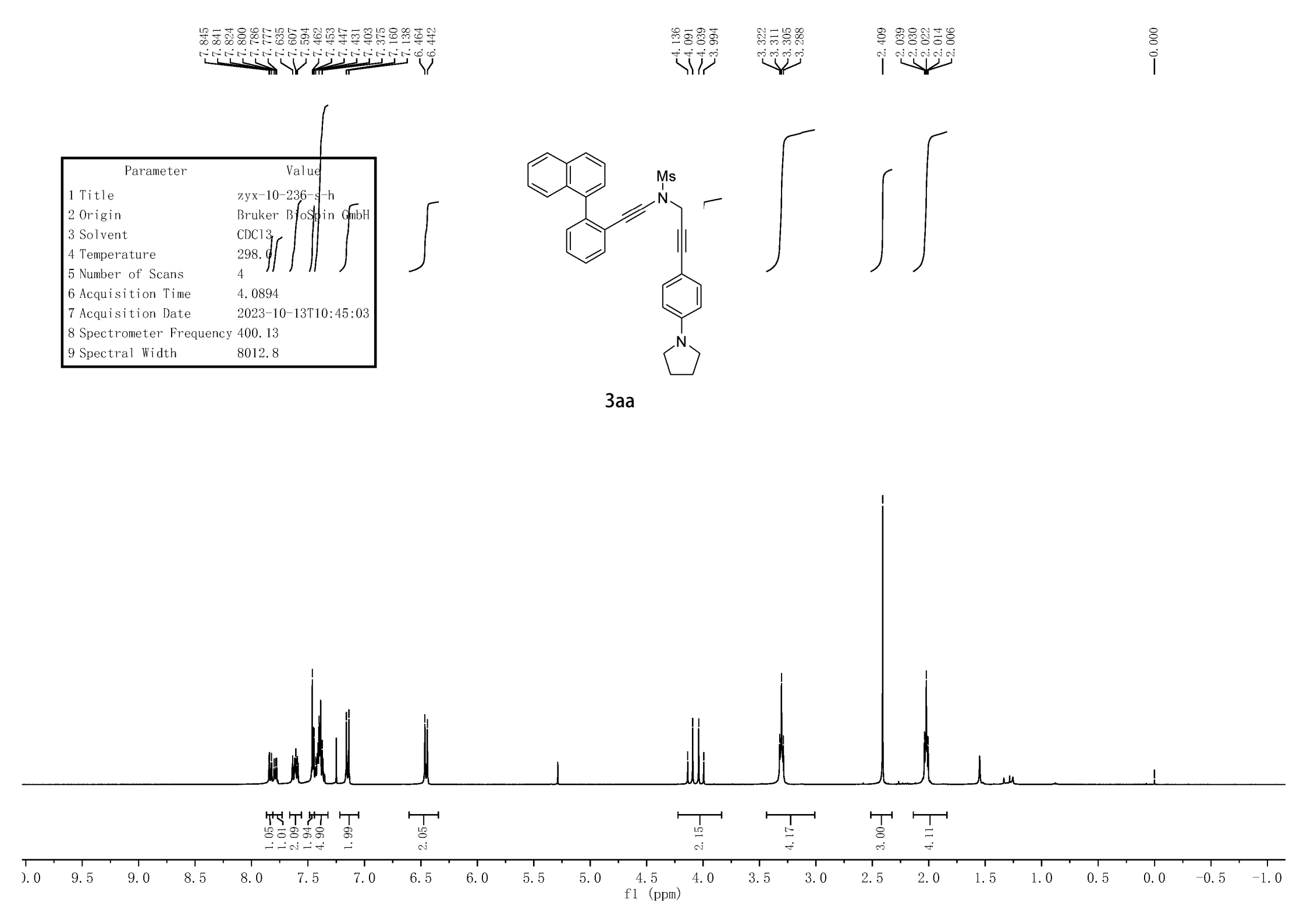


Parameter	Value
1 Title	zyx-6-66-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	104
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-15T15:29:49
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



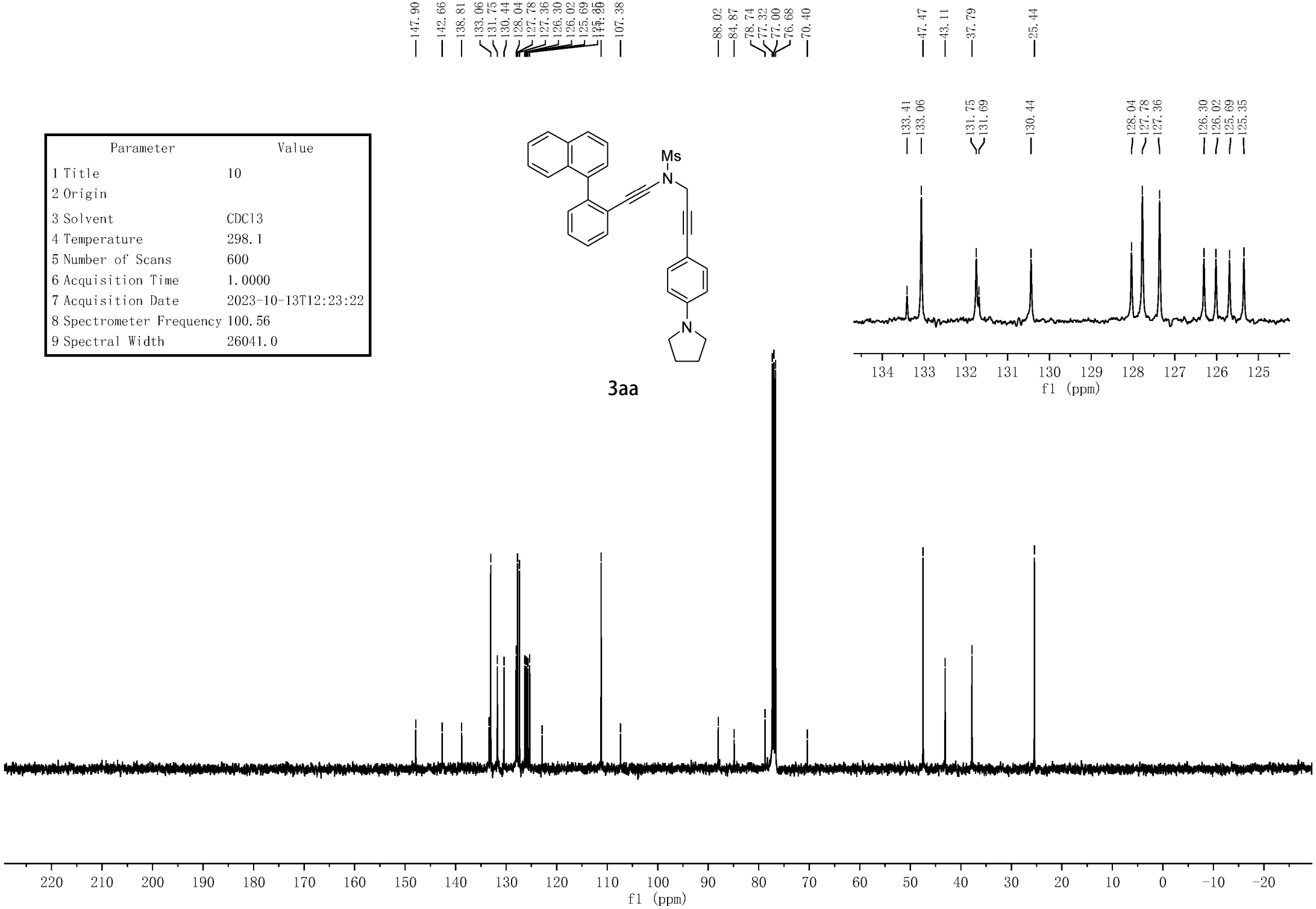
3z

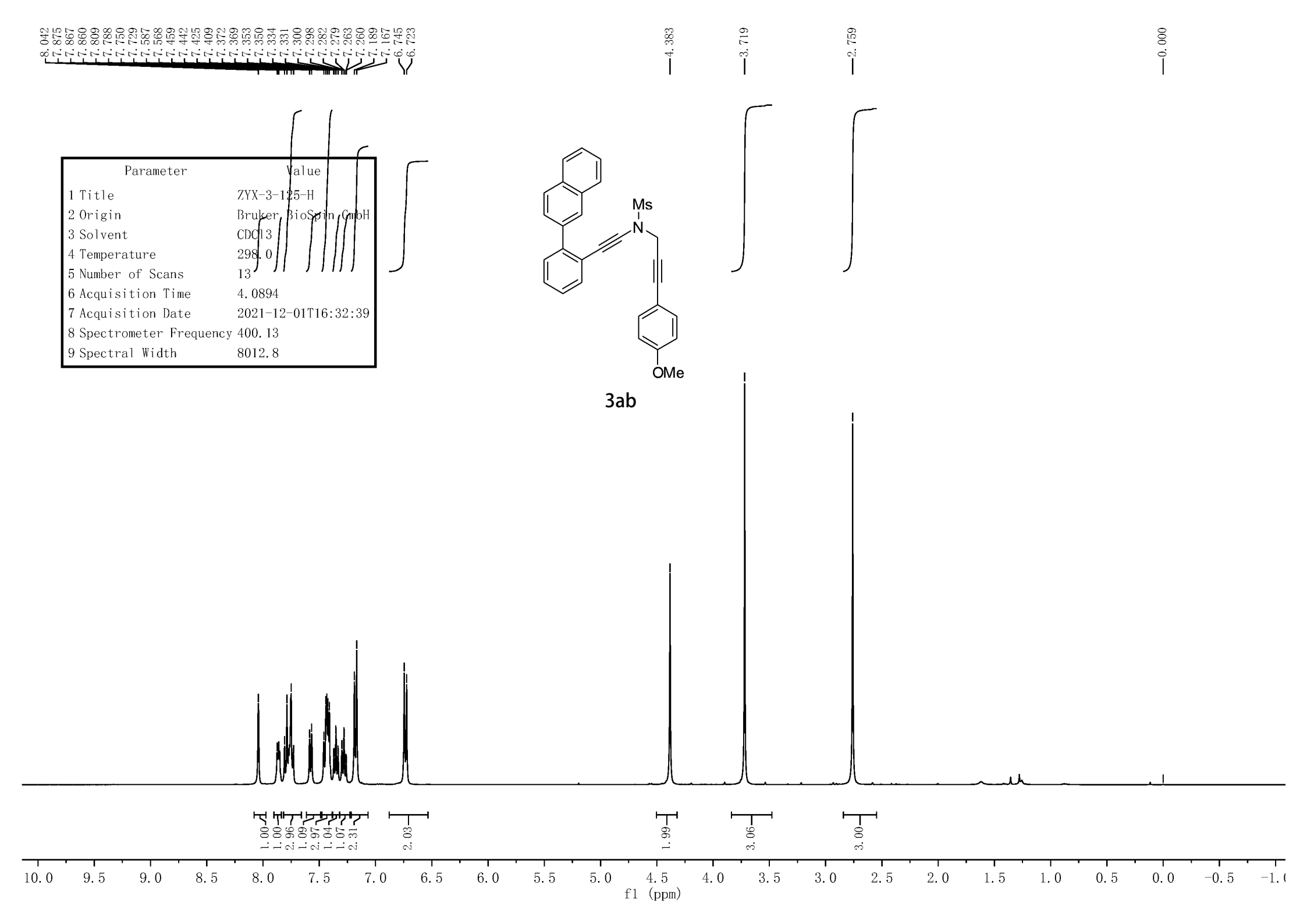



7.845
7.841
7.824
7.800
7.786
7.777
7.635
7.607
7.594
7.462
7.453
7.447
7.431
7.403
7.375
7.160
7.138
6.464
6.442
4.136
4.091
4.039
3.994
3.322
3.311
3.305
3.288
2.409
2.039
2.030
2.022
2.014
2.006
0.000
Parameter Value
1 Title zyx-10-236-s-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 4
6 Acquisition Time 4.0894
7 Acquisition Date 2023-10-13T10:45:03
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
3aa
1.05
1.01
2.09
1.94
4.90
1.99
2.05
2.15
4.17
3.00
4.11
f1 (ppm)

Parameter	Value
1 Title	10
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	600
6 Acquisition Time	1.0000
7 Acquisition Date	2023-10-13T12:23:22
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

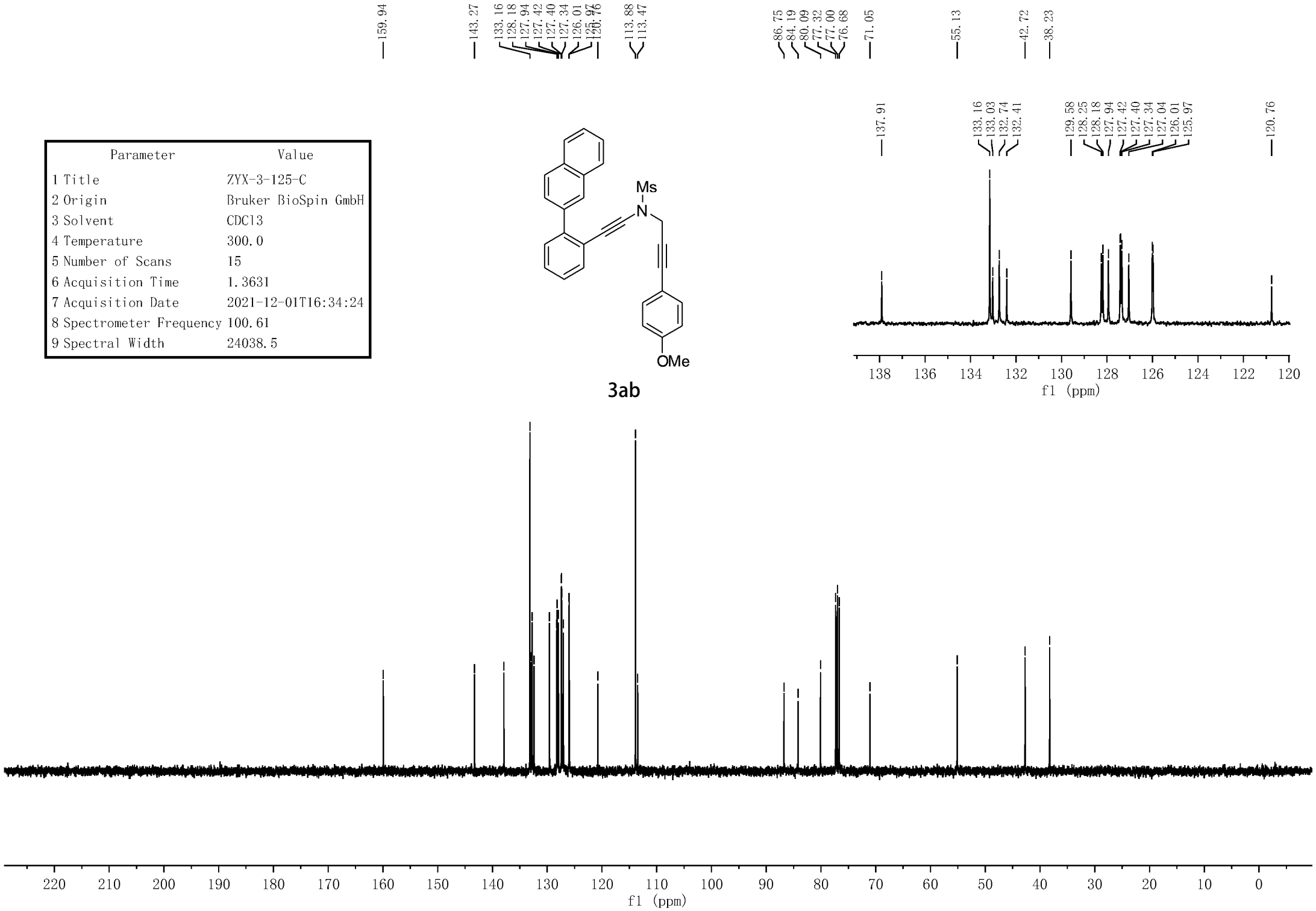
3aa



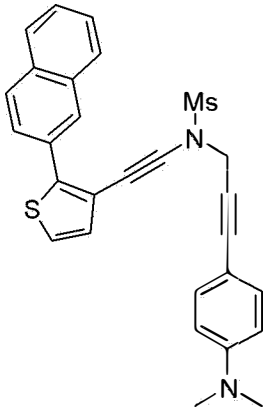

8.042
7.875
7.867
7.860
7.809
7.788
7.750
7.729
7.587
7.568
7.459
7.442
7.425
7.409
7.372
7.369
7.353
7.350
7.334
7.331
7.300
7.298
7.282
7.279
7.263
7.260
7.189
7.167
6.745
6.723
4.383
3.719
2.759
0.000
Parameter Value
1 Title ZYX-3-125-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 13
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-01T16:32:39
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
OMe
3ab
1.00
1.00
2.96
1.09
2.97
1.04
1.07
2.31
2.03
1.99
3.06
3.00
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)

Parameter	Value
1 Title	ZYX-3-125-C
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	2021-12-01T16:34:24
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

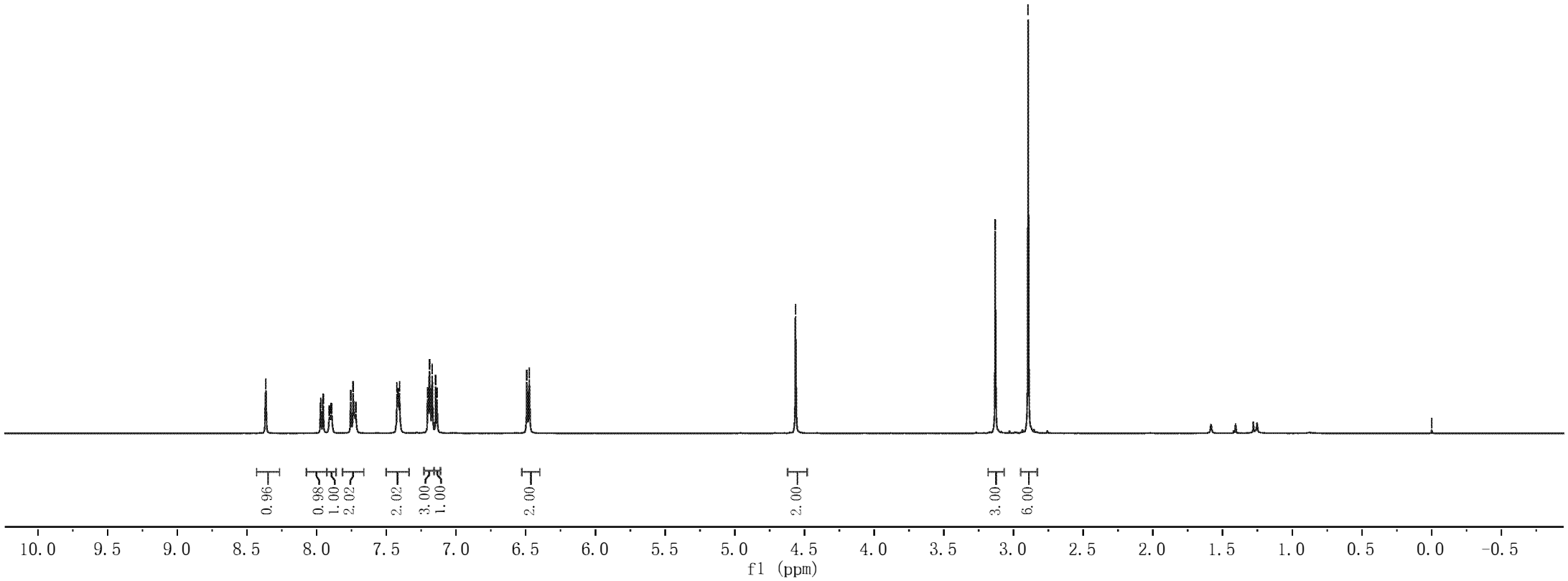
3ab



Parameter	Value
1 Title	zyx-14-44
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	299.0
5 Number of Scans	6
6 Acquisition Time	3.1719
7 Acquisition Date	2024-08-12T11:54:38
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6

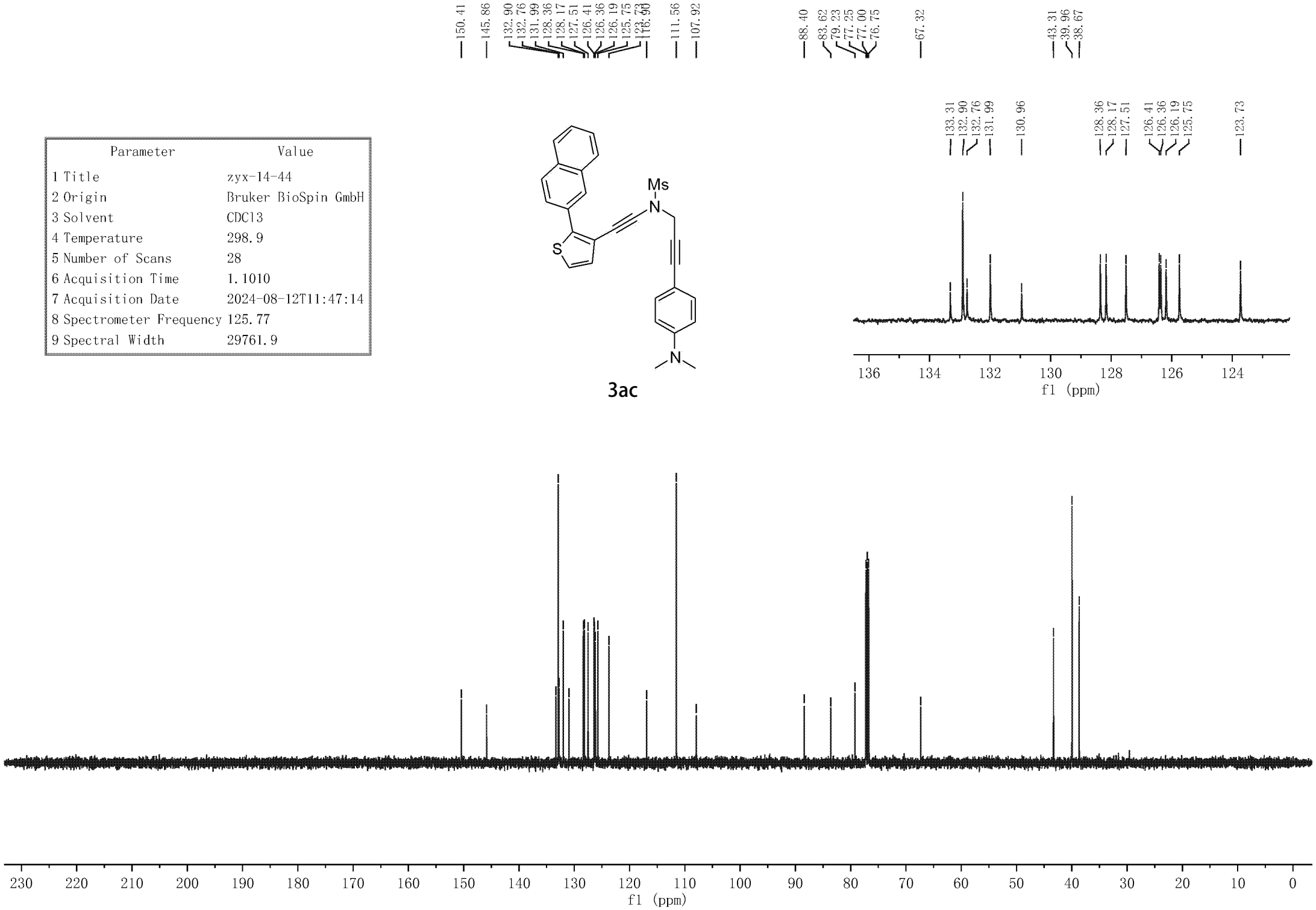


3ac



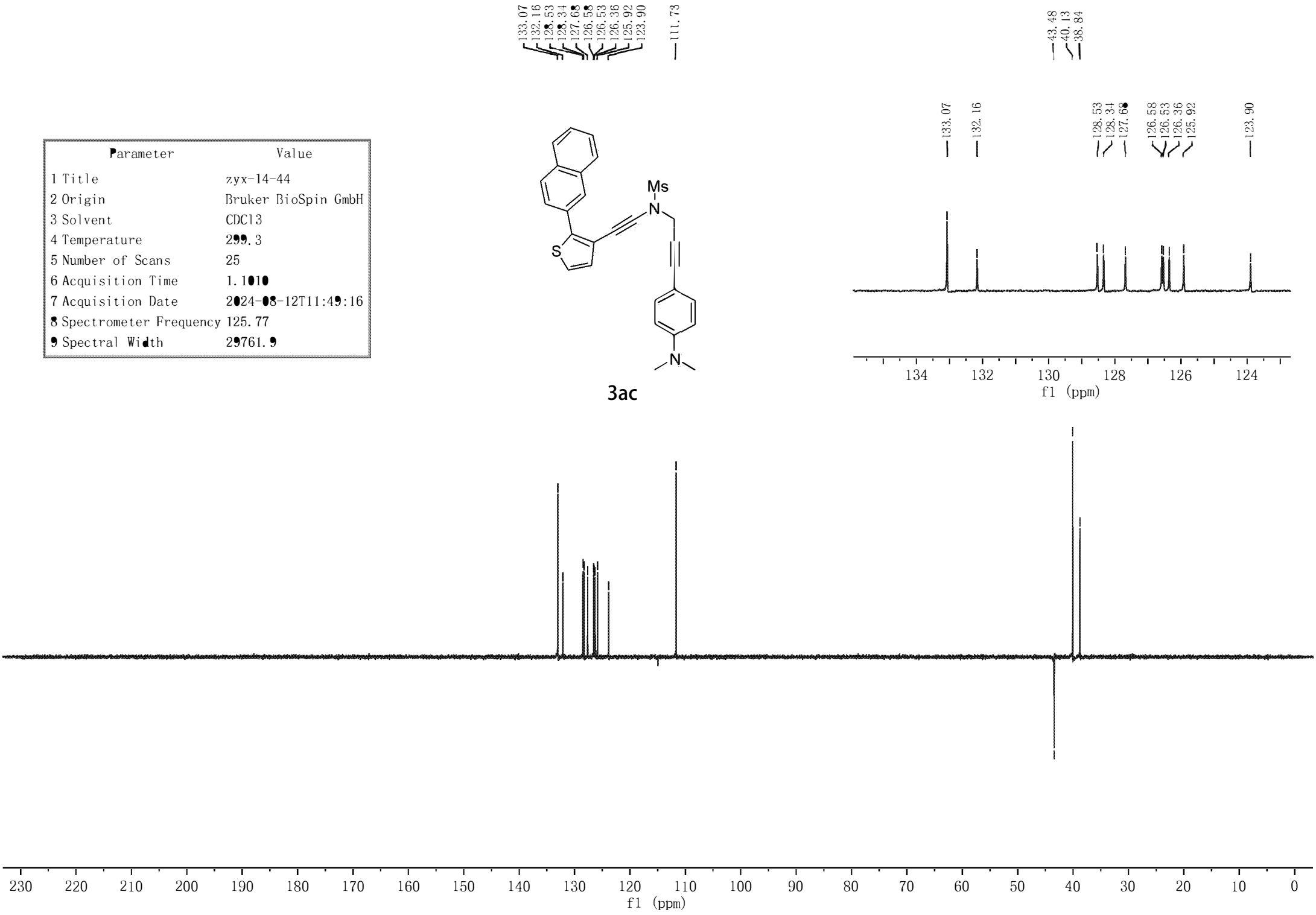
Parameter	Value
1 Title	zyx-14-44
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.9
5 Number of Scans	28
6 Acquisition Time	1.1010
7 Acquisition Date	2024-08-12T11:47:14
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

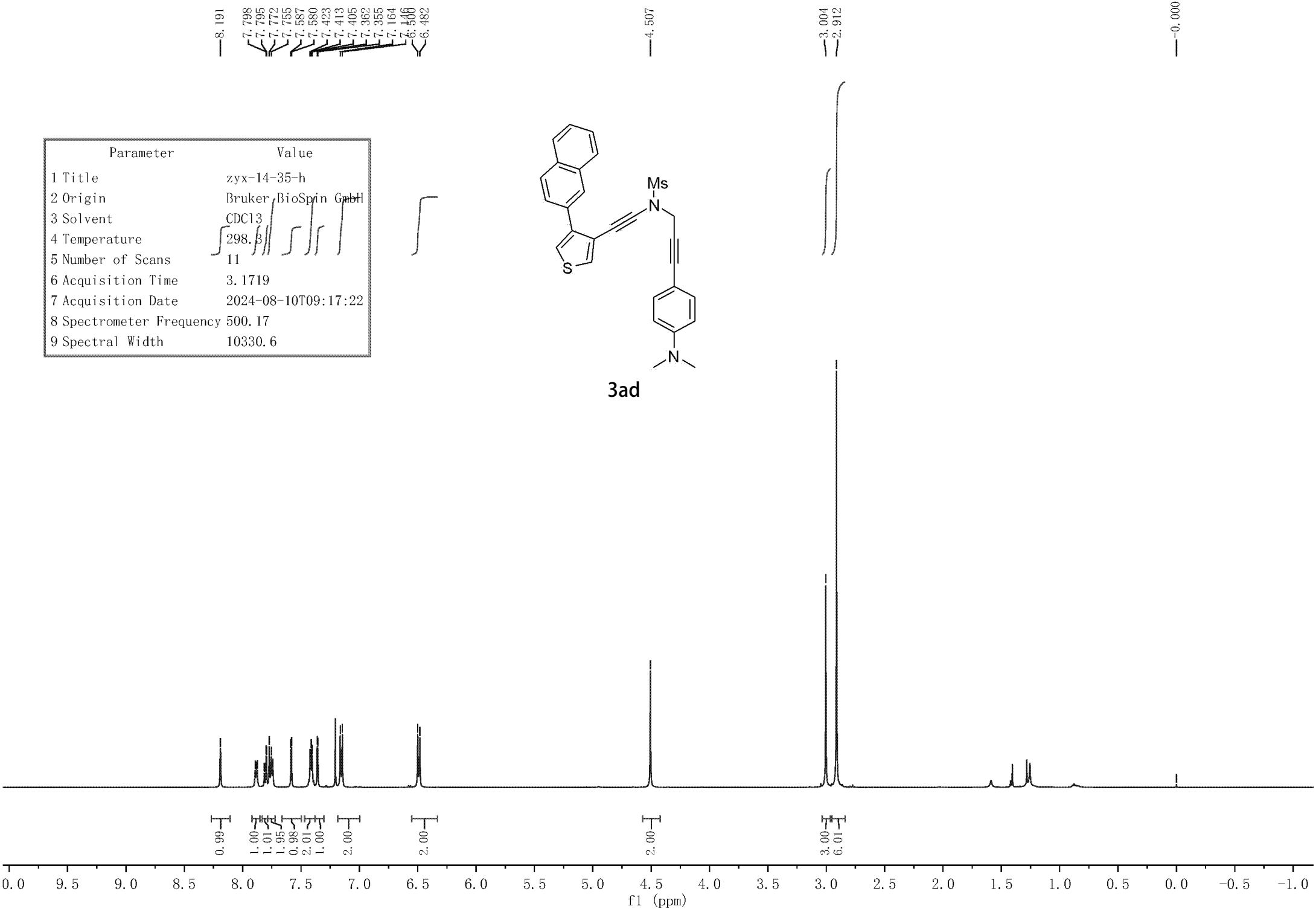
3ac



Parameter	Value
1 Title	zyx-14-44
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	299.3
5 Number of Scans	25
6 Acquisition Time	1.1010
7 Acquisition Date	2024-08-12T11:49:16
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

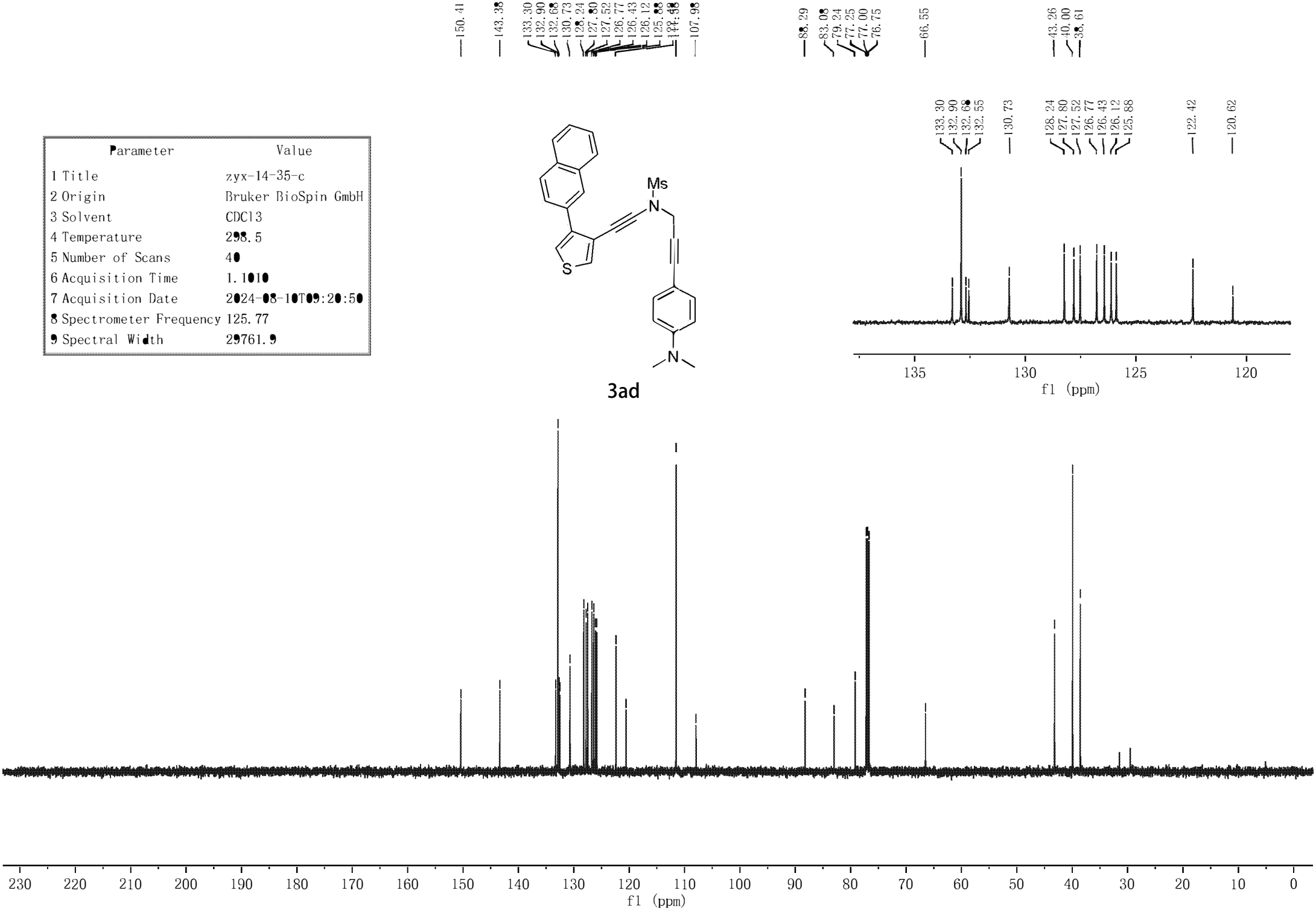
3ac




8.191
7.798
7.795
7.772
7.755
7.587
7.580
7.423
7.413
7.405
7.362
7.355
7.164
7.146
6.500
6.482
4.507
3.004
2.912
-0.000
Parameter Value
1 Title zyx-14-35-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.3
5 Number of Scans 11
6 Acquisition Time 3.1719
7 Acquisition Date 2024-08-10T09:17:22
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Ms
N
S
N
3ad
0.99
1.00
1.01
1.95
0.98
2.01
1.00
2.00
2.00
2.00
3.00
6.01
0.0
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
-1.0
f1 (ppm)

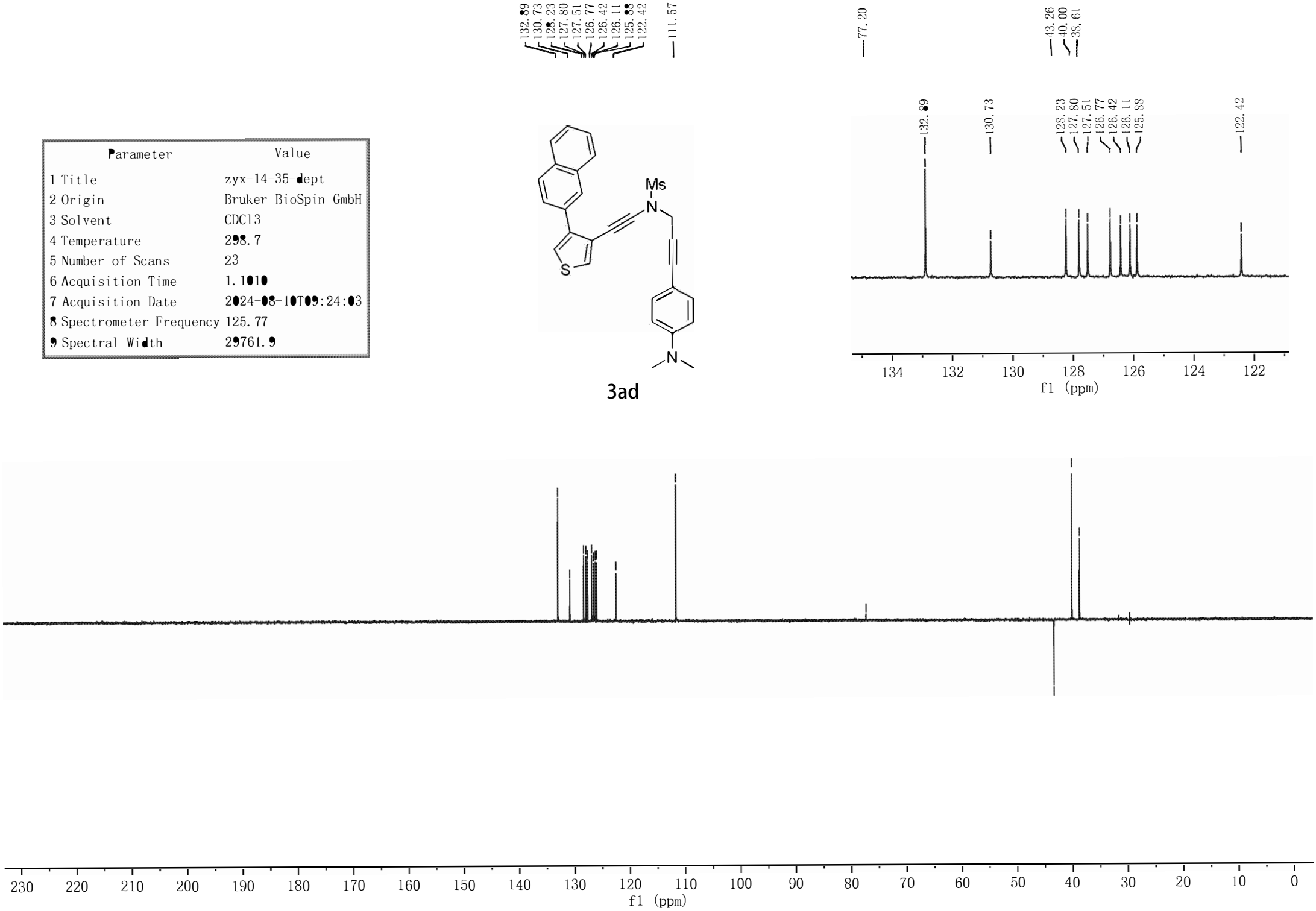
Parameter	Value
1 Title	zyx-14-35-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.5
5 Number of Scans	40
6 Acquisition Time	1.1010
7 Acquisition Date	2024-08-10T09:20:50
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

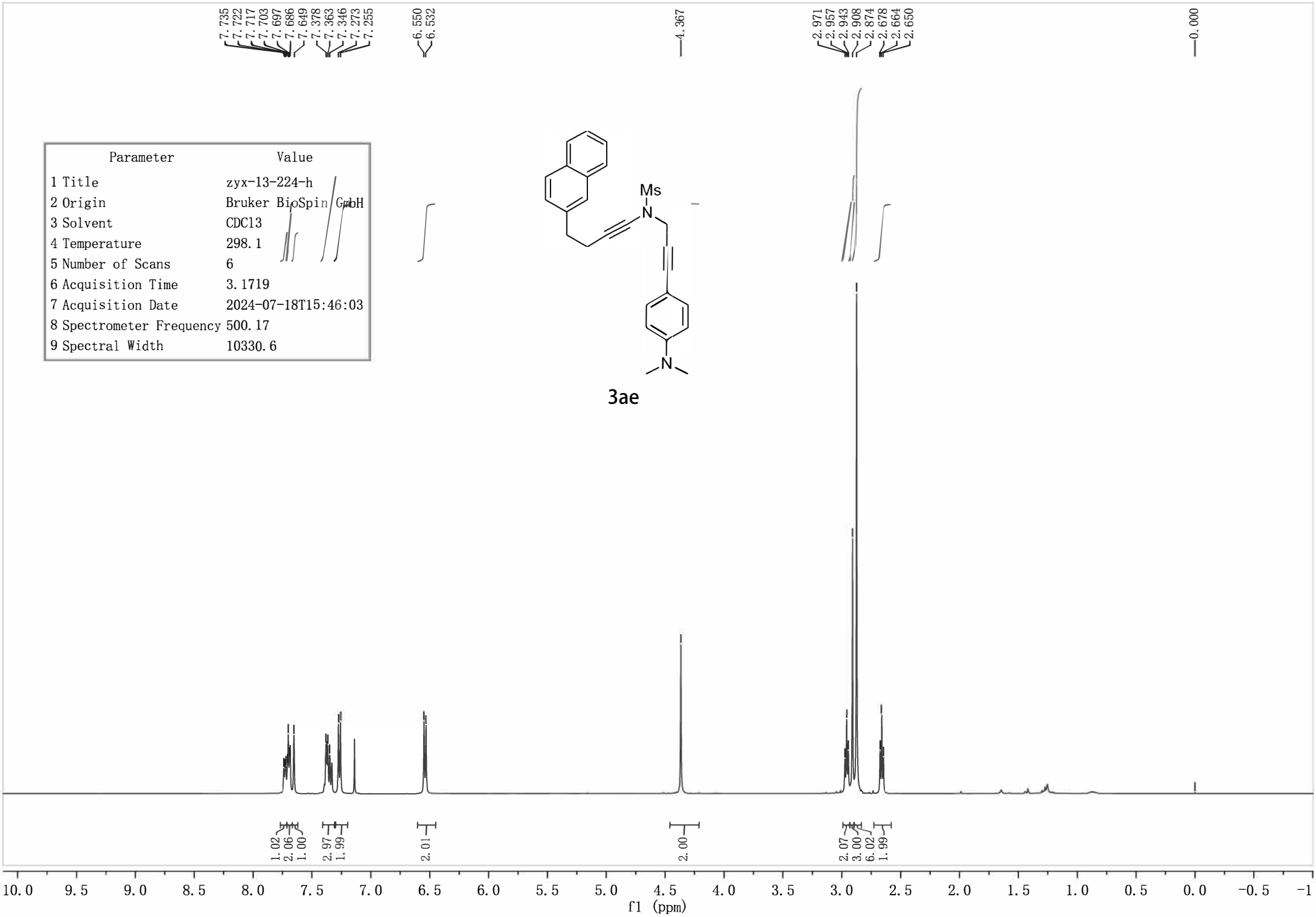
3ad



Parameter	Value
1 Title	zyx-14-35-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.7
5 Number of Scans	23
6 Acquisition Time	1.1010
7 Acquisition Date	2024-08-10T09:24:03
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

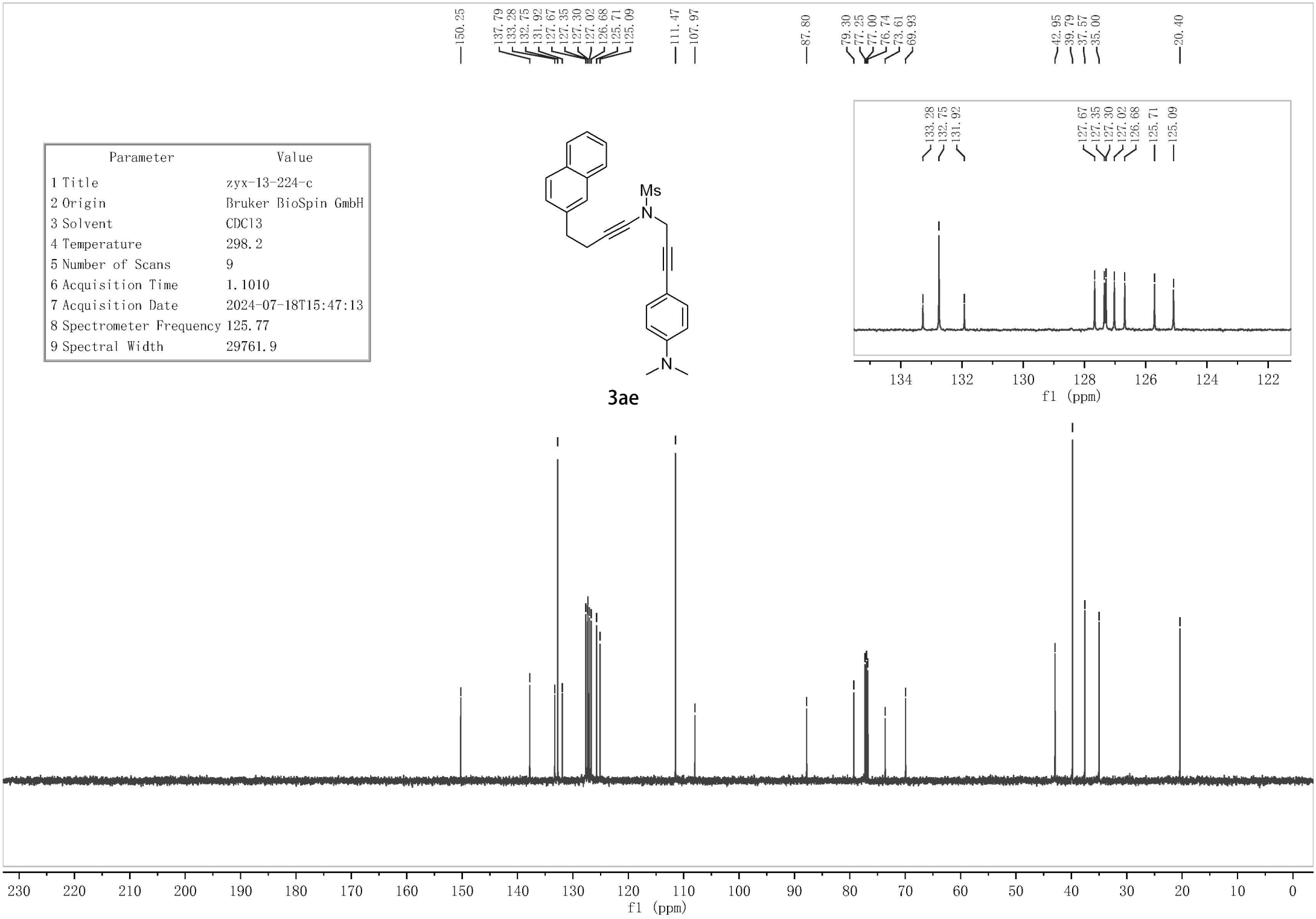
3ad




7.735
7.722
7.717
7.703
7.697
7.686
7.649
7.378
7.363
7.346
7.273
7.255
6.550
6.532
4.367
2.971
2.957
2.943
2.908
2.874
2.678
2.664
2.650
0.000
Parameter Value
1 Title zyx-13-224-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.1
5 Number of Scans 6
6 Acquisition Time 3.1719
7 Acquisition Date 2024-07-18T15:46:03
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Ms
N
N
3ae
1.02
2.06
1.00
2.97
1.99
2.01
2.00
2.07
3.00
6.02
1.99
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
-1
f1 (ppm)

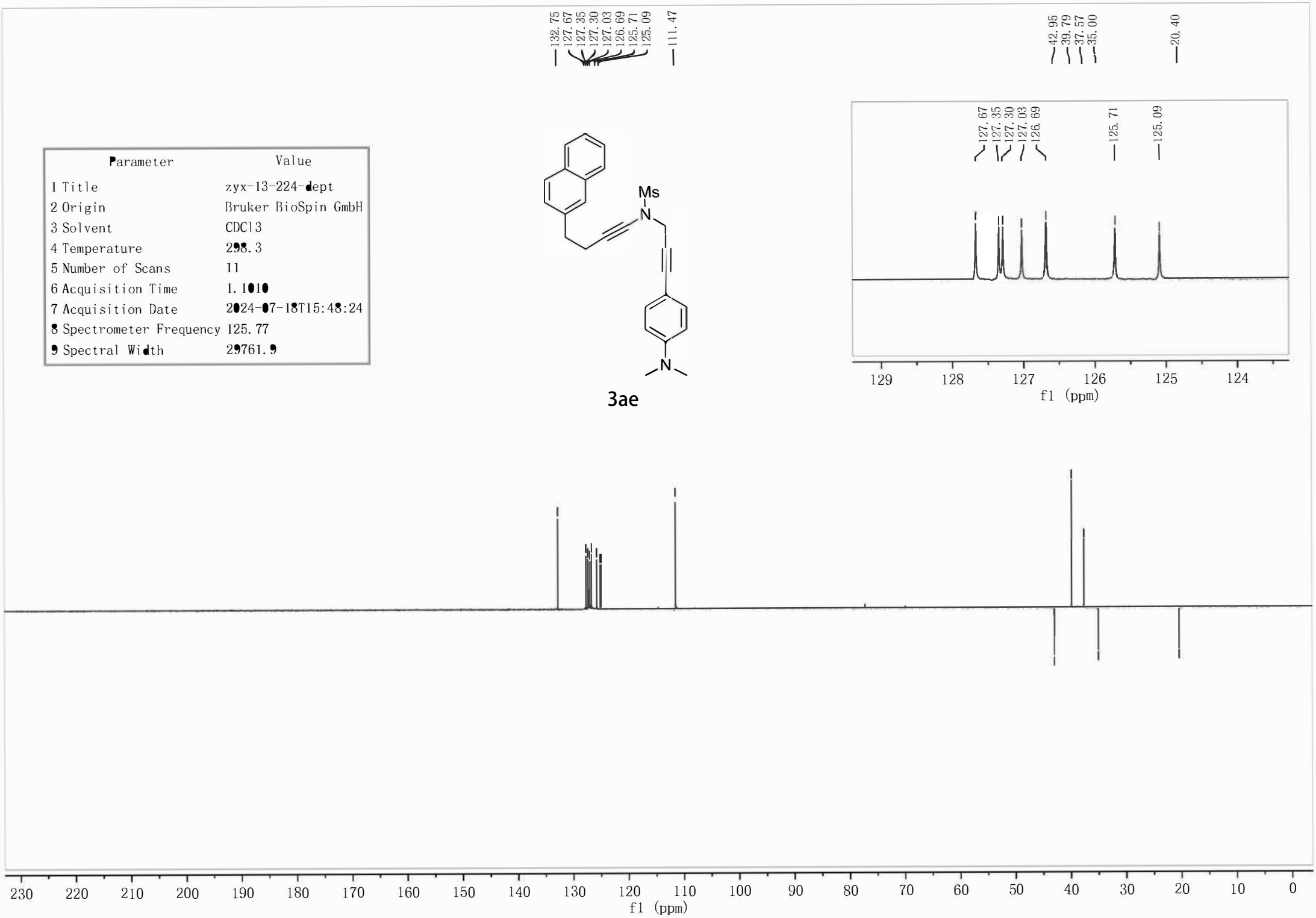
Parameter	Value
1 Title	zyx-13-224-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.2
5 Number of Scans	9
6 Acquisition Time	1.1010
7 Acquisition Date	2024-07-18T15:47:13
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

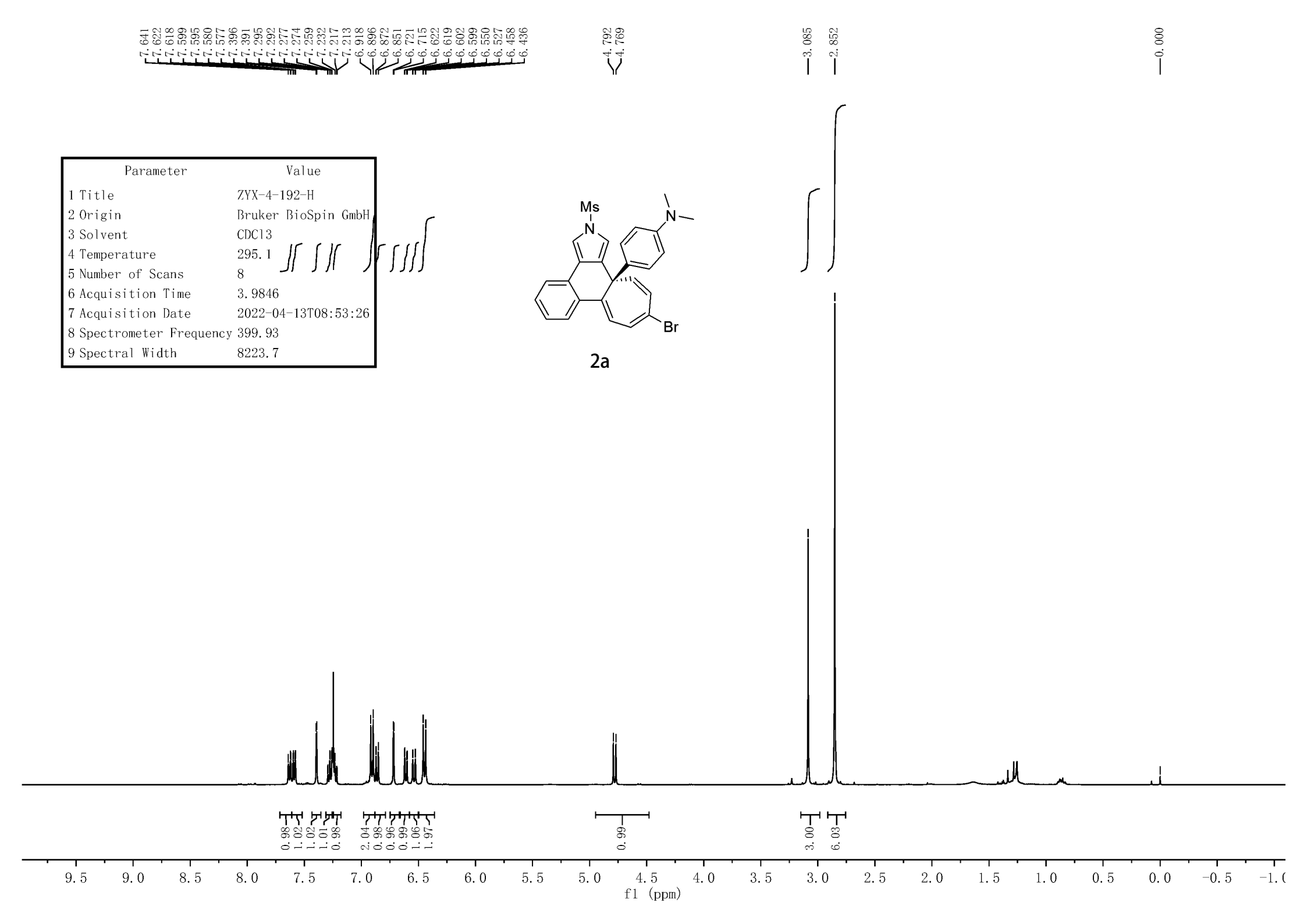
3ae



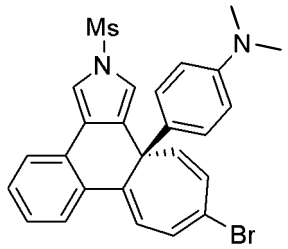
Parameter	Value
1 Title	zyx-13-224-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.3
5 Number of Scans	11
6 Acquisition Time	1.1010
7 Acquisition Date	2024-07-18T15:48:24
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

3ae

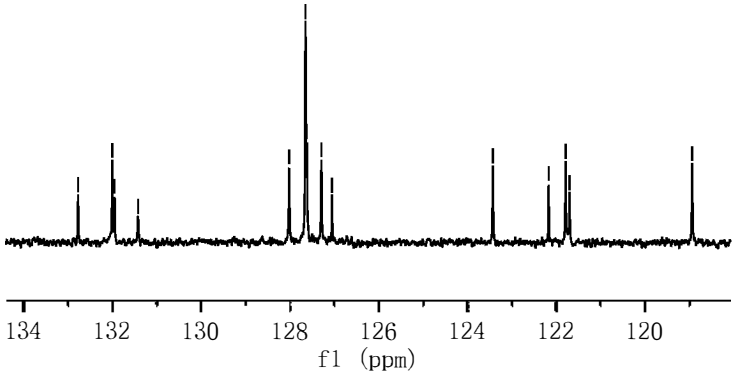


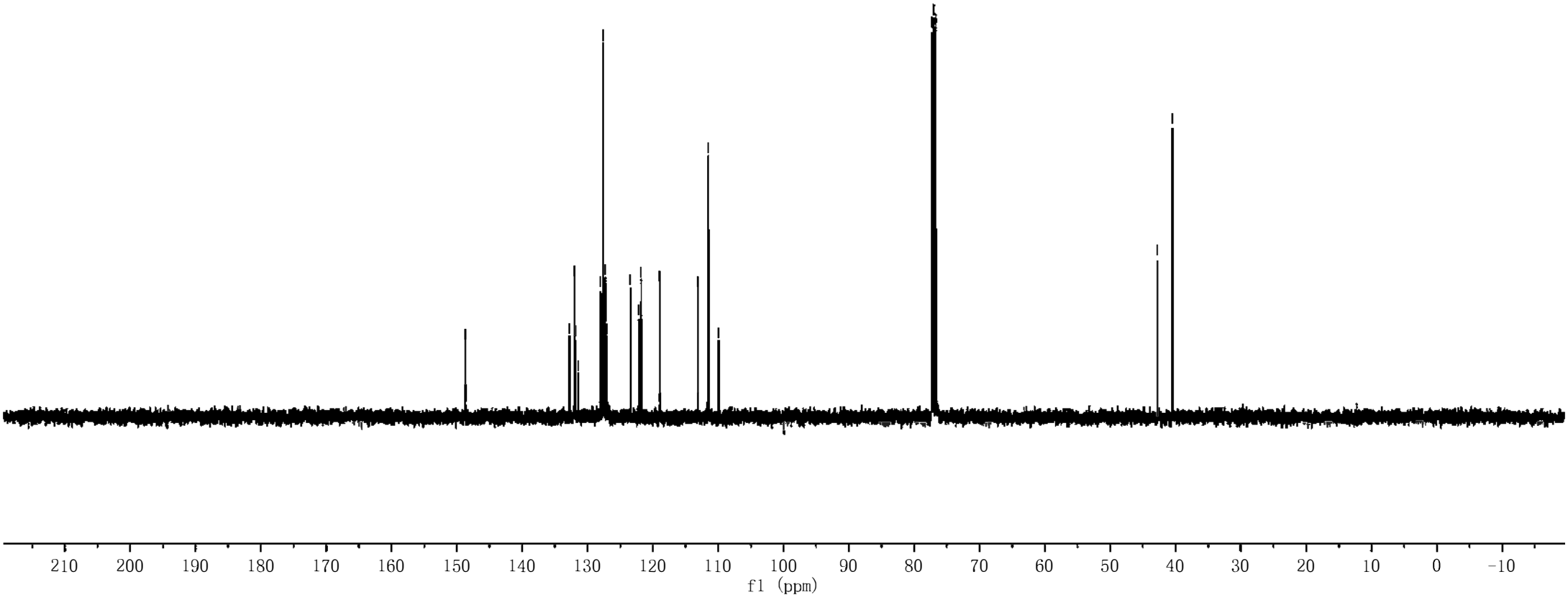

7.641
7.622
7.618
7.599
7.595
7.580
7.577
7.396
7.391
7.295
7.292
7.277
7.274
7.259
7.232
7.217
7.213
6.918
6.896
6.872
6.851
6.721
6.715
6.622
6.619
6.602
6.599
6.550
6.527
6.458
6.436
4.792
4.769
3.085
2.852
0.000
Parameter Value
1 Title ZYX-4-192-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.1
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-13T08:53:26
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
N
Br
2a
0.98
1.02
1.02
1.01
0.98
2.04
0.98
0.96
0.99
1.06
1.97
0.99
3.00
6.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

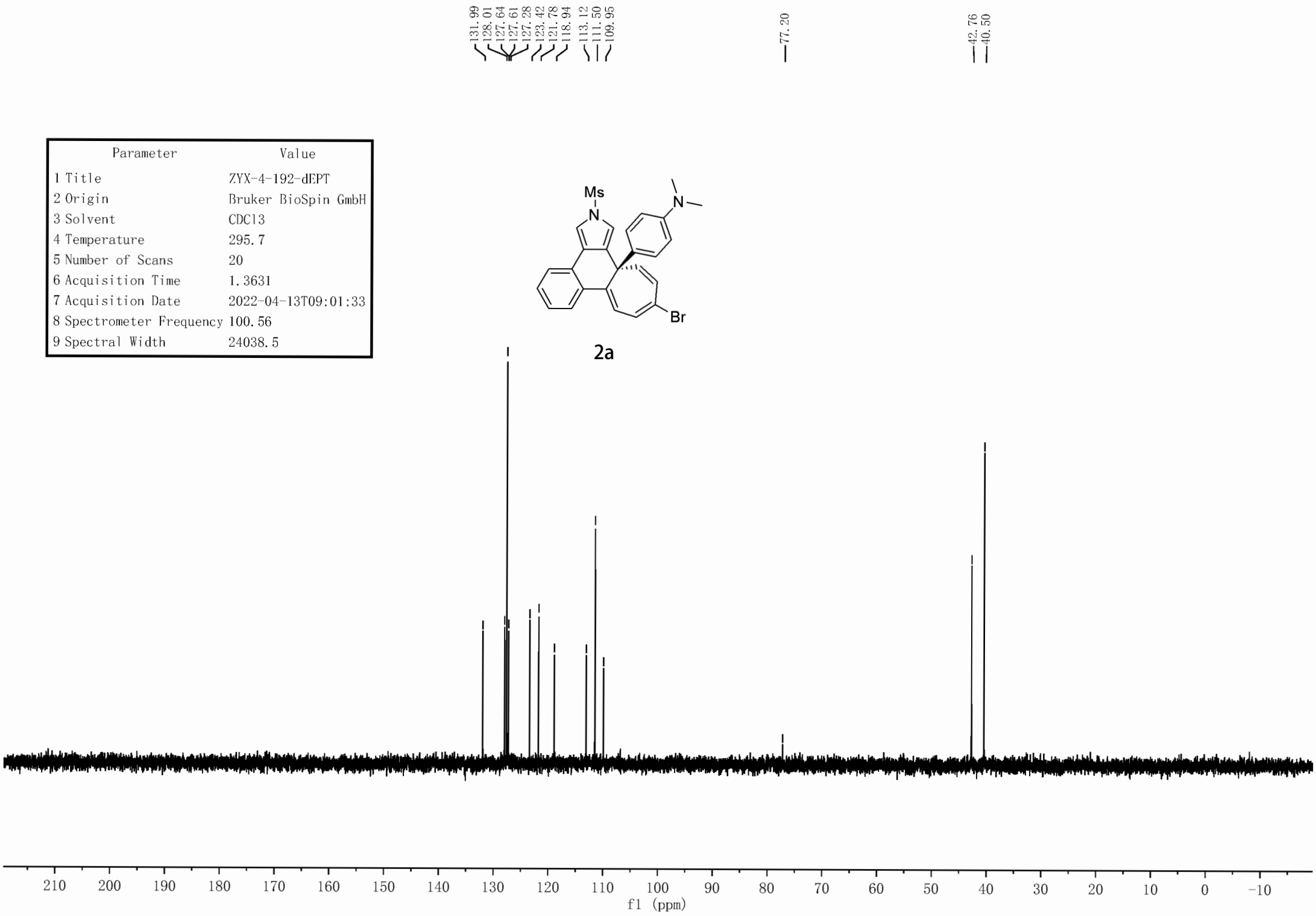
Parameter	Value
1 Title	ZYX-4-192-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	74
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-13T08:56:12
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

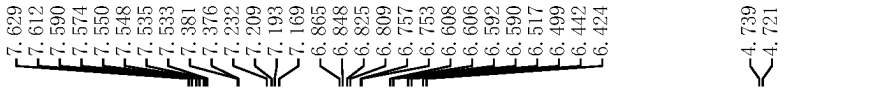


2a

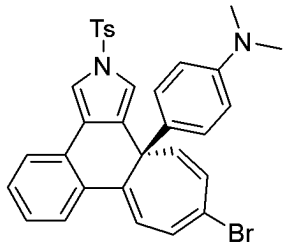




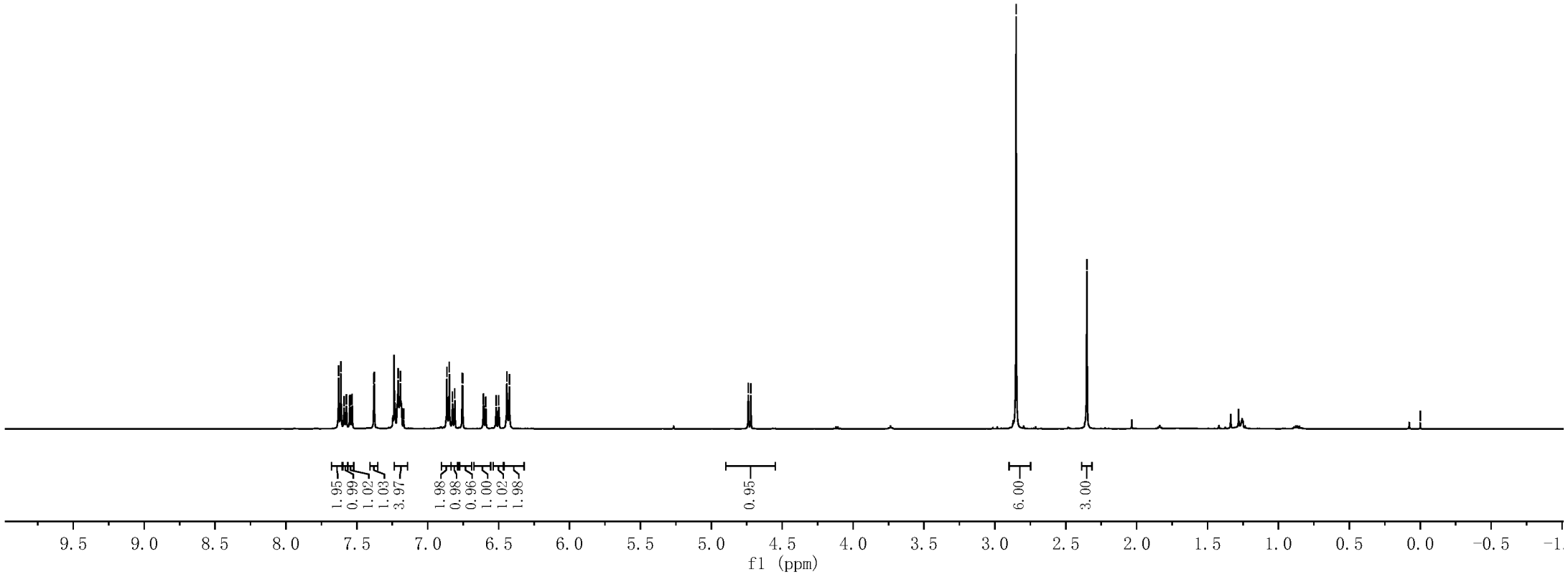

131.99
128.01
127.64
127.61
127.28
123.42
121.78
118.94
113.12
111.50
109.95
77.20
42.76
40.50
Parameter Value
1 Title ZYX-4-192-dEPT
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.7
5 Number of Scans 20
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-13T09:01:33
8 Spectrometer Frequency 100.56
9 Spectral Width 24038.5
Ms
N
N
Br
2a
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	zyx-4-176-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.3
5 Number of Scans	18
6 Acquisition Time	3.1719
7 Acquisition Date	2022-04-02T20:20:54
8 Spectrometer Frequency	500.17
9 Spectral Width	10330.6

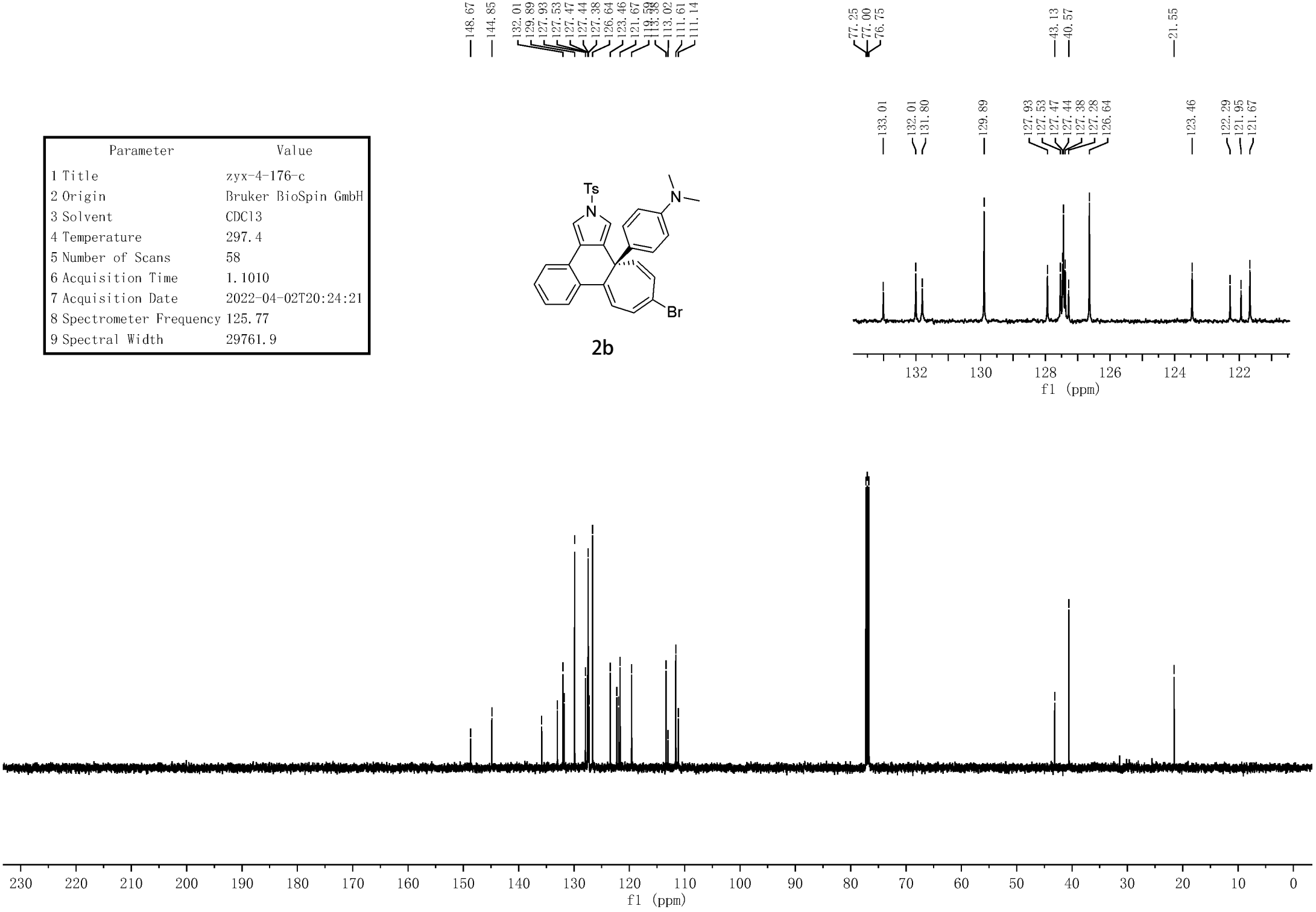


2b



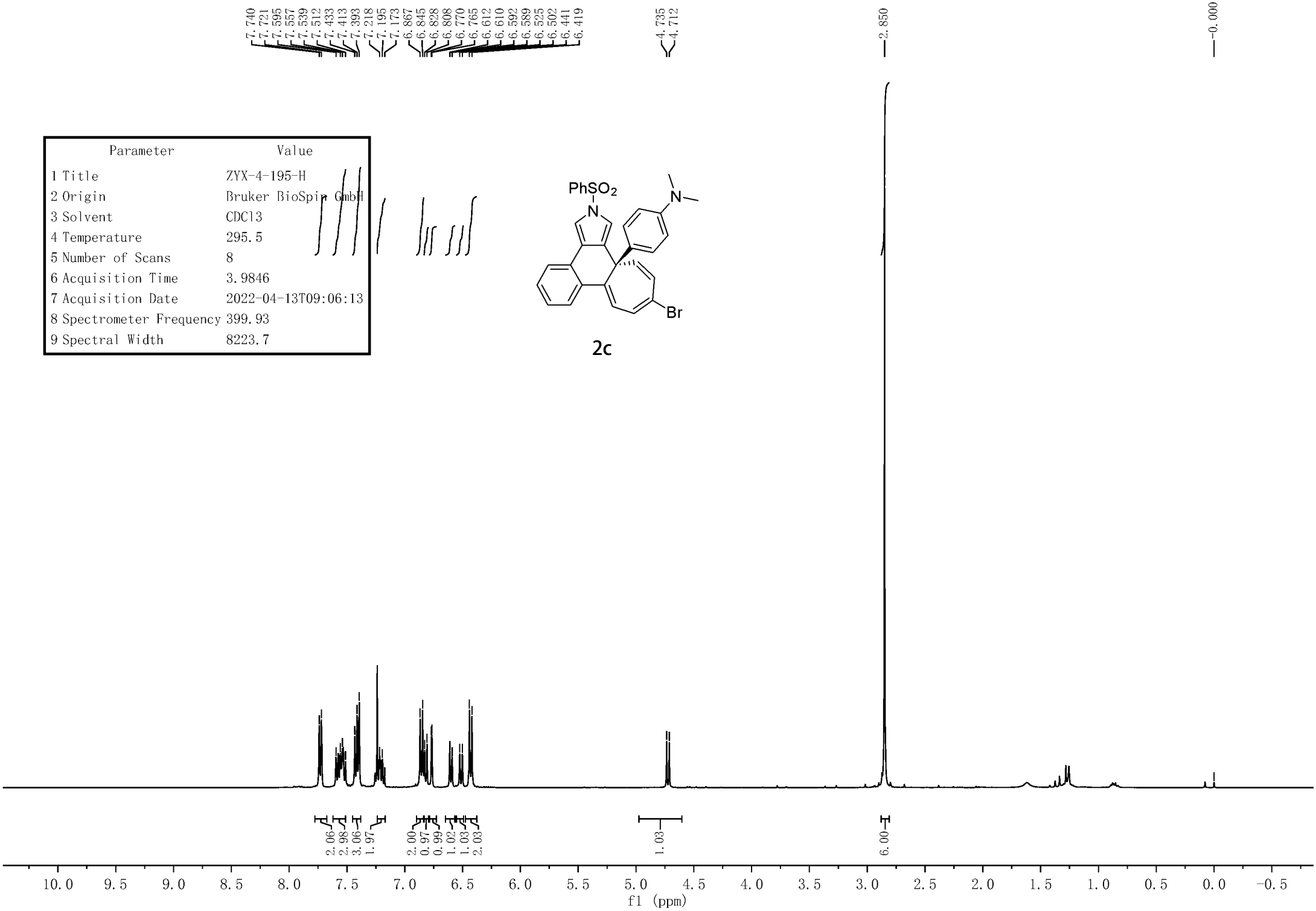
Parameter	Value
1 Title	zyx-4-176-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.4
5 Number of Scans	58
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-02T20:24:21
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

2b



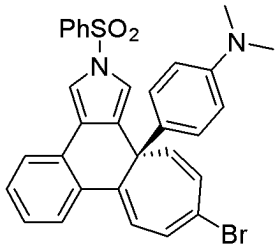
Parameter	Value
1 Title	ZYX-4-195-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	8
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-13T09:06:13
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

2c



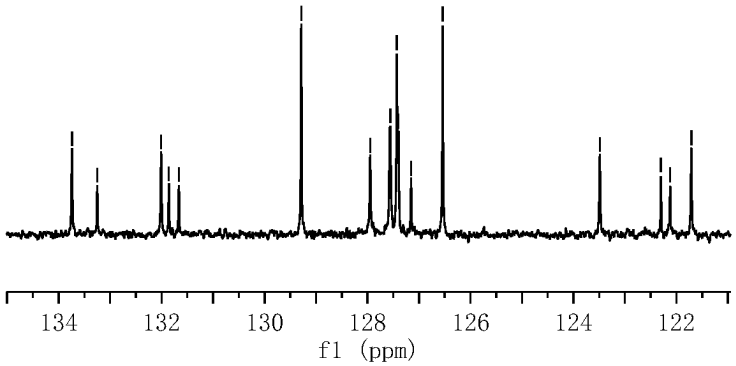
148.73
138.78
133.74
129.29
127.56
127.43
127.40
126.54
121.71
113.44
112.73
111.58
110.87
77.32
77.00
76.68
43.06
40.55

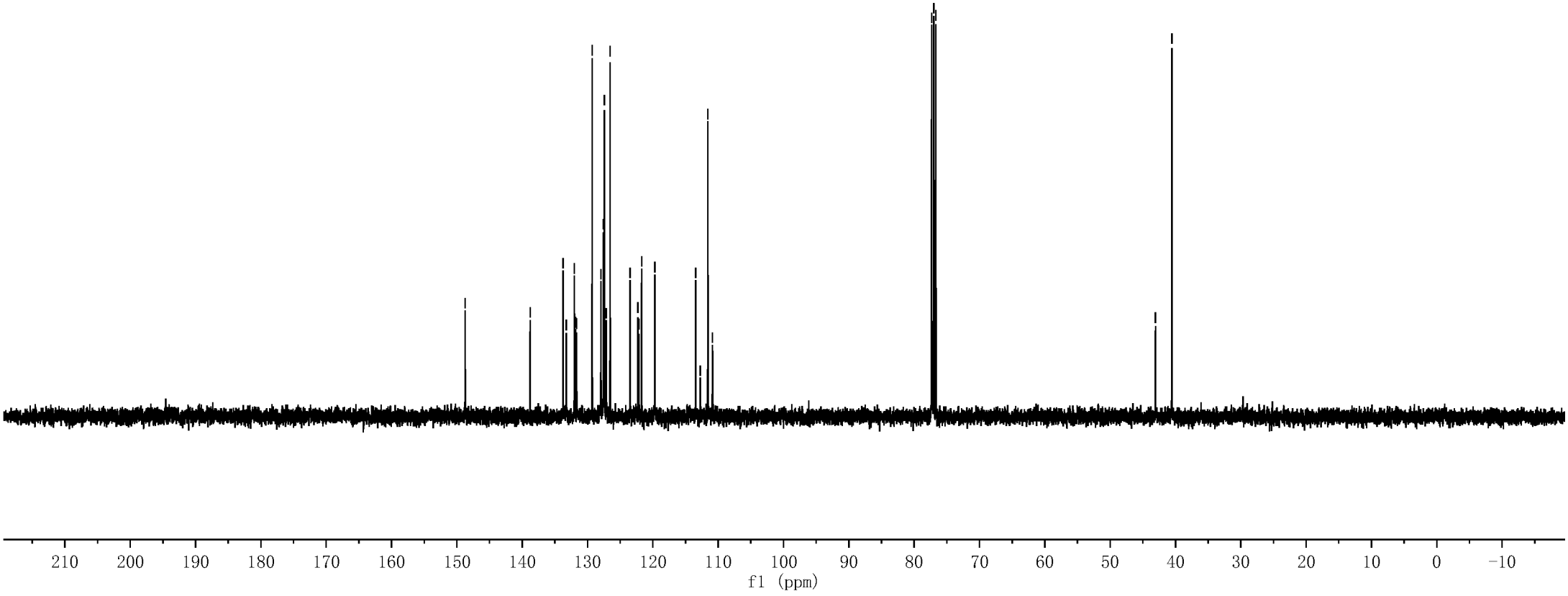
Parameter	Value
1 Title	ZYX-4-195-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	67
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-13T09:07:30
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

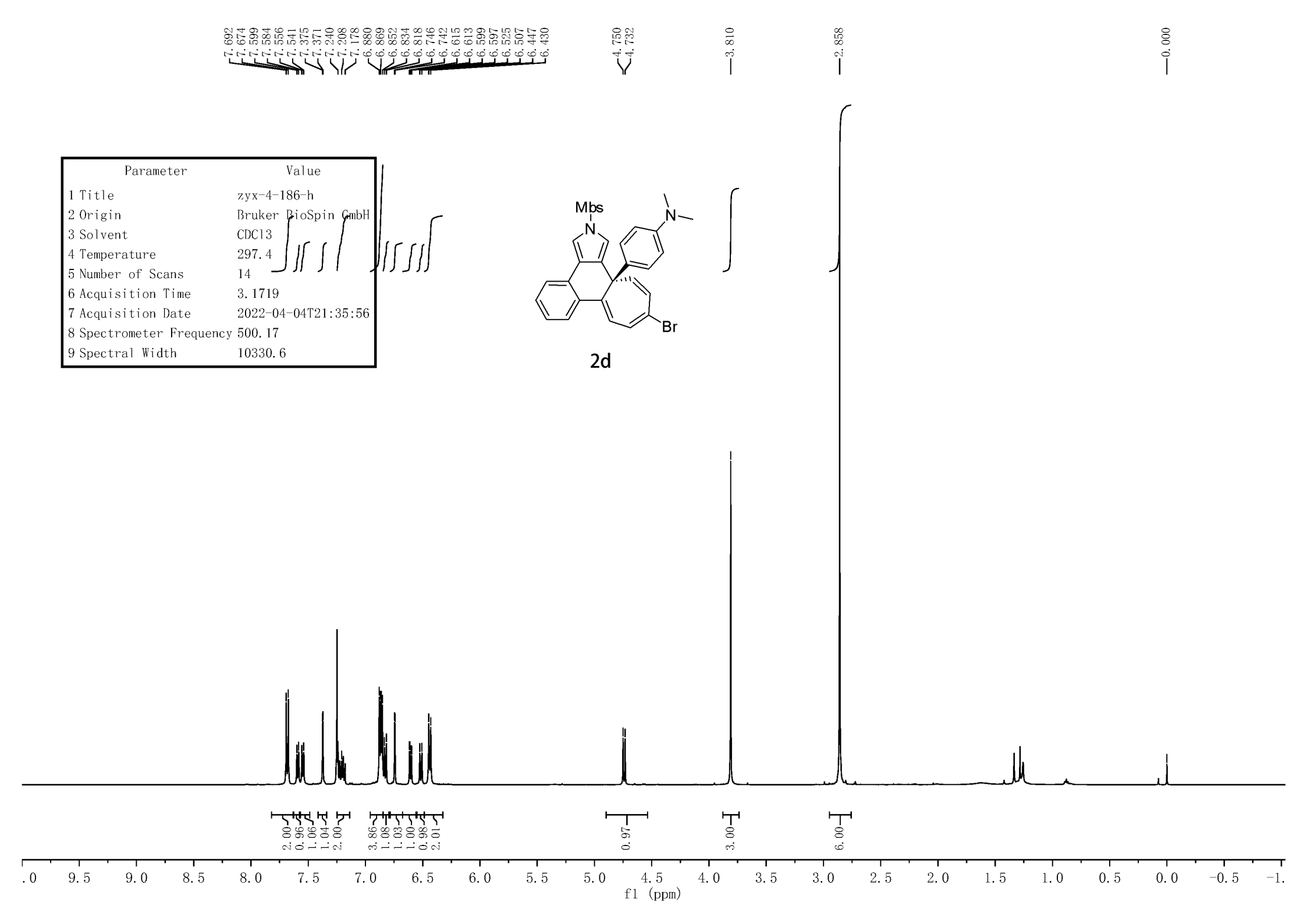


2c

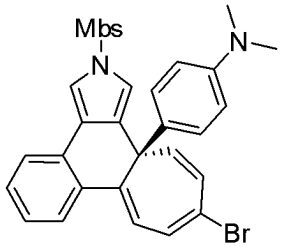
133.74
133.25
132.01
131.86
131.66
129.29
127.95
127.56
127.43
127.40
127.15
126.54
123.49
122.30
122.12
121.71



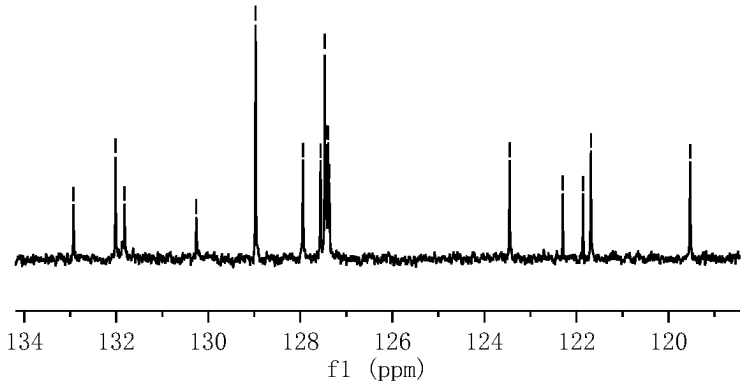


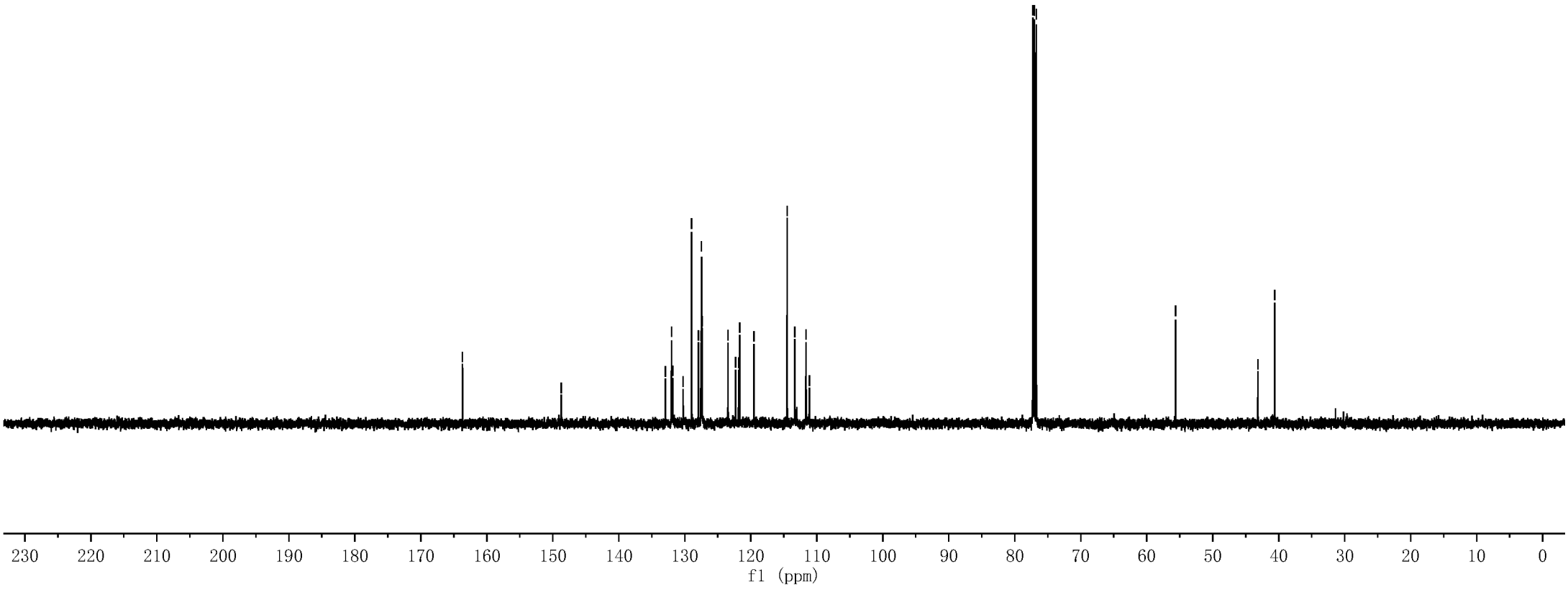

7.692
7.674
7.599
7.584
7.556
7.541
7.375
7.371
7.240
7.208
7.178
6.880
6.869
6.852
6.834
6.818
6.746
6.742
6.615
6.613
6.599
6.597
6.525
6.507
6.447
6.430
4.750
4.732
3.810
2.858
0.000
Parameter Value
1 Title zyx-4-186-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.4
5 Number of Scans 14
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-04T21:35:56
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Mbs
N
N
Br
2d
2.00
0.96
1.06
1.04
2.00
3.86
1.08
1.03
1.00
0.98
2.01
0.97
3.00
6.00
f1 (ppm)

Parameter	Value
1 Title	zyx-4-186--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	96
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-04T21:41:04
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9



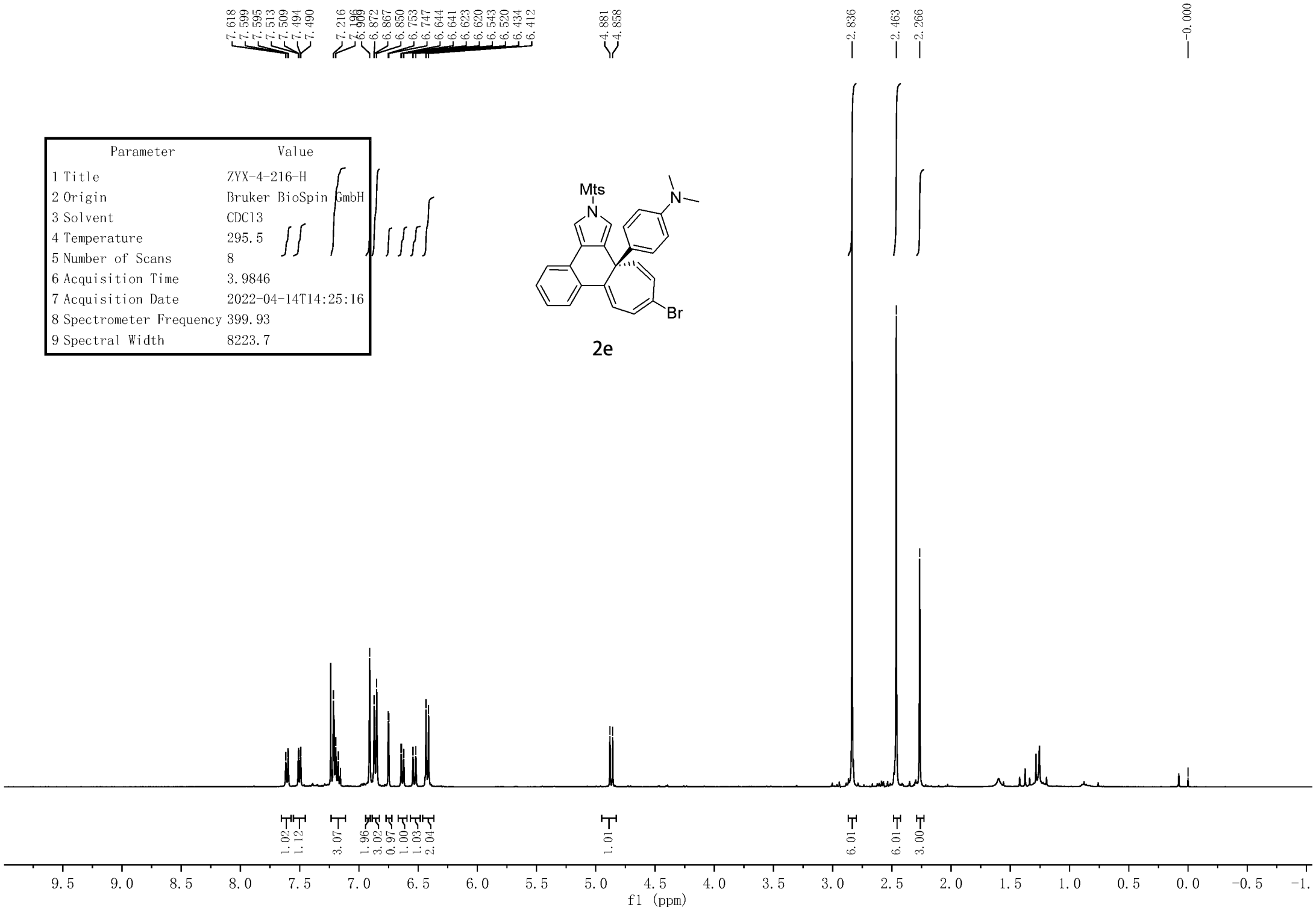
2d





Parameter	Value
1 Title	ZYX-4-216-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	8
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-14T14:25:16
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

2e



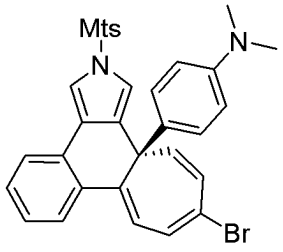
148.75
144.08
140.15
132.61
132.33
132.11
132.09
131.57
130.79
127.91
127.55
127.48
127.45
127.25
127.23
123.33
122.49
121.41
120.72
119.64
115.65
113.35
112.43
111.65

77.32
77.00
76.68

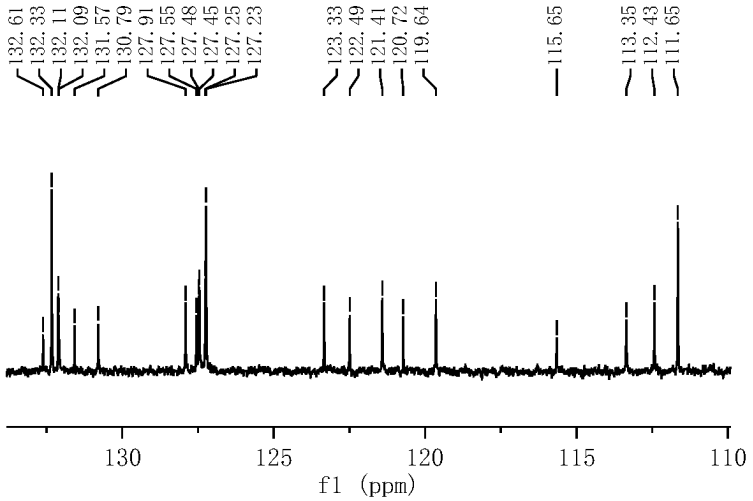
43.67
40.63

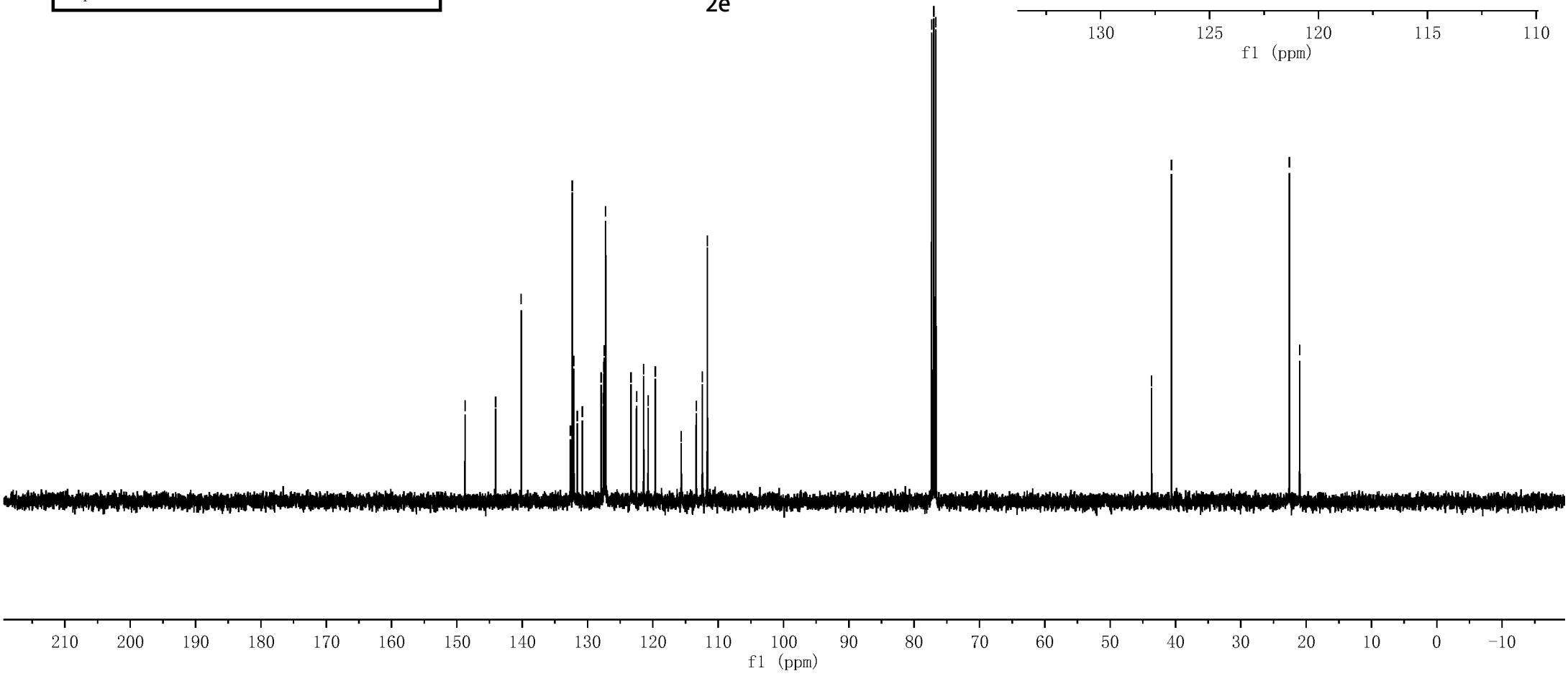
22.57
20.98

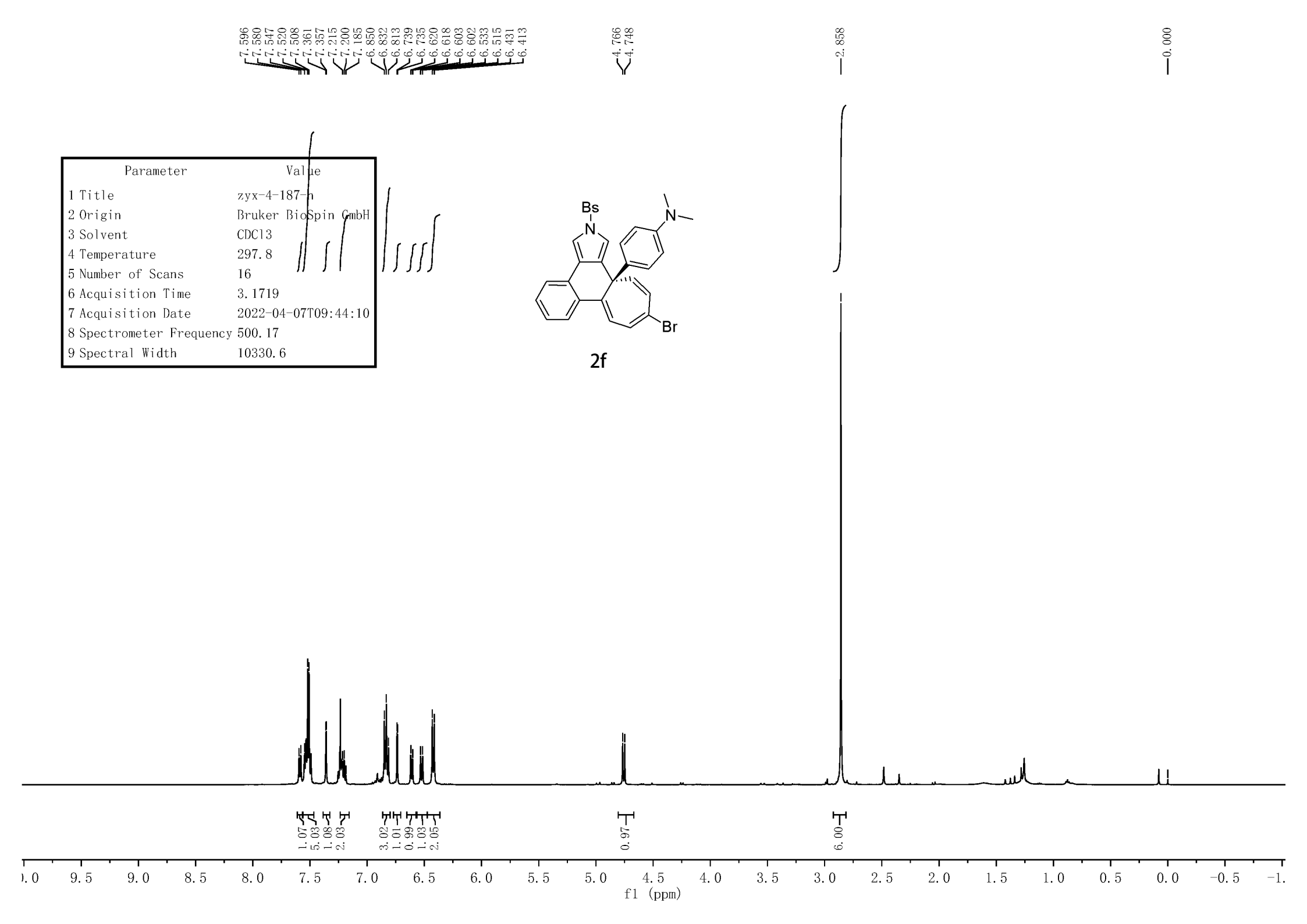
Parameter	Value
1 Title	ZYX-4-216-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.7
5 Number of Scans	61
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-14T14:26:36
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



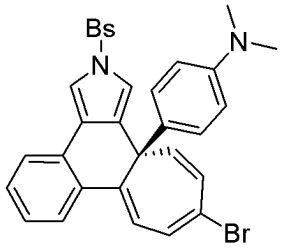
2e





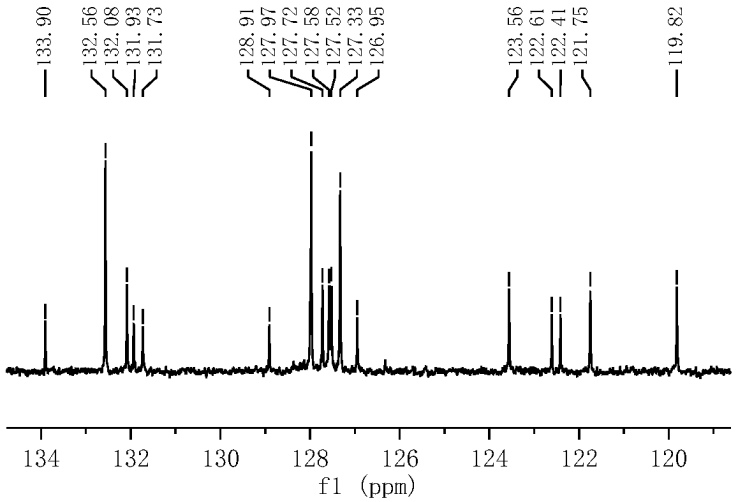

7.596
7.580
7.547
7.520
7.508
7.361
7.357
7.215
7.200
7.185
6.850
6.832
6.813
6.739
6.735
6.620
6.618
6.603
6.602
6.533
6.515
6.431
6.413
4.766
4.748
2.858
0.000
Parameter Value
1 Title zyx-4-187-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.8
5 Number of Scans 16
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-07T09:44:10
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Bs
N
N
Br
2f
1.07
5.03
1.08
2.03
3.02
1.01
0.99
1.03
2.05
0.97
6.00
f1 (ppm)

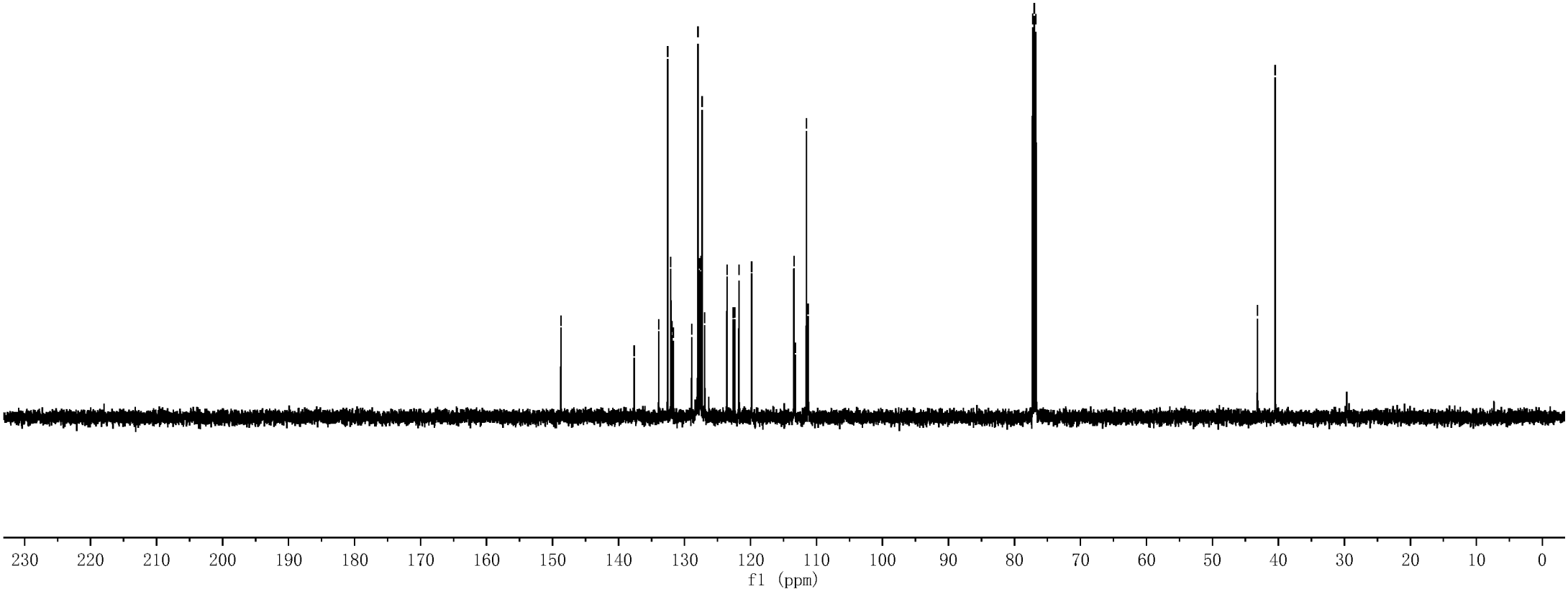
Parameter	Value
1 Title	zyx-4-187-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	40
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-07T09:45:51
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9



2f

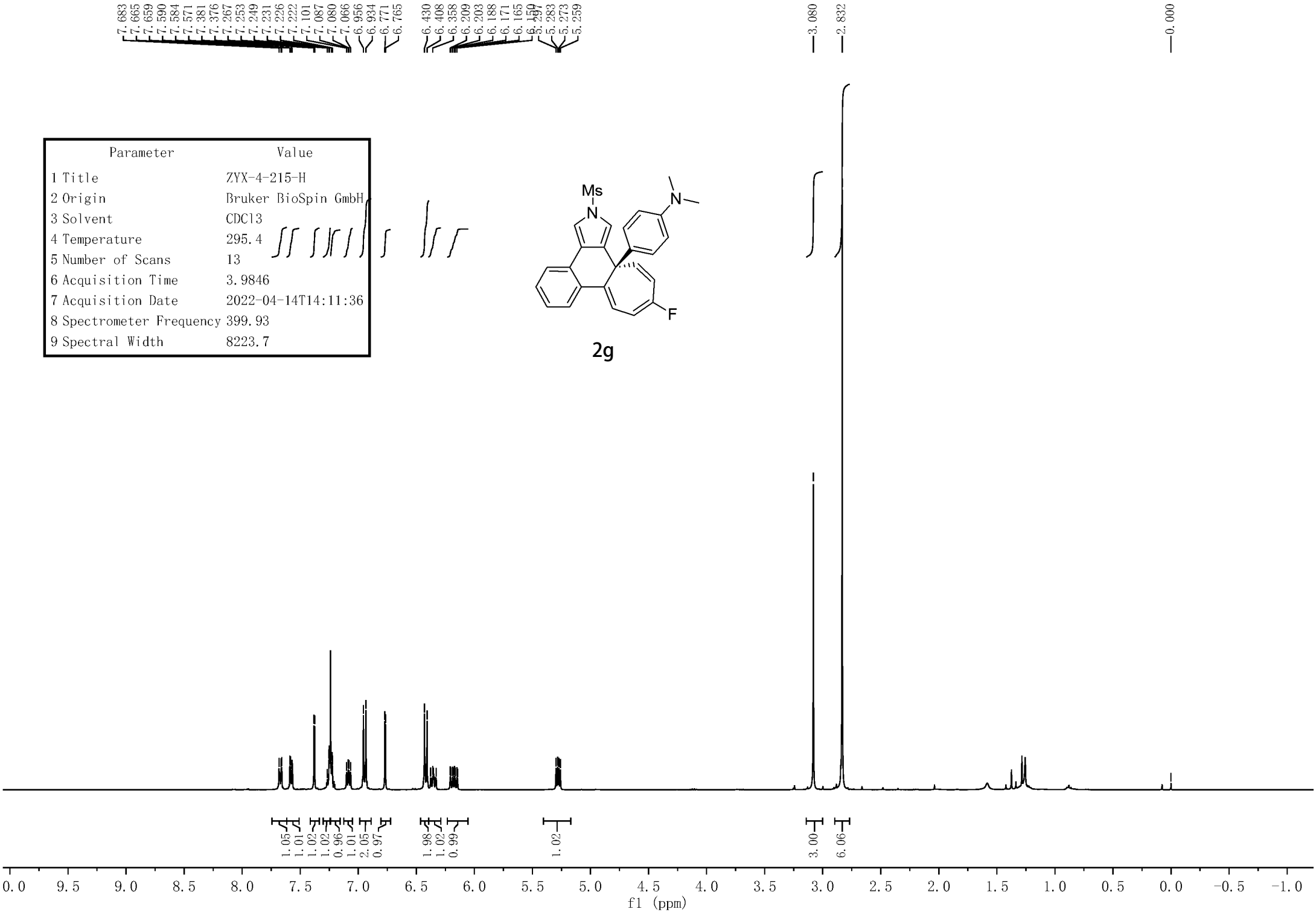
148.72
132.56
132.08
127.97
127.72
127.58
127.52
127.33
126.95
123.56
122.61
122.41
121.75
119.82
113.21
111.52
111.26
77.25
77.00
76.75
43.18
40.51

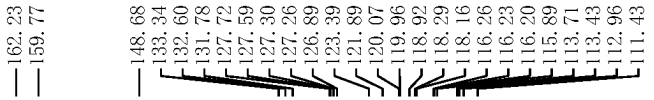




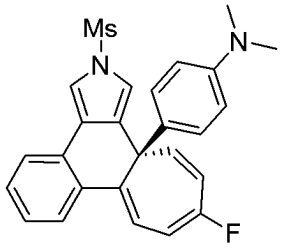
Parameter	Value
1 Title	ZYX-4-215-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.4
5 Number of Scans	13
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-14T14:11:36
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

2g

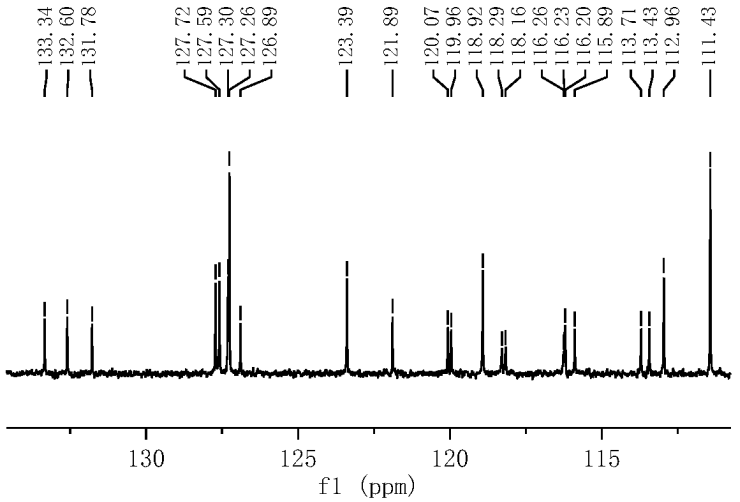


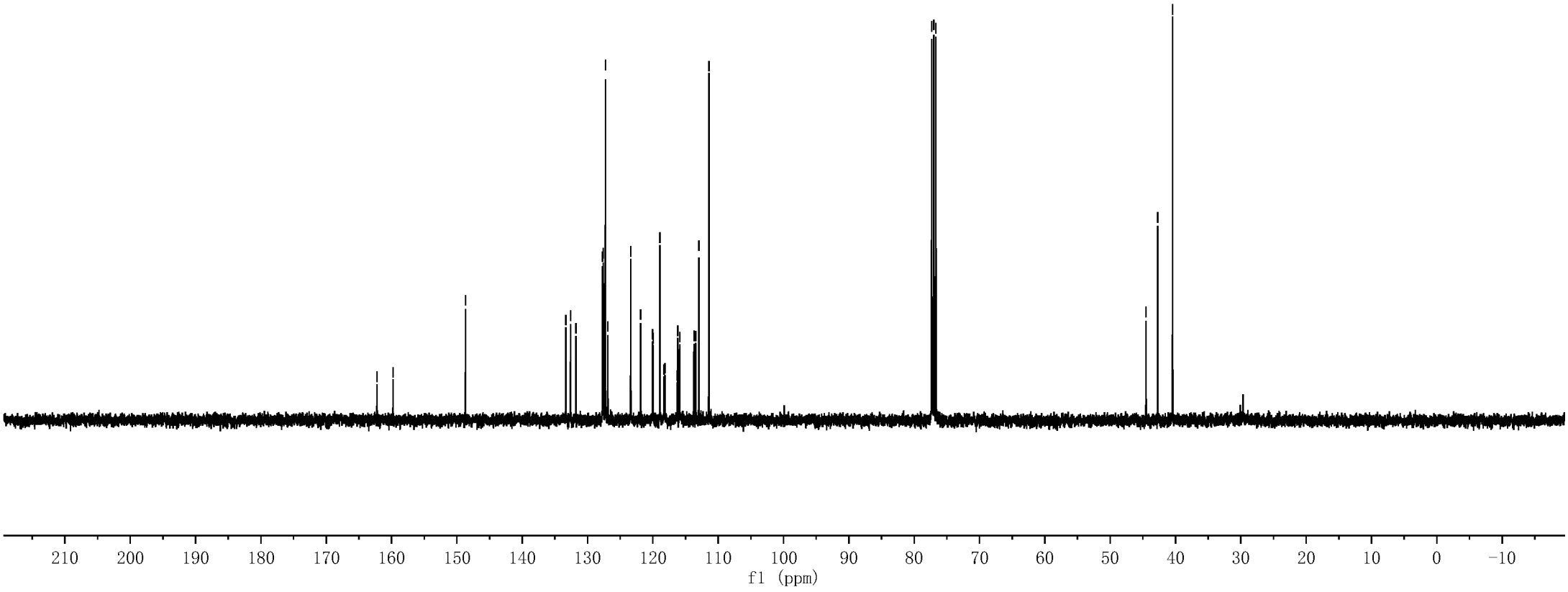


Parameter	Value
1 Title	ZYX-4-215-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.7
5 Number of Scans	106
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-14T14:14:30
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

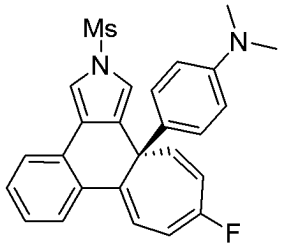


2g

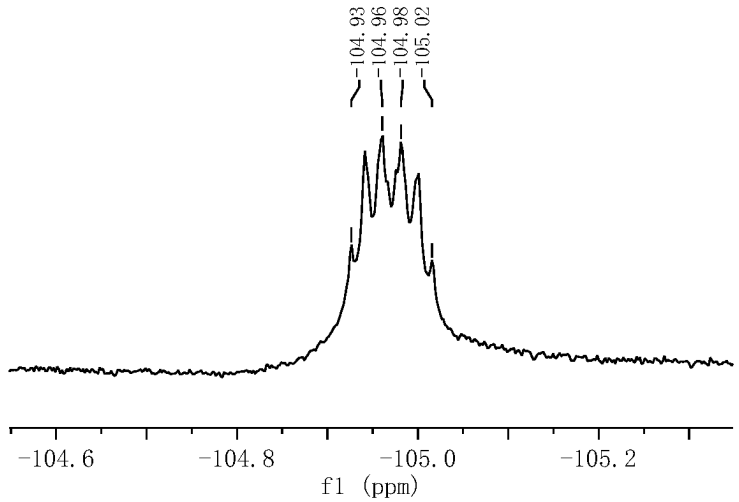


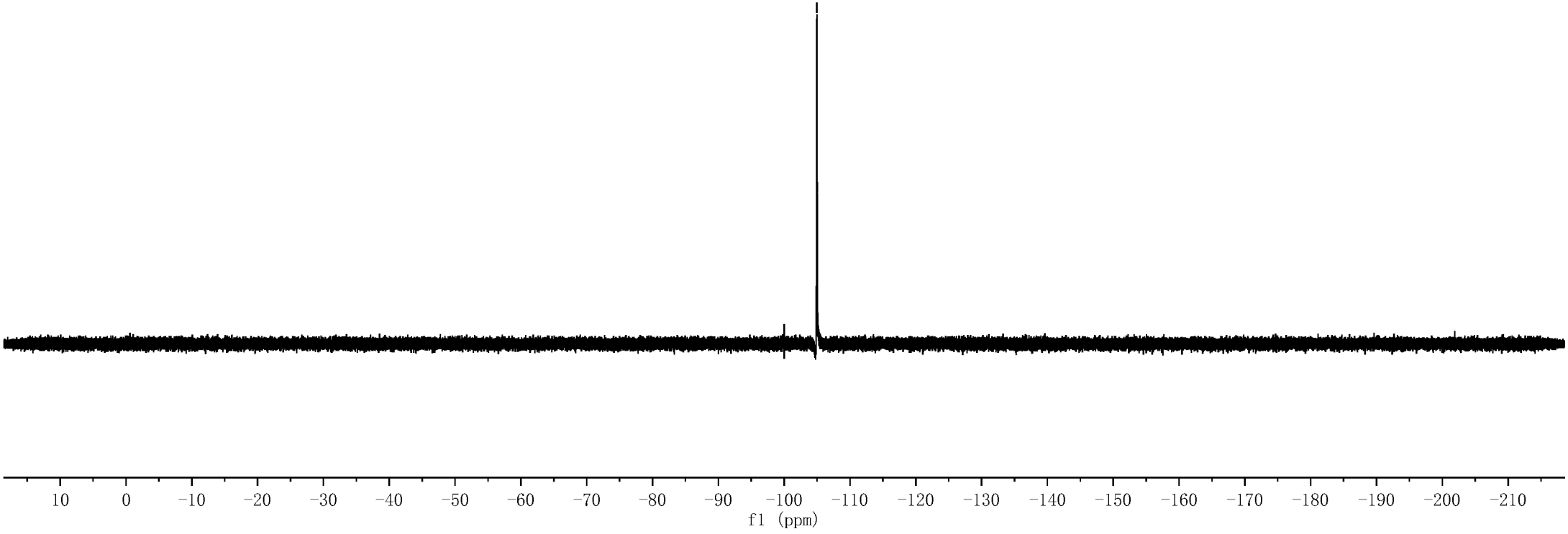


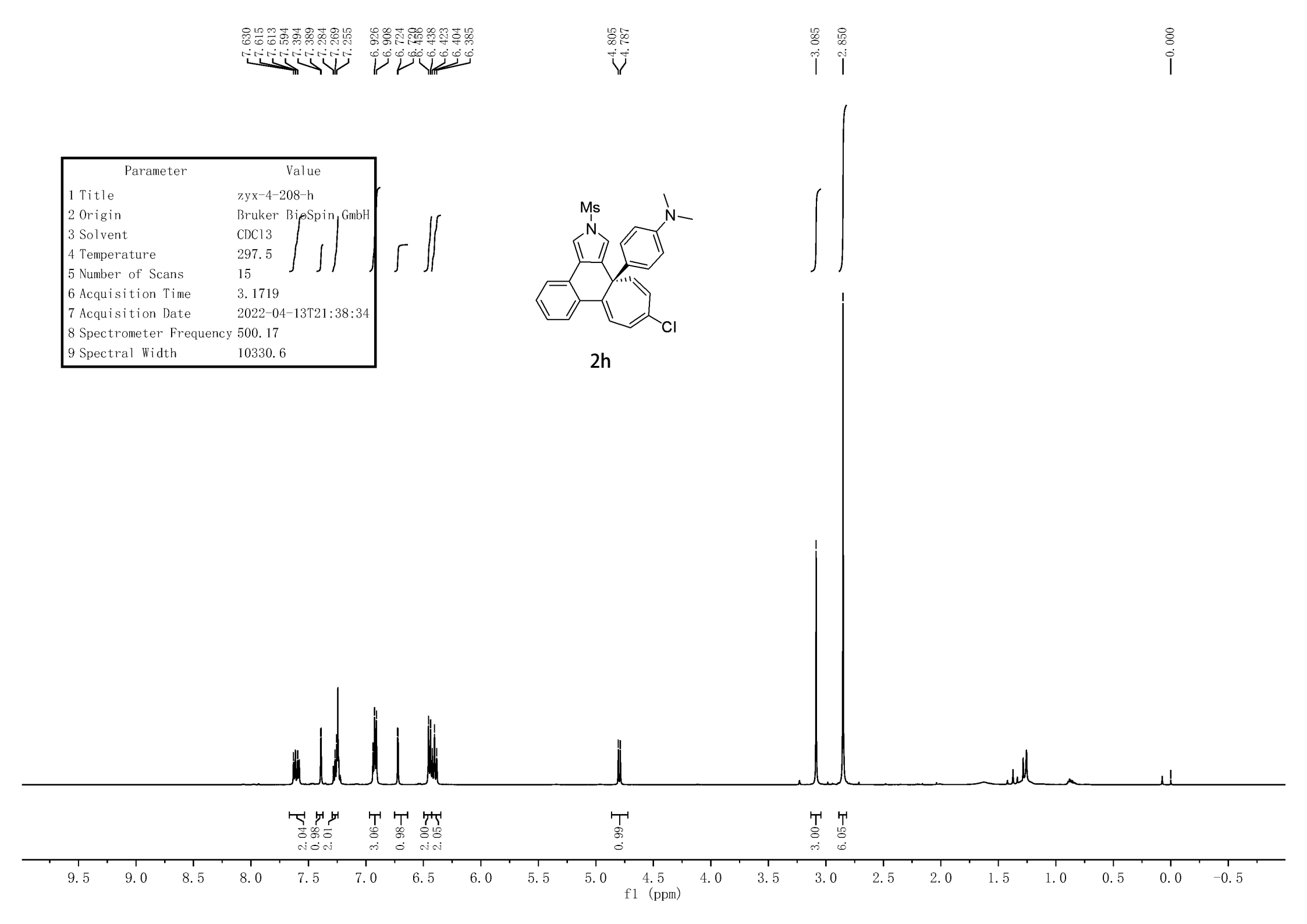
Parameter	Value
1 Title	ZYX-4-215-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.2
5 Number of Scans	40
6 Acquisition Time	0.7340
7 Acquisition Date	2022-04-14T14:06:41
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



2g

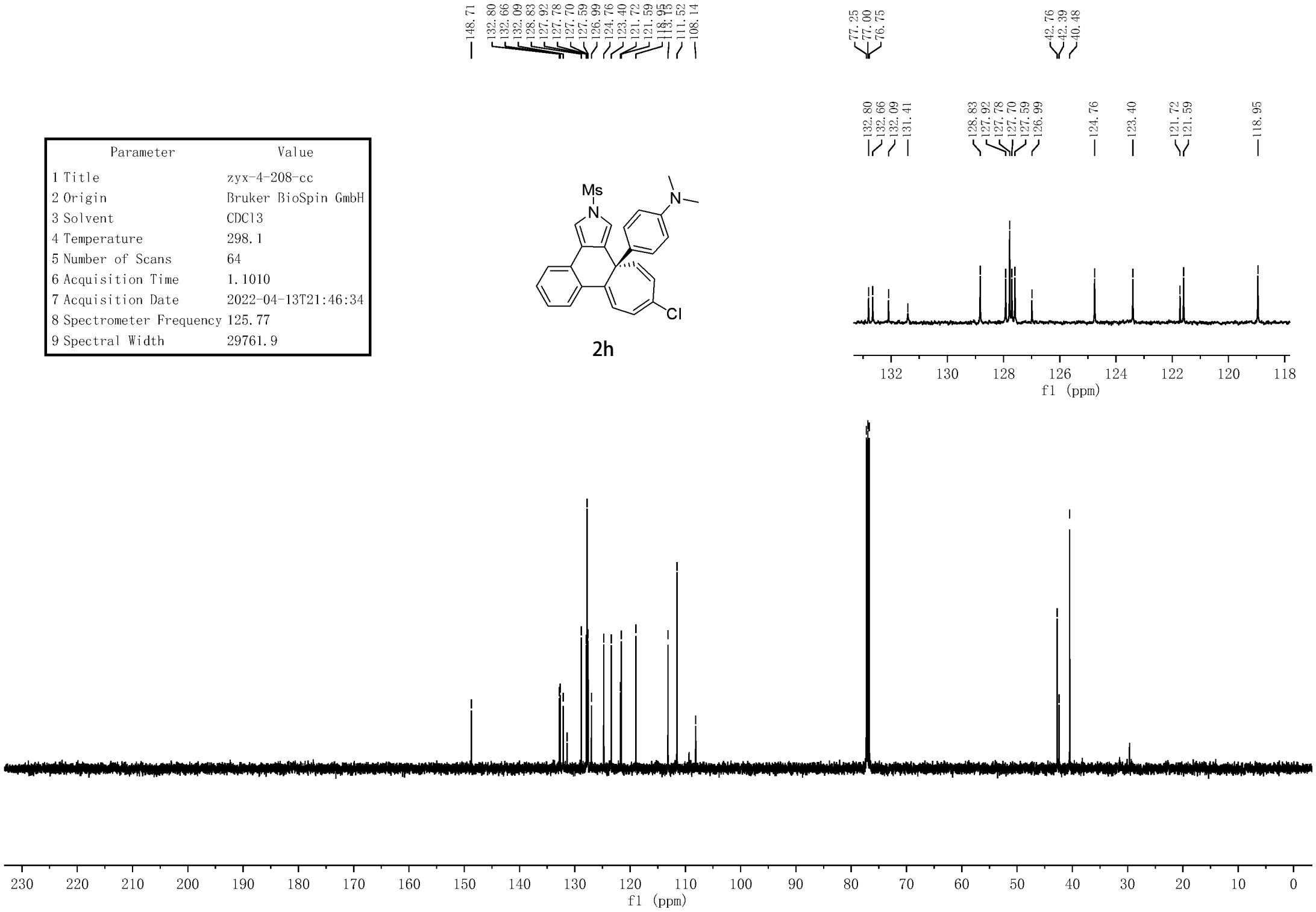




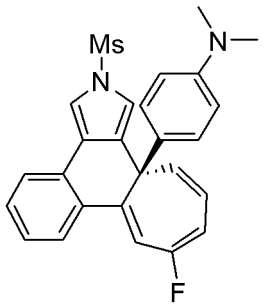

7.630
7.615
7.613
7.594
7.394
7.389
7.284
7.269
7.255
6.926
6.908
6.724
6.720
6.458
6.438
6.423
6.404
6.385
4.805
4.787
3.085
2.850
0.000
Parameter Value
1 Title zyx-4-208-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.5
5 Number of Scans 15
6 Acquisition Time 3.1719
7 Acquisition Date 2022-04-13T21:38:34
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Ms
N
N
Cl
2h
2.04
0.98
2.01
3.06
0.98
2.00
2.05
0.99
3.00
6.05
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)

Parameter	Value
1 Title	zyx-4-208-cc
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.1
5 Number of Scans	64
6 Acquisition Time	1.1010
7 Acquisition Date	2022-04-13T21:46:34
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

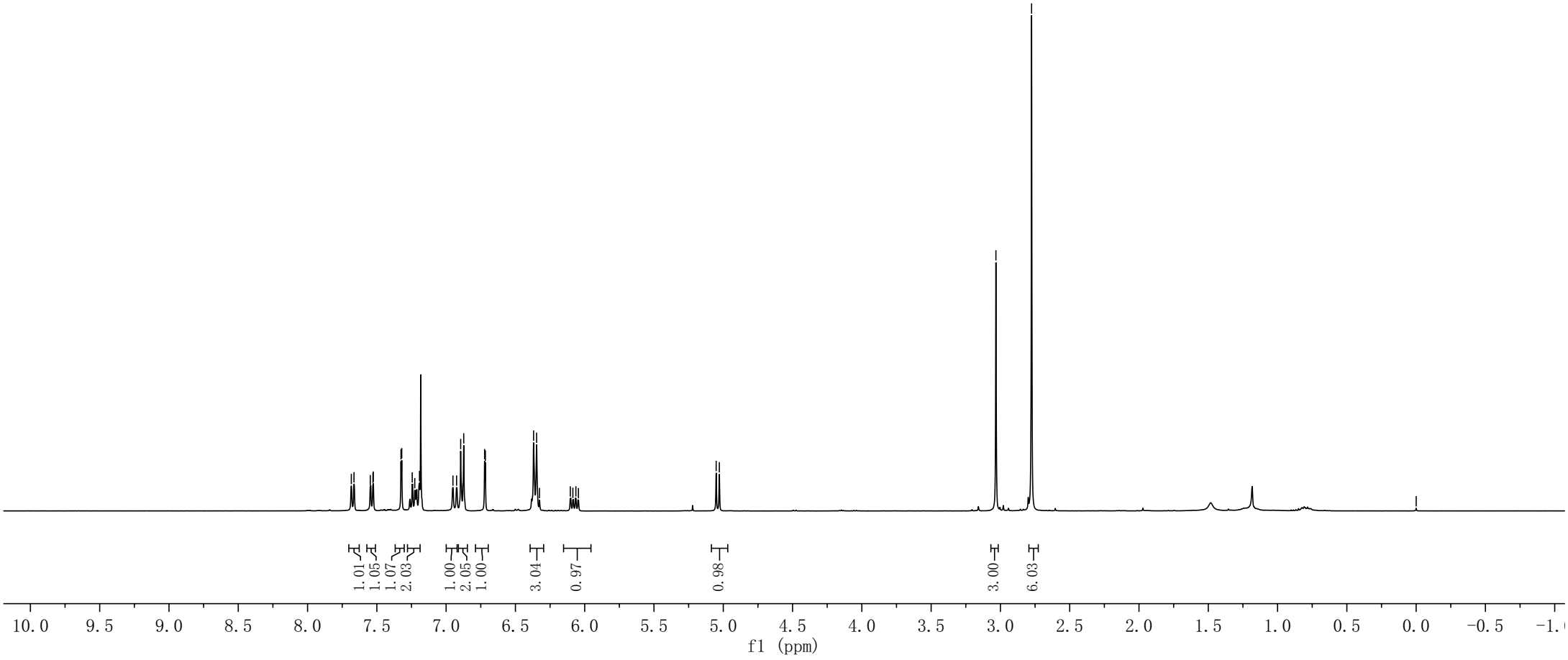
2h



Parameter	Value
1 Title	zyx-11-89-p2
2 Origin	
3 Solvent	CDCl3
4 Temperature	296.8
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2023-11-26T00:43:24
8 Spectrometer Frequency	399.90
9 Spectral Width	8012.0

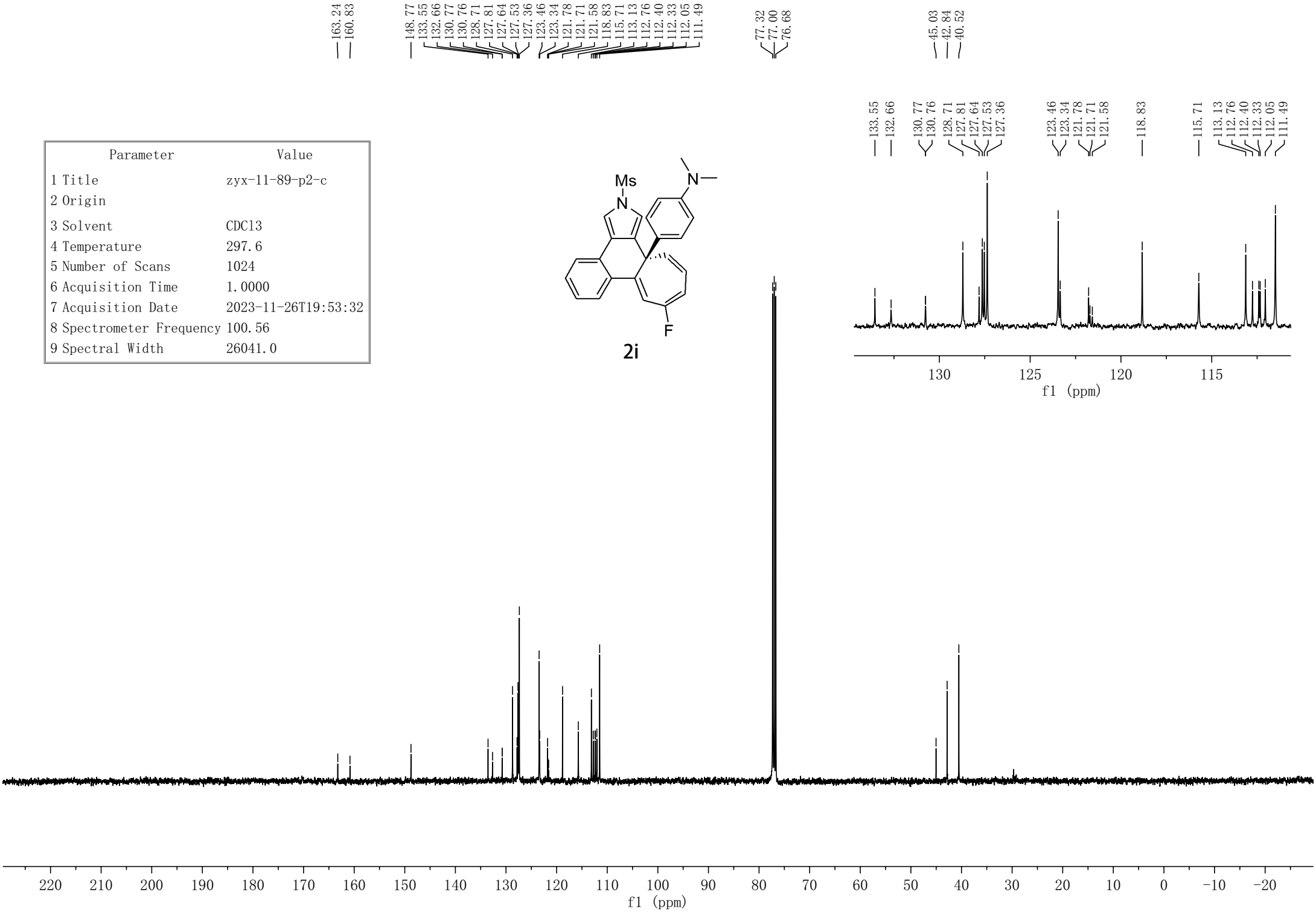


2i



Parameter	Value
1 Title	zyx-11-89-p2-c
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	1024
6 Acquisition Time	1.0000
7 Acquisition Date	2023-11-26T19:53:32
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

2i

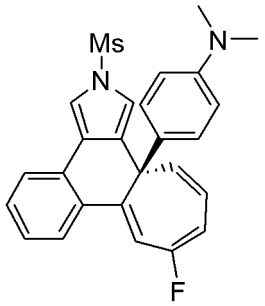


128.70
127.63
127.52
127.36
123.45
123.34
118.83
115.70
113.13
112.75
112.40
112.05
111.49

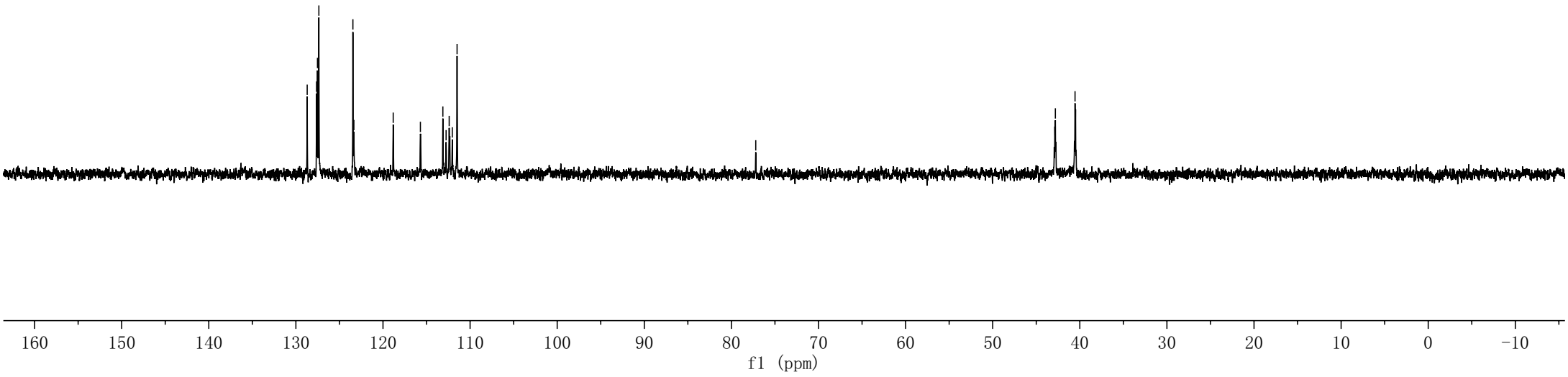
77.20

42.81
40.55

Parameter	Value
1 Title	zyx-11-89-c
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.9
5 Number of Scans	480
6 Acquisition Time	1.0001
7 Acquisition Date	2023-11-26T20:20:57
8 Spectrometer Frequency	100.56
9 Spectral Width	18028.0

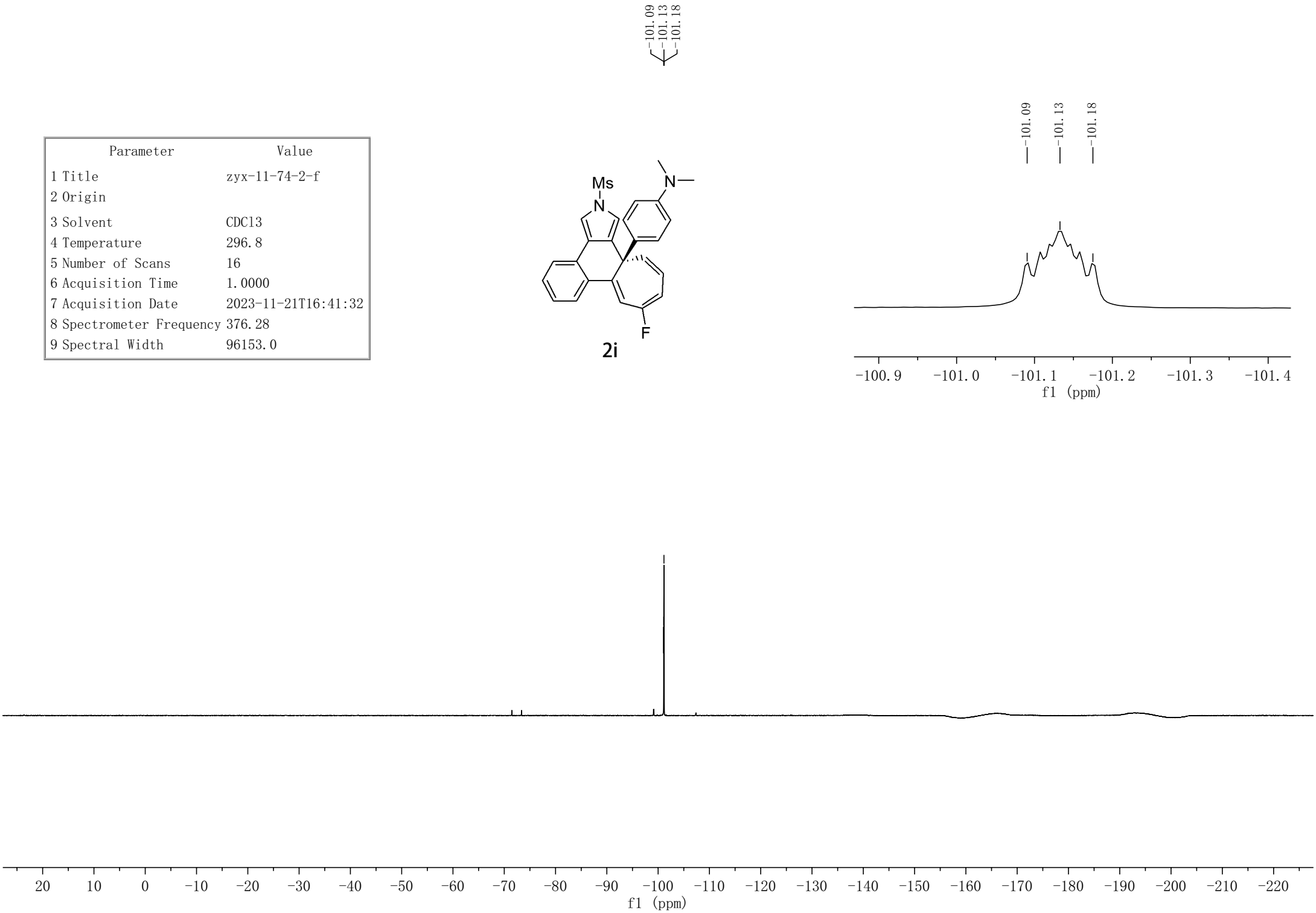


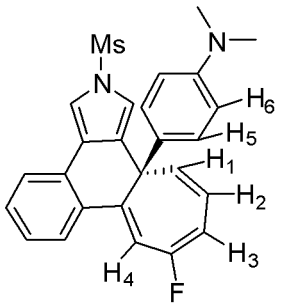
2i



Parameter	Value
1 Title	zyx-11-74-2-f
2 Origin	
3 Solvent	CDCl3
4 Temperature	296.8
5 Number of Scans	16
6 Acquisition Time	1.0000
7 Acquisition Date	2023-11-21T16:41:32
8 Spectrometer Frequency	376.28
9 Spectral Width	96153.0

2i





2i (COSY)
$CDCl_3$, 600 MHz

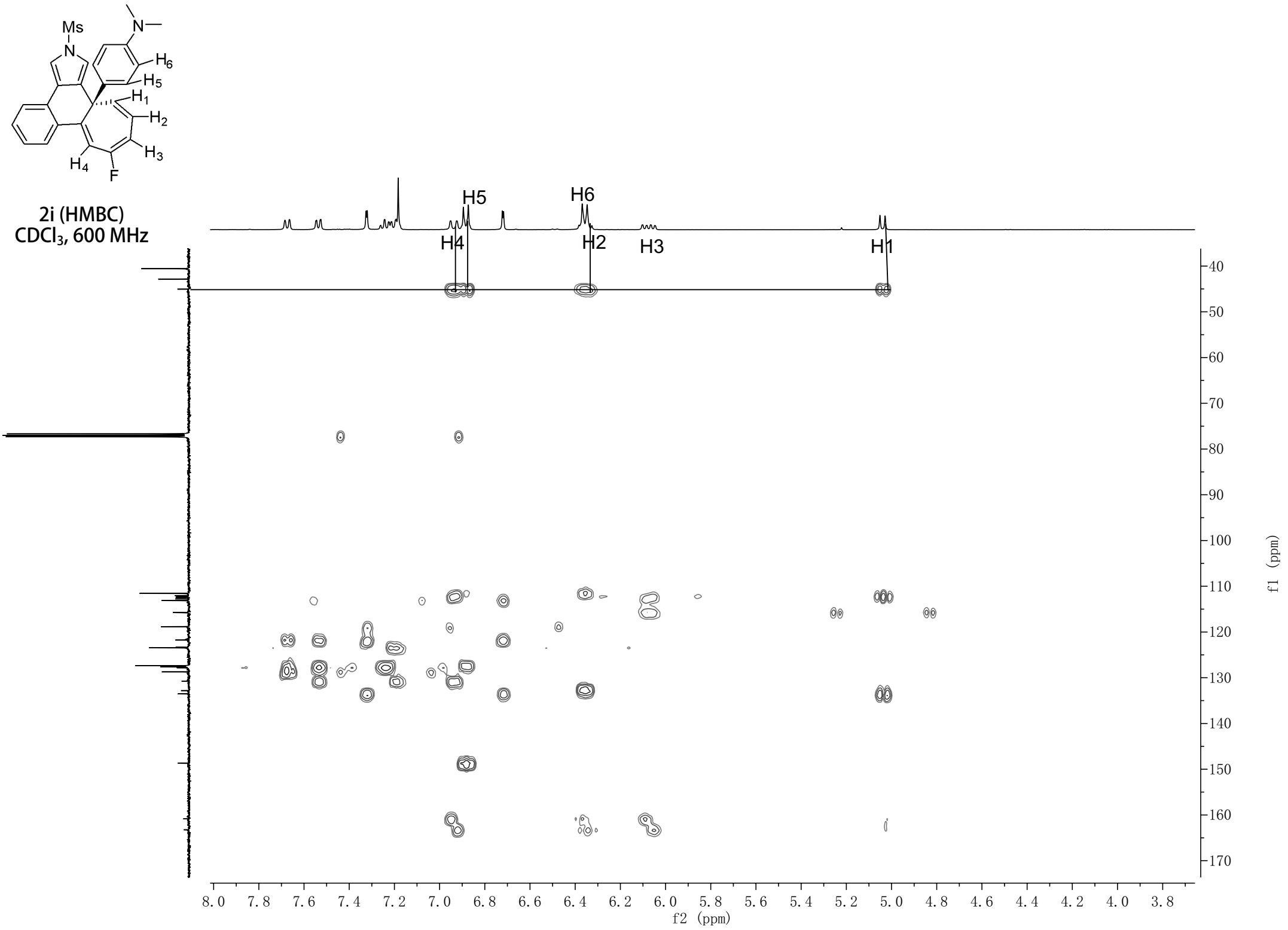
H5
H6
H4
H2
H3
H1

H1
H3
H2
H4

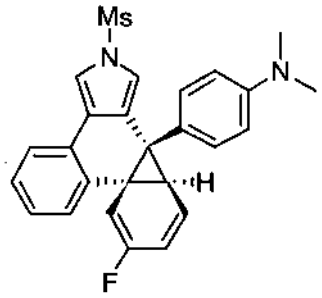
	Parameter	Value (f2, f1)
1	Title	zyx-82-2-h
2	Origin	Bruker BioSpin GmbH
3	Solvent	CDCl3
4	Temperature	298.0
5	Number of Scans	4
6	Acquisition Time	0.0852
7	Spectrometer Frequency	(600.13, 600.13)
8	Spectral Width	(12019.2, 11990.4)
9	Lowest Frequency	(-2466.4, -2454.4)
10	Nucleus	(1H, 1H)
11	Acquired Size	(1024, 128)
12	Spectral Size	(1024, 1024)

7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0
f2 (ppm)

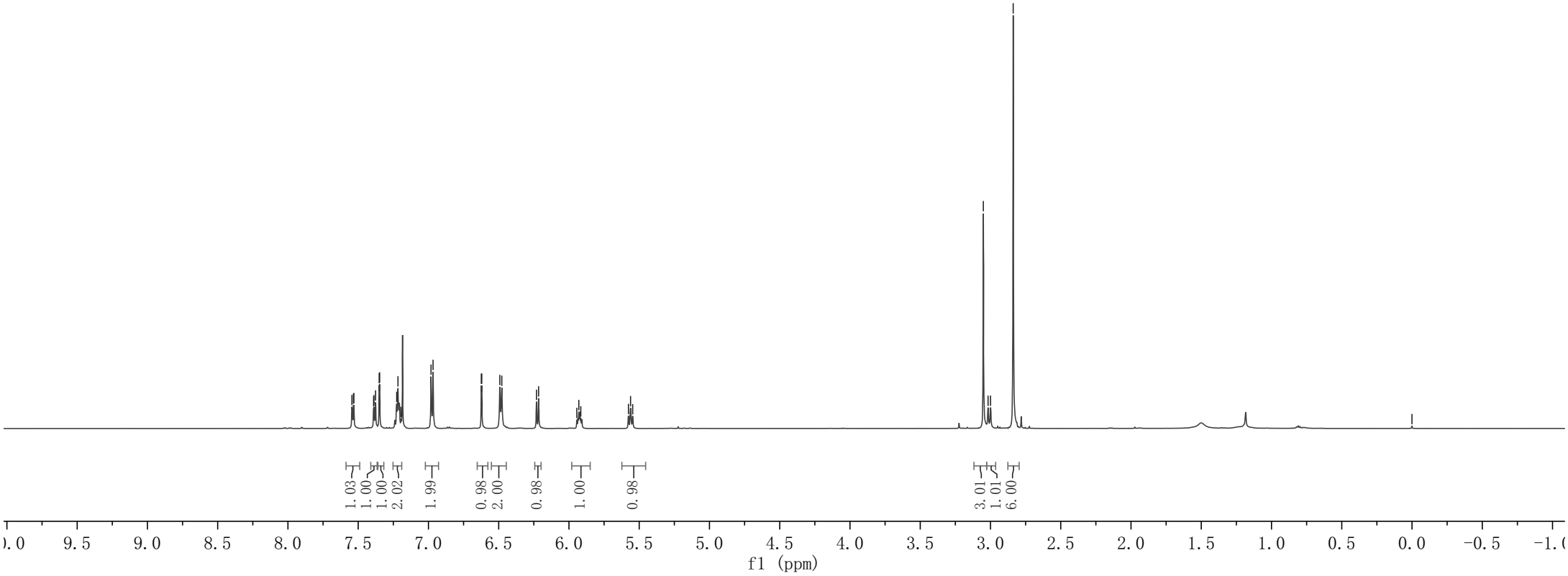
5.0 5.2 5.4 5.6 5.8 6.0 6.2 6.4 6.6 6.8 7.0 7.2 7.4 7.6 7.8
f1 (ppm)


Ms
N
N
H6
H5
H1
H2
H3
H4
F
2i (HMBC)
CDCl3, 600 MHz
H5
H6
H4
H2
H3
H1
40
50
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
f2 (ppm)

Parameter	Value
1 Title	ZYX-11-82
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	2.7263
7 Acquisition Date	2023-11-22T13:00:23
8 Spectrometer Frequency	600.13
9 Spectral Width	12019.2

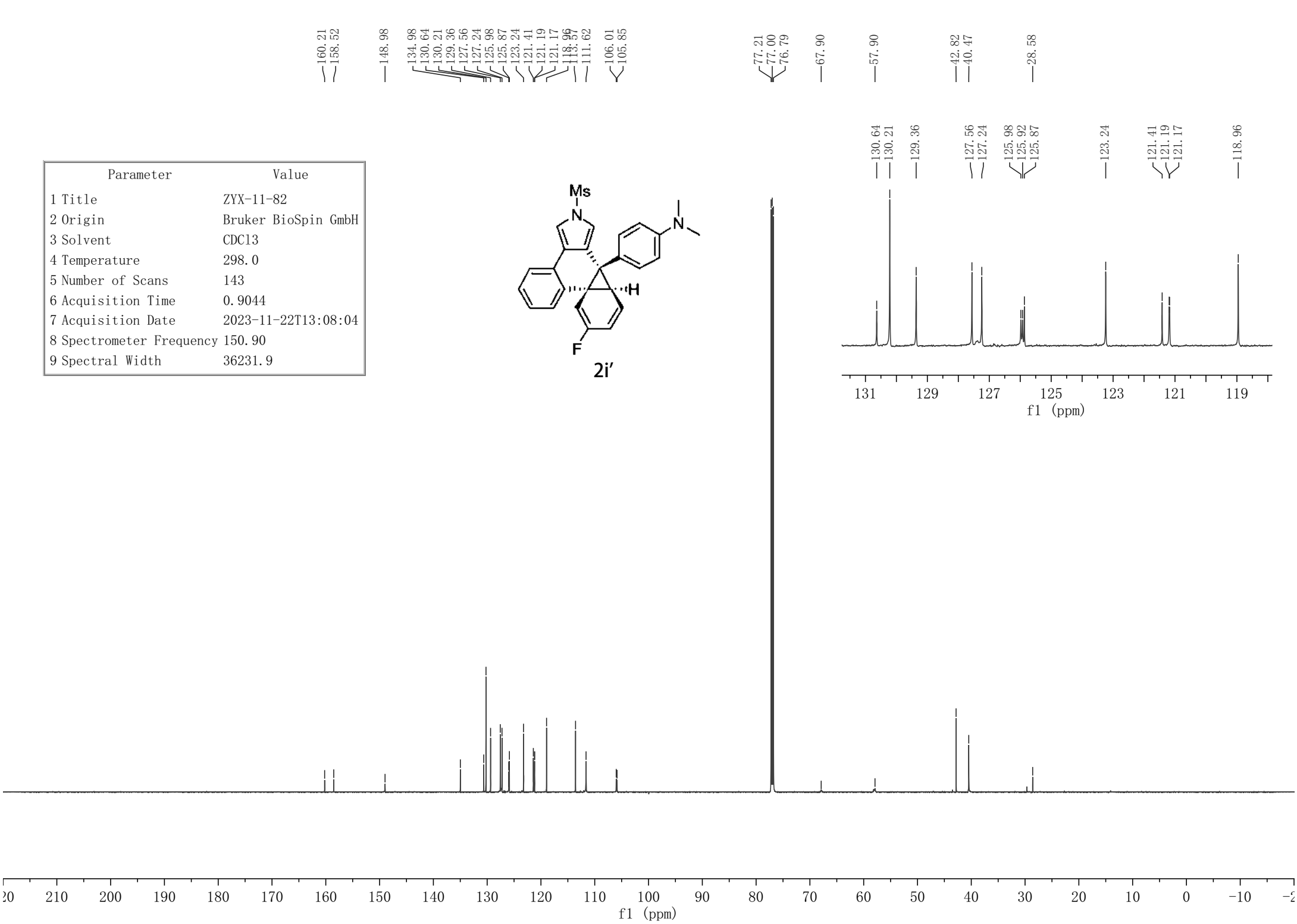


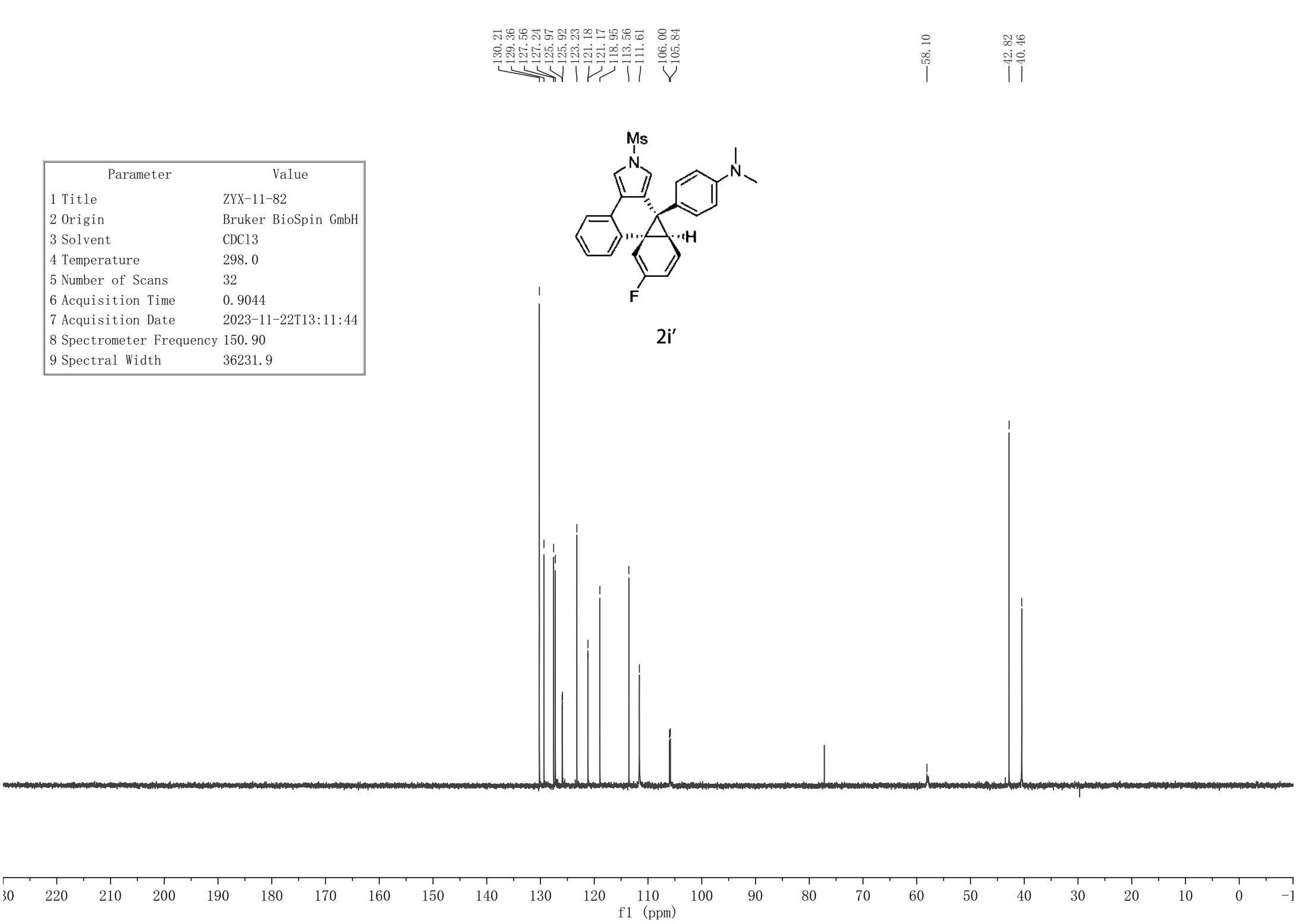
2i′



Parameter	Value
1 Title	ZYX-11-82
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	143
6 Acquisition Time	0.9044
7 Acquisition Date	2023-11-22T13:08:04
8 Spectrometer Frequency	150.90
9 Spectral Width	36231.9

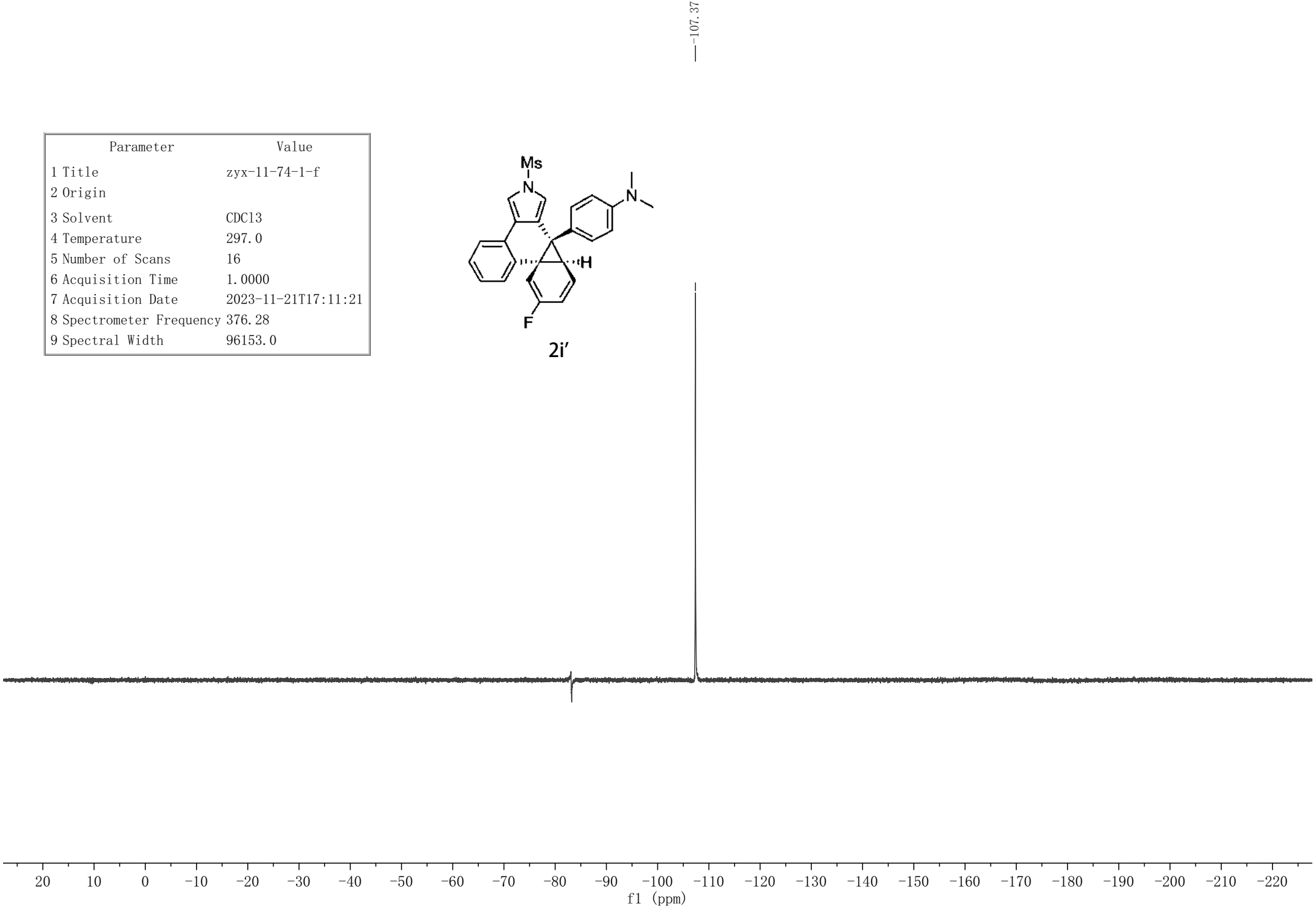
2i′




130.21
129.36
127.56
127.24
125.97
125.92
123.23
121.18
121.17
118.95
113.56
111.61
106.00
105.84
58.10
42.82
40.46
Ms
N
N
H
F
2i'
Parameter	Value
1 Title	ZYX-11-82
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	32
6 Acquisition Time	0.9044
7 Acquisition Date	2023-11-22T13:11:44
8 Spectrometer Frequency	150.90
9 Spectral Width	36231.9
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

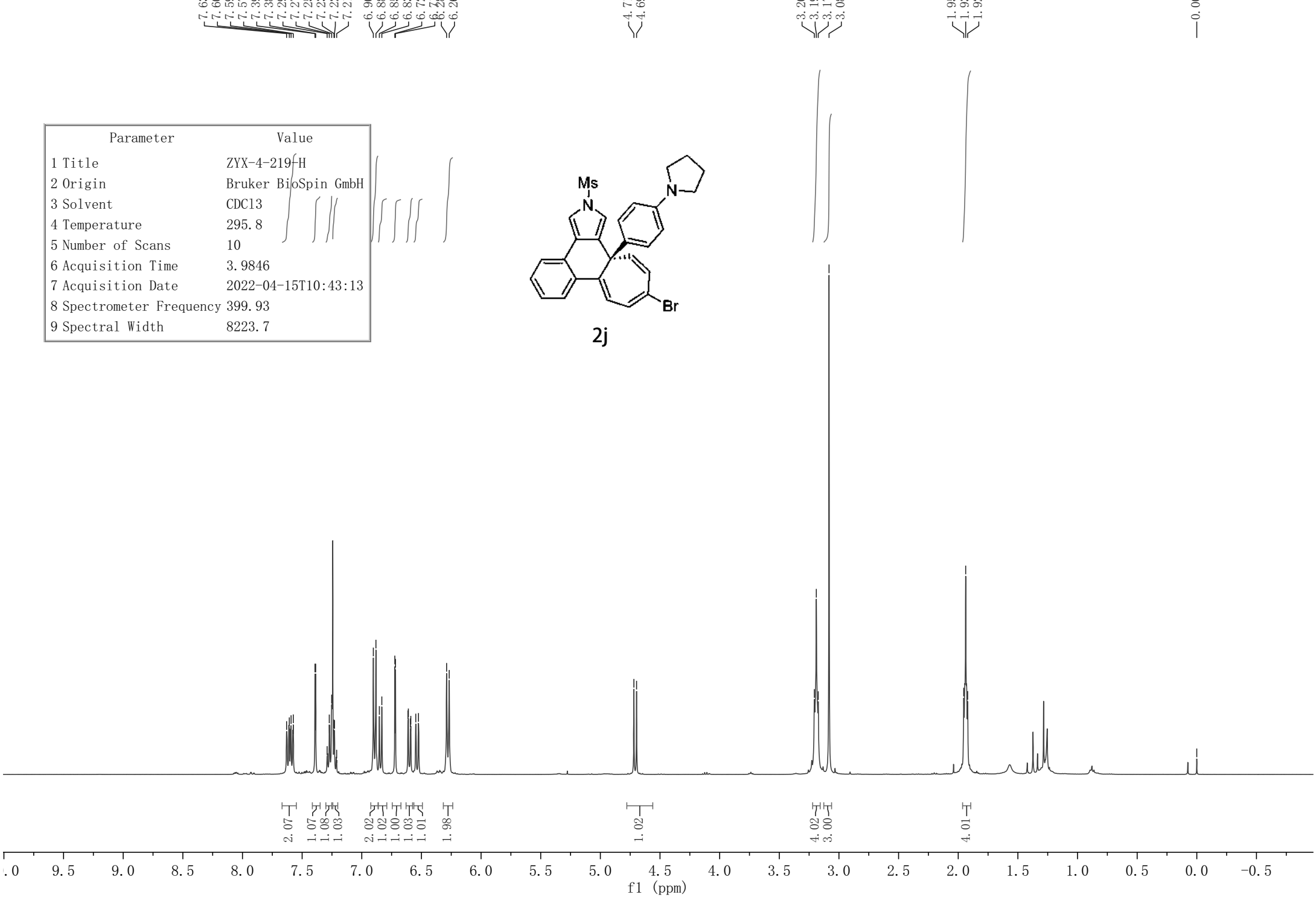
Parameter	Value
1 Title	zyx-11-74-1-f
2 Origin	
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	16
6 Acquisition Time	1.0000
7 Acquisition Date	2023-11-21T17:11:21
8 Spectrometer Frequency	376.28
9 Spectral Width	96153.0

2i'



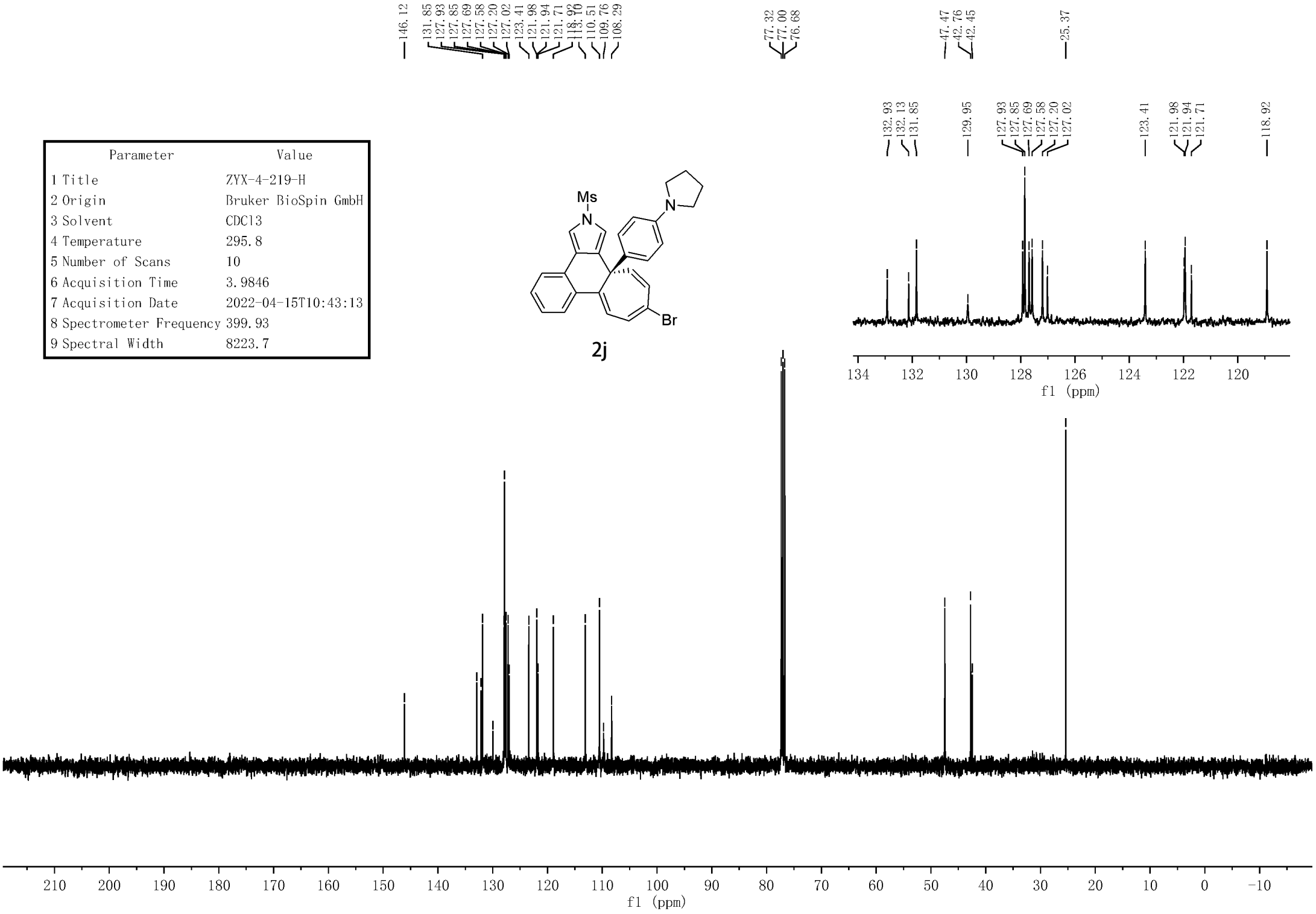
Parameter	Value
1 Title	ZYX-4-219-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-15T10:43:13
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

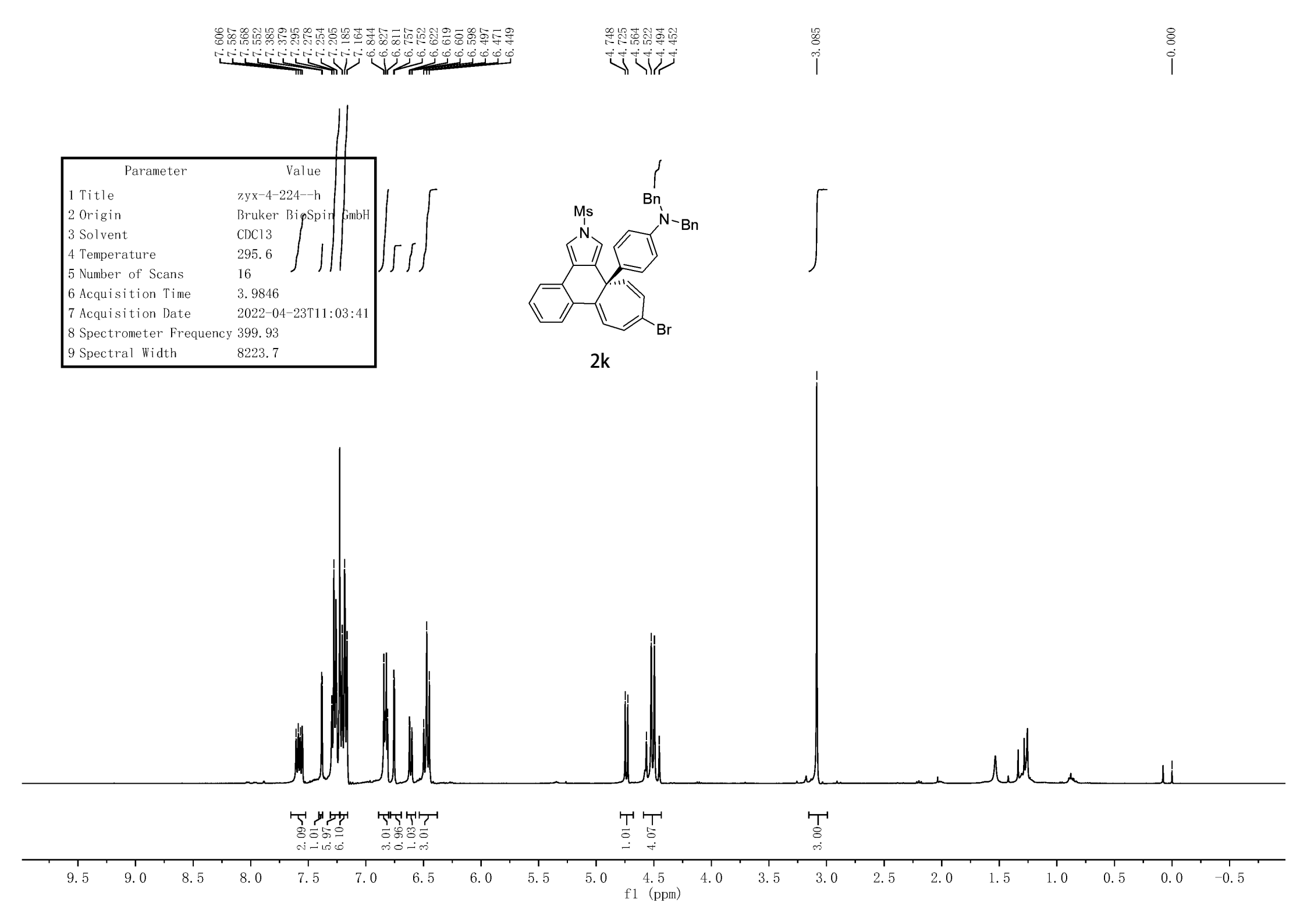
2j



Parameter	Value
1 Title	ZYX-4-219-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	10
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-15T10:43:13
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

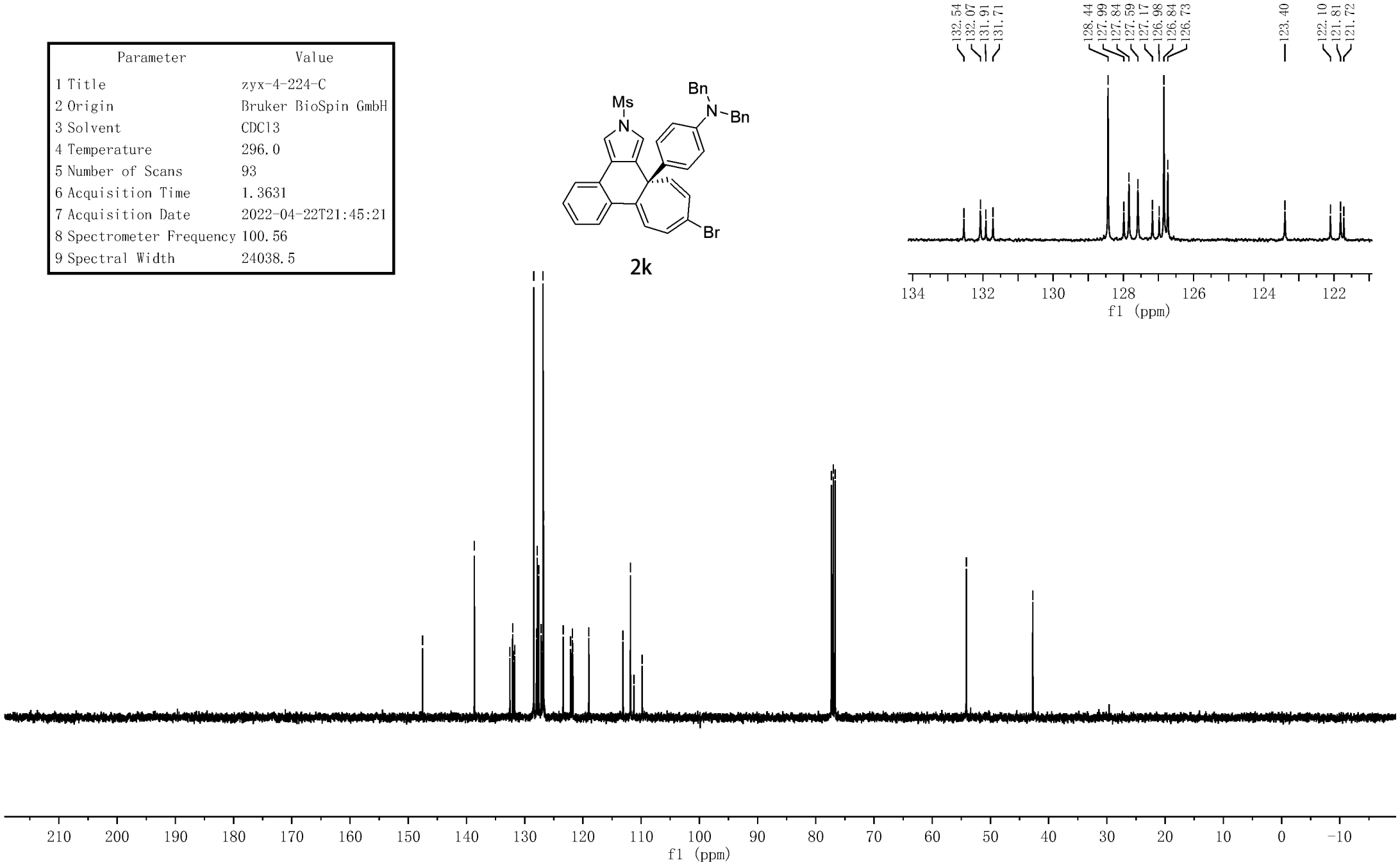
2j

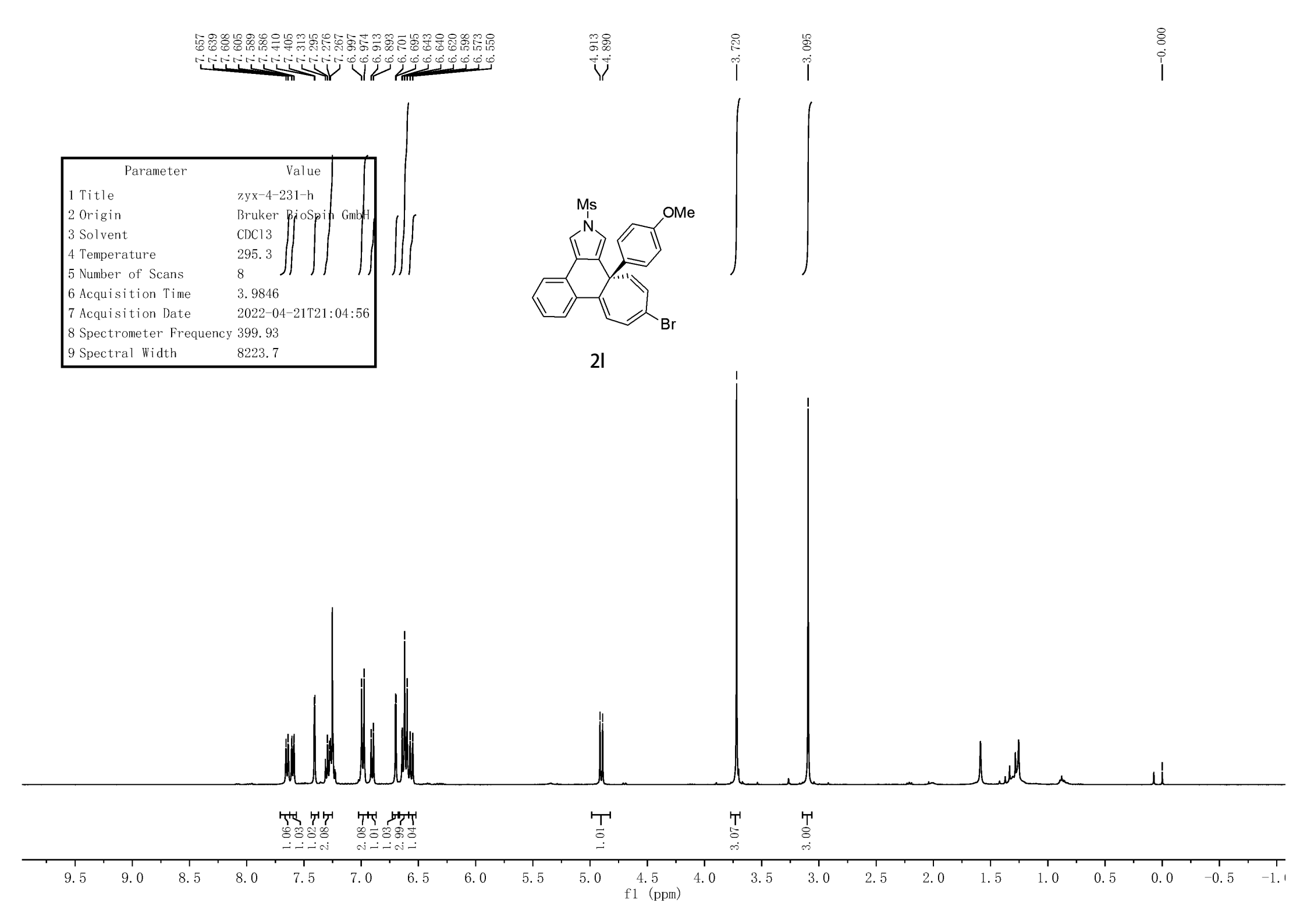


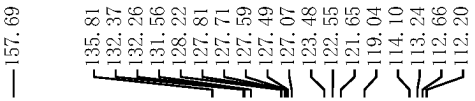

7.606
7.587
7.568
7.552
7.385
7.379
7.295
7.278
7.254
7.205
7.185
7.164
6.844
6.827
6.811
6.757
6.752
6.622
6.619
6.601
6.598
6.497
6.471
6.449
4.748
4.725
4.564
4.522
4.494
4.452
3.085
0.000
Parameter Value
1 Title zyx-4-224--h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.6
5 Number of Scans 16
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-23T11:03:41
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
Bn
N
Bn
Br
2k
2.09
1.01
5.97
6.10
3.01
0.96
1.03
3.01
1.01
4.07
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)

Parameter	Value
1 Title	zyx-4-224-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.0
5 Number of Scans	93
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-22T21:45:21
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

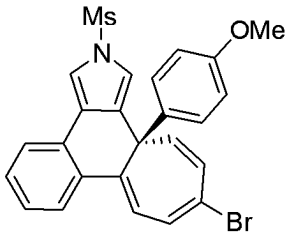
2k



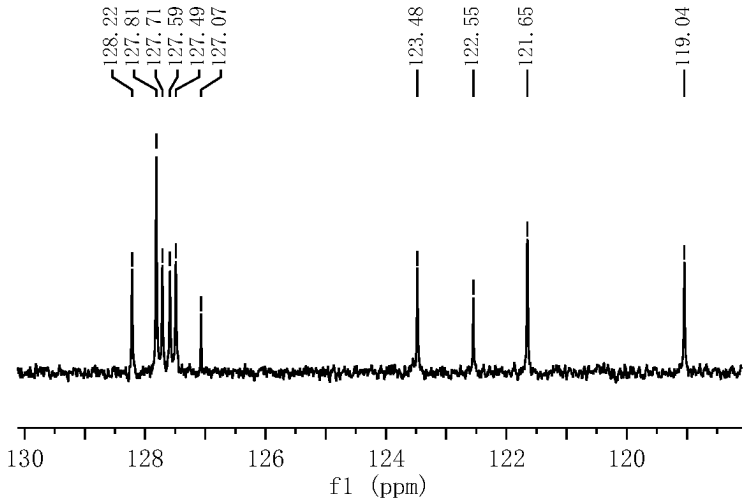

7.657
7.639
7.608
7.605
7.589
7.586
7.410
7.405
7.313
7.295
7.276
7.267
6.997
6.974
6.913
6.893
6.701
6.695
6.643
6.640
6.620
6.598
6.573
6.550
4.913
4.890
3.720
3.095
0.000
Parameter Value
1 Title zyx-4-231-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.3
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-21T21:04:56
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
OMe
Br
2l
1.06
1.03
1.02
2.08
2.08
1.01
1.03
2.99
1.04
1.01
3.07
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)

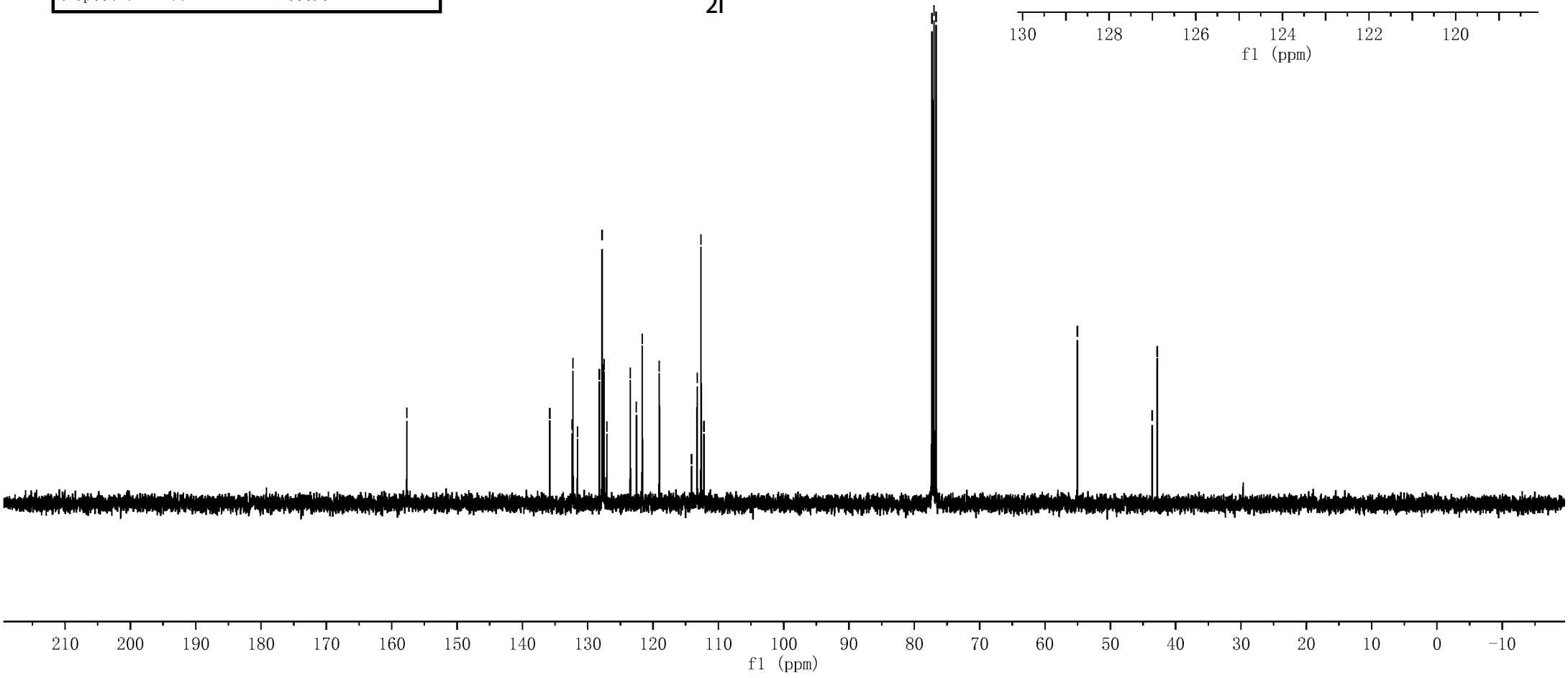


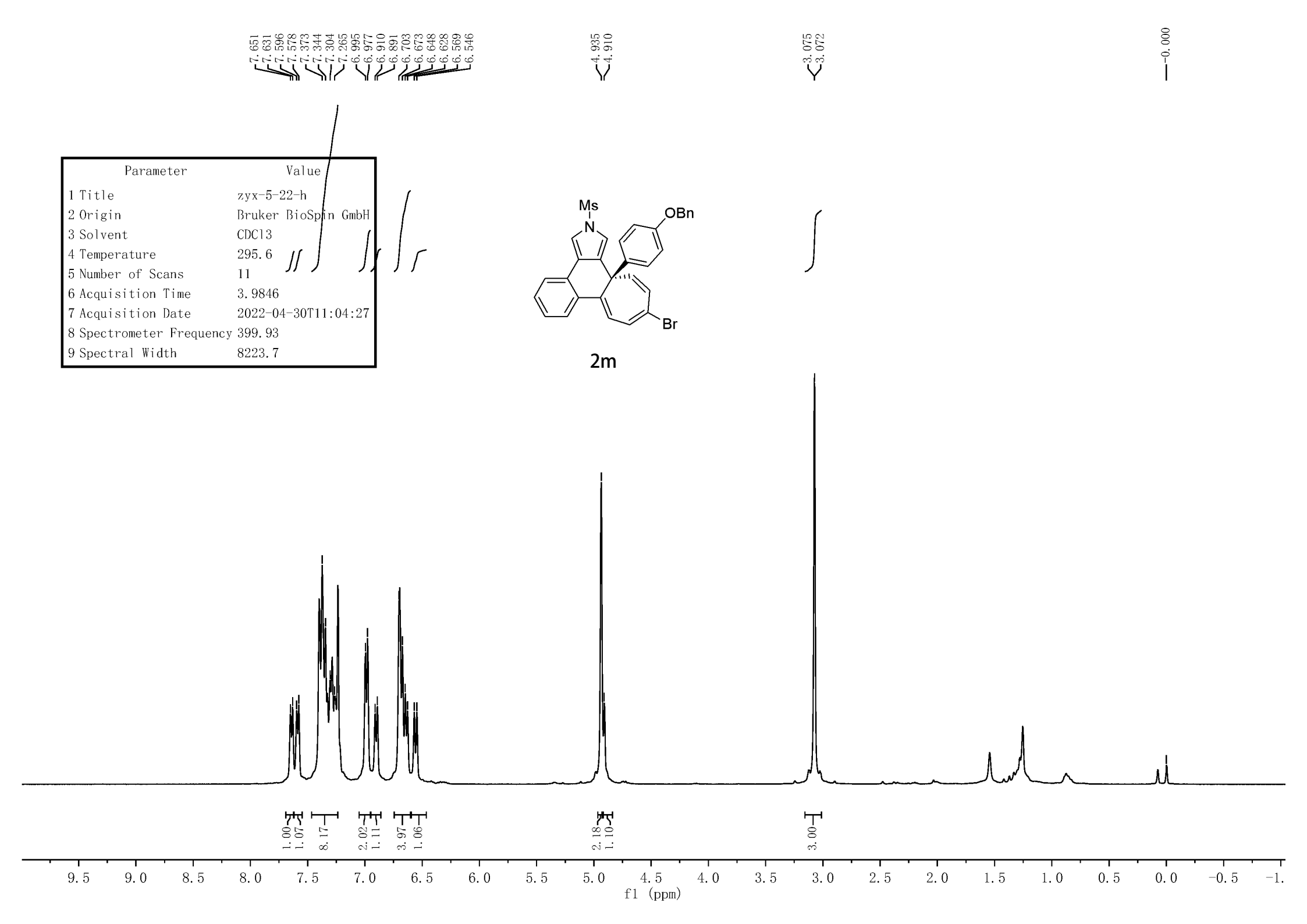
Parameter	Value
1 Title	zyx-4-231-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	86
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-21T21:07:39
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



2l

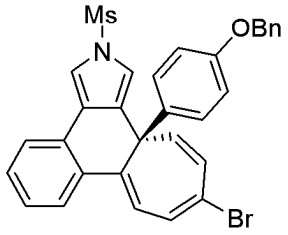




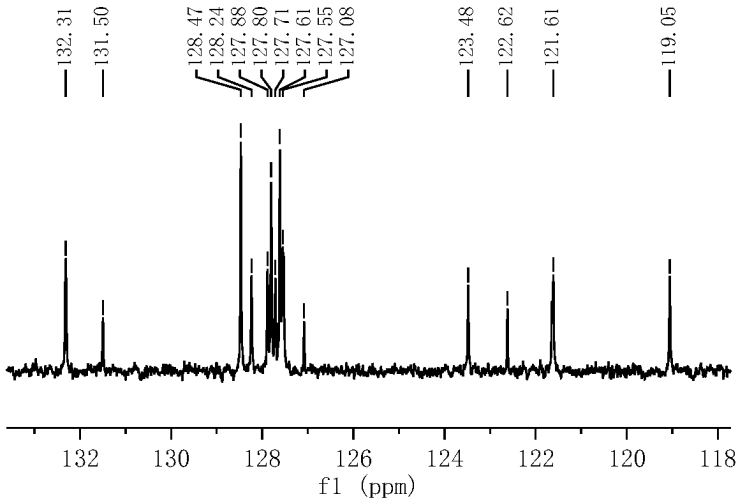

7.651
7.631
7.596
7.578
7.373
7.344
7.304
7.265
6.995
6.977
6.910
6.891
6.703
6.673
6.648
6.628
6.569
6.546
4.935
4.910
3.075
3.072
0.000
Parameter Value
1 Title zyx-5-22-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.6
5 Number of Scans 11
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-30T11:04:27
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
OBn
Br
2m
1.00
1.07
8.17
2.02
1.11
3.97
1.06
2.18
1.10
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 -1.
f1 (ppm)

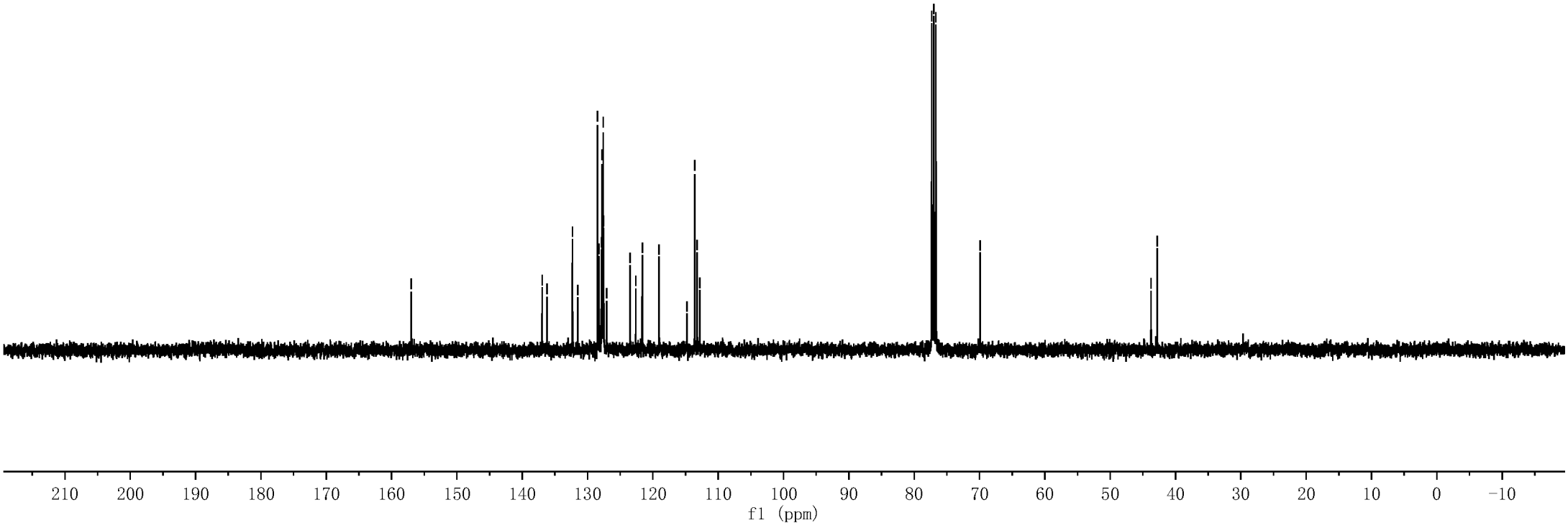
157.00
136.95
136.19
132.31
131.50
128.47
128.24
127.88
127.80
127.71
127.61
127.55
127.08
123.48
122.62
121.61
119.05
114.78
113.59
113.23
112.82
77.32
77.00
76.68
69.91
43.74
42.79

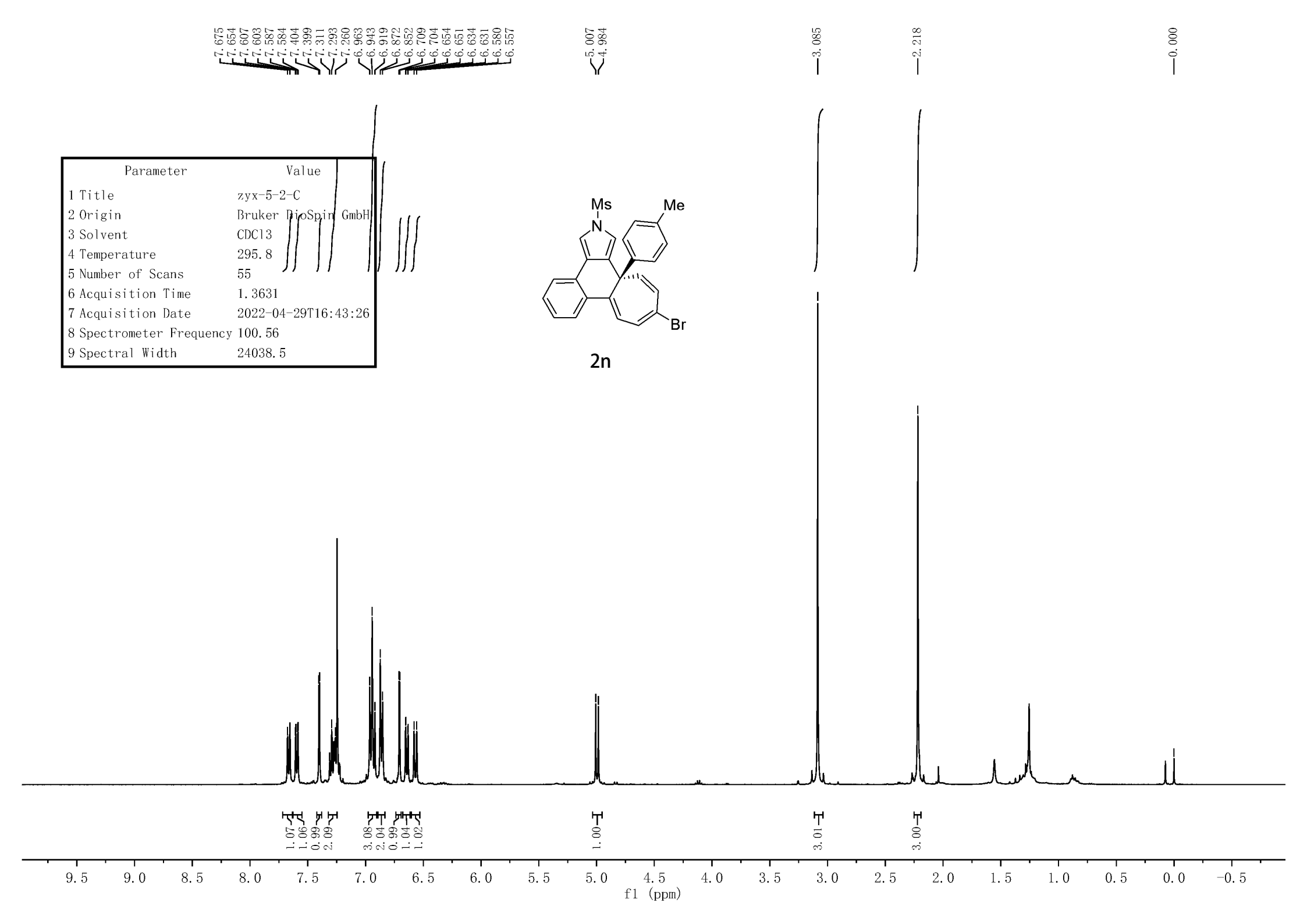
Parameter	Value
1 Title	zyx-5-22-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	73
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-30T11:08:06
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



2m

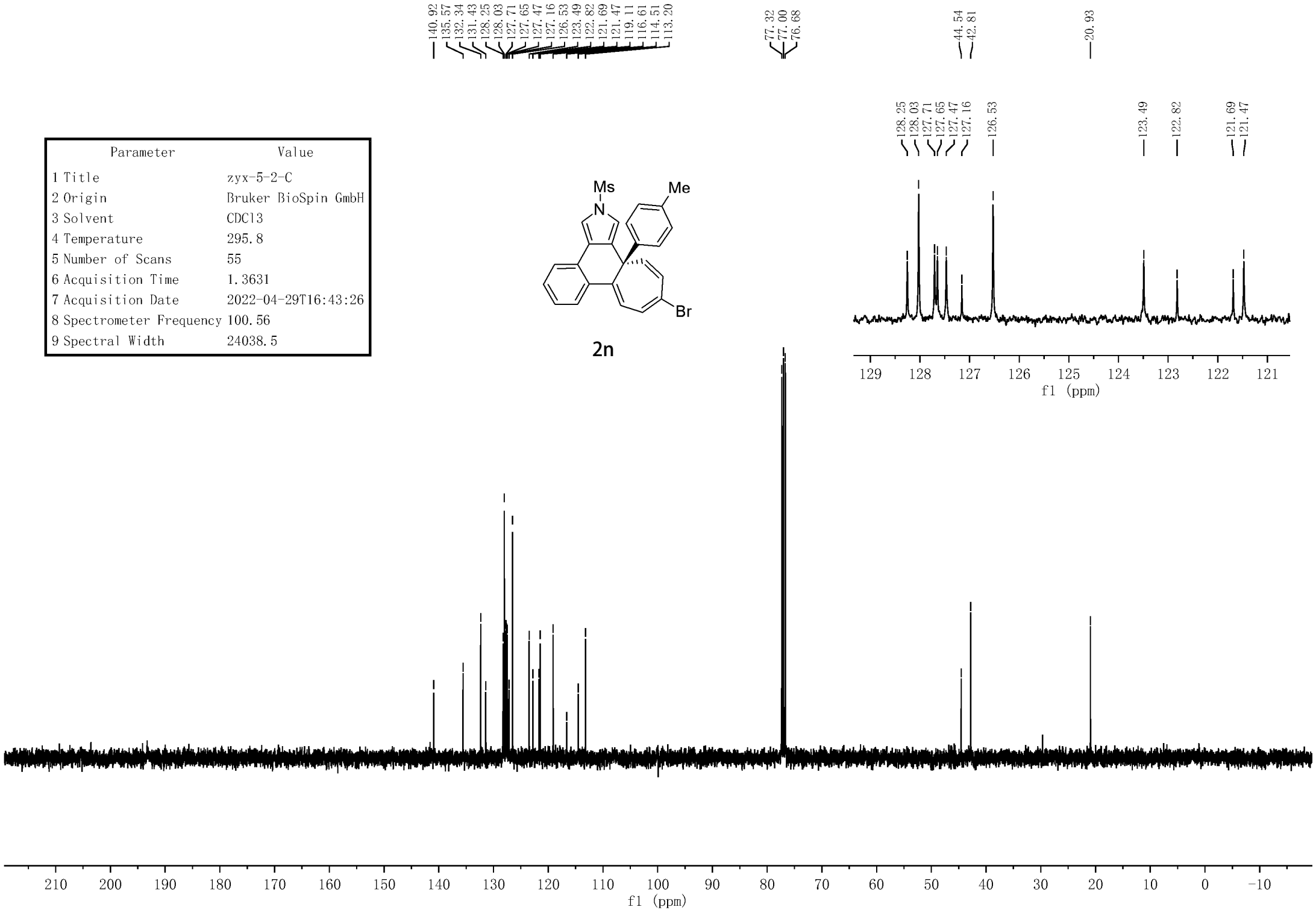


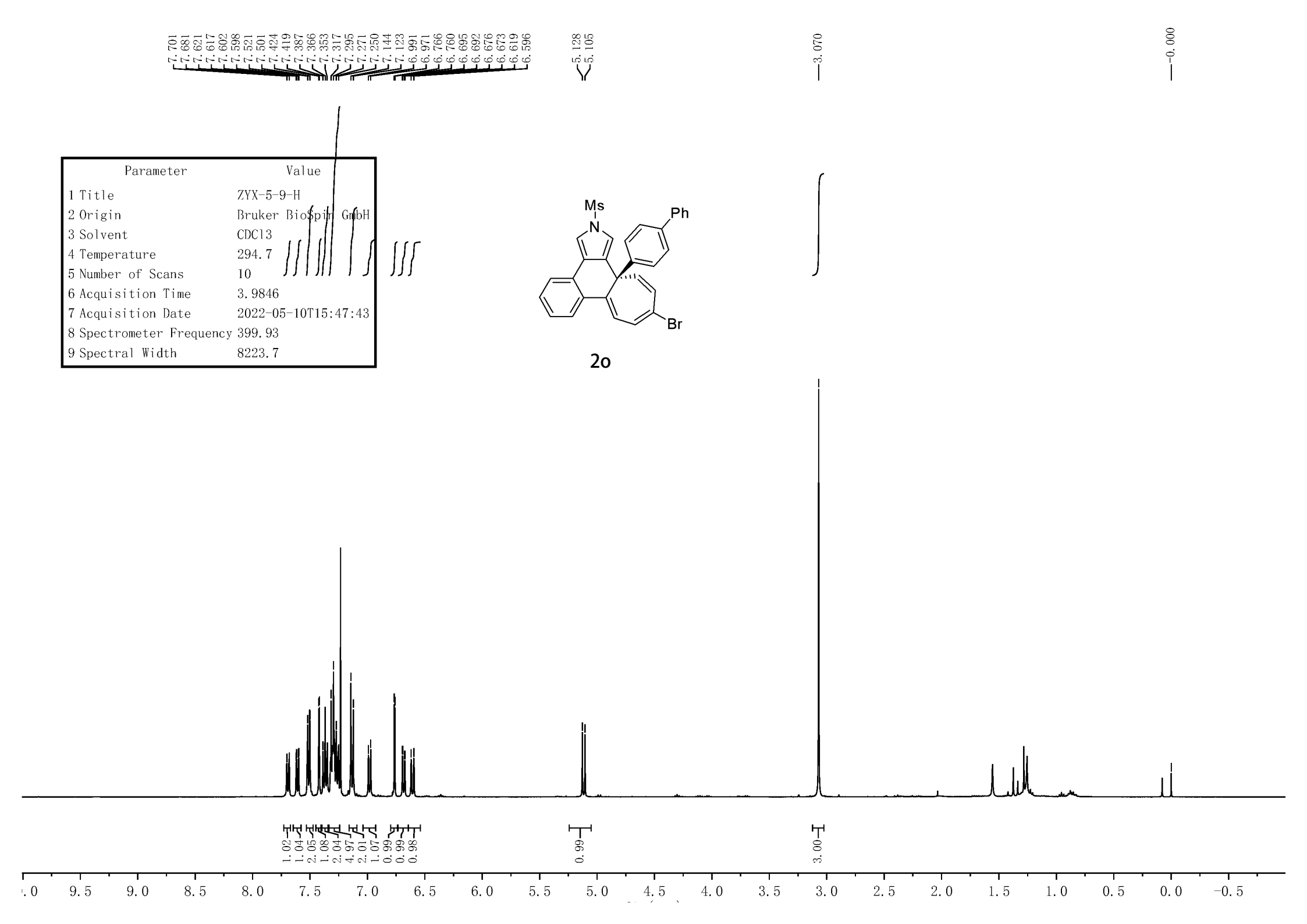



7.675
7.654
7.607
7.603
7.587
7.584
7.404
7.399
7.311
7.293
7.260
6.963
6.943
6.919
6.872
6.852
6.709
6.704
6.654
6.651
6.634
6.631
6.580
6.557
5.007
4.984
3.085
2.218
0.000
Parameter Value
1 Title zyx-5-2-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.8
5 Number of Scans 55
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-29T16:43:26
8 Spectrometer Frequency 100.56
9 Spectral Width 24038.5
Ms
N
Me
Br
2n
1.07
1.06
0.99
2.09
3.08
2.04
0.99
1.04
1.02
1.00
3.01
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)

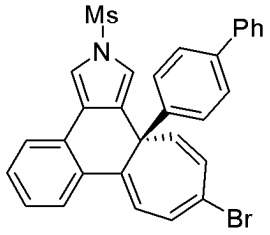
Parameter	Value
1 Title	zyx-5-2-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	55
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-29T16:43:26
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

2n

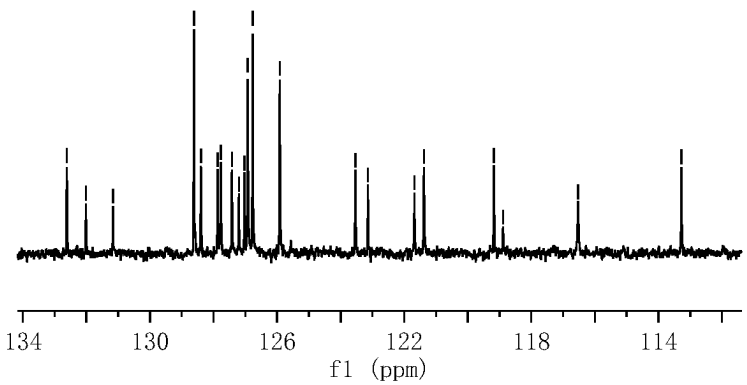


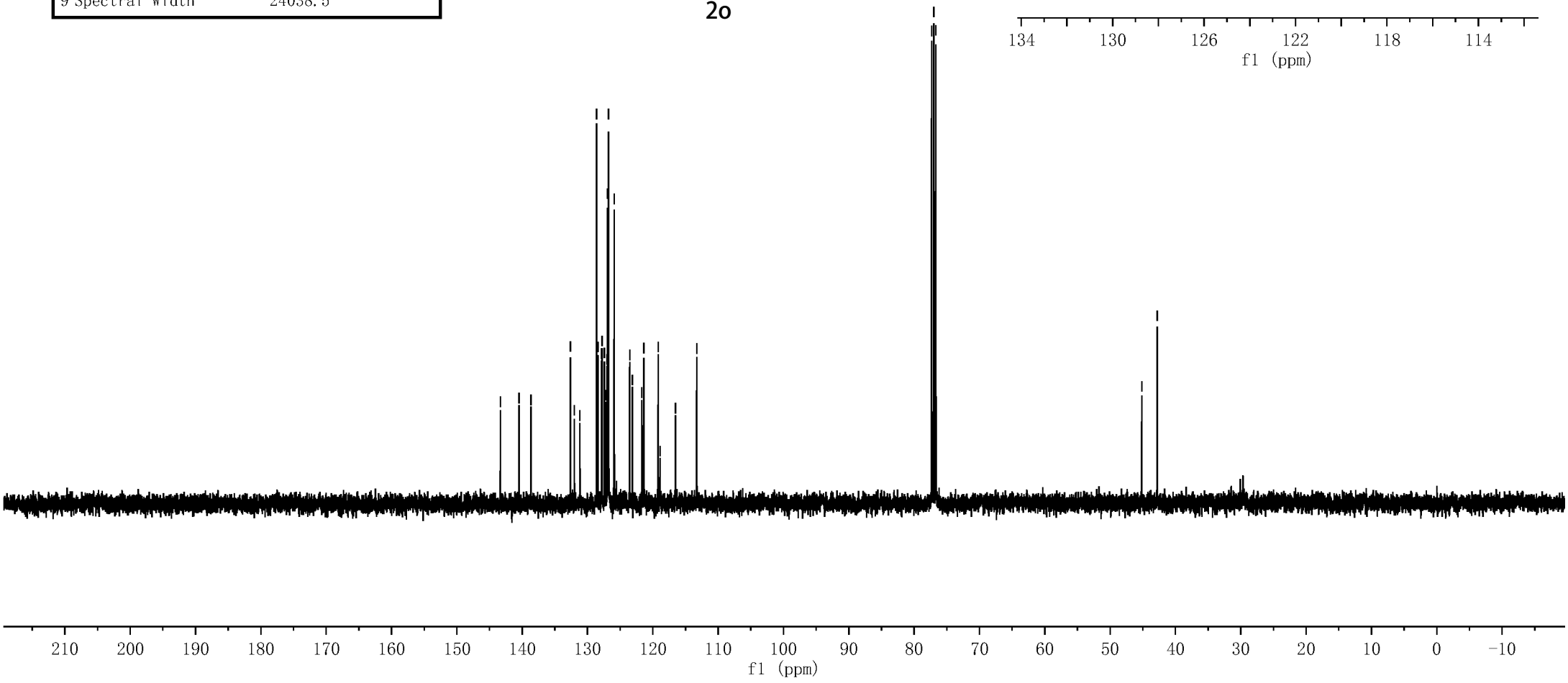

7.701
7.681
7.621
7.617
7.602
7.598
7.521
7.501
7.424
7.419
7.387
7.366
7.353
7.317
7.295
7.271
7.250
7.144
7.123
6.991
6.971
6.766
6.760
6.695
6.692
6.676
6.673
6.619
6.596
5.128
5.105
3.070
0.000
Parameter Value
1 Title ZYX-5-9-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 294.7
5 Number of Scans 10
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-10T15:47:43
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
Ph
Br
2o
1.02
1.04
2.05
1.08
2.04
4.97
2.01
1.07
0.99
0.99
0.98
0.99
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

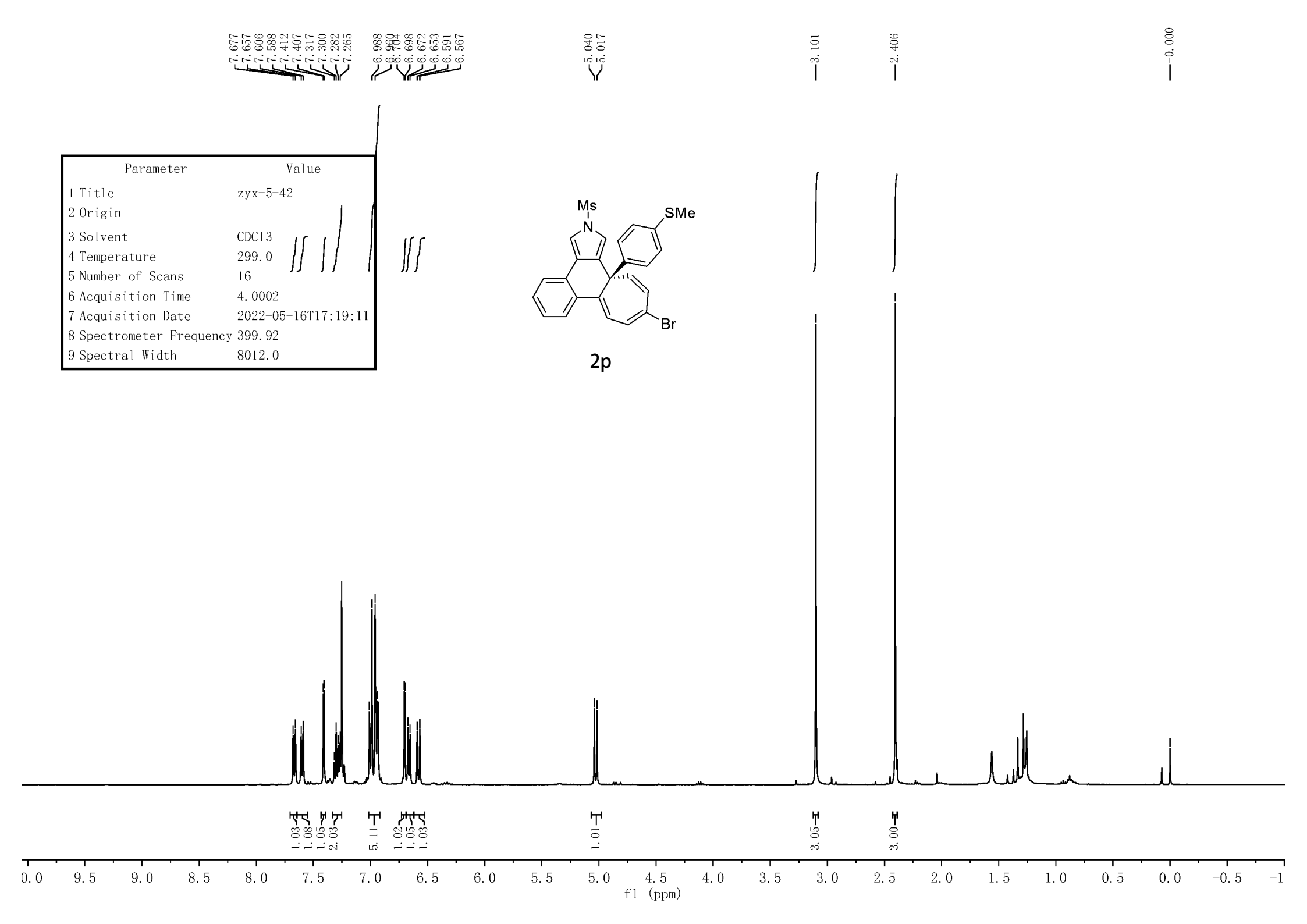
Parameter	Value
1 Title	ZYX-5-9-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	294.9
5 Number of Scans	53
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-10T15:49:00
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



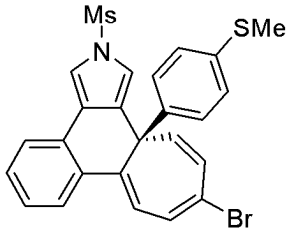
2o



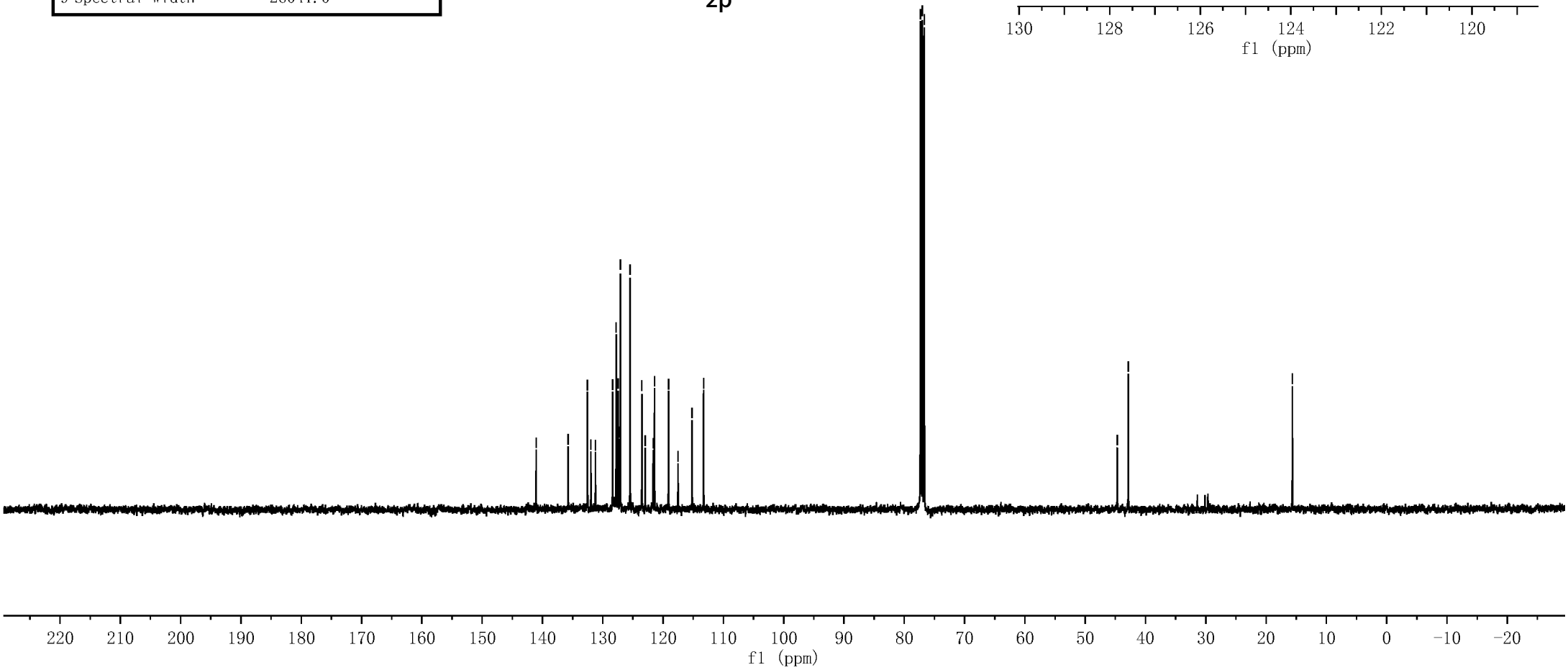


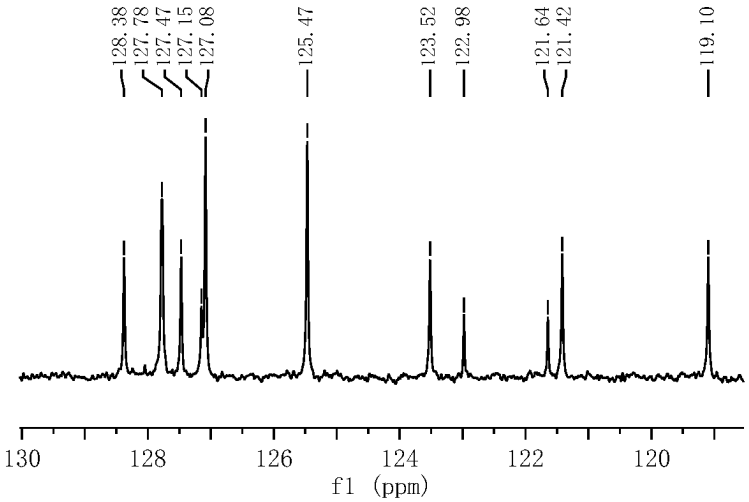

7.677
7.657
7.606
7.588
7.412
7.407
7.317
7.300
7.282
7.265
6.988
6.960
6.704
6.698
6.672
6.653
6.591
6.567
5.040
5.017
3.101
2.406
0.000
Parameter Value
1 Title zyx-5-42
2 Origin
3 Solvent CDCl3
4 Temperature 299.0
5 Number of Scans 16
6 Acquisition Time 4.0002
7 Acquisition Date 2022-05-16T17:19:11
8 Spectrometer Frequency 399.92
9 Spectral Width 8012.0
Ms
N
SMe
Br
2p
1.03
1.08
1.05
2.03
5.11
1.02
1.05
1.03
1.01
3.05
3.00
0.0 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 -1
f1 (ppm)

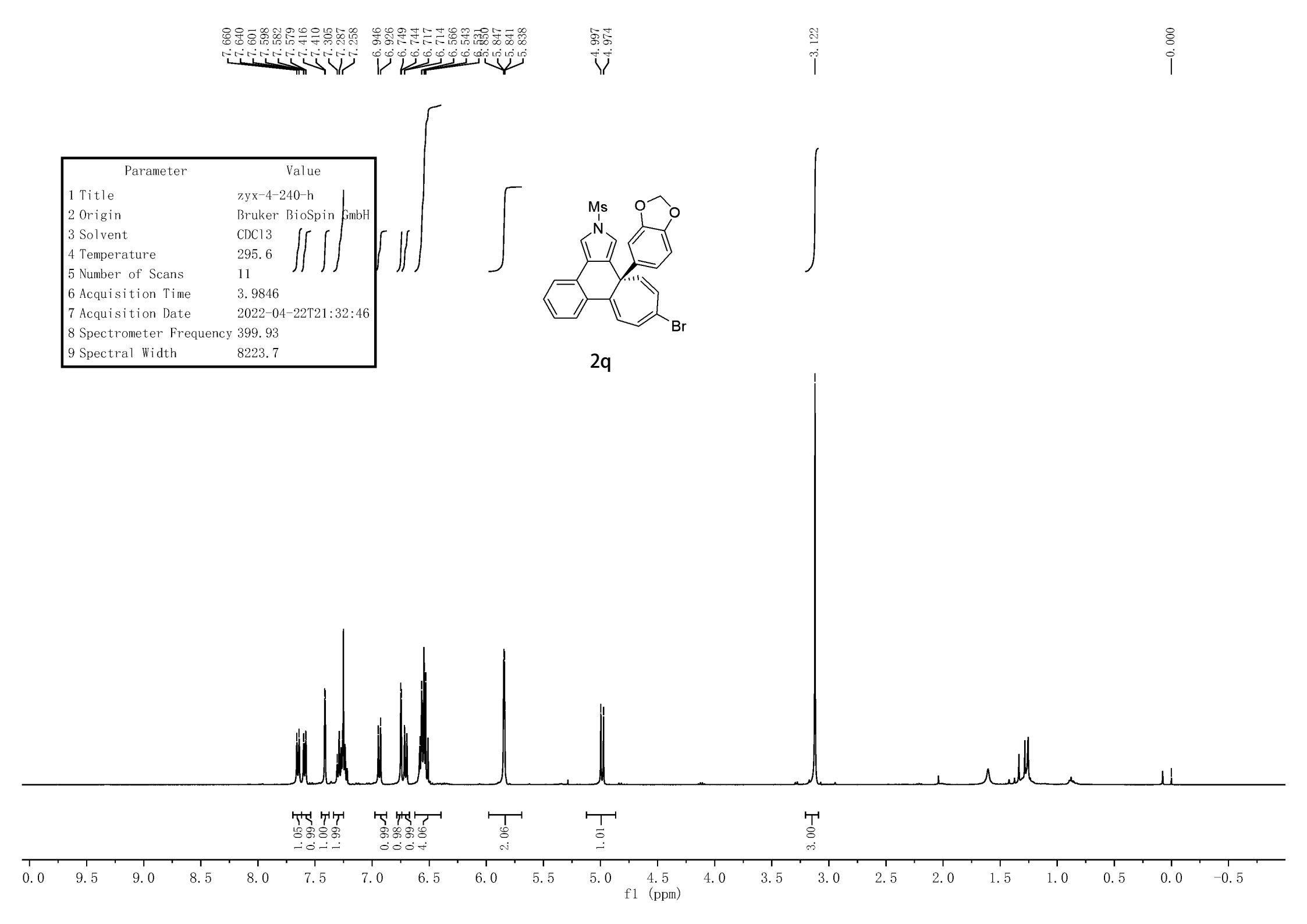
Parameter	Value
1 Title	zyx-5-42
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.8
5 Number of Scans	500
6 Acquisition Time	1.0000
7 Acquisition Date	2022-05-16T17:38:00
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



2p

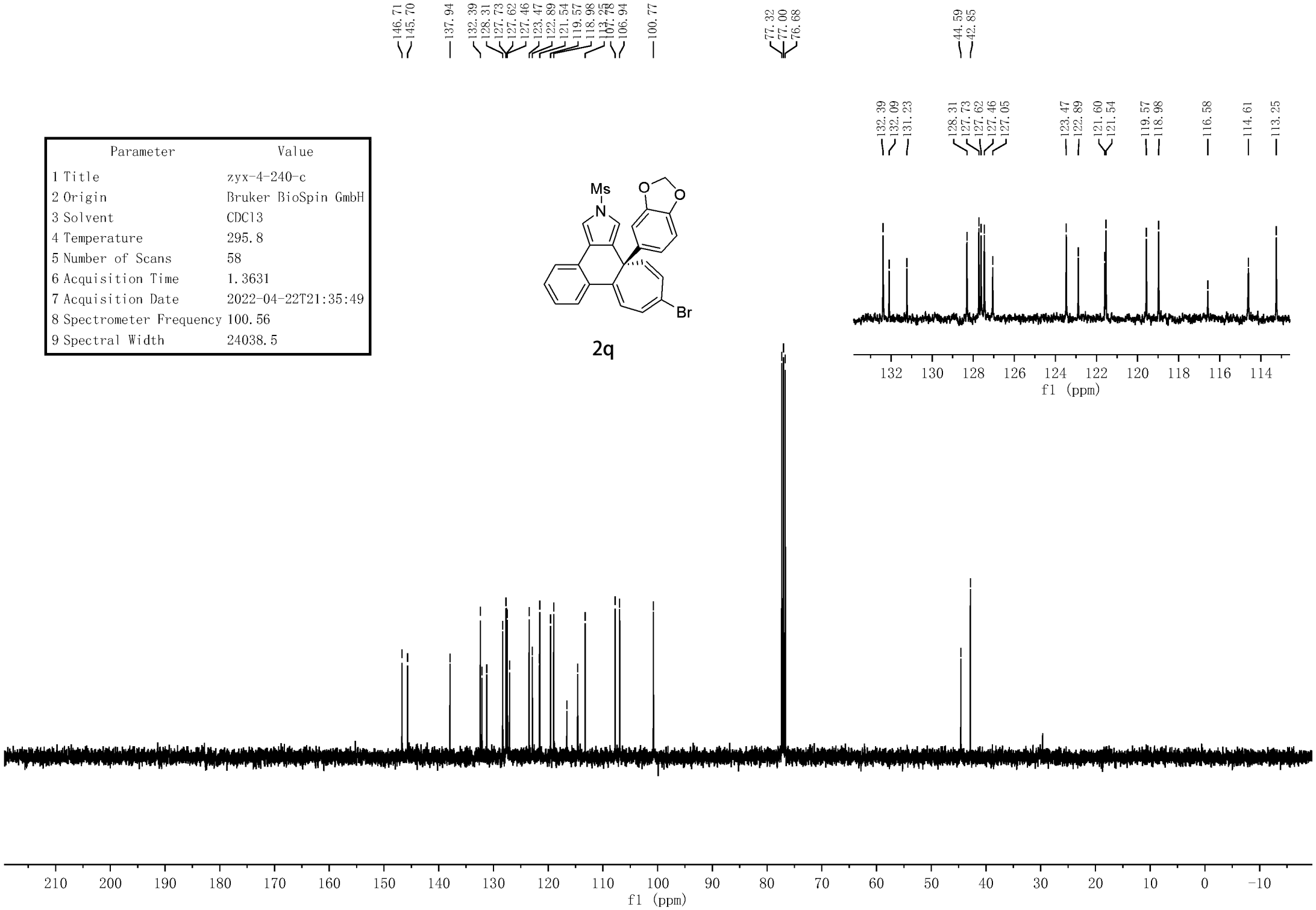


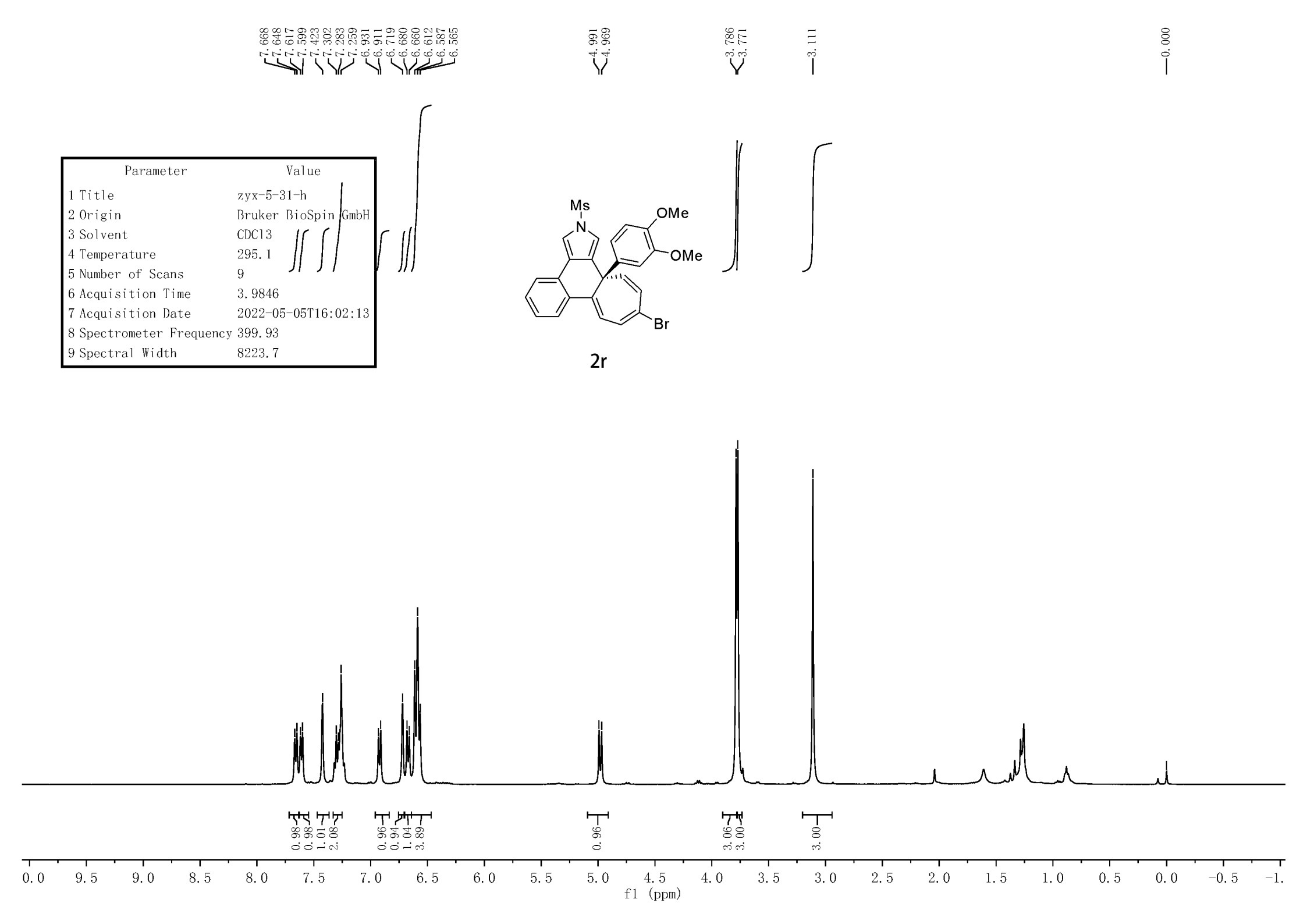



7.660
7.640
7.601
7.598
7.582
7.579
7.416
7.410
7.305
7.287
7.258
6.946
6.926
6.749
6.744
6.717
6.714
6.566
6.543
6.531
6.530
5.847
5.841
5.838
4.997
4.974
3.122
0.000
Parameter Value
1 Title zyx-4-240-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.6
5 Number of Scans 11
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-22T21:32:46
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
O
O
Br
2q
1.05
0.99
1.00
1.99
0.99
0.98
0.99
4.06
2.06
1.01
3.00
0.0
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)

Parameter	Value
1 Title	zyx-4-240-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	58
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-22T21:35:49
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

2q




7.668
7.648
7.617
7.599
7.423
7.302
7.283
7.259
6.931
6.911
6.719
6.680
6.660
6.612
6.587
6.565
4.991
4.969
3.786
3.771
3.111
0.000
Parameter Value
1 Title zyx-5-31-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.1
5 Number of Scans 9
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-05T16:02:13
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
OMe
OMe
Br
2r
0.98
0.98
1.01
2.08
0.96
0.94
1.04
3.89
0.96
3.06
3.00
3.00
0.0
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
-1.
f1 (ppm)

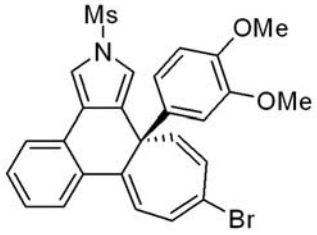
147.55
147.08
136.40
132.39
132.23
131.31
128.26
127.69
127.55
127.11
123.49
122.83
121.57
121.40
119.44
118.93
116.25
114.09
113.24
110.36
110.09

77.32
77.00
76.68

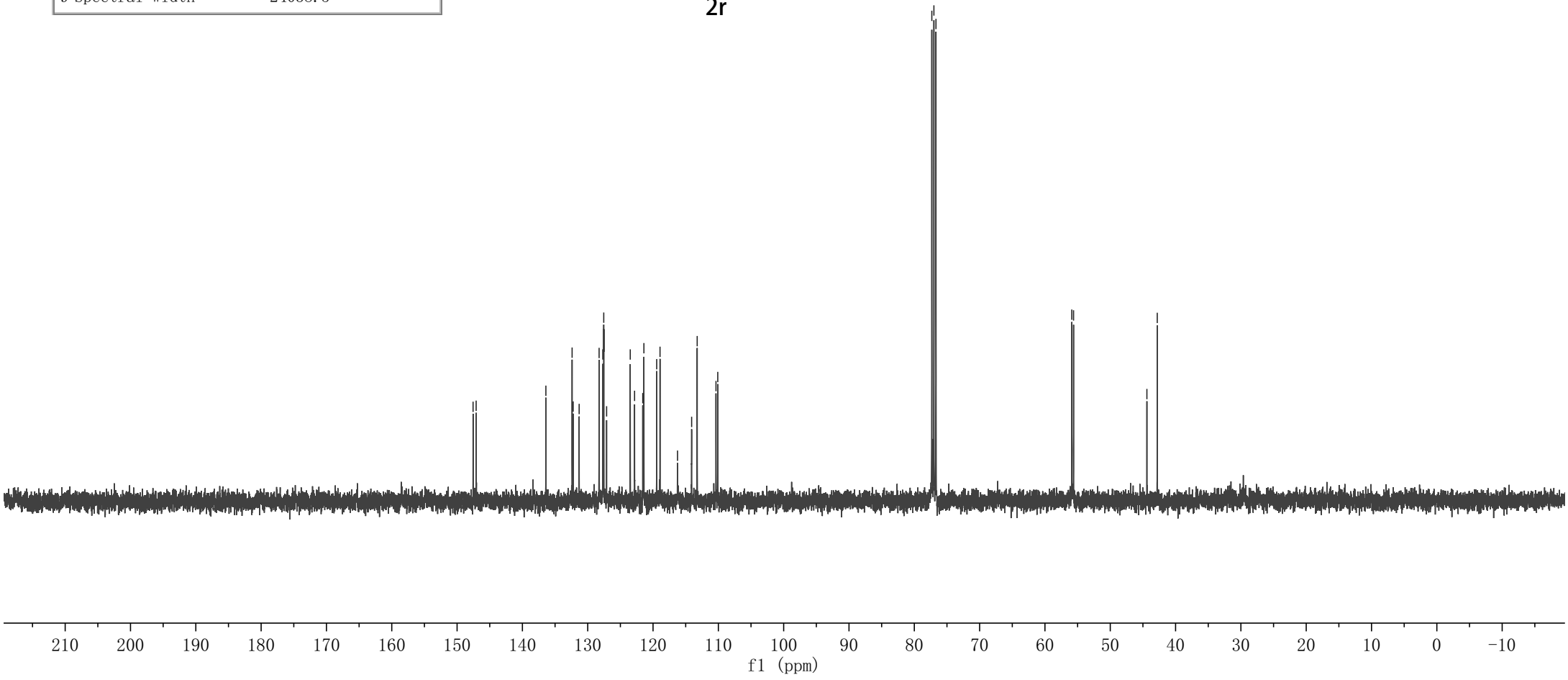
55.89
55.62

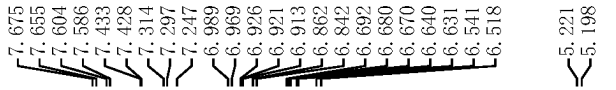
44.39
42.80

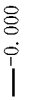
Parameter	Value
1 Title	zyx-5-31--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	61
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-05T16:05:28
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



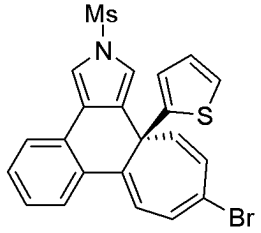
2r



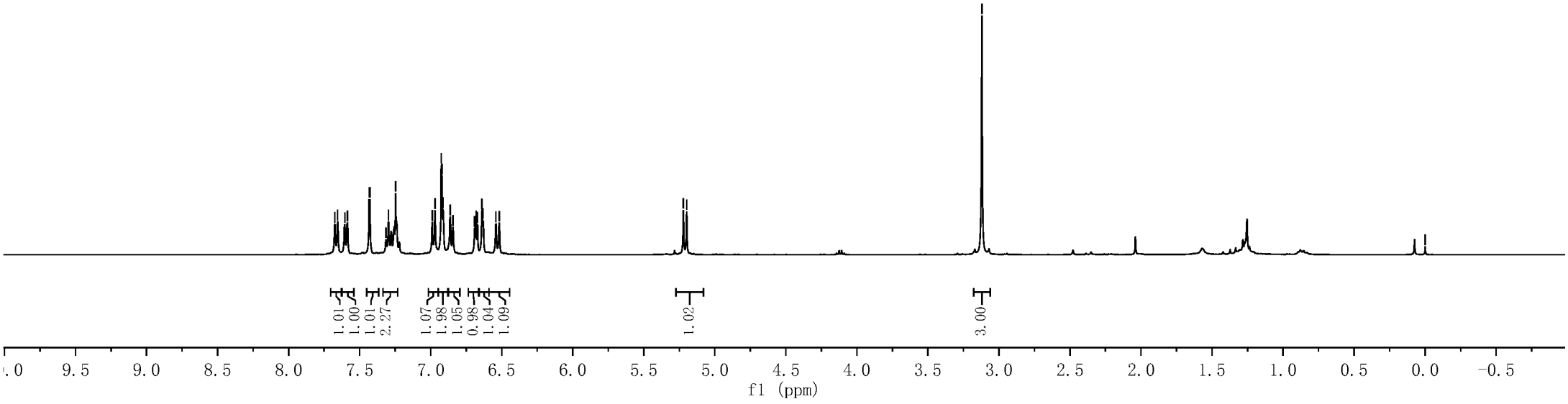


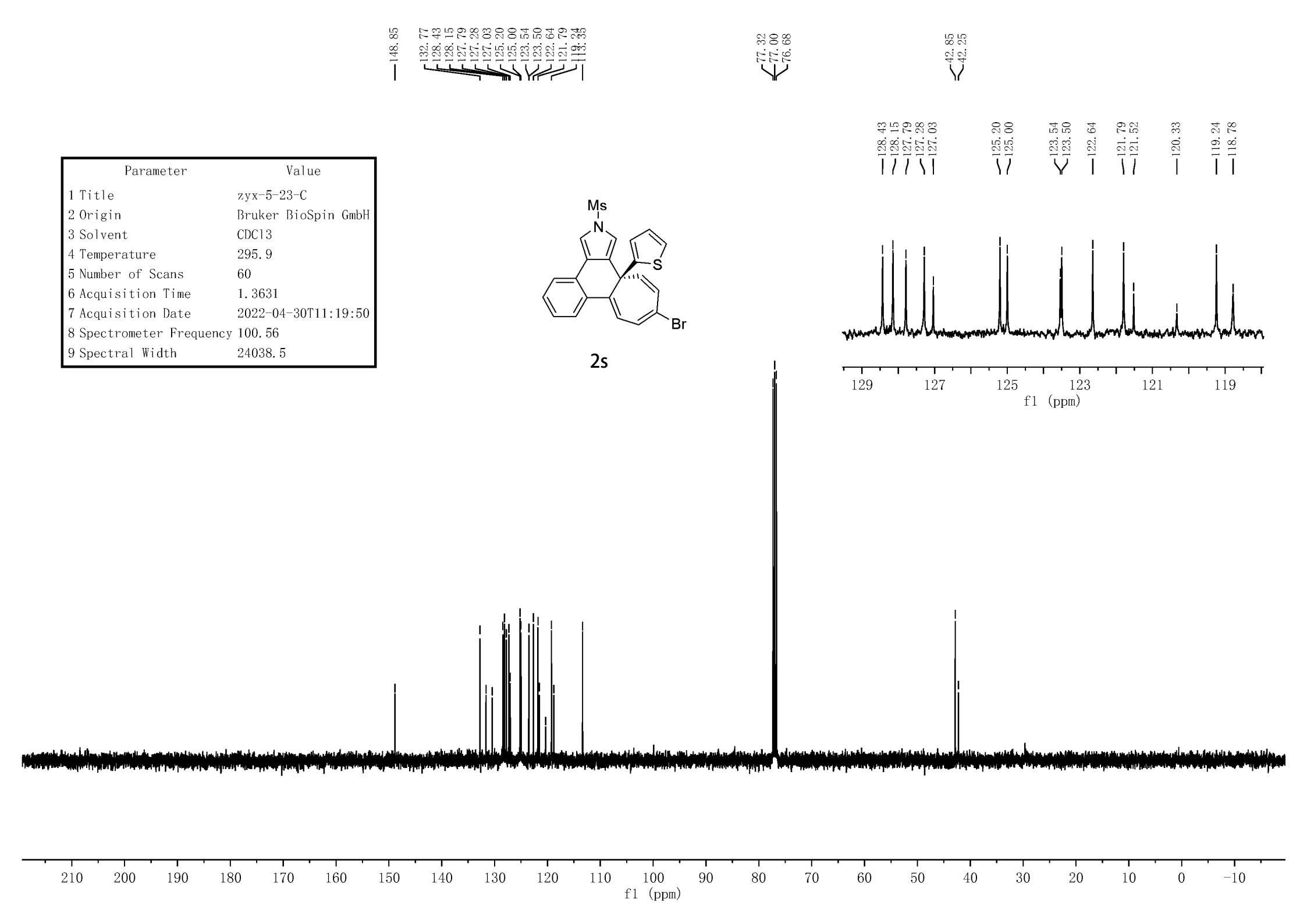


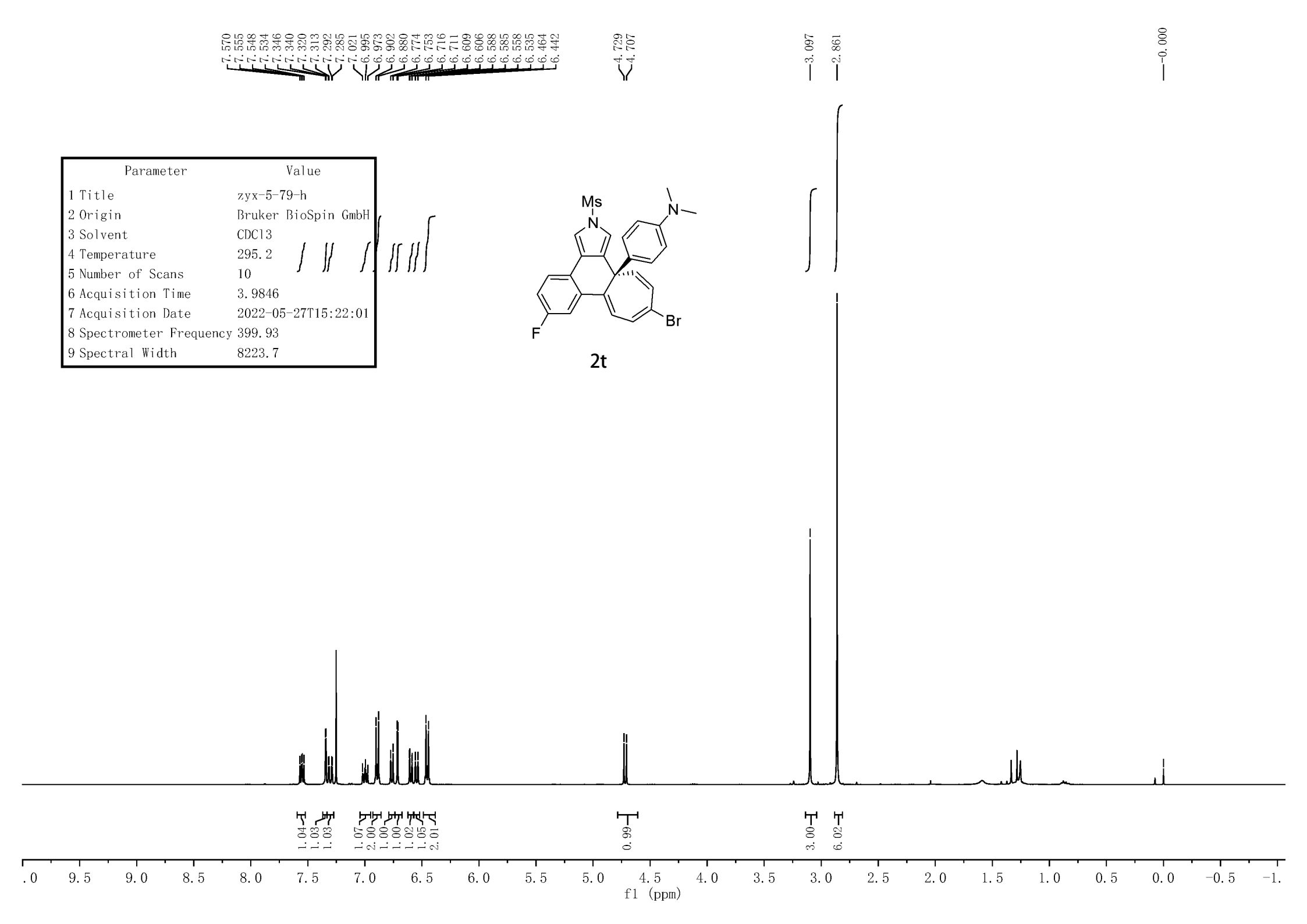
Parameter	Value
1 Title	zyx-5-23-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	13
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-30T11:17:46
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7



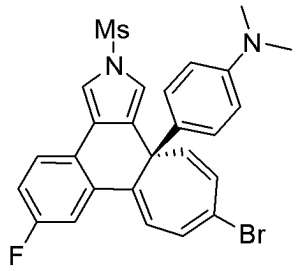
2s



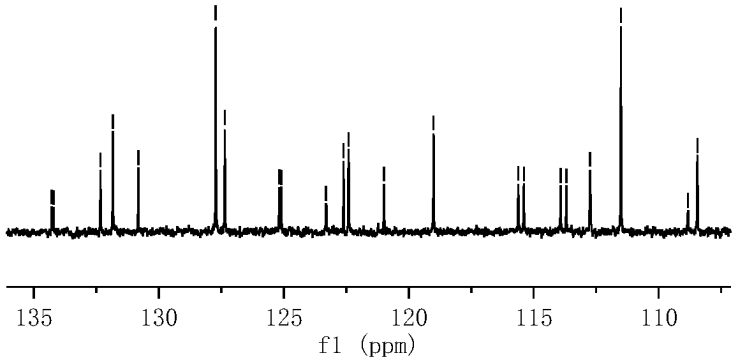

148.85
132.77
128.43
128.15
127.79
127.28
127.03
125.20
125.00
123.54
123.50
122.64
121.79
119.24
118.35
77.32
77.00
76.68
42.85
42.25
Parameter Value
1 Title zyx-5-23-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.9
5 Number of Scans 60
6 Acquisition Time 1.3631
7 Acquisition Date 2022-04-30T11:19:50
8 Spectrometer Frequency 100.56
9 Spectral Width 24038.5
Ms
N
S
Br
2s
128.43
128.15
127.79
127.28
127.03
125.20
125.00
123.54
123.50
122.64
121.79
121.52
120.33
119.24
118.78
129
127
125
123
121
119
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)

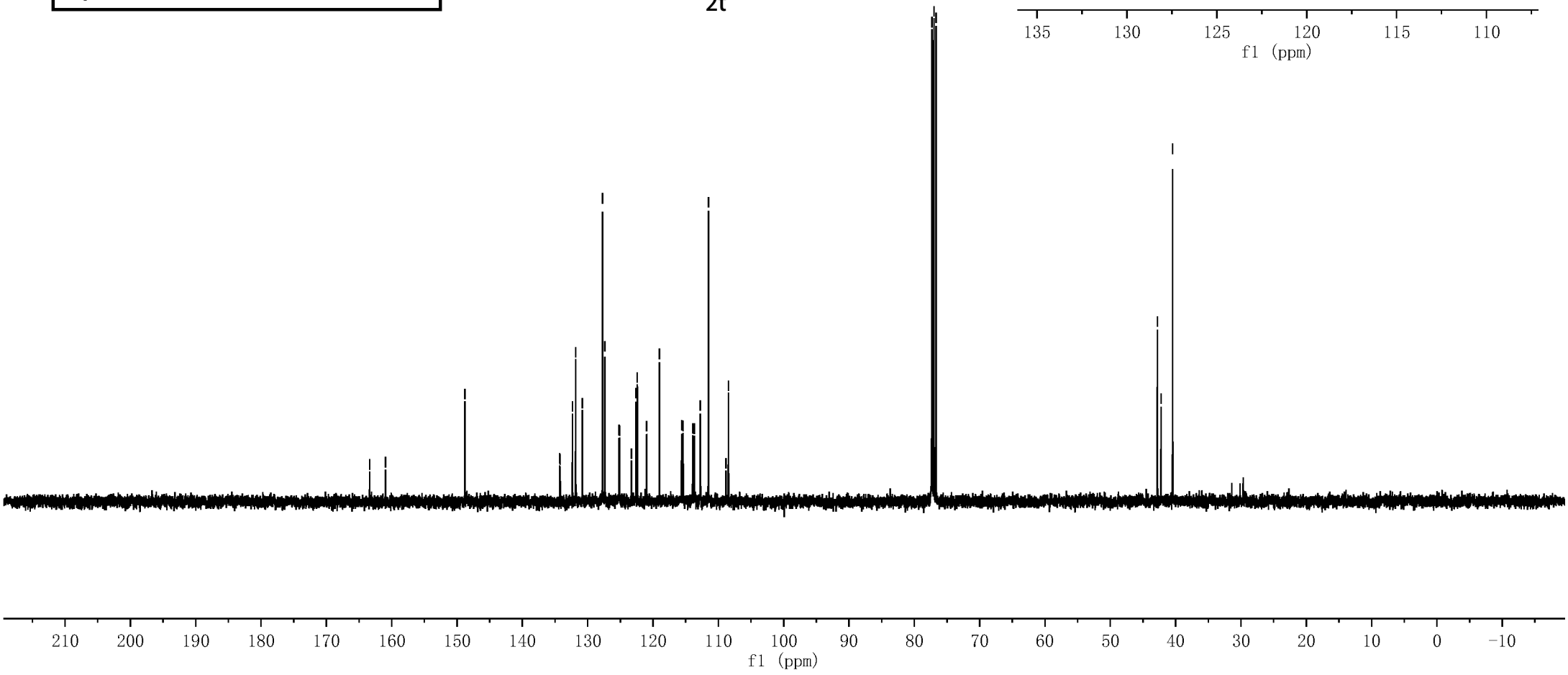

7.570
7.555
7.548
7.534
7.346
7.340
7.320
7.313
7.292
7.285
7.021
6.995
6.973
6.902
6.880
6.774
6.753
6.716
6.711
6.609
6.606
6.588
6.585
6.558
6.535
6.464
6.442
4.729
4.707
3.097
2.861
-0.000
Parameter Value
1 Title zyx-5-79-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.2
5 Number of Scans 10
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-27T15:22:01
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
N
F
Br
2t
1.04
1.03
1.03
1.07
2.00
1.00
1.00
1.02
1.05
2.01
0.99
3.00
6.02
f1 (ppm)

Parameter	Value
1 Title	zyx-5-79-CC
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	147
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-27T15:26:08
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

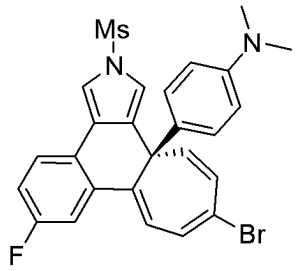


2t

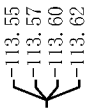


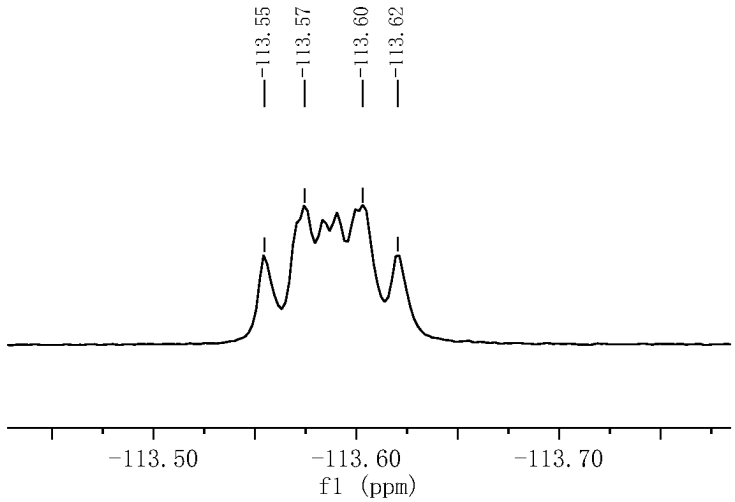


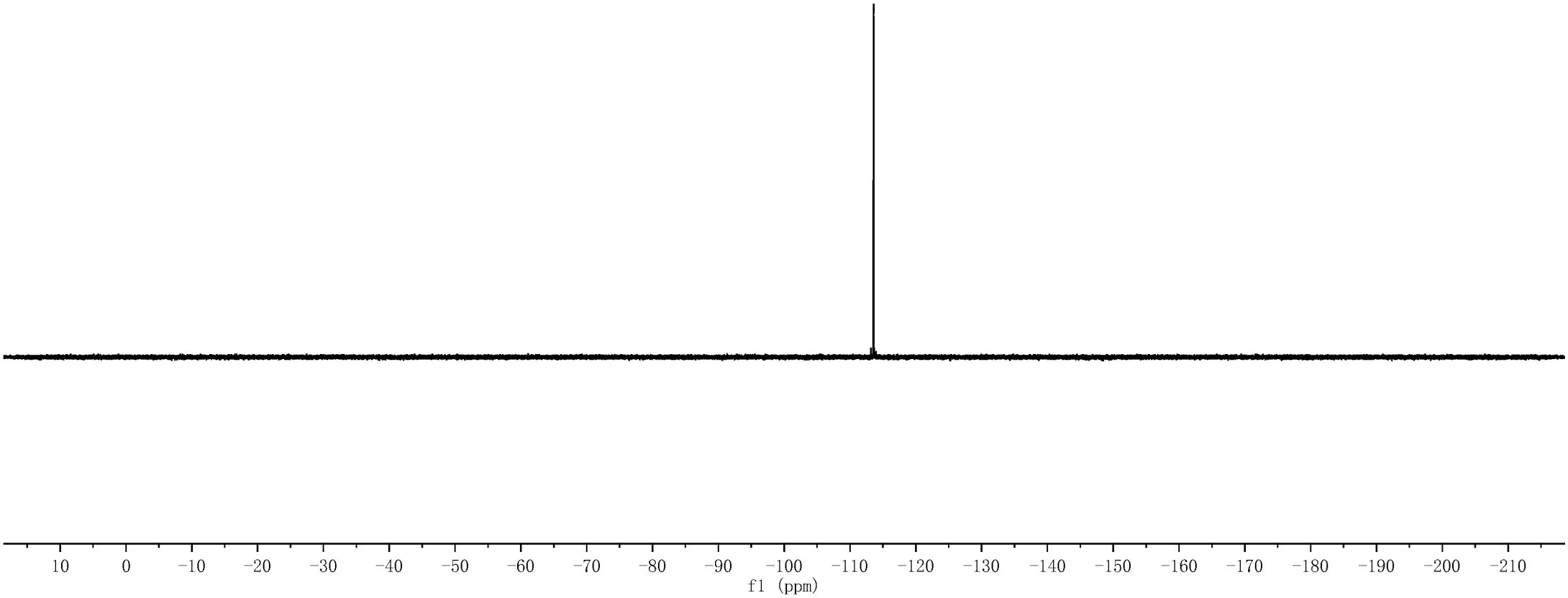
Parameter	Value
1 Title	ZYX-5-79-F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-05-28T11:01:58
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7

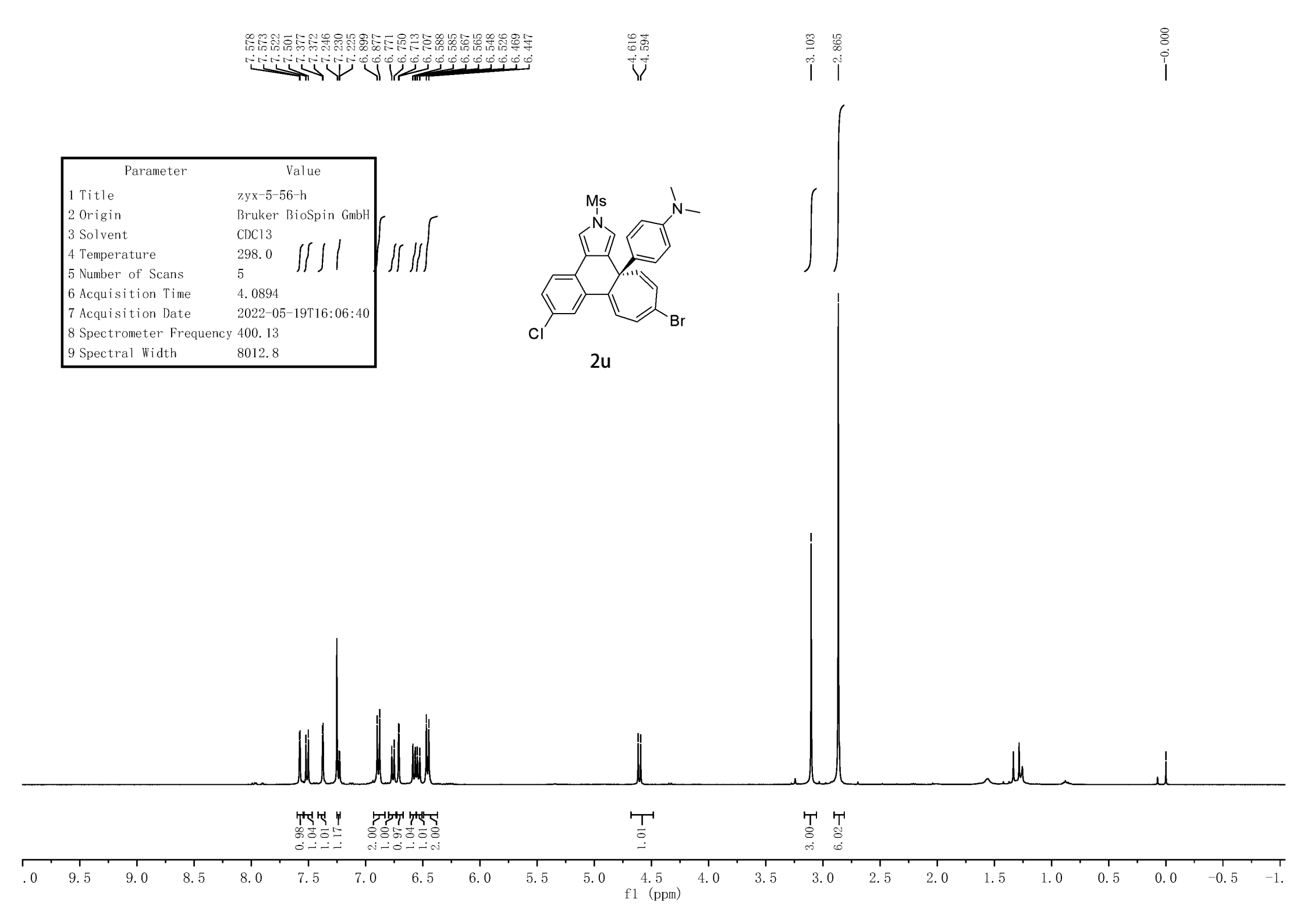


2t



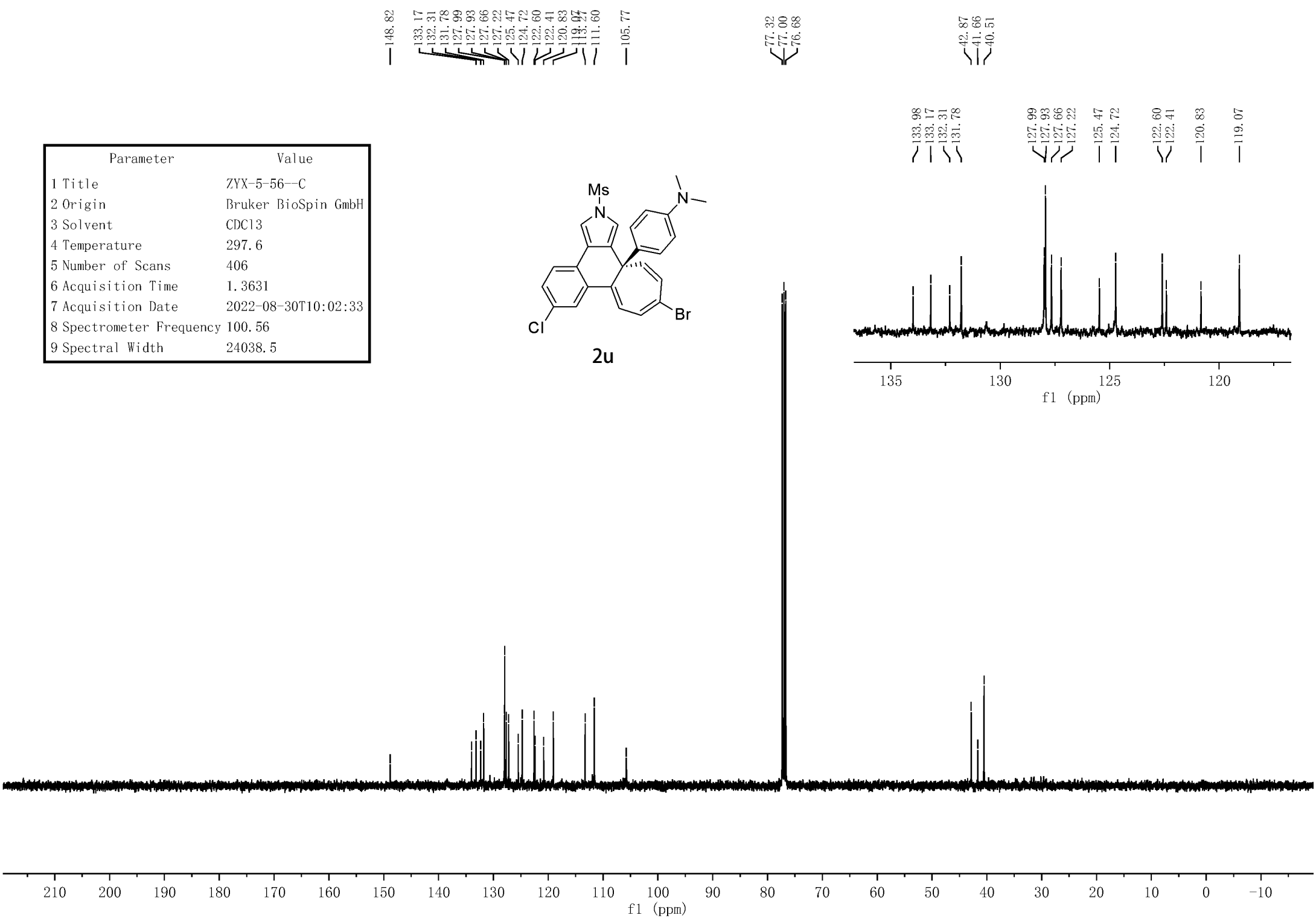


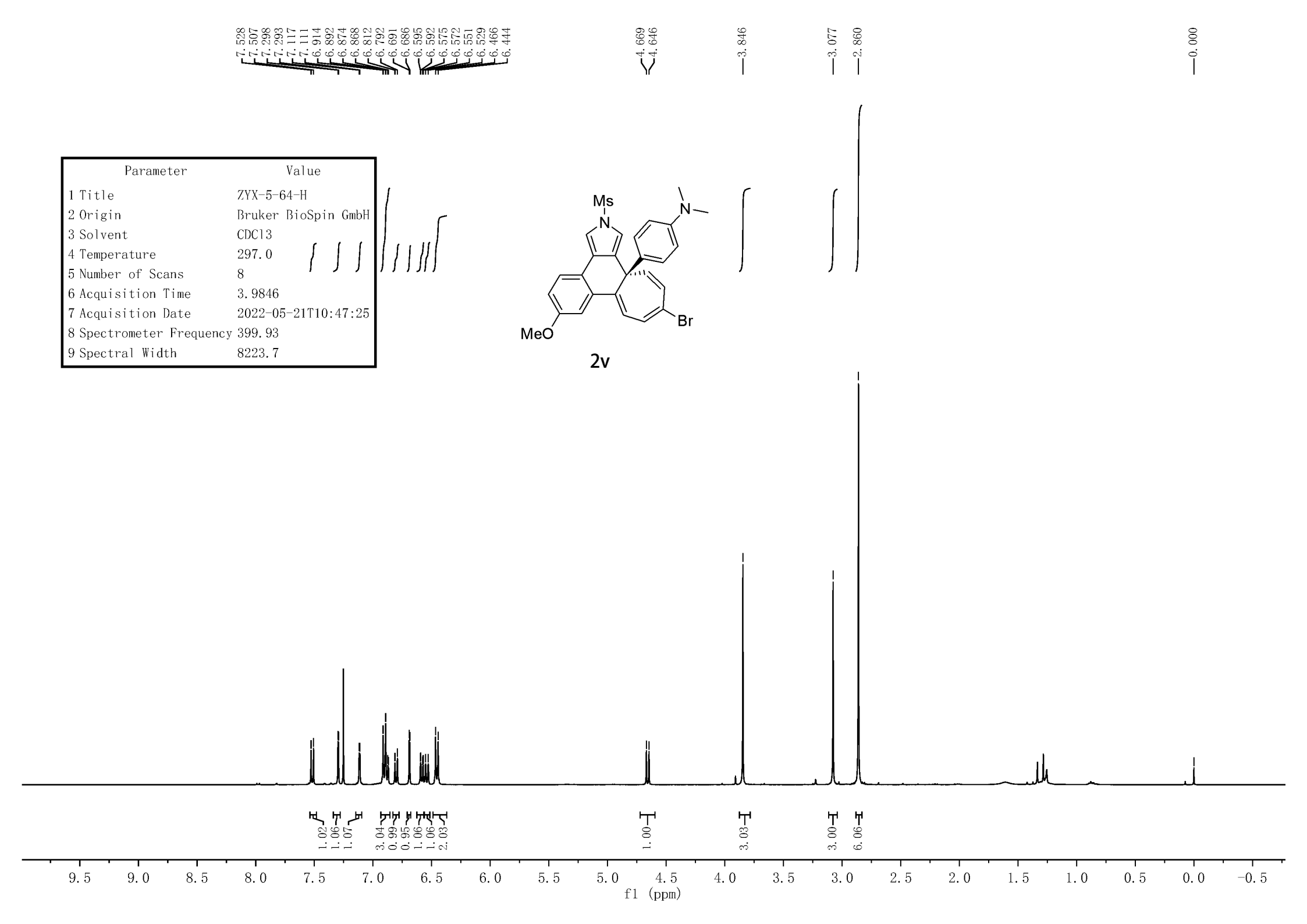



7.578
7.573
7.522
7.501
7.377
7.372
7.246
7.230
7.225
6.899
6.877
6.771
6.750
6.713
6.707
6.588
6.585
6.567
6.565
6.548
6.526
6.469
6.447
4.616
4.594
3.103
2.865
-0.000
Parameter Value
1 Title zyx-5-56-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 5
6 Acquisition Time 4.0894
7 Acquisition Date 2022-05-19T16:06:40
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
Cl
Br
2u
0.98
1.04
1.01
1.17
2.00
1.00
0.97
1.04
1.01
2.00
1.01
3.00
6.02
f1 (ppm)

Parameter	Value
1 Title	ZYX-5-56--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	406
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-30T10:02:33
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

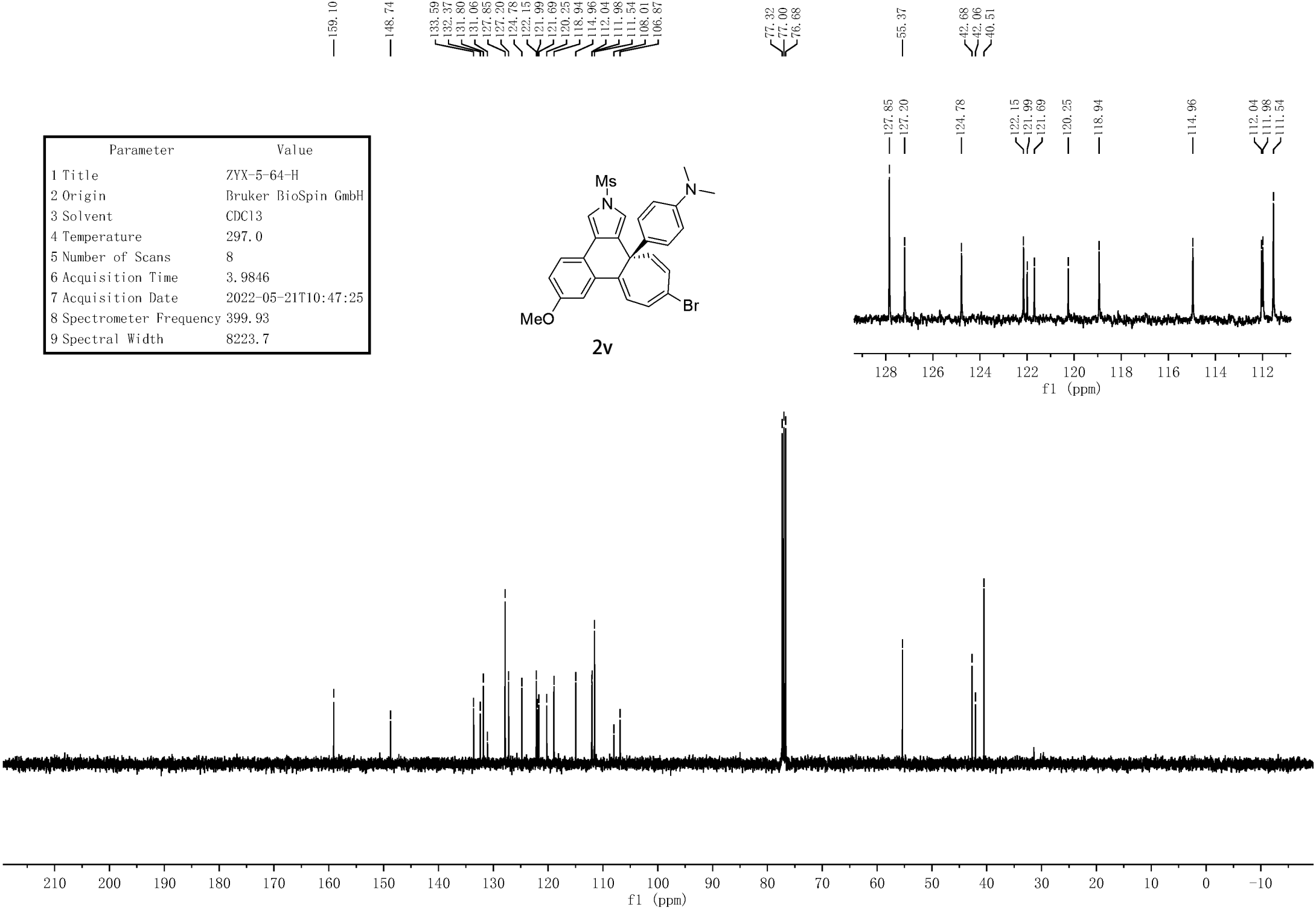
2u



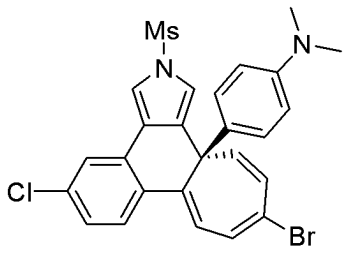

7.528
7.507
7.298
7.293
7.117
7.111
6.914
6.892
6.874
6.868
6.812
6.792
6.691
6.686
6.595
6.592
6.575
6.572
6.551
6.529
6.466
6.444
4.669
4.646
3.846
3.077
2.860
0.000
Parameter Value
1 Title ZYX-5-64-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.0
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-21T10:47:25
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
N
Br
MeO
2v
1.02
1.06
1.07
3.04
0.99
0.95
1.06
1.06
2.03
1.00
3.03
3.00
6.06
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)

Parameter	Value
1 Title	ZYX-5-64-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	8
6 Acquisition Time	3.9846
7 Acquisition Date	2022-05-21T10:47:25
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

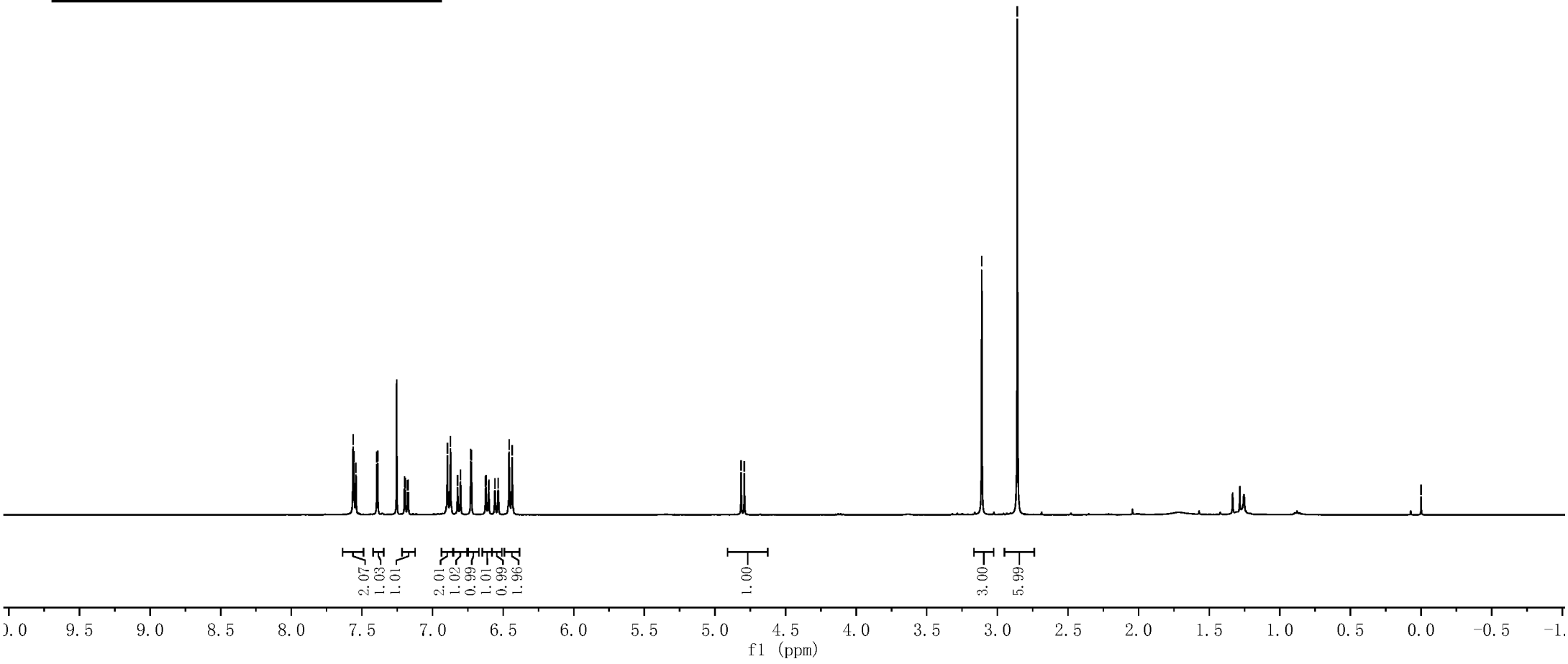
2v



Parameter	Value
1 Title	zyx-5-81--h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.1
5 Number of Scans	11
6 Acquisition Time	3.9846
7 Acquisition Date	2022-05-27T15:17:21
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7



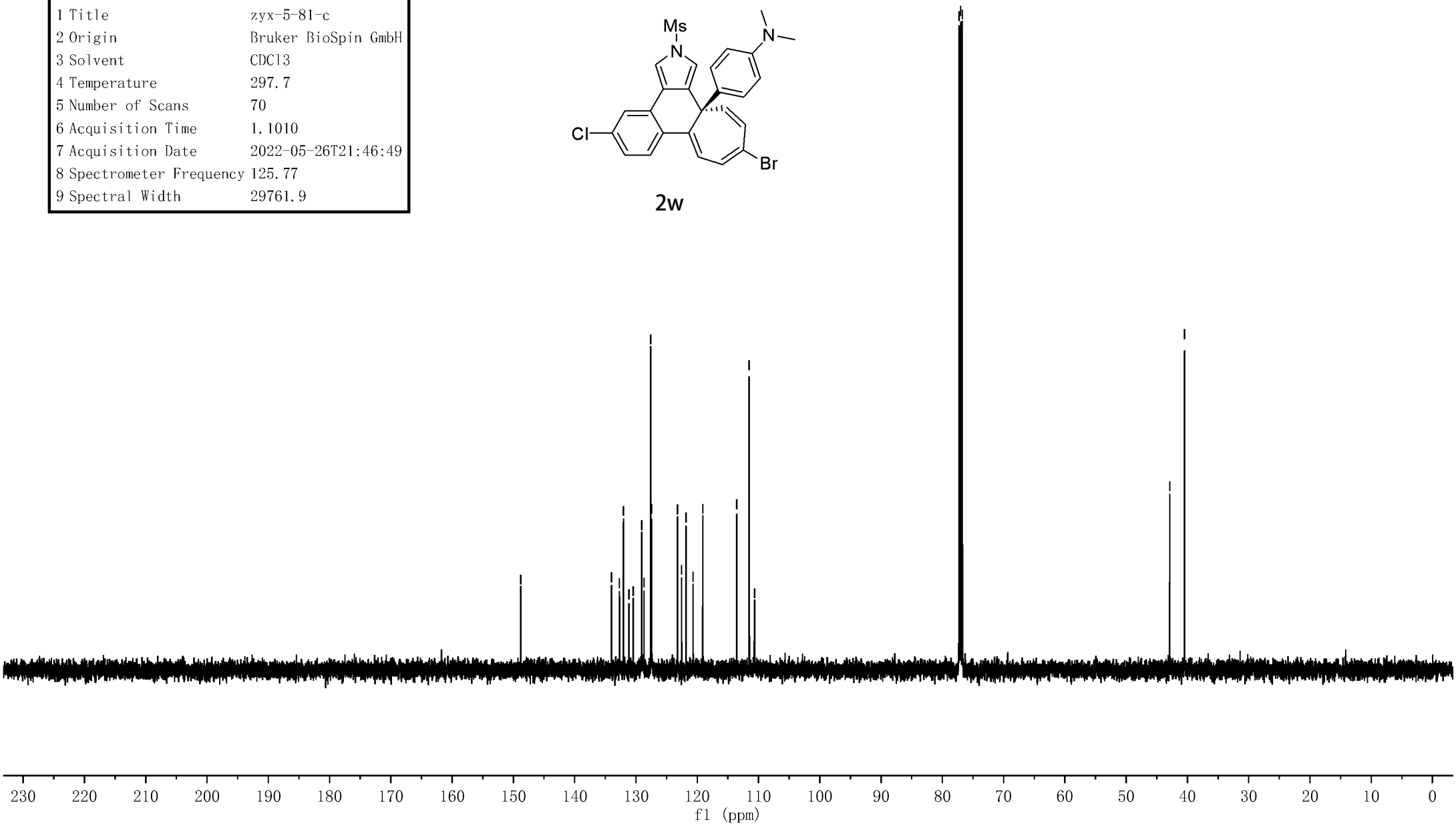
2w

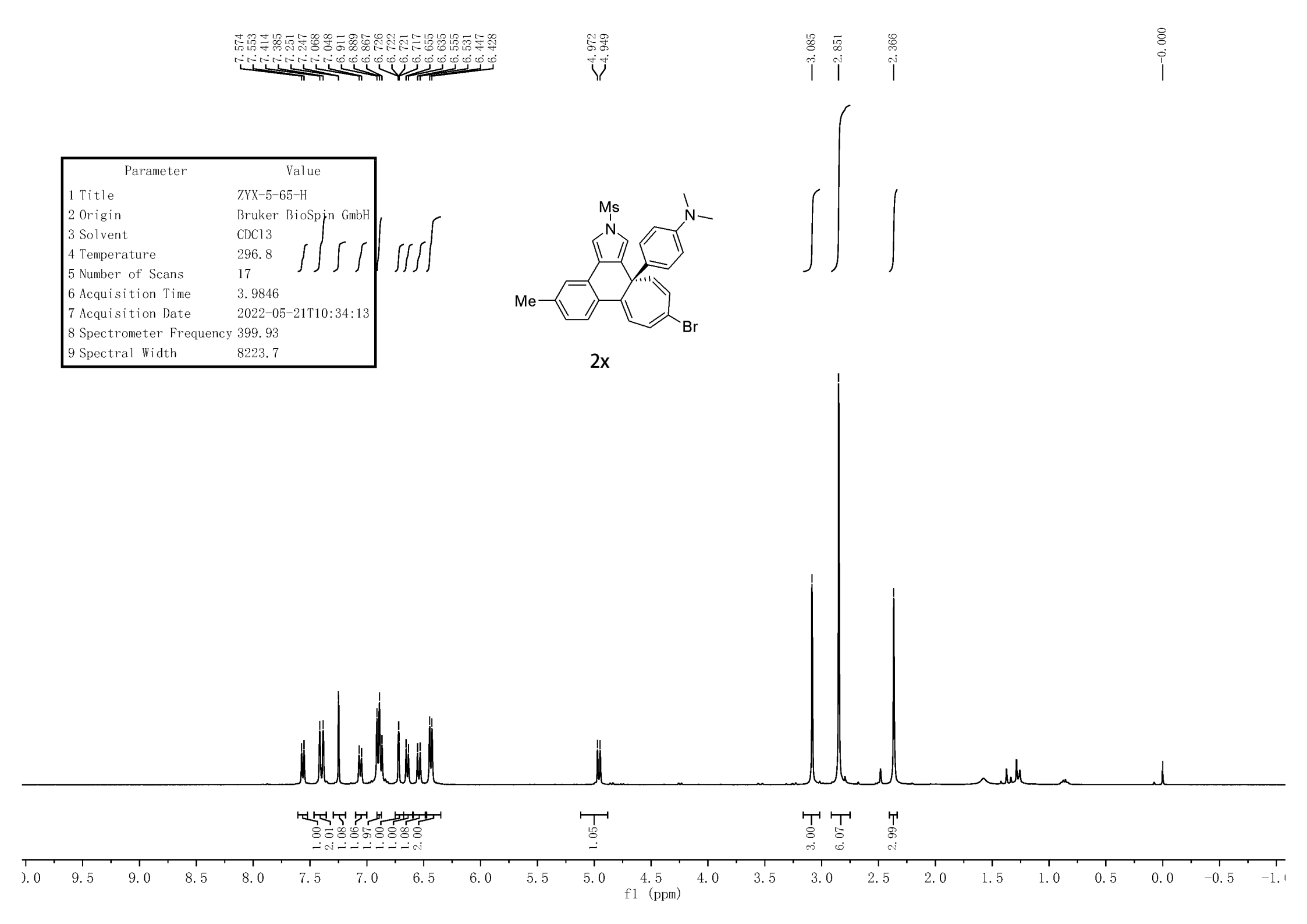


148.82
133.99
132.69
132.03
130.44
129.06
128.68
127.59
127.46
123.21
122.55
121.81
120.68
111.52
110.65
77.25
77.00
76.75
42.88
40.47

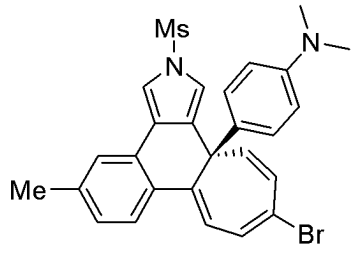
Parameter	Value
1 Title	zyx-5-81-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.7
5 Number of Scans	70
6 Acquisition Time	1.1010
7 Acquisition Date	2022-05-26T21:46:49
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

2w

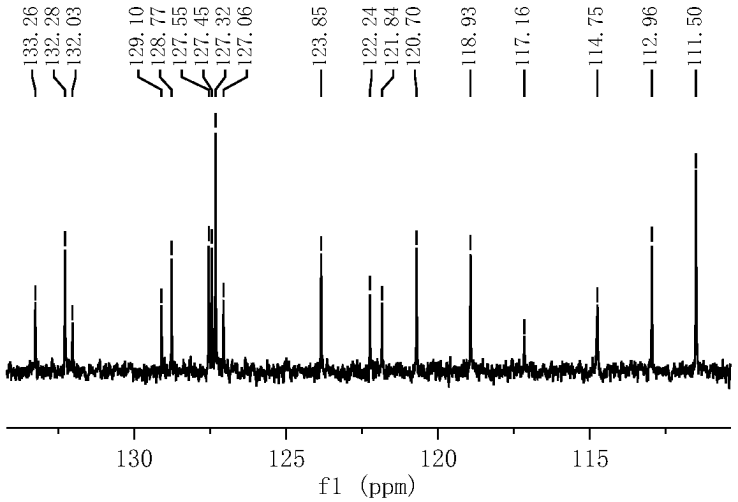


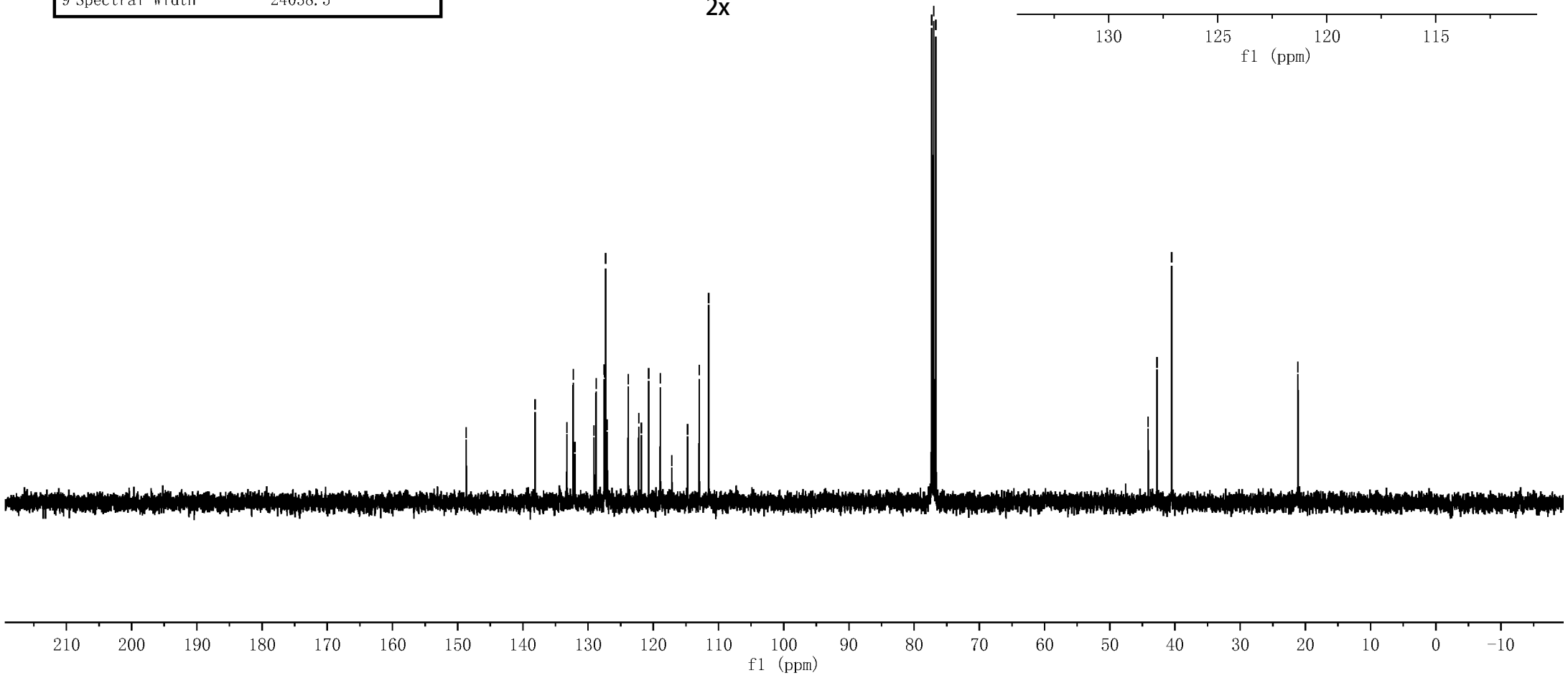

7.574
7.553
7.414
7.385
7.251
7.247
7.068
7.048
6.911
6.889
6.867
6.726
6.722
6.721
6.717
6.655
6.635
6.555
6.531
6.447
6.428
4.972
4.949
3.085
2.851
2.366
-0.000
Parameter Value
1 Title ZYX-5-65-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 296.8
5 Number of Scans 17
6 Acquisition Time 3.9846
7 Acquisition Date 2022-05-21T10:34:13
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
N
Me
Br
2x
1.00
2.01
1.08
1.06
1.97
1.00
1.00
1.08
2.00
1.05
3.00
6.07
2.99
f1 (ppm)

Parameter	Value
1 Title	ZYX-5-65-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.0
5 Number of Scans	85
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-21T10:37:31
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



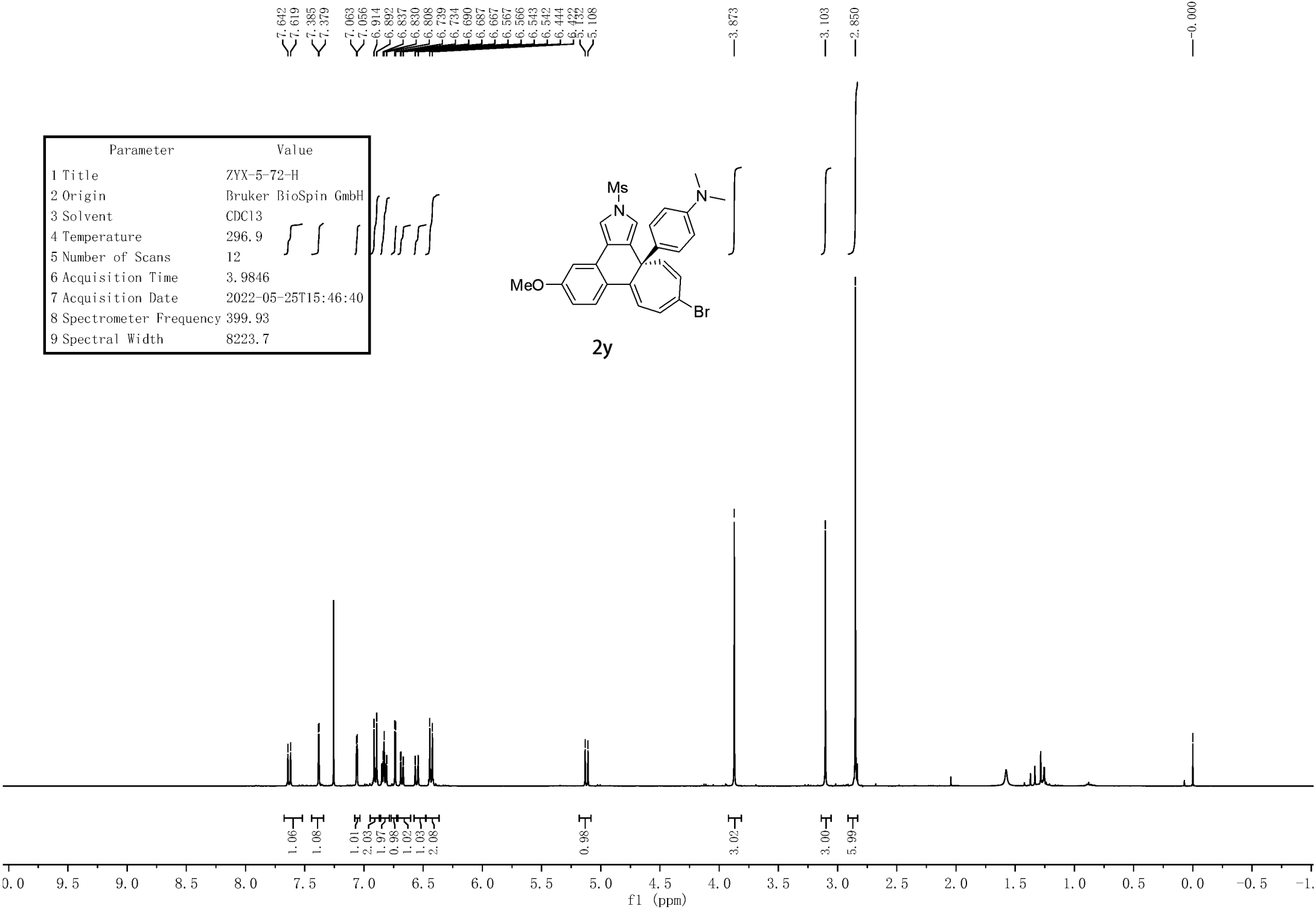
2x





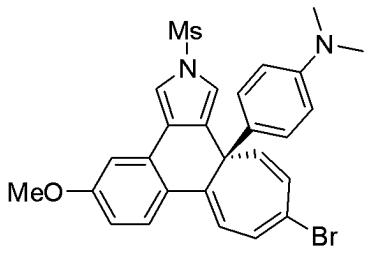
Parameter	Value
1 Title	ZYX-5-72-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.9
5 Number of Scans	12
6 Acquisition Time	3.9846
7 Acquisition Date	2022-05-25T15:46:40
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

2y

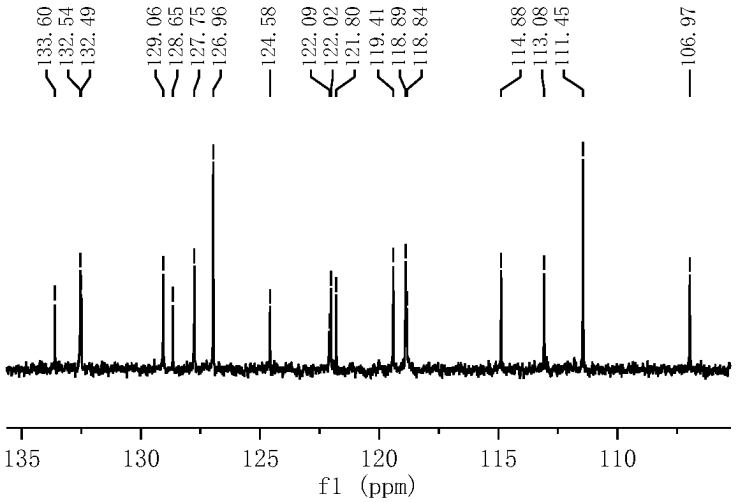


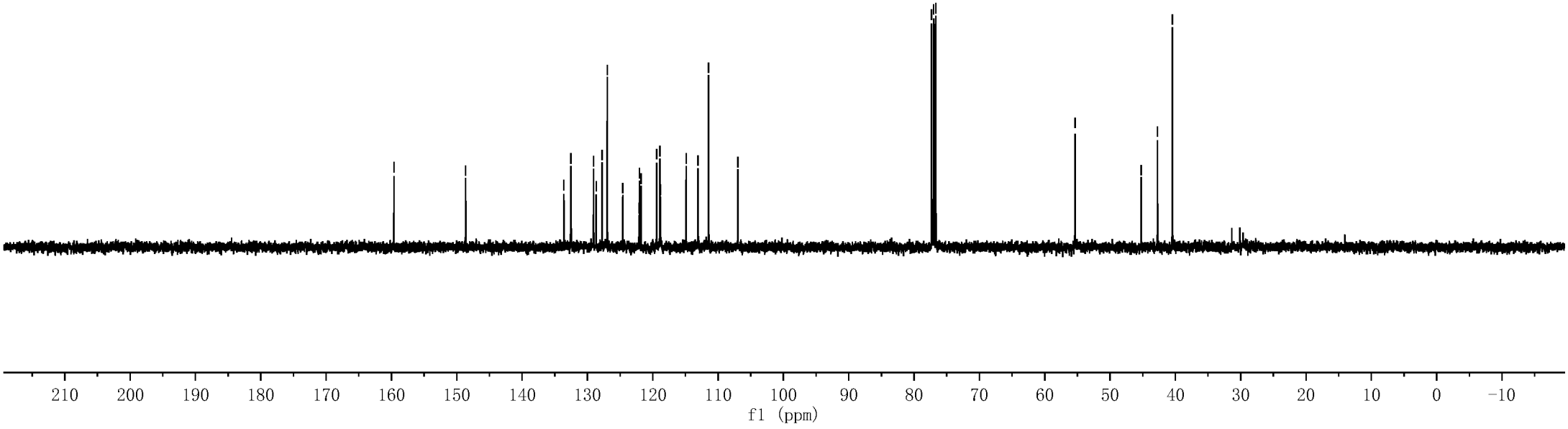
159.61
148.64
133.60
132.54
132.49
129.06
128.65
127.75
126.96
124.58
122.09
122.02
121.80
119.41
118.89
118.84
114.88
113.08
111.45
106.97
77.32
77.00
76.68
55.35
45.24
42.74
40.47

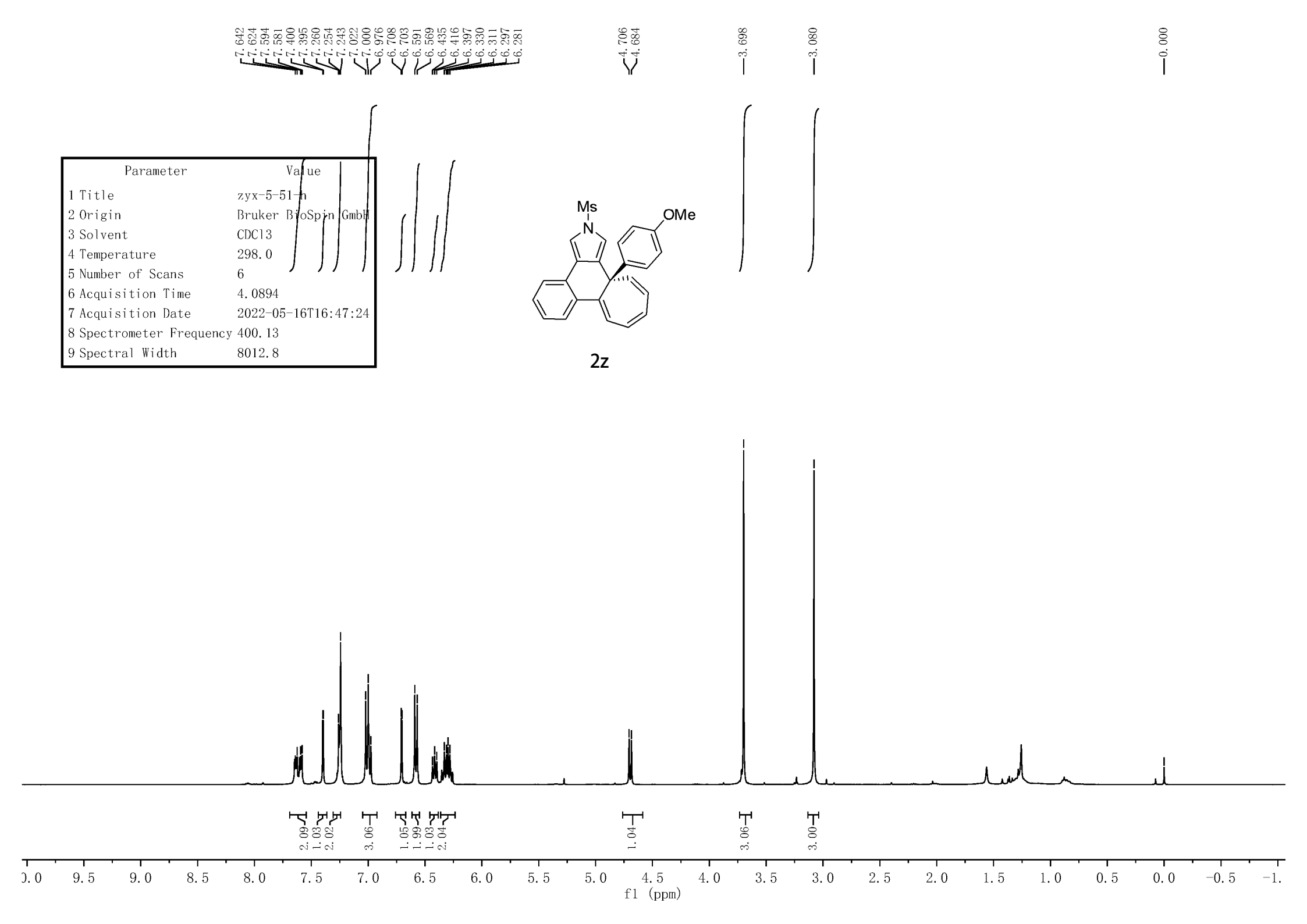
Parameter	Value
1 Title	ZYX-5-88--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.6
5 Number of Scans	47
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-30T16:22:56
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



2y



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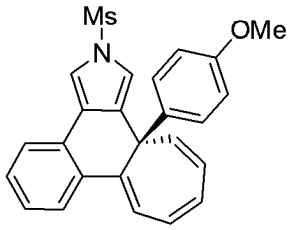
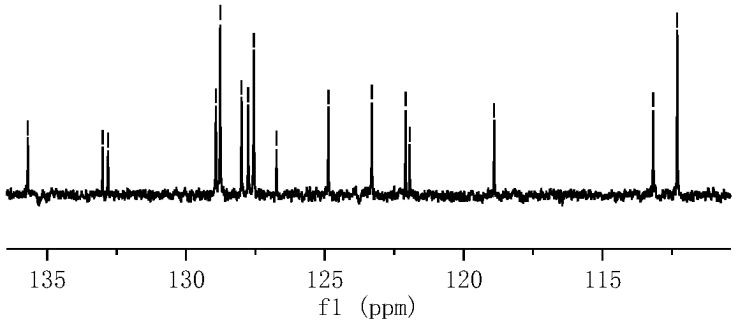
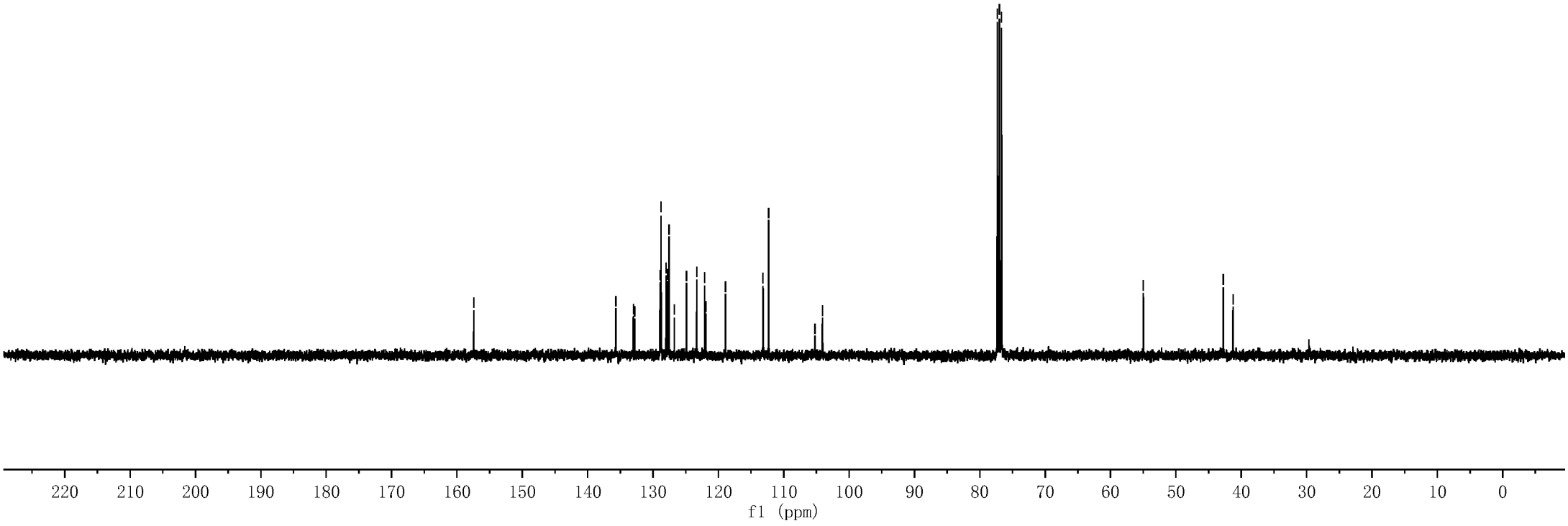
7.624
7.594
7.581
7.400
7.395
7.260
7.254
7.243
7.022
7.000
6.976
6.708
6.703
6.591
6.569
6.435
6.416
6.397
6.330
6.311
6.297
6.281
4.706
4.684
3.698
3.080
0.000
Parameter Value
1 Title zyx-5-51-n
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 6
6 Acquisition Time 4.0894
7 Acquisition Date 2022-05-16T16:47:24
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
OMe
2z
2.09
1.03
2.02
3.06
1.05
1.99
1.03
2.04
1.04
3.06
3.00
f1 (ppm)

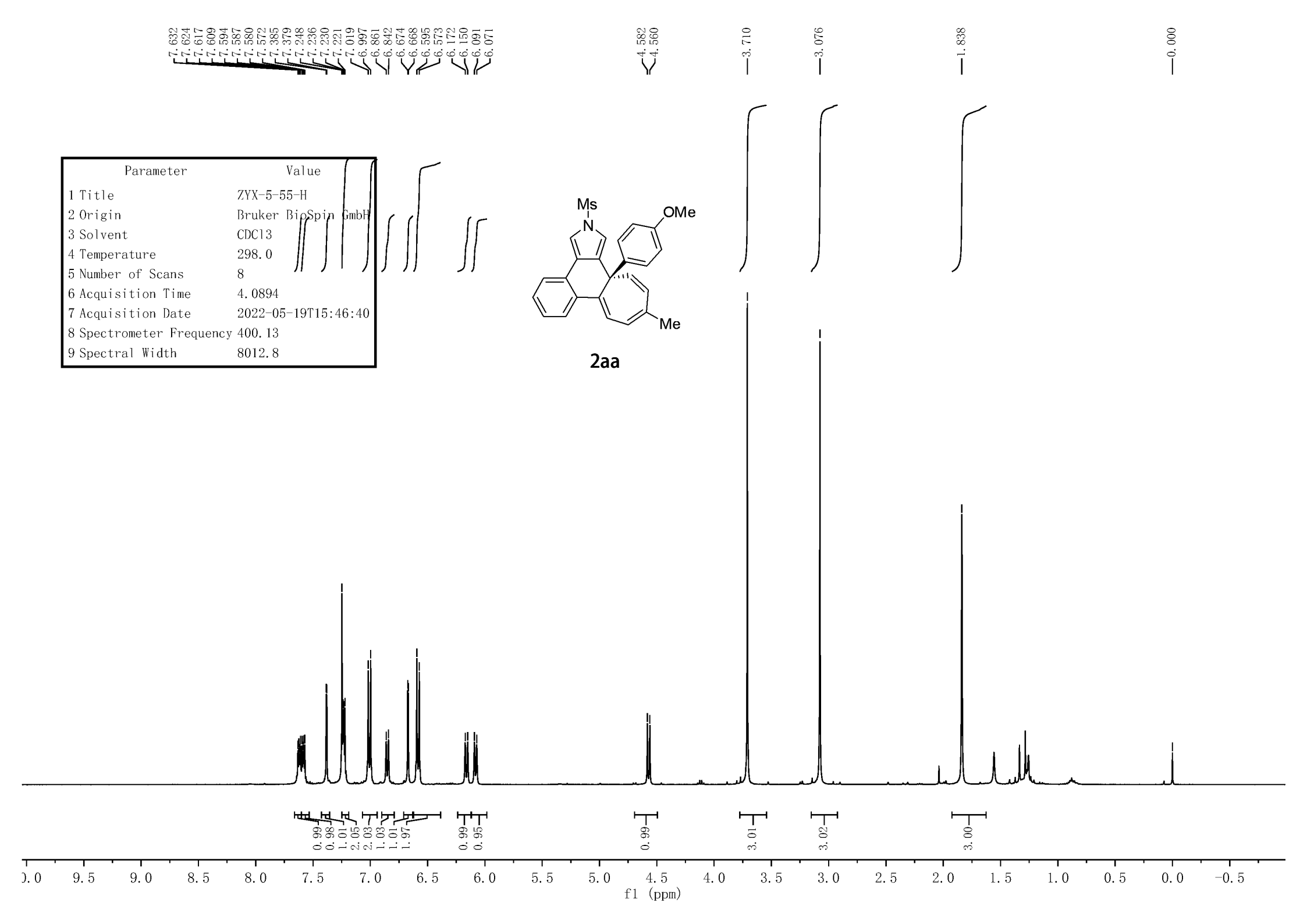
Parameter	Value
1 Title	ZYX-5-51-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	52
6 Acquisition Time	1.3631
7 Acquisition Date	2022-05-16T16:48:36
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



2z



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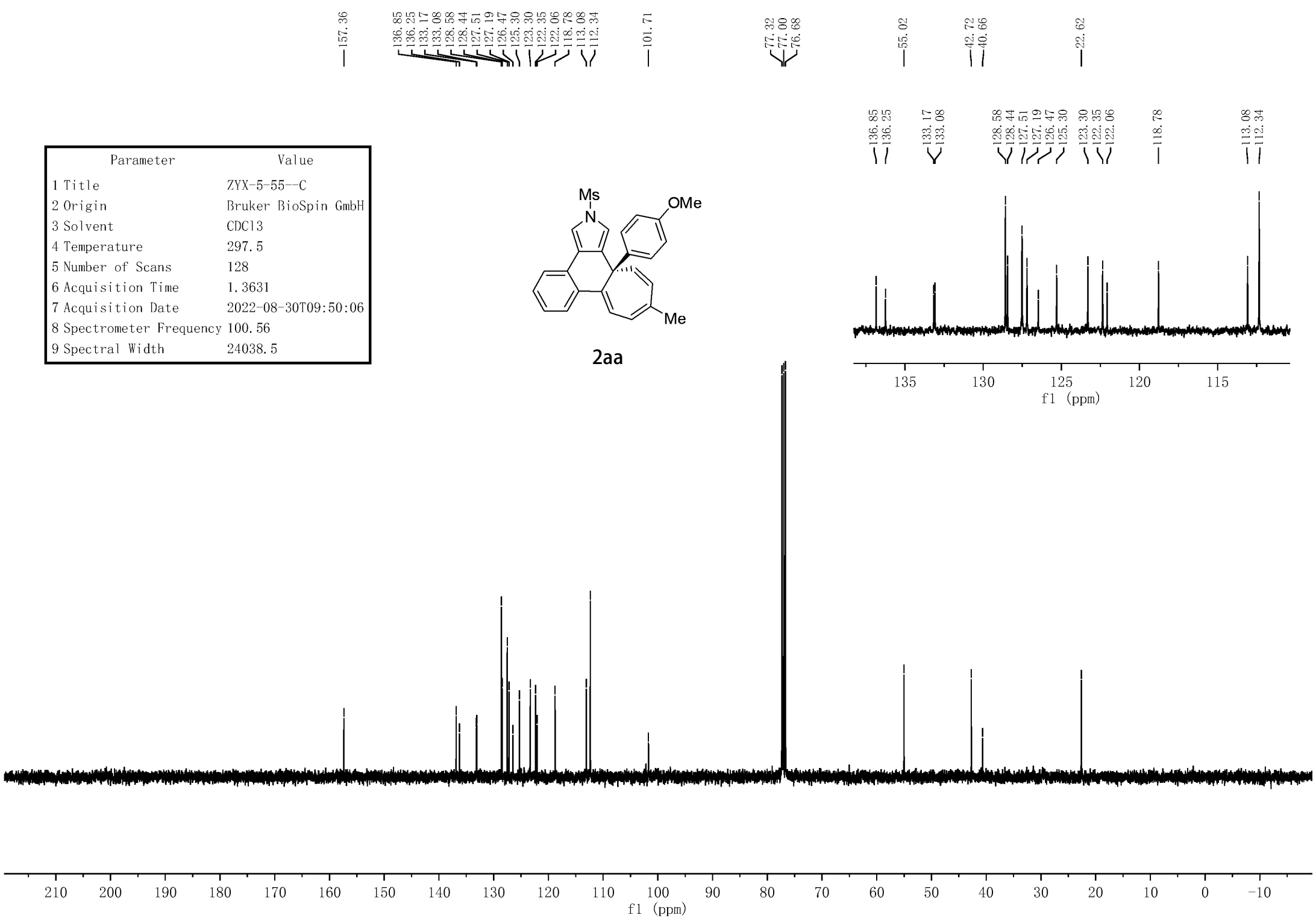
7.624
7.617
7.609
7.594
7.587
7.580
7.572
7.385
7.379
7.248
7.236
7.230
7.221
7.019
6.997
6.861
6.842
6.674
6.668
6.595
6.573
6.172
6.150
6.091
6.071
4.582
4.560
3.710
3.076
1.838
0.000
Parameter Value
1 Title ZYX-5-55-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2022-05-19T15:46:40
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
OMe
Me
2aa
0.99
0.98
1.01
2.05
2.03
1.03
1.01
1.97
0.99
0.95
0.99
3.01
3.02
3.00
f1 (ppm)

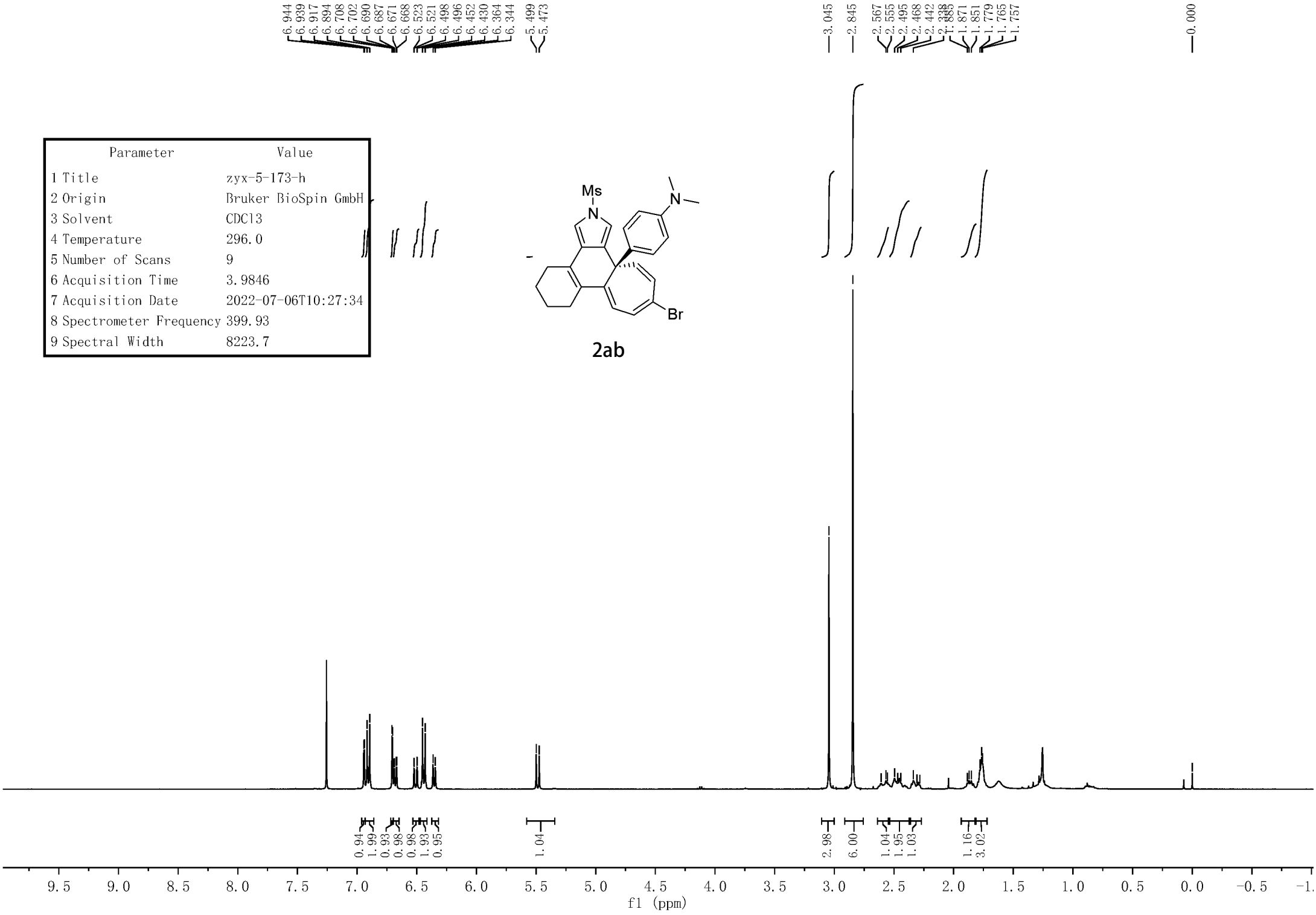
Parameter	Value
1 Title	ZYX-5-55--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.5
5 Number of Scans	128
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-30T09:50:06
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

2aa



Parameter	Value
1 Title	zyx-5-173-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.0
5 Number of Scans	9
6 Acquisition Time	3.9846
7 Acquisition Date	2022-07-06T10:27:34
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

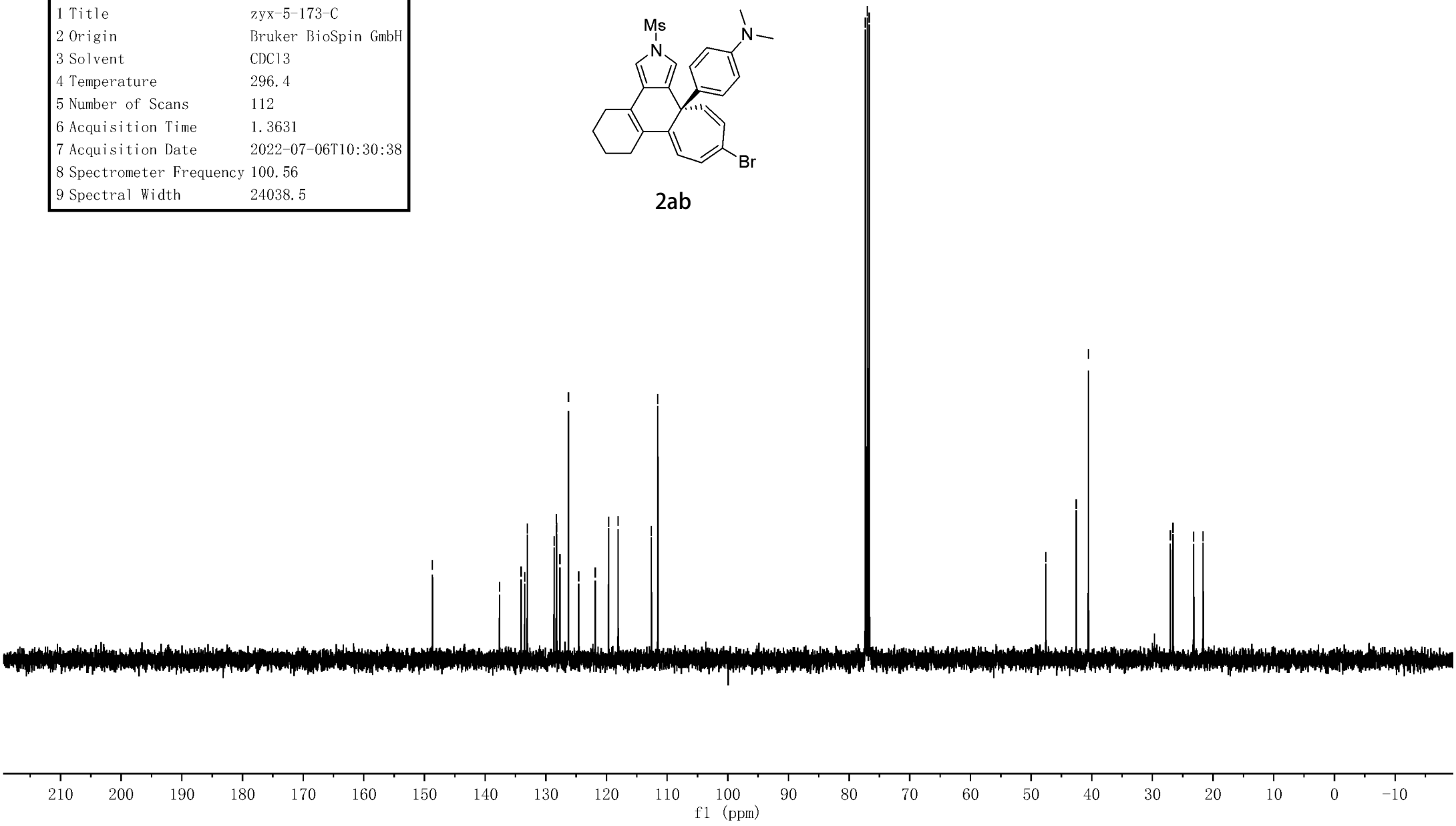
2ab

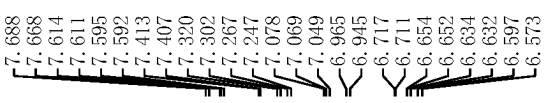


148.69
137.62
134.06
133.48
133.05
128.63
128.27
128.21
127.66
126.28
124.59
121.84
119.64
118.08
112.60
111.54
77.32
77.00
76.68
47.58
42.56
40.55
27.05
26.62
23.20
21.65

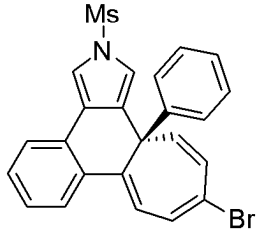
Parameter	Value
1 Title	zyx-5-173-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.4
5 Number of Scans	112
6 Acquisition Time	1.3631
7 Acquisition Date	2022-07-06T10:30:38
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

2ab

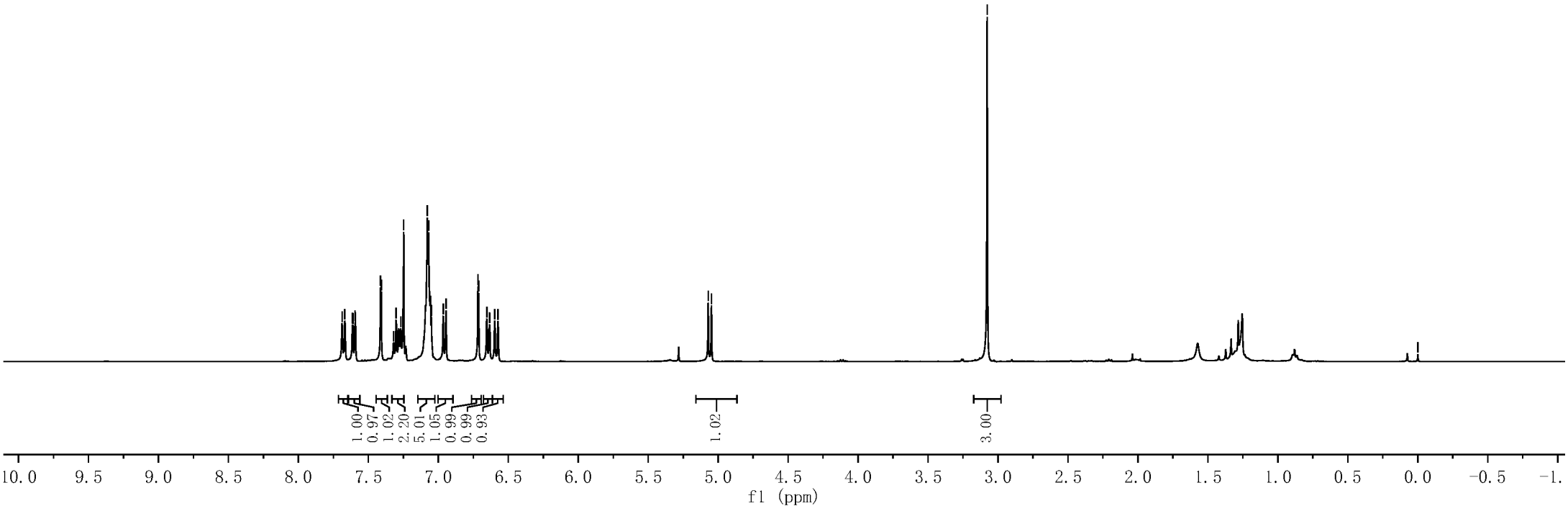




Parameter	Value
1 Title	zyx-4-238-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.6
5 Number of Scans	15
6 Acquisition Time	3.9846
7 Acquisition Date	2022-04-23T11:08:26
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

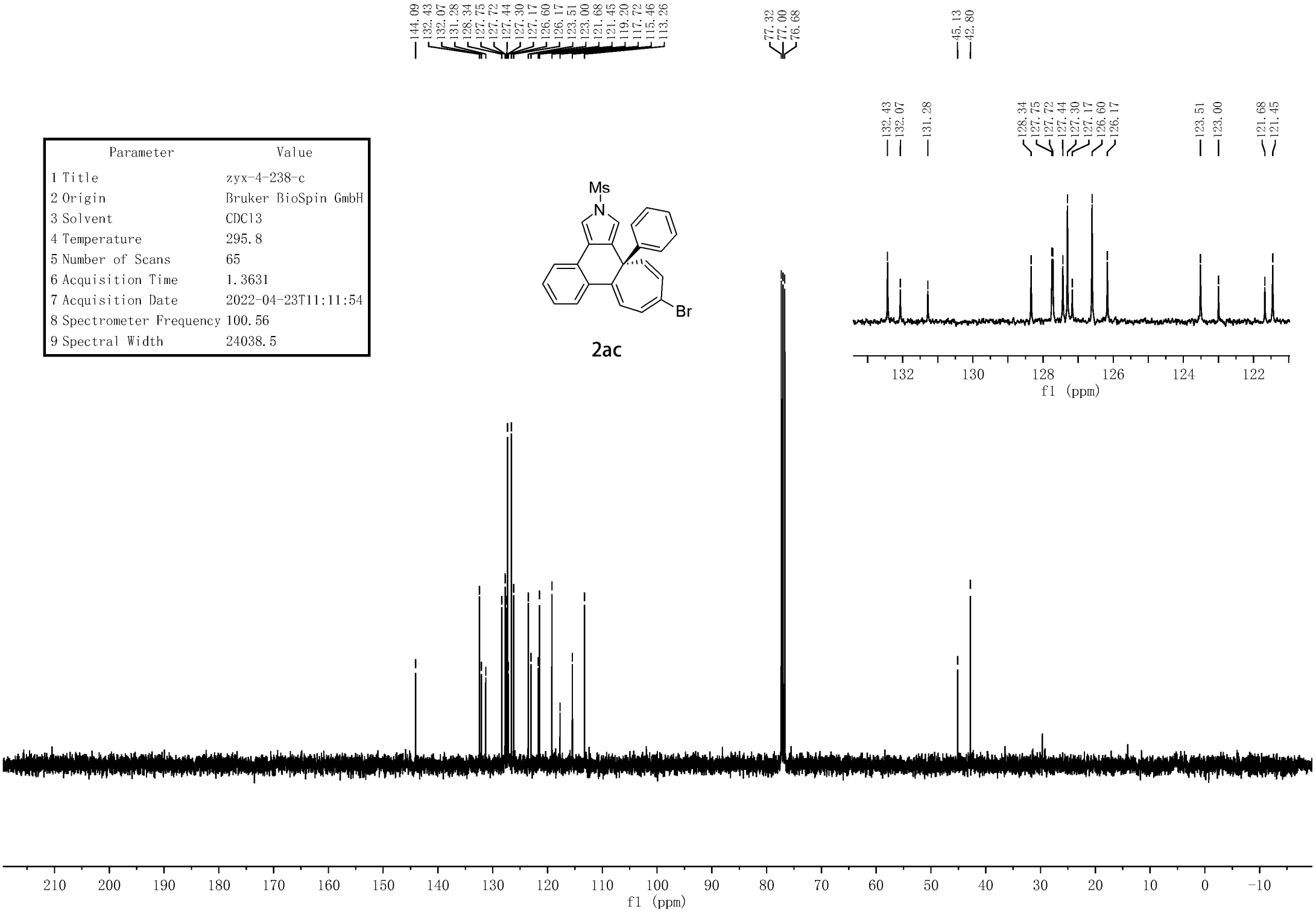


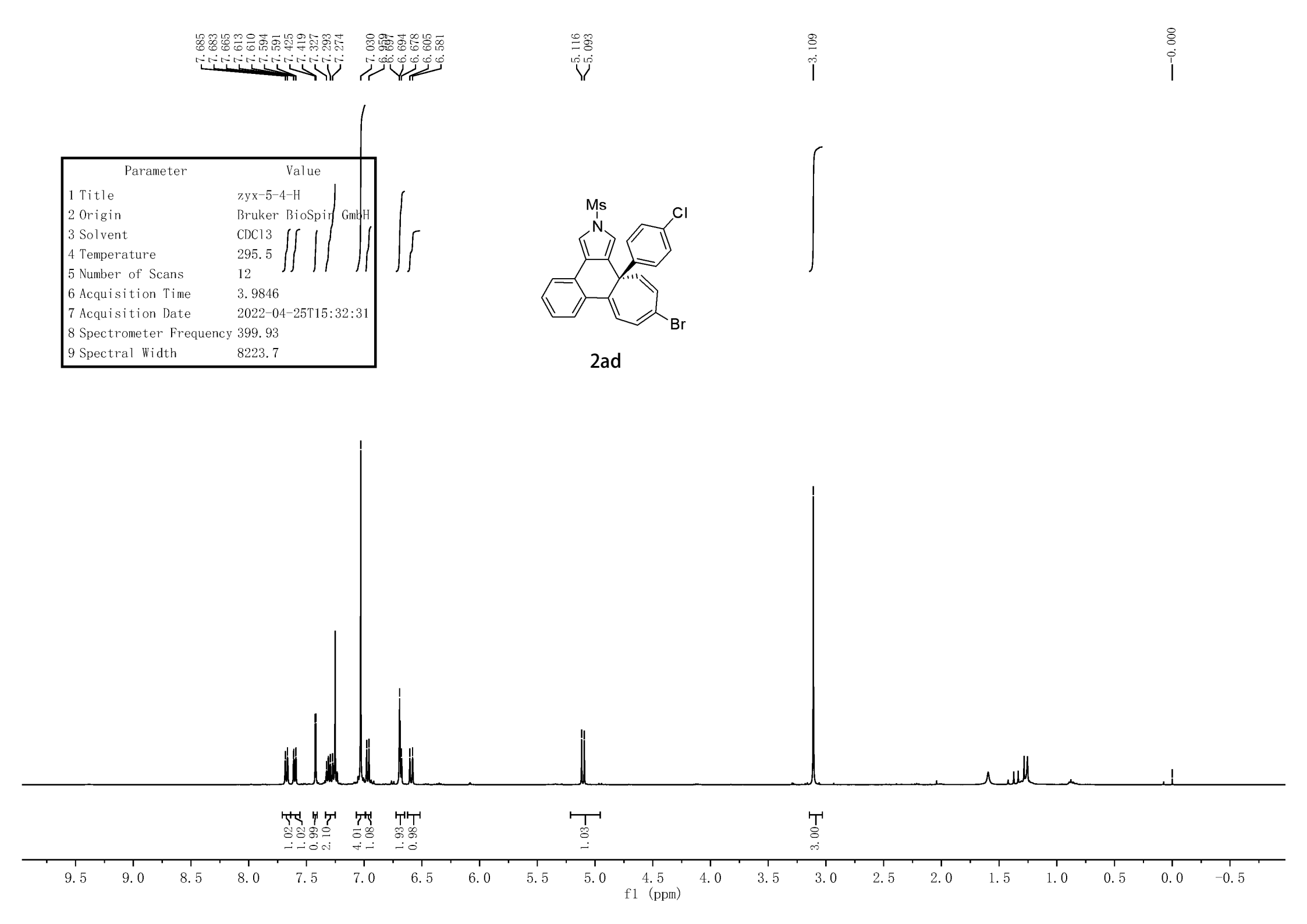
2ac



Parameter	Value
1 Title	zyx-4-238-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	65
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-23T11:11:54
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

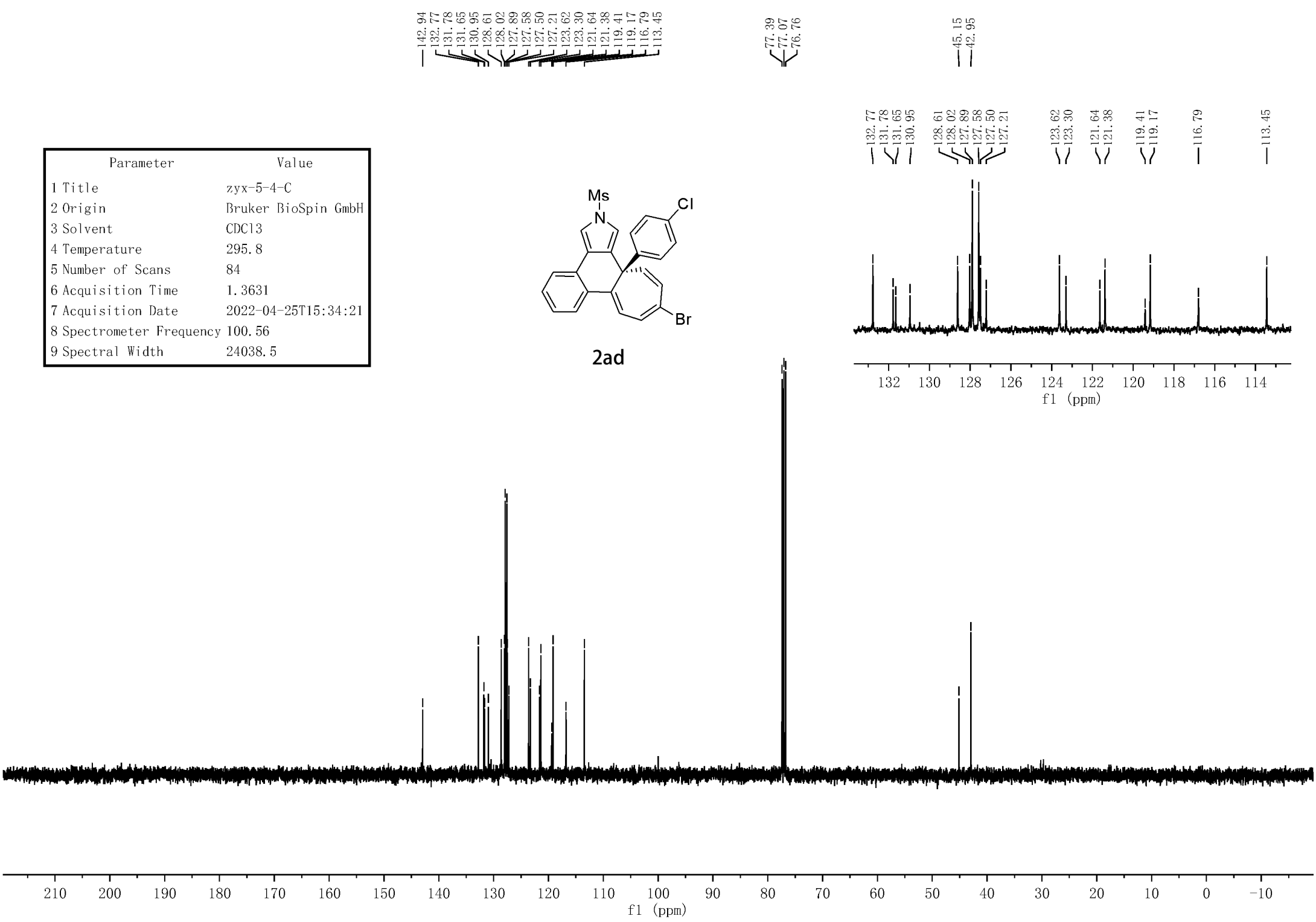
2ac

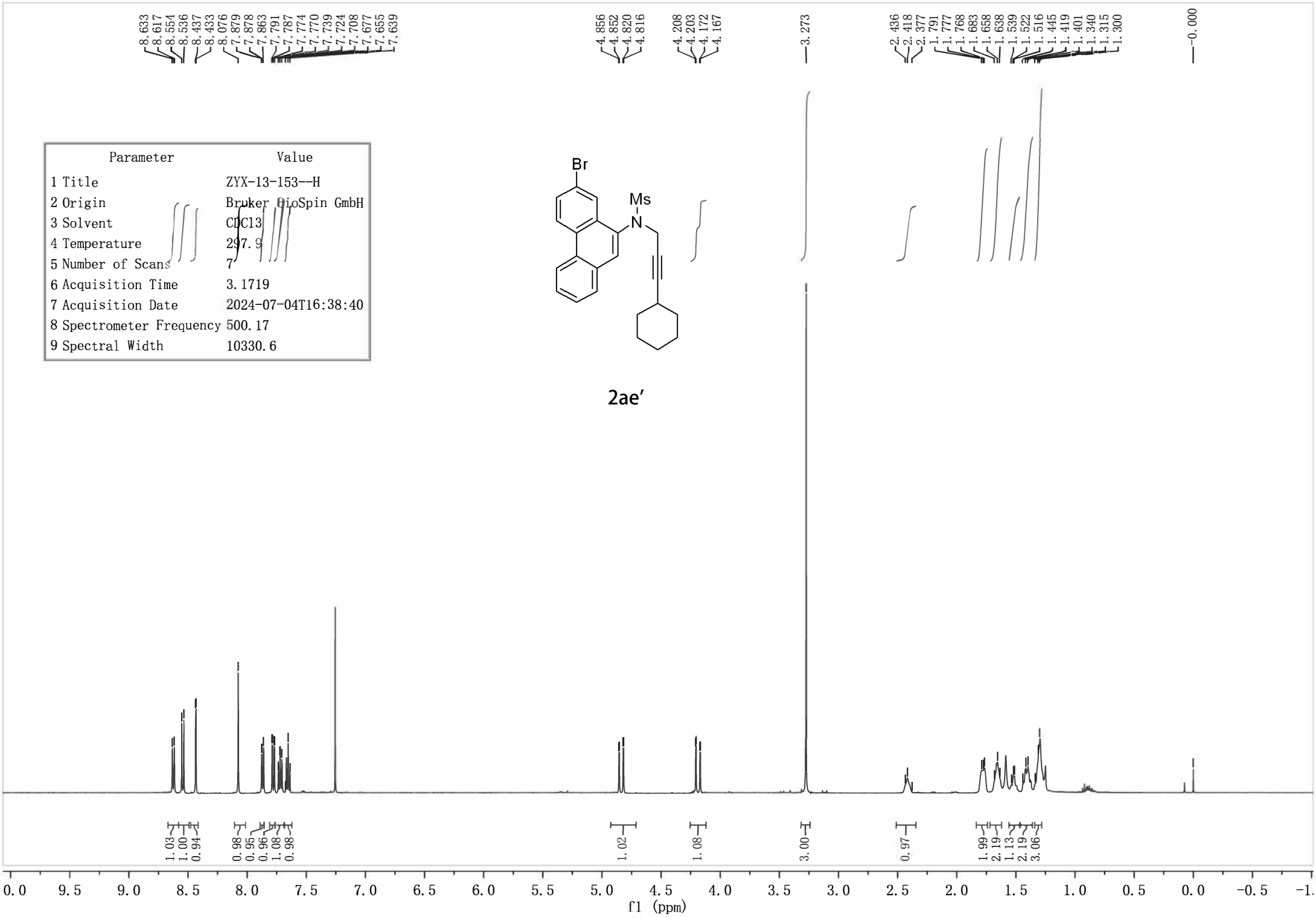



7.685
7.683
7.665
7.613
7.610
7.594
7.591
7.425
7.419
7.327
7.293
7.274
7.030
6.959
6.694
6.678
6.605
6.581
5.116
5.093
3.109
-0.000
Parameter Value
1 Title zyx-5-4-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.5
5 Number of Scans 12
6 Acquisition Time 3.9846
7 Acquisition Date 2022-04-25T15:32:31
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
Cl
Br
2ad
1.02
1.02
0.99
2.10
4.01
1.08
1.93
0.98
1.03
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)

Parameter	Value
1 Title	zyx-5-4-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	84
6 Acquisition Time	1.3631
7 Acquisition Date	2022-04-25T15:34:21
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

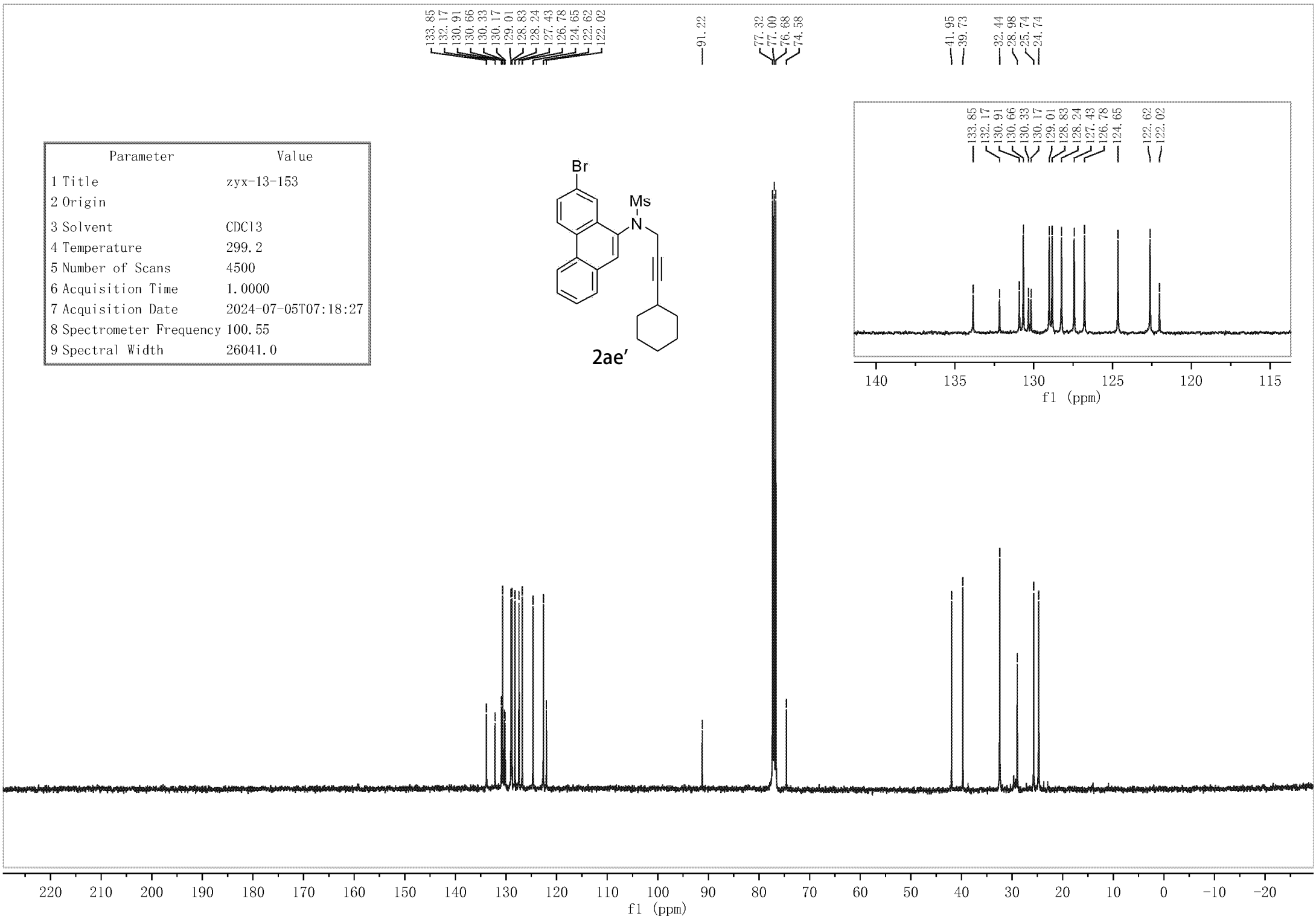
2ad




8.633
8.617
8.554
8.536
8.437
8.433
8.076
7.879
7.878
7.863
7.791
7.787
7.774
7.770
7.739
7.724
7.708
7.677
7.655
7.639
4.856
4.852
4.820
4.816
4.208
4.203
4.172
4.167
3.273
2.436
2.418
2.377
1.791
1.777
1.768
1.683
1.658
1.638
1.539
1.522
1.516
1.445
1.419
1.401
1.340
1.315
1.300
-0.000
Parameter Value
1 Title ZYX-13-153--H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.9
5 Number of Scans 7
6 Acquisition Time 3.1719
7 Acquisition Date 2024-07-04T16:38:40
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Br
Ms
N
2ae'
1.03
1.00
0.94
0.98
0.95
0.96
1.08
0.98
1.02
1.08
3.00
0.97
1.99
2.19
1.13
2.19
3.06
0.0
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)

Parameter	Value
1 Title	zyx-13-153
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.2
5 Number of Scans	4500
6 Acquisition Time	1.0000
7 Acquisition Date	2024-07-05T07:18:27
8 Spectrometer Frequency	100.55
9 Spectral Width	26041.0

2ae′

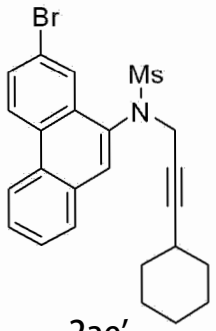


130.65
129.01
128.82
128.23
127.43
126.77
124.65
122.61

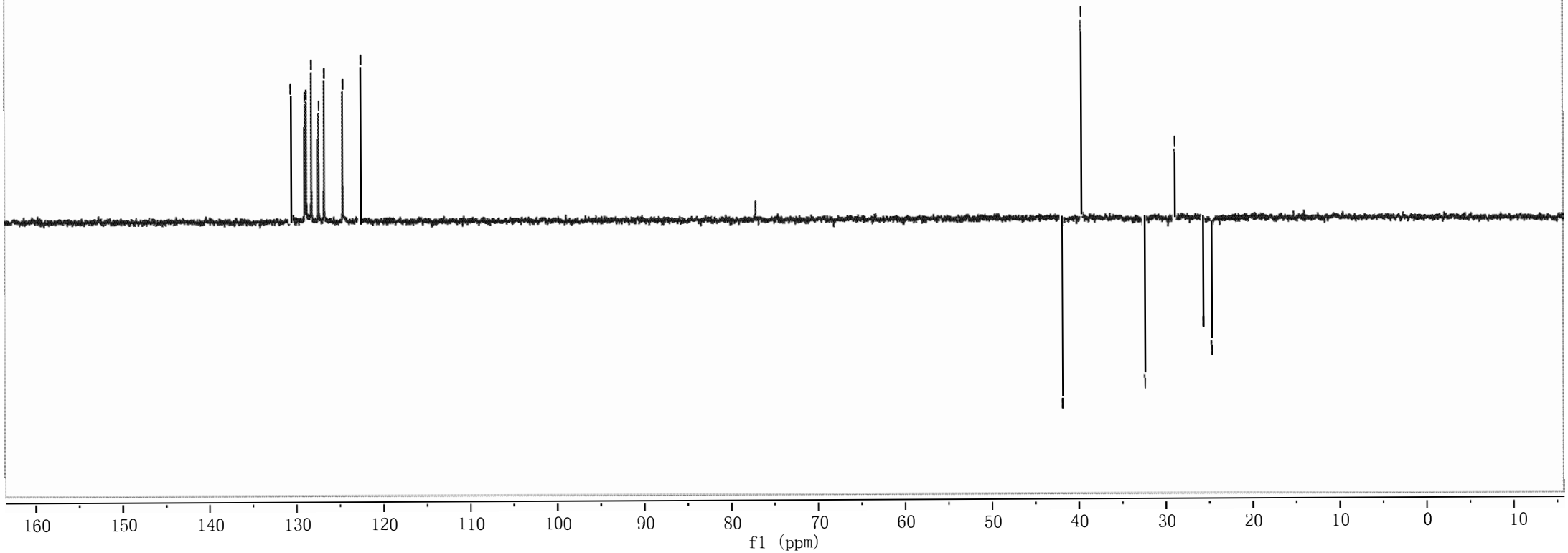
41.95
39.72

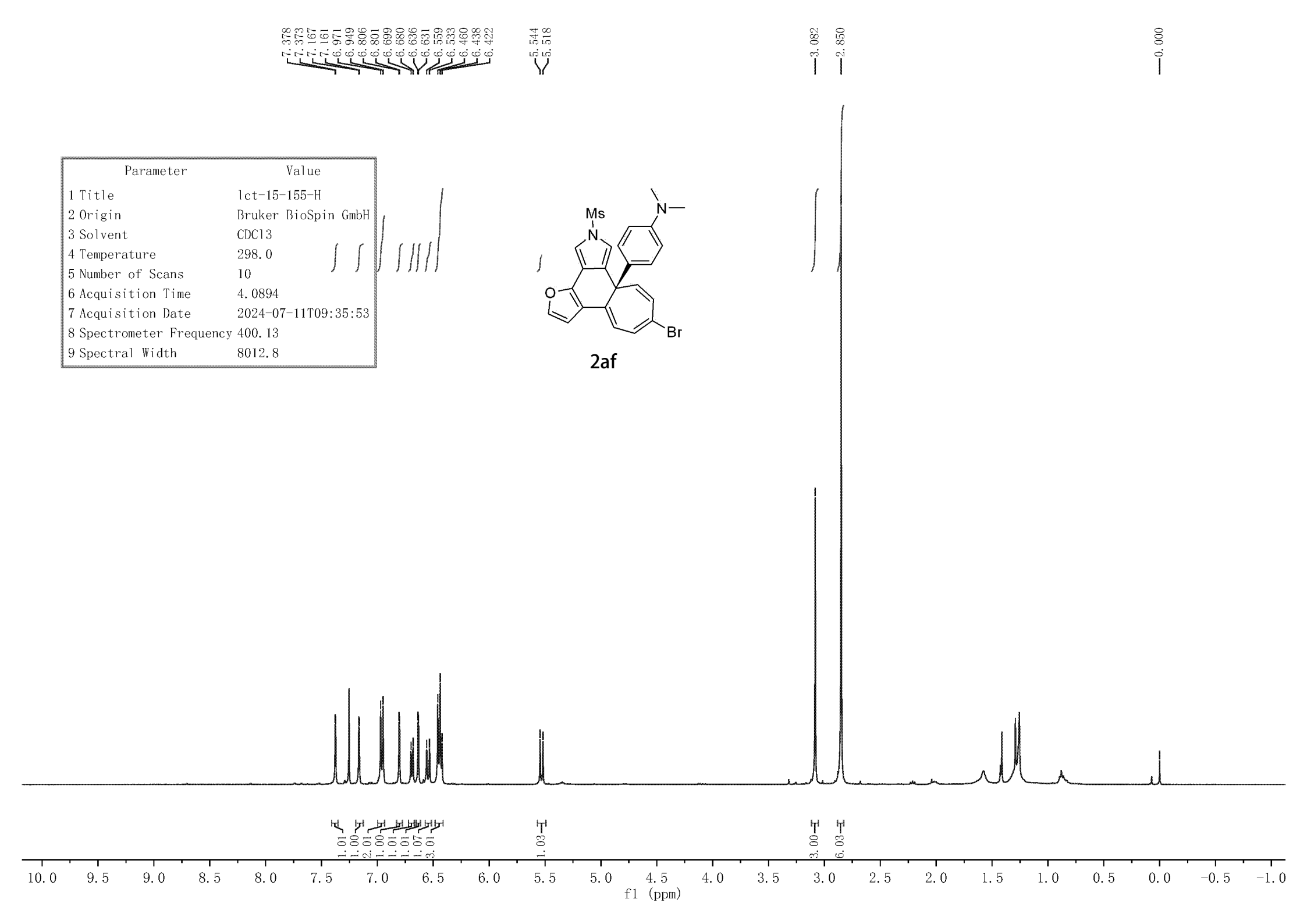
32.44
28.98
25.74
24.74

Parameter	Value
1 Title	zyx-13-153
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.8
5 Number of Scans	1000
6 Acquisition Time	1.0001
7 Acquisition Date	2024-07-05T08:12:17
8 Spectrometer Frequency	100.55
9 Spectral Width	18028.0



2ae'

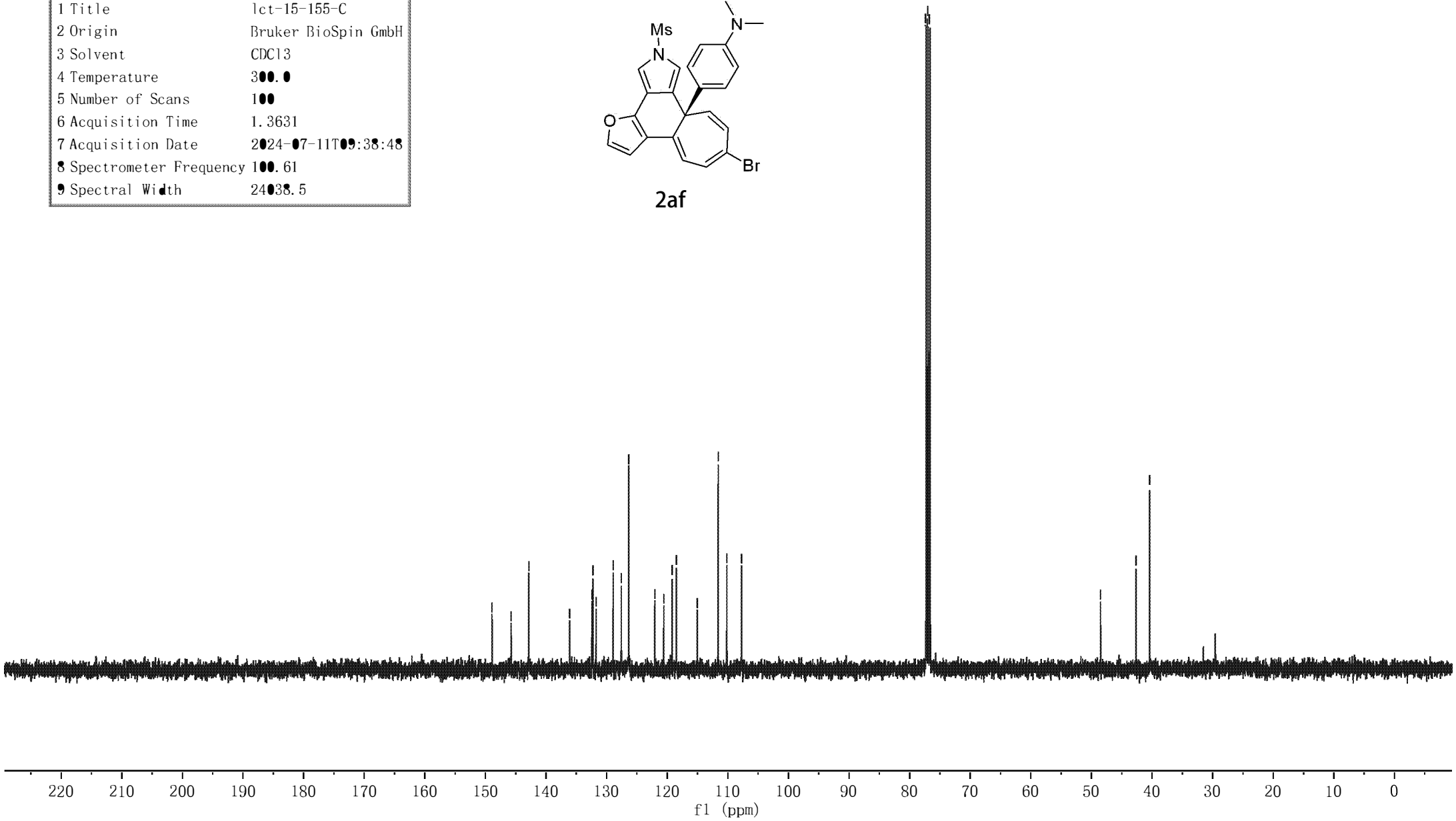



7.378
7.373
7.167
7.161
6.971
6.949
6.806
6.801
6.699
6.680
6.636
6.631
6.559
6.533
6.460
6.438
6.422
5.544
5.518
3.082
2.850
0.000
Parameter Value
1 Title lct-15-155-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 10
6 Acquisition Time 4.0894
7 Acquisition Date 2024-07-11T09:35:53
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
O
Br
2af
1.01
1.00
2.01
1.00
1.01
1.01
1.07
3.01
1.03
3.00
6.03
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
-1.0
f1 (ppm)

148.94
145.78
142.86
136.14
132.46
132.30
131.76
128.96
127.61
126.37
122.08
120.60
119.22
118.52
115.10
111.62
110.21
107.78
77.32
77.00
76.68
48.56
42.71
40.47

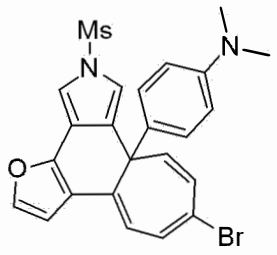
Parameter	Value
1 Title	lct-15-155-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	100
6 Acquisition Time	1.3631
7 Acquisition Date	2024-07-11T09:38:48
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

2af

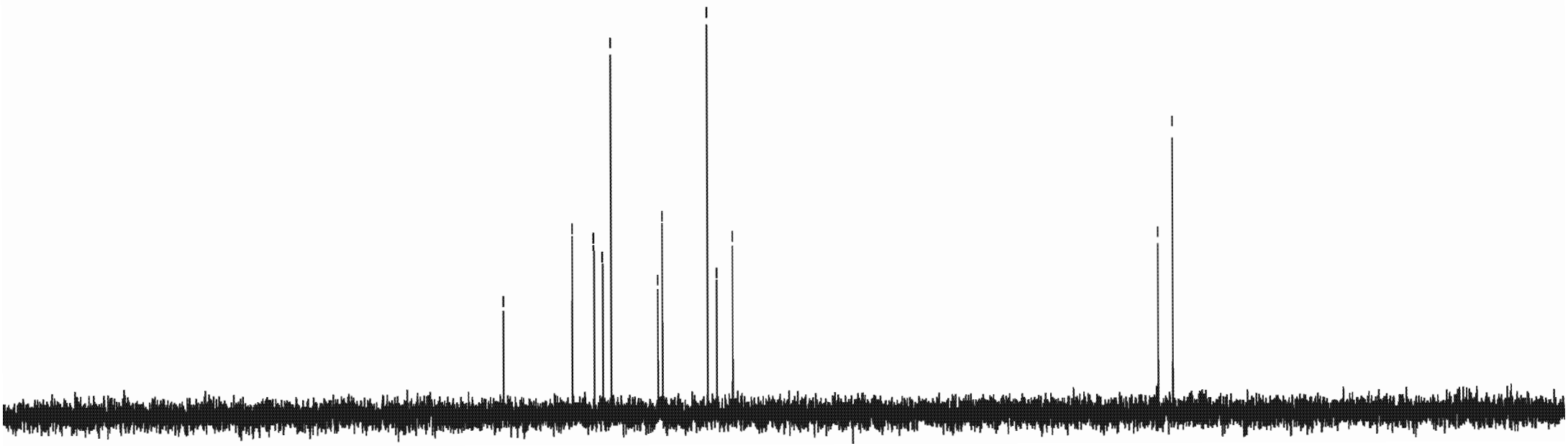


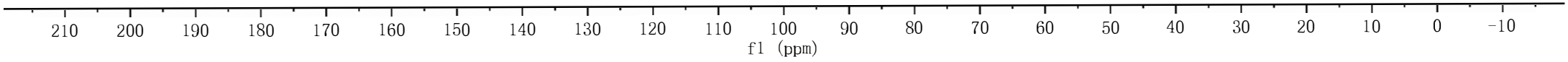
142.86
132.29
128.95
127.61
126.36
119.22
118.52
111.62
110.20
107.78
42.71
40.46

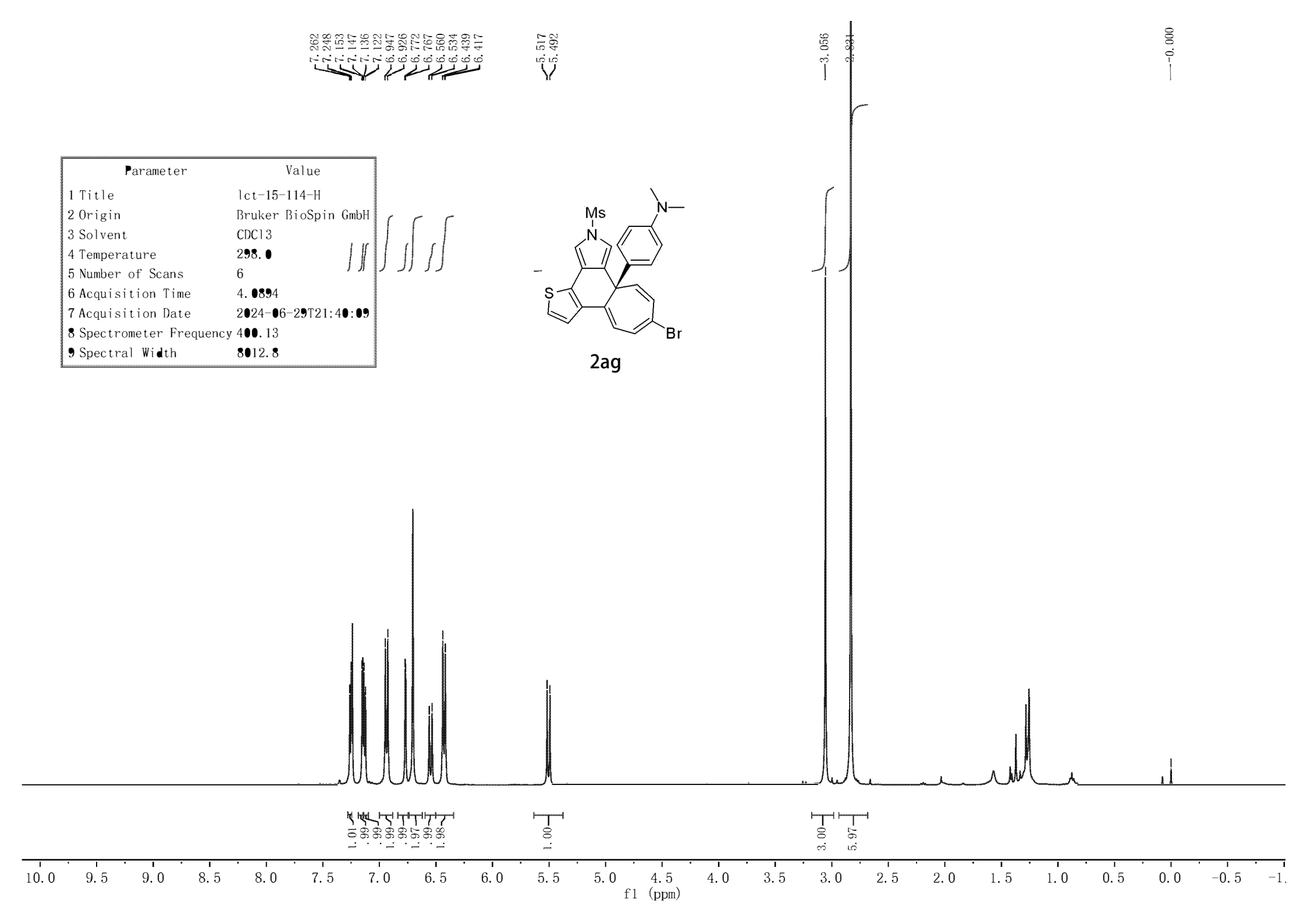
Parameter	Value
1 Title	lct-15-155-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	21
6 Acquisition Time	1.3631
7 Acquisition Date	2024-07-11T09:44:04
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

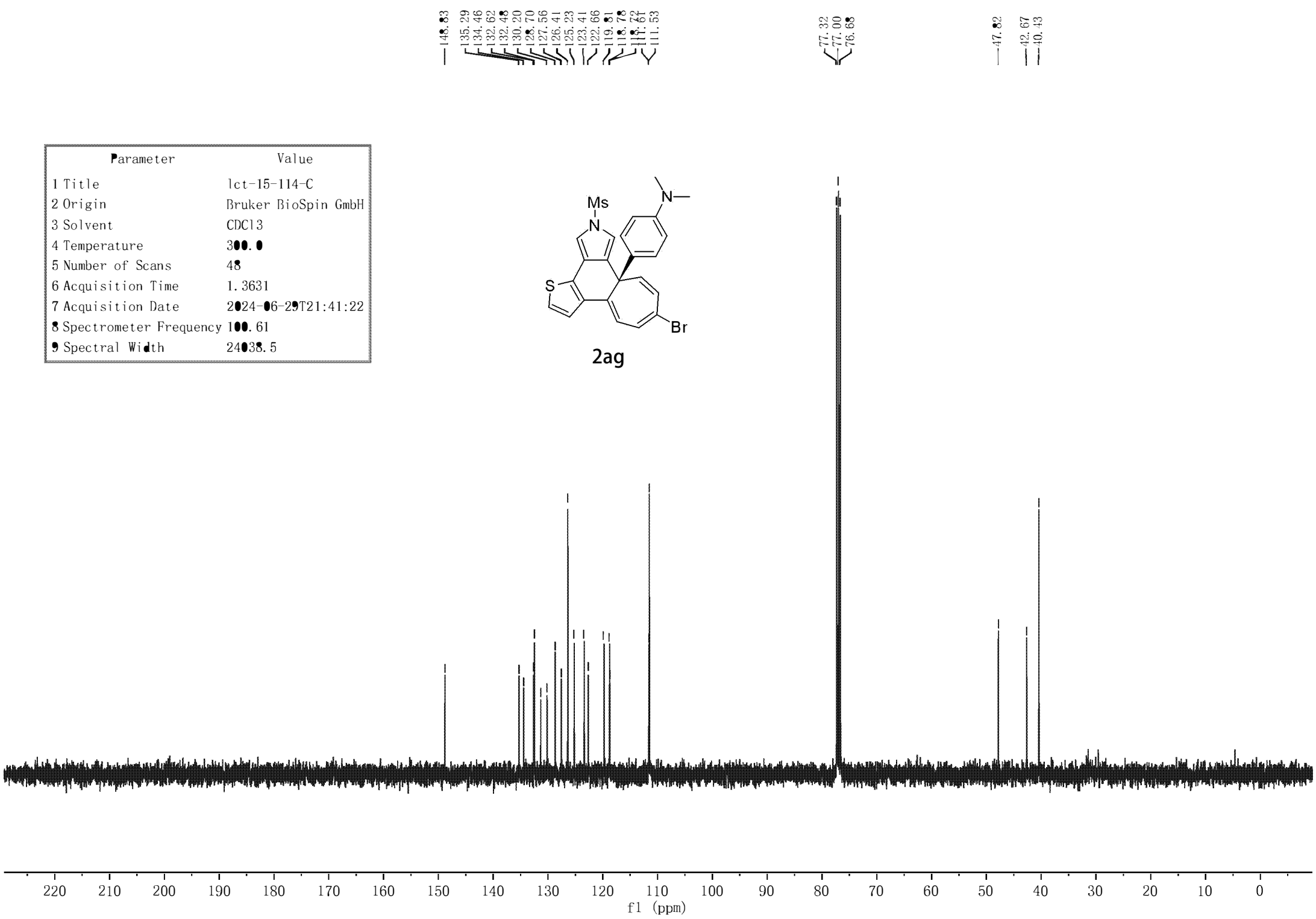


2af

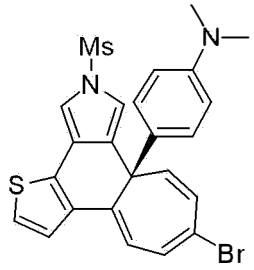




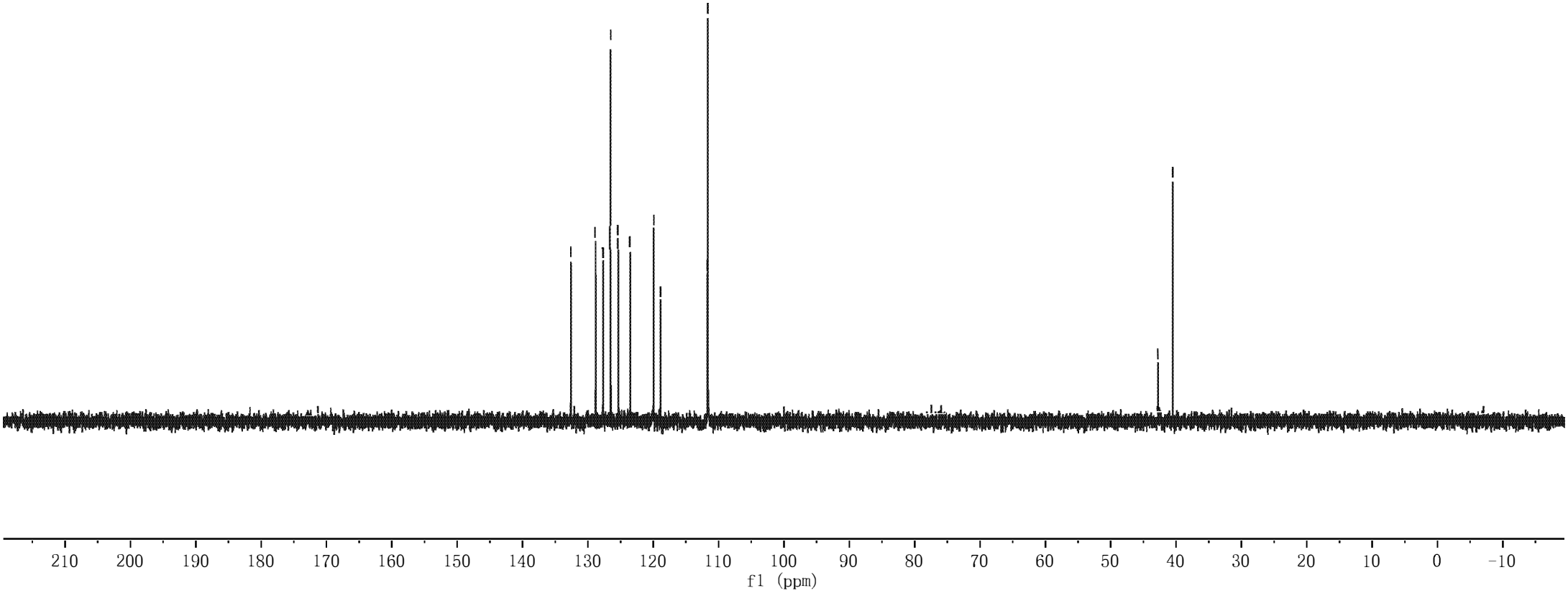

7.262
7.248
7.153
7.147
7.136
7.122
6.947
6.926
6.772
6.767
6.560
6.534
6.439
6.417
5.517
5.492
3.056
2.831
0.000
Parameter Value
1 Title lct-15-114-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 6
6 Acquisition Time 4.0894
7 Acquisition Date 2024-06-29T21:40:09
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
S
Br
2ag
1.01
.99
.99
1.99
.99
1.97
.99
1.98
1.00
3.00
5.97
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)


148.83
135.29
134.46
132.62
132.48
130.20
128.70
127.56
126.41
125.23
123.41
122.66
119.81
118.78
111.53
77.32
77.00
76.68
47.82
42.67
40.43
Parameter Value
1 Title lct-15-114-C
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 48
6 Acquisition Time 1.3631
7 Acquisition Date 2024-06-29T21:41:22
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
N
S
Br
2ag
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

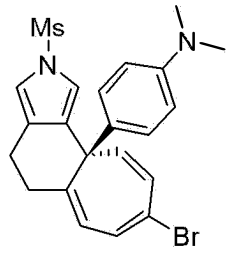
Parameter	Value
1 Title	lct-15-114-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	22
6 Acquisition Time	1.3631
7 Acquisition Date	2024-06-29T21:44:39
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



2ag

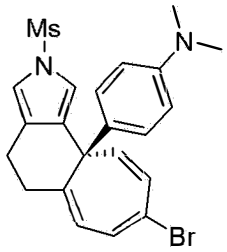


Parameter	Value
1 Title	zyx-13-175-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	4
6 Acquisition Time	4.0894
7 Acquisition Date	2024-07-02T10:06:41
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

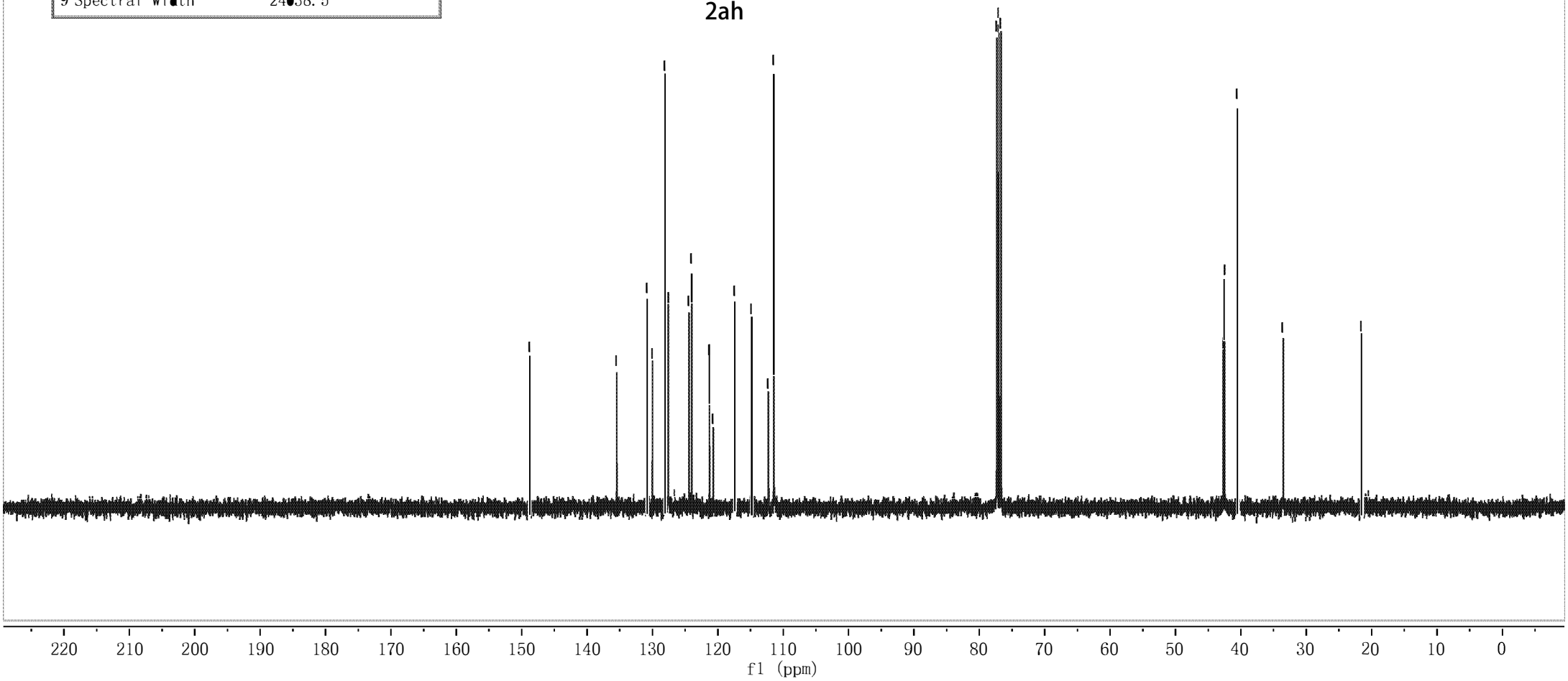


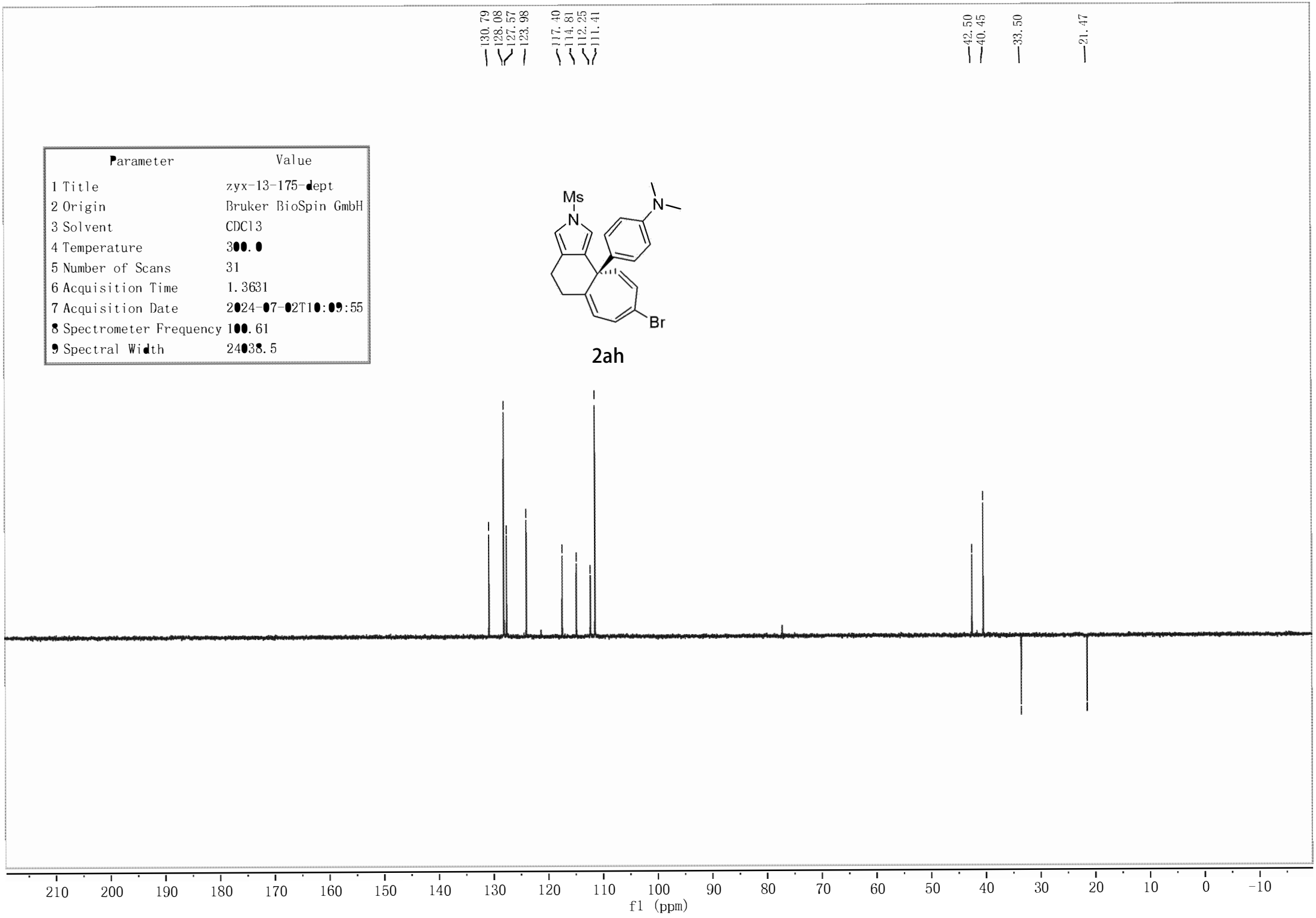
2ah

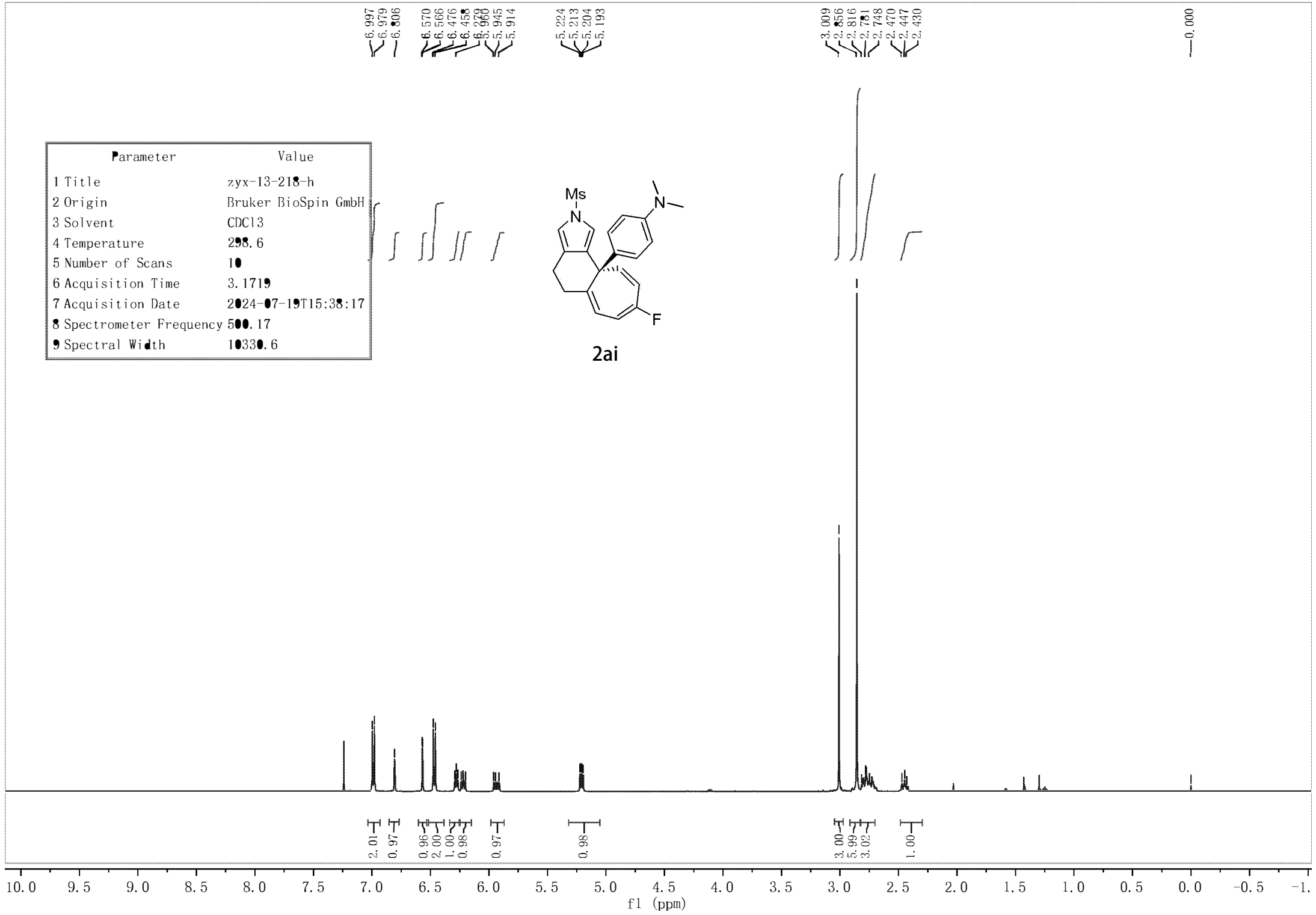
Parameter	Value
1 Title	zyx-13-175-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	29
6 Acquisition Time	1.3631
7 Acquisition Date	2024-07-02T10:07:56
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

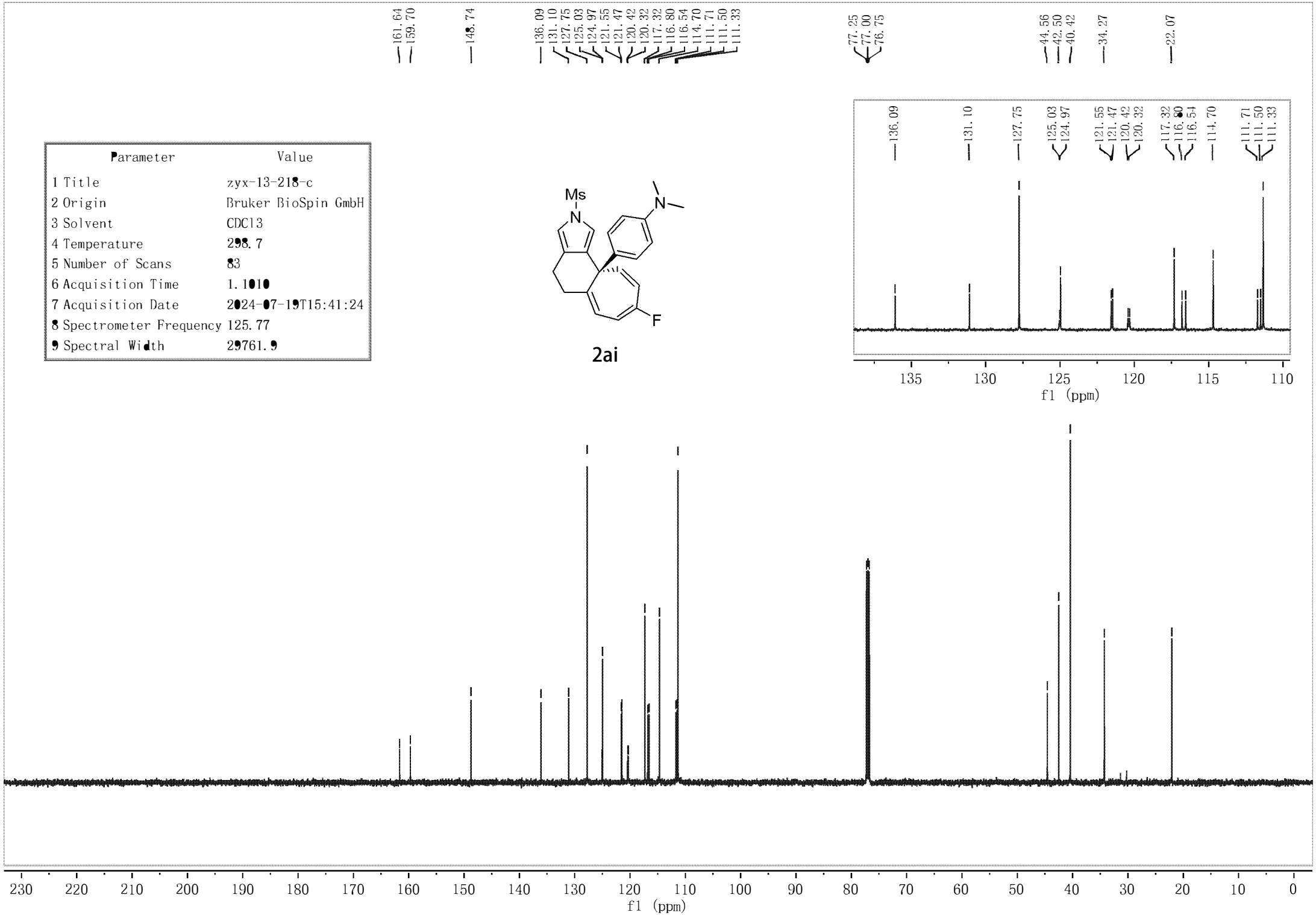


2ah



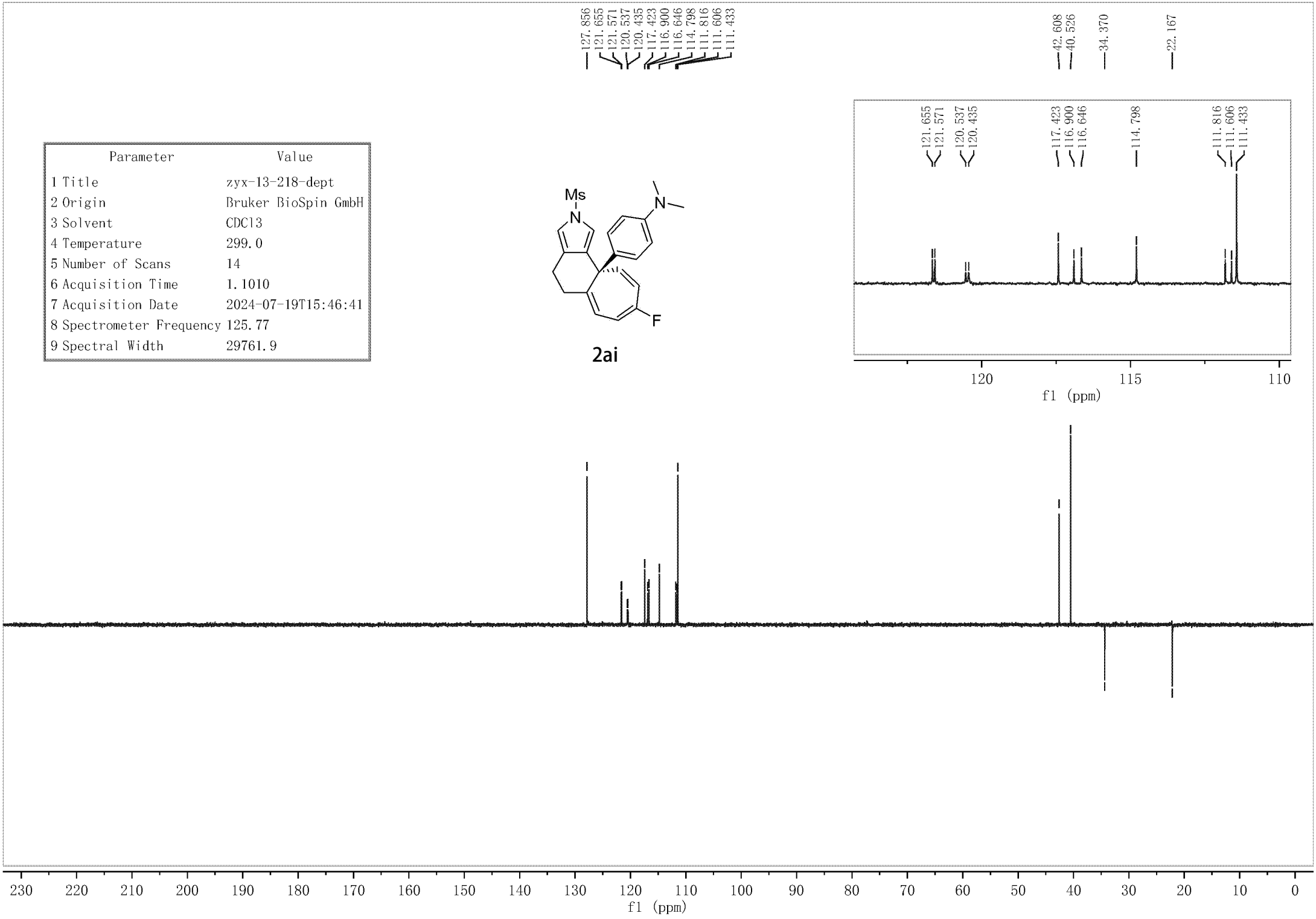

130.79
128.08
127.57
123.98
117.40
114.81
112.25
111.41
42.50
40.45
33.50
21.47
Parameter Value
1 Title zyx-13-175-dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 31
6 Acquisition Time 1.3631
7 Acquisition Date 2024-07-02T10:09:55
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
N
Br
2ah
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)


6.997
6.979
6.806
6.570
6.566
6.476
6.458
6.279
6.260
5.945
5.914
5.224
5.213
5.204
5.193
3.009
2.856
2.816
2.781
2.748
2.470
2.447
2.430
0.000
Parameter Value
1 Title zyx-13-218-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.6
5 Number of Scans 10
6 Acquisition Time 3.1719
7 Acquisition Date 2024-07-19T15:38:17
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Ms
N
N
F
2ai
2.01
0.97
0.96
2.00
1.00
0.98
0.97
0.98
3.00
5.99
3.02
1.00
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
-1.
f1 (ppm)


161.64
159.70
148.74
136.09
131.10
127.75
125.03
124.97
121.55
121.47
120.42
120.32
117.32
116.80
116.54
114.70
111.71
111.50
111.33
77.25
77.00
76.75
44.56
42.50
40.42
34.27
22.07
Parameter Value
1 Title zyx-13-218-c
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.7
5 Number of Scans 83
6 Acquisition Time 1.1010
7 Acquisition Date 2024-07-19T15:41:24
8 Spectrometer Frequency 125.77
9 Spectral Width 29761.9
Ms
N
N
F
2ai
f1 (ppm)
f1 (ppm)

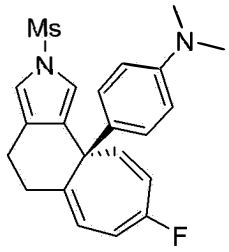
Parameter	Value
1 Title	zyx-13-218-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	299.0
5 Number of Scans	14
6 Acquisition Time	1.1010
7 Acquisition Date	2024-07-19T15:46:41
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

2ai

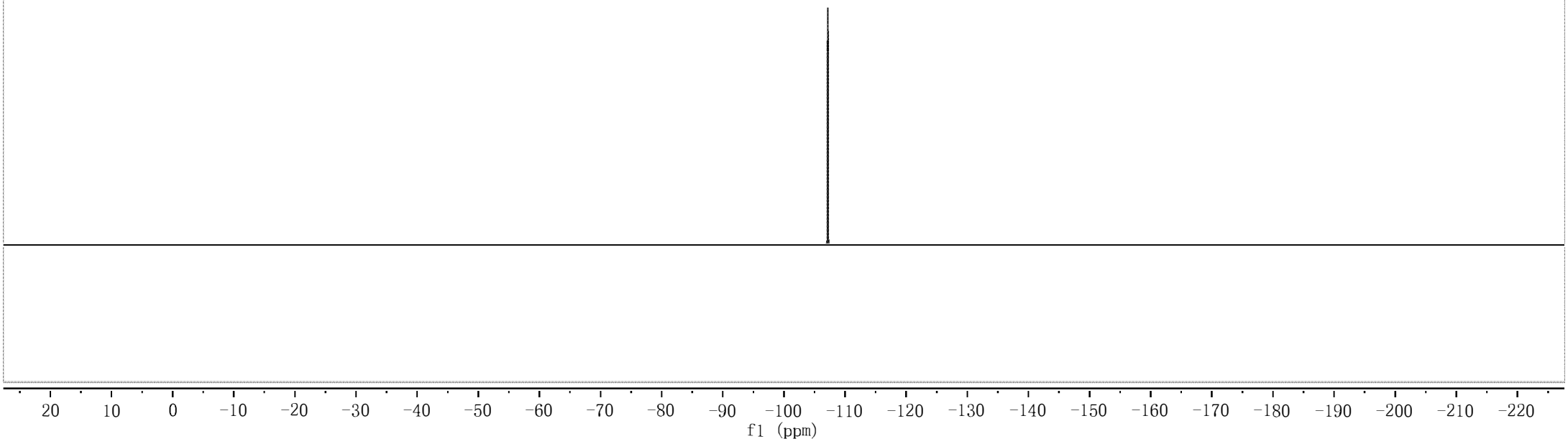


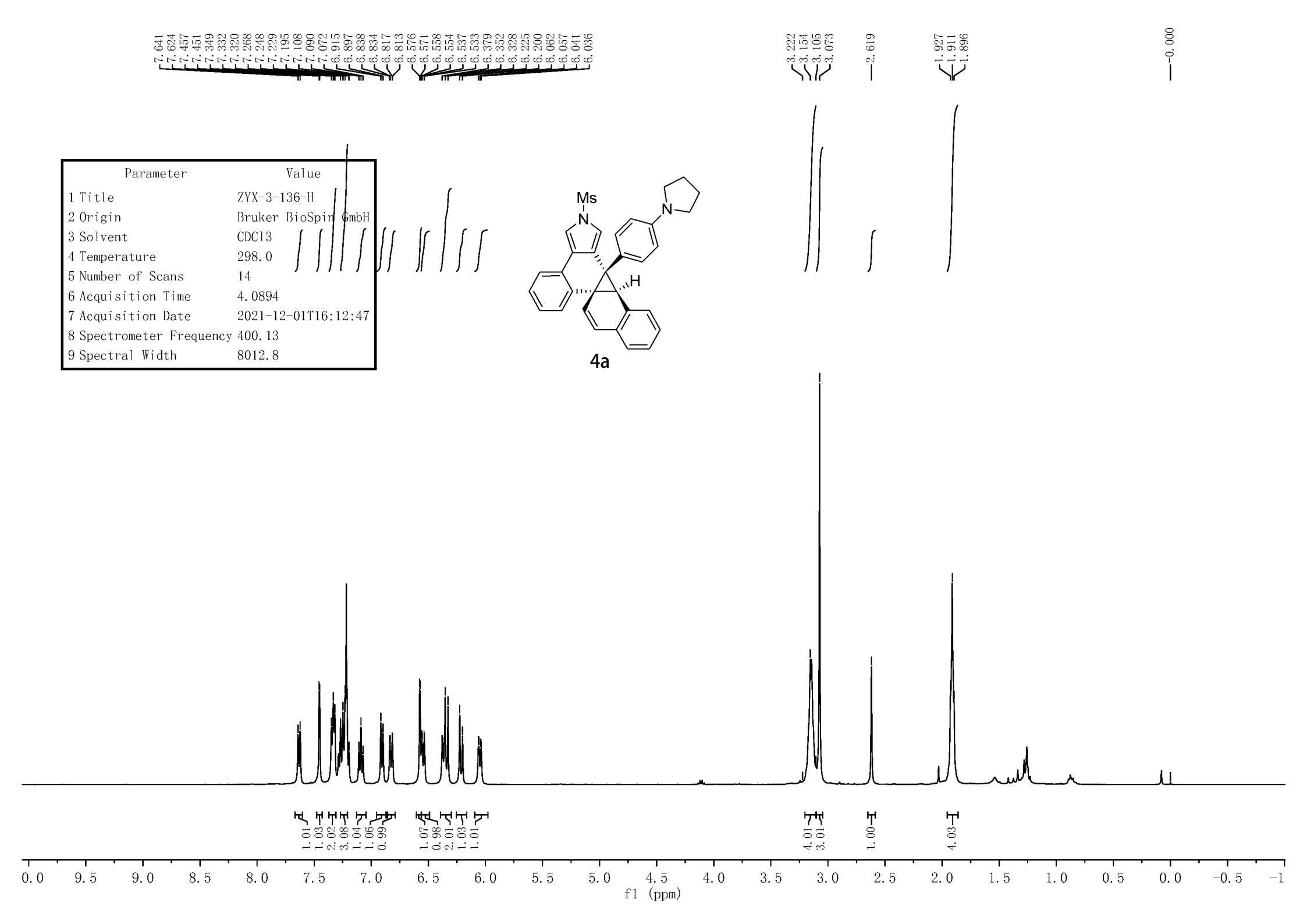
-107.155
-107.172
-107.194
-107.211

Parameter	Value
1 Title	zyx-13-206-f
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.1
5 Number of Scans	16
6 Acquisition Time	1.0000
7 Acquisition Date	2024-07-15T03:13:21
8 Spectrometer Frequency	376.27
9 Spectral Width	96153.0

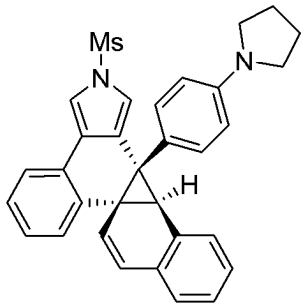


2ai

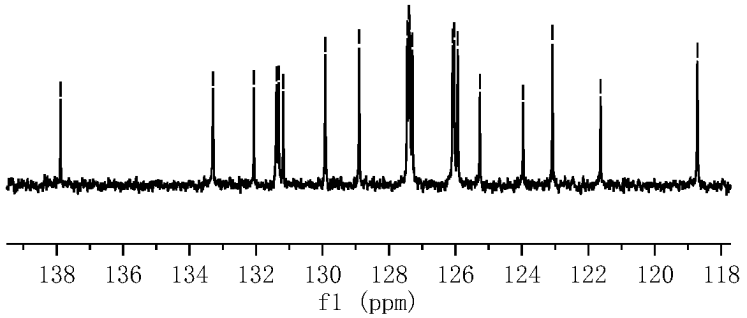


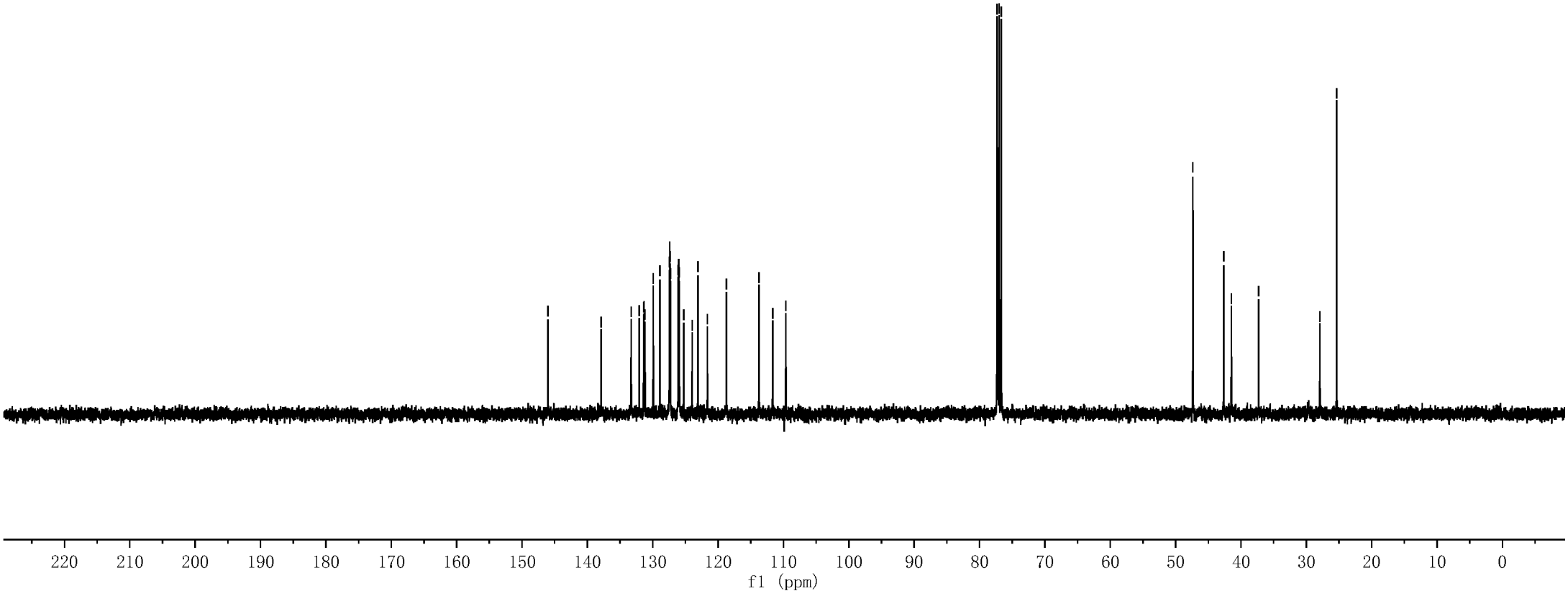

7.641
7.624
7.457
7.451
7.349
7.332
7.320
7.268
7.248
7.229
7.195
7.108
7.090
7.072
6.915
6.897
6.838
6.834
6.817
6.813
6.576
6.571
6.558
6.554
6.537
6.533
6.379
6.352
6.328
6.225
6.200
6.062
6.057
6.041
6.036
3.222
3.154
3.105
3.073
2.619
1.927
1.911
1.896
0.000
Parameter Value
1 Title ZYX-3-136-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 14
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-01T16:12:47
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
4a
1.01
1.03
2.02
3.08
1.04
1.06
0.99
1.07
0.98
2.01
1.03
1.01
4.01
3.01
1.00
4.03
0.0
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
-1
f1 (ppm)

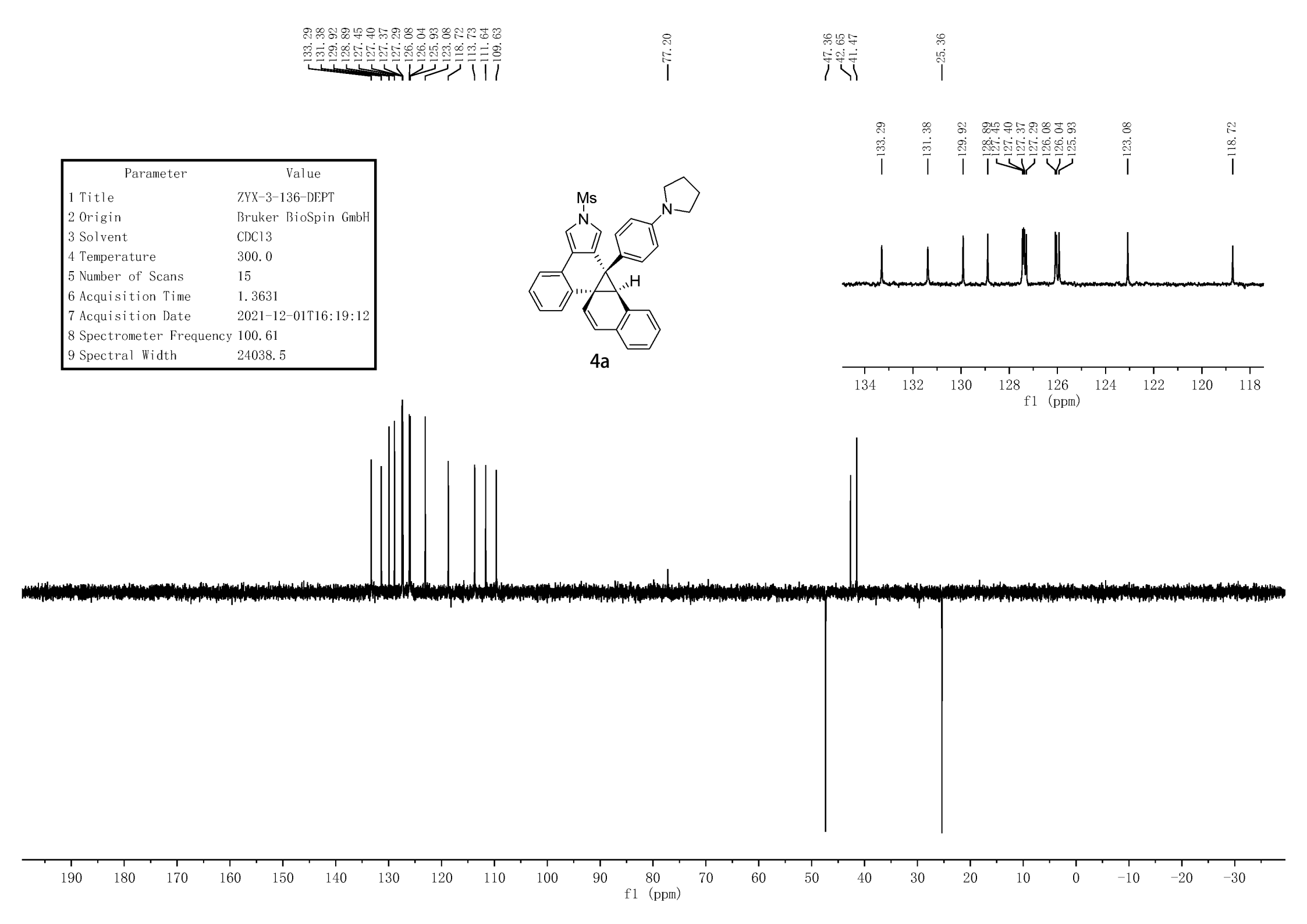
Parameter	Value
1 Title	ZYX-3-136-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	56
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-01T16:15:00
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

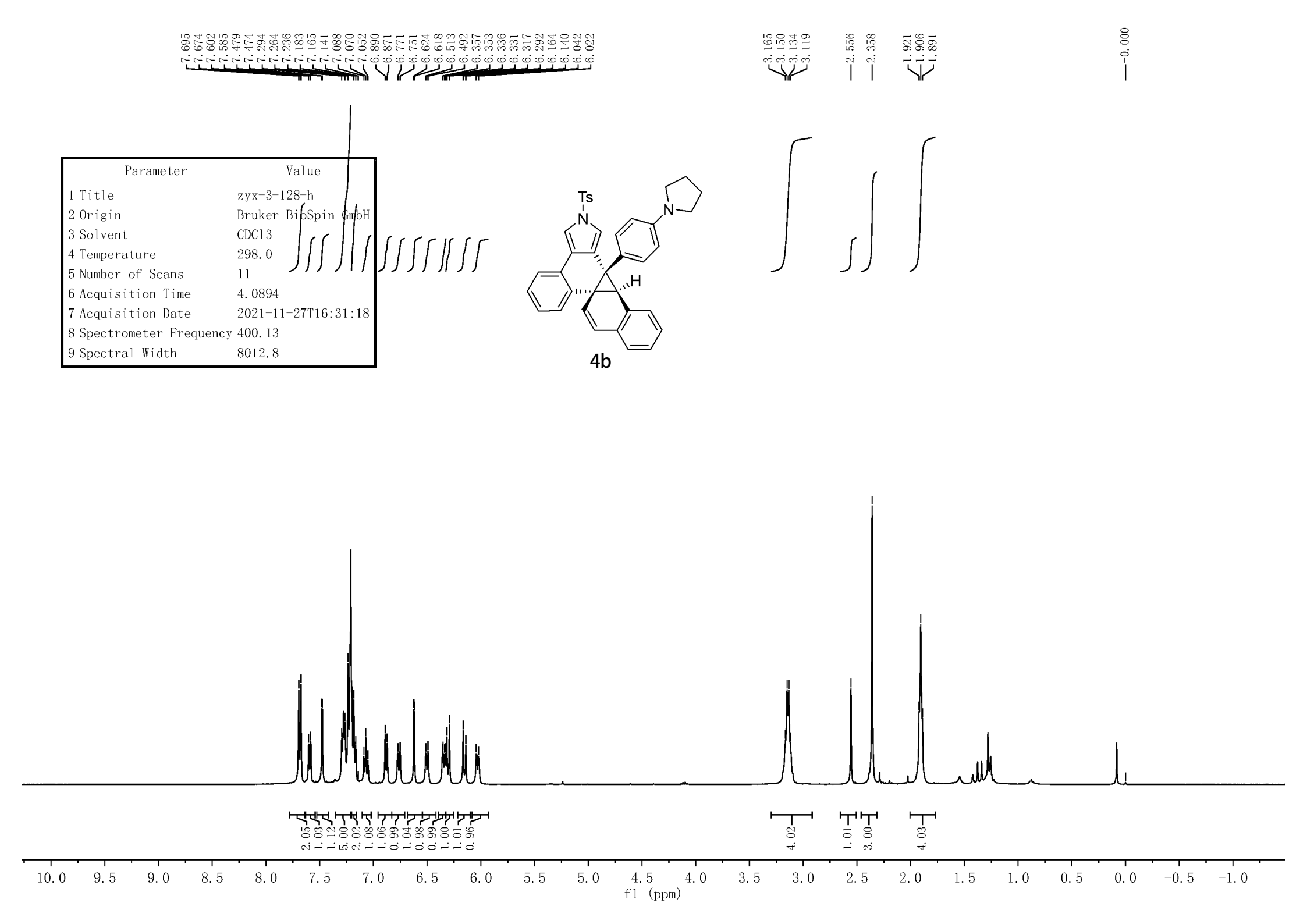


4a



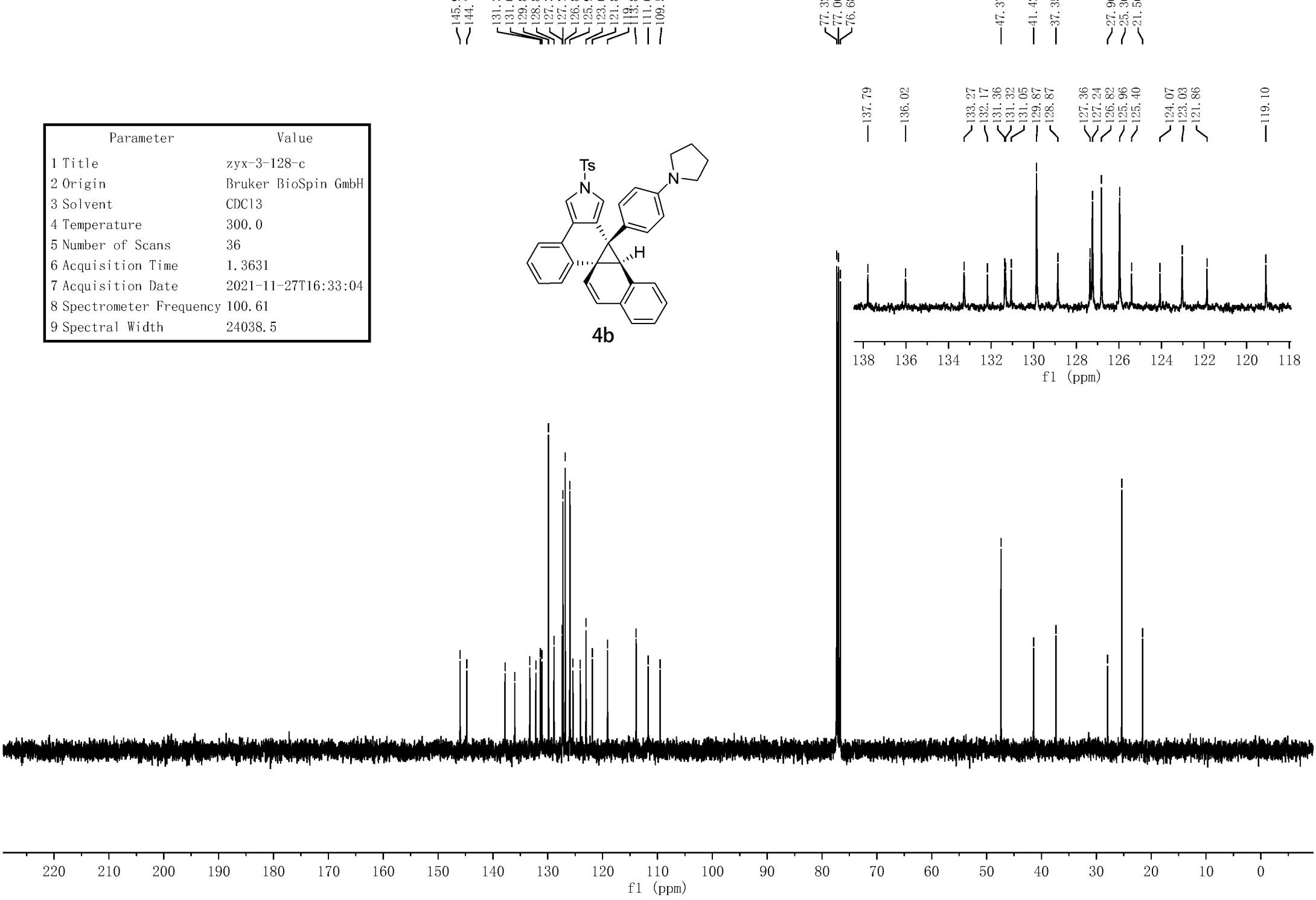



133.29
131.38
129.92
128.89
127.45
127.40
127.37
127.29
126.08
126.04
125.93
123.08
118.72
113.73
111.64
109.63
77.20
47.36
42.65
41.47
25.36
Parameter Value
1 Title ZYX-3-136-DEPT
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 15
6 Acquisition Time 1.3631
7 Acquisition Date 2021-12-01T16:19:12
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
N
H
4a
f1 (ppm)
f1 (ppm)

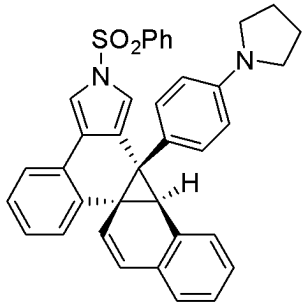

7.695
7.674
7.602
7.585
7.479
7.474
7.294
7.264
7.236
7.183
7.165
7.141
7.088
7.070
7.052
6.890
6.871
6.771
6.751
6.624
6.618
6.513
6.492
6.357
6.353
6.336
6.331
6.317
6.292
6.164
6.140
6.042
6.022
3.165
3.150
3.134
3.119
2.556
2.358
1.921
1.906
1.891
0.000
Parameter Value
1 Title zyx-3-128-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 11
6 Acquisition Time 4.0894
7 Acquisition Date 2021-11-27T16:31:18
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ts
N
N
H
4b
2.05
1.03
1.12
5.00
2.02
1.08
1.06
0.99
1.04
0.98
0.99
1.00
1.01
0.96
4.02
1.01
3.00
4.03
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
-1.0
f1 (ppm)

Parameter	Value
1 Title	zyx-3-128-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	36
6 Acquisition Time	1.3631
7 Acquisition Date	2021-11-27T16:33:04
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

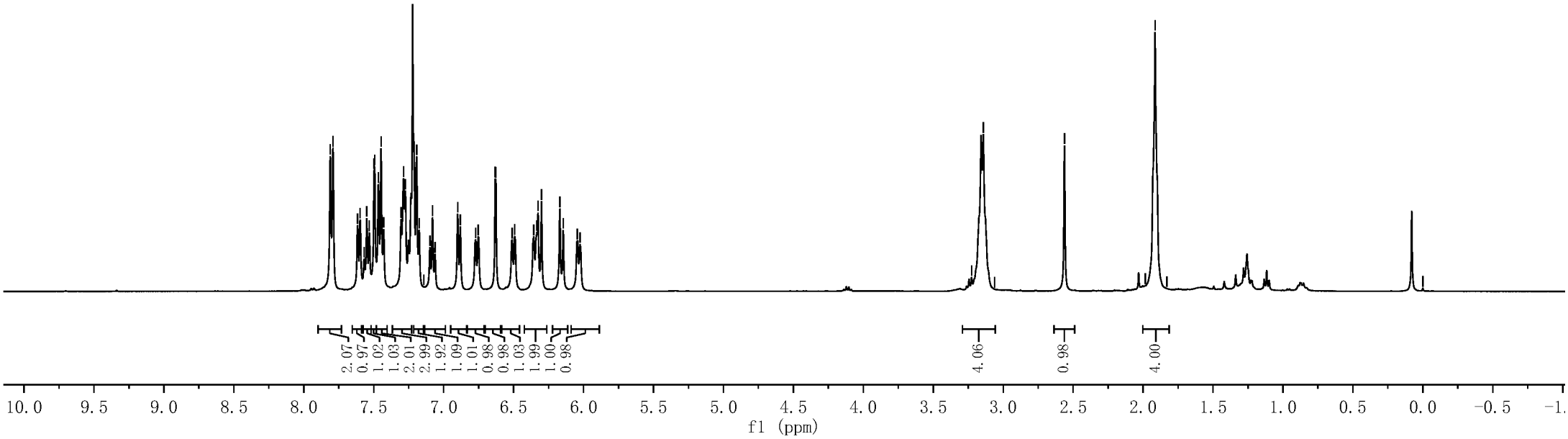
4b



Parameter	Value
1 Title	zyx-3-150-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	16
6 Acquisition Time	4.0894
7 Acquisition Date	2021-12-07T15:56:24
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

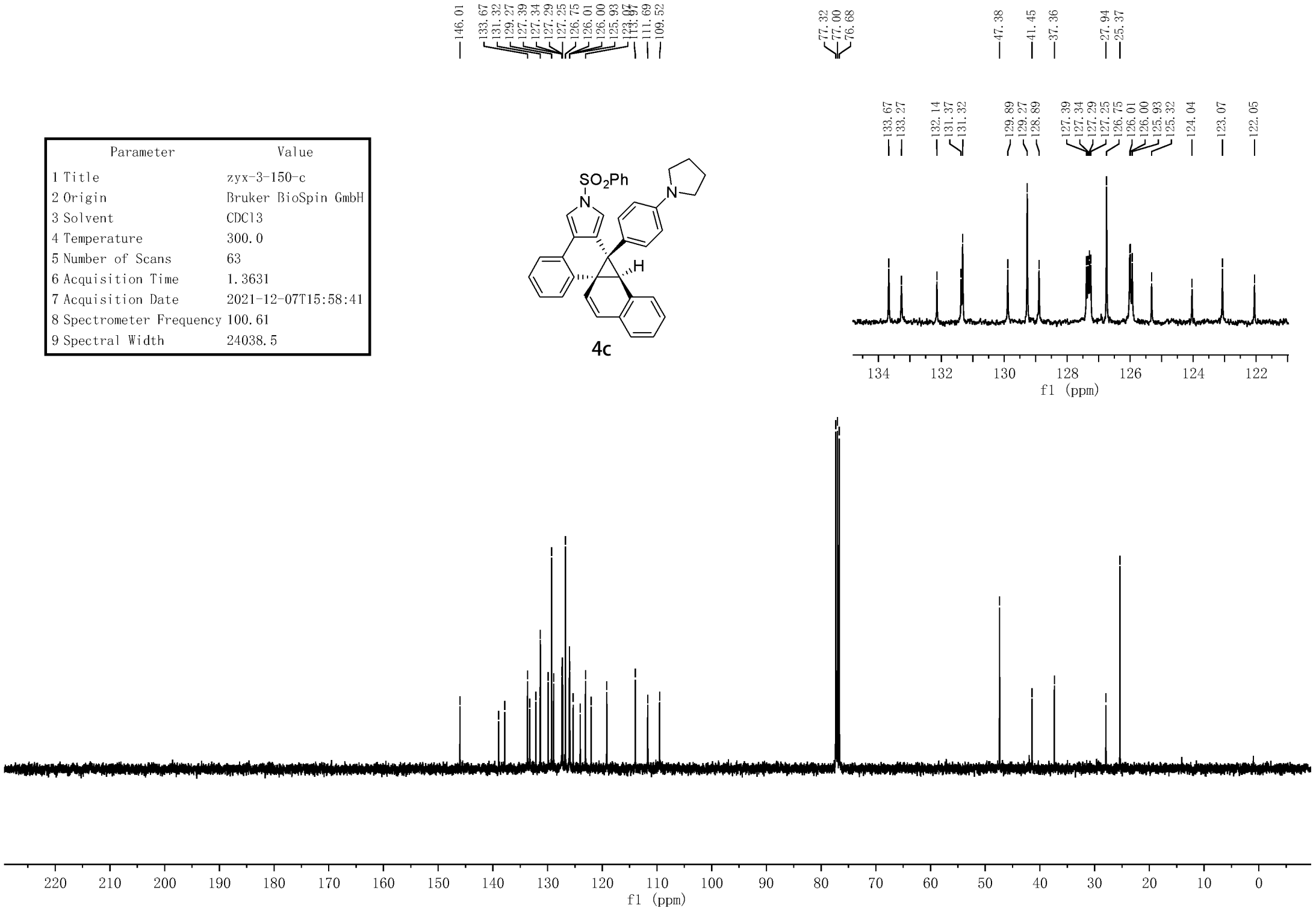


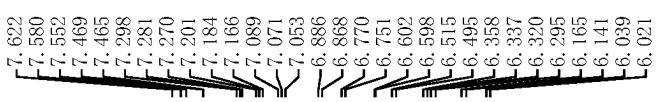
4c

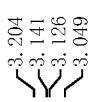


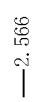
Parameter	Value
1 Title	zyx-3-150-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	63
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-07T15:58:41
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

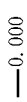
4c



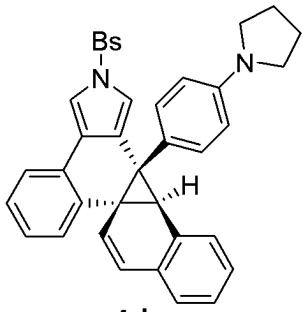




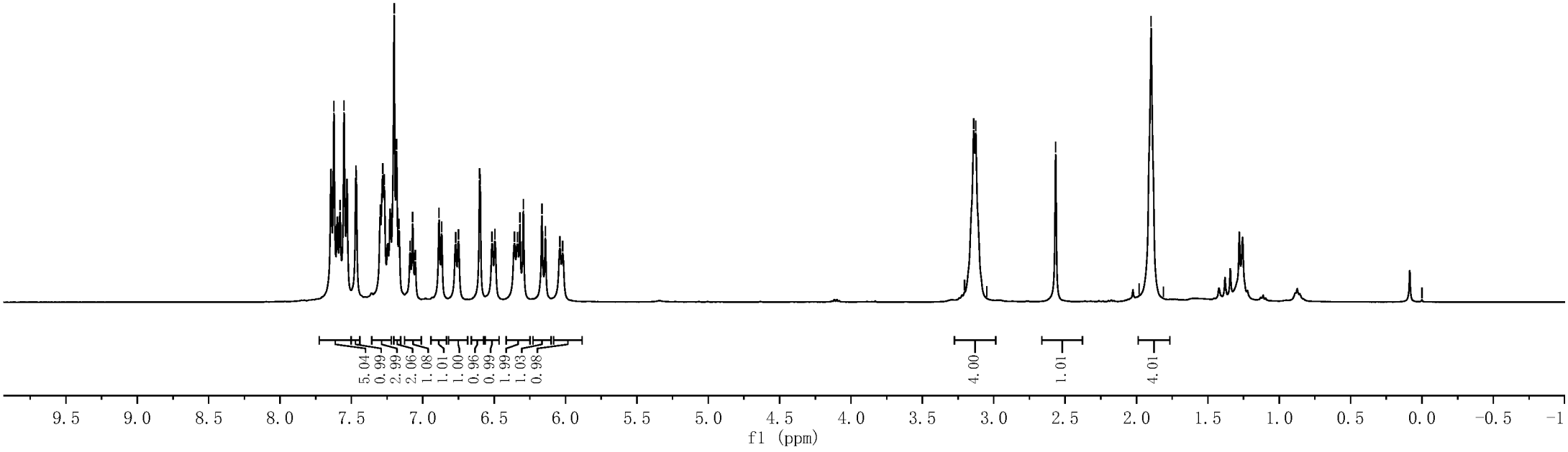




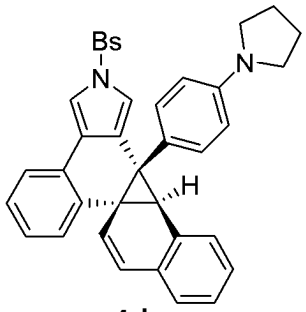
Parameter	Value
1 Title	zyx-3-151-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	12
6 Acquisition Time	4.0894
7 Acquisition Date	2021-12-03T16:13:57
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



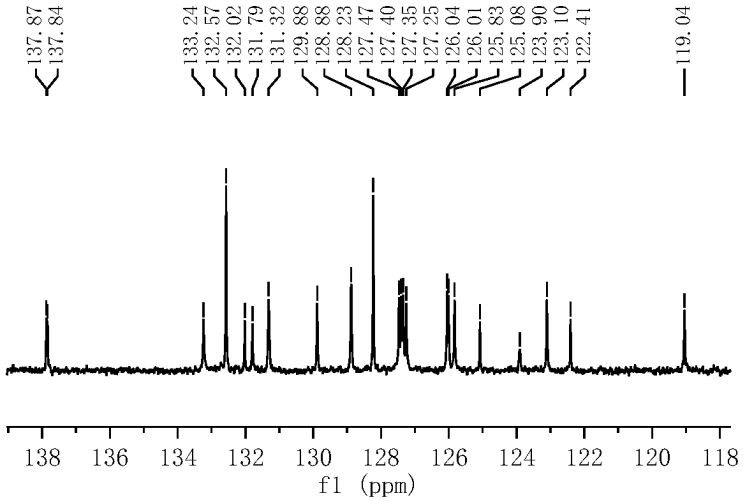
4d

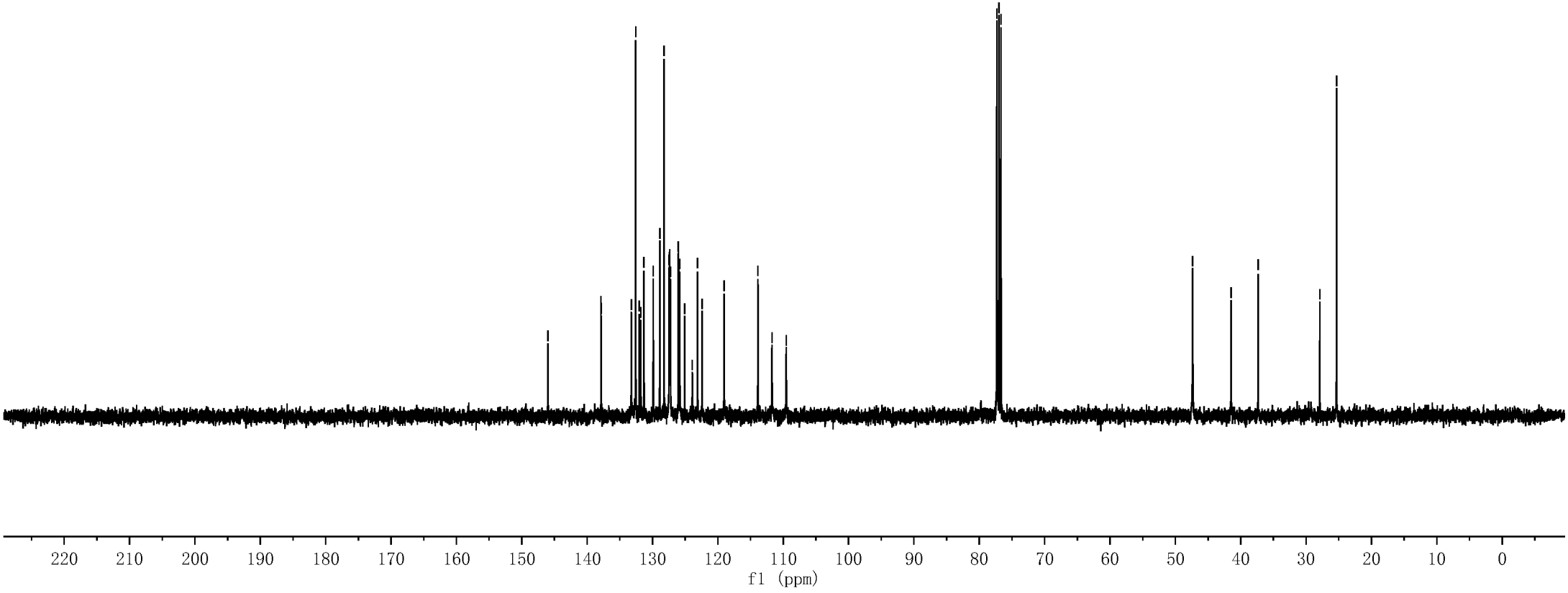


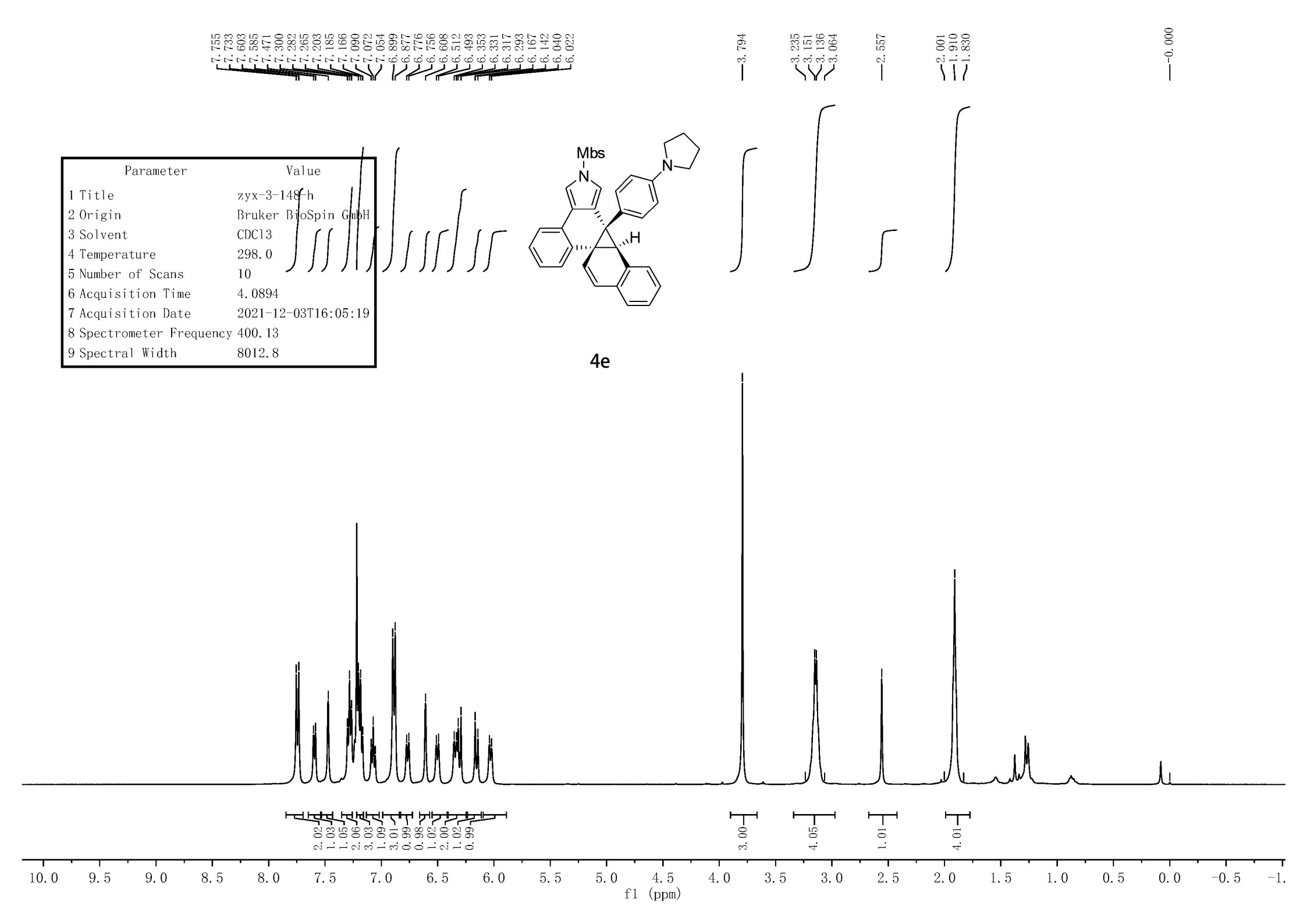
Parameter	Value
1 Title	zyx-3-151-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	53
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-03T16:15:32
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



4d



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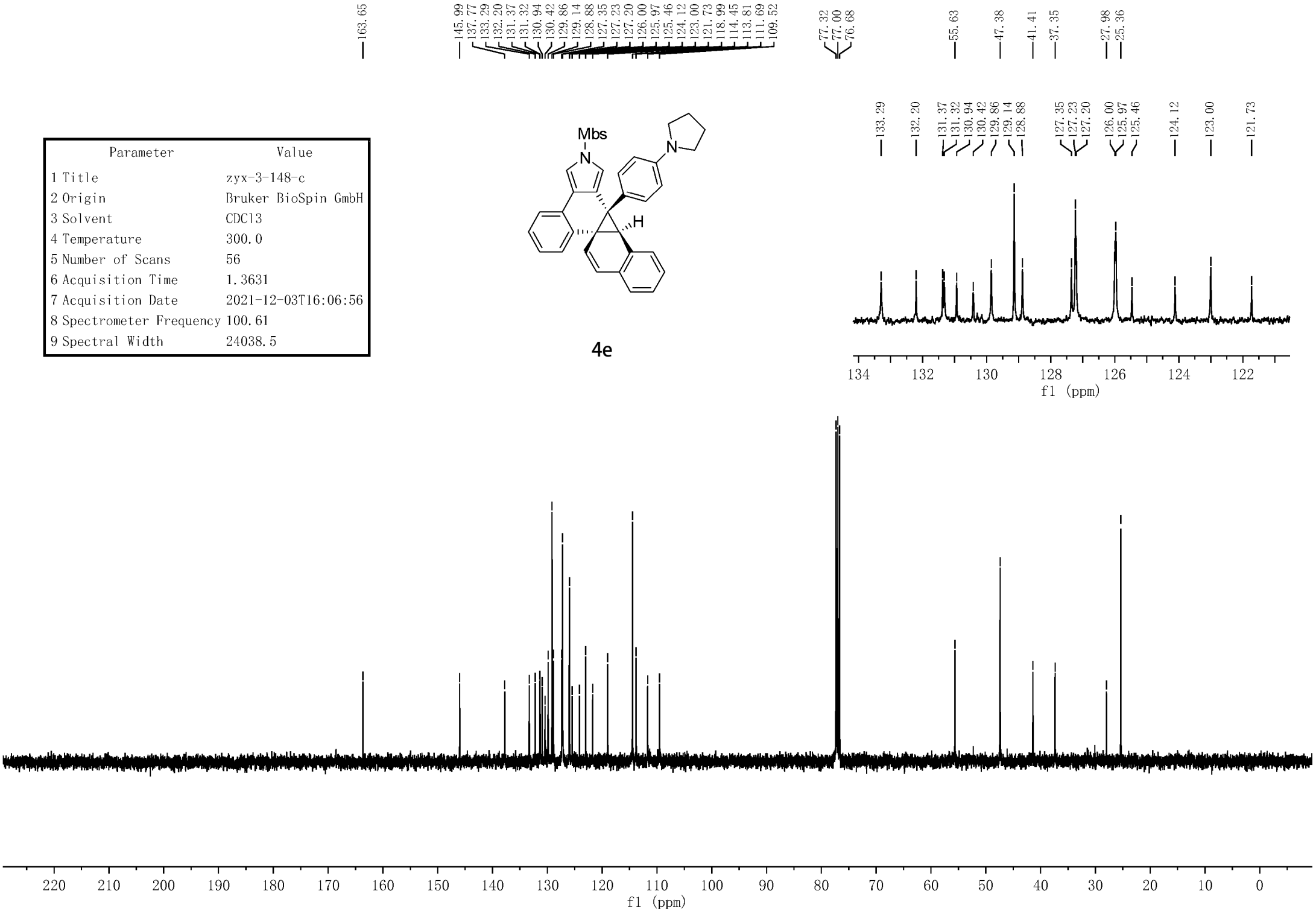
7.282
7.265
7.203
7.185
7.166
7.090
7.072
7.054
6.899
6.877
6.776
6.756
6.608
6.512
6.493
6.353
6.331
6.317
6.293
6.167
6.142
6.040
6.022
3.794
3.235
3.151
3.136
3.064
2.557
2.001
1.910
1.830
-0.000
Parameter Value
1 Title zyx-3-148-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 10
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-03T16:05:19
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Mbs
N
N
H
4e
2.02
1.03
1.05
2.06
3.03
1.09
3.01
0.99
0.98
1.02
2.00
1.02
0.99
3.00
4.05
1.01
4.01
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
-1.
f1 (ppm)

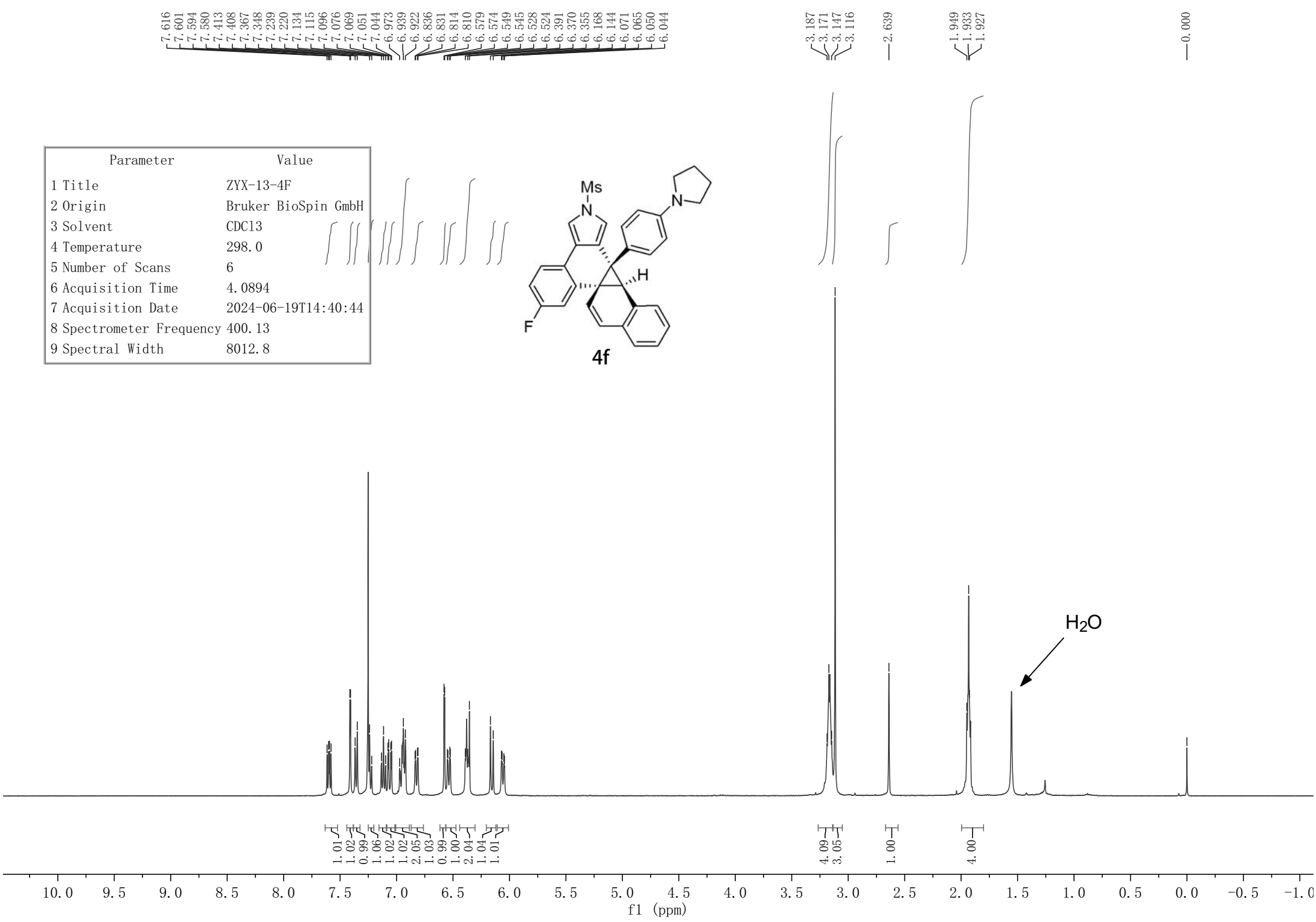
Parameter	Value
1 Title	zyx-3-148-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	56
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-03T16:06:56
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

4e

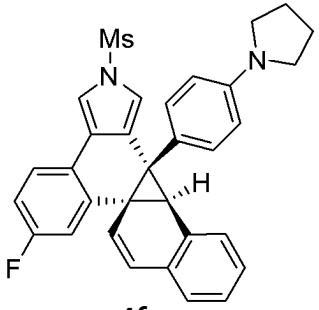


Parameter	Value
1 Title	ZYX-13-4F
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2024-06-19T14:40:44
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

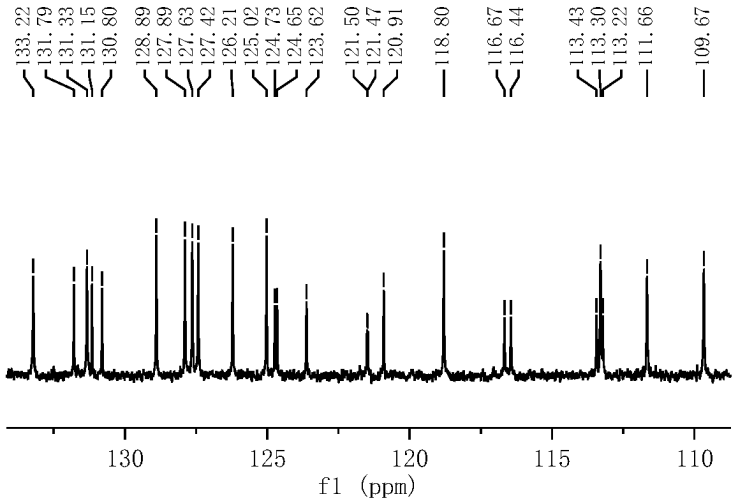
4f

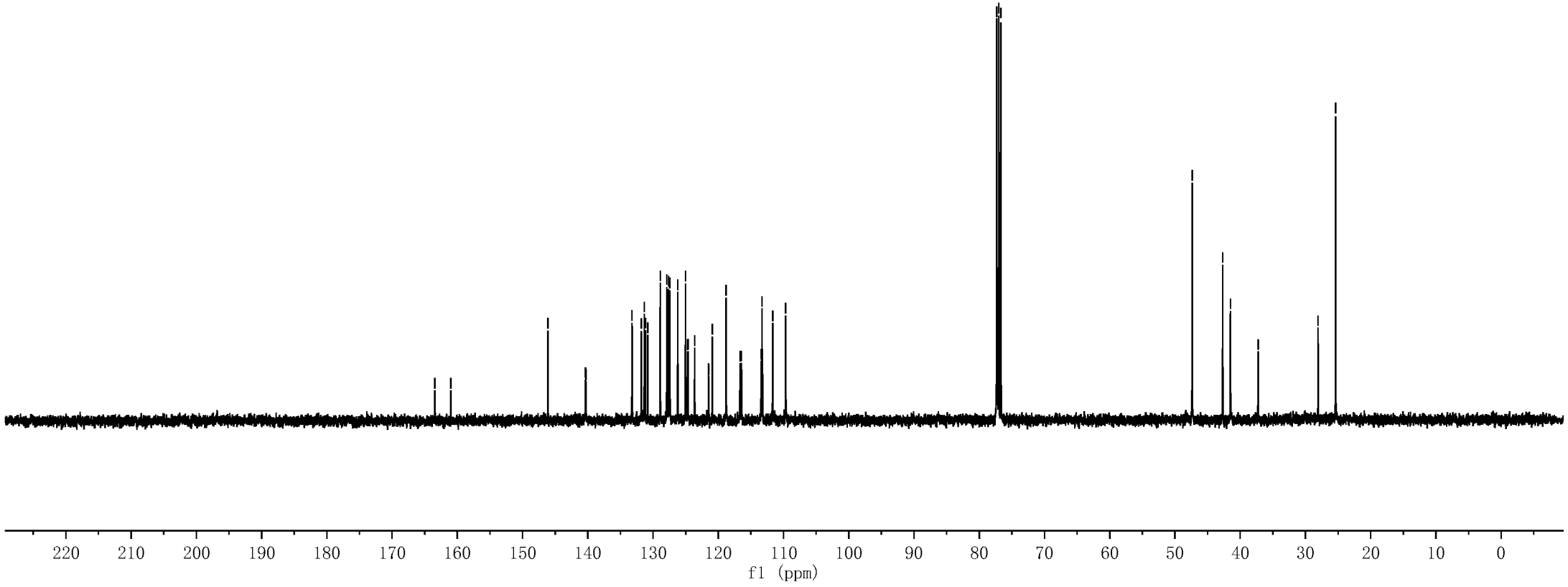


Parameter	Value
1 Title	ZYX-3-215--C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	105
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-25T16:44:02
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

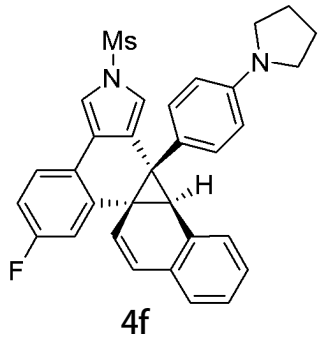


4f

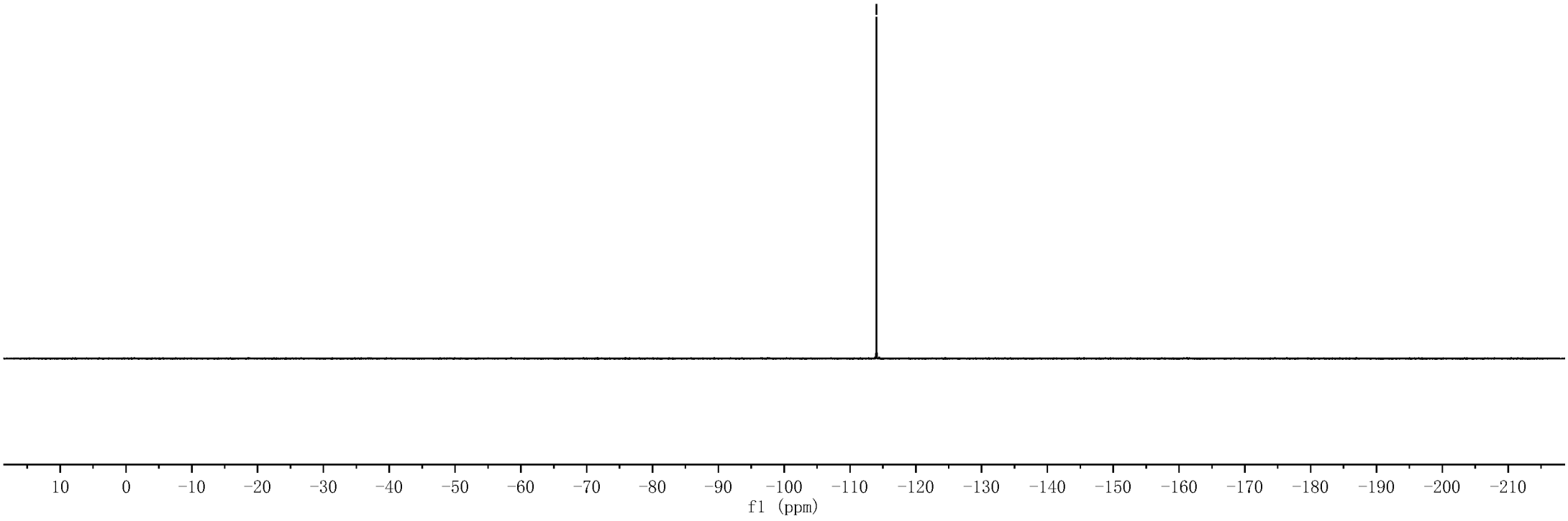


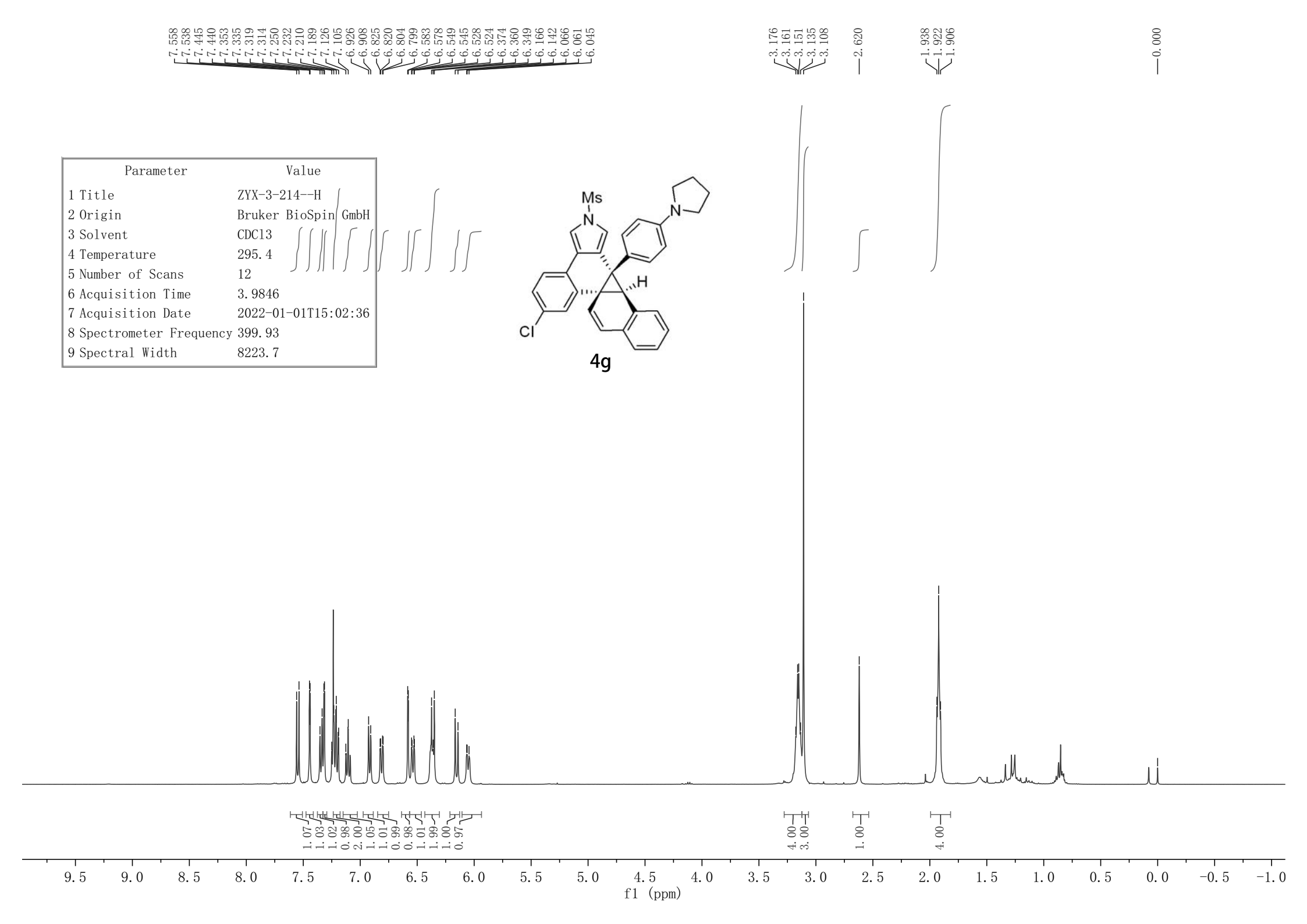


Parameter	Value
1 Title	zyx-3-215-f
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	16
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-19T11:00:19
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



4f

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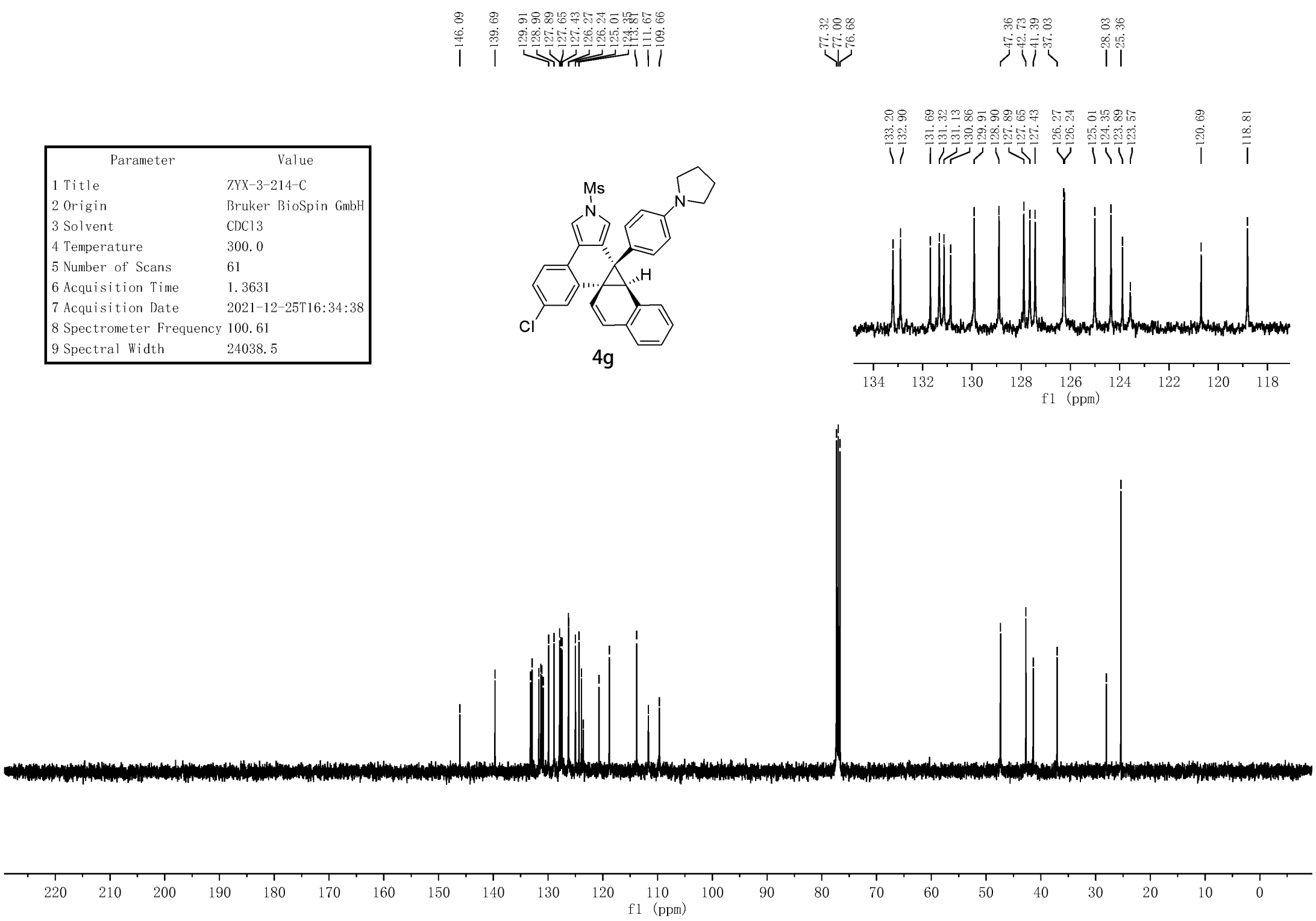
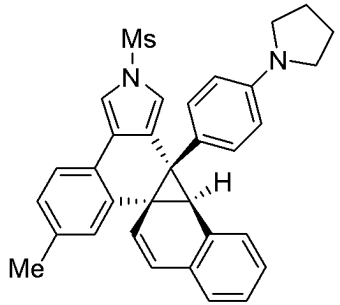
7.538
7.445
7.440
7.353
7.335
7.319
7.314
7.250
7.232
7.210
7.189
7.126
7.105
6.926
6.908
6.825
6.820
6.804
6.799
6.583
6.578
6.549
6.545
6.528
6.524
6.374
6.360
6.349
6.166
6.142
6.066
6.061
6.045
3.176
3.161
3.151
3.135
3.108
2.620
1.938
1.922
1.906
0.000
Parameter Value
1 Title ZYX-3-214--H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.4
5 Number of Scans 12
6 Acquisition Time 3.9846
7 Acquisition Date 2022-01-01T15:02:36
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
N
H
Cl
4g
1.07
1.03
1.02
0.98
2.00
1.05
1.01
0.99
0.98
1.01
1.99
1.00
0.97
4.00
3.00
1.00
4.00
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
-1.0
f1 (ppm)

Parameter	Value
1 Title	ZYX-3-214-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	61
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-25T16:34:38
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

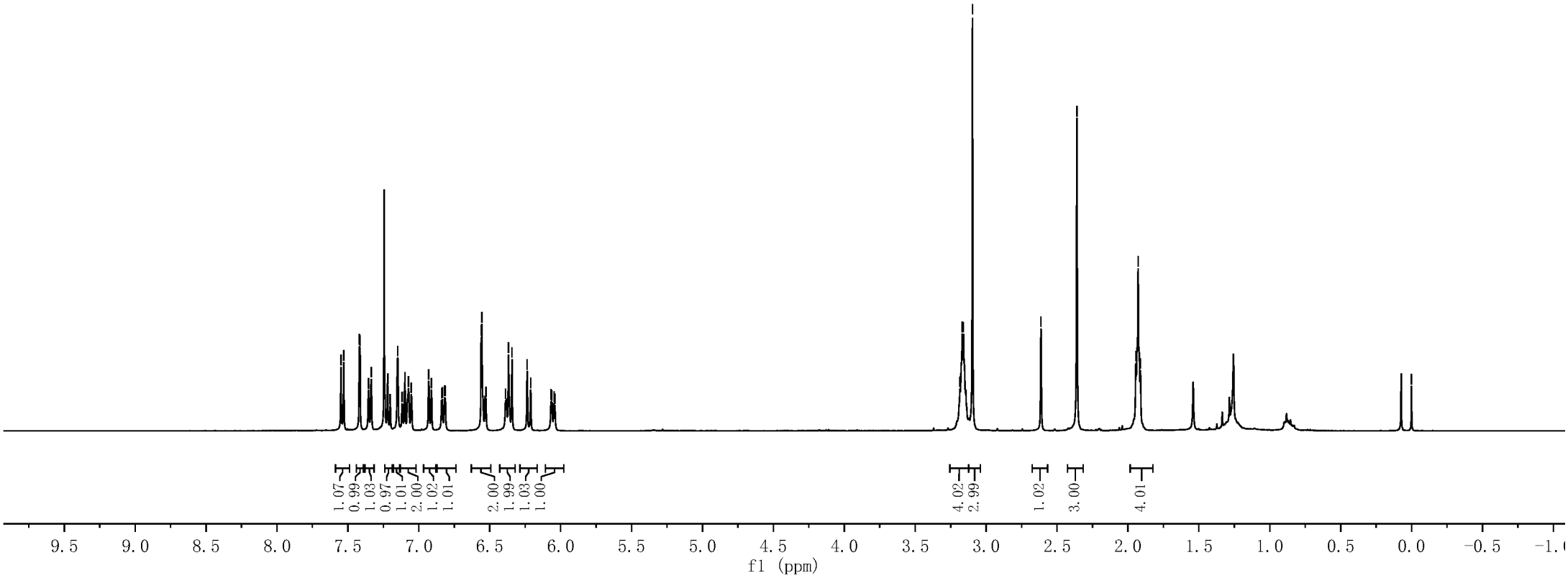
4g



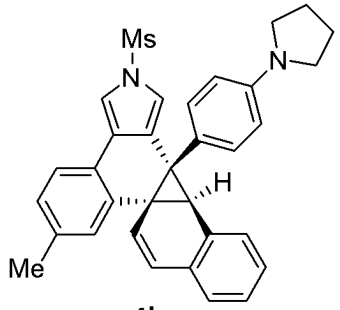
Parameter	Value
1 Title	zyx-3-206----h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	15
6 Acquisition Time	4.0894
7 Acquisition Date	2021-12-23T16:31:47
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



4h



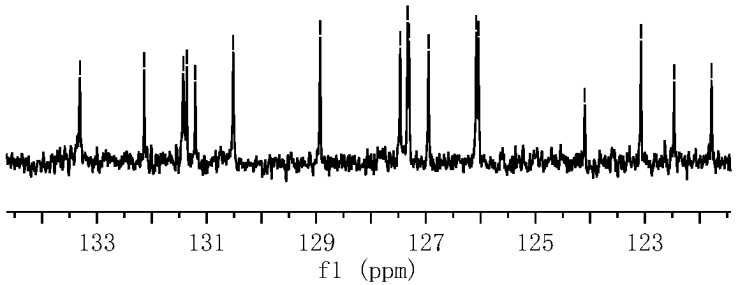
Parameter	Value
1 Title	zyx-3-206----c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	133
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-23T16:33:53
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

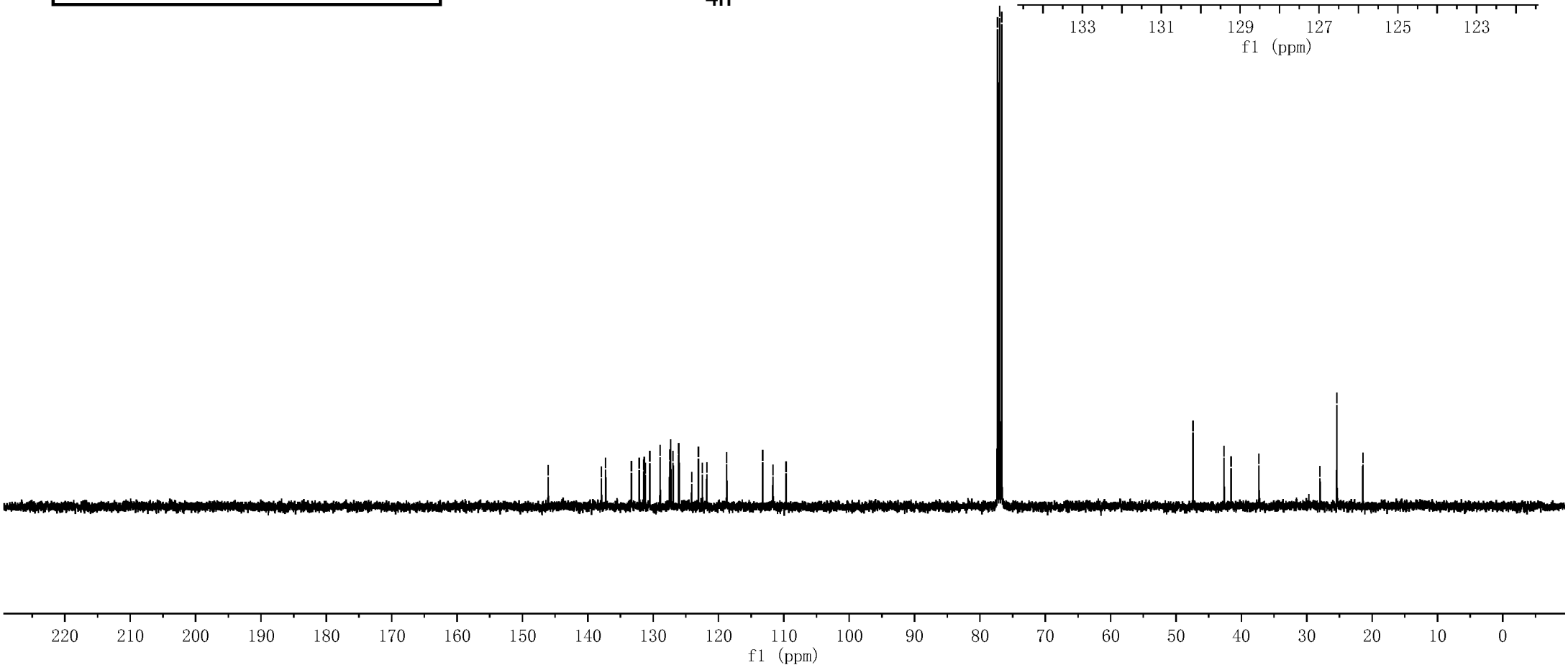


4h

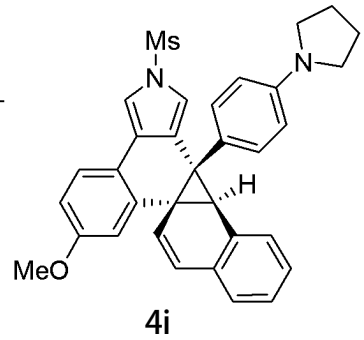
146.05
137.27
131.36
130.51
128.93
127.47
127.33
127.30
126.95
126.08
126.04
123.07
111.67
109.66
77.32
77.20
77.00
76.68
47.40
42.66
41.57
37.32
27.98
25.40
21.41

133.31
132.14
131.43
131.36
131.21
130.51
128.93
127.47
127.33
127.30
126.95
126.08
126.04
124.10
123.07
122.47
121.78

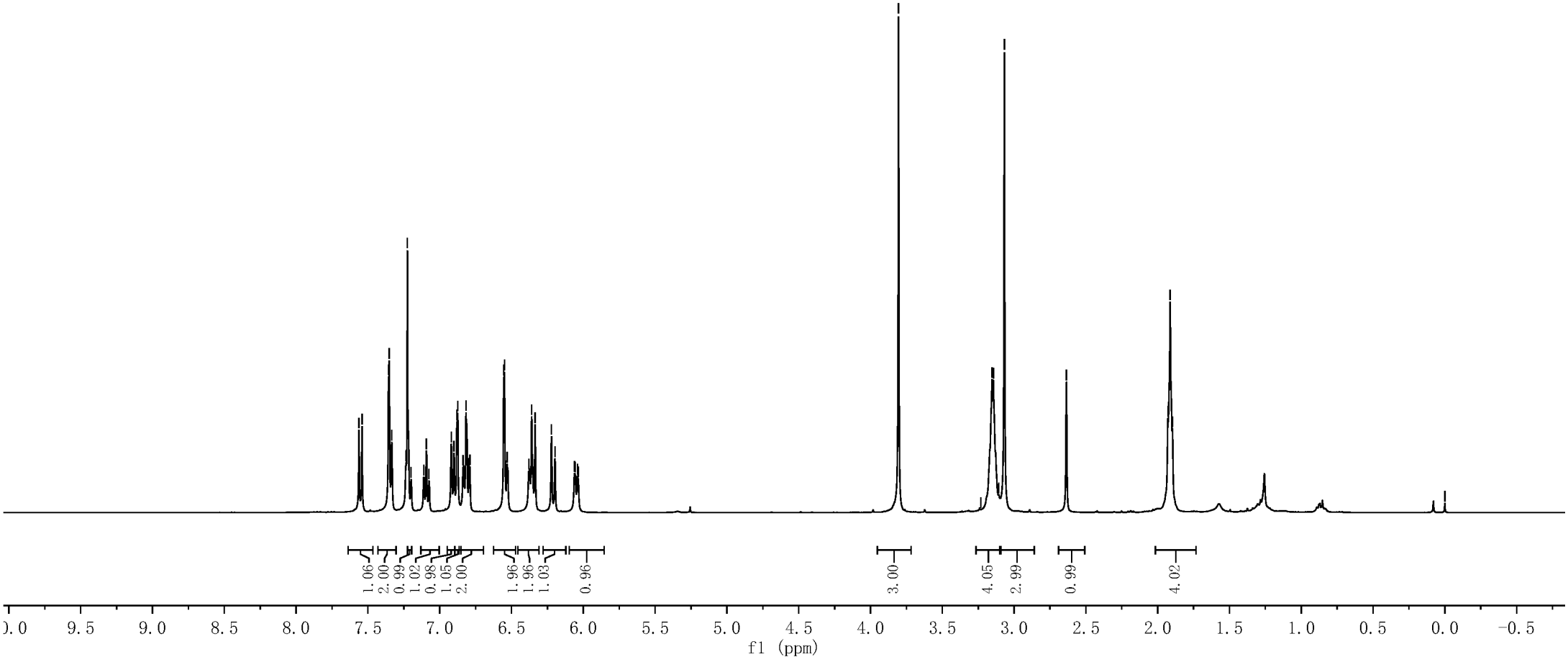




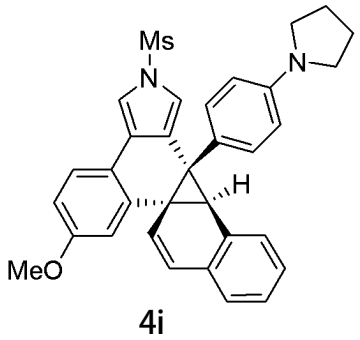
Parameter	Value
1 Title	ZYX-4-61-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-15T16:30:53
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



4i



Parameter	Value
1 Title	zyx-4-61-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	71
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-14T16:40:28
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



4i

159.18
146.03
139.61
133.27
132.09
131.36
131.28
130.83
128.89
127.56
127.50
127.29
126.05
125.69
124.42
123.96
121.64
118.74
118.11
114.77
112.50
112.44
111.64
109.63
77.32
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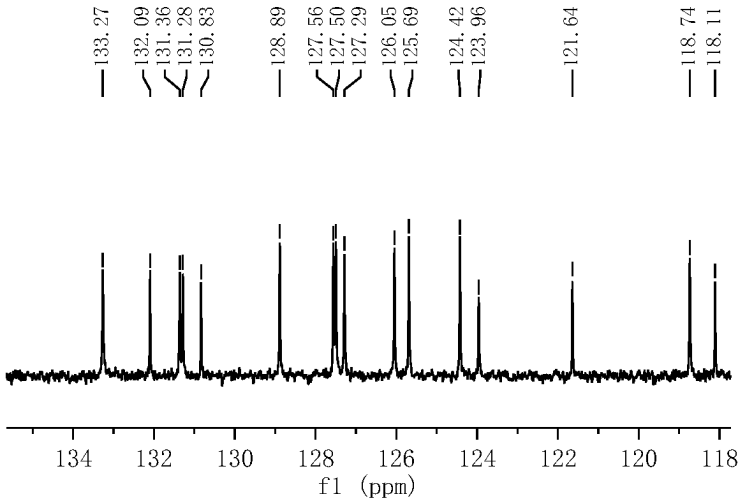
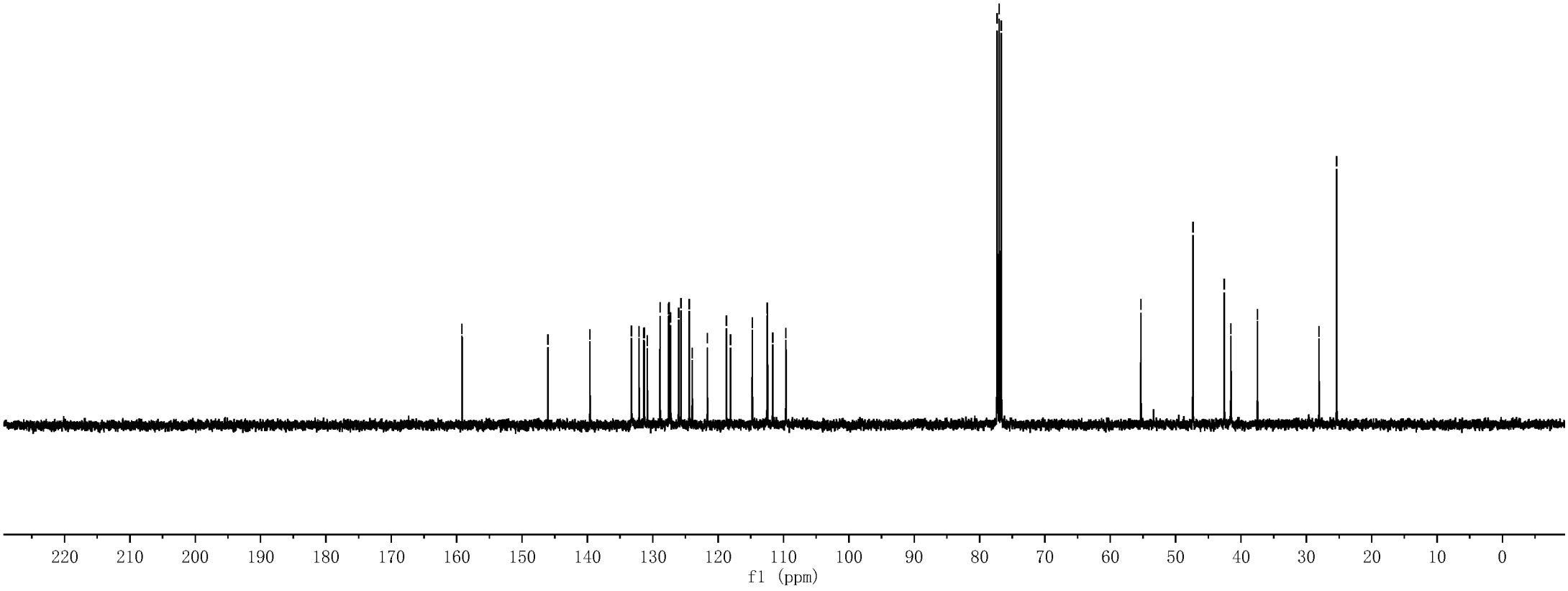
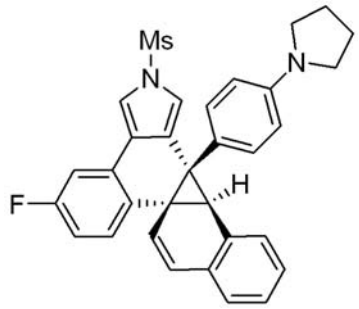
47.36
42.55
41.55
37.48
28.07
25.36

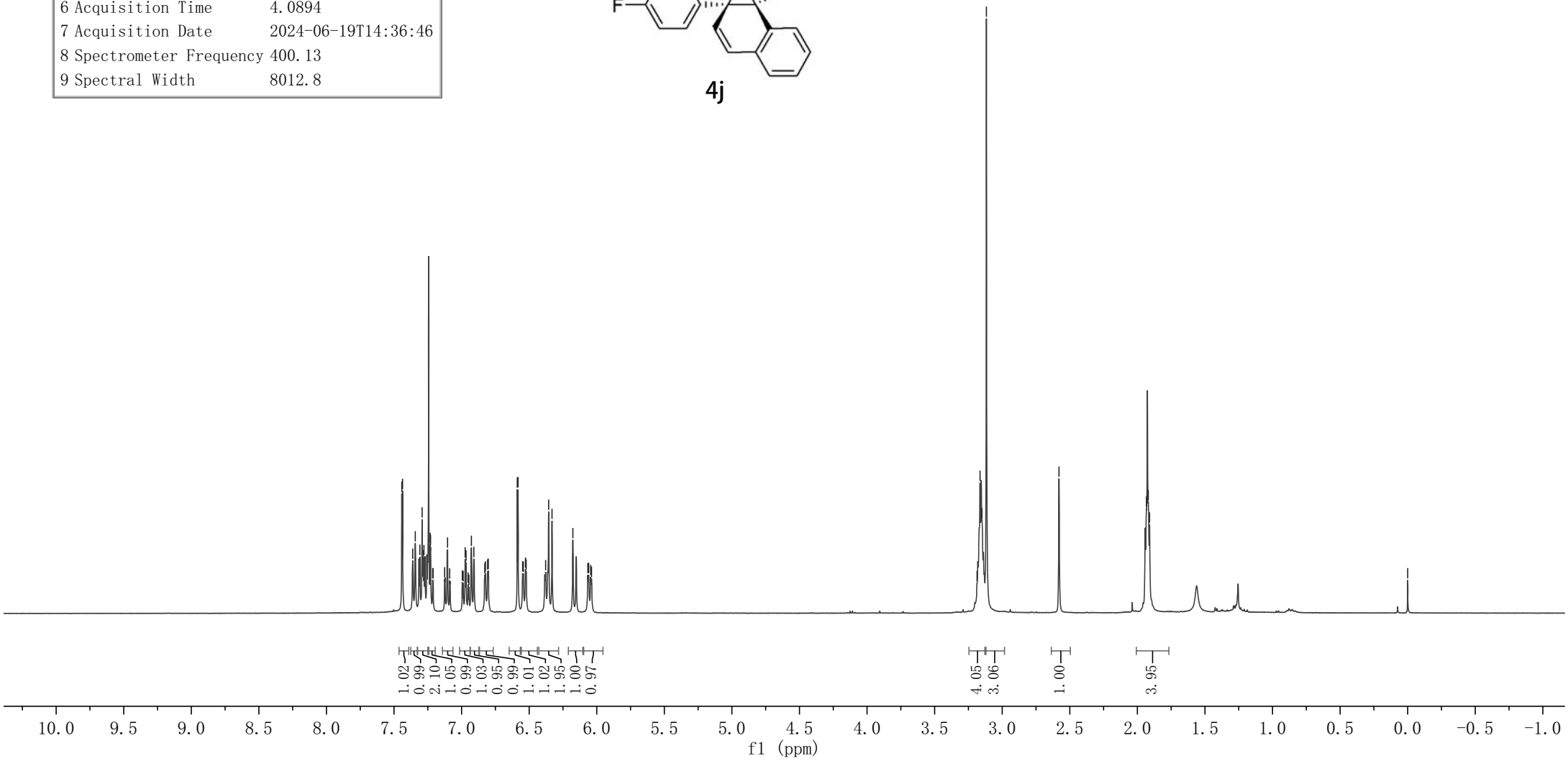




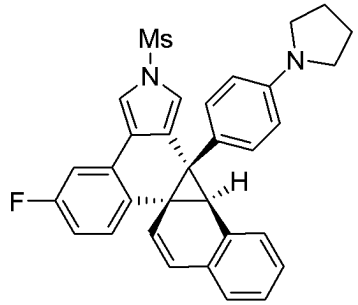
Parameter	Value
1 Title	ZYX-13-4J
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2024-06-19T14:36:46
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



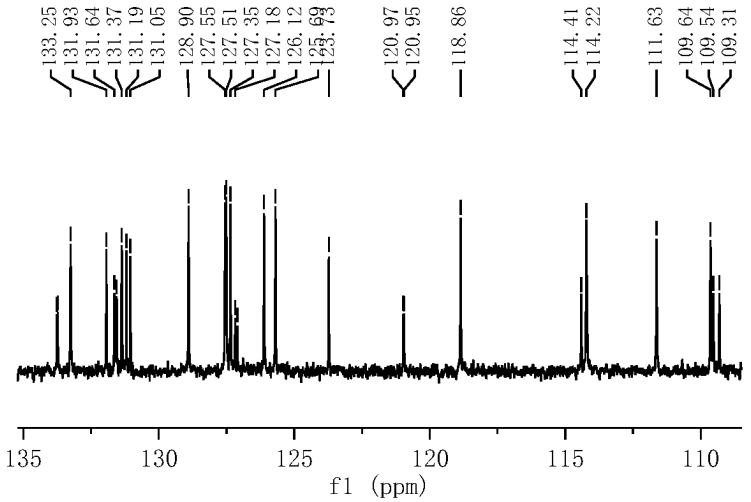
4j

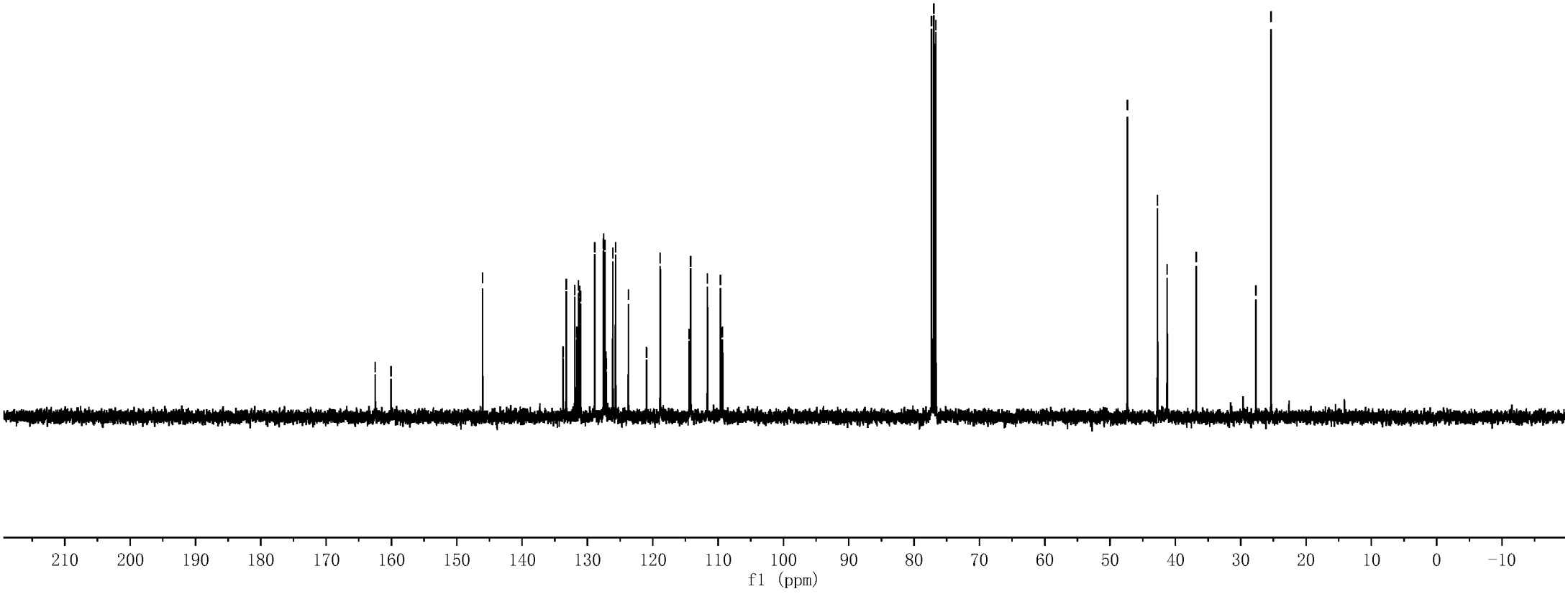


Parameter	Value
1 Title	ZYX-4-20-cc
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.8
5 Number of Scans	78
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-15T16:53:59
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

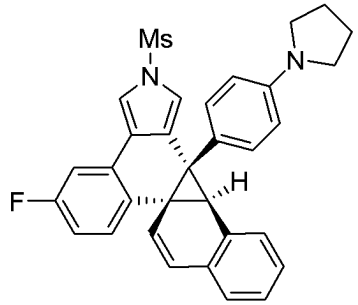


4j

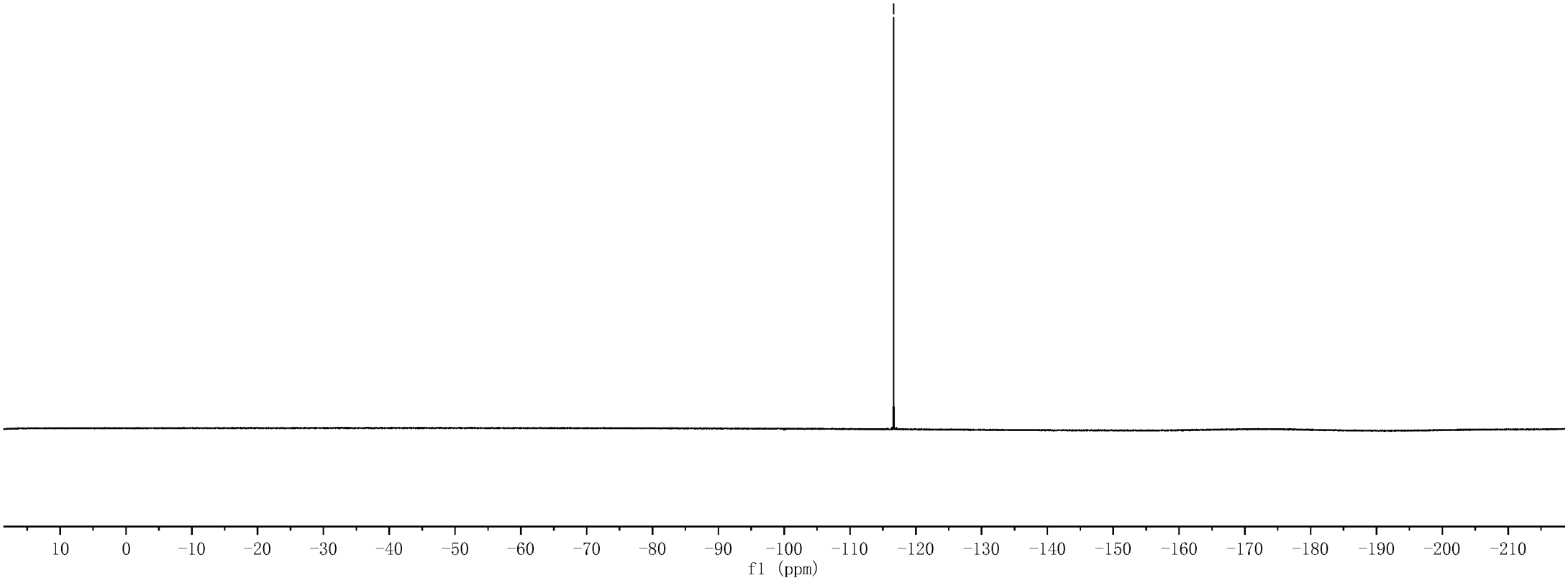




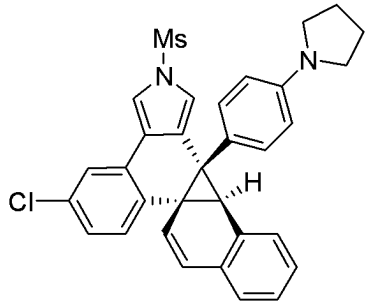
Parameter	Value
1 Title	ZYX-4-20-FF
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	10
6 Acquisition Time	0.7340
7 Acquisition Date	2022-01-15T16:47:06
8 Spectrometer Frequency	376.31
9 Spectral Width	89285.7



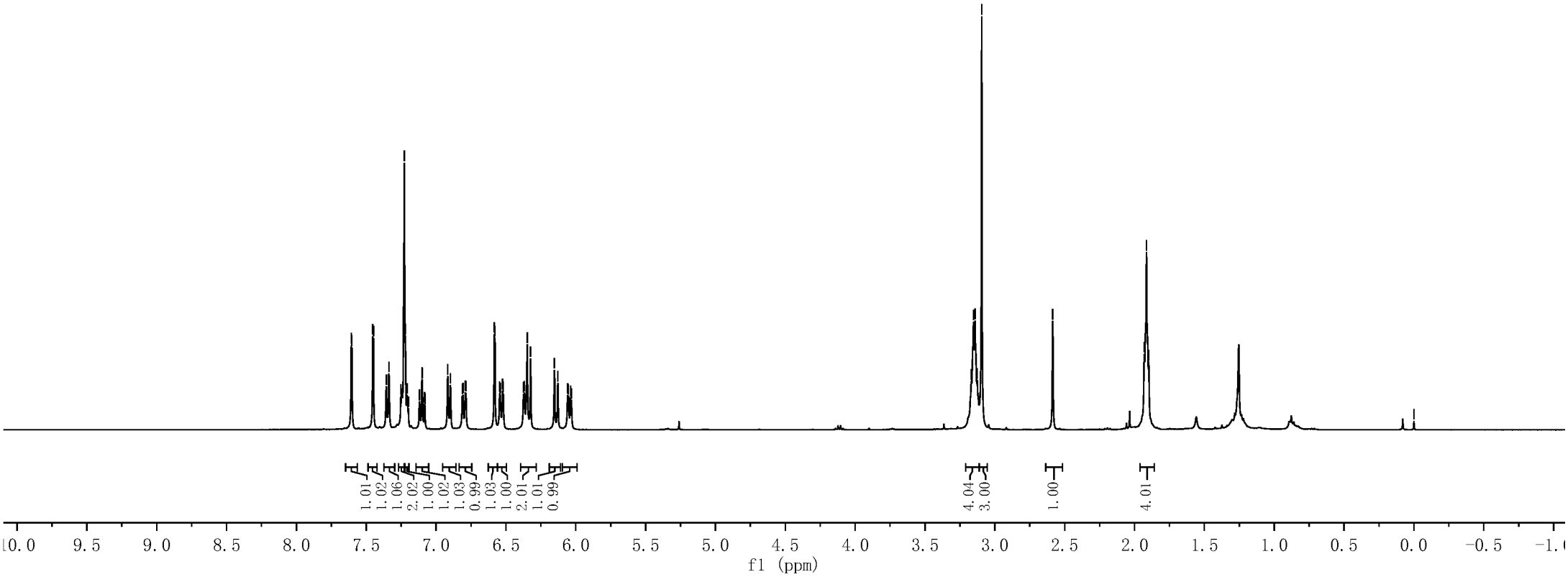
4j



Parameter	Value
1 Title	ZYX-4-9--H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.2
5 Number of Scans	14
6 Acquisition Time	3.9846
7 Acquisition Date	2022-01-19T16:19:13
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

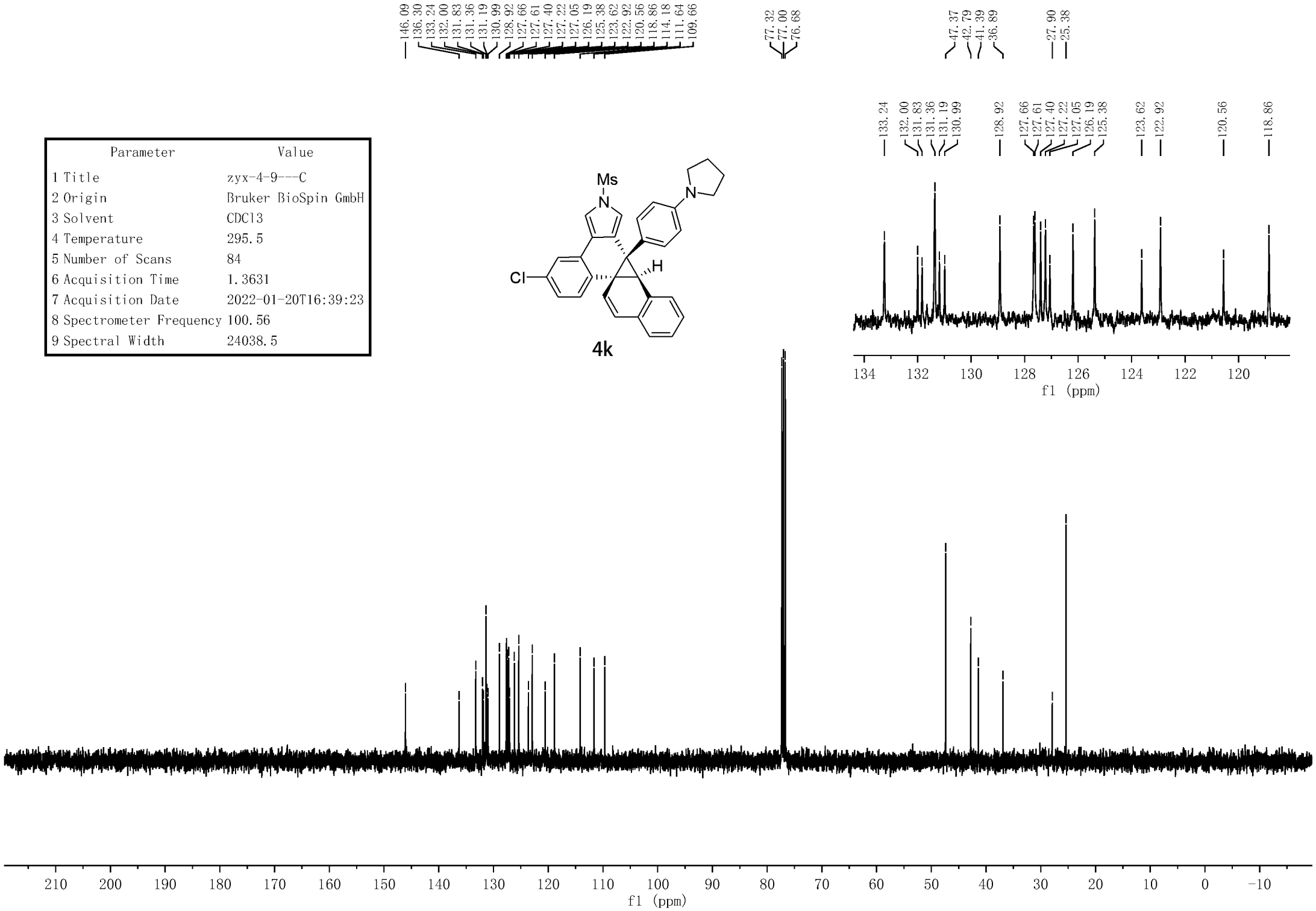


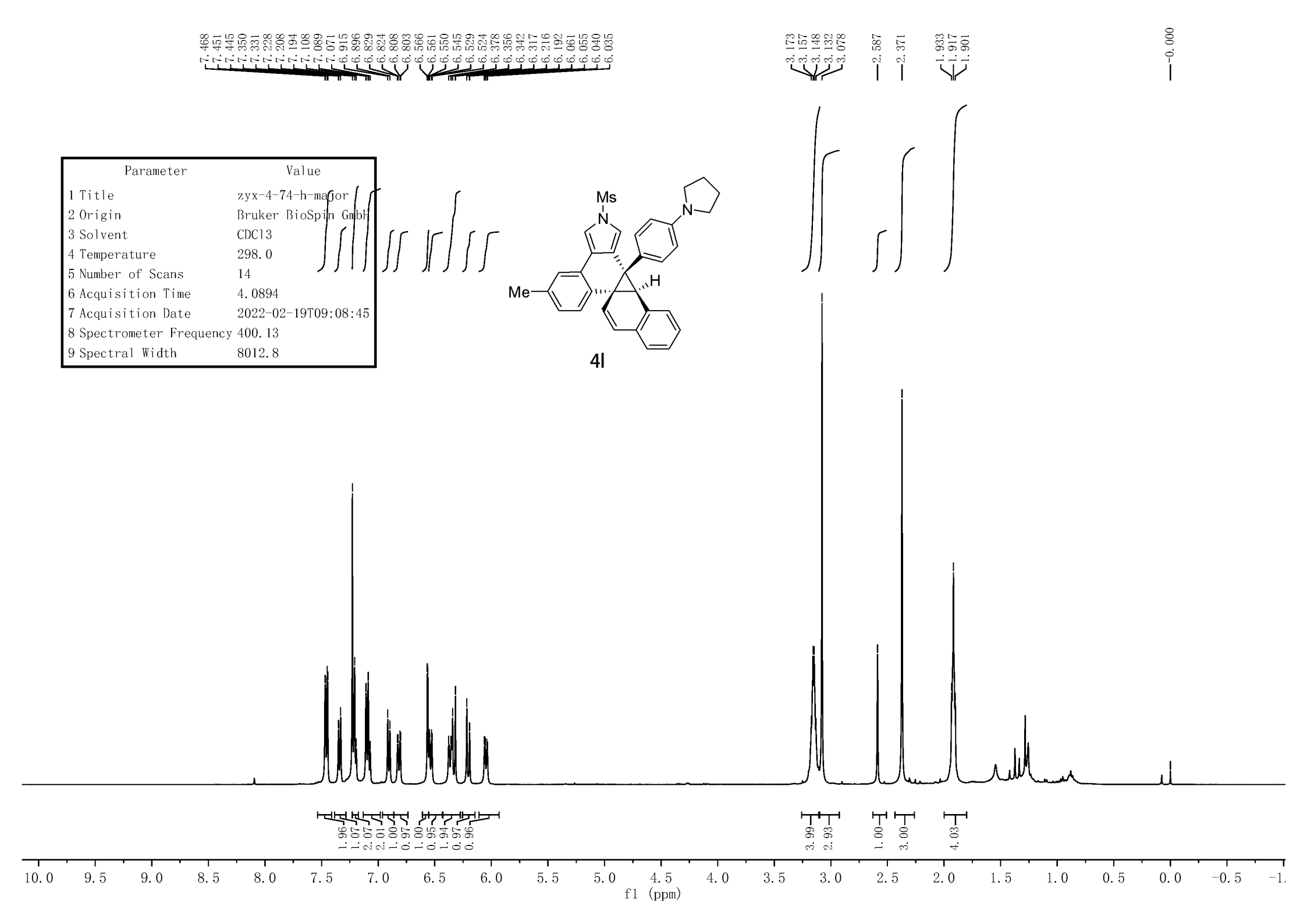
4k



Parameter	Value
1 Title	zyx-4-9---C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	84
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-20T16:39:23
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

4k

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7.194
7.108
7.089
7.071
6.915
6.896
6.829
6.824
6.808
6.803
6.566
6.561
6.550
6.545
6.529
6.524
6.378
6.356
6.342
6.317
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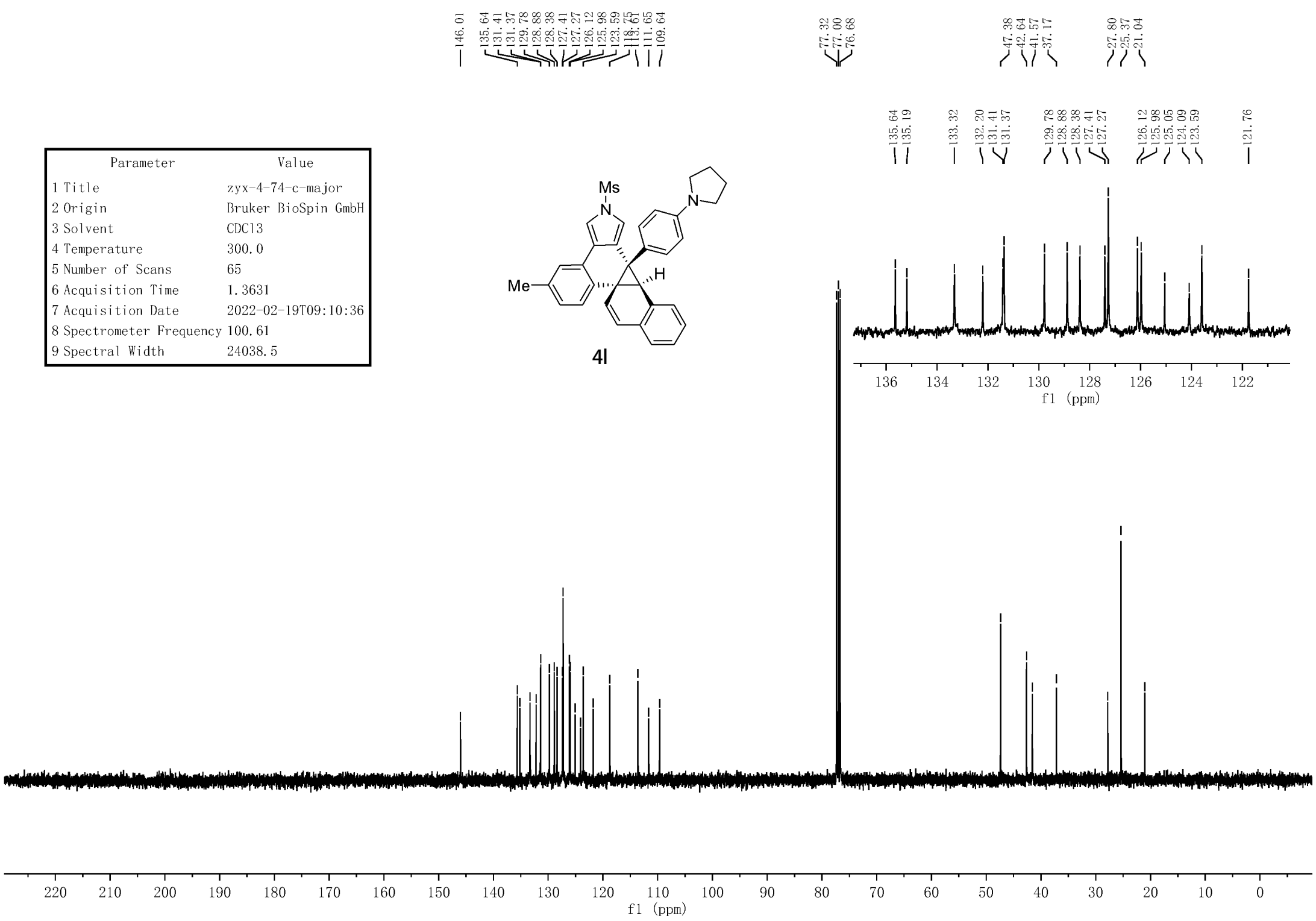
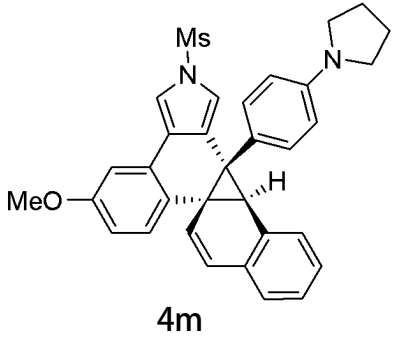
6.055
6.040
6.035
3.173
3.157
3.148
3.132
3.078
2.587
2.371
1.933
1.917
1.901
0.000
Parameter Value
1 Title zyx-4-74-h-major
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 14
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-19T09:08:45
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
Me
H
4l
1.96
1.07
2.07
2.01
1.00
0.97
1.00
0.95
1.94
0.97
0.96
3.99
2.93
1.00
3.00
4.03
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)

Parameter	Value
1 Title	zyx-4-74-c-major
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	65
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-19T09:10:36
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

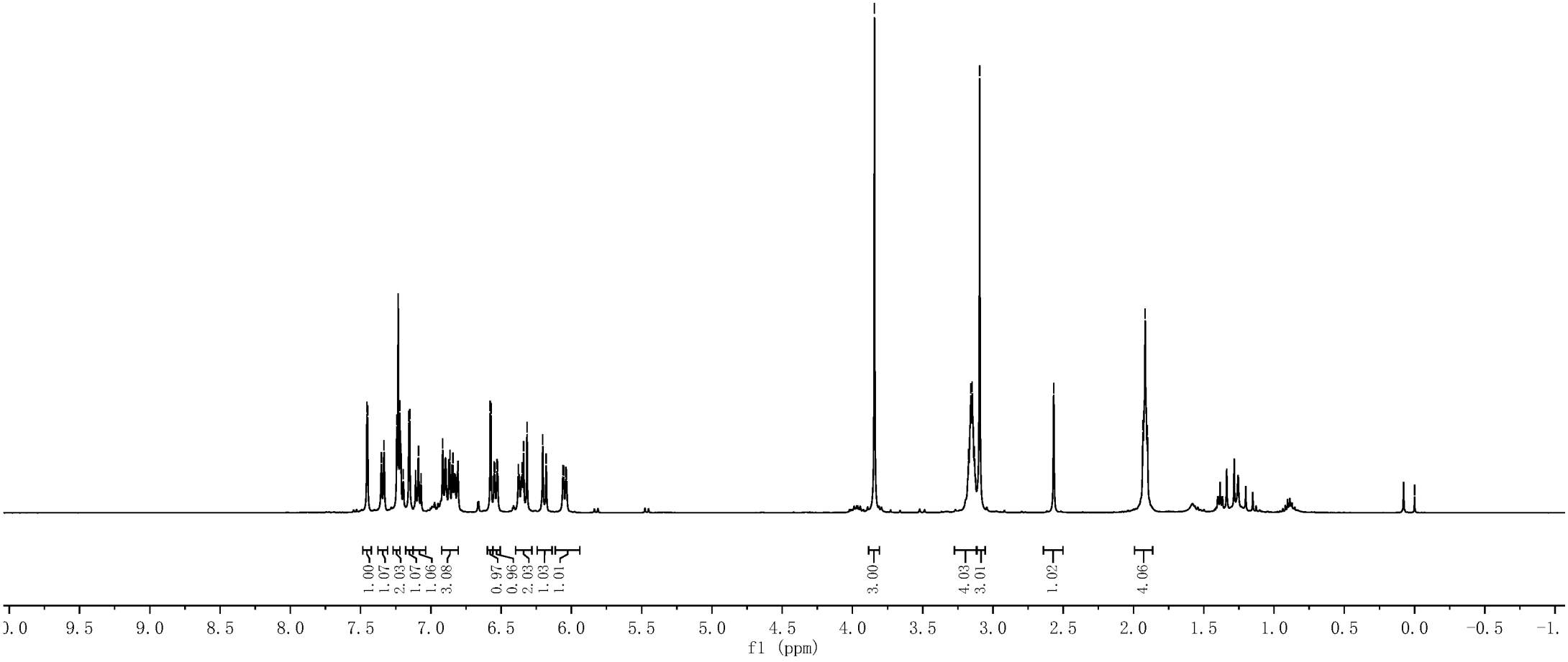
4l



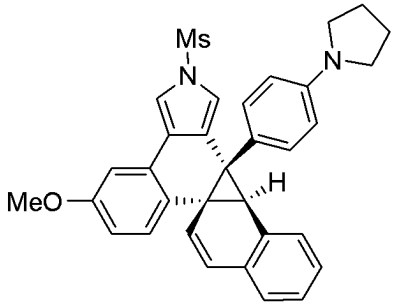
Parameter	Value
1 Title	zyx-3-243-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.5
5 Number of Scans	16
6 Acquisition Time	3.9846
7 Acquisition Date	2022-01-08T15:47:38
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7



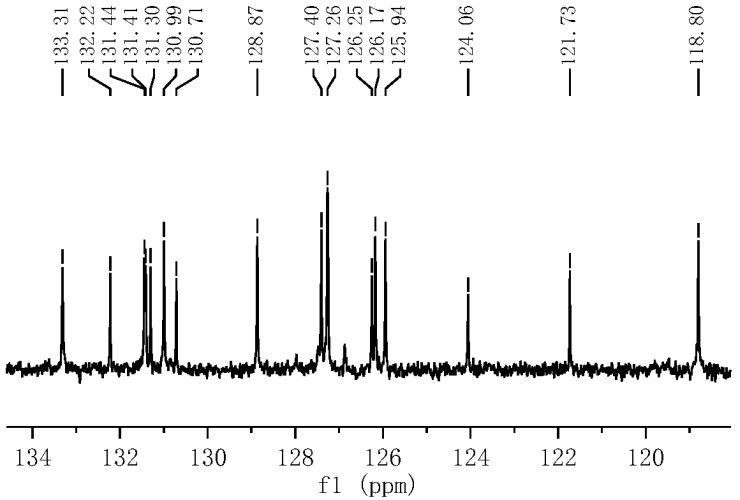
4m

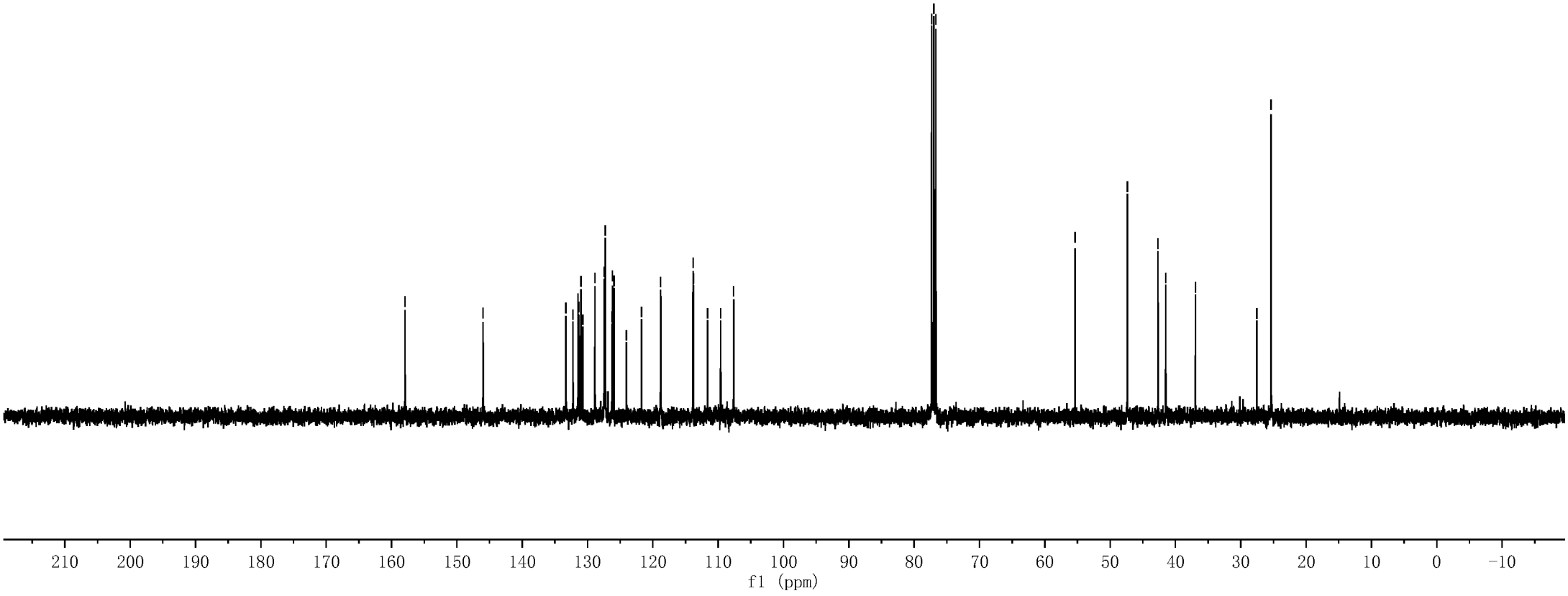


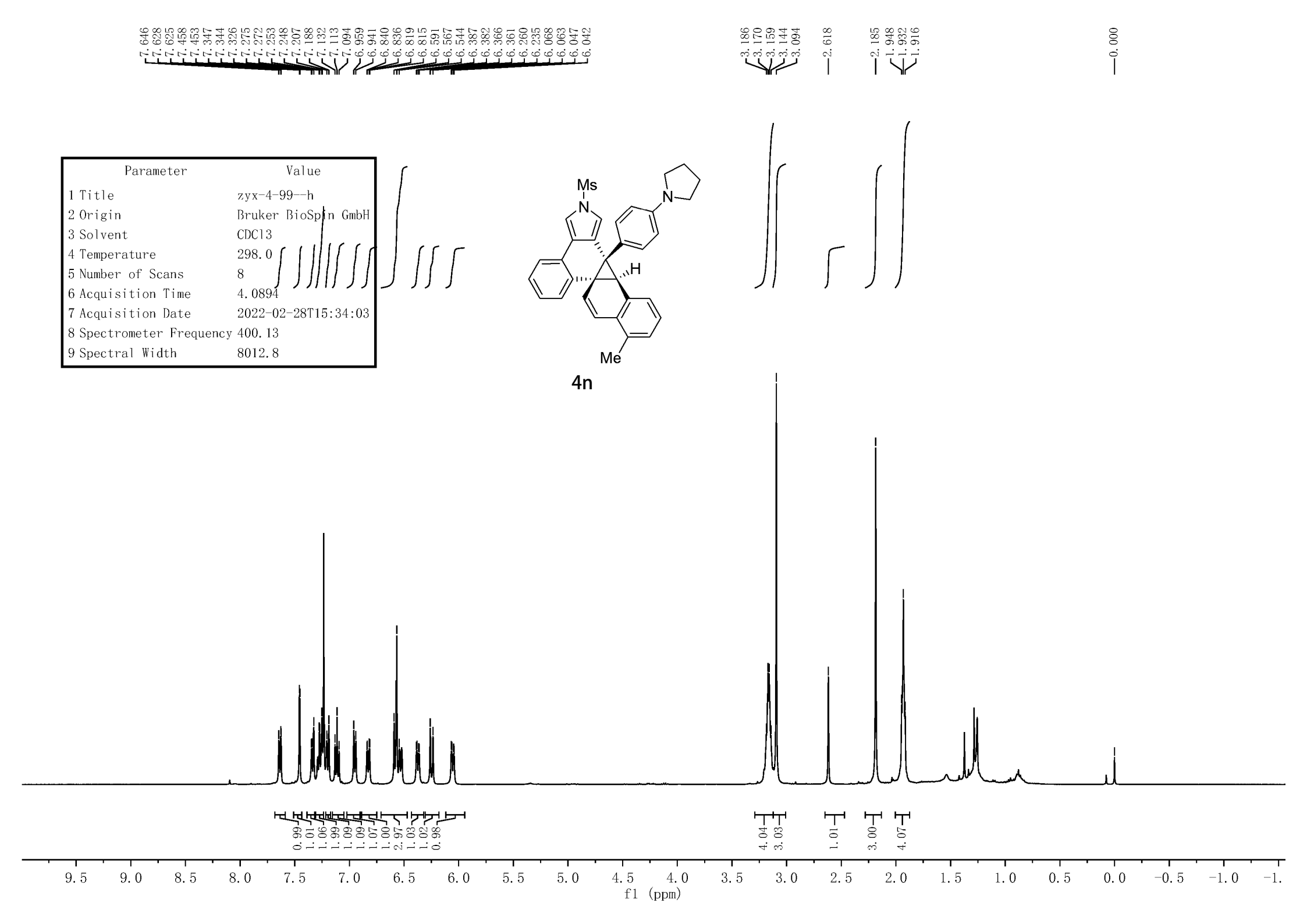
Parameter	Value
1 Title	zyx-3-243-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.7
5 Number of Scans	77
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-08T15:49:43
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



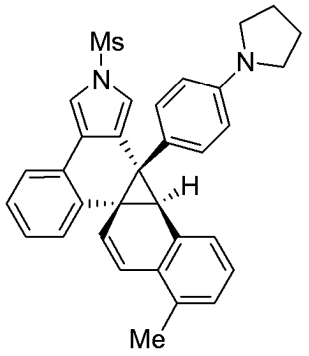
4m



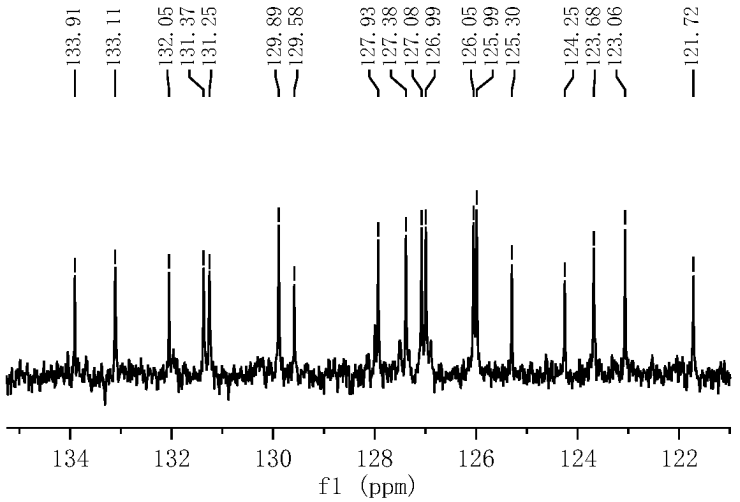


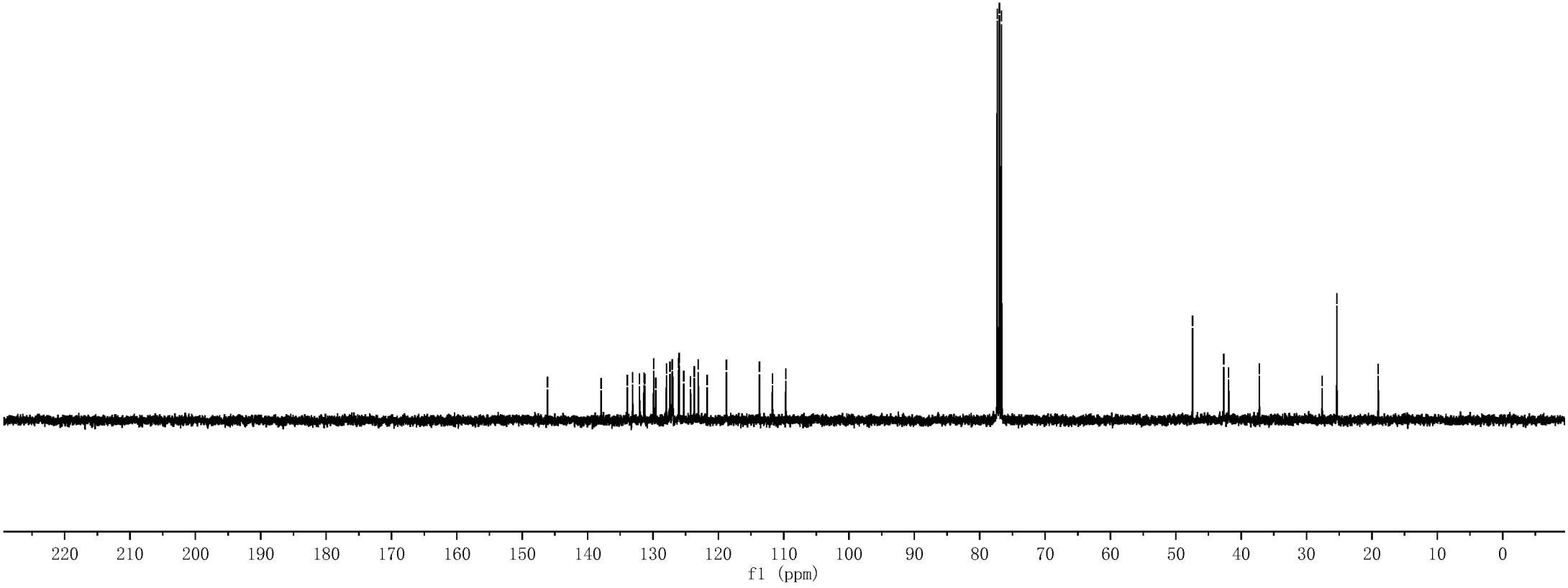

7.646
7.628
7.625
7.458
7.453
7.347
7.344
7.326
7.275
7.272
7.253
7.248
7.207
7.188
7.132
7.113
7.094
6.959
6.941
6.840
6.836
6.819
6.815
6.591
6.567
6.544
6.387
6.382
6.366
6.361
6.260
6.235
6.068
6.063
6.047
6.042
3.186
3.170
3.159
3.144
3.094
2.618
2.185
1.948
1.932
1.916
0.000
Parameter Value
1 Title zyx-4-99--h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-28T15:34:03
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
Me
4n
0.99
1.01
1.06
1.99
1.09
1.09
1.07
1.00
2.97
1.03
1.02
0.98
4.04
3.03
1.01
3.00
4.07
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
-1.0
-1.
f1 (ppm)

Parameter	Value
1 Title	zyx-4-99-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	109
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-26T16:37:46
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

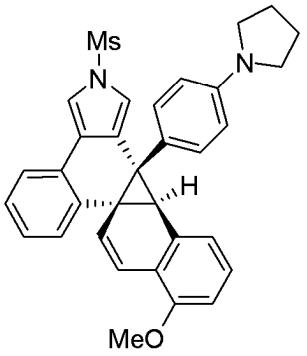


4n

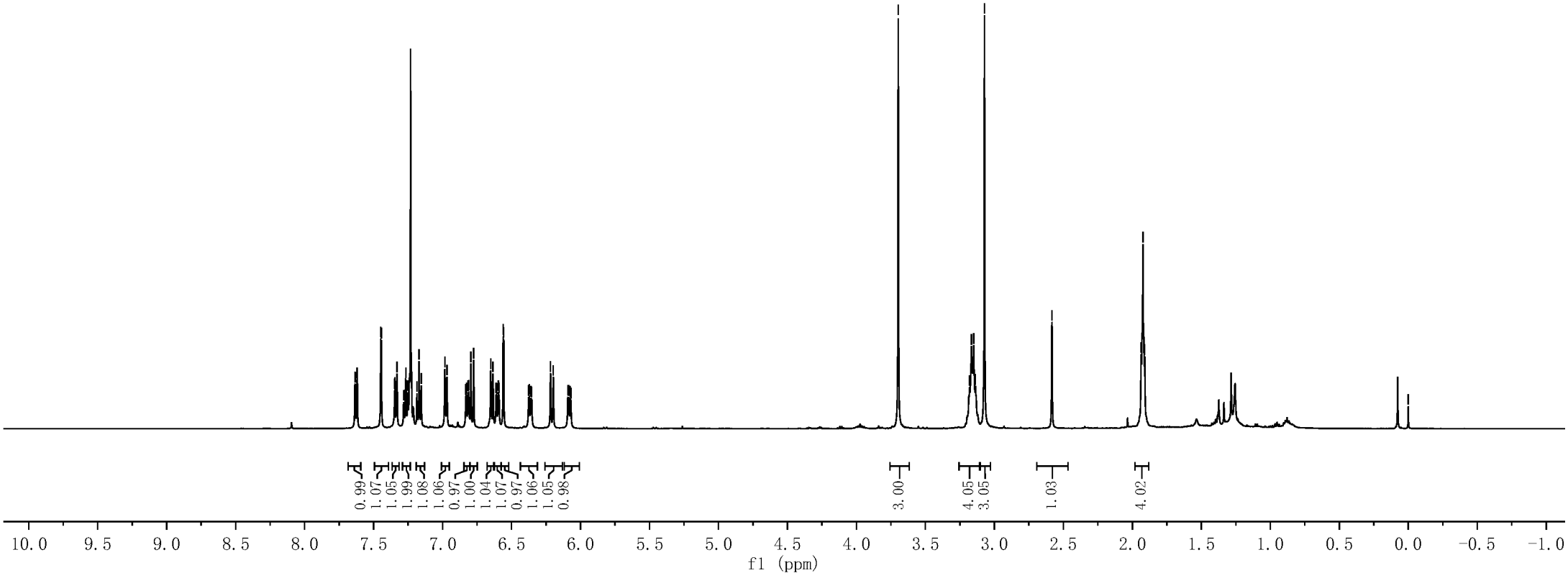




Parameter	Value
1 Title	zyx-4--92--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.7
5 Number of Scans	38
6 Acquisition Time	1.1010
7 Acquisition Date	2022-03-08T10:16:25
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

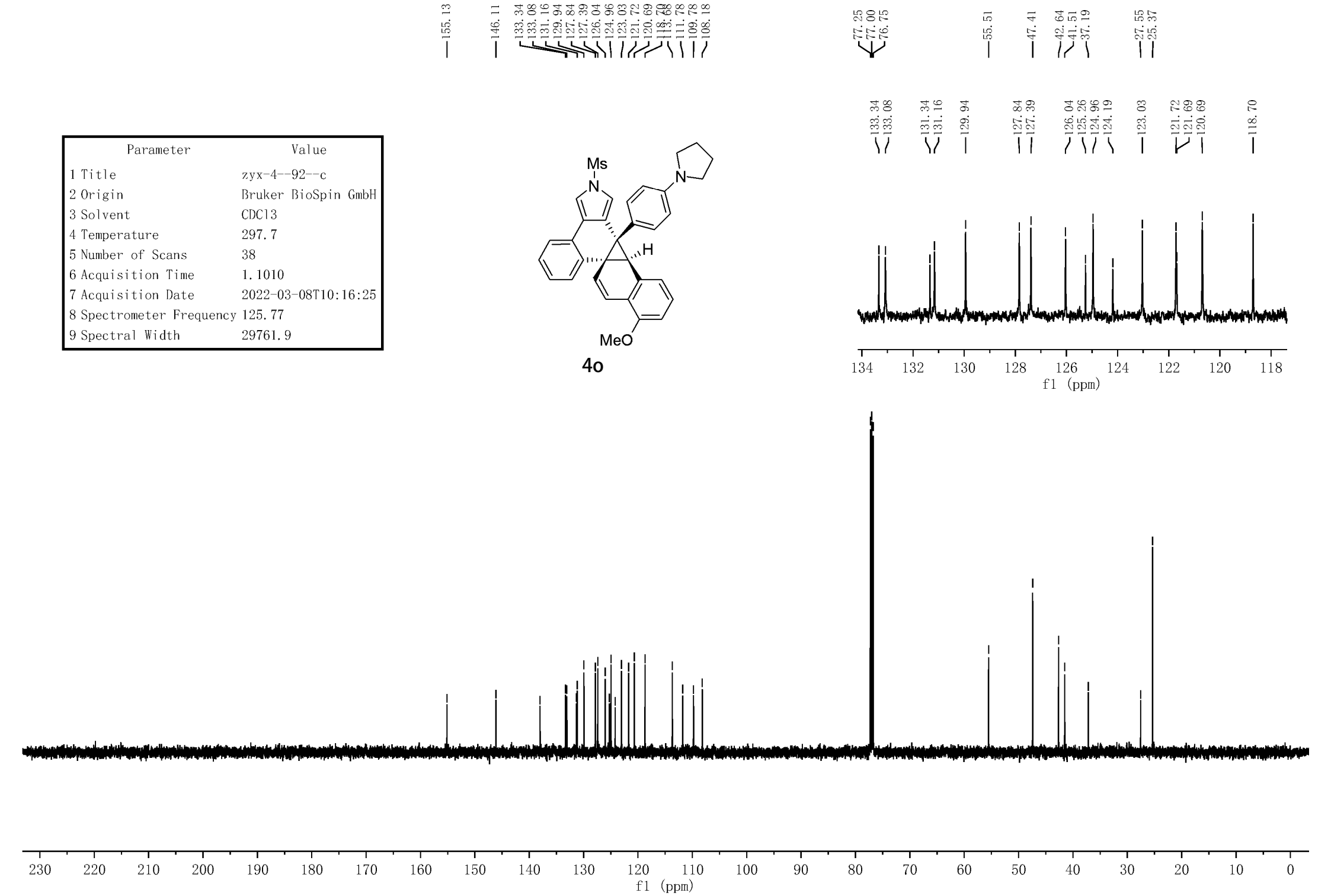


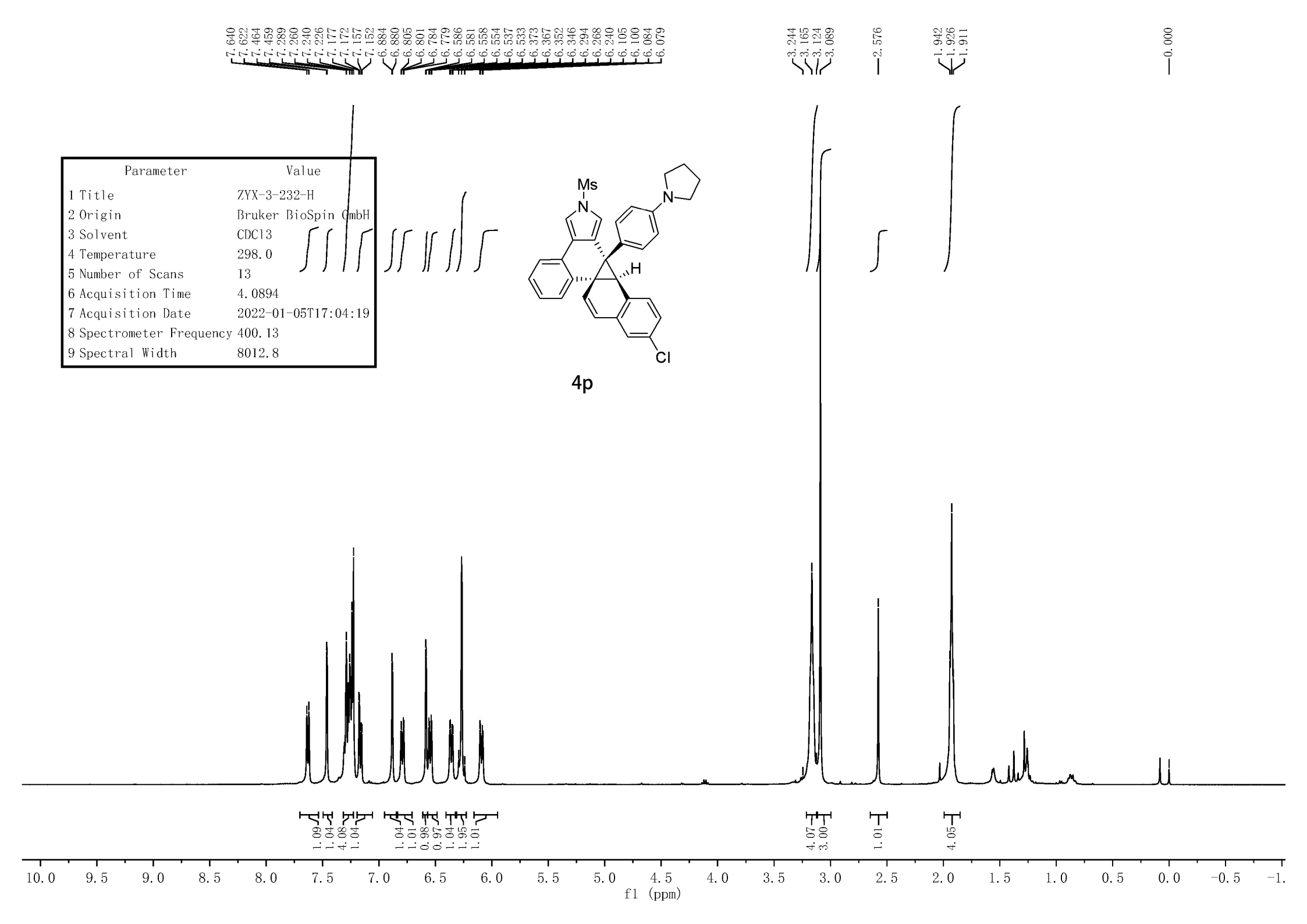
4o



Parameter	Value
1 Title	zyx-4--92--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.7
5 Number of Scans	38
6 Acquisition Time	1.1010
7 Acquisition Date	2022-03-08T10:16:25
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

4o

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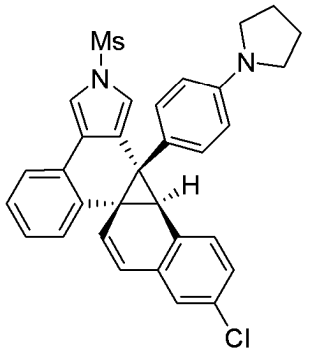
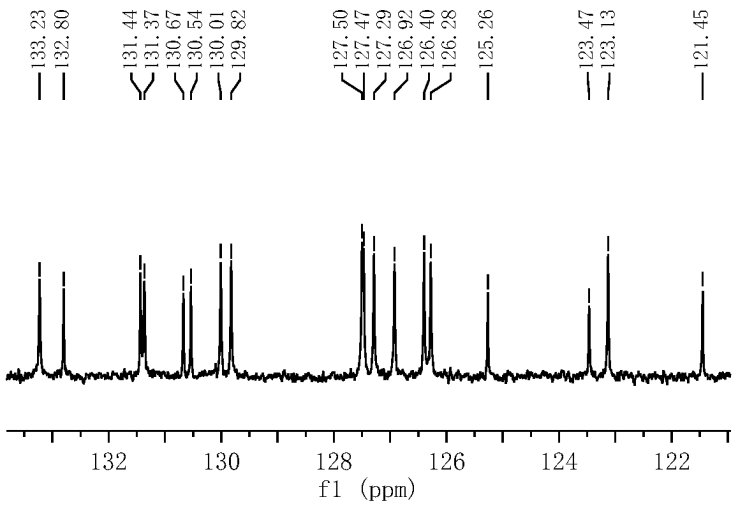
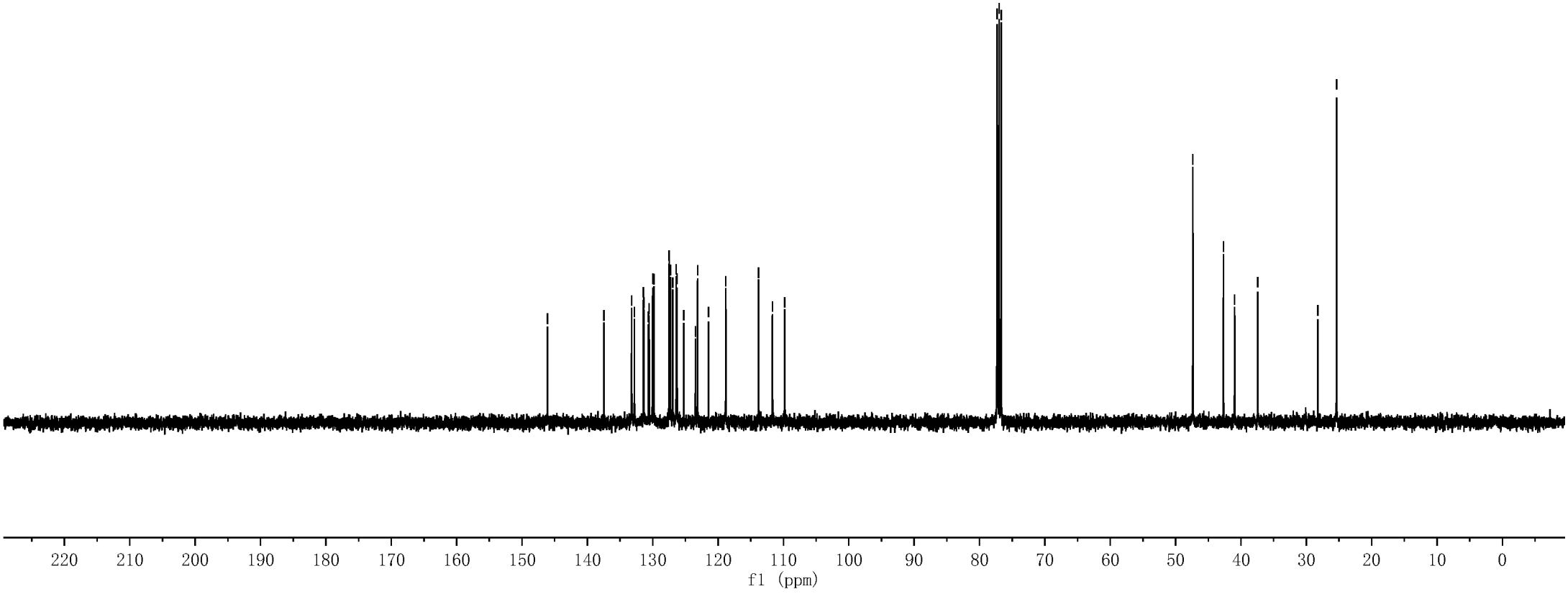
7.622
7.464
7.459
7.289
7.260
7.240
7.226
7.177
7.172
7.157
7.152
6.884
6.880
6.805
6.801
6.784
6.779
6.586
6.581
6.558
6.554
6.537
6.533
6.373
6.367
6.352
6.346
6.294
6.268
6.240
6.105
6.100
6.084
6.079
3.244
3.165
3.124
3.089
2.576
1.942
1.926
1.911
0.000
Parameter Value
1 Title ZYX-3-232-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 13
6 Acquisition Time 4.0894
7 Acquisition Date 2022-01-05T17:04:19
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
Cl
4p
1.09
1.04
4.08
1.04
1.04
1.01
0.98
0.97
1.04
1.95
1.01
4.07
3.00
1.01
4.05
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
-1.
f1 (ppm)

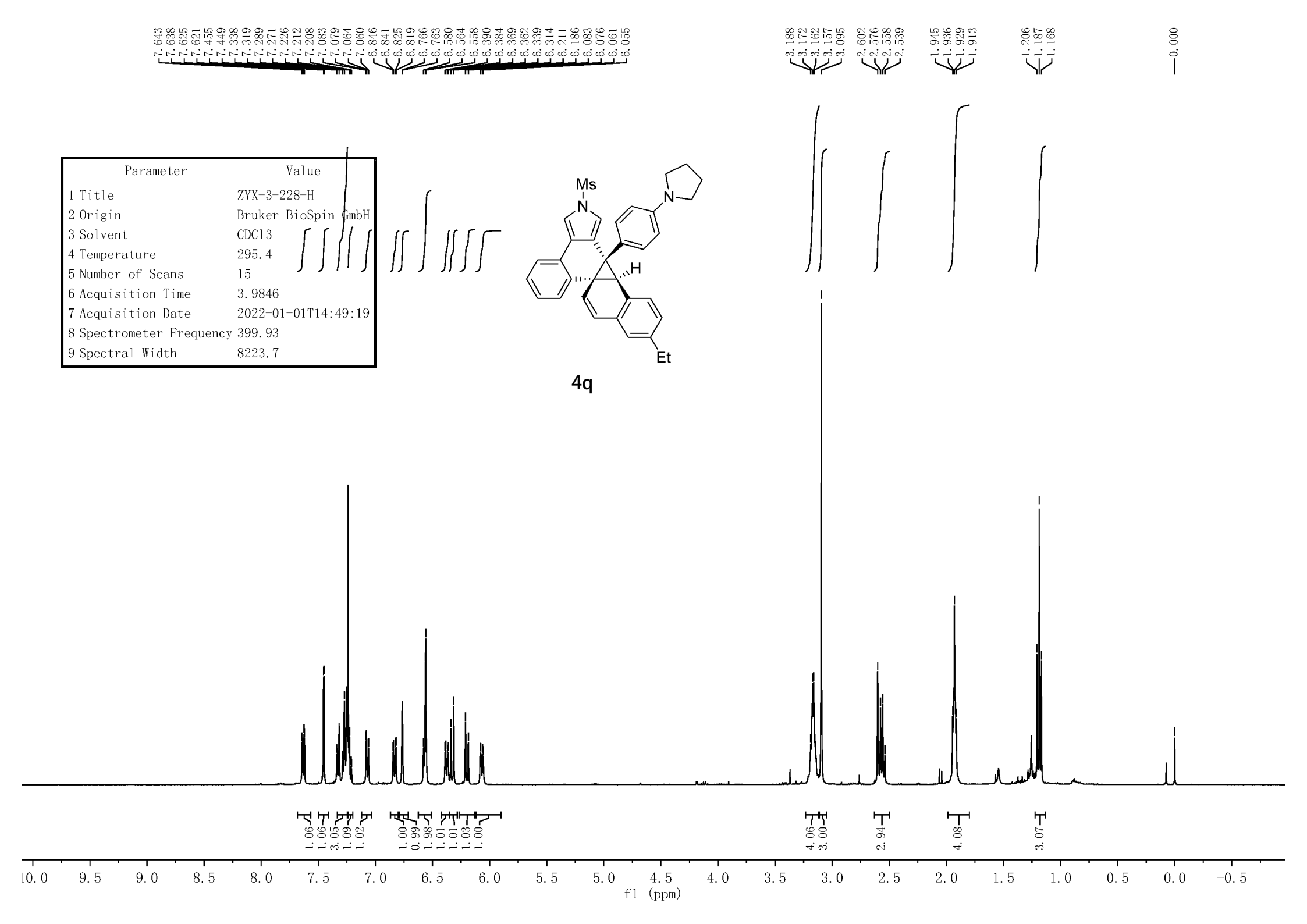
Parameter	Value
1 Title	ZYX-3-232-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	55
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-05T17:06:34
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



4p



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3.188 3.172 3.162 3.157 3.095 2.602 2.576 2.558 2.539 1.945 1.936 1.929 1.913 1.206 1.187 1.168 0.000
Parameter Value
1 Title ZYX-3-228-H
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 295.4
5 Number of Scans 15
6 Acquisition Time 3.9846
7 Acquisition Date 2022-01-01T14:49:19
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
N
H
Et
4q
1.06 1.06 3.05 1.09 1.02 1.00 0.99 1.98 1.01 1.01 1.03 1.00 4.06 3.00 2.94 4.08 3.07
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)

145.98
142.01
138.05
133.29
131.47
131.41
131.19
129.92
129.32
128.81
127.53
127.38
127.17
126.79
126.02
125.90
125.25
124.21
123.04
121.73
118.66
113.70
111.62
109.70

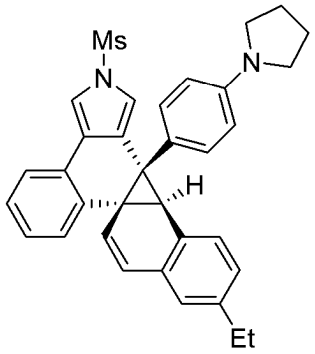
77.32
77.00
76.68

47.39
42.67
41.22
37.21

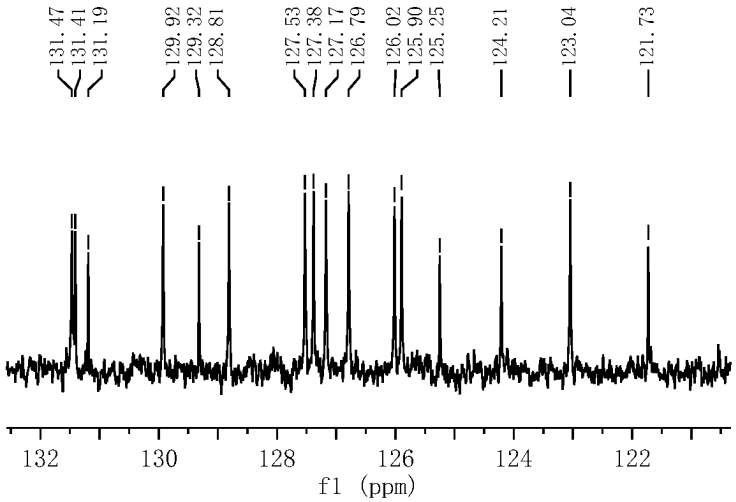
28.43
27.90
25.39

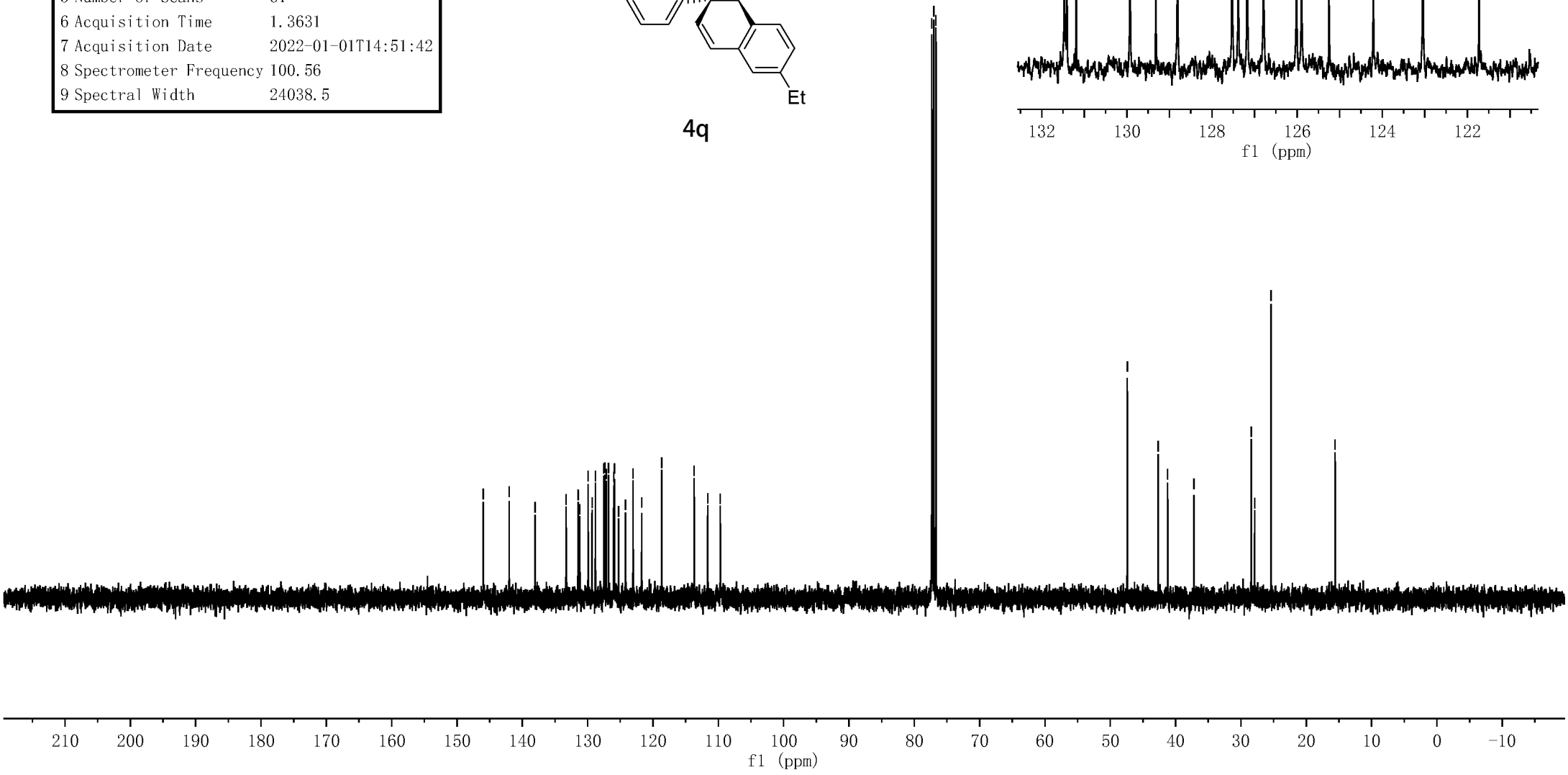
15.58

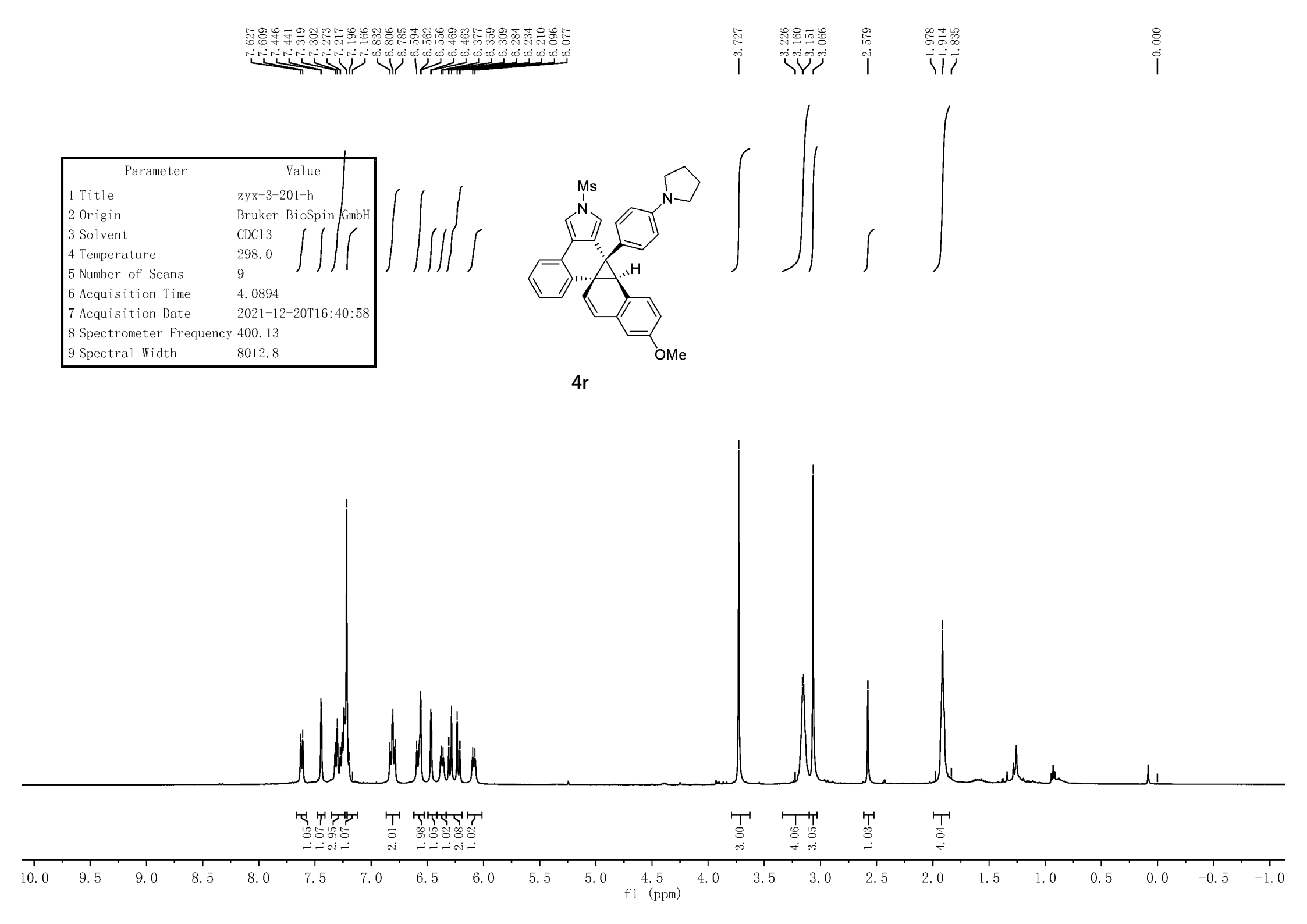
Parameter	Value
1 Title	ZYX-3-228-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.9
5 Number of Scans	61
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-01T14:51:42
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



4q

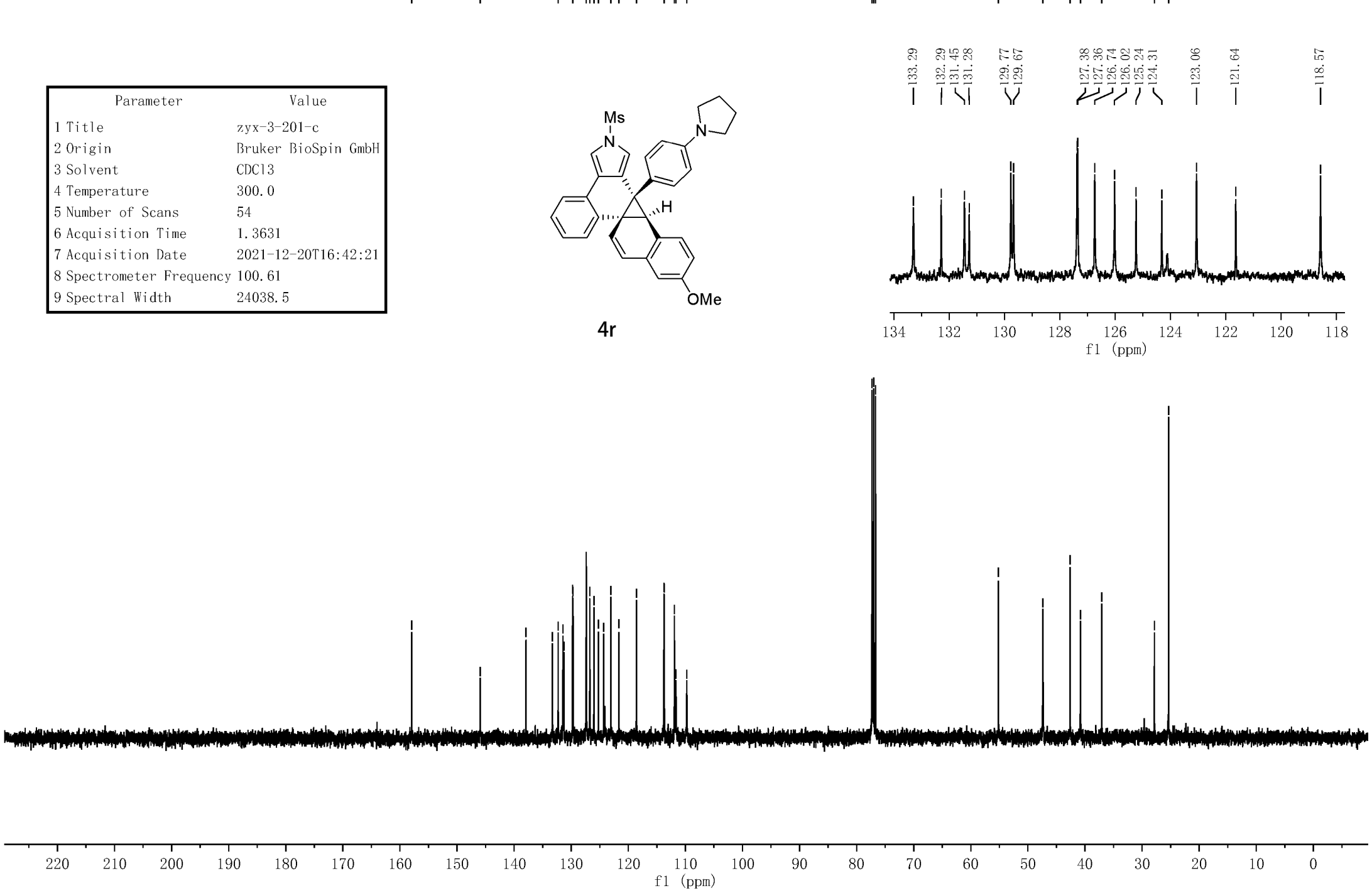


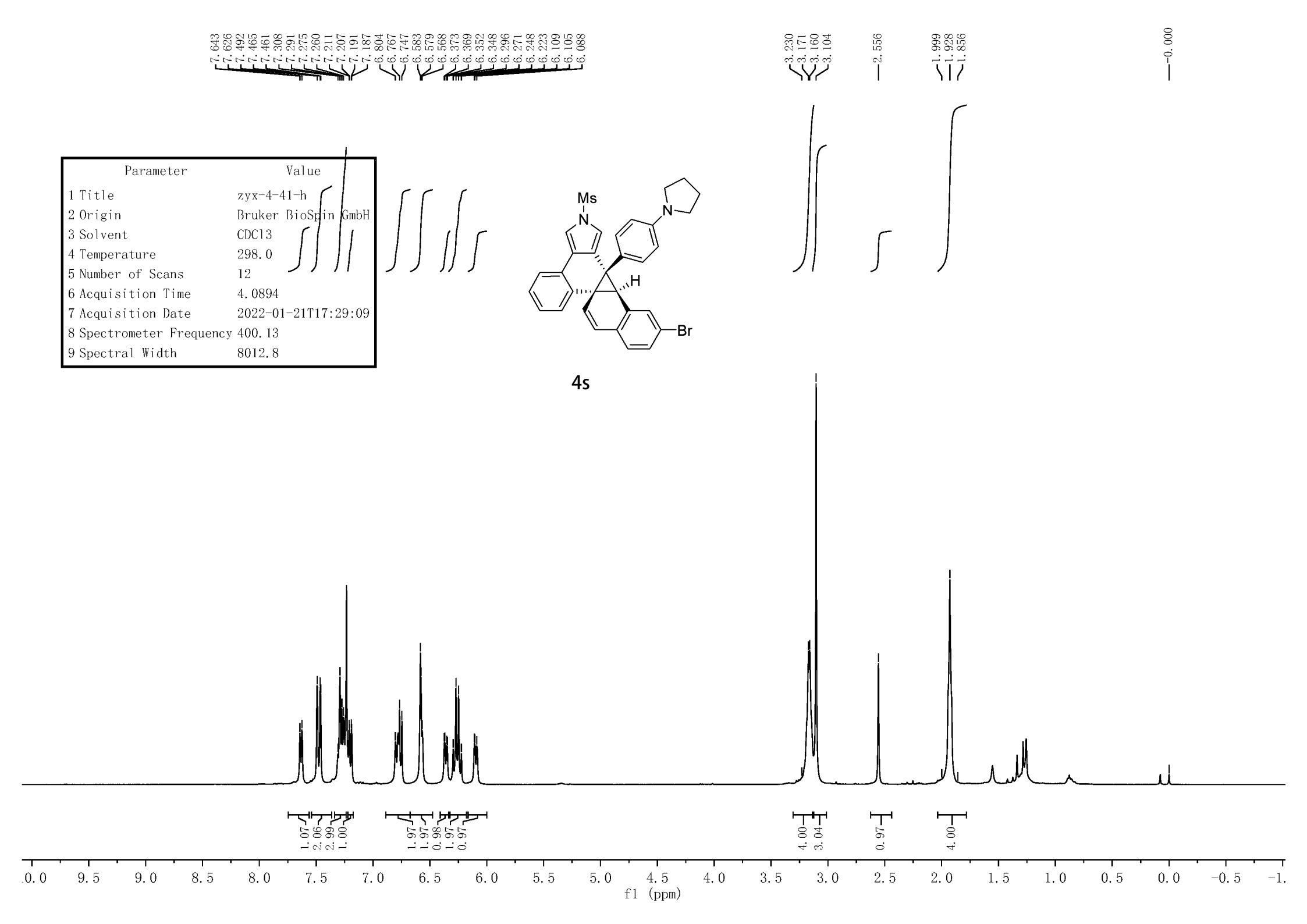



7.627
7.609
7.446
7.441
7.319
7.302
7.273
7.217
7.196
7.166
6.832
6.806
6.785
6.594
6.562
6.556
6.469
6.463
6.377
6.359
6.309
6.284
6.234
6.210
6.096
6.077
3.727
3.226
3.160
3.151
3.066
2.579
1.978
1.914
1.835
0.000
Parameter Value
1 Title zyx-3-201-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 9
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-20T16:40:58
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
OMe
4r
1.05
1.07
2.95
1.07
2.01
1.98
1.05
1.02
2.08
1.02
3.00
4.06
3.05
1.03
4.04
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
-1.0
f1 (ppm)

Parameter	Value
1 Title	zyx-3-201-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	54
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-20T16:42:21
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

4r

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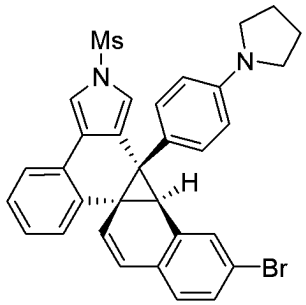
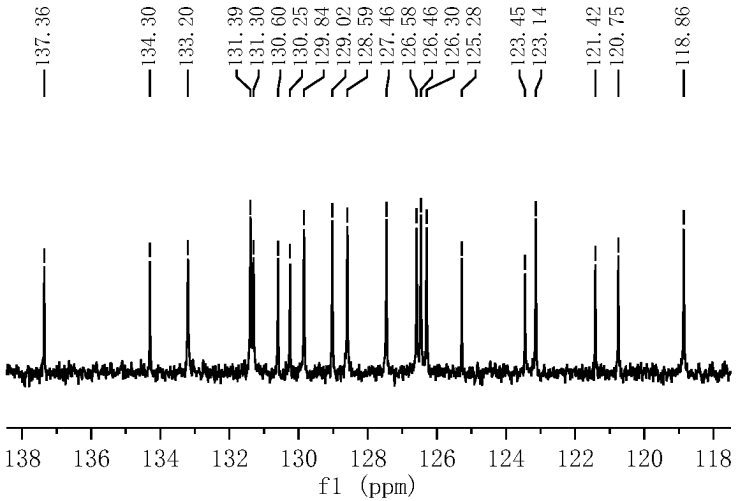
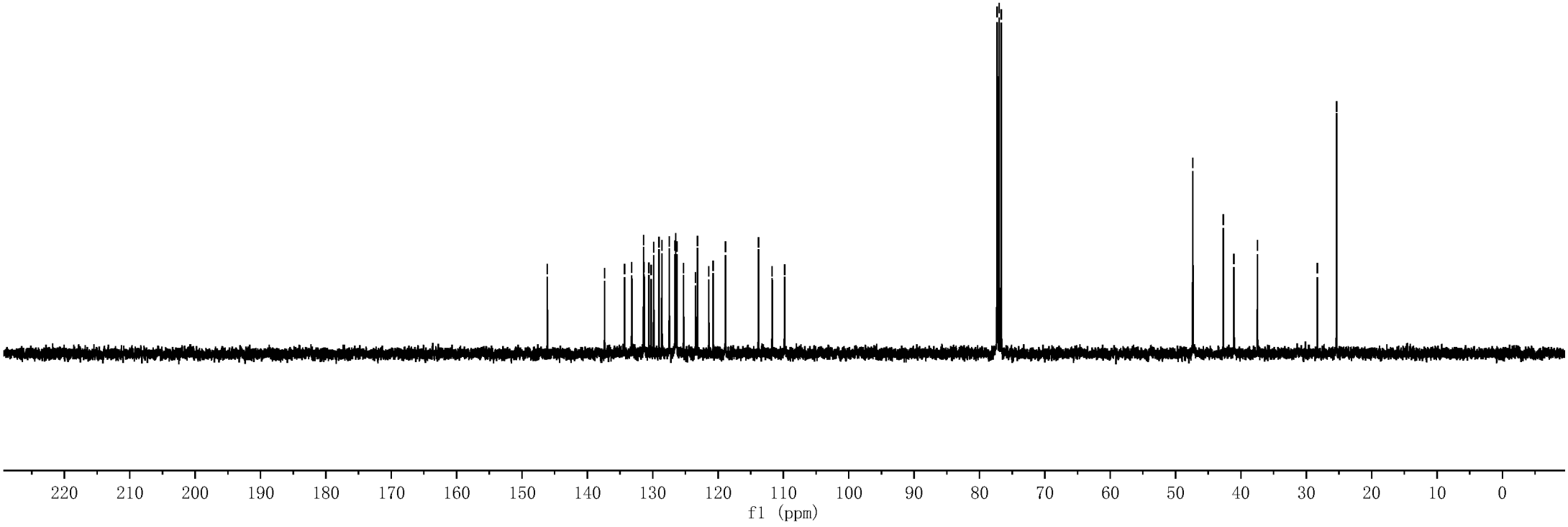
7.626
7.492
7.465
7.461
7.308
7.291
7.275
7.260
7.211
7.207
7.191
7.187
6.804
6.767
6.747
6.583
6.579
6.568
6.373
6.369
6.352
6.348
6.296
6.271
6.248
6.223
6.109
6.105
6.088
3.230
3.171
3.160
3.104
2.556
1.999
1.928
1.856
0.000
Parameter Value
1 Title zyx-4-41-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 12
6 Acquisition Time 4.0894
7 Acquisition Date 2022-01-21T17:29:09
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
Br
4s
1.07
2.06
2.99
1.00
1.97
1.97
0.98
1.97
0.97
4.00
3.04
0.97
4.00
f1 (ppm)

Parameter	Value
1 Title	zyx-4-41-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	40
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-21T16:06:07
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



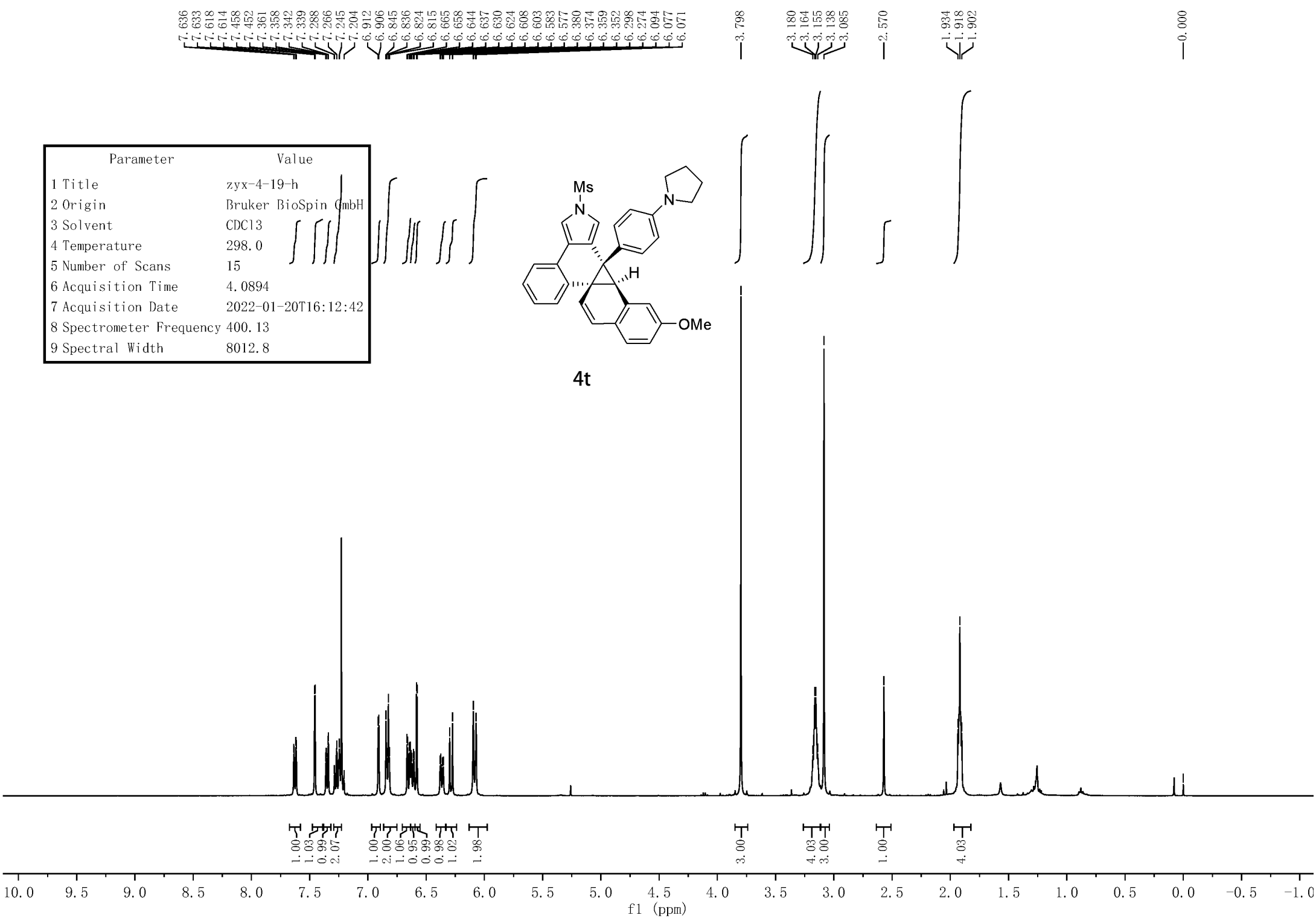
4s



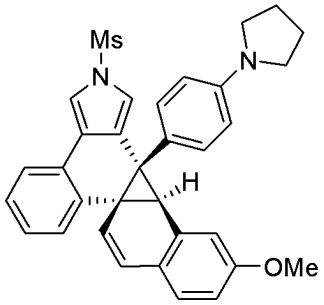


Parameter	Value
1 Title	zyx-4-19-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	15
6 Acquisition Time	4.0894
7 Acquisition Date	2022-01-20T16:12:42
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

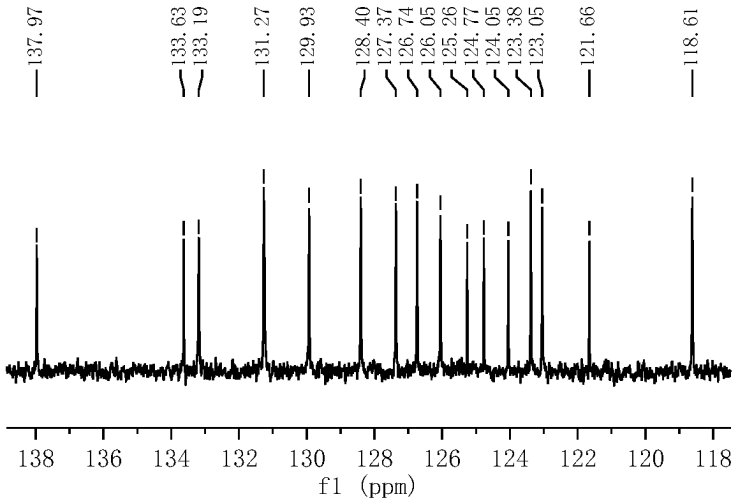
4t

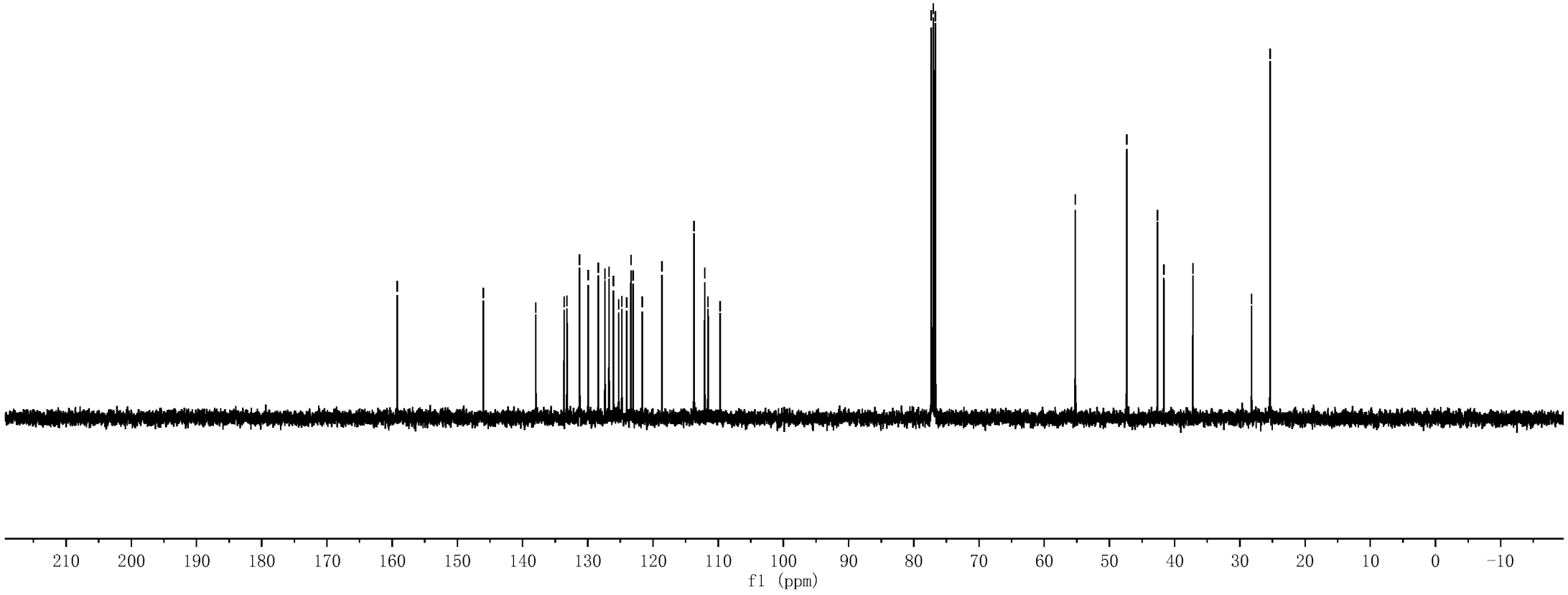


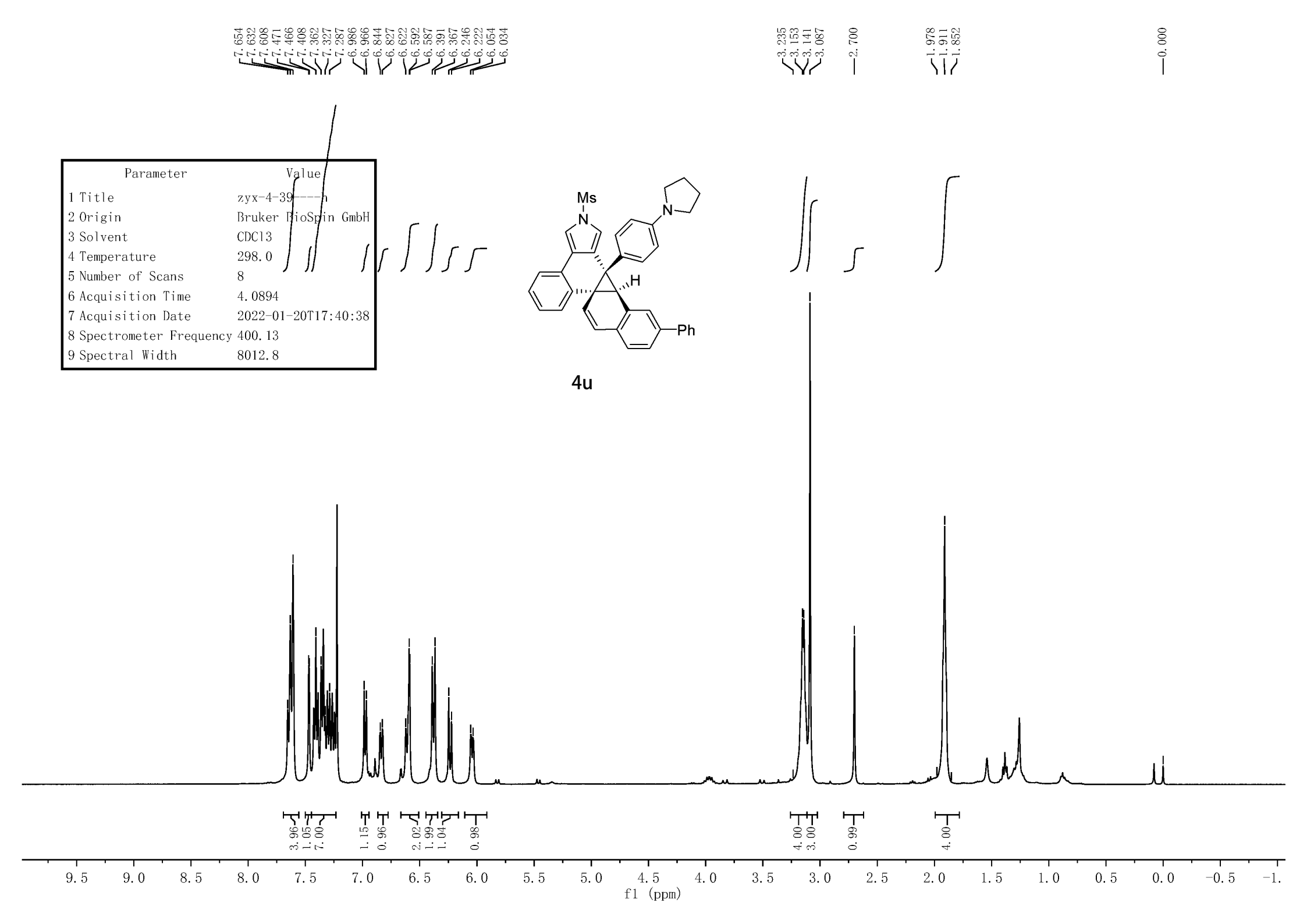
Parameter	Value
1 Title	zyx-4-19---c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	295.9
5 Number of Scans	58
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-20T16:16:58
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



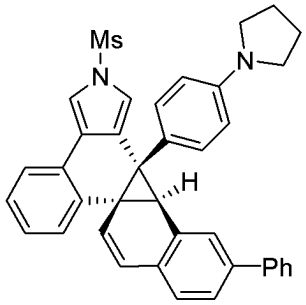
4t



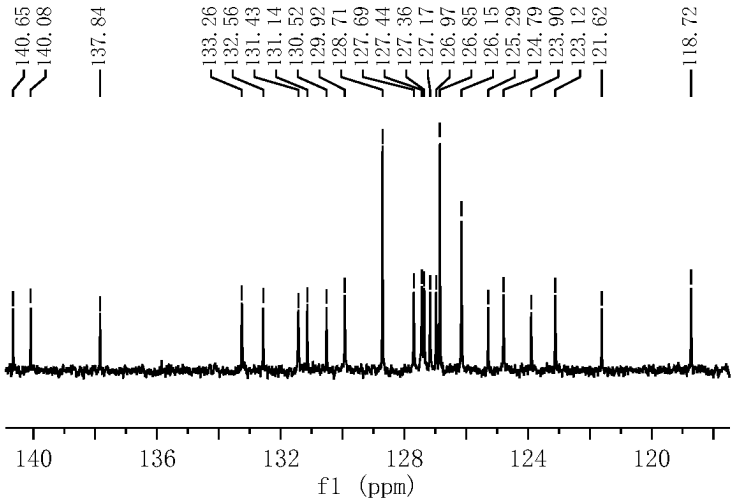


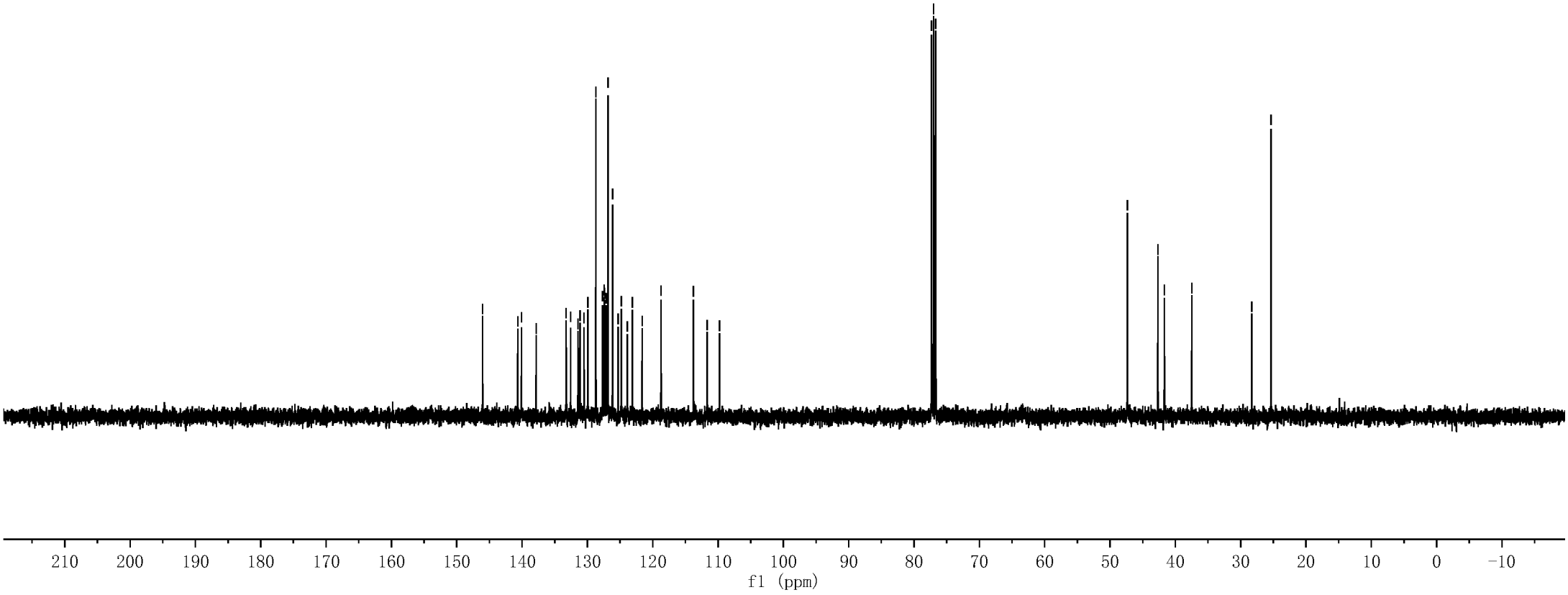

7.654
7.632
7.608
7.471
7.466
7.408
7.362
7.327
7.287
6.986
6.966
6.844
6.827
6.622
6.592
6.587
6.391
6.367
6.246
6.222
6.054
6.034
3.235
3.153
3.141
3.087
2.700
1.978
1.911
1.852
0.000
Parameter Value
1 Title zyx-4-39----h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 8
6 Acquisition Time 4.0894
7 Acquisition Date 2022-01-20T17:40:38
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
Ph
4u
3.96
1.05
7.00
1.15
0.96
2.02
1.99
1.04
0.98
4.00
3.00
0.99
4.00
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
-1.
f1 (ppm)

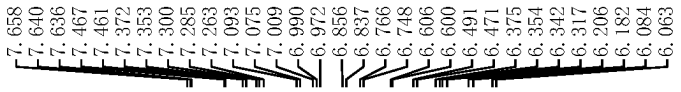
Parameter	Value
1 Title	zyx-4-39---C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.0
5 Number of Scans	53
6 Acquisition Time	1.3631
7 Acquisition Date	2022-01-20T16:26:52
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5

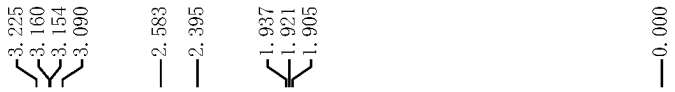


4u

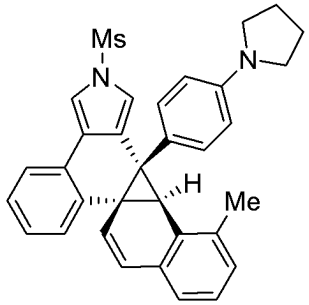




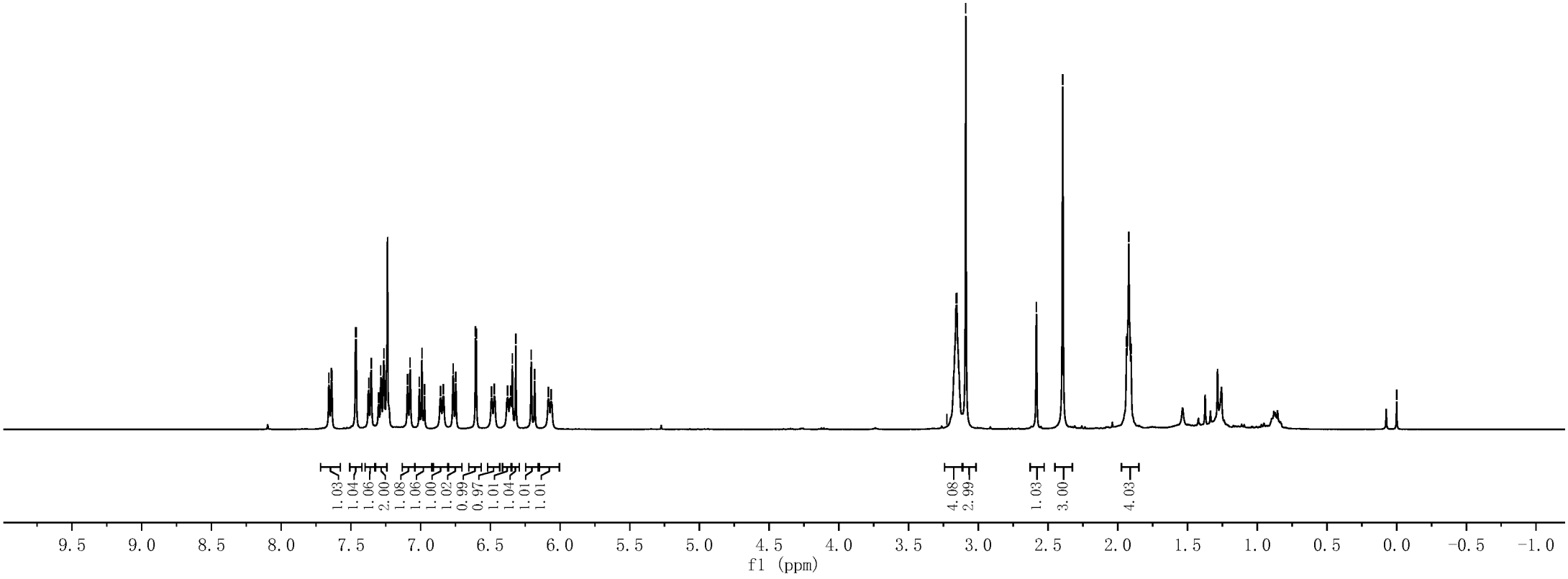




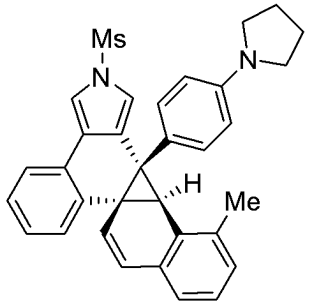
Parameter	Value
1 Title	zyx-4-84---h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	6
6 Acquisition Time	4.0894
7 Acquisition Date	2022-02-23T15:59:42
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



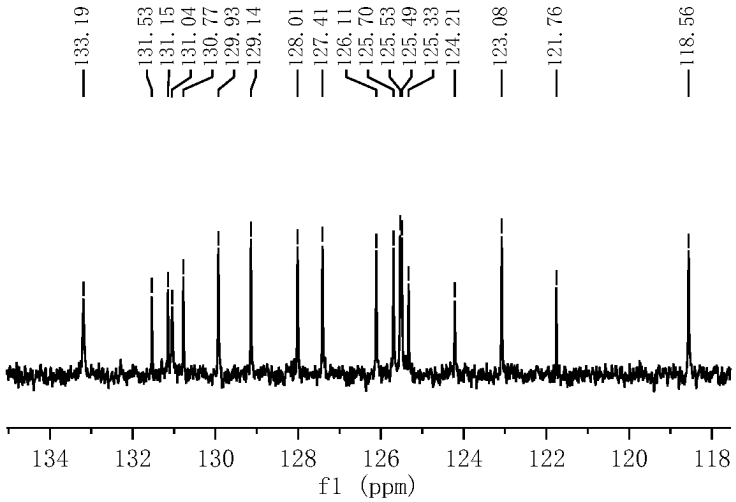
4v

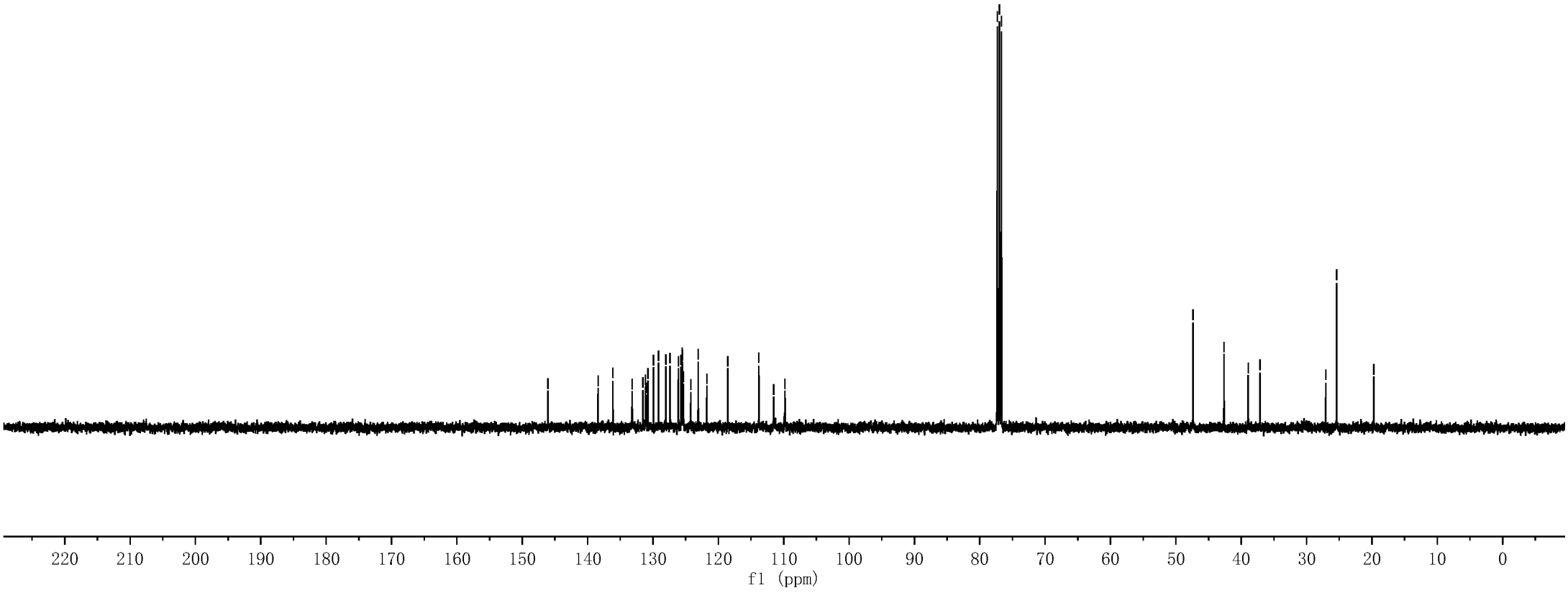


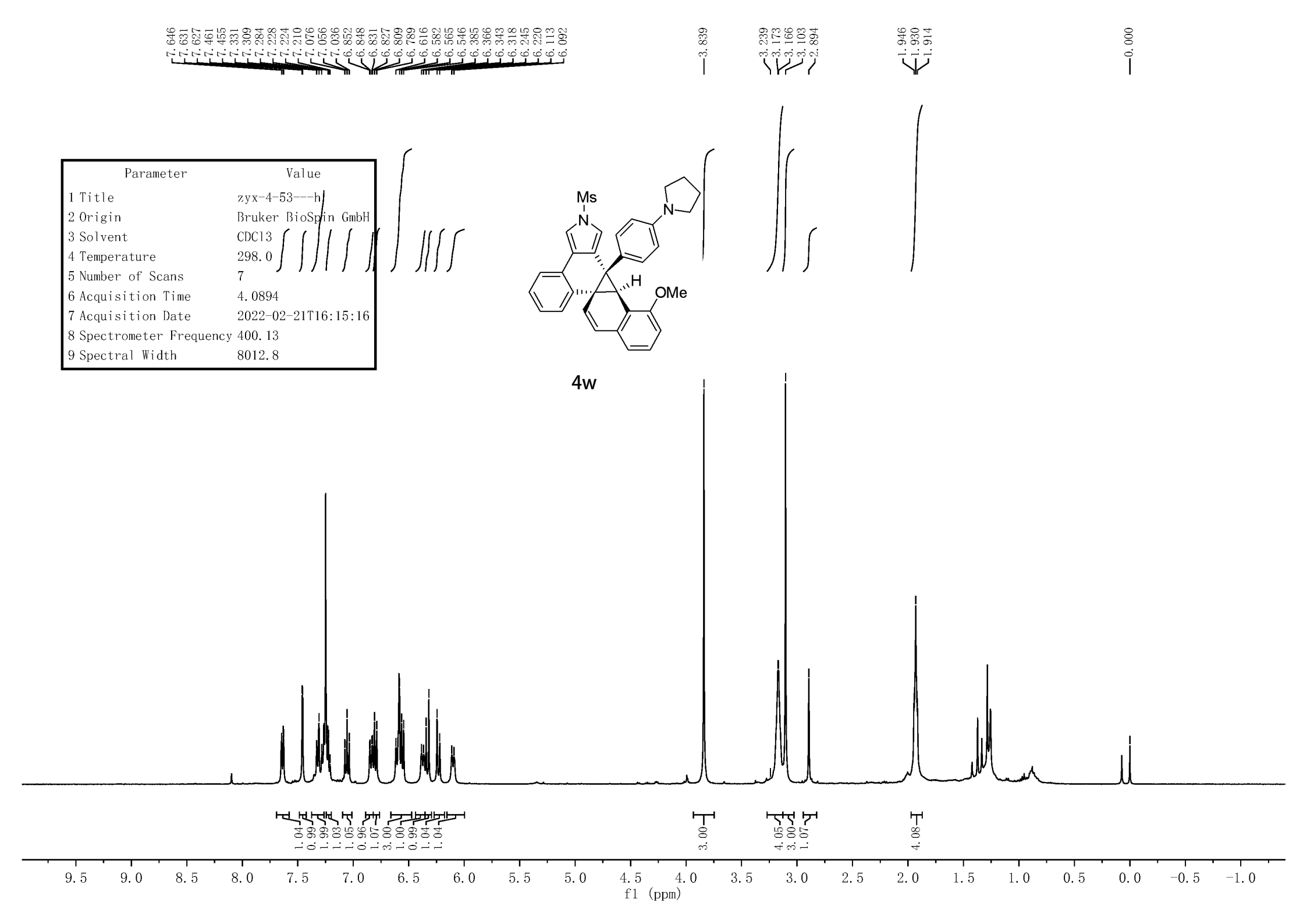
Parameter	Value
1 Title	zyx-4-84---c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	69
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-23T16:01:10
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



4v



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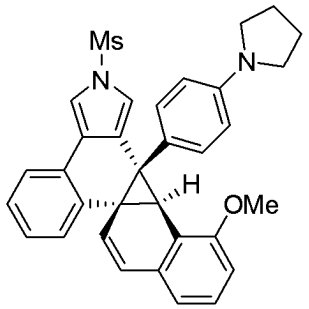
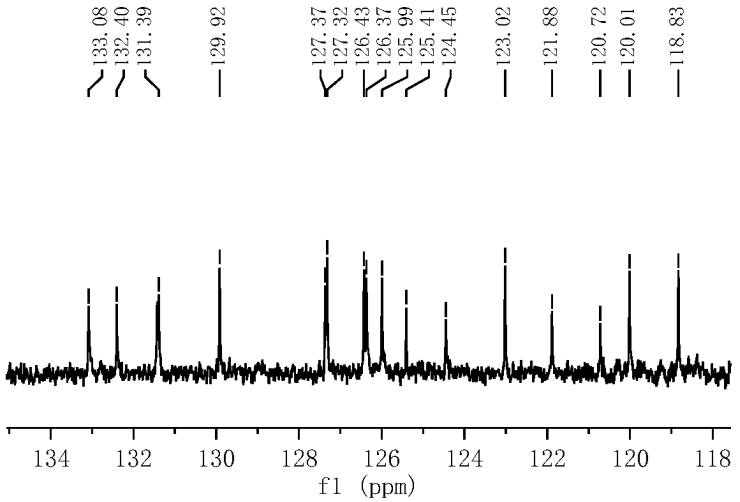
7.631
7.627
7.461
7.455
7.331
7.309
7.284
7.228
7.224
7.210
7.076
7.056
7.036
6.852
6.848
6.831
6.827
6.809
6.789
6.616
6.582
6.565
6.546
6.385
6.366
6.343
6.318
6.245
6.220
6.113
6.092
3.839
3.239
3.173
3.166
3.103
2.894
1.946
1.930
1.914
0.000
Parameter Value
1 Title zyx-4-53---h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 7
6 Acquisition Time 4.0894
7 Acquisition Date 2022-02-21T16:15:16
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
OMe
4w
1.04
0.99
1.99
1.03
1.05
0.96
1.07
3.00
1.00
0.99
1.04
1.04
3.00
4.05
3.00
1.07
4.08
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
-1.0
f1 (ppm)

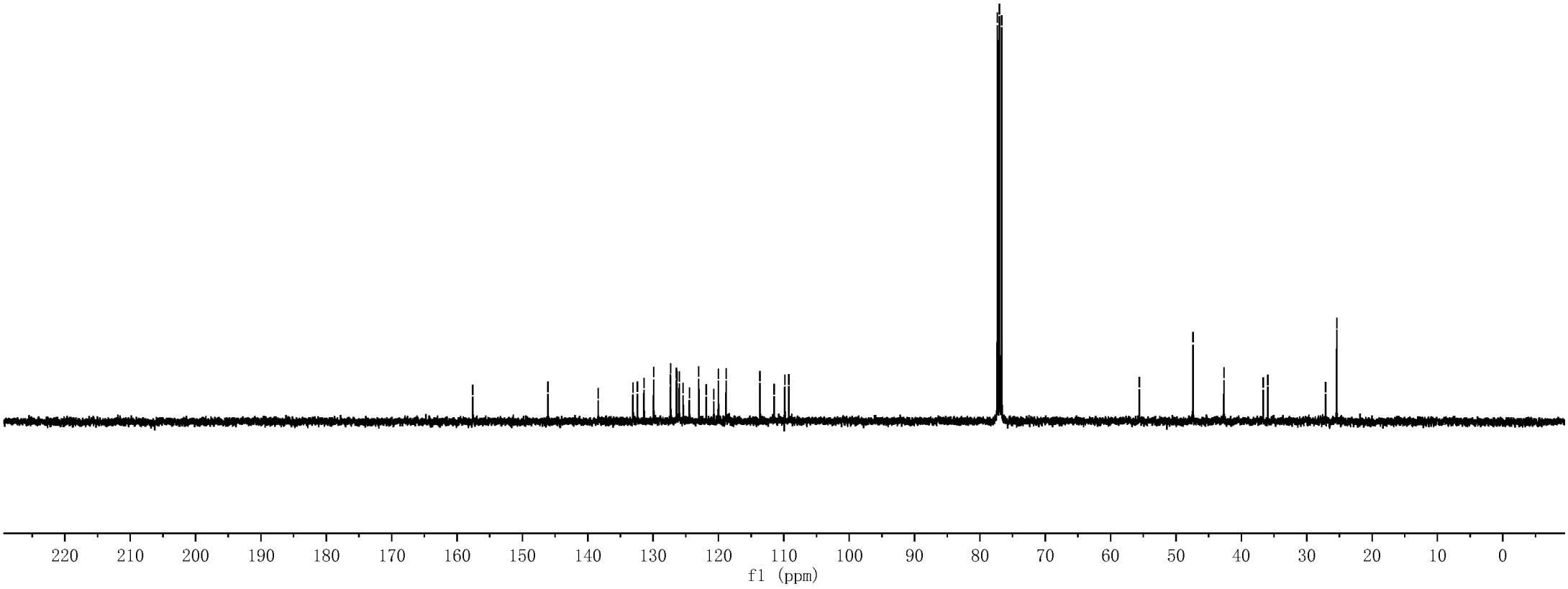
Z

Parameter	Value
1 Title	zyx-4---53-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	130
6 Acquisition Time	1.3631
7 Acquisition Date	2022-02-23T16:09:27
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

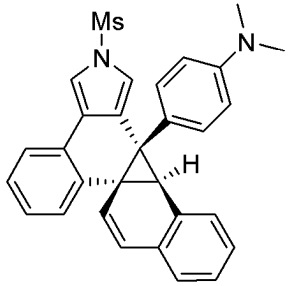


4w

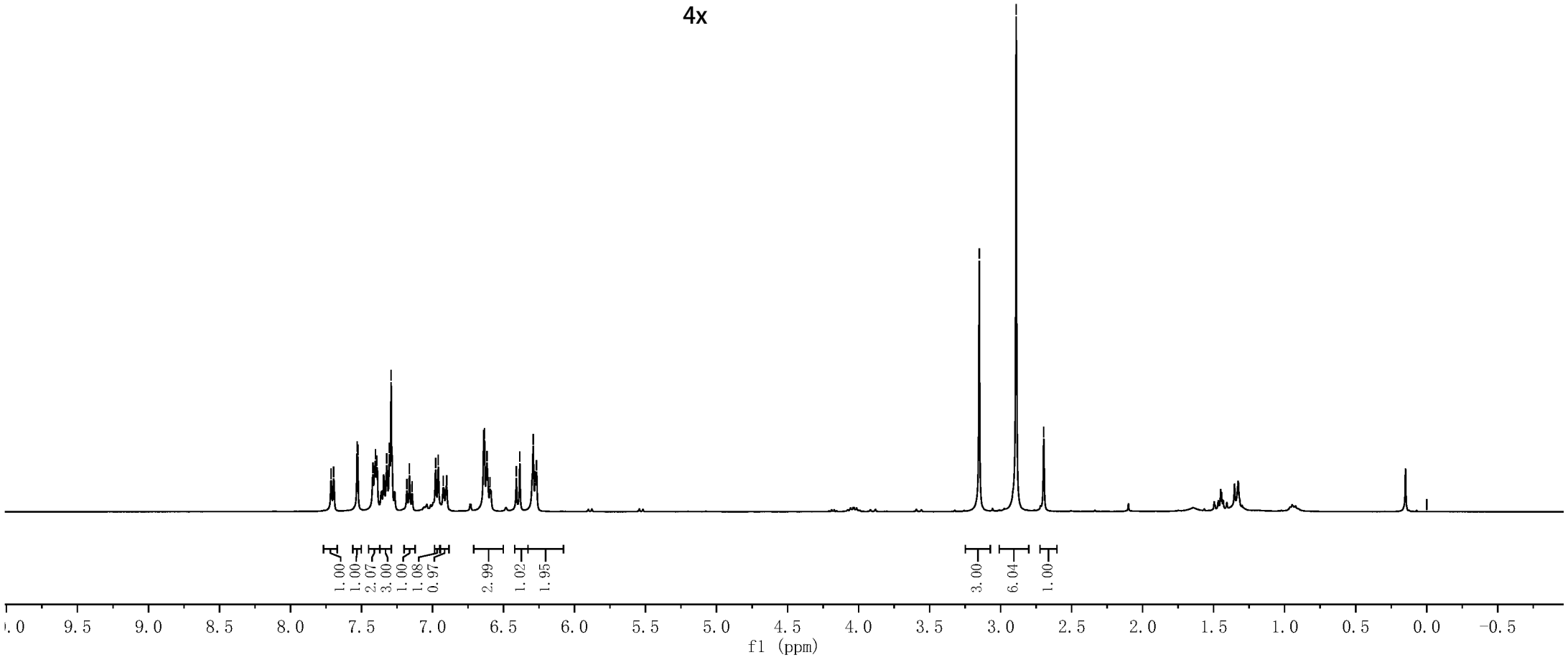




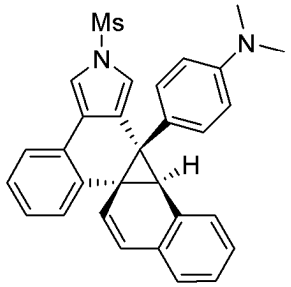
Parameter	Value
1 Title	ZYX-3-165-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	14
6 Acquisition Time	4.0894
7 Acquisition Date	2021-12-10T17:06:07
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



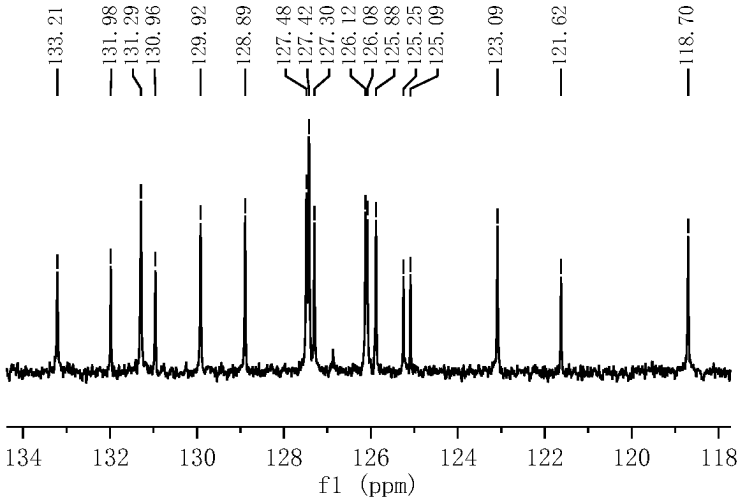
4x

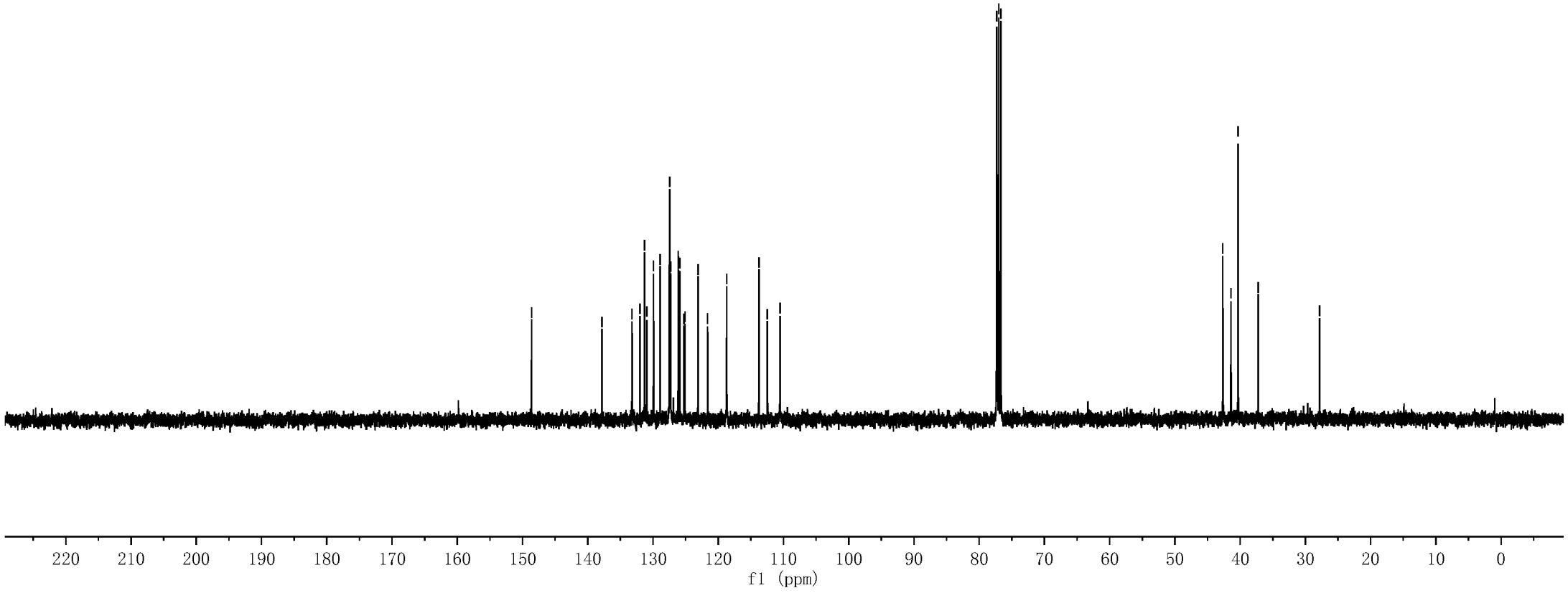


Parameter	Value
1 Title	ZYX-3-165-C
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	60
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-10T17:07:39
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

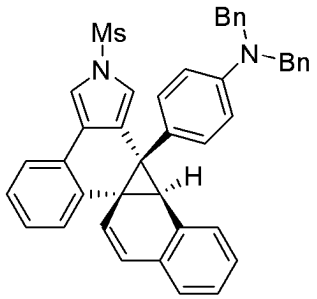


4x

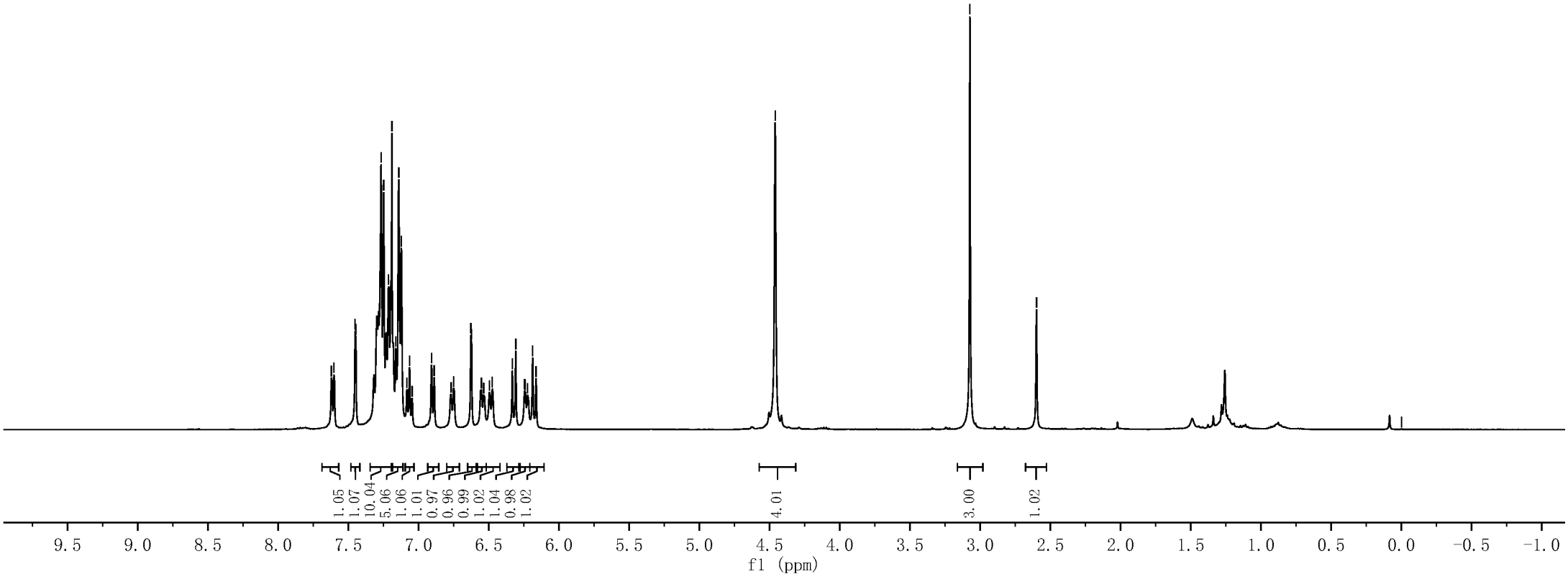




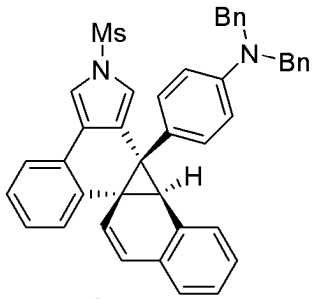
Parameter	Value
1 Title	zyx-3-200-h
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	13
6 Acquisition Time	4.0894
7 Acquisition Date	2021-12-20T16:33:20
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8



4y



Parameter	Value
1 Title	zyx-3-200-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	43
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-20T16:35:06
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



4y

147.68
138.60
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128.41
127.51
127.43
126.83
126.73
126.12
126.08
125.87
123.09
113.73
112.77
110.94
77.32
77.00
76.68
53.91
42.68
41.42
37.27
27.82

133.37
131.97
131.43
131.33
130.76
129.90
128.85
128.41
127.51
127.43
127.16
126.83
126.73
126.12
126.08
125.87
125.41
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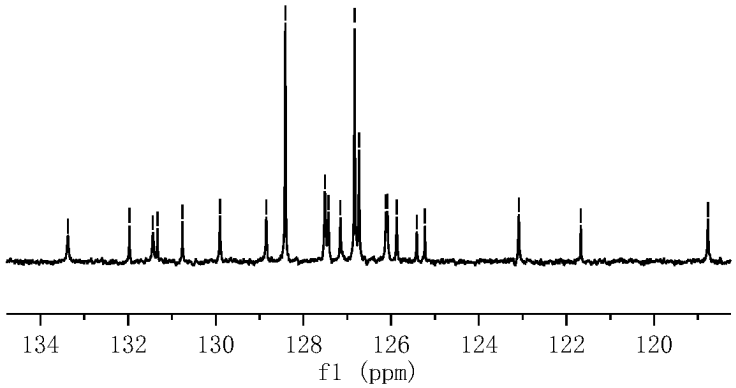
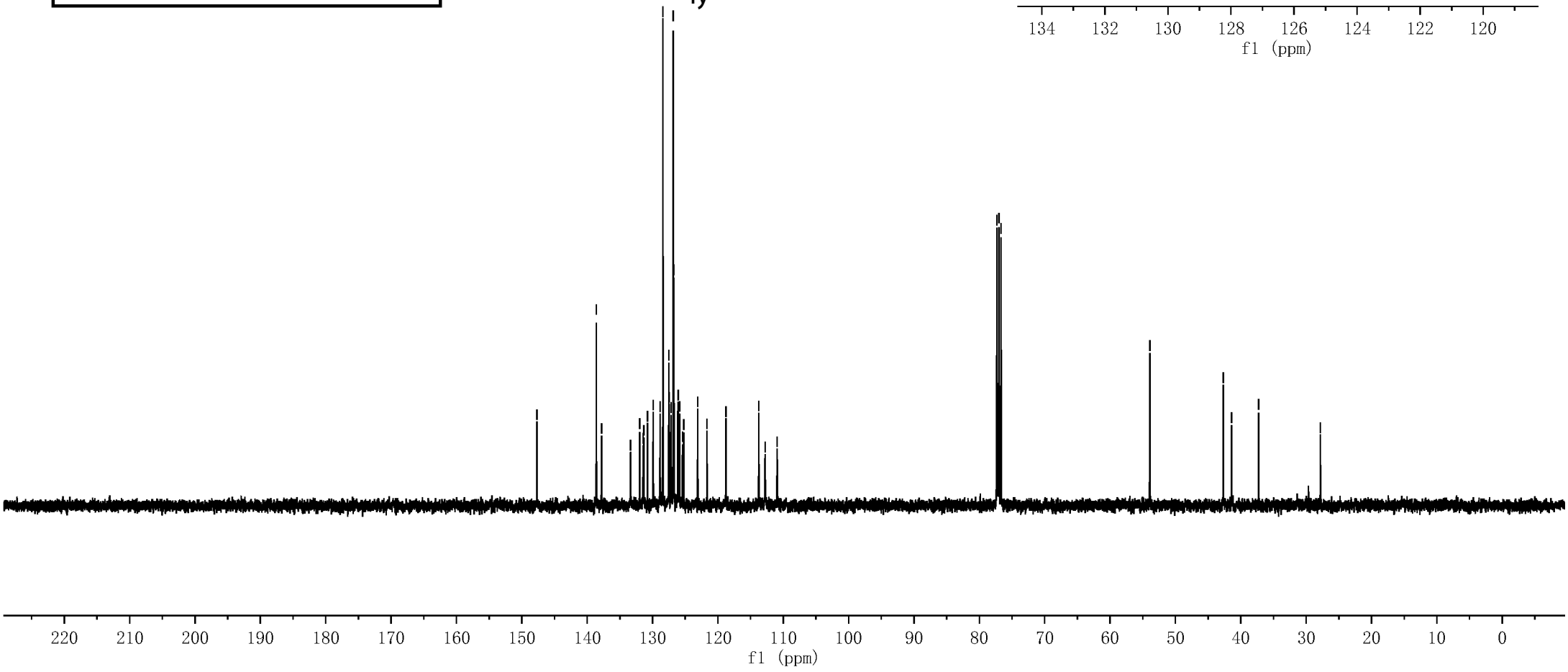
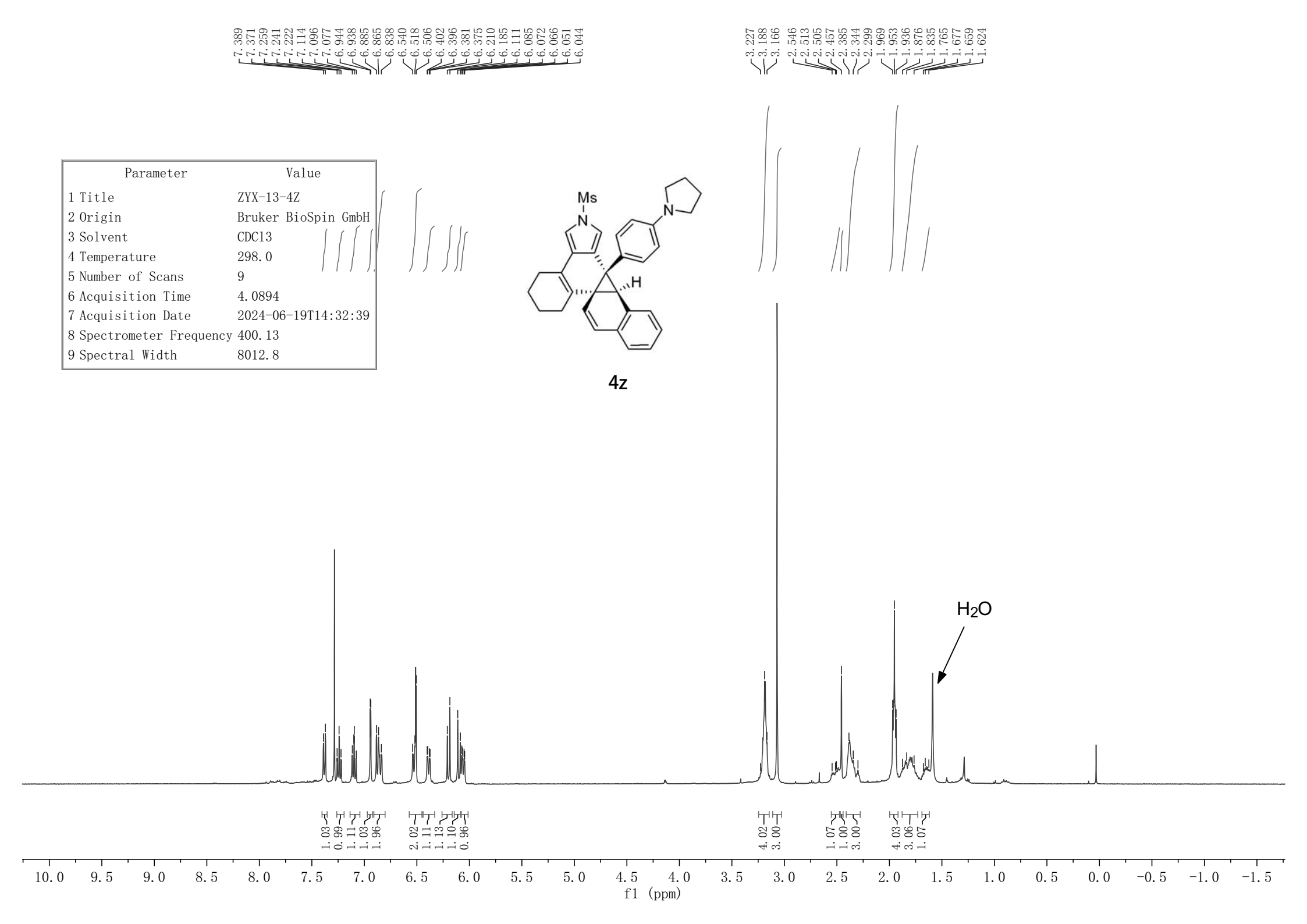
123.09
121.67
118.77



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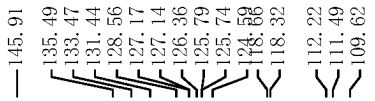
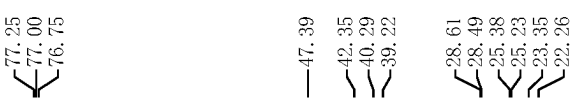
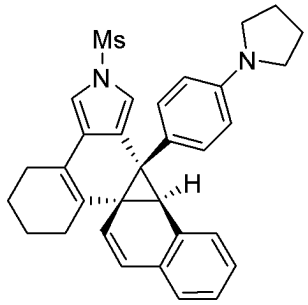
7.114
7.096
7.077
6.944
6.938
6.885
6.865
6.838
6.540
6.518
6.506
6.402
6.396
6.381
6.375
6.210
6.185
6.111
6.085
6.072
6.066
6.051
6.044
3.227
3.188
3.166
2.546
2.513
2.505
2.457
2.385
2.344
2.299
1.969
1.953
1.936
1.876
1.835
1.765
1.677
1.659
1.624
Parameter Value
1 Title ZYX-13-4Z
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 9
6 Acquisition Time 4.0894
7 Acquisition Date 2024-06-19T14:32:39
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
N
H
4z
H2O
1.03
0.99
1.11
1.03
1.96
2.02
1.11
1.13
1.10
0.96
4.02
3.00
1.07
1.00
3.00
4.03
3.06
1.07
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
-1.0
-1.5
f1 (ppm)

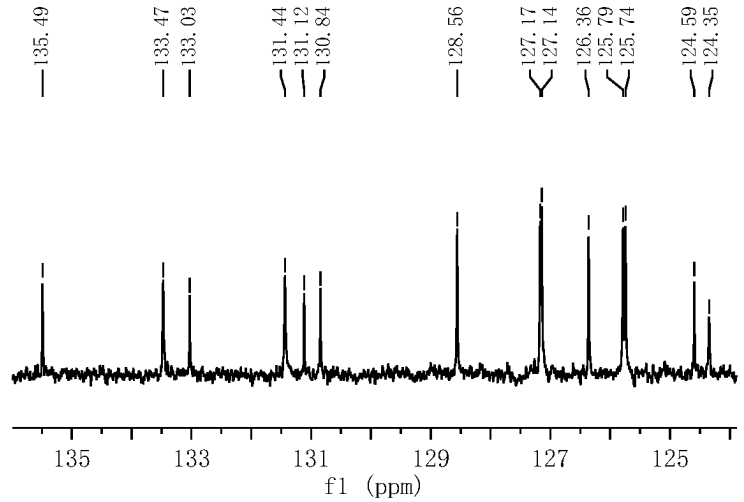
Parameter	Value
1 Title	zyx-6--68-cc
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	299.6
5 Number of Scans	103
6 Acquisition Time	1.1010
7 Acquisition Date	2022-08-17T21:51:10
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

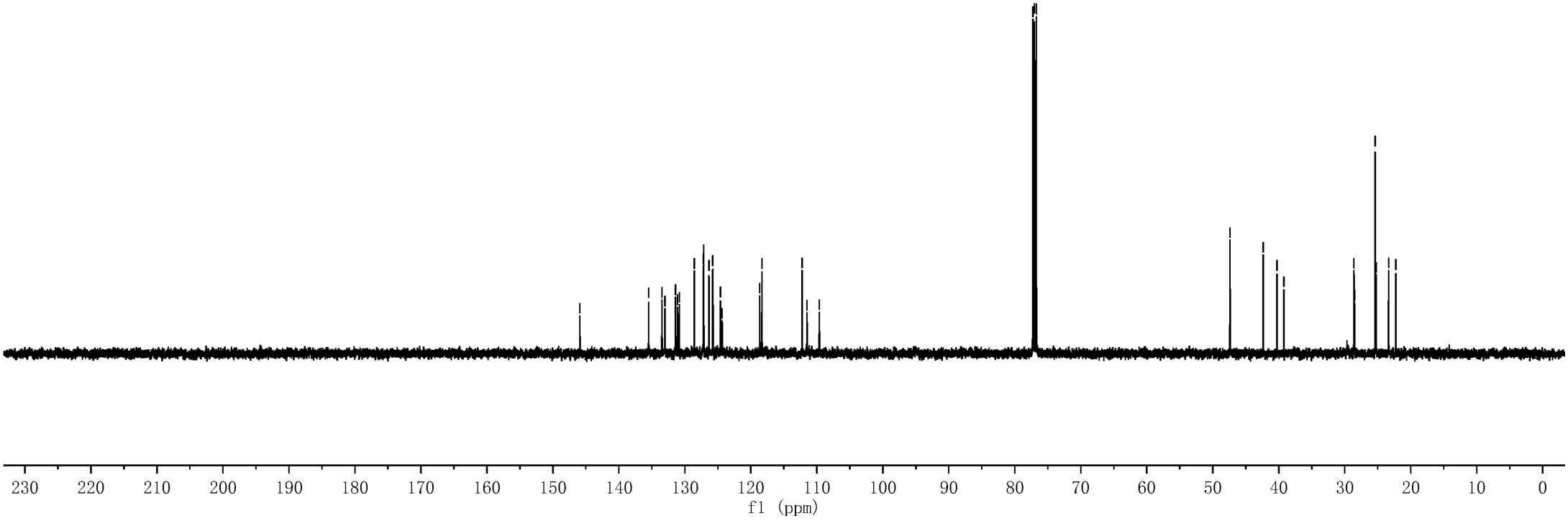


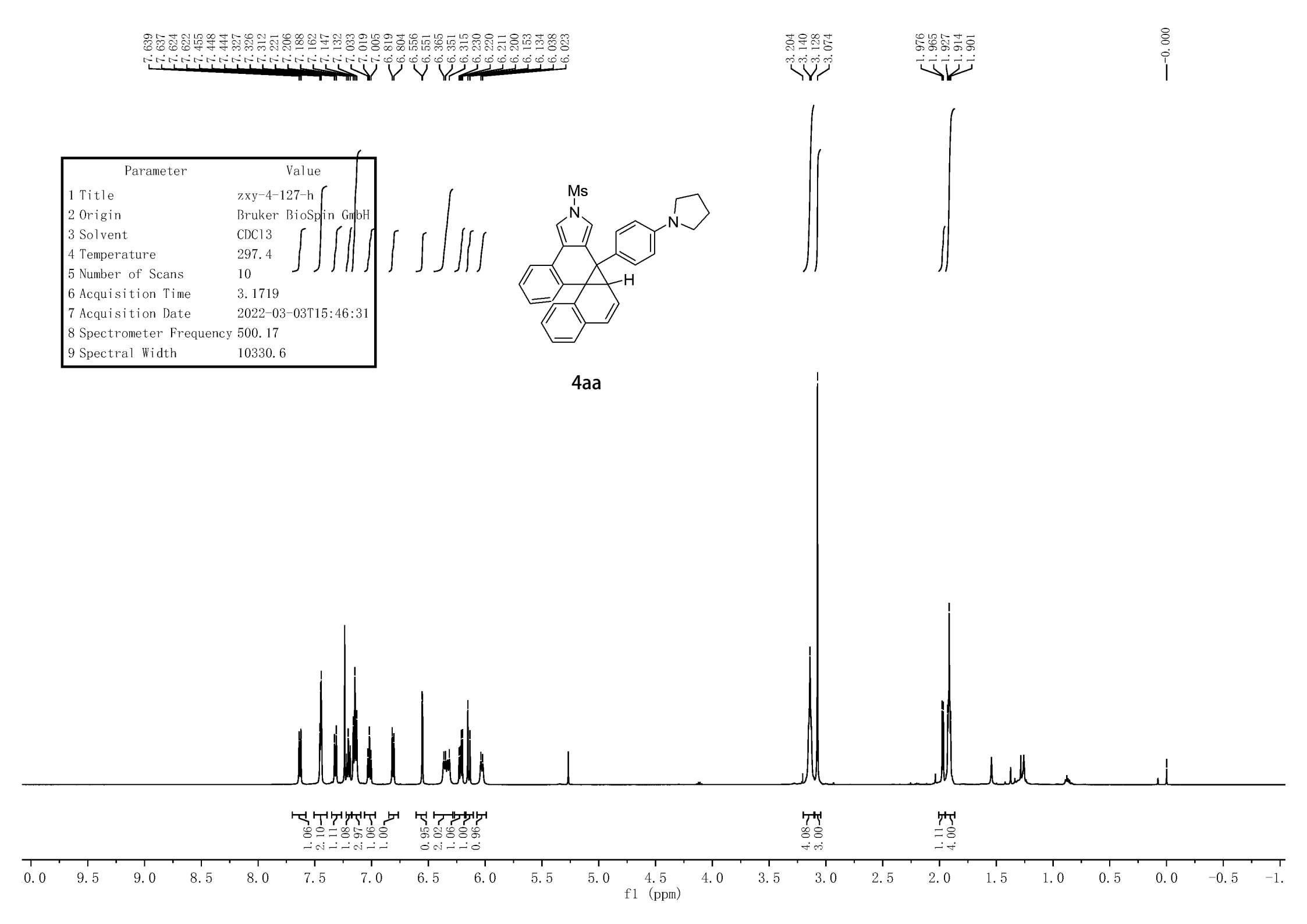




4z



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7.624
7.622
7.455
7.448
7.444
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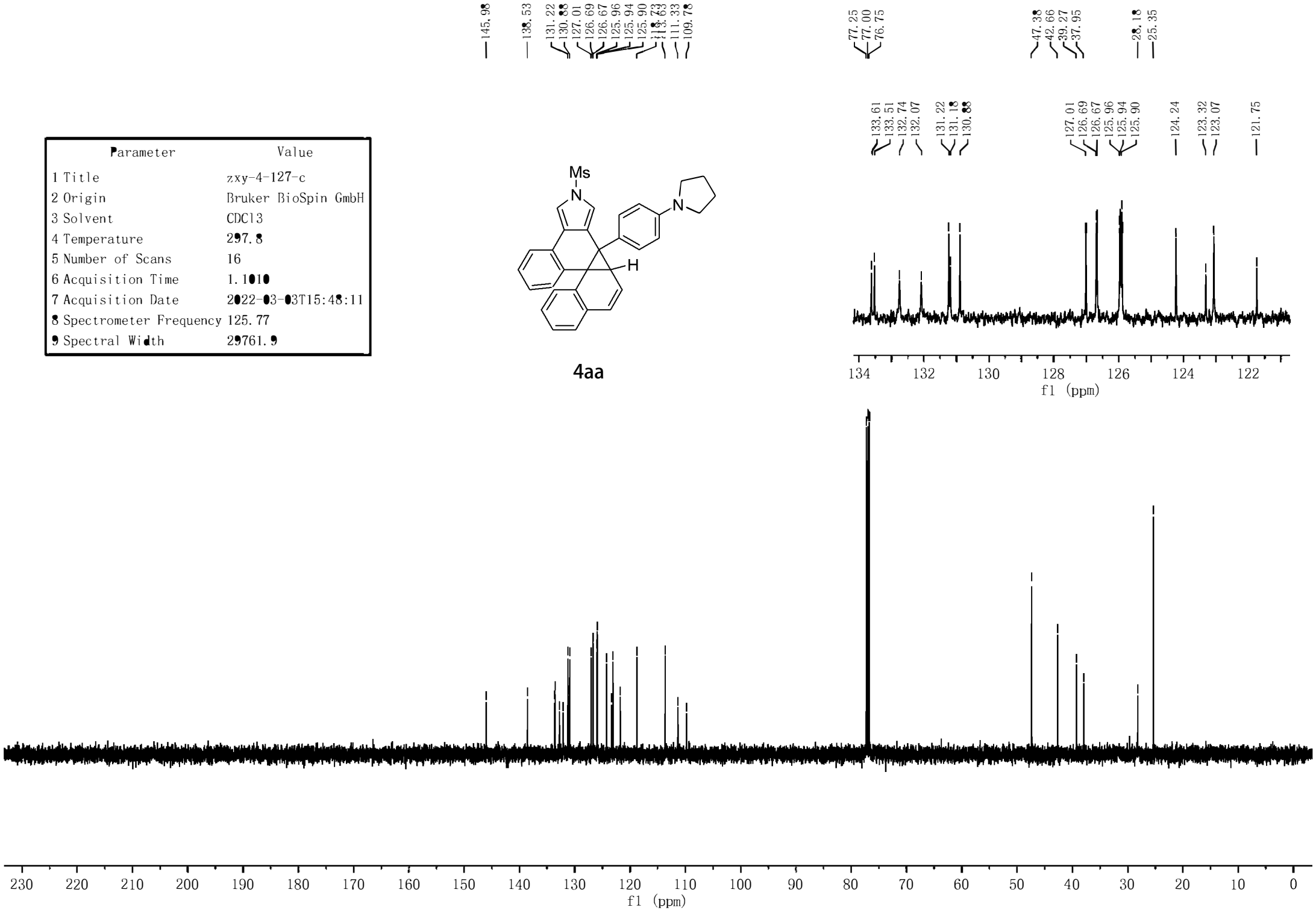
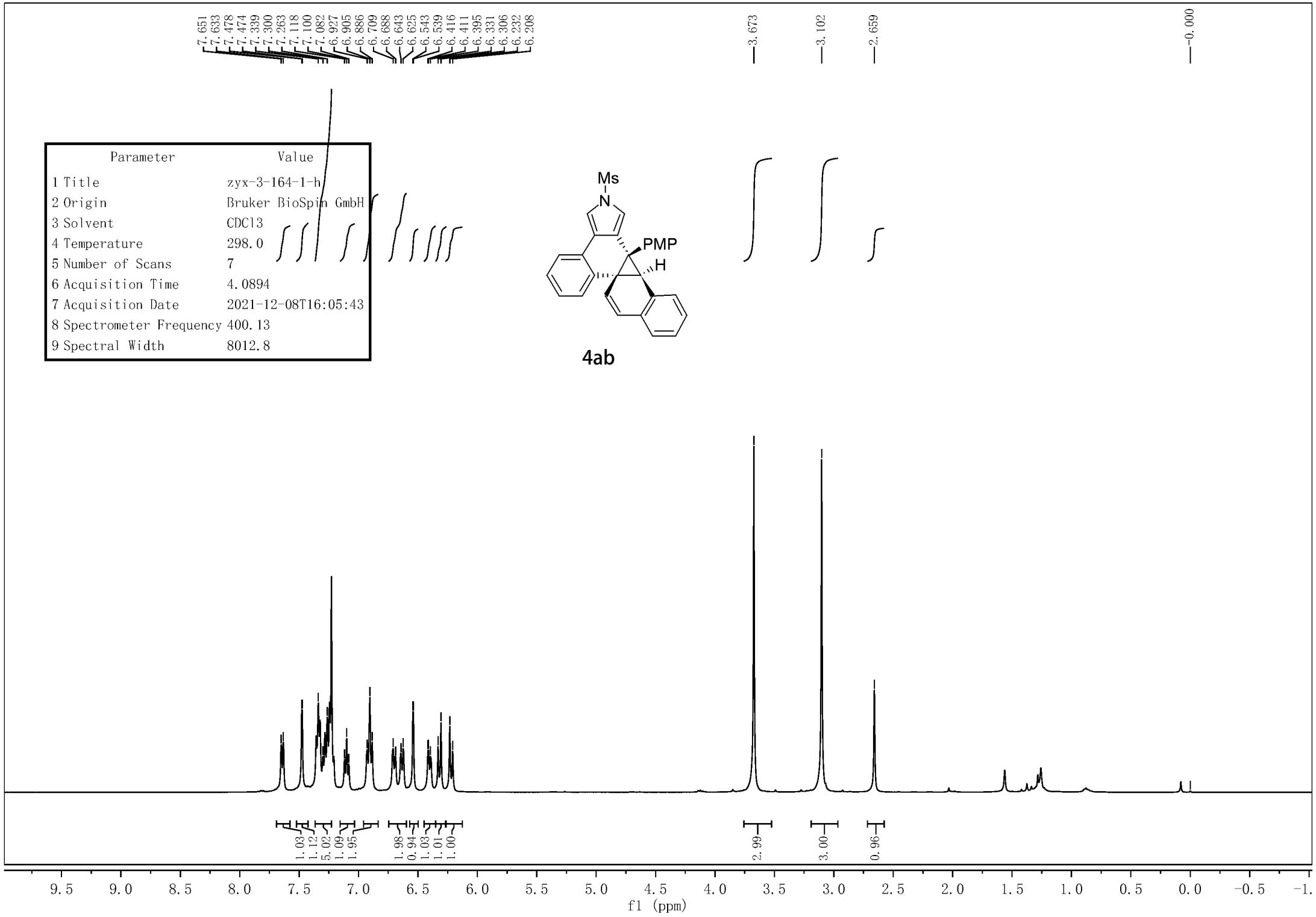
7.326
7.312
7.221
7.206
7.188
7.162
7.147
7.132
7.033
7.019
7.005
6.819
6.804
6.556
6.551
6.365
6.351
6.315
6.230
6.220
6.211
6.200
6.153
6.134
6.038
6.023
3.204
3.140
3.128
3.074
1.976
1.965
1.927
1.914
1.901
0.000
Parameter Value
1 Title zxy-4-127-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.4
5 Number of Scans 10
6 Acquisition Time 3.1719
7 Acquisition Date 2022-03-03T15:46:31
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Ms
N
N
H
4aa
1.06
2.10
1.11
1.08
2.97
1.06
1.00
0.95
2.02
1.06
1.00
0.96
4.08
3.00
1.11
4.00
0.0
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
-1.
f1 (ppm)

Parameter	Value
1 Title	zxy-4-127-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.8
5 Number of Scans	16
6 Acquisition Time	1.1010
7 Acquisition Date	2022-03-03T15:48:11
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

4aa

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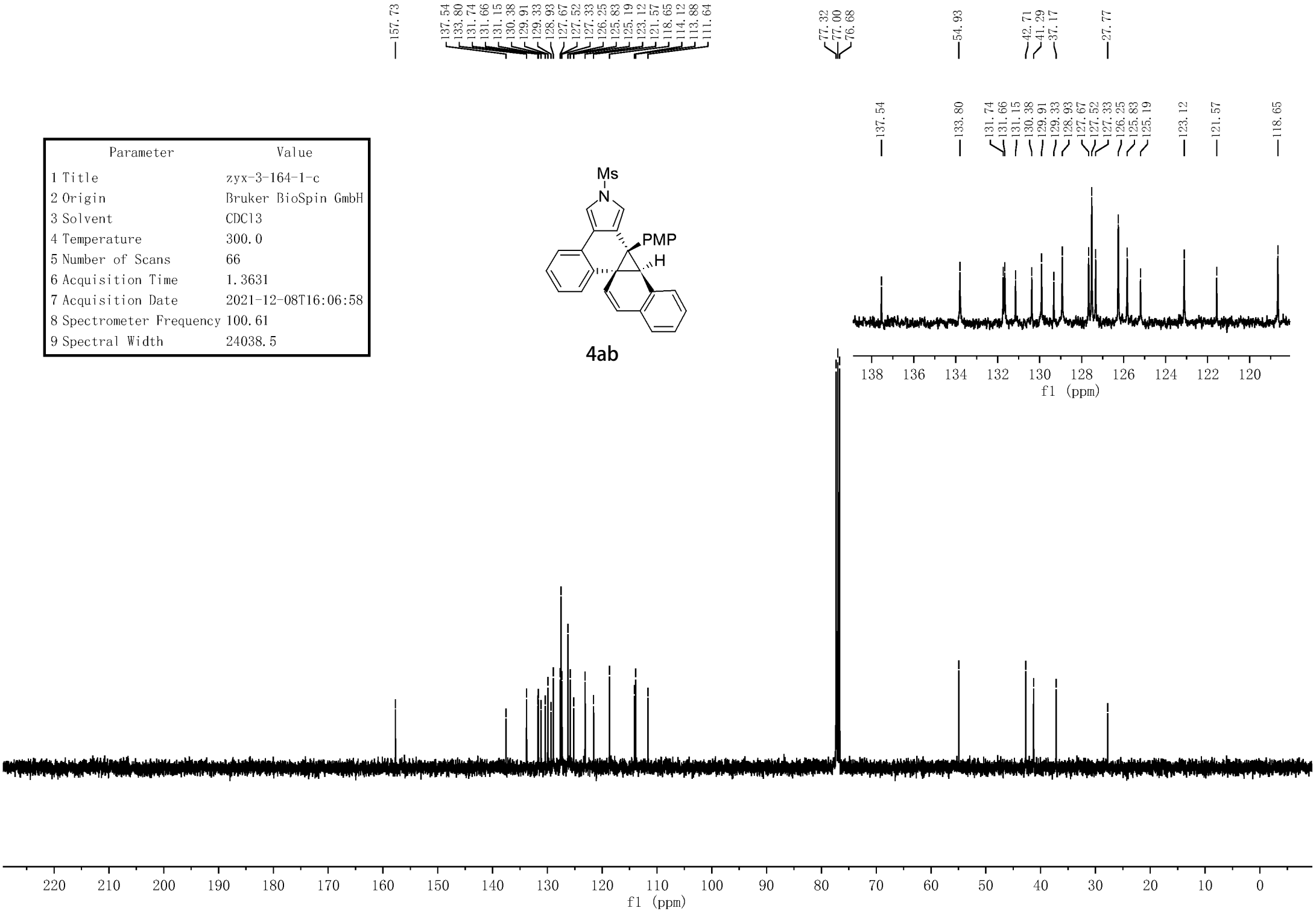
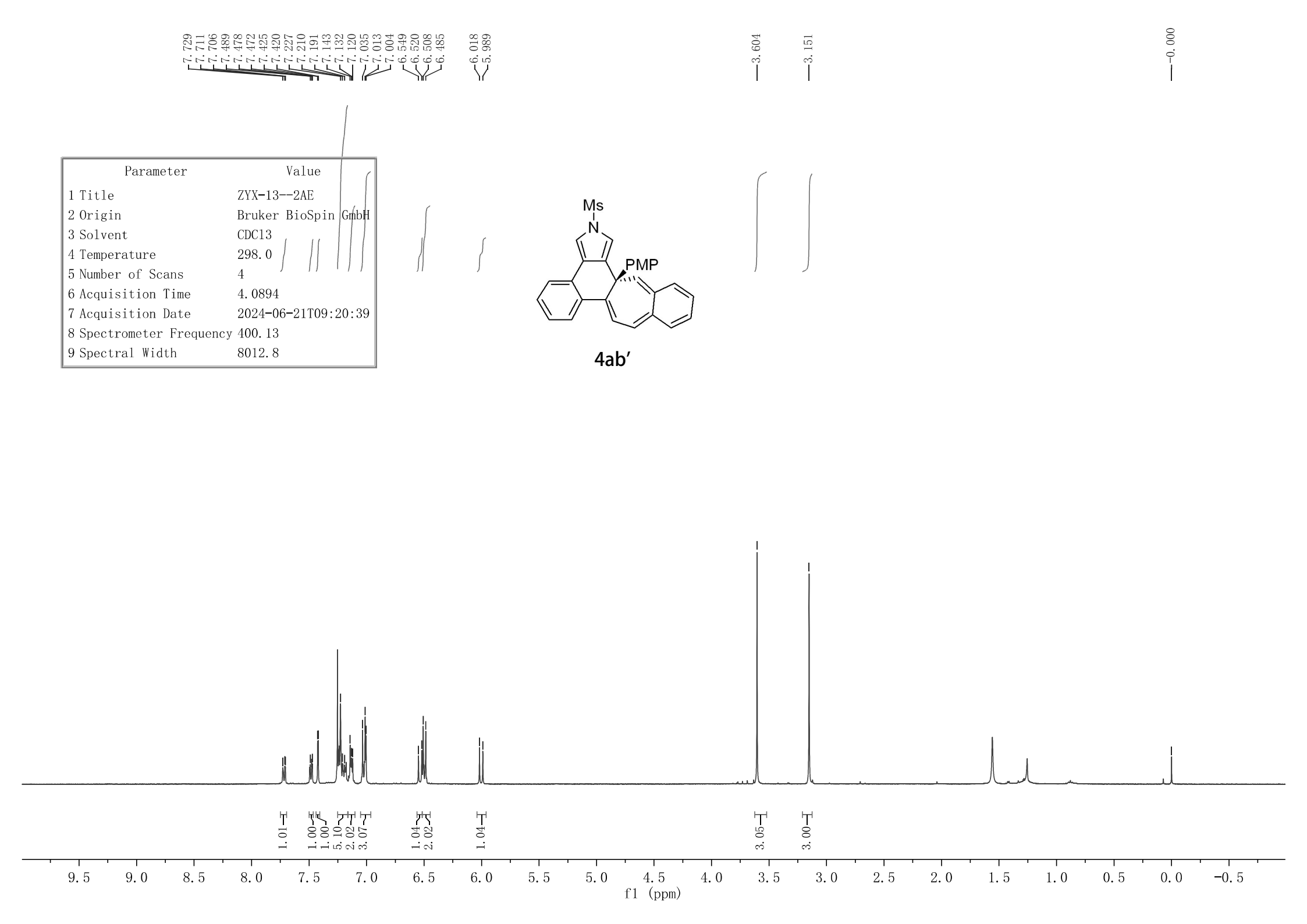
7.633
7.478
7.474
7.339
7.300
7.263
7.118
7.100
7.082
6.927
6.905
6.886
6.709
6.688
6.643
6.625
6.543
6.539
6.416
6.411
6.395
6.331
6.306
6.232
6.208
3.673
3.102
2.659
0.000
Parameter Value
1 Title zyx-3-164-1-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 7
6 Acquisition Time 4.0894
7 Acquisition Date 2021-12-08T16:05:43
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
PMP
H
4ab
1.03
1.12
5.02
1.09
1.95
1.98
0.94
1.03
1.01
1.00
2.99
3.00
0.96
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
-1.
f1 (ppm)

Parameter	Value
1 Title	zyx-3-164-1-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	66
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-08T16:06:58
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

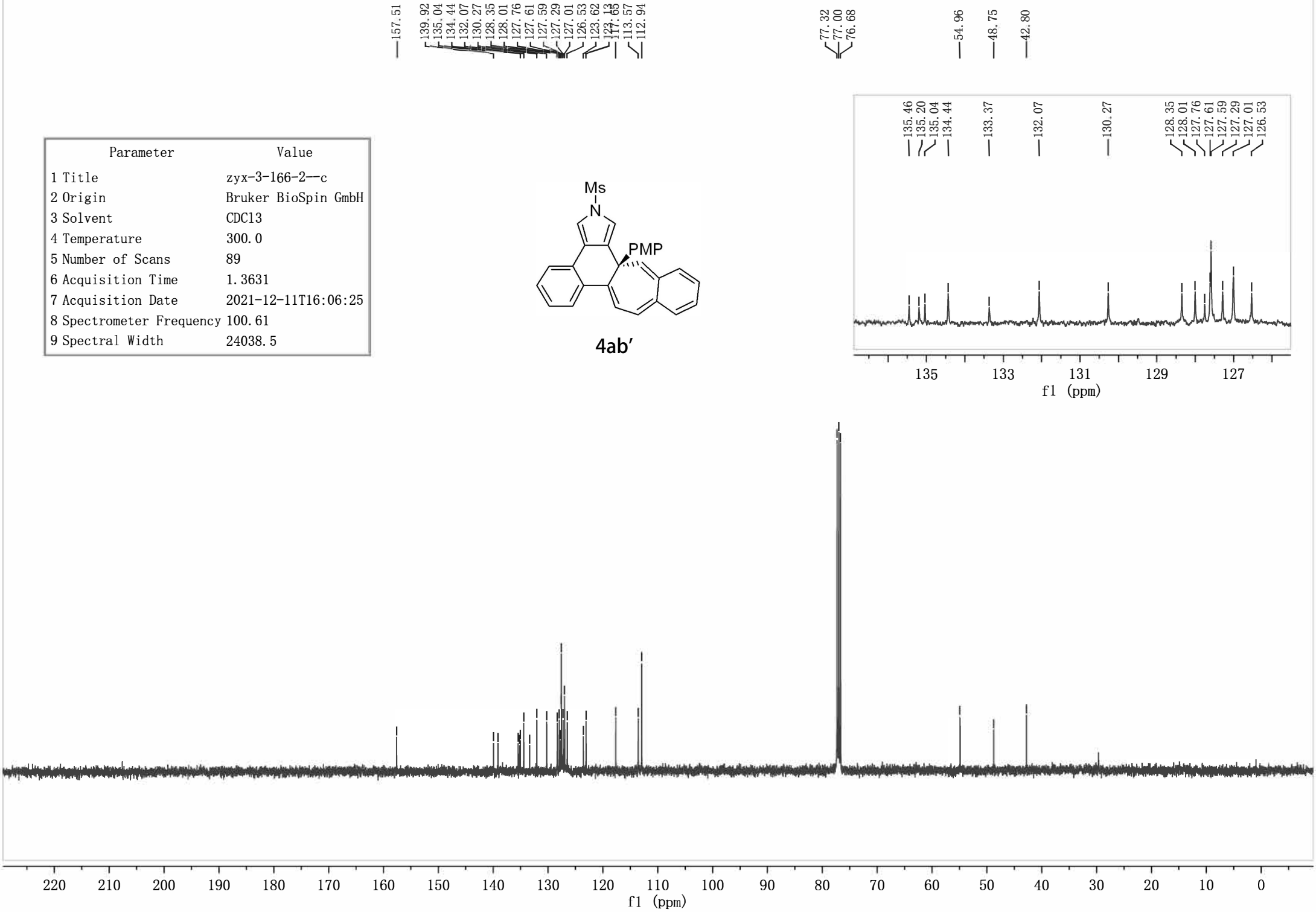
4ab




7.729
7.711
7.706
7.489
7.478
7.472
7.425
7.420
7.227
7.210
7.191
7.143
7.132
7.120
7.035
7.013
7.004
6.549
6.520
6.508
6.485
6.018
5.989
3.604
3.151
-0.000
Parameter Value
1 Title ZYX-13--2AE
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 4
6 Acquisition Time 4.0894
7 Acquisition Date 2024-06-21T09:20:39
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
PMP
4ab'
1.01
1.00
1.00
5.10
2.02
3.07
1.04
2.02
1.04
3.05
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)

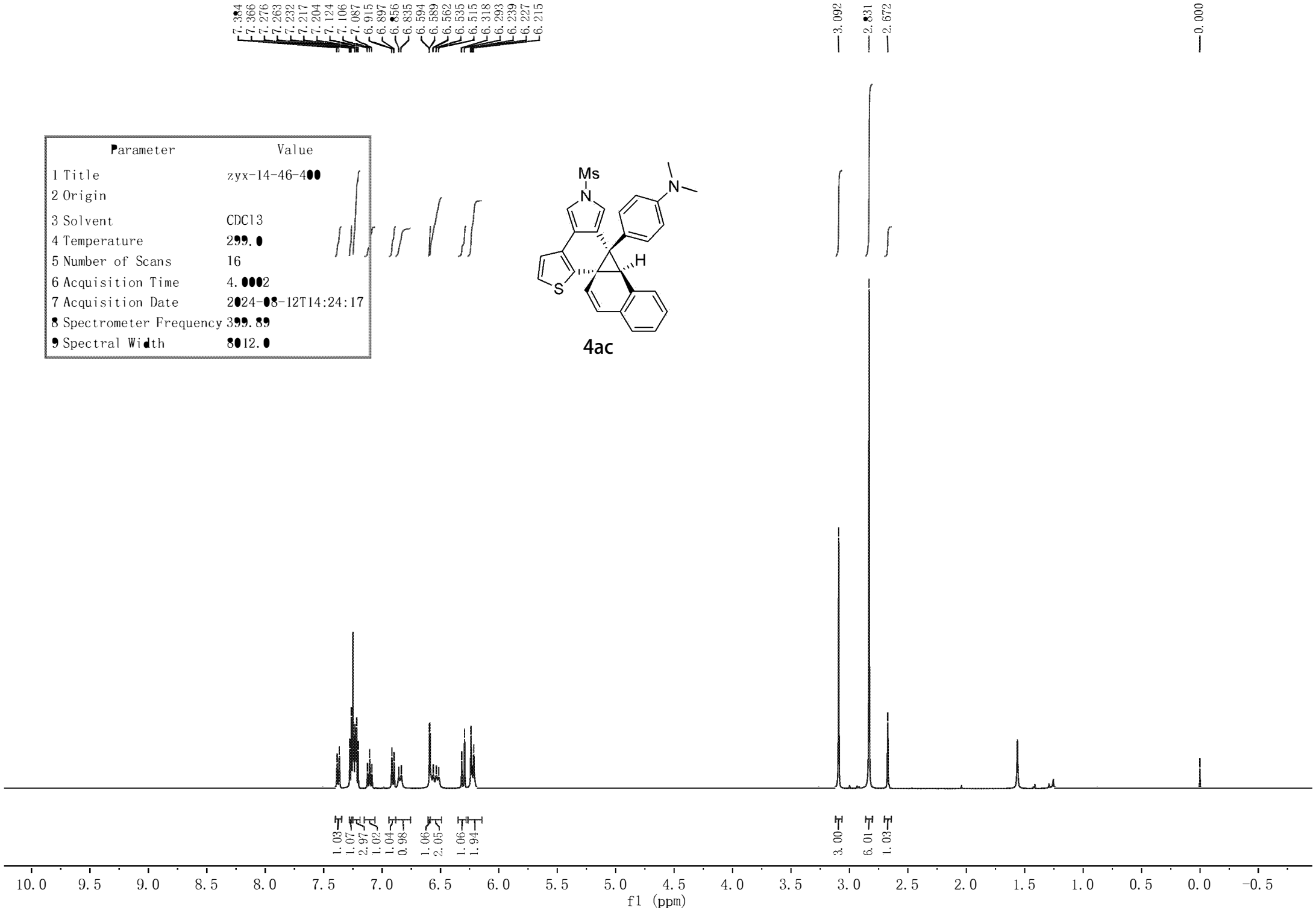
Parameter	Value
1 Title	zyx-3-166-2--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	89
6 Acquisition Time	1.3631
7 Acquisition Date	2021-12-11T16:06:25
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

4ab′

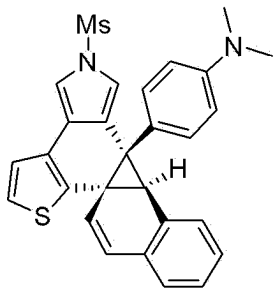


Parameter	Value
1 Title	zyx-14-46-400
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.0
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2024-08-12T14:24:17
8 Spectrometer Frequency	399.89
9 Spectral Width	8012.0

4ac



Parameter	Value
1 Title	zyx-14-46-400
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.8
5 Number of Scans	800
6 Acquisition Time	1.0000
7 Acquisition Date	2024-08-12T14:53:22
8 Spectrometer Frequency	100.55
9 Spectral Width	26041.0



4ac

148.70
142.20
128.83
128.28
127.74
127.57
126.21
124.72
124.35
122.91
112.31
110.62
77.32
77.00
76.68
42.61
41.29
40.34
36.70
29.40

133.33
132.16
131.41
131.11
130.70
128.83
128.28
127.74
127.57
126.21
124.72
124.60
124.35
124.30
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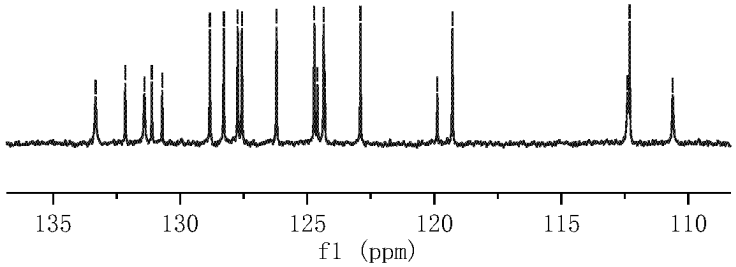
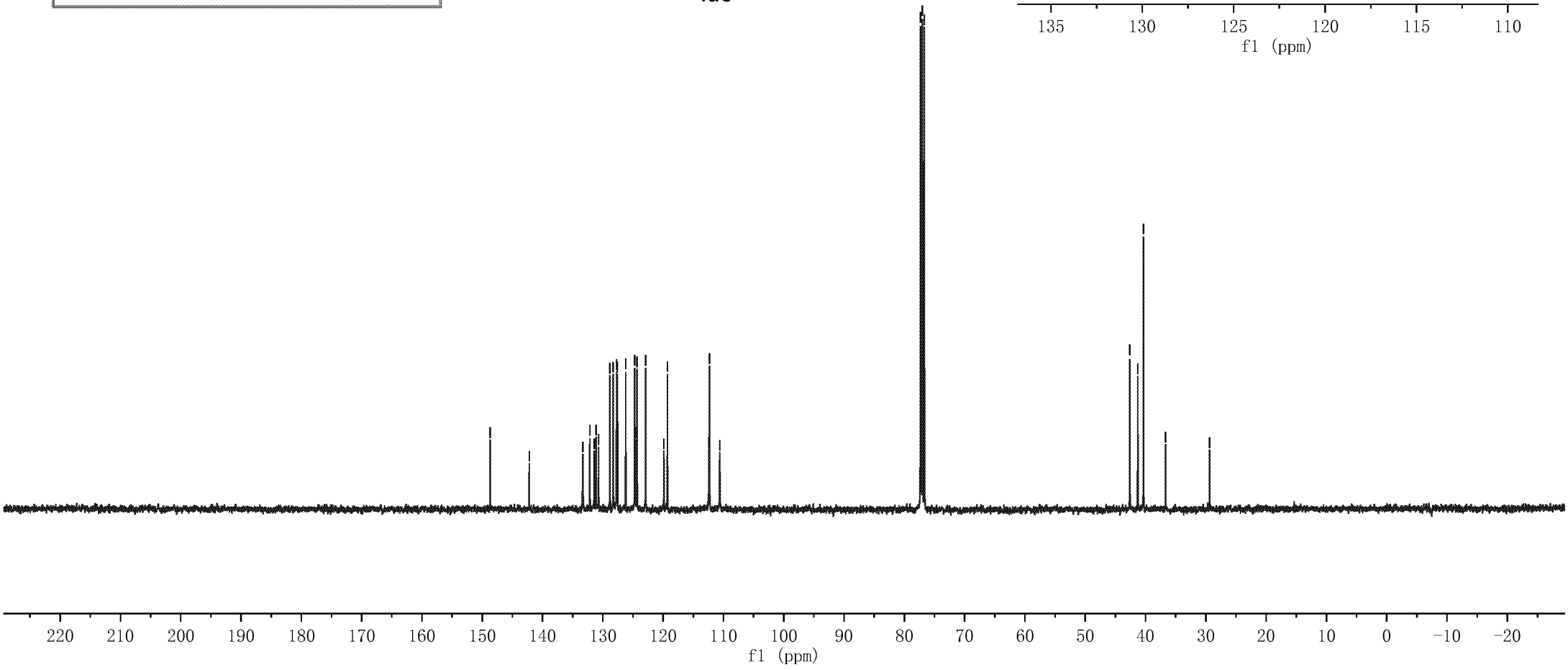
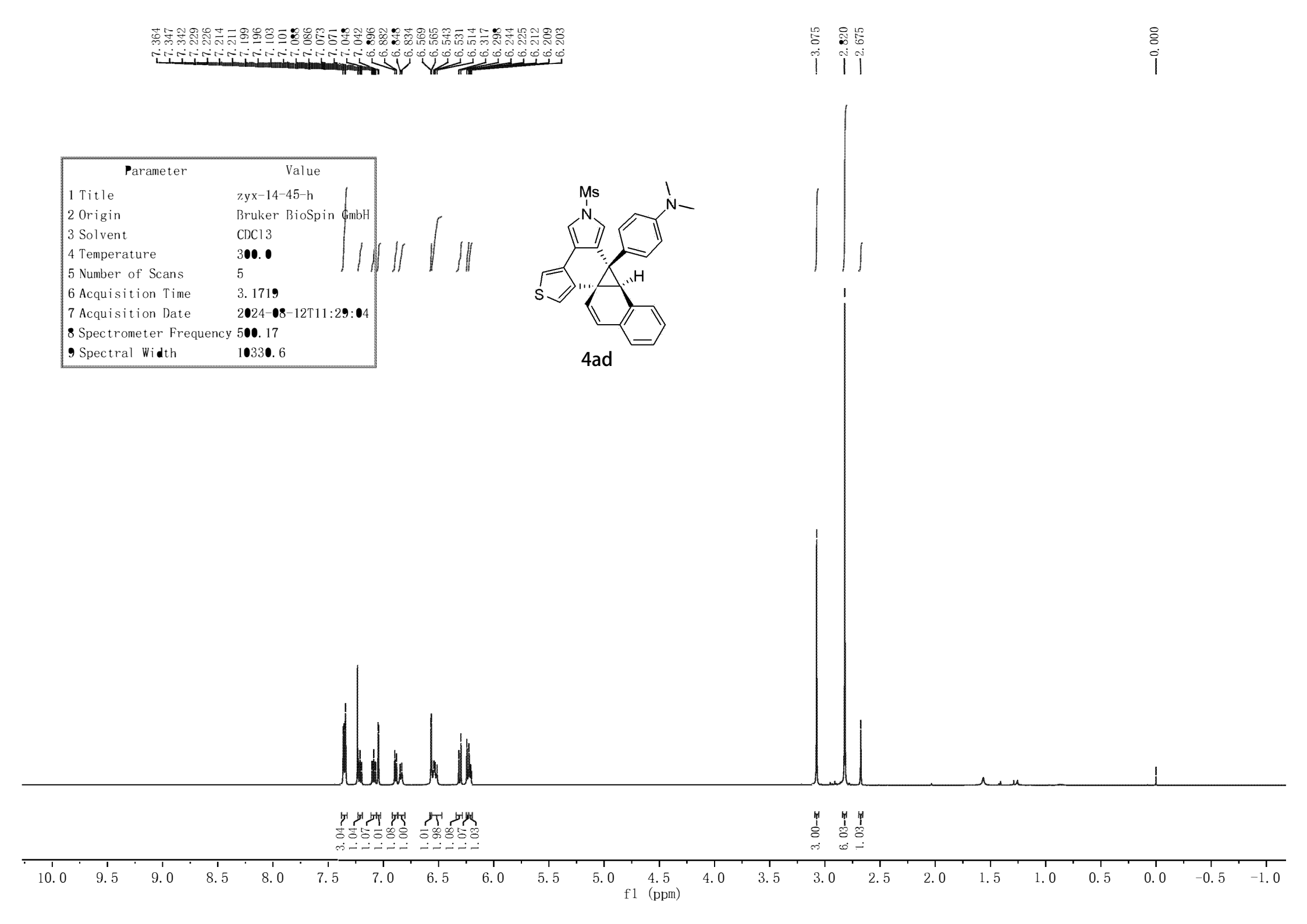
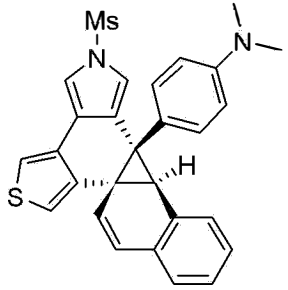
112.39
112.31
110.62



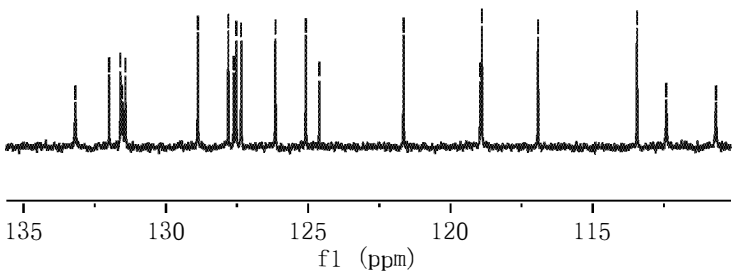


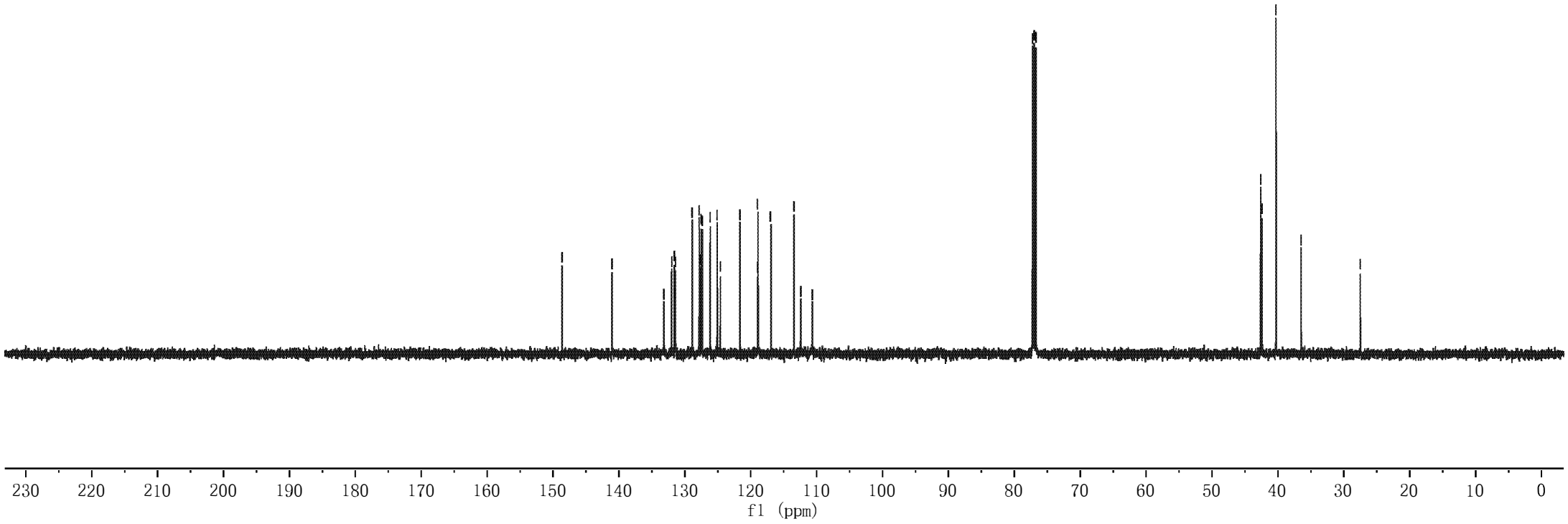

7.364
7.347
7.342
7.229
7.226
7.214
7.211
7.199
7.196
7.103
7.101
7.088
7.086
7.073
7.071
7.048
7.042
6.896
6.882
6.848
6.834
6.569
6.565
6.543
6.531
6.514
6.317
6.298
6.244
6.225
6.212
6.209
6.203
3.075
2.820
2.675
0.000
Parameter Value
1 Title zyx-14-45-h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 5
6 Acquisition Time 3.1719
7 Acquisition Date 2024-08-12T11:29:04
8 Spectrometer Frequency 500.17
9 Spectral Width 10330.6
Ms
N
N
H
S
4ad
3.04
1.04
1.07
1.01
1.08
1.00
1.01
1.98
1.08
1.07
1.03
3.00
6.03
1.03
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
-1.0
f1 (ppm)

Parameter	Value
1 Title	zyx-14-45-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	299.0
5 Number of Scans	68
6 Acquisition Time	1.1010
7 Acquisition Date	2024-08-12T11:34:46
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

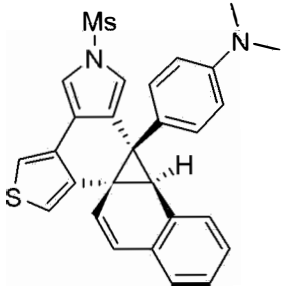


4ad

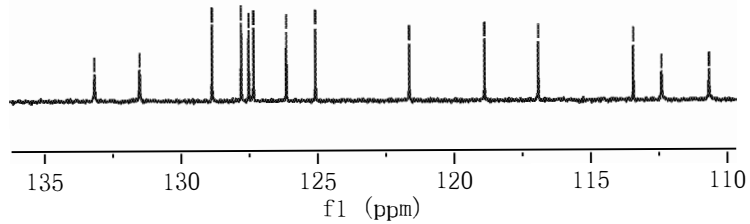


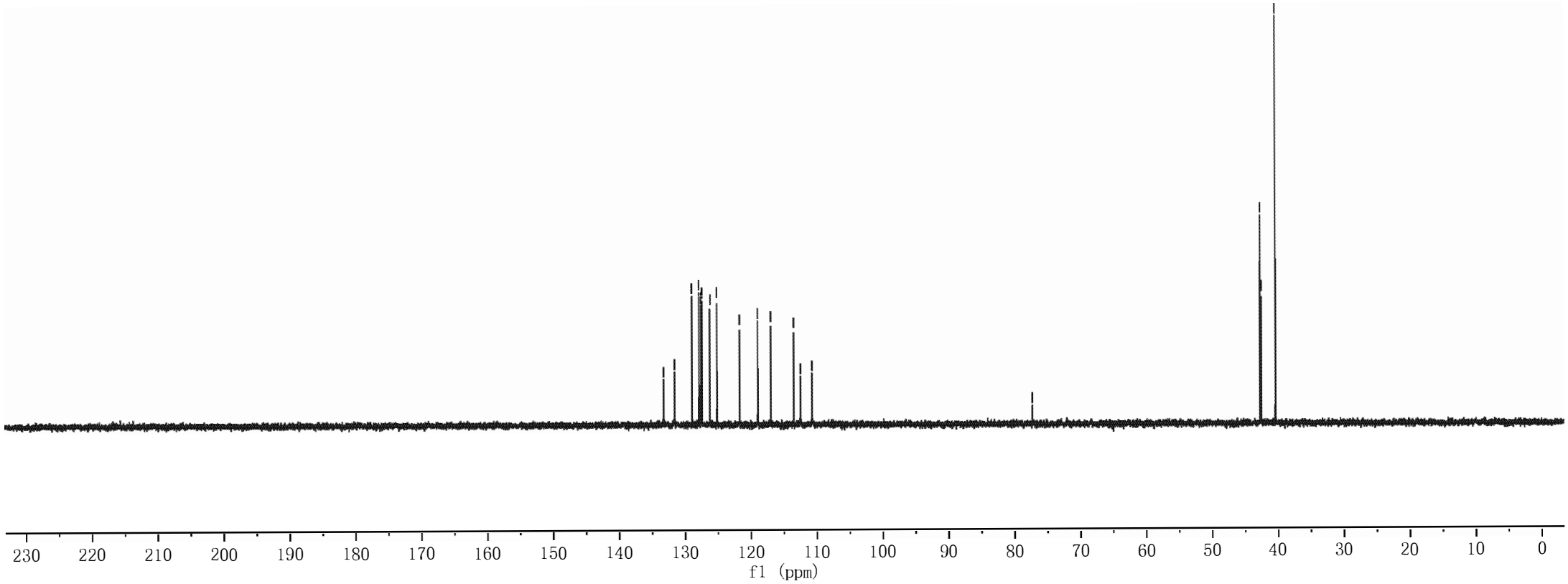


Parameter	Value
1 Title	zyx-14-45-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	299.1
5 Number of Scans	36
6 Acquisition Time	1.1010
7 Acquisition Date	2024-08-12T11:38:48
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9



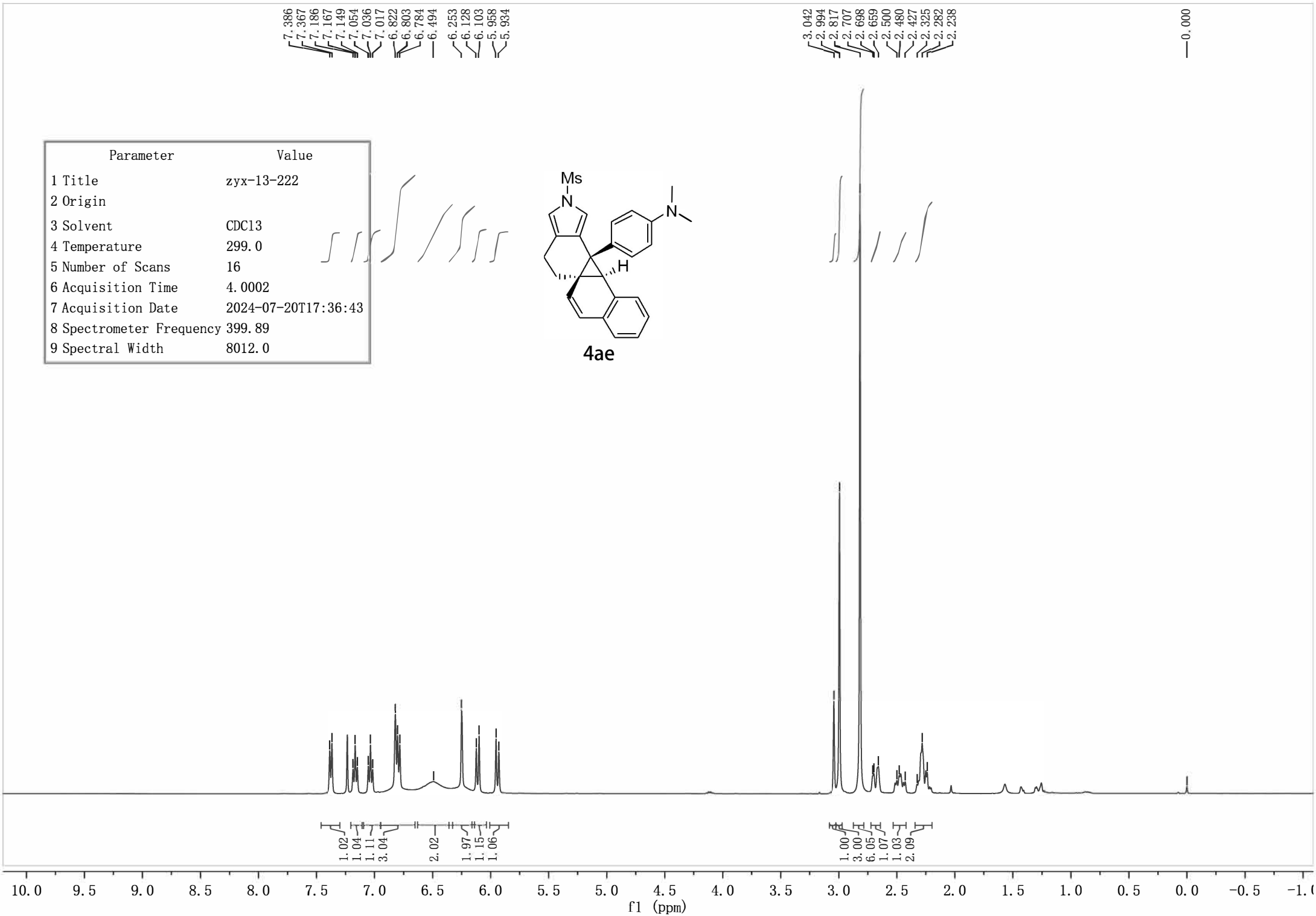
4ad





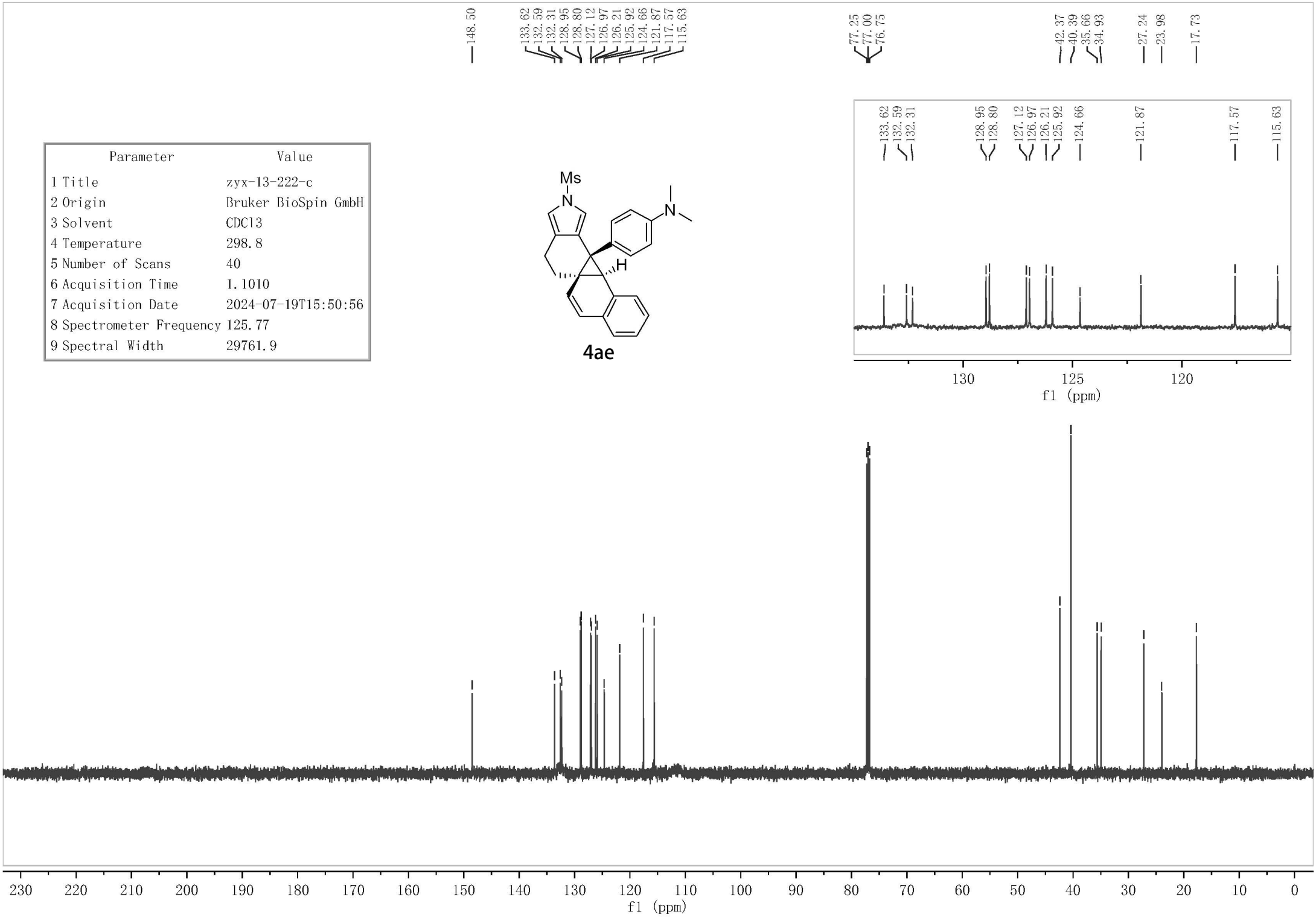
Parameter	Value
1 Title	zyx-13-222
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.0
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2024-07-20T17:36:43
8 Spectrometer Frequency	399.89
9 Spectral Width	8012.0

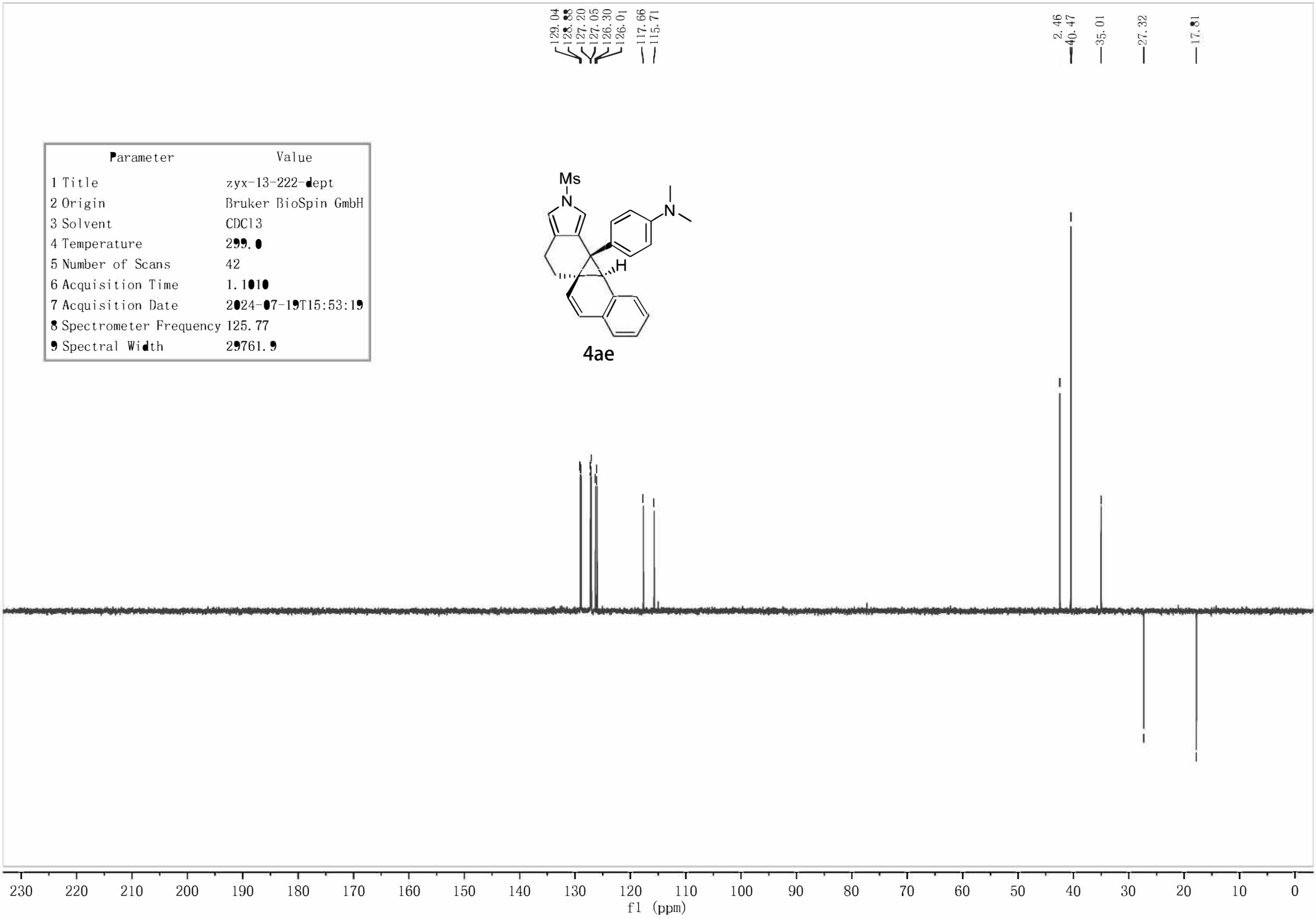
4ae



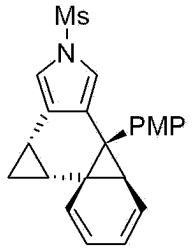
Parameter	Value
1 Title	zyx-13-222-c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.8
5 Number of Scans	40
6 Acquisition Time	1.1010
7 Acquisition Date	2024-07-19T15:50:56
8 Spectrometer Frequency	125.77
9 Spectral Width	29761.9

4ae

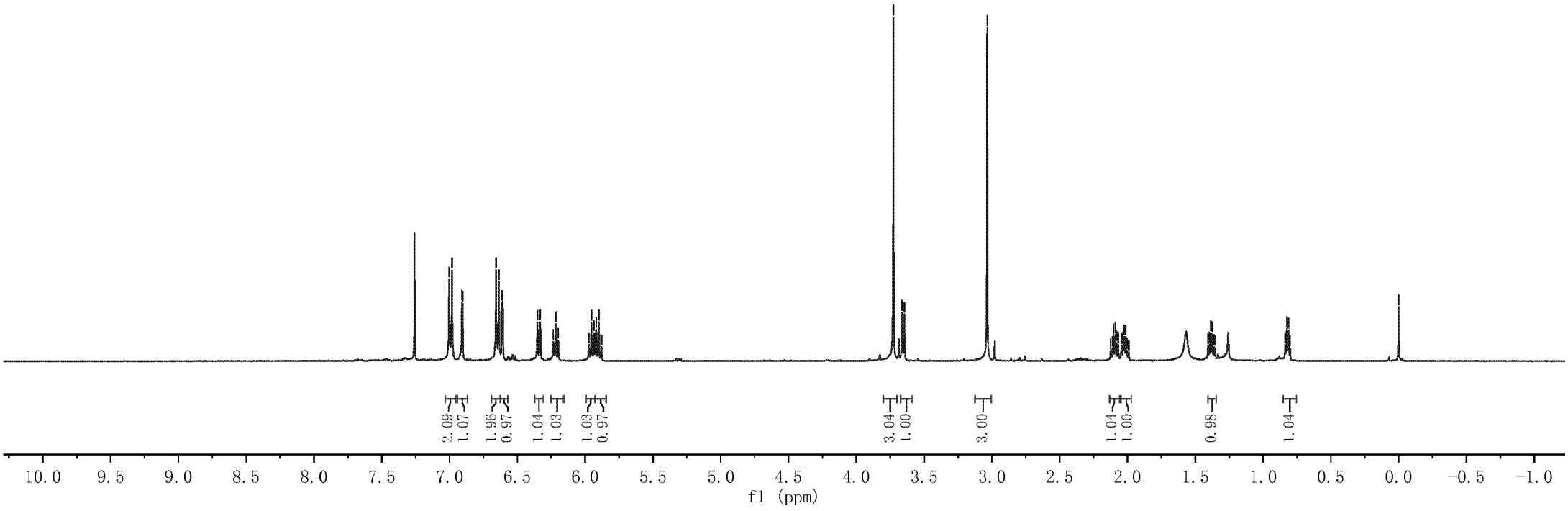



129.04
128.88
127.20
127.05
126.30
126.01
117.66
115.71
2.46
40.47
35.01
27.32
17.81
Parameter Value
1 Title zyx-13-222-dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 299.0
5 Number of Scans 42
6 Acquisition Time 1.1010
7 Acquisition Date 2024-07-19T15:53:19
8 Spectrometer Frequency 125.77
9 Spectral Width 29761.9
Ms
N
N
H
4ae
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Parameter	Value
1 Title	ZYX-13-236-H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	3
6 Acquisition Time	4.0894
7 Acquisition Date	2024-07-27T22:13:02
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

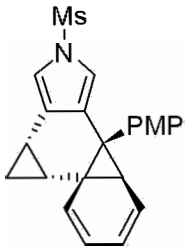


4aj

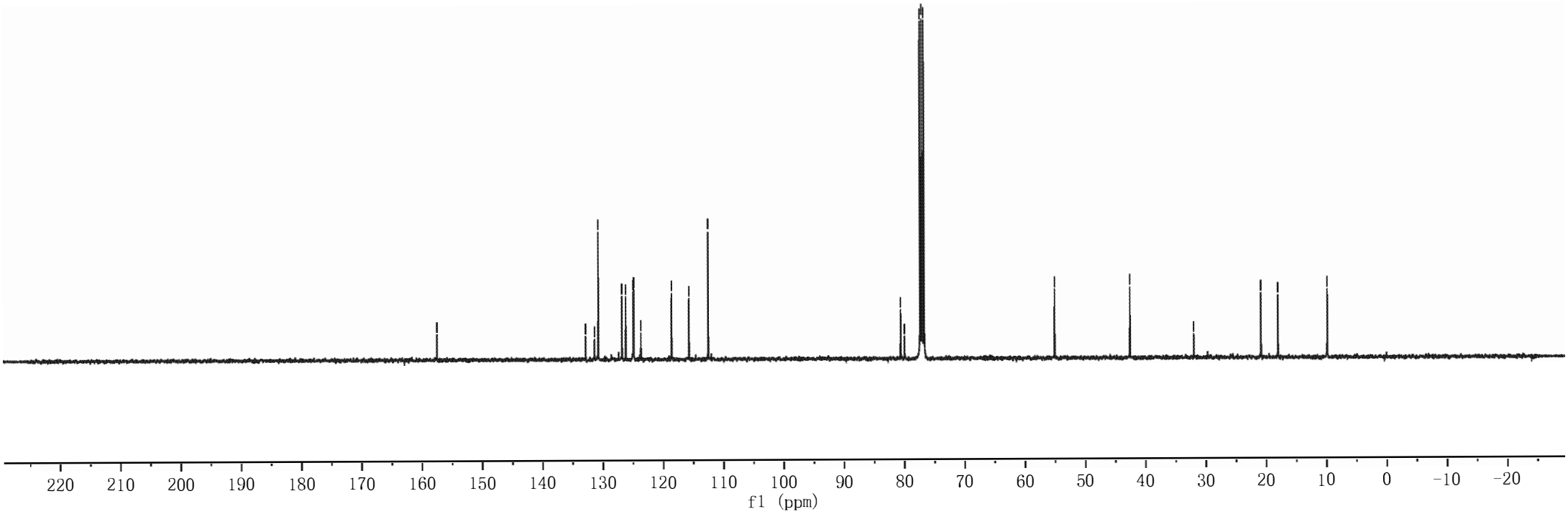


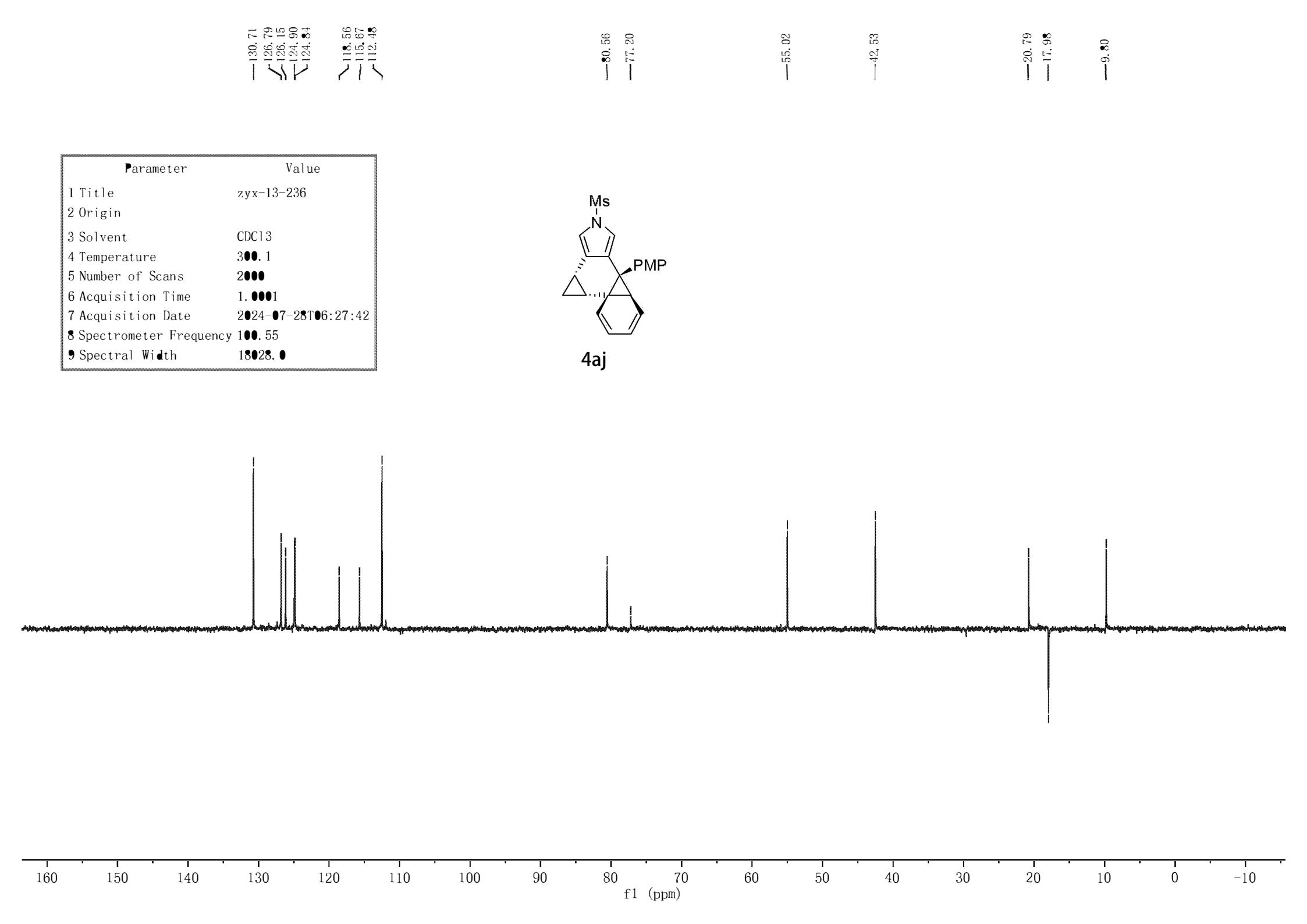
157.47
132.81
131.34
130.71
126.79
126.15
124.90
124.84
123.64
118.56
115.67
112.48
80.56
79.91
77.32
77.00
76.68
55.02
42.53
31.94
20.79
17.98
9.80

Parameter	Value
1 Title	zyx-13-236-c
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.6
5 Number of Scans	4000
6 Acquisition Time	1.0000
7 Acquisition Date	2024-07-28T19:31:59
8 Spectrometer Frequency	100.55
9 Spectral Width	26041.0

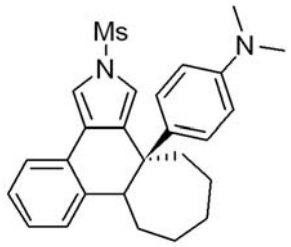


4aj

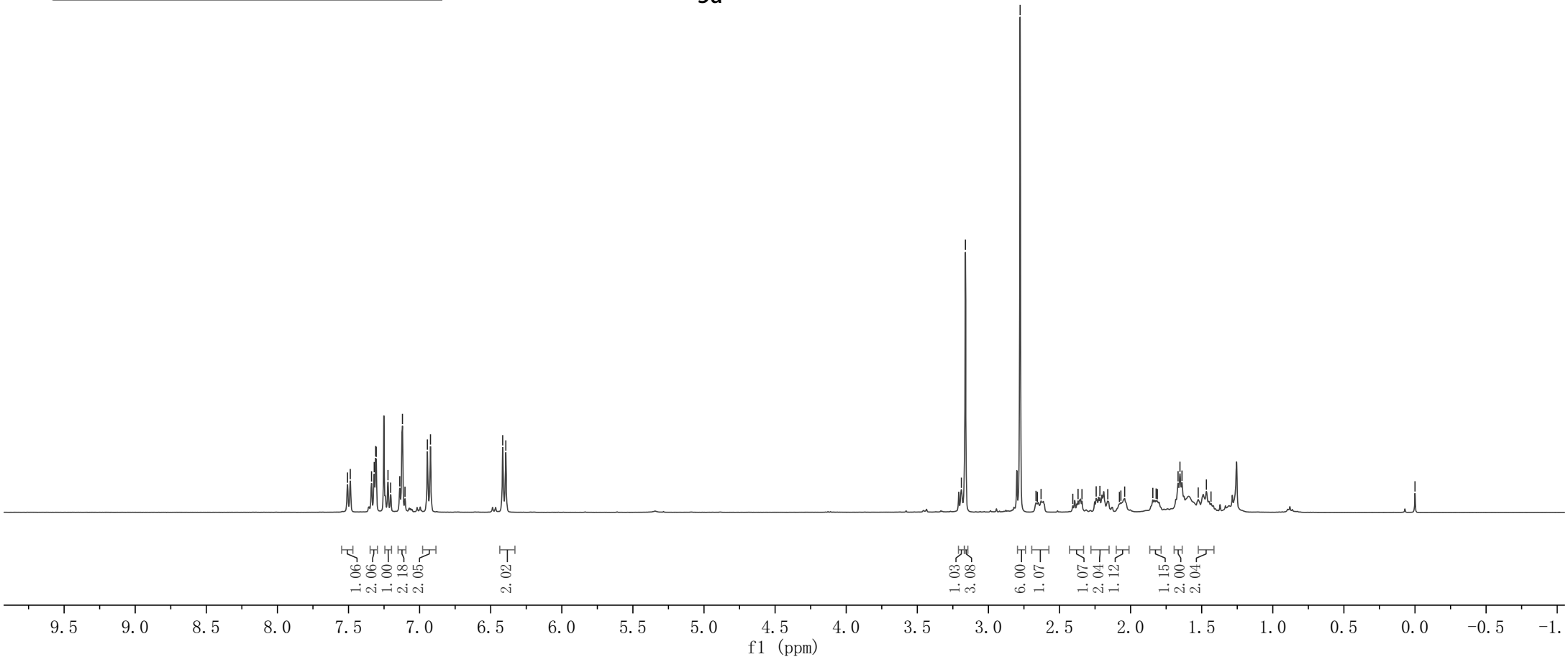



130.71
126.79
126.15
124.90
124.84
118.56
115.67
112.48
80.56
77.20
55.02
42.53
20.79
17.98
9.80
Parameter Value
1 Title zyx-13-236
2 Origin
3 Solvent CDCl3
4 Temperature 300.1
5 Number of Scans 2000
6 Acquisition Time 1.0001
7 Acquisition Date 2024-07-28T06:27:42
8 Spectrometer Frequency 100.55
9 Spectral Width 18028.0
Ms
N
PMP
4aj
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Parameter	Value
1 Title	ZYX-6-74
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.9
5 Number of Scans	25
6 Acquisition Time	4.0002
7 Acquisition Date	2022-08-20T13:22:52
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0



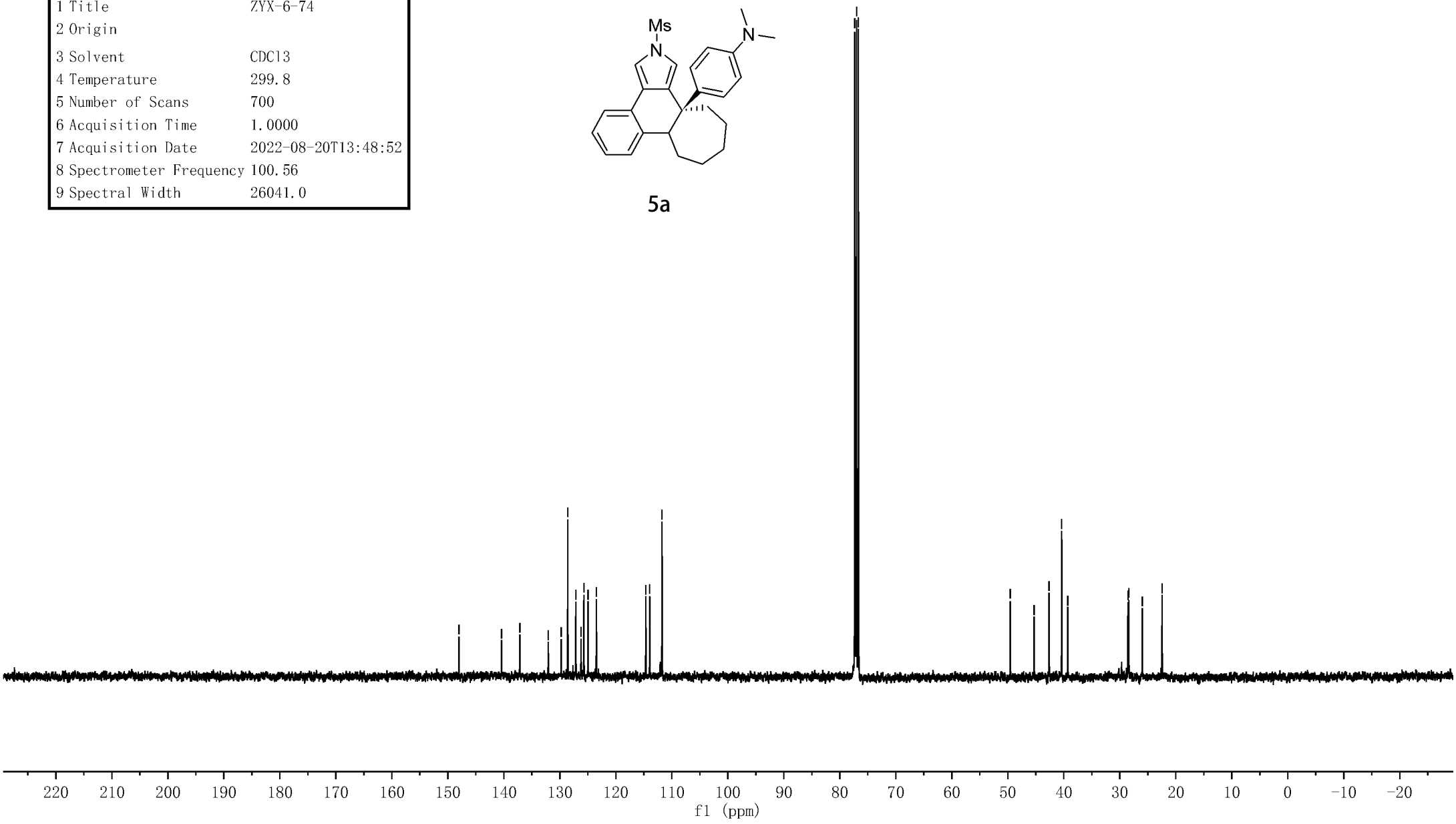
5a



148.00
140.42
137.13
132.07
129.74
128.58
127.15
126.22
125.71
124.96
123.47
114.65
113.95
111.75
77.32
77.00
76.68
49.55
45.32
42.63
40.38
39.29
28.54
28.39
25.98
22.45

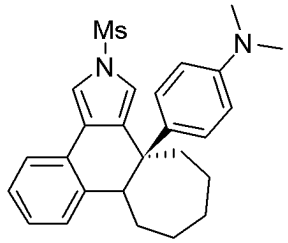
Parameter	Value
1 Title	ZYX-6-74
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.8
5 Number of Scans	700
6 Acquisition Time	1.0000
7 Acquisition Date	2022-08-20T13:48:52
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

5a

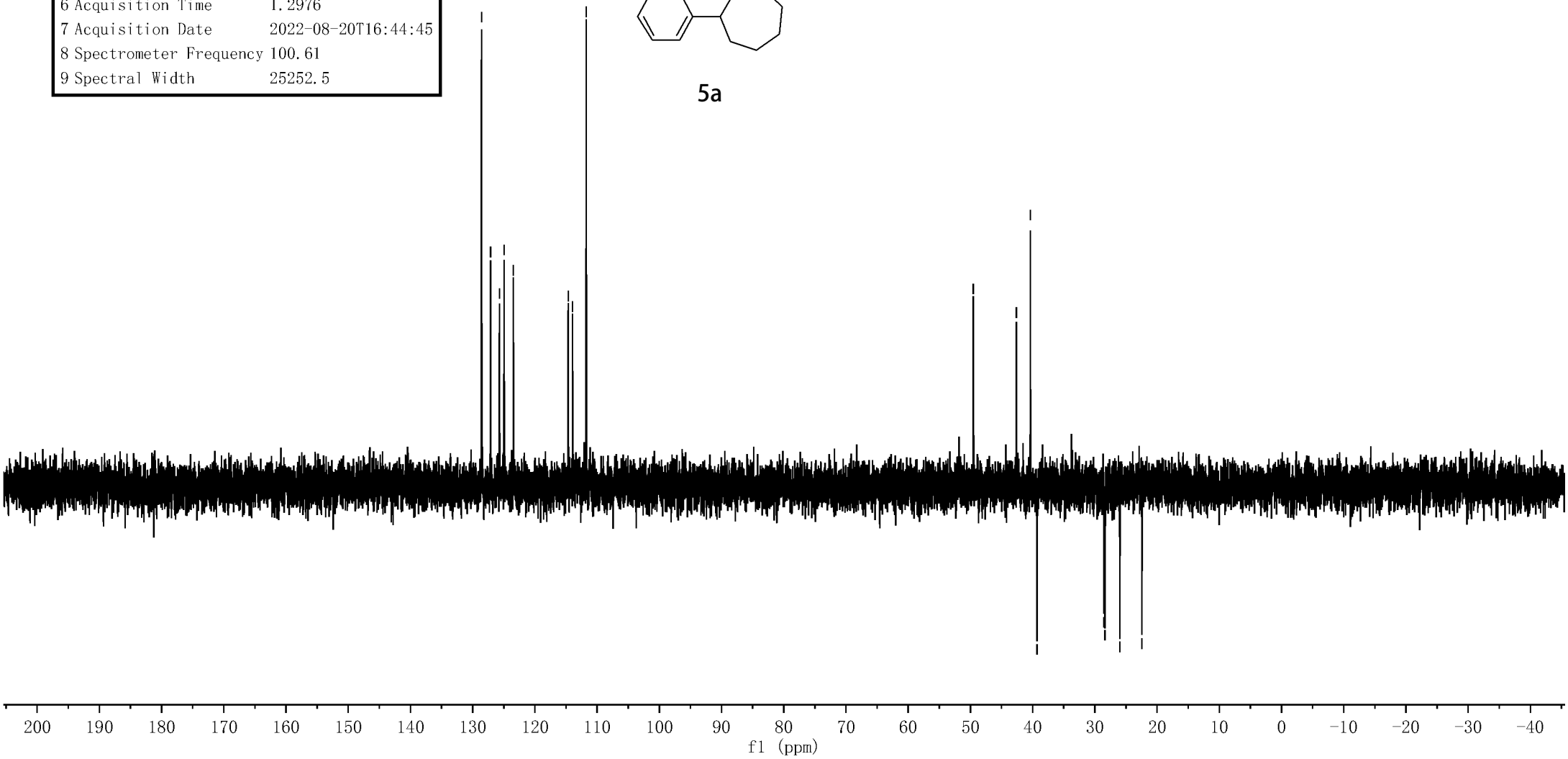


128.57
127.14
125.70
124.95
123.46
114.64
113.95
111.75
49.55
42.61
40.37
39.28
28.52
28.37
25.99
22.44

Parameter	Value
1 Title	zyx-6-74--dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	73
6 Acquisition Time	1.2976
7 Acquisition Date	2022-08-20T16:44:45
8 Spectrometer Frequency	100.61
9 Spectral Width	25252.5

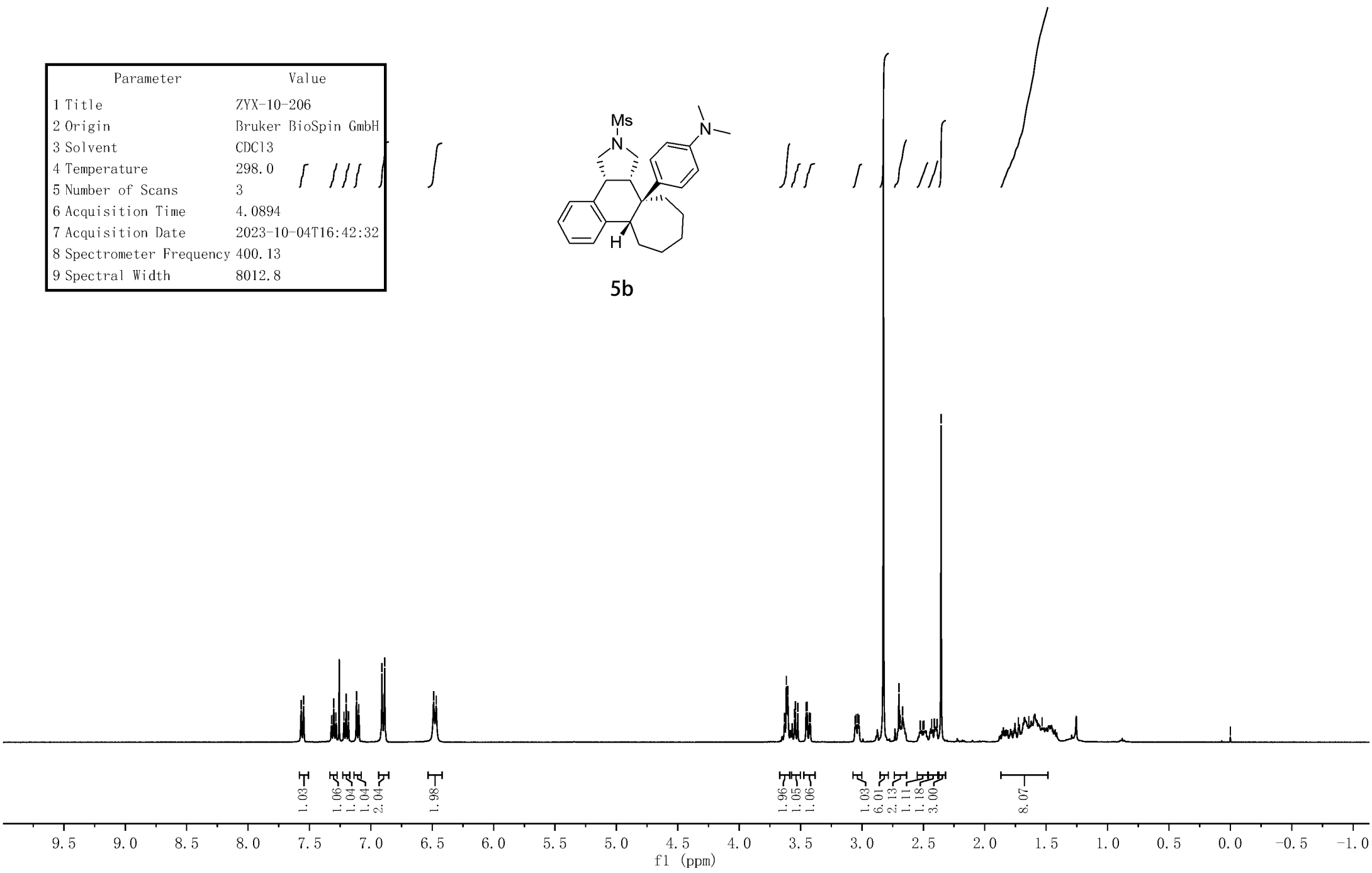


5a

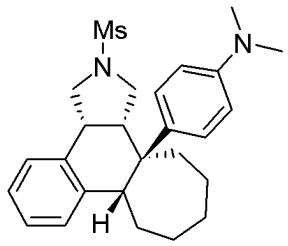


Parameter	Value
1 Title	ZYX-10-206
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	3
6 Acquisition Time	4.0894
7 Acquisition Date	2023-10-04T16:42:32
8 Spectrometer Frequency	400.13
9 Spectral Width	8012.8

5b



Parameter	Value
1 Title	ZYX-10-206
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	166
6 Acquisition Time	1.3631
7 Acquisition Date	2023-10-04T16:43:10
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

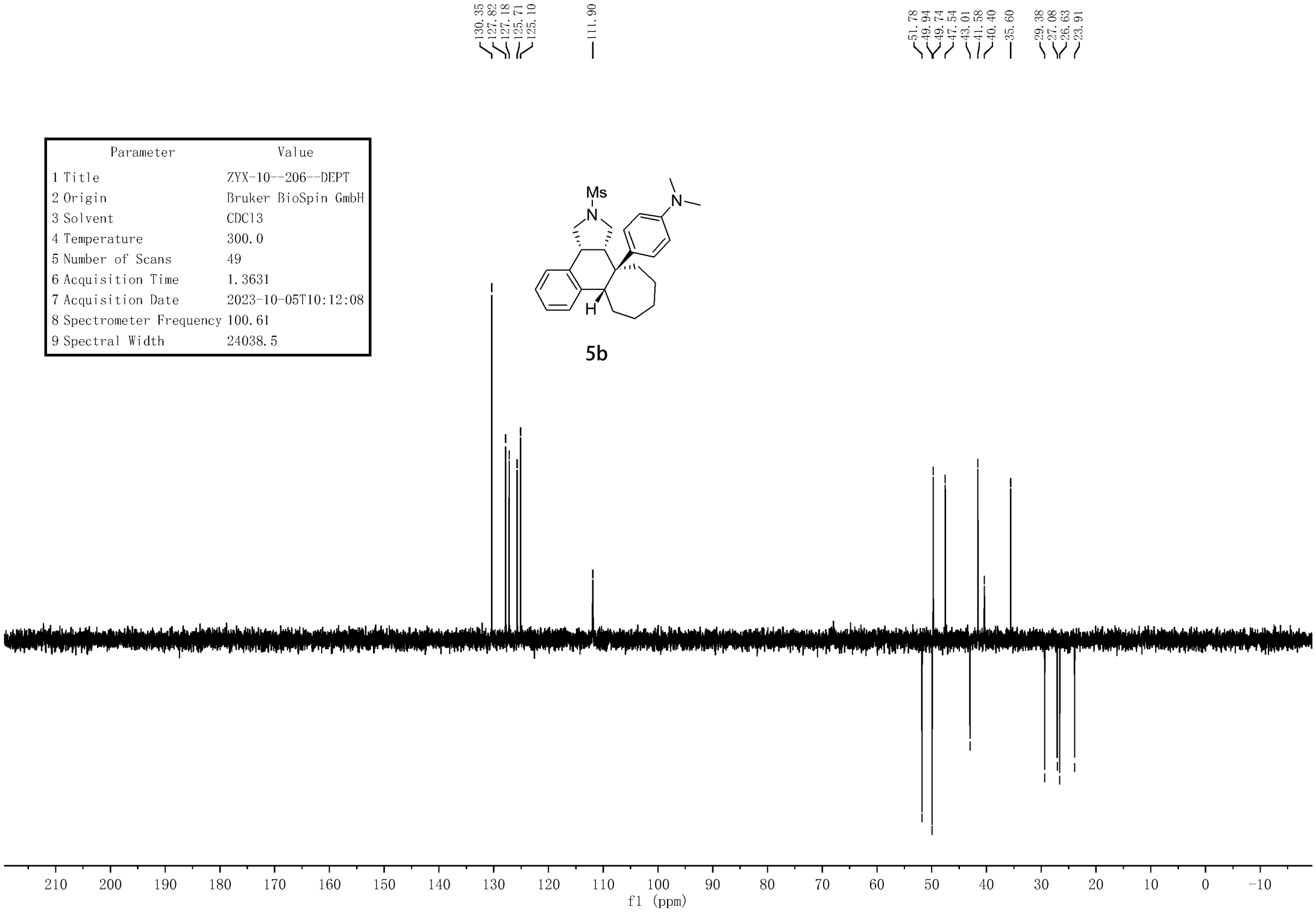


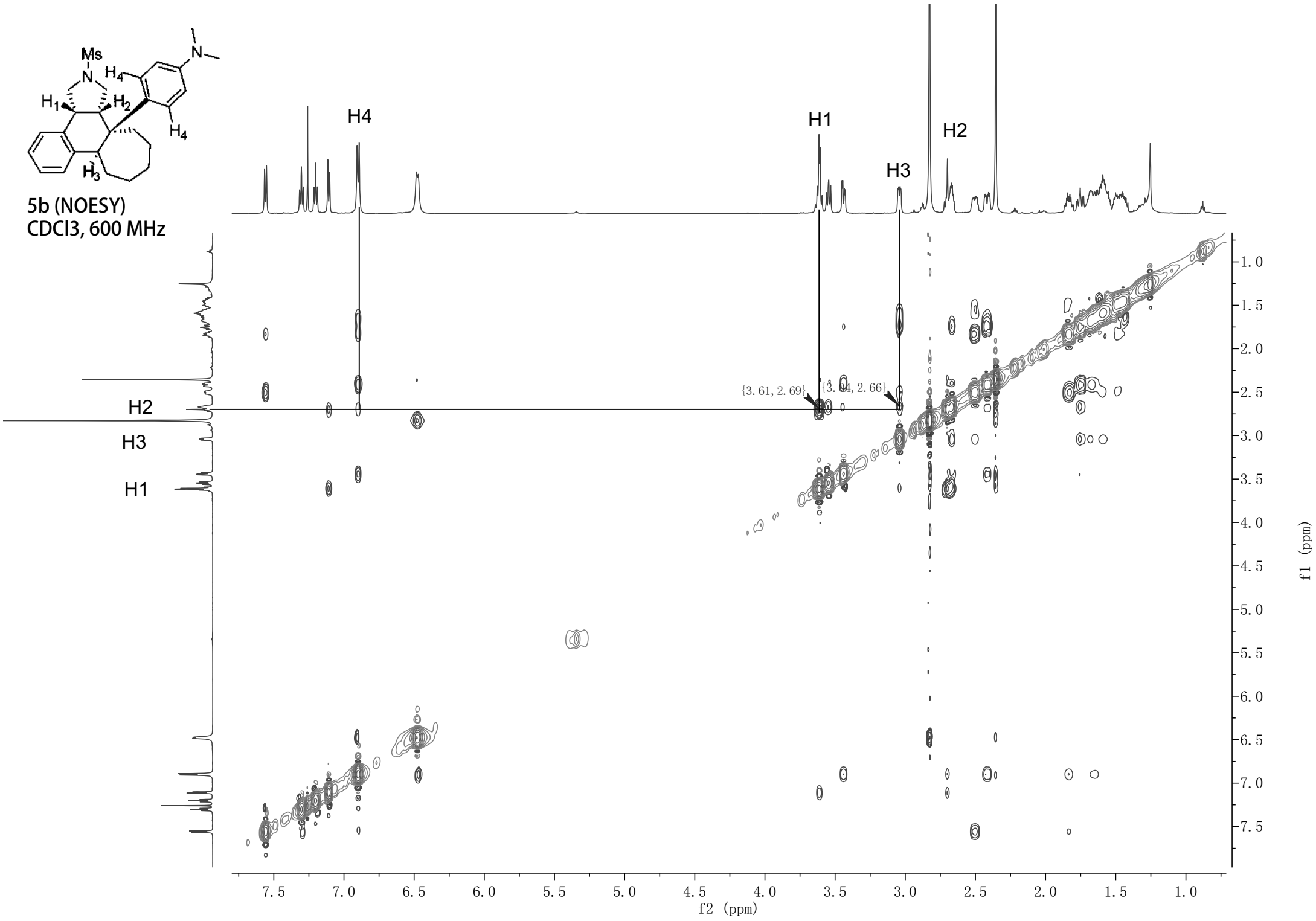
5b

142.15
134.43
130.35
127.81
127.17
125.70
125.09
111.90
77.32
77.00
76.68
51.78
49.93
49.75
47.56
44.60
43.00
41.58
40.39
35.61
29.37
27.07
26.63
23.90

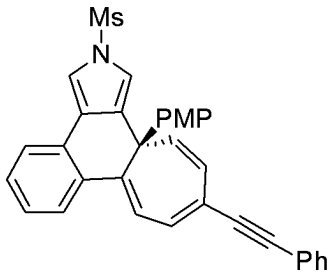
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

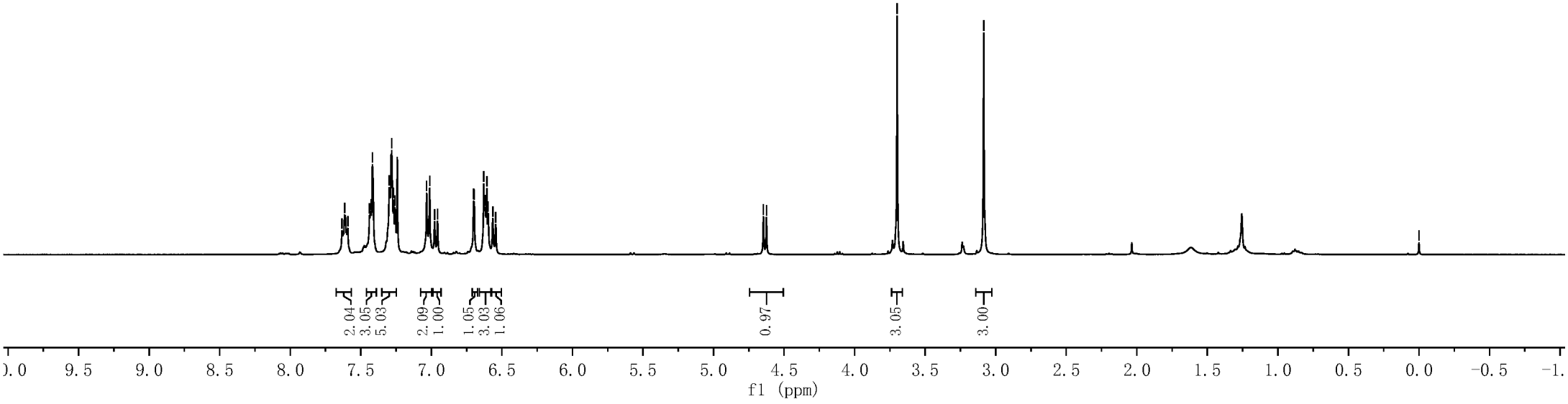

130.35
127.82
127.18
125.71
125.10
111.90
51.78
49.94
49.74
47.54
43.01
41.58
40.40
35.60
29.38
27.08
26.63
23.91
Parameter Value
1 Title ZYX-10--206--DEPT
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 49
6 Acquisition Time 1.3631
7 Acquisition Date 2023-10-05T10:12:08
8 Spectrometer Frequency 100.61
9 Spectral Width 24038.5
Ms
N
N
H
5b
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)


Ms
N
H4
H1
H2
H4
H3
5b (NOESY)
CDCl3, 600 MHz
H4
H1
H3
H2
{3.61, 2.69}
{3.61, 2.66}
H2
H3
H1
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
f2 (ppm)
f1 (ppm)

Parameter	Value
1 Title	zyx-6-43--H
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.6
5 Number of Scans	8
6 Acquisition Time	3.9846
7 Acquisition Date	2022-08-09T16:02:41
8 Spectrometer Frequency	399.93
9 Spectral Width	8223.7

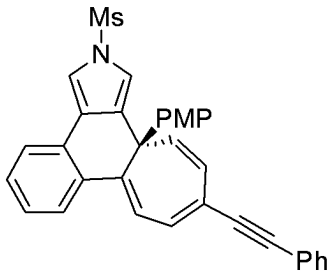


5c



157.64
135.28
132.63
132.58
132.54
131.45
128.71
128.23
128.11
128.03
127.95
127.94
127.66
126.90
123.38
122.31
121.72
118.97
113.33
112.71
104.70
101.83
90.59
90.06
77.32
77.00
76.68
55.01
42.76
41.51

Parameter	Value
1 Title	zyx-6-43--c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	119
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-09T16:24:33
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5



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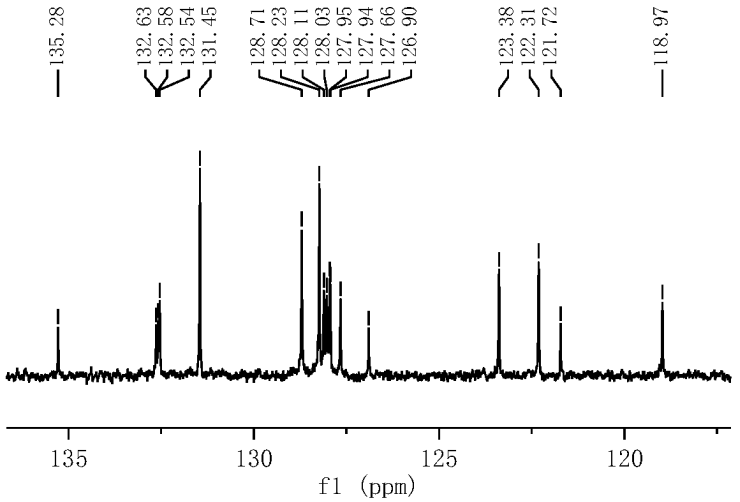
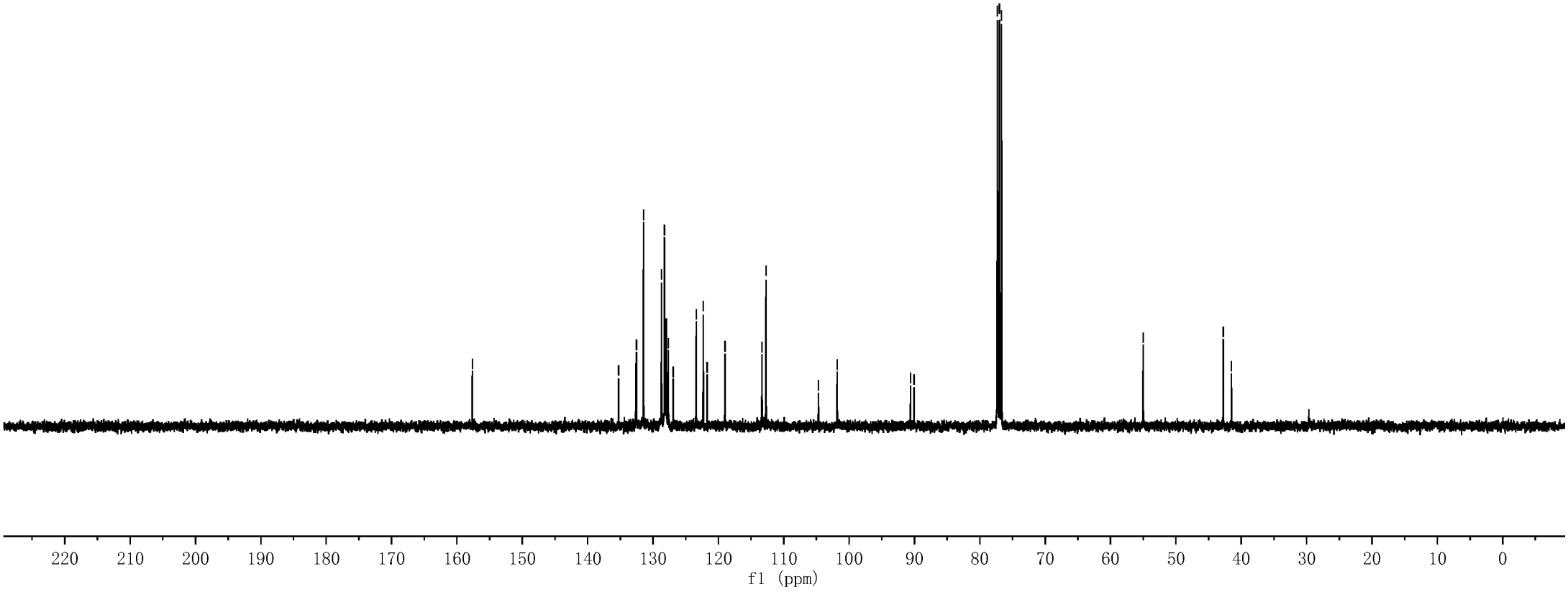
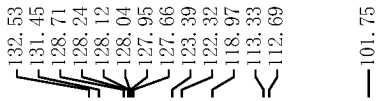
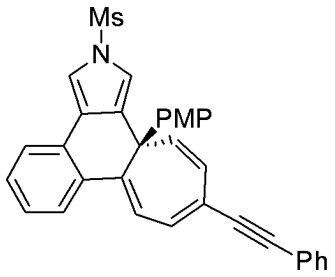


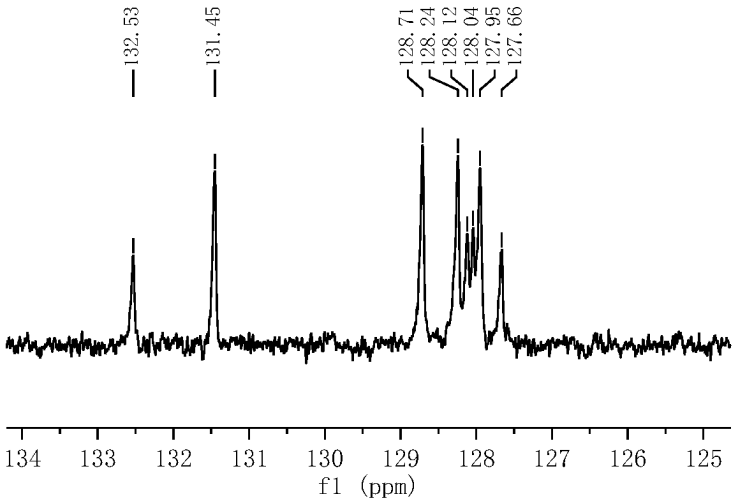


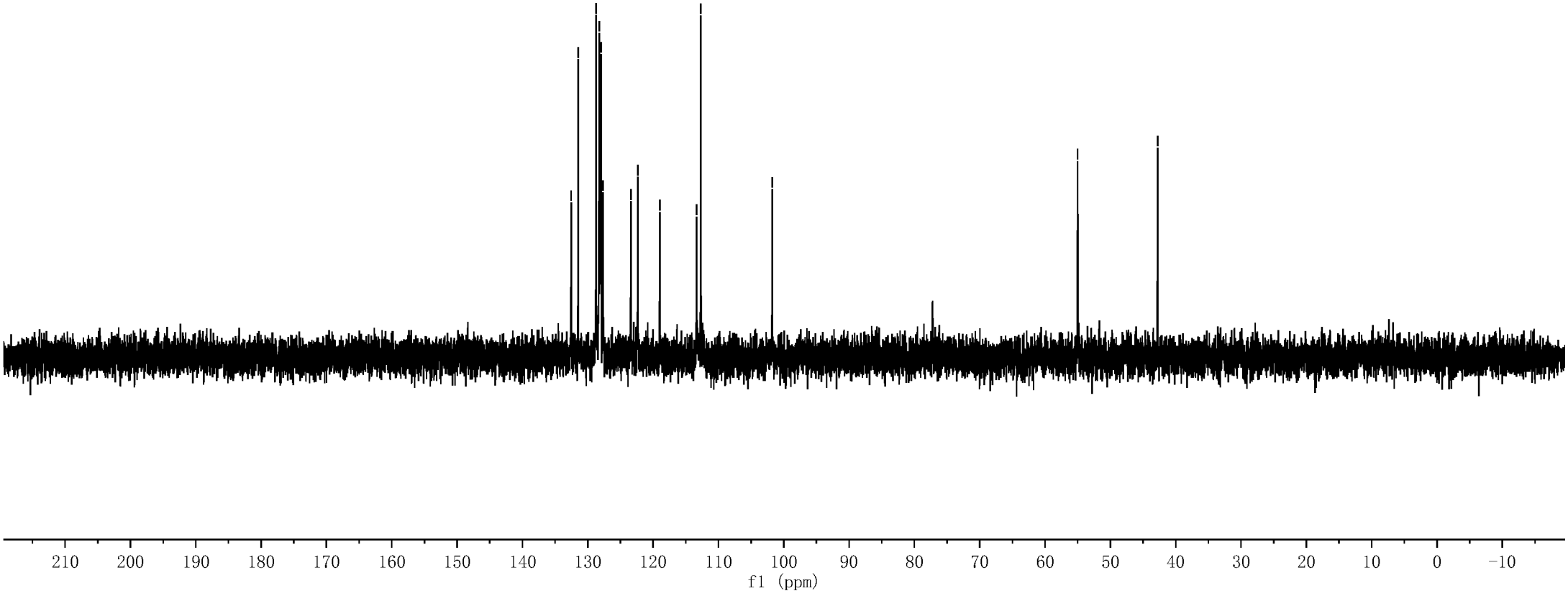


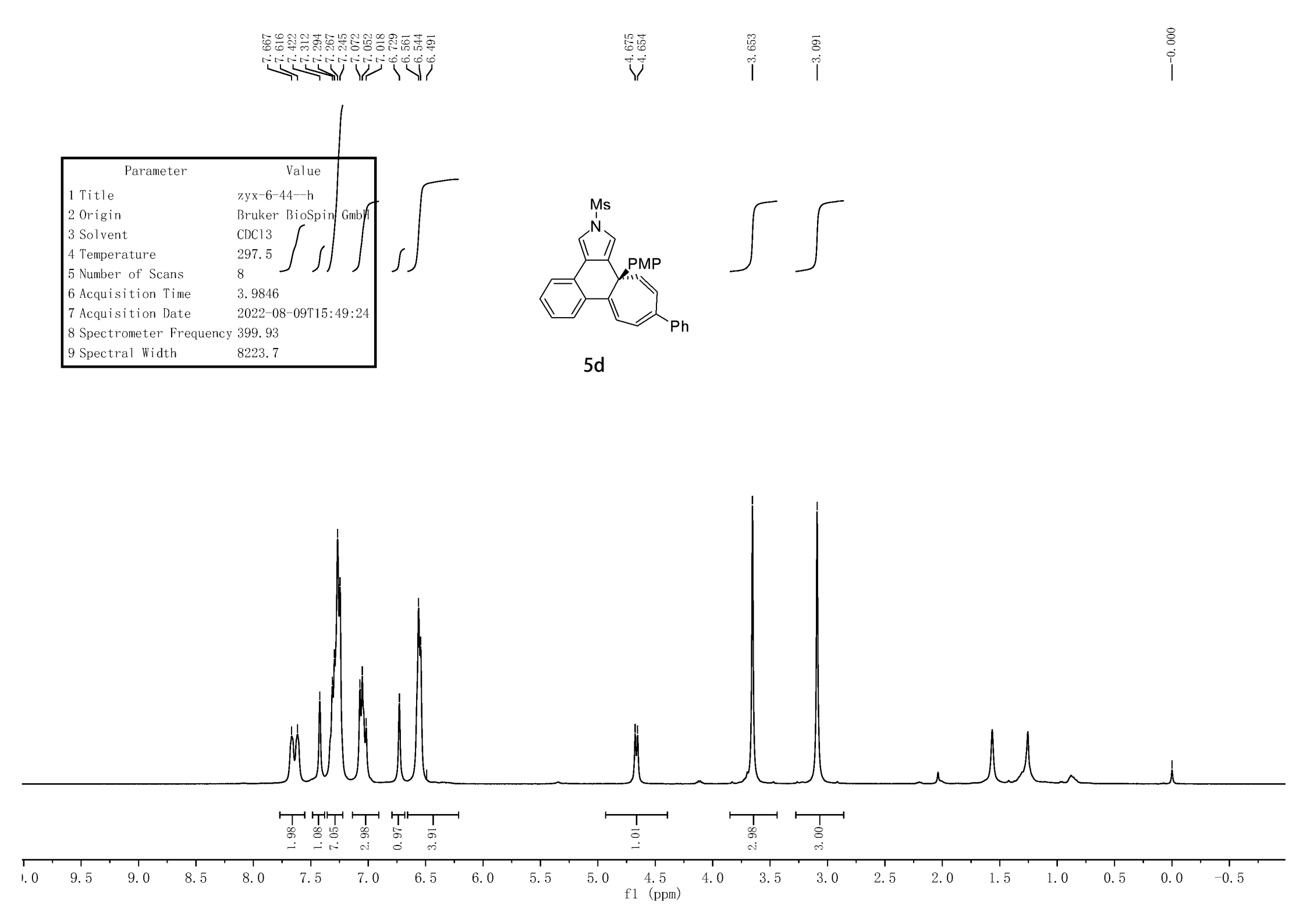
Parameter	Value
1 Title	ZYX-6-43-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.1
5 Number of Scans	52
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-30T09:30:25
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



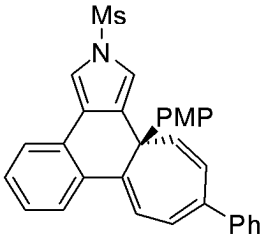
5c



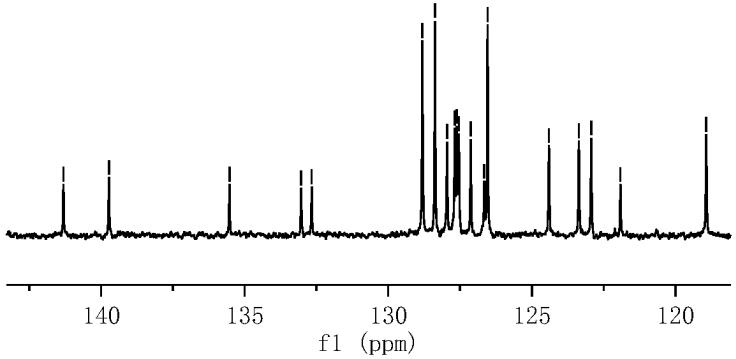


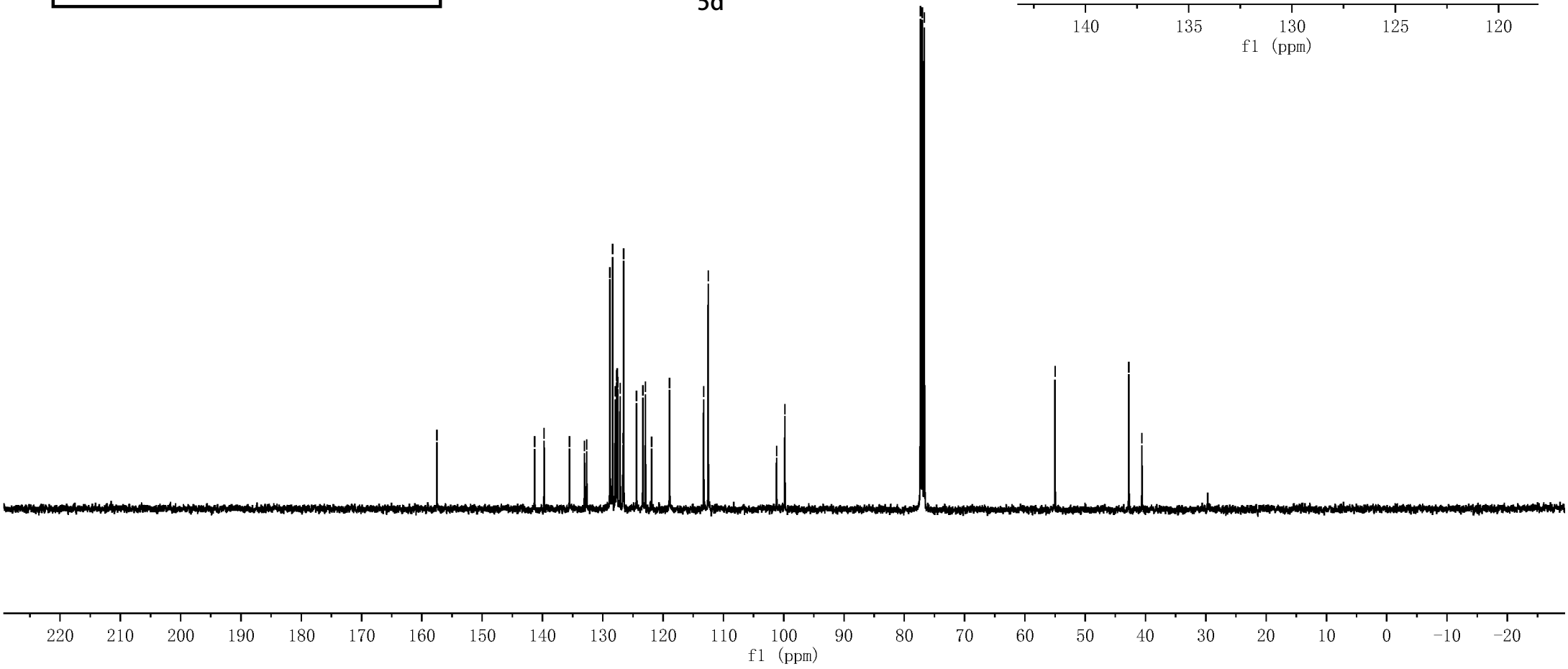

7.667
7.616
7.422
7.312
7.294
7.267
7.245
7.072
7.052
7.018
6.729
6.561
6.544
6.491
4.675
4.654
3.653
3.091
0.000
Parameter Value
1 Title zyx-6-44--h
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 297.5
5 Number of Scans 8
6 Acquisition Time 3.9846
7 Acquisition Date 2022-08-09T15:49:24
8 Spectrometer Frequency 399.93
9 Spectral Width 8223.7
Ms
N
PMP
Ph
5d
1.98
1.08
7.05
2.98
0.97
3.91
1.01
2.98
3.00
f1 (ppm)

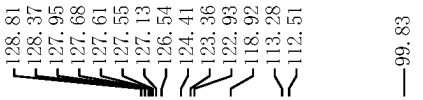
Parameter	Value
1 Title	ZYX-6-44---C
2 Origin	
3 Solvent	CDCl3
4 Temperature	299.5
5 Number of Scans	800
6 Acquisition Time	1.0000
7 Acquisition Date	2022-08-09T16:59:39
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0



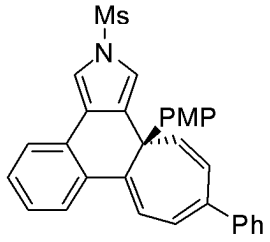
5d



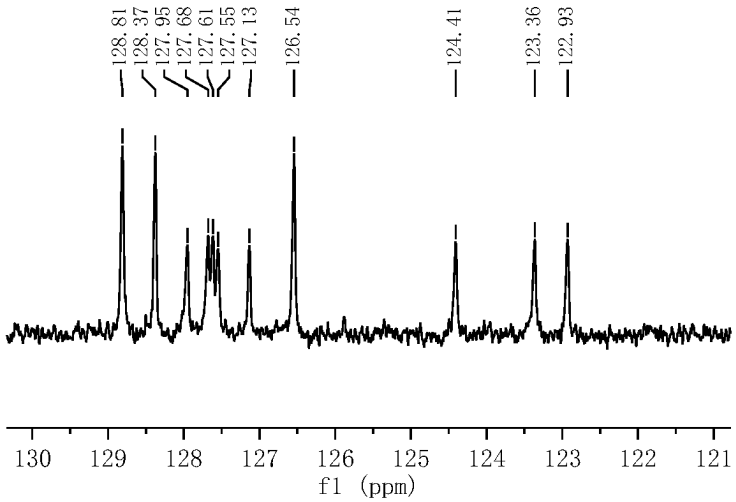


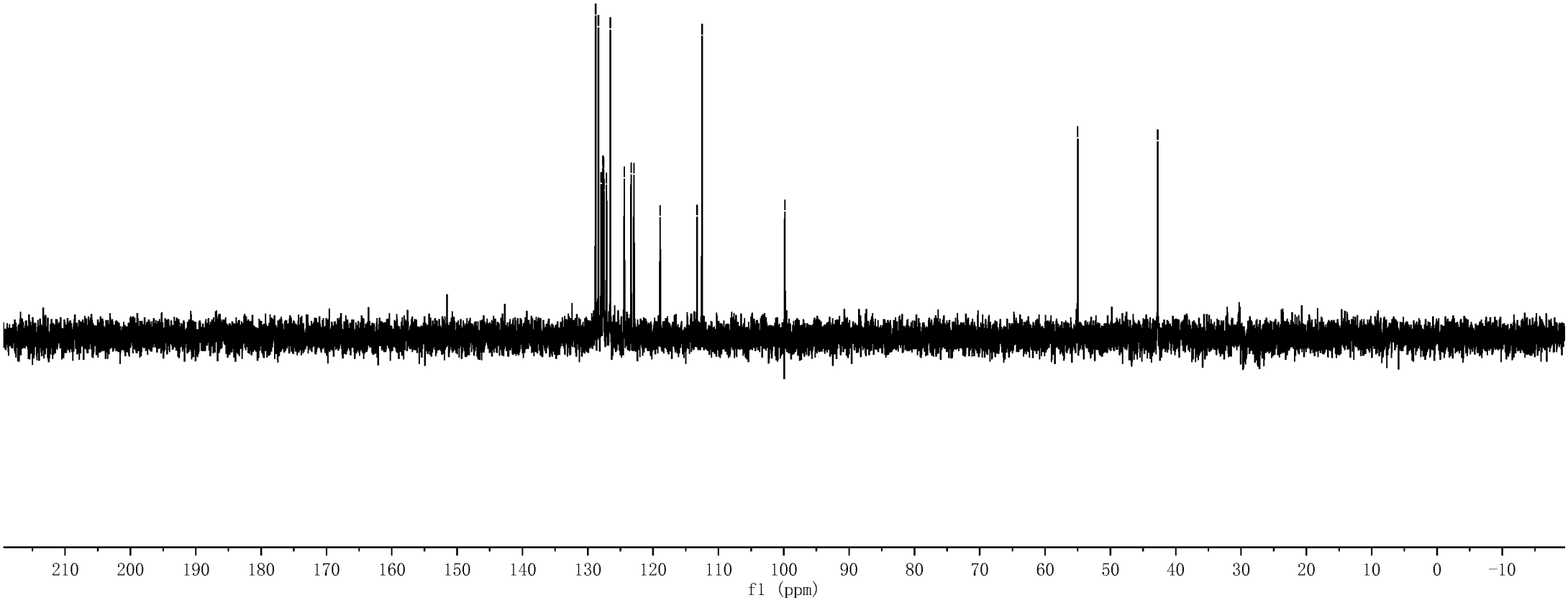


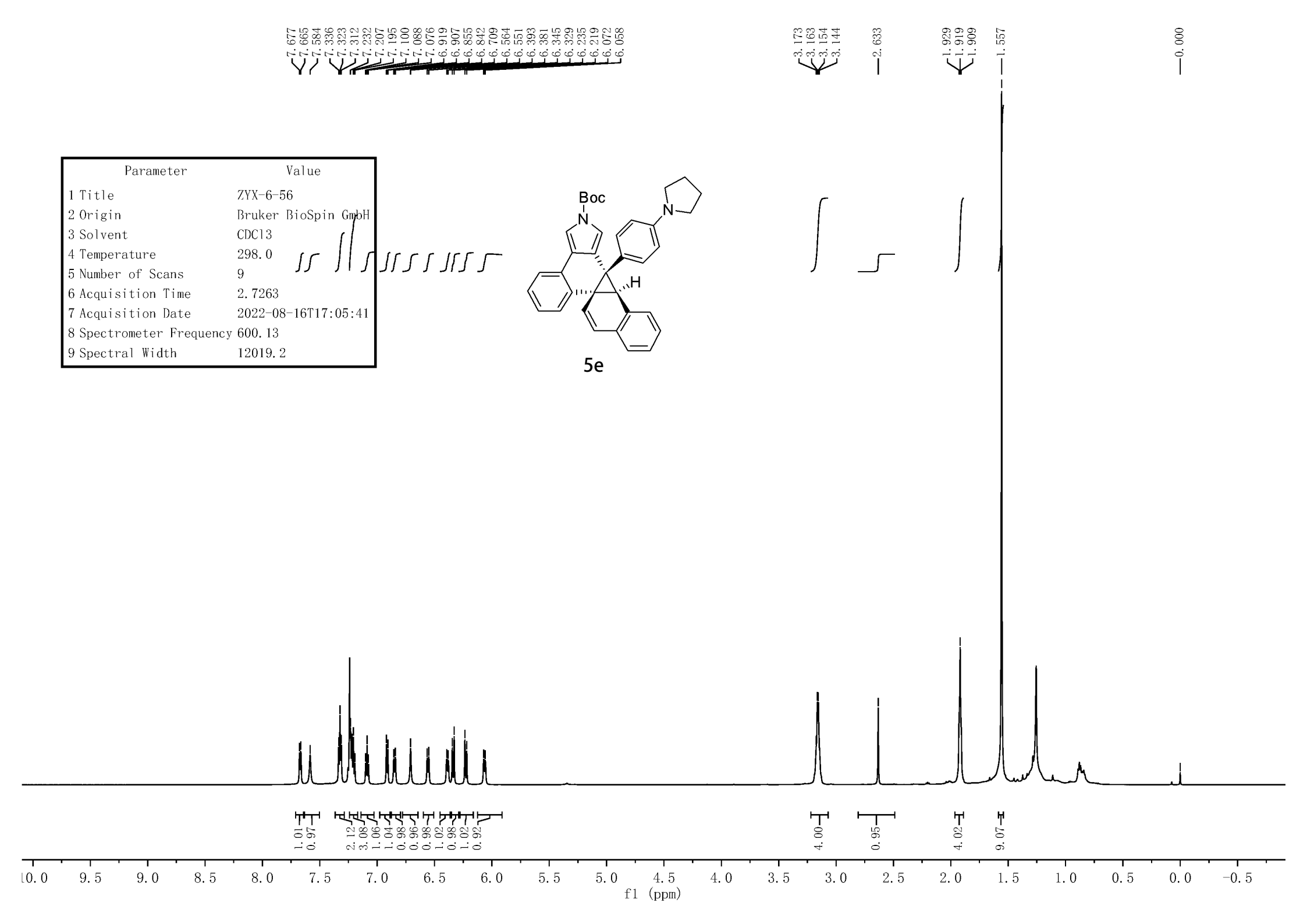
Parameter	Value
1 Title	ZYX-6-44-DEPT
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	297.3
5 Number of Scans	61
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-30T09:34:37
8 Spectrometer Frequency	100.56
9 Spectral Width	24038.5



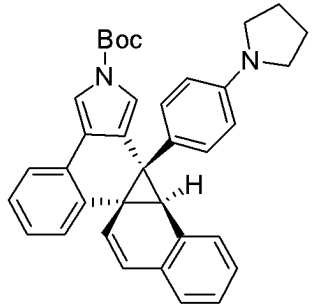
5d






7.677
7.665
7.584
7.336
7.323
7.312
7.232
7.207
7.195
7.100
7.088
7.076
6.919
6.907
6.855
6.842
6.709
6.564
6.551
6.393
6.381
6.345
6.329
6.235
6.219
6.072
6.058
3.173
3.163
3.154
3.144
2.633
1.929
1.919
1.909
1.557
0.000
Parameter Value
1 Title ZYX-6-56
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 9
6 Acquisition Time 2.7263
7 Acquisition Date 2022-08-16T17:05:41
8 Spectrometer Frequency 600.13
9 Spectral Width 12019.2
Boc
N
N
H
5e
1.01
0.97
2.12
3.08
1.06
1.04
0.98
0.96
0.98
1.02
0.98
1.02
0.92
4.00
0.95
4.02
9.07
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)

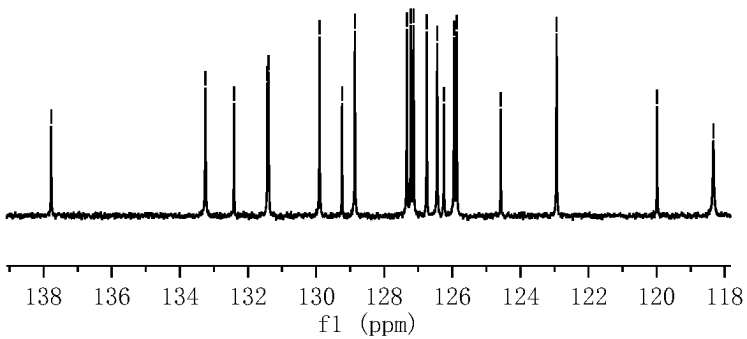
Parameter	Value
1 Title	ZYX-6-56
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	25
6 Acquisition Time	0.9044
7 Acquisition Date	2022-08-16T17:02:18
8 Spectrometer Frequency	150.90
9 Spectral Width	36231.9

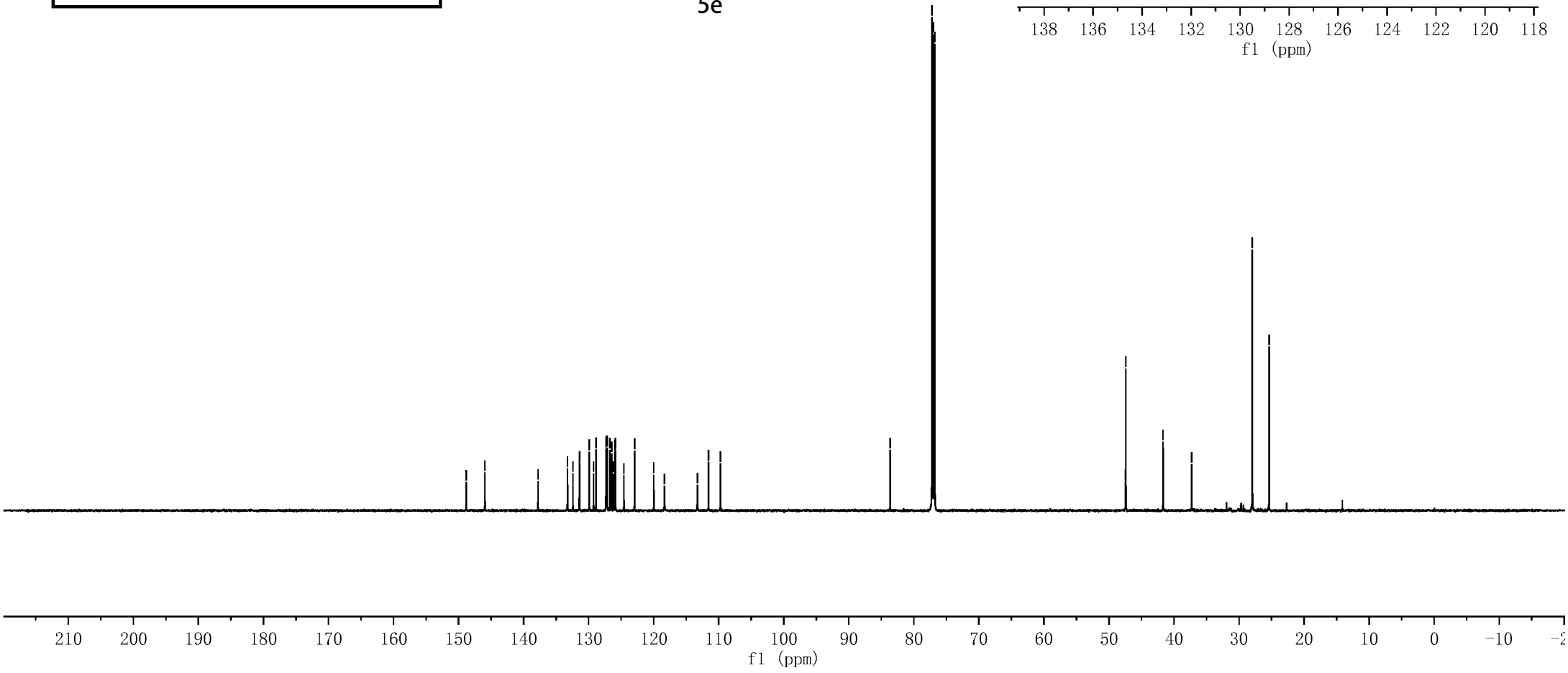


5e

148.82
145.95
131.43
131.40
129.90
128.86
127.33
127.22
127.14
126.75
126.44
125.95
125.87
123.27
111.57
109.73
83.65
77.21
77.00
76.79
47.41
41.68
37.30
27.97
27.93
25.38

137.78
133.25
132.41
131.43
131.40
129.90
129.24
128.86
127.33
127.22
127.14
126.75
122.94
119.99
118.34

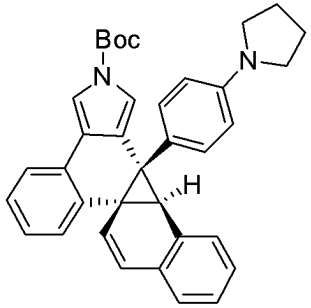




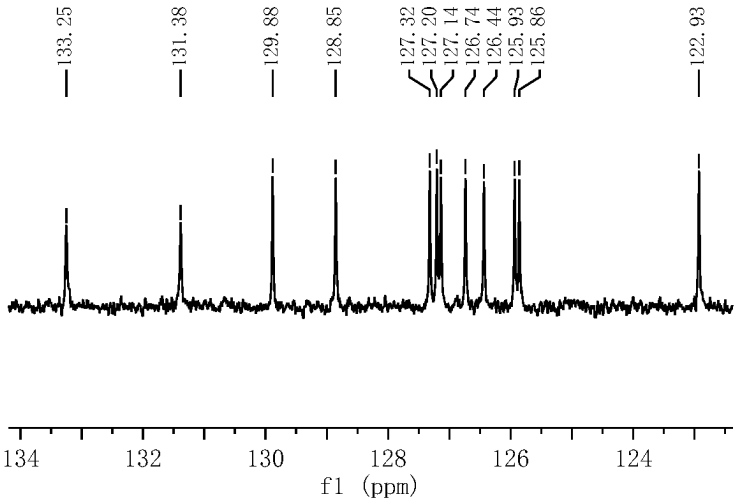
133.25
131.38
129.88
128.85
127.32
127.20
127.14
126.74
126.44
125.93
125.86
122.93
118.35
113.26
111.58
109.73

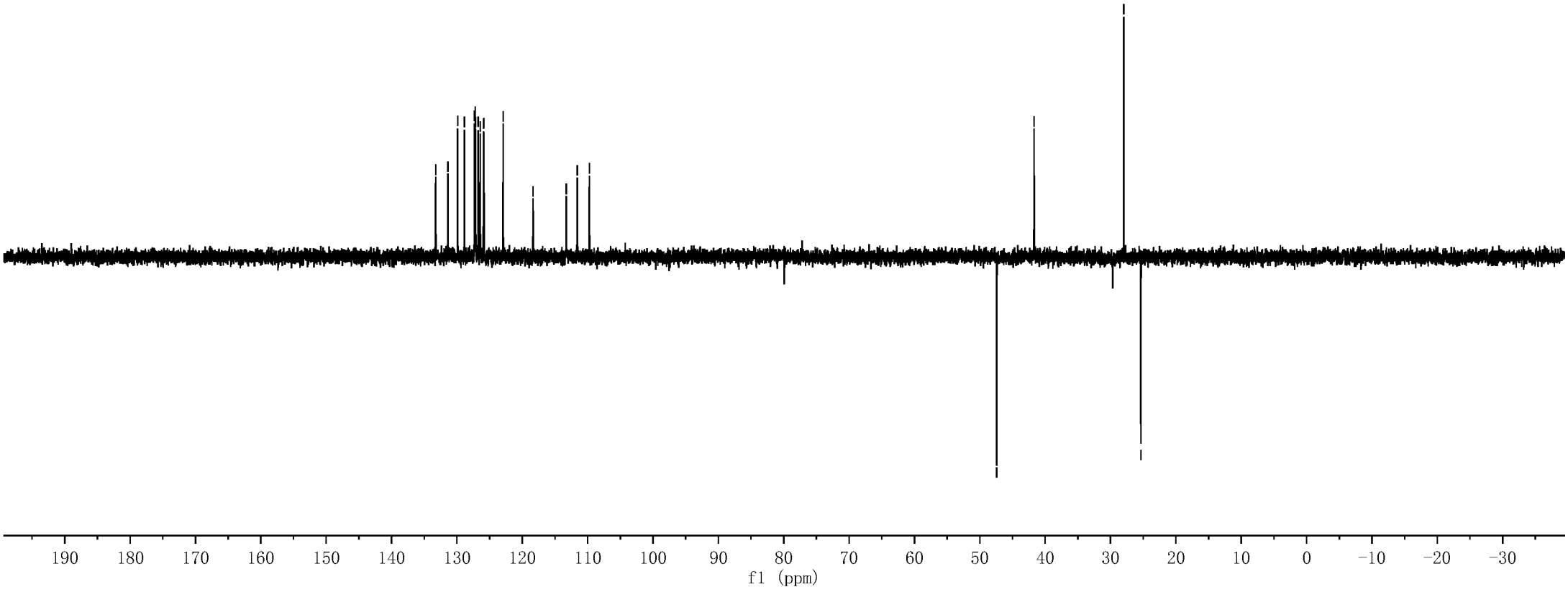
47.41
41.69
27.97
25.36

Parameter	Value
1 Title	zyx-6----56-dept
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	36
6 Acquisition Time	1.3631
7 Acquisition Date	2022-08-17T09:46:21
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

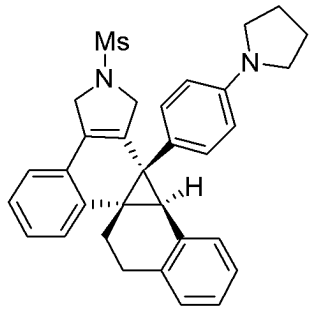


5e

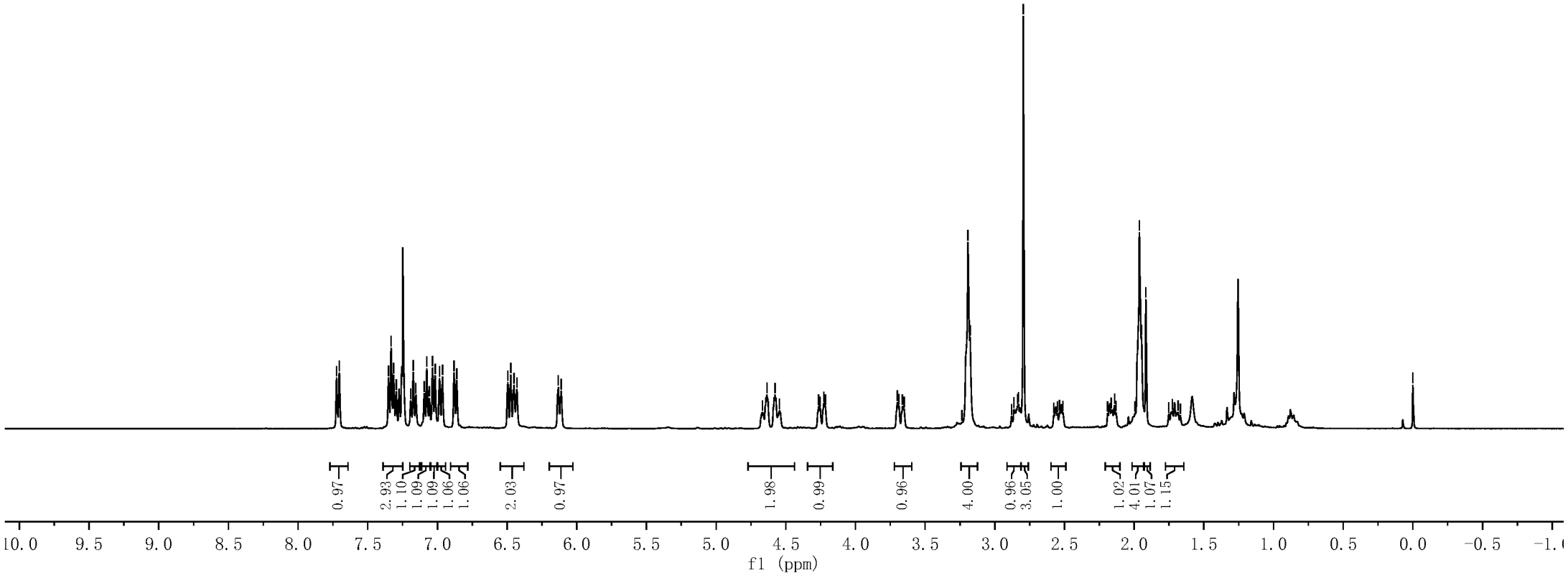




Parameter	Value
1 Title	ZXY-6---95
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.2
5 Number of Scans	16
6 Acquisition Time	4.0002
7 Acquisition Date	2022-09-07T14:07:31
8 Spectrometer Frequency	399.92
9 Spectral Width	8012.0

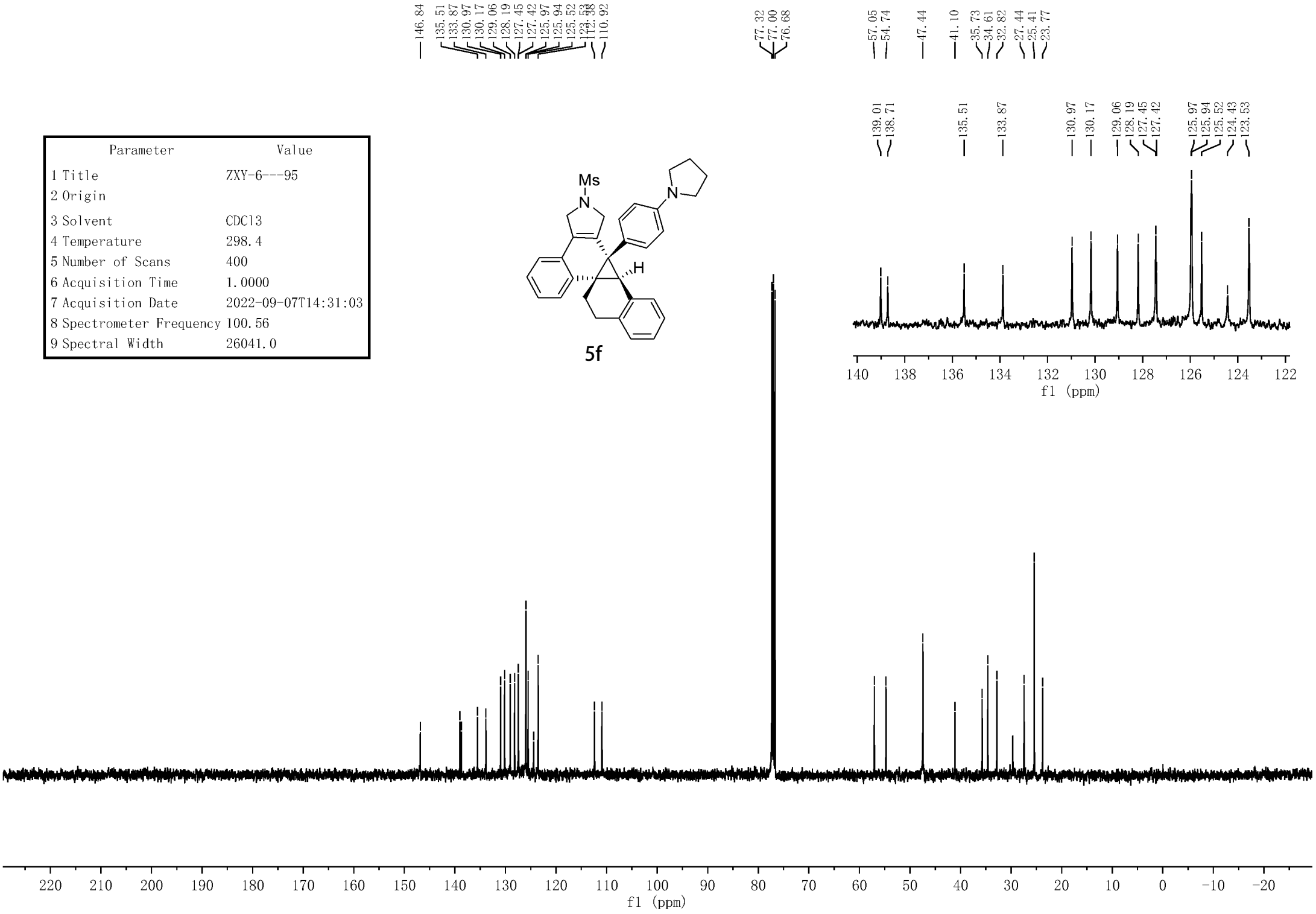


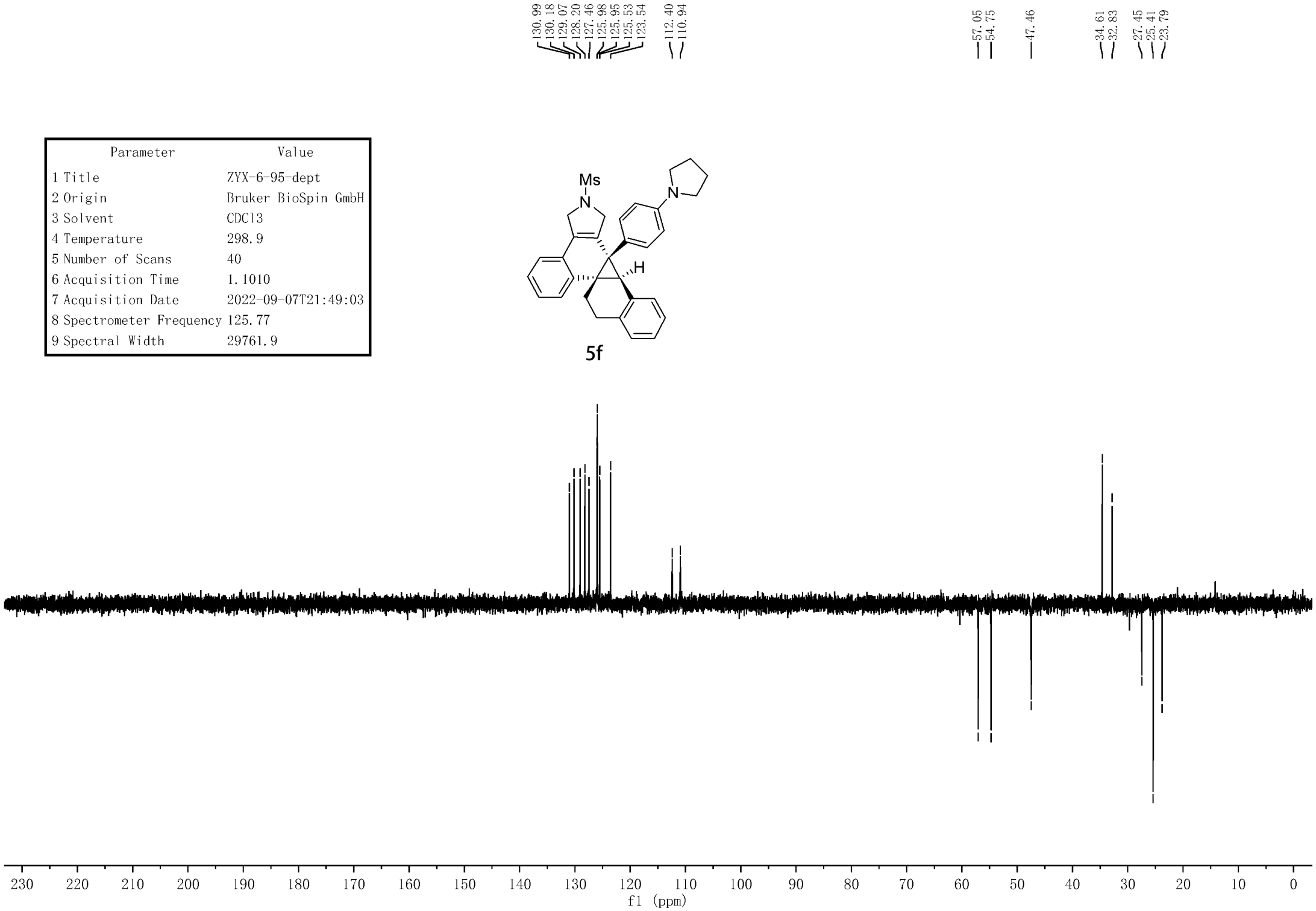
5f

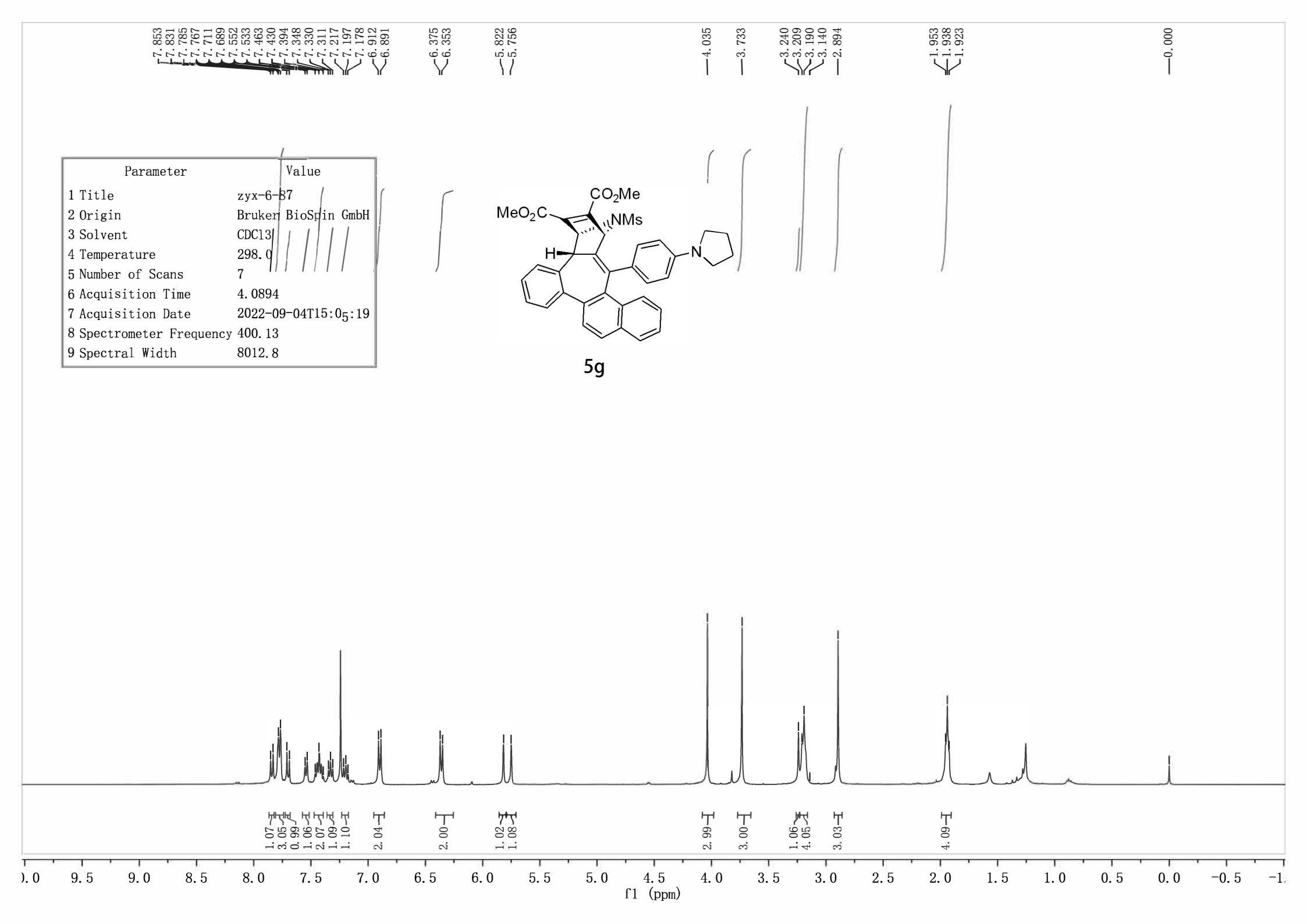


Parameter	Value
1 Title	ZXY-6---95
2 Origin	
3 Solvent	CDCl3
4 Temperature	298.4
5 Number of Scans	400
6 Acquisition Time	1.0000
7 Acquisition Date	2022-09-07T14:31:03
8 Spectrometer Frequency	100.56
9 Spectral Width	26041.0

5f

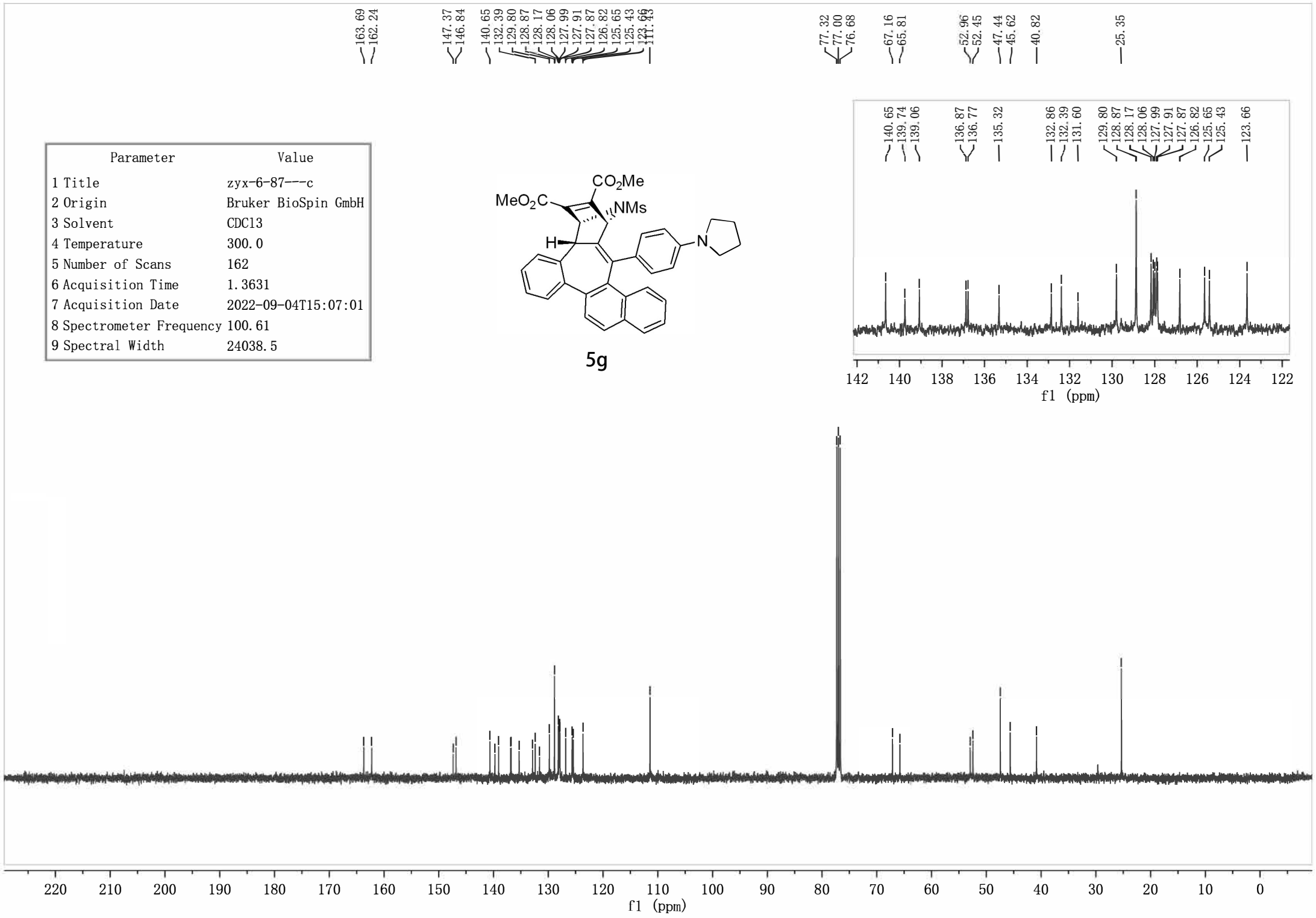


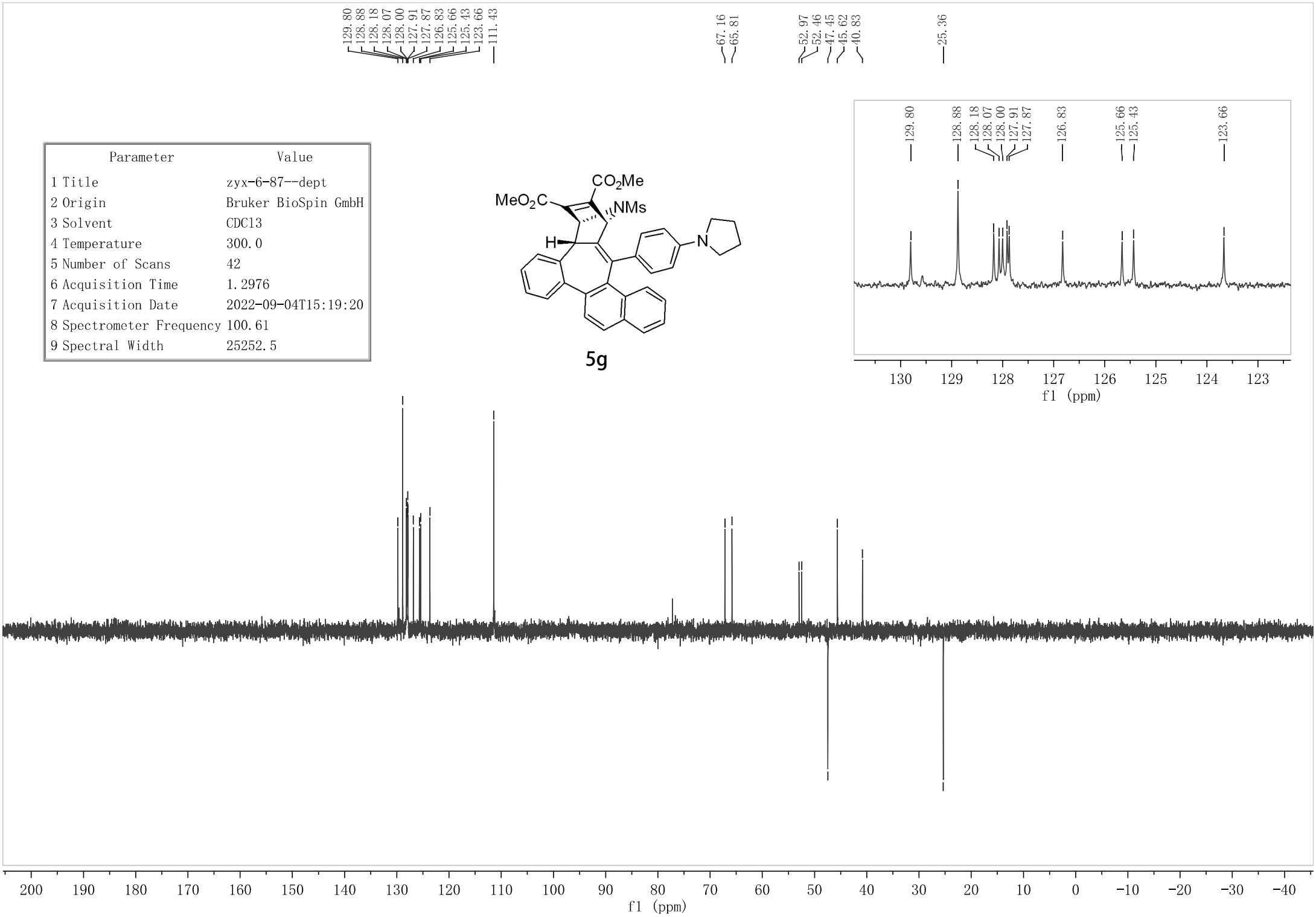

130.99
130.18
129.07
128.20
127.46
125.98
125.95
125.53
123.54
112.40
110.94
57.05
54.75
47.46
34.61
32.83
27.45
25.41
23.79
Parameter Value
1 Title ZYX-6-95-dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.9
5 Number of Scans 40
6 Acquisition Time 1.1010
7 Acquisition Date 2022-09-07T21:49:03
8 Spectrometer Frequency 125.77
9 Spectral Width 29761.9
Ms
N
N
H
5f
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

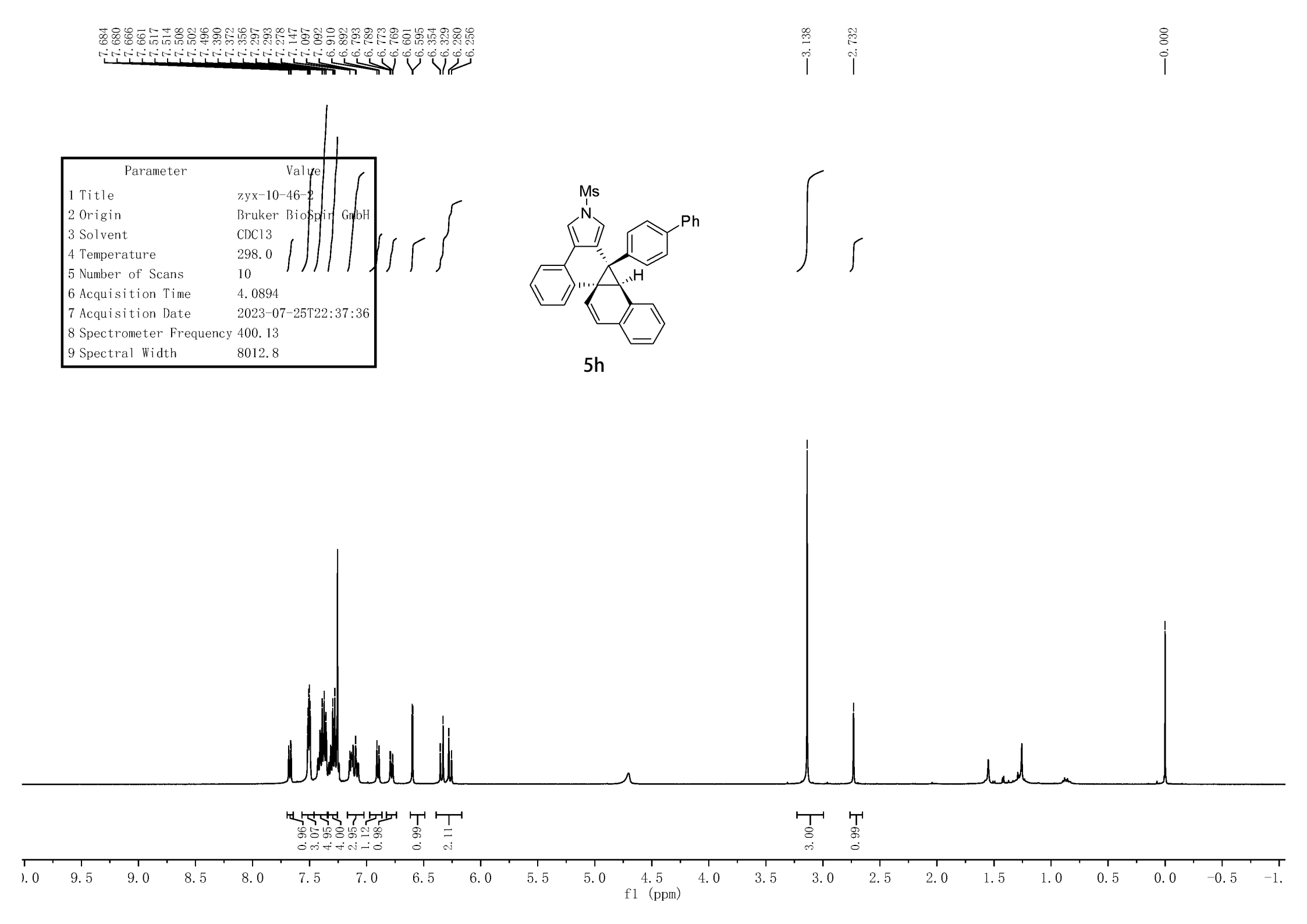

7.853
7.831
7.785
7.767
7.711
7.689
7.552
7.533
7.463
7.430
7.394
7.348
7.330
7.311
7.217
7.197
7.178
6.912
6.891
6.375
6.353
5.822
5.756
4.035
3.733
3.240
3.209
3.190
3.140
2.894
1.953
1.938
1.923
0.000
Parameter
Value
1 Title
zyx-6-87
2 Origin
Bruker BioSpin GmbH
3 Solvent
CDCl3
4 Temperature
298.0
5 Number of Scans
7
6 Acquisition Time
4.0894
7 Acquisition Date
2022-09-04T15:05:19
8 Spectrometer Frequency
400.13
9 Spectral Width
8012.8
CO2Me
MeO2C
NMs
H
N
5g
1.07
3.05
0.99
1.06
2.07
1.09
1.10
2.04
2.00
1.02
1.08
2.99
3.00
1.06
4.05
3.03
4.09
f1 (ppm)

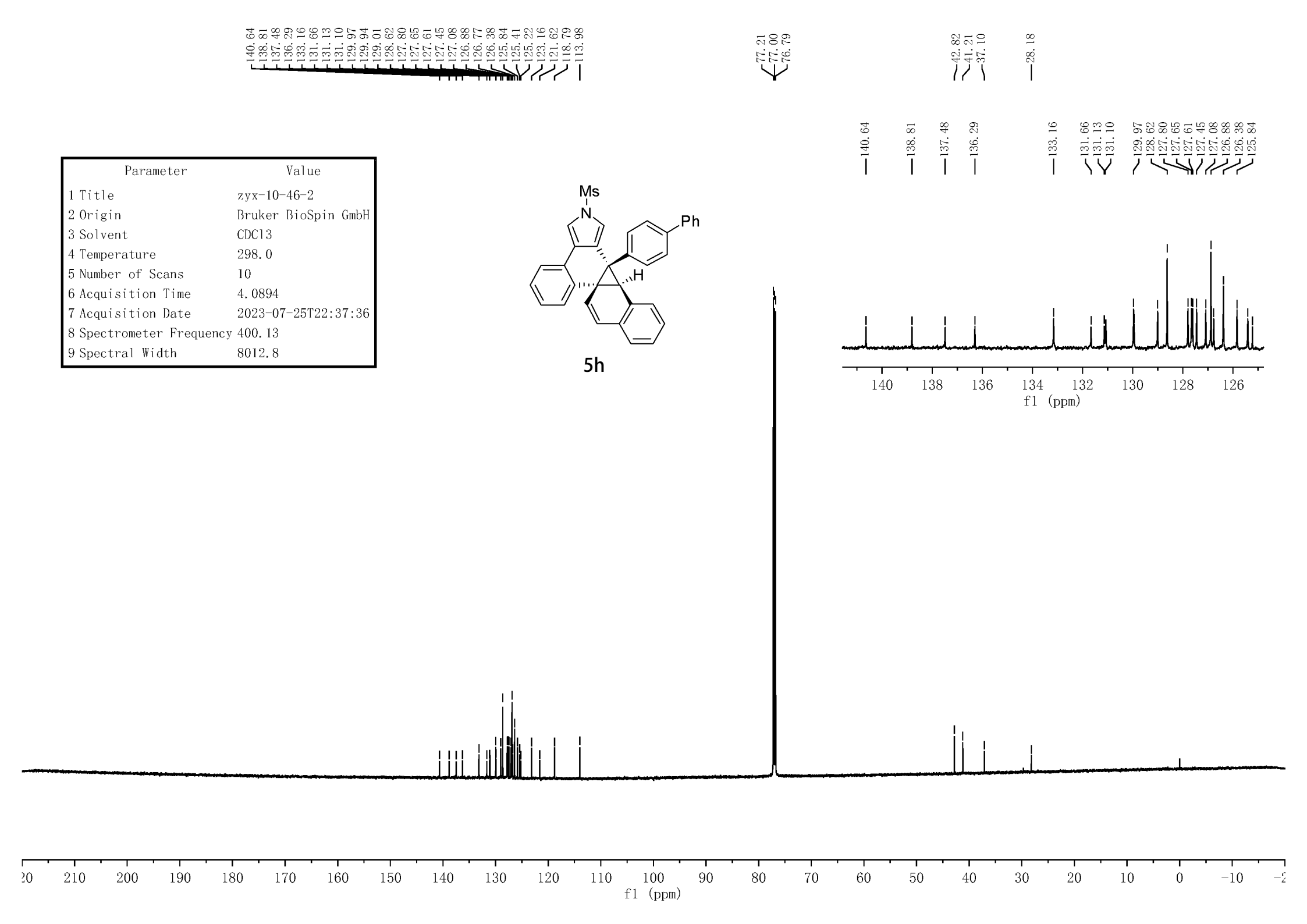
Parameter	Value
1 Title	zyx-6-87---c
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	300.0
5 Number of Scans	162
6 Acquisition Time	1.3631
7 Acquisition Date	2022-09-04T15:07:01
8 Spectrometer Frequency	100.61
9 Spectral Width	24038.5

5g




129.80
128.88
128.18
128.07
128.00
127.91
127.87
126.83
125.66
125.43
123.66
111.43
67.16
65.81
52.97
52.46
47.45
45.62
40.83
25.36
Parameter Value
1 Title zyx-6-87--dept
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 300.0
5 Number of Scans 42
6 Acquisition Time 1.2976
7 Acquisition Date 2022-09-04T15:19:20
8 Spectrometer Frequency 100.61
9 Spectral Width 25252.5
CO2Me
MeO2C
NMs
H
N
5g
f1 (ppm)
f1 (ppm)

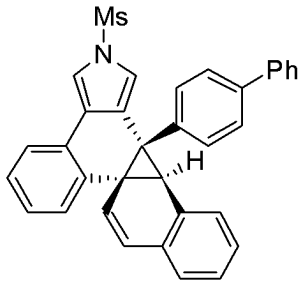

7.684
7.680
7.666
7.661
7.517
7.514
7.508
7.502
7.496
7.390
7.372
7.356
7.297
7.293
7.278
7.147
7.097
7.092
6.910
6.892
6.793
6.789
6.773
6.769
6.601
6.595
6.354
6.329
6.280
6.256
3.138
2.732
0.000
Parameter Value
1 Title zyx-10-46-2
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 10
6 Acquisition Time 4.0894
7 Acquisition Date 2023-07-25T22:37:36
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
Ph
H
5h
0.96
3.07
4.95
4.00
2.95
1.12
0.98
0.99
2.11
3.00
0.99
f1 (ppm)


140.64
138.81
137.48
136.29
133.16
131.66
131.13
131.10
129.97
129.94
129.01
128.62
127.80
127.65
127.61
127.45
127.08
126.88
126.77
126.38
125.84
125.41
125.22
123.16
121.62
118.79
113.98
77.21
77.00
76.79
42.82
41.21
37.10
28.18
Parameter Value
1 Title zyx-10-46-2
2 Origin Bruker BioSpin GmbH
3 Solvent CDCl3
4 Temperature 298.0
5 Number of Scans 10
6 Acquisition Time 4.0894
7 Acquisition Date 2023-07-25T22:37:36
8 Spectrometer Frequency 400.13
9 Spectral Width 8012.8
Ms
N
Ph
H
5h
f1 (ppm)

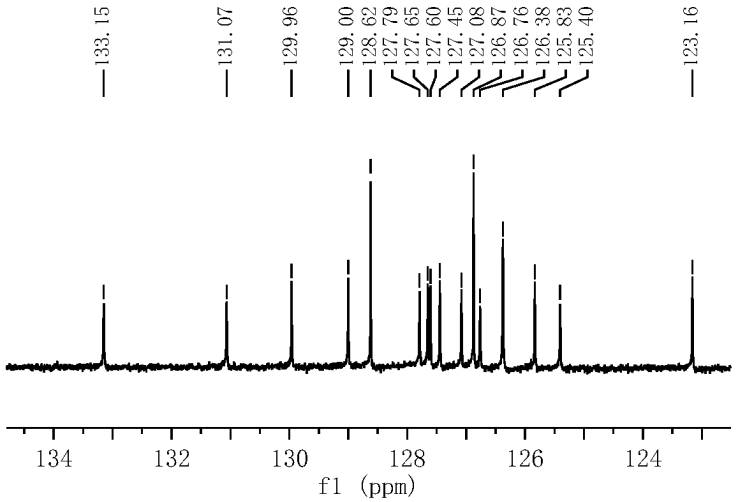
133.15
131.07
129.96
129.00
128.62
127.79
127.65
127.60
127.45
127.08
126.87
126.76
126.38
125.83
125.40
123.16
118.78
113.97

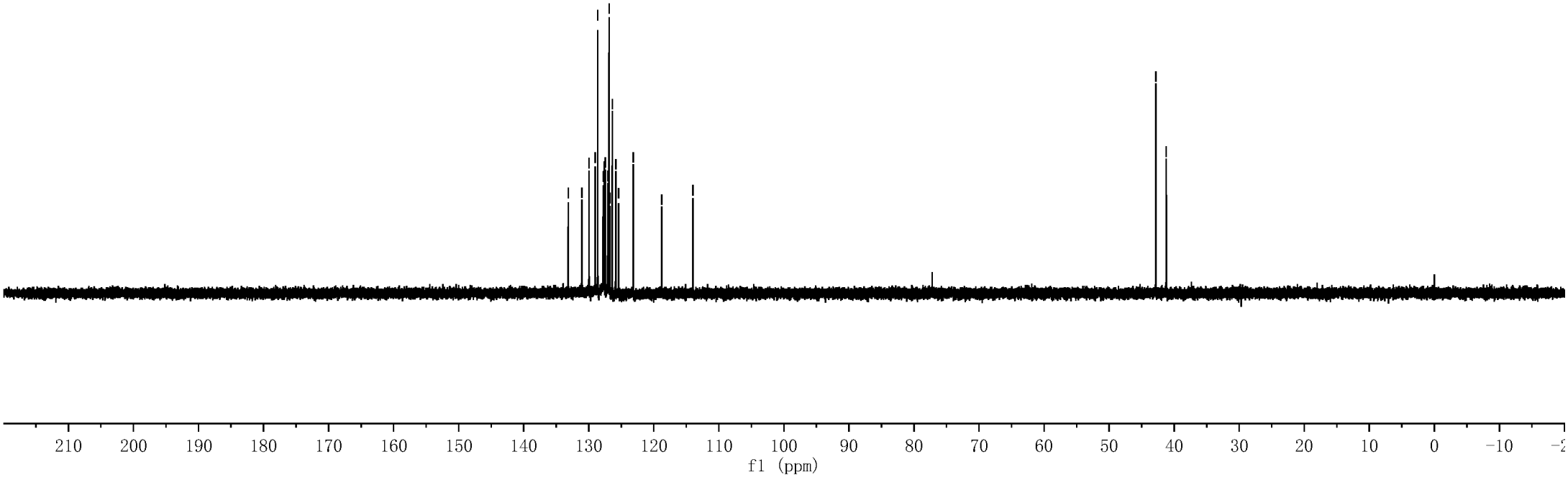
42.82
41.22

Parameter	Value
1 Title	ZYX-10-42
2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	298.0
5 Number of Scans	32
6 Acquisition Time	0.9044
7 Acquisition Date	2023-07-25T20:51:19
8 Spectrometer Frequency	150.92
9 Spectral Width	36231.9



5h





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