Supporting Information

Gold(I)-Catalyzed Pathway-Switchable Tandem Cycloisomerizations to Indolizino[8,7-*b*]indole and Indolo[2,3-*a*]quinolizine Derivatives

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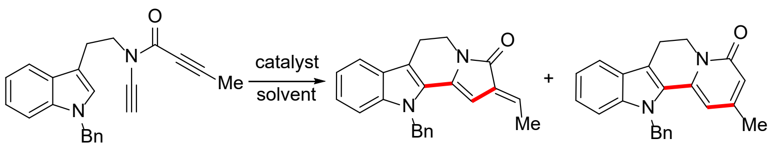
Contents

1. General Information

Unless otherwise noted, reagents were obtained commercially and used without further purification. Tetrahydrofuran (THF) and Toluene (Tol) were distilled from sodium under a nitrogen atmosphere. Dichloromethane (DCM) and 1,2-dichloroethane (DCE) were distilled from calcium hydride under a nitrogen atmosphere. TLC analysis of reaction mixtures was performed on Dynamic Adsorbents silica gel F-254 TLC plates. Flash chromatography was carried out on Zeoprep 60 (200-300 mesh) silica gel. ^{1}H and ^{13}C NMR spectra were recorded with Bruker Avance-III 600 spectrometers and referenced to $CDCl_3$ and DMSO-d_6. HR-ESI-MS was recorded on a Bruker micro-TOFQ-Q instrument. IR spectra were recorded on a Bruker IFS 55 spectrometer. Melting points (mp) were tested on Thomas Hoover capillary melting point apparatus.

2. Detailed Information on Reaction Condition Screening

2.1 Table S1. Condition Screening for the Cycloisomerization of Substrate 1 Leading to the Optimal Condition (C1)[a]

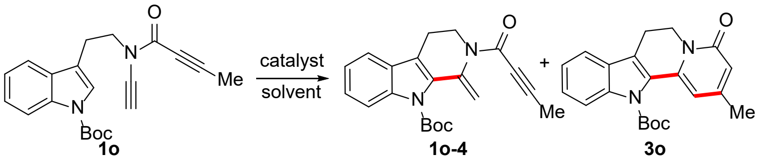


1 **2** **3**

entry	catalyst	loading (mol%)	solvent	yield [**2**+**3**] (%)	ratio [**2**:**3**]
1	$Ph_3PAuNTf_2$	10	DCM	44	1:1.1
2	$Ph_3PAuCl/AgBF_4$	10	DCM	27	1:1.25
3	$Ph_3PAuCl/AgOTf$	10	DCM	35	1:1.69
4	$PPh_3AuCl/AgSbF_6$	10	DCM	50	1:1.17
5	$IPrAuCl/AgSbF_6$	10	DCM	38	1:1.53
6	$AgSbF_6$	10	DCM	0	-
7	$JohnPhosAu(MeCN)SbF_6$	10	DCM	73	1:1.28
8	$JohnPhosAu(MeCN)SbF_6$	10	THF	88	1.05:1
9	$JohnPhosAu(MeCN)SbF_6$	10	DCE	80	1:1.29
10	$JohnPhosAu(MeCN)SbF_6$	10	toluene	43	1:1
11	**$JohnPhosAu(MeCN)SbF_6$**	**8**	**THF**	**90**[a]	**1.25:1**
12	$JohnPhosAu(MeCN)SbF_6$	5	THF	25	1.5:1

Note: [a] The reaction was run at room temperature.

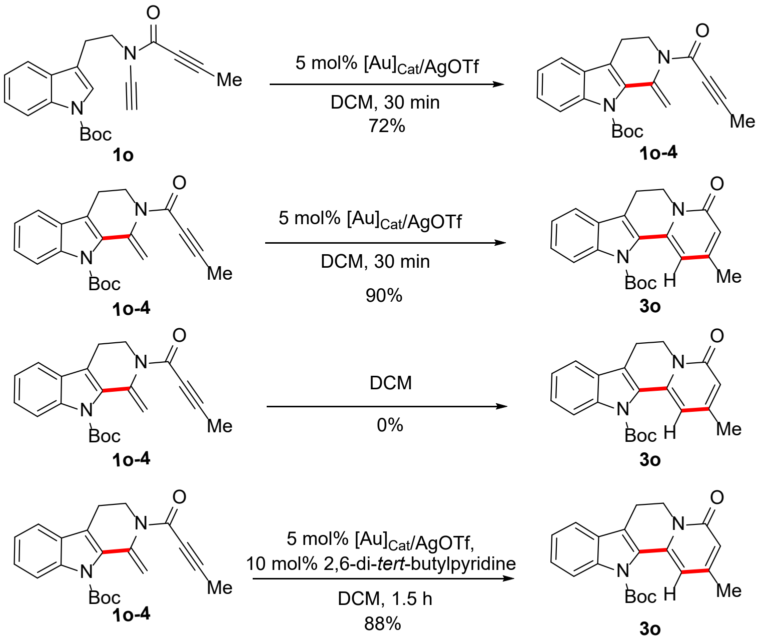
2.2 Table S2. Condition Screening for the Cycloisomerization of Substrate 1o Leading to the Optimal Condition (C2)[a]



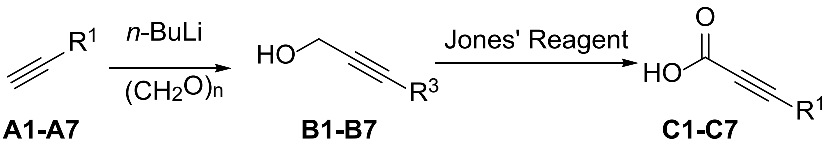
entry	catalyst	loading (mol%)	solvent	yield [**1o-4**] (%)	yield [**3o**] (%)
1	JohnPhosAu(MeCN)SbF_6	10	DCM	15	10
2	$Ph_3PAuNTf_2$	10	DCM	10	0
3	$Ph_3PAuCl/AgSbF_6$	10	DCM	12	0
4	Ph_3PAuCl/AgOTf	10	DCM	52	14
5	IPrAuCl/AgOTf	10	DCM	15	10
6	**[Au]$_{cat}$[b]/AgOTf**	**10**	**DCM**	**0**	**72**
7	[Au]$_{cat}$/AgOTf	10	DCE	46	15
8	[Au]$_{cat}$/AgOTf	10	toluene	0	0
9	[Au]$_{cat}$/AgOTf	10	THF	0	22

Note: [a] The reaction was run at room temperature. [b] [Au]$_{cat}$: [tris(2,4-di-*tert*-butylphenyl) phosphite]gold chloride.

3. Control Experiment



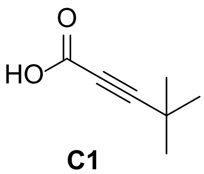
4. General Procedures for the Preparation of Substrates C1-C7 and Characterization Data



To a solution of compounds **A1**-**A7** (75 mmol) in anhydrous THF (50 mL) was added *n*-BuLi (83 mmol, 2.5 mol/L, 33 mL) at −78 °C under the N_2 atmosphere, and the mixture was stirred at the same temperature for 1 h. To this solution was slowly added Paraformaldehyde (150 mmol, 4.5 g) at −78 °C, and the mixture was first stirred at the same temperature for 30 min, and then warmed up to room temperature, and stirred for 1 h. The reaction was quenched by addition of water. After removal of the solvent *in vacuo*, the residue was extracted with ethyl acetate for 3 times, and the combined organic extracts were first washed with water and saturated brine, and then dried over anhydrous Na_2SO_4. The extract was concentrated *in vacuo*, to give crude products **B1**-**B7** as yellow oil.

To a solution crude products **B1**-**B7** (20.8 mmol) in acetone was added Jones reagent (41.6 mmol, 1 mol/L, 41.6 mL) at 0 °C for 30 min, and the mixture was stirred at the room temperature for 3 h. The reaction was quenched by addition of water. After removal of the solvent *in vacuo*, the residue was extracted with ethyl acetate for 3 times, and the combined organic extracts were first washed with water and saturated brine, and then dried over anhydrous Na_2SO_4. The extract was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel (DCM/MeOH) to give **C1-C7**.

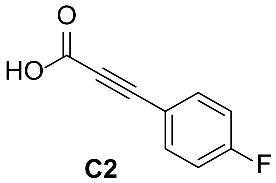
4,4-Dimethylpent-2-ynoic acid (C1)[S1]



C1

White oil in 65% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 1.23 (s, 9H).

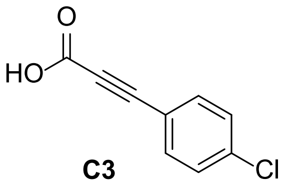
3-(4-Fluorophenyl)propiolic acid (C2)[S2]



C2

White oil in 72% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, DMSO-d_6) δ 7.79 – 7.55 (m, 2H), 7.30 (t, J = 8.9 Hz, 2H).

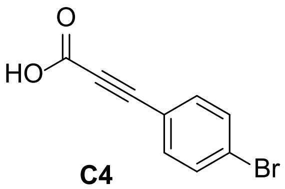
3-(4-Chlorophenyl)propiolic acid (C3)[S2]



C3

White oil in 70% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, DMSO-d_6) δ 7.54 – 7.49 (m, 2H), 7.49 – 7.43 (m, 2H).

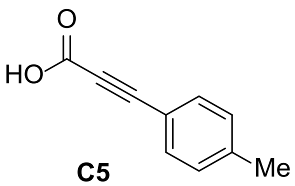
3-(4-Bromophenyl)propiolic acid (C4)[S2]



C4

White oil in 70% yield; R_f =0.2 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, DMSO-d_6) δ 7.60 – 7.54 (m, 2H), 7.41 – 7.34 (m, 2H).

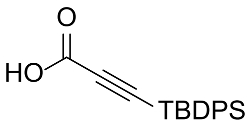
3-(*p*-Tolyl)propiolic acid (C5)[S3]



C5

White oil in 77% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, DMSO-d_6) δ 7.36 (d, J = 7.9 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 2.32 (s, 3H).

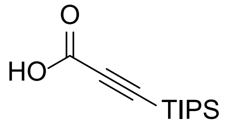
3-(*tert*-Butyldiphenylsilyl)propiolic acid (C6)



C6

White oil in 78% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^1H NMR (400 MHz, DMSO-d_6) δ 7.72 (dd, J = 7.6, 1.6 Hz, 4H), 7.58 – 7.37 (m, 6H), 1.05 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 152.8, 134.5, 130.3, 129.8, 127.7, 99.6, 85.7, 26.1, 17.6; IR (thin film, cm^{-1}): 3409, 3071, 3050, 2929, 2857, 2772, 2715, 2173, 1694, 1610, 1469, 1365, 1172, 1051; HRMS (ESI): *m/z* Calcd. for $C_{19}H_{21}O_2Si$ $[M+H]^+$ 309.1305, Found 309.1306.

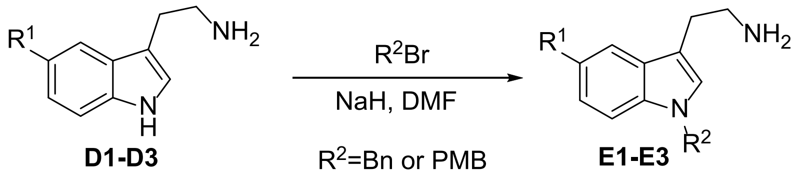
3-(triisopropylsilyl)propiolic acid (C7)



C7

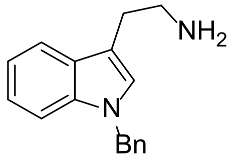
White oil in 65% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^1H NMR (600 MHz, DMSO-d_6) δ 1.15 – 1.08 (m, 3H), 1.06 (d, J = 6.1 Hz, 18H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 153.53, 98.60, 87.80, 18.25, 10.37; IR (thin film, cm^{-1}): 3500, 3300, 2962, 2926, 2842, 2795, 1714, 1625, 1465, 1377; HRMS (ESI): *m/z* Calcd. for $C_{12}H_{23}O_2Si$ $[M+H]^+$ 227.1462, Found 227.1463.

5. General Procedures for the Preparation of E1-E3 and Characterization Data



To a solution of NaH (72 mmol, 2.88 g) in DMF was added a solution of tryptamines **D1**-**D3** (60 mmol) in DMF 0 °C under the N_2 atmosphere, and the mixture was stirred at room temperature for 30 min. To this mixture was add BnBr or PMBBr (66 mmol) at 0 °C, and the mixture was stirred at room temperature for 2 h. The reaction was quenched by addition of water, then the residue was extracted with ethyl acetate for 3 times, and the combined organic extracts were first washed with water and saturated brine, and then dried over anhydrous Na_2SO_4. The extract was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel (DCM/MeOH) to provide the products **E1**-**E3**.

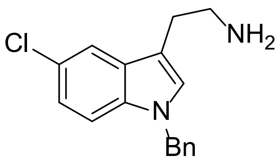
2-(1-Benzyl-1*H*-indol-3-yl)ethan-1-amine (E1)[S4]



E1

White solid in 75% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.59 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.37 (s, 1H), 7.30 (t, *J* = 7.2 Hz, 2H), 7.26 – 7.16 (m, 3H), 7.10 (dd, *J* = 11.2, 4.0 Hz, 1H), 7.02 (dd, *J* = 10.9, 3.9 Hz, 1H), 5.36 (s, 2H), 2.99 (dt, *J* = 11.9, 6.2 Hz, 4H).

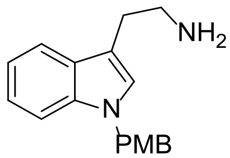
2-(1-Benzyl-5-chloro-1*H*-indol-3-yl)ethan-1-amine (E2)[S5]



E2

White solid in 85% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (s, 2H), 7.68 (d, *J* = 1.9 Hz, 1H), 7.53 – 7.42 (m, 2H), 7.31 (dd, *J* = 11.2, 4.4 Hz, 2H), 7.25 (t, *J* = 5.0 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.11 (dd, *J* = 8.7, 2.0 Hz, 1H), 5.38 (s, 2H), 3.09 – 2.93 (m, 4H).

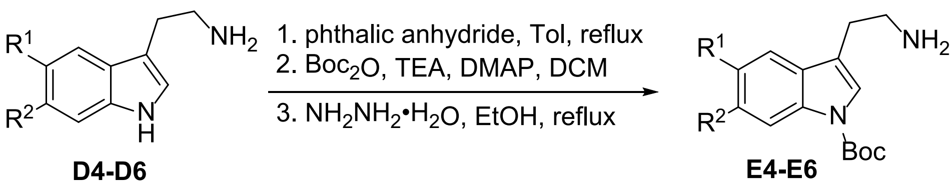
2-(1-(4-Methoxybenzyl)-1*H*-indol-3-yl)ethan-1-amine (E3)[S4]



E3

White solid in 80% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.92 (s, 1H), 6.79 (d, *J* = 8.6 Hz, 2H), 5.16 (s, 2H), 3.73 (s, 3H), 3.00 (t, *J* = 6.5 Hz, 2H), 2.90 (t, *J* = 6.5 Hz, 2H), 2.33 (s, 2H).

6. General Procedures for the Preparation of E4-E6 and Characterization Data

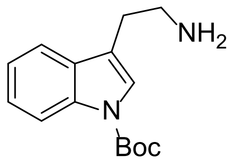


To a solution of compounds **D4-D6** (10 mmol) in toluene was added phthalic anhydride (11 mmol, 1.63 g) under the N_2 atmosphere, and the mixture was stirred overnight at reflux temperature. The solution was concentrated *in vacuo*, which was recrystallized from CH_2Cl_2 and hexane to give the yellow solid.

To the solution of the yellow solid obtained above in DCM was added di-*tert*-butyl dicarbonate (12 mmol, 2.62 g) and 4-dimethylaminopyridine (1 mmol, 122 mg) under the N_2 atmosphere at 0 °C, and the mixture was stirred at room temperature for 20 min. The reaction was quenched by addition of water, then the residue was added more DCM, and was first washed with water and saturated brine, and then dried over anhydrous Na_2SO_4. The extract was concentrated *in vacuo* to give yellow solid without further purification.

A solution of the yellow solid and hydrazine monohydrate (50 mmol, 2.50 g, 2.43 mL) in ethanol was stirred overnight at reflux temperature. The reaction was quenched by addition of 2 N NaOH, then the residue was extracted with ethyl acetate for 3 times, and the combined organic extracts were first washed with water and saturated brine, then dried over anhydrous Na_2SO_4. The extract was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel (DCM/MeOH).

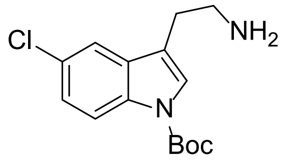
***tert*-Butyl 3-(2-aminoethyl)-1*H*-indole-1-carboxylate (E4)**



E4

White solid in 78% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^{1}H NMR (400 MHz, DMSO-*d₆*) δ 8.05 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.59 (s, 1H), 7.39 – 7.31 (m, 1H), 7.30 – 7.22 (m, 1H), 3.43 (s, 2H), 3.08 (dd, *J* = 11.2, 4.5 Hz, 2H), 3.04 – 2.95 (m, 2H), 1.62 (s, 9H).

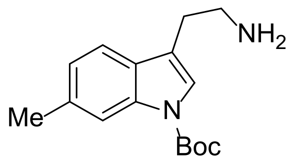
***tert*-Butyl 3-(2-aminoethyl)-5-chloro-1*H*-indole-1-carboxylate (E5)**



E5

White solid in 82% yield; R_f = 0.2 (DCM/MeOH = 10:1); ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.02 (d, J = 8.8 Hz, 1H), 7.78 (d, J = 1.6 Hz, 1H), 7.66 (s, 1H), 7.36 (d, J = 8.8 Hz, 1H), 3.53 (s, 2H), 3.08 – 3.01 (m, 2H), 3.01 – 2.92 (m, 2H), 1.62 (s, 9H).

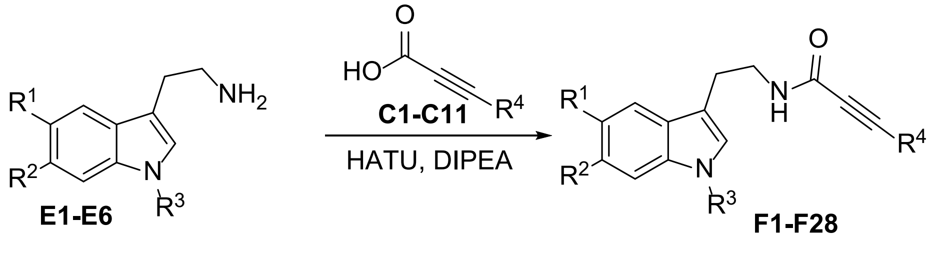
***tert*-Butyl 3-(2-aminoethyl)-6-methyl-1*H*-indole-1-carboxylate (E6)**



E6

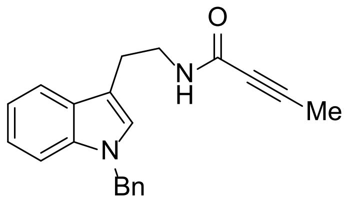
White solid in 83% yield; R_f = 0.2 (DCM/MeOH = 10:1); Mp 211.7 – 213.1 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.98 (d, J = 64.6 Hz, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.49 (s, 1H), 7.10 (d, J = 7.7 Hz, 1H), 3.34 (s, 2H), 3.12 – 3.01 (m, 2H), 3.00 – 2.90 (m, 2H), 2.43 (s, 3H), 1.62 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 149.0, 135.3, 133.9, 127.6, 123.89, 123.06, 118.8, 116.1, 115.0, 83.4, 38.6, 27.7, 23.0, 21.6; IR (thin film, cm^{-1}): 3424, 3128, 2984, 2936, 1732, 1635, 1599, 1514, 1491, 1453, 1384, 1366, 1319; HRMS (ESI): *m/z* Calcd. for $C_{16}H_{23}N_2O_2$ [M+H]$^+$ 275.1754, Found 275.1758.

7. General Procedures for the Preparation of F1-F21 and Characterization Data



To a solution of acids **C1**-**C11** (5.7 mmol) and HATU (6.3 mmol, 2.40 g) in DCM (50 mL) was added DIPEA (11.4 mmol, 1.47 g) at 0 °C, and the reaction was stirred at room temperature for 20 min. Then a solution of **E1**-**E6** (5.7 mmol) in DCM was added at 0 °C, and the reaction was stirred at room temperature for another 3 h. The reaction was quenched by addition of water, then the residue was added more DCM, and was first washed with water and saturated brine, and then dried over anhydrous Na_2SO_4. The extract was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel (EtOAc/petroleum ether) to give the products **F1**-**F28**.

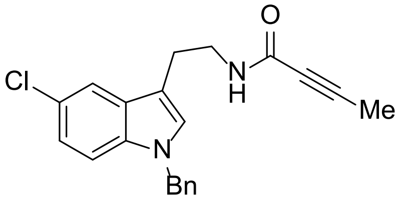
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)but-2-ynamide (F1)**



F1

White solid in 67% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 110.5 – 112.1 °C; The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.59 (t, *J* = 5.6 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.31 (S, 1H), 7.29 (t, *J* = 7.4 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.18 (d, *J* = 7.2 Hz, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 5.35 (s, 2H), 3.37 – 3.32 (m, 2H), 2.83 (t, *J* = 7.5 Hz, 2H), 1.94 (s, 3H); (minor rotamer) δ 8.05 (t, *J* = 6.2 Hz, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.31 (s, 1H), 7.29 (t, *J* = 7.4 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.18 (d, *J* = 7.2 Hz, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 5.36 (s, 2H), 3.49 (dd, *J* = 14.4, 6.7 Hz, 2H), 2.87 (t, *J*= 7.5Hz , 2H), 1.84 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) (major rotamer) δ 152.5, 138.4, 136.0, 128.5, 127.8, 127.6, 127.0, 126.6, 121.3, 118.6, 118.6, 111.5, 110.1, 82.1, 75.8, 48.9, 24.7, 3.0; IR (thin film, cm^{-1}): 3435, 3252, 2921, 2849, 2257, 1622, 1538, 1468; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{21}N_2O$ $[M+H]^+$ 317.1648, Found 317.1649.

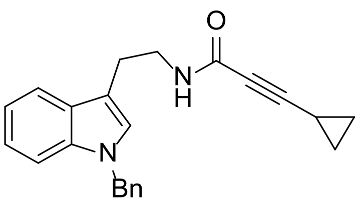
N-(2-(1-Benzyl-5-chloro-1H-indol-3-yl)ethyl)but-2-ynamide (F2)



F2

Yellow oil in 71% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 12.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.57 (t, J = 5.7 Hz, 1H), 7.58 (d, J = 2.0 Hz, 1H), 7.44 – 7.41 (m, 1H), 7.39 (s, 1H), 7.29 (dd, J = 10.2, 4.5 Hz, 2H), 7.23 (t, J = 7.3 Hz, 1H), 7.17 (d, J = 7.2 Hz, 2H), 7.10 – 7.06 (m, 1H), 5.36 (s, 2H), 3.34 – 3.29 (m, 2H), 2.81 (t, J = 7.3 Hz, 2H), 1.94 (s, 3H); (minor rotamer) δ 8.04 (t, J = 6.3 Hz, 1H), 7.60 (d, J = 2.0 Hz, 1H), 7.42 (dd, J = 8.7, 4.6 Hz, 1H), 7.39 (s, 1H), 7.29 (dd, J = 10.2, 4.5 Hz, 2H), 7.23 (t, J = 7.3 Hz, 1H), 7.17 (d, J = 7.2 Hz, 2H), 7.10 – 7.07 (m, 1H), 5.38 (s, 2H), 3.47 (dd, J = 14.1, 6.8 Hz, 2H), 2.86 – 2.83 (m, 2H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.9, 152.5, 138.1, 138.0, 134.6, 134.5, 129.0, 129.0, 128.9, 128.6, 128.5, 127.4, 127.0, 126.9, 123.5, 121.1, 118.0, 117.9, 111.8, 111.7, 111.5, 110.9, 87.7, 82.2, 75.8, 73.3, 65.7, 49.1, 43.3, 39.6, 24.4, 23.7, 14.0, 3.0; IR (thin film, cm^{-1}): 3438, 3249, 3061, 3026, 2989, 2916, 2835, 2257, 1620, 1542, 1491, 1472, 1451, 1384, 1353; HRMS (ESI): m/z Calcd. for $C_{21}H_{19}ClN_2ONa$ [M+Na]$^+$ 373.1078, Found 373.1078.

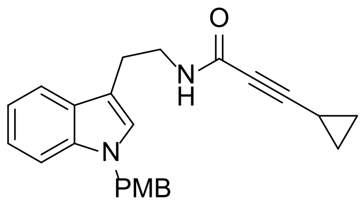
N-(2-(1-Benzyl-1H-indol-3-yl)ethyl)-3-cyclopropylpropiolamide (F3)



F3

Brown oil in 58% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.54 (t, J = 5.6 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.31 – 7.27 (m, 3H), 7.23 (t, J = 7.3 Hz, 1H), 7.18 (d, J = 7.2 Hz, 2H), 7.08 (t, J = 7.2 Hz, 1H), 7.00 (t, J = 7.4 Hz, 1H), 5.35 (s, 2H), 3.35 – 3.30 (m, 2H), 2.82 (t, J = 7.5 Hz, 2H), 1.45 (tt, J = 8.3, 5.0 Hz, 1H), 0.92 – 0.88 (m, 2H), 0.75 – 0.71 (m, 2H); (minor rotamer) δ 8.03 (t, J = 6.2 Hz, 1H), 7.56 (d, J = 7.9 Hz, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.33 – 7.26 (m, 3H), 7.23 (t, J = 7.3 Hz, 1H), 7.18 (d, J = 7.2 Hz, 2H), 7.08 (t, J = 7.2 Hz, 1H), 7.00 (t, J = 7.4 Hz, 1H), 5.36 (s, 3H), 3.45 (dd, J = 14.5, 6.8 Hz, 2H), 2.87 – 2.84 (m, 2H), 1.48 – 1.43 (m, 1H), 0.85 (dt, J = 6.6, 4.0 Hz, 2H), 0.63 – 0.60 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 152.5, 138.4, 138.4, 128.6, 128.5, 127.8, 127.3, 127.03, 127.0, 126.6, 121.3, 118.6, 118.6, 111.6, 111.5, 111.0, 110.2, 110.1, 89.0, 71.6, 48.9, 26.6, 24.7, 8.7, 8.4, -1.1, -1.2; IR (thin film, cm^{-1}): 3437, 2987, 2953, 2923, 2852, 1654, 1629, 1606, 1548, 1530, 1490; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{22}N_2ONa$ [M+Na]$^+$ 365.1624, Found 365.1631.

3-Cyclopropyl-*N*-(2-(1-(4-methoxybenzyl)-1*H*-indol-3-yl)ethyl)propiolamide (F4)

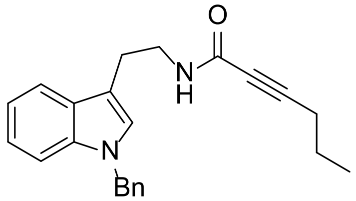


F4

Brown oil in 55% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.54 (t, J = 5.5 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.41 (d, J = 8.2 Hz, 1H), 7.28 (s, 1H), 7.16 (d, J = 8.6 Hz, 2H), 7.08 (t, J = 7.4 Hz, 1H), 7.00 (t, J = 7.4 Hz, 1H), 6.85 (d, J = 8.6 Hz, 2H), 5.25 (s, 2H), 3.69 (s, 3H), 3.35 – 3.30 (m, 2H), 2.81 (t, J = 7.5 Hz, 2H), 1.48 – 1.43 (m, 1H), 0.92 – 0.88 (m, 2H), 0.75 – 0.71 (m, 2H); (minor rotamer) δ 8.04 (t, J = 6.3 Hz, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.37 (dd, J = 8.1, 3.6 Hz, 1H), 7.23 (s, 1H), 7.13 (d, J = 7.2 Hz, 1H), 7.08 (t, J = 7.4 Hz, 1H), 7.05 – 7.02 (m, 2H), 7.00 (t, J = 7.4 Hz, 1H), 6.79 (d, J = 8.5 Hz, 1H), 5.27 (s, 2H), 3.72 (s, 3H), 3.45 (dd, J = 14.4, 6.8 Hz, 2H), 2.87 – 2.82 (m, 2H), 1.43 – 1.38 (m, 1H), 0.87 – 0.84 (m, 2H), 0.63 (dt, J = 6.7, 4.0 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 158.4, 154.4, 153.6, 136.0, 135.9, 130.2, 130.1, 129.5, 128.4, 128.4, 127.8, 127.7, 127.3, 126.9, 121.3, 118.7, 118.7, 118.4, 118.3, 113.9, 113.8, 110.3, 110.2, 109.8, 109.6, 100.8, 98.3, 76.9, 75.5, 68.7, 67.5, 65.6, 63.5, 55.0, 51.6, 48.5, 48.4, 47.1, 23.5, 22.6, 9.2, 9.0, -0.9, -1.1; IR (thin film, cm^{-1}): 3430, 3325, 2927, 2900, 2833, 1719, 1611, 1511, 1464, 1332;

HRMS (ESI): *m/z* Calcd. for $C_{24}H_{24}N_2O_2Na$ $[M+Na]^+$ 395.1730, Found 395.1732.

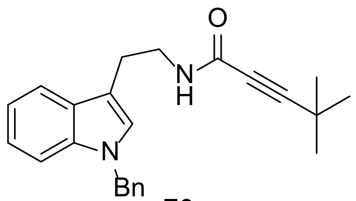
_N_-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)hex-2-ynamide (F5)



F5

Yellow oil in 58% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^1H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.60 (t, *J* = 5.6 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.31 (s, 1H), 7.29 (t, *J* = 7.4 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.18 (d, *J* = 7.3 Hz, 2H), 7.09 (t, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 5.35 (s, 2H), 3.36 (q, *J* = 7.4 Hz, 2H), 2.85 (t, *J* = 7.4 Hz, 2H), 2.30 (t, *J* = 7.0 Hz, 2H), 1.54-1.46 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); (minor rotamer) ^1H NMR (600 MHz, DMSO-d_6) δ 8.09 (t, *J* = 6.2 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.31 (s, 1H), 7.29 (t, *J* = 7.4 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.18 (d, *J* = 7.3 Hz, 2H), 7.09 (t, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 5.36 (s, 2H), 3.52 (dd, *J* = 14.3, 6.8 Hz, 2H), 2.90 – 2.87 (m, 2H), 2.20 (t, *J* = 7.0 Hz, 2H), 1.40 (dq, *J* = 14.3, 7.2 Hz, 2H), 0.87 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.9, 152.5, 138.3, 138.3, 136.1, 136.0, 128.5, 127.8, 127.7, 127.2, 127.0, 126.9, 126.9, 126.6, 121.2, 118.6, 118.6, 118.5, 111.5, 111.0, 110.1, 110.0, 91.4, 85.5, 76.6, 74.2, 48.9, 43.4, 26.6, 24.7, 20.9, 20.8, 19.6, 19.6, 13.3 , 13.3; IR (thin film, cm^{-1}): 3278, 3056, 2963, 2933, 2244, 1721, 1535, 1497, 1466, 1274; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{25}N_2O$ $[M+H]^+$ 345.1961, Found 345.1970.

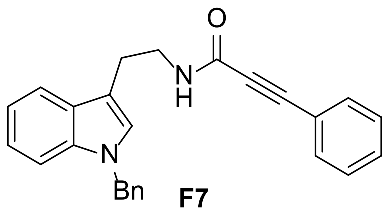
_N_-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-4,4-dimethylpent-2-ynamide (F6)



F6

White oil in 72% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^1H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.56 (t, *J* = 5.5 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.31 (s, 1H), 7.29 (t, J = 7.4 Hz, 2H), 7.23 (t, J = 7.3 Hz, 1H), 7.19 (d, J = 7.4 Hz, 2H), 7.08 (t, J = 7.5 Hz, 1H), 7.01 (t, J = 7.4 Hz, 1H), 5.35 (s, 2H), 3.37 – 3.33 (m, 2H), 2.84 (t, J = 7.5 Hz, 2H), 1.23 (s, 9H); (minor rotamer) δ 8.08 (t, J = 6.2 Hz, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.31 (s, 1H), 7.29 (t, J = 7.4 Hz, 2H), 7.23 (t, J = 7.3 Hz, 1H), 7.19 (d, J = 7.4 Hz, 2H), 7.08 (t, J = 7.5 Hz, 1H), 7.01 (t, J = 7.4 Hz, 1H), 5.36 (s, 2H), 3.50 (dd, J = 14.1, 6.8 Hz, 2H), 2.90 – 2.86 (m, 2H), 1.12 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 155.0, 152.6, 138.4, 138.3, 128.5, 127.8, 127.7, 127.3, 127.0, 127.0, 126.9, 126.6, 121.3, 118.7, 118.6, 118.5, 111.5, 111.0, 110.2, 110.1, 92.7, 75.0, 72.6, 54.3, 48.9, 43.5, 30.0, 29.8, 27.5, 27.1, 26.9, 26.5, 24.7; IR (thin film, cm^{-1}): 3409, 3057, 3030, 2970, 2929, 2715, 2602, 1950, 1880, 1724, 1630, 1467, 1453; HRMS (ESI): *m/z* Calcd. for $C_{24}H_{26}N_2ONa$ [M+Na]$^+$ 381.1937, Found 381.1941.

***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-phenylpropiolamide (F7)**

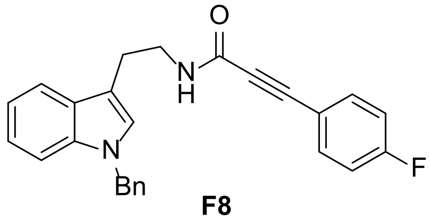


F7

Brown oil in 68% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.93 (t, J = 5.7 Hz, 1H), 7.60 – 7.55 (m, 3H), 7.53 – 7.49 (m, 1H), 7.46 (t, J = 7.3 Hz, 2H), 7.40 (t, J = 5.4 Hz, 1H), 7.35 (s, 1H), 7.27 (t, J = 7.4 Hz, 2H), 7.23 – 7.18 (m, 3H), 7.09 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 7.4 Hz, 1H), 5.36 (s, 2H), 3.45 (dd, J = 13.6, 7.1 Hz, 2H), 2.91 (t, J = 7.5 Hz, 2H); (minor rotamer) δ 8.35 (t, J = 6.3 Hz, 1H), 7.59 – 7.55 (m, 3H), 7.52 – 7.49 (m, 1H), 7.40 (t, J = 5.4 Hz, 2H), 7.36 (d, J = 8.6 Hz, 1H), 7.33 (s, 1H), 7.23 (d, J = 7.9 Hz, 2H), 7.15 (d, J = 7.1 Hz, 3H), 7.06 (d, J = 7.5 Hz, 1H), 6.91 (t, J = 7.4 Hz, 1H), 3.62 (dd, J = 14.1, 6.8 Hz, 2H), 2.97 – 2.94 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 152.3, 138.4, 138.3, 136.1, 136.1, 132.1, 132.1, 130.3, 130.2, 129.0, 128.8, 128.5, 128.4, 127.8, 127.2, 127.2, 127.0, 126.9, 126.7, 121.3, 119.9, 119.7, 118.7, 118.6, 118.6, 111.5, 111.0, 110.2, 110.1, 88.1, 84.2, 82.9, 48.9, 43.6, 26.6, 24.6; IR (thin film, cm^{-1}): 3438, 3276, 2928, 2849, 1630, 1488, 1466, 1382;

HRMS (ESI): *m/z* Calcd. for $C_{26}H_{23}N_2O$ $[M+H]^+$ 401.1624, Found 401.1621.

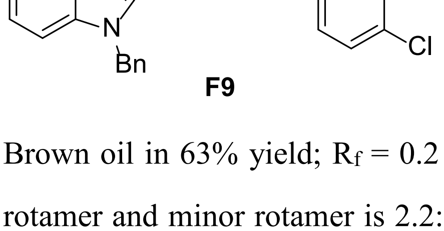
N-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-(4-fluorophenyl)propiolamide (F8)



F8

Brown oil in 70% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.92 (t, J = 5.5 Hz, 1H), 7.64 (dd, J = 8.0, 5.7 Hz, 2H), 7.57 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.34 (s, 1H), 7.32 (t, J = 8.8 Hz, 2H), 7.27 (t, J = 7.4 Hz, 2H), 7.20 (dd, J = 14.9, 7.5 Hz, 3H), 7.09 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 7.4 Hz, 1H), 5.36 (s, 2H), 3.44 (dd, J = 13.6, 6.8 Hz, 2H), 2.90 (t, J = 7.4 Hz, 2H); (minor rotamer) δ 8.35 – 8.32 (m, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.32 (t, J = 8.8 Hz, 2H), 7.27 (t, J = 7.4 Hz, 2H), 7.24 (s, 1H), 7.20 (dd, J = 14.9, 7.5 Hz, 3H), 7.15 (d, J = 7.5 Hz, 2H), 7.09 (t, J = 7.5 Hz, 1H), 6.91 (t, J = 7.4 Hz, 1H), 5.36 (s, 2H), 3.60 (dd, J = 13.5, 6.7 Hz, 2H), 2.95 – 2.92 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 163.7, 162.0, 154.6, 152.2, 138.4, 138.3, 136.1, 136.1, 134.7, 134.7, 134.6, 128.5, 128.4, 127.8, 127.8, 127.3, 127.2, 127.1, 127.0, 126.9, 126.7, 121.3, 118.6, 118.5, 116.4, 116.4, 116.3, 116.2, 116.1, 111.4, 111.0, 110.2, 110.1, 84.0, 81.9, 81.53, 54.9, 48.9, 43.6, 26.6, 24.7; IR (thin film, cm^{-1}): 3436, 2985, 2924, 1722, 1629, 1530, 1488, 1464, 1384; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{22}FN_2O$ $[M+H]^+$ 419.1530, Found 419.1545.

N-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-(4-chlorophenyl)propiolamide (F9)

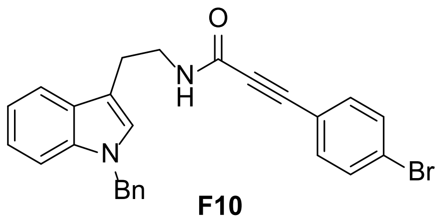


F9

Brown oil in 63% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 2.2:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.71 (t, J = 5.5 Hz, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.61 (d, J = 7.9 Hz, 1H), 7.54 –

7.51 (m, 2H), 7.40 (d, J = 8.5 Hz, 2H), 7.33 (s, 1H), 7.26 (dt, J = 7.2, 6.7 Hz, 3H), 7.17 (d, J = 6.9 Hz, 2H), 7.09 (t, J = 7.6 Hz, 1H), 7.04 – 6.99 (m, 1H), 5.35 (d, J = 6.1 Hz, 2H), 3.57 (dd, J = 13.4, 7.0 Hz, 2H), 2.98 (t, J = 7.4 Hz, 2H); (minor rotamer) δ 8.33 (t, J = 5.7 Hz, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.58 (t, J = 7.3 Hz, 1H), 7.54 – 7.51 (m, 1H), 7.40 (d, J = 8.5 Hz, 3H), 7.29 – 7.23 (m, 2H), 7.22 – 7.20 (m, 3H), 7.17 (d, J = 6.9 Hz, 2H), 7.09 (t, J = 7.6 Hz, 1H), 5.35 (d, J = 6.1 Hz, 2H), 3.34 (dd, J = 13.5, 7.0 Hz, 2H), 2.79 (t, J = 7.3 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 165.1, 162.5, 139.7, 138.4, 138.4, 136.1, 135.9, 135.2, 134.1, 133.8, 133.4, 130.4, 129.2, 129.1, 128.5, 128.4, 128.3, 127.9, 127.8, 127.8, 127.3, 127.3, 127.0, 127.0, 126.6, 124.8, 121.3, 118.7, 118.7, 118.6, 111.8, 111.6, 110.1, 49.0, 48.9, 40.2, 25.0, 24.7; IR (thin film, cm^{-1}): 3439, 2988, 2924, 2853, 1631, 1486, 1466, 1003; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{21}ClN_2ONa$ [M+Na]$^+$ 435.1235, Found 435.1243.

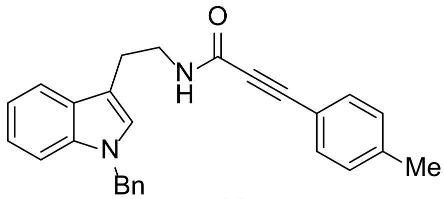
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-(4-bromophenyl)propiolamide (F10)**



F10

Brown oil in 70% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.96 (t, J = 5.7 Hz, 1H), 7.70 – 7.65 (m, 2H), 7.57 (d, J = 7.9 Hz, 1H), 7.52 – 7.49 (m, 2H), 7.40 (d, J = 8.2 Hz, 1H), 7.34 (s, 1H), 7.27 (t, J = 7.4 Hz, 2H), 7.20 (d, J = 7.3 Hz, 1H), 7.19 (d, J = 7.3 Hz, 2H), 7.11 – 7.07 (m, 1H), 7.02 (t, J = 7.2 Hz, 1H), 5.36 (s, 1H), 3.44 (dd, J = 13.6, 7.2 Hz, 2H), 2.90 (t, J = 7.4 Hz, 2H); (minor rotamer) δ 8.37 (t, J = 6.4 Hz, 1H), 7.59 (d, J = 1.8 Hz, 2H), 7.57 (d, J = 7.9 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.31 (s, 1H), 7.27 (t, J = 7.4 Hz, 2H), 7.23 (d, J = 1.5 Hz, 1H), 7.19 (d, J = 7.3 Hz, 2H), 7.14 (d, J = 7.0 Hz, 2H), 7.05 (d, J = 8.0 Hz, 1H), 6.92 (t, J = 7.3 Hz, 1H), 5.35 (s, 2H), 3.60 (dd, J = 13.8, 6.9 Hz, 2H), 2.94 – 2.92 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.5, 152.1, 138.4, 138.3, 136.1, 136.1, 134.1, 133.9, 132.1, 131.9, 128.5, 128.4, 127.8, 127.8, 127.3, 127.2, 127.2, 127.0, 126.8, 126.7, 123.9, 123.9, 123.9, 121.3, 119.2, 118.9, 118.6, 118.5, 111.4, 111.0, 110.2, 110.1, 86.9, 85.1, 82.7, 81.8, 48.9, 43.6, 26.6, 24.7; IR (thin film, cm^{-1}): 3439, 3285, 2988, 2955, 2927, 1630, 1463, 1385; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{21}BrN_2ONa$ $[M+Na]^+$ 479.0729, Found 479.0728.

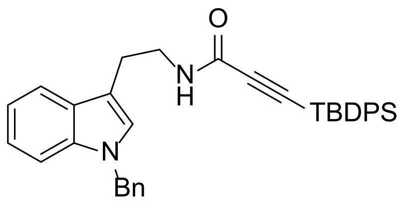
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-(*p*-tolyl)propiolamide (F11)**



F11

Brown oil in 69% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^1H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.88 (t, J = 5.7 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.45 (d, J = 8.1 Hz, 2H), 7.40 (d, J = 8.2 Hz, 1H), 7.34 (s, 1H), 7.27 (t, J = 7.4 Hz, 4H), 7.23 – 7.18 (m, 3H), 7.09 (dd, J = 11.2, 3.9 Hz, 1H), 7.02 (t, J = 7.3 Hz, 1H), 5.36 (s, 2H), 3.44 (dd, J = 13.6, 7.2 Hz, 2H), 2.90 (t, J = 7.5 Hz, 2H), 2.34 (s, 3H); (minor rotamer) δ 8.30 (t, J = 6.4 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.37 (d, J = 8.3 Hz, 2H), 7.32 (s, 1H), 7.24 (d, J = 7.6 Hz, 3H), 7.23 – 7.18 (m, 1H), 7.15 (d, J = 6.9 Hz, 3H), 7.09 (dd, J = 11.2, 3.9 Hz, 1H), 6.93 (t, J = 7.5 Hz, 1H), 5.35 (s, 2H), 3.61 (dd, J = 14.2, 6.7 Hz, 2H), 2.95 – 2.93 (m, 2H), 2.33 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 152.4, 151.9, 140.4, 140.3, 138.4, 138.3, 136.1, 136.1, 132.1, 132.0, 129.6, 129.5, 128.5, 128.4, 127.6, 127.84, 127.77, 127.24, 127.20, 127.0, 126.95, 126.9, 126.7, 121.3, 121.2, 118.7, 118.6, 118.5, 116.9, 116.7, 111.5, 111.0, 110.16, 110.10, 88.5, 83.8, 83.2, 81.4, 68.6, 48.9, 43.6, 26.6, 24.7, 21.2; IR (thin film, cm^{-1}): 3437, 3275, 2985, 2922, 2855, 1631, 1466, 1452, 1384; HRMS (ESI): *m/z* Calcd. for $C_{27}H_{24}N_2ONa$ $[M+Na]^+$ 415.1781, Found 415.1785.

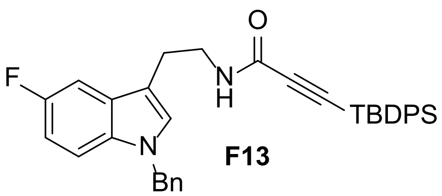
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-(*tert*-butyldiphenylsilyl)propiolamide (F12)**



F12

Brown oil in 57% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 5.5:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 7.67 – 7.65 (m, 1H), 7.65 – 7.61 (m, 4H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.28 (d, *J* = 8.9 Hz, 1H), 7.24 (d, *J* = 9.6 Hz, 1H), 7.18 – 7.15 (m, 2H), 7.15 – 7.13 (m, 2H), 7.11 (d, *J* = 7.1 Hz, 1H), 7.10 – 7.07 (m, 1H), 7.00 (dd, *J* = 13.4, 7.4 Hz, 3H), 6.88 (s, 1H), 5.97 (t, *J* = 5.4 Hz, 1H), 5.15 (s, 2H), 3.55 (q, *J* = 6.8 Hz, 1H), 2.92 (t, *J* = 6.8 Hz, 1H), 0.99 (s, 9H); (minor rotamer) δ 7.52 (d, *J* = 10.5 Hz, 1H), 7.44 (d, *J* = 7.9 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 3H), 7.28 (d, *J* = 8.9 Hz, 5H), 7.24 (d, *J* = 9.6 Hz, 2H), 7.15 – 7.13 (m, 3H), 7.10 – 7.06 (m, 2H), 6.96 (dd, *J* = 9.4, 5.7 Hz, 2H), 6.77 (s, 1H), 5.77 (t, *J* = 6.1 Hz, 1H), 5.12 (s, 2H), 3.71 (dd, *J* = 13.5, 6.8 Hz, 2H), 2.97 – 2.93 (m, 2H), 1.01 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.1, 152.6, 137.5, 136.9, 136.9, 136.1, 135.7, 135.7, 131.8, 131.7, 130.1, 130.1, 128.9, 128.2, 128.0, 127.8, 127.8, 126.9, 126.9, 126.5, 126.3, 122.2, 122.2, 119.5, 119.0, 118.8, 111.9, 111.0, 110.0, 110.0, 101.6, 99.1, 93.6, 86.7, 50.1, 50.1, 43.9, 40.6, 27.5, 27.1, 26.8, 25.2, 18.8, 18.8; IR (thin film, cm^{-1}): 3056, 2930, 1715, 1637, 1463, 1432; HRMS (ESI): *m/z* Calcd. for $C_{36}H_{37}N_2OSi$ $[M+H]^+$ 541.2670, Found 541.2679.

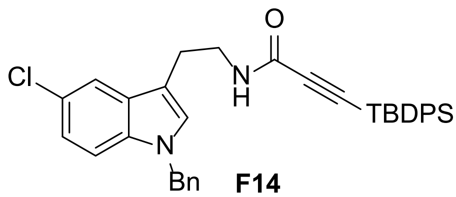
_N_-(2-(1-benzyl-5-fluoro-1_H_-indol-3-yl)ethyl)-3-(_tert_-butyldiphenylsilyl)propiolamide (F13)



F13

Brown oil in 49% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 12.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 9.05 (t, *J* = 5.8 Hz, 1H), 7.76 (d, *J* = 6.5 Hz, 4H), 7.51 – 7.42 (m, 7H), 7.41 (dd, *J* = 8.9, 4.4 Hz, 1H), 7.35 (dd, *J* = 9.9, 2.5 Hz, 1H), 7.29 – 7.24 (m, 2H), 7.22 – 7.17 (m, 3H), 6.94 (td, *J* = 9.2, 2.6 Hz, 1H), 5.36 (s, 2H), 3.42 (td, *J* = 7.5, 5.7 Hz, 2H), 2.88 (t, *J* = 7.4 Hz, 2H), 1.05 (s, 9H); (minor rotamer) δ 8.51 (t, *J* = 6.3 Hz, 1H), 7.67 (d, *J* = 6.7 Hz, 4H), 7.51 – 7.47 (m, 3H), 7.46 (dt, *J* = 3.2, 1.2 Hz, 2H), 7.44 (dd, *J* = 4.9, 3.2 Hz, 3H), 7.41 (dd, *J* = 8.9, 4.4 Hz, 1H), 7.35 (dd, J = 9.9, 2.5 Hz, 1H), 7.31 – 7.28 (m, 2H), 7.22 (dd, J = 7.5, 1.6 Hz, 3H), 6.90 (m, 1H), 5.31 (s, 2H), 3.67 (dd, J = 14.2, 6.8 Hz, 2H), 2.94 (t, J = 7.3 Hz, 2H), 0.96 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 157.7, 156.2, 151.5, 138.1, 135.2, 135.0, 132.7, 131.3, 130.2, 128.7, 128.5, 128.5, 128.1, 128.1, 127.3, 127.03, 127.00, 111.7, 111.7, 111.2, 111.2, 109.4, 109.3, 103.5, 103.4, 102.8, 83.9, 49.2, 39.9, 26.7, 24.4, 18.1; IR (thin film, cm^{-1}): 3678, 3048, 2929, 2856, 1637, 1485, 1453, 1428, 1393, 1260, 1182, 1111, 1028; HRMS (ESI): *m/z* Calcd. for $C_{36}H_{36}FN_2OSi$ [M+H]$^+$ 559.2575, Found 559.2571.

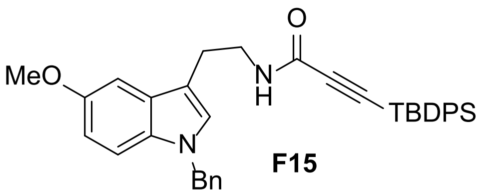
***N*-(2-(1-benzyl-5-chloro-1*H*-indol-3-yl)ethyl)-3-(*tert*-butyldiphenylsilyl)propiolamide (F14)**



F14

Brown oil in 55% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 15:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 9.04 (t, *J* = 5.8 Hz, 1H), 7.75 (d, *J* = 6.4 Hz, 4H), 7.63 (s, 1H), 7.53 – 7.40 (m, 8H), 7.26 (t, *J* = 7.5 Hz, 2H), 7.19 (dd, *J* = 14.6, 7.3 Hz, 3H), 7.09 (d, *J* = 6.7 Hz, 1H), 5.36 (s, 2H), 3.41 (dd, *J* = 13.4, 7.2 Hz, 2H), 2.89 (t, *J* = 7.4 Hz, 2H), 1.05 (s, 9H); (minor rotamer) δ 8.50 (t, *J* = 6.3 Hz, 1H), 7.67 (dd, *J* = 10.4, 3.6 Hz, 4H), 7.60 – 7.57 (m, 1H), 7.38 (dd, *J* = 13.7, 6.2 Hz, 8H), 7.30 (dd, *J* = 12.8, 5.1 Hz, 2H), 7.22 (d, *J* = 7.6 Hz, 3H), 7.07 (d, *J* = 2.0 Hz, 1H), 5.31 (s, 2H), 3.66 (dd, *J* = 14.0, 6.8 Hz, 2H), 2.94 (dd, *J* = 12.4, 5.1 Hz, 2H). 0.95 (d, *J* = 6.6 Hz, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 151.6, 135.2, 135.1, 134.6, 131.4, 130.2, 129.0, 128.6, 128.5, 128.2, 128.2, 127.4, 127.2, 123.6, 121.3, 118.0, 111.8, 111.6, 102.8, 84.0, 49.2, 40.0, 26.7, 24.4, 18.2; IR (thin film, cm^{-1}): 3676, 3028, 2929, 1638, 1521, 1470, 1428, 1355, 1269, 1171, 1110; HRMS (ESI): *m/z* Calcd. for $C_{36}H_{36}ClN_2OSi$ [M+H]$^+$ 575.2280, Found 575.2277.

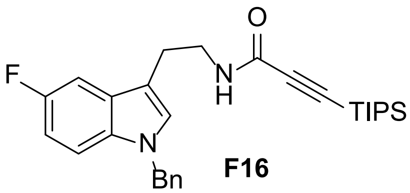
***N*-(2-(1-benzyl-5-methoxy-1*H*-indol-3-yl)ethyl)-3-(*tert*-butyldiphenylsilyl)propiolamide (F15)**



F15

Brown oil in 53% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 – 7.69 (m, 4H), 7.45 – 7.33 (m, 7H), 7.24 (s, 1H), 7.23 – 7.19 (m, 1H), 7.14 (t, J = 8.9 Hz, 1H), 7.08 (dd, J = 14.8, 4.8 Hz, 3H), 6.96 (s, 1H), 6.85 (dd, J = 8.9, 2.3 Hz, 1H), 6.06 (s, 1H), 5.23 (s, 2H), 3.82 (d, J = 4.1 Hz, 3H), 3.65 (q, J = 6.7 Hz, 2H), 3.00 (t, J = 6.9 Hz, 2H), 1.10 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.2, 152.6, 137.6, 135.7, 132.1, 131.8, 130.1, 128.9, 128.9, 128.4, 128.1, 128.1, 127.8, 126.9, 126.9, 112.5, 111.4, 110.9, 100.6, 86.9, 56.0, 50.3, 40.6, 27.1, 25.2, 18.8; IR (thin film, cm^{-1}): 3677, 3030, 2926, 1643, 1519, 1465, 1428, 1356, 1269, 1192, 1113; HRMS (ESI): m/z Calcd. for $C_{37}H_{39}N_2O_2Si$ $[M+H]^+$ 571.2275, Found 571.2277.

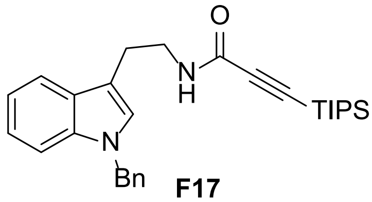
***N*-(2-(1-benzyl-5-fluoro-1*H*-indol-3-yl)ethyl)-3-(triisopropylsilyl)propiolamide (F16)**



F16

Brown oil in 73% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.74 (t, J = 5.8 Hz, 1H), 7.39 (q, J = 4.4 Hz, 2H), 7.33 – 7.26 (m, 4H), 7.23 (t, J = 7.4 Hz, 1H), 7.18 (d, J = 6.7 Hz, 2H), 6.92 (td, J = 9.2, 2.5 Hz, 1H), 5.34 (s, 2H), 3.35 (dd, J = 13.4, 7.5 Hz, 5H), 2.83 (t, J = 7.4 Hz, 2H), 1.06 (d, J = 3.7 Hz, 21H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 158.2, 156.6, 152.2, 133.2, 129.0, 129.0, 128.9, 128.5, 128.5, 127.9, 127.5, 127.4, 112.2, 112.2, 111.7, 111.6, 109.9, 109.7, 104.0, 103.8, 101.5, 85.8, 49.6, 24.9, 18.8, 10.9; IR (thin film, cm^{-1}): 3677, 3221, 3053, 2942, 2865, 2891, 1787, 1708, 1631, 1495, 1465, 1288, 1246, 1171, 1056; HRMS (ESI): m/z Calcd. for $C_{29}H_{38}FN_2OSi$ $[M+H]^+$ 477.2732, Found 477.2731.

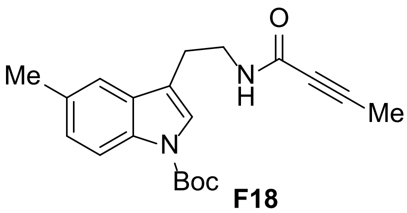
***N*-(2-(1-benzyl-1*H*-indol-3-yl)ethyl)-3-(triisopropylsilyl)propiolamide (F17)**



F17

Brown oil in 77% yield; $R_f = 0.2$ (EtOAc/petroleum ether = 1:8); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.76 (t, J = 5.8 Hz, 1H), 7.56 (d, J = 7.9 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.29 (dd, J = 15.6, 8.4 Hz, 2H), 7.22 (m, 1H), 7.20 – 7.14 (m, 2H), 7.11 – 7.03 (m, 1H), 7.04 – 6.95 (m, 1H), 5.35 (d, J = 4.2 Hz, 2H), 3.43 – 3.35 (m, 2H), 3.34 (s, 3H), 2.87 (t, J = 7.5 Hz, 2H), 1.07 (d, J = 3.8 Hz, 21H); ^{13}C NMR (150 MHz, DMS-d_6) δ 154.0, 151.7, 138.3, 138.2, 136.1, 136.0, 128.7, 128.6, 128.5, 127.8, 127.2, 127.2, 126.9, 126.5, 126.4, 121.3, 121.2, 118.6, 118.6, 111.5, 110.9, 110.0, 101.1, 85.8, 48.9, 26.4, 24.6, 18.3, 18.3, 18.2, 18.2, 10.5, 10.44, 10.40; IR (thin film, cm^{-1}): 3675, 3211, 3030, 2924, 2864, 2881, 1785, 1701, 1559, 1465, 1289, 1115; HRMS (ESI): *m/z* Calcd. for $C_{29}H_{39}N_2OSi$ $[M+H]^+$ 459.2826, Found 459.2827.

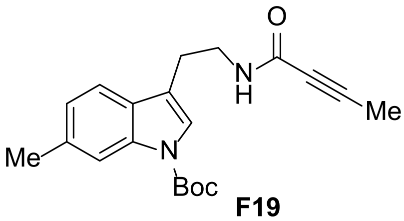
***tert*-butyl 3-(2-(but-2-ynamido)ethyl)-5-methyl-1*H*-indole-1-carboxylate (F18)**



F18

Yellow oil in 53% yield; $R_f = 0.2$ (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) ^{1}H NMR (600 MHz, DMSO) δ 8.60 (t, J = 5.6 Hz, 1H), 7.94 (t, J = 38.3 Hz, 1H), 7.41 (d, J = 33.2 Hz, 2H), 7.13 (dd, J = 8.4, 0.9 Hz, 1H), 3.43 – 3.26 (m, 2H), 2.78 (t, J = 7.0 Hz, 2H), 2.39 (s, 3H), 1.94 (s, 2H), 1.61 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 152.5, 149.0, 133.0, 131.4, 130.4, 125.6, 123.0, 119.1, 117.7, 114.4, 83.3, 82.2, 75.7, 38.7, 27.7, 24.4, 20.9; IR (thin film, cm^{-1}): 3677, 2978, 2931, 2256, 1731, 1630, 1528, 1473, 1383, 1285, 1158, 1084; HRMS (ESI): *m/z* Calcd. for $C_{20}H_{24}N_2O3Si$ $[M+H]^+$ 341.1860, Found 341.1862.

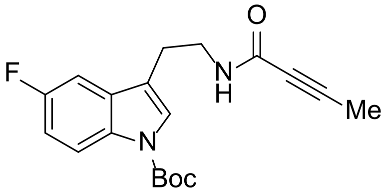
***tert*-Butyl 3-(2-(but-2-ynamido)ethyl)-6-methyl-1*H*-indole-1-carboxylate (F19)**



F19

Brown oil in 69% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.00 (s, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.34 (s, 1H), 7.08 (d, J = 7.9 Hz, 1H), 5.81 (s, 1H), 3.62 (dd, J = 13.1, 6.6 Hz, 2H), 2.90 (t, J = 6.9 Hz, 2H), 2.48 (s, 3H), 1.92 (s, 3H), 1.67 (s, 9H); (minor rotamer) δ 7.40 (d, J = 8.0 Hz, 1H), 7.38 (s, 1H), 7.34 (s, 1H), 7.08 (d, J = 7.9 Hz, 1H), 5.68 (s, 1H), 3.72 (dd, J = 13.5, 6.8 Hz, 2H), 2.93 – 2.88 (m, 2H), 2.48 (s, 3H), 1.94 (s, 3H), 1.67 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.2, 153.6, 149.9, 136.2, 134.8, 128.0, 124.2, 124.1, 123.1, 122.8, 118.6, 118.3, 117.4, 116.6, 115.9, 115.8, 100.1, 90.0, 83.6, 83.5, 75.0, 72.7, 42.9, 39.4, 28.4, 28.3, 26.9, 25.1, 22.1, 4.1, 3.8, 0.1; IR (thin film, cm^{-1}): 3436, 3321, 2987, 2835, 1723, 1629, 1605, 1489, 1460, 1441, 1384, 1307; HRMS (ESI): *m/z* Calcd. for $C_{20}H_{24}N_2O_3Na$ $[M+Na]^+$ 363.1679, Found 363.1685.

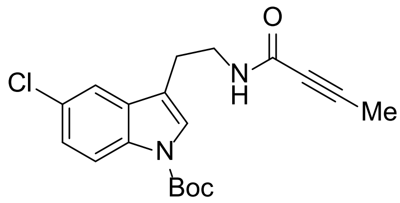
***tert*-butyl 3-(2-(but-2-ynamido)ethyl)-5-fluoro-1*H*-indole-1-carboxylate (F20)**



F20

Yellow oil in 61% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.60 (t, J = 5.6 Hz, 1H), 8.00 (d, J = 3.8 Hz, 1H), 7.56 (s, 1H), 7.42 (d, J = 9.1 Hz, 1H), 7.15 (t, J = 9.1 Hz, 1H), 3.46 – 3.25 (m, 2H), 2.78 (t, J = 7.0 Hz, 2H), 1.94 (s, 3H), 1.61 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6): δ 159.3, 157.7, 152.5, 148.8, 131.4, 131.3, 131.2, 124.7, 117.9, 117.8, 116.0, 115.9, 111.9, 111.8, 104.9, 104.8, 83.7, 82.3, 75.6, 54.9, 38.4, 27.6, 24.0, 2.4; IR (thin film, cm^{-1}): 3677, 3210, 3039, 2934, 2260, 2226, 1731, 1621, 1545, 1445, 1388; HRMS (ESI): *m/z* Calcd. for $C_{19}H_{21}N_2O_3$ $[M+H]^+$ 345.1609, Found 345.1605.

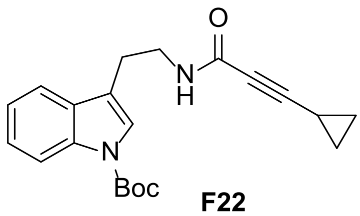
***tert*-Butyl 3-(2-(but-2-ynamido)ethyl)-5-chloro-1*H*-indole-1-carboxylate (F21)**



F21

Yellow oil in 64% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 5:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.06 (s, 1H), 7.49 (d, *J* = 1.4 Hz, 1H), 7.44 (s, 1H), 7.28 (d, *J* = 1.7 Hz, 1H), 5.84 (s, 1H), 3.60 (dd, *J* = 13.1, 6.7 Hz, 2H), 2.88 (t, *J* = 6.9 Hz, 2H), 1.93 (s, 3H), 1.66 (s, 9H); (minor rotamer) δ 8.06 (s, 1H), 7.49 (d, *J* = 1.4 Hz, 1H), 7.44 (s, 1H), 7.28 (d, *J* = 1.7 Hz, 1H), 5.79 (s, 1H), 3.70 (dd, *J* = 13.7, 6.9 Hz, 2H), 2.91 – 2.87 (m, 2H), 1.96 (s, 3H), 1.66 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.3, 153.7, 149.5, 134.1, 131.6, 128.5, 128.4, 125.2, 124.9, 124.7, 118.7, 118.5, 116.9, 116.7, 116.5, 116.0, 90.3, 84.3, 83.8, 74.9, 72.5, 42.7, 39.4, 29.8, 28.3, 28.3, 26.9, 25.0, 4.0, 3.8; IR (thin film, cm^{-1}): 3436, 3294, 2985, 2926, 2835, 1732, 1692, 1608, 1488, 1453, 1382; HRMS (ESI): *m/z* Calcd. for $C_{19}H_{21}ClN_2O_3Na$ $[M+Na]^+$ 383.1133 Found 383.1140.

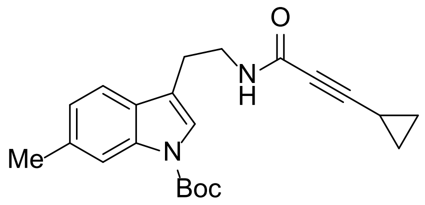
***tert*-Butyl 3-(2-(3-cyclopropylpropiolamido)ethyl)-1*H*-indole-1-carboxylate (F22)**



F22

Yellow oil in 74% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.58 (t, *J* = 5.6 Hz, 1H), 8.03 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.49 (s, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 3.38 – 3.32 (m, 2H), 2.80 (t, *J* = 7.0 Hz, 2H), 1.62 (s, 9H), 1.48 – 1.42 (m, 1H), 0.89 (td, *J* = 6.7, 4.0 Hz, 2H), 0.74 – 0.71 (m, 2H); (minor rotamer) δ 8.20 (t, *J* = 5.4 Hz, 1H), 8.03 (d, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.49 (s, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 3.49 (dd, *J* = 13.4, 6.7 Hz, 2H), 2.85 – 2.81 (m, 2H), 1.62 (s, 9H), 1.41 – 1.36 (m, 1H), 0.87 – 0.83 (m, 2H), 0.63 (dt, *J* = 6.9, 4.2 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.9, 152.5, 149.1, 134.8, 130.2, 124.4, 123.4, 123.0, 122.5, 119.2, 119.1, 118.0, 117.5, 114.8, 114.7, 95.0, 89.2, 83.5, 83.5, 71.5, 69.1, 54.9, 42.4, 38.6, 27.7, 25.9, 24.2, 8.7, 8.4, 6.1, -1.3, -1.2; IR (thin film, cm^{-1}): 3434, 3285, 2977, 2931, 2875, 1729, 1629, 1535, 1453, 1372; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{24}N_2O_3Na$ $[M+Na]^+$ 375.1679, Found 375.1681.

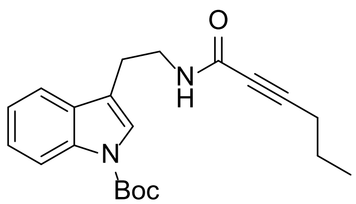
***tert*-Butyl 3-(2-(3-cyclopropylpropiolamido)ethyl)-6-methyl-1*H*-indole-1-carboxylate (F23)**



F23

Yellow oil in 69% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 5:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.00 (s, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.33 (s, 1H), 7.08 (d, J = 7.9 Hz, 1H), 5.76 (s, 1H), 3.61 (dd, J = 13.0, 6.5 Hz, 2H), 2.89 (t, J = 6.8 Hz, 2H), 2.48 (s, 3H), 1.67 (s, 9H), 1.33 – 1.28 (m, 1H), 0.90 – 0.85 (m, 2H), 0.84 – 0.80 (m, 2H); (minor rotamer) δ 8.00 (s, 1H), 7.43 (d, J = 7.9 Hz, 1H), 7.33 (s, 1H), 7.08 (d, J = 7.9 Hz, 1H), 5.36 – 5.34 (m, 1H), 3.69 (dd, J = 13.5, 6.8 Hz, 2H), 2.93 – 2.89 (m, 2H), 2.48 (s, 3H), 1.67 (s, 9H), 0.97 (dt, J = 7.9, 4.1 Hz, 1H), 0.90 – 0.85 (m, 2H), 0.71 (td, J = 7.0, 3.9 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.7, 153.7, 149.9, 134.8, 128.1, 124.2, 124.1, 122.8, 122.7, 118.8, 118.7, 118.4, 117.9, 117.4, 116.6, 115.9, 115.8, 91.0, 83.6, 70.9, 42.9, 39.5, 39.4, 29.9, 29.5, 28.4, 28.3, 27.4, 26.8, 25.5, 25.2, 22.8, 22.1, 15.0, 14.3, 9.3, 8.9, 7.25, 0.1, -0.3, -0.6; IR (thin film, cm^{-1}): 3427, 3321, 2977, 2931, 2868, 2224, 1726, 1632, 1545, 1487, 1476, 1451, 1381; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{26}N_2O_3Na$ $[M+Na]^+$ 389.1836, Found 389.1839.

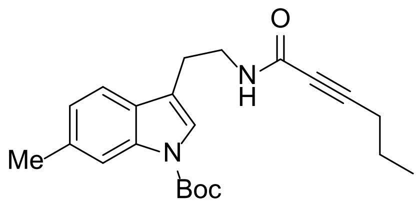
***tert*-Butyl 3-(2-(hex-2-ynamido)ethyl)-1*H*-indole-1-carboxylate (F24)**



F24

White oil in 63% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 6.7:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.14 (s, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.43 (s, 1H), 7.35 – 7.31 (m, 1H), 7.26 – 7.23 (m, 1H), 5.90 (s, 1H), 3.62 (q, *J* = 6.8 Hz, 2H), 2.96 – 2.91 (m, 2H), 2.24 (t, *J* = 7.1 Hz, 2H), 1.67 (s, 9H), 1.60 – 1.52 (m, 2H), 1.01 – 0.96 (m, 3H); (minor rotamer) δ 8.14 (s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.43 (s, 1H), 7.35 – 7.31 (m, 1H), 7.26 – 7.22 (m, 1H), 5.82 (t, *J* = 6.0 Hz, 1H), 3.73 (q, *J* = 6.8 Hz, 2H), 2.97 – 2.91 (m, 2H), 2.28 – 2.23 (m, 2H), 1.67 (s, 9H), 1.60 – 1.52 (m, 2H), 1.01 – 0.96 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.3, 153.7, 149.8, 135.7, 130.4, 124.7, 124.7, 123.7, 123.4, 122.7, 122.6, 119.0, 118.7, 117.5, 116.7, 115.6, 115.4, 94.0, 87.5, 83.8, 75.7, 73.4, 43.0, 40.0, 29.8, 28.3, 28.3, 26.7, 25.1, 21.4, 21.4, 20.9, 20.6, 13.7, 13.6; IR (thin film, cm^{-1}): 3372, 3291, 3053, 2969, 2934, 2873, 2246, 1730, 1631, 1453, 1383; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{26}N_2O_3Na$ $[M+Na]^+$ 377.1836, Found 377.1839.

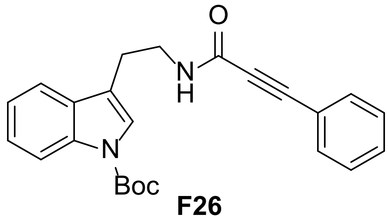
***tert*-Butyl 3-(2-(hex-2-ynamido)ethyl)-6-methyl-1*H*-indole-1-carboxylate (F25)**



F25

Yellow solid in 59% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 92.3 – 93.8 °C; The ratio of major rotamer and minor rotamer is 6.7:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.00 (s, 1H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.34 (s, 1H), 7.08 (d, *J* = 7.7 Hz, 1H), 5.87 (s, 1H), 3.61 (dd, *J* = 12.9, 6.5 Hz, 2H), 2.90 (t, *J* = 6.8 Hz, 2H), 2.48 (s, 3H), 2.24 (t, *J* = 7.0 Hz, 2H), 1.66 (s, 9H), 1.60 – 1.51 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H); (minor rotamer) δ 8.00 (s, 1H), 7.38 (d, *J* = 8.2 Hz, 1H), 7.34 (s, 1H), 7.08 (d, *J* = 7.7 Hz, 1H), 5.77 (s, 1H), 3.71 (dd, *J* = 13.3, 6.6 Hz, 2H), 2.90 (t, *J* = 6.8 Hz, 2H), 2.48 (s, 3H), 2.30 – 2.26 (m, 2H), 1.66 (s, 9H), 1.60 – 1.52 (m, 2H), 1.01 – 0.96 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.3, 153.3, 149.9, 136.2, 134.8, 128.1, 124.1, 124.1, 123.0, 122.7, 118.6, 118.3, 117.4, 116.6, 115.9, 115.7, 94.0, 87.5, 83.7, 83.6, 75.8, 73.4, 43.0, 39.5, 29.8, 28.3, 26.8, 25.1, 22.1, 21.4, 21.4, 20.9, 20.6, 13.7, 13.6; IR (thin film, cm^{-1}): 3433, 3296, 2968, 2932, 2872, 2245, 1728, 1630, 1530, 1490, 1440, 1382; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{28}N_2O_3Na$ $[M+Na]^+$ 391.1992, Found 391.1997.

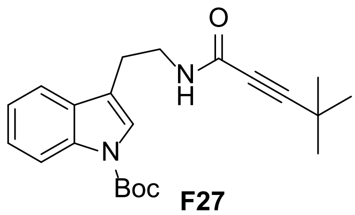
***tert*-Butyl 3-(2-(3-phenylpropiolamido)ethyl)-1*H*-indole-1-carboxylate (F26)**



F26

Yellow oil in 70% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); The ratio of major rotamer and minor rotamer is 6.7:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.47 (m, 2H), 7.46 (s, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.36 – 7.29 (m, 3H), 7.25 (t, *J* = 7.3 Hz, 1H), 6.13 (s, 1H), 3.69 (q, *J* = 6.8 Hz, 2H), 2.97 (t, *J* = 6.8 Hz, 2H), 1.66 (s, 9H); (minor rotamer) δ 7.52 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.38 (q, *J* = 7.1 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.25 (t, *J* = 7.3 Hz, 3H), 7.17 (t, *J* = 7.5 Hz, 1H), 5.98 (t, *J* = 6.2 Hz, 1H), 3.81 (dd, *J* = 13.7, 6.9 Hz, 2H), 3.02 – 2.98 (m, 2H), 1.66 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.1, 153.6, 149.8, 135.7, 132.7, 132.6, 130.4, 130.3, 130.2, 128.7, 128.6, 124.8, 124.7, 123.7, 123.4, 122.7, 120.3, 120.2, 119.0, 118.7, 117.4, 116.6, 115.6, 115.5, 91.0, 84.9, 83.8, 83.1, 80.7, 43.2, 39.6, 28.3, 26.8, 25.1; IR (thin film, cm^{-1}): 3435, 3300, 3057, 2981, 2933, 2214, 1727, 1630, 1546, 1489, 1476, 1452, 1383, 1306; HRMS (ESI): *m/z* Calcd. for $C_{24}H_{24}N_2O_3Na$ $[M+Na]^+$ 411.1679, Found 411.1687.

***tert*-Butyl 3-(2-(4,4-dimethylpent-2-ynamido)ethyl)-1*H*-indole-1-carboxylate (F27)**

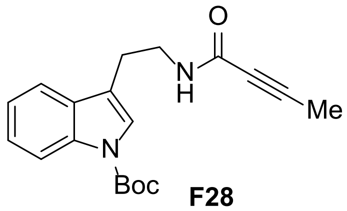


F27

White solid in 76% yield (EtOAc/petroleum ether = 1:5); Mp 77.2 – 78.9 °C; The ratio of major rotamer and minor rotamer is 10:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.57 (t, *J* = 5.7 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.49 (s, 1H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.4 Hz, 1H), 3.37 (dd, *J* =

13.2, 7.1 Hz, 2H), 2.81 (t, J = 7.0 Hz, 2H), 1.61 (s, 9H), 1.22 (s, 9H); (minor rotamer) δ 8.09 (t, J = 6.3 Hz, 1H), 7.64 (d, J = 7.6 Hz, 1H), 7.60 (d, J = 7.7 Hz, 1H), 7.47 (s, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.25 (t, J = 7.4 Hz, 1H), 3.51 (dd, J = 13.4, 6.7 Hz, 2H), 2.85 (t, J = 7.0 Hz, 2H), 1.60 (s, 9H), 1.12 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 155.0, 152.6, 149.1, 134.8, 130.2, 124.4, 123.3, 123.0, 122.5, 119.2, 119.1, 118.0, 117.6, 114.7, 98.5, 92.8, 83.5, 83.4, 74.9, 72.4, 54.9, 42.7, 38.6, 30.0, 29.7, 27.7, 27.4, 27.0, 26.9, 25.7, 24.2; IR (thin film, cm^{-1}): 3439, 3295, 2970, 2926, 2866, 1730, 1630, 1476, 1453, 1382; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{28}N_2O_3Na$ [M+Na]$^+$ 391.1992, Found 391.1989.

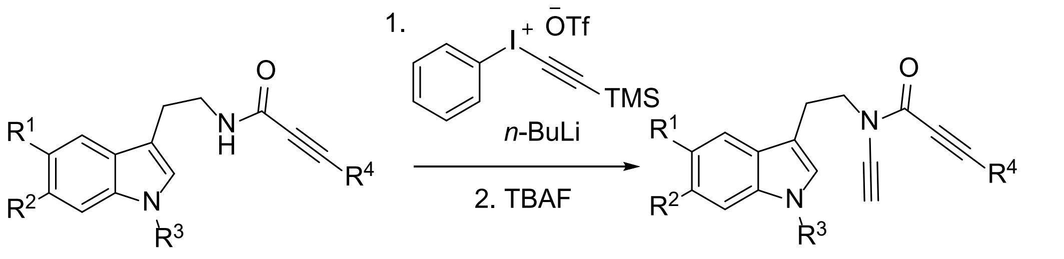
***tert*-Butyl 3-(2-(but-2-ynamido)ethyl)-1*H*-indole-1-carboxylate (F28)**



F28

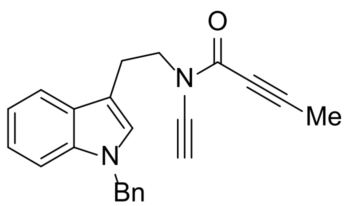
White solid in 77% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 117.6 – 119.1 °C; The ratio of major rotamer and minor rotamer is 6.7:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.13 (s, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.43 (s, 1H), 7.32 (t, J = 7.7 Hz, 1H), 7.24 (t, J = 7.5 Hz, 1H), 5.97 (s, 1H), 3.62 (q, J = 6.8 Hz, 2H), 2.92 (t, J = 6.8 Hz, 2H), 1.90 (s, 3H), 1.67 (s, 9H); (minor rotamer) δ 8.13 (s, 1H), 7.54 – 7.51 (m, 1H), 7.43 (s, 1H), 7.32 (t, J = 7.7 Hz, 1H), 7.24 (t, J = 7.5 Hz, 1H), 5.97 (s, 1H), 3.71 (q, J = 6.8 Hz, 1H), 2.94 – 2.91 (m, 1H), 1.91 (s, 1H), 1.67 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.3, 153.6, 149.8, 135.6, 130.3, 124.7, 123.7, 123.3, 122.7, 122.6, 119.0, 118.7, 117.4, 116.7, 115.5, 115.4, 89.9, 83.8, 83.5, 75.0, 72.6, 42.8, 39.4, 28.3, 26.7, 3.9, 3.7; IR (thin film, cm^{-1}): 3440, 3219, 3047, 2982, 2938, 2861, 2260, 1733, 1718, 1626, 1545, 1452, 1384, 1356; HRMS (ESI): *m/z* Calcd. for $C_{19}H_{22}N_2O_3Na$ [M+Na]$^+$ 349.1523, Found 349.1528.

8. General Procedures for the Preparation of 1, 1a-1aa and Characterization Data



To a solution of compounds **F1-F28** (3.6 mmol) in anhydrous Tol (30 mL) was added *n*-BuLi (4.3 mmol, 2.5 mol/L, 1.72 mL) at −78 °C under the N_2 atmosphere, and the mixture was stirred at the same temperature for 10 min, and then warmed up to room temperature, and stirred for 20 min. The mixture was added a solution of phenyl(trimethylsilylethynyl)iodonium triflate (6.5 mmol, 2.93 g) in anhydrous DCM, and was stirred for 12 h. then mixture was added TBAF (1 mmol, 1 mol/L, 1 mL) at −10 °C, and stirred for 5 min. The reaction was quenched by addition of a saturated solution of NH_4Cl. The residue was extracted with ethyl acetate for 3 times, and the combined organic extracts were first washed with water and saturated brine, and then dried over anhydrous Na_2SO_4. The extract was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel (EtOAc/petroleum ether).

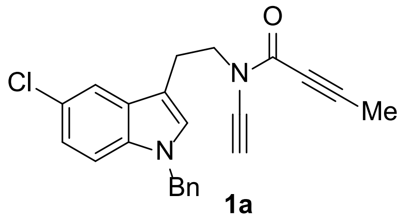
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-*N*-ethynylbut-2-ynamide (1)**



1

Brown oil in 78% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.56 (d, J = 7.8 Hz, 1H), 7.38 (t, J = 8.9 Hz, 1H), 7.33 (s, 1H), 7.28 (t, J = 7.4 Hz, 2H), 7.22 (t, J = 7.3 Hz, 1H), 7.15 (d, J = 7.0 Hz, 2H), 7.09 (t, J = 7.6 Hz, 1H), 7.03 (q, J = 7.5 Hz, 1H), 5.36 (s, 2H), 4.11 (s, 1H), 3.76 (t, J = 7.4 Hz, 2H), 3.00 (t, J = 7.4 Hz, 2H), 2.05 (s, 3H); (minor rotamer) δ 7.60 (d, J = 7.8 Hz, 1H), 7.38 (t, J = 8.9 Hz, 1H), 7.31 (s, 1H), 7.28 (t, J = 7.4 Hz, 2H), 7.22 (t, J = 7.3 Hz, 1H), 7.15 (d, J = 7.0 Hz, 2H), 7.09 (t, J = 7.6 Hz, 1H), 7.03 (q, J = 7.4 Hz, 1H), 5.37 (s, 2H), 3.96 (t, J = 6.7 Hz, 2H), 3.08 (t, J = 6.7 Hz, 2H), 1.64 (s, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.4, 153.8, 138.3, 138.3, 136.1, 136.0, 128.5, 128.4, 127.9, 127.65, 127.60, 127.2, 127.1, 126.9, 126.8, 121.4, 121.3, 118.8, 118.4, 110.2, 110.2, 109.9, 109.7, 93.8, 91.4, 76.9, 75.5, 72.9, 71.5, 65.5, 63.5, 51.5, 48.9, 48.9, 47.2, 23.6, 22.6, 3.4, 3.0; IR (thin film, cm^{-1}): 3440, 2988, 2952, 2853, 2239, 1658, 1465, 1384; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{21}N_2O$ $[M+H]^+$ 341.1648, Found 341.1651.

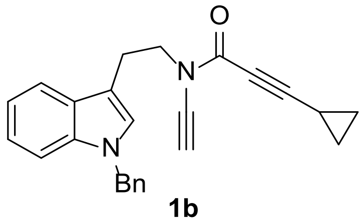
***N*-(2-(1-Benzyl-5-chloro-1*H*-indol-3-yl)ethyl)-*N*-ethynylbut-2-ynamide (1a)**



1a

Yellow oil in 40% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.2:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.61 (d, J = 1.9 Hz, 1H), 7.40 (t, J = 8.2 Hz, 2H), 7.28 (t, J = 7.4 Hz, 2H), 7.23 (t, J = 7.2 Hz, 1H), 7.13 (d, J = 7.3 Hz, 2H), 7.09 (dd, J = 8.7, 2.0 Hz, 1H), 5.38 (s, 2H), 4.09 (s, 1H), 3.74 (t, J = 7.1 Hz, 2H), 2.98 (t, J = 7.1 Hz, 2H), 2.05 (s, 3H); (minor rotamer) δ 7.67 (d, J = 1.6 Hz, 1H), 7.40 (t, J = 8.2 Hz, 2H), 7.28 (t, J = 7.4 Hz, 2H), 7.23 (t, J = 7.2 Hz, 1H), 7.13 (d, J = 7.3 Hz, 2H), 7.09 (dd, J = 8.7, 2.0 Hz, 1H), 5.39 (s, 2H), 4.11 (s, 1H), 3.95 (t, J = 6.5 Hz, 2H), 3.06 (t, J = 6.5 Hz, 2H), 1.68 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.4, 153.4, 138.0, 138.0, 134.7, 134.5, 129.5, 129.1, 128.9, 128.8, 128.5, 128.5, 127.3, 126.8, 126.8, 123.7, 121.3, 121.2, 117.9, 117.8, 111.9, 111.8, 110.0, 109.6, 93.7, 91.5, 76.82, 75.4, 72.9, 71.4, 65.6, 63.5, 51.3, 49.09, 49.06, 47.2, 23.3, 22.3, 3.4, 3.0; IR (thin film, cm^{-1}): 3437, 3329, 2987, 2926, 2869, 2832, 1735, 1679, 1607, 1488, 1470, 1396; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{19}ClN_2ONa$ $[M+Na]^+$ 397.1078, Found 397.1073.

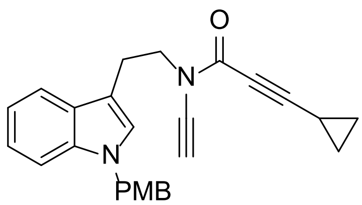
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-cyclopropyl-*N*-ethynylpropiolamide (1b)**



1b

Brown oil in 45% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.55 (d, J = 7.8 Hz, 1H), 7.38 (dd, J = 7.9, 4.0 Hz, 1H), 7.32 (s, 1H), 7.29 – 7.26 (m, 2H), 7.22 (t, J = 7.3 Hz, 1H), 7.15 (d, J = 7.3 Hz, 2H), 7.09 (dd, J = 13.5, 6.5 Hz, 1H), 7.03 (dt, J = 14.7, 7.5 Hz, 1H), 5.36 (s, 2H), 4.10 (s, 1H), 3.74 (t, J = 7.4 Hz, 2H), 2.99 (t, J = 7.3 Hz, 2H), 1.59 – 1.54 (m, 1H), 1.01 – 0.97 (m, 2H), 0.81 (dt, J = 6.8, 3.9 Hz, 2H); (minor rotamer) δ 7.59 (d, J = 7.8 Hz, 1H), 7.38 (dd, J = 7.9, 4.0 Hz, 1H), 7.29 (s, 1H), 7.29 – 7.26 (m, 2H), 7.22 (t, J = 7.3 Hz, 1H), 7.15 (d, J = 7.3 Hz, 2H), 7.09 (dd, J = 13.5, 6.5 Hz, 1H), 7.03 (dt, J = 14.7, 7.5 Hz, 1H), 5.38 (s, 2H), 4.11 (s, 1H), 3.91 (t, J = 6.7 Hz, 2H), 3.08 (t, J = 6.7 Hz, 2H), 1.29 – 1.25 (m, 1H), 0.80 – 0.76 (m, 2H), 0.50 – 0.45 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.4, 153.7, 138.3, 138.3, 136.0, 136.0, 128.49, 128.46, 127.8, 127.7, 127.5, 127.2, 127.22, 127.1, 126.9, 126.8, 121.4, 118.8, 118.8, 118.4, 118.3, 110.2, 110.2, 110.0, 109.7, 100.0, 98.2, 76.9, 75.5, 68.7, 67.5, 65.6, 63.4, 51.5, 48.9, 48.2, 47.1, 23.5, 22.6, 9.3, 9.0, -0.9, -1.1; IR (thin film, cm^{-1}): 3438, 3254, 3082, 3040, 2989, 2953, 2225, 1650, 1466, 1364; HRMS (ESI): m/z Calcd. for $C_{25}H_{22}N_2ONa$ $[M+Na]^+$ 389.1624, Found 389.1632.

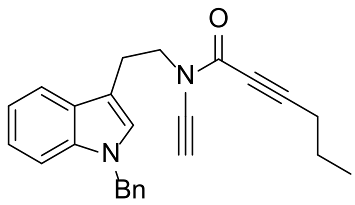
3-Cyclopropyl-*N*-ethynyl-*N*-(2-(1-(4-methoxybenzyl)-1*H*-indol-3-yl)ethyl) propiolamide (1c)



1c

Brown oil in 30% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.53 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.30 (s, 1H), 7.13 (d, J = 8.6 Hz, 2H), 7.09 (dd, J = 13.7, 6.6 Hz, 1H), 7.01 (dt, J = 14.8, 7.6 Hz, 1H), 6.84 (d, J = 8.6 Hz, 2H), 5.27 (s, 2H), 4.11 (s, 1H), 3.73 (t, J = 7.4 Hz, 2H), 3.69 (s, 3H), 2.97 (t, J = 7.4 Hz, 2H), 1.60 – 1.555 (m, 1H), 0.99 (td, J = 6.9, 4.0 Hz, 2H), 0.81 (dt, J = 7.0, 4.0 Hz, 2H); (minor rotamer) δ 7.57 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.27 (s, 1H), 7.13 (d, J = 8.6 Hz, 1H), 7.09 (dd, J = 13.7, 6.6 Hz, 1H), 7.01 (dt, J = 14.8, 7.6 Hz, 2H), 6.84 (d, J = 8.6 Hz, 2H), 5.29 (s, 2H), 4.11 (s, 1H), 3.90 (t, J = 6.8 Hz, 3H), 3.71 (s, 3H), 3.06 (t, J = 6.8 Hz, 2H), 1.32 – 1.27 (m, 1H), 0.81 (dt, J = 7.0, 4.0 Hz, 2H), 0.50 (dt, J = 6.6, 4.0 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 158.5, 154.4, 153.6, 136.0, 135.9, 130.2, 130.1, 129.5, 128.0, 128.3, 127.7, 127.6, 127.2, 126.8, 121.6, 118.7, 118.6, 118.5, 118.2, 113.8, 113.82, 110.3, 110.2, 109.8, 109.6, 100.8, 98.2, 76.8, 75.5, 68.7, 67.4, 65.6, 63.5, 55.03, 51.6, 48.5, 48.4, 47.0, 23.5, 22.6, 9.2, 9.0, -0.9, -1.1; IR (thin film, cm^{-1}): 3437, 3321, 2987, 2890, 2835, 1685, 1611, 1464; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{25}N_2O_2$ $[M+H]^+$ 397.1911, Found 397.1901.

***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-*N*-ethynylhex-2-ynamide (1d)**

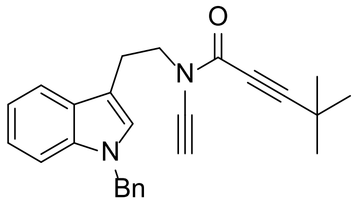


1d

Brown oil in 58% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.57 (d, J = 7.8 Hz, 1H), 7.38 (t, J = 8.6 Hz, 1H), 7.33 (s, 1H), 7.27 (d, J = 7.6 Hz, 2H), 7.22 (t, J = 7.2 Hz, 1H), 7.15 (d, J = 7.2 Hz, 2H), 7.09 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 7.4 Hz, 1H), 5.36 (s, 2H), 4.12 (s, 1H), 3.77 (t, J = 7.4 Hz, 2H), 3.01 (t, J = 7.3 Hz, 2H), 2.41 (t, J = 6.8 Hz, 2H), 1.56 – 1.48 (m, 2H), 0.97 (t, J = 7.4 Hz, 3H); (minor rotamer) δ 7.59 (d, J = 7.9 Hz, 1H), 7.38 (t, J = 8.6 Hz, 1H), 7.29 (s, 1H), 7.27 (d, J = 7.6 Hz, 2H), 7.22 (t, J = 7.2 Hz, 1H), 7.15 (d, J = 7.2 Hz, 6H), 7.09 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 7.4 Hz, 1H), 5.37 (s, 2H), 4.12 (s, 1H), 3.96 (t, J = 6.6 Hz, 2H), 3.09 (t, J = 6.6 Hz, 2H), 1.98 (t, J = 7.0 Hz, 2H), 1.23 (dq, J = 14.3, 7.2 Hz, 2H), 0.76 (t, J = 7.3

Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.9, 154.3, 138.8, 138.7, 136.6, 136.5, 128.9, 128.9, 128.3, 128.1, 128.0, 127.8, 127.7, 127.5, 127.4, 127.3, 121.8, 121.8, 119.2, 119.2, 118.9, 118.8, 110.7, 110.6, 110.4, 110.1, 97.7, 95.2, 77.3, 75.9, 74.3, 72.8, 66.0, 64.0, 52.0, 49.4, 47.7, 24.0, 23.1, 21.1, 20.9, 20.4, 20.1, 13.7; IR (thin film, cm^{-1}): 3435, 2986, 2960, 2932, 1721, 1652, 1627, 1463, 1529, 1173, 1003; HRMS (ESI): *m/z* Calcd. for $C_{25}H_{25}N_2O$ $[M+H]^+$ 369.1961, Found 369.1969.

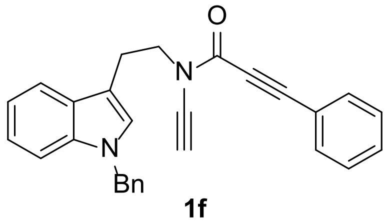
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-*N*-ethynyl-4,4-dimethylpent-2-ynamide (1e)**



1e

Brown oil in 71% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^1H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.56 (d, *J* = 7.9 Hz, 1H), 7.38 (t, *J* = 9.1 Hz, 1H), 7.34 (s, 1H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.15 (d, *J* = 7.2 Hz, 2H), 7.11 – 7.07 (m, 1H), 7.04 – 7.00 (m, 1H), 5.36 (s, 2H), 4.13 (s, 1H), 3.76 (t, *J* = 7.5 Hz, 2H), 3.01 (t, *J* = 7.4 Hz, 2H), 1.25 (s, 9H); (minor rotamer) δ 7.60 (d, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 9.1 Hz, 1H), 7.29 (s, 1H), 7.26 (d, *J* = 3.4 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.13 (d, *J* = 7.2 Hz, 2H), 7.11 – 7.06 (m, 1H), 7.04 – 7.00 (m, 1H), 5.38 (s, 2H), 4.14 (s, 1H), 3.94 (t, *J* = 6.7 Hz, 2H), 3.10 (t, *J* = 6.6 Hz, 2H), 0.96 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.5, 153.9, 138.3, 138.2, 136.1, 136.0, 128.5, 128.4, 127.7, 127.6, 127.4, 127.2, 127.2, 127.0, 126.9, 126.8, 121.4, 118.7, 118.4, 118.4, 110.2, 110.1, 109.9, 109.6, 103.7, 101.0, 76.8, 75.3, 72.2, 70.8, 65.7, 63.6, 51.6, 48.9, 47.1, 29.4, 29.1, 27.6, 27.2, 23.2, 22.6; IR (thin film, cm^{-1}): 3435, 3058, 2969, 2927, 2866, 2222, 1658, 1466, 1361, 1174; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{26}N_2ONa$ $[M+Na]^+$ 383.2118, Found 383.2110.

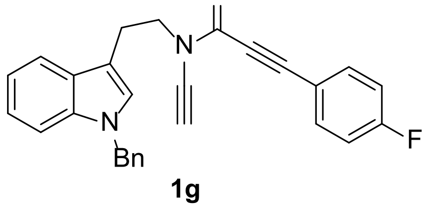
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-*N*-ethynyl-3-phenylpropiolamide (1f)**



1f

Brown oil in 84% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.60 (dd, *J* = 8.5, 7.2 Hz, 2H), 7.57 (dt, *J* = 2.6, 1.6 Hz, 1H), 7.49 (dd, *J* = 10.5, 4.6 Hz, 2H), 7.39 (t, *J* = 5.7 Hz, 1H), 7.36 (s, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.19 (dd, *J* = 9.6, 5.2 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 2H), 7.11 – 7.08 (m, 1H), 7.05 – 7.01 (m, 1H), 5.37 (s, 2H), 4.25 (s, 1H), 3.84 (t, *J* = 7.4 Hz, 2H), 3.07 (t, *J* = 7.4 Hz, 2H); (minor rotamer) δ 7.60 (dd, *J* = 8.5, 7.2 Hz, 2H), 7.49 (dd, *J* = 10.5, 4.6 Hz, 1H), 7.39 (t, *J* = 5.7 Hz, 1H), 7.35 (s, 1H), 7.28 – 7.24 (m, 2H), 7.23 (d, *J* = 1.1 Hz, 1H), 7.19 (dd, *J* = 9.6, 5.2 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.11 – 7.08 (m, 2H), 7.05 – 7.01 (m, 1H), 6.89 (t, *J* = 7.3 Hz, 1H), 5.34 (s, 2H), 4.21 (s, 1H), 4.07 (t, *J* = 6.6 Hz, 2H), 3.16 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.5, 153.8, 138.3, 138.2, 136.1, 136.1, 132.5, 132.3, 131.2, 131.0, 129.1, 128.8, 128.5, 128.4, 127.7, 127.7, 127.6, 127.2, 127.1, 126.9, 126.7, 121.4, 121.3, 118.8, 118.8, 118.5, 118.4, 110.2, 110.2, 109.9, 109.7, 92.9, 90.3, 81.2, 79.7, 76.6, 75.4, 66.0, 64.2, 54.9, 52.0, 48.9, 47.3, 23.4, 22.6; IR (thin film, cm^{-1}): 3439, 2985, 2926, 2854, 1721, 1629, 1607, 1488, 1463, 1384; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{22}N_2ONa$ $[M+Na]^+$ 425.1624, Found 425.1626.

***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-*N*-ethynyl-3-(4-fluorophenyl)propiolamide (1g)**

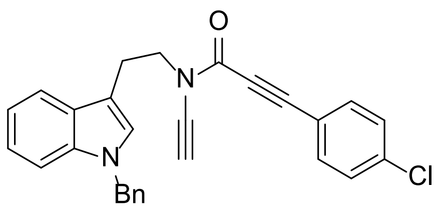


1g

Brown oil in 42% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.70 – 7.65 (m, 2H), 7.60 (t, *J* = 8.8 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.37 – 7.33

(m, 2H), 7.28 – 7.23 (m, 2H), 7.20 (dd, J = 12.0, 5.4 Hz, 2H), 7.15 (d, J = 7.2 Hz, 2H), 7.11 – 7.08 (m, 1H), 7.03 (t, J = 7.1 Hz, 1H), 5.37 (s, 2H), 4.25 (s, 1H), 3.84 (t, J = 7.3 Hz, 2H), 3.07 (t, J = 7.3 Hz, 2H); (minor rotamer) δ 7.60 (t, J = 8.8 Hz, 1H), 7.37 – 7.33 (m, 2H), 7.32 – 7.29 (m, 2H), 7.28 – 7.23 (m, 2H), 7.20 (dd, J = 12.0, 5.4 Hz, 2H), 7.18 (d, J = 1.5 Hz, 1H), 7.11 – 7.08 (m, 2H), 7.03 (t, J = 7.1 Hz, 1H), 6.90 (t, J = 7.4 Hz, 1H), 5.34 (s, 2H), 4.21 (s, 1H), 4.06 (t, J = 6.4 Hz, 2H), 3.15 (t, J = 6.4 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 164.3, 164.1, 162.7, 162.4, 154.4, 153.7, 138.3, 138.2, 136.1, 136.0, 135.2, 135.2, 135.0, 135.0, 128.4, 128.3, 127.8, 127.7, 127.63, 127.2, 127.1, 127.1, 126.9, 126.7, 121.39, 121.37, 118.83, 118.80, 118.43, 118.41, 116.7, 116.5, 116.2, 116.1, 115.34, 115.32, 115.01, 114.99, 110.22, 110.19, 109.9, 109.8, 92.0, 89.4, 81.1, 79.6, 76.6, 75.3, 66.0, 64.2, 52.0, 48.9, 47.3, 23.34, 22.6; IR (thin film, cm^{-1}): 3437, 2983, 2214, 2136, 1598, 1492, 1665, 1384, 1054; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{22}FN_2O$ [M+H]$^+$ 421.1711, Found 421.1720.

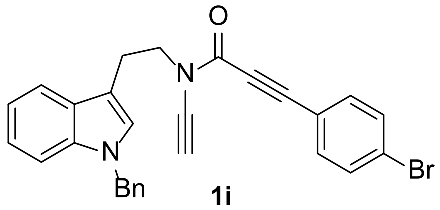
***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-(4-chlorophenyl)-*N*-ethynylpropiolamide (1h)**



1h

Red solid in 45% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); Mp 110.5 – 112.3 °C; The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.64 – 7.60 (m, 2H), 7.60 – 7.56 (m, 2H), 7.39 (d, J = 8.2 Hz, 1H), 7.36 (s, 1H), 7.26 (t, J = 7.5 Hz, 2H), 7.22 – 7.14 (m, 4H), 7.11 – 7.07 (m, 1H), 7.03 (t, J = 7.4 Hz, 1H), 5.37 (s, 2H), 4.25 (s, 1H), 3.84 (t, J = 7.3 Hz, 2H), 3.06 (t, J = 7.3 Hz, 2H); (minor rotamer) δ 7.60 – 7.56 (m, 2H), 7.41 (d, J = 8.5 Hz, 2H), 7.30 (d, J = 7.7 Hz, 2H), 7.22 – 7.13 (m, 4H), 7.11 – 7.07 (m, 2H), 7.03 (t, J = 7.4 Hz, 1H), 6.90 (t, J = 7.4 Hz, 1H), 5.34 (s, 2H), 4.22 (s, 1H), 4.05 (t, J = 6.4 Hz, 2H), 3.15 (t, J = 6.4 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.3, 153.6, 138.3, 138.2, 136.2, 136.1, 136.1, 135.8, 134.2, 134.0, 129.4, 128.9, 128.5, 128.4, 127.8, 127.6, 127.2, 127.1, 126.9, 126.7, 121.4, 121.4, 118.8, 118.8, 118.4, 118.4, 117.7, 117.4, 110.3, 110., 109.9, 109.8, 91.6, 89.0, 82.0, 80.5, 76.5, 75.3, 66.1, 64.3, 52.0, 48.9, 47.3, 23.3, 22.3; IR (thin film, cm^{-1}): 3442, 2988, 2225, 1639, 1523, 1468, 1441, 1273; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{21}ClN_2ONa$ $[M+Na]^+$ 459.1235, Found 459.1247.

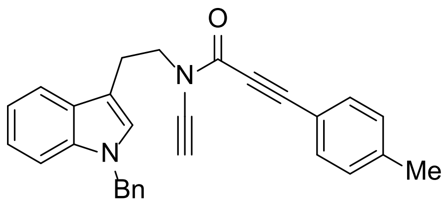
N-(2-(1-Benzyl-1H-indol-3-yl)ethyl)-3-(4-bromophenyl)-N-ethynylpropiolamide (1i)



1i

Brown oil in 42% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.71 (d, J = 8.1 Hz, 1H), 7.59 (t, J = 7.7 Hz, 1H), 7.54 (t, J = 6.7 Hz, 2H), 7.39 (d, J = 8.1 Hz, 1H), 7.36 (s, 1H), 7.30 (d, J = 4.7 Hz, 1H), 7.26 (t, J = 7.3 Hz, 2H), 7.20 (d, J = 7.0 Hz, 1H), 7.15 (d, J = 7.4 Hz, 2H), 7.11 – 7.06 (m, 1H), 7.03 (t, J = 7.2 Hz, 1H), 5.37 (s, 2H), 4.25 (s, 1H), 3.84 (t, J = 7.1 Hz, 2H), 3.06 (t, J = 7.1 Hz, 2H); (minor rotamer) δ 7.71 (d, J = 8.1 Hz, 2H), 7.59 (t, J = 7.7 Hz, 1H), 7.54 (t, J = 6.7 Hz, 1H), 7.20 (d, J = 7.0 Hz, 4H), 7.11 – 7.06 (m, 4H), 7.03 (t, J = 7.2 Hz, 1H), 6.90 (t, J = 7.3 Hz, 1H), 5.33 (s, 2H), 4.22 (s, 1H), 4.05 (t, J = 5.7 Hz, 2H), 3.15 (t, J = 5.7 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.4, 153.6, 138.3, 138.2, 136.1, 136.1, 134.3, 134.1, 132.3, 131.8, 128.5, 128.4, 127.8, 127.7, 127.2, 127.1, 126.9, 126.7, 125.1, 124.8, 121.4, 118.9, 118.8, 118.4, 118.4, 118.0, 117.7, 110.3, 110.2, 109.9, 109.8, 91.70, 89.2, 82.1, 80.6, 76.5, 75.3, 66.1, 64.3, 52.0, 48.9, 47.4, 23.4, 22.6; IR (thin film, cm^{-1}): 3425, 3295, 3027, 2922, 2852, 1731, 1614, 1466; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{21}BrN_2ONa$ $[M+Na]^+$ 503.0729, Found 503.0720.

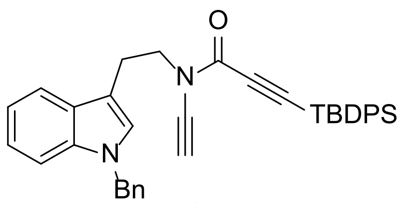
N-(2-(1-Benzyl-1H-indol-3-yl)ethyl)-N-ethynyl-3-(p-tolyl)propiolamide (1j)



1j

Brown oil in 40% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 2.5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.59 (d, *J* = 7.8 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.36 (s, 1H), 7.31 (dd, *J* = 13.9, 7.2 Hz, 2H), 7.26 (t, *J* = 7.5 Hz, 2H), 7.19 (t, *J* = 8.4 Hz, 2H), 7.15 (t, *J* = 7.5 Hz, 2H), 7.09 (dd, *J* = 9.2, 5.1 Hz, 1H), 7.03 (t, *J* = 7.3 Hz, 1H), 5.37 (s, 2H), 4.24 (s, 1H), 3.84 (t, *J* = 7.3 Hz, 2H), 3.06 (t, *J* = 7.3 Hz, 2H), 2.36 (s, 3H); (minor rotamer) δ 7.62 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.31 (dd, *J* = 13.9, 7.2 Hz, 2H), 7.21 (s, 1H), 7.19 (t, *J* = 8.4 Hz, 2H), 7.15 (t, *J* = 7.5 Hz, 2H), 7.09 (dd, *J* = 9.2, 5.1 Hz, 2H), 7.06 (d, *J* = 7.5 Hz, 1H), 6.92 (t, *J* = 7.4 Hz, 1H), 5.34 (s, 2H), 4.19 (s, 1H), 4.06 (t, *J* = 6.6 Hz, 2H), 3.16 (t, *J* = 6.6 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.6, 153.9, 141.6, 141.3, 138.3, 138.2, 136.1, 136.1, 132.5, 132.4, 129.8, 129.4, 128.5, 128.4, 127.7, 127.6, 127.5, 127.2, 127.1, 127.1, 126.9, 126.2, 121.3, 118.81, 118.79, 118.4, 115.7, 115.4, 110.2, 110.1, 109.9, 109.8, 93.5, 90.8, 80.9, 79.5, 76.7, 75.4, 65.9, 64.1, 51.9, 48.9, 47.2, 23.4, 22.6, 21.2, 21.2; IR (thin film, cm^{-1}): 3442, 3295, 2988, 2933, 2860, 2824, 1630, 1490, 1384; HRMS (ESI): *m/z* Calcd. for $C_{29}H_{24}N_2ONa$ $[M+Na]^+$ 439.1781, Found 439.1782.

***N*-(2-(1-Benzyl-1*H*-indol-3-yl)ethyl)-3-(*tert*-butyldiphenylsilyl)-*N*-ethynyl propiolamide (1k)**

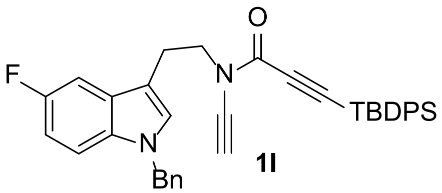


1k

Brown oil in 65% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 5:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.76 (d, *J* = 6.7 Hz, 4H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.48 (dt, *J* = 14.1, 6.9 Hz, 5H), 7.40

– 7.37 (m, 2H), 7.36 (s, 1H), 7.24 (t, *J* = 7.5 Hz, 2H), 7.15 (t, *J* = 8.7 Hz, 3H), 7.08 (dd, *J* = 13.5, 5.9 Hz, 1H), 7.02 (dd, *J* = 13.2, 5.6 Hz, 1H), 5.36 (s, 2H), 4.35 (s, 1H), 3.84 (t, *J* = 7.3 Hz, 2H), 3.08 (t, *J* = 7.3 Hz, 2H), 1.06 (s, 9H); (minor rotamer) δ 7.76 (d, *J* = 6.7 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 4H), 7.48 (dt, *J* = 14.1, 6.9 Hz, 6H), 7.40 – 7.37 (m, 1H), 7.36 (s, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.15 (t, *J* = 8.7 Hz, 2H), 7.08 (dd, *J* = 13.5, 5.9 Hz, 2H), 7.02 (dd, *J* = 13.2, 5.6 Hz, 1H), 6.83 (t, *J* = 7.5 Hz, 1H), 5.28 (s, 2H), 4.28 (s, 1H), 4.12 (t, *J* = 7.2 Hz, 2H), 3.19 (t, *J* = 7.2 Hz, 2H), 0.92 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 153.5, 152.9, 138.3, 138.1, 136.3, 136.0, 135.1, 135.0, 134.5, 130.7, 130.4, 130.3, 129.7, 129.2, 128.6, 128.4, 128.3, 128.3, 127.9, 127.7, 127.5, 127.5, 127.2, 127.08, 126.9, 126.8, 126.7, 121.4, 121.3, 118.8, 118.4, 118.3, 110.2, 110.1, 110.0, 109.6, 98.9, 97.8, 96.2, 93.1, 76.5, 74.8, 66.8, 64.3, 51.8, 48.9, 48.9, 47.7, 26.7, 26.5, 26.5, 23.5, 22.5, 22.4, 18.2, 18.1. IR (thin film, cm^{-1}): 3437, 3315, 2930, 1886, 1663, 1720, 1487, 1361; HRMS (ESI): *m/z* Calcd. for $C_{38}H_{37}N_2OSi$ $[M+H]^+$ 565.2670, Found 565.2668.

***N*-(2-(1-benzyl-5-fluoro-1*H*-indol-3-yl)ethyl)-3-(*tert*-butyldiphenylsilyl)-*N*-ethynyl propiolamide (1l)**

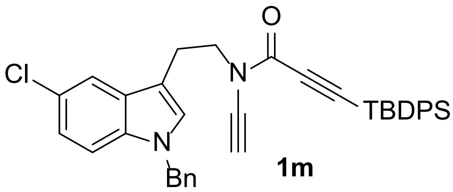


1l

Yellow oil in 39% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:18); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.75 (dd, *J* = 7.8, 1.4 Hz, 4H), 7.56 – 7.39 (m, 7H), 7.41 – 7.34 (m, 3H), 7.32 – 7.19 (m, 2H), 7.15 (dd, *J* = 14.4, 7.3 Hz, 4H), 6.93 (td, *J* = 9.2, 2.4 Hz, 1H), 5.36 (s, 2H), 4.33 (s, 1H), 3.83 (t, *J* = 7.2 Hz, 2H), 3.05 (t, *J* = 7.1 Hz, 2H), 1.05 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 157.8, 157.7, 156.3, 156.2, 153.5, 152.8, 138.0, 137.9, 135.1, 135.0, 134.98 134.4, 132.7, 132.7, 130.6, 130.4, 130.3, 129.1, 128.5, 128.4, 128.3, 128.2, 128.0, 127.9, 127.4, 127.2, 126.8, 126.7, 126.59 126.3, 125.58, 125.1, 125.0, 111.3, 111.2, 110.2, 110.1, 109.5, 109.3, 108.5, 108.5, 107.9, 107.7, 103.3, 103.2, 101.6, 101.5, 98.8, 97.1, 93.1, 76.5, 74.9, 73.1, 65.2, 64.30 62.6, 50.0, 49.1, 47.6, 45.9, 38.4, 24.9, 24.9, 21.3, 20.1, 16.5, 16.3; IR (thin film, cm^{-1}):

3432, 2985, 2935, 2925, 1856, 1720, 1487, 1465, 1361, 1105; HRMS (ESI): *m/z* Calcd. for $C_{38}H_{36}FN_2OSi$ $[M+H]^+$ 583.2575, Found 583.2575.

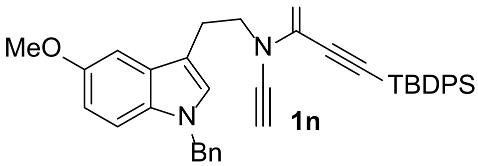
***N*-(2-(1-benzyl-5-chloro-1*H*-indol-3-yl)ethyl)-3-(*tert*-butyldiphenylsilyl)-*N*-ethynylpropiolamide (1m)**



1m

Yellow oil in 38% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:18); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.78 – 7.72 (m, 4H), 7.66 (d, *J* = 1.5 Hz, 1H), 7.52 – 7.43 (m, 7H), 7.41 (d, *J* = 8.7 Hz, 1H), 7.39 – 7.34 (m, 2H), 7.23 (t, *J* = 7.7 Hz, 1H), 7.16 (d, *J* = 7.3 Hz, 2H), 7.12 (d, *J* = 7.2 Hz, 1H), 7.09 (dd, *J* = 8.7, 2.0 Hz, 1H), 5.37 (s, 2H), 4.33 (s, 1H), 3.82 (t, *J* = 7.2 Hz, 2H), 3.06 (t, *J* = 7.1 Hz, 2H), 1.05 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 153.5, 152.8, 137.9, 137.8, 135.1, 134.9, 134.5, 134.4, 130.6, 130.4, 130.3, 128.9, 128.8, 128.5, 128.4, 128.5, 127.5, 127.2, 126.7, 126.7, 123.9, 123.7, 121.4, 121.3, 117.8, 111.8, 111.7, 109.9, 109.6, 98.8, 97.8, 96.3, 93.1, 76.3, 74.7, 66.9, 64.2, 51.7, 49.1, 47.6, 26.6, 26.4, 23.1, 22.2, 18.2, 17.9; IR (thin film, cm^{-1}): 3675, 2930, 2858, 2140, 1731, 1660, 1520, 1471, 1390, 1369, 1273, 1082; HRMS (ESI): *m/z* Calcd. for $C_{38}H_{36}ClN_2OSi$ $[M+H]^+$ 599.2280, Found 559.2281.

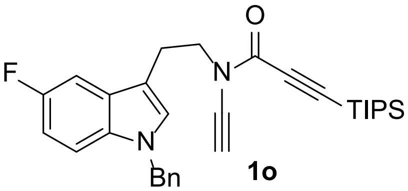
***N*-(2-(1-benzyl-5-methoxy-1*H*-indol-3-yl)ethyl)-3-(*tert*-butyldiphenylsilyl)-*N*-ethynylpropiolamide (1n)**



1n

Yellow oil in 49% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:22); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 – 7.71 (m, 4H), 7.54 – 7.43 (m, 7H), 7.31 (s, 1H), 7.27 – 7.21 (m, 3H), 7.16 (dt, *J* = 14.7, 7.4 Hz, 2H), 7.14 – 7.07 (m, 3H), 6.73 (dd, *J* = 8.9, 2.4 Hz, 1H), 5.31 (s, 2H), 4.35 (s, 1H), 3.83 (t, *J* = 7.3 Hz, 2H), 3.73 (s, 3H), 3.04 (t, *J* = 7.2 Hz, 2H), 1.05 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.5, 153.4, 153.3, 152.8, 138.4, 138.2, 136.3, 135.1, 135.0, 134.4, 131.5, 131.2, 130.9, 130.6, 130.4, 130.3, 129.1, 128.4, 128.3, 128.2, 128.1, 127.5, 127.5, 127.1, 126.7, 126.7, 111.5, 111.4, 110.9, 110.8, 109.6, 109.3, 100.2, 98.9, 93.1, 76.6, 65.0, 64.3, 55.2, 55.1, 49.1, 49.0, 47.7, 40.0, 26.6, 26.5, 26.9, 22.4, 18.2, 18.0; IR (thin film, cm^{-1}): 3676, 2929, 2857, 2139, 1720, 1636, 1549, 1522, 1487, 1360, 1276, 1228, 1111; HRMS (ESI): *m/z* Calcd. for $C_{39}H_{39}N_2O_2Si$ $[M+H]^+$ 595.2775, Found 595.2775.

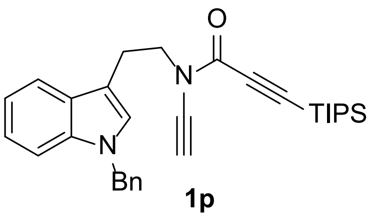
***N*-(2-(1-benzyl-5-fluoro-1*H*-indol-3-yl)ethyl)-*N*-ethynyl-3-(triisopropylsilyl)propiolamide (1o)**



1o

Brown oil in 40% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); ^1H NMR (600 MHz, DMSO-d_6) δ 7.40 (s, 1H), 7.37 (dd, *J* = 8.9, 4.4 Hz, 2H), 7.35 – 7.30 (m, 1H), 7.27 (q, *J* = 7.4 Hz, 3H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.16 – 7.12 (m, 2H), 6.92 (td, *J* = 9.2, 2.4 Hz, 1H), 5.36 (d, *J* = 4.3 Hz, 2H), 4.15 (s, 1H), 3.76 (t, *J* = 7.2 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 1.06 (d, *J* = 6.2 Hz, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 166.9, 157.7, 156.2, 153.0, 138.0, 132.7, 132.6, 131.7, 131.5, 129.0, 128.6, 128.4, 128.4, 128.0, 127.9, 127.2, 126.1, 126.7, 111.5, 111.4, 110.3, 110.1, 109.7, 109.5, 109.3, 103.3, 103.2, 103.1, 103.0, 98.1, 97.1, 96.0, 95.2, 76.5, 74.8, 66.6, 65.0, 63.9, 51.4, 49.1, 49.1, 48.5, 47.4, 30.0, 23.0, 22.3, 18.6, 18.2, 18.1, 18.1, 17.8, 17.4, 17.3, 13.5, 12.0, 10.3, 10.2; IR (thin film, cm^{-1}): 3676, 2944, 2865, 2140, 1723, 1665, 1625, 1580, 1487, 1357, 1167, 1071; HRMS (ESI): *m/z* Calcd. for $C_{31}H_{38}FN_2OSi$ $[M+H]^+$ 501.2732, Found 501.2733.

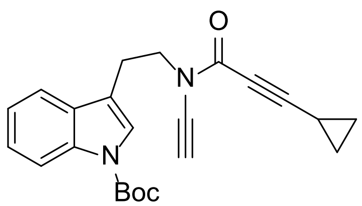
***N*-(2-(1-benzyl-1*H*-indol-3-yl)ethyl)-*N*-ethynyl-3-(triisopropylsilyl)propiolamide (1p)**



1p

Brown oil in 46% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.57 (d, *J* = 7.9 Hz, 1H), 7.41 – 7.35 (m, 1H), 7.33 (s, 1H), 7.27 (dt, *J* = 7.4, 2.5 Hz, 3H), 7.24 – 7.19 (m, 2H), 7.17 – 7.12 (m, 3H), 7.11 – 7.06 (m, 1H), 7.01 (dd, *J* = 11.0, 3.8 Hz, 1H), 5.36 (s, 2H), 4.16 (s, 1H), 3.77 (t, *J* = 7.4 Hz, 2H), 3.02 (t, *J* = 7.4 Hz, 2H), 1.07 (d, *J* = 6.2 Hz, 18H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 153.5, 153.0, 138.3, 138.2, 136.1, 136.0, 128.5, 128.4, 127.6, 127.4, 127.2, 127.0, 126.9, 126.8, 121.3, 118.7, 118.3, 118.2, 110.1, 110.0, 109.5, 98.2, 97.1, 96.7, 95.2, 76.5, 74.9, 66.5, 63.9, 51.8, 48.4, 47.4, 23.42 22.5, 18.2, 18.1, 17.8, 10.4, 10.2; IR (thin film, cm^{-1}): 3677, 2944, 2865, 2140, 1723, 1665, 1630, 1550, 1525, 1467, 1357, 1278, 1074; HRMS (ESI): *m/z* Calcd. for $C_{31}H_{39}N_2OSi$ $[M+H]^+$ 483.2826, Found 483.2825.

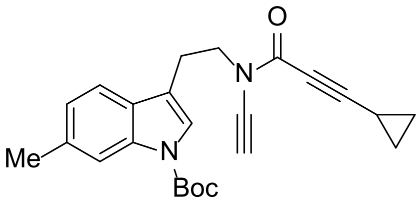
***tert*-Butyl 3-(2-(3-cyclopropyl-*N*-ethynylpropiolamido)ethyl)-1*H*-indole-1-carboxylate (1q)**



1q

Yellow oil in 44% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.52 (s, 1H), 7.33 (dd, *J* = 14.2, 6.9 Hz, 1H), 7.28 – 7.23 (m, 1H), 4.13 (s, 1H), 3.77 (t, *J* = 7.2 Hz, 2H), 2.97 (t, *J* = 7.2 Hz, 2H), 1.62 (s, 9H), 1.60 – 1.55 (m, 1H), 1.02 – 0.97 (m, 2H), 0.83 – 0.80 (m, 2H); (minor rotamer) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.51 (s, 1H), 7.33 (dd, *J* = 14.2, 6.9 Hz, 1H), 7.28 – 7.23 (m, 1H), 4.13 (s, 1H), 3.95 (t, *J* = 6.6 Hz, 2H), 3.05 (t, *J* = 6.6 Hz, 2H), 1.62 (s, 9H), 1.36 (dt, *J* = 8.4, 6.4 Hz, 1H), 0.90 – 0.86 (m, 2H), 0.61 (dd, *J* = 4.3, 2.5 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 167.0, 154.3, 153.7, 149.0, 134.7, 131.7, 131.5, 130.1, 130.0, 128.7, 124.5, 123.8, 123.4, 122.6, 119.0, 116.6, 116.5, 114.8, 114.8, 101.0, 98.5, 83.7, 83.6, 76.7, 75.3, 68.6, 67.4, 65.8, 65.0, 63.7, 54.9, 50.7, 46.1, 30.0, 27.7, 23.0, 22.2, 18.7, 13.6, 9.3, 9.1, -0.9, -1.0; IR (thin film, cm^{-1}): 3434, 3296, 3051, 2985, 2936, 1726, 1649, 1477, 1455, 1383, 1368; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{25}N_2O_3$ $[M+H]^+$ 399.1679, Found 399.1672.

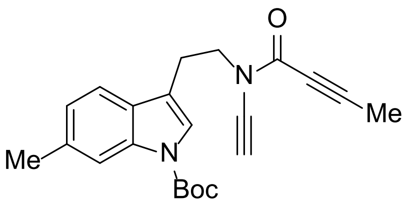
***tert*-Butyl 3-(2-(3-cyclopropyl-*N*-ethynylpropiolamido)ethyl)-6-methyl-1*H*-indole-1-carboxylate (1r)**



1r

Brown oil in 69% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 7.99 (s, 1H), 7.44 (t, *J* = 9.3 Hz, 1H), 7.34 (s, 1H), 7.08 (d, *J* = 7.7 Hz, 1H), 3.84 – 3.80 (m, 2H), 3.04 – 2.99 (m, 2H), 2.97 (s, 1H), 2.47 (s, 3H), 1.66 (s, 9H), 1.45 – 1.40 (m, 1H), 0.99 – 0.95 (m, 2H), 0.94 (s, 2H); (minor rotamer) δ 7.99 (s, 1H), 7.44 (t, *J* = 9.3 Hz, 1H), 7.34 (s, 1H), 7.08 (d, *J* = 7.7 Hz, 1H), 3.98 (t, *J* = 6.9 Hz, 2H), 3.11 (d, *J* = 9.9 Hz, 2H), 2.97 (s, 1H), 2.47 (s, 3H), 1.66 (s, 9H), 1.22 (s, 1H), 0.88 (s, 2H), 0.75 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.3, 154.8, 149.9, 136.1, 134.7, 134.7, 128.1, 124.1, 123.2, 122.8, 118.5, 118.2, 116.6, 116.1, 115.9, 115.7, 101.6, 98.9, 83.7, 83.4, 77.3, 75.1, 69.1, 67.9, 63.6, 60.9, 51.2, 47.2, 29.8, 28.3, 24.3, 23.2, 22.1, 9.6, 9.5, -0.1, -0.3; IR (thin film, cm^{-1}): 3435, 3329, 2982, 2926, 2854, 2223, 1730, 1630, 1619, 1487, 1454; HRMS (ESI): *m/z* Calcd. for $C_{24}H_{27}N_2O_3$ $[M+H]^+$ 391.2016, Found 391.2027.

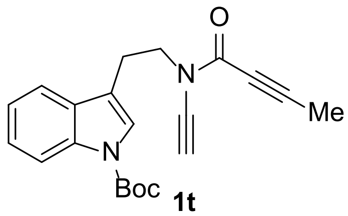
***tert*-Butyl 3-(2-(*N*-ethynylbut-2-ynamido)ethyl)-6-methyl-1*H*-indole-1-carboxylate (1s)**



1s

Brown oil in 53% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 7.99 (s, 1H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.35 (s, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 3.85 – 3.81 (m, 2H), 3.04 – 3.00 (m, 2H), 2.99(s, 1H), 2.47 (s, 3H), 2.05 (s, 3H), 1.65 (s, 9H); (minor rotamer) δ 7.99 (s, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.27 (s, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 4.02 (t, *J* = 7.1 Hz, 2H), 3.12 – 3.09 (m, 3H), 2.47 (s, 3H), 1.75 (s, 3H), 1.65 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.7, 155.4, 154.8, 149.9, 136.1, 134.7, 134.7, 128.1, 128.1, 124.1, 124.0, 123.9, 123.4, 122.8, 122.7, 118.7, 118.5, 118.1, 116.5, 116.0, 115.9, 115.7, 94.1, 91.2, 83.7, 83.5, 75.0, 73.1, 71.8, 66.1, 63.6, 61.0, 60.9, 51.2, 47.4, 28.3, 26.3, 24.3, 23.2, 22.1, 4.3, 4.0; IR (thin film, cm^{-1}): 3434, 3296, 2980, 2929, 2828, 2240, 1731, 1657, 1593, 1453, 1395, 1370; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{24}N_2O_3Na$ $[M+Na]^+$ 387.1679, Found 387.1677.

***tert*-Butyl 3-(2-(*N*-ethynylbut-2-ynamido)ethyl)-1*H*-indole-1-carboxylate (1t)**

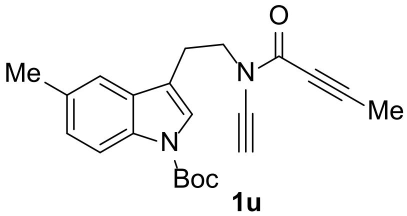


1t

Yellow solid in 68% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); Mp 118.6 – 120.3 °C; The ratio of major rotamer and minor rotamer is 3:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.04 (d, *J* = 7.8 Hz, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.52 (s, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.29 – 7.24 (m, 1H), 4.13 (s, 1H), 3.79 (t, *J* = 7.3 Hz, 2H), 2.98 (t, *J* = 7.3 Hz, 2H), 2.06 (s, 3H), 1.62 (s, 9H); (minor rotamer) δ 8.04 (d, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.51 (s, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.30 – 7.23 (m, 1H), 4.13 (s, 1H), 4.00 (t, *J* = 6.7 Hz, 1H), 3.07 (t, *J* = 6.7 Hz, 1H), 1.78 (s, 3H), 1.62 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.4, 153.8, 149.0, 134.7, 130.2, 123.0, 124.5, 123.9, 123.4, 122.6, 119.0, 119.0, 116.6, 116.3, 114.8, 94.1, 91.7, 83.7, 83.6, 76.6, 75.2, 72.8, 71.3, 65.7, 63.6, 54.9, 50.5, 46.3, 27.7, 23.2, 22.2, 3.4, 3.2; IR (thin film, cm^{-1}): 3438, 3296, 2987, 2920, 2869, 2835, 1750, 1690, 1629, 1606, 1489, 1455, 1384; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{22}N_2O_3Na$ $[M+Na]^+$ 373.1523, Found 373.1518.

***tert*-butyl 3-(2-(*N*-ethynylbut-2-ynamido)ethyl)-5-methyl-1*H*-indole-1-**

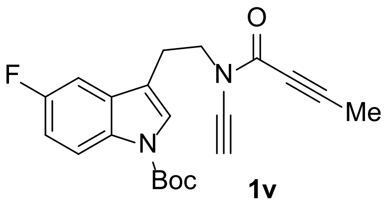
carboxylate (1u)



1u

Yellow oil in 62% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.90 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.34 (m, 2H), 7.14 (d, *J* = 8.2 Hz, 1H), 4.13 (s, 1H), 3.78 (t, *J* = 7.2 Hz, 2H), 2.95 (t, *J* = 7.1 Hz, 2H), 2.40 (s, 3H), 2.06 (s, 3H), 1.61 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.8, 154.2, 149.4, 133.4, 132.0, 130.8, 130.6, 126.1, 124.3, 123.8, 119.3, 119.2, 116.8, 116.4, 114.9, 114.9, 94.5, 92.0, 83.9, 83.8, 77.1, 75.6, 73.2, 71.7, 64.1, 50.8, 46.7, 28.1, 28.1, 22.6, 21.4, 3.8; IR (thin film, cm^{-1}): 3423, 2243, 1723, 1648, 1546, 1450, 1375, 1292, 1224, 1160, 1112; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{25}N_2O_3$ $[M+H]^+$ 365.1860, Found 365.1860.

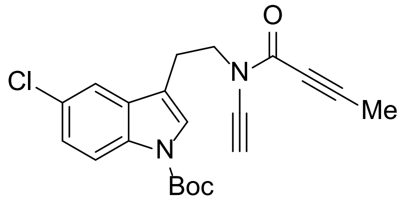
***tert*-butyl 3-(2-(*N*-ethynylbut-2-ynamido)ethyl)-5-fluoro-1*H*-indole-1-carboxylate (1v)**



1v

Yellow oil in 64% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.00 (d, *J* = 3.6 Hz, 1H), 7.57 (d, *J* = 5.5 Hz, 1H), 7.43 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.16 (td, *J* = 9.1, 2.6 Hz, 1H), 4.12 (s, 1H), 3.78 (t, *J* = 7.1 Hz, 2H), 2.95 (t, *J* = 7.0 Hz, 2H), 2.06 (s, 3H), 1.61 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ δ 159.3, 157.7, 154.3, 153.8, 148.7, 131.2, 131.1, 131.0, 125.7, 125.2, 116.5, 116.5, 116.2, 116.0, 115.9, 112.1, 111.9, 104.9, 104.8, 104.7, 104.6, 94.0, 91.7, 84.0, 83.9, 76.6, 75.1, 72.3, 71.3, 65.7, 63.6, 54.2, 50.9, 46.2, 27.6, 23.0, 22.1, 3.4, 3.1; IR (thin film, cm^{-1}): 3632, 2972, 2242, 2215, 2136, 1722, 1600, 1450, 1332, 1160, 1024; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{22}FN_2O_3$ $[M+H]^+$ 369.1609, Found 369.1609

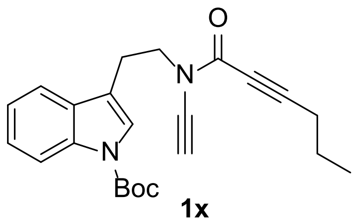
***tert*-Butyl 5-chloro-3-(2-(*N*-ethynylbut-2-ynamido)ethyl)-1*H*-indole-1-carboxylate (1w)**



1w

Yellow oil in 64% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3.3:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.04 (s, 1H), 7.54 (d, J = 1.7 Hz, 1H), 7.45 (s, 1H), 7.25 (d, J = 1.6 Hz, 1H), 3.85 – 3.80 (m, 2H), 3.00 (dd, J = 9.7, 5.6 Hz, 3H), 2.05 (s, 3H), 1.65 (s, 9H); (minor rotamer) δ 8.04 (s, 1H), 7.50 (s, 1H), 7.45 (s, 1H), 7.27 (s, 1H), 4.01 (t, J = 7.1 Hz, 2H), 3.11 – 3.07 (m, 3H), 1.82 (s, 3H), 1.65 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.2, 154.8, 149.4, 149.3, 134.0, 131.6, 128.4, 128.3, 125.7, 124.8, 124.7, 118.6, 118.3, 116.7, 116.4, 116.0, 115.1, 94.4, 91.4, 84.4, 84.1, 77.0, 74.7, 73.0, 71.7, 63.8, 61.2, 50.8, 47.2, 28.3, 24.1, 22.9, 4.2, 4.0; IR (thin film, cm^{-1}): 3439, 3316, 2977, 2931, 2860, 2237, 1727, 1658, 1628, 1492, 1475, 1450, 1369; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{22}ClN_2O_3$ $[M+H]^+$ 385.1313, Found 385.1318.

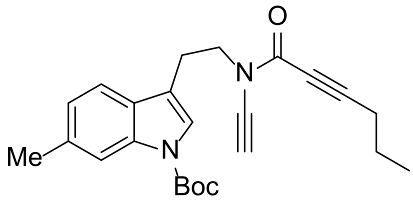
***tert*-Butyl 3-(2-(*N*-ethynylhex-2-ynamido)ethyl)-1*H*-indole-1-carboxylate (1x)**



1x

Yellow oil in 66% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3.7:1; ^{1}H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 8.13 (s, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.45 (s, 1H), 7.32 (t, J = 7.3 Hz, 1H), 7.27 – 7.23 (m, 1H), 3.88 – 3.83 (m, 2H), 3.08 – 3.04 (m, 2H), 2.98 (s, 1H), 2.38 (t, J = 7.0 Hz, 2H), 1.66 (s, 9H), 1.63 (dt, J = 14.4, 7.2 Hz, 2H), 1.04 (t, J = 7.4 Hz, 3H); (minor rotamer) δ 8.13 (s, 1H), 7.54 (d, J = 7.7 Hz, 1H), 7.45 (s, 1H), 7.32 (t, J = 7.3 Hz, 1H), 7.28 – 7.19 (m, 1H), 4.03 (t, J = 7.2 Hz, 2H), 3.14 (t, J = 7.2 Hz, 2H), 3.11 (s, 1H), 2.09 (t, J = 7.0 Hz, 2H), 1.66 (s, 9H), 1.45 (td, J = 14.5, 7.3 Hz, 2H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.4, 154.9, 149.8, 135.6, 130.4, 124.7, 124.6, 124.0, 123.5, 122.7, 122.6, 118.9, 118.6, 116.6, 116.1, 115.6, 115.4, 98.0, 95.2, 83.9, 83.6, 77.3, 75.0, 74.0, 72.5, 63.7, 61.0, 51.3, 47.3, 29.8, 28.3, 24.2, 23.2, 21.2, 21.1, 21.0, 20.8, 13.64 13.59; IR (thin film, cm^{-1}): 3436, 3291, 2961, 2928, 2870, 2835, 2222, 1727, 1657, 1610, 1476, 1451, 1369; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{27}N_2O_3$ $[M+H]^+$ 379.2016, Found 379.2021.

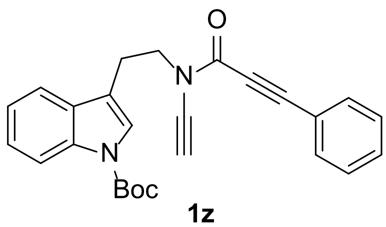
***tert*-Butyl 3-(2-(*N*-ethynylhex-2-ynamido)ethyl)-6-methyl-1*H*-indole-1-carboxylate (1y)**



1y

Yellow oil in 67% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3:1; ^1H NMR (600 MHz, $CDCl_3$) (major rotamer) δ 7.99 (s, 1H), 7.46 (d, J = 7.9 Hz, 1H), 7.35 (s, 1H), 7.08 (d, J = 7.6 Hz, 1H), 3.86 – 3.80 (m, 2H), 3.05 – 3.01 (m, 2H), 2.98 (s, 1H), 2.48 (s, 3H), 2.38 (t, J = 6.8 Hz, 2H), 1.66 (s, 9H), 1.64 – 1.61 (m, 2H), 1.04 (t, J = 7.3 Hz, 3H); (minor rotamer) δ 7.99 (s, 1H), 7.41 (d, J = 7.9 Hz, 1H), 7.35 (s, 1H), 7.08 (d, J = 7.6 Hz, 1H), 4.02 (t, J = 7.0 Hz, 2H), 3.13 – 3.09 (m, 2H), 2.48 (s, 3H), 2.10 (t, J = 6.8 Hz, 2H), 1.66 (s, 9H), 1.46 (dd, J = 14.5, 7.2 Hz, 2H), 0.92 (t, J = 7.3 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.4, 154.9, 149.8, 136.1, 134.7, 134.7, 128.1, 124.1, 124.0, 123.3, 122.8, 118.5, 118.2, 116.5, 116.1, 115.8, 115.7, 98.0, 95.1, 83.7, 83.4, 77.3, 75.0, 74.0, 72.5, 63.6, 61.0, 51.3, 47.3, 29.8, 28.3, 24.3, 23.2, 22.1, 21.2, 21.1, 21.0, 20.9, 14.3, 13.8, 13.6; IR (thin film, cm^{-1}): 3433, 3299, 2965, 2932, 2871, 2230, 1724, 1659, 1615, 1487, 1477, 1442, 1381; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{29}N_2O_3$ $[M+H]^+$ 393.2173, Found 393.2181.

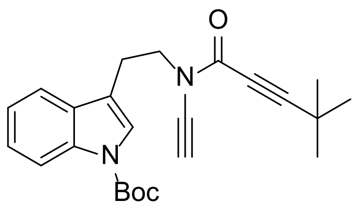
***tert*-Butyl 3-(2-(*N*-ethynyl-3-phenylpropiolamido)ethyl)-1*H*-indole-1-carboxylate (1z)**



1z

Yellow oil in 68% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.05 (d, *J* = 8.1 Hz, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.63 – 7.59 (m, 2H), 7.55 (d, *J* = 4.8 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.44 – 7.39 (m, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.26 (dd, *J* = 12.4, 5.2 Hz, 1H), 4.28 (s, 1H), 3.87 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 1.59 (s, 9H); (minor rotamer) δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 2H), 7.55 (d, *J* = 4.8 Hz, 2H), 7.52 (dd, *J* = 6.5, 2.2 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.26 (dd, *J* = 12.4, 5.2 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 4.23 (s, 1H), 4.11 (t, *J* = 6.6 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H), 1.55 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.3, 153.8, 149.0, 148.9, 134.8, 132.5, 132.4, 131.3, 131.2, 130.1, 123.0, 129.1, 128.9, 124.5, 124.4, 123.9, 123.5, 122.6, 122.5, 119.0, 118.8, 118.5, 116.5, 116.4, 114.8, 114.7, 93.1, 90.5, 83.6, 81.1, 79.7, 76.4, 75.1, 66.2, 64.3, 51.2, 46.4, 27.7, 27.6, 23.1, 22.2, 14.1; IR (thin film, cm^{-1}): 3434, 3305, 3054, 2978, 2932, 2213, 1727, 1659, 1627, 1490, 1451, 1368; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{24}N_2O_3Na$ $[M+Na]^+$ 435.1679, Found 435.1675.

***tert*-Butyl 3-(2-(*N*-ethynyl-4,4-dimethylpent-2-ynamido)ethyl)-1*H*-indole-1-carboxylate (1aa)**

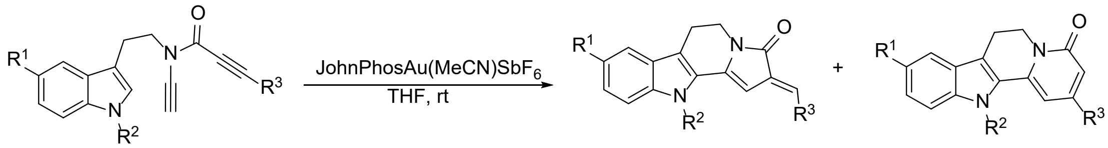


1aa

Brown oil in 62% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); The ratio of major rotamer and minor rotamer is 3:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 8.04 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.52 (s, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.25 (dd, *J* = 14.5, 7.3 Hz, 1H), 4.15 (s, 1H), 3.79 (t, *J* = 7.2 Hz, 2H), 2.98 (t, *J* = 7.2 Hz, 2H), 1.61 (s, 9H), 1.24 (s, 9H); (minor rotamer) δ 8.04 (d, *J* = 8.0 Hz, 1H), 7.62 (t,

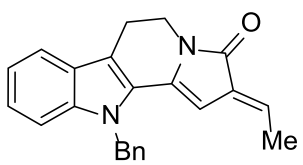
J = 7.7 Hz, 1H), 7.49 (s, 1H), 7.33 (t, J = 7.7 Hz, 1H), 7.25 (dd, J = 14.5, 7.3 Hz, 1H), 4.17 (s, 1H), 3.96 (t, J = 6.5 Hz, 2H), 3.07 (t, J = 6.5 Hz, 2H), 1.61 (s, 9H), 1.05 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.4, 153.9, 149.0, 134.7, 130.1, 123.0, 124.5, 124.5, 123.8, 123.4, 122.6, 119.0, 116.6, 116.6, 114.8, 103.8, 101.2, 83.6, 83.6, 76.6, 75.2, 72.1, 70.7, 65.9, 63.8, 54.9, 51.2, 46.1, 29.4, 29.2, 27.9, 27.5, 27.3, 22.8, 22.2, 18.7, 13.6; IR (thin film, cm^{-1}): 3437, 3296, 2971, 2930, 2867, 2223, 1730, 1664, 1629, 1453, 1369; HRMS (ESI): *m/z* Calcd. for $C_{24}H_{29}N_2O_3$ $[M+H]^+$ 393.2173, Found 393.2177.

9. The Procedures for the Prepartion of 2, 2a-2p, 3, 3a-3p on Condition C1 and Characterization Data



To a solution of compounds **1**, **1a-1p** (1 mmol) in anhydrous THF was added a solution of JohnPhosAu(MeCN)SbF_6 (0.08 mmol) in anhydrous THF (1 mL) under the N_2 atmosphere, and the mixture was stirred for about 15 min, until the total conversion of the reactant. Then mixture was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel.

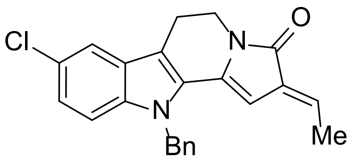
(*E*)-11-Benzyl-2-ethylidene-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2)



2

Brown oil in 50% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.65 (d, J = 7.9 Hz, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.29 (t, J = 7.6 Hz, 2H), 7.26 – 7.20 (m, 2H), 7.13 (t, J = 7.4 Hz, 1H), 7.07 (d, J = 7.4 Hz, 2H), 6.51 (q, J = 7.5 Hz, 1H), 6.18 (s, 1H), 5.69 (s, 2H), 3.75 (t, J = 6.3 Hz, 2H), 3.09 (t, J = 6.3 Hz, 2H), 1.95 (d, J = 7.6 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 166.4, 139.7, 138.5, 134.6, 133.3, 132.1, 129.1, 127.7, 126.6, 126.3, 125.7, 124.6, 120.6, 120.0, 115.0, 110.8, 94.2, 47.4, 37.2, 20.5, 15.8; IR (thin film, cm^{-1}): 3428, 2986, 2952, 1738, 1722, 1683, 1601, 1492, 1271; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{21}N_2O$ $[M+H]^+$ 341.1648, Found 341.1659.

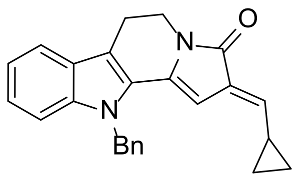
(*E*)-11-Benzyl-8-chloro-2-ethylidene-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*] indol-3-one (2a)



2a

Yellow solid in 46% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 202.4 – 204.2 °C; ^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 7.74 (d, *J* = 1.4 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.26 – 7.20 (m, 2H), 7.06 (d, *J* = 7.5 Hz, 2H), 6.54 (q, *J* = 7.6 Hz, 1H), 6.24 (s, 1H), 5.70 (s, 2H), 3.73 (t, *J* = 6.3 Hz, 2H), 3.07 (t, *J* = 6.3 Hz, 2H), 1.95 (d, *J* = 7.6 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-*d*$_6$) δ 165.8, 137.7, 137.6, 134.0, 132.6, 132.5, 128.7, 127.3, 126.30 126.1, 124.8, 123.8, 118.8, 114.0, 112.0, 94.6, 47.0, 36.6, 19.9, 15.4; IR (thin film, cm^{-1}): 3435, 2929, 2860, 2837, 1738, 1690, 1611, 1472, 1438, 1382; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{20}ClN_2O$ $[M+H]^+$ 375.1259 Found 375.1252.

(*E*)-11-Benzyl-2-(cyclopropylmethylene)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*] indol-3-one (2b)

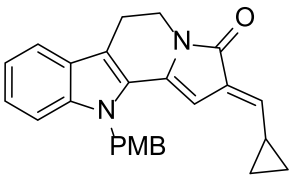


2b

Yellow oil in 48% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 7.64 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.22 (dd, *J* = 13.0, 7.0 Hz, 2H), 7.12 (t, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 7.4 Hz, 2H), 6.35 (s, 1H), 5.97 (d, *J* = 11.1 Hz, 1H), 5.69 (s, 2H), 3.75 (t, *J* = 6.3 Hz, 2H), 3.09 (t, *J* = 6.3 Hz, 2H), 1.92 – 1.85 (m, 1H), 1.07 – 1.01 (m, 2H), 0.80 – 0.77 (m, 2H); ^{13}C

NMR (150 MHz, DMSO-d_6) δ 165.8, 142.6, 139.0, 138.0, 131.9, 131.0, 128.7, 128.69, 127.2, 126.2, 126.1, 125.3, 123.9, 120.1, 119.5, 114.0, 110.3, 94.3, 46.9, 36.8, 20.1, 13.5, 9.8; IR (thin film, cm^{-1}): 3437, 2983, 2927, 2843, 1720, 1647, 1639, 1458, 1235, 1190, 1029; HRMS (ESI): *m/z* Calcd. for $C_{25}H_{23}N_2O$ $[M+H]^+$ 367.1805, Found 367.1810.

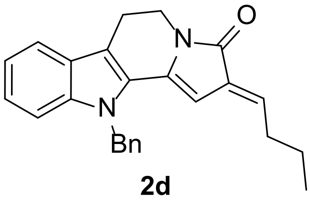
(*E*)-2-(Cyclopropylmethylene)-11-(4-methoxybenzyl)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2c)



2c

Green solid in 44% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 148.8 – 150.1 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.63 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.24 – 7.20 (m, 1H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.87 – 6.83 (m, 2H), 6.40 (s, 1H), 5.98 (d, *J* = 11.1 Hz, 1H), 5.61 (s, 2H), 3.74 (t, *J* = 6.3 Hz, 2H), 3.67 (s, 3H), 3.08 (t, *J* = 6.3 Hz, 2H), 1.95 – 1.90 (m, 1H), 1.05 (td, *J* = 6.6, 3.9 Hz, 2H), 0.81 – 0.77 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 165.7, 158.4, 142.5, 139.0, 131.9, 131.0, 129.8, 127.5, 126.0, 125.3, 123.8, 112.0, 119.4, 114.1, 114.1, 113.9, 110.4, 94.3, 55.0, 46.3, 36.7, 20.1, 13.6, 9.8; IR (thin film, cm^{-1}): 3430, 2987, 2927, 2872, 1731, 1687, 1633, 1610, 1512, 1461, 1396, 1350; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{25}N_2O_2$ $[M+H]^+$ 397.1911, Found 397.1900.

(*E*)-11-Benzyl-2-butylidene-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2d)

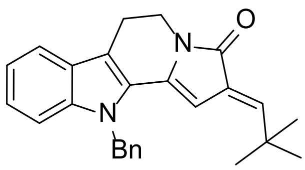


2d

Yellow oil in 62% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.65 (d, *J* = 7.9 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.26 – 7.23 (m, 1H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.12 (t, *J* = 7.3 Hz, 1H), 7.07 (d, *J*

= 7.3 Hz, 2H), 6.45 (t, J = 8.1 Hz, 1H), 6.14 (s, 1H), 5.68 (s, 2H), 3.75 (t, J = 6.3 Hz, 2H), 3.09 (t, J = 6.3 Hz, 2H), 2.29 (dd, J = 15.2, 7.4 Hz, 2H), 1.47 – 1.41 (m, 2H), 0.85 (t, J = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 166.0, 139.2, 138.0, 136.1, 133.6, 132.9, 128.6, 127.2, 126.2, 125.8, 125.2, 124.1, 120.1, 119.6, 114.6, 110.3, 94.0, 46.9, 36.72, 31.0, 21.6, 20.0, 13.6; IR (thin film, cm^{-1}): 2958, 2927, 2870, 2227, 1683, 1644, 1602, 1494, 1453, 1349; HRMS (ESI): *m/z* Calcd. for $C_{25}H_{25}N_2O$ [M+H]$^+$ 369.1961, Found 369.1975.

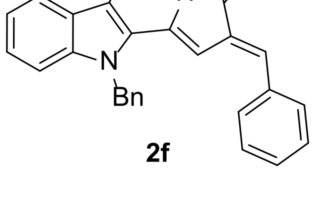
(*E*)-11-Benzyl-2-(2,2-dimethylpropylidene)-2,5,6,11-tetrahydro-3*H*-indolizino [8,7-*b*]indol-3-one (2e)



2e

Orange solid in 74% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 84.2 – 85.6 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.67 (d, J = 7.9 Hz, 1H), 7.62 (d, J = 8.4 Hz, 1H), 7.29 (dd, J = 16.5, 8.6 Hz, 3H), 7.23 (t, J = 7.4 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 7.03 (d, J = 7.5 Hz, 2H), 6.43 (s, 1H), 5.95 (s, 1H), 5.66 (s, 2H), 3.73 (t, J = 6.3 Hz, 2H), 3.09 (t, J = 6.3 Hz, 2H), 1.10 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 167.1, 145.7, 139.5, 138.0, 133.1, 129.5, 128.8, 127.2, 125.8, 125.8, 125.0, 124.3, 120.1, 119.6, 114.7, 110.1, 94.2, 54.9, 47.0, 36.8, 34.2, 29.8, 20.0; IR (thin film, cm^{-1}): 3427, 2956, 1675, 1630, 1601, 1461, 1384, 1174; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{26}N_2ONa$ [M+Na]$^+$ 405.1937, Found 405.1936.

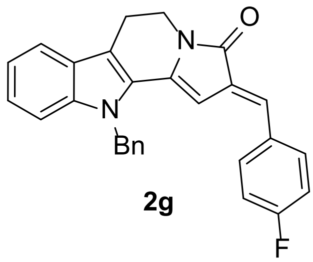
(*E*)-11-Benzyl-2-benzylidene-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2f)



2f

Yellow oil in 64% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.71 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 8.3 Hz, 1H), 7.54 (d, J = 7.6 Hz, 2H), 7.46 (t, J = 7.5 Hz, 2H), 7.40 (t, J = 7.3 Hz, 1H), 7.36 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.6 Hz, 1H), 7.25 (t, J = 7.4 Hz, 1H), 7.18 (d, J = 7.7 Hz, 1H), 7.16 (s, 1H), 7.12 (d, J = 7.8 Hz, 2H), 6.27 (s, 1H), 5.75 (s, 2H), 3.82 (t, J = 6.3 Hz, 2H), 3.16 (t, J = 6.3 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 167.5, 139.9, 138.2, 135.5, 135.4, 130.4, 130.0, 129.5, 129.4, 129.0, 128.8, 127.3, 125.9, 125.7, 125.0, 124.7, 120.3, 119.9, 115.8, 110.3, 94.7, 47.0, 36.9, 20.2; IR (thin film, cm^{-1}): 3424, 2946, 2928, 2836, 1678, 1493, 1452, 1370, 1295; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{23}N_2O$ [M+H]$^+$ 403.1805, Found 403.1799.

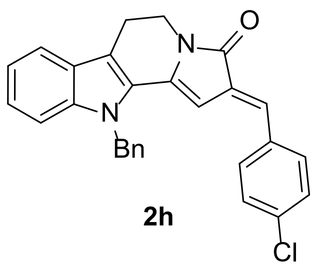
(*E*)-11-Benzyl-2-(4-fluorobenzylidene)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*] indol-3-one (2g)



2g

Red solid in 72% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 102.4 – 104.1 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.70 (d, J = 7.9 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.61 (dd, J = 8.5, 5.7 Hz, 2H), 7.36 (t, J = 7.7 Hz, 2H), 7.30 (dt, J = 11.4, 8.1 Hz, 3H), 7.24 (t, J = 7.4 Hz, 1H), 7.17 (d, J = 7.7 Hz, 1H), 7.16 (s, 1H), 7.11 (d, J = 7.7 Hz, 2H), 6.24 (s, 1H), 5.74 (s, 2H), 3.80 (t, J = 6.3 Hz, 2H), 3.14 (t, J = 6.2 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 167.5, 163.4, 161.7, 140.0, 138.3, 135.6, 132.3, 132.2, 132.12, 132.10, 130.2, 130.1, 128.9, 128.4, 127.4, 126.0, 125.7, 125.1, 124.8, 120.4, 119.9, 116.2, 116.1, 115.9, 110.3, 94.4, 47.1, 36.9, 20.2; IR (thin film, cm^{-1}): 3059, 2925, 2857, 1686, 1625, 1599, 1505, 1455, 1354; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{22}FN_2O$ [M+H]$^+$ 421.1711, Found 421.1707.

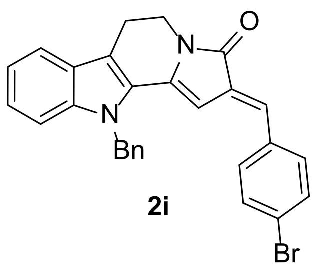
(*E*)-11-Benzyl-2-(4-chlorobenzylidene)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*] indol-3-one (2h)



2h

Brown oil in 78% yield; $R_f = 0.2$ (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.71 (d, J = 7.9 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.57 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.36 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.6 Hz, 1H), 7.25 (t, J = 7.3 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 7.14 (s, 1H), 7.11 (d, J = 7.6 Hz, 2H), 6.25 (s, 1H), 5.75 (s, 2H), 3.81 (t, J = 6.3 Hz, 2H), 3.15 (t, J = 6.3 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 167.4, 138.2, 135.9, 134.4, 133.9, 131.5, 130.9, 129.0, 128.9, 127.9, 127.3, 126.0, 125.6, 125.0, 124.8, 120.4, 119.9, 116.2, 110.4, 94.4, 54.9, 47.0, 36.9, 20.2; IR (thin film, cm^{-1}): 3439, 2954, 2927, 2888, 2852, 1630, 1488, 1457, 1385, 1003; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{22}ClN_2O$ [M+H]$^+$ 437.1415, Found 437.1411.

(*E*)-11-Benzyl-2-(4-bromobenzylidene)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*] indol-3-one (2i)

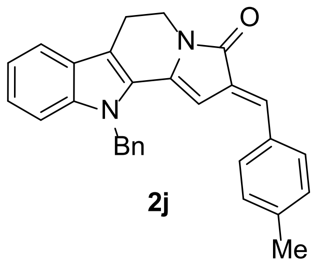


2i

Brown oil in 75% yield; $R_f = 0.2$ (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.71 (d, J = 7.9 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.64 (d, J = 8.3 Hz, 2H), 7.49 (d, J = 8.2 Hz, 2H), 7.36 (t, J = 7.5 Hz, 2H), 7.32 (t, J = 7.6 Hz, 1H), 7.25 (t, J = 7.3 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 7.11 (d, J = 5.0 Hz, 3H), 6.24 (s, 1H), 5.75 (s, 2H), 3.81 (t, J = 6.2 Hz, 2H), 3.15 (t, J = 6.2 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 167.5, 140.0, 138.2, 136.0, 134.7, 132.0, 131.8, 131.0, 128.9, 128.0, 127.3, 126.0, 125.6, 125.0, 124.8, 122.7, 120.3, 119.9, 116.2, 110.4, 94.4, 47.0, 36.9, 20.2; IR (thin film, cm^{-1}): 3413, 2951, 2926, 2842, 1649, 1587, 1486, 1452; HRMS

(ESI): m/z Calcd. for $C_{28}H_{22}BrN_2O$ $[M+H]^+$ 481.0910, Found 481.0913.

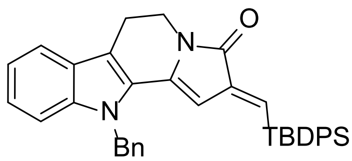
(*E*)-11-Benzyl-2-(4-methylbenzylidene)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*] indol-3-one (2j)



2j

Red solid in 65% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); Mp 102.9 – 104.2 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.70 (d, J = 7.9 Hz, 1H), 7.65 (d, J = 8.3 Hz, 1H), 7.43 (d, J = 7.9 Hz, 2H), 7.37 (t, J = 7.6 Hz, 2H), 7.31 (t, J = 7.6 Hz, 1H), 7.26 (t, J = 7.5 Hz, 3H), 7.17 (t, J = 7.4 Hz, 1H), 7.12 (d, J = 9.1 Hz, 3H), 6.25 (s, 1H), 5.74 (s, 2H), 3.80 (t, J = 6.3 Hz, 2H), 3.14 (t, J = 6.3 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 167.6, 139.9, 139.6, 138.3, 135.0, 132.7, 130.1, 129.8, 129.7, 129.6, 128.9, 127.3, 125.9, 125.8, 125.1, 124.6, 120.3, 119.8, 115.6, 110.2, 94.8, 47.1, 36.9, 21.1, 20.2; IR (thin film, cm^{-1}): 3435, 2945, 2927, 2867, 2835, 1677, 1451, 1407, 1383; HRMS (ESI): m/z Calcd. for $C_{29}H_{25}N_2O$ $[M+H]^+$ 417.1961, Found 417.1956.

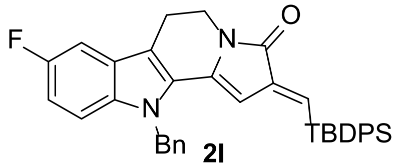
(*E*)-11-Benzyl-2-((*tert*-butyldiphenylsilyl)methylene)-2,5,6,11-tetrahydro-3*H*-indo lizino[8,7-*b*]indol-3-one (2k)



2k

Yellow oil in 63% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (d, J = 7.9 Hz, 1H), 7.56 – 7.52 (m, 4H), 7.38 – 7.34 (m, 2H), 7.28 (t, J = 7.4 Hz, 4H), 7.25 – 7.21 (m, 2H), 7.18 (d, J = 8.3 Hz, 1H), 7.17 – 7.13 (m, 1H), 7.12 (d, J = 7.2 Hz, 1H), 7.08 (t, J = 7.4 Hz, 2H), 6.58 (d, J = 7.3 Hz, 2H), 5.11 (s, 1H), 4.95 (s, 2H), 3.90 (t, J = 6.3 Hz, 2H), 3.14 (t, J = 6.3 Hz, 2H), 1.06 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.9, 148.3, 139.9, 136.7, 136.3, 135.6, 134.0, 129.5, 128.8, 128.8, 127.8, 127.4, 126.3, 125.9, 125.7, 124.7, 120.5, 119.8, 115.7, 109.9, 97.8, 47.7, 37.4, 27.6, 20.8, 18.7; IR (thin film, cm^{-1}): 2927, 2855, 1700, 1614, 1571, 1460; HRMS (ESI): *m/z* Calcd. for $C_{38}H_{37}N_2OSi$ $[M+H]^+$ 565.2670, Found 565.2676.

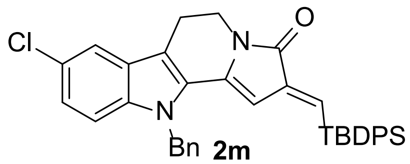
(*E*)-11-benzyl-2-((*tert*-butyldiphenylsilyl)methylene)-8-fluoro-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2l)



2l

Yellow oil in 72% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 6.8 Hz, 4H), 7.35 (d, *J* = 7.4 Hz, 2H), 7.30 – 7.19 (m, 4H), 7.15 – 7.05 (m, 1H), 6.96 (td, *J* = 9.0, 2.4 Hz, 1H), 6.56 (d, *J* = 7.4 Hz, 3H), 5.11 (s, 1H), 4.92 (s, 2H), 3.89 (t, *J* = 6.3 Hz, 2H), 3.07 (t, *J* = 6.3 Hz, 2H), 1.06 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.8, 148.1, 136.4, 136.3, 136.0, 135.3, 133.9, 129.7, 129.5, 128.8, 128.2, 127.8, 127.7, 127.8, 125.8, 125.8, 113.3, 113.1, 110.7, 110.6, 104.5, 104.4, 98.1, 47.9, 37.3, 29.8, 27.6, 27.2, 20.7, 18.7; IR (thin film, cm^{-1}): 3676, 2926, 2854, 1561, 1524, 1491, 1339, 1181; HRMS (ESI): *m/z* Calcd. for $C_{38}H_{36}FN_2OSi$ $[M+H]^+$ 583.2575, Found 583.2575.

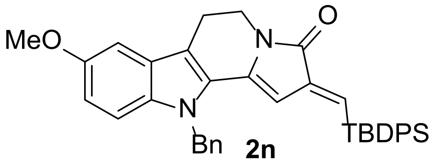
(*E*)-11-benzyl-2-((*tert*-butyldiphenylsilyl)methylene)-8-chloro-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2m)



2m

Green oil in 68% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 8.2, 4.4 Hz, 4H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.21 (m, 4H), 7.12 (ddd, *J* = 28.7, 8.2, 2.1 Hz, 1H), 7.08 (dd, *J* = 8.2, 5.8 Hz, 1H), 6.54 (d, *J* = 7.4 Hz, 1H), 5.11 (s, 1H), 4.91 (s, 2H), 3.88 (t, *J* = 6.3 Hz, 2H), 3.07 (t, *J* = 6.3 Hz, 2H), 1.05 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.7, 148.0, 138.1, 136.2, 136.2, 135.2, 133.9, 129.9, 129.5, 128.8, 127.8, 127.6, 127.4, 126.6, 126.3, 125.8, 124.9, 119.1, 114.8, 110.9, 98.4, 47.8, 37.3, 29.8, 27.6, 20.7, 18.7; IR (thin film, cm^{-1}): 3679, 2926, 2854, 1586, 1573, 1519, 1427, 1334, 1294, 1156, 1094; HRMS (ESI): *m/z* Calcd. for $C_{38}H_{36}ClN_2OSi$ $[M+H]^+$ 599.2280, Found 559.2280.

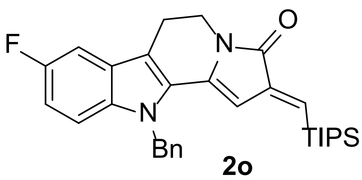
(*E*)-11-benzyl-2-((*tert*-butyldiphenylsilyl)methylene)-8-methoxy-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2n)



2n

Green oil in 59% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 4H), 7.37 – 7.31 (m, 2H), 7.30 – 7.26 (m, 4H), 7.21 (d, *J* = 0.8 Hz, 1H), 7.11 (d, *J* = 7.2 Hz, 1H), 7.06 (dt, *J* = 18.2, 5.0 Hz, 3H), 6.97 (d, *J* = 2.3 Hz, 1H), 6.88 (dd, *J* = 9.0, 2.4 Hz, 2H), 5.07 (s, 1H), 4.90 (s, 2H), 3.89 (t, *J* = 6.3 Hz, 2H), 3.85 (s, 3H), 3.09 (t, *J* = 6.3 Hz, 2H), 1.06 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.9, 154.7, 148.2, 136.7, 136.3, 135.6, 135.2, 134.0, 129.4, 128.7, 128.6, 127.8, 127.4, 126.6, 125.9, 125.8, 115.5, 115.0, 110.7, 100.6, 97.5, 65.7, 55.9, 47.7, 37.4, 29.8, 27.6, 20.8, 18.7; IR (thin film, cm^{-1}): 3685, 2926, 2822, 1673, 1545, 1448, 1334, 1300, 1150, 1091; HRMS (ESI): *m/z* Calcd. for $C_{39}H_{39}N_2O_2Si$ $[M+H]^+$ 595.2275, Found 595.2275.

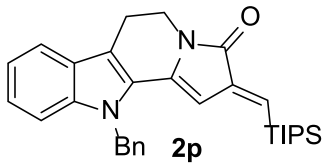
(*E*)-11-benzyl-8-fluoro-2-((triisopropylsilyl)methylene)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2o)



2o

Green oil in 78% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (t, *J* = 16.3 Hz, 1H), 7.37 – 7.29 (m, 4H), 7.28 (d, *J* = 7.2 Hz, 1H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.05 (d, *J* = 7.4 Hz, 2H), 6.79 (s, 1H), 5.55 (s, 1H), 5.50 (s, 2H), 3.91 (t, *J* = 6.3 Hz, 2H), 3.17 (t, *J* = 6.3 Hz, 2H), 0.96 (d, *J* = 6.5 Hz, 18H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.7, 146.7, 140.1, 137.1, 135.3, 132.7, 129.1, 127.6, 126.7, 125.7, 125.4, 124.7, 120.6, 119.8, 115.3, 109.6, 98.1, 47.9, 37.3, 32.0, 29.8, 22.8, 20.9, 18.7, 11.8; IR (thin film, cm^{-1}): 3651, 3629, 2924, 2854, 2367, 2310, 1734, 1640, 1561, 1460, 1181, 1097; HRMS (ESI): *m/z* Calcd. for $C_{31}H_{38}FN_2OSi$ $[M+H]^+$ 501.2732, Found 501.2730.

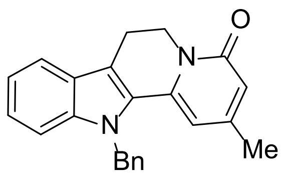
(*E*)-11-benzyl-2-((triisopropylsilyl)methylene)-2,5,6,11-tetrahydro-3*H*-indolizino[8,7-*b*]indol-3-one (2p)



2p

Yellow oil in 75% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^1H NMR (600 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.9 Hz, 1H), 7.48 – 7.27 (m, 4H), 7.28 (d, *J* = 1.3 Hz, 1H), 7.25 – 7.08 (m, 1H), 7.09 – 6.96 (m, 2H), 6.79 (d, *J* = 1.1 Hz, 1H), 5.55 (s, 1H), 5.50 (s, 2H), 3.91 (t, *J* = 6.3 Hz, 2H), 3.17 (t, *J* = 6.3 Hz, 2H), 1.02 – 0.84 (m, 21H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.8, 146.8, 140.1, 137.1, 135.4, 132.7, 129.1, 127.6, 126.7, 125.7, 125.4, 125.4, 124.7, 120.6, 119.8, 115.3, 109.6, 98.1, 47.9, 37.3, 29.8, 20.9, 18.7, 11.8; IR (thin film, cm^{-1}): 3694, 3620, 2922, 2849, 2385, 2256, 1745, 1628, 1523, 1460, 1238, 1227, 1181; HRMS (ESI): *m/z* Calcd. for $C_{31}H_{39}N_2OSi$ $[M+H]^+$ 483.2826, Found 483.2827.

12-Benzyl-2-methyl-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3)

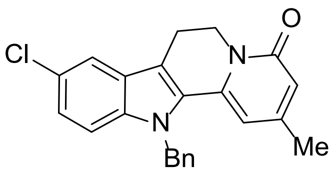


3

Brown oil in 40% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^1H NMR (600 MHz, DMSO-d_6) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.26 (dt, *J* = 14.9, 7.4 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.06 (d, *J* = 7.5 Hz, 2H), 6.24 (d, *J* = 0.9 Hz, 1H), 6.17 (s, 1H), 5.68 (s, 2H), 4.20 (t, *J* = 6.5 Hz, 2H), 3.02 (t, *J* = 6.5 Hz, 2H), 2.00 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 161.3, 149.3, 140.2, 138.0, 136.0, 128.8, 128.8, 127.3, 126.0, 124.5, 124.4, 120.5, 119.7, 116.6, 116.3, 111.0, 103.8, 47.9, 20.8, 19.4; IR (thin film, cm^{-1}): 2962, 2944, 2833, 1656, 1450, 1410, 1113, 1019; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{21}N_2O$ $[M+H]^+$ 341.1648, Found

341.1656.

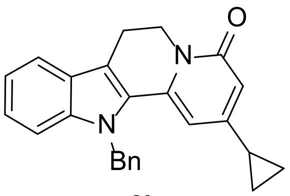
12-Benzyl-9-chloro-2-methyl-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3a)



3a

Brown oil in 41% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, J = 1.7 Hz, 1H), 7.37 (t, J = 7.4 Hz, 2H), 7.32 (t, J = 7.3 Hz, 1H), 7.22 (dd, J = 8.8, 1.9 Hz, 1H), 7.14 (dd, J = 11.1, 8.2 Hz, 3H), 6.33 (s, 1H), 6.03 (d, J = 1.3 Hz, 1H), 5.51 (s, 2H), 4.37 (t, J = 6.6 Hz, 2H), 3.03 (t, J = 6.6 Hz, 2H), 2.00 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.8, 149.5, 139.1, 137.0, 135.8, 131.0, 129.35, 128.0, 126.8, 126.0, 125.9, 125.1, 119.2, 118.0, 116.1, 111.7, 105.1, 49.1, 40.1, 21.5, 20.1; IR (thin film, cm^{-1}): 3436, 2986, 2951, 2922, 2835, 1733, 1662, 1591, 1491, 1450, 1397; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{20}ClN_2O$ $[M+H]^+$ 375.1259, Found 375.1268.

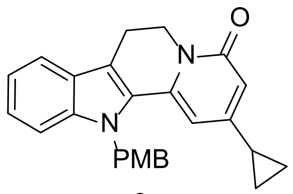
12-Benzyl-2-cyclopropyl-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3b)



3b

Gray solid in 45% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 248.1 – 249.7 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (d, J = 7.9 Hz, 1H), 7.39 (t, J = 7.4 Hz, 2H), 7.33 (t, J = 7.3 Hz, 1H), 7.30 (dd, J = 11.1, 4.0 Hz, 1H), 7.27 – 7.24 (m, 1H), 7.22 (t, J = 7.4 Hz, 1H), 7.17 (d, J = 7.4 Hz, 2H), 6.27 (d, J = 1.5 Hz, 1H), 5.71 (d, J = 1.5 Hz, 1H), 5.51 (s, 2H), 4.38 (t, J = 6.6 Hz, 2H), 3.07 (t, J = 6.6 Hz, 2H), 1.52 – 1.47 (m, 1H), 0.84 – 0.79 (m, 2H), 0.32 – 0.28 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 156.2, 140.9, 137.4, 136.5, 129.9, 129.4, 127.8, 125.7, 125.0, 124.9, 121.0, 119.8, 116.7, 114.0, 110.4, 100.0, 48.9, 40.1, 20.2, 15.1, 9.5; IR (thin film, cm^{-1}): 3433, 3255, 3078, 2999, 2954, 2924, 2853, 2220, 1549, 1385; HRMS (ESI): *m/z* Calcd. for $C_{25}H_{23}N_2O$ $[M+H]^+$ 367.1805, Found 367.1792.

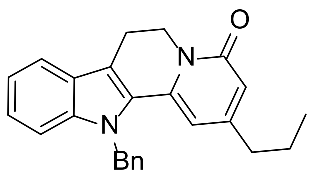
2-Cyclopropyl-12-(4-methoxybenzyl)-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3c)



3c

White solid in 32% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 173.8 – 175.5 °C ; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.9 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.25 (d, *J* = 6.8 Hz, 1H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 2H), 6.26 (s, 1H), 5.80 (d, *J* = 1.3 Hz, 1H), 5.45 (s, 2H), 4.37 (t, *J* = 6.6 Hz, 2H), 3.81 (s, 3H), 3.06 (t, *J* = 6.6 Hz, 2H), 1.54 –1.50 (m, 1H), 0.85 (dt, *J* = 6.7, 4.9 Hz, 2H), 0.40 – 0.36 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.7, 159.2, 156.2, 140.8, 136.5, 129.9, 129.3, 126.9, 125.0, 124.2, 120.9, 119.8, 116.6, 114.7, 113.8, 110.4, 100.3, 55.5, 48.4, 40.1, 20.2, 15.2, 9.6; IR (thin film, cm^{-1}): 3437, 2988, 2953, 2925, 2893, 1657, 1611, 1589, 1460, 1397, 1350, 1323, 1005; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{25}N_2O_2$ $[M+H]^+$ 397.1911, Found 397.1913.

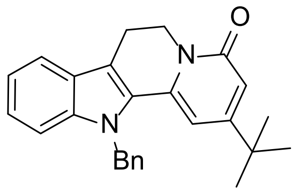
12-Benzyl-2-propyl-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3d)



3d

Yellow oil in 11% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.9 Hz, 1H), 7.37 (dd, *J* = 10.2, 4.6 Hz, 2H), 7.32 – 7.28 (m, 3H), 7.23 – 7.21 (m, 1H), 7.17 (d, *J* = 7.2 Hz, 2H), 6.31 – 6.29 (m, 1H), 6.04 (d, *J* = 1.6 Hz, 1H), 5.52 (s, 2H), 4.39 (t, *J* = 6.6 Hz, 2H), 3.11 – 3.06 (m, 2H), 2.21 (t, *J* = 7.5 Hz, 2H), 1.35 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.80 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.1, 153.2, 140.9, 137.5, 136.2, 129.9, 129.2, 127.8, 125.9, 125.0, 124.8, 120.9, 119.7, 116.8, 116.7, 110.5, 104.0, 49.0, 40.2, 37.3, 22.1, 20.2, 13.6. IR (thin film, cm^{-1}): 2955, 2926, 2860, 1657, 1582, 1543, 1455, 1350, 1023; HRMS (ESI): *m/z* Calcd. for $C_{25}H_{25}N_2O$ $[M+H]^+$ 369.1961, Found 369.1963.

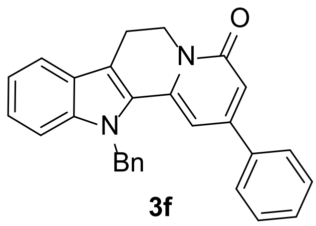
12-Benzyl-2-(*tert*-butyl)-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3e)



3e

Brown oil in 9% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.9 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.31 (dd, *J* = 11.5, 7.1 Hz, 3H), 7.24 – 7.21 (m, 1H), 7.19 (d, *J* = 7.8 Hz, 2H), 6.43 (s, 1H), 6.17 (s, 1H), 5.55 (s, 2H), 4.39 (t, *J* = 6.5 Hz, 2H), 3.11 – 3.08 (m, 2H), 0.94 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.4, 162.1, 140.8, 137.3, 135.8, 130.2, 129.3, 127.8, 125.7, 125.1, 124.7, 120.9, 119.7, 116.3, 113.9, 110.3, 102.0, 48.9, 40.14, 34.8, 29.5, 20.2, 0.1; IR (thin film, cm^{-1}): 2962, 2942, 2845, 2835, 1647, 1455, 1112, 1018; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{27}N_2O$ $[M+H]^+$ 383.2118, Found 383.2116.

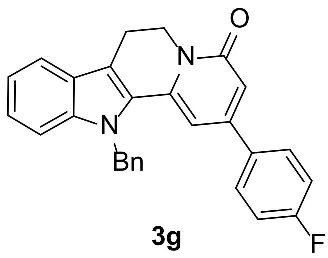
12-Benzyl-2-phenyl-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3f)



3f

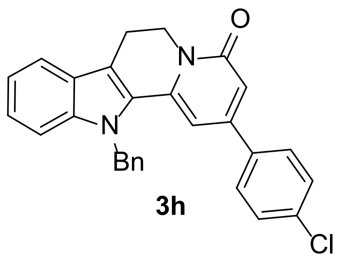
Yellow oil in 10% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.38 – 7.32 (m, 4H), 7.30 (dd, *J* = 13.7, 6.2 Hz, 2H), 7.24 (d, *J* = 6.8 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 2H), 7.15 (d, *J* = 7.7 Hz, 2H), 6.75 (s, 1H), 6.48 (s, 1H), 4.47 (t, *J* = 6.5 Hz, 2H), 3.15 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.2, 149.9, 141.0, 137.5, 137.2, 136.9, 130.0, 129.4, 129.4, 128.9, 127.8, 126.5, 125.9, 125.1, 125.0, 121.0, 119.9, 116.8, 114.5, 110.4, 101.8, 49.0, 40.3, 20.2; IR (thin film, cm^{-1}): 2925, 2855, 1652, 1573, 1529, 1529, 1457, 1351; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{23}N_2O$ $[M+H]^+$ 403.1805, Found 403.1795.

12-Benzyl-2-(4-fluorophenyl)-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3g)



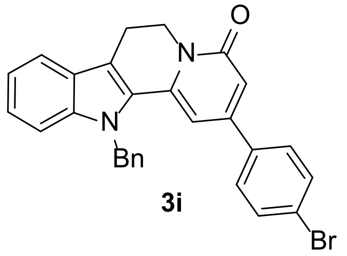
Yellow solid in 14% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 245.3 – 247.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 2H), 7.39 – 7.36 (m, 1H), 7.33 (dd, *J* = 12.4, 7.6 Hz, 2H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 2H), 7.09 (dd, *J* = 8.7, 5.3 Hz, 2H), 6.97 (t, *J* = 8.6 Hz, 2H), 6.69 (d, *J* = 1.6 Hz, 1H), 6.40 (d, *J* = 1.6 Hz, 1H), 5.58 (s, 2H), 4.46 (t, *J* = 6.6 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.4, 163.1, 162.7, 148.9, 141.1, 137.5, 137.1, 133.3, 133.2, 129.9, 129.4, 128.6, 128.0, 127.8, 125.9, 125.2, 124.9, 121.1, 119.9, 117.0, 116.0, 115.8, 114.2, 110.3, 101.6, 49.0, 40.3, 20.2; IR (thin film, cm^{-1}): 3375, 2925, 1649, 1529, 1509, 1233, 1158; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{22}FN_2O$ $[M+H]^+$ 421.1711, Found 421.1718.

12-Benzyl-2-(4-chlorophenyl)-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3h)



Brown oil in 12% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.39 (d, *J* = 7.0 Hz, 1H), 7.35 (dt, *J* = 13.7, 6.1 Hz, 3H), 7.25 (m, 2H), 7.21 (d, *J* = 7.3 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 1.3 Hz, 1H), 6.40 (d, *J* = 1.3 Hz, 1H), 5.58 (s, 2H), 4.46 (t, *J* = 6.5 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.1, 148.6, 141.1, 137.5, 137.2, 135.6, 135.6, 129.9, 129.4, 129.1, 127.9, 127.5, 125.9, 125.2, 124.9, 121.17, 119.9, 117.0, 114.4, 110.39 101.3, 49.0, 40.3, 20.2; IR (thin film, cm^{-1}): 3436, 2982, 2925, 2855, 1734, 1715, 1653, 1576, 1525, 1490, 1455, 1355; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{22}ClN_2O$ $[M+H]^+$ 437.1415, Found 437.1406.

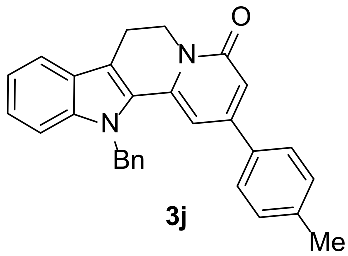
12-Benzyl-2-(4-bromophenyl)-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3i)



3i

Yellow oil in 9% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.44 – 7.38 (m, 5H), 7.36 – 7.31 (m, 2H), 7.26 – 7.24 (m, 1H), 7.20 (d, *J* = 7.0 Hz, 2H), 6.99 – 6.96 (m, 2H), 6.70 (d, *J* = 1.9 Hz, 1H), 6.40 (d, *J* = 1.9 Hz, 1H), 5.58 (s, 2H), 4.46 (t, *J* = 6.6 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.0, 148.6, 141.0, 137.4, 137.1, 135.9, 131.9, 129.7, 129.3, 127.8, 127.7, 125.8, 125.1, 124.8, 123.7, 121.0, 119.8, 116.9, 114.3, 110.2, 101.1, 48.8, 40.1, 20.0; IR (thin film, cm^{-1}): 3436, 2924, 2853, 1653, 1573, 1489, 1455; HRMS (ESI): *m/z* Calcd. for $C_{28}H_{22}BrN_2O$ $[M+H]^+$ 481.0910, Found 481.0920.

12-Benzyl-2-(*p*-tolyl)-7,12-dihydroindolo[2,3-*a*]quinolizin-4(6*H*)-one (3j)



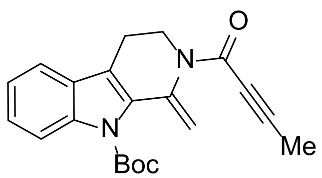
3j

Yellow oil in 13% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.41 (t, *J* = 7.3 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.26 – 7.23 (m, 1H), 7.21 (d, *J* = 7.2 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.74 (d, *J* = 1.7 Hz, 1H), 6.49 (d, *J* = 1.7 Hz, 1H), 5.59 (s, 2H), 4.46 (t, *J* = 6.6 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.3, 149.8, 141.0, 139.7, 137.5, 136.8, 134.1, 130.0, 129.6, 129.4, 127.8, 126.3, 125.9, 125.0, 125.0, 121.0, 119.9, 116.8, 114.0, 110.4, 101.8, 49.0, 40.3, 21.3, 20.2; IR (thin film, cm^{-1}): 3433, 2966, 2924, 2856, 2837, 1731, 1647, 1560, 1458, 1376; HRMS (ESI): *m/z* Calcd. for $C_{29}H_{25}N_2O$ $[M+H]^+$ 417.1961, Found 417.1962.

10. The Procedure for the Preparation of 1o-4 and Characterization Data

To a solution of AgOTf (0.08 mmol, 21 mg) in anhydrous DCM was added a solution of [tris(2,4-di-*tert*-butylphenyl) phosphite]gold chloride (0.08 mmol, 70 mg) in anhydrous DCM under the N_2 atmosphere, and the mixture was stirred for about 30 min. The mixture was added to a solution of compound **1o** (1 mmol, 350 mg) in anhydrous DCM under the N_2 atmosphere, and the mixture was stirred for about 20 min, until the total conversion of the reactant. Then mixture was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel (EtOAc/petroleum ether = 1:5) to give **1o-4** as yellow oil in 72% yield.

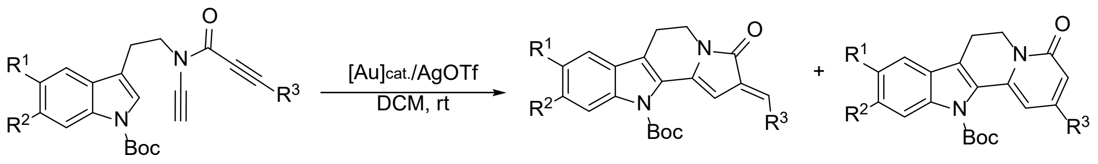
***tert*-Butyl 2-(but-2-ynoyl)-1-methylene-1,2,3,4-tetrahydro-9*H*-pyrido[3,4-*b*] indole-9-carboxylate (1o-4)**



1o-4

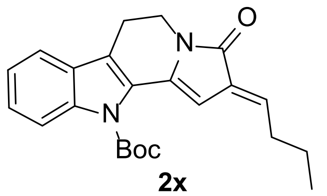
The ratio of major rotamer and minor rotamer is 2:1; ^{1}H NMR (600 MHz, DMSO-d_6) (major rotamer) δ 7.96 (s, 1H), 7.55 (d, J = 7.7 Hz, 1H), 7.42 – 7.36 (m, 1H), 7.27 (dd, J = 11.1, 3.9 Hz, 1H), 5.55 (s, 2H), 3.98 (s, 2H), 2.85 (s, 2H), 1.96 (s, 3H), 1.61 (s, 9H); (minor rotamer) δ 7.96 (s, 1H), 7.55 (d, J = 7.7 Hz, 1H), 7.42 – 7.36 (m, 1H), 7.27 (dd, J = 11.1, 3.9 Hz, 1H), 5.55 (s, 2H), 4.17 (s, 2H), 2.85 (s, 2H), 1.61 (s, 12H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 151.8, 149.7, 137.9, 135.0, 129.6, 127.4, 126.3, 126.2, 123.3, 123.2, 120.8, 120.6, 119.6, 115.2, 114.4, 112.4, 91.0, 85.1, 84.5, 74.0, 67.3, 41.5, 27.5, 27.2, 20.5, 18.7, 3.7, 3.0; IR (thin film, cm^{-1}): 3423, 2972, 2965, 2926, 2840, 2826, 1710, 1659, 1593, 1471, 1465, 1393, 1369, 1343; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{23}N_2O_3$ $[M+H]^+$ 351.1703, Found 351.1705.

11. General Procedures for the Preparation of 2q-2aa and 3q-3aa on Condition C2 and Characterization Data



To a solution of AgOTf (0.1 mmol) in anhydrous DCM was added a solution of [tris(2,4-di-*tert*-butylphenyl) phosphite]gold chloride (0.1 mmol) in anhydrous DCM under the N_2 atmosphere, and the mixture was stirred for about 30 min. The mixture was added to a solution of compounds **1q-1aa** (1 mmol) in anhydrous DCM under the N_2 atmosphere, and the mixture was stirred for about 1.5 h, until the total conversion of the reactant. Then mixture was concentrated *in vacuo*, and the residue was purified by a flash column chromatography on silica gel (DCM/MeOH) to give the products.

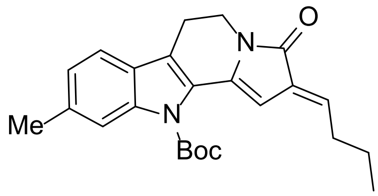
***tert*-Butyl (*E*)-2-butylidene-3-oxo-2,3,5,6-tetrahydro-11*H*-indolizino[8,7-*b*]indole-11-carboxylate (2x)**



2x

Brown oil in 12% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 6.54 (t, *J* = 8.1 Hz, 1H), 6.33 (s, 1H), 3.78 (t, *J* = 6.1 Hz, 2H), 3.04 (t, *J* = 6.1 Hz, 2H), 2.37 (dd, *J* = 15.0, 7.4 Hz, 2H), 1.66 (s, 9H), 1.53 (dd, *J* = 14.4, 7.5 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 165.5, 149.3, 137.6, 137.0, 133.2, 132.4, 127.2, 126.7, 125.8, 123.4, 122.3, 119.9, 115.2, 98.0, 84.9, 35.6, 31.2, 27.6, 21.7, 20.5, 13.7; IR (thin film, cm^{-1}): 3431, 2958, 2929, 2869, 2834, 1705, 1606, 1491, 1449, 1397, 1368; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{27}N_2O_3$ [M+H]$^+$ 379.2016, Found 379.2018.

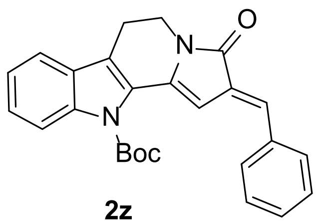
***tert*-Butyl (*E*)-2-butylidene-9-methyl-3-oxo-2,3,5,6-tetrahydro-11*H*-indolizino[8,7-*b*]indole-11-carboxylate (2y)**



2y

Yellow oil in 12% yield; $R_f = 0.2$ (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.88 (s, 1H), 7.56 (d, J = 7.9 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 6.52 (t, J = 8.3 Hz, 1H), 6.27 (s, 1H), 3.76 (t, J = 6.2 Hz, 2H), 3.01 (t, J = 6.2 Hz, 2H), 2.46 (s, 3H), 2.36 (dd, J = 15.2, 7.5 Hz, 2H), 1.66 (s, 9H), 1.53 (dd, J = 14.7, 7.3 Hz, 2H), 0.93 (t, J = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 165.5, 149.3, 138.1, 136.6, 136.5, 133.2, 132.5, 125.2, 125.1, 124.8, 122.5, 119.6, 115.4, 97.5, 84.8, 35.5, 31.2, 27.6, 21.9, 21.7, 20.6, 13.7; IR (thin film, cm^{-1}): 3434, 2980, 2931, 2862, 2833, 1735, 1687, 1611, 1530, 1468, 1455, 1380; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{27}N_2O_3$ $[M+H]^+$ 393.2173, Found 393.2178.

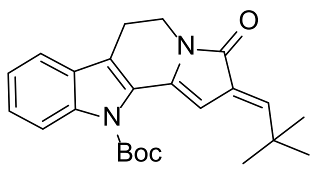
***tert*-Butyl (*E*)-2-benzylidene-3-oxo-2,3,5,6-tetrahydro-11*H*-indolizino[8,7-*b*] indole-11-carboxylate (2z)**



2z

Brown oil in 33% yield; $R_f = 0.2$ (EtOAc/petroleum ether = 1:5); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.06 (d, J = 8.4 Hz, 1H), 7.74 (d, J = 7.6 Hz, 2H), 7.71 (d, J = 7.7 Hz, 1H), 7.51 – 7.45 (m, 3H), 7.42 (t, J = 7.3 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 7.30 (s, 1H), 6.79 (s, 1H), 3.85 (t, J = 6.2 Hz, 2H), 3.10 (t, J = 6.2 Hz, 2H), 1.64 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 166.9, 149.2, 137.9, 135.5, 135.1, 130.5, 130.4, 129.9, 129.6, 129.0, 127.1, 127.0, 125.7, 123.5, 123.4, 120.2, 115.2, 98.6, 85.0, 35.7, 27.6, 20.6; IR (thin film, cm^{-1}): 3424, 2984, 2926, 2835, 1737, 1690, 1607, 1491, 1443, 1397, 1366; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{25}N_2O_3$ $[M+H]^+$ 413.1860 Found, 413.1858.

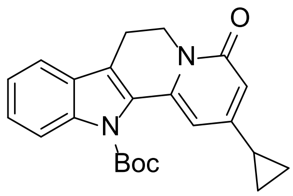
***tert*-Butyl (*E*)-2-(2,2-dimethylpropylidene)-3-oxo-2,3,5,6-tetrahydro-11*H*-indolizino[8,7-*b*]indole-11-carboxylate (2aa)**



2aa

Yellow oil in 60% yield; R_f = 0.2 (EtOAc/petroleum ether = 1:20); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.00 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 7.7 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.31 (t, J = 7.4 Hz, 1H), 6.54 (s, 1H), 6.46 (s, 1H), 3.77 (t, J = 6.2 Hz, 2H), 3.02 (t, J = 6.2 Hz, 2H), 1.65 (s, 9H), 1.23 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 166.7, 149.3, 146.5, 137.6, 132.8, 129.2, 127.2, 126.7, 125.8, 123.4, 122.5, 120.0, 115.0, 98.0, 84.8, 35.6, 34.5, 29.8, 27.6, 20.6; IR (thin film, cm^{-1}): 3432, 2984, 2955, 2926, 1738, 1703, 1607, 1492, 1442, 1366, 1311; HRMS (ESI): *m/z* Calcd. for $C_{24}H_{29}N_2O_3$ $[M+H]^+$ 393.2173, Found 393.2173.

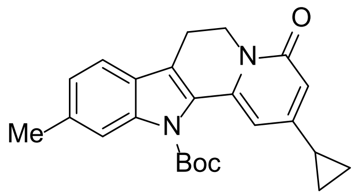
***tert*-Butyl 2-cyclopropyl-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3q)**



3q

Yellow solid in 70% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 177.7 – 179.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.7 Hz, 1H), 7.41 (t, J = 7.5 Hz, 1H), 7.29 (t, J = 7.5 Hz, 1H), 6.21 (d, J = 1.4 Hz, 1H), 6.07 (d, J = 1.4 Hz, 1H), 4.43 (t, J = 6.4 Hz, 2H), 2.93 (t, J = 6.4 Hz, 2H), 1.73 – 1.68 (m, 1H), 1.64 (s, 9H), 1.04 – 0.99 (m, 2H), 0.80 – 0.76 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.3, 155.5, 150.2, 140.0, 136.2, 129.9, 127.1, 127.0, 125.9, 123.7, 119.7, 115.5, 112.7, 104.3, 84.9, 38.9, 28.1, 20.7, 15.3, 9.5; IR (thin film, cm^{-1}): 3439, 2965, 2926, 2835, 1733, 1650, 1586, 1453, 1392, 1368; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{25}N_2O_3$ $[M+H]^+$ 377.1860, Found 377.1865.

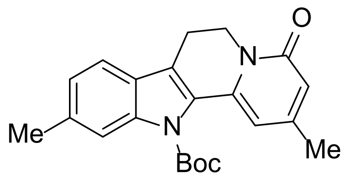
***tert*-Butyl 2-cyclopropyl-10-methyl-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12 (4*H*)-carboxylate (3r)**



3r

Yellow oil in 68% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.40 (d, J = 7.9 Hz, 1H), 7.12 (d, J = 7.9 Hz, 1H), 6.17 (d, J = 1.6 Hz, 1H), 6.05 (d, J = 1.6 Hz, 1H), 4.41 (t, J = 6.5 Hz, 2H), 2.90 (t, J = 6.5 Hz, 2H), 2.50 (s, 3H), 1.73 – 1.68 (m, 1H), 1.62 (s, 9H), 1.03 – 0.99 (m, 2H), 0.80 – 0.76 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.4, 155.6, 150.3, 140.5, 137.6, 136.5, 129.3, 126.1, 125.2, 124.8, 119.3, 115.9, 112.2, 104.3, 84.7, 38.8, 28.1, 22.4, 20.7, 15.3, 9.5; IR (thin film, cm^{-1}): 3437, 2985, 2928, 2836, 1731, 1650, 1589, 1531, 1459, 1395, 1368; HRMS (ESI): *m/z* Calcd. for $C_{24}H_{27}N_2O_3$ $[M+H]^+$ 391.2016, Found 391.2009.

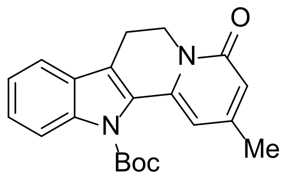
***tert*-Butyl 2,10-dimethyl-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3s)**



3s

Yellow solid in 66% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 167.8 – 169.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.40 (d, J = 7.9 Hz, 1H), 7.12 (d, J = 7.9 Hz, 1H), 6.33 (s, 1H), 6.13 (d, J = 1.6 Hz, 1H), 4.42 (t, J = 6.5 Hz, 2H), 2.90 (t, J = 6.5 Hz, 2H), 2.50 (s, 3H), 2.21 (s, 3H), 1.59 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.3, 150.2, 149.0, 140.6, 137.6, 136.5, 129.1, 126.0, 125.2, 124.7, 119.2, 116.8, 115.8, 107.1, 84.6, 38.8, 28.0, 22.4, 21.5, 20.7; IR (thin film, cm^{-1}): 3443, 2962, 2924, 2854, 1731, 1655, 1593, 1471, 1454, 1393, 1369, 1343; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{25}N_2O_3$ $[M+H]^+$ 365.1860, Found 365.1858.

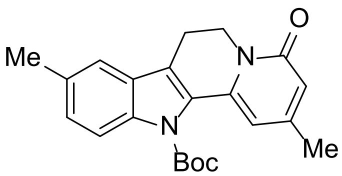
***tert*-Butyl 2-methyl-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3t)**



3t

White solid in 72% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 173.2 – 174.8 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, J = 8.4 Hz, 1H), δ 7.53 (d, J = 7.7 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.29 (t, J = 7.5 Hz, 1H), 6.35 (s, 1H), 6.17 (d, J = 1.4 Hz, 1H), 4.44 (t, J = 6.5 Hz, 2H), 2.93 (t, J = 6.5 Hz, 2H), 2.21 (s, 3H), 1.61 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.3, 150.1, 149.0, 140.0, 136.2, 129.7, 127.1, 126.9, 125.8, 123.7, 119.6, 117.2, 115.6, 107.4, 84.7, 38.8, 28.1, 21.6, 20.6; IR (thin film, cm^{-1}): 3434, 3002, 2960, 2923, 2854, 2831, 1705, 1611, 1460, 1387, 1330; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{23}N_2O_3$ $[M+H]^+$ 351.1703, Found 351.1710.

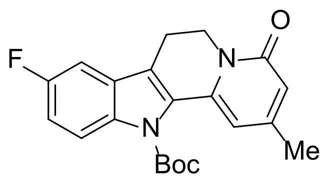
***tert*-butyl 2,9-dimethyl-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3u)**



3u

Yellow oil in 63% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.91 (d, J = 8.5 Hz, 1H), 7.47 (s, 1H), 7.28 (d, J = 8.7 Hz, 1H), 6.20 (d, J = 9.5 Hz, 2H), 4.24 (t, J = 6.4 Hz, 2H), 2.92 (t, J = 6.4 Hz, 2H), 2.40 (s, 3H), 2.17 (d, J = 1.1 Hz, 3H), 1.55 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 161.2, 149.9, 149.2, 138.0, 136.2, 133.3, 129.5, 128.9, 127.1, 126.1, 120.3, 116.5, 115.0, 107.0, 85.0, 38.6, 27.9, 21.3, 21.2, 20.2; IR (thin film, cm^{-1}): 3425, 3002, 2960, 2928, 2834, 1745, 1611, 1465, 1400, 1236; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{25}N_2O_3$ $[M+H]^+$ 365.1860, Found 365.1863.

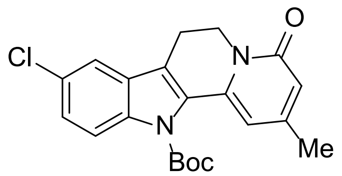
***tert*-butyl 9-fluoro-2-methyl-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3v)**



3v

Yellow oil in 60% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.02 (dd, J = 9.1, 4.4 Hz, 1H), 7.55 (d, J = 8.5 Hz, 1H), 7.30 (td, J = 9.2, 2.5 Hz, 1H), 6.24 (d, J = 5.6 Hz, 2H), 4.24 (t, J = 6.4 Hz, 2H), 2.93 (t, J = 6.4 Hz, 2H), 2.17 (s, 3H), 1.55 (s, 9H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 160.7, 159.7, 158.1, 149.2, 148.8, 135.6, 135.3, 130.5, 127.5, 127.5, 125.3, 125.2, 116.6, 116.3, 116.2, 114.7, 114.6, 107.0, 105.9, 105.7, 85.0, 38.2, 27.4, 20.8, 19.8; IR (thin film, cm^{-1}): 3430, 2962, 2926, 2854, 1725, 1644, 1538, 1488, 1423, 1314; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{22}FN_2O_3$ $[M+H]^+$ 369.1609, Found 369.1609.

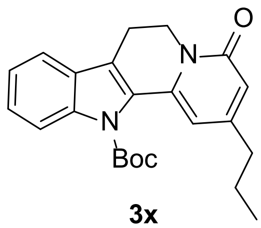
***tert*-Butyl 9-chloro-2-methyl-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3w)**



3w

Yellow oil in 71% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, J = 8.9 Hz, 1H), 7.48 (d, J = 1.9 Hz, 1H), 7.34 (dd, J = 8.9, 2.0 Hz, 1H), 6.37 (s, 1H), 6.18 (d, J = 1.1 Hz, 1H), 4.42 (t, J = 6.4 Hz, 2H), 2.89 (t, J = 6.4 Hz, 2H), 2.21 (s, 3H), 1.60 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 149.8, 148.9, 138.3, 135.8, 130.9, 129.4, 128.1, 127.1, 124.7, 119.2, 117.7, 116.7, 107.9, 85.3, 38.8, 28.0, 21.5, 20.5; IR (thin film, cm^{-1}): 3436, 2984, 2925, 2830, 1736, 1660, 1603, 1492, 1442, 1397, 1367; HRMS (ESI): *m/z* Calcd. for $C_{21}H_{22}ClN_2O_3$ $[M+H]^+$ 385.1313, Found 385.1311.

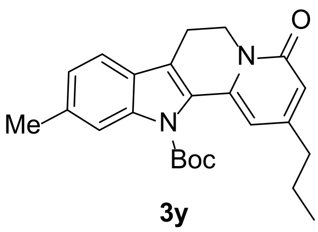
***tert*-Butyl 4-oxo-2-propyl-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3x)**



3x

White solid in 75% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 178.7 – 179.8 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.7 Hz, 1H), 7.42 – 7.39 (m, 1H), 7.31 – 7.27 (m, 1H), 6.36 – 6.33 (m, 1H), 6.18 (d, J = 1.6 Hz, 1H), 4.45 (t, J = 6.5 Hz, 2H), 2.94 (t, J = 6.5 Hz, 2H), 2.44 (t, J = 7.6 Hz, 2H), 1.68 – 1.62 (m, 2H), 1.62 (s, 9H), 0.97 (t, J = 7.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 153.3, 150.2, 140.0, 136.3, 129.9, 127.0, 127.0, 125.7, 123.7, 119.6, 116.5, 115.5, 106.8, 84.7, 38.9, 37.6, 28.1, 22.4, 20.6, 13.8; IR (thin film, cm^{-1}): 3441, 2958, 2930, 2807, 1732, 1655, 1592, 1535, 1454, 1392, 1368, 1350; HRMS (ESI): *m/z* Calcd. for $C_{23}H_{27}N_2O_3$ [M+H]$^+$ 379.2016, Found 379.2015.

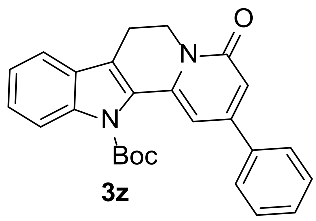
***tert*-Butyl 10-methyl-4-oxo-2-propyl-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3y)**



3y

Brown oil in 68% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.40 (d, J = 7.9 Hz, 1H), 7.12 (d, J = 7.9 Hz, 1H), 6.34 (s, 1H), 6.14 (d, J = 1.6 Hz, 1H), 4.43 (t, J = 6.5 Hz, 2H), 2.91 (t, J = 6.5 Hz, 2H), 2.50 (s, 3H), 2.43 (t, J = 7.6 Hz, 2H), 1.68 – 1.62 (m, 2H), 1.60 (s, 9H), 0.97 (t, J = 7.3 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 153.3, 150.3, 140.6, 137.6, 136.6, 129.3, 126.0, 125.2, 124.8, 119.3, 116.1, 115.8, 106.5, 84.6, 38.9, 37.7, 28.1, 22.4, 20.7, 13.8; IR (thin film, cm^{-1}): 3421, 2980, 2935, 2873, 2811, 1688, 1592, 1480, 1462, 1382, 1375; HRMS (ESI): *m/z* Calcd. for $C_{22}H_{28}N_2O_3Na$ [M+Na]$^+$ 415.1992, Found 415.1996.

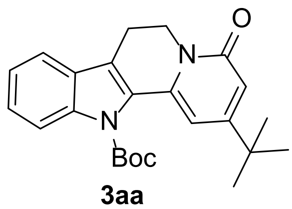
***tert*-Butyl 4-oxo-2-phenyl-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3z)**



3z

Yellow solid in 58% yield; R_f = 0.2 (DCM/MeOH = 50:1); Mp 319.2 – 319.9 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 1H), 7.64 – 7.59 (m, 2H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.49 – 7.40 (m, 4H), 7.32 (t, *J* = 7.5 Hz, 1H), 6.77 (d, *J* = 1.8 Hz, 1H), 6.64 (d, *J* = 1.8 Hz, 1H), 4.52 (t, *J* = 6.5 Hz, 2H), 3.01 (t, *J* = 6.5 Hz, 2H), 1.58 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.6, 150.2, 150.1, 140.1, 138.0, 137.0, 130.0, 129.4, 129.1, 127.3, 127.0, 126.7, 126.1, 123.8, 119.8, 115.7, 114.8, 104.9, 85.0, 39.1, 28.1, 20.7; IR (thin film, cm^{-1}): 3440, 2981, 2835, 1732, 1652, 1591, 1491, 1452, 1394, 1369, 1352; HRMS (ESI): *m/z* Calcd. for $C_{26}H_{25}N_2O_3$ $[M+H]^+$ 413.1860, Found 413.1865.

***tert*-Butyl 2-(*tert*-butyl)-4-oxo-6,7-dihydroindolo[2,3-*a*]quinolizine-12(4*H*)-carboxylate (3aa)**



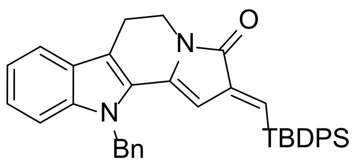
3aa

White oil in 14% yield; R_f = 0.2 (DCM/MeOH = 50:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.52 (d, *J* = 1.6 Hz, 1H), 6.41 (d, *J* = 1.6 Hz, 1H), 4.45 (t, *J* = 6.4 Hz, 2H), 2.95 (t, *J* = 6.4 Hz, 2H), 1.68 (s, 9H), 1.27 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.8, 161.6, 150.4, 139.8, 135.8, 130.4, 127.2, 127.0, 125.7, 123.7, 119.7, 115.6, 114.0, 104.4, 84.9, 38.9, 35.0, 30.0, 28.2, 20.7; IR (thin film, cm^{-1}): 3437, 2984, 2926, 1737, 1656, 1597, 1488, 1450, 1396, 1353; HRMS (ESI): *m/z* Calcd. for $C_{24}H_{29}N_2O_3$ $[M+H]^+$ 393.2173, Found 393.2174.

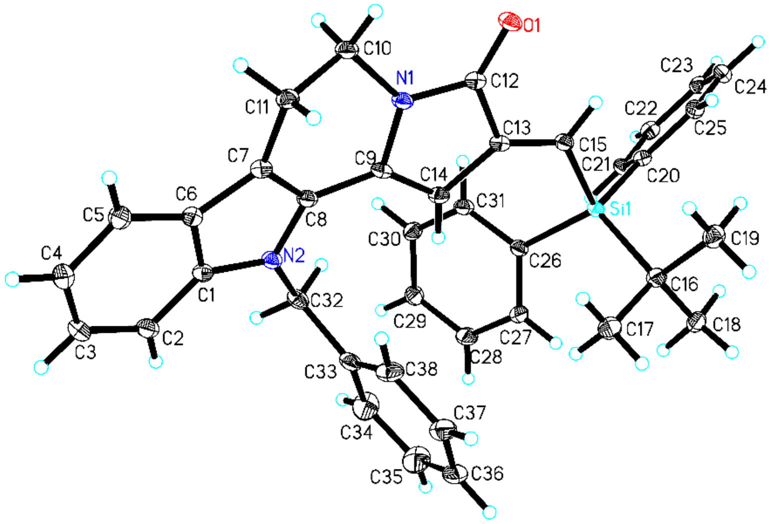
12. X-Ray Crystal Structure Analyses of Compounds 2k and 3t

12.1 X-Ray Crystal Structure Analyses of Compound 2k

Identification code	exp_1493
Empirical formula	$C_{38}H_{36}N_2OSi$
Formula weight	564.78
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.0141(5)
b/Å	16.8417(6)
c/Å	18.3913(8)
α/°	88.276(3)
β/°	83.244(4)
γ/°	77.357(4)
Volume/Å^3	3005.5(2)
Z	4
ρ_{calc}g/cm^3	1.248
μ/mm^{-1}	0.940
F(000)	1200.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	4.838 to 147.256
Index ranges	$-10 \le h \le 12$, $-20 \le k \le 20$, $-22 \le l \le 22$
Reflections collected	21813
Independent reflections	11721 [R_{int} = 0.0568, R_{sigma} = 0.0690]
Data/restraints/parameters	11721/0/763
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0635, wR_2 = 0.1769
Final R indexes [all data]	R_1 = 0.0785, wR_2 = 0.1928
Largest diff. peak/hole / e Å^{-3}	0.47/-0.43



2k

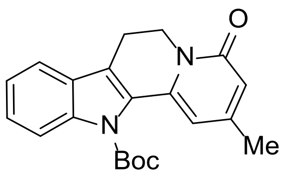


CCDC 1880231 contains the supplementary crystallographic data for compound **2k**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

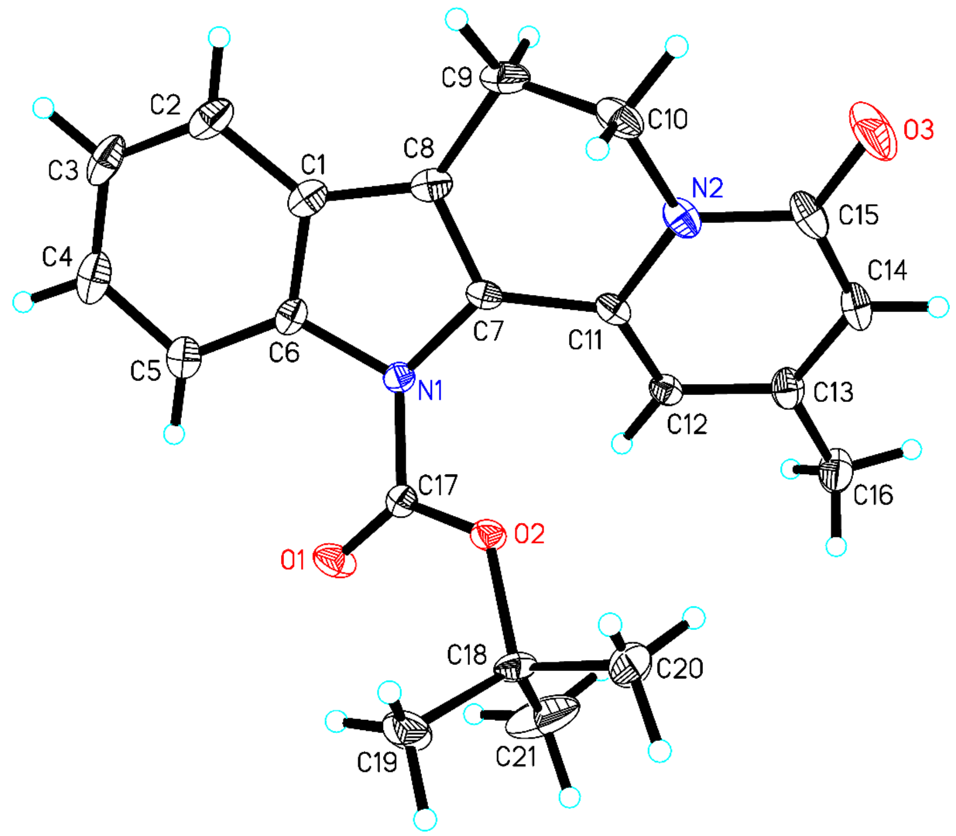
12.2 X-Ray Crystal Structure Analyses of compound 3t

Identification code	exp_1421
Empirical formula	$C_{21}H_{22}N_2O_3$
Formula weight	350.40
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.426(2)
b/Å	7.9081(7)
c/Å	14.0205(16)
α/°	90

$\beta/°$	106.829(13)
$\gamma/°$	90
Volume/$Å^3$	1849.4(4)
Z	4
$\rho_{calc}g/cm^3$	1.258
μ/mm^{-1}	0.085
F(000)	744.0
Crystal size/mm^3	0.14 × 0.13 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.884 to 49.998
Index ranges	-20 ≤ h ≤ 20, -9 ≤ k ≤ 9, -16 ≤ l ≤ 16
Reflections collected	11542
Independent reflections	3258 [R_{int} = 0.0498, R_{sigma} = 0.0428]
Data/restraints/parameters	3258/0/239
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0835, wR_2 = 0.2124
Final R indexes [all data]	R_1 = 0.0954, wR_2 = 0.2233
Largest diff. peak/hole / e $Å^{-3}$	0.69/-0.27



3t



CCDC 1880232 contains the supplementary crystallographic data for compound **3t**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

13. Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E.

Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

14. Computational Methods

All of the DFT calculations in this study were performed using the GAUSSIAN 09 series of programs. DFT method B3LYP with a standard 6-31G (d) basis set (LANL2DZ basis set for Au) was used for the geometry optimizations. The M11-L functional, proposed by Truhlar et al., was used with a 6-31+G (d, p) basis set (LANL2DZ basis set for Au) to calculate the single point energies. The solvent effects were taken into consideration using single point calculations based on the gas-phase stationary points with a SMD continuum solvation model. The energies presented in this paper are the M11-L calculated Gibbs free energies in tetrahydrofuran solvent.

15. B3LYP Geometries for All the Optimized Compounds and Transition States

1k-1

Energy: -2007345.5788517

Number of Imaginary Frequencies: 0

Si	0.88256	4.22910	0.58092
O	2.86329	1.67734	-3.48319
N	5.18152	-2.85152	-0.12297
N	2.05492	-0.18130	-2.37844
C	3.98862	-3.01140	-0.79953
C	1.82182	2.06846	-1.41867
C	0.49851	3.40153	2.23393
C	1.44095	-0.66862	-1.35137
C	2.30333	1.25898	-2.49800
C	4.56396	-2.77598	2.29605
C	-1.81597	5.25014	0.55867
H	-1.81900	5.05039	1.62652
C	0.73357	-1.14488	-0.41244
H	1.09991	-1.55066	0.52556
C	1.44134	2.88093	-0.59033
C	4.05870	-3.59718	3.31072
H	4.27454	-4.66341	3.29732

C	4.06257	-2.46042	-2.05628
C	-0.67938	4.93993	-0.21168
C	6.06713	-2.18047	-0.95591
C	0.61073	2.00735	2.39381
H	0.92818	1.39225	1.55589
C	0.08535	4.15281	3.35340
H	-0.01650	5.23219	3.28080
C	4.28161	-1.40339	2.32918
H	4.67320	-0.75747	1.54756
C	0.32231	1.39118	3.61396
H	0.42173	0.31289	3.70714
C	5.39553	-1.92134	-2.18409
C	7.39407	-1.78698	-0.74078
H	7.90655	-1.98619	0.19571
C	3.02136	-1.68903	4.37742
H	2.44084	-1.26413	5.19200
C	5.45191	-3.36758	1.21265
H	6.50198	-3.15330	1.43325
H	5.35403	-4.46038	1.20794
C	-0.73601	5.19694	-1.59651
H	0.11475	4.95801	-2.22964
C	-2.98584	6.06382	-1.39756
H	-3.86909	6.50439	-1.85221
C	-2.95535	5.81022	-0.02480
H	-3.81537	6.05319	0.59395
C	3.29520	-3.05788	4.35023
H	2.92271	-3.70621	5.13868
C	2.34101	5.47935	0.67018
C	-1.87402	5.75151	-2.18380
H	-1.89135	5.94390	-3.25320
C	-0.08612	2.15627	4.70782
H	-0.30879	1.67922	5.65847
C	3.51382	-0.86311	3.36170
H	3.30741	0.20353	3.38129
C	8.04921	-1.13060	-1.77607
H	9.07926	-0.81568	-1.63705
C	2.67008	6.00416	-0.74444
H	2.95895	5.19830	-1.42908
H	3.51344	6.70594	-0.68985
H	1.82573	6.54401	-1.18742
C	6.09056	-1.26257	-3.21535
H	5.61505	-1.06899	-4.17344
C	-0.20450	3.54074	4.57425
H	-0.51956	4.14558	5.42011

C	1.96234	6.67760	1.56942
H	1.05562	7.18690	1.22133
H	2.77569	7.41584	1.55965
H	1.81265	6.38041	2.61326
C	2.96089	-2.44655	-3.07601
H	2.09923	-3.01188	-2.70193
H	3.27576	-2.94997	-4.00129
C	3.58236	4.77152	1.25619
H	3.39547	4.38396	2.26436
H	4.41929	5.47989	1.32412
H	3.91261	3.93637	0.62670
C	2.51042	-1.04573	-3.51493
H	3.32053	-0.48845	-3.98306
H	1.68264	-1.10604	-4.22948
C	7.40613	-0.87295	-3.00361
H	7.95128	-0.36605	-3.79429
Au	-1.36118	-1.10019	-0.64699
P	-3.72371	-0.92622	-0.87094
C	-3.55842	1.13493	0.96990
H	-3.98237	0.46488	1.72574
H	-3.78163	2.16473	1.27378
H	-2.46984	1.01714	0.97404
C	-2.62821	-3.08496	1.46842
C	-4.68746	-2.00527	0.28439
C	-4.09590	-2.85755	1.25133
C	-1.95796	-4.09795	0.76132
H	-2.48346	-4.64051	-0.01976
C	-4.12217	-3.00001	-2.68947
H	-3.14494	-3.37206	-2.35984
H	-4.27426	-3.34008	-3.72110
H	-4.89505	-3.45979	-2.06724
C	-0.63101	-2.76579	2.82120
H	-0.12102	-2.26041	3.63651
C	-0.64068	-4.43723	1.07845
H	-0.14650	-5.23608	0.53201
C	-5.67681	1.20364	-0.35256
H	-6.20716	1.00489	-1.28744
H	-5.78742	2.27372	-0.13849
H	-6.17234	0.65965	0.45534
C	-1.94892	-2.42564	2.50578
H	-2.46323	-1.65931	3.07921
C	-4.18687	-1.45742	-2.66094
C	0.02671	-3.77363	2.11153
H	1.04449	-4.04625	2.37686

C	-3.50120	1.82572	-1.45145
H	-2.43491	1.60916	-1.57788
H	-3.58572	2.85917	-1.09568
H	-3.98548	1.77796	-2.43195
C	-4.93717	-3.60430	2.09628
H	-4.47701	-4.25280	2.83583
C	-6.09511	-1.96699	0.20043
H	-6.57283	-1.33016	-0.53178
C	-6.32427	-3.54431	2.00182
H	-6.94068	-4.13873	2.66983
C	-3.11972	-0.90860	-3.63483
H	-3.08986	0.18346	-3.65873
H	-3.36103	-1.25503	-4.64732
H	-2.11739	-1.27259	-3.38686
C	-6.90840	-2.72321	1.03964
H	-7.98829	-2.66570	0.94057
C	-4.17015	0.88576	-0.42739
C	-5.57217	-0.99022	-3.14825
H	-6.39227	-1.38194	-2.54228
H	-5.72443	-1.36338	-4.16848
H	-5.65182	0.09969	-3.18822
H	3.16449	-3.52848	-0.32584

1k-2

Energy: -2007341.4814972

Number of Imaginary Frequencies: 0

Si	1.56332	3.45660	0.58232
O	0.65057	1.48891	-4.10486
N	4.01096	-3.20637	-1.00041
N	0.95452	-0.49472	-3.03665
C	2.82342	-3.26230	-1.53766
C	0.97979	1.58935	-1.79110
C	1.03408	2.53069	2.14851
C	1.25447	-1.31424	-1.91652
C	0.82461	0.88481	-3.05157
C	4.81302	-3.57957	1.33129
C	0.61888	6.11931	1.21998
H	1.21587	6.04975	2.12552
C	0.49601	-1.52804	-0.83476
H	0.92265	-2.20119	-0.08684
C	1.19159	2.32951	-0.84388
C	5.96410	-3.95019	2.03659
H	6.67789	-4.63904	1.59020
C	2.53205	-2.08833	-2.38717

C	0.58697	5.04852	0.30265
C	4.69859	-2.02639	-1.43434
C	1.08693	1.12303	2.18723
H	1.36793	0.56990	1.29482
C	0.62159	3.19719	3.31772
H	0.53794	4.28014	3.32674
C	3.90115	-2.69194	1.91620
H	3.00859	-2.38294	1.37758
C	0.75733	0.41635	3.34633
H	0.79043	-0.67091	3.34232
C	3.83613	-1.32188	-2.28410
C	5.98885	-1.61540	-1.12218
H	6.62623	-2.17217	-0.44495
C	5.28915	-2.55437	3.89293
H	5.47613	-2.15256	4.88428
C	4.56030	-4.18418	-0.03758
H	5.48757	-4.57503	-0.46757
H	3.84053	-5.00845	0.00292
C	-0.19037	5.21346	-0.86056
H	-0.23090	4.41690	-1.59833
C	-0.86549	7.43157	-0.16722
H	-1.42200	8.34720	-0.34809
C	-0.09892	7.29434	0.99161
H	-0.05559	8.10322	1.71607
C	6.19656	-3.44527	3.31716
H	7.09025	-3.74159	3.85817
C	3.47003	3.74738	0.56591
C	-0.90725	6.38904	-1.09391
H	-1.49483	6.49083	-2.00256
C	0.36488	1.10098	4.49896
H	0.10808	0.55349	5.40211
C	4.14340	-2.17557	3.18911
H	3.43969	-1.47224	3.62498
C	6.42183	-0.42774	-1.71612
H	7.42146	-0.06164	-1.50585
C	3.87485	4.42969	-0.75798
H	3.61903	3.81469	-1.62895
H	4.96076	4.60104	-0.77765
H	3.38622	5.40263	-0.88159
C	4.28464	-0.13986	-2.86692
H	3.65516	0.43984	-3.53347
C	0.29401	2.49485	4.47996
H	-0.01980	3.03671	5.36821
C	3.88129	4.64890	1.75003

H	3.44945	5.65248	1.66955
H	4.97381	4.76850	1.76632
H	3.58508	4.22285	2.71641
C	2.08343	-2.42714	-3.85184
H	1.45072	-3.31928	-3.83198
H	2.93487	-2.62080	-4.50908
C	4.20126	2.39429	0.69161
H	3.95395	1.88027	1.62789
H	5.28910	2.55466	0.68163
H	3.95941	1.72036	-0.13865
C	1.25955	-1.18741	-4.29272
H	1.80669	-0.51438	-4.95796
H	0.34447	-1.49249	-4.81058
C	5.58276	0.29581	-2.57353
H	5.94506	1.21667	-3.01980
Au	-1.42660	-0.88165	-0.51058
P	-3.70998	-0.12145	-0.31845
C	-3.02032	1.20709	2.00924
H	-3.57482	0.46341	2.59257
H	-2.96713	2.12427	2.60876
H	-1.99757	0.84662	1.86349
C	-3.15727	-3.04926	1.26142
C	-4.90716	-1.25015	0.54822
C	-4.54191	-2.48567	1.14107
C	-2.77780	-4.14361	0.46842
H	-3.45023	-4.49541	-0.30921
C	-4.68820	-1.37698	-2.61040
H	-3.83087	-2.04951	-2.48767
H	-4.93245	-1.34145	-3.67948
H	-5.54370	-1.81022	-2.08474
C	-1.08159	-3.28657	2.50692
H	-0.43926	-2.96532	3.32265
C	-1.56332	-4.79693	0.68627
H	-1.29788	-5.65396	0.07233
C	-5.11112	2.11462	0.98860
H	-5.70532	2.32446	0.09530
H	-4.96469	3.06808	1.51164
H	-5.69176	1.46857	1.65199
C	-2.29253	-2.62858	2.28354
H	-2.58234	-1.80112	2.92390
C	-4.36515	0.05362	-2.12596
C	-0.71376	-4.37392	1.71115
H	0.21513	-4.90389	1.90780
C	-2.89074	2.56407	-0.10243

H	-1.90854	2.17684	-0.39243
H	-2.72558	3.43758	0.53957
H	-3.40514	2.91694	-1.00189
C	-5.54981	-3.29478	1.69879
H	-5.25871	-4.23854	2.15062
C	-6.26994	-0.88688	0.56779
H	-6.57966	0.05280	0.13201
C	-6.88872	-2.91714	1.69890
H	-7.63776	-3.56740	2.14156
C	-3.22431	0.61244	-3.00739
H	-2.91274	1.61751	-2.71371
H	-3.57870	0.66725	-4.04450
H	-2.34106	-0.03260	-2.98672
C	-7.25113	-1.69747	1.13179
H	-8.28841	-1.37552	1.12292
C	-3.72456	1.52266	0.67123
C	-5.60135	0.95191	-2.32114
H	-6.48138	0.59591	-1.78075
H	-5.86313	0.95385	-3.38692
H	-5.40918	1.99035	-2.03655
H	2.14435	-4.07696	-1.31449

1k-4

Energy: -2007372.6892249

Number of Imaginary Frequencies: 0

Si	-0.20292	2.81441	0.40809
O	0.32111	-1.62861	-2.45745
N	-5.31986	-0.85486	-0.93940
N	-1.92380	-1.17783	-2.48915
C	-4.14832	-1.23423	-1.60621
C	-0.40273	0.13630	-1.12778
C	-1.85274	3.55839	-0.14406
C	-3.06878	-0.38237	-2.11283
C	-0.64695	-0.96168	-2.08020
C	-5.65700	0.41443	1.20355
C	1.75483	4.92620	0.18648
H	1.44562	5.22539	1.18380
C	-3.04385	0.93677	-2.37422
H	-3.86500	1.60334	-2.15361
C	-0.10272	1.08711	-0.39066
C	-6.61036	1.17279	1.89387
H	-7.37439	1.71195	1.33713
C	-4.18003	-2.59963	-1.84824
C	1.18624	3.79048	-0.42253

C	-6.09368	-1.99258	-0.75831
C	-3.07601	3.27654	0.49707
H	-3.11795	2.57422	1.32332
C	-1.87630	4.47271	-1.21640
H	-0.95531	4.72614	-1.73294
C	-4.69317	-0.29048	1.93541
H	-3.95878	-0.89681	1.41120
C	-4.26382	3.89040	0.09584
H	-5.18630	3.66654	0.62480
C	-5.40956	-3.10152	-1.32225
C	-7.34535	-2.13412	-0.14410
H	-7.85903	-1.29071	0.30458
C	-5.63610	0.52883	4.01157
H	-5.63114	0.56619	5.09716
C	-5.64980	0.42315	-0.31912
H	-6.62917	0.75014	-0.68973
H	-4.92507	1.16110	-0.65876
C	1.61327	3.47100	-1.72692
H	1.19248	2.60960	-2.24006
C	3.12582	5.35888	-1.75947
H	3.86818	5.96323	-2.27336
C	2.71625	5.69820	-0.46870
H	3.13885	6.56796	0.02671
C	-6.59915	1.23457	3.28954
H	-7.34968	1.82295	3.80988
C	-0.03949	2.61368	2.31781
C	2.56819	4.24476	-2.39004
H	2.87228	3.98054	-3.39950
C	-4.26194	4.79180	-0.97176
H	-5.18519	5.27321	-1.28249
C	-4.68561	-0.23624	3.33021
H	-3.94112	-0.79834	3.88785
C	-7.90862	-3.40422	-0.12213
H	-8.88081	-3.54396	0.34161
C	1.43538	2.36643	2.70358
H	1.82452	1.44988	2.24212
H	1.51645	2.24257	3.79235
H	2.09147	3.19345	2.41439
C	-6.00474	-4.37666	-1.28653
H	-5.49956	-5.23577	-1.71979
C	-3.06526	5.07754	-1.63035
H	-3.05255	5.78035	-2.45888
C	-0.54364	3.89179	3.03009
H	0.03753	4.78180	2.76335

H	-0.45500	3.76351	4.11738
H	-1.59369	4.10393	2.80605
C	-3.10221	-3.33782	-2.58577
H	-3.53079	-4.05081	-3.30123
H	-2.49011	-3.93085	-1.88986
C	-0.86706	1.40624	2.81675
H	-1.93962	1.50967	2.62517
H	-0.74572	1.31043	3.90489
H	-0.53372	0.46575	2.36537
C	-2.21365	-2.34514	-3.34556
H	-1.26170	-2.78163	-3.64428
H	-2.73068	-1.97548	-4.23782
C	-7.24807	-4.51598	-0.68863
H	-7.72363	-5.49163	-0.65238
Au	1.93066	-0.12398	-0.28114
P	4.19466	-0.81749	-0.17298
C	3.68866	-2.40221	-2.40208
H	3.77019	-3.29408	-1.77115
H	3.93606	-2.70485	-3.42729
H	2.65169	-2.05683	-2.39578
C	2.07216	-2.81790	1.57814
C	4.53698	-2.28474	0.90345
C	3.55718	-3.00347	1.63402
C	1.38664	-2.34229	2.70884
H	1.95367	-1.98915	3.56603
C	5.05190	0.58483	2.09204
H	4.00000	0.53702	2.39344
H	5.47788	1.49727	2.52659
H	5.57243	-0.27075	2.52984
C	-0.07068	-3.30939	0.53824
H	-0.62783	-3.70799	-0.30425
C	-0.00865	-2.34701	2.75086
H	-0.52050	-1.98809	3.63934
C	6.11161	-1.87416	-2.11154
H	6.89102	-1.18367	-1.78177
H	6.28476	-2.07529	-3.17575
H	6.23187	-2.82212	-1.58162
C	1.32489	-3.29927	0.49137
H	1.83438	-3.69945	-0.37902
C	5.21527	0.64769	0.55810
C	-0.74218	-2.83631	1.66692
H	-1.82759	-2.86563	1.70801
C	4.52625	-0.07519	-2.87820
H	3.53641	0.38511	-2.78763

H	4.64849	-0.39533	-3.91994
H	5.28457	0.68871	-2.68150
C	3.98486	-4.02989	2.49801
H	3.22957	-4.57800	3.05298
C	5.89051	-2.65343	1.05878
H	6.65873	-2.12667	0.50964
C	5.32534	-4.37096	2.64275
H	5.61244	-5.17301	3.31637
C	4.60610	1.96961	0.04551
H	4.64697	2.06038	-1.04244
H	5.17844	2.80449	0.46791
H	3.56489	2.09326	0.35213
C	6.28782	-3.68063	1.90907
H	7.34054	-3.93196	1.99711
C	4.68501	-1.30731	-1.96362
C	6.71647	0.65318	0.20402
H	7.24787	-0.23770	0.54476
H	7.17935	1.50966	0.70928
H	6.89132	0.78114	-0.86789
H	-2.18056	1.38373	-2.85287

1k-5

Energy: -2007402.5967905

Number of Imaginary Frequencies: 0

Si	-0.19643	2.49372	0.33021
O	0.30912	-2.19893	-1.32964
N	-5.54194	-1.13707	-0.88541
N	-1.99910	-2.12647	-1.31616
C	-4.32171	-1.79310	-1.08028
C	-0.91693	-0.19613	-0.53750
C	-1.92331	3.15228	-0.18645
C	-3.00083	-1.30394	-0.99402
C	-0.68433	-1.55399	-1.06684
C	-6.34489	0.65533	0.66772
C	1.54968	4.72383	-0.35661
H	1.32388	5.12850	0.62517
C	-2.43472	0.01487	-0.55419
H	-2.84945	0.31618	0.41329
C	0.06799	0.65909	-0.14975
C	-7.35598	1.61747	0.77460
H	-7.76979	2.06749	-0.12532
C	-4.55791	-3.16945	-1.27158
C	1.02358	3.47816	-0.74746
C	-6.53608	-2.08275	-0.96514

C	-3.04563	3.18425	0.66559
H	-2.96599	2.82843	1.68816
C	-2.11152	3.63536	-1.49843
H	-1.27325	3.65729	-2.18895
C	-5.82752	0.07981	1.83468
H	-5.05703	-0.68474	1.76836
C	-4.28218	3.67753	0.24114
H	-5.11872	3.70201	0.93376
C	-5.94953	-3.36873	-1.19426
C	-7.92857	-1.92281	-0.85830
H	-8.37703	-0.95453	-0.66857
C	-7.31093	1.43360	3.18604
H	-7.68593	1.73181	4.16066
C	-5.79906	0.29557	-0.70489
H	-6.50249	0.61458	-1.48239
H	-4.86784	0.83134	-0.89725
C	1.34369	3.02626	-2.04444
H	0.96687	2.06627	-2.38964
C	2.65898	5.00793	-2.48900
H	3.28283	5.59632	-3.15643
C	2.36180	5.47645	-1.20856
H	2.75507	6.43250	-0.87318
C	-7.83505	2.00838	2.02703
H	-8.62196	2.75407	2.09483
C	0.09307	2.69044	2.24204
C	2.14278	3.77984	-2.90754
H	2.36252	3.40771	-3.90520
C	-4.43889	4.14198	-1.06689
H	-5.39631	4.53532	-1.39879
C	-6.30826	0.46590	3.08646
H	-5.90221	0.00884	3.98443
C	-8.70758	-3.06090	-0.97688
H	-9.78666	-2.97078	-0.89397
C	1.59459	2.54610	2.57679
H	1.97268	1.55280	2.31295
H	1.74620	2.68059	3.65768
H	2.20948	3.29136	2.06156
C	-6.77930	-4.51178	-1.30451
H	-6.34679	-5.49309	-1.47510
C	-3.34841	4.11465	-1.93800
H	-3.45286	4.48438	-2.95489
C	-0.39162	4.06253	2.76588
H	0.15574	4.89909	2.31915
H	-0.22855	4.11661	3.85161

H	-1.45580	4.23710	2.58425
C	-3.42228	-4.14367	-1.38377
H	-3.67805	-4.98498	-2.03605
H	-3.20635	-4.57169	-0.39339
C	-0.66256	1.57182	2.99868
H	-1.74831	1.61472	2.85148
H	-0.48483	1.67034	4.07922
H	-0.31686	0.57683	2.69904
C	-2.18490	-3.43798	-1.94779
H	-1.26429	-4.00131	-1.79096
H	-2.30041	-3.26603	-3.02594
C	-8.14322	-4.34647	-1.19743
H	-8.80276	-5.20432	-1.28109
Au	2.06115	0.01844	-0.15728
P	4.38093	-0.62407	-0.49214
C	3.98284	-2.68363	-2.34809
H	4.68132	-3.36105	-1.84909
H	3.88634	-3.01028	-3.39154
H	2.99857	-2.78560	-1.87774
C	3.11210	-2.26300	2.19180
C	5.11261	-1.99168	0.53672
C	4.48936	-2.55343	1.67840
C	2.94861	-1.57110	3.40230
H	3.81555	-1.12518	3.88236
C	5.20877	1.28001	1.33771
H	4.15565	1.53084	1.49006
H	5.80771	2.16139	1.59984
H	5.47864	0.47797	2.03322
C	0.73602	-2.77066	2.20927
H	-0.11831	-3.25964	1.74816
C	1.69459	-1.47721	4.00714
H	1.58886	-0.94445	4.94807
C	5.84465	-1.11957	-3.02280
H	6.20203	-0.08817	-3.09160
H	5.74049	-1.49323	-4.04946
H	6.61877	-1.72500	-2.54652
C	1.98741	-2.85369	1.59601
H	2.09923	-3.40359	0.66688
C	5.50335	0.89295	-0.12795
C	0.58573	-2.08853	3.41772
H	-0.38493	-2.04146	3.90417
C	3.47021	-0.37558	-3.15852
H	2.44156	-0.52895	-2.82032
H	3.53167	-0.69223	-4.20791

H	3.68433	0.69601	-3.12056
C	5.19156	-3.51805	2.42752
H	4.70520	-3.93879	3.30258
C	6.39868	-2.45741	0.19187
H	6.90115	-2.04772	-0.67293
C	6.46193	-3.95628	2.07023
H	6.96783	-4.70755	2.66987
C	5.07680	2.05091	-1.05080
H	5.34034	1.86273	-2.09644
H	5.60264	2.96316	-0.74236
H	4.00296	2.25178	-0.99508
C	7.06799	-3.42634	0.93328
H	8.05643	-3.75497	0.62550
C	4.46991	-1.21818	-2.33110
C	7.02106	0.66371	-0.26328
H	7.39247	-0.07267	0.45363
H	7.52983	1.61188	-0.04796
H	7.32318	0.35645	-1.26731
H	-2.72458	0.80021	-1.26516

1k-5'

Energy: -2007393.9014922

Number of Imaginary Frequencies: 0

Si	-1.05004	2.10190	0.54357
O	0.34604	-2.84369	-0.98829
N	-5.40592	-1.52516	-0.65563
N	-1.82275	-2.45560	-0.46034
C	-4.16876	-2.15998	-0.45787
C	-0.10041	-0.60343	-0.22778
C	-1.95600	3.05216	-0.83740
C	-2.85417	-1.60756	-0.45517
C	-0.43271	-1.99159	-0.60166
C	-6.16189	0.87996	-0.42315
C	0.94071	4.09622	0.07828
H	0.23158	4.49713	-0.63963
C	-2.55171	-0.14432	-0.43398
H	-3.31358	0.35557	0.17051
C	-1.12973	0.27080	-0.05266
C	-6.15567	2.18284	-0.94013
H	-5.75295	2.37191	-1.93278
C	-4.39049	-3.49263	-0.08225
C	0.66963	2.87264	0.72162
C	-6.38853	-2.46673	-0.42864
C	-2.78911	4.16577	-0.62212

H	-2.98773	4.51070	0.38783
C	-1.72640	2.67247	-2.17700
H	-1.06467	1.83474	-2.39291
C	-6.66588	0.66114	0.86348
H	-6.67140	-0.33862	1.28585
C	-3.37133	4.86015	-1.68612
H	-4.00312	5.72174	-1.48615
C	-5.78475	-3.69990	-0.03601
C	-7.78268	-2.34413	-0.55449
H	-8.24935	-1.40901	-0.84433
C	-7.17202	3.01871	1.09052
H	-7.56761	3.84482	1.67422
C	-5.68570	-0.25028	-1.32511
H	-6.44662	-0.45789	-2.08829
H	-4.79382	0.05323	-1.87587
C	1.62599	2.40081	1.64506
H	1.47769	1.45326	2.15285
C	3.01061	4.35867	1.30187
H	3.90029	4.93610	1.53868
C	2.09674	4.82953	0.35960
H	2.27281	5.77467	-0.14728
C	-6.66078	3.24429	-0.19029
H	-6.65048	4.24760	-0.60594
C	-1.91660	2.22456	2.29249
C	2.77494	3.13734	1.93830
H	3.48441	2.75844	2.66938
C	-3.13625	4.45596	-3.00142
H	-3.58471	4.99826	-3.82945
C	-7.16751	1.72678	1.61616
H	-7.55725	1.54191	2.61316
C	-8.54760	-3.46135	-0.25966
H	-9.62860	-3.39465	-0.33917
C	-1.33737	1.14666	3.23866
H	-1.49695	0.13138	2.85620
H	-1.82945	1.21233	4.21954
H	-0.26371	1.27230	3.40809
C	-6.59648	-4.81845	0.26747
H	-6.14853	-5.75812	0.57659
C	-2.30752	3.35833	-3.24571
H	-2.10504	3.04427	-4.26650
C	-1.62195	3.61353	2.91062
H	-0.54959	3.79406	3.02589
H	-2.08040	3.67469	3.90760
H	-2.03303	4.43718	2.31601

C	-3.23053	-4.37449	0.24688
H	-3.44291	-5.42370	0.01702
H	-3.00017	-4.32656	1.32171
C	-3.44868	2.03257	2.24590
H	-3.94904	2.68050	1.51998
H	-3.87557	2.25855	3.23319
H	-3.73099	0.99781	2.02199
C	-2.03646	-3.91920	-0.58527
H	-1.10805	-4.40185	-0.28890
H	-2.20224	-4.13730	-1.64788
C	-7.96500	-4.68862	0.15121
H	-8.61141	-5.53151	0.37387
H	-2.72681	0.24533	-1.45144
Au	1.98201	-0.37586	-0.34063
P	4.30298	-0.45938	-1.02407
C	3.85821	-3.14234	-1.65152
H	4.52722	-3.45150	-0.84094
H	3.84365	-3.95557	-2.38873
H	2.84446	-3.02899	-1.25833
C	3.99180	-1.40086	2.22462
C	5.60175	-0.91287	0.22749
C	5.33587	-1.25278	1.57892
C	3.17219	-2.51086	1.96968
H	3.46142	-3.22726	1.20864
C	5.36673	2.10486	-0.57730
H	4.68062	2.10766	0.27439
H	5.47251	3.14336	-0.91522
H	6.34560	1.76108	-0.23290
C	2.44860	-0.72059	3.98317
H	2.18188	-0.02741	4.77661
C	2.00949	-2.72449	2.71300
H	1.40136	-3.60261	2.51230
C	5.75847	-2.17125	-2.93091
H	6.21164	-1.32601	-3.45248
H	5.64640	-2.98056	-3.66365
H	6.45438	-2.52612	-2.16613
C	3.61632	-0.51355	3.24676
H	4.25759	0.33394	3.47407
C	4.82542	1.25723	-1.74677
C	1.64244	-1.83077	3.72039
H	0.74588	-2.00517	4.30900
C	3.39693	-1.49885	-3.49096
H	2.38934	-1.28791	-3.11775
H	3.32884	-2.35209	-4.17747

H	3.73916	-0.63868	-4.07437
C	6.42483	-1.49371	2.43978
H	6.21197	-1.75669	3.47170
C	6.94879	-0.84988	-0.18583
H	7.18042	-0.58477	-1.20864
C	7.74496	-1.42322	2.00810
H	8.55603	-1.62131	2.70297
C	3.54497	1.93423	-2.28849
H	3.05884	1.34410	-3.07133
H	3.81716	2.90440	-2.72360
H	2.81372	2.11643	-1.49643
C	8.00984	-1.10161	0.67867
H	9.03111	-1.04043	0.31405
C	4.36671	-1.85920	-2.34586
C	5.86810	1.23912	-2.88256
H	6.82371	0.79714	-2.58977
H	6.07515	2.27726	-3.17227
H	5.50620	0.72314	-3.77611

1k-1-ts

Energy: -2007333.2207116

Number of Imaginary Frequencies: -1

Si	1.73704	3.50440	0.60751
O	1.29917	1.55851	-4.10817
N	3.95291	-3.30310	-0.98208
N	1.10487	-0.46914	-3.07421
C	2.88946	-3.44781	-1.78815
C	1.32870	1.59020	-1.77129
C	1.48978	2.55662	2.22435
C	1.13738	-1.24901	-1.97334
C	1.24926	0.94300	-3.05718
C	4.44695	-3.64949	1.46263
C	-0.29359	5.35809	1.49828
H	-0.10046	4.97904	2.49811
C	0.49107	-1.52952	-0.87698
H	0.92368	-2.17017	-0.11531
C	1.46580	2.30379	-0.79026
C	5.36141	-4.20435	2.36690
H	6.01225	-5.01622	2.04932
C	2.76937	-2.36850	-2.69213
C	0.41204	4.83542	0.39825
C	4.65978	-2.14401	-1.35872
C	1.05515	1.21791	2.21293
H	0.88774	0.71365	1.26443

C	1.69353	3.16275	3.48115
H	2.02649	4.19530	3.54246
C	3.62310	-2.59900	1.88243
H	2.92669	-2.13847	1.18701
C	0.82371	0.52021	3.40152
H	0.47124	-0.50718	3.35955
C	3.96709	-1.55447	-2.43977
C	5.84156	-1.62049	-0.83609
H	6.34667	-2.07876	0.00680
C	4.62137	-2.67422	4.08647
H	4.69312	-2.29169	5.10050
C	4.35541	-4.24516	0.06802
H	5.32338	-4.67155	-0.21936
H	3.62678	-5.06329	0.03918
C	0.10263	5.34278	-0.88003
H	0.60914	4.94906	-1.75763
C	-1.54026	6.85063	0.05810
H	-2.28745	7.62891	-0.07205
C	-1.25691	6.35634	1.33261
H	-1.78398	6.74767	2.19887
C	5.44319	-3.72518	3.67484
H	6.15620	-4.16530	4.36593
C	3.52986	4.17062	0.38017
C	-0.85993	6.33894	-1.04963
H	-1.07903	6.71497	-2.04544
C	1.03164	1.14223	4.63442
H	0.84947	0.60167	5.55951
C	3.71565	-2.10916	3.18664
H	3.08565	-1.27891	3.49245
C	6.34445	-0.47112	-1.44277
H	7.26494	-0.03276	-1.07022
C	3.66716	4.83248	-1.00839
H	3.44850	4.13314	-1.82368
H	4.69673	5.19095	-1.14707
H	3.00406	5.69807	-1.11645
C	4.49517	-0.40255	-3.03497
H	4.00475	0.07401	-3.87827
C	1.47063	2.46690	4.67105
H	1.63566	2.96074	5.62480
C	3.85446	5.22179	1.46433
H	3.13808	6.05211	1.46486
H	4.84945	5.64968	1.27893
H	3.87667	4.78428	2.46838
C	2.06346	-2.48368	-4.03065

H	1.36499	-3.32542	-3.99042
H	2.77961	-2.69545	-4.83216
C	4.52903	2.99862	0.48989
H	4.46829	2.49779	1.46327
H	5.55641	3.37192	0.37411
H	4.36362	2.24420	-0.28841
C	1.29593	-1.17355	-4.34968
H	1.83841	-0.50420	-5.01860
H	0.32530	-1.38847	-4.80728
C	5.68252	0.12620	-2.52917
H	6.10641	1.01526	-2.98611
Au	-1.47454	-0.89390	-0.59389
P	-3.73555	-0.11578	-0.42212
C	-2.93396	1.49262	1.68333
H	-3.45776	0.82239	2.37415
H	-2.86581	2.47685	2.16245
H	-1.91418	1.12107	1.54412
C	-3.08641	-2.86654	1.40665
C	-4.87209	-1.12404	0.64341
C	-4.46618	-2.27856	1.35937
C	-2.75935	-3.95732	0.58551
H	-3.47285	-4.29505	-0.16106
C	-4.76811	-1.67839	-2.48037
H	-3.88727	-2.30840	-2.30870
H	-5.05999	-1.79343	-3.53157
H	-5.58714	-2.05524	-1.86136
C	-0.95800	-3.14277	2.55162
H	-0.27121	-2.84109	3.33798
C	-1.54419	-4.62793	0.74044
H	-1.31791	-5.48104	0.10617
C	-5.05886	2.28671	0.63662
H	-5.69014	2.37559	-0.25139
H	-4.88469	3.30233	1.01287
H	-5.61244	1.74664	1.40878
C	-2.17098	-2.46838	2.39361
H	-2.42278	-1.64439	3.05527
C	-4.46441	-0.18939	-2.20599
C	-0.64139	-4.22501	1.72716
H	0.29172	-4.76342	1.87105
C	-2.88512	2.56699	-0.59254
H	-1.91937	2.13520	-0.87589
H	-2.68296	3.51165	-0.07409
H	-3.44010	2.80938	-1.50444
C	-5.42542	-2.98025	2.11268

H	-5.10410	-3.86235	2.65862
C	-6.22664	-0.73776	0.72156
H	-6.56698	0.13855	0.18730
C	-6.75616	-2.57900	2.17602
H	-7.46797	-3.14659	2.76833
C	-3.38213	0.27678	-3.20587
H	-3.09824	1.32243	-3.06522
H	-3.78106	0.17657	-4.22312
H	-2.47579	-0.33318	-3.13788
C	-7.16027	-1.44664	1.47242
H	-8.19328	-1.11290	1.50357
C	-3.68958	1.64247	0.34456
C	-5.73449	0.64846	-2.44837
H	-6.57212	0.34849	-1.81464
H	-6.05362	0.50079	-3.48774
H	-5.55723	1.71971	-2.31623
H	2.22198	-4.29234	-1.67018

1k-4-ts

Energy: -2007369.9529949

Number of Imaginary Frequencies: -1

Si	-0.23362	2.77640	0.36579
O	0.38673	-1.44883	-2.40737
N	-5.32990	-1.37572	-0.83893
N	-1.91284	-1.44236	-2.34121
C	-4.06859	-1.69718	-1.35147
C	-0.67595	0.17919	-1.05861
C	-1.78418	3.56034	-0.40164
C	-3.02474	-0.79917	-1.77086
C	-0.66209	-0.97223	-1.99123
C	-6.07449	0.59351	0.54352
C	1.78502	4.85709	0.30937
H	1.38963	5.18007	1.26754
C	-2.88430	0.55686	-1.59530
H	-3.50779	1.11448	-0.91051
C	-0.03721	1.00427	-0.33426
C	-6.99108	1.63858	0.72641
H	-7.64497	1.93195	-0.09255
C	-3.93609	-3.08366	-1.42300
C	1.25677	3.71863	-0.32948
C	-5.98175	-2.56127	-0.55549
C	-3.05492	3.54375	0.20822
H	-3.19868	3.06370	1.17046
C	-1.67901	4.20412	-1.65183

H	-0.71598	4.26300	-2.15079
C	-5.25594	0.21504	1.61180
H	-4.55802	-0.60808	1.48977
C	-4.16389	4.13824	-0.39772
H	-5.12653	4.11122	0.10480
C	-5.13431	-3.65074	-0.91022
C	-7.26487	-2.76700	-0.02763
H	-7.90155	-1.93701	0.26054
C	-6.25600	1.91916	3.01431
H	-6.33163	2.42604	3.97200
C	-5.99546	-0.07766	-0.82102
H	-7.00753	-0.22337	-1.21654
H	-5.48246	0.56901	-1.53864
C	1.80511	3.36936	-1.58063
H	1.42973	2.49892	-2.11290
C	3.33858	5.23964	-1.50640
H	4.13311	5.82646	-1.95903
C	2.81588	5.60428	-0.26460
H	3.20379	6.47585	0.25558
C	-7.08036	2.29975	1.95137
H	-7.80161	3.10192	2.08068
C	-0.29634	2.66479	2.29244
C	2.82677	4.12086	-2.16627
H	3.21941	3.83412	-3.13845
C	-4.03296	4.76156	-1.64037
H	-4.89376	5.22764	-2.11230
C	-5.34798	0.87387	2.84187
H	-4.71532	0.56067	3.66789
C	-7.68405	-4.07972	0.13635
H	-8.67101	-4.27240	0.54655
C	1.10471	2.33227	2.85163
H	1.45784	1.35626	2.49849
H	1.06240	2.28546	3.94909
H	1.85471	3.08286	2.58143
C	-5.59062	-4.97372	-0.73020
H	-4.95855	-5.81717	-0.99356
C	-2.78636	4.79225	-2.26690
H	-2.67098	5.28366	-3.22928
C	-0.77446	4.00107	2.90976
H	-0.09003	4.83043	2.70171
H	-0.82906	3.89795	4.00228
H	-1.76623	4.29755	2.55586
C	-2.72457	-3.74030	-2.01777
H	-3.00375	-4.64806	-2.56519

H	-2.01134	-4.05143	-1.24041
C	-1.26040	1.53852	2.73427
H	-2.29524	1.71225	2.42239
H	-1.26276	1.47153	3.83172
H	-0.95202	0.56307	2.34490
C	-2.05310	-2.75729	-2.98681
H	-1.05472	-3.07645	-3.28474
H	-2.66739	-2.63088	-3.88459
C	-6.85731	-5.17468	-0.21094
H	-7.22708	-6.18473	-0.06319
Au	1.94178	0.04056	-0.09578
P	4.17966	-0.75631	-0.17956
C	3.96610	-2.30510	-2.50731
H	4.49078	-3.15589	-2.06447
H	4.05808	-2.38422	-3.59781
H	2.90119	-2.37714	-2.26285
C	2.18724	-2.71791	1.73416
C	4.51907	-2.40255	0.60427
C	3.58358	-3.13286	1.37723
C	1.94033	-2.01103	2.92121
H	2.77680	-1.65285	3.51455
C	4.77246	0.59973	2.16679
H	3.73729	0.95123	2.19386
H	5.38652	1.31807	2.72396
H	4.83083	-0.36023	2.69089
C	-0.21079	-3.00143	1.44992
H	-1.04682	-3.40695	0.88623
C	0.63393	-1.80040	3.36596
H	0.46204	-1.26447	4.29512
C	6.05342	-0.88542	-2.44931
H	6.49724	0.08909	-2.22750
H	6.13291	-1.03701	-3.53286
H	6.65968	-1.66186	-1.97802
C	1.09525	-3.21098	1.00259
H	1.27532	-3.77902	0.09423
C	5.31330	0.49915	0.72415
C	-0.44532	-2.30027	2.63427
H	-1.46082	-2.15806	2.99321
C	3.82370	0.17016	-2.83400
H	2.73819	0.06221	-2.75572
H	4.08907	0.09248	-3.89601
H	4.10011	1.17192	-2.49478
C	3.96634	-4.38477	1.89496
H	3.24261	-4.93563	2.48824

C	5.79416	-2.96967	0.39404
H	6.53115	-2.43626	-0.19054
C	5.22870	-4.92526	1.67394
H	5.48663	-5.89446	2.09074
C	5.18138	1.87316	0.03750
H	5.63539	1.88463	-0.95823
H	5.70808	2.62119	0.64280
H	4.13909	2.19470	-0.05378
C	6.15243	-4.20882	0.91587
H	7.14526	-4.60674	0.72791
C	4.56164	-0.95075	-2.06537
C	6.80096	0.10205	0.80277
H	6.95147	-0.81484	1.37795
H	7.33948	0.90375	1.32300
H	7.26810	-0.01641	-0.17729
H	-2.32394	1.14775	-2.31128

1k-4'-ts
Energy: -2007362.2956663
Number of Imaginary Frequencies: -1

Si	-1.17622	2.02245	0.86595
O	0.50389	-2.47214	-1.79474
N	-5.33115	-1.58028	-0.63025
N	-1.72076	-2.18251	-1.39081
C	-4.00872	-2.05883	-0.67936
C	-0.05721	-0.54746	-0.53395
C	-1.97601	3.11582	-0.45037
C	-2.83487	-1.35330	-1.15182
C	-0.38247	-1.77981	-1.31246
C	-6.46136	0.68739	-0.86737
C	0.59804	4.22606	1.25547
H	-0.14357	4.79269	0.69990
C	-2.75662	0.00404	-1.35877
H	-3.57580	0.64339	-1.06008
C	-0.74521	0.41198	-0.05268
C	-6.76256	1.78249	-1.69018
H	-6.55530	1.72817	-2.75709
C	-3.96235	-3.35715	-0.19048
C	0.43917	2.83658	1.42522
C	-6.10800	-2.59754	-0.09000
C	-3.26059	3.67902	-0.34889
H	-3.88059	3.48653	0.52060
C	-1.22748	3.40179	-1.61182
H	-0.22532	2.99282	-1.72484

C	-6.73740	0.77482	0.50109
H	-6.50728	-0.06202	1.15264
C	-3.77512	4.49509	-1.36000
H	-4.77131	4.91431	-1.25421
C	-5.27807	-3.71238	0.21758
C	-7.49455	-2.63992	0.11254
H	-8.13025	-1.79351	-0.12607
C	-7.61036	3.01675	0.21002
H	-8.06226	3.91286	0.62579
C	-5.91988	-0.57396	-1.52353
H	-6.73488	-1.07089	-2.06670
H	-5.17133	-0.31158	-2.27451
C	1.43374	2.14826	2.14901
H	1.36226	1.07483	2.29966
C	2.65688	4.20444	2.52628
H	3.50282	4.73086	2.95987
C	1.69400	4.90275	1.79739
H	1.78829	5.97599	1.65582
C	-7.33605	2.93686	-1.15834
H	-7.57272	3.77169	-1.81243
C	-2.23005	1.58130	2.41919
C	2.52487	2.82429	2.69821
H	3.26894	2.27247	3.26678
C	-3.01643	4.76386	-2.49907
H	-3.41579	5.39968	-3.28444
C	-7.30681	1.93453	1.03643
H	-7.51842	1.98557	2.10095
C	-8.02898	-3.80308	0.65278
H	-9.09925	-3.86095	0.82798
C	-1.42439	0.63800	3.34183
H	-1.13278	-0.28931	2.83400
H	-2.04423	0.36011	4.20534
H	-0.51916	1.11390	3.73090
C	-5.84788	-4.87688	0.77087
H	-5.22581	-5.73178	1.02076
C	-1.73839	4.21331	-2.62457
H	-1.13979	4.41937	-3.50784
C	-2.52734	2.88601	3.19759
H	-1.60953	3.40431	3.49573
H	-3.08316	2.64622	4.11440
H	-3.13795	3.59088	2.62305
C	-2.70562	-4.16414	-0.29979
H	-2.93612	-5.22682	-0.43761
H	-2.07496	-4.08655	0.59795

C	-3.55442	0.88063	2.06012
H	-4.19119	1.47966	1.40406
H	-4.12619	0.68779	2.97878
H	-3.38439	-0.08506	1.57309
C	-1.94685	-3.64389	-1.52569
H	-0.97186	-4.10870	-1.65093
H	-2.53309	-3.82050	-2.43395
C	-7.21570	-4.91048	0.98454
H	-7.67508	-5.79742	1.41011
H	-2.03792	0.43476	-2.04106
Au	2.08609	-0.26665	-0.42340
P	4.39899	-0.17144	-1.00043
C	4.03604	-2.63298	-2.25883
H	4.64807	-3.11404	-1.48812
H	4.09893	-3.25565	-3.16011
H	2.99144	-2.62040	-1.93596
C	3.84342	-1.80027	1.92693
C	5.59588	-0.89026	0.21872
C	5.23126	-1.52031	1.43719
C	3.04986	-2.80972	1.35859
H	3.40255	-3.34131	0.48140
C	5.25346	2.24254	0.14510
H	4.46849	2.05491	0.88410
H	5.37146	3.33012	0.06343
H	6.19271	1.82917	0.52177
C	2.16069	-1.51642	3.66615
H	1.82779	-1.01924	4.57311
C	1.82910	-3.16678	1.93649
H	1.24077	-3.96379	1.49010
C	5.99935	-1.37331	-3.14089
H	6.46701	-0.42320	-3.40756
H	5.95638	-1.97993	-4.05385
H	6.64782	-1.89946	-2.43564
C	3.38408	-1.16465	3.09287
H	4.00192	-0.40209	3.55980
C	4.88156	1.68311	-1.24325
C	1.38028	-2.52217	3.09055
H	0.43950	-2.81256	3.54985
C	3.66289	-0.60262	-3.69117
H	2.62835	-0.49163	-3.34945
H	3.65469	-1.26900	-4.56225
H	4.02739	0.37192	-4.02973
C	6.25645	-1.94718	2.30339
H	5.97179	-2.43289	3.23190

C	6.96847	-0.73861	-0.06903
H	7.27289	-0.25894	-0.98962
C	7.60396	-1.78412	1.99978
H	8.36335	-2.13291	2.69353
C	3.63109	2.43660	-1.75325
H	3.25623	2.03887	-2.70081
H	3.89946	3.48781	-1.91666
H	2.81643	2.41023	-1.02336
C	7.96422	-1.17704	0.79853
H	9.00899	-1.04013	0.53587
C	4.56250	-1.22248	-2.60242
C	6.03571	1.95247	-2.22952
H	6.97582	1.47928	-1.93681
H	6.21959	3.03383	-2.25050
H	5.79378	1.64826	-3.25138

1o-1

Energy: -2238174.2870804

Number of Imaginary Frequencies: 0

O	-4.06011	4.37952	0.44831
C	-3.70436	3.25405	0.71506
N	-3.43698	2.32524	-0.40263
C	-3.78406	2.78370	-1.77902
C	-5.23685	2.40801	-2.13567
C	-5.47852	0.92896	-2.15886
C	-6.07970	0.18989	-1.18201
C	-2.99552	1.13292	-0.19681
C	-2.40219	0.02111	-0.01720
H	-2.90461	-0.93163	0.11428
N	-6.10906	-1.15987	-1.54075
C	-6.70594	-2.10901	-0.68564
O	-6.71521	-3.31742	-1.24480
C	-7.33686	-4.48115	-0.54879
C	-8.82528	-4.20601	-0.32379
C	-7.13286	-5.61195	-1.55813
C	-6.58251	-4.76210	0.75303
O	-7.13073	-1.79023	0.40694
C	-5.49987	-1.29534	-2.80531
C	-5.27080	-2.41541	-3.60904
C	-4.62808	-2.21299	-4.82886
C	-4.22413	-0.93300	-5.24611
C	-4.45320	0.17898	-4.44307
C	-5.09401	0.00320	-3.20763
C	-3.51357	2.71184	2.01334

C	-3.42463	2.34140	3.16999
Au	-0.31050	0.10508	0.02556
P	2.03436	0.19717	0.04270
O	2.69305	1.65421	-0.20794
C	1.96807	2.86397	-0.08355
C	2.09007	3.84615	-1.08740
C	2.96856	3.67590	-2.34684
C	2.94406	4.93418	-3.24035
C	4.44294	3.43457	-1.93914
C	2.45064	2.49596	-3.20468
C	1.36162	5.02254	-0.85851
C	0.55648	5.26388	0.26968
C	-0.18132	6.60864	0.41026
C	-1.15158	6.79714	-0.78042
C	-1.00192	6.68974	1.71209
C	0.85211	7.76126	0.41930
C	0.48756	4.25395	1.23110
C	1.19755	3.06404	1.05790
O	2.61066	-0.72577	-1.13052
C	3.93195	-1.10077	-1.48915
C	4.06968	-2.06838	-2.50380
C	2.87294	-2.71625	-3.23881
C	3.33758	-3.73629	-4.29995
C	1.96790	-3.48092	-2.24126
C	2.04507	-1.63412	-3.97516
C	5.39205	-2.40510	-2.82581
C	6.53021	-1.84701	-2.21855
C	7.93383	-2.30062	-2.65920
C	8.12306	-2.00485	-4.16642
C	9.04876	-1.57234	-1.88402
C	8.08562	-3.82056	-2.41014
C	6.31736	-0.88656	-1.22800
C	5.02359	-0.51201	-0.86442
O	2.79717	-0.21865	1.41320
C	2.39666	-1.25882	2.28080
C	2.79209	-1.18781	3.63334
C	3.69941	-0.07337	4.20299
C	3.94345	-0.24798	5.71696
C	5.08021	-0.12759	3.50231
C	3.06533	1.32357	4.00234
C	2.34790	-2.24470	4.43965
C	1.57824	-3.33236	3.98946
C	1.15321	-4.43090	4.98080
C	0.29817	-3.80461	6.10844

C	0.31803	-5.53334	4.30180
C	2.41141	-5.08944	5.59594
C	1.25485	-3.36253	2.63281
C	1.67020	-2.33604	1.78261
C	-3.32348	1.90145	4.51989
C	-4.34366	2.40678	5.55048
C	-2.94376	2.90570	5.61633
H	-3.64275	3.86453	-1.78692
H	-3.06987	2.31182	-2.45616
H	-5.91050	2.90120	-1.42644
H	-5.44418	2.84890	-3.11916
H	-9.31555	-3.95349	-1.26995
H	-9.30234	-5.10839	0.07348
H	-8.97852	-3.39098	0.38534
H	-6.06761	-5.77792	-1.75000
H	-7.55884	-6.54027	-1.16479
H	-7.62843	-5.38188	-2.50664
H	-6.71414	-3.95254	1.47278
H	-6.96310	-5.68856	1.19629
H	-5.51338	-4.89764	0.55502
H	-5.58634	-3.40216	-3.30074
H	-4.44350	-3.06722	-5.47378
H	-3.73406	-0.81258	-6.20779
H	-4.14935	1.16848	-4.77551
H	3.32654	5.81870	-2.71921
H	3.58720	4.76438	-4.11010
H	1.93973	5.15933	-3.61669
H	4.56805	2.51775	-1.36050
H	5.06550	3.35119	-2.83758
H	4.82300	4.27285	-1.34414
H	1.41236	2.66571	-3.51399
H	3.05847	2.40202	-4.11203
H	2.50083	1.54277	-2.67592
H	1.42763	5.80559	-1.60199
H	-1.92169	6.01691	-0.78387
H	-1.65840	7.76611	-0.70488
H	-0.63165	6.76919	-1.74397
H	-0.36877	6.58734	2.60104
H	-1.49615	7.66519	1.77279
H	-1.78611	5.92468	1.75087
H	1.43844	7.79505	-0.50486
H	0.34152	8.72574	0.52287
H	1.55167	7.65627	1.25629
H	-0.09966	4.37937	2.13310

H	1.17599	2.30576	1.83395
H	3.90141	-4.56573	-3.85872
H	2.45839	-4.16404	-4.79325
H	3.95442	-3.27281	-5.07766
H	1.49230	-2.80829	-1.52385
H	1.17172	-4.00162	-2.78662
H	2.54136	-4.23166	-1.68566
H	2.66642	-1.09306	-4.69770
H	1.22406	-2.10759	-4.52691
H	1.60981	-0.90698	-3.28573
H	5.54857	-3.14544	-3.59863
H	8.02629	-0.93266	-4.37189
H	9.11987	-2.32372	-4.49286
H	7.38849	-2.53245	-4.78400
H	8.99171	-1.76437	-0.80636
H	10.02655	-1.92557	-2.22878
H	9.01683	-0.48825	-2.04319
H	7.34954	-4.40421	-2.97331
H	9.08200	-4.15767	-2.71916
H	7.96148	-4.05973	-1.34778
H	7.14968	-0.41156	-0.72252
H	4.88012	0.23990	-0.09805
H	4.44631	-1.19228	5.95127
H	4.59216	0.56099	6.06874
H	3.01299	-0.19745	6.29425
H	4.99787	0.01651	2.42243
H	5.73200	0.65917	3.90036
H	5.56907	-1.09198	3.68023
H	2.05908	1.36462	4.43741
H	3.67628	2.08308	4.50373
H	3.00350	1.59607	2.94826
H	2.62380	-2.22782	5.48539
H	-0.60857	-3.34065	5.70264
H	-0.00751	-4.57590	6.82500
H	0.84858	-3.03736	6.66337
H	0.88078	-6.04724	3.51409
H	0.03149	-6.28655	5.04347
H	-0.60481	-5.13631	3.86268
H	3.03008	-4.36652	6.13799
H	2.11962	-5.87288	6.30512
H	3.03386	-5.54854	4.81979
H	0.69169	-4.18561	2.20865
H	1.44993	-2.40541	0.72276
H	-2.97033	0.88150	4.65111

H	-5.11622	3.07741	5.18882
H	-4.67732	1.67337	6.27791
H	-2.28623	2.52797	6.39329
H	-2.74337	3.92463	5.30129
H	-6.53423	0.48612	-0.24848

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Energy: -2238169.0168166

Number of Imaginary Frequencies: 0

O	-2.81804	3.17645	2.87201
C	-2.82985	2.25486	2.06396
N	-3.25714	2.47573	0.74913
C	-3.93864	3.72819	0.41541
C	-5.13641	3.28360	-0.45715
C	-4.80691	1.83895	-0.94217
C	-5.51449	0.72649	-0.30405
C	-3.37063	1.55150	-0.29370
C	-2.49709	0.63576	-0.74575
H	-2.89109	-0.02383	-1.51909
N	-5.94042	-0.17149	-1.18846
C	-6.55455	-1.40900	-0.71665
O	-6.92329	-2.14569	-1.73683
C	-7.60568	-3.48482	-1.52799
C	-8.92275	-3.25431	-0.78941
C	-7.83718	-3.95031	-2.96339
C	-6.64745	-4.41142	-0.78169
O	-6.65677	-1.60078	0.46945
C	-5.64352	0.28570	-2.52582
C	-5.92928	-0.28975	-3.75939
C	-5.50571	0.40948	-4.89380
C	-4.82479	1.62752	-4.78952
C	-4.54858	2.18707	-3.53797
C	-4.96688	1.50753	-2.40017
C	-2.46755	0.91061	2.43243
C	-2.16895	-0.15457	2.93777
Au	-0.51760	0.43586	-0.29066
P	1.82870	0.22779	0.01592
O	2.67524	1.58576	0.27614
C	2.08369	2.77880	0.75539
C	2.43189	4.00636	0.15697
C	3.42919	4.13043	-1.01593
C	3.64581	5.59976	-1.43566
C	4.81073	3.56618	-0.60209
C	2.89329	3.37518	-2.25641

C	1.81217	5.13532	0.71185
C	0.90199	5.10571	1.78346
C	0.26839	6.41568	2.28732
C	-0.55815	7.05316	1.14436
C	-0.66841	6.18200	3.48827
C	1.37924	7.39982	2.72479
C	0.61281	3.85986	2.34292
C	1.20951	2.70478	1.83501
O	2.45511	-0.37823	-1.33650
C	3.76730	-0.74805	-1.71007
C	3.93017	-1.33093	-2.98376
C	2.76285	-1.55998	-3.97232
C	3.24372	-2.20983	-5.28744
C	1.70558	-2.50920	-3.35626
C	2.10187	-0.20941	-4.34400
C	5.24515	-1.68602	-3.31436
C	6.35896	-1.49324	-2.47883
C	7.75806	-1.92272	-2.95681
C	8.12493	-1.14378	-4.24283
C	8.84365	-1.64254	-1.89994
C	7.75953	-3.44072	-3.25791
C	6.12676	-0.90188	-1.23594
C	4.83819	-0.52880	-0.85277
O	2.42586	-0.66122	1.25006
C	1.95879	-1.91687	1.67252
C	2.33050	-2.36362	2.96055
C	3.24616	-1.55888	3.91180
C	3.44368	-2.27453	5.26500
C	4.64581	-1.39577	3.26939
C	2.64344	-0.16665	4.21823
C	1.84578	-3.62879	3.32080
C	1.04756	-4.44775	2.50124
C	0.60046	-5.83336	3.00302
C	-0.22376	-5.68013	4.30339
C	-0.27110	-6.57066	1.96795
C	1.84841	-6.70334	3.28924
C	0.72683	-3.95558	1.23540
C	1.18810	-2.70423	0.82168
C	-1.81272	-1.41844	3.50514
C	-2.64654	-1.98922	4.65440
C	-1.26913	-1.48323	4.93097
H	-4.22664	4.23652	1.33509
H	-3.26317	4.38384	-0.14558
H	-6.06672	3.29199	0.11734

H	-5.28104	3.93809	-1.31974
H	-9.54773	-2.53270	-1.32569
H	-9.47013	-4.20145	-0.74101
H	-8.75931	-2.90165	0.23058
H	-6.88958	-4.05453	-3.50145
H	-8.33151	-4.92656	-2.95255
H	-8.48002	-3.24988	-3.50595
H	-6.46133	-4.06637	0.23706
H	-7.09293	-5.41037	-0.72965
H	-5.69472	-4.49547	-1.31496
H	-6.45472	-1.22996	-3.84363
H	-5.71344	-0.00642	-5.87477
H	-4.50715	2.14368	-5.69004
H	-4.01373	3.12893	-3.45952
H	4.05624	6.20598	-0.62054
H	4.36513	5.63161	-2.26091
H	2.72238	6.07283	-1.78875
H	4.76640	2.50343	-0.35775
H	5.52454	3.69220	-1.42479
H	5.20330	4.10417	0.26844
H	1.92324	3.78007	-2.56895
H	3.59117	3.49166	-3.09414
H	2.77538	2.30638	-2.07166
H	2.04928	6.09952	0.28201
H	-1.36545	6.38243	0.82570
H	-1.01165	7.99304	1.48109
H	0.05868	7.27611	0.26692
H	-0.12851	5.76585	4.34674
H	-1.10137	7.13718	3.80606
H	-1.49401	5.50481	3.24427
H	2.05573	7.65254	1.90139
H	0.93545	8.33475	3.08692
H	1.98145	6.97474	3.53558
H	-0.07765	3.76239	3.17147
H	0.99903	1.74607	2.29822
H	3.68871	-3.19770	-5.12387
H	2.38494	-2.34364	-5.95407
H	3.97232	-1.58481	-5.81532
H	1.22022	-2.06556	-2.48433
H	0.92712	-2.72782	-4.09750
H	2.16027	-3.45994	-3.05523
H	2.83235	0.46984	-4.79784
H	1.30120	-0.37763	-5.07483
H	1.66537	0.28777	-3.47498

H	5.41748	-2.13788	-4.28197
H	8.13876	-0.06373	-4.05733
H	9.11975	-1.44057	-4.59556
H	7.41501	-1.33557	-5.05440
H	8.65691	-2.18706	-0.96709
H	9.81892	-1.96612	-2.27947
H	8.92065	-0.57464	-1.66548
H	7.03704	-3.70545	-4.03732
H	8.75059	-3.75726	-3.60394
H	7.51227	-4.01982	-2.36082
H	6.93989	-0.71819	-0.54378
H	4.68078	-0.06437	0.11227
H	3.92427	-3.25269	5.15439
H	4.09483	-1.66338	5.89852
H	2.49867	-2.41118	5.80380
H	4.59852	-0.85654	2.32120
H	5.30319	-0.83566	3.94495
H	5.10573	-2.37304	3.08403
H	1.62996	-0.25798	4.62703
H	3.26010	0.34706	4.96488
H	2.60327	0.46659	3.33148
H	2.11544	-4.01069	4.29665
H	-1.12946	-5.08665	4.12710
H	-0.53414	-6.66346	4.67589
H	0.34969	-5.19254	5.09880
H	0.27103	-6.75251	1.03309
H	-0.57252	-7.54520	2.36705
H	-1.18574	-6.01356	1.73214
H	2.49202	-6.25608	4.05393
H	1.54707	-7.69503	3.64687
H	2.44938	-6.83687	2.38282
H	0.13523	-4.54001	0.54025
H	0.96001	-2.36357	-0.18235
H	-1.40299	-2.14129	2.80284
H	-3.49017	-1.39829	4.99661
H	-2.81781	-3.06152	4.63737
H	-0.47407	-2.20171	5.10337
H	-1.16600	-0.54347	5.46428
H	-5.65689	0.55009	0.75413

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Energy: -2238194.2766832

Number of Imaginary Frequencies: 0

O	1.51220	-1.99328	-1.60005

C	2.35542	-1.09572	-1.63917
N	3.56620	-1.22292	-2.25433
C	3.95265	-2.61574	-2.60008
C	5.40927	-2.71867	-3.08140
C	6.30189	-1.81087	-2.29147
C	5.85591	-0.57730	-1.91318
C	4.51810	-0.14507	-2.32790
C	4.16703	1.03864	-2.84999
H	4.85963	1.87010	-2.85911
N	6.90927	0.15652	-1.32276
C	6.71529	1.34228	-0.59044
O	7.88484	1.89470	-0.27121
C	7.96738	3.14702	0.52940
C	7.33809	2.92356	1.90650
C	9.47764	3.36225	0.64744
C	7.31459	4.29383	-0.24659
O	5.60833	1.77621	-0.32548
C	8.06262	-0.67656	-1.34311
C	9.36551	-0.46267	-0.88601
C	10.28854	-1.49481	-1.05094
C	9.93722	-2.71463	-1.65271
C	8.64078	-2.92888	-2.10349
C	7.69333	-1.90766	-1.94406
C	2.10656	0.16111	-0.91718
C	2.09179	1.14597	-0.16865
Au	-0.06473	0.10153	-0.10110
P	-2.30870	-0.32116	0.34379
O	-2.65048	-1.61721	1.23332
C	-1.69946	-2.30601	2.03170
C	-1.63804	-3.71185	1.96988
C	-2.53326	-4.57174	1.05062
C	-2.26722	-6.08056	1.23847
C	-4.02724	-4.32779	1.37714
C	-2.24639	-4.23759	-0.43322
C	-0.69379	-4.29851	2.82453
C	0.15445	-3.59060	3.69480
C	1.14625	-4.35833	4.58772
C	2.09529	-5.20164	3.70290
C	2.00576	-3.41182	5.44696
C	0.36057	-5.29481	5.53737
C	0.03329	-2.20030	3.71336
C	-0.89716	-1.56298	2.89112
O	-3.05353	-0.54662	-1.04954
C	-4.42682	-0.70249	-1.38497

C	-4.75039	-0.73882	-2.75530
C	-3.70111	-0.65954	-3.88983
C	-4.36311	-0.71405	-5.28332
C	-2.90620	0.66760	-3.81704
C	-2.72572	-1.85902	-3.79712
C	-6.11708	-0.88161	-3.03441
C	-7.12561	-0.99621	-2.06200
C	-8.59395	-1.15289	-2.49729
C	-8.74305	-2.42761	-3.36220
C	-9.54543	-1.27770	-1.29170
C	-9.02047	0.08336	-3.32486
C	-6.72746	-0.96690	-0.72426
C	-5.38231	-0.82103	-0.38478
O	-3.11046	0.81572	1.17333
C	-2.99328	2.21096	0.97781
C	-3.32968	3.06522	2.04959
C	-3.87473	2.56668	3.40768
C	-4.17004	3.73378	4.37355
C	-5.20517	1.80473	3.18569
C	-2.85019	1.64371	4.10874
C	-3.18095	4.43440	1.78860
C	-2.75362	4.97932	0.56442
C	-2.63273	6.50590	0.40648
C	-1.60636	7.04824	1.43007
C	-2.16326	6.90706	-1.00505
C	-4.00956	7.16488	0.66299
C	-2.47599	4.08142	-0.46705
C	-2.60291	2.70547	-0.26312
C	2.39556	2.34709	0.55706
C	1.79860	2.64089	1.92925
C	1.37159	3.46191	0.75710
H	3.80399	-3.22589	-1.70325
H	3.26117	-2.98741	-3.36155
H	5.71924	-3.76572	-2.99924
H	5.46981	-2.46078	-4.14811
H	7.79894	2.06359	2.40392
H	7.51218	3.80723	2.52990
H	6.26249	2.75486	1.83309
H	9.93639	3.45349	-0.34203
H	9.67782	4.28209	1.20589
H	9.95162	2.53049	1.17853
H	6.23815	4.14701	-0.34814
H	7.49075	5.23541	0.28454
H	7.75762	4.38156	-1.24426

H	9.65992	0.47215	-0.43328
H	11.30853	-1.34261	-0.71012
H	10.68650	-3.49204	-1.76813
H	8.36360	-3.86931	-2.57150
H	-2.47147	-6.41276	2.26249
H	-2.93142	-6.64351	0.57449
H	-1.23873	-6.35729	0.98095
H	-4.32827	-3.29391	1.19803
H	-4.65216	-4.97146	0.74718
H	-4.24178	-4.57239	2.42375
H	-1.19057	-4.40397	-0.67552
H	-2.84832	-4.88462	-1.08195
H	-2.49424	-3.20431	-0.68147
H	-0.61243	-5.37698	2.81419
H	2.67210	-4.56258	3.02429
H	2.80235	-5.75670	4.33035
H	1.55091	-5.93124	3.09425
H	1.39517	-2.80822	6.12827
H	2.69680	-3.99883	6.06136
H	2.60777	-2.73397	4.83032
H	-0.24427	-6.02262	4.98637
H	1.05338	-5.85438	6.17665
H	-0.31253	-4.72279	6.18605
H	0.64149	-1.59344	4.37366
H	-1.01683	-0.48595	2.94613
H	-5.04699	0.12547	-5.45140
H	-3.58367	-0.66124	-6.05070
H	-4.91342	-1.64758	-5.44247
H	-2.28061	0.71849	-2.92277
H	-2.24504	0.75099	-4.68770
H	-3.57983	1.53227	-3.82303
H	-3.26816	-2.80879	-3.86294
H	-2.01285	-1.82210	-4.62961
H	-2.15241	-1.85672	-2.86729
H	-6.41827	-0.91029	-4.07285
H	-8.44967	-3.32141	-2.79994
H	-9.78605	-2.55162	-3.67598
H	-8.12859	-2.38442	-4.26789
H	-9.51486	-0.38902	-0.65063
H	-10.57554	-1.38998	-1.64648
H	-9.31308	-2.15471	-0.67660
H	-8.40763	0.20526	-4.22429
H	-10.06387	-0.01755	-3.64553
H	-8.93485	1.00171	-2.73282

H	-7.45112	-1.05832	0.07688
H	-5.09405	-0.80524	0.65934
H	-4.92329	4.42236	3.97550
H	-4.56395	3.32690	5.31055
H	-3.26927	4.30780	4.61913
H	-5.07339	0.92563	2.55095
H	-5.60684	1.46847	4.14875
H	-5.95245	2.45551	2.71806
H	-1.88237	2.14706	4.22333
H	-3.21003	1.38113	5.11017
H	-2.70015	0.71271	3.56091
H	-3.42112	5.12482	2.58591
H	-0.61530	6.60911	1.26426
H	-1.51452	8.13638	1.33479
H	-1.90107	6.82981	2.46187
H	-2.86775	6.58167	-1.77898
H	-2.08533	7.99750	-1.07113
H	-1.17629	6.49226	-1.24140
H	-4.37995	6.96225	1.67327
H	-3.93414	8.25262	0.55007
H	-4.75911	6.80112	-0.04873
H	-2.17546	4.42958	-1.44836
H	-2.43003	2.03074	-1.09370
H	3.43237	2.63450	0.39021
H	1.09652	1.91678	2.33182
H	2.47532	3.07380	2.65950
H	1.75319	4.47378	0.65975
H	0.37423	3.30999	0.35597
H	3.17650	1.20534	-3.25782

1o-5’

Energy: -2238245.3045798

Number of Imaginary Frequencies: 0

O	1.68914	-1.76671	-0.39374
C	2.61883	-0.98903	-0.42999
N	3.97955	-1.49833	-0.68238
C	4.27106	-2.91980	-0.87713
C	5.31662	-3.08883	-1.98394
C	6.42621	-2.10088	-1.77871
C	6.22417	-0.90839	-1.08744
C	4.89917	-0.54226	-0.71186
C	4.24619	0.78073	-0.43830
H	4.69794	1.22066	0.45608
N	7.40713	-0.13436	-1.13907

C	7.65696	0.94886	-0.25321
O	8.78468	1.56459	-0.56787
C	9.29726	2.72015	0.24750
C	9.55235	2.25625	1.68185
C	10.60374	3.06248	-0.46780
C	8.29908	3.87514	0.15920
O	6.88486	1.21880	0.64321
C	8.35137	-0.86131	-1.89028
C	9.67426	-0.56720	-2.24086
C	10.35839	-1.50481	-3.00746
C	9.76774	-2.71651	-3.42718
C	8.46326	-3.01444	-3.07978
C	7.74639	-2.08369	-2.30050
C	2.77144	0.44814	-0.28393
C	1.74314	1.31472	-0.02612
Au	-0.19664	0.61615	0.16637
P	-2.41941	-0.20251	0.33763
O	-2.71801	-1.35903	1.44211
C	-1.86595	-1.60530	2.54007
C	-1.51457	-2.93386	2.85531
C	-1.98851	-4.15659	2.03909
C	-1.45396	-5.48072	2.62495
C	-3.53462	-4.23943	2.05487
C	-1.47405	-4.06168	0.58183
C	-0.69985	-3.08333	3.98649
C	-0.23377	-2.02393	4.78529
C	0.65928	-2.31980	6.00409
C	1.94954	-3.03514	5.53642
C	1.06691	-1.03513	6.75058
C	-0.10215	-3.23155	6.99604
C	-0.62351	-0.73361	4.42378
C	-1.44145	-0.52868	3.31203
O	-2.83170	-0.89501	-1.05796
C	-4.06183	-1.39568	-1.54050
C	-4.13210	-1.72637	-2.90987
C	-2.93536	-1.60209	-3.88203
C	-3.31475	-2.02995	-5.31609
C	-2.43877	-0.13762	-3.96398
C	-1.77856	-2.52253	-3.41920
C	-5.37441	-2.20813	-3.34542
C	-6.50086	-2.37519	-2.52160
C	-7.81700	-2.90229	-3.12236
C	-7.58604	-4.31091	-3.72003
C	-8.93647	-3.00477	-2.06867

C	-8.29461	-1.94301	-4.23897
C	-6.35506	-2.04907	-1.17250
C	-5.14185	-1.56531	-0.68250
O	-3.63330	0.81990	0.72269
C	-3.74204	2.14981	0.27336
C	-4.49742	3.05905	1.04560
C	-5.28021	2.65458	2.31575
C	-6.00176	3.85921	2.95683
C	-6.36501	1.61495	1.93848
C	-4.33977	2.06257	3.39191
C	-4.54371	4.37039	0.55271
C	-3.92086	4.80652	-0.63004
C	-4.03696	6.28052	-1.05898
C	-3.43091	7.18522	0.04077
C	-3.28959	6.56140	-2.37674
C	-5.52654	6.64753	-1.26271
C	-3.22935	3.84893	-1.37254
C	-3.14852	2.52864	-0.92692
C	2.04150	2.74523	0.11349
C	1.26381	3.61175	1.11409
C	1.03195	3.80834	-0.33965
H	4.65086	-3.31690	0.07279
H	3.32256	-3.40991	-1.10162
H	5.69497	-4.11612	-1.96505
H	4.86820	-2.93890	-2.97728
H	10.22283	1.39045	1.69515
H	10.03892	3.06589	2.23594
H	8.62421	1.99790	2.19447
H	10.42044	3.32393	-1.51475
H	11.07609	3.91976	0.02160
H	11.30471	2.22222	-0.43031
H	7.35809	3.63088	0.65472
H	8.72839	4.75578	0.64841
H	8.10067	4.13421	-0.88627
H	10.14538	0.35713	-1.94329
H	11.38304	-1.29087	-3.29689
H	10.34522	-3.41325	-4.02618
H	7.99805	-3.94352	-3.39495
H	-1.79772	-5.64977	3.65149
H	-1.82253	-6.31345	2.01651
H	-0.35885	-5.52589	2.61340
H	-3.99805	-3.36482	1.59489
H	-3.86467	-5.12550	1.49948
H	-3.90823	-4.32787	3.08163

H	-0.38181	-3.97389	0.55579
H	-1.75638	-4.96651	0.03013
H	-1.89434	-3.20749	0.04957
H	-0.40784	-4.08696	4.26601
H	2.51528	-2.40562	4.83926
H	2.59477	-3.25630	6.39508
H	1.73232	-3.98279	5.03218
H	0.19618	-0.49677	7.14204
H	1.70497	-1.29039	7.60370
H	1.63343	-0.35081	6.10815
H	-0.38542	-4.18634	6.54067
H	0.52506	-3.45233	7.86798
H	-1.01782	-2.74546	7.35102
H	-0.31413	0.12885	5.00244
H	-1.76701	0.47555	3.06244
H	-4.10898	-1.40413	-5.73836
H	-2.43702	-1.92588	-5.96319
H	-3.63487	-3.07649	-5.36575
H	-2.01302	0.20137	-3.01746
H	-1.65700	-0.05461	-4.72876
H	-3.25447	0.53945	-4.24273
H	-2.10801	-3.56699	-3.37528
H	-0.94826	-2.46229	-4.13404
H	-1.39610	-2.24181	-2.43569
H	-5.47491	-2.47150	-4.38987
H	-7.25571	-5.01586	-2.94853
H	-8.51575	-4.69546	-4.15607
H	-6.82830	-4.30077	-4.51075
H	-9.16731	-2.03083	-1.62203
H	-9.85289	-3.37559	-2.54065
H	-8.67809	-3.70056	-1.26214
H	-7.56066	-1.85600	-5.04726
H	-9.23009	-2.30889	-4.67864
H	-8.47664	-0.93788	-3.84179
H	-7.17821	-2.16354	-0.47722
H	-5.04782	-1.32572	0.36911
H	-6.73473	4.31283	2.28089
H	-6.54608	3.51663	3.84328
H	-5.30063	4.63656	3.28176
H	-5.93179	0.71381	1.49868
H	-6.92746	1.31995	2.83259
H	-7.07468	2.03817	1.21855
H	-3.52547	2.75851	3.62798
H	-4.90201	1.88157	4.31550

H	-3.90851	1.11173	3.07782
H	-5.10433	5.10074	1.12063
H	-2.37099	6.95431	0.19925
H	-3.50954	8.23994	-0.24865
H	-3.94625	7.06531	0.99954
H	-3.69460	5.97566	-3.20994
H	-3.39172	7.61982	-2.63980
H	-2.21807	6.34483	-2.29296
H	-6.11015	6.51496	-0.34572
H	-5.62132	7.69677	-1.56669
H	-5.98128	6.02576	-2.04220
H	-2.75484	4.10418	-2.31299
H	-2.64027	1.79303	-1.53993
H	3.08199	3.04353	-0.00839
H	0.49402	3.11593	1.69700
H	1.84714	4.34774	1.66002
H	1.45104	4.68570	-0.82434
H	0.09819	3.45313	-0.76425
H	4.46413	1.47467	-1.26190

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Energy: -2238239.5270122

Number of Imaginary Frequencies: 0

O	1.58739	1.07174	2.52638
C	2.30729	0.54010	1.70683
N	3.74697	0.47292	2.07884
C	4.10616	0.95510	3.43346
C	5.10572	0.00625	4.08971
C	6.22989	-0.21967	3.13237
C	6.03224	-0.04510	1.76873
C	4.69830	0.05442	1.25018
C	4.31464	-0.38706	-0.12021
H	4.78208	0.32015	-0.82150
N	7.22469	-0.37588	1.07764
C	7.53165	0.16727	-0.20311
O	8.66163	-0.33808	-0.66854
C	9.24260	0.12030	-1.97879
C	9.53836	1.61853	-1.90631
C	10.53040	-0.69836	-2.06164
C	8.27972	-0.24738	-3.10828
O	6.79836	0.97314	-0.73944
C	8.16507	-0.78974	2.04809
C	9.48918	-1.22055	1.91881
C	10.16706	-1.56889	3.08377

C	9.56797	-1.49459	4.35892
C	8.25997	-1.06414	4.49207
C	7.55133	-0.70414	3.32900
C	1.89011	-0.03755	0.43045
C	2.84097	-0.49811	-0.41750
Au	-0.15170	0.06989	0.10470
P	-2.48938	0.25463	-0.18023
O	-3.10841	1.70077	-0.58706
C	-2.34152	2.74989	-1.14003
C	-2.52256	4.06324	-0.65889
C	-3.50191	4.42856	0.47851
C	-3.50840	5.94443	0.76888
C	-4.94636	4.03203	0.08625
C	-3.08823	3.71544	1.78854
C	-1.74978	5.04393	-1.29671
C	-0.84467	4.79807	-2.34423
C	-0.05160	5.96558	-2.95958
C	0.83066	6.61935	-1.86890
C	0.86702	5.50178	-4.10635
C	-1.03202	7.02016	-3.52648
C	-0.71866	3.47843	-2.77994
C	-1.46920	2.46361	-2.18504
O	-3.22182	-0.09539	1.20962
C	-4.58268	-0.21644	1.57080
C	-4.86194	-0.61912	2.89321
C	-3.76824	-0.91140	3.94720
C	-4.37686	-1.33391	5.30172
C	-2.85476	-2.07107	3.47915
C	-2.91538	0.35573	4.20424
C	-6.22316	-0.73142	3.20817
C	-7.27540	-0.47282	2.31315
C	-8.73379	-0.63247	2.78033
C	-9.00676	0.33194	3.95946
C	-9.74036	-0.31491	1.65778
C	-8.97248	-2.08986	3.24330
C	-6.92750	-0.07146	1.02253
C	-5.58866	0.05816	0.65207
O	-3.21667	-0.65753	-1.32763
C	-2.84188	-1.97663	-1.64316
C	-3.07899	-2.45011	-2.95233
C	-3.80648	-1.62713	-4.04049
C	-3.91347	-2.39990	-5.37242
C	-5.24900	-1.31700	-3.56860
C	-3.05990	-0.30583	-4.33982

C	-2.65817	-3.76381	-3.20105
C	-2.05791	-4.60876	-2.25082
C	-1.62605	-6.03017	-2.65447
C	-0.57103	-5.94234	-3.78344
C	-1.00508	-6.80473	-1.47620
C	-2.85392	-6.82592	-3.15838
C	-1.89752	-4.09962	-0.96191
C	-2.29439	-2.79578	-0.65966
C	2.57864	-1.08136	-1.77068
C	1.45038	-2.02871	-2.07567
C	2.86737	-2.54698	-2.05252
H	4.54882	1.95241	3.32068
H	3.17683	1.05115	3.98974
H	5.46348	0.45659	5.02193
H	4.63463	-0.94979	4.36301
H	10.18427	1.84399	-1.05114
H	10.06825	1.92046	-2.81587
H	8.62341	2.20836	-1.82969
H	10.31491	-1.77129	-2.03913
H	11.04882	-0.47279	-2.99866
H	11.20481	-0.45512	-1.23421
H	7.35199	0.32388	-3.04730
H	8.75725	-0.02792	-4.06898
H	8.04805	-1.31757	-3.08465
H	9.96607	-1.29968	0.95358
H	11.19246	-1.91757	3.00336
H	10.13982	-1.78015	5.23593
H	7.78694	-1.00219	5.46747
H	-3.82263	6.53180	-0.10118
H	-4.22049	6.14878	1.57545
H	-2.52874	6.30848	1.09870
H	-5.05191	2.95673	-0.06661
H	-5.64063	4.32743	0.88184
H	-5.25258	4.54348	-0.83370
H	-2.07190	4.00127	2.08408
H	-3.76805	4.00418	2.59902
H	-3.12530	2.62900	1.69874
H	-1.85750	6.06590	-0.95884
H	1.54445	5.89684	-1.45585
H	1.39941	7.45648	-2.29116
H	0.23281	7.01000	-1.03880
H	0.29779	5.05434	-4.92925
H	1.41196	6.36073	-4.51294
H	1.61059	4.77167	-3.76553

H	-1.68960	7.42753	-2.75147
H	-0.47583	7.85810	-3.96310
H	-1.66465	6.58721	-4.30950
H	-0.05206	3.21701	-3.59346
H	-1.38497	1.44755	-2.55494
H	-4.96871	-2.25274	5.22234
H	-3.56596	-1.52707	6.01230
H	-5.00938	-0.55036	5.73322
H	-2.28626	-1.80591	2.58530
H	-2.13579	-2.31745	4.26992
H	-3.44186	-2.97190	3.26597
H	-3.54390	1.18441	4.54999
H	-2.17262	0.14983	4.98469
H	-2.37907	0.68105	3.31052
H	-6.48407	-1.03710	4.21240
H	-8.85323	1.37446	3.65815
H	-10.04256	0.22705	4.30363
H	-8.35162	0.13036	4.81359
H	-9.61904	-0.98457	0.79852
H	-10.76201	-0.44236	2.03204
H	-9.64667	0.71844	1.30447
H	-8.31812	-2.36839	4.07630
H	-10.00855	-2.21631	3.57925
H	-8.79243	-2.79618	2.42484
H	-7.68714	0.14795	0.28154
H	-5.34117	0.37546	-0.35304
H	-4.47815	-3.33264	-5.26800
H	-4.44357	-1.77889	-6.10226
H	-2.92948	-2.63507	-5.79451
H	-5.25987	-0.74583	-2.63742
H	-5.77417	-0.73061	-4.33208
H	-5.81269	-2.24287	-3.40729
H	-2.01236	-0.49655	-4.60419
H	-3.53069	0.20168	-5.18995
H	-3.08815	0.37925	-3.49232
H	-2.81281	-4.15965	-4.19569
H	0.31612	-5.39204	-3.44800
H	-0.25331	-6.94674	-4.08765
H	-0.96368	-5.43551	-4.67138
H	-1.71436	-6.93007	-0.65006
H	-0.70867	-7.80558	-1.80861
H	-0.10836	-6.30776	-1.08761
H	-3.31897	-6.35588	-4.03135
H	-2.55565	-7.84039	-3.44852

H	-3.61701	-6.90714	-2.37607
H	-1.47511	-4.70575	-0.16884
H	-2.19392	-2.43313	0.35718
H	2.85985	-0.40427	-2.57964
H	0.79471	-2.33045	-1.26538
H	0.94873	-1.92618	-3.03331
H	3.35405	-2.80613	-2.98867
H	3.14582	-3.18058	-1.21320
H	4.82217	-1.33843	-0.33140

1o-1-ts

Energy: -2238164.9659293

Number of Imaginary Frequencies: -1

O	-3.30564	3.30777	2.75733
C	-3.14767	2.33089	2.04365
N	-3.36270	2.43914	0.63819
C	-3.97022	3.65334	0.09209
C	-5.31323	3.18559	-0.51823
C	-5.13420	1.79513	-1.10196
C	-5.58612	0.61135	-0.47919
C	-3.37680	1.40093	-0.23467
C	-2.59782	0.44139	-0.67836
H	-3.03302	-0.33543	-1.30363
N	-5.69592	-0.39773	-1.38130
C	-6.06496	-1.71467	-0.93626
O	-6.17928	-2.53202	-1.96475
C	-6.59510	-3.96833	-1.77392
C	-7.99365	-4.00441	-1.15833
C	-6.60148	-4.49328	-3.20862
C	-5.54527	-4.68115	-0.92141
O	-6.22953	-1.92967	0.24218
C	-5.39313	0.10636	-2.68393
C	-5.39445	-0.51956	-3.92981
C	-5.06757	0.26738	-5.03465
C	-4.74932	1.62794	-4.90337
C	-4.74469	2.23925	-3.65162
C	-5.06985	1.47000	-2.53249
C	-2.73351	1.04982	2.53282
C	-2.37090	0.03463	3.09667
Au	-0.57453	0.35835	-0.30771
P	1.76513	0.24379	0.00011
O	2.54708	1.64537	0.22246
C	1.90026	2.81481	0.68895
C	2.15173	4.04251	0.04434

C	3.08499	4.18983	-1.17815
C	3.17758	5.65387	-1.65743
C	4.51894	3.73537	-0.81033
C	2.54971	3.35403	-2.36657
C	1.49724	5.15066	0.60136
C	0.63979	5.10105	1.71509
C	-0.02285	6.39214	2.23030
C	-0.90986	6.99434	1.11441
C	-0.90890	6.13684	3.46486
C	1.07051	7.41482	2.62238
C	0.43719	3.85459	2.31037
C	1.07260	2.71982	1.80318
O	2.42924	-0.38049	-1.32121
C	3.76560	-0.69503	-1.66715
C	3.97229	-1.33925	-2.90374
C	2.82852	-1.70375	-3.87858
C	3.36097	-2.37712	-5.16141
C	1.85126	-2.70315	-3.21219
C	2.06167	-0.43056	-4.31579
C	5.30915	-1.63131	-3.20782
C	6.40289	-1.32498	-2.37994
C	7.82897	-1.69527	-2.82634
C	8.16128	-0.96187	-4.14813
C	8.88552	-1.29828	-1.77753
C	7.92270	-3.22380	-3.04970
C	6.12587	-0.67841	-1.17424
C	4.81428	-0.36141	-0.81930
O	2.36921	-0.58846	1.26712
C	1.88705	-1.81108	1.76773
C	2.28076	-2.19678	3.06887
C	3.25931	-1.37813	3.94237
C	3.48345	-2.02962	5.32334
C	4.63810	-1.30609	3.24037
C	2.72295	0.05117	4.19551
C	1.76220	-3.42066	3.51470
C	0.91767	-4.25854	2.76343
C	0.42771	-5.58960	3.36288
C	-0.37831	-5.31305	4.65464
C	-0.48022	-6.36458	2.38860
C	1.64489	-6.48341	3.70229
C	0.58941	-3.83500	1.47486
C	1.07967	-2.62530	0.97864
C	-1.93984	-1.16323	3.74332
C	-2.68800	-1.65612	4.98574

C	-1.31945	-1.08460	5.13987
H	-4.09256	4.37889	0.89472
H	-3.30923	4.06600	-0.67663
H	-6.07687	3.16252	0.26512
H	-5.65838	3.87868	-1.29051
H	-8.69888	-3.42837	-1.76651
H	-8.34291	-5.04195	-1.13091
H	-7.99541	-3.61370	-0.13929
H	-5.60750	-4.41407	-3.66079
H	-6.89385	-5.54780	-3.21077
H	-7.31652	-3.93979	-3.82553
H	-5.52877	-4.29819	0.10056
H	-5.78225	-5.74974	-0.88623
H	-4.54946	-4.57160	-1.36430
H	-5.64451	-1.56496	-4.03947
H	-5.06614	-0.18776	-6.02042
H	-4.50518	2.20881	-5.78727
H	-4.49443	3.29139	-3.55116
H	3.58762	6.31649	-0.88733
H	3.84843	5.70375	-2.52153
H	2.20579	6.04937	-1.97436
H	4.55759	2.68181	-0.52761
H	5.18519	3.87729	-1.66951
H	4.91270	4.33061	0.02152
H	1.53416	3.66700	-2.63749
H	3.19109	3.50196	-3.24341
H	2.53375	2.28502	-2.14848
H	1.66387	6.11516	0.14025
H	-1.70596	6.29587	0.82972
H	-1.38123	7.92095	1.46254
H	-0.33327	7.23252	0.21412
H	-0.32735	5.74351	4.30673
H	-1.36038	7.07969	3.79284
H	-1.72301	5.43503	3.25248
H	1.71117	7.67997	1.77454
H	0.60955	8.33882	2.99082
H	1.71279	7.01708	3.41618
H	-0.20737	3.74478	3.17436
H	0.93672	1.76290	2.29642
H	3.88153	-3.31804	-4.95120
H	2.51678	-2.61083	-5.81890
H	4.03929	-1.72318	-5.72042
H	1.35598	-2.26809	-2.34150
H	1.07445	-2.99691	-3.92867

H	2.37618	-3.61081	-2.89326
H	2.73864	0.28821	-4.79132
H	1.28946	-0.69764	-5.04763
H	1.57119	0.06527	-3.47515
H	5.51487	-2.12503	-4.14806
H	8.11124	0.12519	-4.01779
H	9.17463	-1.21774	-4.47936
H	7.47065	-1.23506	-4.95310
H	8.72006	-1.80435	-0.81939
H	9.88180	-1.58349	-2.13221
H	8.89834	-0.21705	-1.59825
H	7.22656	-3.56987	-3.82118
H	8.93459	-3.49764	-3.37069
H	7.69974	-3.77082	-2.12651
H	6.92117	-0.40697	-0.49002
H	4.62342	0.15084	0.11540
H	3.92163	-3.03053	5.24563
H	4.18293	-1.41328	5.89751
H	2.55697	-2.10062	5.90529
H	4.57368	-0.82803	2.26082
H	5.33940	-0.72879	3.85453
H	5.05740	-2.30904	3.10226
H	1.72255	0.02239	4.64439
H	3.38579	0.57640	4.89292
H	2.67546	0.64026	3.27922
H	2.04188	-3.75387	4.50552
H	-1.26512	-4.70343	4.44070
H	-0.71893	-6.25451	5.10099
H	0.21921	-4.78814	5.40764
H	0.04566	-6.63056	1.46462
H	-0.81219	-7.29754	2.85675
H	-1.37700	-5.79260	2.12187
H	2.31085	-6.00966	4.43102
H	1.30893	-7.43538	4.12982
H	2.23300	-6.70263	2.80419
H	-0.03210	-4.44172	0.82648
H	0.84410	-2.34008	-0.04095
H	-1.54032	-1.93097	3.08410
H	-3.53463	-1.06507	5.31985
H	-2.82068	-2.73073	5.06687
H	-0.48870	-1.75851	5.32389
H	-1.22132	-0.09854	5.58276
H	-5.83573	0.42941	0.55653

1o-4'-ts

Energy: -2238192.2038626

Number of Imaginary Frequencies: -1

O	1.34687	-1.53934	-1.98394
C	2.29812	-0.76527	-2.01229
N	3.55639	-1.10629	-2.43983
C	3.84372	-2.55220	-2.55130
C	5.29442	-2.80221	-2.97345
C	6.21763	-1.89656	-2.21809
C	5.84447	-0.61845	-1.88356
C	4.56640	-0.10857	-2.36457
C	4.24554	1.13557	-2.80216
H	4.89458	1.97890	-2.61735
N	6.94629	0.06590	-1.32059
C	6.82062	1.27871	-0.60917
O	8.01377	1.73287	-0.23578
C	8.15352	2.98332	0.56691
C	7.43023	2.81817	1.90522
C	9.66711	3.07446	0.76772
C	7.63720	4.17187	-0.24713
O	5.74185	1.80286	-0.40814
C	8.04138	-0.83798	-1.30608
C	9.35609	-0.69208	-0.85400
C	10.21091	-1.78503	-0.98605
C	9.78470	-3.00101	-1.54890
C	8.47872	-3.14791	-1.99464
C	7.59794	-2.06252	-1.86783
C	2.16256	0.60821	-1.50917
C	1.68361	1.58499	-0.86795
Au	-0.15809	0.54047	-0.27365
P	-2.23639	-0.26795	0.40276
O	-2.28754	-1.47278	1.47295
C	-1.21320	-1.84850	2.31592
C	-0.92814	-3.21742	2.49053
C	-1.70602	-4.35016	1.78485
C	-1.18914	-5.74482	2.19717
C	-3.20544	-4.28669	2.16652
C	-1.53759	-4.23536	0.25036
C	0.12348	-3.49471	3.37539
C	0.87315	-2.52368	4.06337
C	1.99872	-2.96144	5.01829
C	3.05287	-3.78158	4.23682
C	2.71070	-1.75840	5.66585
C	1.40179	-3.83508	6.14806

C	0.53346	-1.18686	3.85071
C	-0.51176	-0.85324	2.98808
O	-2.98516	-0.82954	-0.89296
C	-4.30553	-1.30537	-1.10950
C	-4.65203	-1.64948	-2.43110
C	-3.67304	-1.56582	-3.62668
C	-4.34439	-2.00755	-4.94482
C	-3.18107	-0.11200	-3.83371
C	-2.46141	-2.50183	-3.39381
C	-5.96914	-2.10011	-2.59803
C	-6.91035	-2.22498	-1.56168
C	-8.33099	-2.72943	-1.87505
C	-8.25253	-4.14726	-2.49054
C	-9.21193	-2.80261	-0.61316
C	-9.00807	-1.76847	-2.88172
C	-6.49211	-1.87747	-0.27603
C	-5.19407	-1.41970	-0.04854
O	-3.21883	0.79165	1.13883
C	-3.41111	2.13485	0.74328
C	-3.84867	3.06182	1.71333
C	-4.18930	2.68240	3.17283
C	-4.66557	3.90325	3.98863
C	-5.33882	1.64416	3.18651
C	-2.95065	2.10493	3.89694
C	-4.00516	4.37655	1.25312
C	-3.77736	4.79972	-0.06857
C	-3.98677	6.27739	-0.44589
C	-3.04535	7.16404	0.40415
C	-3.68687	6.54432	-1.93331
C	-5.45623	6.67797	-0.17072
C	-3.38586	3.82573	-0.98762
C	-3.21253	2.49965	-0.58539
C	1.96073	2.96802	-0.51233
C	1.48218	3.56315	0.80870
C	0.85065	4.01686	-0.46368
H	3.64635	-3.01163	-1.57571
H	3.13630	-2.98266	-3.26453
H	5.53076	-3.85620	-2.79376
H	5.40889	-2.63718	-4.05415
H	7.79067	1.92598	2.42820
H	7.64129	3.68758	2.53718
H	6.35024	2.74005	1.76990
H	10.18620	3.12670	-0.19455
H	9.91045	3.97593	1.33867

H	10.04150	2.20799	1.32244
H	6.55788	4.11466	-0.39689
H	7.86653	5.10029	0.28676
H	8.13284	4.21286	-1.22290
H	9.70916	0.23581	-0.43069
H	11.23892	-1.68622	-0.64981
H	10.48460	-3.82627	-1.63742
H	8.14209	-4.08306	-2.43296
H	-1.30153	-5.92706	3.27182
H	-1.77269	-6.50940	1.67378
H	-0.13792	-5.89510	1.92667
H	-3.67769	-3.35922	1.83756
H	-3.74152	-5.11980	1.69713
H	-3.33398	-4.37341	3.25157
H	-0.48028	-4.29515	-0.03261
H	-2.06549	-5.05951	-0.24369
H	-1.94254	-3.30237	-0.14416
H	0.37507	-4.53323	3.54396
H	3.50247	-3.18215	3.43649
H	3.85523	-4.10539	4.91007
H	2.62124	-4.67927	3.78173
H	2.02493	-1.15262	6.26924
H	3.50361	-2.11512	6.33207
H	3.17722	-1.10799	4.91666
H	0.91670	-4.73531	5.75643
H	2.19187	-4.15625	6.83701
H	0.65558	-3.27656	6.72433
H	1.05678	-0.38703	4.36119
H	-0.79602	0.18652	2.86580
H	-5.19572	-1.37131	-5.21174
H	-3.61431	-1.93571	-5.75787
H	-4.68688	-3.04732	-4.90575
H	-2.56954	0.23467	-2.99753
H	-2.56526	-0.05461	-4.73911
H	-4.02570	0.57551	-3.95848
H	-2.79206	-3.53596	-3.24449
H	-1.80558	-2.48371	-4.27260
H	-1.86364	-2.20376	-2.52982
H	-6.28469	-2.37395	-3.59561
H	-7.78698	-4.85328	-1.79337
H	-9.25874	-4.51485	-2.72345
H	-7.67246	-4.16093	-3.41948
H	-9.33638	-1.82030	-0.14292
H	-10.20960	-3.16597	-0.88180

H	-8.80127	-3.49258	0.13300
H	-8.45342	-1.70357	-3.82401
H	-10.02041	-2.11777	-3.11643
H	-9.08590	-0.75653	-2.46802
H	-7.16352	-1.95560	0.57078
H	-4.88908	-1.15737	0.95714
H	-5.57093	4.35559	3.56938
H	-4.90566	3.57831	5.00633
H	-3.89396	4.67772	4.06579
H	-5.06189	0.71893	2.67622
H	-5.60116	1.39314	4.22100
H	-6.23400	2.04862	2.70094
H	-2.10852	2.80638	3.85528
H	-3.18591	1.92773	4.95281
H	-2.63689	1.15291	3.46715
H	-4.33339	5.12076	1.96618
H	-1.99433	6.91258	0.21936
H	-3.19056	8.22100	0.15231
H	-3.23305	7.05082	1.47710
H	-4.34739	5.97100	-2.59379
H	-3.84292	7.60536	-2.15561
H	-2.64874	6.30382	-2.19154
H	-5.72478	6.55379	0.88364
H	-5.61666	7.73051	-0.43177
H	-6.14723	6.07125	-0.76674
H	-3.22750	4.07139	-2.03132
H	-2.95996	1.75124	-1.32787
H	2.93616	3.29873	-0.86125
H	0.90932	2.91755	1.46719
H	2.18289	4.22089	1.31379
H	1.10887	4.99568	-0.85678
H	-0.16199	3.69181	-0.68283
H	3.39269	1.28686	-3.45322

1o-4-ts

Energy: -2238193.8917563

Number of Imaginary Frequencies: -1

O	-1.23116	2.16785	-2.49685
C	-2.15771	1.94482	-1.72886
N	-3.47922	2.14907	-2.07003
C	-3.78662	2.29967	-3.50407
C	-4.26698	0.94700	-4.03665
C	-5.25486	0.35859	-3.07371
C	-5.47196	0.83368	-1.79734

C	-4.59865	1.86469	-1.21457
C	-4.67379	2.55743	-0.05616
H	-3.96436	3.35849	0.12045
N	-6.50177	0.04760	-1.19037
C	-7.26703	0.42271	-0.06434
O	-7.92651	-0.62713	0.42685
C	-8.92947	-0.46501	1.52112
C	-10.03170	0.50090	1.08055
C	-9.47496	-1.88549	1.67920
C	-8.21984	-0.00991	2.79912
O	-7.28908	1.55309	0.37920
C	-6.88330	-0.95244	-2.12459
C	-7.82636	-1.98328	-2.04866
C	-7.98886	-2.79827	-3.16716
C	-7.24164	-2.60776	-4.34313
C	-6.30672	-1.58573	-4.41866
C	-6.12619	-0.75337	-3.30217
C	-1.88241	1.38506	-0.36406
C	-2.52613	1.13015	0.69174
Au	0.15568	0.82181	-0.03986
P	2.38210	0.16518	0.21542
O	3.50046	1.31812	0.36948
C	3.19308	2.67494	0.64510
C	3.82499	3.68947	-0.10090
C	4.84254	3.41518	-1.23048
C	5.39525	4.72303	-1.83597
C	6.05094	2.62260	-0.67331
C	4.16932	2.62779	-2.38017
C	3.47777	4.99732	0.26723
C	2.57662	5.33190	1.29390
C	2.28034	6.81157	1.59889
C	1.71923	7.49986	0.33159
C	1.24691	6.97493	2.73000
C	3.58726	7.51827	2.03288
C	2.00176	4.27849	2.00663
C	2.31747	2.95661	1.68867
O	2.82425	-0.68579	-1.06458
C	3.98575	-1.45139	-1.34948
C	3.97723	-2.21209	-2.53540
C	2.79999	-2.22682	-3.53939
C	3.07652	-3.17011	-4.72938
C	1.49957	-2.72490	-2.86108
C	2.57817	-0.80796	-4.11901
C	5.14281	-2.95551	-2.76961

C	6.26538	-2.97236	-1.92403
C	7.48847	-3.83219	-2.29107
C	8.05154	-3.37269	-3.65736
C	8.61350	-3.71575	-1.24451
C	7.06545	-5.31807	-2.38177
C	6.20755	-2.18381	-0.77356
C	5.07334	-1.42417	-0.48642
O	2.72089	-0.71622	1.53927
C	1.90619	-1.73933	2.06519
C	2.01979	-2.04564	3.43876
C	3.02754	-1.35835	4.38854
C	2.92895	-1.90719	5.82752
C	4.47147	-1.62262	3.89328
C	2.76868	0.16530	4.46158
C	1.17657	-3.06877	3.89432
C	0.27529	-3.78818	3.08892
C	-0.58616	-4.90309	3.70964
C	-1.45735	-4.31657	4.84609
C	-1.52287	-5.55677	2.67542
C	0.33582	-6.00362	4.28824
C	0.23615	-3.46033	1.73272
C	1.05261	-2.44780	1.22413
C	-2.99170	0.74294	1.96816
C	-2.59501	-0.65619	2.50594
C	-3.99564	-0.41732	2.09294
H	-4.56931	3.05833	-3.60081
H	-2.88593	2.64983	-4.00500
H	-4.72687	1.07315	-5.02495
H	-3.40954	0.27281	-4.17435
H	-10.46936	0.17575	0.13074
H	-10.82686	0.50345	1.83368
H	-9.65722	1.51969	0.96970
H	-8.66984	-2.59042	1.90990
H	-10.20158	-1.91207	2.49728
H	-9.97999	-2.21763	0.76648
H	-7.80682	0.99399	2.68938
H	-8.93705	-0.00223	3.62676
H	-7.41641	-0.70881	3.05937
H	-8.40421	-2.15834	-1.15451
H	-8.71364	-3.60601	-3.12208
H	-7.39855	-3.26569	-5.19244
H	-5.72380	-1.42935	-5.32176
H	5.92042	5.33336	-1.09295
H	6.11591	4.47345	-2.62172

H	4.60962	5.33296	-2.29580
H	5.76167	1.64309	-0.28742
H	6.78832	2.46453	-1.46899
H	6.54200	3.17905	0.13331
H	3.31290	3.18039	-2.78349
H	4.88642	2.47714	-3.19558
H	3.82397	1.64309	-2.06201
H	3.93812	5.81000	-0.27828
H	0.78848	7.02234	0.00410
H	1.50528	8.55492	0.53851
H	2.42605	7.46380	-0.50380
H	1.59916	6.54232	3.67351
H	1.06174	8.03970	2.90754
H	0.28604	6.51210	2.47524
H	4.35353	7.47624	1.25182
H	3.39250	8.57503	2.25029
H	4.00330	7.05727	2.93593
H	1.31767	4.46384	2.82631
H	1.89952	2.14631	2.27728
H	3.21669	-4.20934	-4.41124
H	2.21799	-3.14776	-5.40891
H	3.95547	-2.86218	-5.30591
H	1.14465	-2.02881	-2.09752
H	0.70596	-2.82379	-3.61126
H	1.64788	-3.70749	-2.39822
H	3.48378	-0.44576	-4.61840
H	1.77232	-0.83198	-4.86245
H	2.29991	-0.08505	-3.34894
H	5.18282	-3.55769	-3.66722
H	8.36475	-2.32307	-3.62054
H	8.92423	-3.97752	-3.93040
H	7.31432	-3.47422	-4.46091
H	8.28753	-4.05277	-0.25370
H	9.45955	-4.34407	-1.54295
H	8.98385	-2.68808	-1.15445
H	6.29586	-5.47977	-3.14405
H	7.92784	-5.94201	-2.64404
H	6.66884	-5.67322	-1.42373
H	7.04010	-2.14329	-0.08122
H	5.05245	-0.81373	0.40815
H	3.14849	-2.97917	5.87849
H	3.66570	-1.39461	6.45460
H	1.94257	-1.73266	6.27251
H	4.64224	-1.21828	2.89316

H	5.18974	-1.15210	4.57490
H	4.68435	-2.69721	3.86891
H	1.73519	0.37474	4.76383
H	3.43202	0.61905	5.20689
H	2.96179	0.65774	3.50787
H	1.23093	-3.33302	4.94196
H	-2.13333	-3.54120	4.46492
H	-2.07048	-5.10445	5.29881
H	-0.85089	-3.87212	5.64220
H	-0.96558	-6.03432	1.86174
H	-2.12207	-6.33393	3.16175
H	-2.21831	-4.83166	2.23574
H	0.99396	-5.61609	5.07291
H	-0.26445	-6.80956	4.72632
H	0.96705	-6.43812	3.50512
H	-0.40684	-3.99655	1.04424
H	1.04026	-2.24322	0.15964
H	-3.06838	1.53784	2.70620
H	-1.94802	-1.25769	1.87605
H	-2.34768	-0.67255	3.56295
H	-4.75708	-0.28004	2.85461
H	-4.34722	-0.85323	1.16341
H	-5.46983	2.40640	0.65387

16. References

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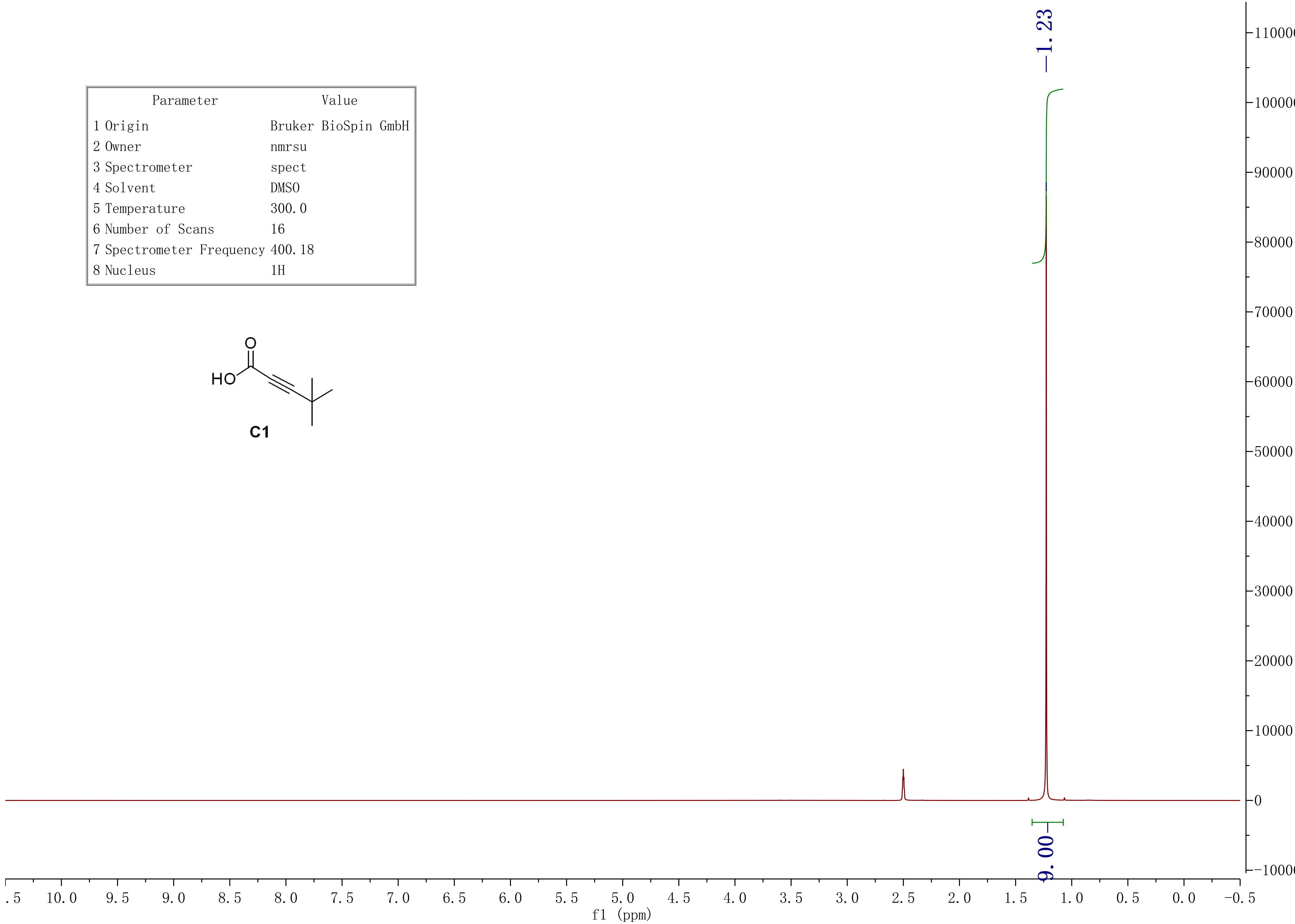
S2. Grugel, C.-P.; Breit B. *Org. Lett.* **2018**, *20*, 1066−1069.

S3. Meng, M.-T.; Wang, G.-F.; Yang, L.-F; Cheng, K.; Qi, C.-Z. *Adv. Synth. Catal.* **2018**, *360*, 1218−1231.

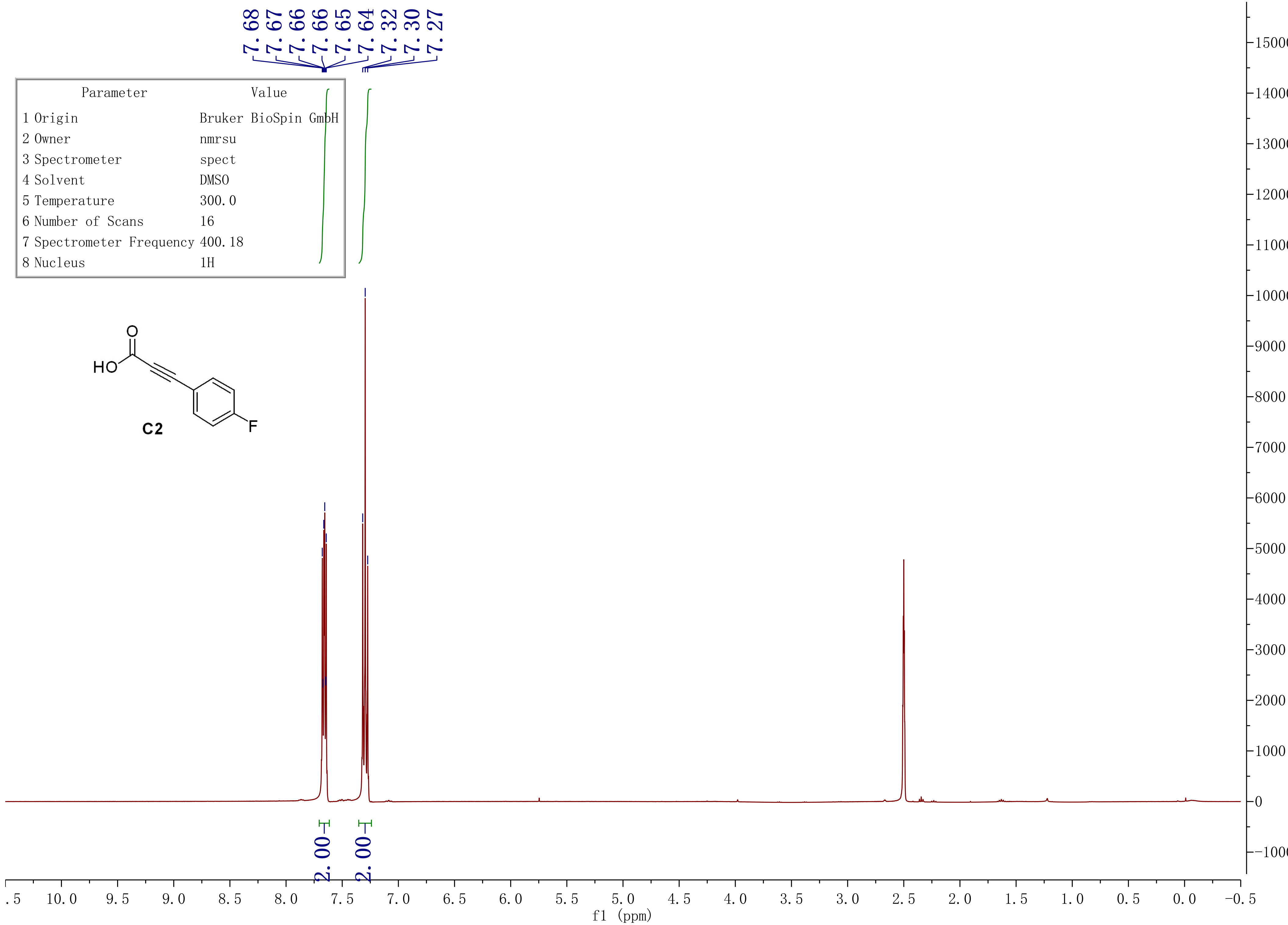
S4. Wang, Y.; Wang, X.; Lin, J.; Yao, B.; Wang, G.; Zhao, Y.; Zhang, X.; Lin, B.; Liu, Y.; Cheng, M. Liu, Y. *Adv. Synth. Catal.* **2018**, *360*, 1483−1492.

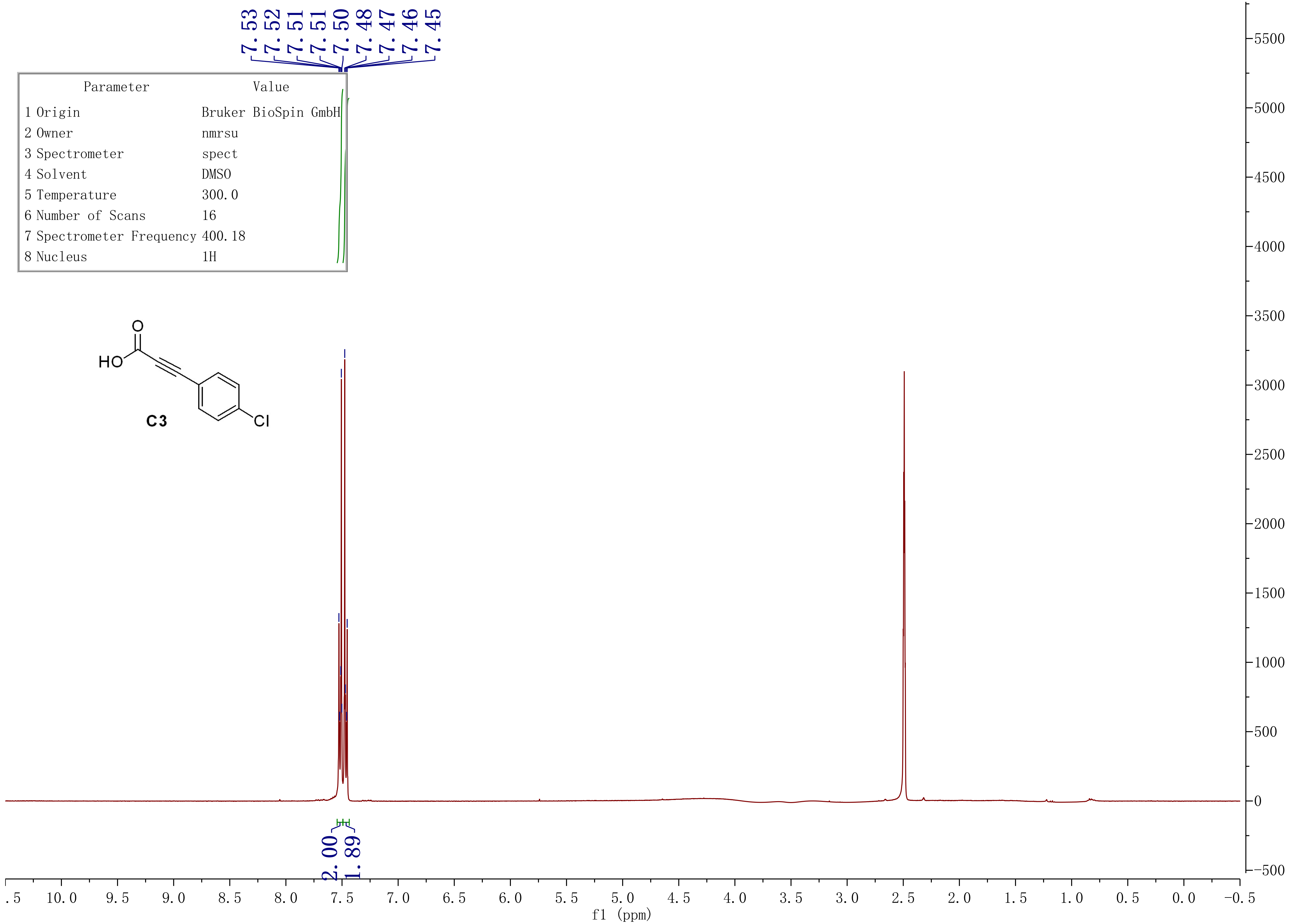
S5. Wang, Y.; Lin, J.-S.; Wang, X.-Y.; Wang, G.-H.; Zhang, X.-H.; Yao, B.; Zhao, Y.-D.; Yu, P.-F.; Lin, B.; Liu, Y.-X.; Cheng, M.-S. *Chem. Eur. J.* **2018**, *24*, 4026−4032.

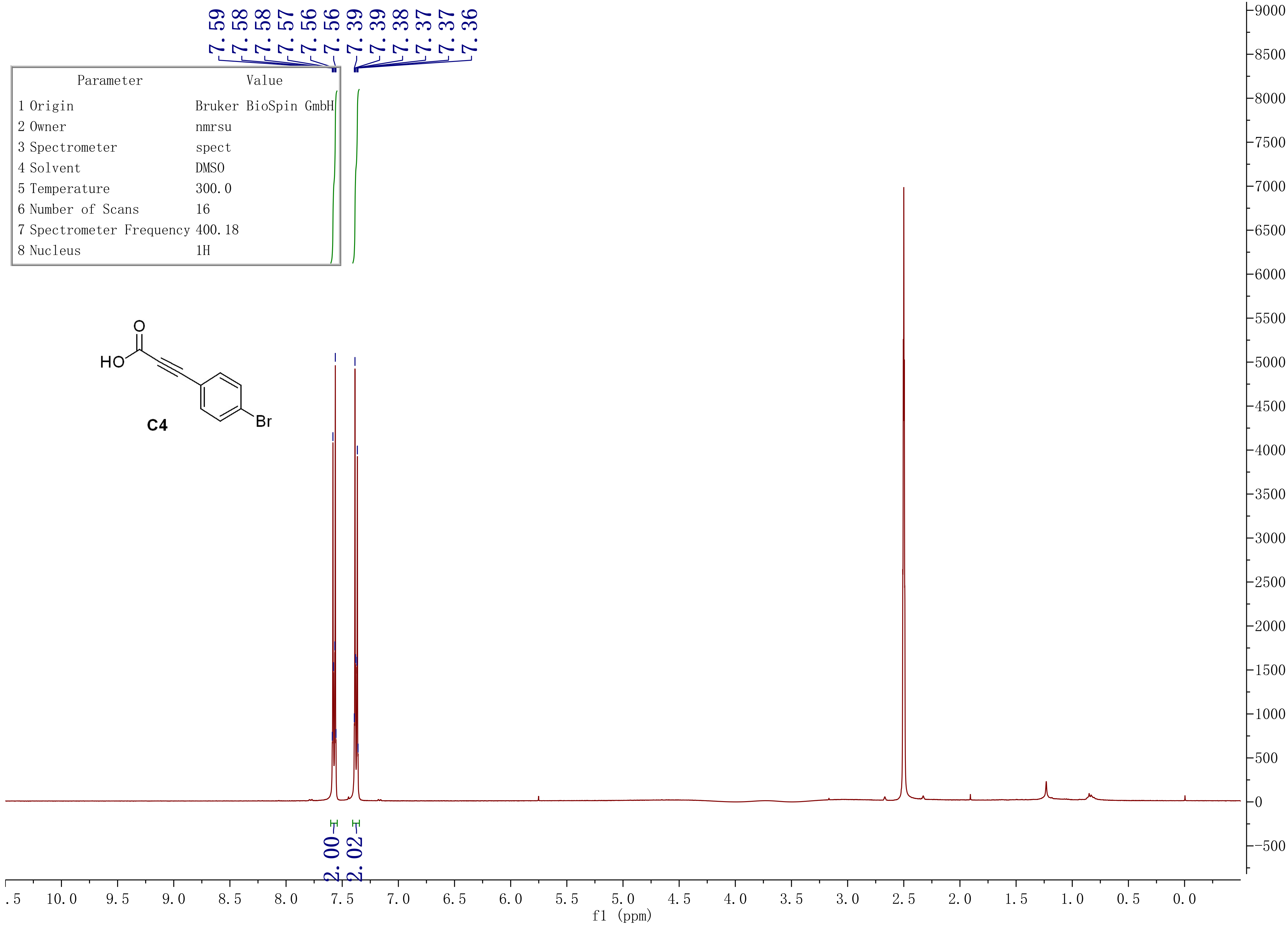
17. NMR Spectra



Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
HO
O
C1
1.23
9.00
f1 (ppm)

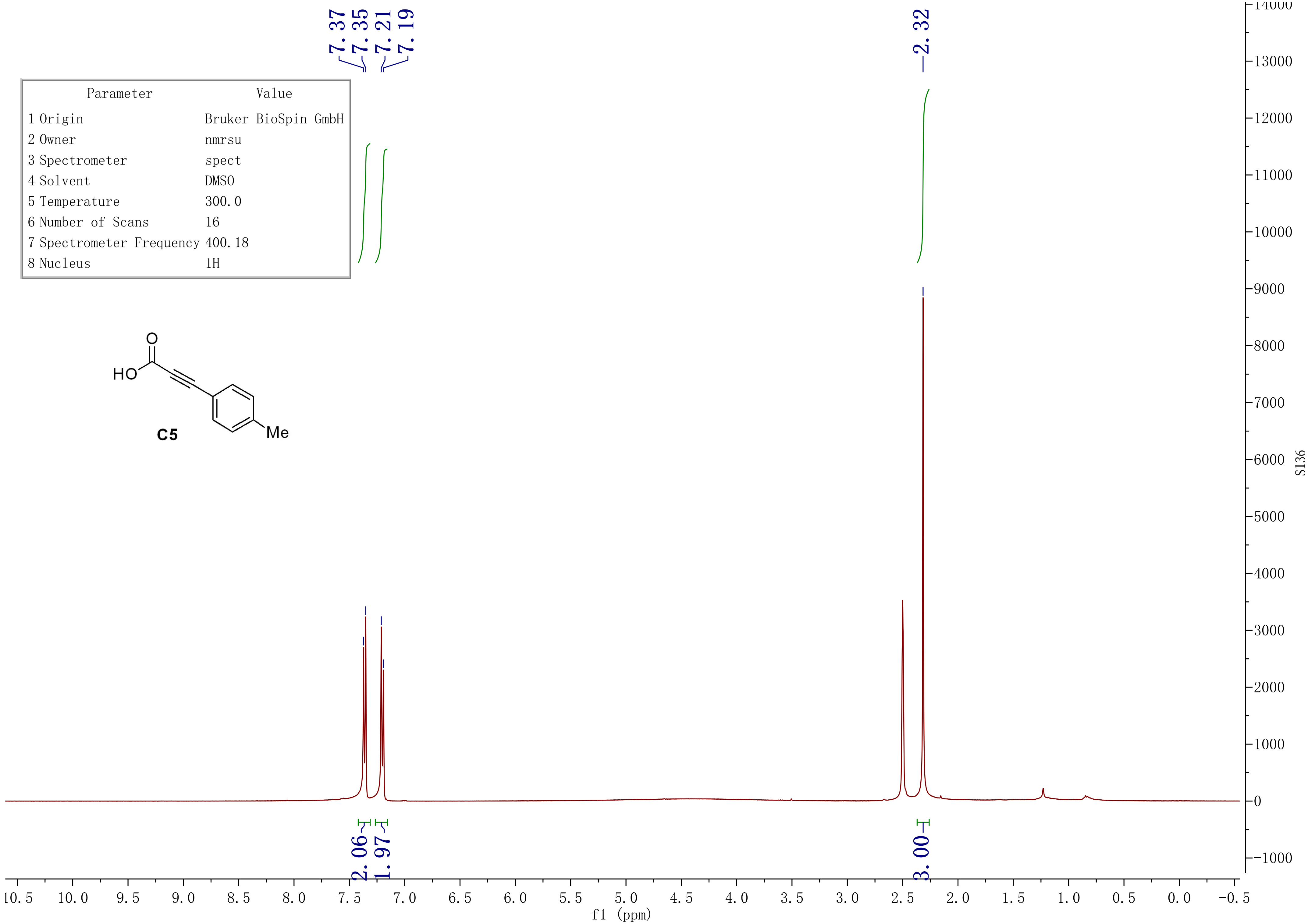

7.68
7.67
7.66
7.66
7.65
7.64
7.32
7.30
7.27
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
HO
O
F
C2
2.00
2.00
f1 (ppm)

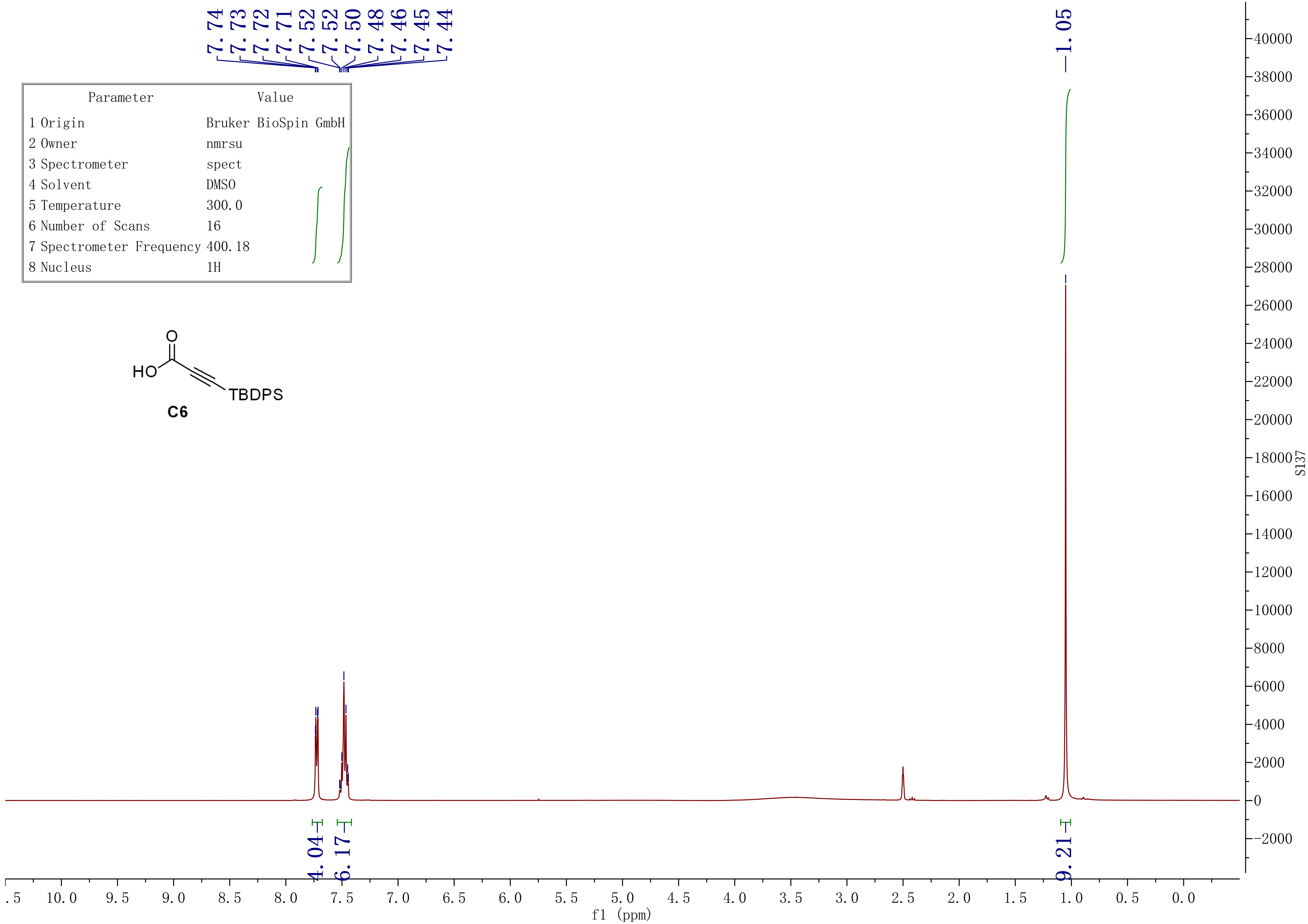

7.53
7.52
7.51
7.51
7.50
7.48
7.47
7.46
7.45
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
HO
O
Cl
C3
2.00
1.89
f1 (ppm)



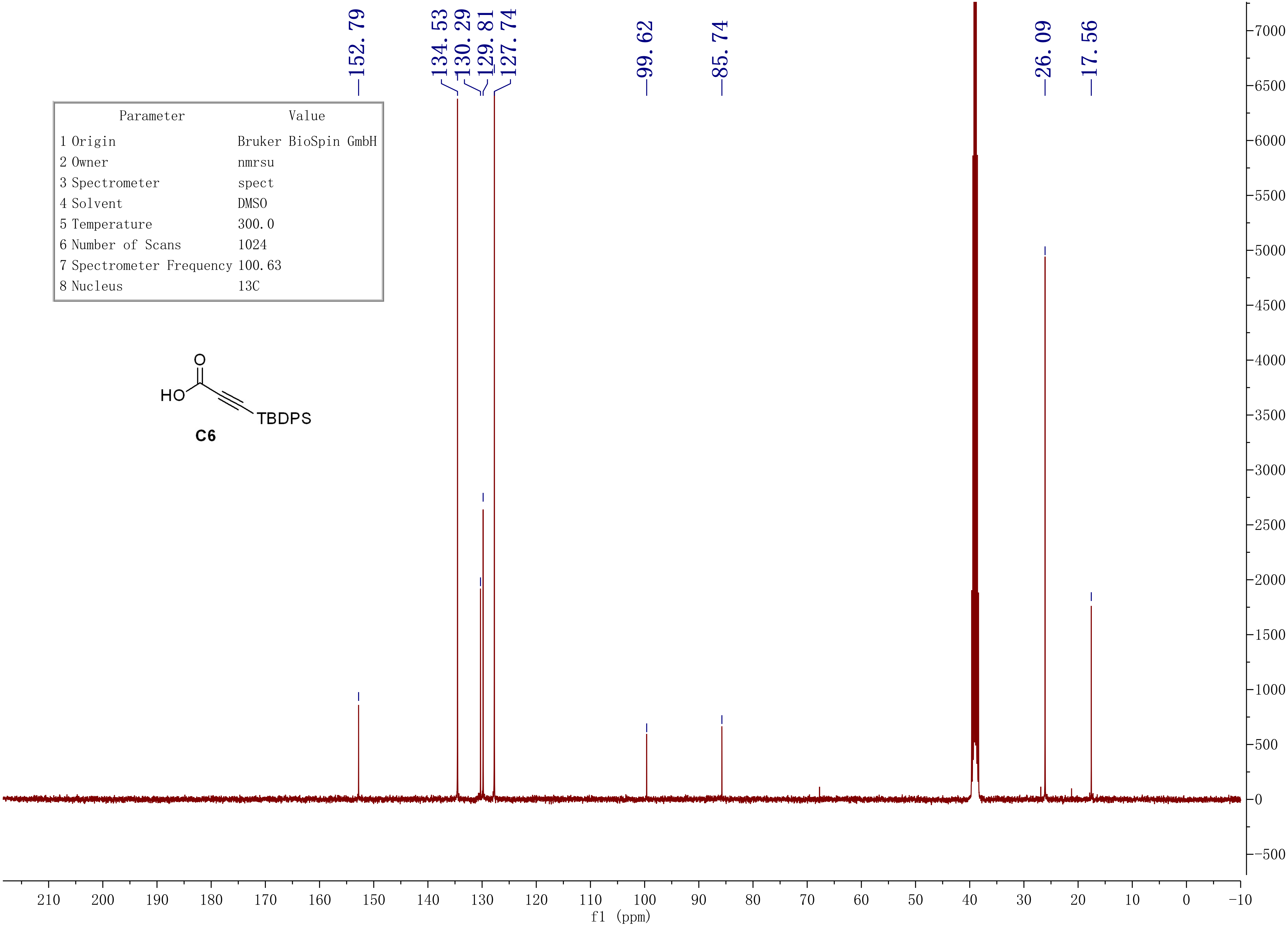
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
7.59
7.58
7.58
7.57
7.56
7.56
7.39
7.39
7.38
7.37
7.37
7.36
HO
O
Br
C4
2.00
2.02
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	16
7 Spectrometer Frequency	400.18
8 Nucleus	1H

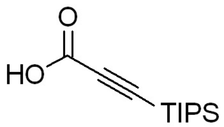




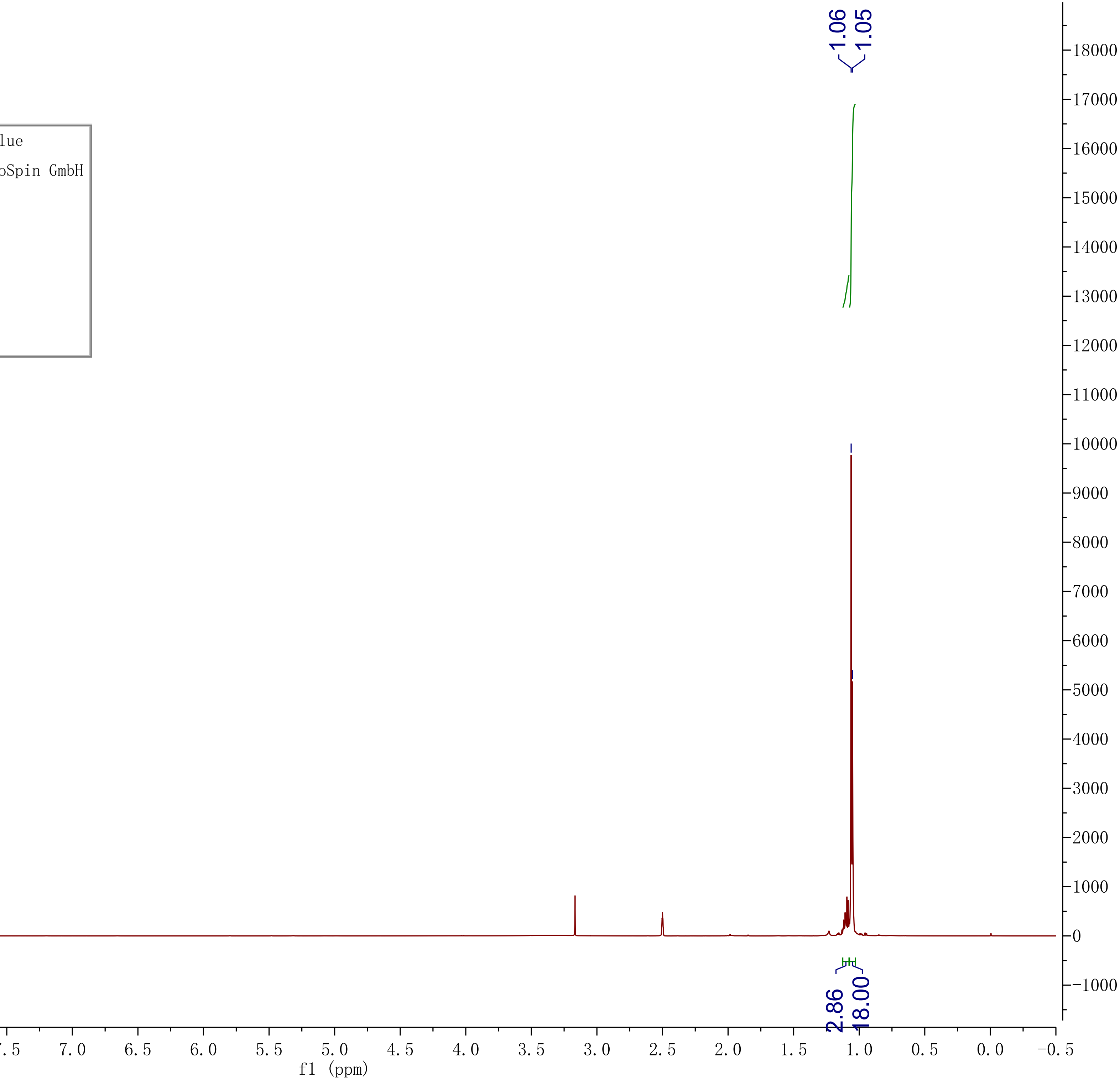
7.74
7.73
7.72
7.71
7.52
7.52
7.50
7.48
7.46
7.45
7.44
1.05
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
HO
O
TBDPS
C6
4.04
6.17
9.21
f1 (ppm)


152.79
134.53
130.29
129.81
127.74
99.62
85.74
26.09
17.56
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 1024
7 Spectrometer Frequency 100.63
8 Nucleus 13C
HO
O
TBDPS
C6
f1 (ppm)

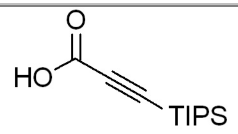
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	600.20
8 Nucleus	1H



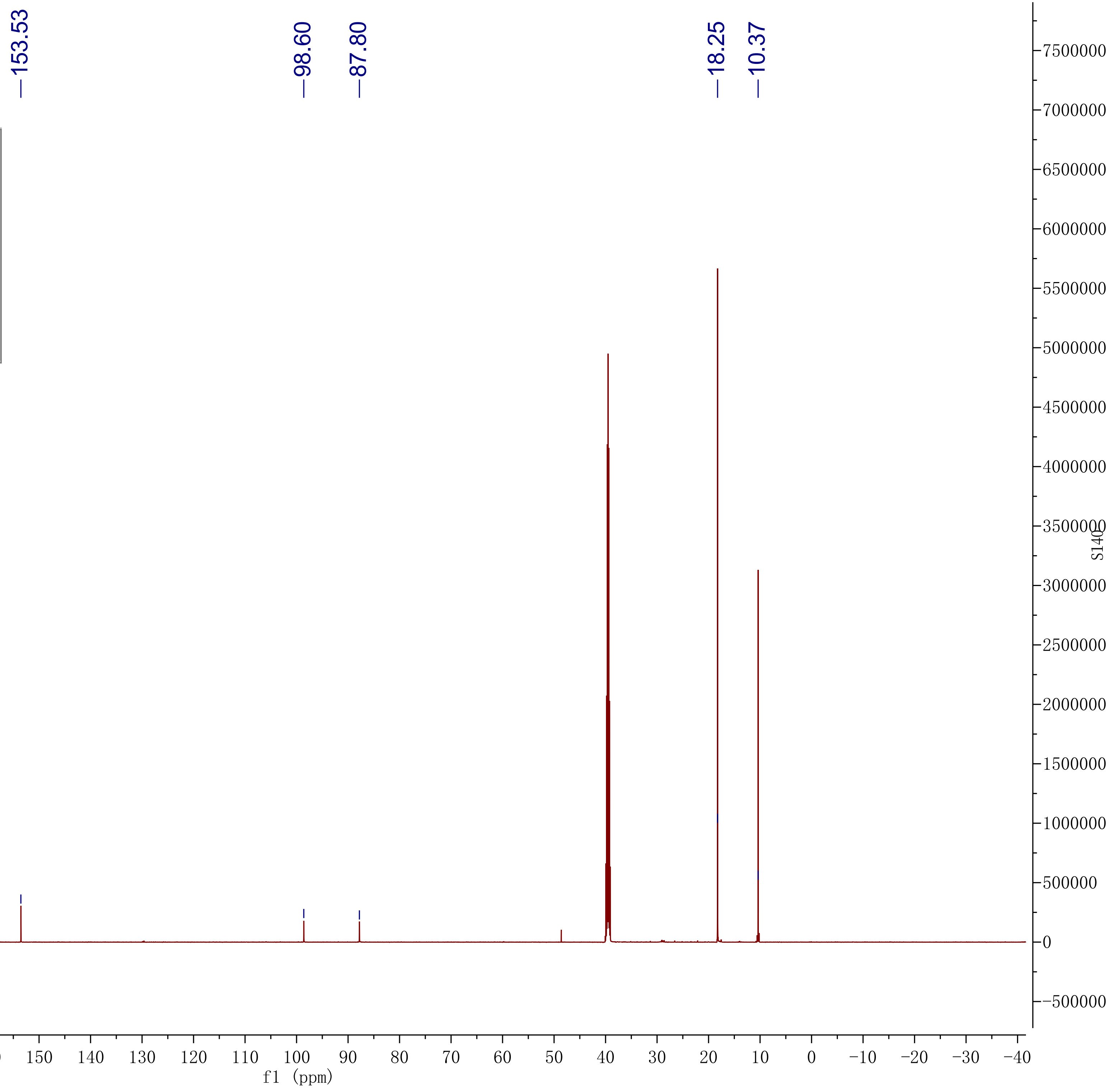
C7

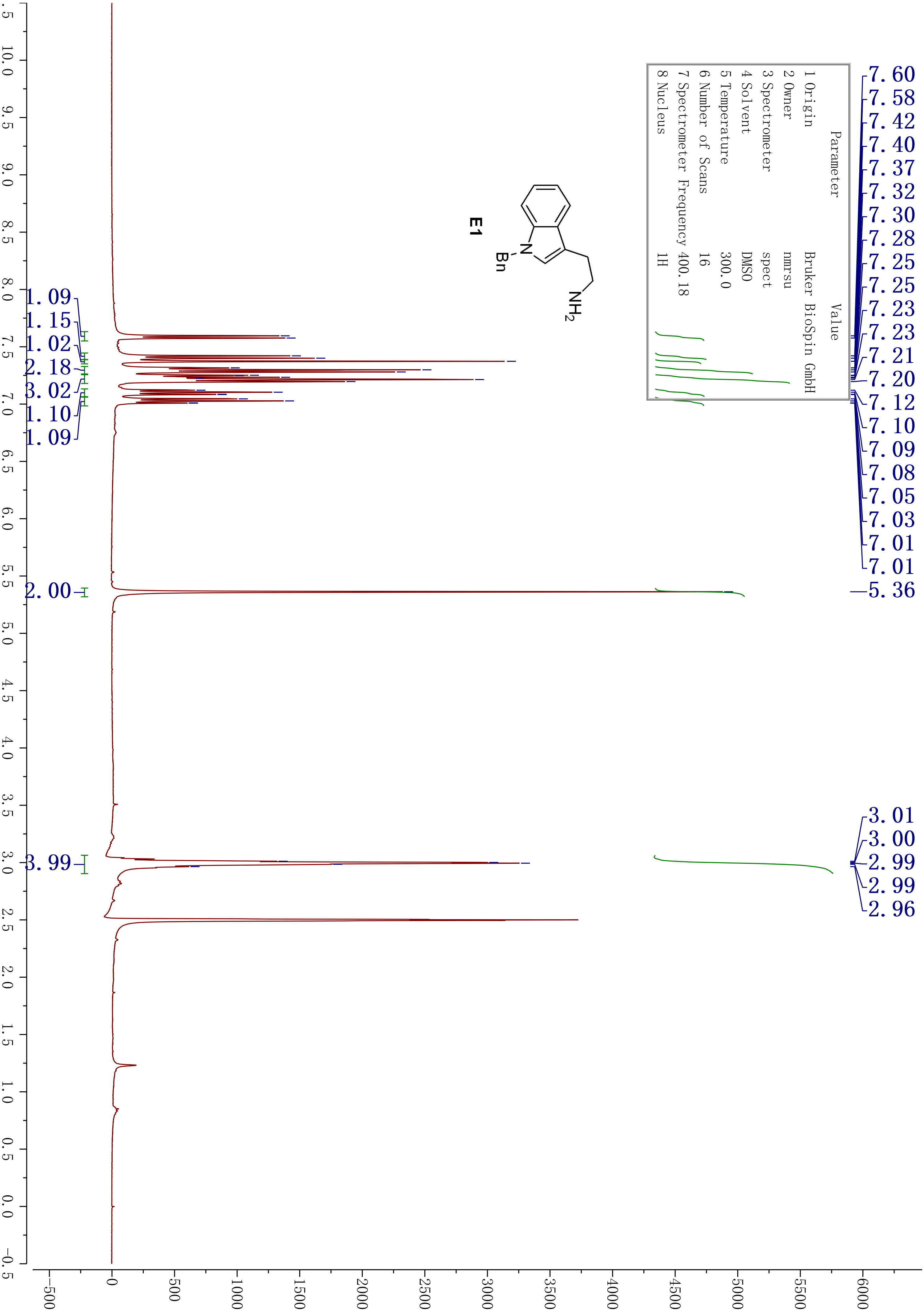


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C

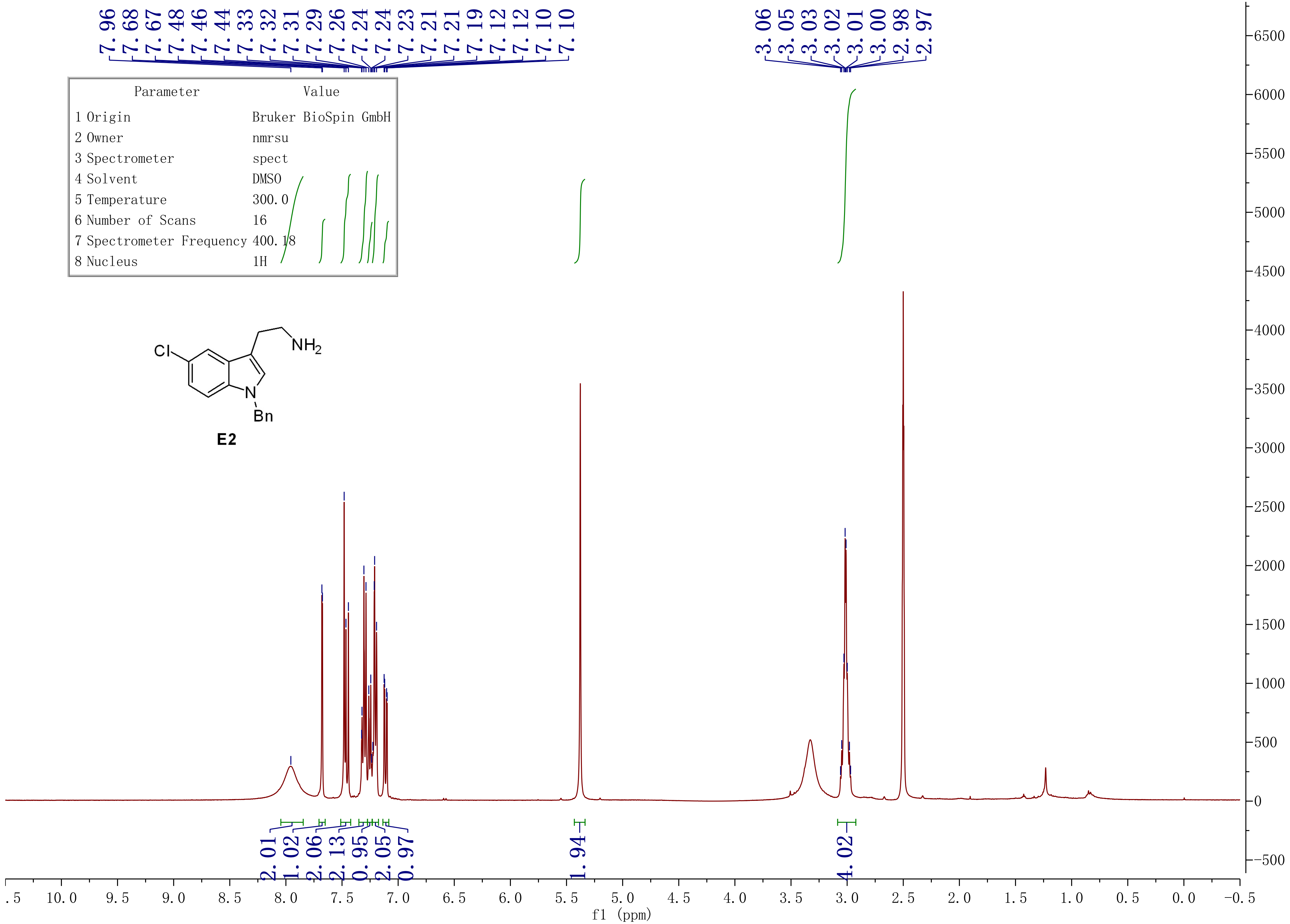


C7

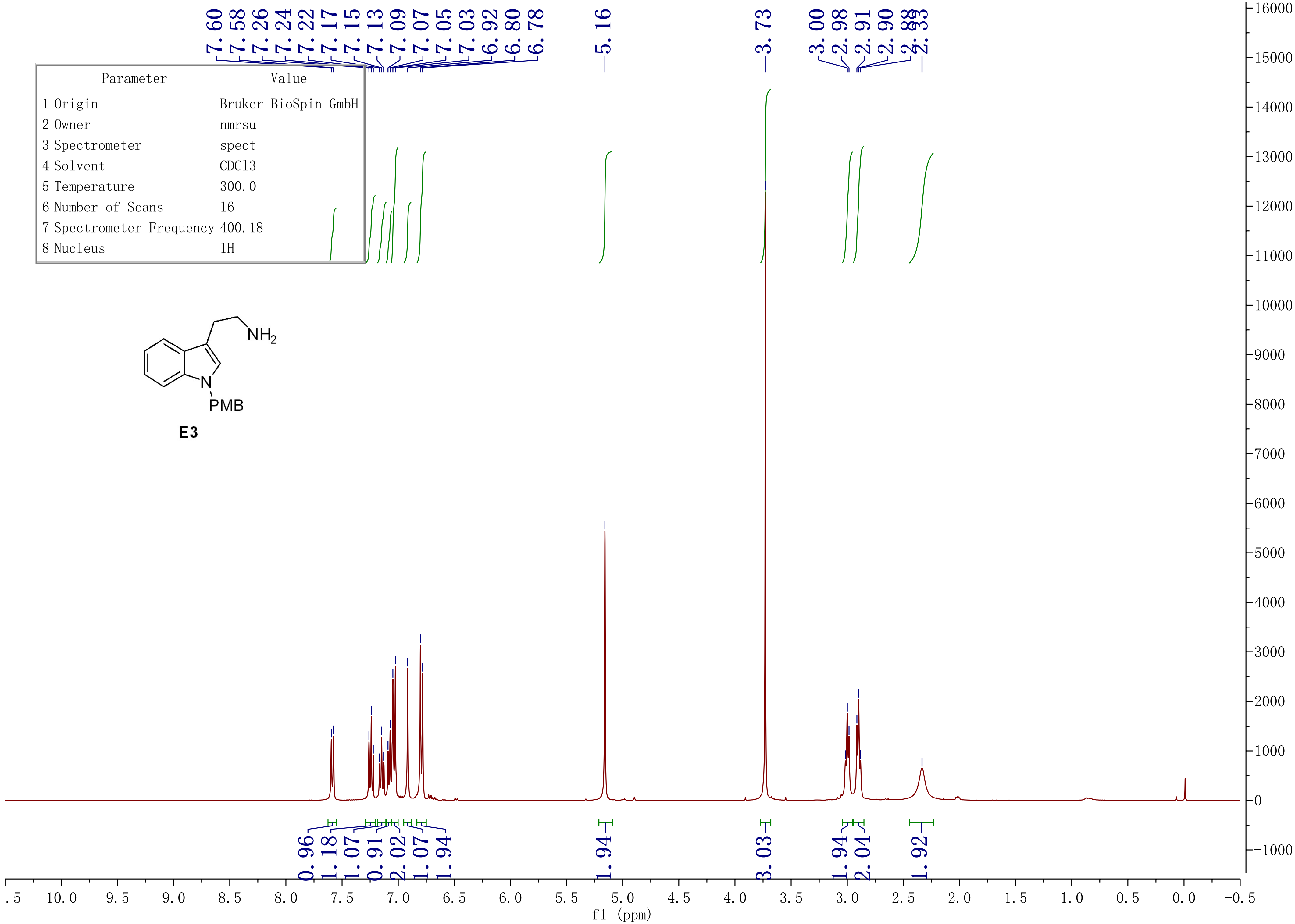




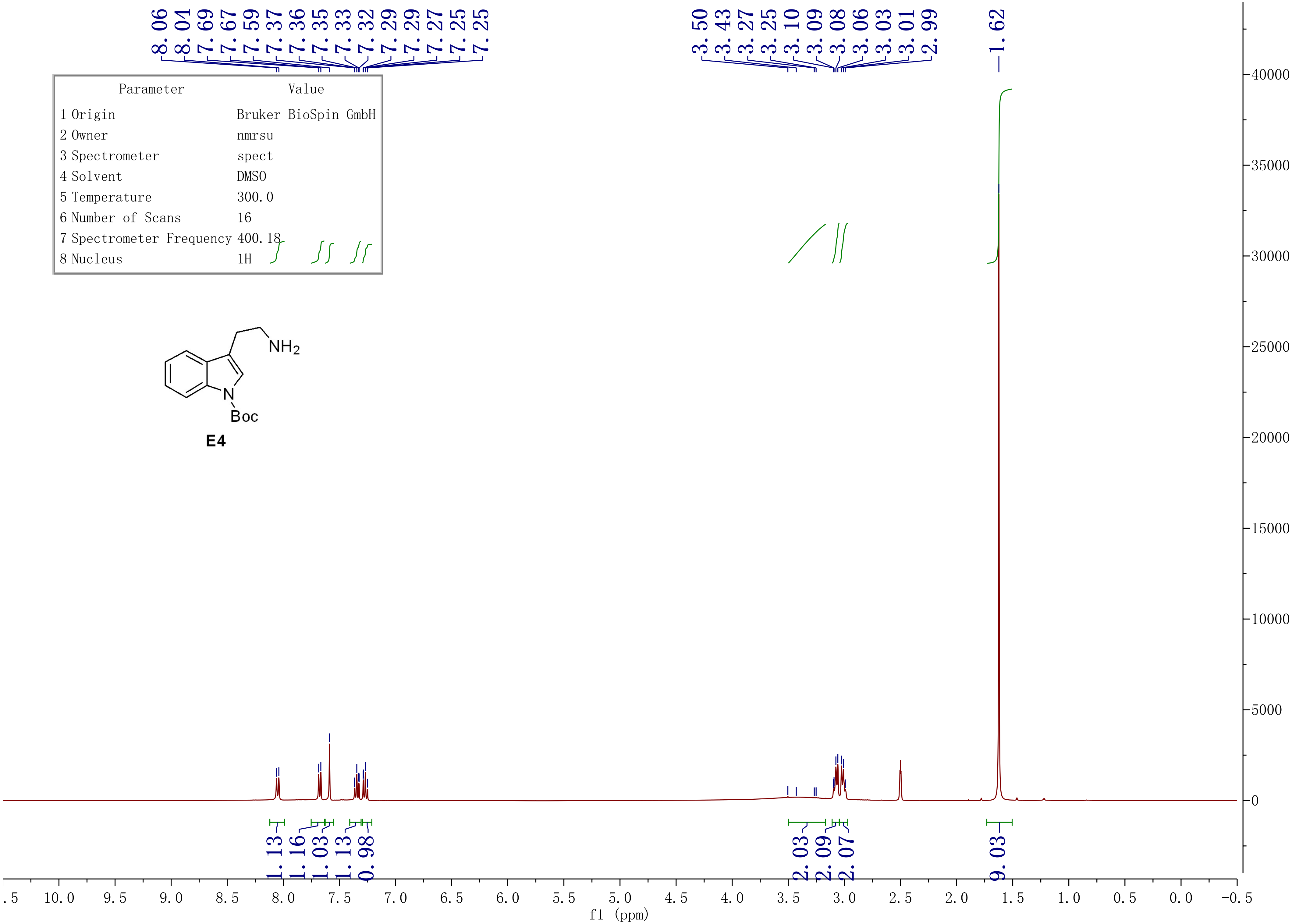
E1
N
Bn
NH2
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
7.60
7.58
7.42
7.40
7.37
7.32
7.30
7.28
7.25
7.25
7.23
7.23
7.21
7.20
7.12
7.10
7.09
7.08
7.05
7.03
7.01
7.01
5.36
3.01
3.00
2.99
2.99
2.96
1.09
1.15
1.02
2.18
3.02
1.10
1.09
2.00
3.99
f1 (ppm)

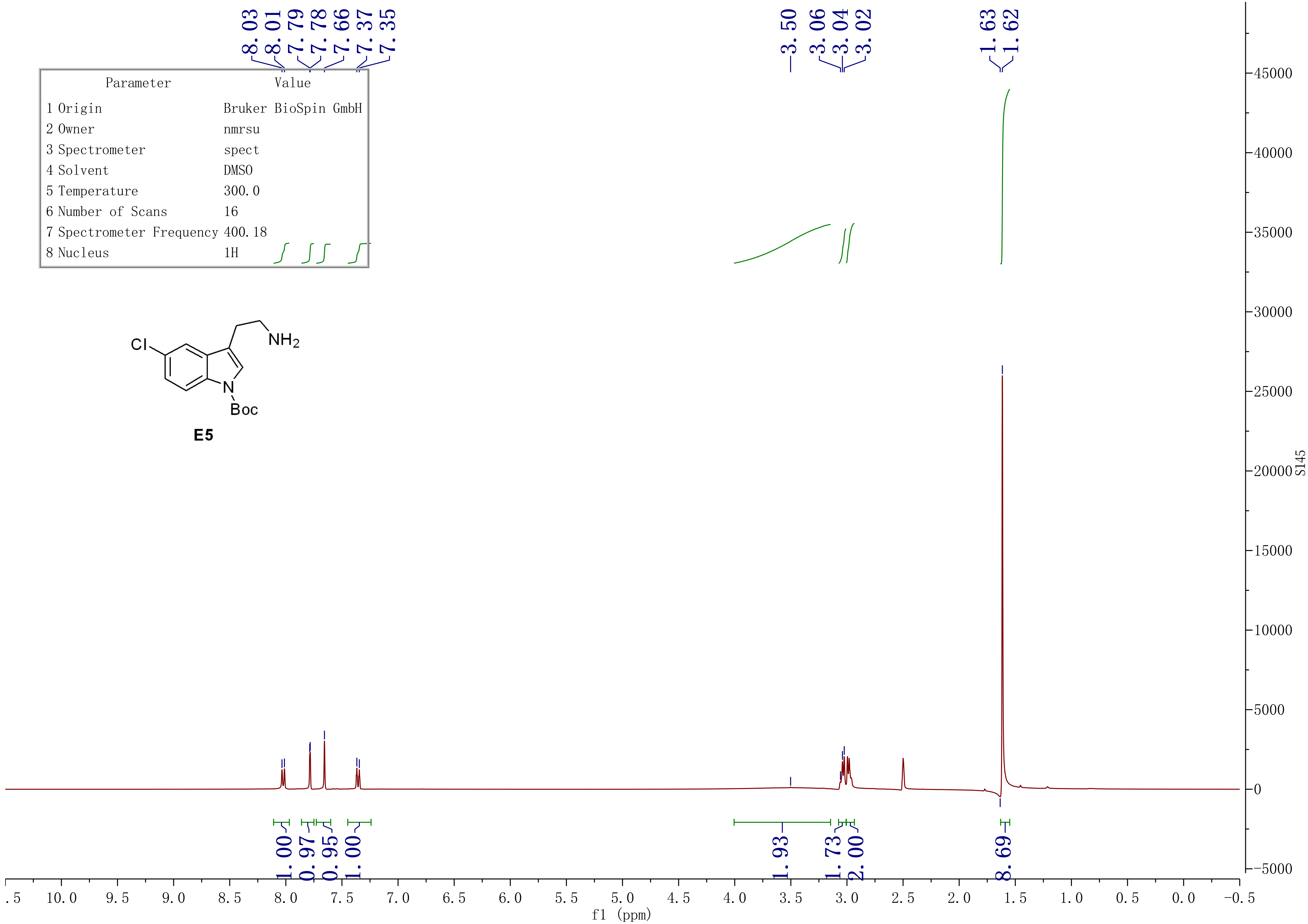


Parameter | Value
1 Origin | Bruker BioSpin GmbH
2 Owner | nmrsu
3 Spectrometer | spect
4 Solvent | DMSO
5 Temperature | 300.0
6 Number of Scans | 16
7 Spectrometer Frequency | 400.18
8 Nucleus | 1H
E2
f1 (ppm)



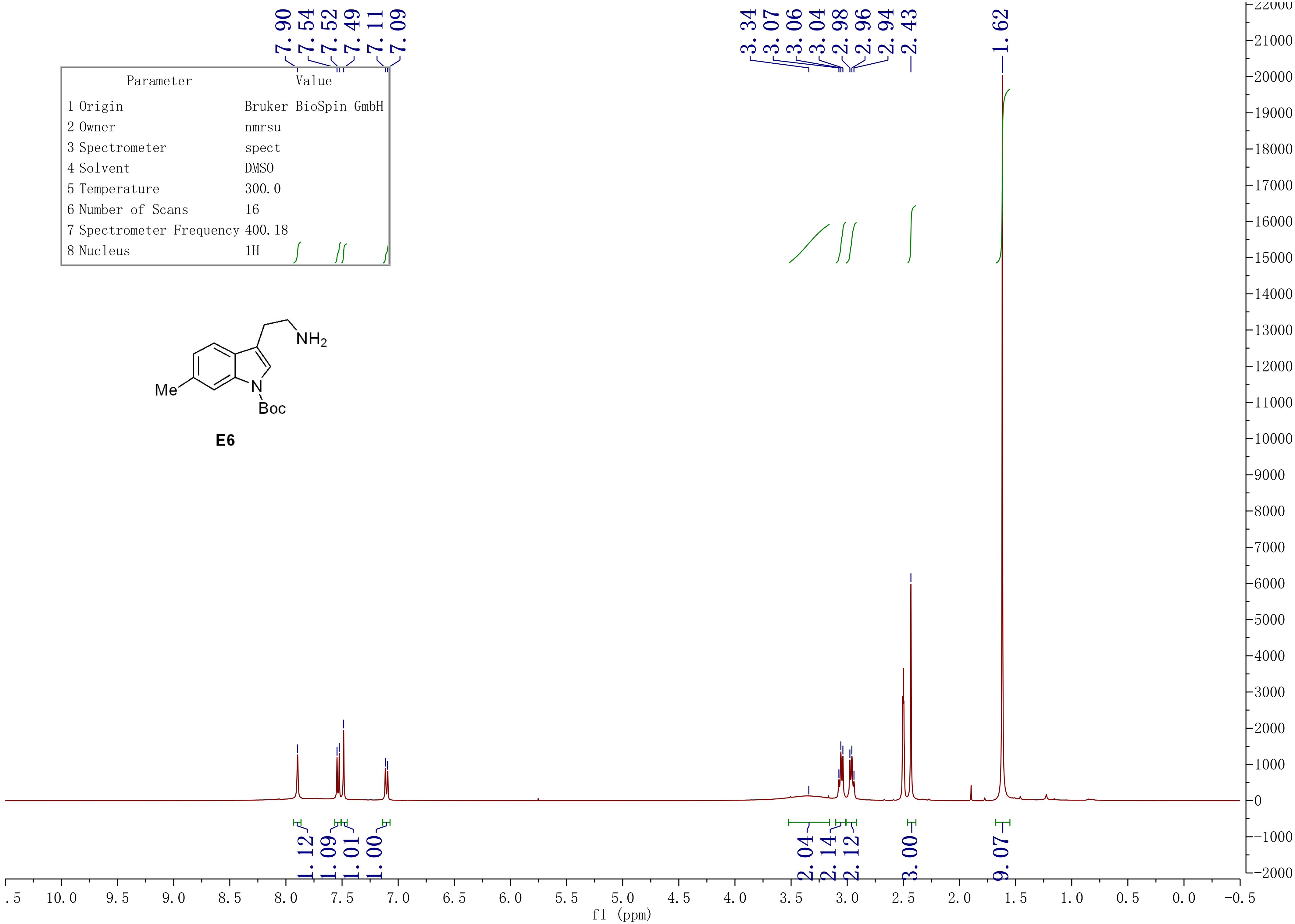
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
7.60 7.58 7.26 7.24 7.22 7.17 7.15 7.13 7.09 7.07 7.05 7.03 6.92 6.80 6.78
5.16
3.73
3.00 2.98 2.91 2.90 2.88 2.33
NH2
N
PMB
E3
0.96 1.18 1.07 0.91 2.02 1.07 1.94
1.94
3.03
1.94 2.04
1.92
f1 (ppm)

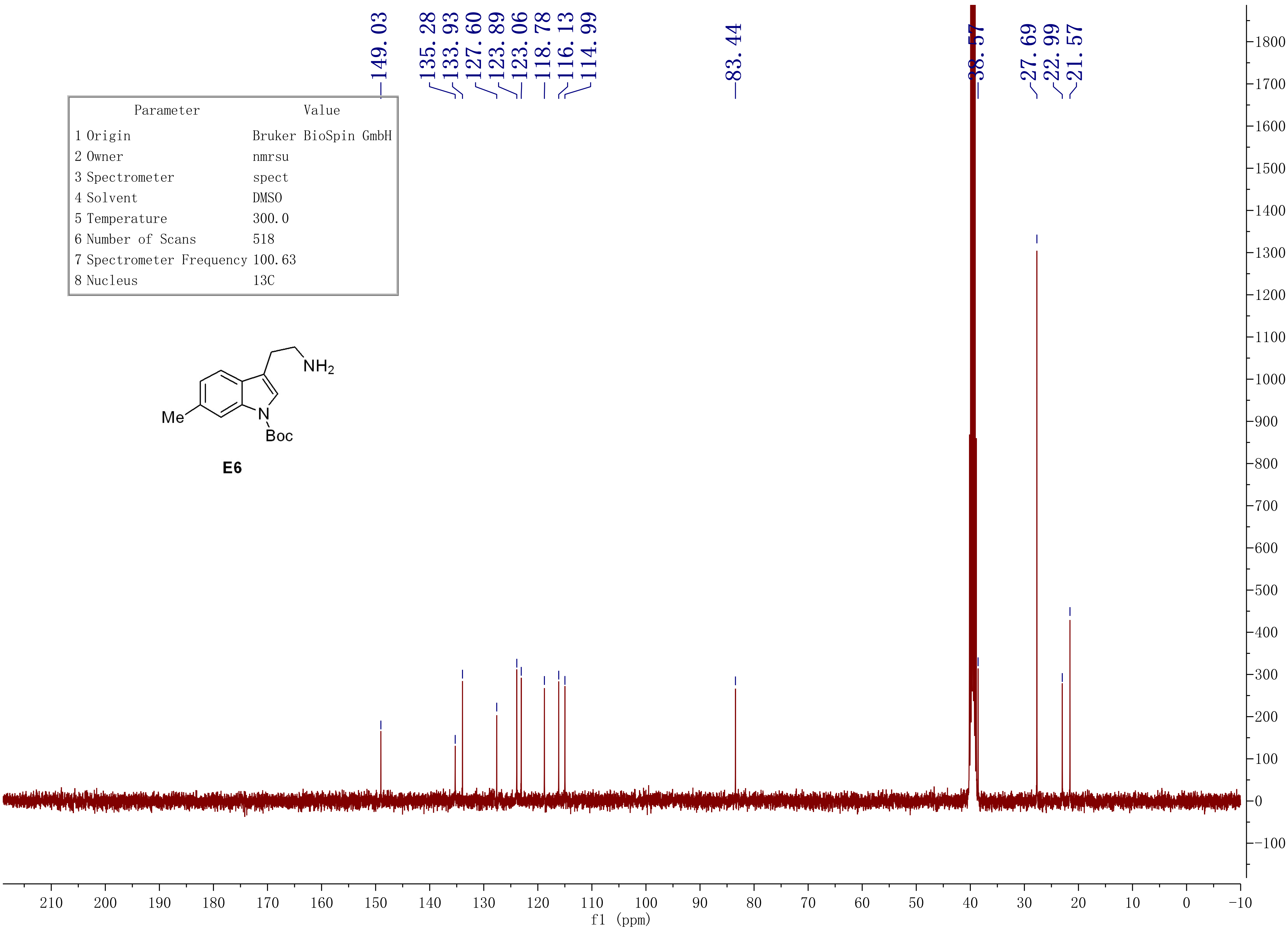

8.06
8.04
7.69
7.67
7.59
7.37
7.36
7.35
7.33
7.32
7.29
7.29
7.27
7.25
7.25
3.50
3.43
3.27
3.25
3.10
3.09
3.08
3.06
3.03
3.01
2.99
1.62
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
NH2
N
Boc
E4
1.13
1.16
1.03
1.13
0.98
2.03
2.09
2.07
9.03
f1 (ppm)



Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 400.18
8 Nucleus 1H
8.03
8.01
7.79
7.78
7.66
7.37
7.35
3.50
3.06
3.04
3.02
1.63
1.62
1.00
0.97
0.95
1.00
1.93
1.73
2.00
8.69
f1 (ppm)
Cl
NH2
N
Boc

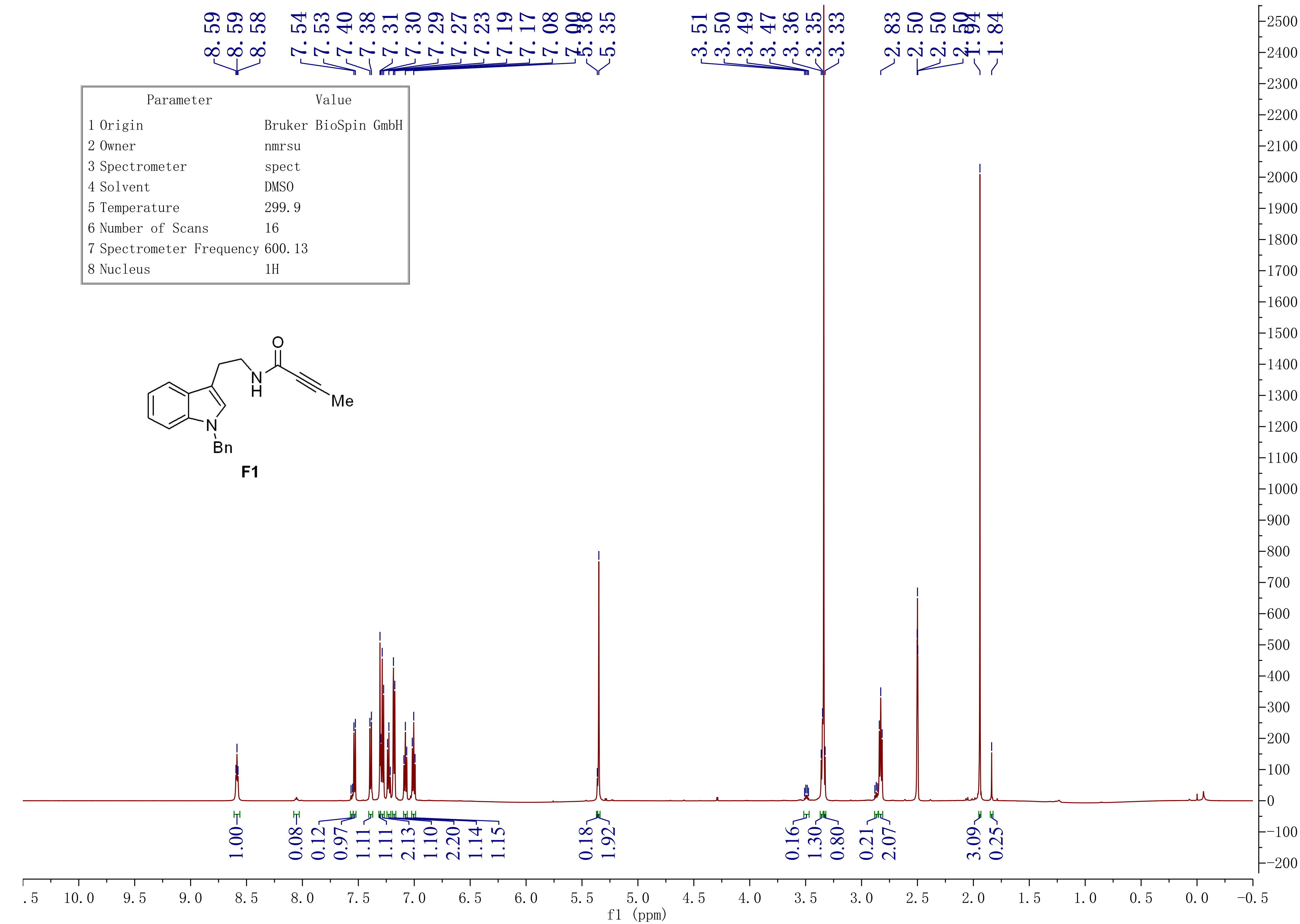
E5

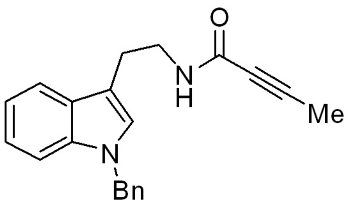

Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
DMSO
5 Temperature
300.0
6 Number of Scans
16
7 Spectrometer Frequency
400.18
8 Nucleus
1H
NH2
Me
N
Boc
E6
7.90
7.54
7.52
7.49
7.11
7.09
3.34
3.07
3.06
3.04
2.98
2.96
2.94
2.43
1.62
1.12
1.09
1.01
1.00
2.04
2.14
2.12
3.00
9.07
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	518
7 Spectrometer Frequency	100.63
8 Nucleus	13C

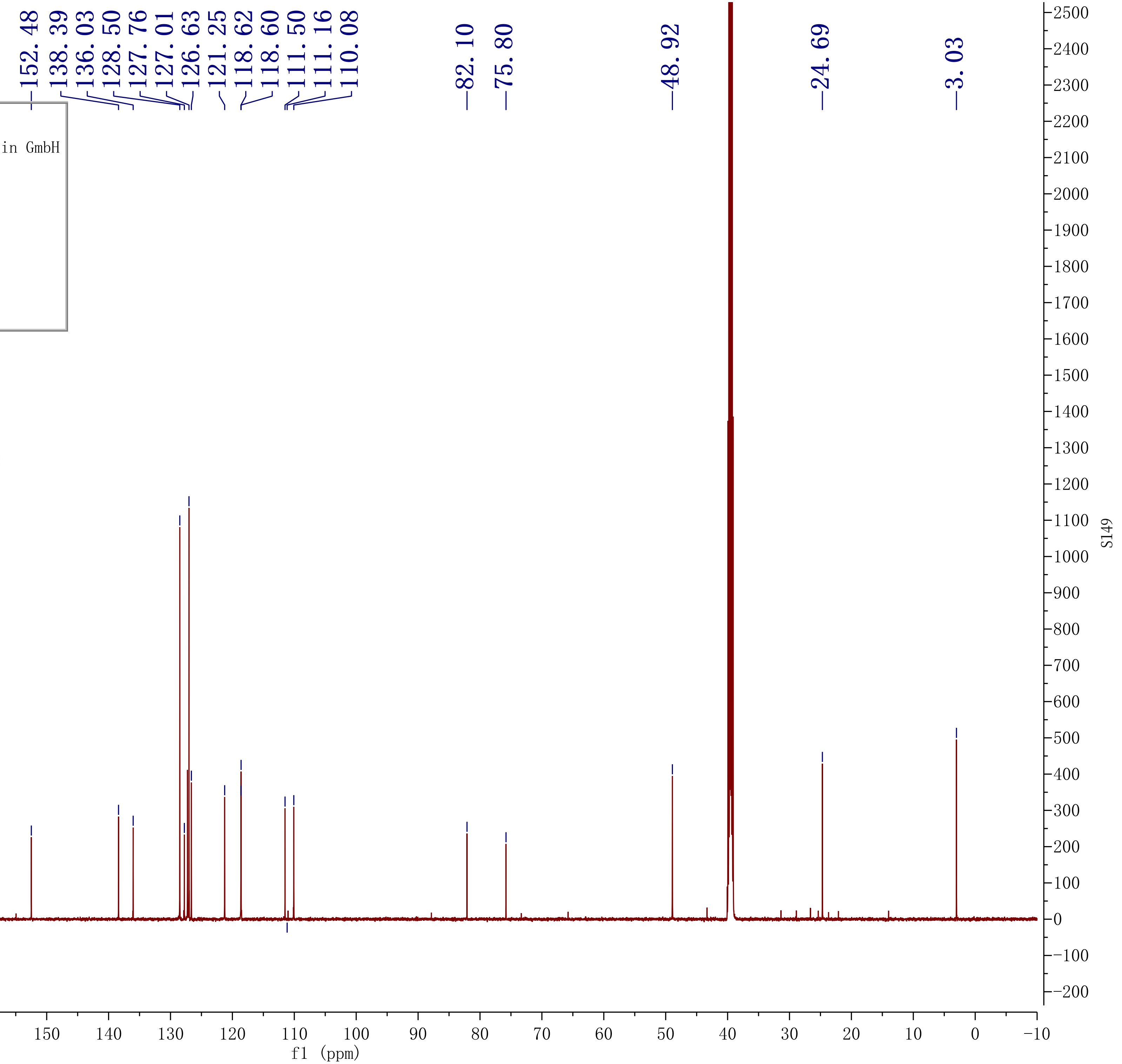
E6


8.59
8.59
8.58
7.54
7.53
7.40
7.38
7.31
7.30
7.29
7.27
7.23
7.19
7.17
7.08
7.00
5.36
5.35
3.51
3.50
3.49
3.47
3.36
3.35
3.33
2.83
2.50
2.50
2.50
1.94
1.84
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
Me
N
Bn
F1
1.00
0.08
0.12
0.97
1.11
1.11
2.13
1.10
2.20
1.14
1.15
0.18
1.92
0.16
1.30
0.80
0.21
2.07
3.09
0.25
f1 (ppm)

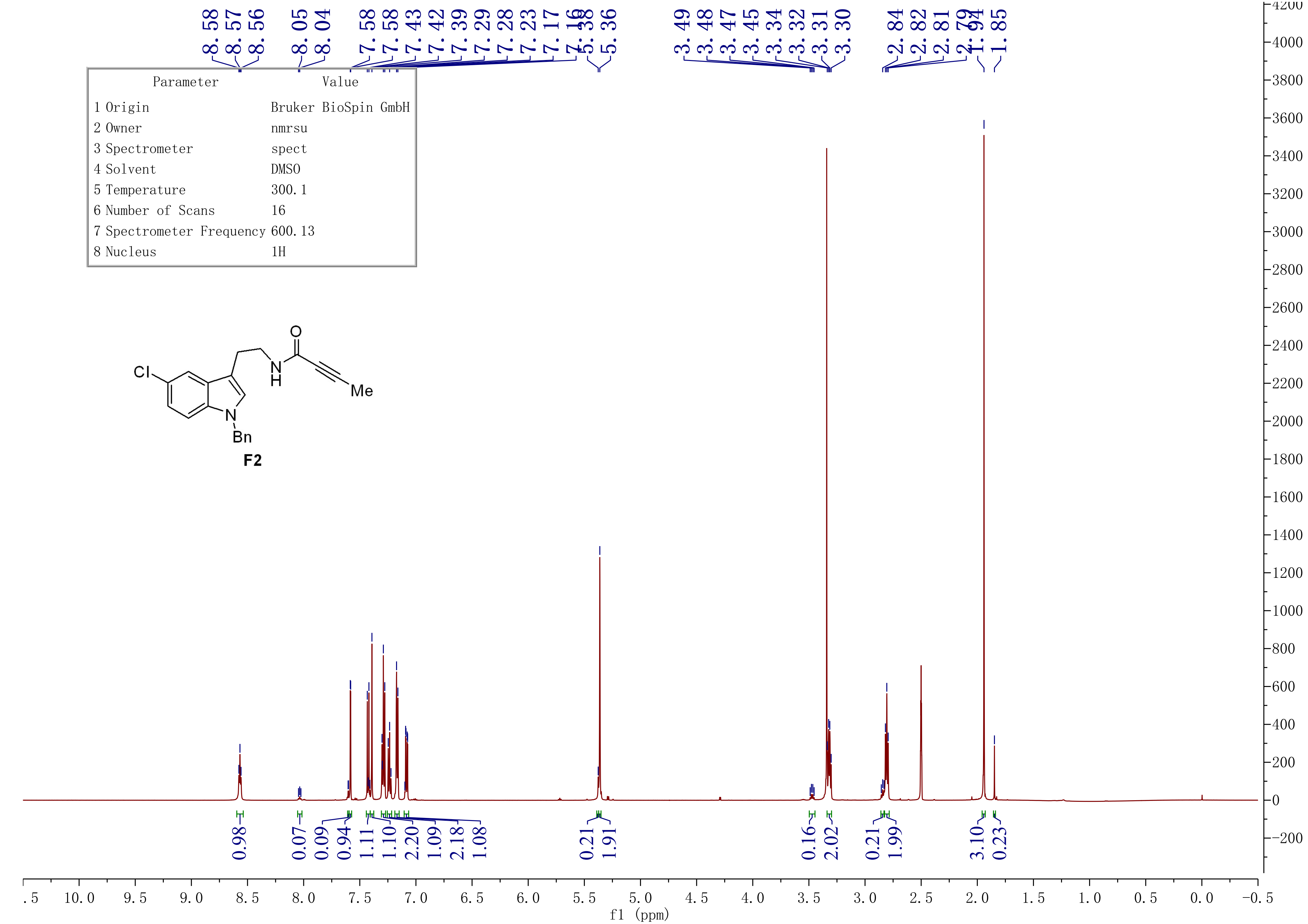


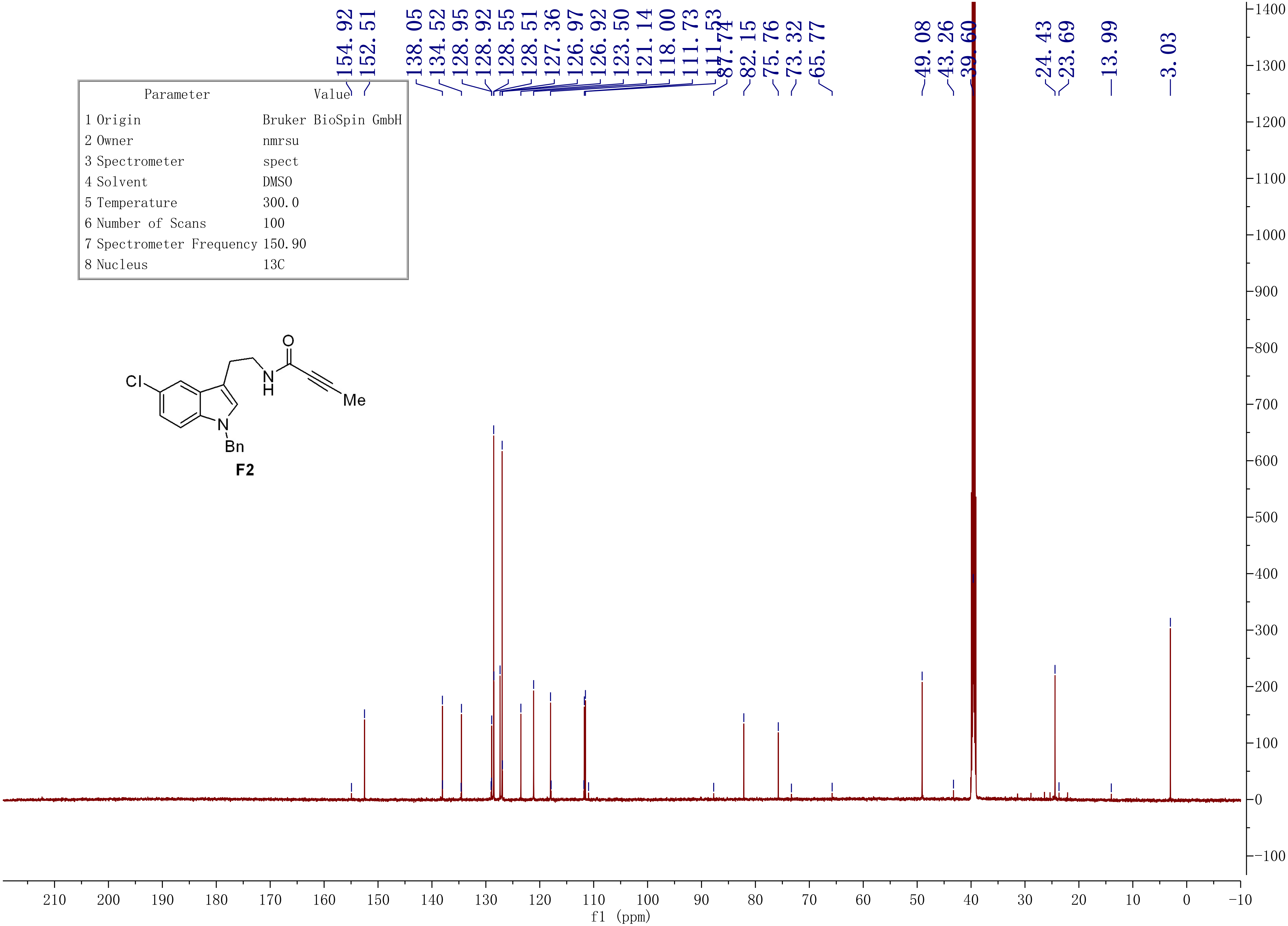
F1

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	256
7 Spectrometer Frequency	150.90
8 Nucleus	13C



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.1
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H





Parameter	Value
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2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
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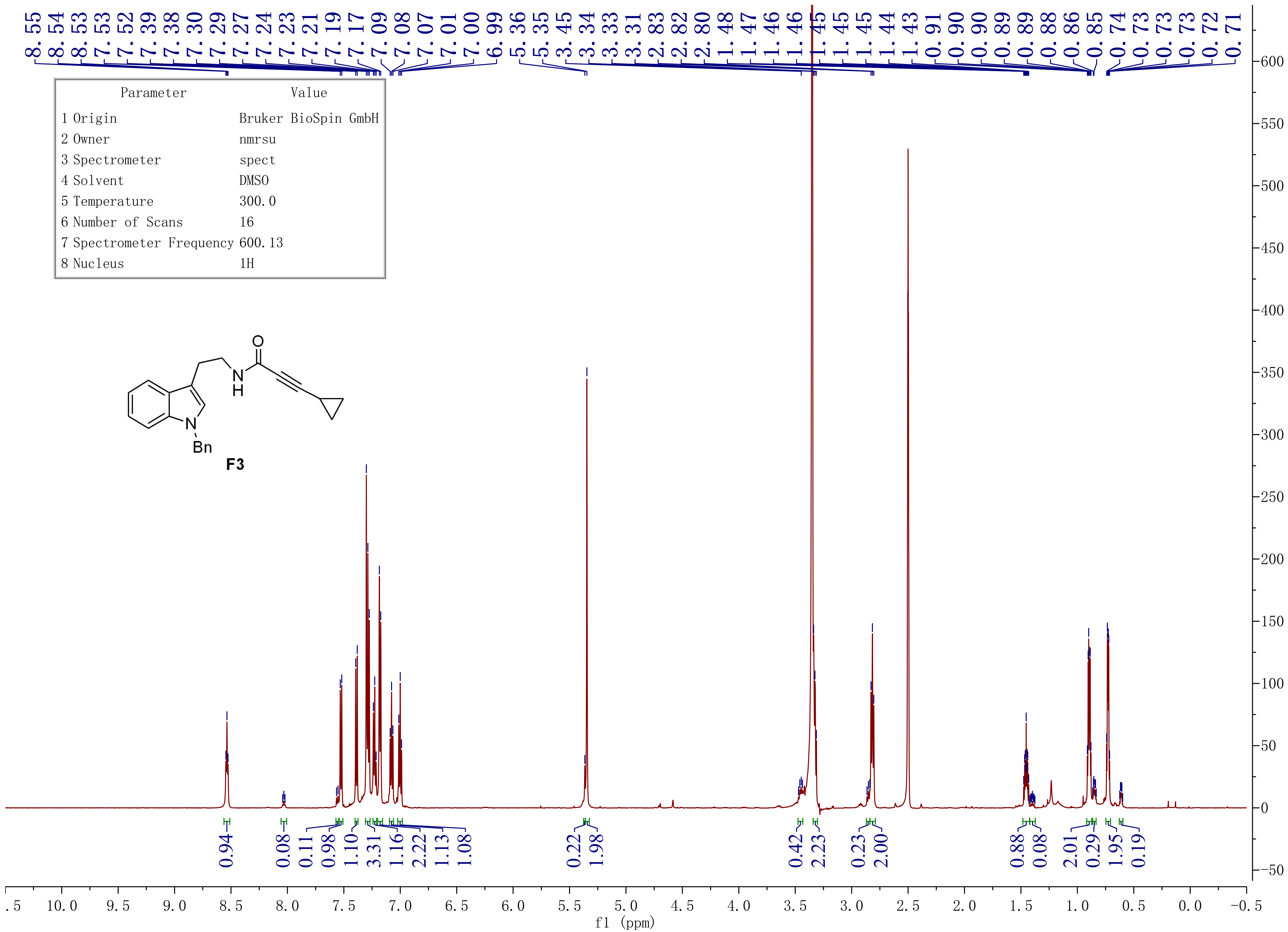
7 Spectrometer Frequency	150.90
8 Nucleus	13C

F2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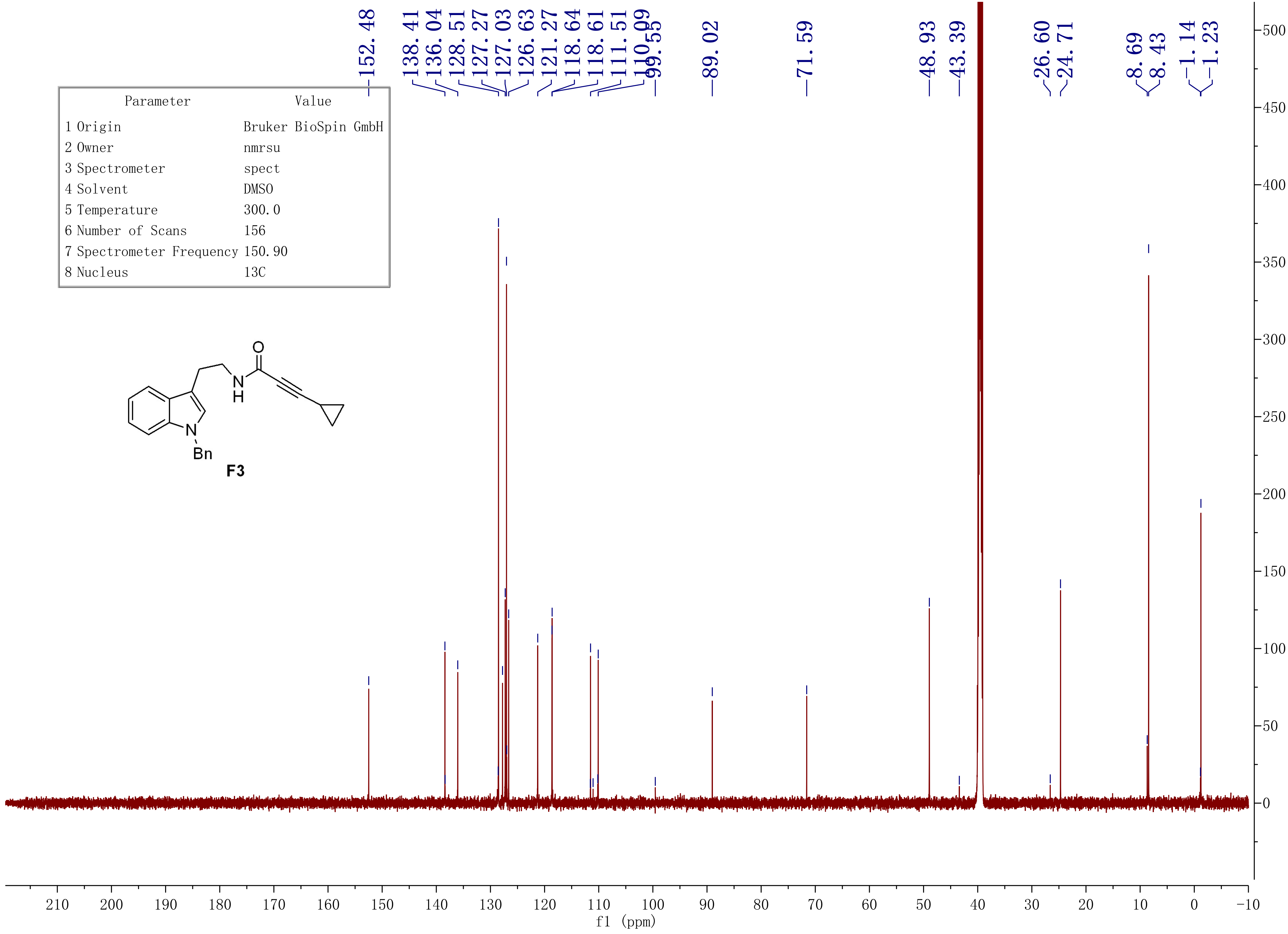
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Bn
F3
f1 (ppm)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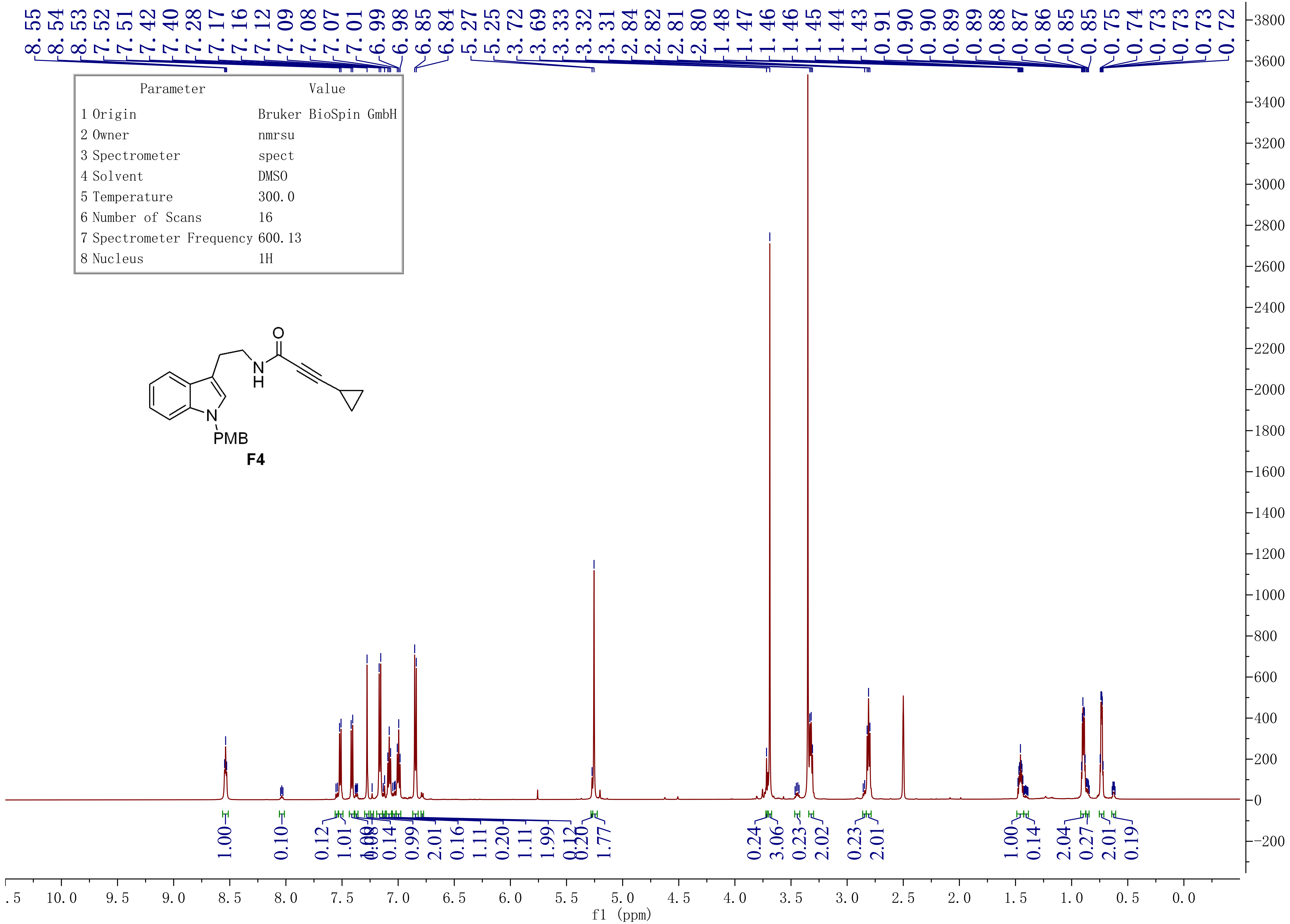
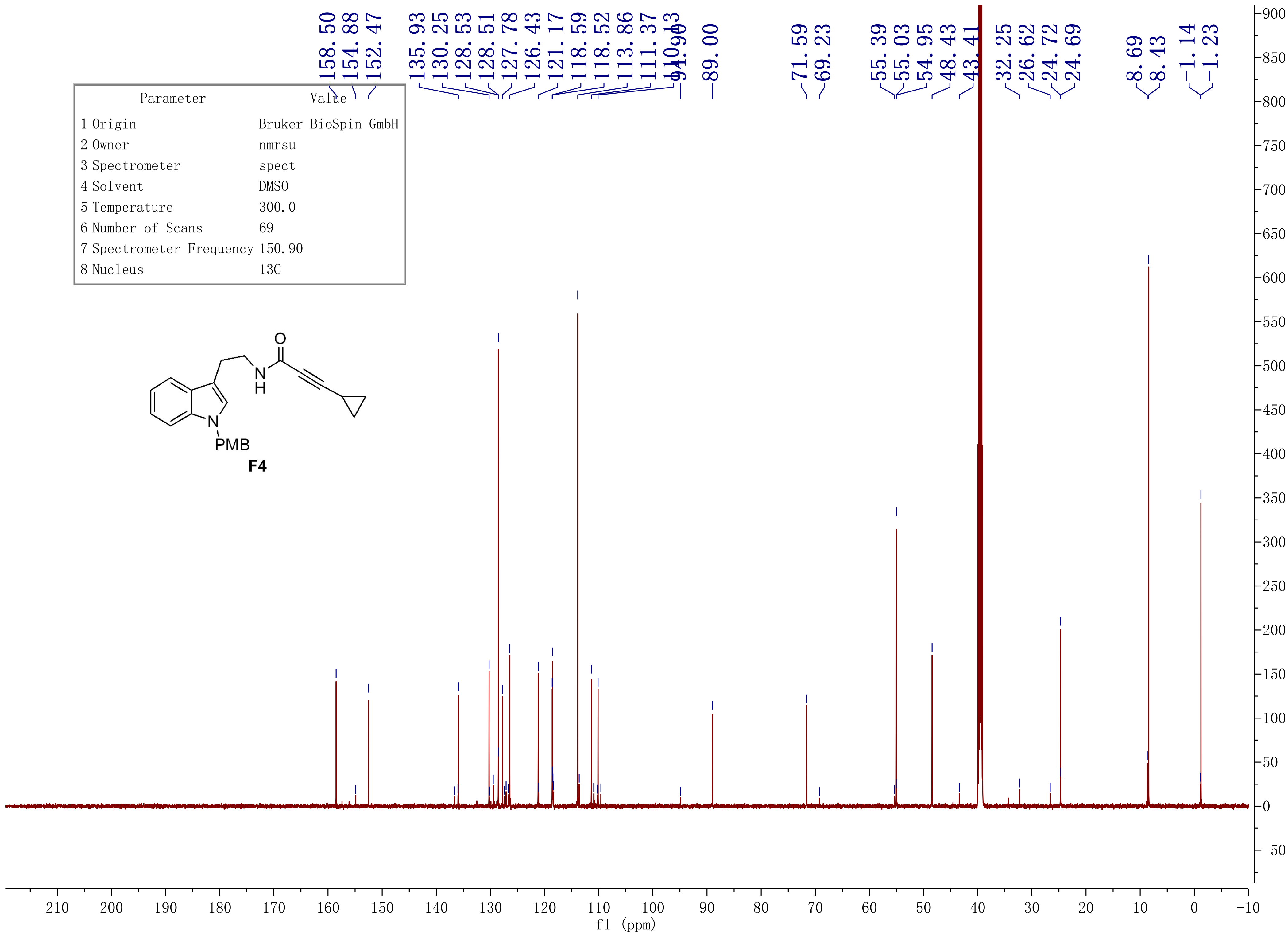
138.41
136.04
128.51
127.27
127.03
126.63
121.27
118.64
118.61
111.51
110.09
99.55
89.02
71.59
48.93
43.39
26.60
24.71
8.69
8.43
-1.14
-1.23
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 156
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
N
Bn
F3
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
PMB
F4
f1 (ppm)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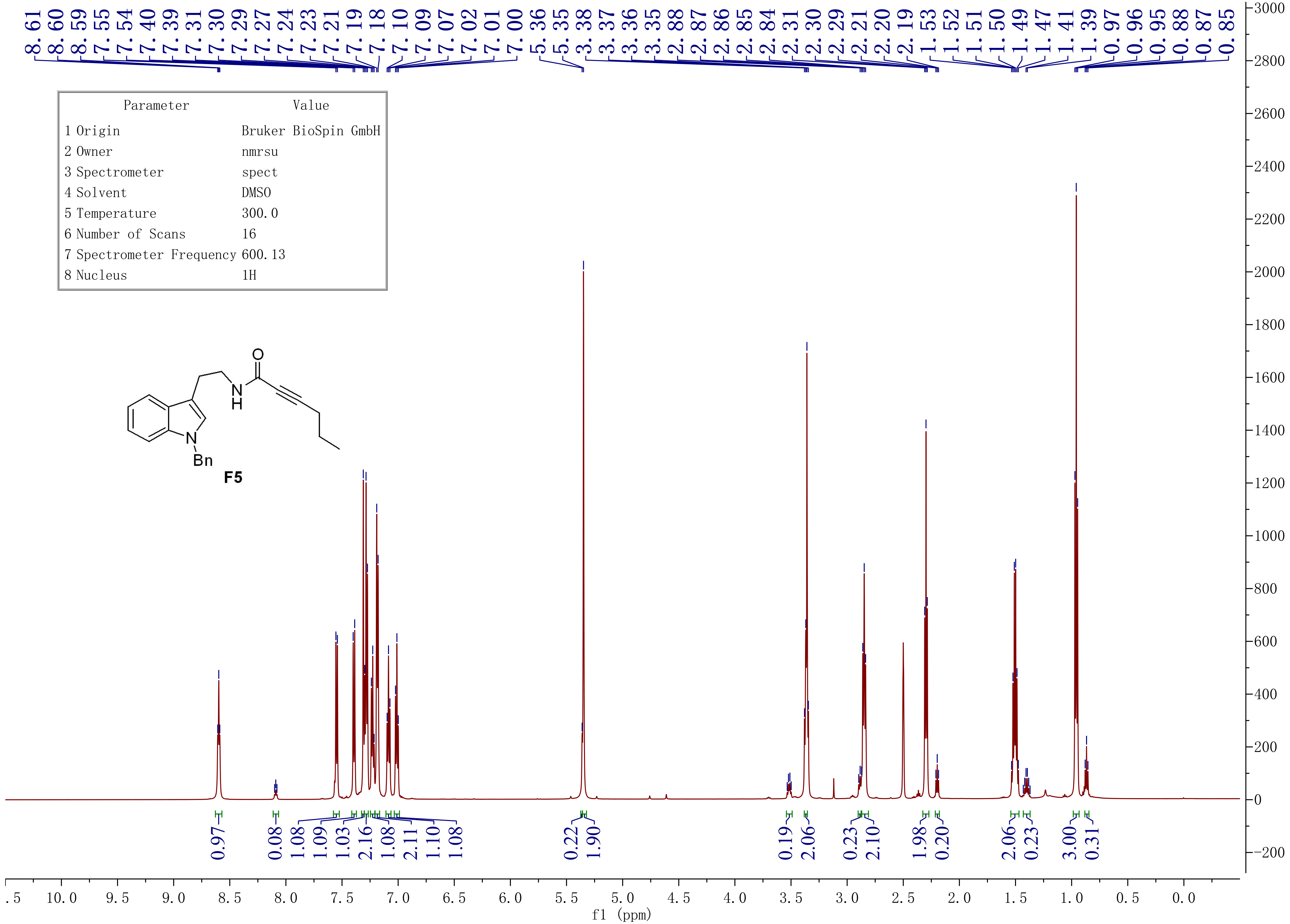
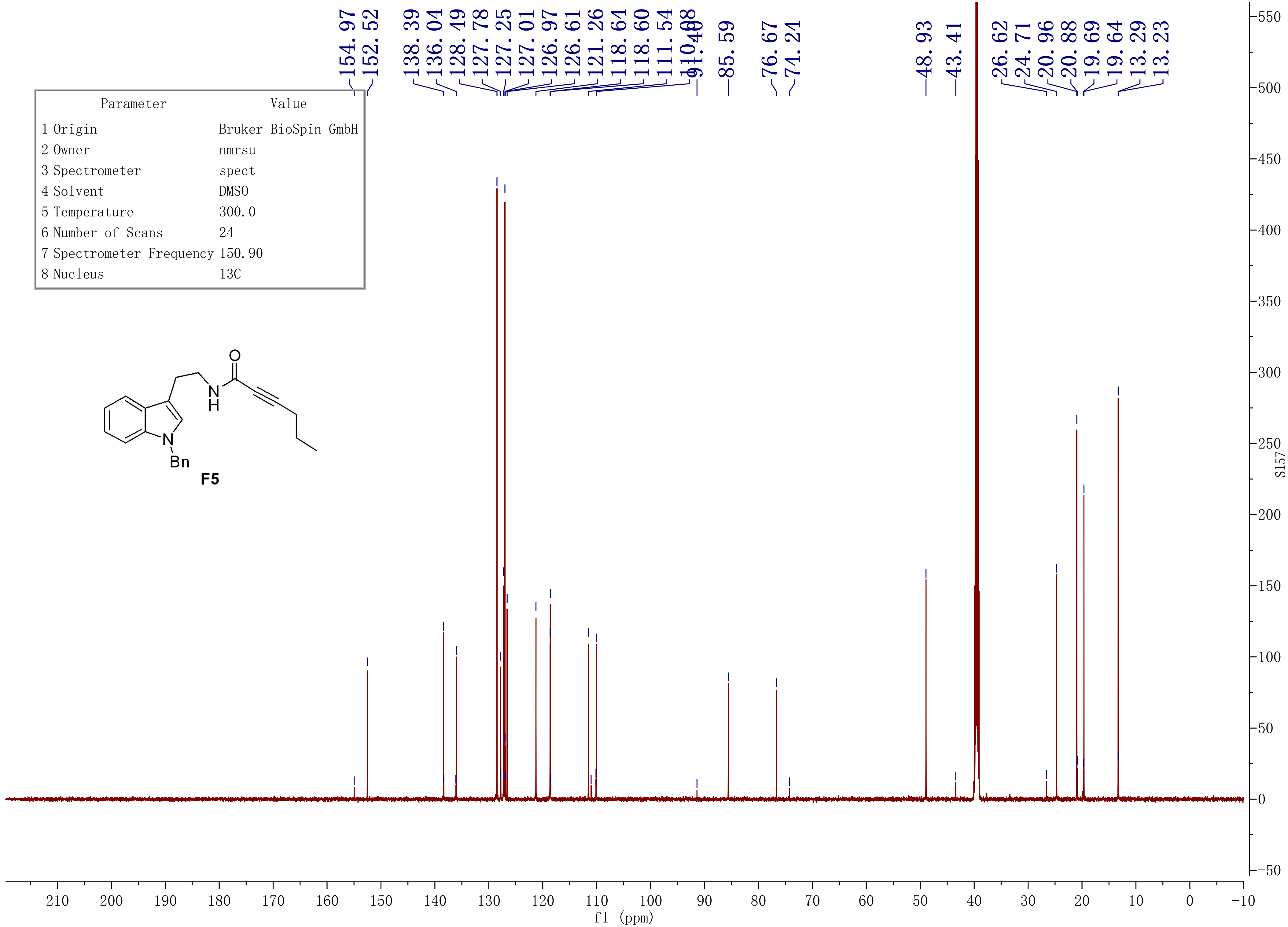
118.52
113.86
111.37
110.13
94.90
89.00
71.59
69.23
55.39
55.03
54.95
48.43
43.41
32.25
26.62
24.72
24.69
8.69
8.43
-1.14
-1.23
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 69
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
N
PMB
F4
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H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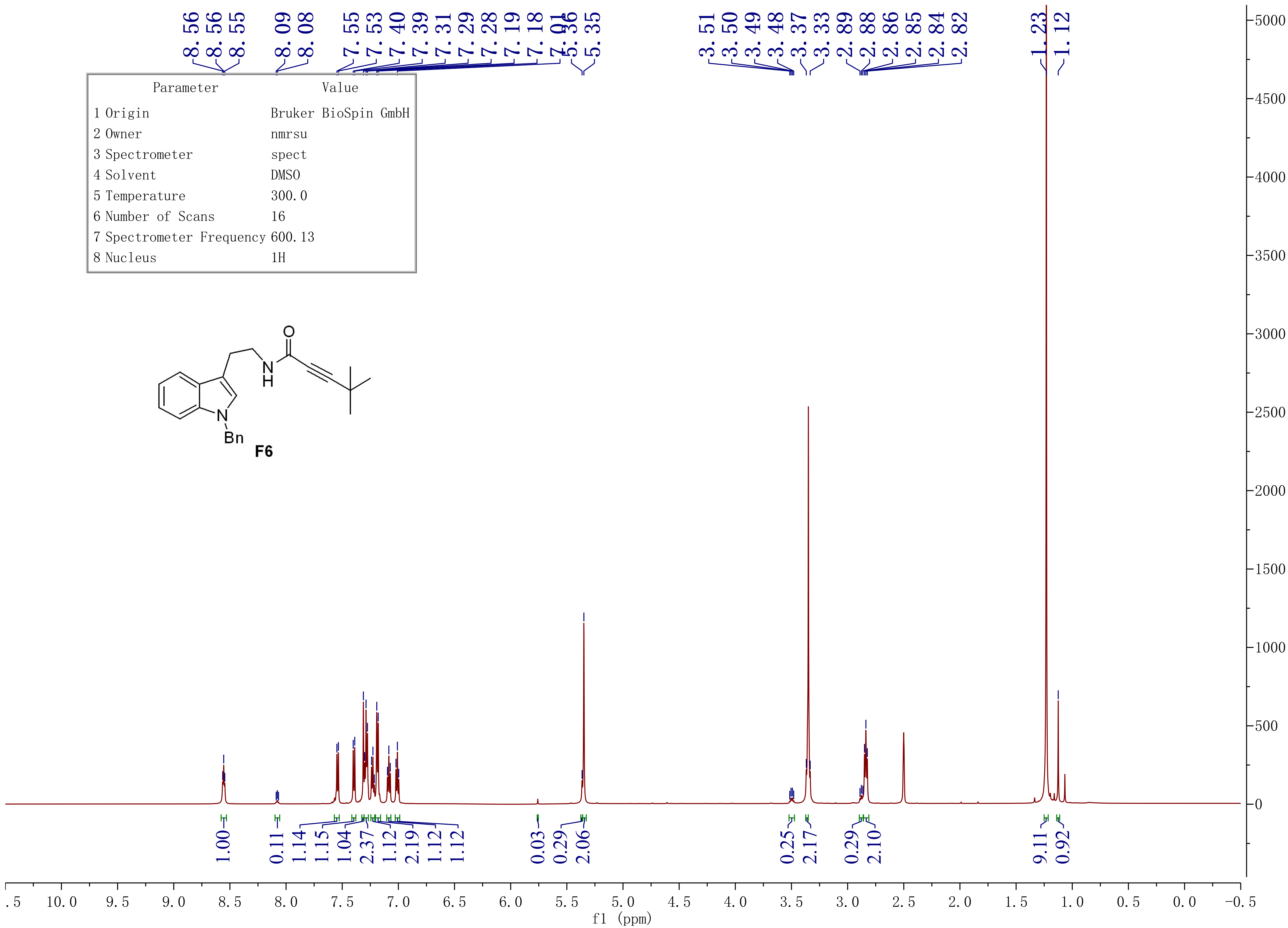
136.04
128.49
127.78
127.25
127.01
126.97
126.61
121.26
118.64
118.60
111.54
110.08
91.40
85.59
76.67
74.24
48.93
43.41
26.62
24.71
20.96
20.88
19.69
19.64
13.29
13.23
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 24
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
N
Bn
F5
f1 (ppm)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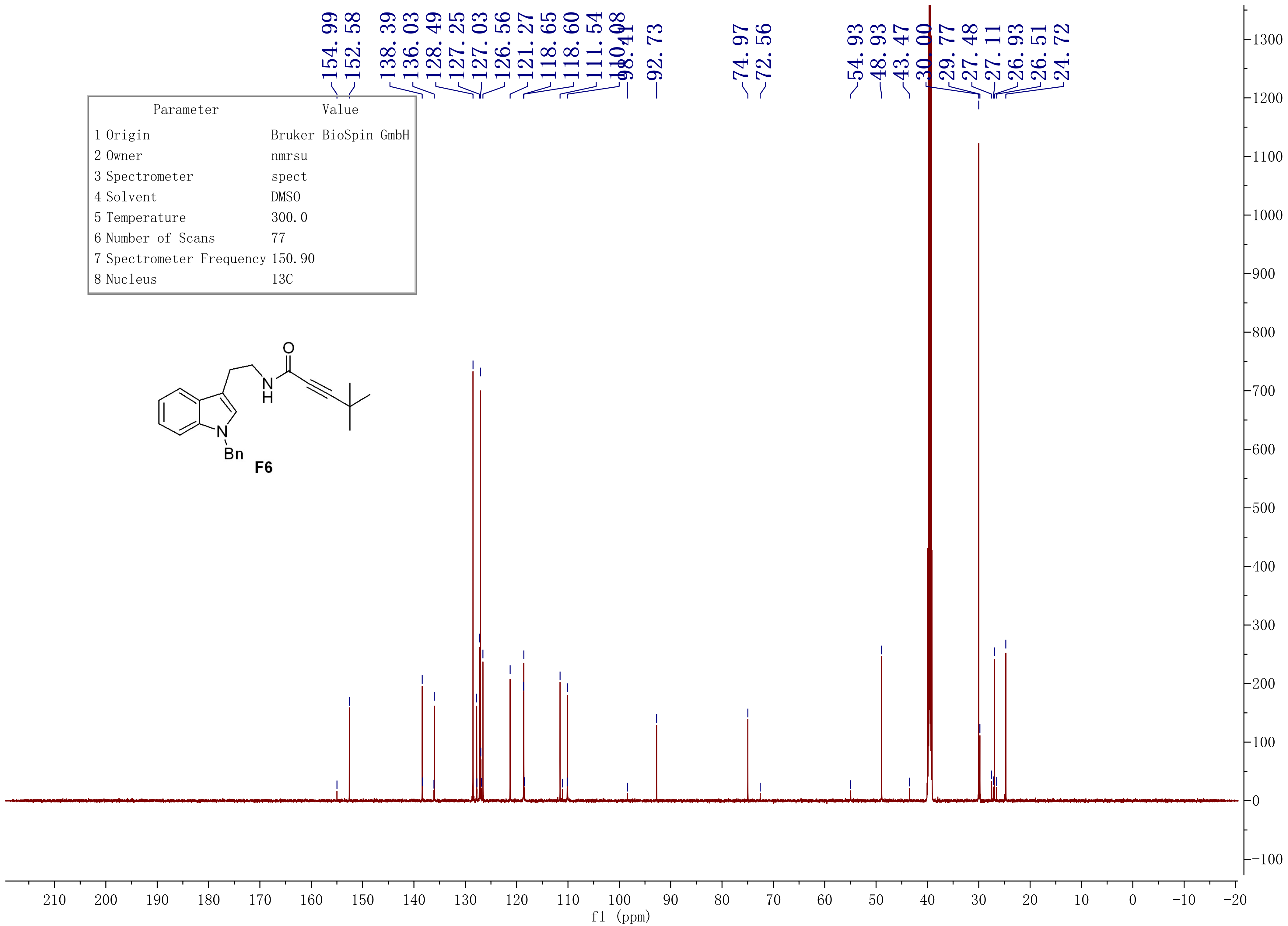
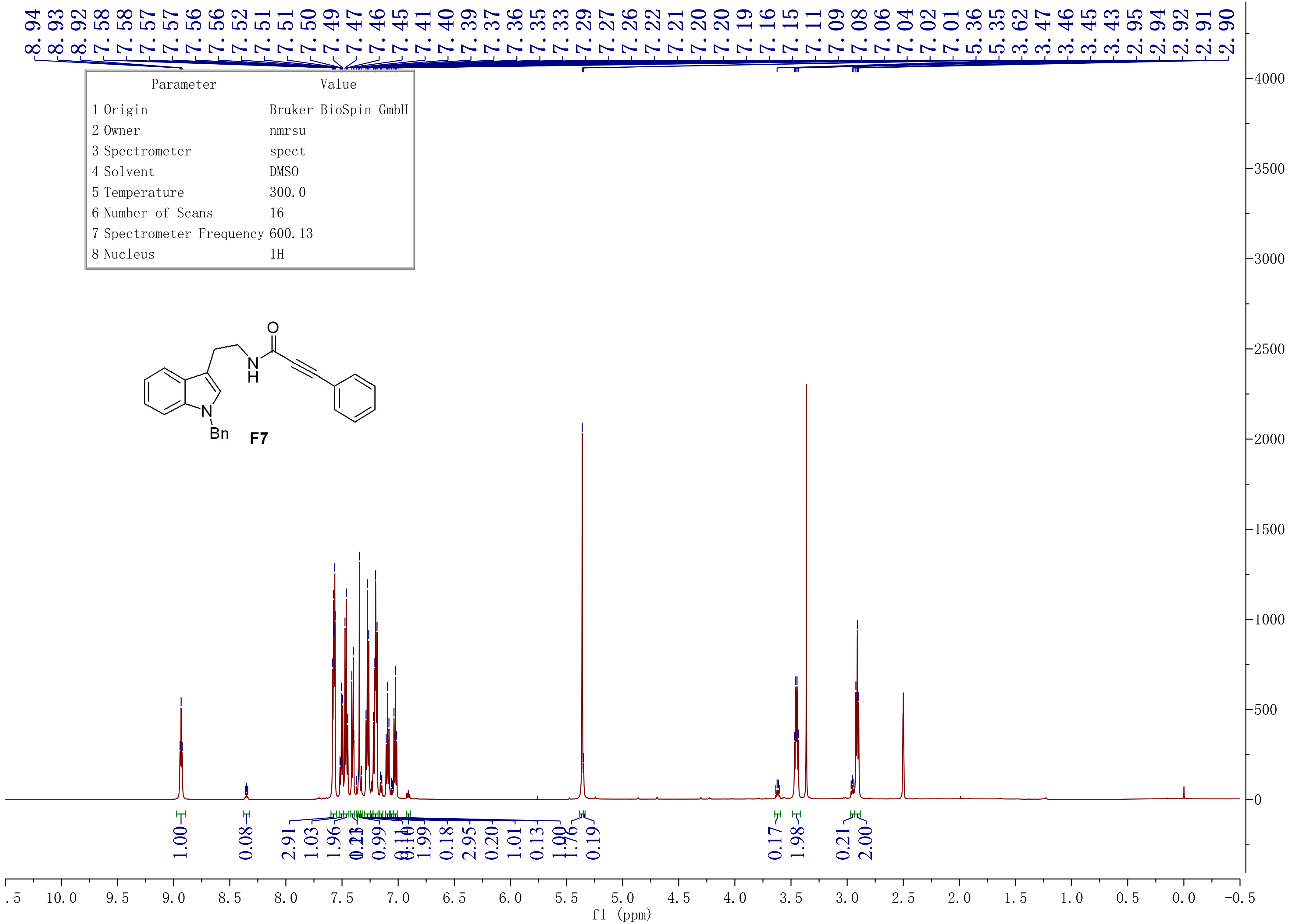
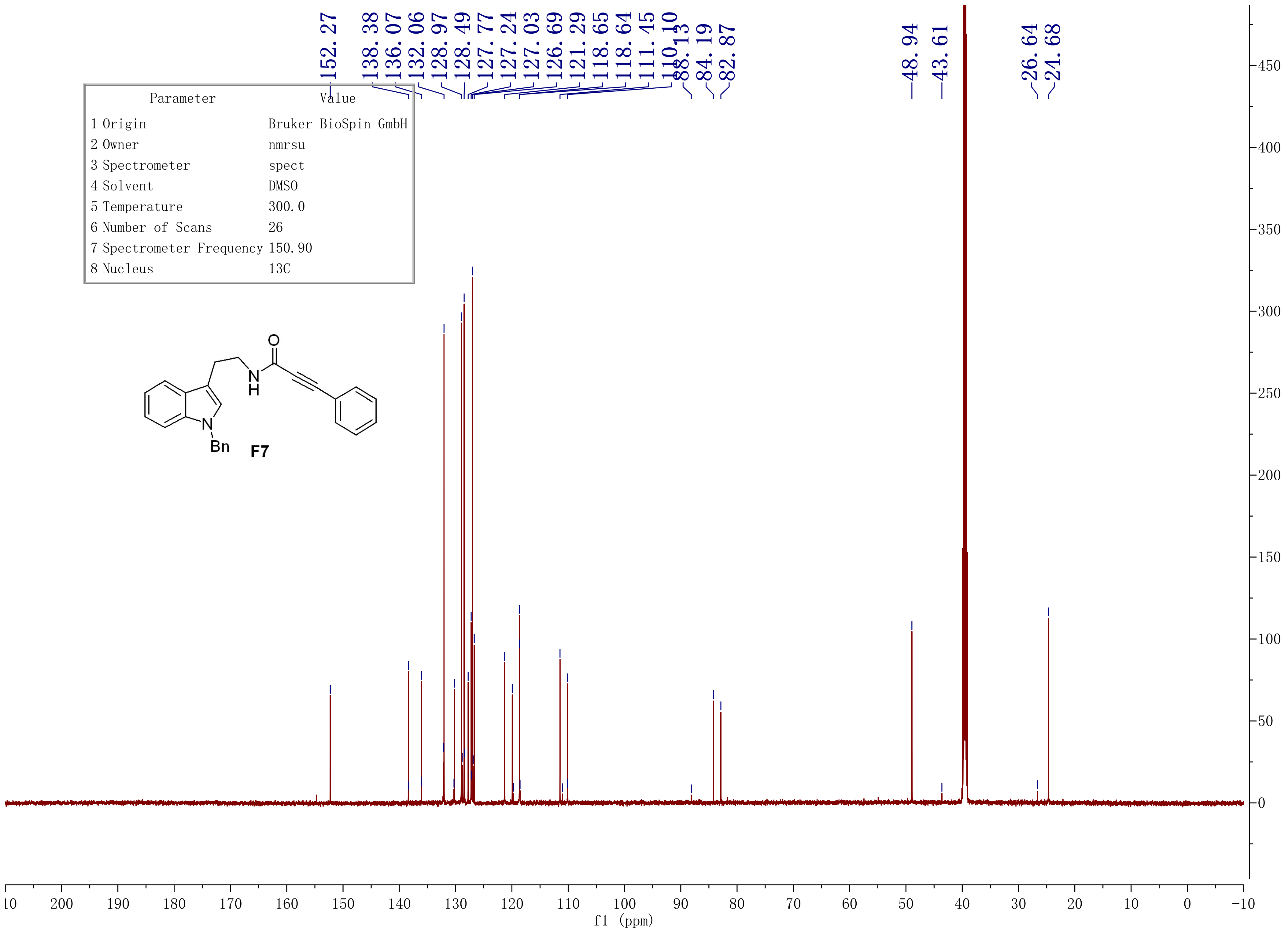
8.56
8.55
8.09
8.08
7.55
7.53
7.40
7.39
7.31
7.29
7.28
7.19
7.18
7.01
5.36
5.35
3.51
3.50
3.49
3.48
3.37
3.33
2.89
2.88
2.86
2.85
2.84
2.82
1.23
1.12
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
DMSO
5 Temperature
300.0
6 Number of Scans
16
7 Spectrometer Frequency
600.13
8 Nucleus
1H
O
N
H
N
Bn
F6
1.00
0.11
1.14
1.15
1.04
2.37
1.12
2.19
1.12
1.12
0.03
0.29
2.06
0.25
2.17
0.29
2.10
9.11
0.92
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	77
7 Spectrometer Frequency	150.90
8 Nucleus	13C


8.94 8.93 8.92 7.58 7.58 7.57 7.57 7.56 7.56 7.52 7.51 7.51 7.50 7.49 7.47 7.46 7.45 7.41 7.40 7.39 7.37 7.36 7.35 7.33 7.29 7.27 7.26 7.22 7.21 7.20 7.20 7.19 7.16 7.15 7.11 7.09 7.08 7.06 7.04 7.02 7.01 5.36 5.35 3.62 3.47 3.46 3.45 3.43 2.95 2.94 2.92 2.91 2.90
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
N
Bn
F7
1.00 0.08 2.91 1.03 1.96 0.23 0.11 0.99 0.11 0.10 1.99 0.18 2.95 0.20 1.01 0.13 1.00 1.76 0.19 0.17 1.98 0.21 2.00
f1 (ppm)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138.38
136.07
132.06
128.97
128.49
127.77
127.24
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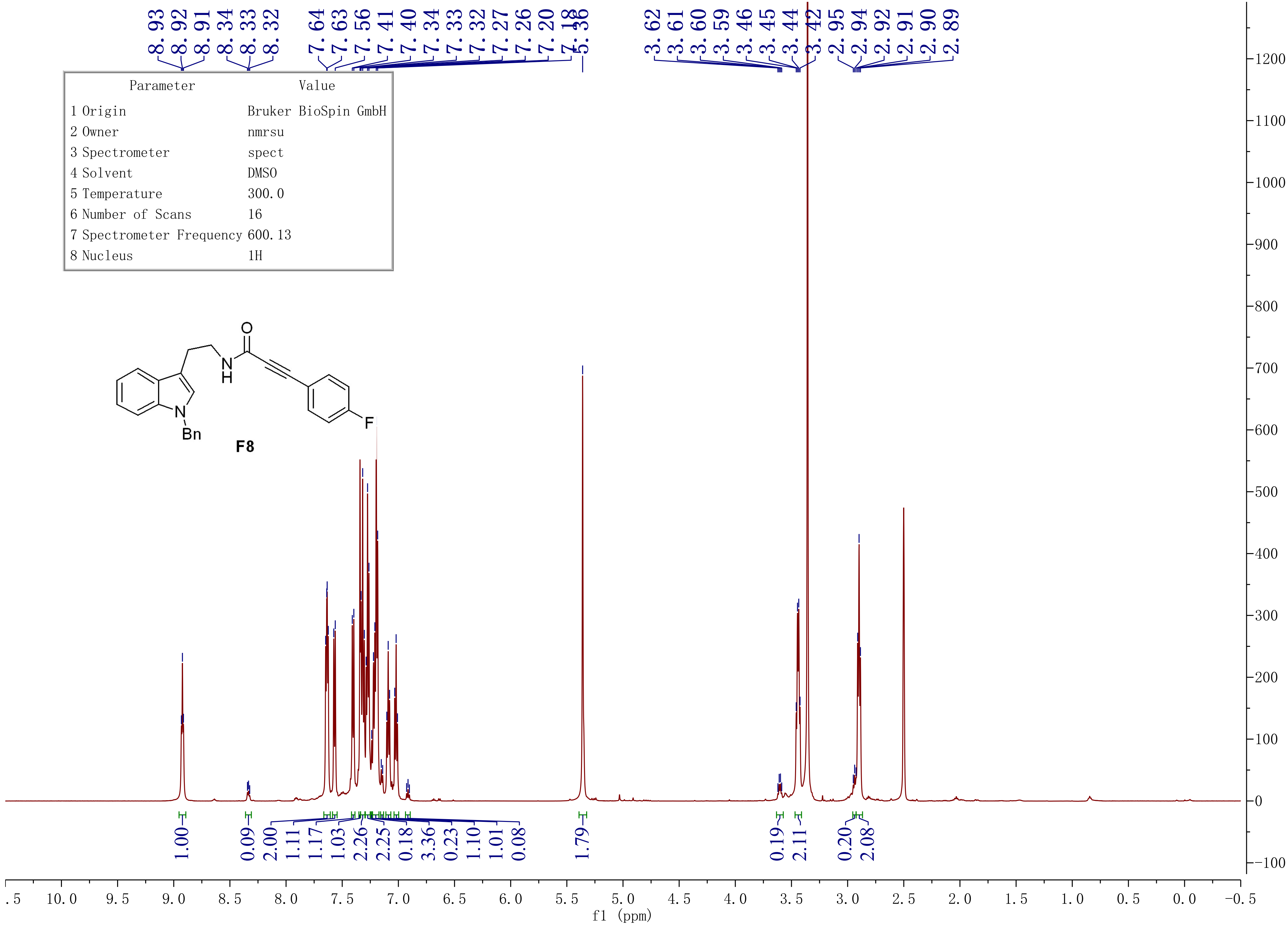
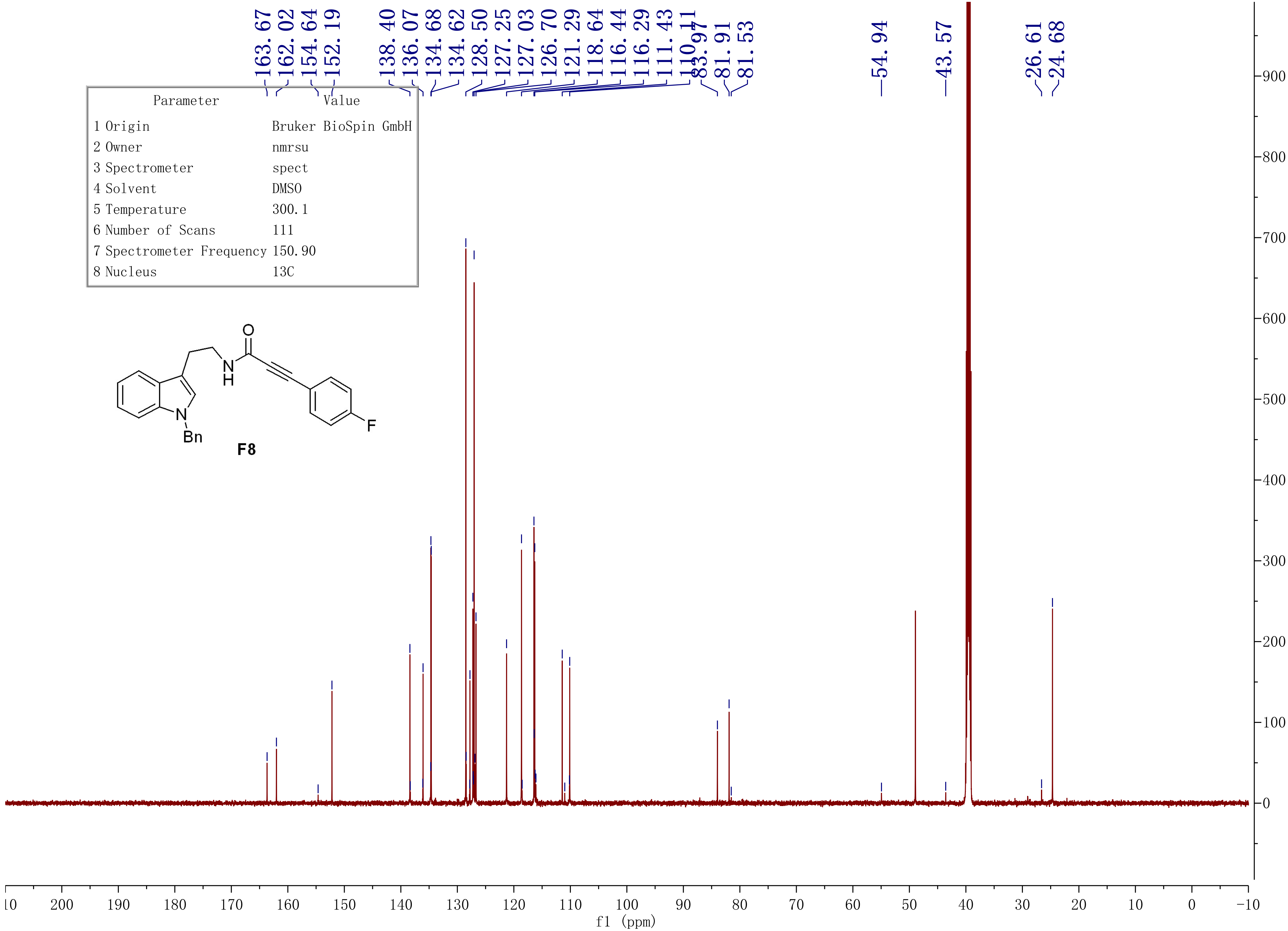
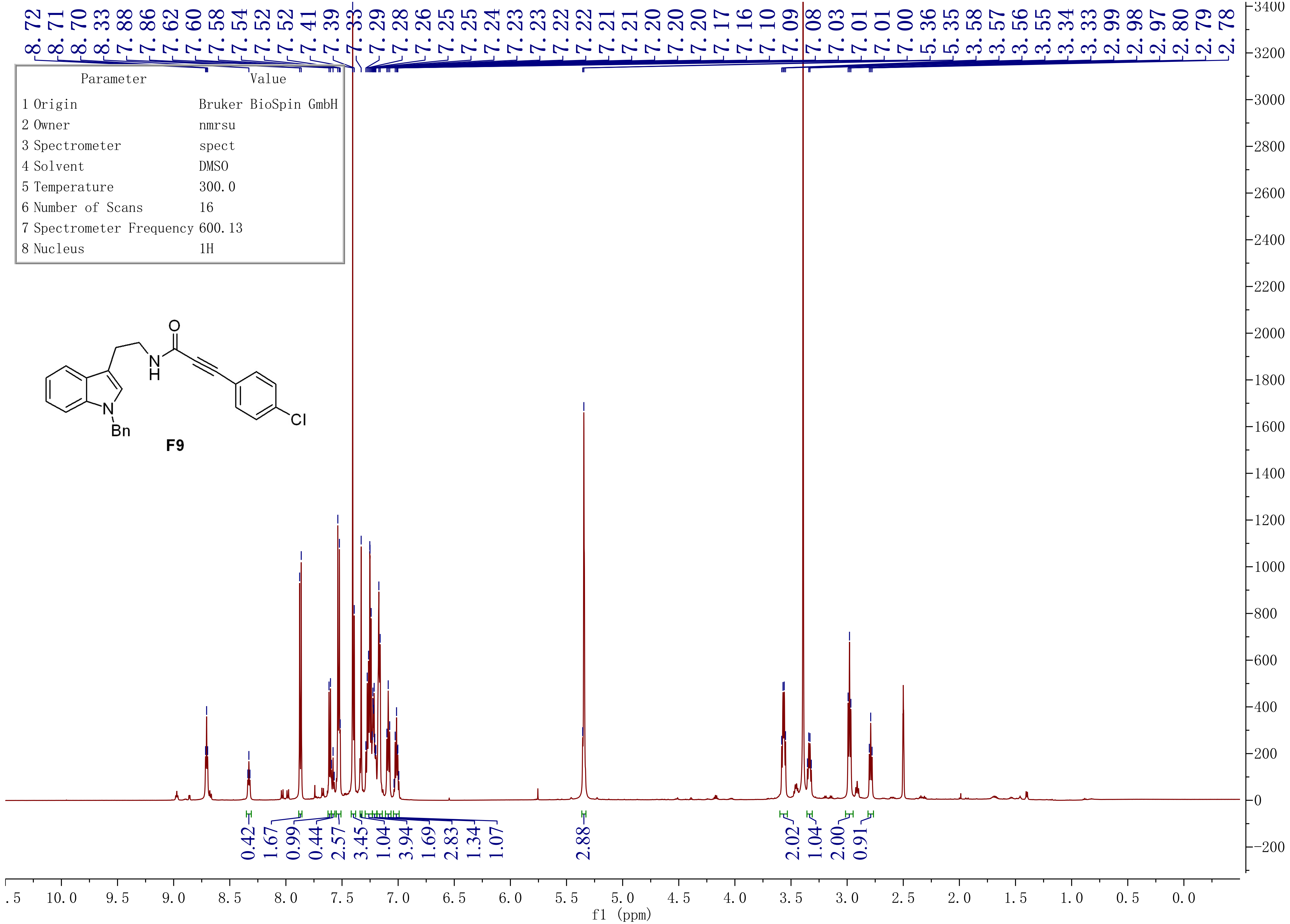
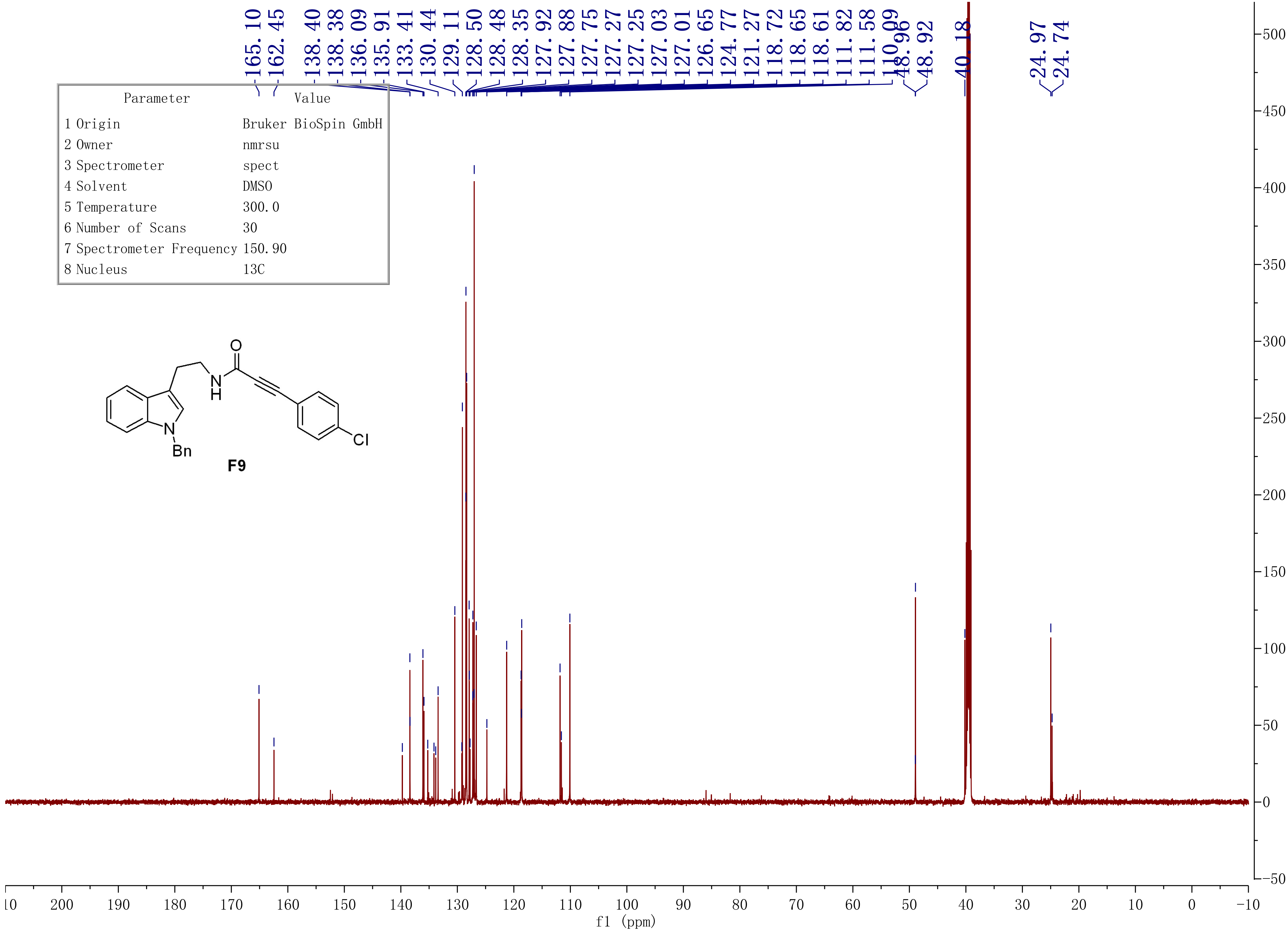
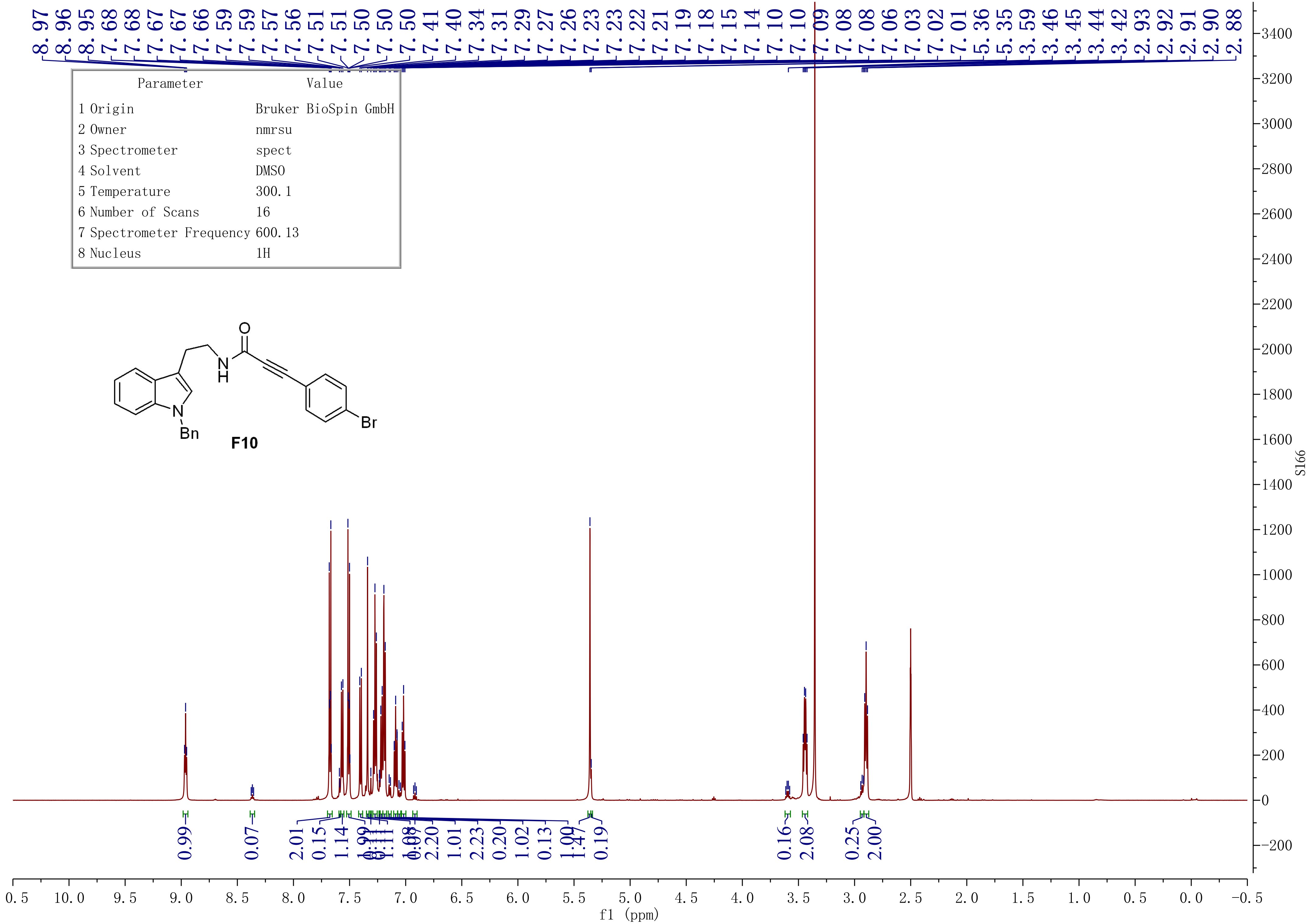
126.69
121.29
118.65
118.64
111.45
110.10
88.13
84.19
82.87
48.94
43.61
26.64
24.68
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 26
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
N
Bn
F7
f1 (ppm)

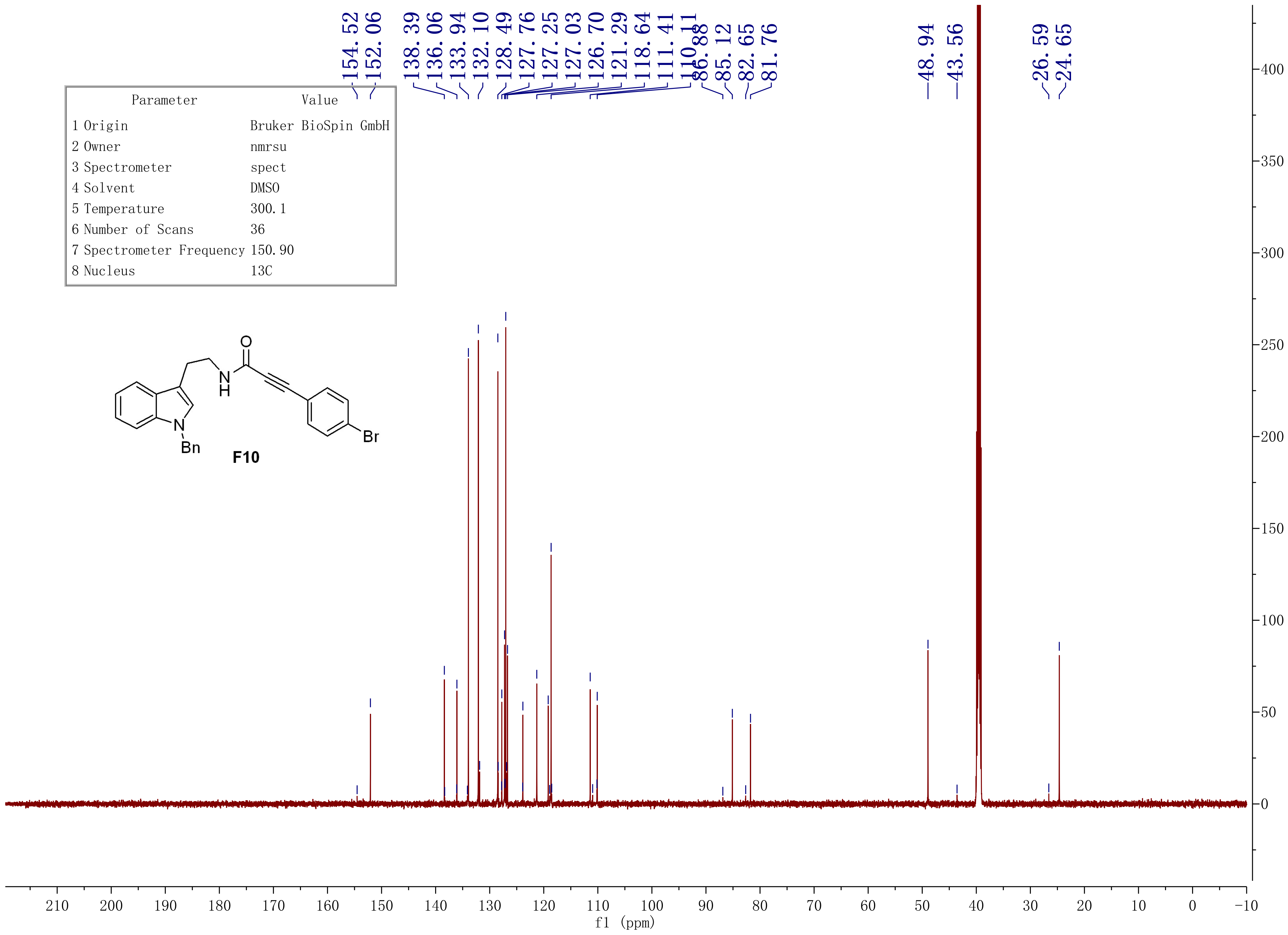

8.93
8.92
8.91
8.34
8.33
8.32
7.64
7.63
7.56
7.41
7.40
7.34
7.33
7.32
7.27
7.26
7.20
7.18
5.36
3.62
3.61
3.60
3.59
3.46
3.45
3.44
3.42
2.95
2.94
2.92
2.91
2.90
2.89
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
N
Bn
F
F8
1.00
0.09
2.00
1.11
1.17
1.03
2.26
2.25
0.18
3.36
0.23
1.10
1.01
0.08
1.79
0.19
2.11
0.20
2.08
f1 (ppm)

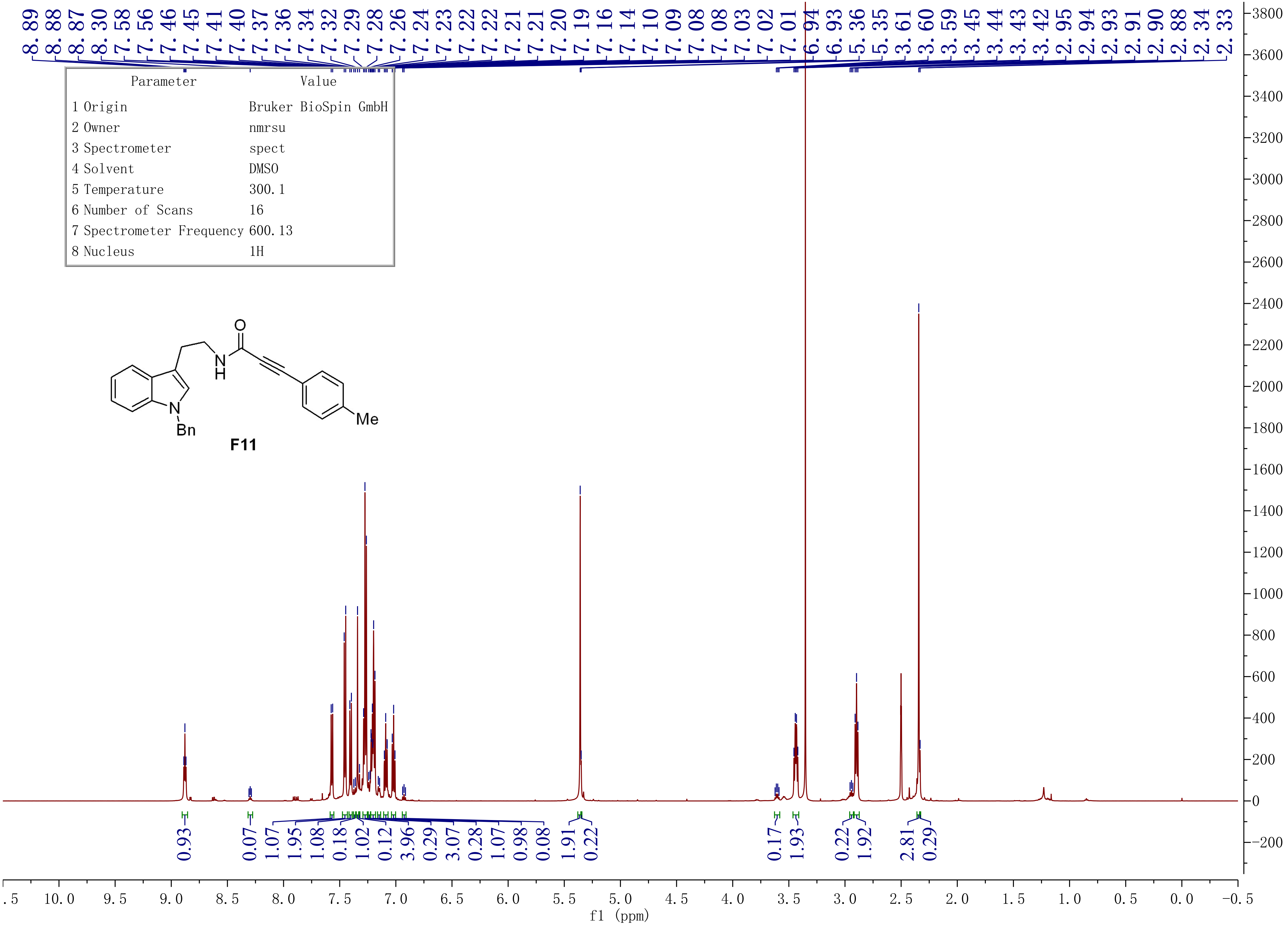

163.67
162.02
154.64
152.19
138.40
136.07
134.68
134.62
128.50
127.25
127.03
126.70
121.29
118.64
116.44
116.29
111.43
110.11
83.97
81.91
81.53
54.94
43.57
26.61
24.68
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 111
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
N
Bn
F
F8
f1 (ppm)


8.72 8.71 8.70 8.33 7.88 7.86 7.62 7.60 7.58 7.54 7.52 7.52 7.41 7.39 7.33 7.29 7.28 7.26 7.25 7.25 7.24 7.23 7.23 7.22 7.22 7.21 7.21 7.20 7.20 7.20 7.17 7.16 7.10 7.09 7.08 7.03 7.01 7.01 7.00 5.36 5.35 3.58 3.57 3.56 3.55 3.34 3.33 2.99 2.98 2.97 2.80 2.79 2.78
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
N
Bn
Cl
F9
0.42 1.67 0.99 0.44 2.57 3.45 1.04 3.94 1.69 2.83 1.34 1.07 2.88 2.02 1.04 2.00 0.91
f1 (ppm)

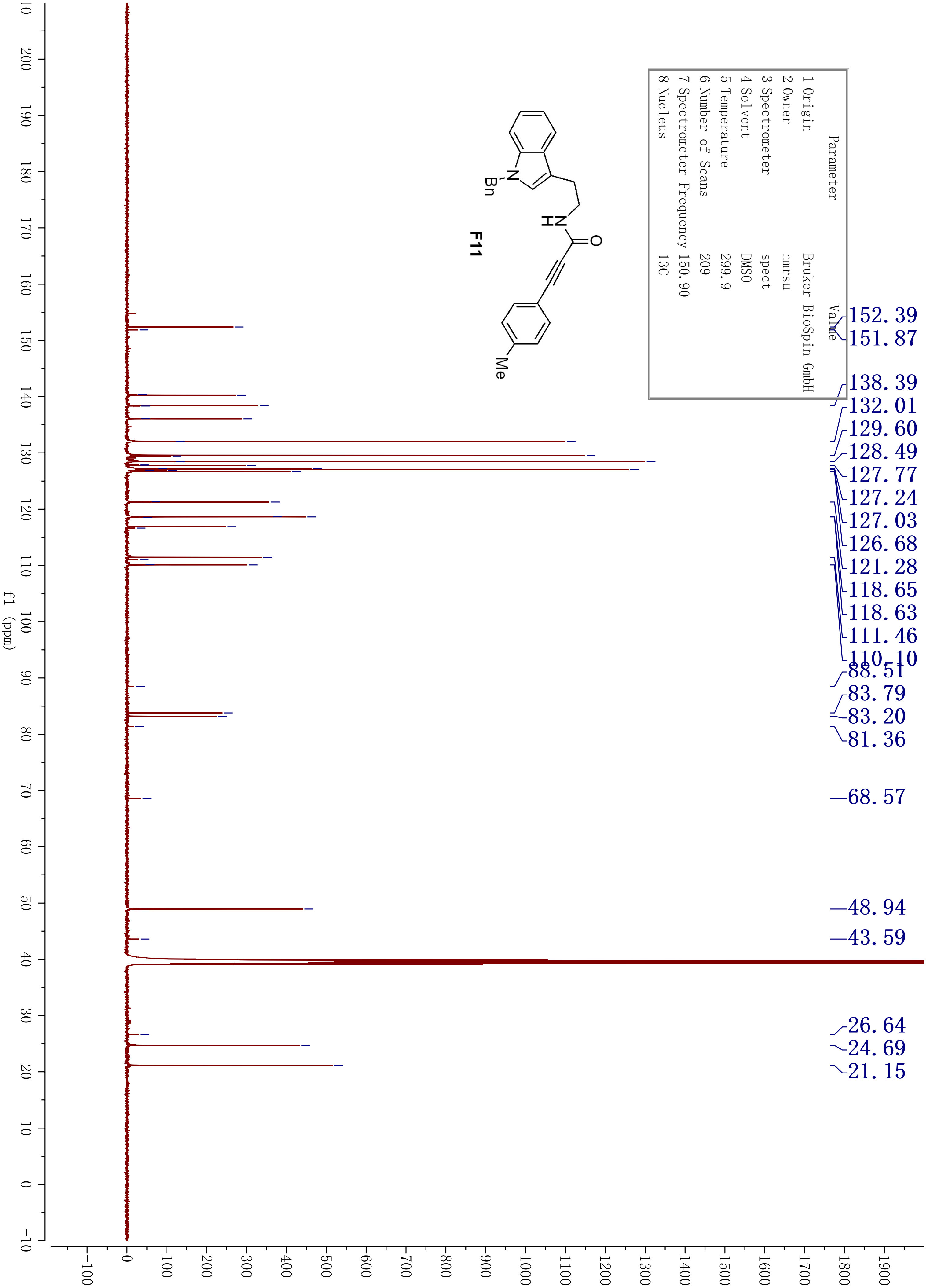

165.10
162.45
138.40
138.38
136.09
135.91
133.41
130.44
129.11
128.50
128.48
128.35
127.92
127.88
127.75
127.27
127.25
127.03
127.01
126.65
124.77
121.27
118.72
118.65
118.61
111.82
111.58
110.09
48.96
48.92
40.18
24.97
24.74
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 30
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
N
Bn
Cl
F9
f1 (ppm)

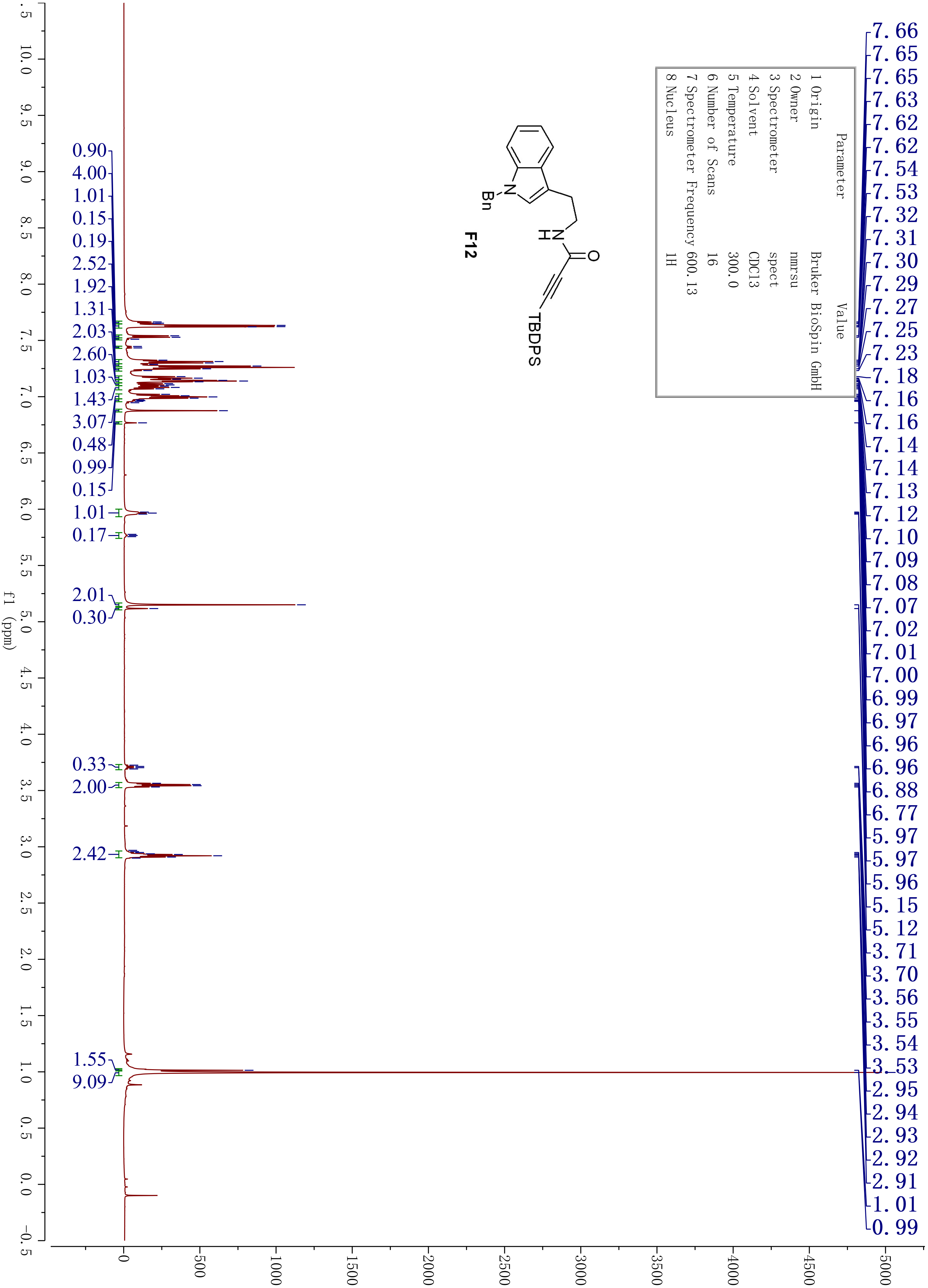

8.97 8.96 8.95 7.68 7.68 7.67 7.67 7.66 7.59 7.59 7.57 7.56 7.51 7.51 7.50 7.50 7.50 7.41 7.40 7.34 7.31 7.29 7.27 7.26 7.23 7.23 7.22 7.21 7.19 7.18 7.15 7.14 7.10 7.10 7.09 7.08 7.08 7.06 7.03 7.02 7.01 5.36 5.35 3.59 3.46 3.45 3.44 3.42 2.93 2.92 2.91 2.90 2.88
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
N
Bn
Br
F10
0.99 0.07 2.01 0.15 1.14 1.99 0.11 1.11 1.08 0.07 2.20 1.01 2.23 0.20 1.02 0.13 1.00 1.47 0.19 0.16 2.08 0.25 2.00
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 36
7 Spectrometer Frequency 150.90
8 Nucleus 13C
154.52
152.06
138.39
136.06
133.94
132.10
128.49
127.76
127.25
127.03
126.70
121.29
118.64
111.41
110.11
86.88
85.12
82.65
81.76
48.94
43.56
26.59
24.65
N
H
O
N
Bn
Br
F10
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)
400 350 300 250 200 150 100 50 0

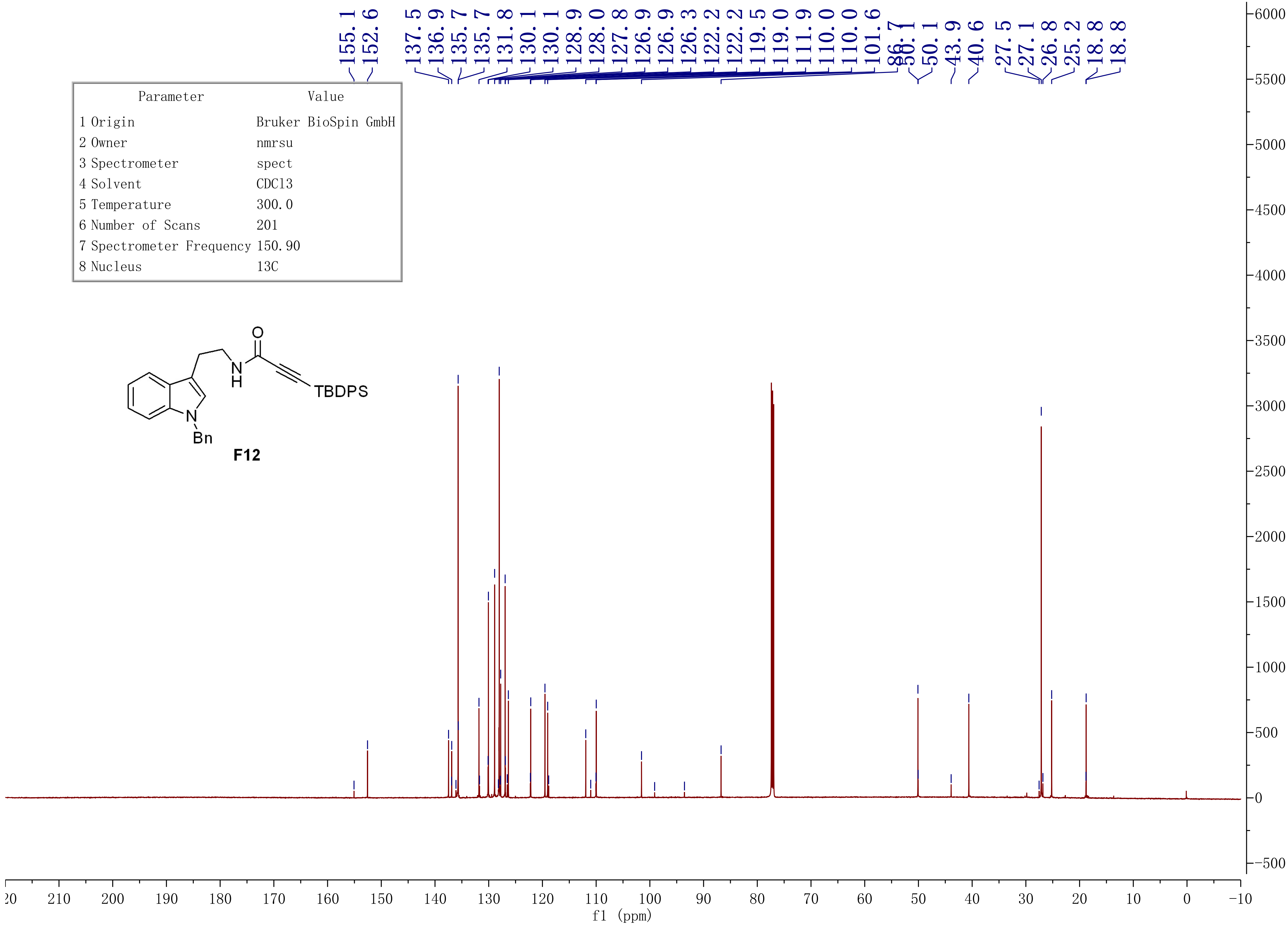


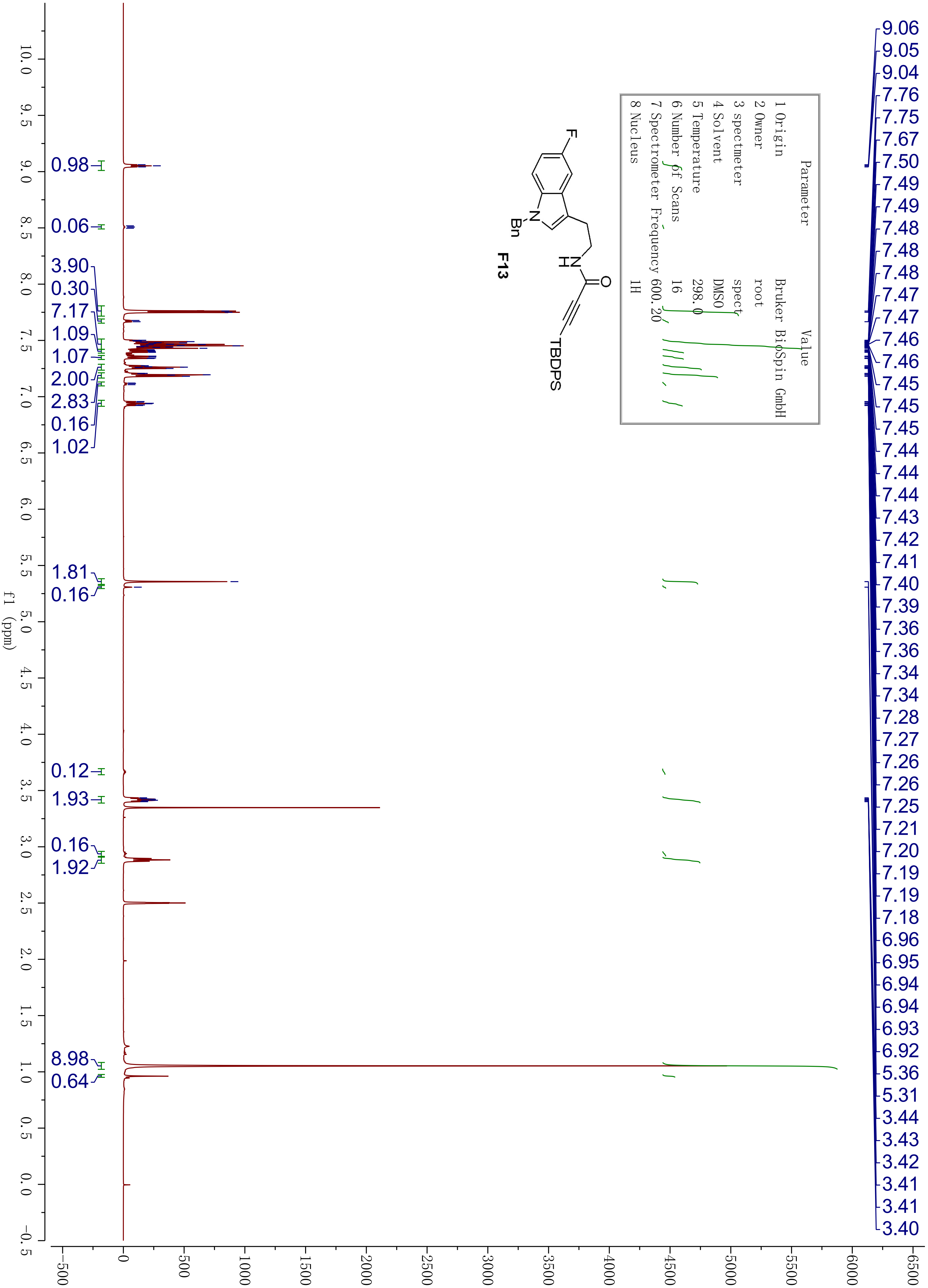
8.89 8.88 8.87 8.30 7.58 7.56 7.46 7.45 7.41 7.40 7.37 7.36 7.34 7.32 7.29 7.28 7.26 7.24 7.23 7.22 7.22 7.21 7.21 7.20 7.19 7.16 7.14 7.10 7.09 7.08 7.08 7.03 7.02 7.01 6.94 6.93 5.36 5.35 3.61 3.60 3.59 3.45 3.44 3.43 3.42 2.95 2.94 2.93 2.91 2.90 2.88 2.34 2.33
Parameter | Value
1 Origin | Bruker BioSpin GmbH
2 Owner | nmrsu
3 Spectrometer | spect
4 Solvent | DMSO
5 Temperature | 300.1
6 Number of Scans | 16
7 Spectrometer Frequency | 600.13
8 Nucleus | 1H
O
N
H
N
Bn
Me
F11
0.93 0.07 1.07 1.95 1.08 0.18 1.02 0.12 3.96 0.29 3.07 0.28 1.07 0.98 0.08 1.91 0.22 0.17 1.93 0.22 1.92 2.81 0.29
f1 (ppm)

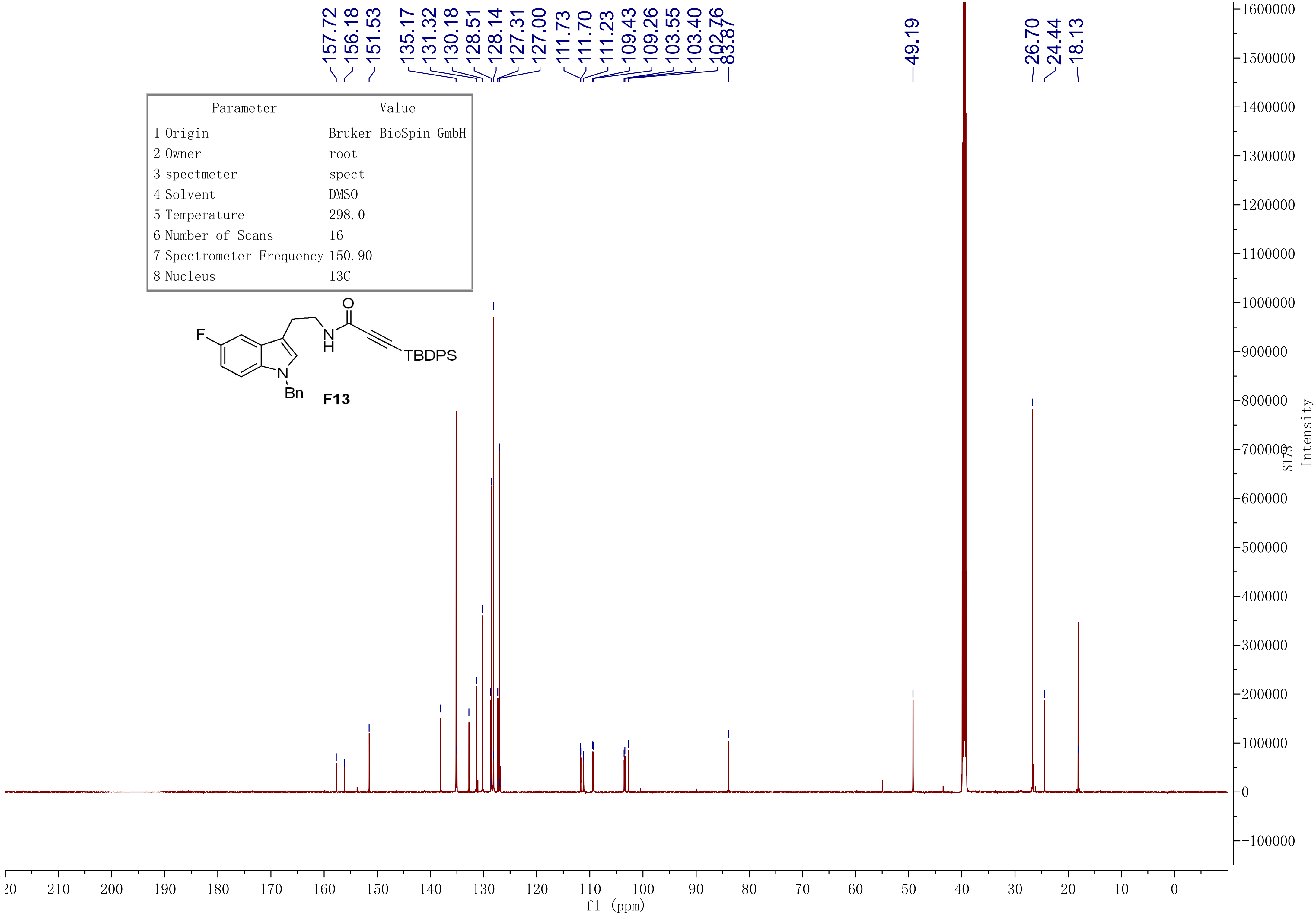

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 209
7 Spectrometer Frequency 150.90
8 Nucleus 13C
F11
Bn
N
H
O
Me
152.39
151.87
138.39
132.01
129.60
128.49
127.77
127.24
127.03
126.68
121.28
118.65
118.63
111.46
110.10
88.51
83.79
83.20
81.36
68.57
48.94
43.59
26.64
24.69
21.15
f1 (ppm)

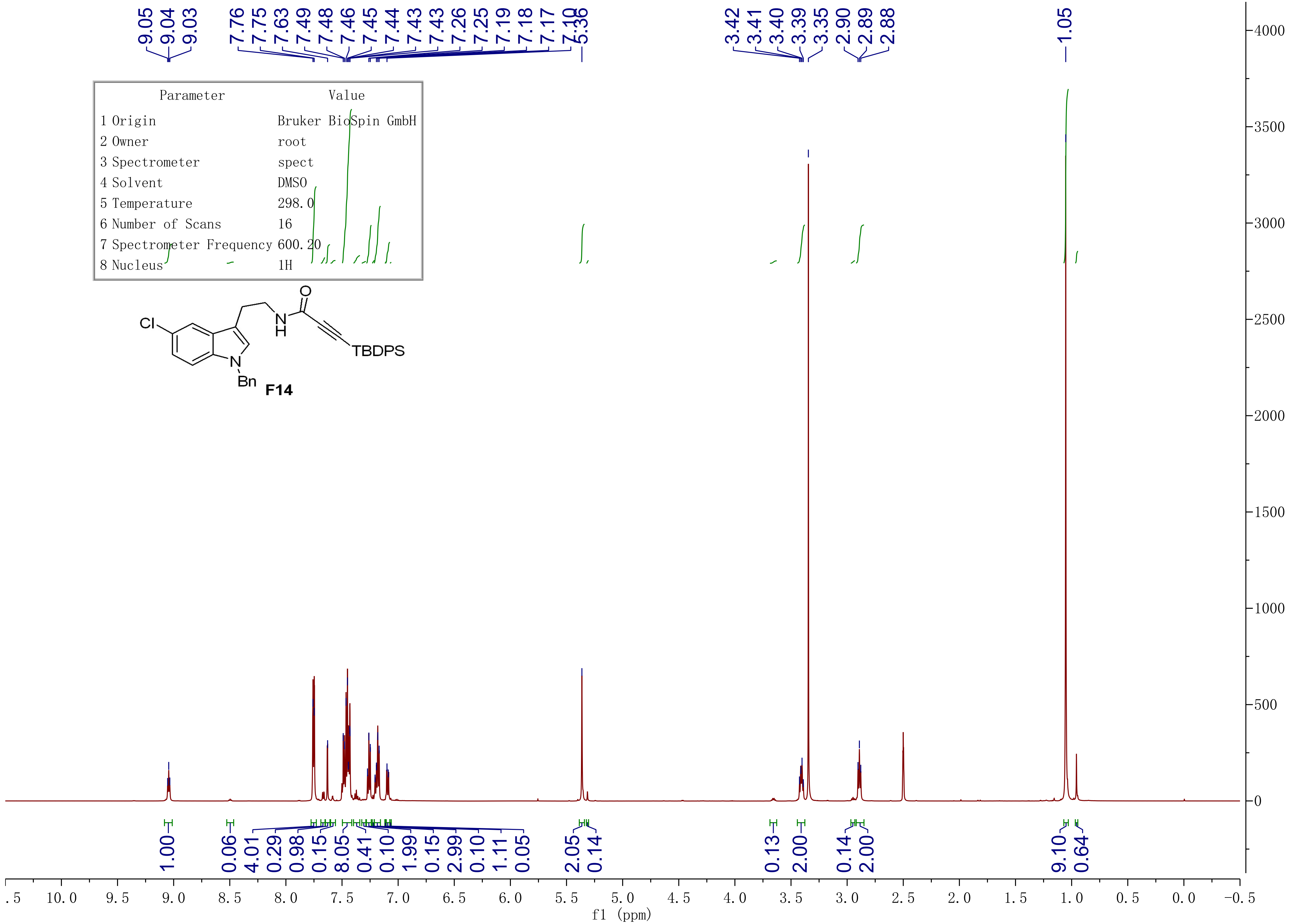


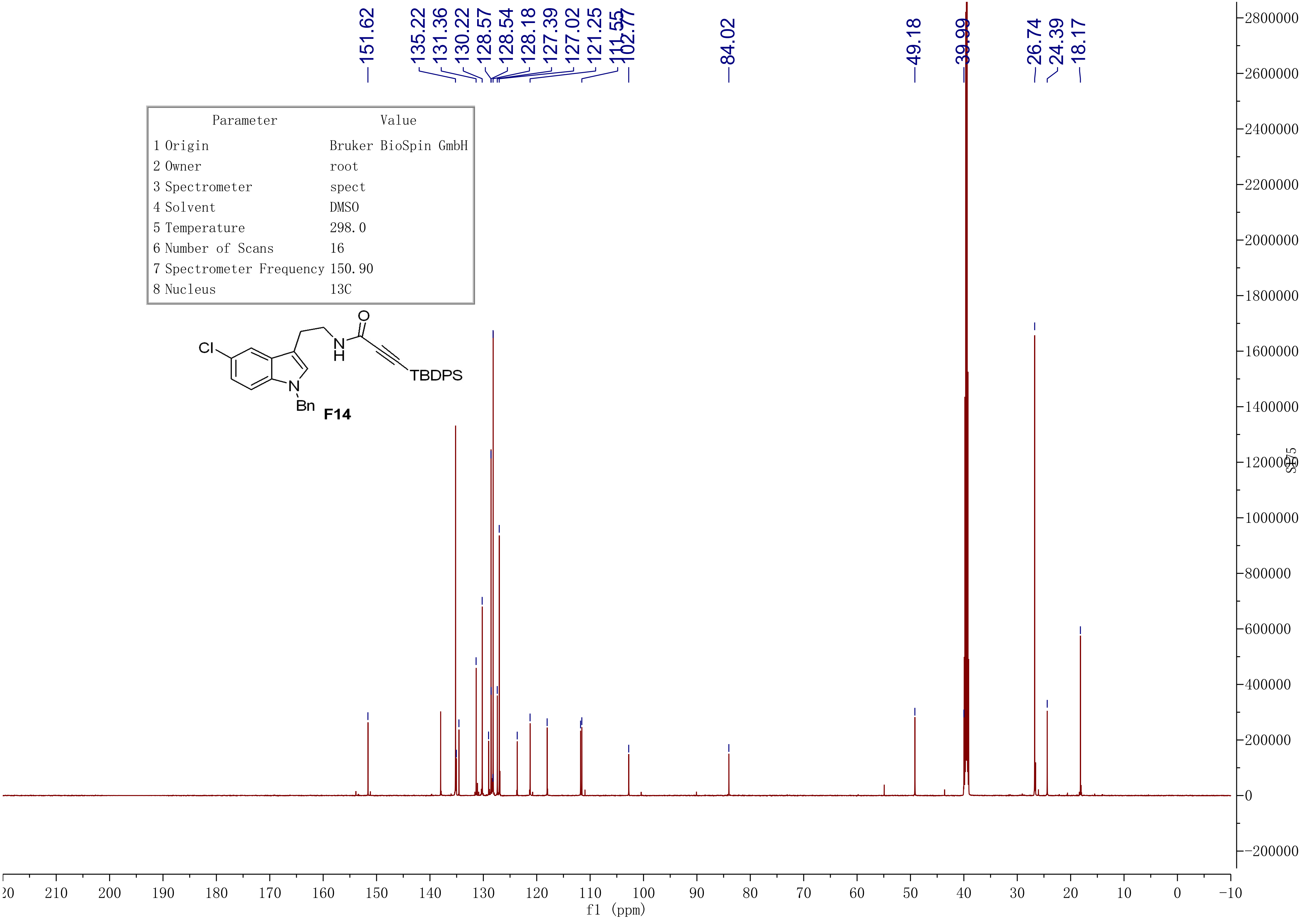
F12
Bn
TBDPS
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
7.66 7.65 7.65 7.63 7.62 7.62 7.54 7.53 7.32 7.31 7.30 7.29 7.27 7.25 7.23 7.18 7.16 7.16 7.14 7.14 7.13 7.12 7.10 7.09 7.08 7.07 7.02 7.01 7.00 6.99 6.97 6.96 6.96 6.88 6.77 5.97 5.97 5.96 5.15 5.12 3.71 3.70 3.56 3.55 3.54 3.53 2.95 2.94 2.93 2.92 2.91 1.01 0.99
0.90 4.00 1.01 0.15 0.19 2.52 1.92 1.31 2.03 2.60 1.03 1.43 3.07 0.48 0.99 0.15 1.01 0.17 2.01 0.30 0.33 2.00 2.42 1.55 9.09
f1 (ppm)


155.1
152.6
137.5
136.9
135.7
135.7
131.8
130.1
130.1
128.9
128.0
127.8
126.9
126.9
126.3
122.2
122.2
119.5
119.0
111.9
110.0
110.0
101.6
86.7
50.1
50.1
43.9
40.6
27.5
27.1
26.8
25.2
18.8
18.8
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 201
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
TBDPS
N
Bn
F12
f1 (ppm)

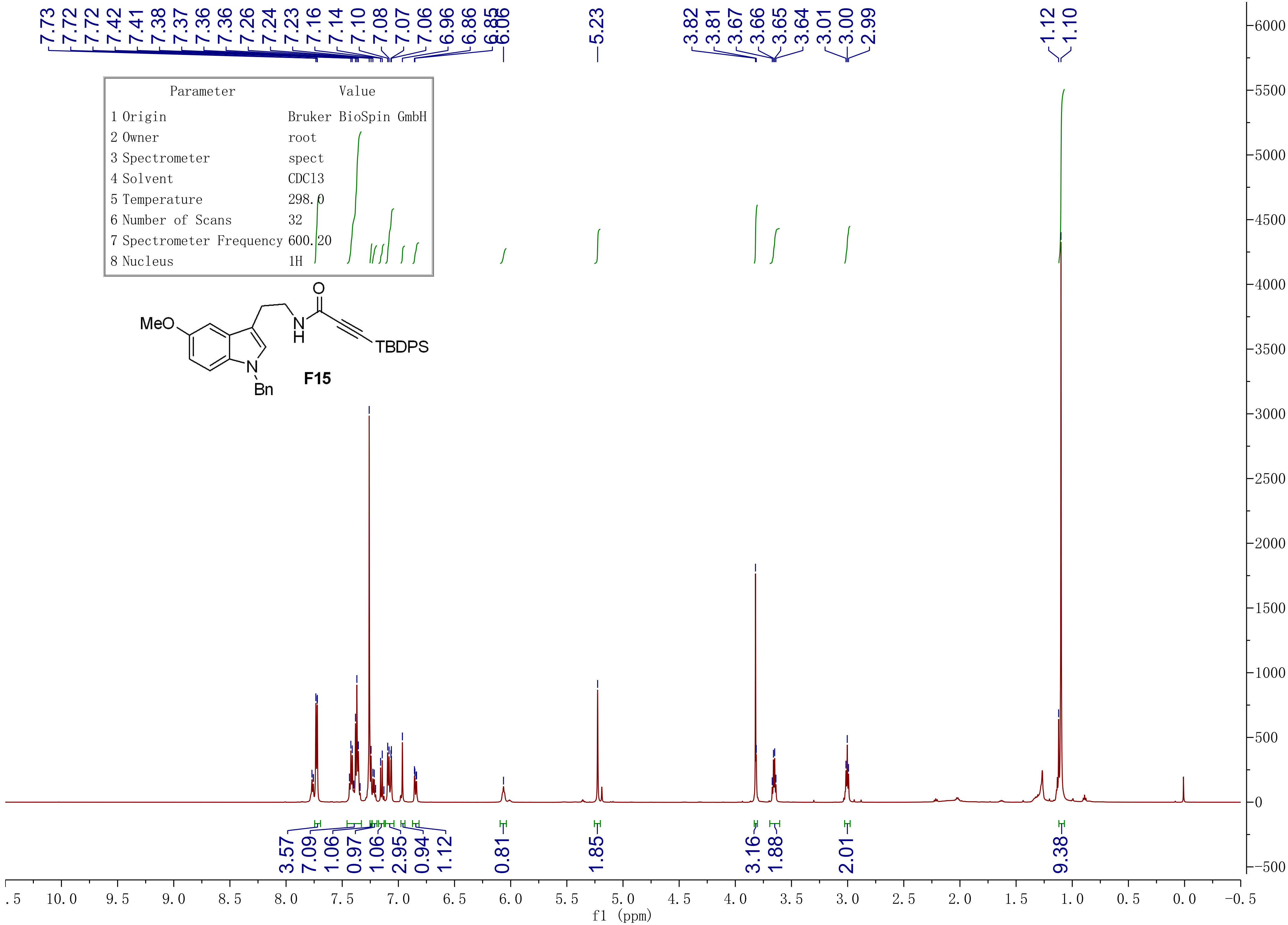

F13
TBDPS
Bn
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 spectmeter spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
9.06
9.05
9.04
7.76
7.75
7.67
7.50
7.49
7.49
7.48
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.45
7.45
7.44
7.44
7.44
7.43
7.42
7.41
7.40
7.39
7.36
7.36
7.34
7.34
7.28
7.27
7.26
7.26
7.25
7.21
7.20
7.19
7.19
7.18
6.96
6.95
6.94
6.94
6.93
6.92
5.36
5.31
3.44
3.43
3.42
3.41
3.41
3.40
0.98
0.06
3.90
0.30
7.17
1.09
1.07
2.00
2.83
0.16
1.02
1.81
0.16
0.12
1.93
0.16
1.92
8.98
0.64
f1 (ppm)

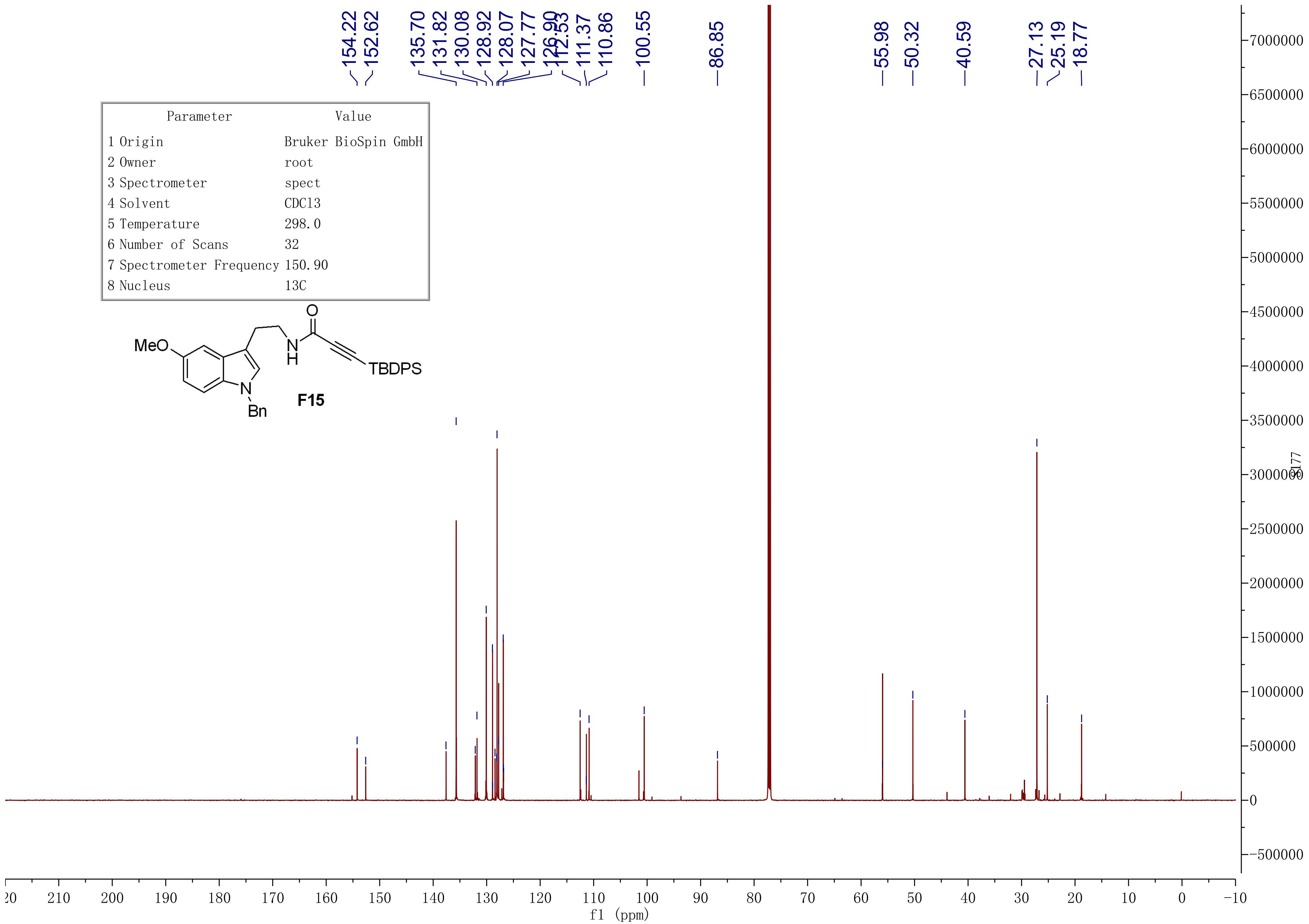

157.72
156.18
151.53
135.17
131.32
130.18
128.51
128.14
127.31
127.00
111.73
111.70
111.23
109.43
109.26
103.55
103.40
102.76
83.87
49.19
26.70
24.44
18.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 spectmeter spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 150.90
8 Nucleus 13C
F
N
H
O
TBDPS
Bn
F13
f1 (ppm)
Intensity

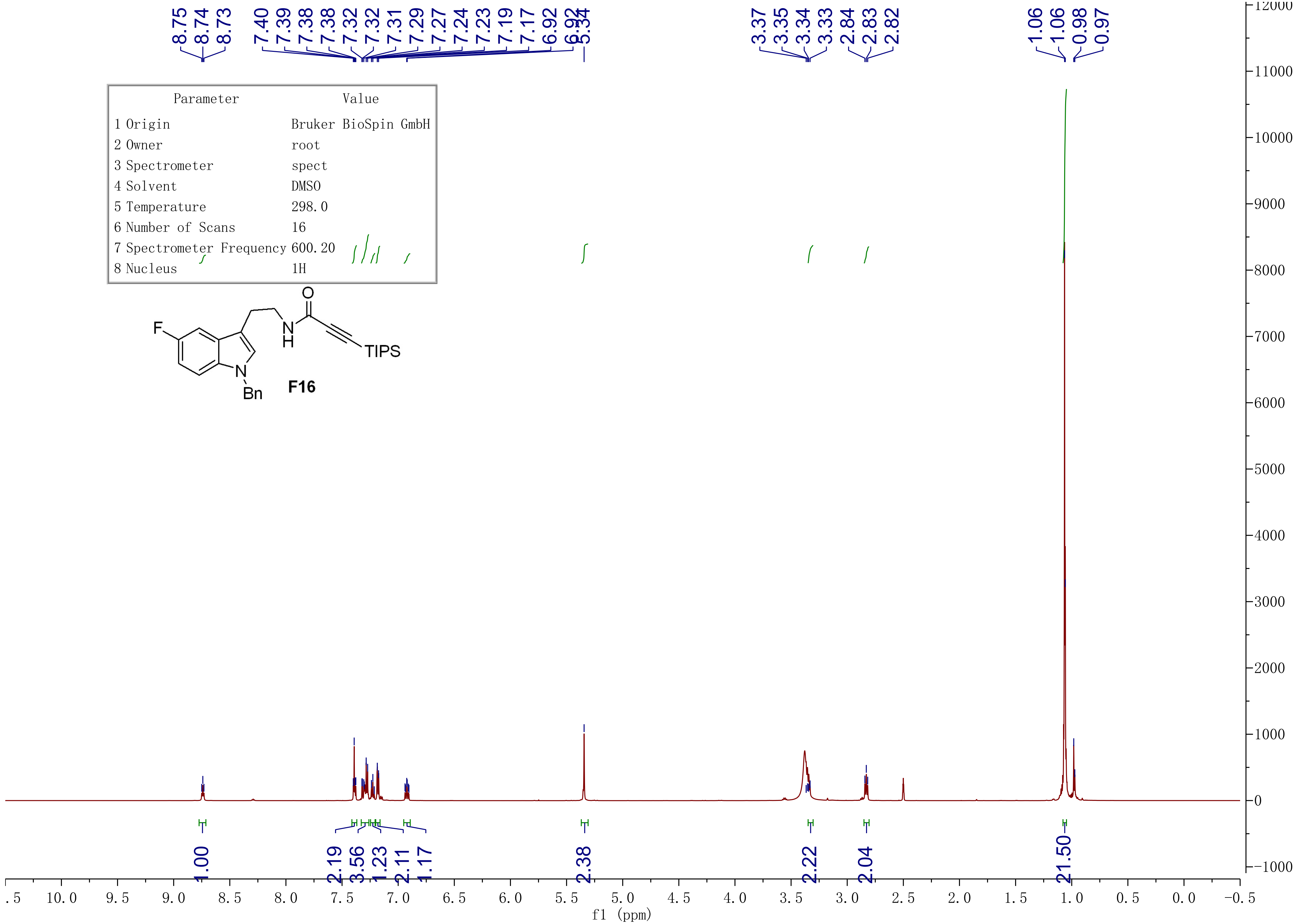

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
Cl
N
H
O
TBDPS
N
Bn
F14
9.05
9.04
9.03
7.76
7.75
7.63
7.49
7.48
7.46
7.45
7.44
7.43
7.43
7.26
7.25
7.19
7.18
7.17
7.10
5.36
3.42
3.41
3.40
3.39
3.35
2.90
2.89
2.88
1.05
1.00
0.06
4.01
0.29
0.98
0.15
8.05
0.41
0.10
1.99
0.15
2.99
0.10
1.11
0.05
2.05
0.14
0.13
2.00
0.14
2.00
9.10
0.64
f1 (ppm)

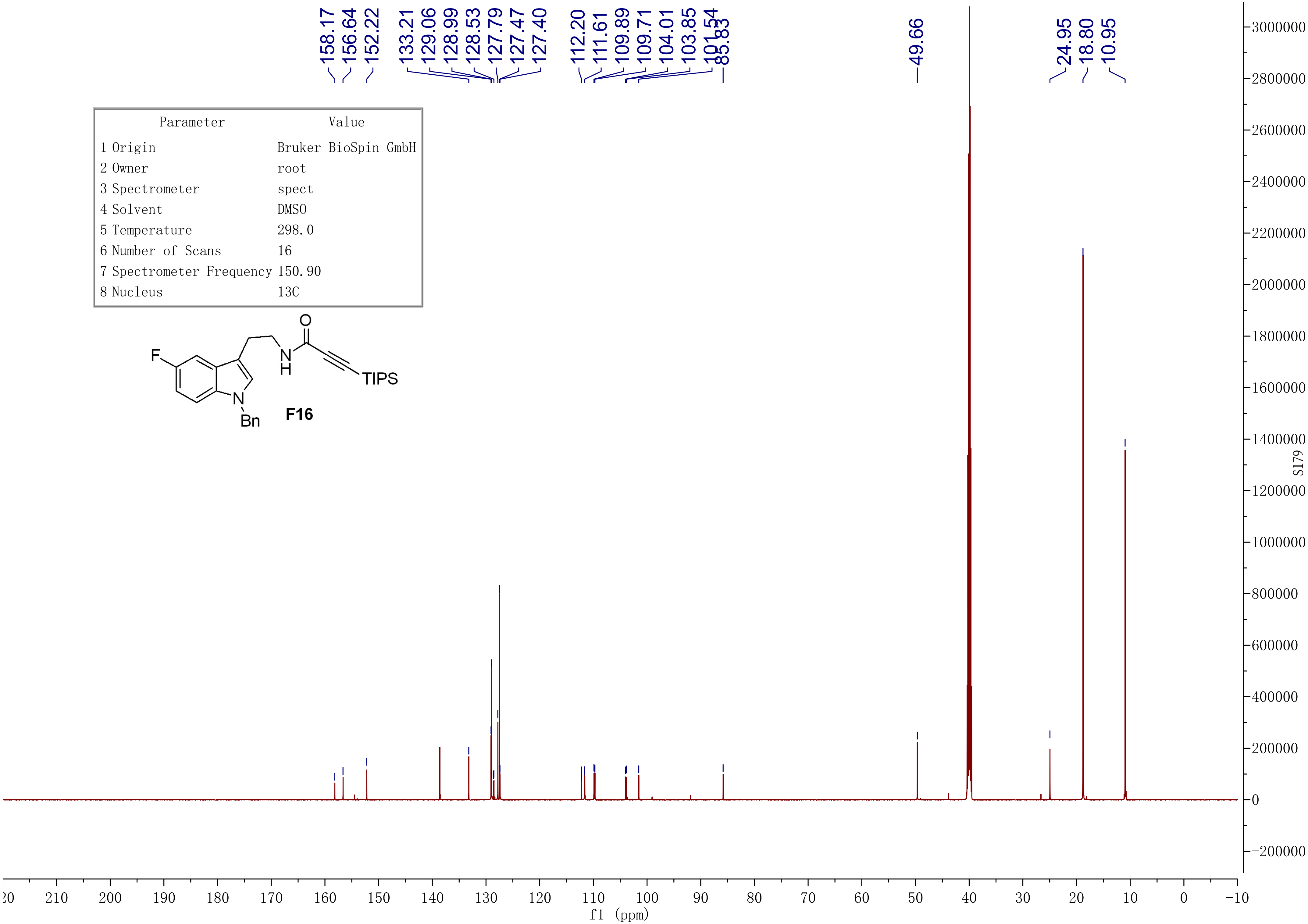


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C


7.73 7.72 7.72 7.42 7.41 7.38 7.37 7.36 7.36 7.26 7.24 7.23 7.16 7.14 7.10 7.08 7.07 7.06 6.96 6.86 6.85 6.06
5.23
3.82 3.81 3.67 3.66 3.65 3.64 3.01 3.00 2.99
1.12 1.10
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 32
7 Spectrometer Frequency 600.20
8 Nucleus 1H
MeO
N
H
O
TBDPS
N
Bn
F15
3.57 7.09 1.06 0.97 1.06 2.95 0.94 1.12
0.81
1.85
3.16 1.88
2.01
9.38
f1 (ppm)

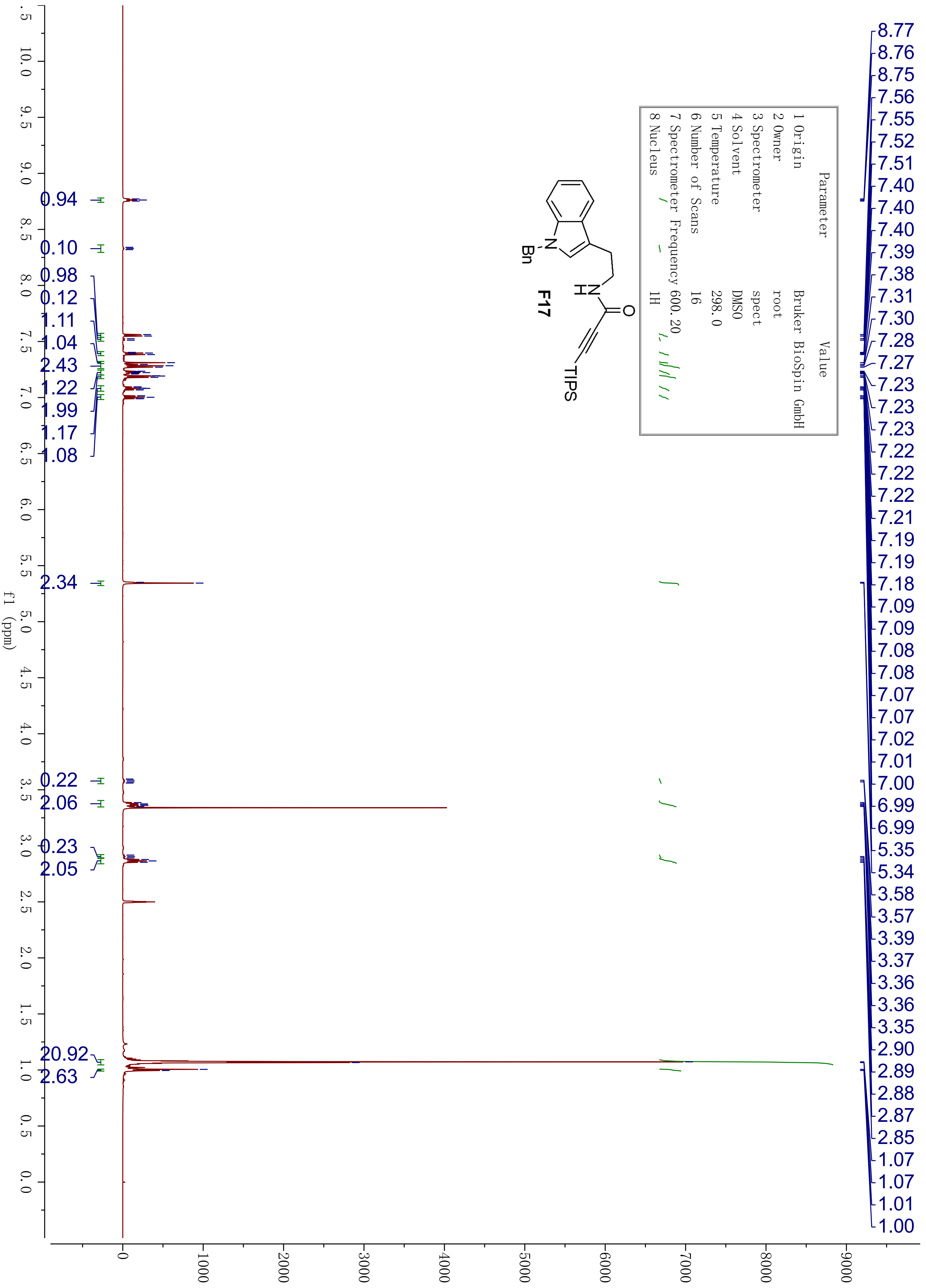

154.22
152.62
135.70
131.82
130.08
128.92
128.07
127.77
126.90
112.53
111.37
110.86
100.55
86.85
55.98
50.32
40.59
27.13
25.19
18.77
Parameter | Value
1 Origin | Bruker BioSpin GmbH
2 Owner | root
3 Spectrometer | spect
4 Solvent | CDCl3
5 Temperature | 298.0
6 Number of Scans | 32
7 Spectrometer Frequency | 150.90
8 Nucleus | 13C
MeO
N
H
O
TBDPS
N
Bn
F15
f1 (ppm)


8.75
8.74
8.73
7.40
7.39
7.38
7.38
7.32
7.32
7.31
7.29
7.27
7.24
7.23
7.19
7.17
6.92
6.92
5.34
3.37
3.35
3.34
3.33
2.84
2.83
2.82
1.06
1.06
0.98
0.97
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
F
O
N
H
TIPS
N
Bn
F16
1.00
2.19
3.56
1.23
2.11
1.17
2.38
2.22
2.04
21.50
f1 (ppm)

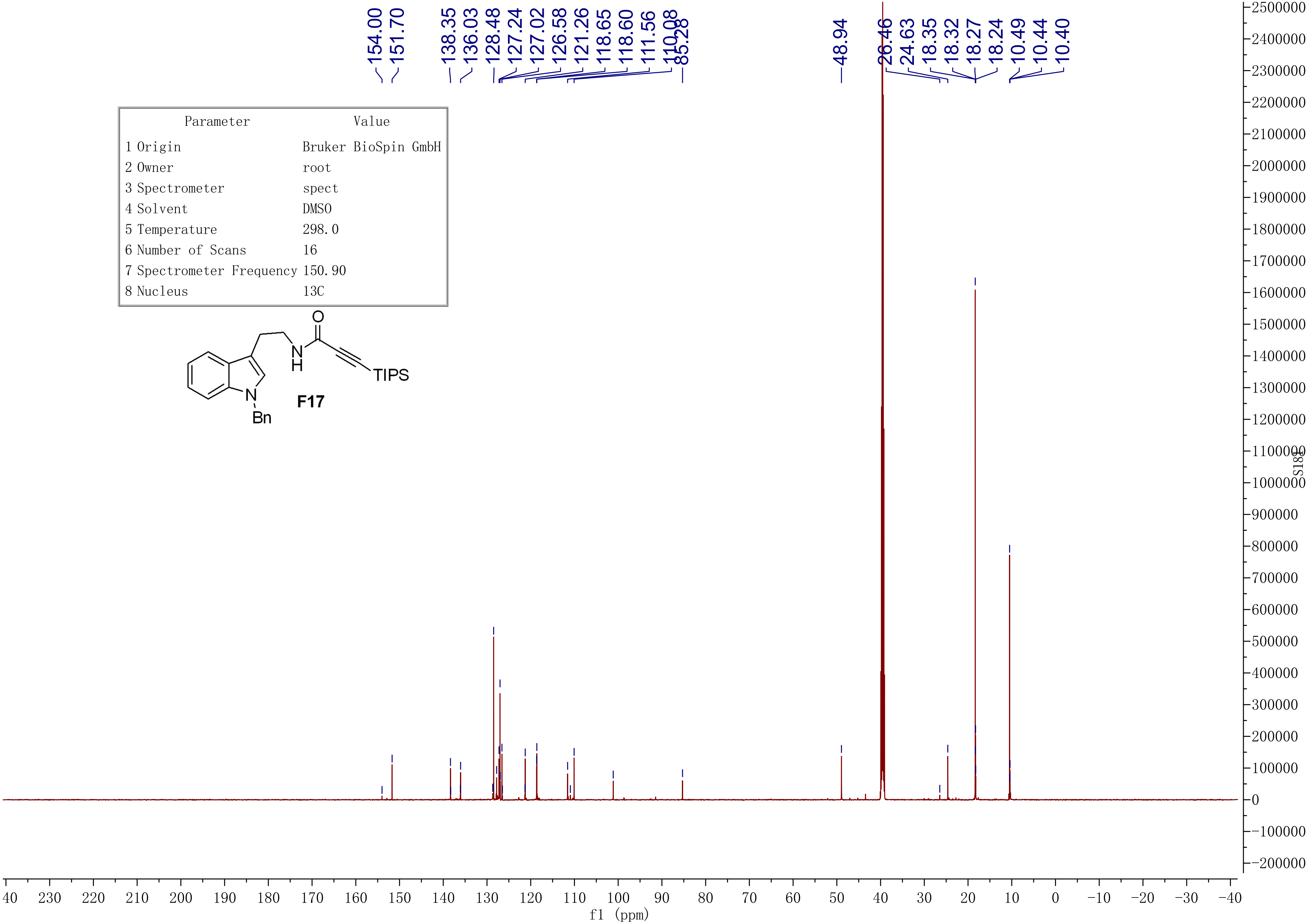


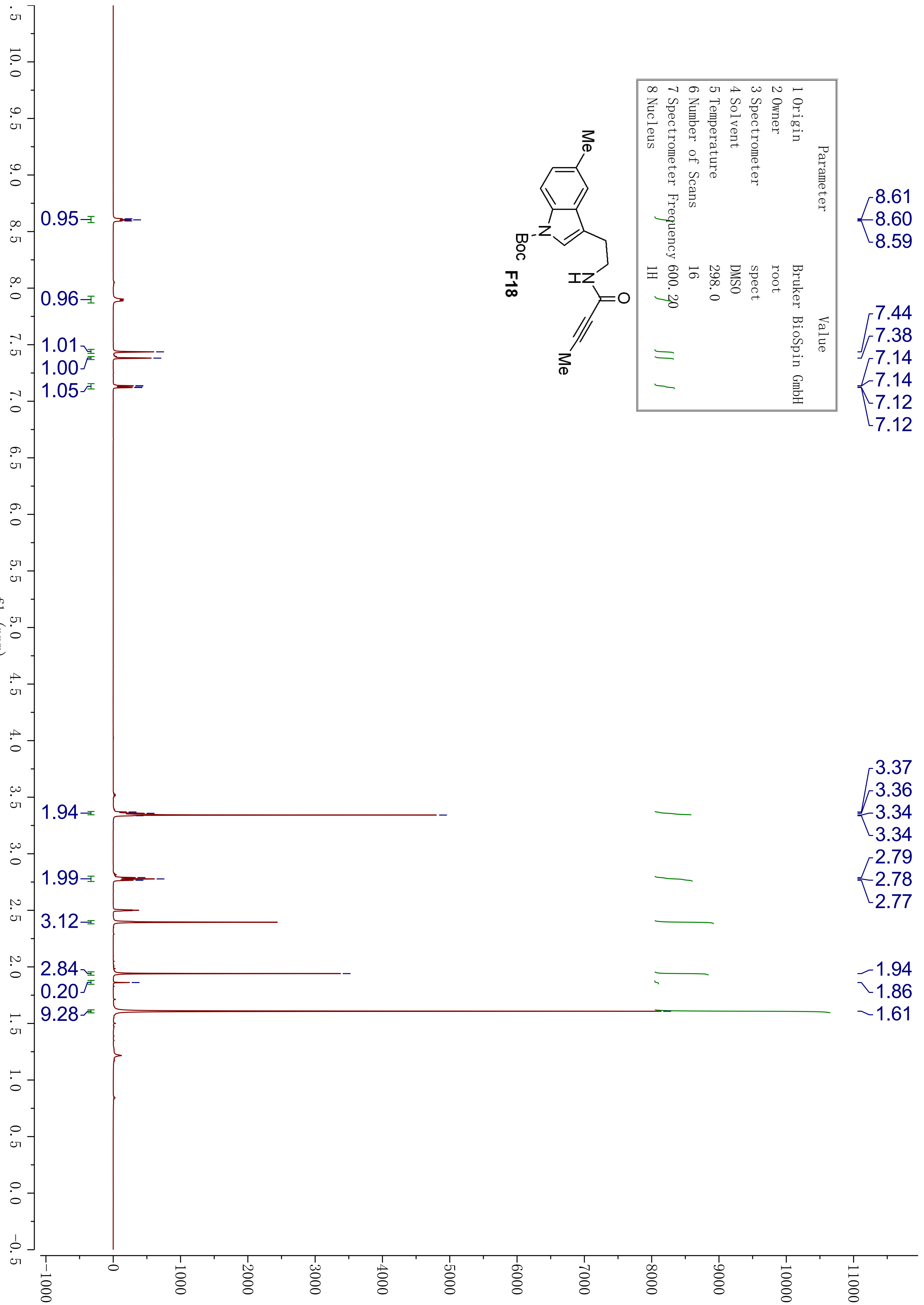
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C

F16

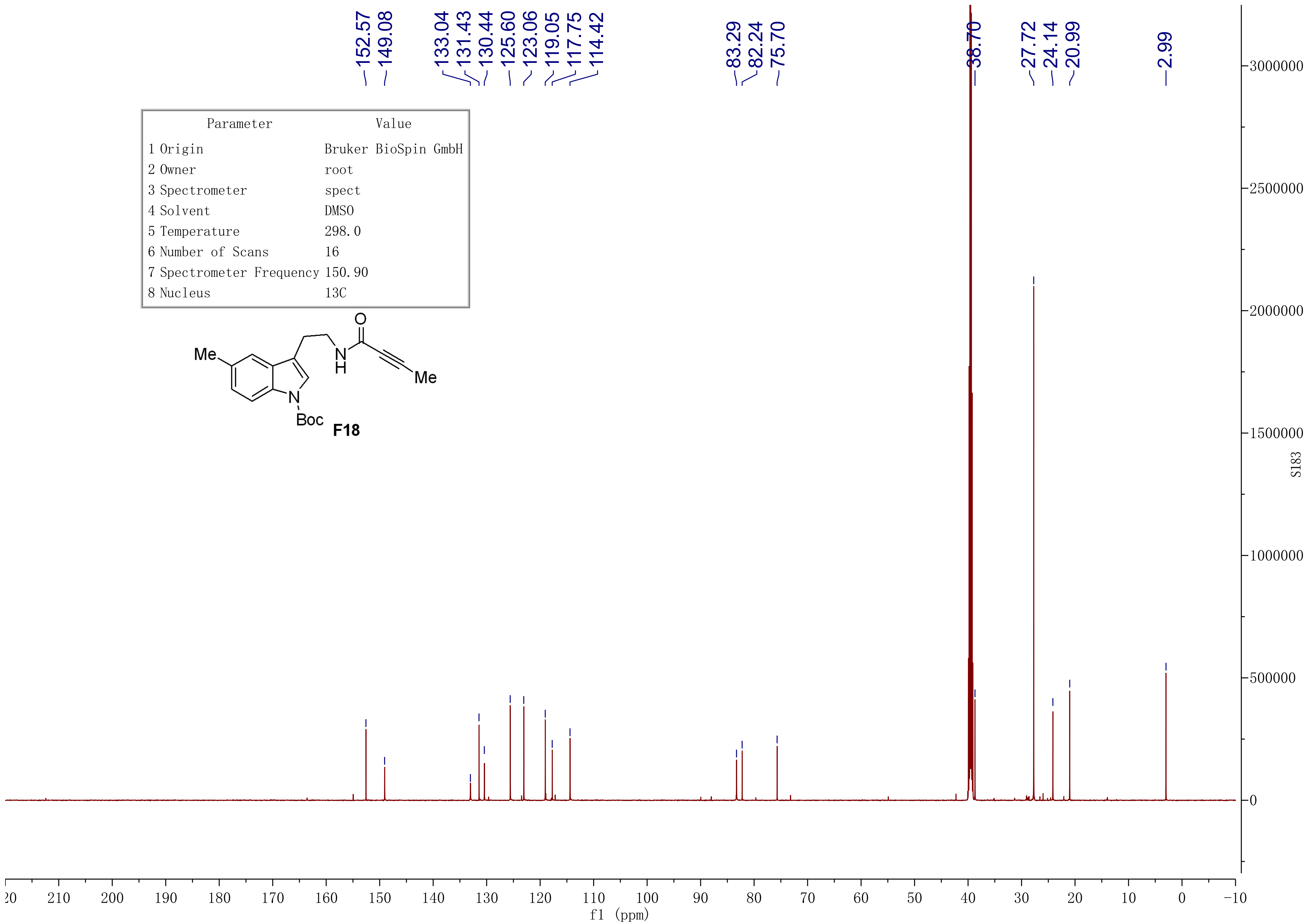

8.77
8.76
8.75
7.56
7.55
7.52
7.51
7.40
7.40
7.40
7.39
7.38
7.31
7.30
7.28
7.27
7.23
7.23
7.23
7.22
7.22
7.22
7.21
7.19
7.19
7.18
7.09
7.09
7.08
7.08
7.07
7.07
7.02
7.01
7.00
6.99
6.99
5.35
5.34
3.58
3.57
3.39
3.37
3.36
3.36
3.35
2.90
2.89
2.88
2.87
2.85
1.07
1.07
1.01
1.00
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
O
N
H
TIPS
N
Bn
F17
0.94
0.10
0.98
0.12
1.11
1.04
2.43
1.22
1.99
1.17
1.08
2.34
0.22
2.06
0.23
2.05
20.92
2.63
f1 (ppm)

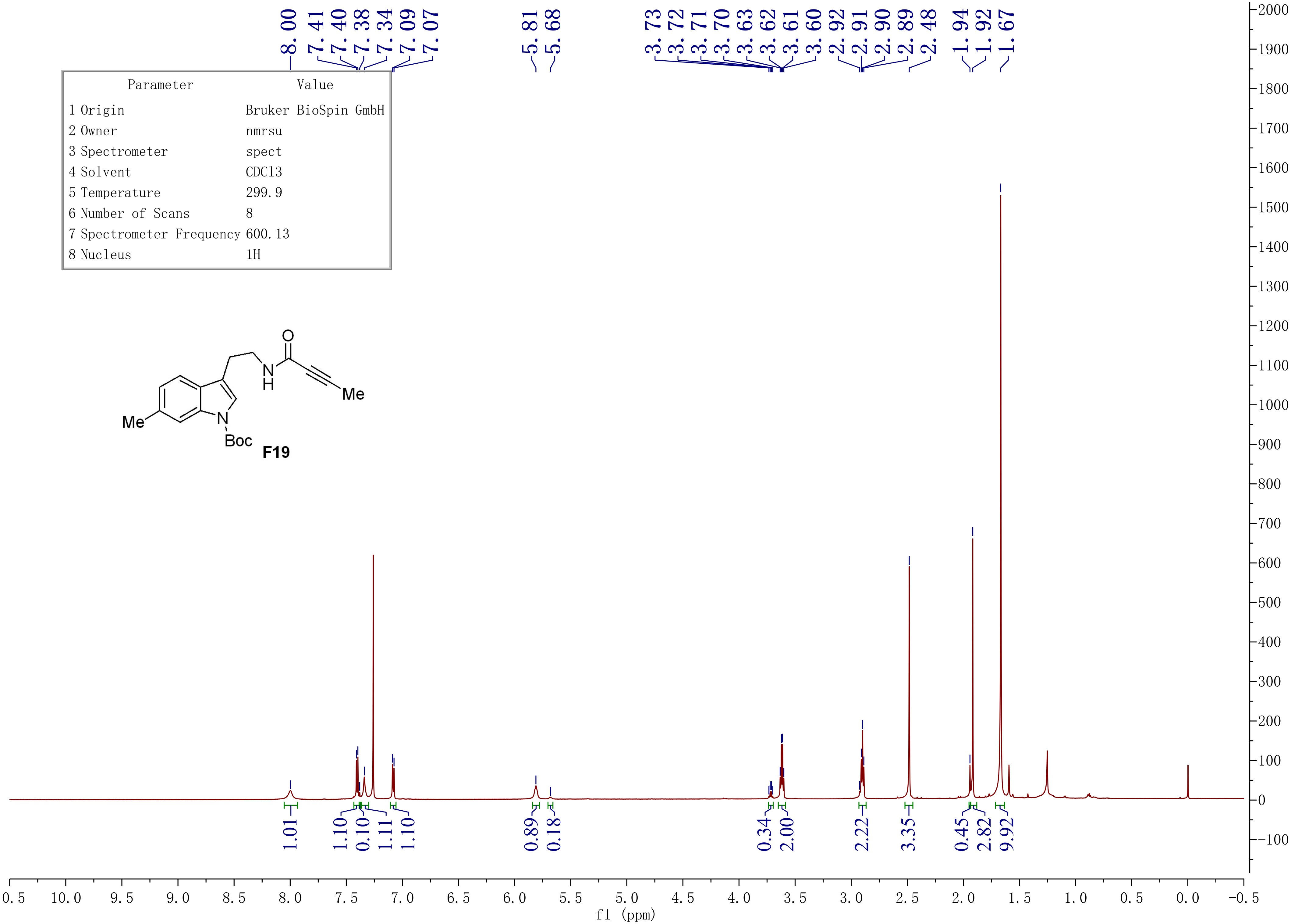
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C



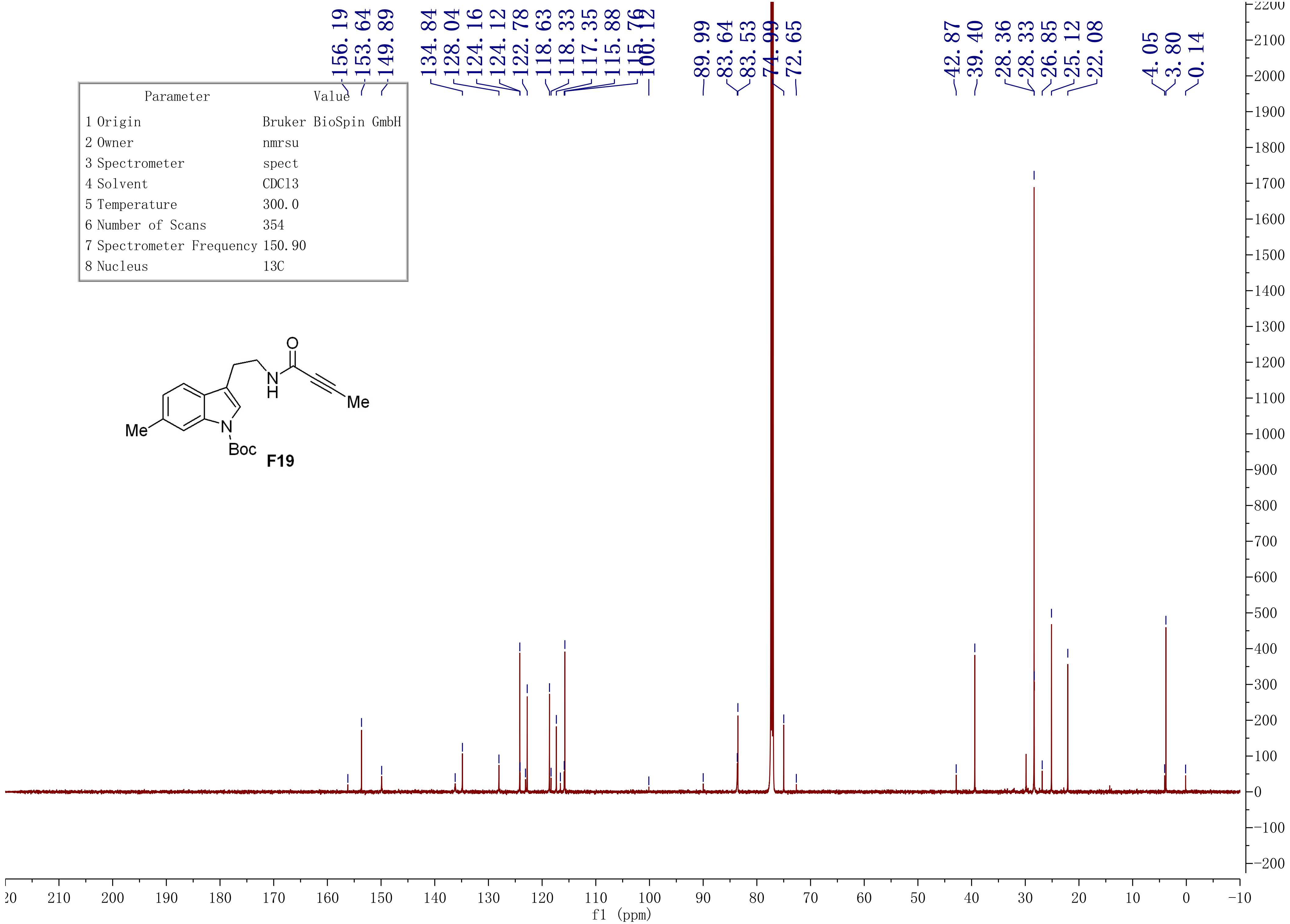


Parameter | Value
1 Origin | Bruker BioSpin GmbH
2 Owner | root
3 Spectrometer | spect
4 Solvent | DMSO
5 Temperature | 298.0
6 Number of Scans | 16
7 Spectrometer Frequency | 600.20
8 Nucleus | 1H
Me
N
Boc
F18
N
H
O
Me
8.61
8.60
8.59
7.44
7.38
7.14
7.14
7.12
7.12
3.37
3.36
3.34
3.34
2.79
2.78
2.77
1.94
1.86
1.61
0.95
0.96
1.01
1.00
1.05
1.94
1.99
3.12
2.84
0.20
9.28
f1 (ppm)


152.57
149.08
133.04
131.43
130.44
125.60
123.06
119.05
117.75
114.42
83.29
82.24
75.70
38.70
27.72
24.14
20.99
2.99
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Me
O
N
H
Me
N
Boc
F18
f1 (ppm)

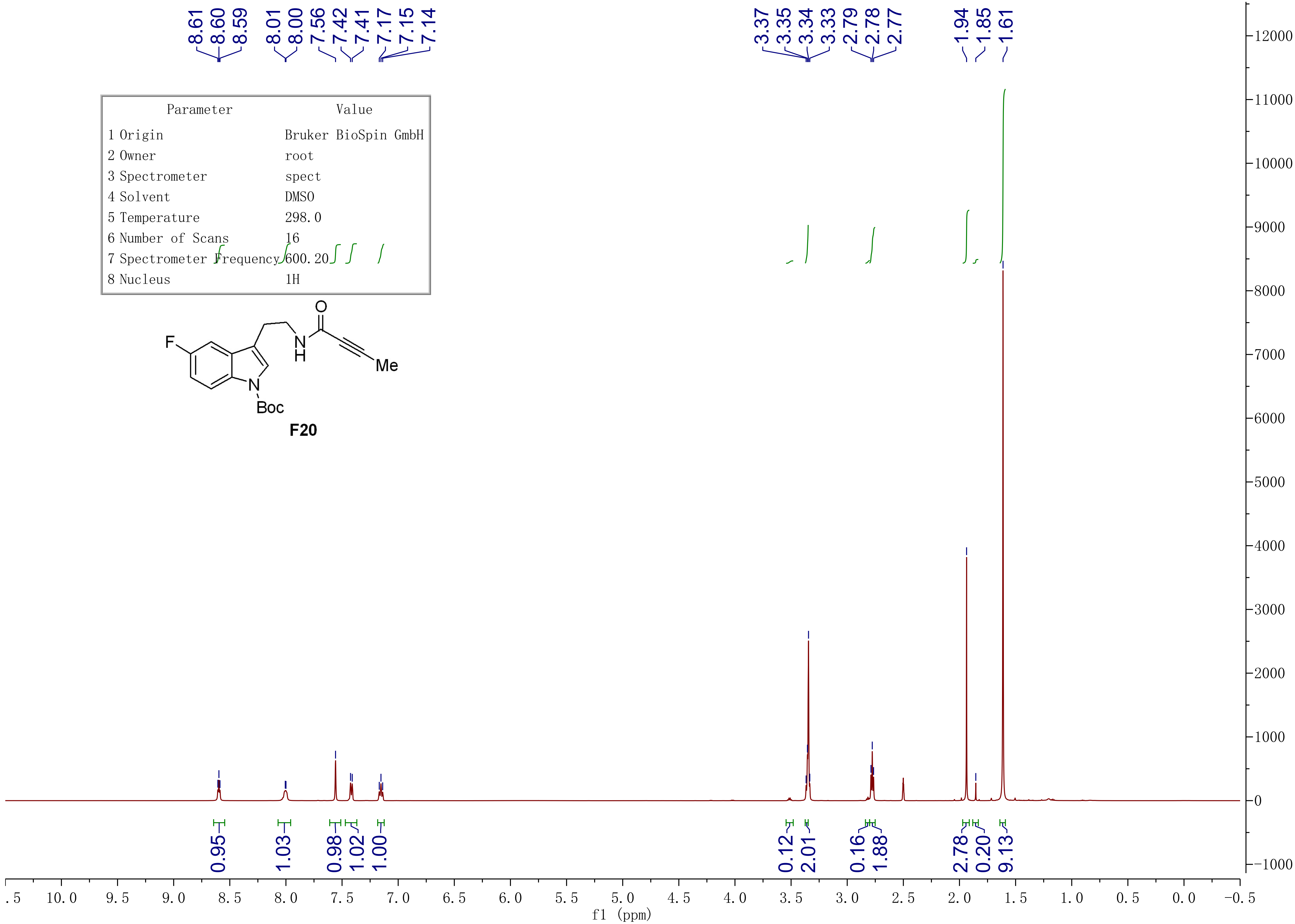


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
8.00 7.41 7.40 7.38 7.34 7.09 7.07
5.81 5.68
3.73 3.72 3.71 3.70 3.63 3.62 3.61 3.60 2.92 2.91 2.90 2.89 2.48
1.94 1.92 1.67
1.01 1.10 0.10 1.11 1.10 0.89 0.18 0.34 2.00 2.22 3.35 0.45 2.82 9.92
O
N
H
Me
Me
N
Boc
F19
f1 (ppm)

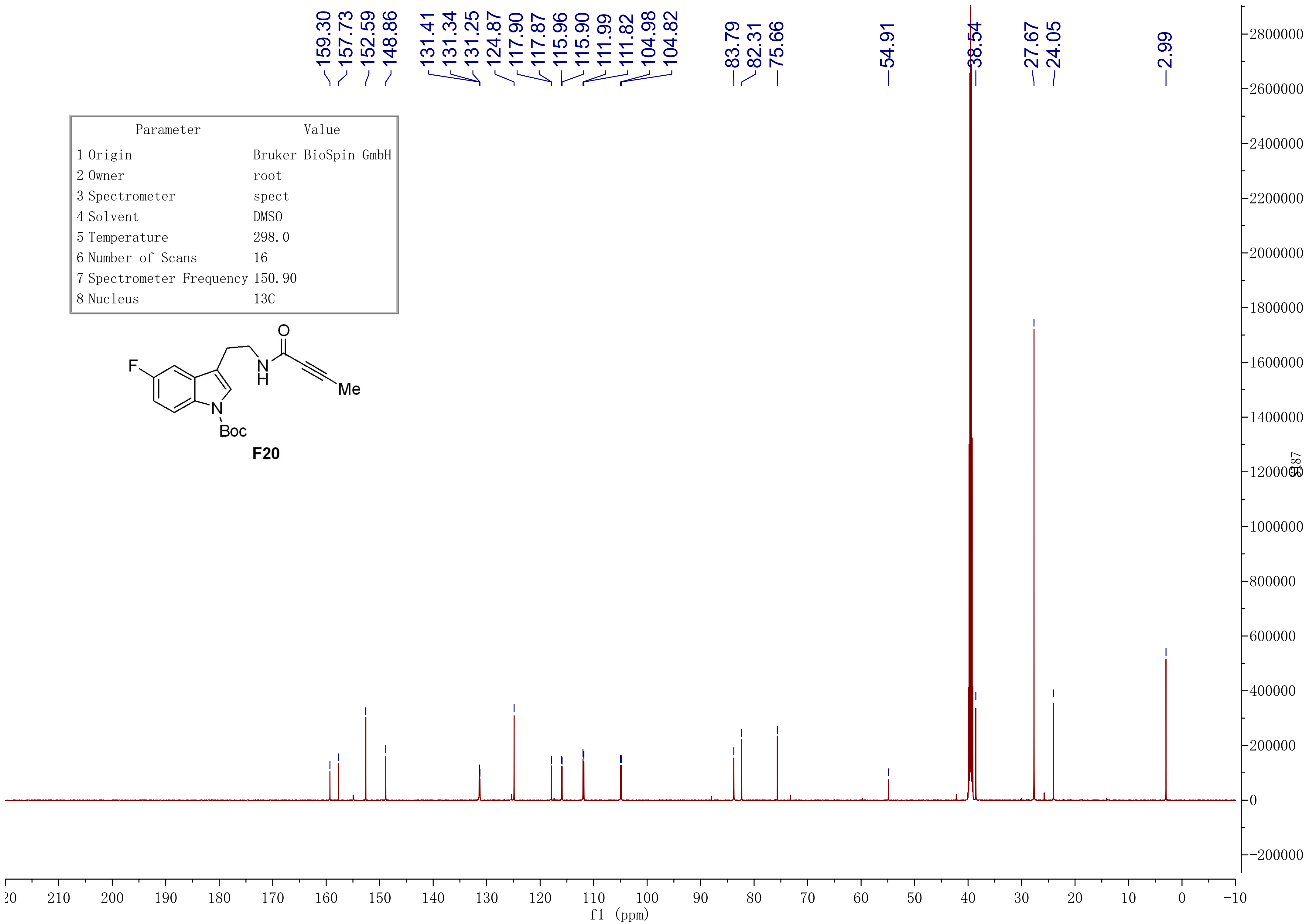


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	354
7 Spectrometer Frequency	150.90
8 Nucleus	13C

F19

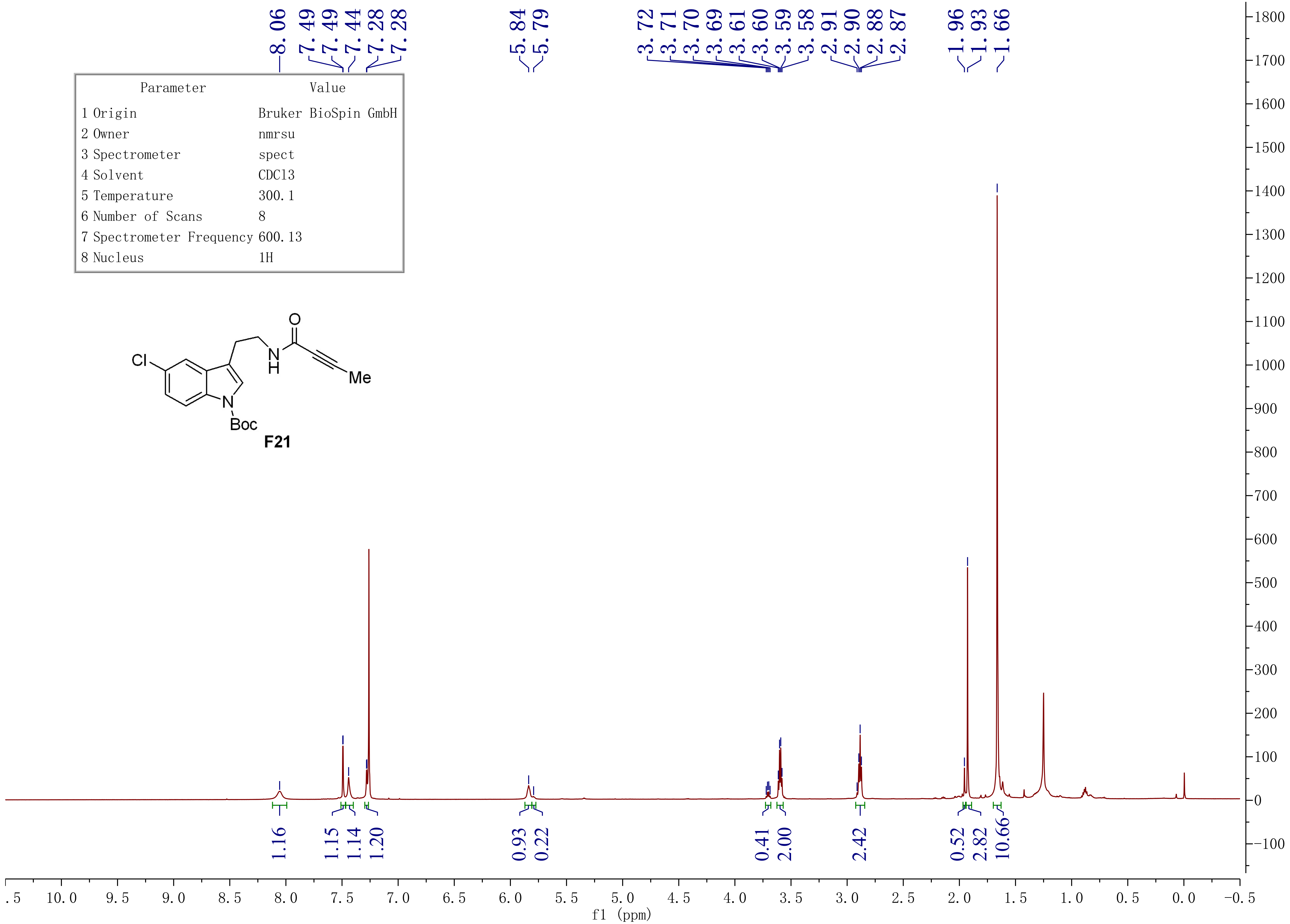


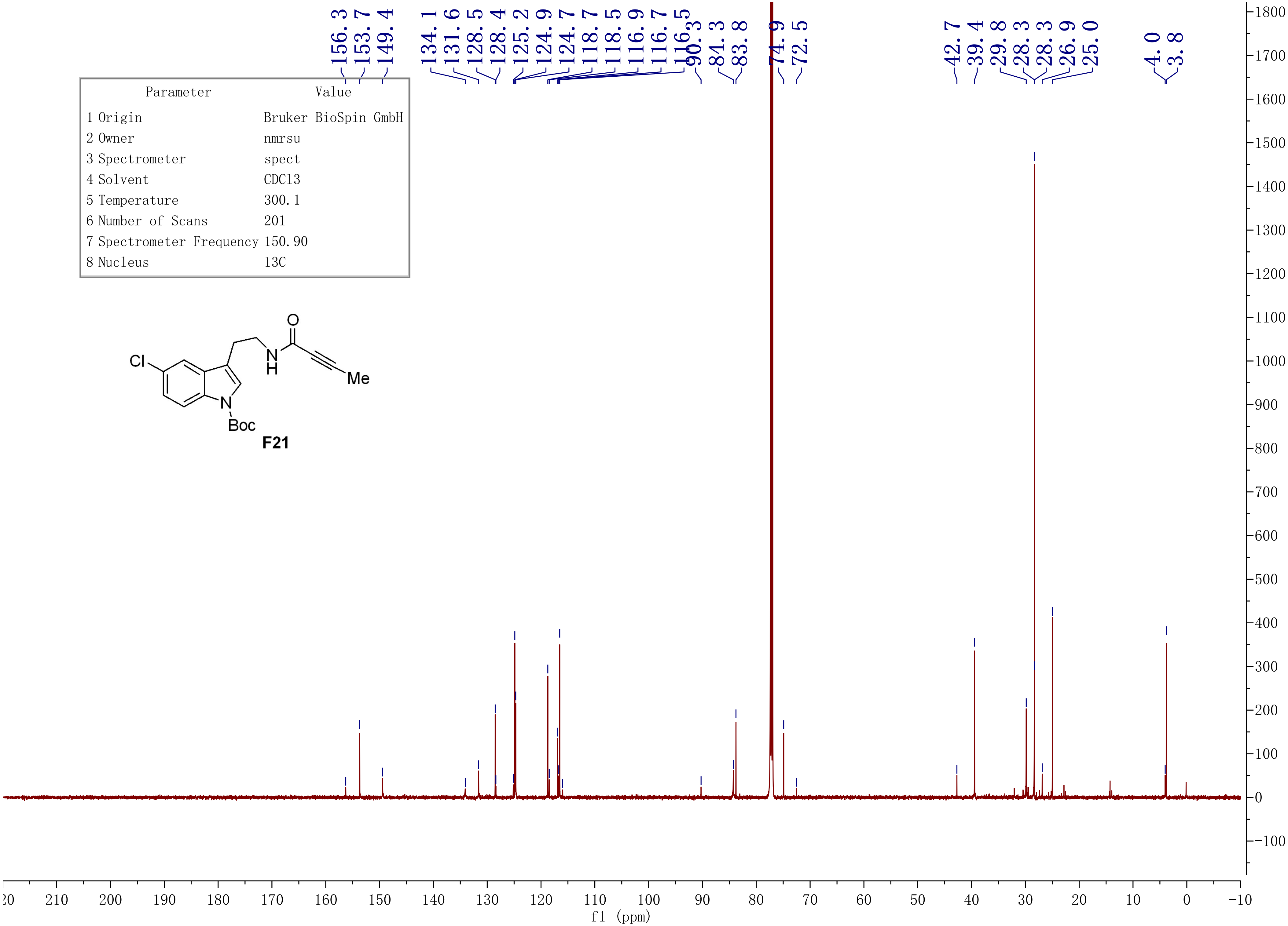
8.61
8.60
8.59
8.01
8.00
7.56
7.42
7.41
7.17
7.15
7.14
3.37
3.35
3.34
3.33
2.79
2.78
2.77
1.94
1.85
1.61
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
root
3 Spectrometer
spect
4 Solvent
DMSO
5 Temperature
298.0
6 Number of Scans
16
7 Spectrometer Frequency
600.20
8 Nucleus
1H
F
N
H
O
Me
N
Boc
F20
0.95
1.03
0.98
1.02
1.00
0.12
2.01
0.16
1.88
2.78
0.20
9.13
f1 (ppm)

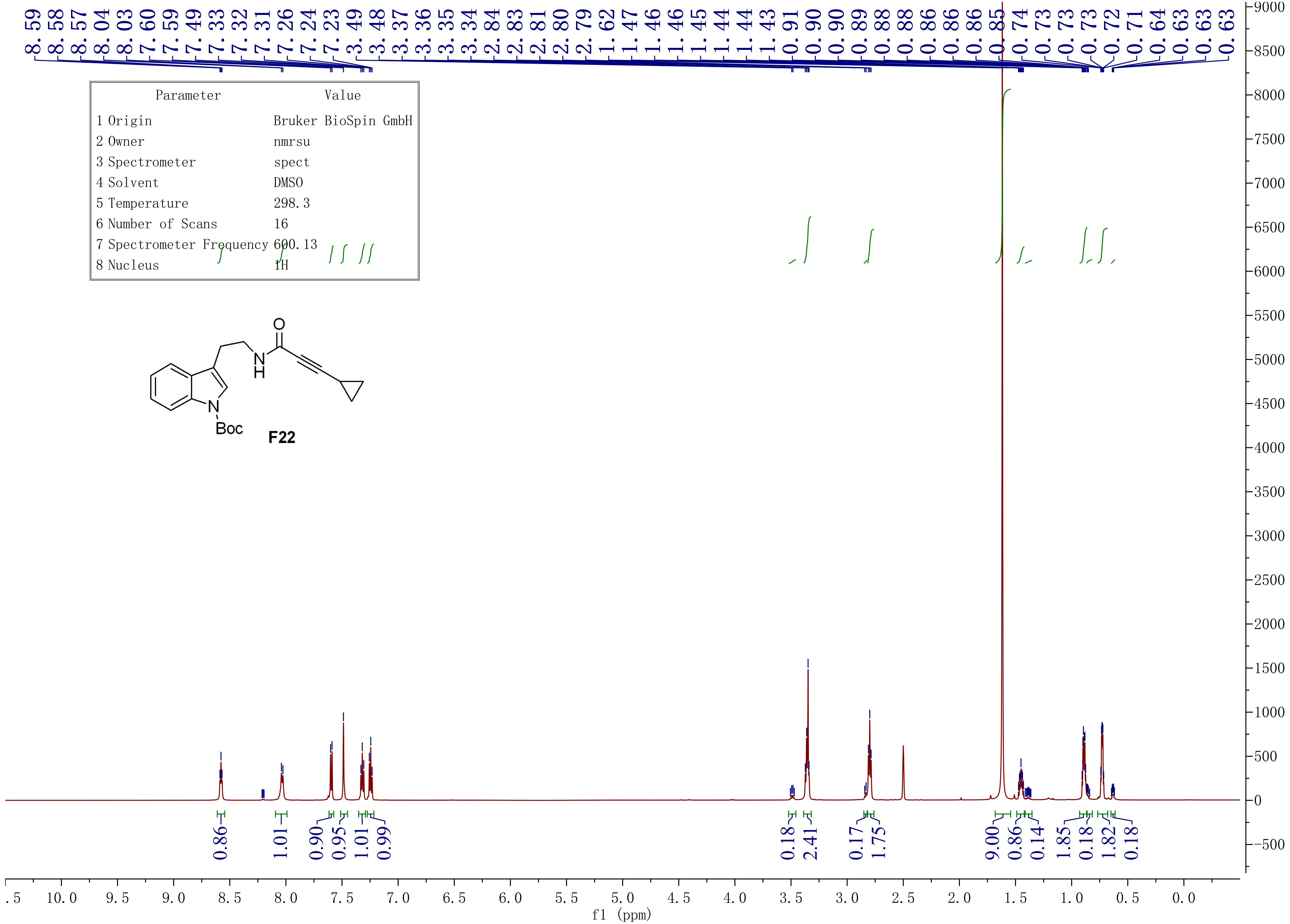


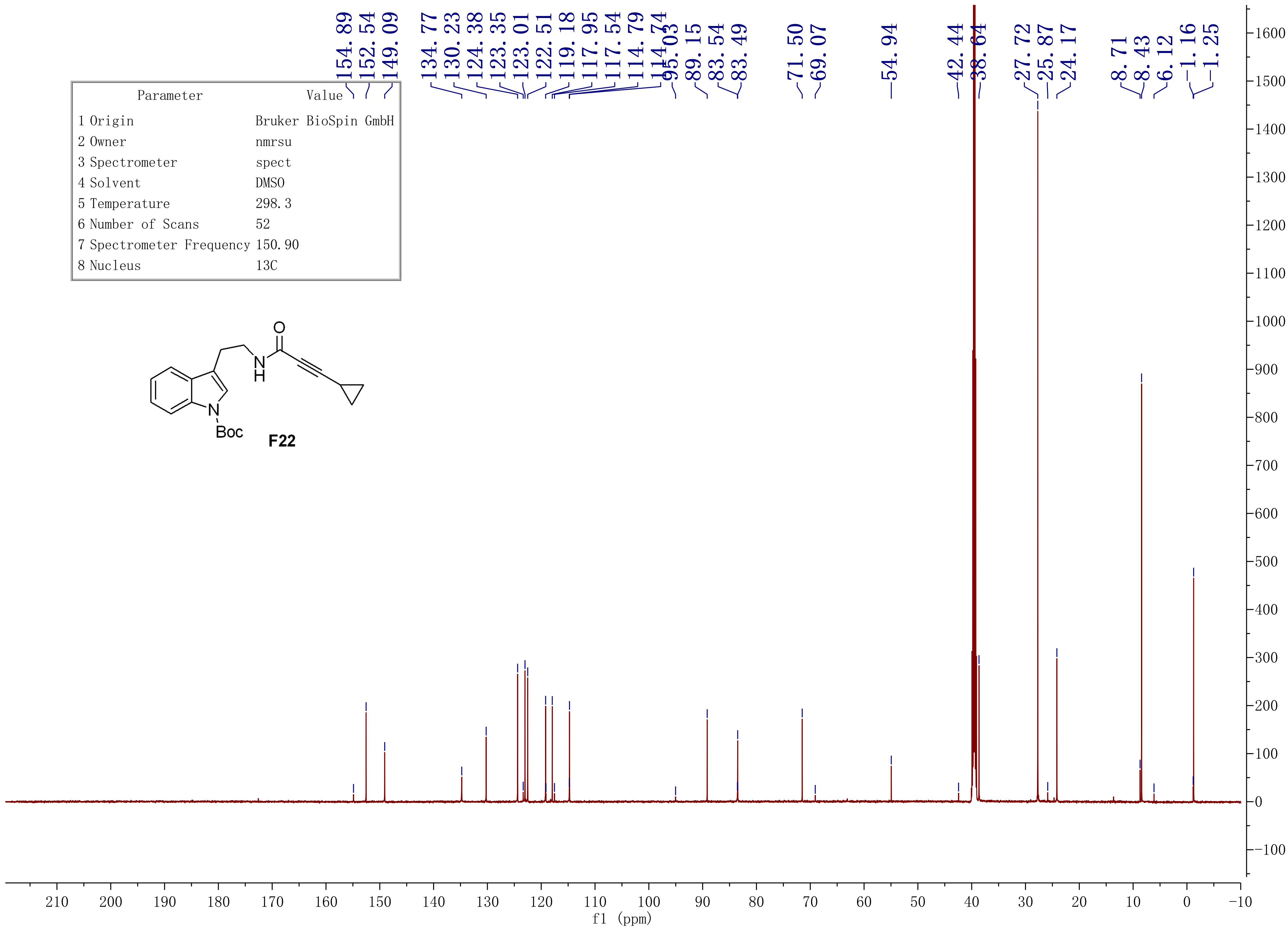
159.30
157.73
152.59
148.86
131.41
131.34
131.25
124.87
117.90
117.87
115.96
115.90
111.99
111.82
104.98
104.82
83.79
82.31
75.66
54.91
38.54
27.67
24.05
2.99
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 150.90
8 Nucleus 13C
F
O
N
H
Me
N
Boc
F20
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.1
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H

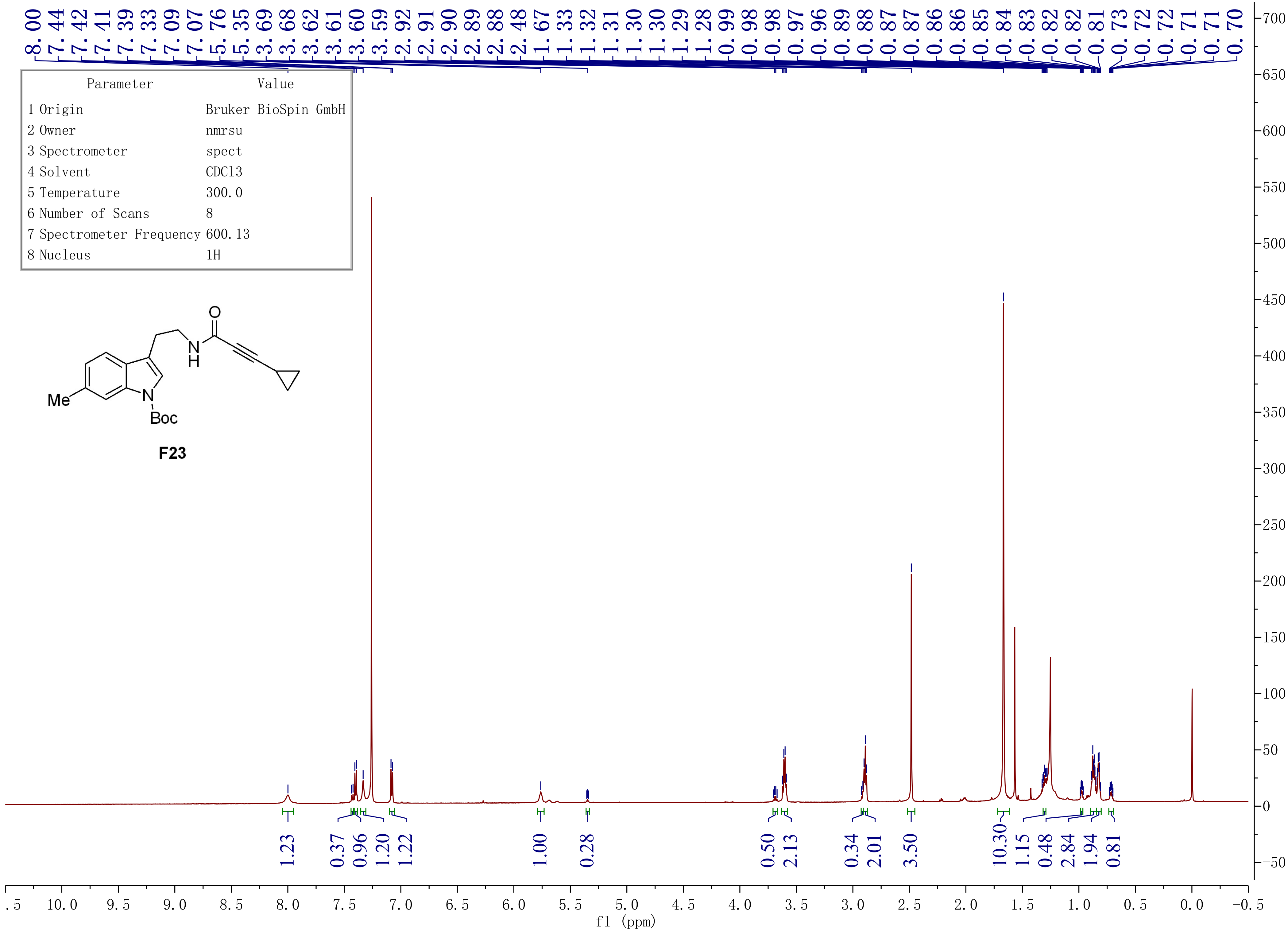



156.3
153.7
149.4
134.1
131.6
128.5
128.4
125.2
124.9
124.7
118.7
118.5
116.9
116.7
116.5
90.3
84.3
83.8
74.9
72.5
42.7
39.4
29.8
28.3
28.3
26.9
25.0
4.0
3.8
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 201
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Cl
O
N
H
Me
N
Boc
F21
f1 (ppm)

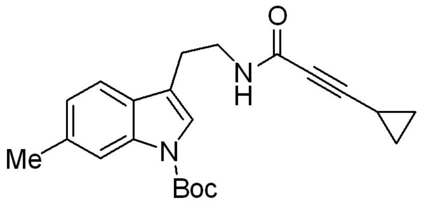

8.59 8.58 8.57 8.04 8.03 7.60 7.59 7.49 7.33 7.32 7.31 7.26 7.24 7.23 3.49 3.48 3.37 3.36 3.35 3.34 2.84 2.83 2.81 2.80 2.79 1.62 1.47 1.46 1.46 1.45 1.44 1.44 1.43 0.91 0.90 0.90 0.89 0.88 0.88 0.86 0.86 0.86 0.85 0.74 0.73 0.73 0.73 0.72 0.71 0.64 0.63 0.63 0.63
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.3
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
N
Boc
F22
0.86 1.01 0.90 0.95 1.01 0.99 0.18 2.41 0.17 1.75 9.00 0.86 0.14 1.85 0.18 1.82 0.18
f1 (ppm)



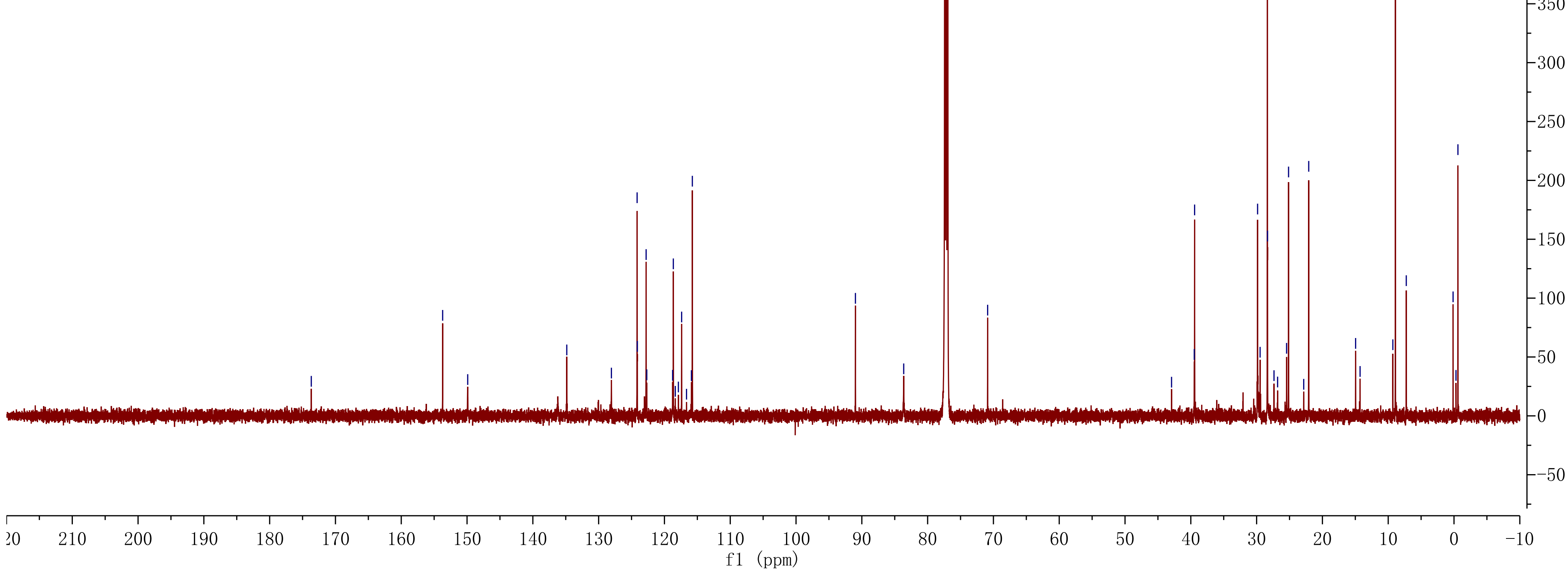
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.3
6 Number of Scans 52
7 Spectrometer Frequency 150.90
8 Nucleus 13C
154.89
152.54
149.09
134.77
130.23
124.38
123.35
123.01
122.51
119.18
117.95
117.54
114.79
114.74
95.03
89.15
83.54
83.49
71.50
69.07
54.94
42.44
38.64
27.72
25.87
24.17
8.71
8.43
6.12
-1.16
-1.25
O
N
H
N
Boc
F22
f1 (ppm)

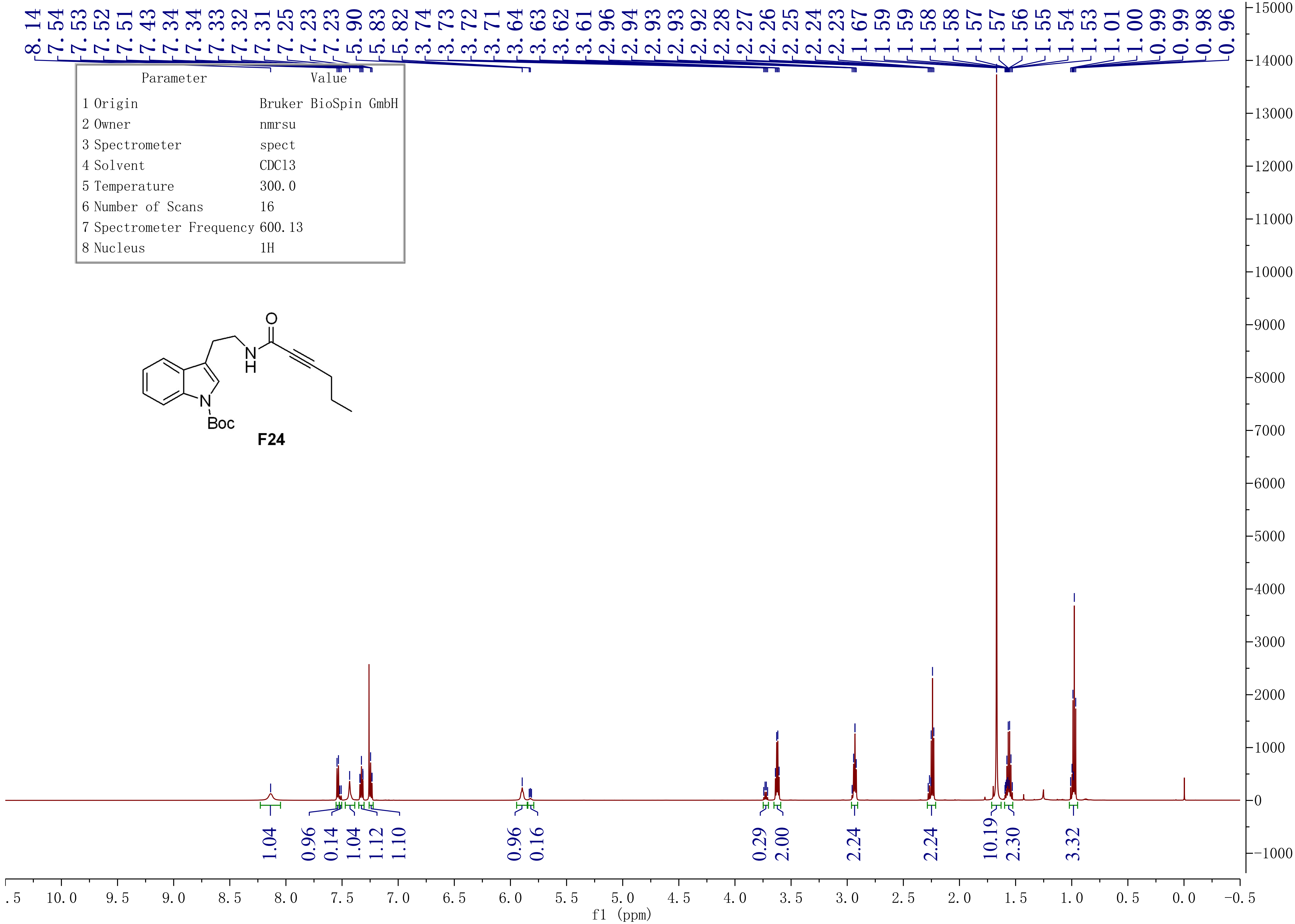

8.00 7.44 7.42 7.41 7.39 7.33 7.09 7.07 5.76 5.35 3.69 3.68 3.62 3.61 3.60 3.59 2.92 2.91 2.90 2.89 2.88 2.48 1.67 1.33 1.32 1.31 1.30 1.30 1.29 1.28 0.99 0.98 0.98 0.97 0.96 0.89 0.88 0.87 0.87 0.86 0.86 0.85 0.84 0.83 0.82 0.82 0.81 0.73 0.72 0.72 0.71 0.71 0.70
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
Me
N
Boc
F23
1.23 0.37 0.96 1.20 1.22 1.00 0.28 0.50 2.13 0.34 2.01 3.50 10.30 1.15 0.48 2.84 1.94 0.81
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.1
6 Number of Scans	400
7 Spectrometer Frequency	150.90
8 Nucleus	13C

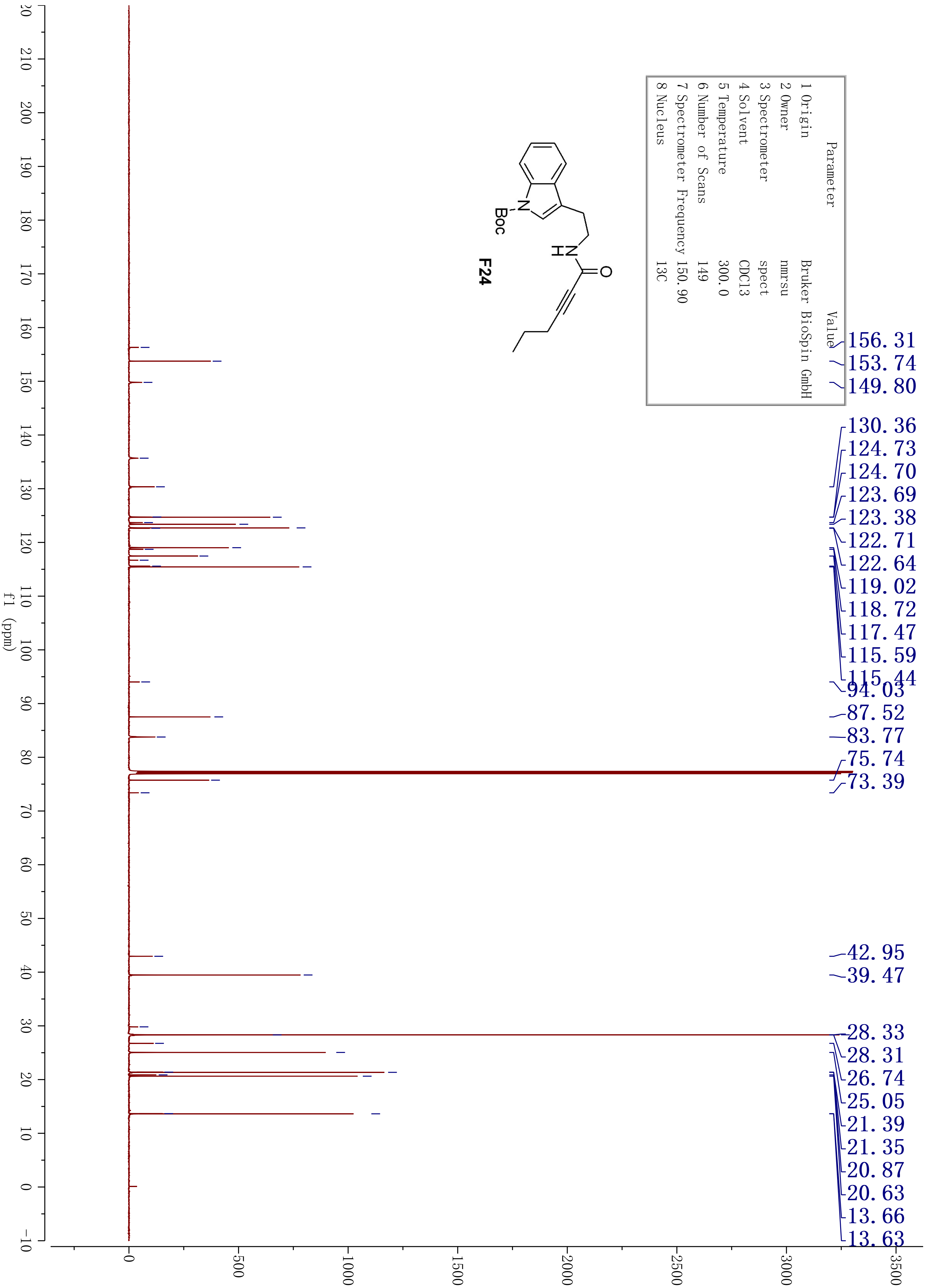


F23

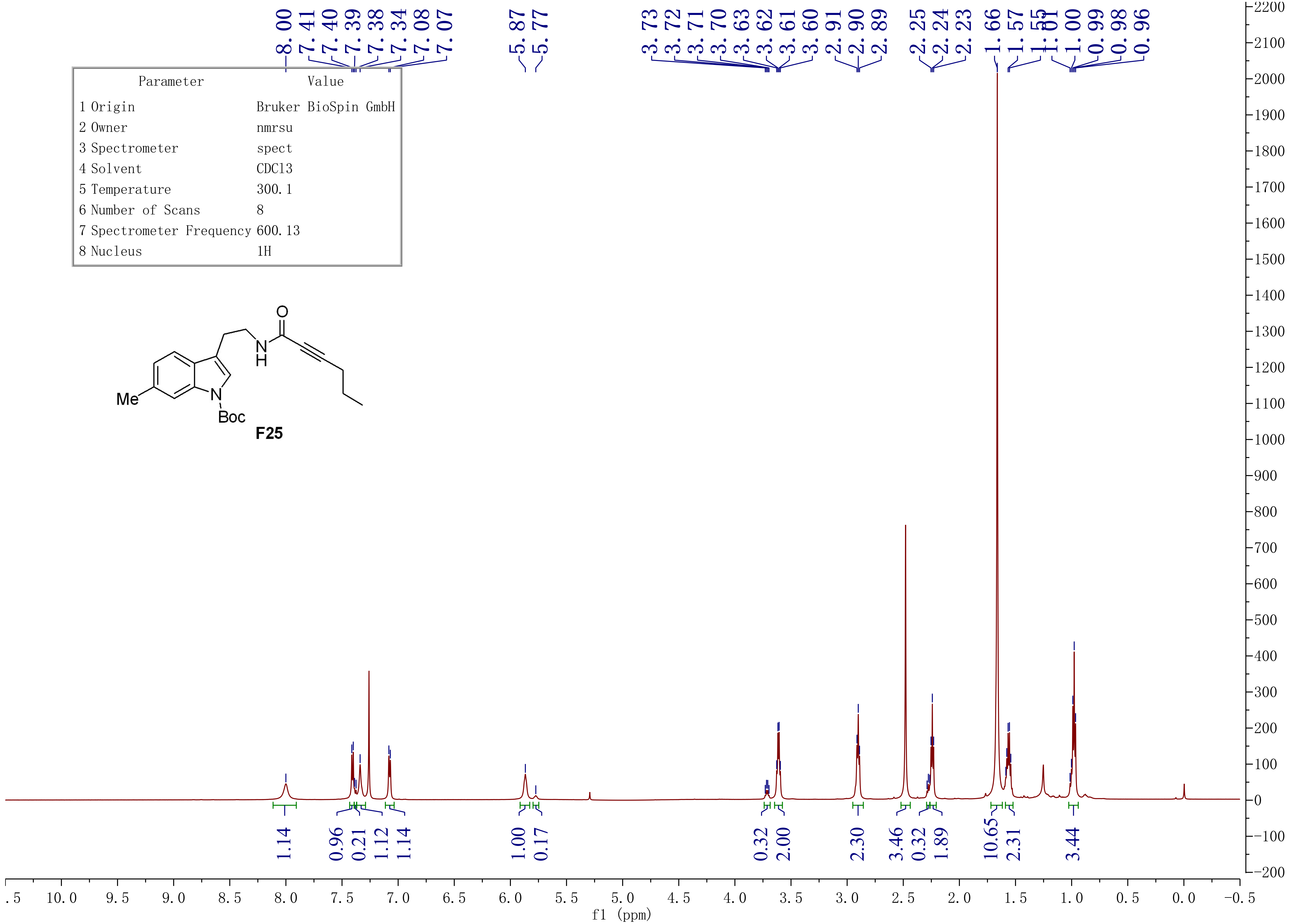


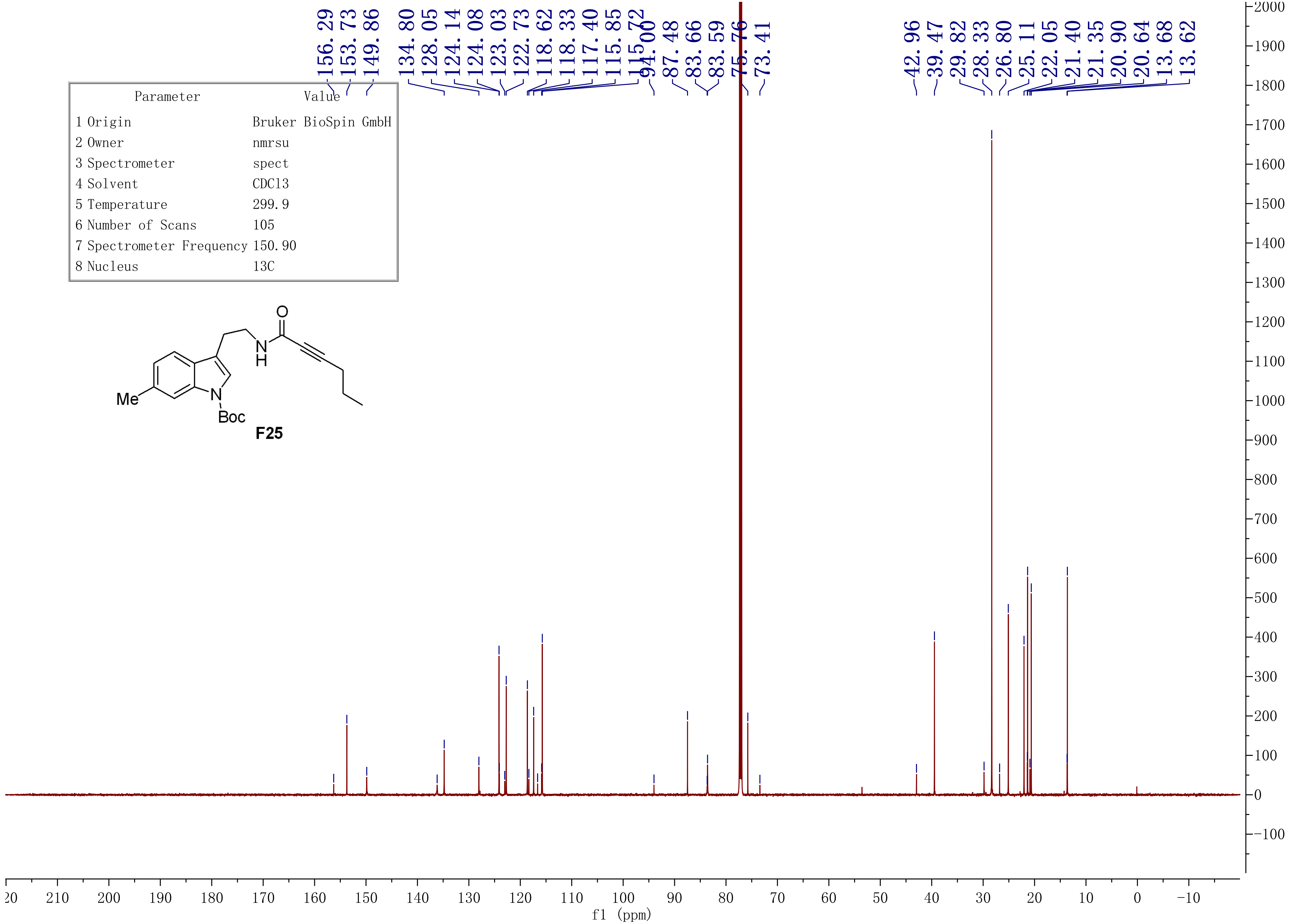


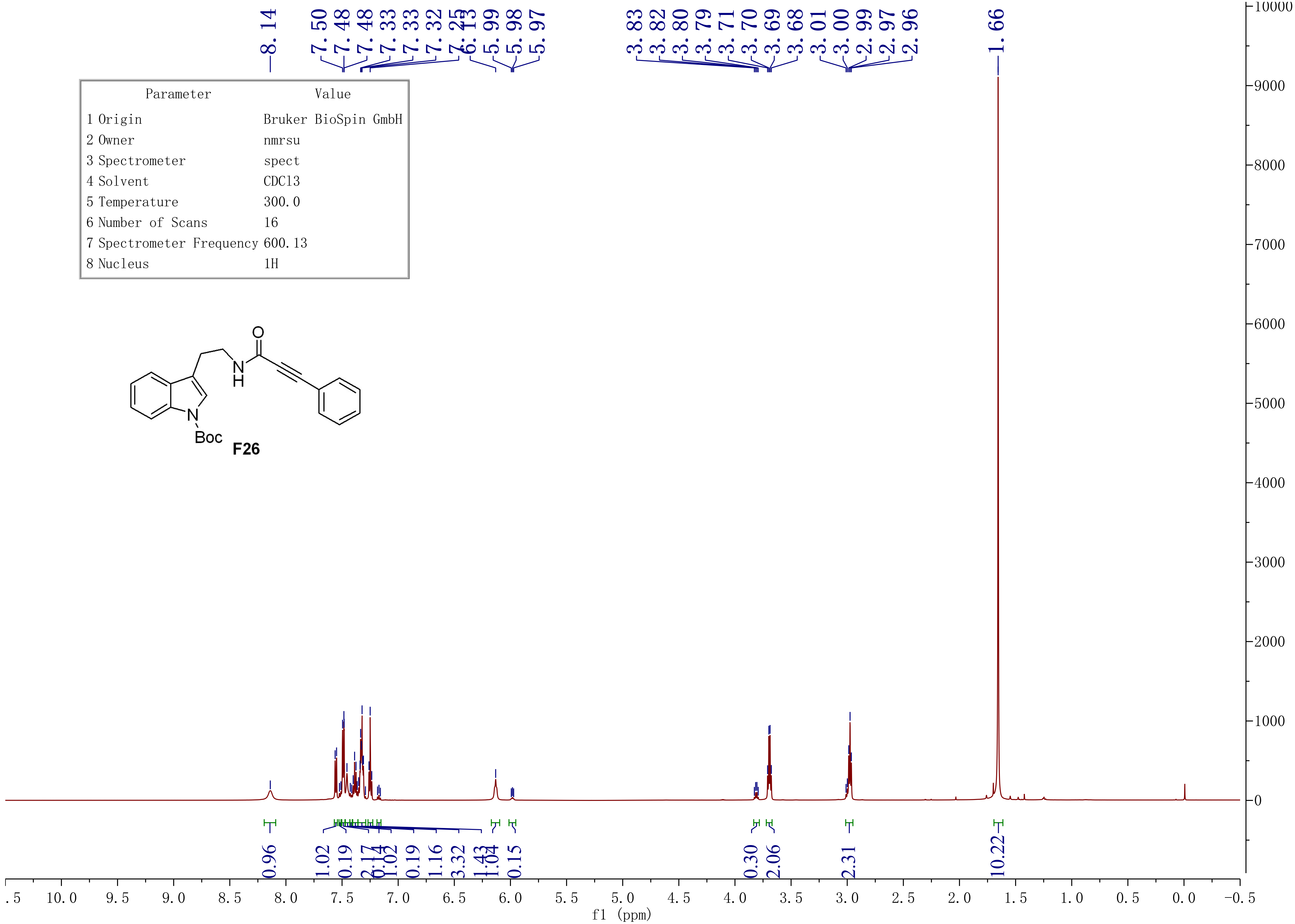
8.14 7.54 7.53 7.52 7.51 7.43 7.34 7.34 7.33 7.32 7.31 7.25 7.23 7.23 5.90 5.83 5.82 3.74 3.73 3.72 3.71 3.64 3.63 3.62 3.61 2.96 2.94 2.93 2.93 2.92 2.28 2.27 2.26 2.25 2.24 2.23 1.67 1.59 1.59 1.58 1.58 1.57 1.57 1.56 1.55 1.54 1.53 1.01 1.00 0.99 0.99 0.98 0.96
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
H
N
Boc
F24
1.04 0.96 0.14 1.04 1.12 1.10 0.96 0.16 0.29 2.00 2.24 2.24 10.19 2.30 3.32
f1 (ppm)



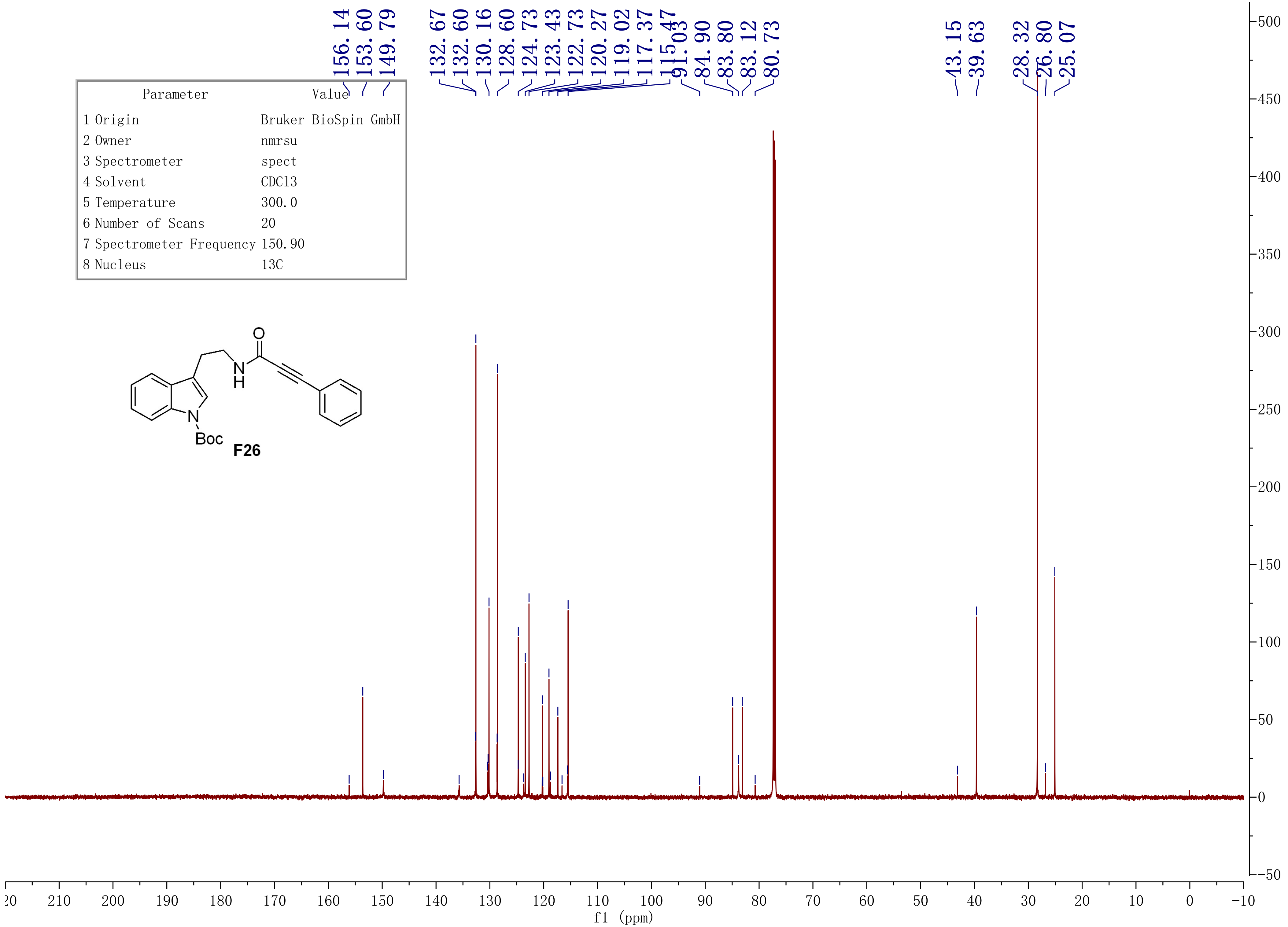
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
CDCl3
5 Temperature
300.0
6 Number of Scans
149
7 Spectrometer Frequency
150.90
8 Nucleus
13C
F24
Boc
N
H
O
156.31
153.74
149.80
130.36
124.73
124.70
123.69
123.38
122.71
122.64
119.02
118.72
117.47
115.59
115.44
94.03
87.52
83.77
75.74
73.39
42.95
39.47
28.33
28.31
26.74
25.05
21.39
21.35
20.87
20.63
13.66
13.63
f1 (ppm)

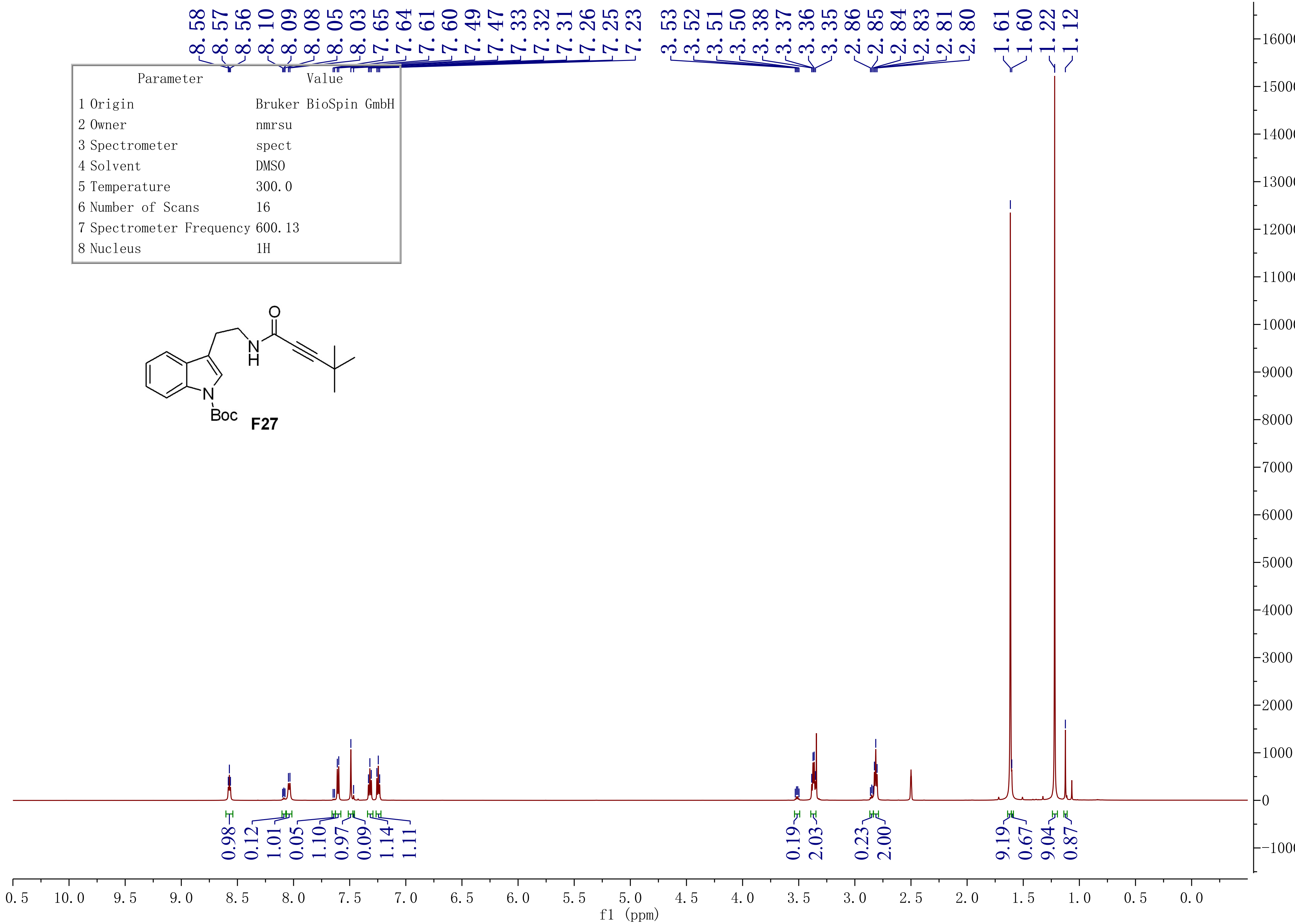

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Me
N
Boc
N
H
O
F25
8.00 7.41 7.40 7.39 7.38 7.34 7.08 7.07
5.87 5.77
3.73 3.72 3.71 3.70 3.63 3.62 3.61 3.60 2.91 2.90 2.89
2.25 2.24 2.23 1.66 1.57 1.55 1.01 1.00 0.99 0.98 0.96
1.14 0.96 0.21 1.12 1.14 1.00 0.17 0.32 2.00 2.30 3.46 0.32 1.89 10.65 2.31 3.44
f1 (ppm)


156.29
153.73
149.86
134.80
128.05
124.14
124.08
123.03
122.73
118.62
118.33
117.40
115.85
115.72
94.00
87.48
83.66
83.59
75.76
73.41
42.96
39.47
29.82
28.33
26.80
25.11
22.05
21.40
21.35
20.90
20.64
13.68
13.62
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 105
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
H
Me
N
Boc
F25
f1 (ppm)

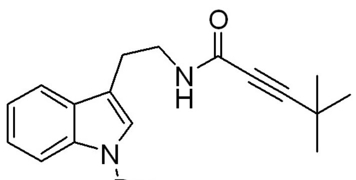

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
8.14
7.50
7.48
7.48
7.33
7.33
7.32
7.25
6.13
5.99
5.98
5.97
3.83
3.82
3.80
3.79
3.71
3.70
3.69
3.68
3.01
3.00
2.99
2.97
2.96
1.66
0.96
1.02
0.19
2.17
0.14
1.02
0.19
1.16
3.32
1.43
1.04
0.15
0.30
2.06
2.31
10.22
Boc
F26
f1 (ppm)

S198

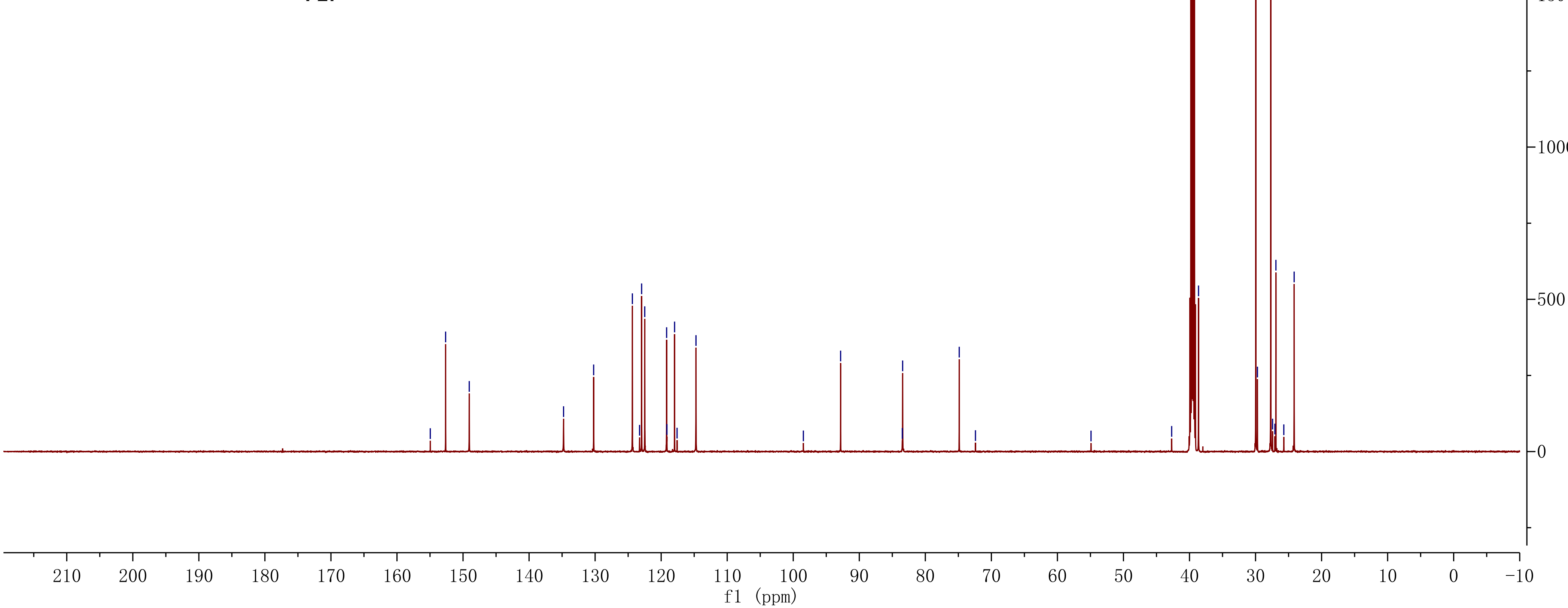

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 20
7 Spectrometer Frequency 150.90
8 Nucleus 13C
156.14
153.60
149.79
132.67
132.60
130.16
128.60
124.73
123.43
122.73
120.27
119.02
117.37
115.47
91.03
84.90
83.80
83.12
80.73
43.15
39.63
28.32
26.80
25.07
N
H
O
N
Boc
F26
f1 (ppm)

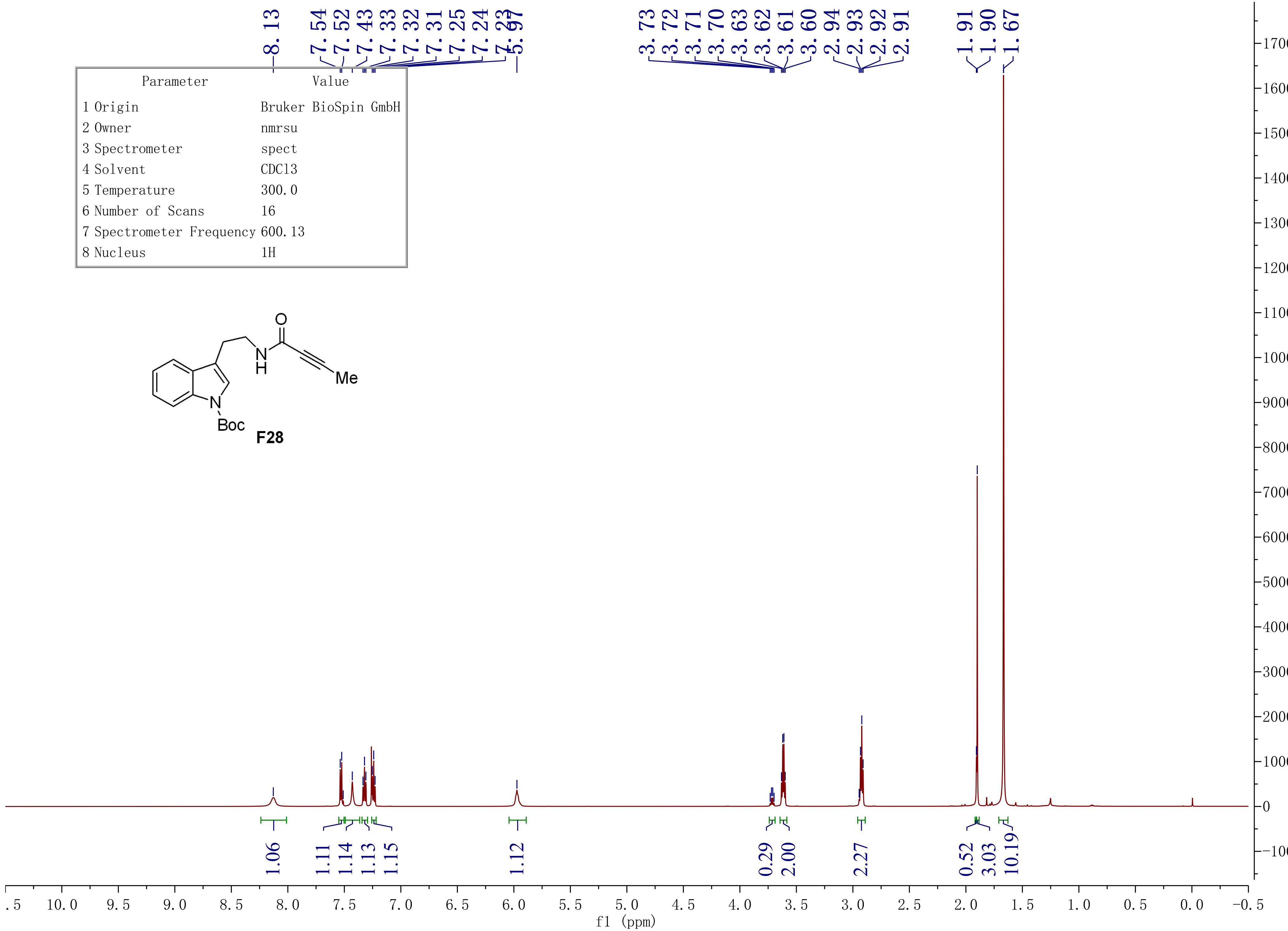

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Boc
F27
f1 (ppm)

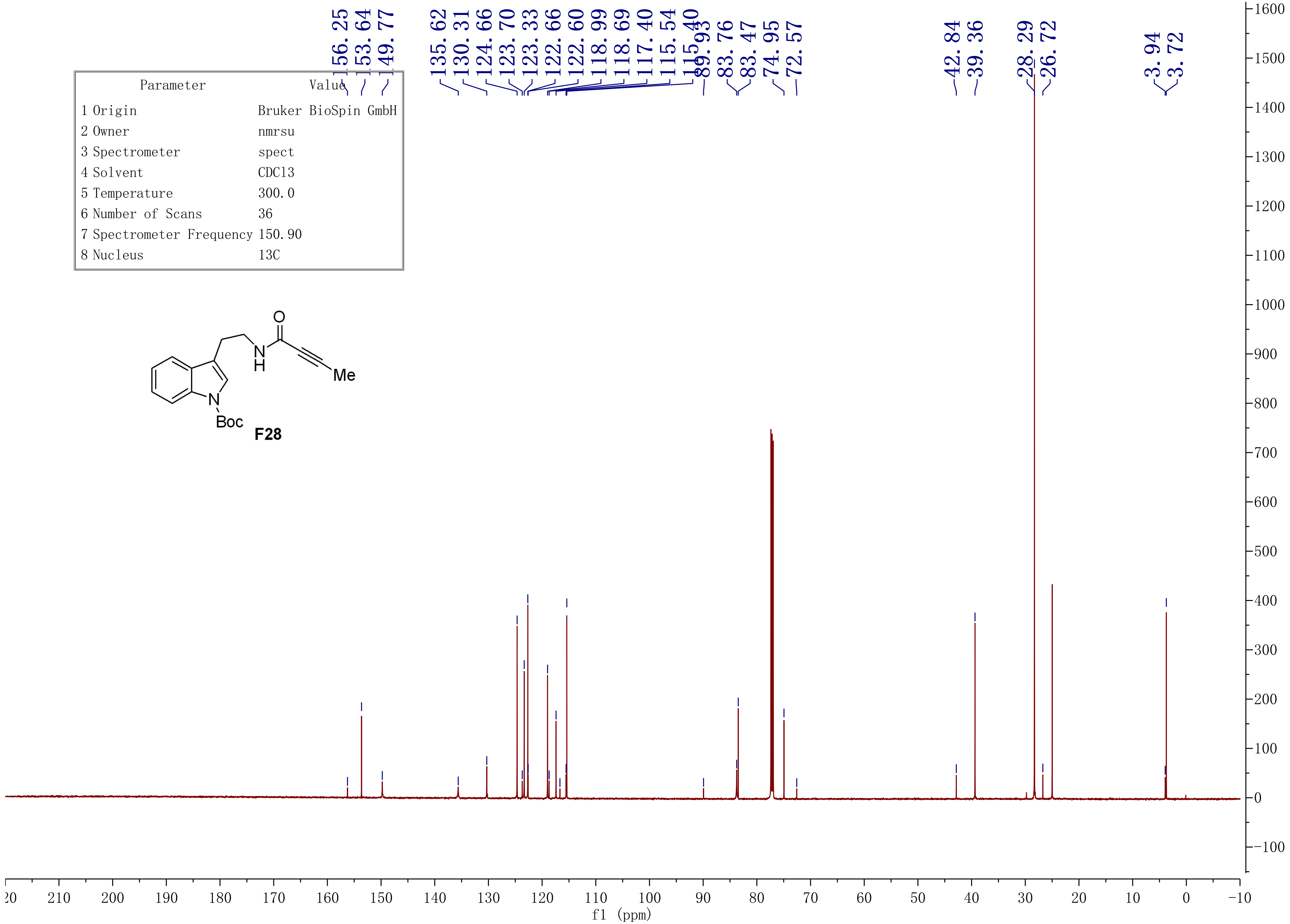
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	90
7 Spectrometer Frequency	150.90
8 Nucleus	13C



F27

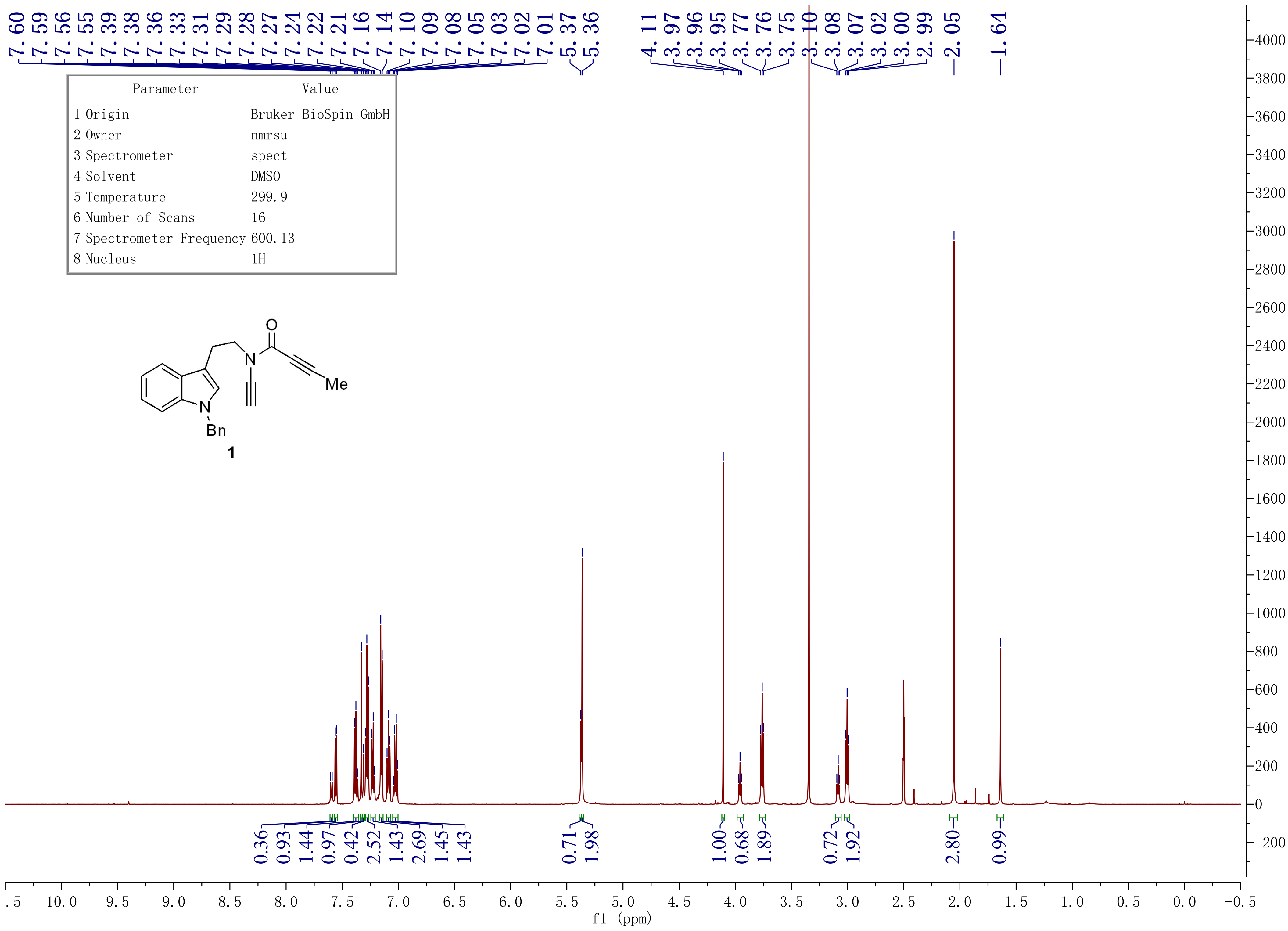



Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
H
O
Me
N
Boc
F28
8.13
7.54
7.52
7.43
7.33
7.32
7.31
7.25
7.24
7.23
5.97
3.73
3.72
3.71
3.70
3.63
3.62
3.61
3.60
2.94
2.93
2.92
2.91
1.91
1.90
1.67
1.06
1.11
1.14
1.13
1.15
1.12
0.29
2.00
2.27
0.52
3.03
10.19
f1 (ppm)

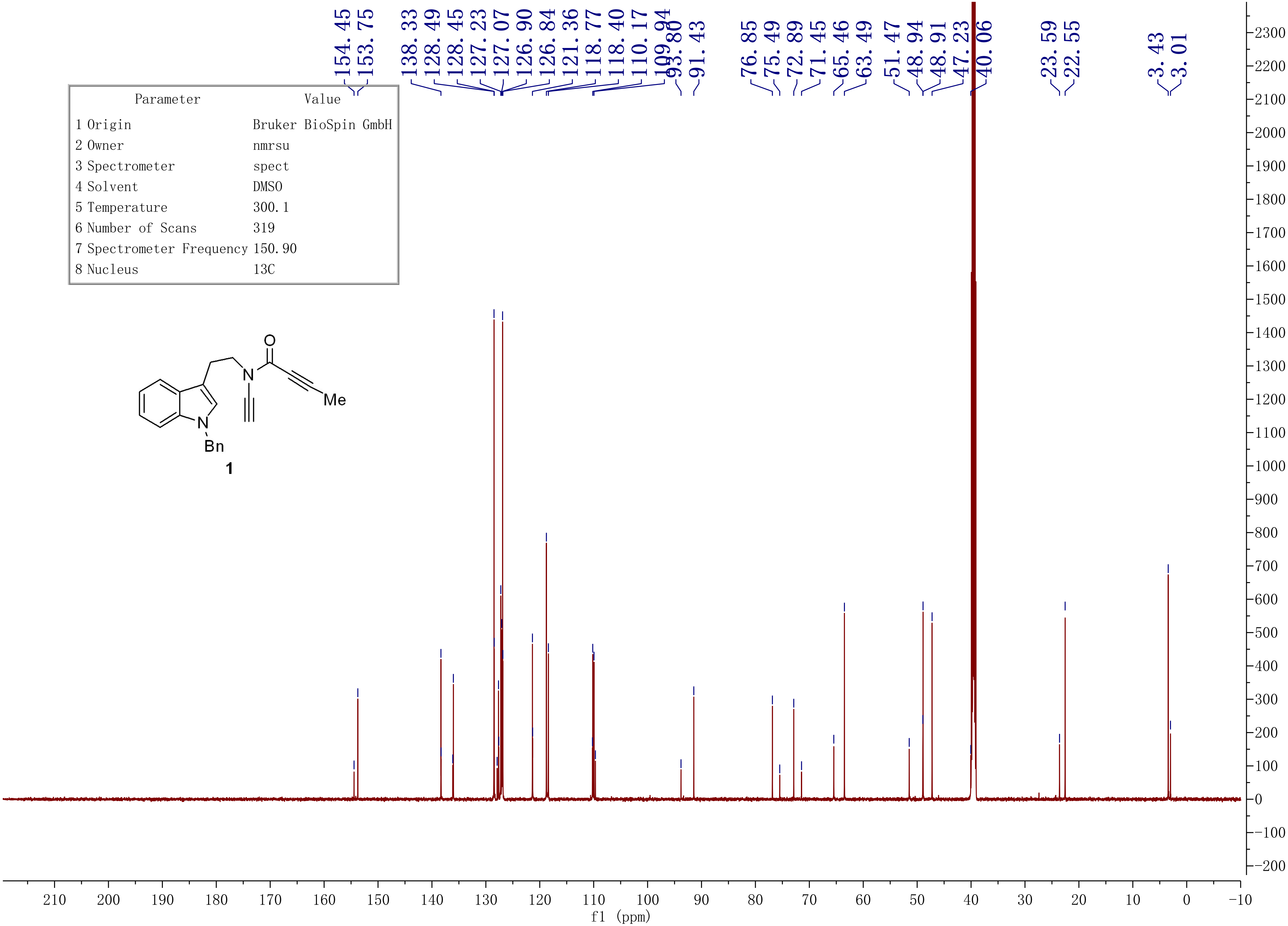


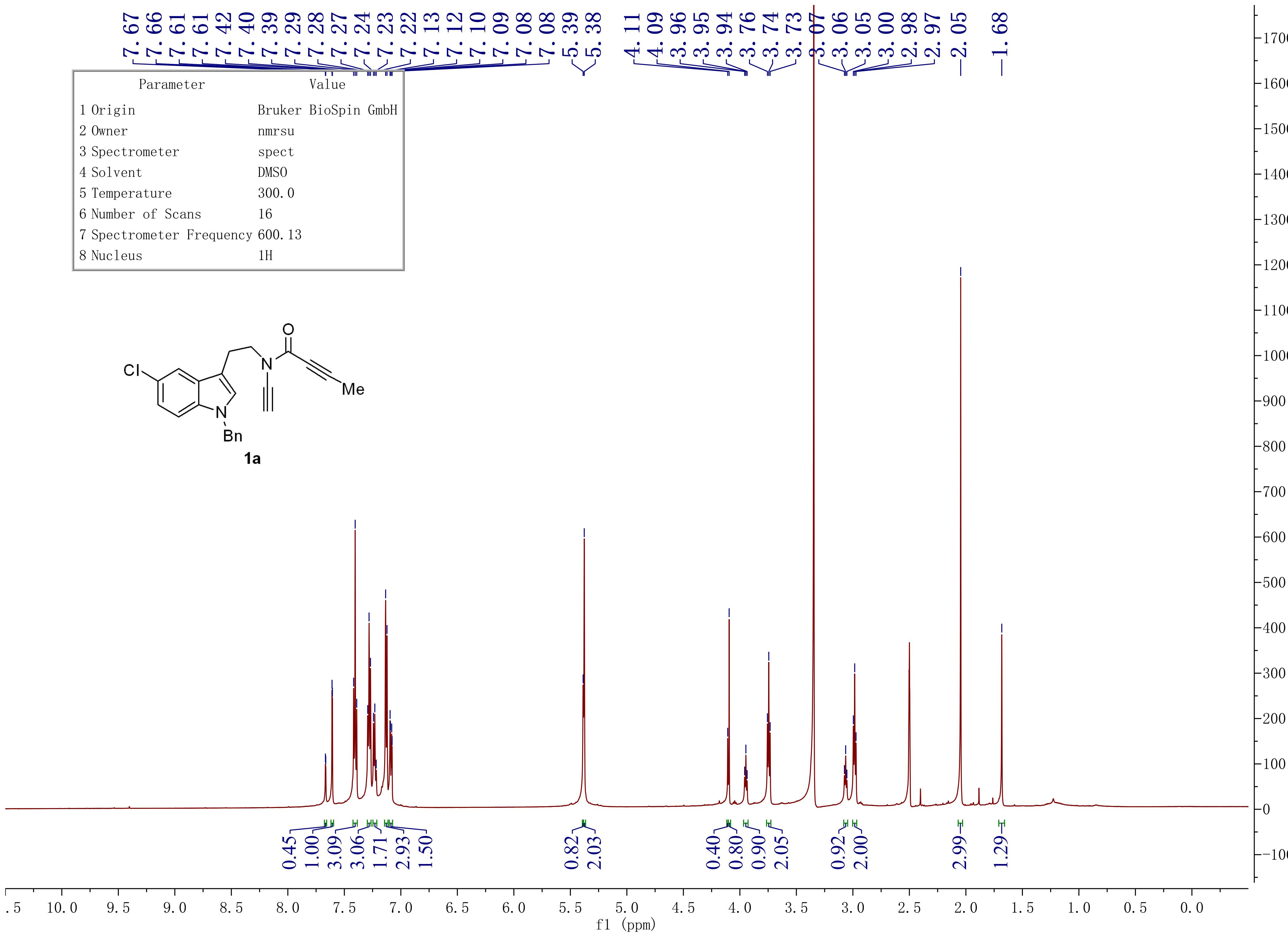
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	36
7 Spectrometer Frequency	150.90
8 Nucleus	13C

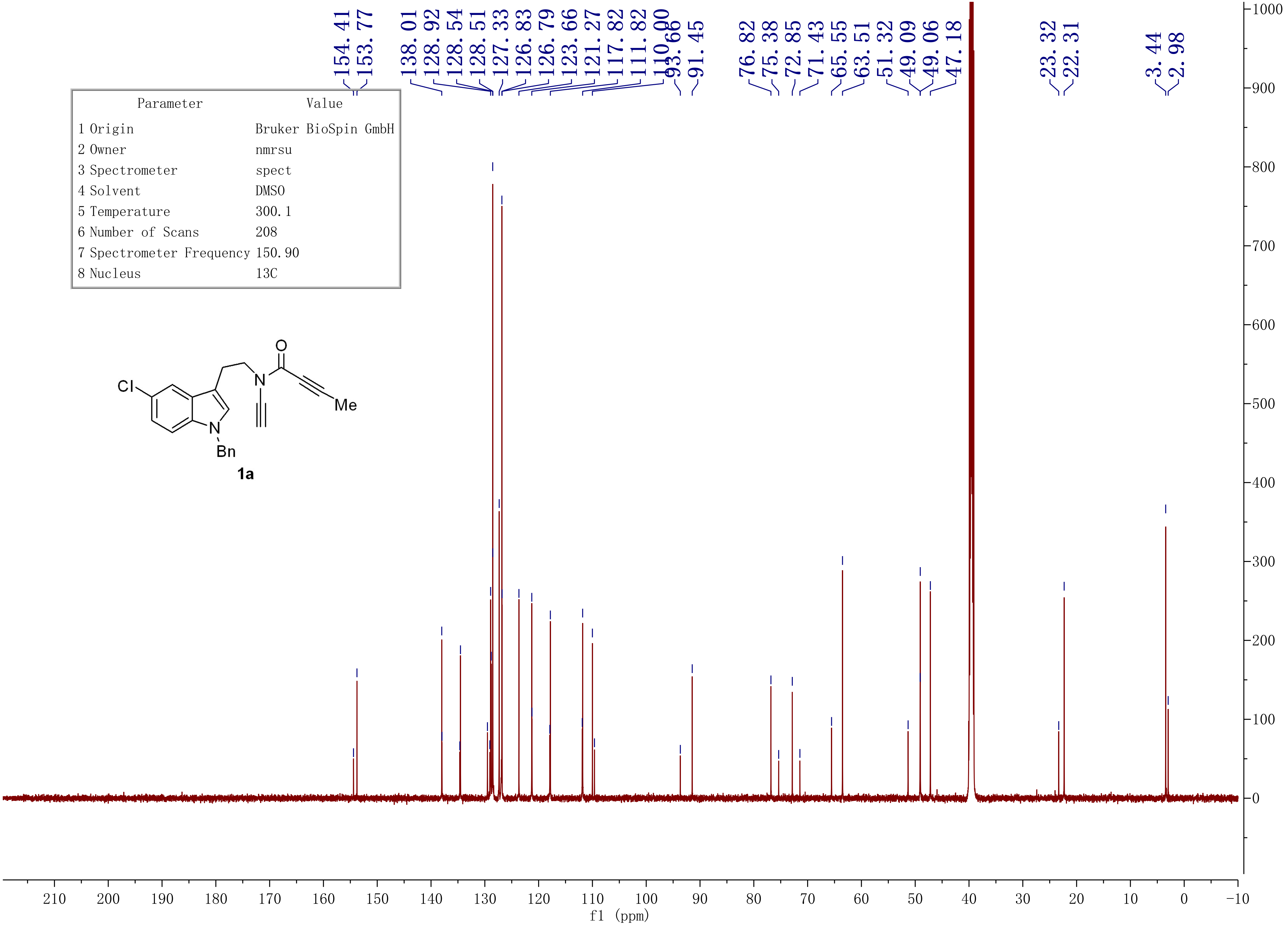
F28



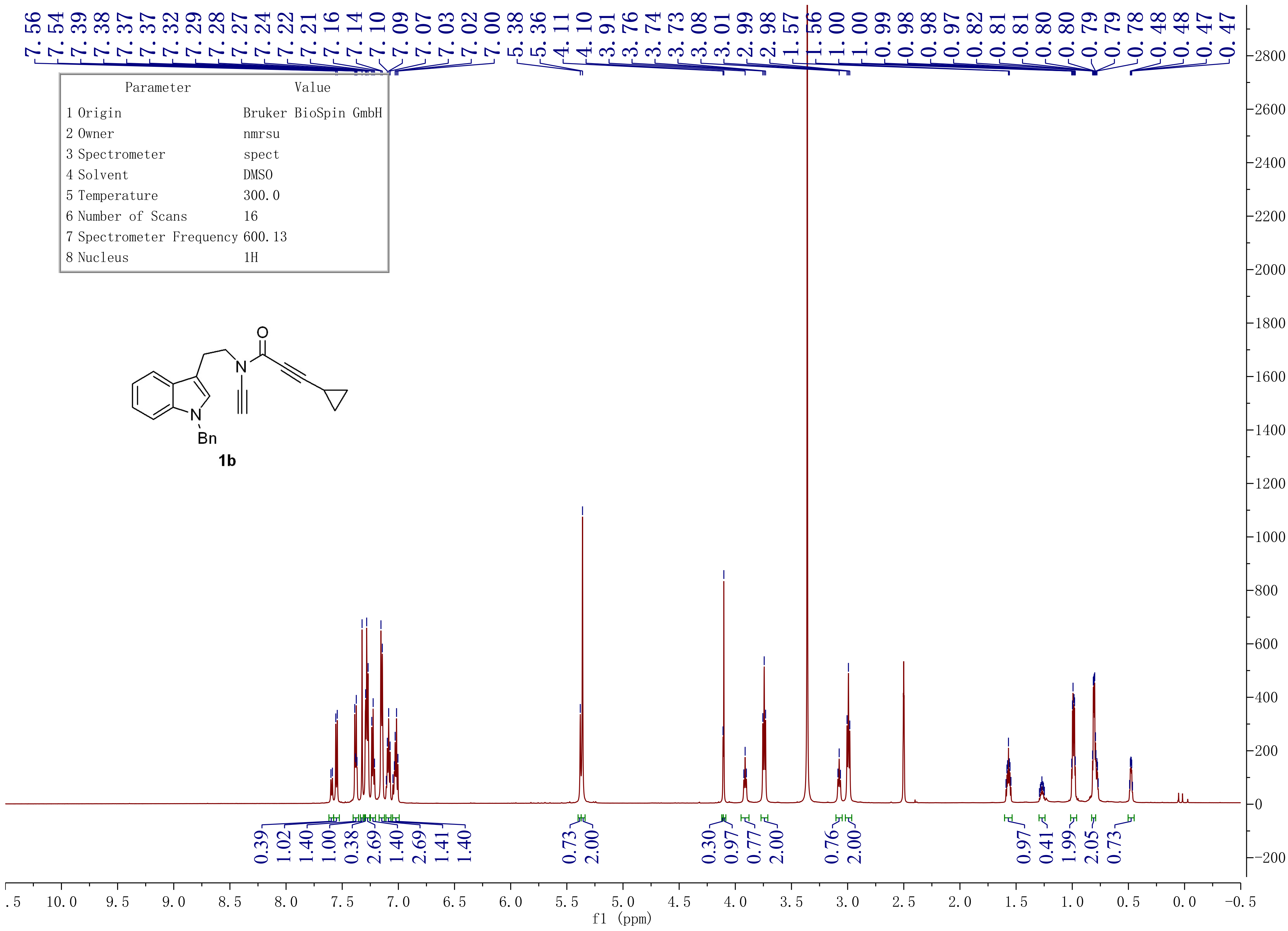
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
Me
N
Bn
1
f1 (ppm)

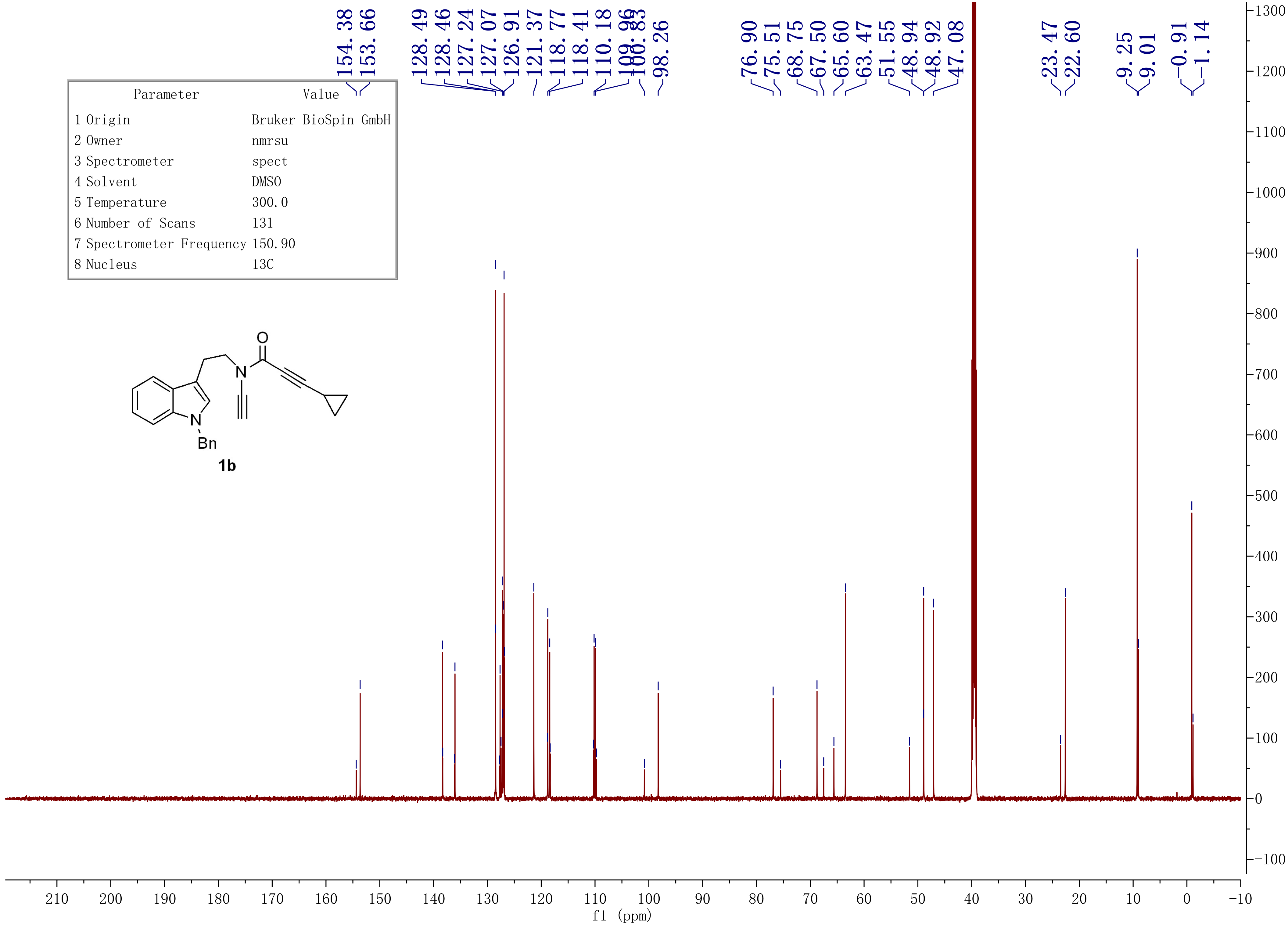

154.45
153.75
138.33
128.49
128.45
127.23
127.07
126.90
126.84
121.36
118.77
118.40
110.17
109.94
93.80
91.43
76.85
75.49
72.89
71.45
65.46
63.49
51.47
48.94
48.91
47.23
40.06
23.59
22.55
3.43
3.01
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 319
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
Me
N
Bn
1
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
7.67 7.66 7.61 7.61 7.42 7.40 7.39 7.29 7.28 7.27 7.24 7.23 7.22 7.13 7.12 7.10 7.09 7.08 7.08 5.39 5.38 4.11 4.09 3.96 3.95 3.94 3.76 3.74 3.73 3.07 3.06 3.05 3.00 2.98 2.97 2.05 1.68
Cl
N
O
Me
Bn
1a
0.45 1.00 3.09 3.06 1.71 2.93 1.50 0.82 2.03 0.40 0.80 0.90 2.05 0.92 2.00 2.99 1.29
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.1
6 Number of Scans	208
7 Spectrometer Frequency	150.90
8 Nucleus	13C


7.56 7.54 7.39 7.38 7.37 7.37 7.32 7.29 7.28 7.27 7.24 7.22 7.21 7.16 7.14 7.10 7.09 7.07 7.03 7.02 7.00 5.38 5.36 4.11 4.10 3.91 3.76 3.74 3.73 3.08 3.01 2.99 2.98 1.57 1.56 1.00 1.00 0.99 0.98 0.98 0.97 0.82 0.81 0.81 0.80 0.80 0.79 0.79 0.78 0.48 0.48 0.47 0.47
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
N
Bn
1b
0.39 1.02 1.40 1.00 0.38 2.69 1.40 2.69 1.41 1.40
0.73 2.00
0.30 0.97 0.77 2.00
0.76 2.00
0.97 0.41 1.99 2.05 0.73
f1 (ppm)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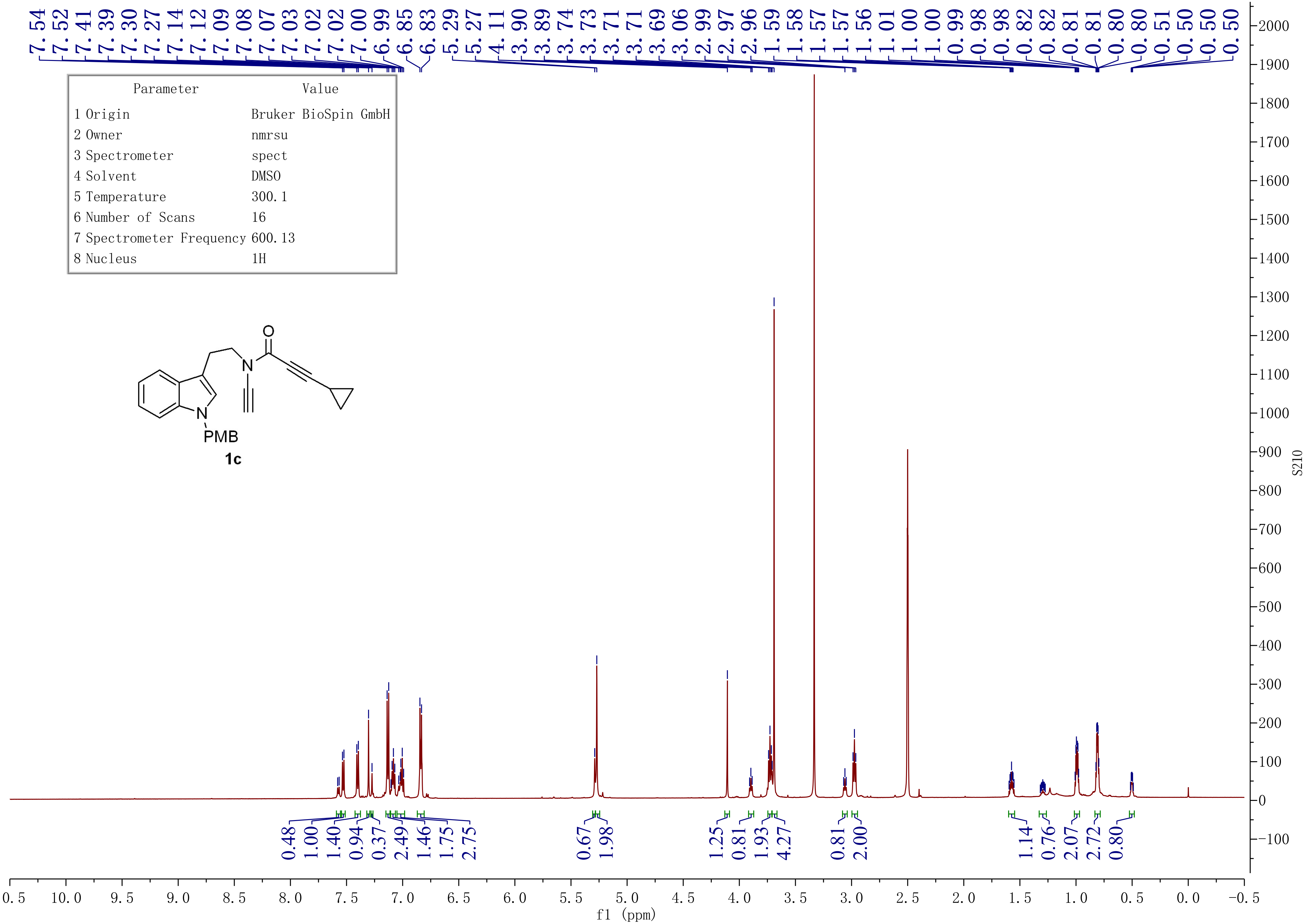
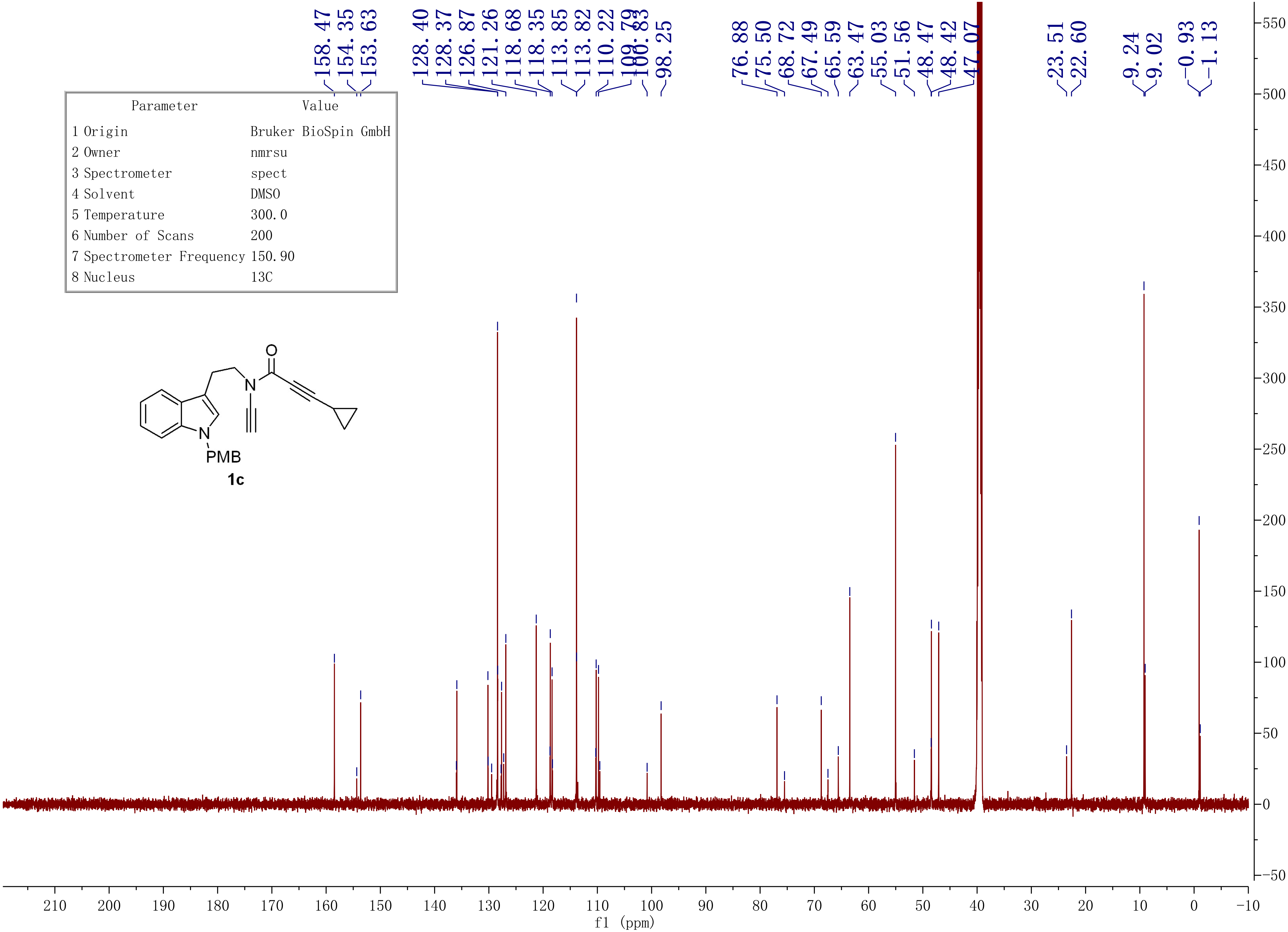
127.07
126.91
121.37
118.77
118.41
110.18
109.96
100.83
98.26
76.90
75.51
68.75
67.50
65.60
63.47
51.55
48.94
48.92
47.08
23.47
22.60
9.25
9.01
-0.91
-1.14
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 131
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
N
Bn
1b
f1 (ppm)



7.54 7.52 7.41 7.39 7.30 7.27 7.14 7.12 7.09 7.08 7.07 7.03 7.02 7.02 7.02 7.00 6.99 6.85 6.83 5.29 5.27 4.11 3.90 3.89 3.74 3.73 3.71 3.71 3.69 3.06 2.99 2.97 2.96 1.59 1.58 1.57 1.57 1.56 1.01 1.00 1.00 0.99 0.98 0.98 0.82 0.82 0.81 0.81 0.80 0.80 0.51 0.50 0.50 0.50
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
N
PMB
1c
0.48 1.00 1.40 0.94 0.37 2.49 1.46 1.75 2.75
0.67 1.98
1.25 0.81 1.93 4.27
0.81 2.00
1.14 0.76 2.07 2.72 0.80
f1 (ppm)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154.35
153.63
128.40
128.37
126.87
121.26
118.68
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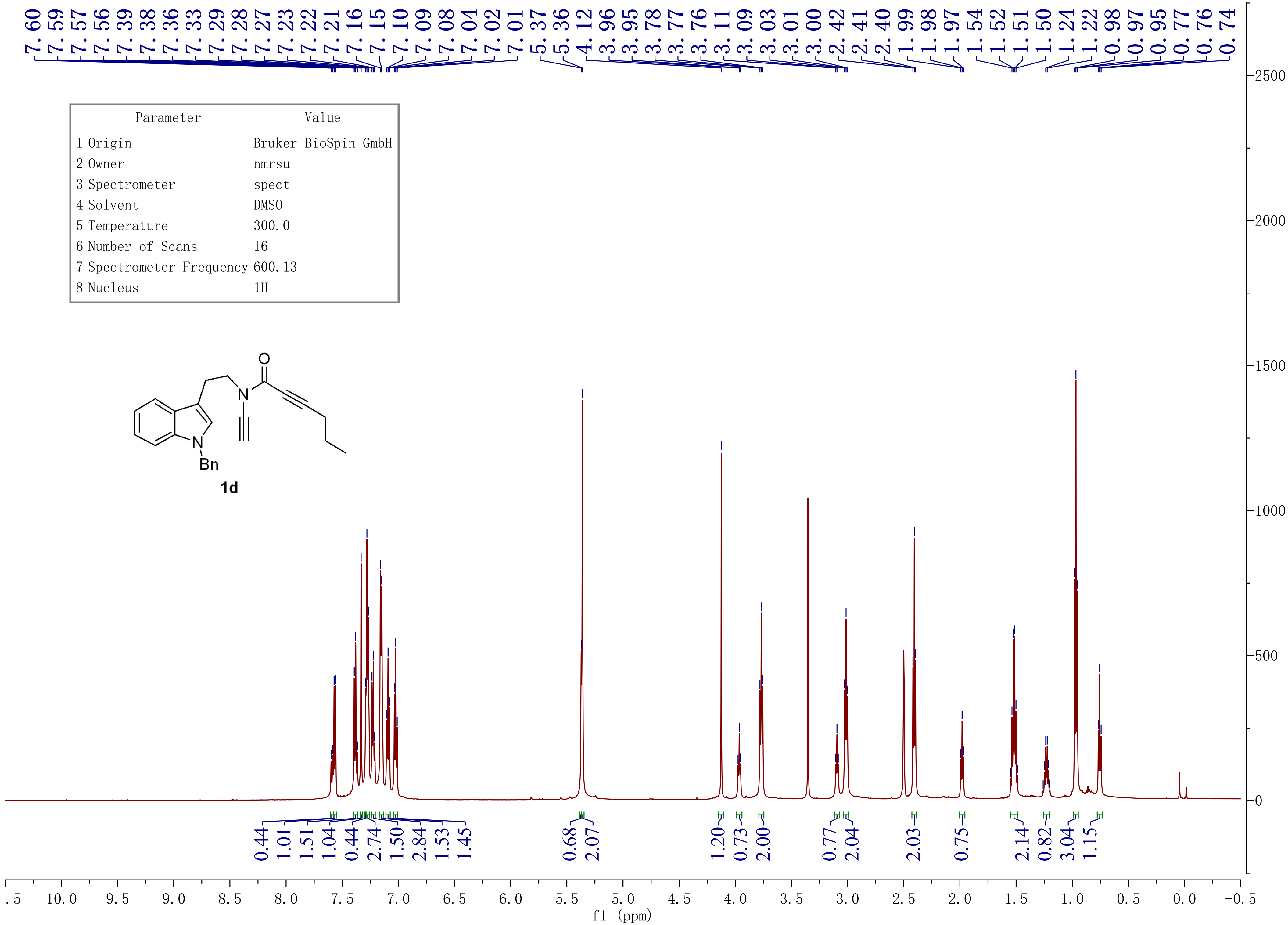
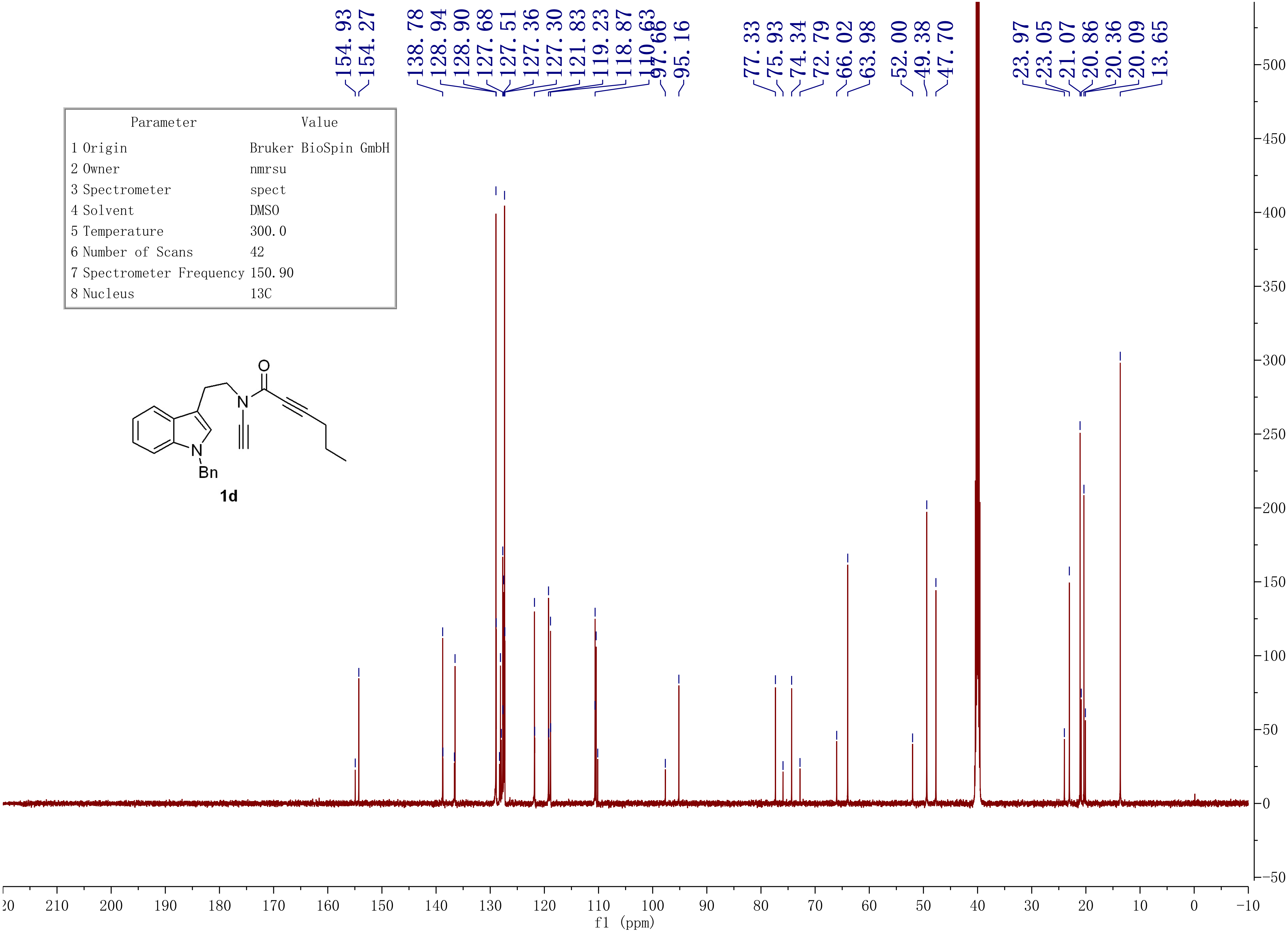
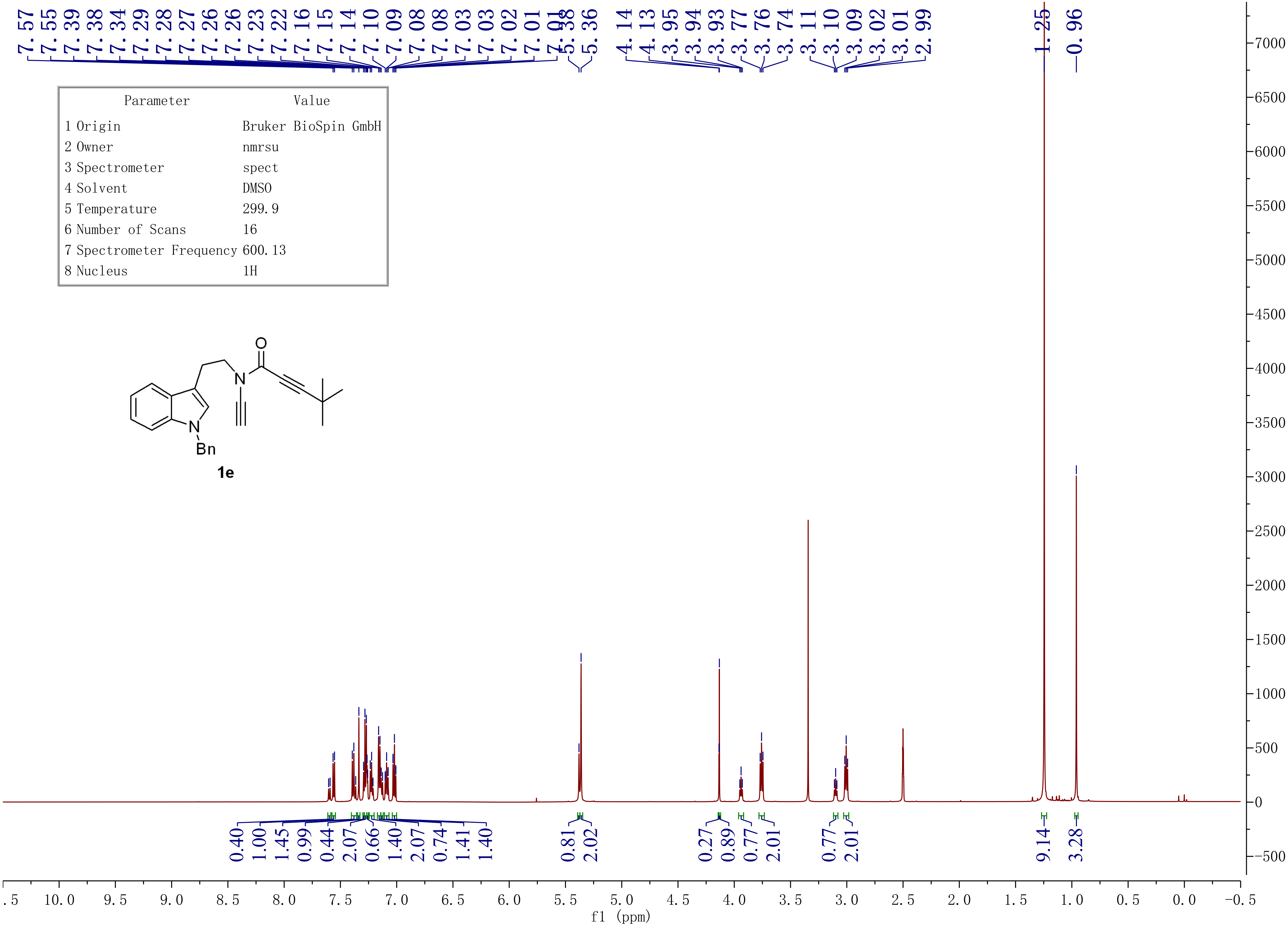
113.85
113.82
110.22
109.79
100.83
98.25
76.88
75.50
68.72
67.49
65.59
63.47
55.03
51.56
48.47
48.42
47.07
23.51
22.60
9.24
9.02
-0.93
-1.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 200
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
N
PMB
1c
f1 (ppm)



Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Bn
1d
7.60 7.59 7.57 7.56 7.39 7.38 7.36 7.33 7.29 7.28 7.27 7.23 7.22 7.21 7.16 7.15 7.10 7.09 7.08 7.04 7.02 7.01 5.37 5.36 4.12 3.96 3.95 3.78 3.77 3.76 3.11 3.09 3.03 3.01 3.00 2.42 2.41 2.40 1.99 1.98 1.97 1.54 1.52 1.51 1.50 1.24 1.22 0.98 0.97 0.95 0.77 0.76 0.74
0.44 1.01 1.51 1.04 0.44 2.74 1.50 2.84 1.53 1.45 0.68 2.07 1.20 0.73 2.00 0.77 2.04 2.03 0.75 2.14 0.82 3.04 1.15
f1 (ppm)

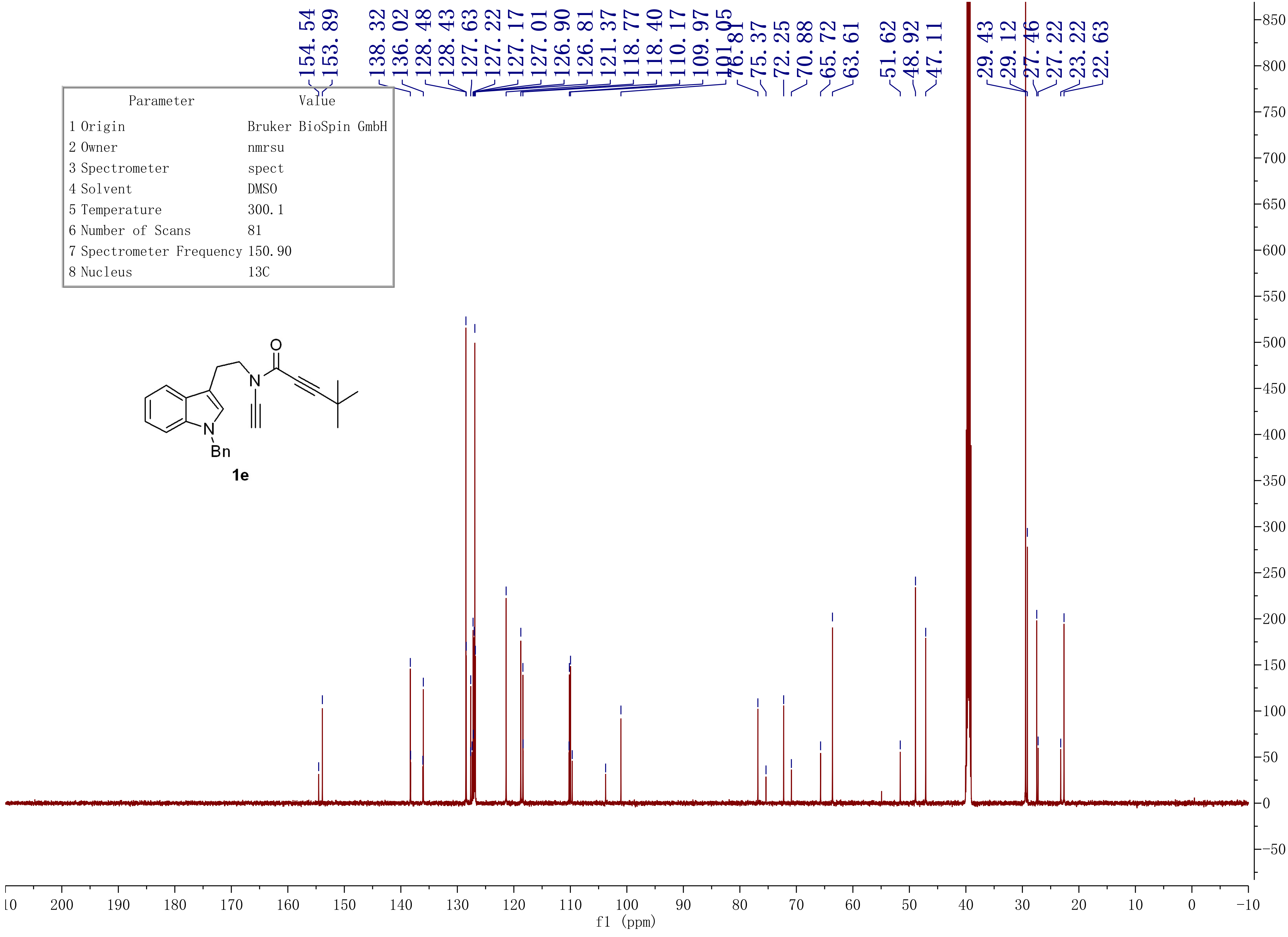


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	42
7 Spectrometer Frequency	150.90
8 Nucleus	13C

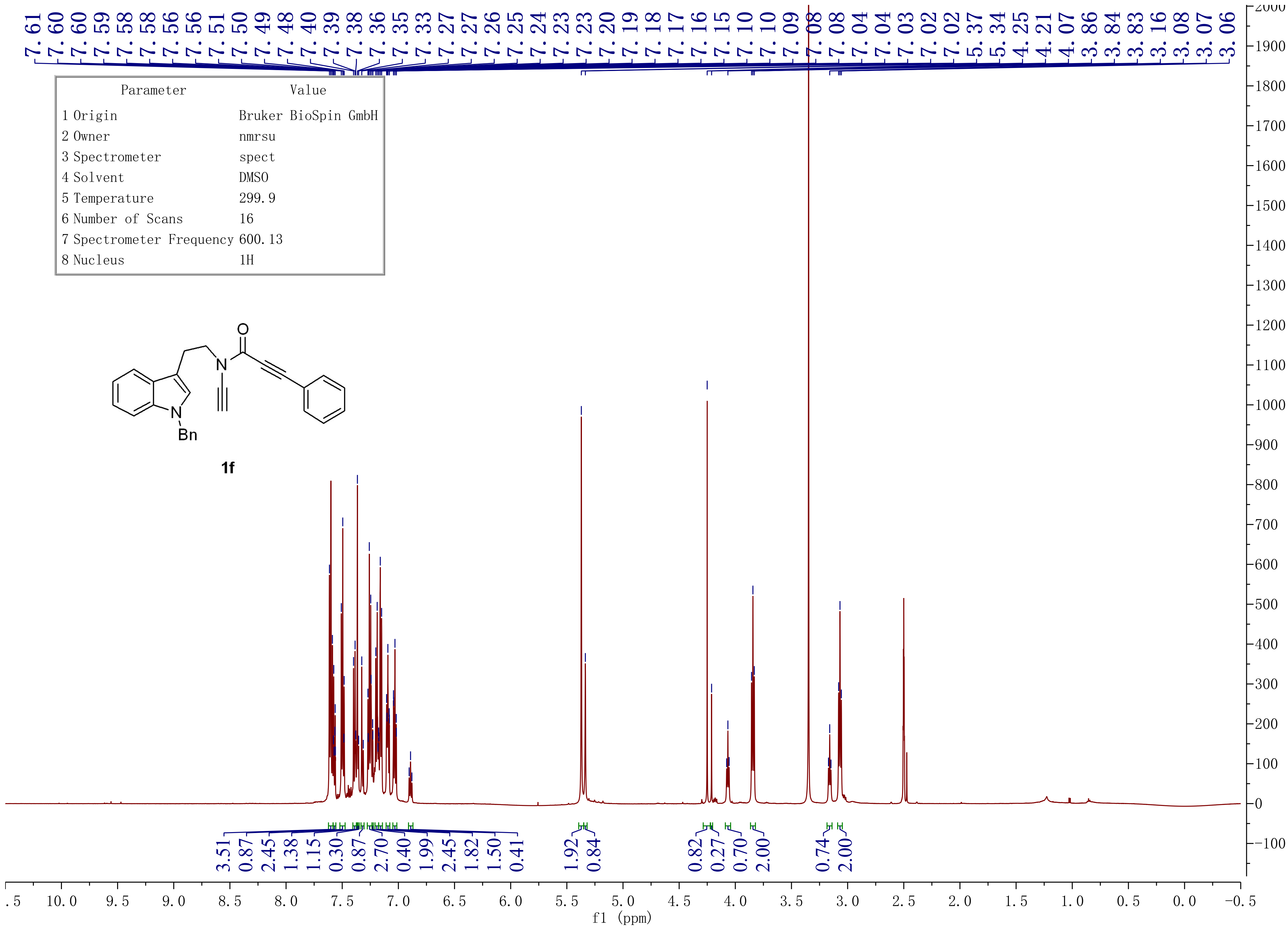


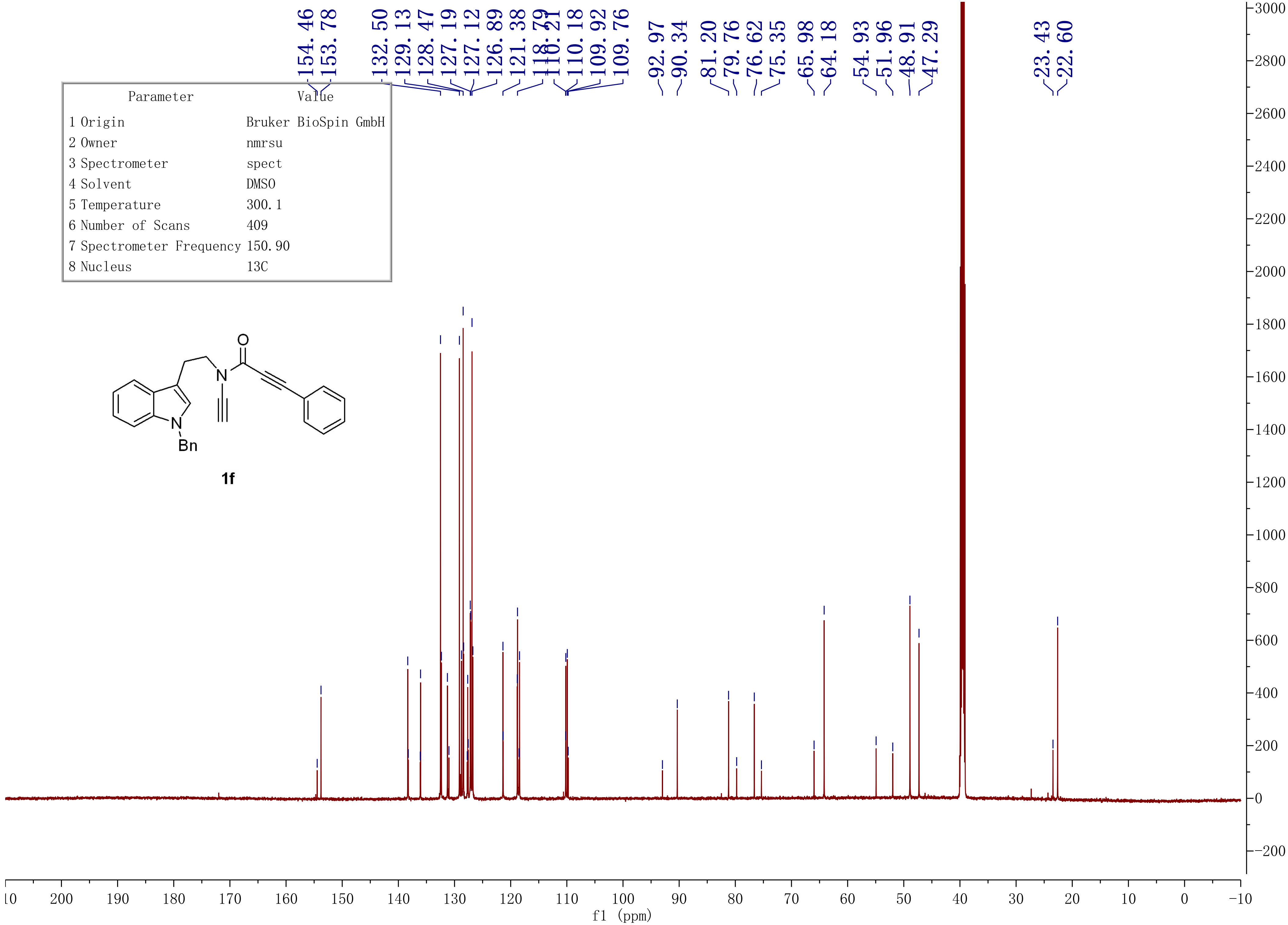
1e

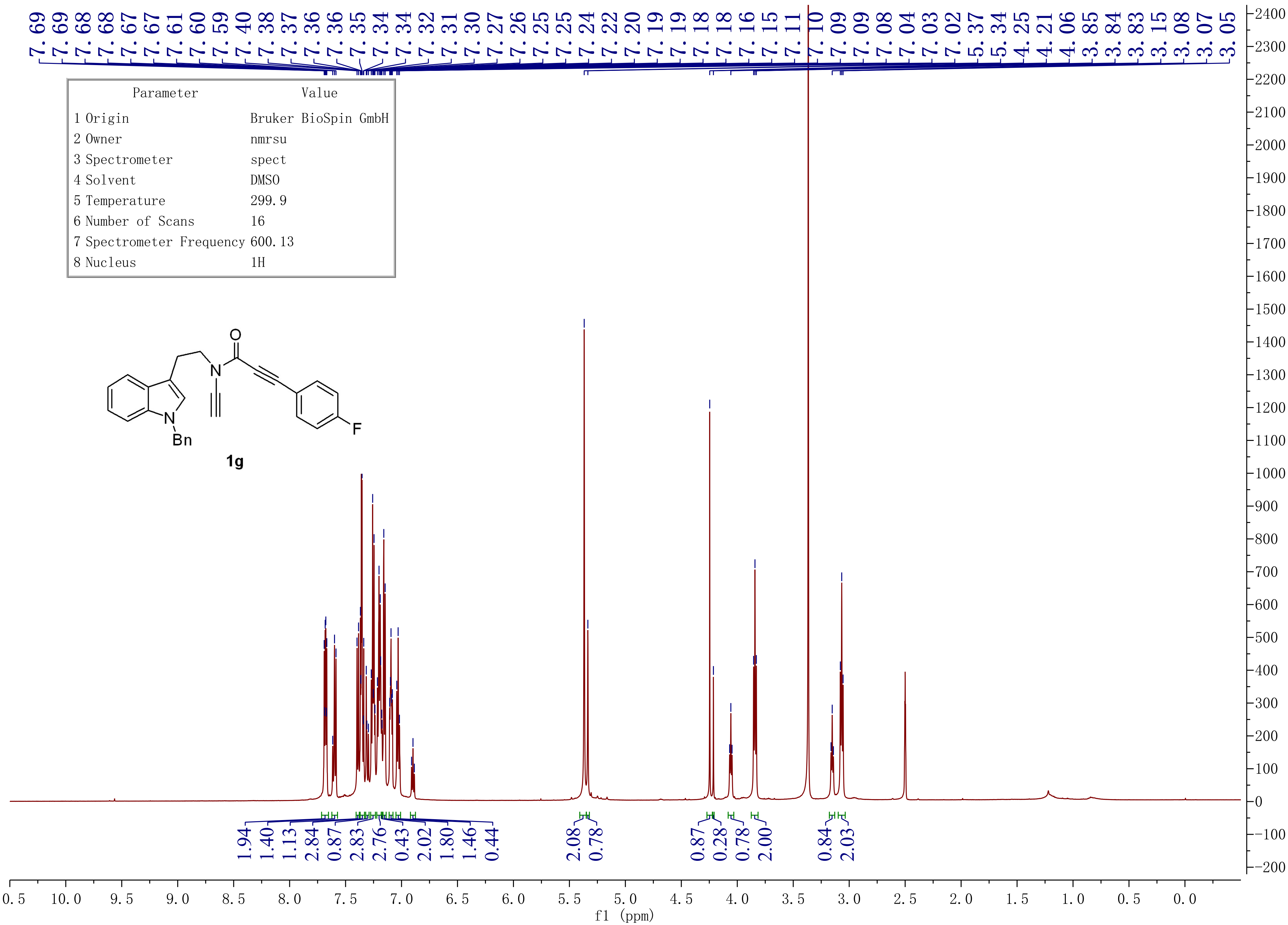
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	299.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H



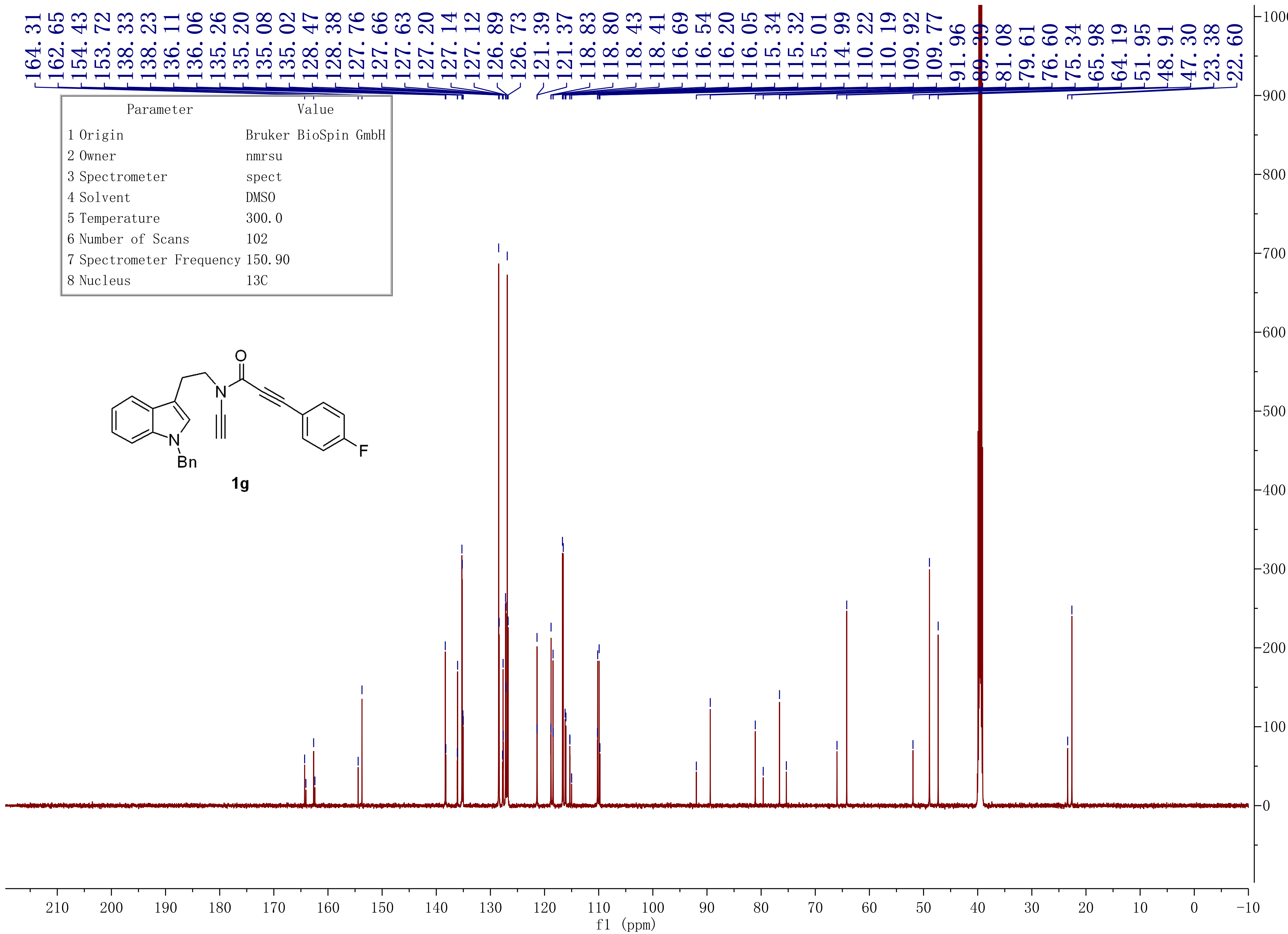
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 81
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
N
Bn
1e
154.54
153.89
138.32
136.02
128.48
128.43
127.63
127.22
127.17
127.01
126.90
126.81
121.37
118.77
118.40
110.17
109.97
101.05
76.81
75.37
72.25
70.88
65.72
63.61
51.62
48.92
47.11
29.43
29.12
27.46
27.22
23.22
22.63
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Bn
1f
7.61 7.60 7.60 7.59 7.58 7.58 7.56 7.56 7.51 7.50 7.49 7.48 7.40 7.39 7.38 7.36 7.35 7.33 7.27 7.27 7.26 7.25 7.24 7.23 7.23 7.20 7.19 7.18 7.17 7.16 7.15 7.10 7.10 7.09 7.08 7.08 7.04 7.04 7.03 7.02 7.02 5.37 5.34 4.25 4.21 4.07 3.86 3.84 3.83 3.16 3.08 3.07 3.06
3.51 0.87 2.45 1.38 1.15 0.30 0.87 2.70 0.40 1.99 2.45 1.82 1.50 0.41
1.92 0.84
0.82 0.27 0.70 2.00
0.74 2.00
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 409
7 Spectrometer Frequency 150.90
8 Nucleus 13C
1f
Bn
154.46
153.78
132.50
129.13
128.47
127.19
127.12
126.89
121.38
118.79
110.21
110.18
109.92
109.76
92.97
90.34
81.20
79.76
76.62
75.35
65.98
64.18
54.93
51.96
48.91
47.29
23.43
22.60
f1 (ppm)



7.69
7.69
7.68
7.68
7.67
7.67
7.61
7.60
7.59
7.40
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.32
7.31
7.30
7.27
7.26
7.25
7.25
7.24
7.22
7.20
7.19
7.19
7.18
7.18
7.16
7.15
7.11
7.10
7.09
7.09
7.08
7.04
7.03
7.02
5.37
5.34
4.25
4.21
4.06
3.85
3.84
3.83
3.15
3.08
3.07
3.05
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
N
Bn
F
1g
1.94
1.40
1.13
2.84
0.87
2.83
2.76
0.43
2.02
1.80
1.46
0.44
2.08
0.78
0.87
0.28
0.78
2.00
0.84
2.03
f1 (ppm)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162.65
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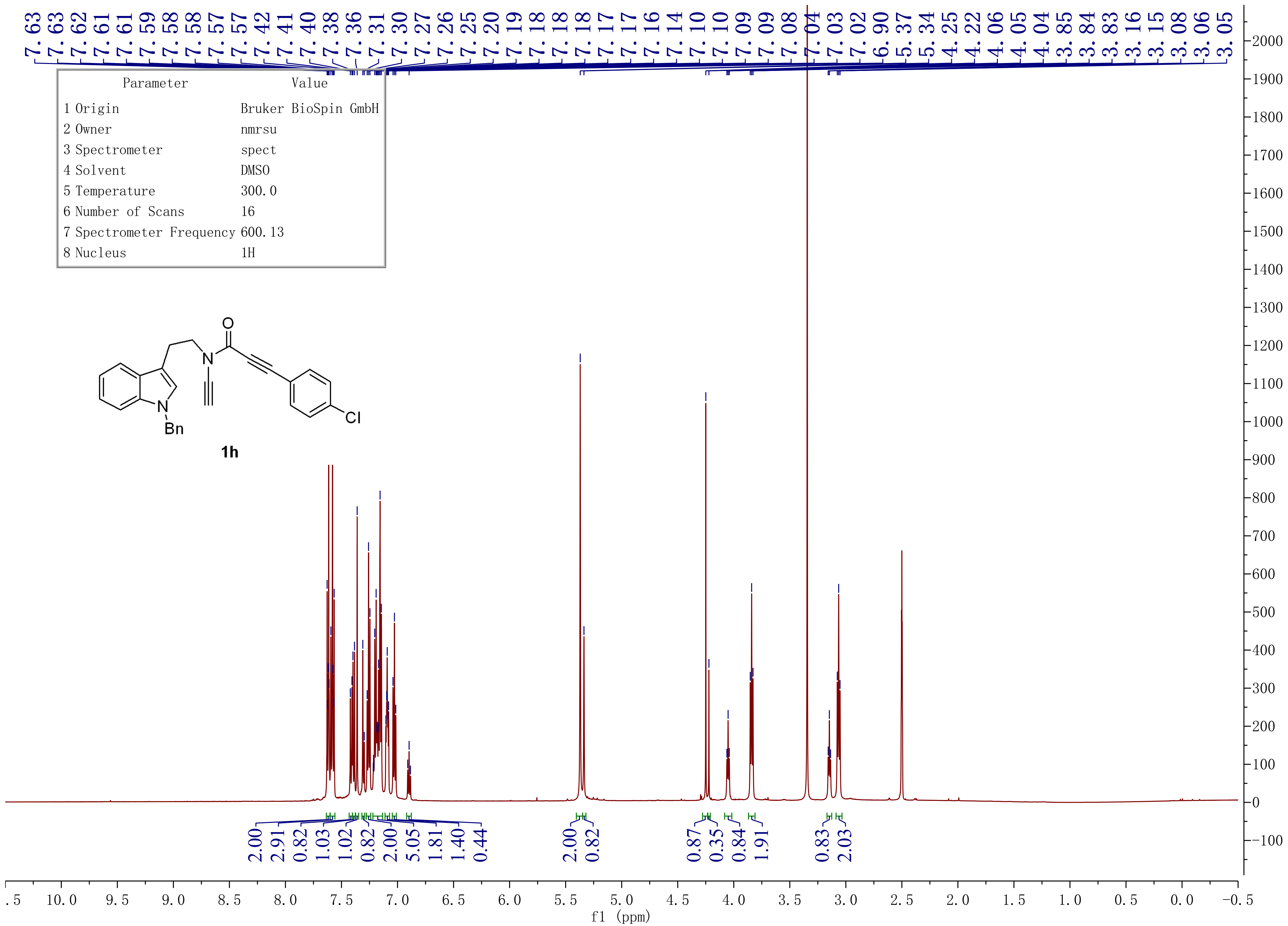
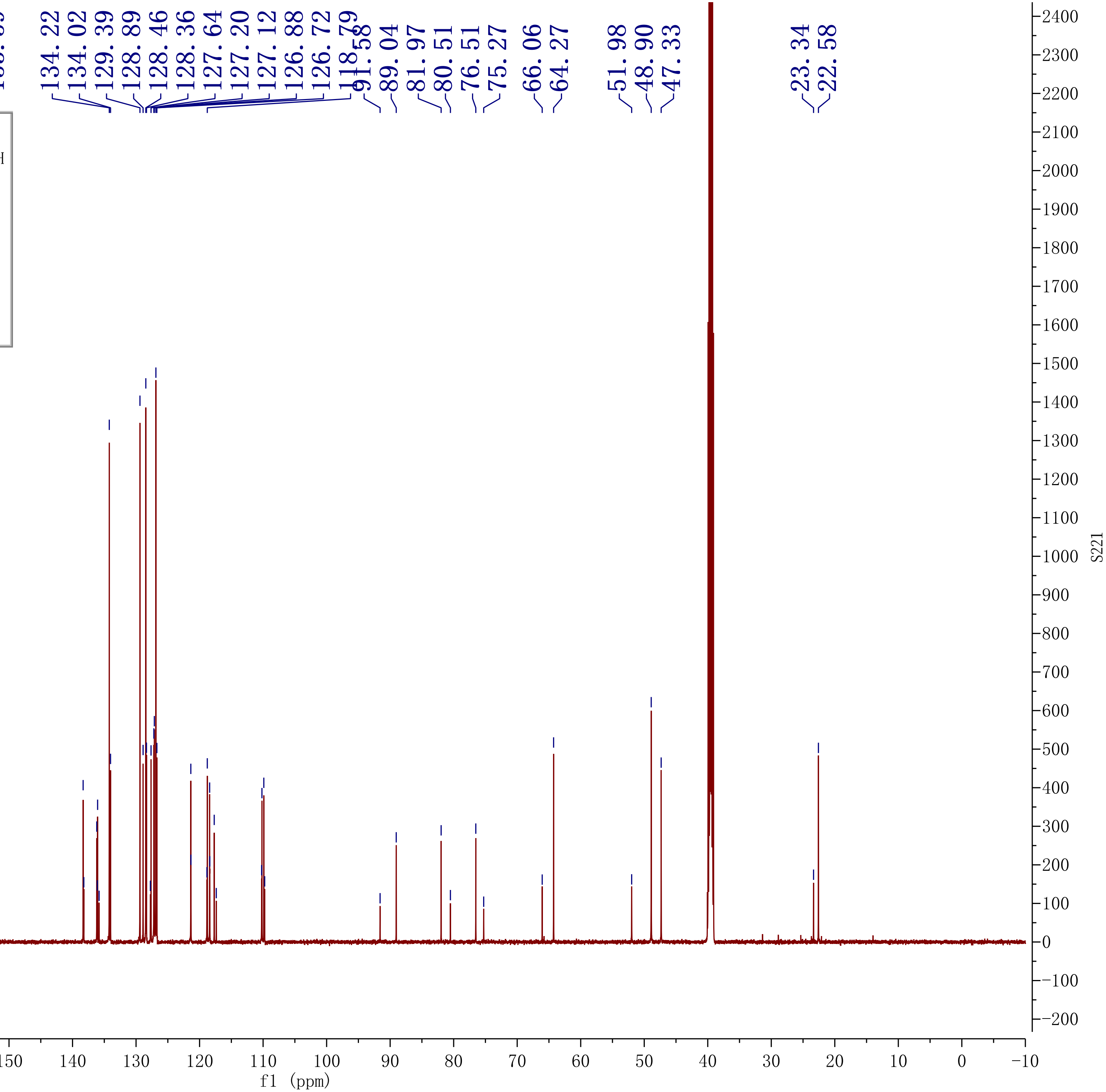
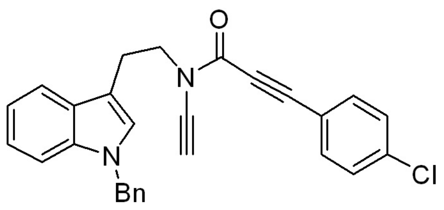
153.72
138.33
138.23
136.11
136.06
135.26
135.20
135.08
135.02
128.47
128.38
127.76
127.66
127.63
127.20
127.14
127.12
126.89
126.73
121.39
121.37
118.83
118.80
118.43
118.41
116.69
116.54
116.20
116.05
115.34
115.32
115.01
114.99
110.22
110.19
109.92
109.77
91.96
89.39
81.08
79.61
76.60
75.34
65.98
64.19
51.95
48.91
47.30
23.38
22.60
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 102
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
N
Bn
F
1g
f1 (ppm)



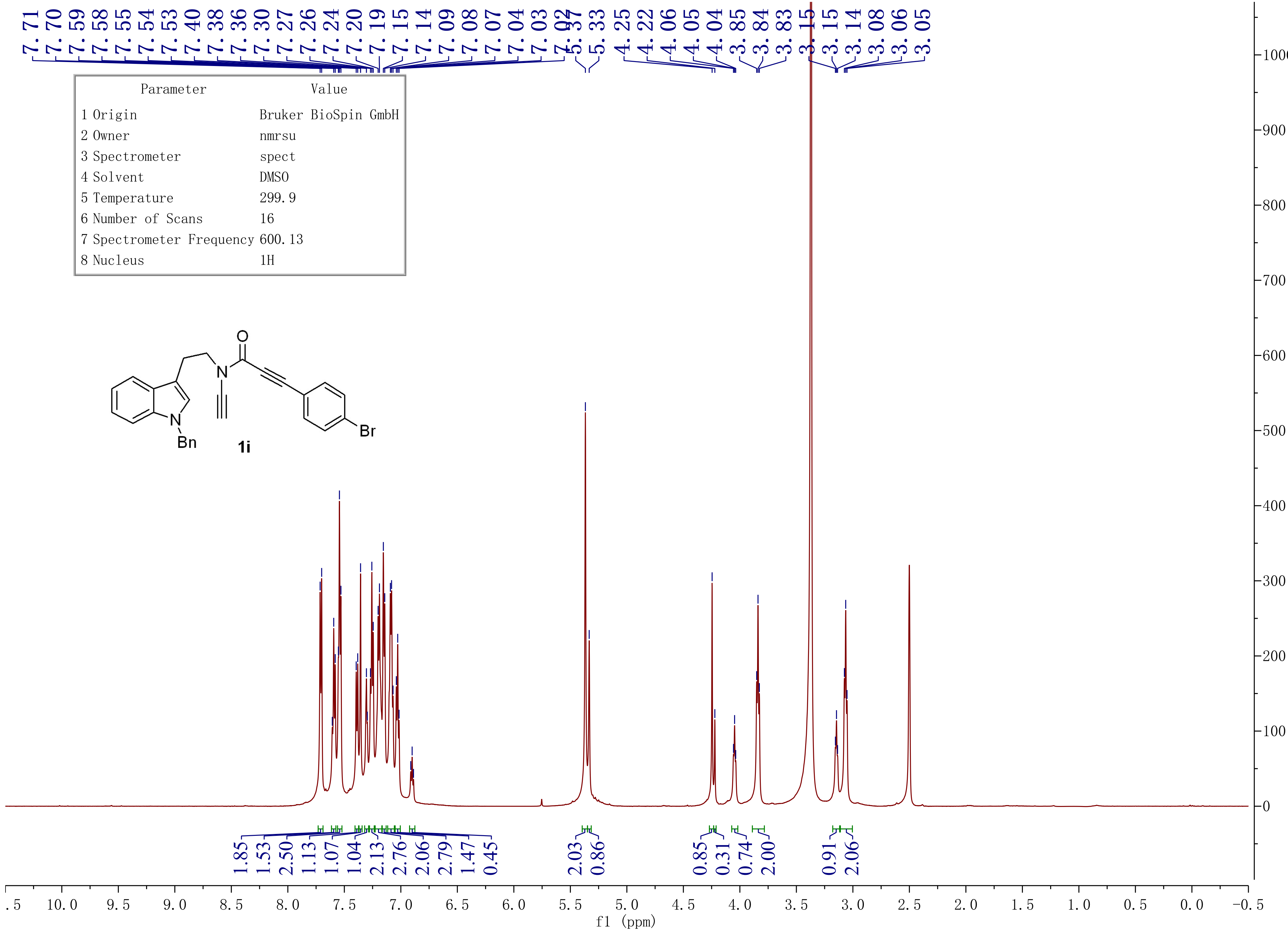
7.63
7.63
7.62
7.61
7.61
7.59
7.58
7.58
7.57
7.57
7.42
7.41
7.40
7.38
7.36
7.31
7.30
7.27
7.26
7.25
7.20
7.19
7.18
7.18
7.18
7.17
7.17
7.16
7.14
7.10
7.10
7.09
7.09
7.08
7.04
7.03
7.02
6.90
5.37
5.34
4.25
4.22
4.06
4.05
4.04
3.85
3.84
3.83
3.16
3.15
3.08
3.06
3.05
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
DMSO
5 Temperature
300.0
6 Number of Scans
16
7 Spectrometer Frequency
600.13
8 Nucleus
1H
O
N
N
Bn
Cl
1h
2.00
2.91
0.82
1.03
1.02
0.82
2.00
5.05
1.81
1.40
0.44
2.00
0.82
0.87
0.35
0.84
1.91
0.83
2.03
f1 (ppm)

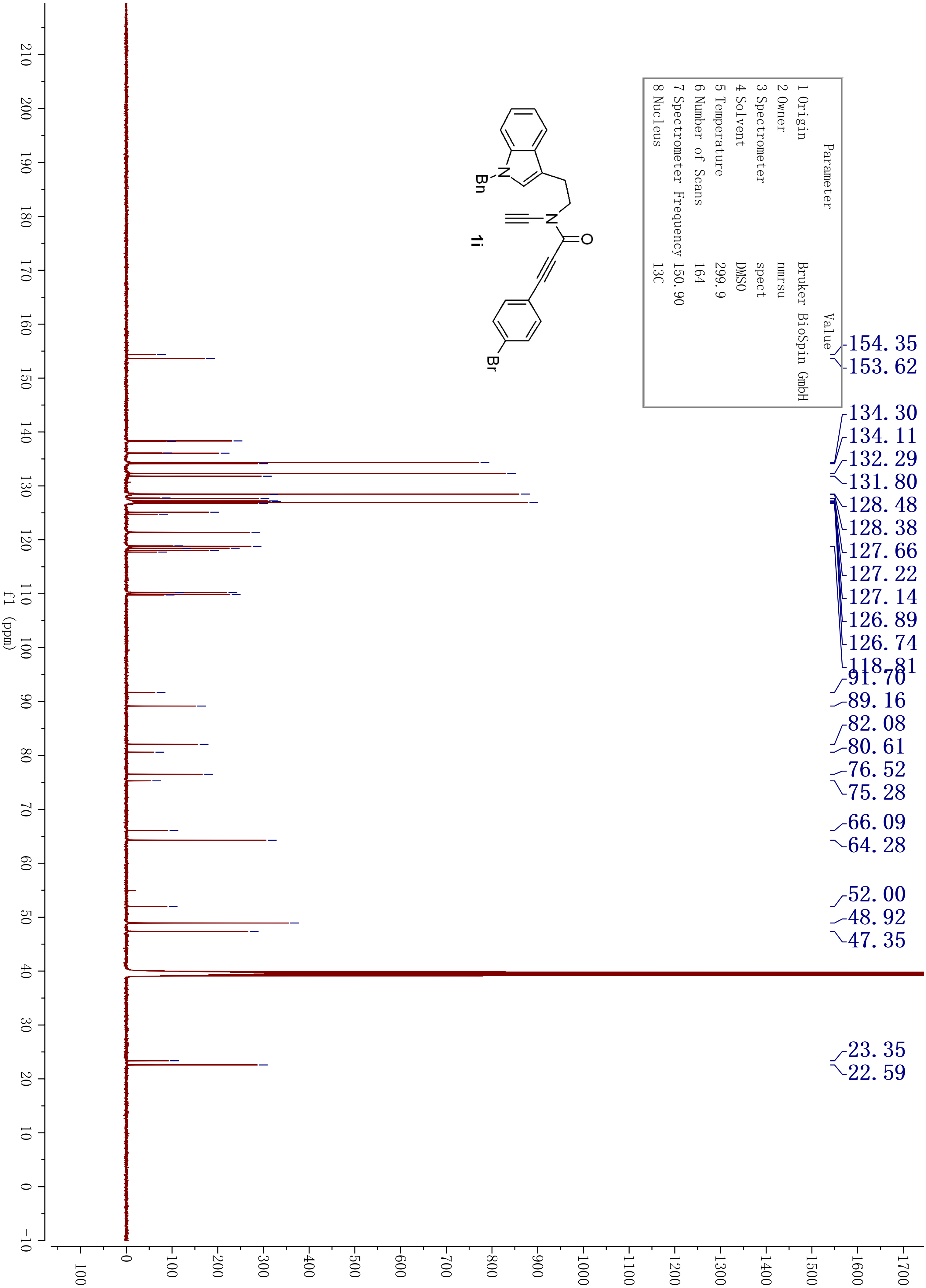


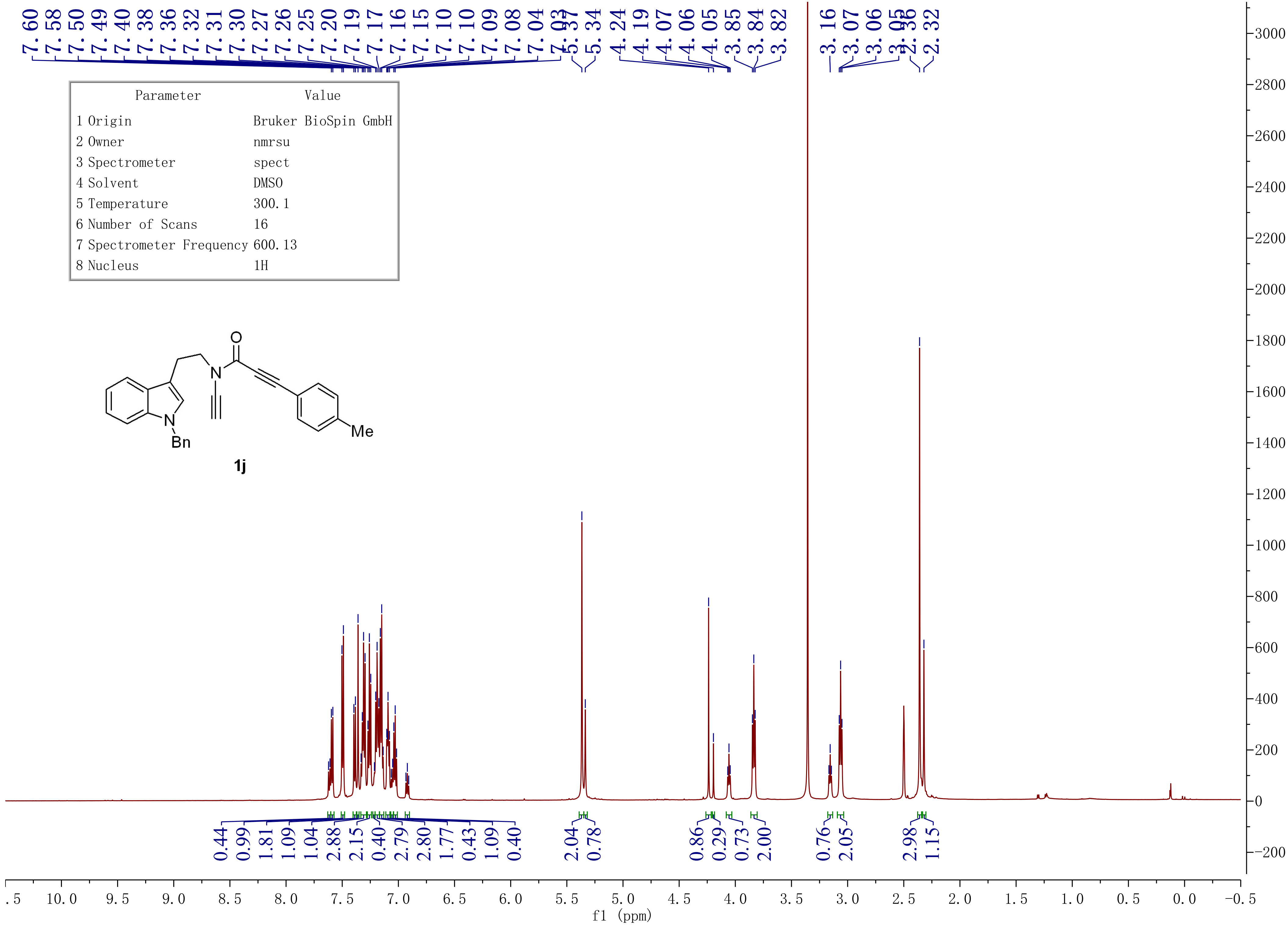
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.1
6 Number of Scans	325
7 Spectrometer Frequency	150.90
8 Nucleus	13C



1h


7.71 7.70 7.59 7.58 7.55 7.54 7.53 7.40 7.38 7.36 7.30 7.27 7.26 7.24 7.20 7.19 7.15 7.14 7.09 7.08 7.07 7.04 7.03 7.02
5.37 5.33
4.25 4.22 4.06 4.05 4.04 3.85 3.84 3.83 3.15 3.15 3.14 3.08 3.06 3.05
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Bn
O
N
Br
1i
1.85 1.53 2.50 1.13 1.07 1.04 2.13 2.76 2.06 2.79 1.47 0.45
2.03 0.86
0.85 0.31 0.74 2.00
0.91 2.06
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 164
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Bn
N
O
Br
1i
154.35
153.62
134.30
134.11
132.29
131.80
128.48
128.38
127.66
127.22
127.14
126.89
126.74
118.81
91.70
89.16
82.08
80.61
76.52
75.28
66.09
64.28
52.00
48.92
47.35
23.35
22.59
f1 (ppm)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7.58
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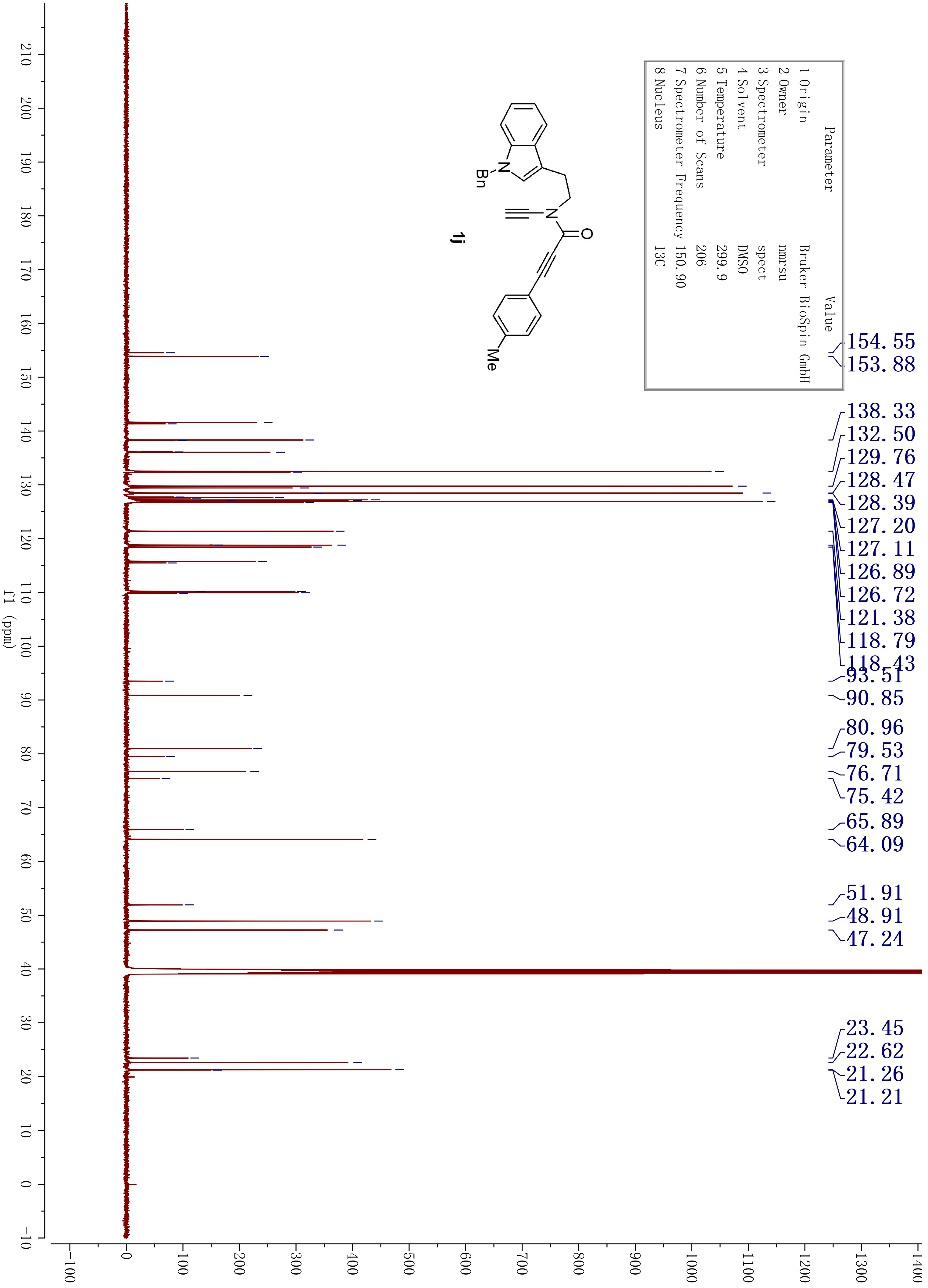
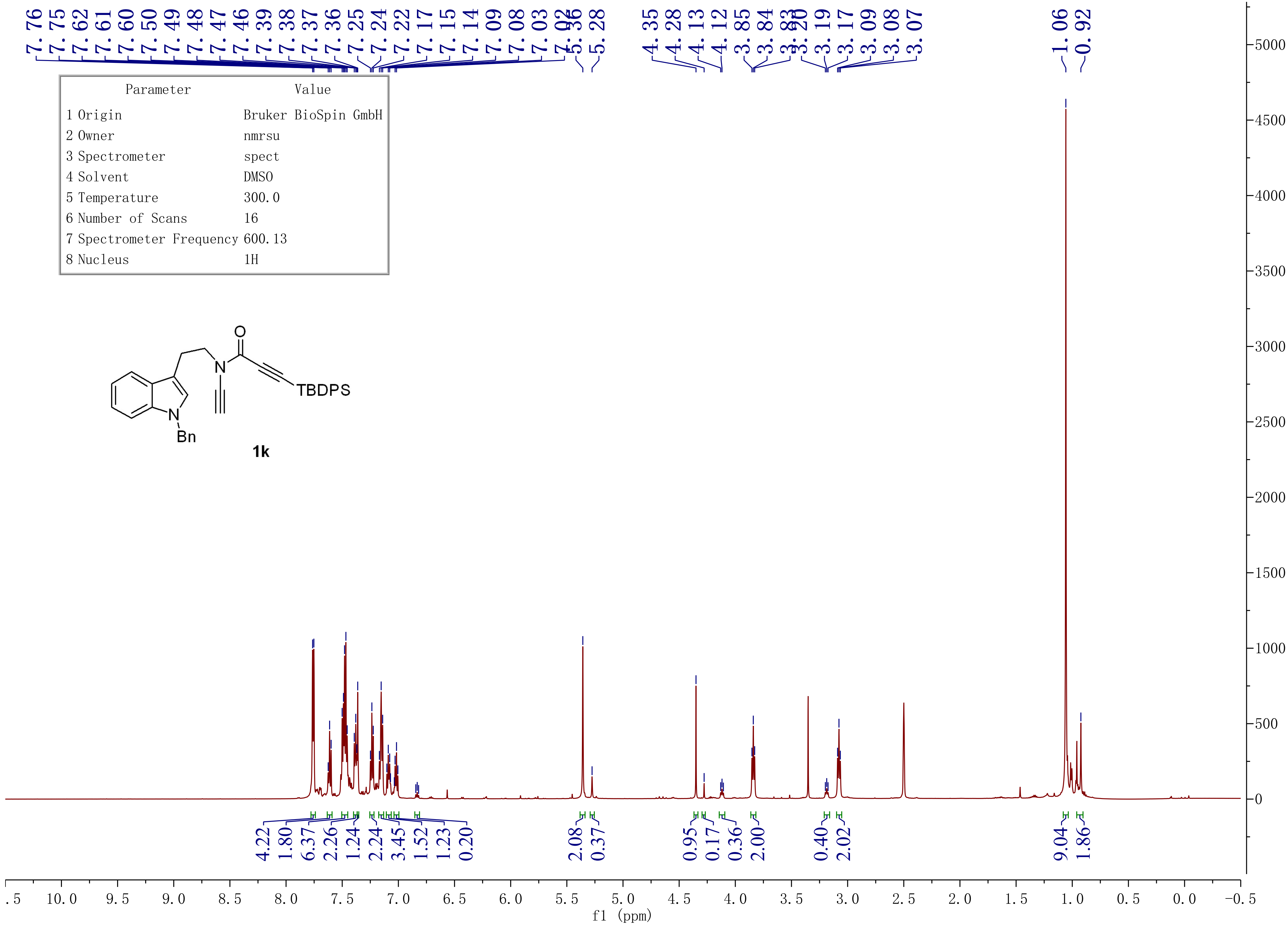
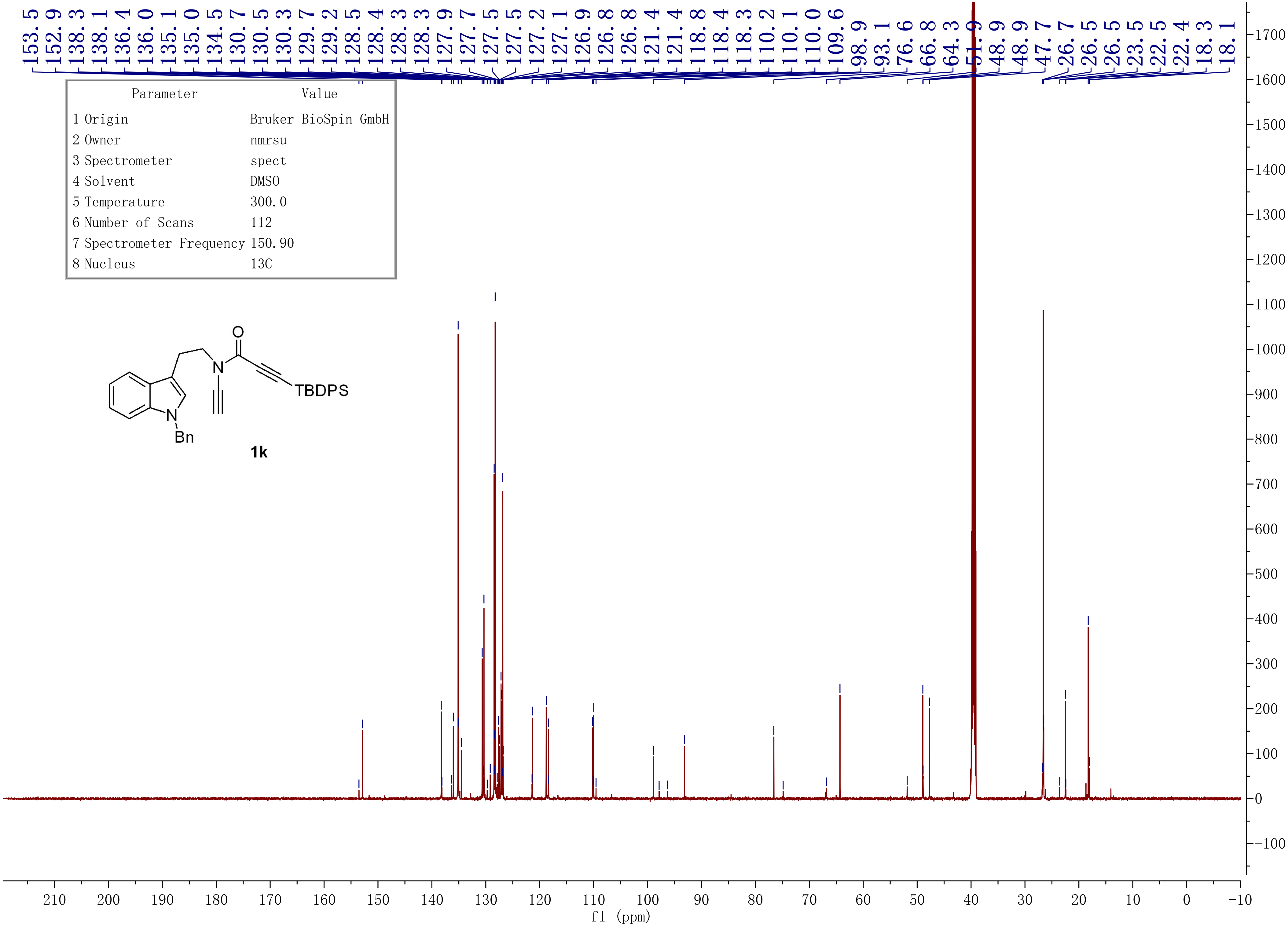
7.49
7.40
7.38
7.36
7.32
7.31
7.30
7.27
7.26
7.25
7.20
7.19
7.17
7.16
7.15
7.10
7.10
7.09
7.08
7.04
7.03
5.37
5.34
4.24
4.19
4.07
4.06
4.05
3.85
3.84
3.82
3.16
3.07
3.06
3.05
2.36
2.32
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
N
Bn
Me
1j
0.44
0.99
1.81
1.09
1.04
2.88
2.15
0.40
2.79
2.80
1.77
0.43
1.09
0.40
2.04
0.78
0.86
0.29
0.73
2.00
0.76
2.05
2.98
1.15
f1 (ppm)



Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 206
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Bn
N
N
O
Me
1j
154.55
153.88
138.33
132.50
129.76
128.47
128.39
127.20
127.11
126.89
126.72
121.38
118.79
118.43
93.51
90.85
80.96
79.53
76.71
75.42
65.89
64.09
51.91
48.91
47.24
23.45
22.62
21.26
21.21
f1 (ppm)



Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
TBDPS
Bn
1k
7.76 7.75 7.62 7.61 7.60 7.50 7.49 7.48 7.47 7.46 7.39 7.38 7.37 7.36 7.25 7.24 7.22 7.17 7.15 7.14 7.09 7.08 7.03 7.02
5.36 5.28
4.35 4.28 4.13 4.12 3.85 3.84 3.83 3.20 3.19 3.17 3.09 3.08 3.07
1.06 0.92
4.22 1.80 6.37 2.26 1.24 2.24 3.45 1.52 1.23 0.20
2.08 0.37
0.95 0.17 0.36 2.00
0.40 2.02
9.04 1.86
f1 (ppm)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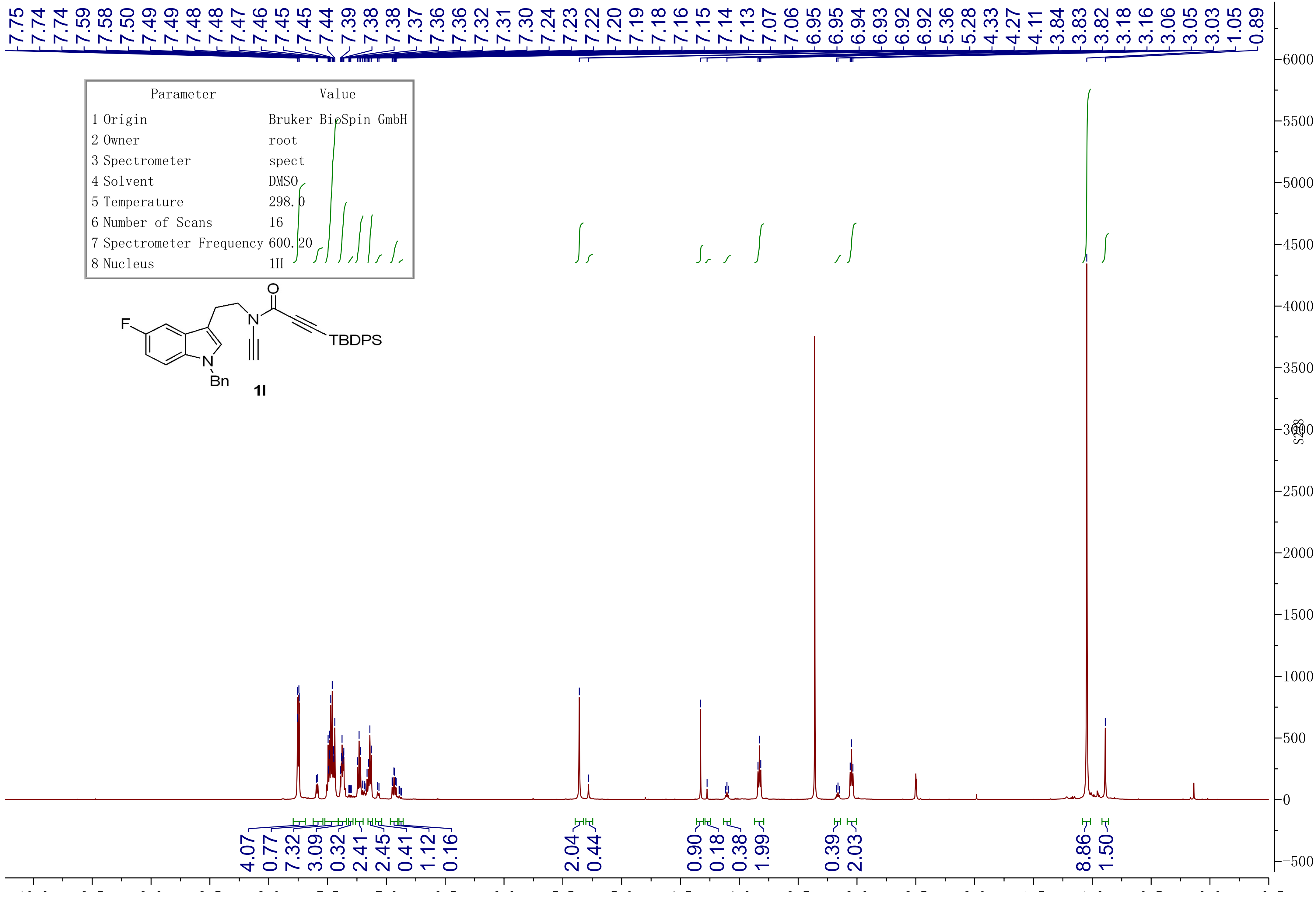
138.1
136.4
136.0
135.1
135.0
134.5
130.7
130.5
130.3
129.7
129.2
128.5
128.4
128.3
128.3
127.9
127.7
127.5
127.5
127.2
127.1
126.9
126.8
126.8
121.4
121.4
118.8
118.4
118.3
110.2
110.1
110.0
109.6
98.9
93.1
76.6
66.8
64.3
51.9
48.9
48.9
47.7
26.7
26.5
26.5
23.5
22.5
22.4
18.3
18.1
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 112
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
TBDPS
N
Bn
1k
f1 (ppm)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7.74
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7.58
7.50
7.49
7.49
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7.48
7.47
7.46
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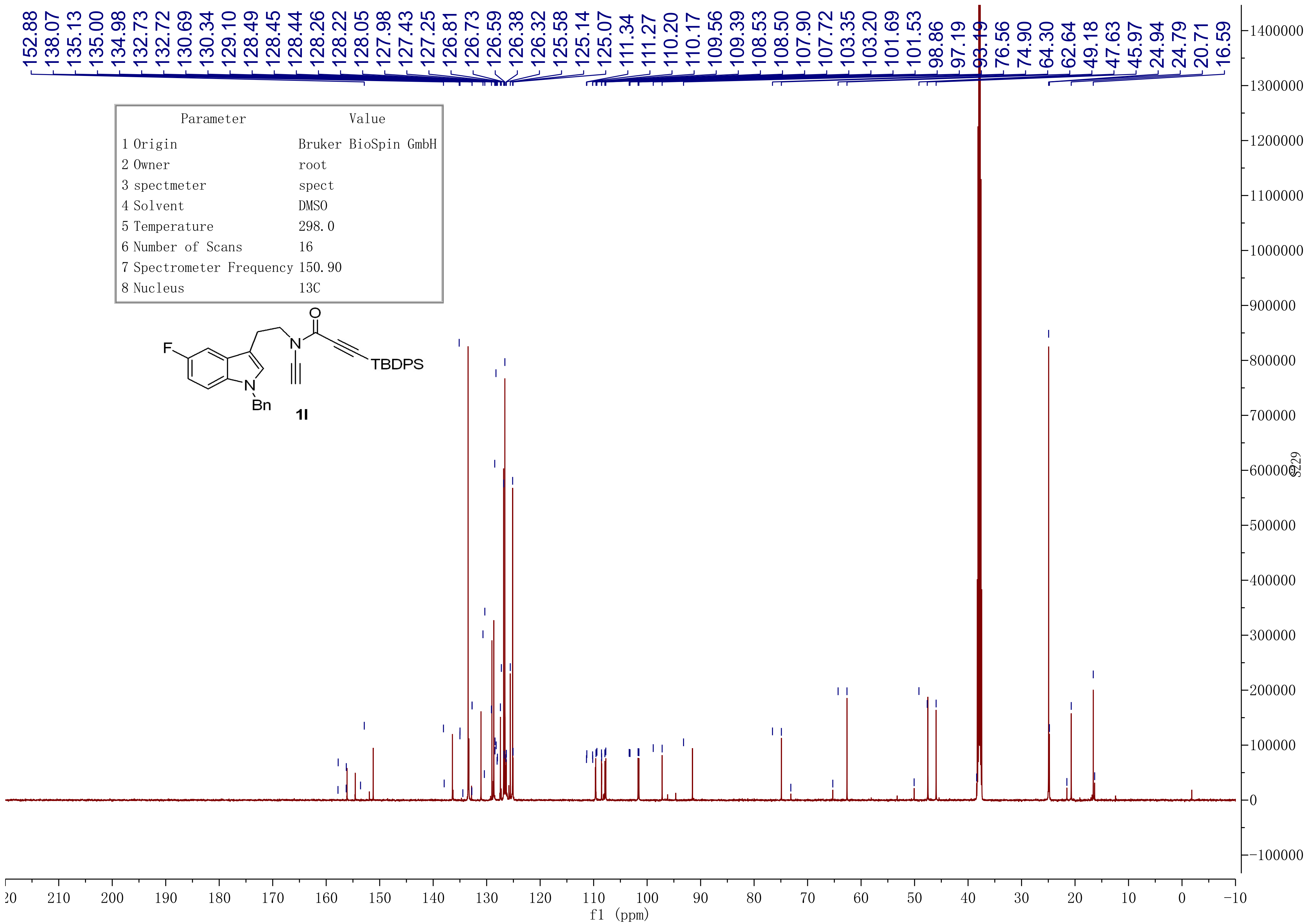
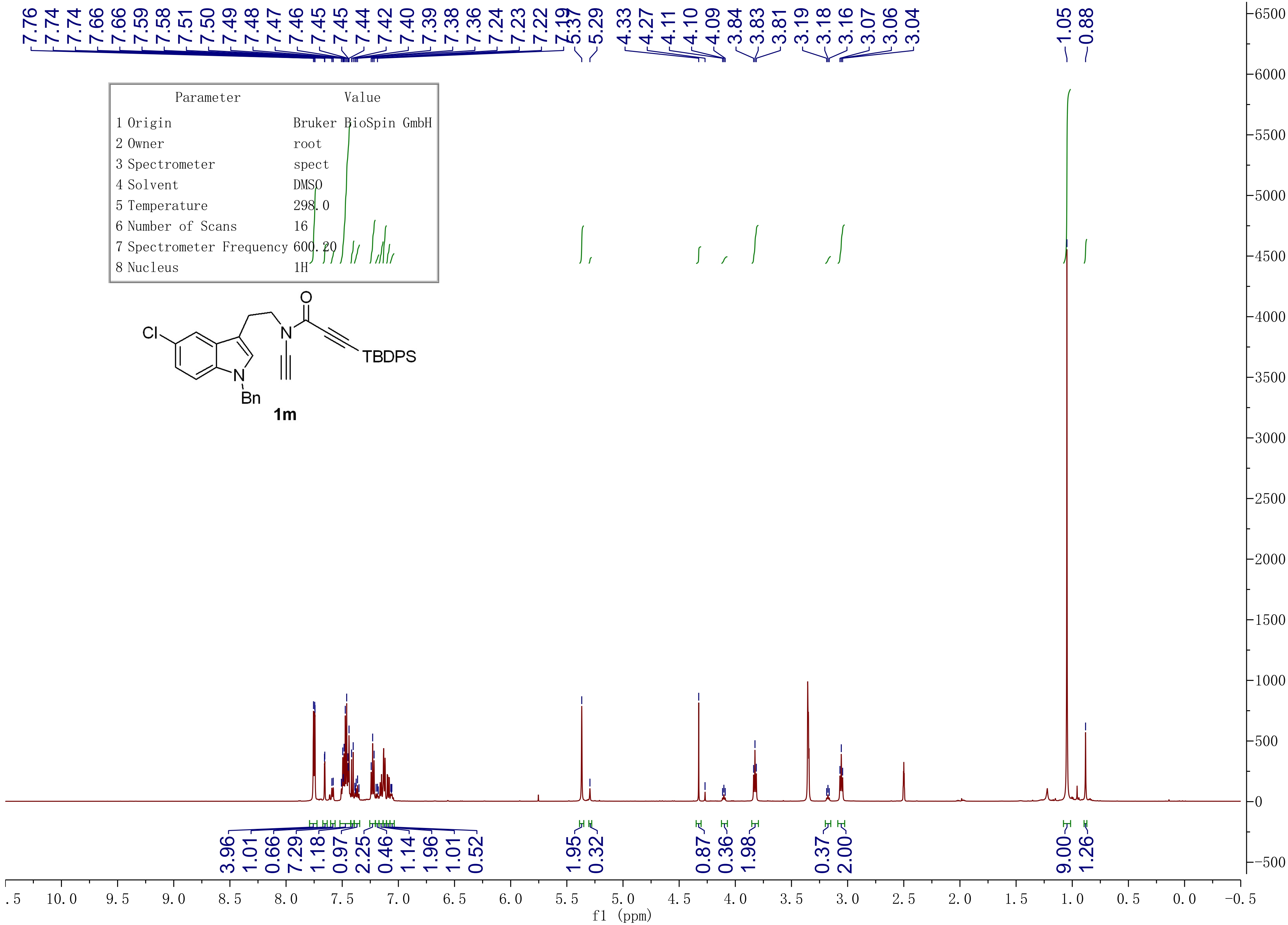
7.45
7.44
7.39
7.38
7.38
7.37
7.36
7.36
7.32
7.31
7.30
7.24
7.23
7.22
7.20
7.19
7.18
7.16
7.15
7.14
7.13
7.07
7.06
6.95
6.95
6.94
6.93
6.92
6.92
5.36
5.28
4.33
4.27
4.11
3.84
3.83
3.82
3.18
3.16
3.06
3.05
3.03
1.05
0.89
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
F
N
Bn
O
N
TBDPS
1l
4.07
0.77
7.32
3.09
0.32
2.41
2.45
0.41
1.12
0.16
2.04
0.44
0.90
0.18
0.38
1.99
0.39
2.03
8.86
1.50
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500

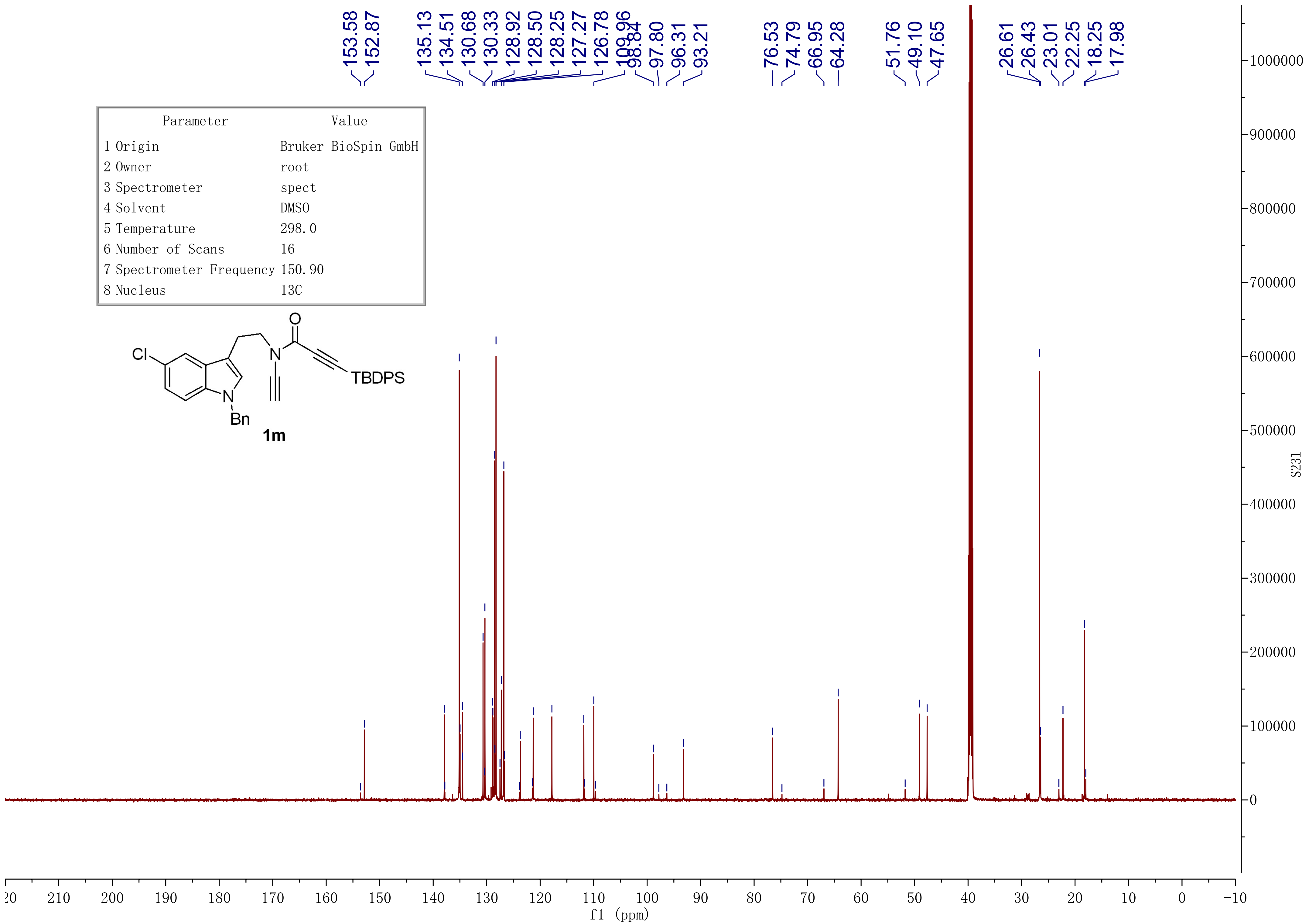


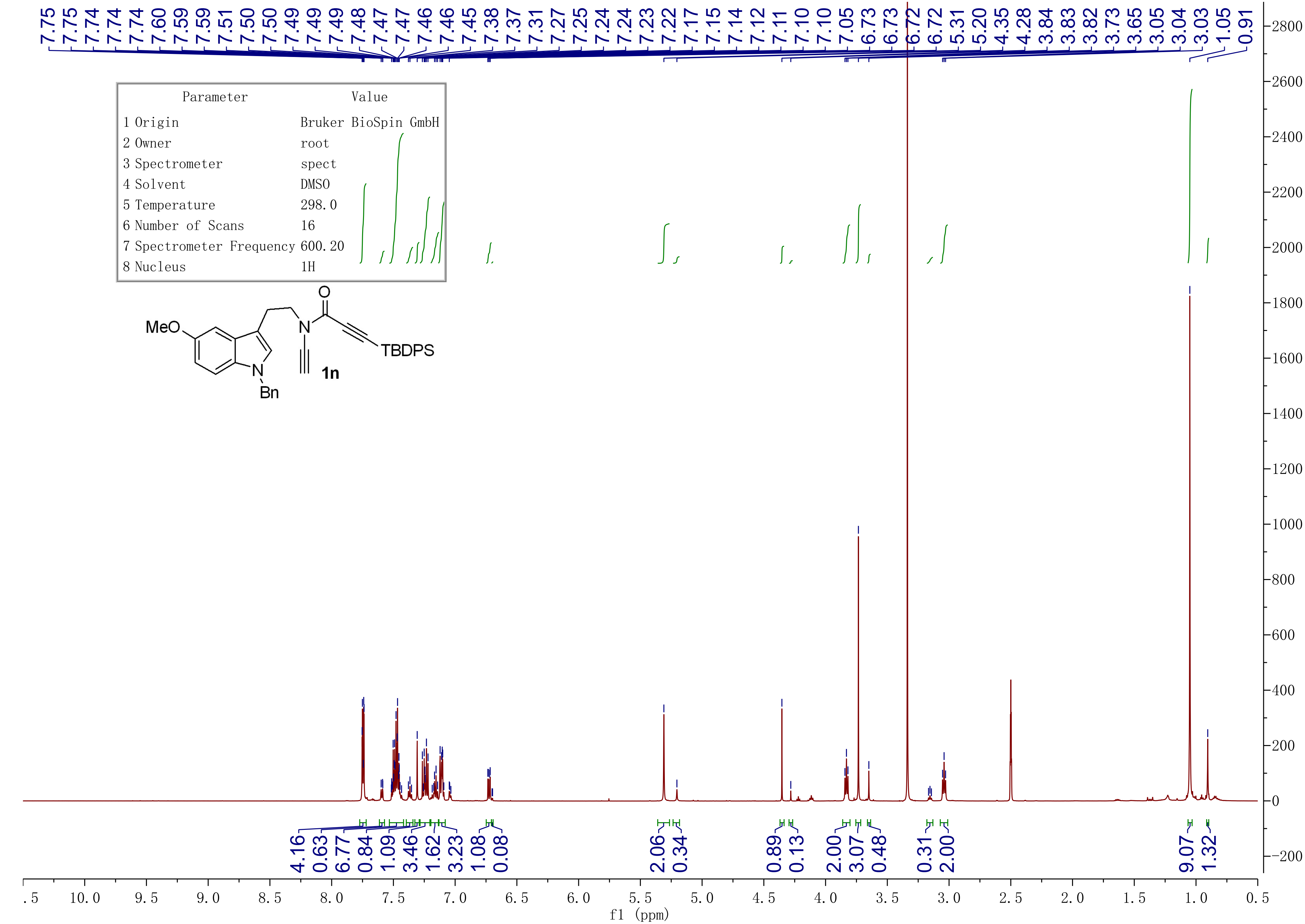
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 spectmeter	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C

1l

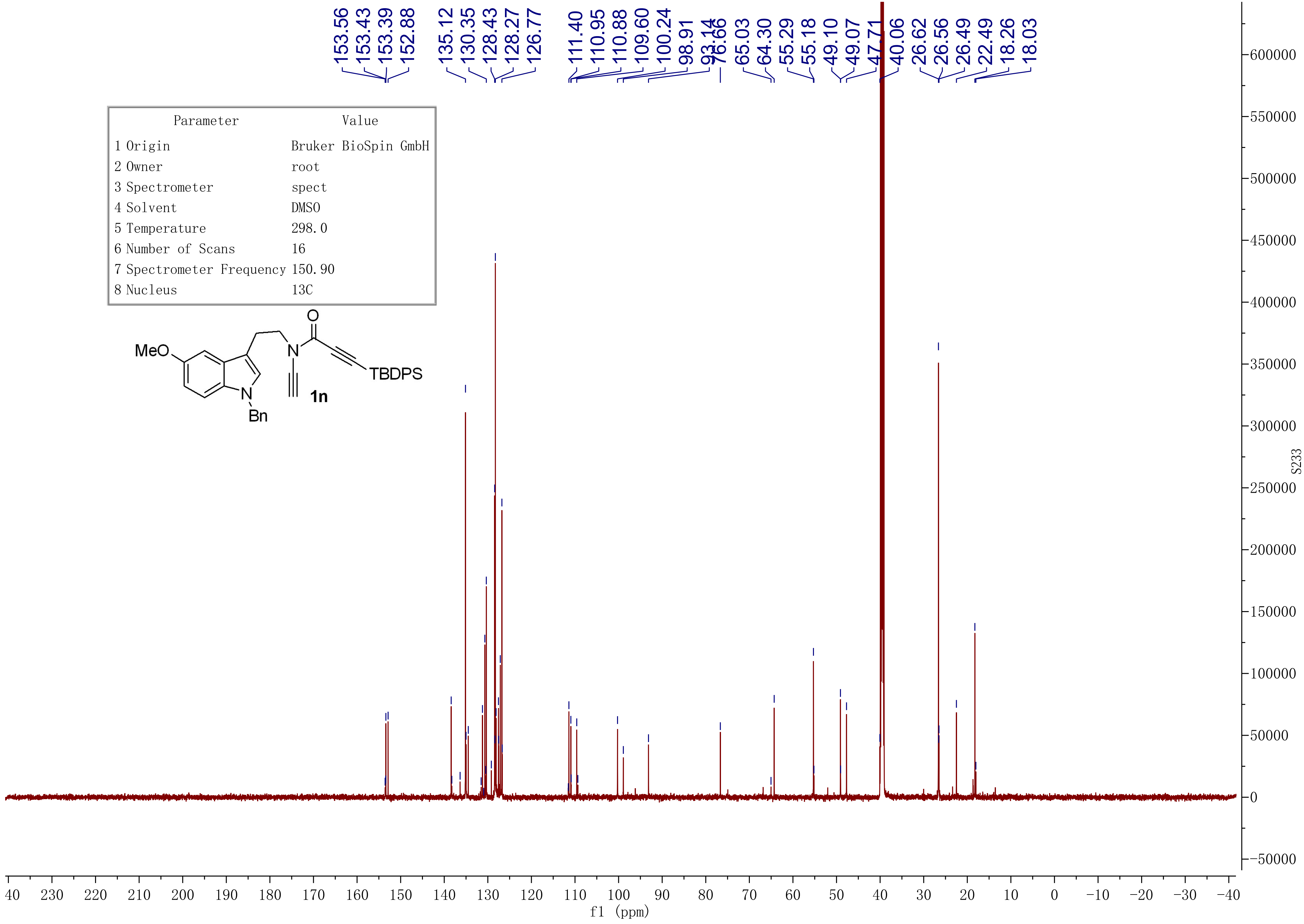

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
Cl
N
Bn
N
O
TBDPS
1m
7.76 7.74 7.74 7.66 7.66 7.59 7.58 7.51 7.50 7.49 7.48 7.47 7.46 7.45 7.45 7.44 7.42 7.40 7.39 7.38 7.36 7.24 7.23 7.22 7.19 5.37 5.29 4.33 4.27 4.11 4.10 4.09 3.84 3.83 3.81 3.19 3.18 3.16 3.07 3.06 3.04 1.05 0.88
3.96 1.01 0.66 7.29 1.18 0.97 2.25 0.46 1.14 1.96 1.01 0.52 1.95 0.32 0.87 0.36 1.98 0.37 2.00 9.00 1.26
f1 (ppm)

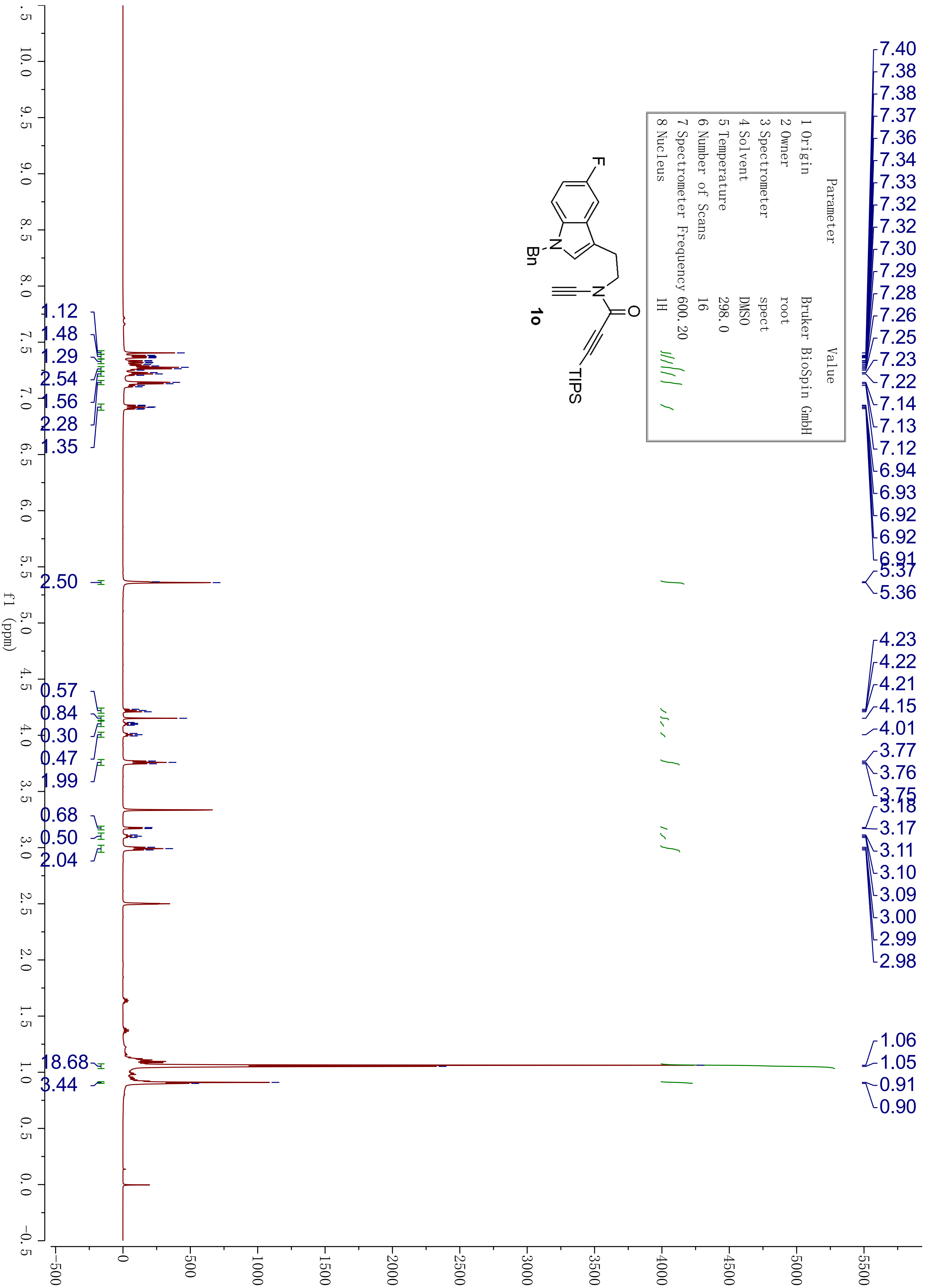
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C



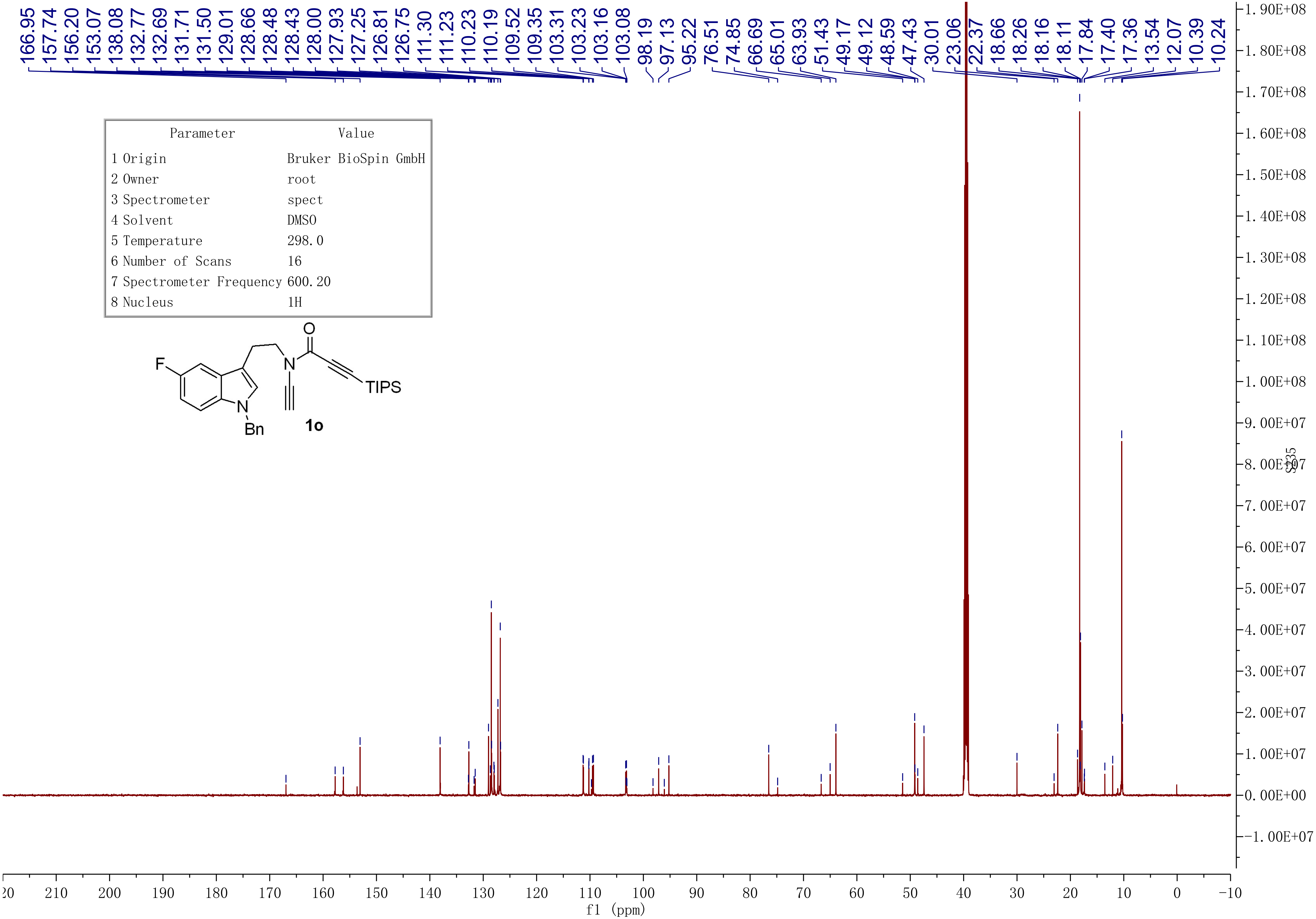


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	600.20
8 Nucleus	1H

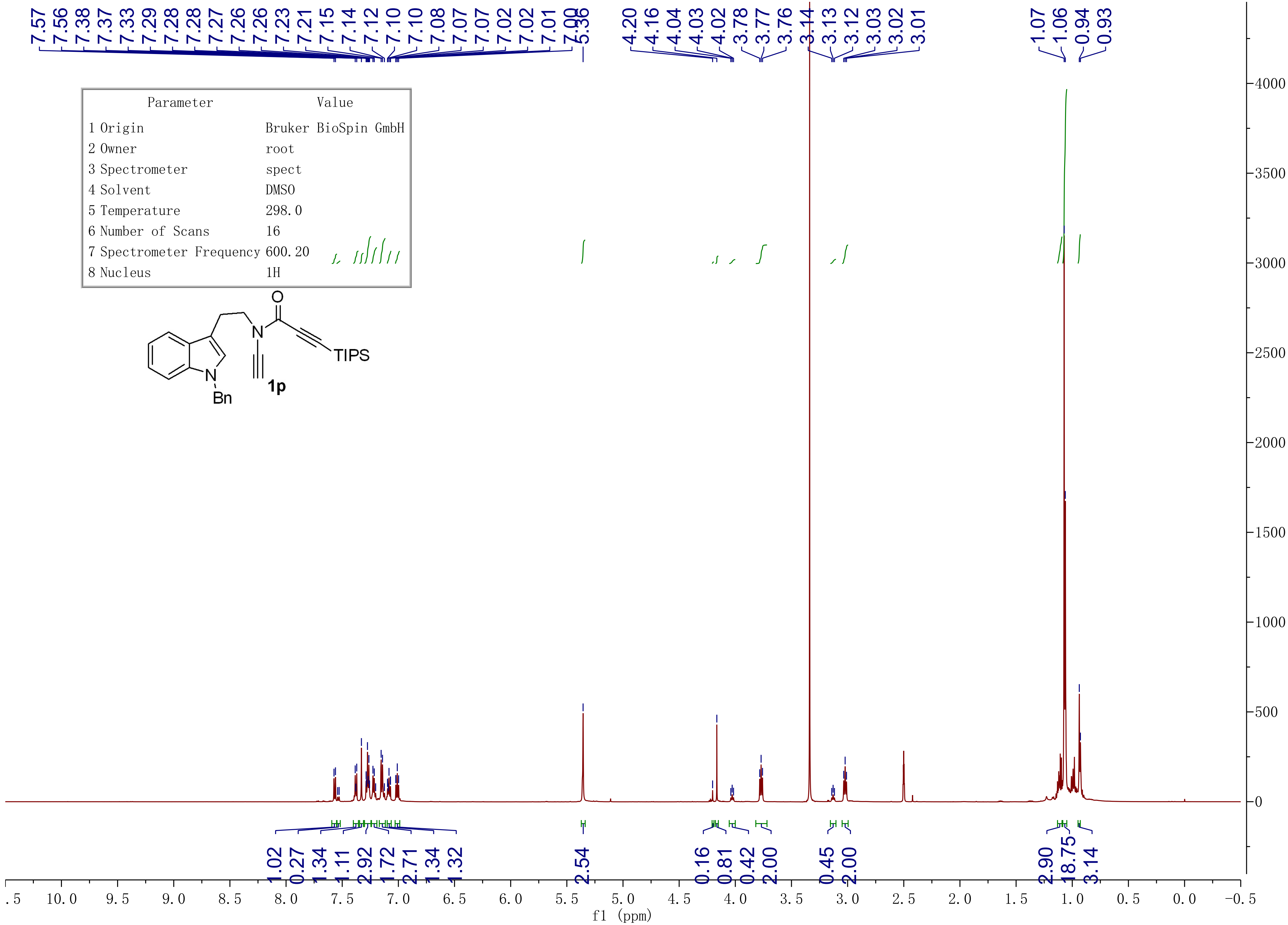

153.56
153.43
153.39
152.88
135.12
130.35
128.43
128.27
126.77
111.40
110.95
110.88
109.60
100.24
98.91
93.14
76.66
65.03
64.30
55.29
55.18
49.10
49.07
47.71
40.06
26.62
26.56
26.49
22.49
18.26
18.03
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 150.90
8 Nucleus 13C
MeO
N
Bn
N
O
TBDPS
1n
f1 (ppm)



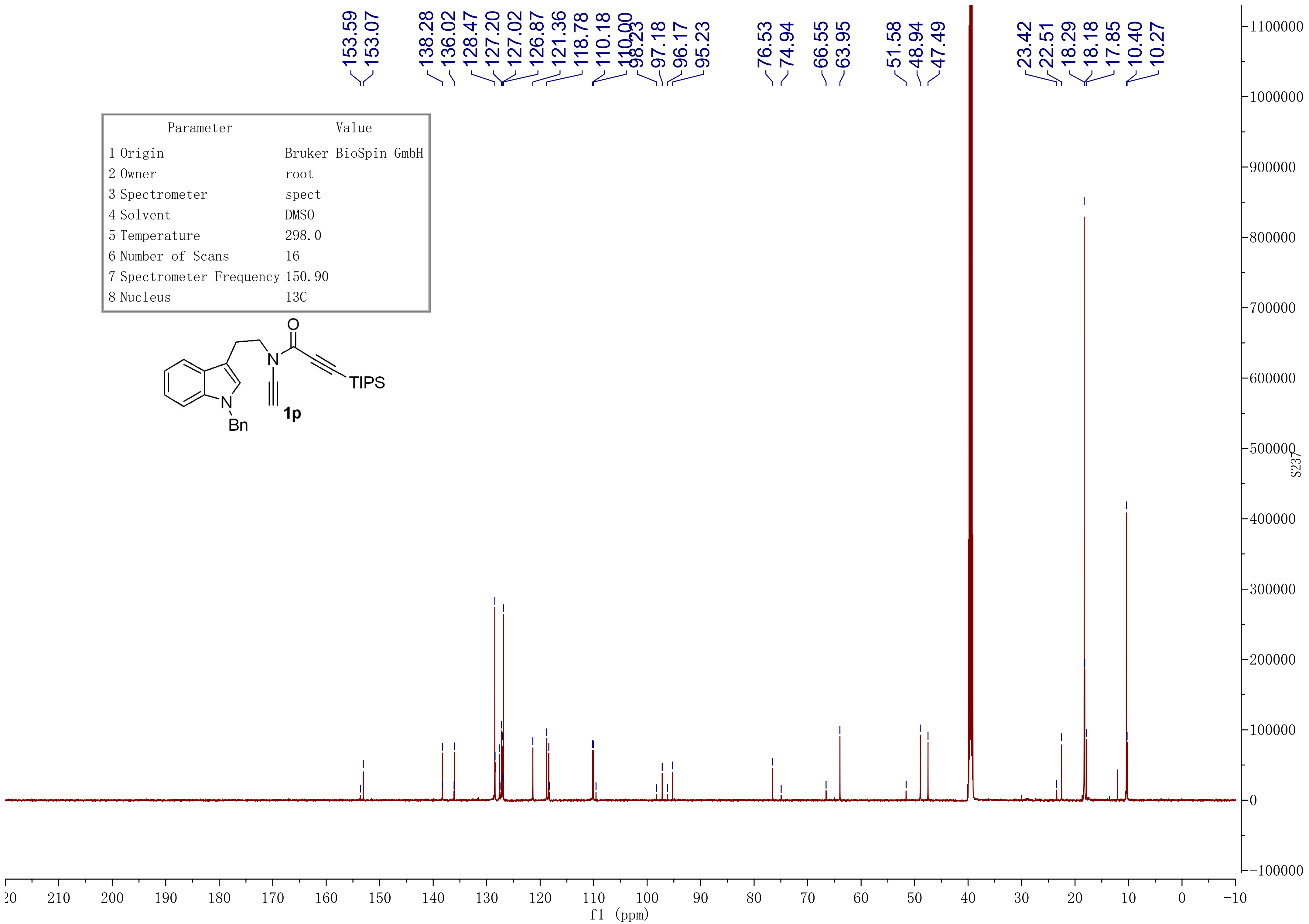
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
F
N
Bn
O
TIPS
1o
f1 (ppm)

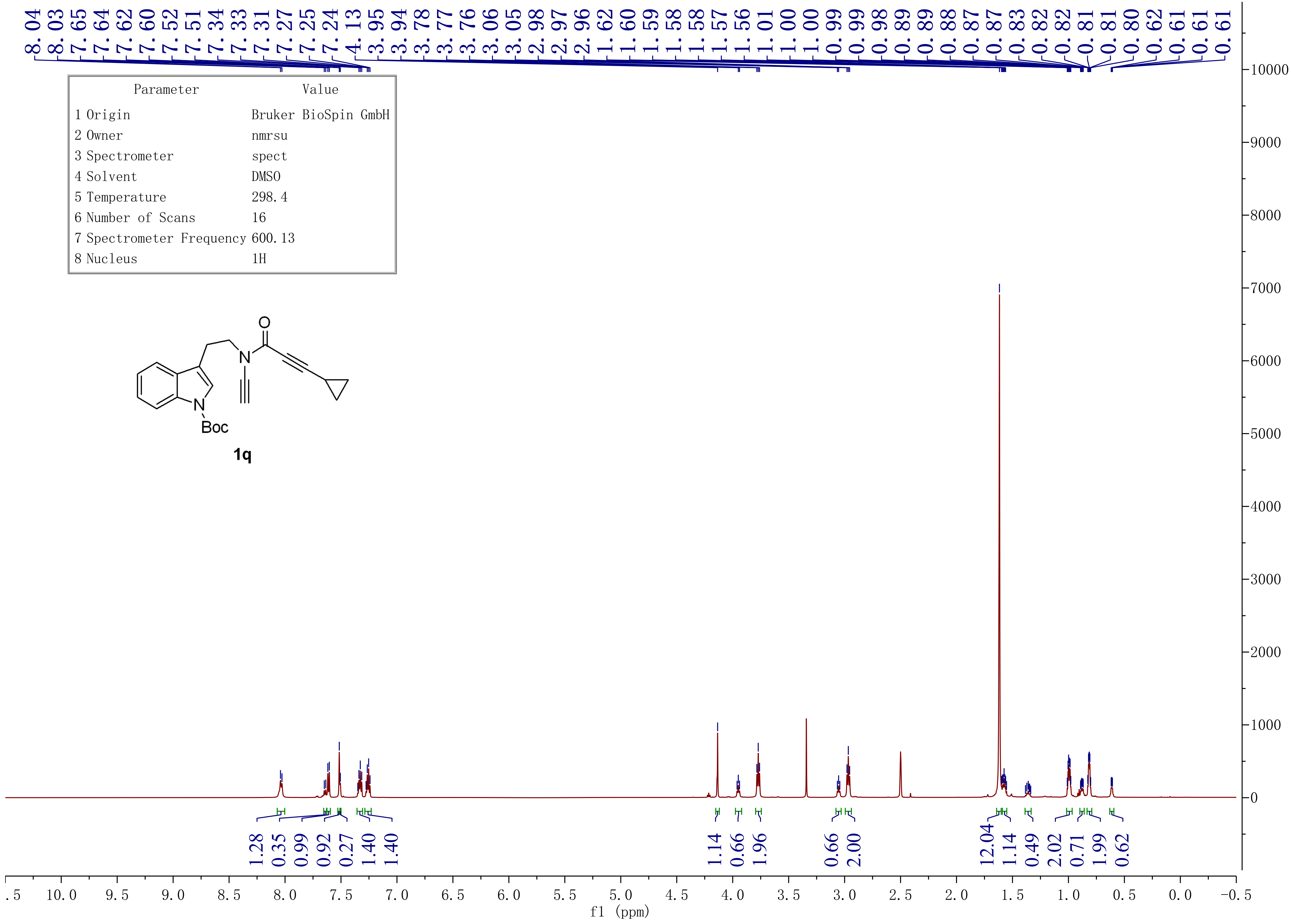


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	600.20
8 Nucleus	1H

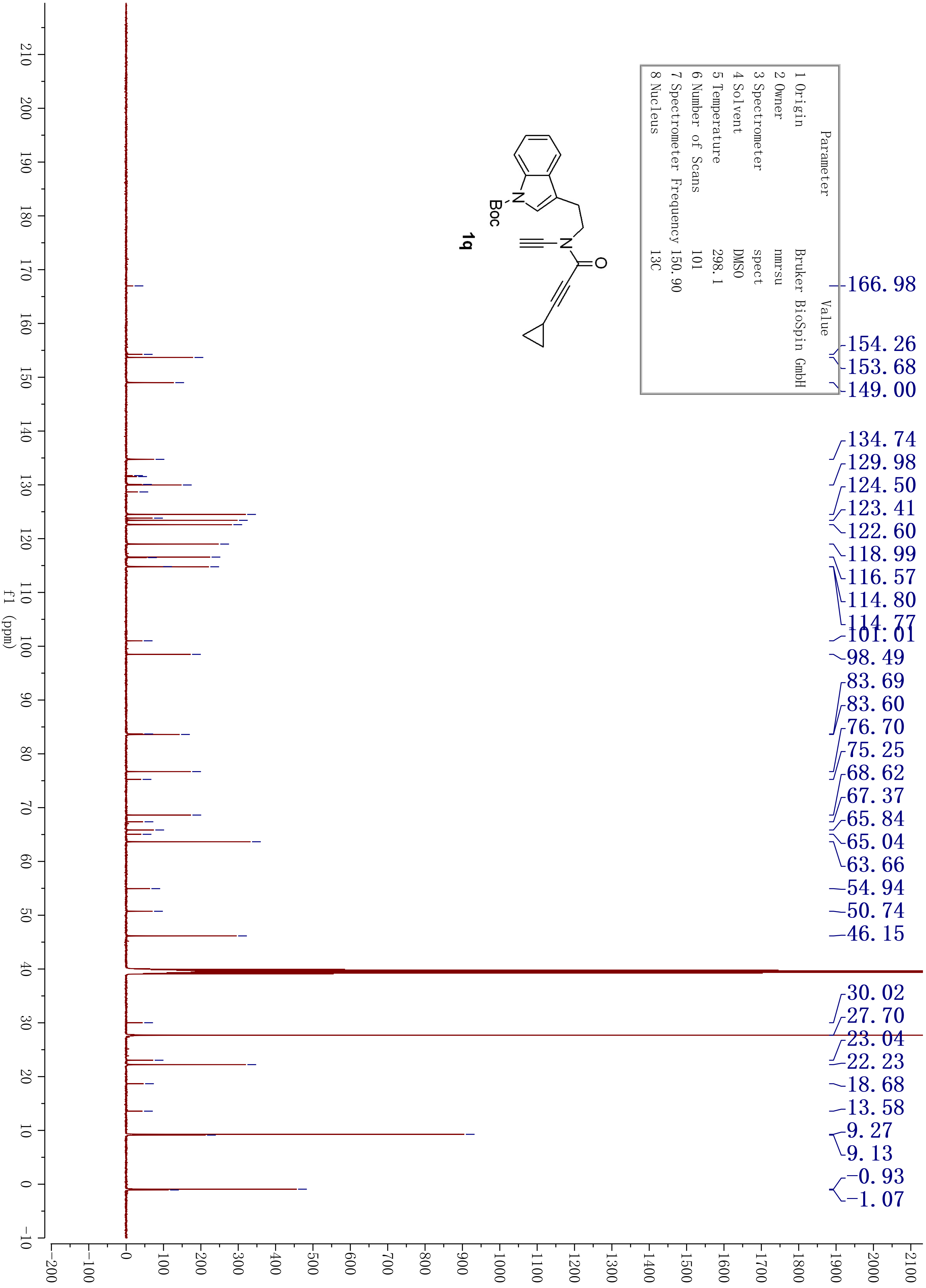


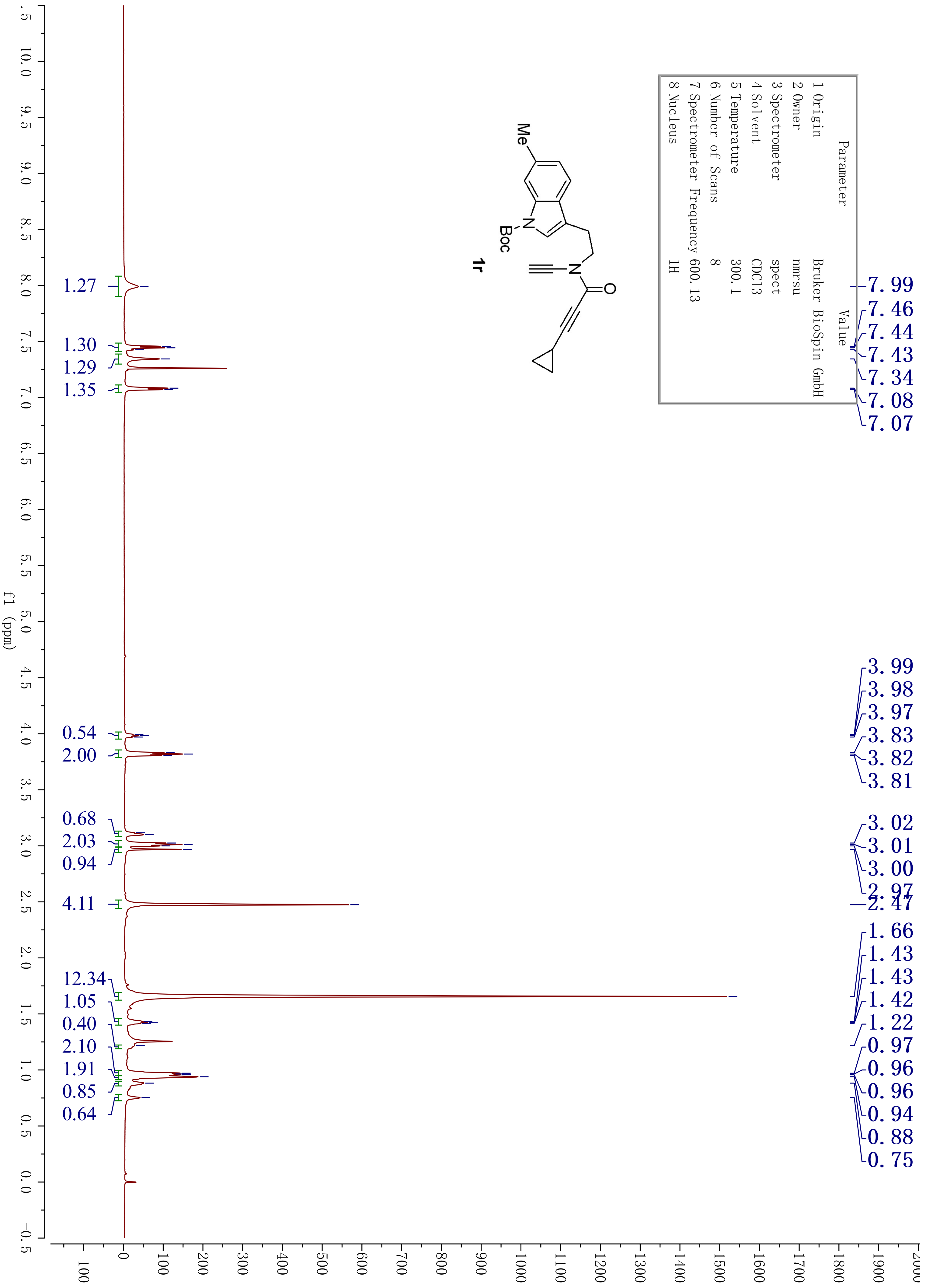
7.57 7.56 7.38 7.37 7.33 7.29 7.28 7.28 7.27 7.26 7.26 7.23 7.21 7.15 7.14 7.12 7.10 7.10 7.08 7.07 7.07 7.02 7.02 7.01 7.00 5.36
4.20 4.16 4.04 4.03 4.02 3.78 3.77 3.76 3.14 3.13 3.12 3.03 3.02 3.01
1.07 1.06 0.94 0.93
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
O
N
TIPS
N
Bn
1p
1.02 0.27 1.34 1.11 2.92 1.72 2.71 1.34 1.32
2.54
0.16 0.81 0.42 2.00
0.45 2.00
2.90 18.75 3.14
f1 (ppm)

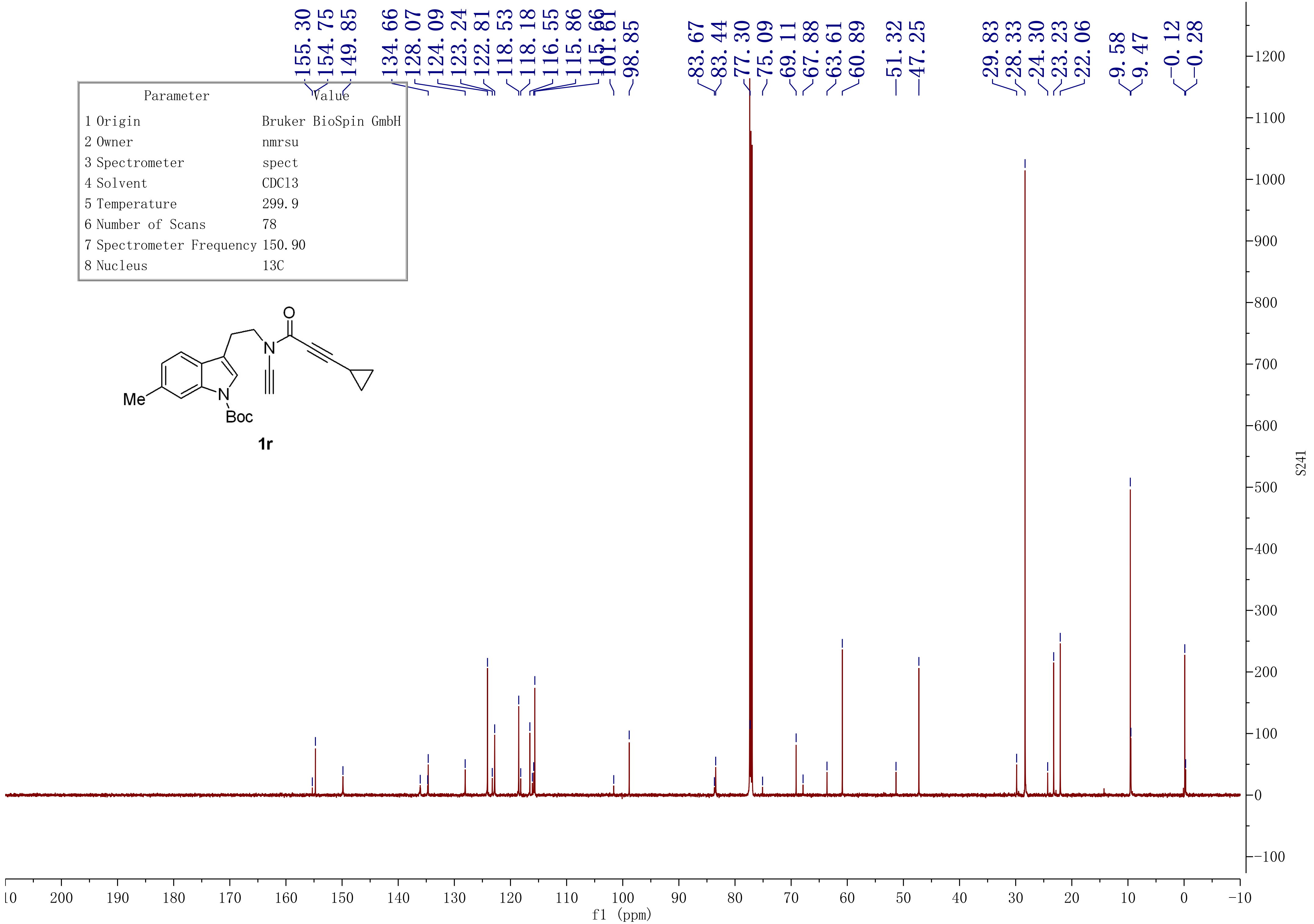

153.59
153.07
138.28
136.02
128.47
127.20
127.02
126.87
121.36
118.78
110.18
110.00
98.23
97.18
96.17
95.23
76.53
74.94
66.55
63.95
51.58
48.94
47.49
23.42
22.51
18.29
18.18
17.85
10.40
10.27
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
TIPS
N
Bn
1p
f1 (ppm)



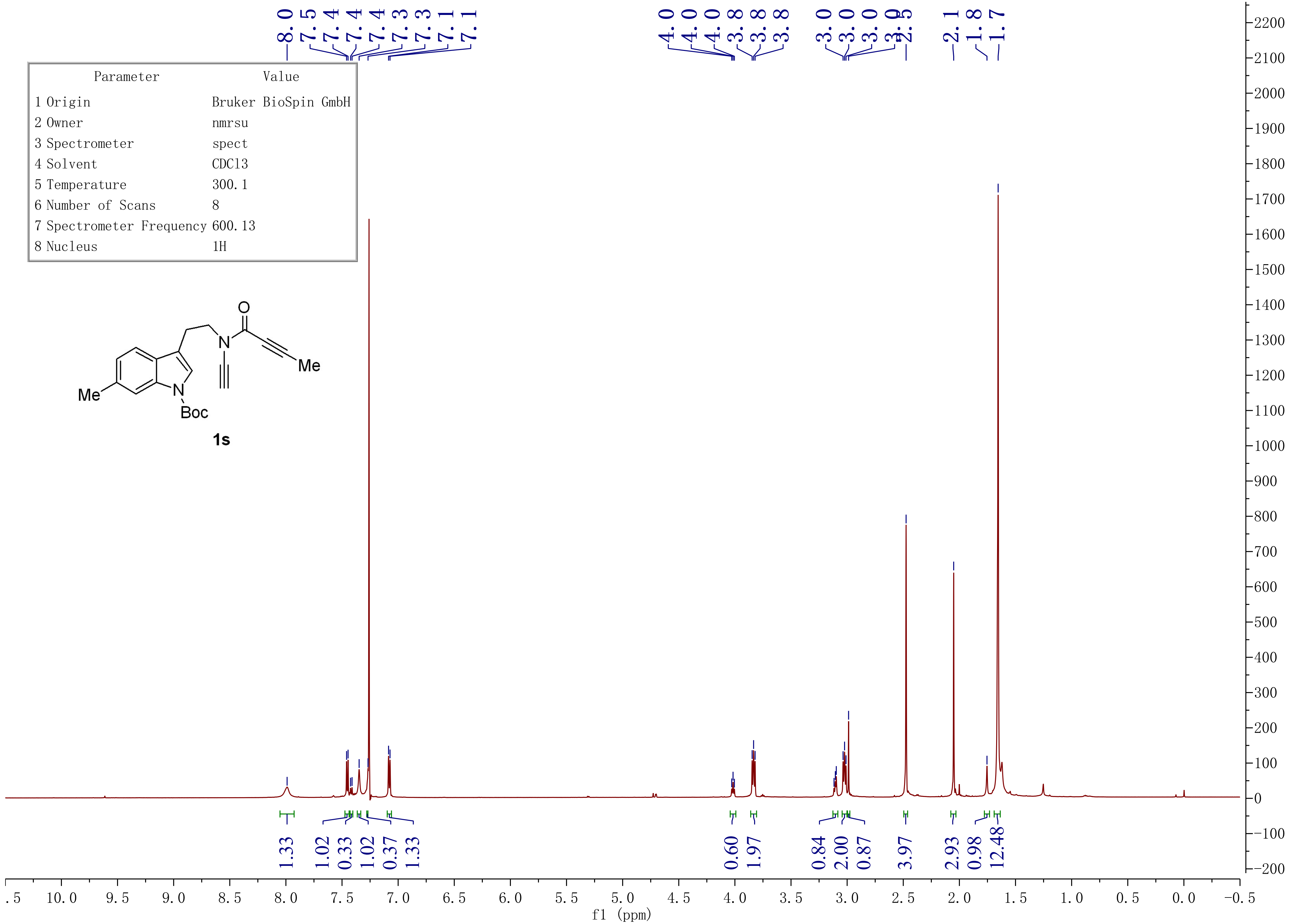
8.04 8.03 7.65 7.64 7.62 7.60 7.52 7.51 7.34 7.33 7.31 7.27 7.25 7.24 4.13 3.95 3.94 3.78 3.77 3.76 3.06 3.05 2.98 2.97 2.96 1.62 1.60 1.59 1.58 1.58 1.57 1.56 1.01 1.00 1.00 0.99 0.99 0.98 0.89 0.89 0.88 0.87 0.87 0.83 0.82 0.82 0.81 0.81 0.80 0.62 0.61 0.61 0.61
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.4
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
N
Boc
1q
1.28 0.35 0.99 0.92 0.27 1.40 1.40 1.14 0.66 1.96 0.66 2.00 12.04 1.14 0.49 2.02 0.71 1.99 0.62
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.1
6 Number of Scans 101
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Boc
1q
166.98
154.26
153.68
149.00
134.74
129.98
124.50
123.41
122.60
118.99
116.57
114.80
114.77
101.01
98.49
83.69
83.60
76.70
75.25
68.62
67.37
65.84
65.04
63.66
54.94
50.74
46.15
30.02
27.70
23.04
22.23
18.68
13.58
9.27
9.13
-0.93
-1.07
f1 (ppm)

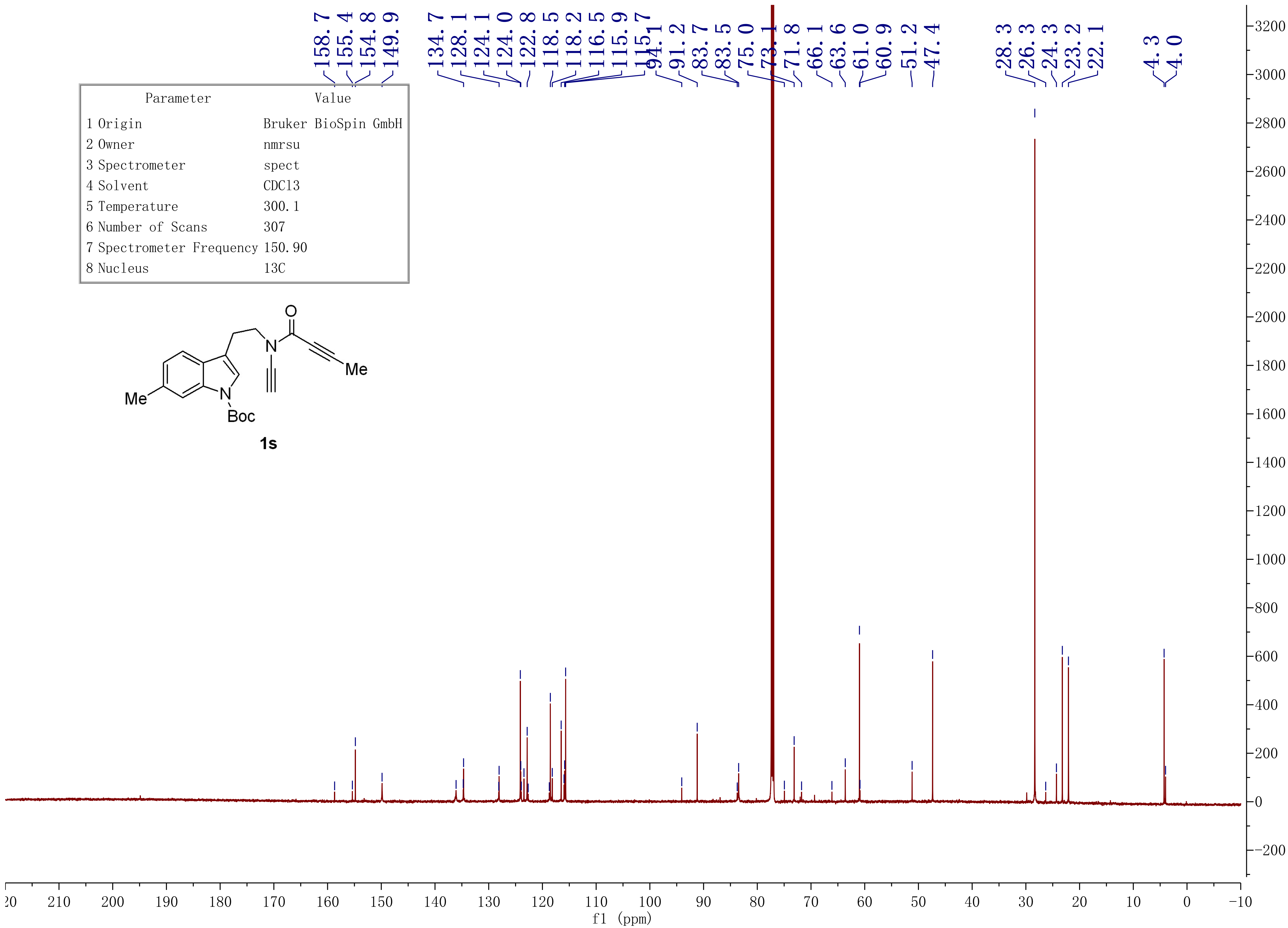

1r
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
f1 (ppm)

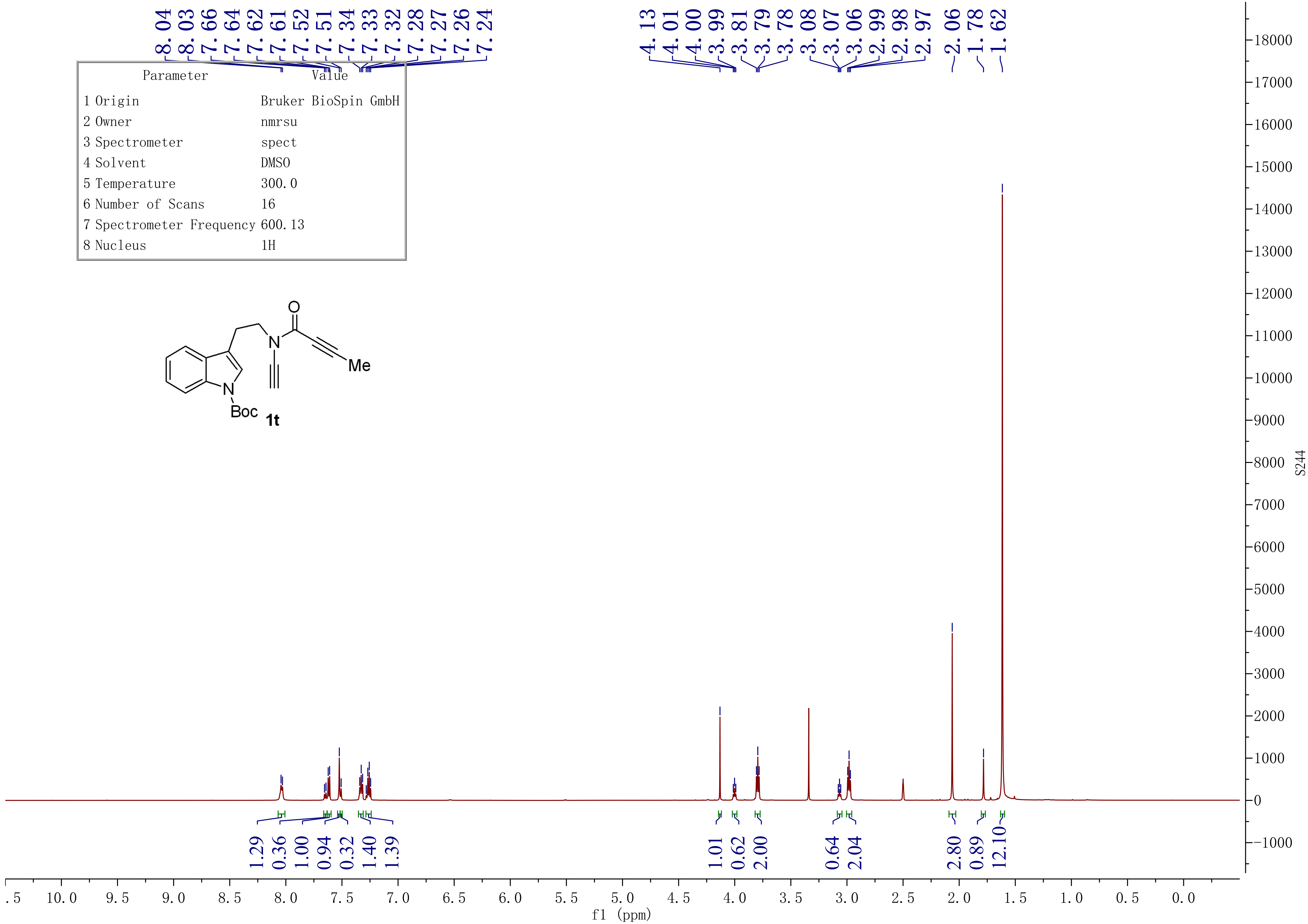


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	299.9
6 Number of Scans	78
7 Spectrometer Frequency	150.90
8 Nucleus	13C

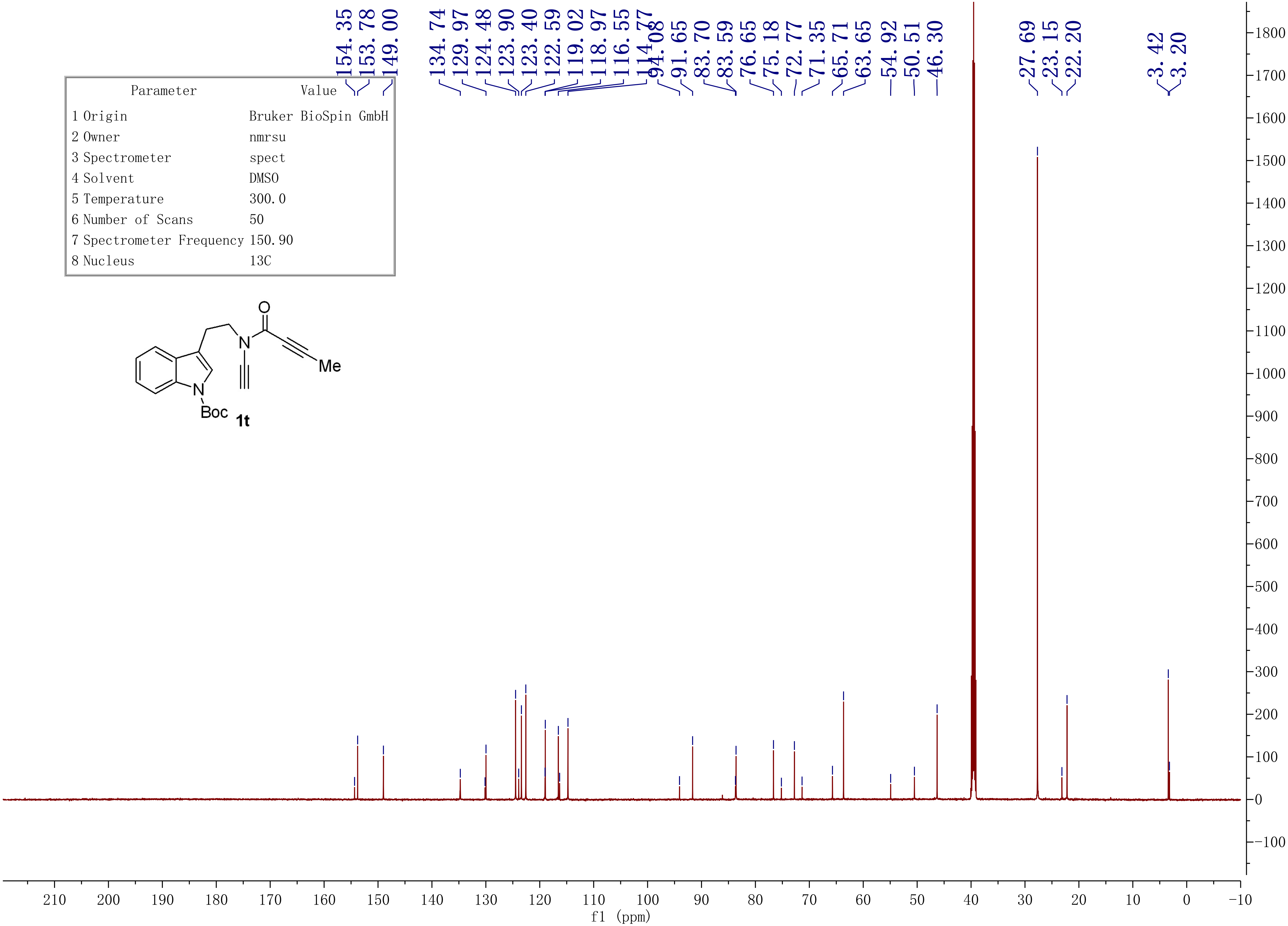


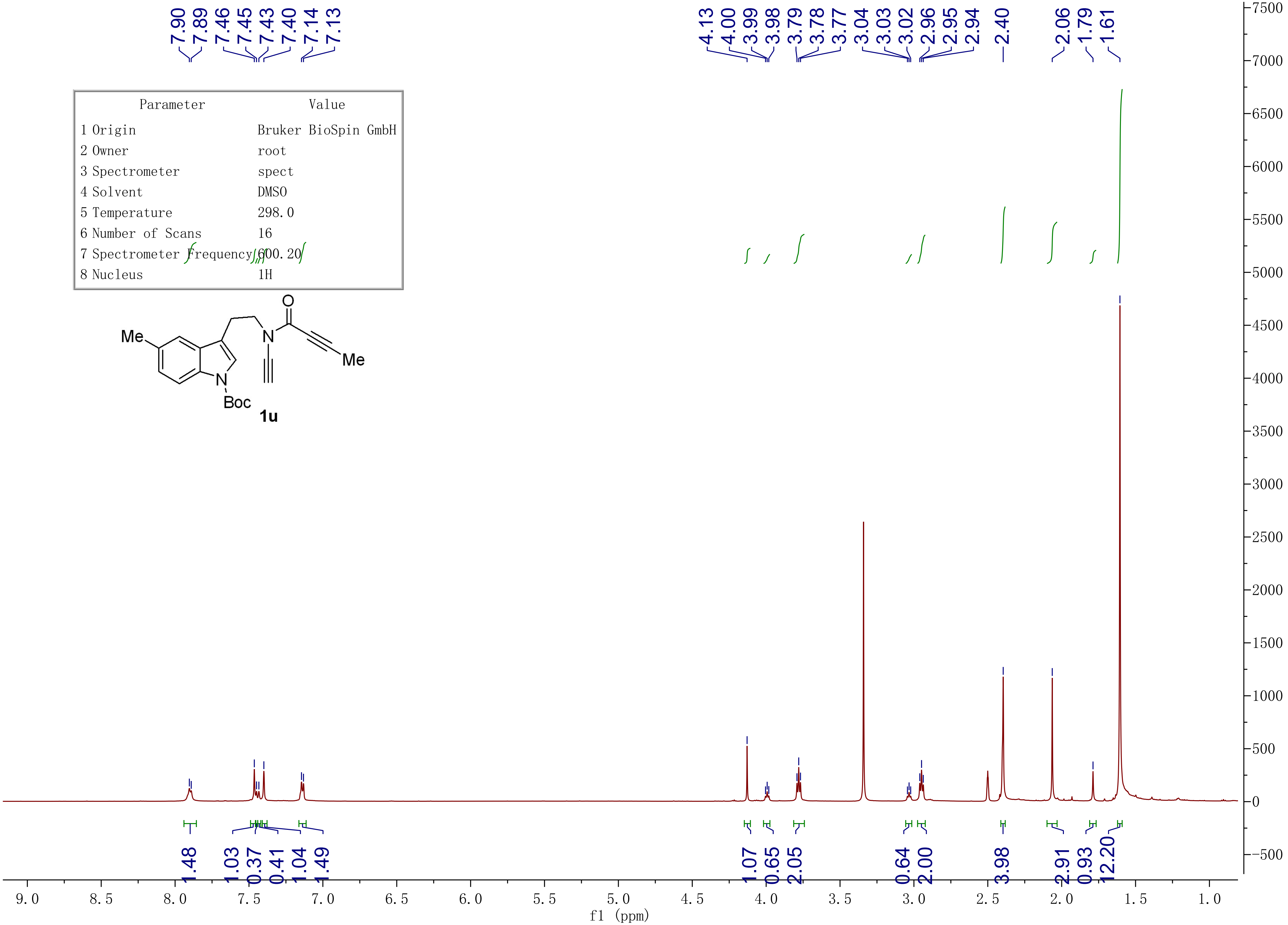
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Me
N
Boc
O
Me
1s
8.0
7.5
7.4
7.4
7.4
7.3
7.3
7.1
7.1
4.0
4.0
4.0
3.8
3.8
3.8
3.0
3.0
3.0
3.0
2.5
2.1
1.8
1.7
1.33
1.02
0.33
1.02
0.37
1.33
0.60
1.97
0.84
2.00
0.87
3.97
2.93
0.98
12.48
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 307
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Me
N
Boc
O
N
Me
1s
158.7
155.4
154.8
149.9
134.7
128.1
124.1
124.0
122.8
118.5
118.2
116.5
115.9
115.7
94.1
91.2
83.7
83.5
75.0
73.1
71.8
66.1
63.6
61.0
60.9
51.2
47.4
28.3
26.3
24.3
23.2
22.1
4.3
4.0
f1 (ppm)


8.04
8.03
7.66
7.64
7.62
7.61
7.52
7.51
7.34
7.33
7.32
7.28
7.27
7.26
7.24
4.13
4.01
4.00
3.99
3.81
3.79
3.78
3.08
3.07
3.06
2.99
2.98
2.97
2.06
1.78
1.62
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
Me
N
Boc
1t
1.29
0.36
1.00
0.94
0.32
1.40
1.39
1.01
0.62
2.00
0.64
2.04
2.80
0.89
12.10
f1 (ppm)

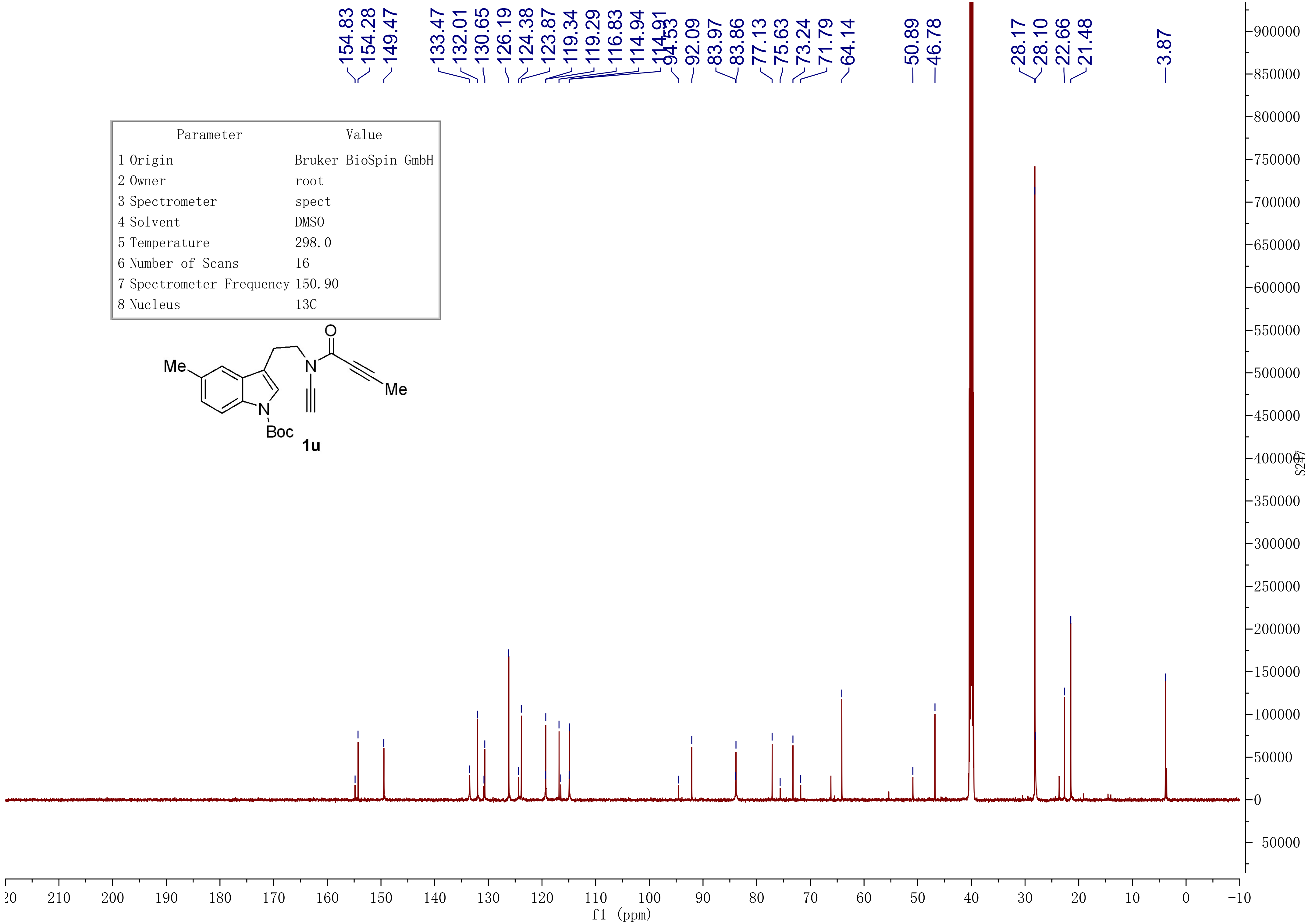
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	50
7 Spectrometer Frequency	150.90
8 Nucleus	13C





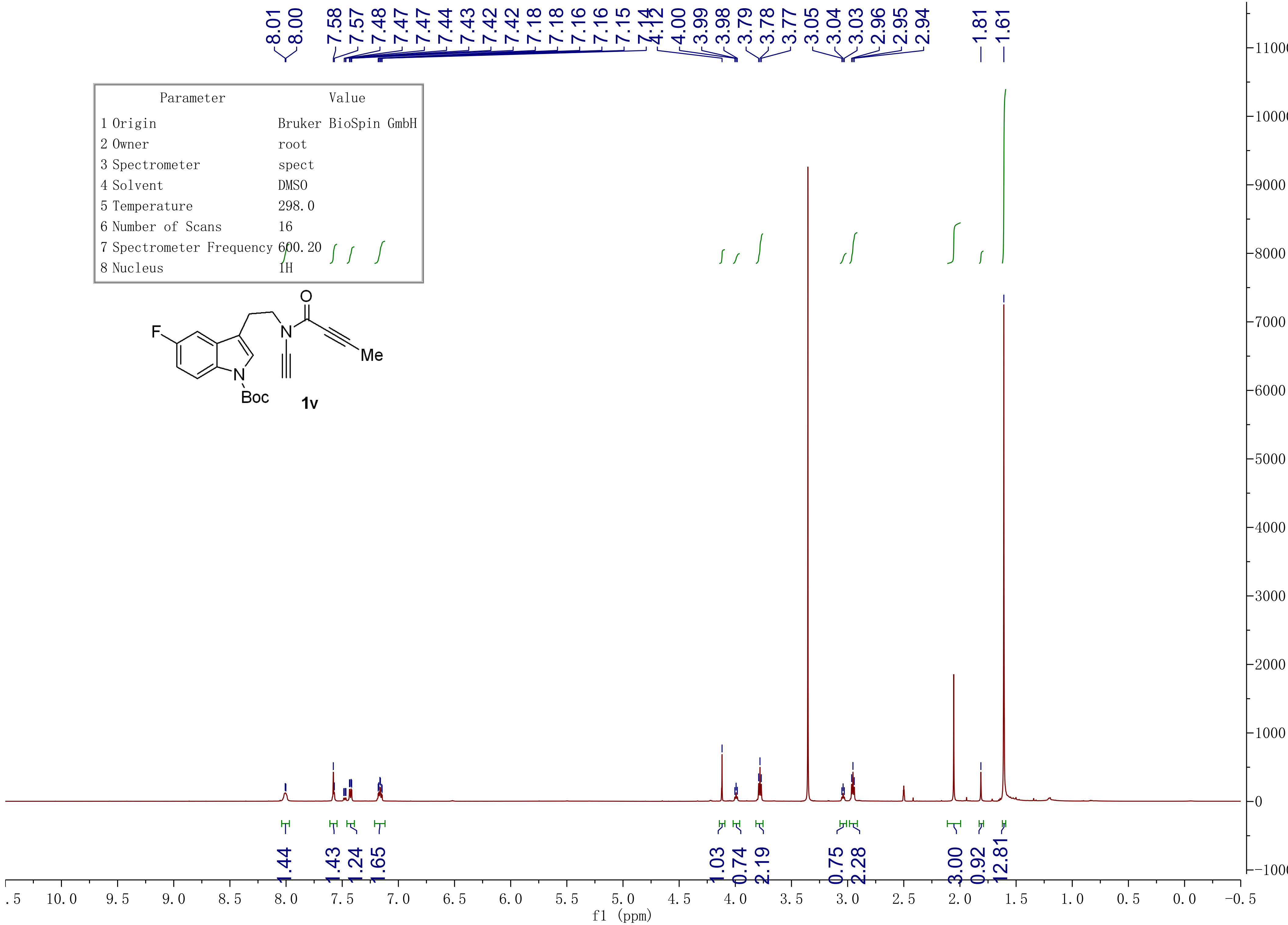
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	600.20
8 Nucleus	1H

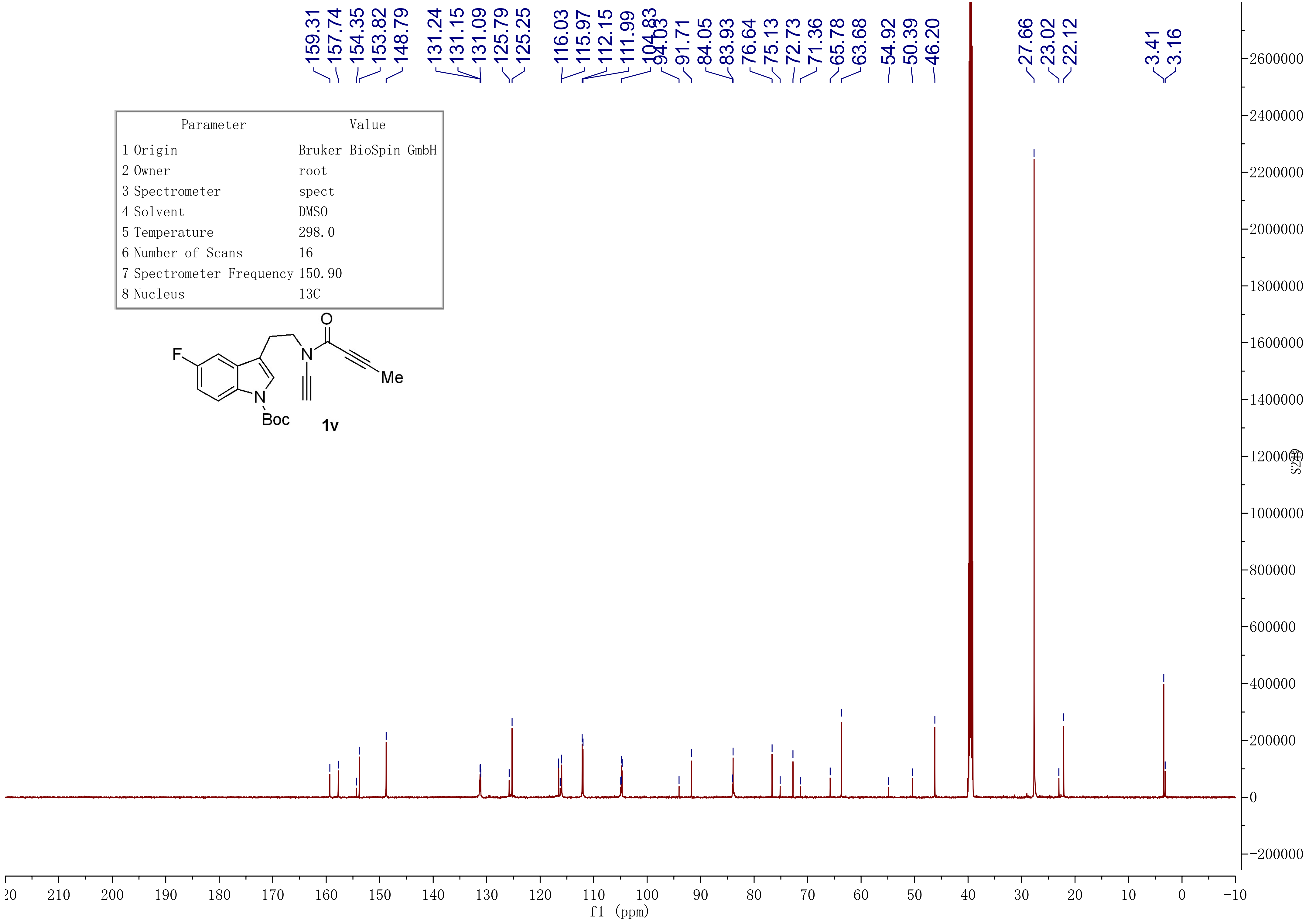
1u



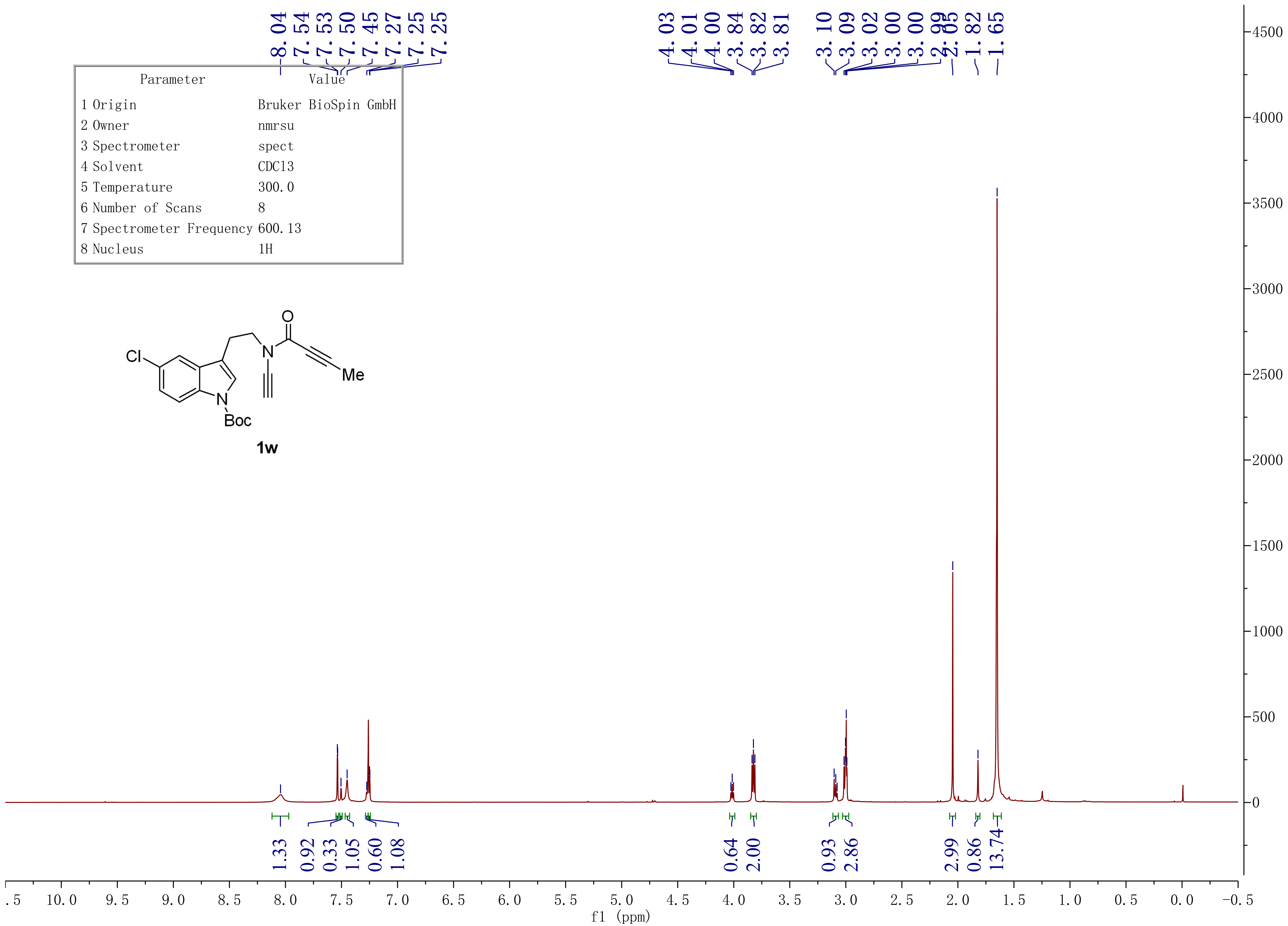
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C

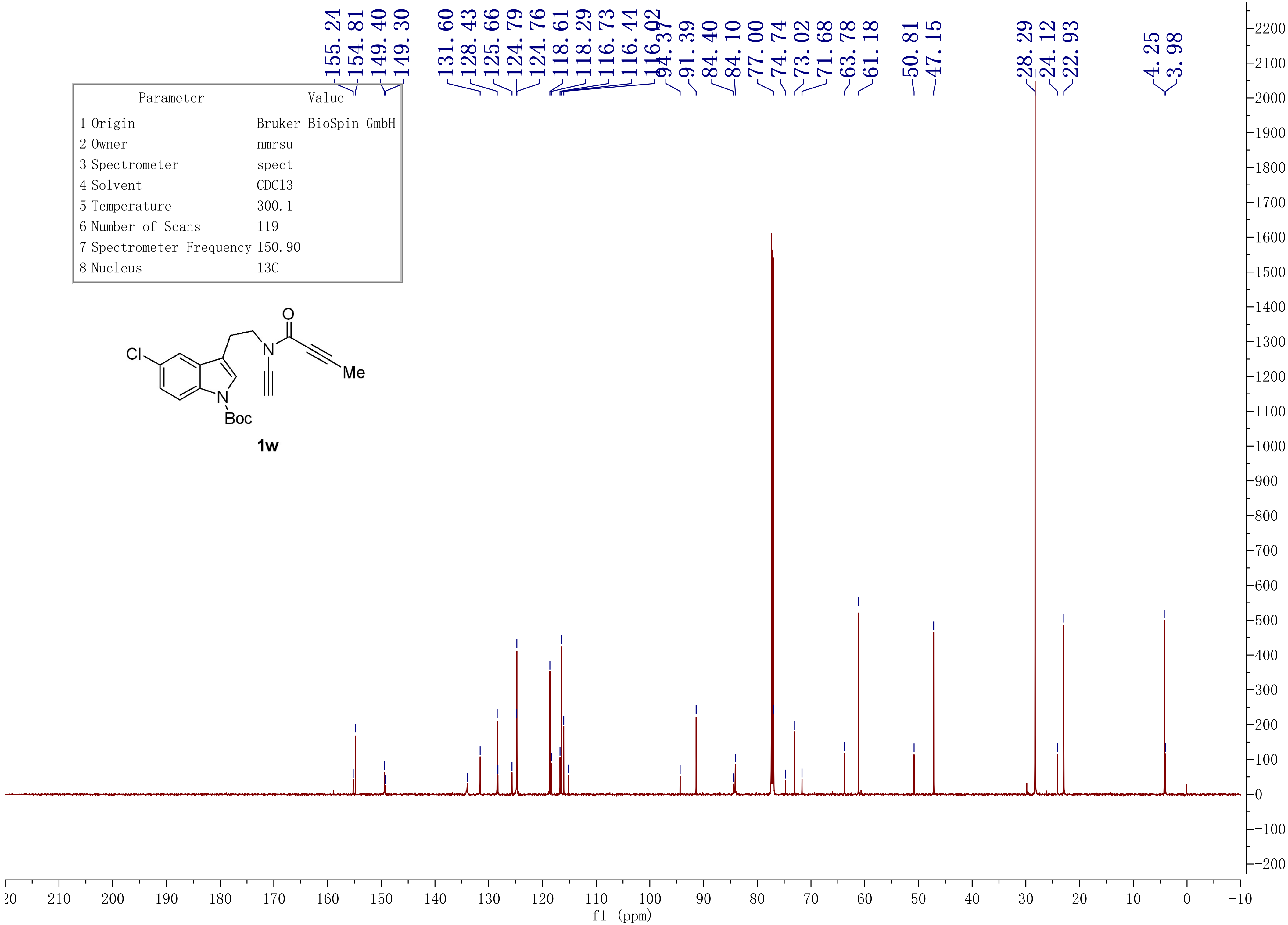
1u


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
F
N
Boc
N
O
Me
1v
8.01
8.00
7.58
7.57
7.48
7.47
7.47
7.44
7.43
7.42
7.42
7.18
7.18
7.16
7.16
7.15
7.14
4.12
4.00
3.99
3.98
3.79
3.78
3.77
3.05
3.04
3.03
2.96
2.95
2.94
1.81
1.61
1.44
1.43
1.24
1.65
1.03
0.74
2.19
0.75
2.28
3.00
0.92
12.81
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Cl
N
Boc
N
O
Me
1w
8.04 7.54 7.53 7.50 7.45 7.27 7.25 7.25
4.03 4.01 4.00 3.84 3.82 3.81
3.10 3.09 3.02 3.00 3.00 2.99 2.05 1.82 1.65
1.33 0.92 0.33 1.05 0.60 1.08
0.64 2.00
0.93 2.86
2.99 0.86 13.74
f1 (ppm)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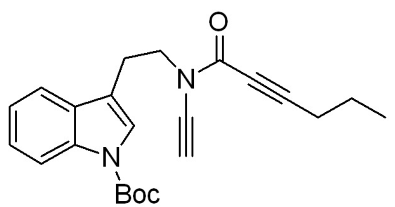
154.81
149.40
149.30
131.60
128.43
125.66
124.79
124.76
118.61
118.29
116.73
116.44
116.02
94.37
91.39
84.40
84.10
77.00
74.74
73.02
71.68
63.78
61.18
50.81
47.15
28.29
24.12
22.93
4.25
3.98
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
CDCl3
5 Temperature
300.1
6 Number of Scans
119
7 Spectrometer Frequency
150.90
8 Nucleus
13C
Cl
N
Boc
N
O
Me
1w
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.1
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H



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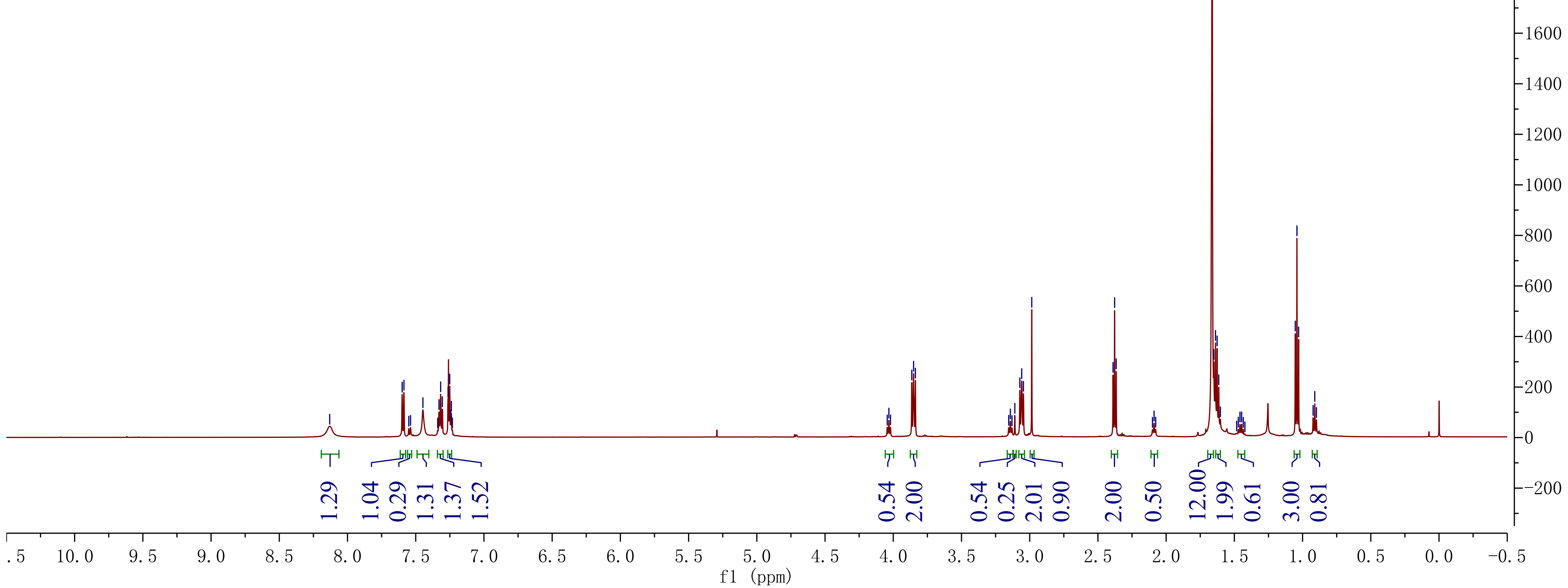
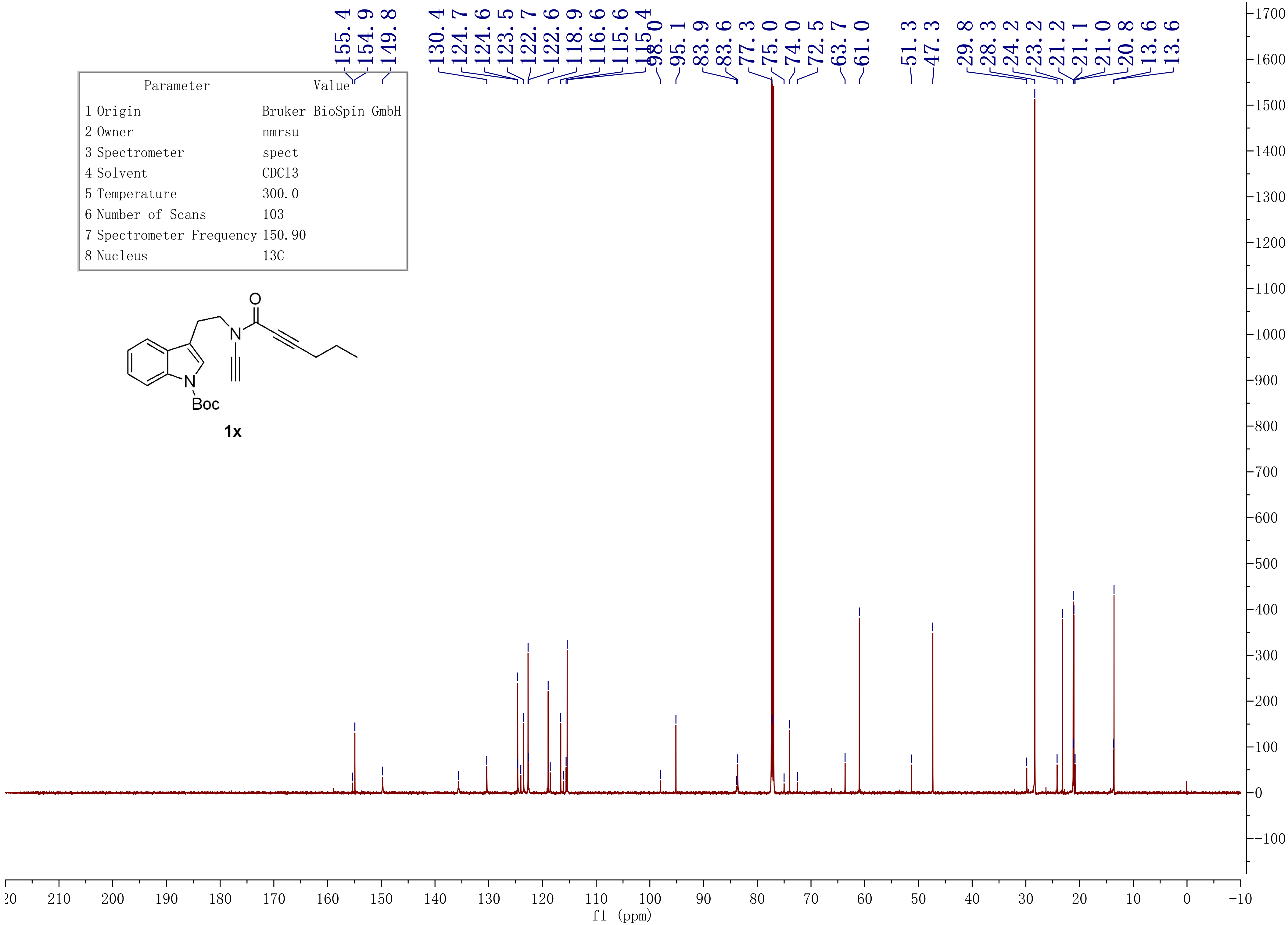
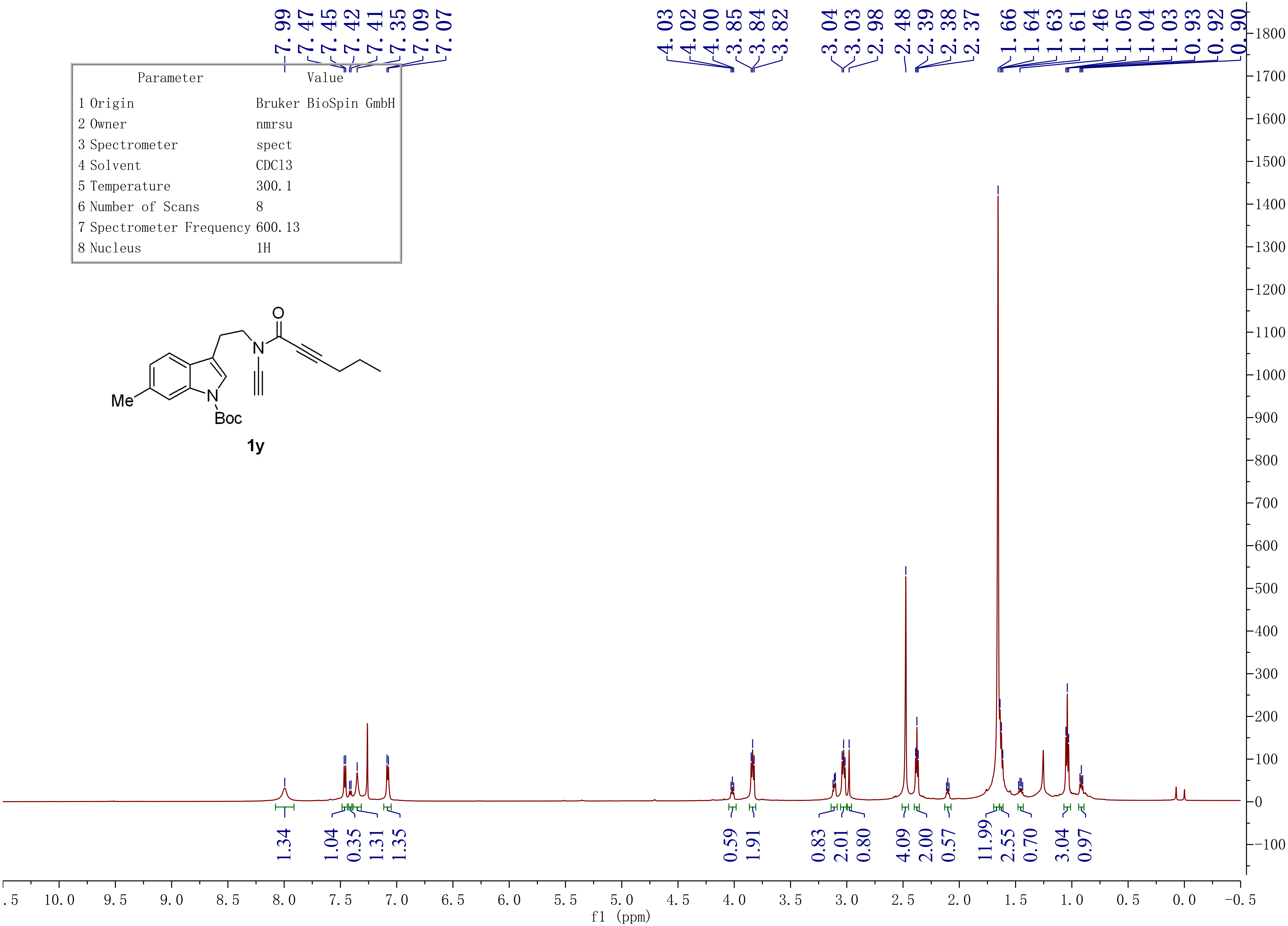
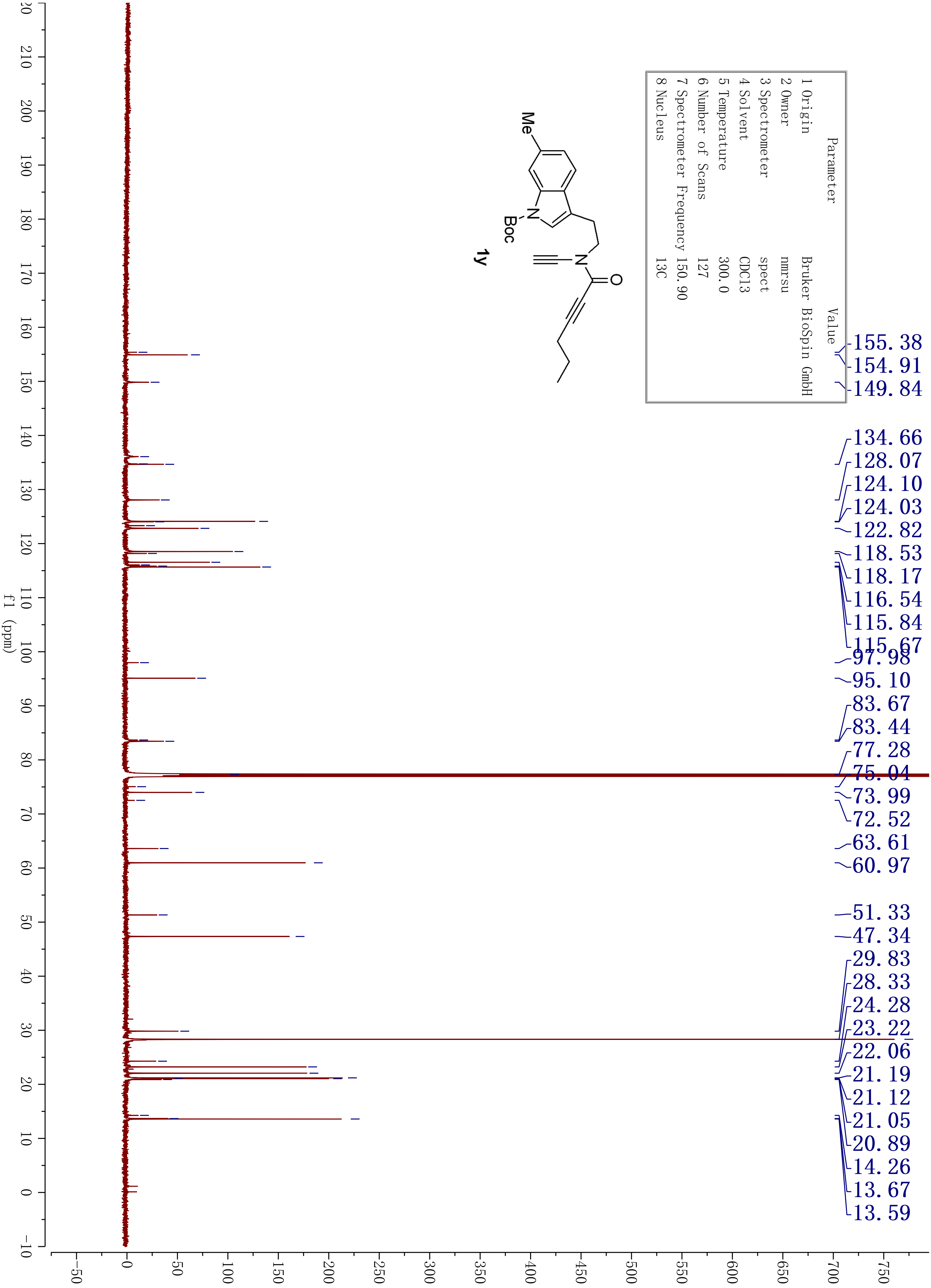
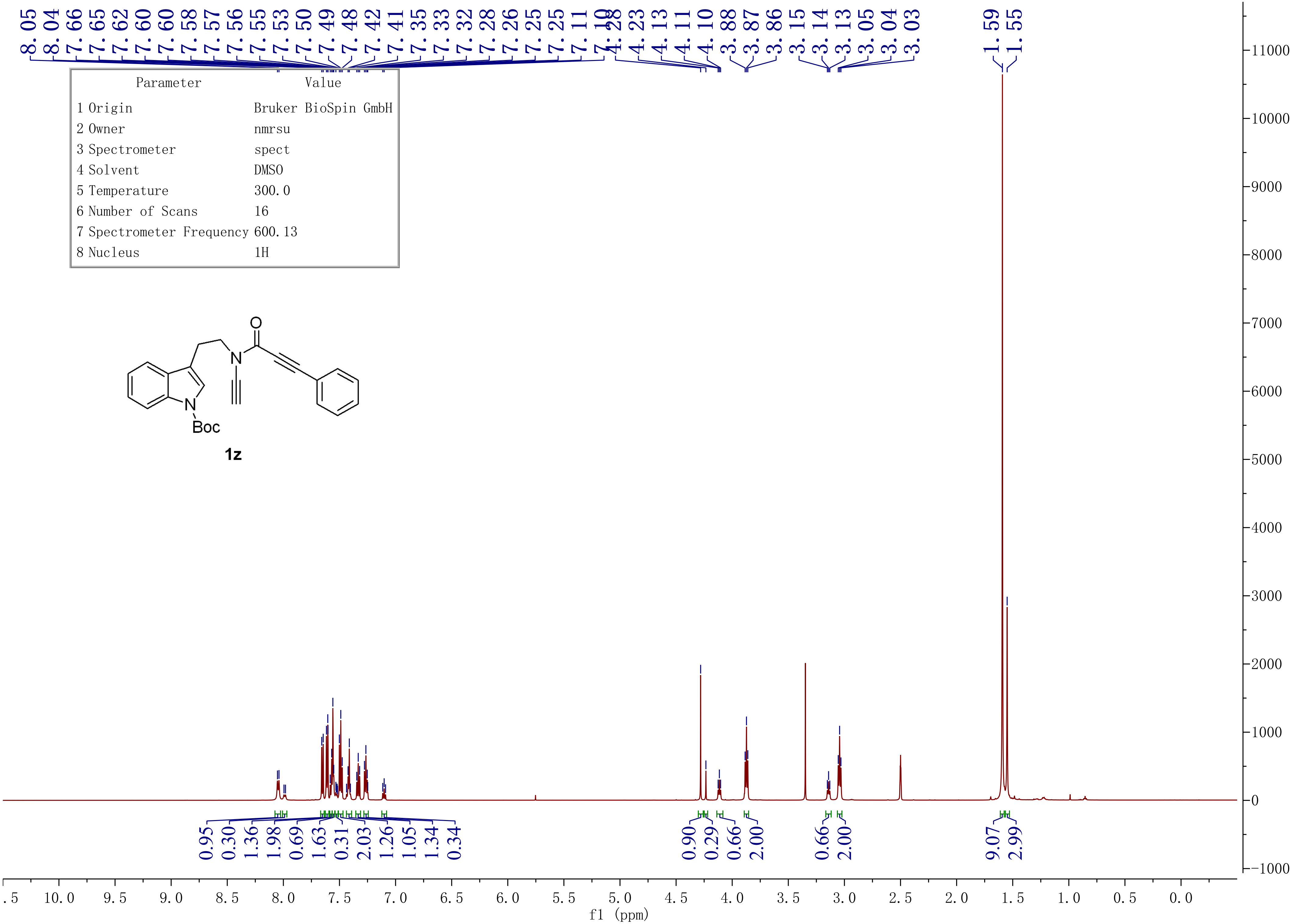
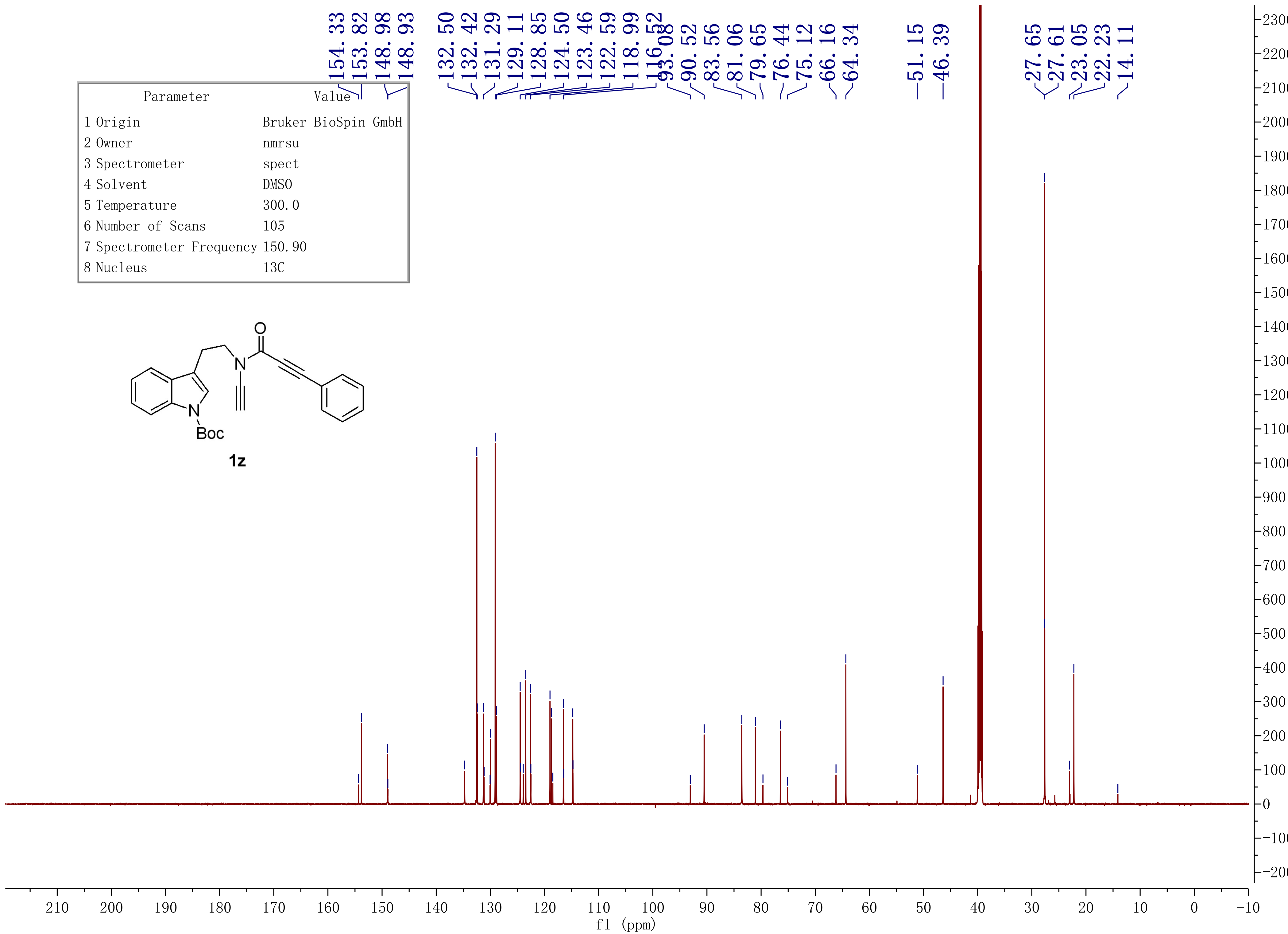


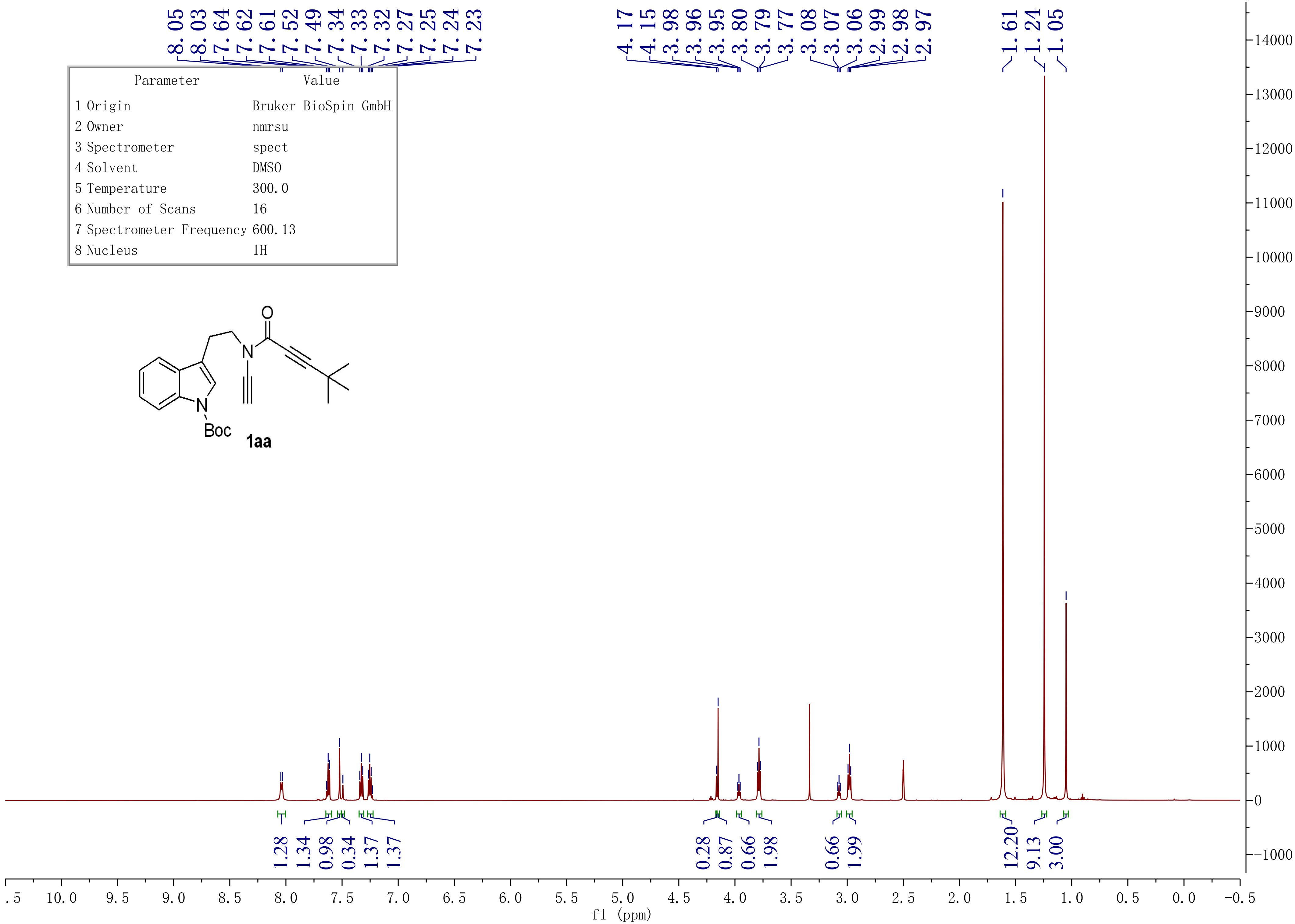

155.4
154.9
149.8
130.4
124.7
124.6
123.5
122.7
122.6
118.9
116.6
115.6
115.4
98.0
95.1
83.9
83.6
77.3
75.0
74.0
72.5
63.7
61.0
51.3
47.3
29.8
28.3
24.2
23.2
21.2
21.1
21.0
20.8
13.6
13.6
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 103
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
N
Boc
1x
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Me
N
Boc
N
O
1y
7.99 7.47 7.45 7.42 7.41 7.35 7.09 7.07
4.03 4.02 4.00 3.85 3.84 3.82
3.04 3.03 2.98 2.48 2.39 2.38 2.37
1.66 1.64 1.63 1.61 1.46 1.05 1.04 1.03 0.93 0.92 0.90
1.34 1.04 0.35 1.31 1.35 0.59 1.91 0.83 2.01 0.80 4.09 2.00 0.57 11.99 2.55 0.70 3.04 0.97
f1 (ppm)

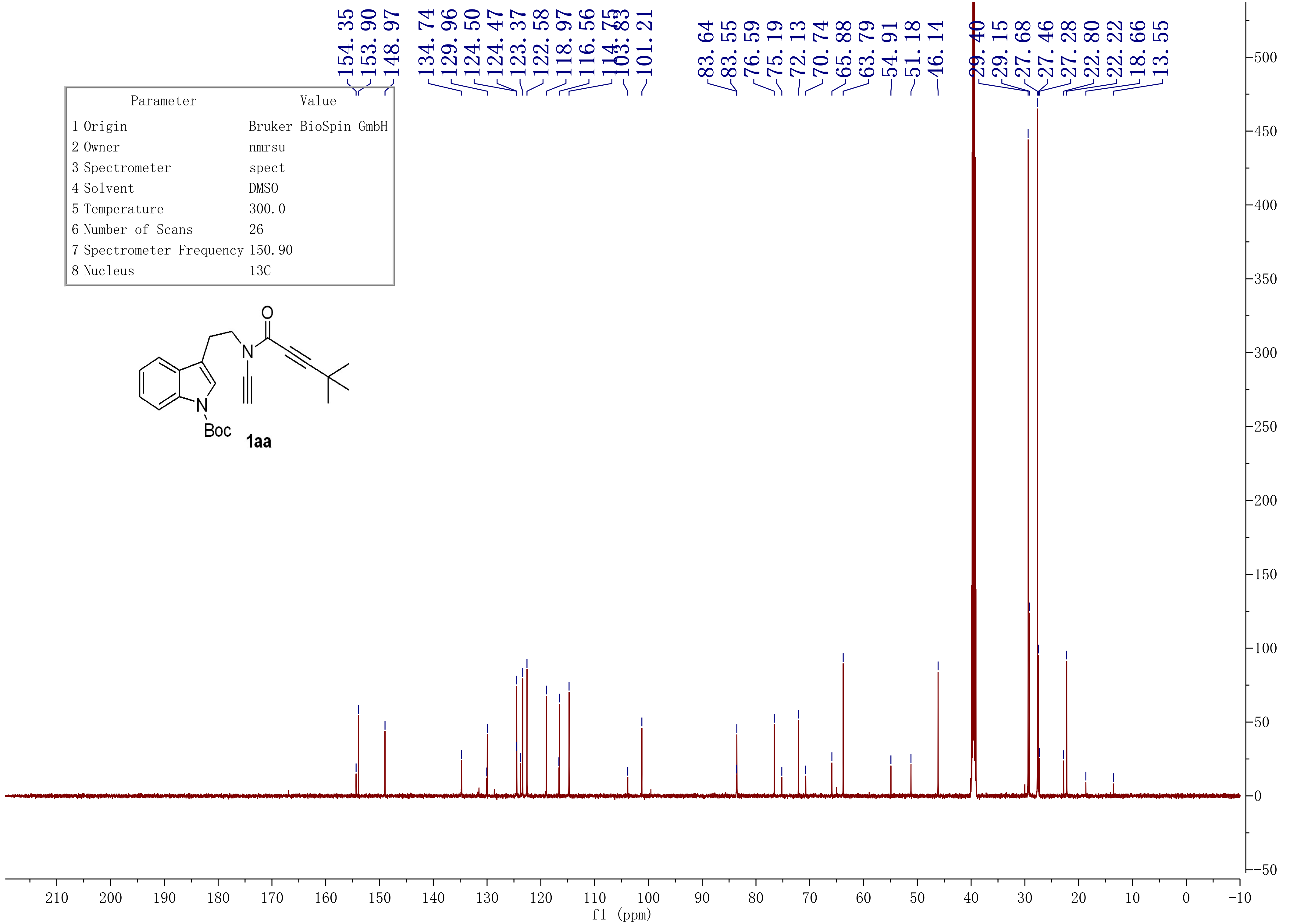

1y
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 127
7 Spectrometer Frequency 150.90
8 Nucleus 13C
155.38
154.91
149.84
134.66
128.07
124.10
124.03
122.82
118.53
118.17
116.54
115.84
115.67
97.98
95.10
83.67
83.44
77.28
75.04
73.99
72.52
63.61
60.97
51.33
47.34
29.83
28.33
24.28
23.22
22.06
21.19
21.12
21.05
20.89
14.26
13.67
13.59
f1 (ppm)

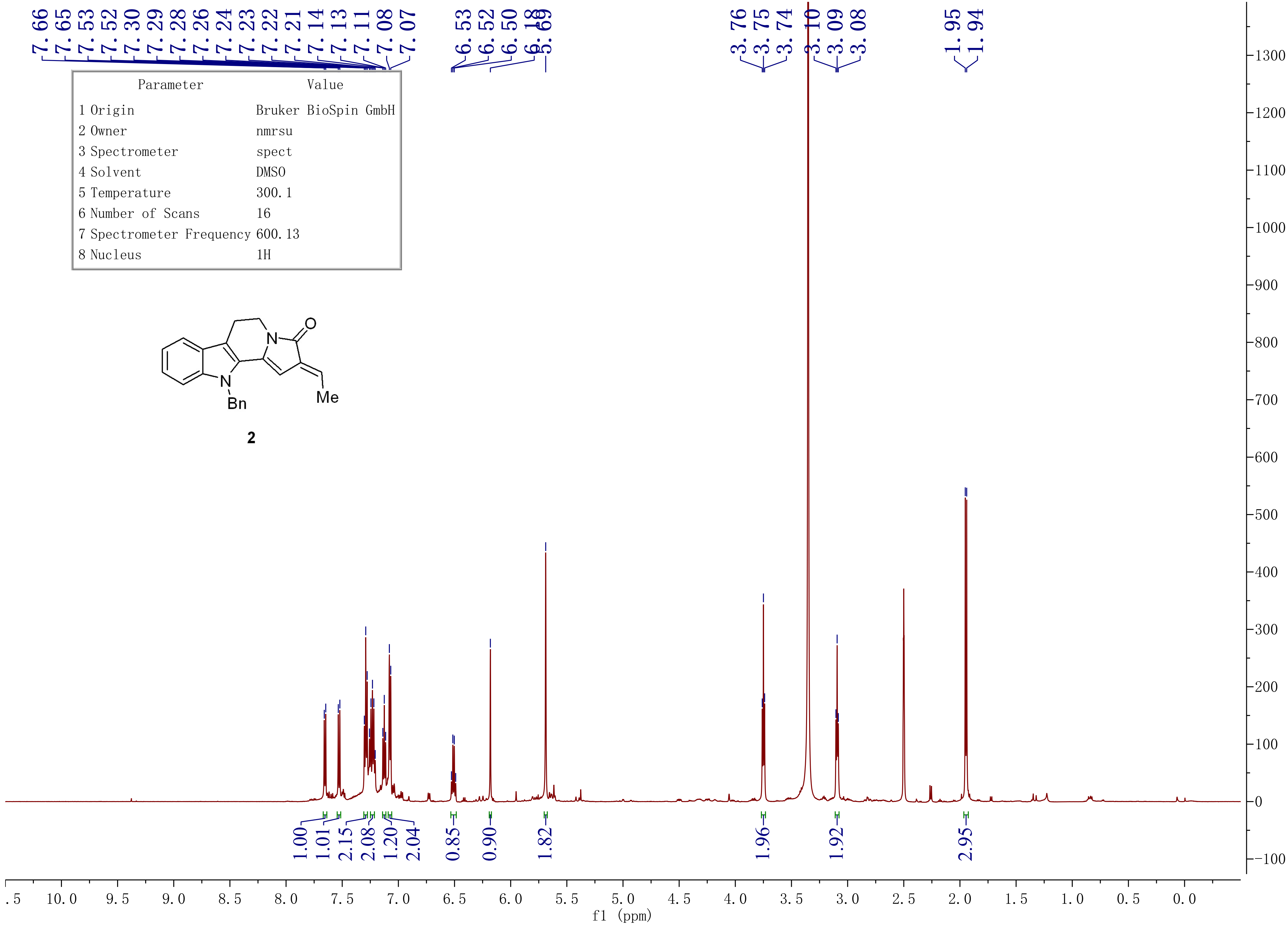

8.05 8.04 7.66 7.65 7.62 7.60 7.60 7.58 7.57 7.56 7.55 7.53 7.50 7.49 7.48 7.42 7.41 7.35 7.33 7.32 7.28 7.26 7.25 7.25 7.11 7.10 4.28 4.23 4.13 4.11 4.10 3.88 3.87 3.86 3.15 3.14 3.13 3.05 3.04 3.03 1.59 1.55
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
N
Boc
1z
0.95 0.30 1.36 1.98 0.69 1.63 0.31 2.03 1.26 1.05 1.34 0.34
0.90 0.29 0.66 2.00
0.66 2.00
9.07 2.99
f1 (ppm)

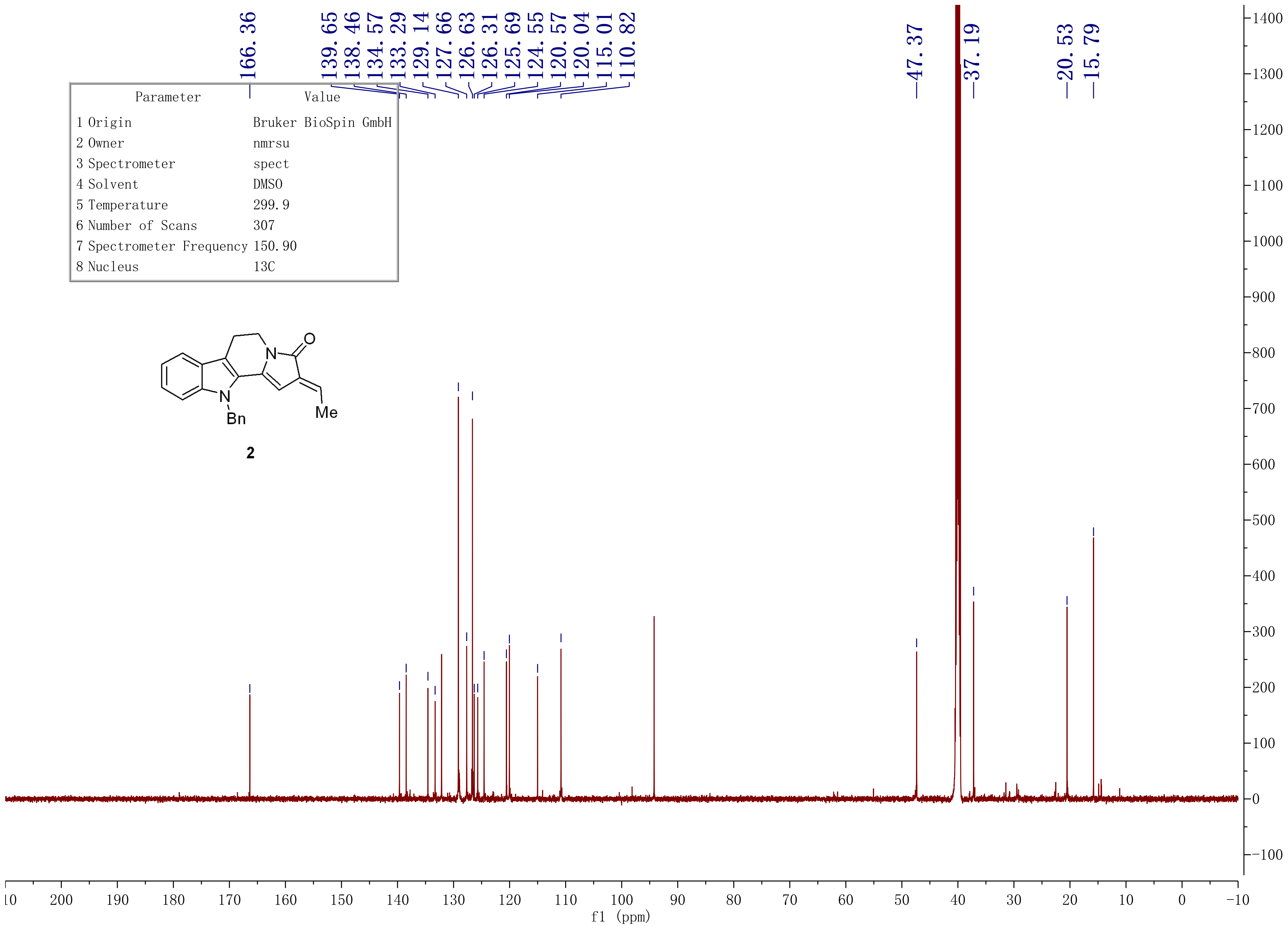

154.33
153.82
148.98
148.93
132.50
132.42
131.29
129.11
128.85
124.50
123.46
122.59
118.99
116.52
93.08
90.52
83.56
81.06
79.65
76.44
75.12
66.16
64.34
51.15
46.39
27.65
27.61
23.05
22.23
14.11
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 105
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
O
N
Boc
1z
f1 (ppm)



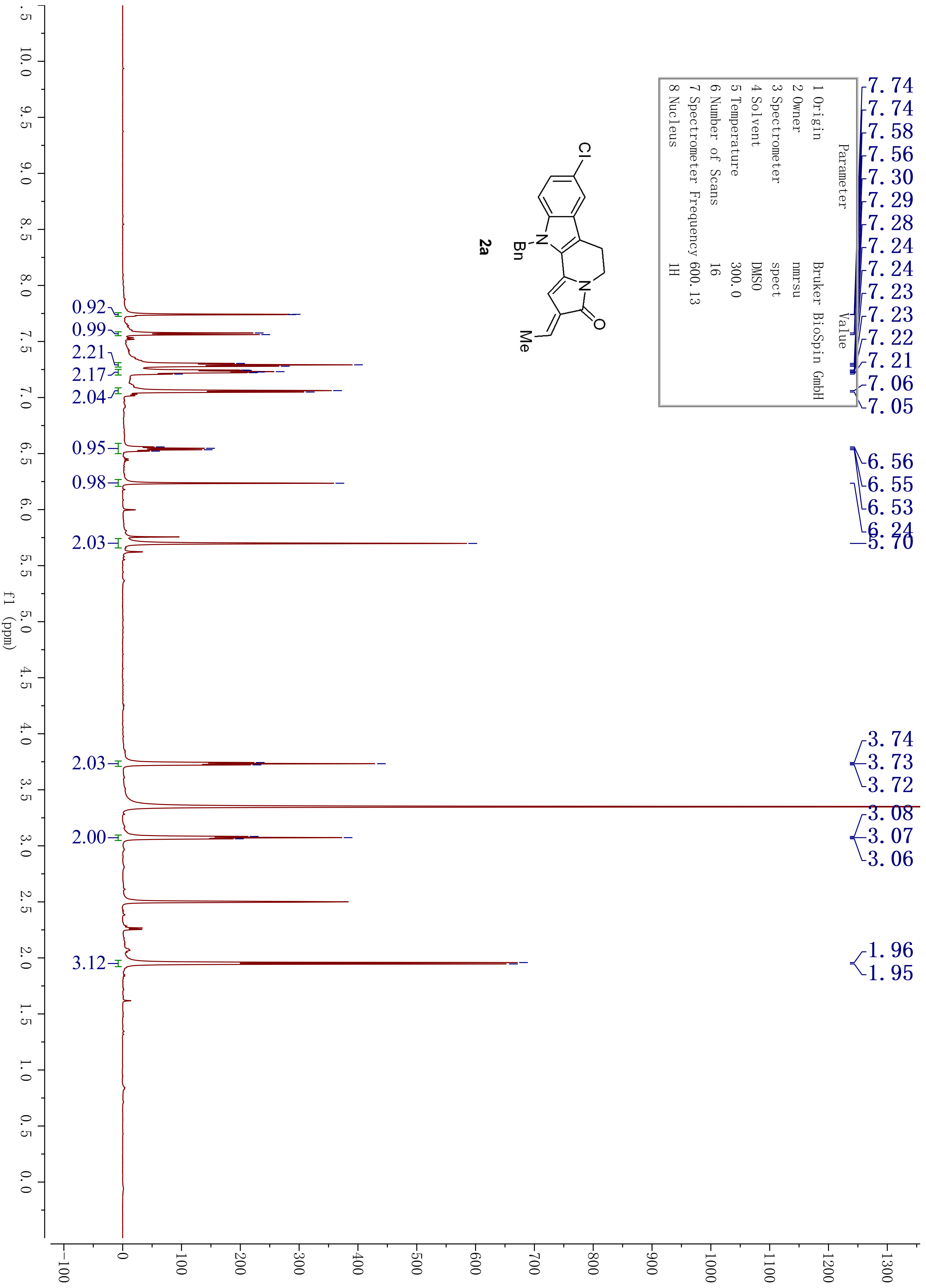
8.05 8.03 7.64 7.62 7.61 7.52 7.49 7.34 7.33 7.32 7.27 7.25 7.24 7.23
4.17 4.15 3.98 3.96 3.95 3.80 3.79 3.77 3.08 3.07 3.06 2.99 2.98 2.97
1.61 1.24 1.05
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Boc
1aa
1.28 1.34 0.98 0.34 1.37 1.37
0.28 0.87 0.66 1.98
0.66 1.99
12.20 9.13 3.00
f1 (ppm)

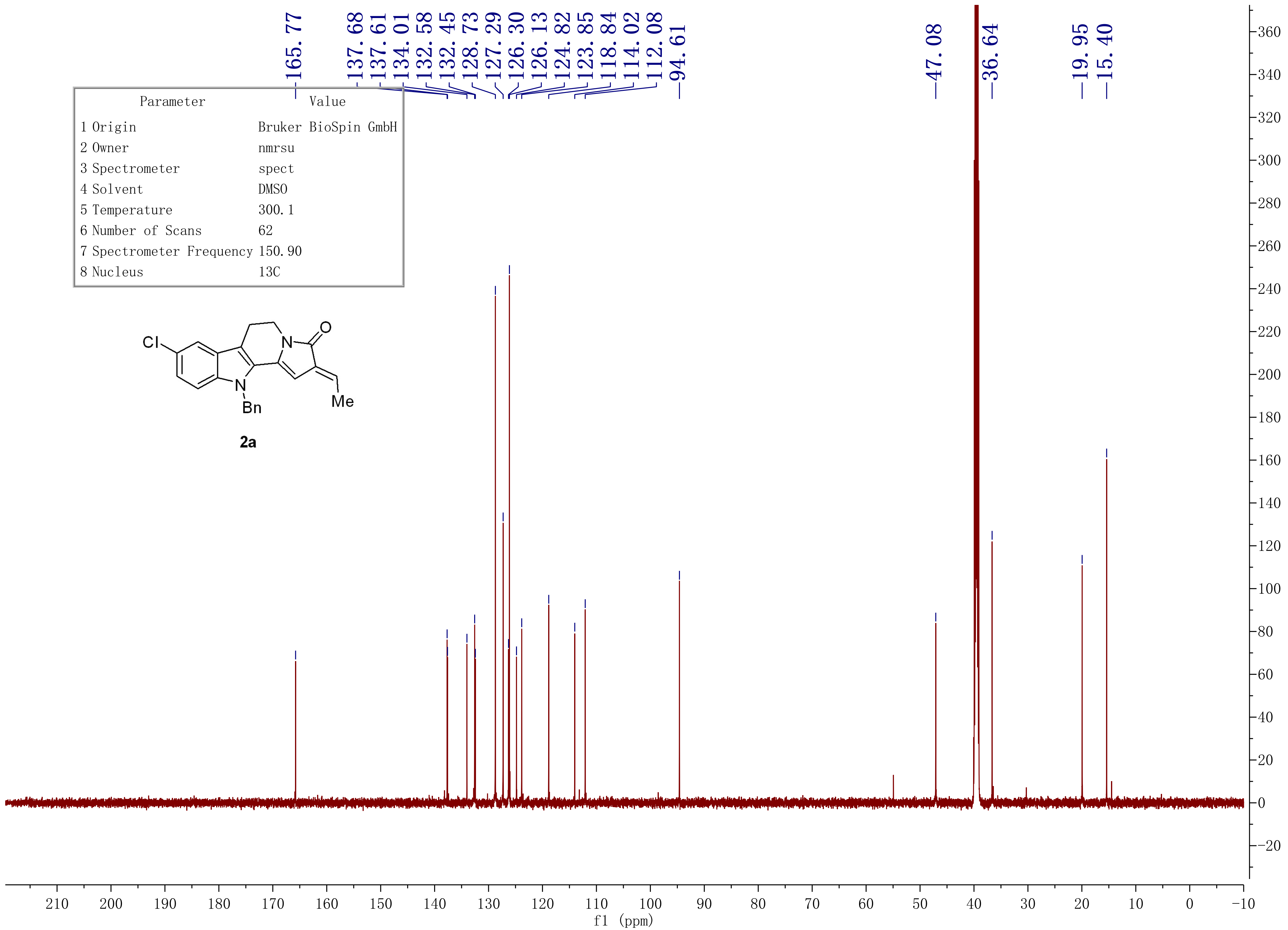

154.35
153.90
148.97
134.74
129.96
124.50
124.47
123.37
122.58
118.97
116.56
114.75
103.83
101.21
83.64
83.55
76.59
75.19
72.13
70.74
65.88
63.79
54.91
51.18
46.14
29.40
29.15
27.68
27.46
27.28
22.80
22.22
18.66
13.55
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 26
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
O
N
Boc
1aa
f1 (ppm)


7.66 7.65 7.53 7.52 7.30 7.29 7.28 7.26 7.24 7.23 7.22 7.21 7.14 7.13 7.11 7.08 7.07
6.53 6.52 6.50 6.18 5.69
3.76 3.75 3.74 3.10 3.09 3.08
1.95 1.94
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Bn
N
O
Me
2
1.00 1.01 2.15 2.08 1.20 2.04 0.85 0.90 1.82 1.96 1.92 2.95
f1 (ppm)



166.36
139.65
138.46
134.57
133.29
129.14
127.66
126.63
126.31
125.69
124.55
120.57
120.04
115.01
110.82
47.37
37.19
20.53
15.79
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 307
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Bn
N
O
Me
2
f1 (ppm)


2a
Cl
N
Bn
N
O
Me
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
DMSO
5 Temperature
300.0
6 Number of Scans
16
7 Spectrometer Frequency
600.13
8 Nucleus
1H
7.74
7.74
7.58
7.56
7.30
7.29
7.28
7.24
7.24
7.23
7.23
7.22
7.21
7.06
7.05
6.56
6.55
6.53
6.24
5.70
3.74
3.73
3.72
3.08
3.07
3.06
1.96
1.95
0.92
0.99
2.21
2.17
2.04
0.95
0.98
2.03
2.03
2.00
3.12
f1 (ppm)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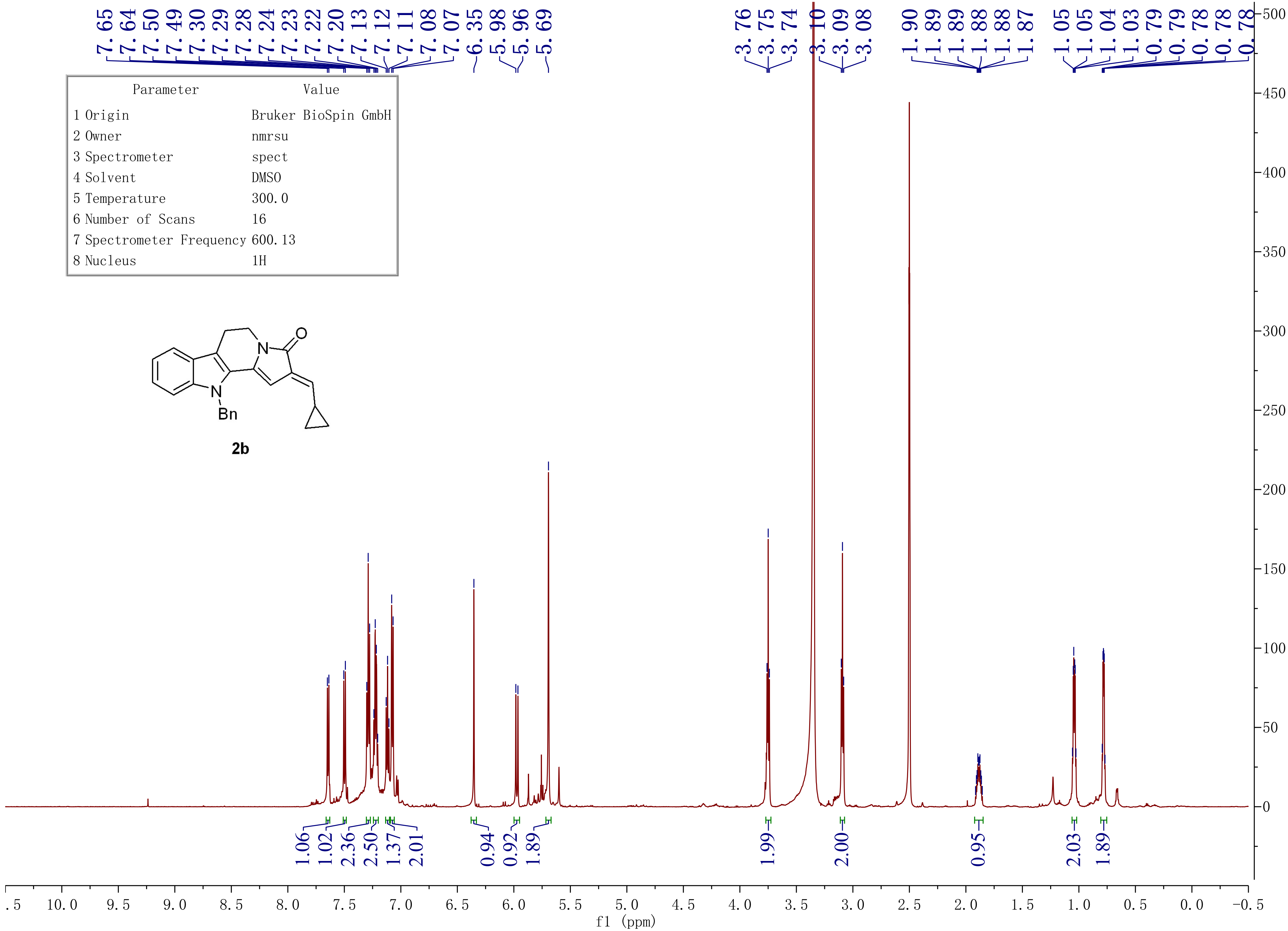
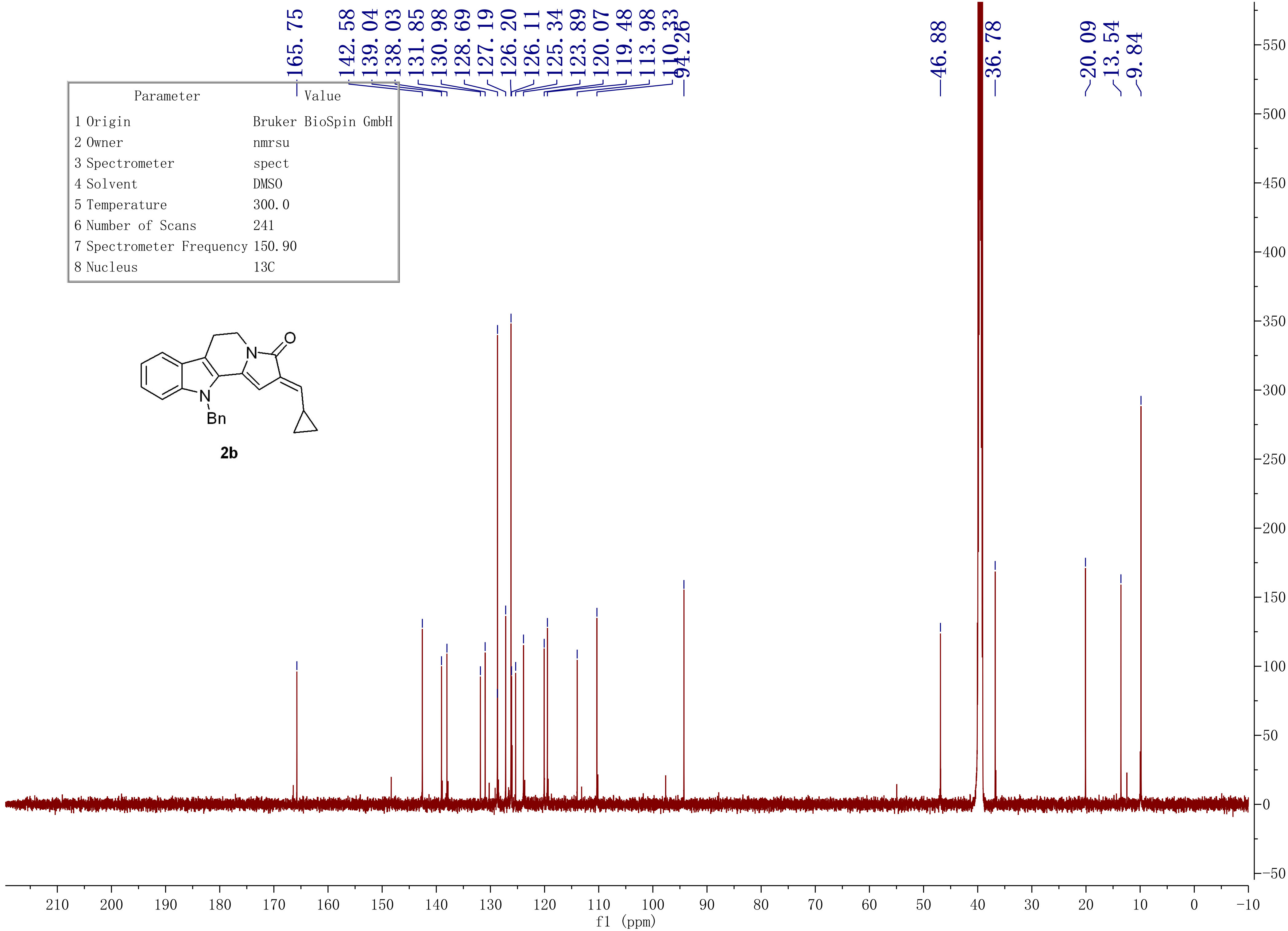
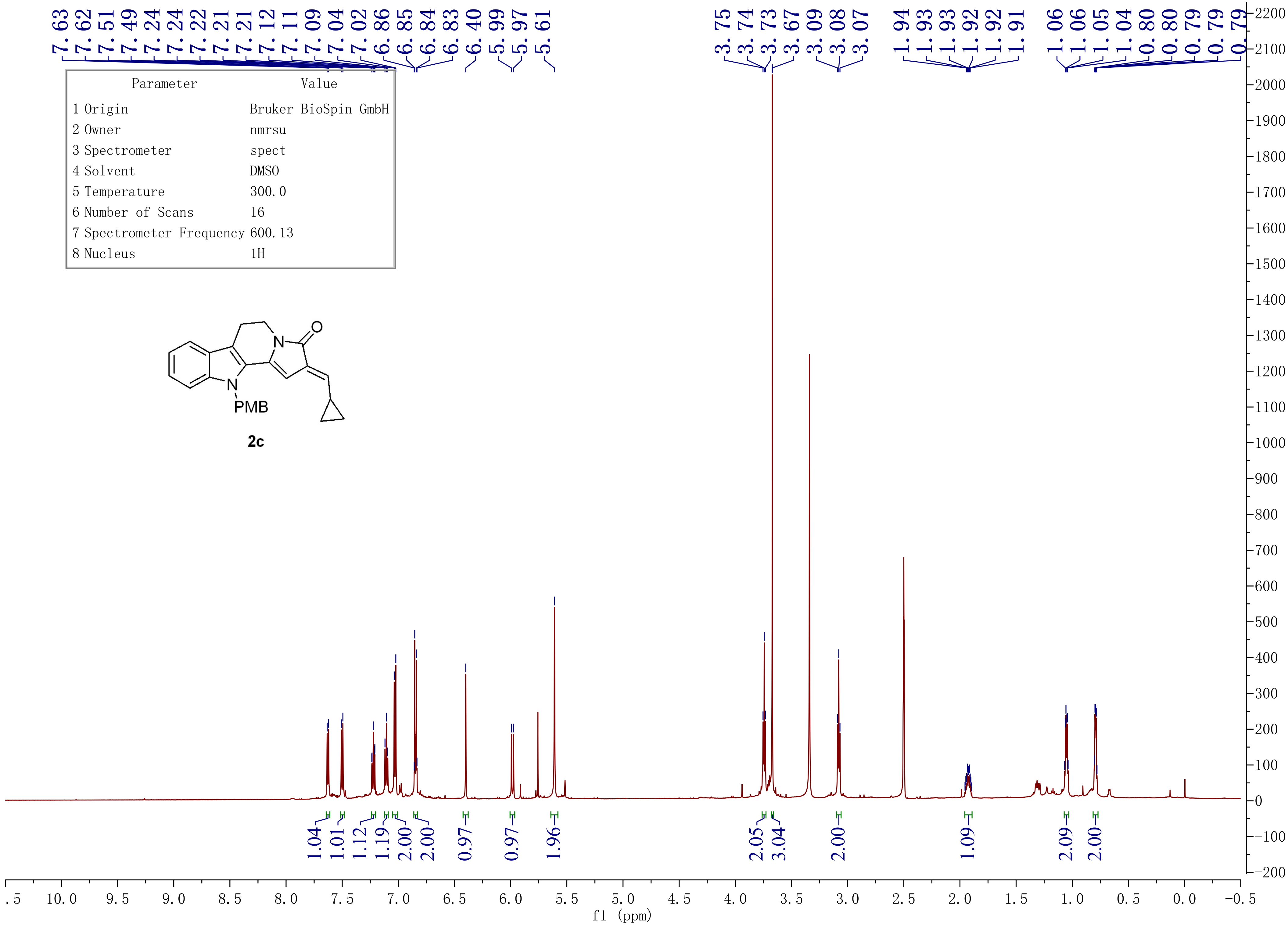
137.68
137.61
134.01
132.58
132.45
128.73
127.29
126.30
126.13
124.82
123.85
118.84
114.02
112.08
94.61
47.08
36.64
19.95
15.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 62
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Cl
N
Bn
N
O
Me
2a
f1 (ppm)

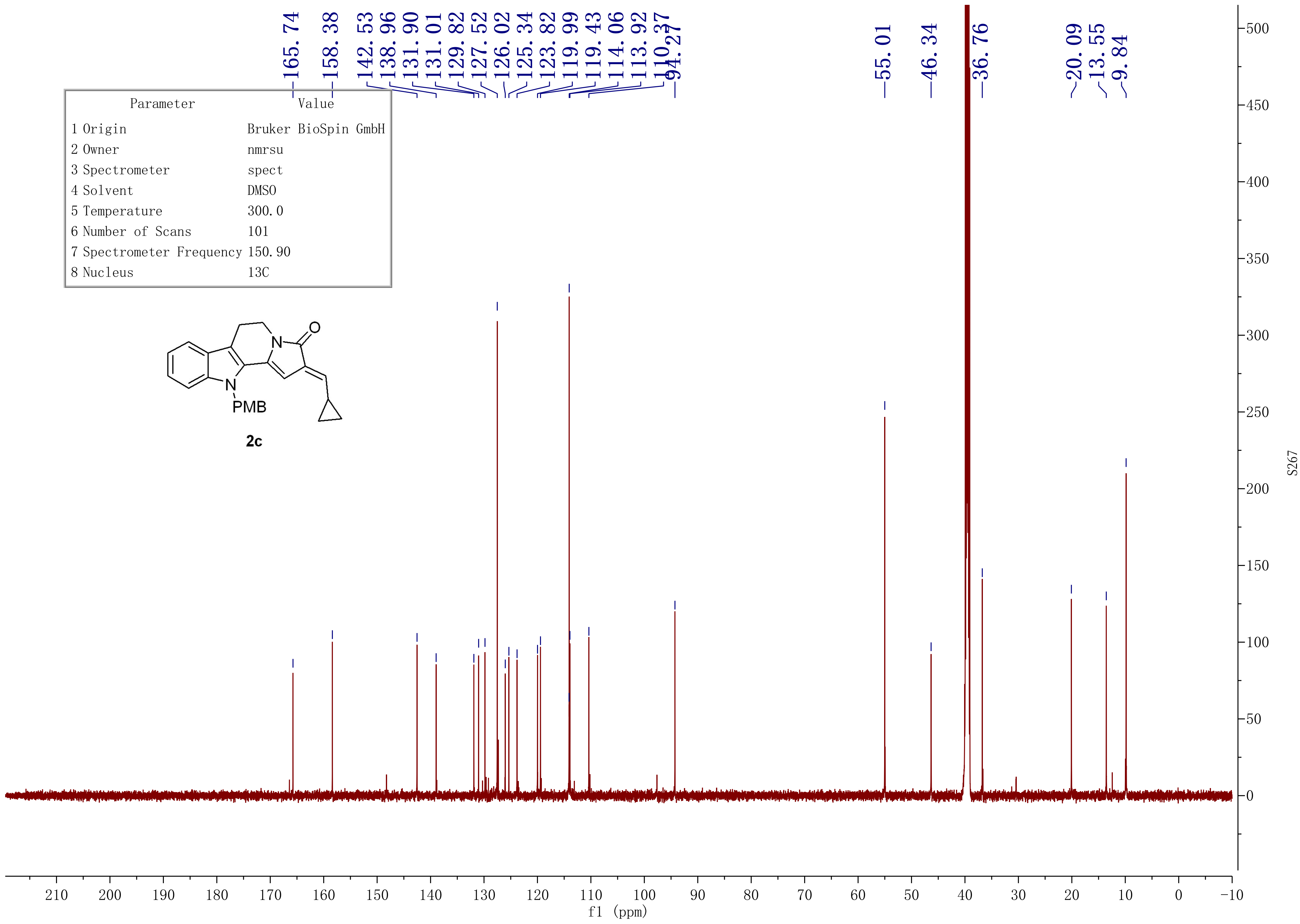

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Bn
N
O
2b
7.65 7.64 7.50 7.49 7.30 7.29 7.28 7.24 7.23 7.22 7.20 7.13 7.12 7.11 7.08 7.07 6.35 5.98 5.96 5.69
3.76 3.75 3.74 3.10 3.09 3.08 1.90 1.89 1.89 1.88 1.88 1.87 1.05 1.05 1.04 1.03 0.79 0.79 0.78 0.78 0.78
1.06 1.02 2.36 2.50 1.37 2.01 0.94 0.92 1.89 1.99 2.00 0.95 2.03 1.89
f1 (ppm)

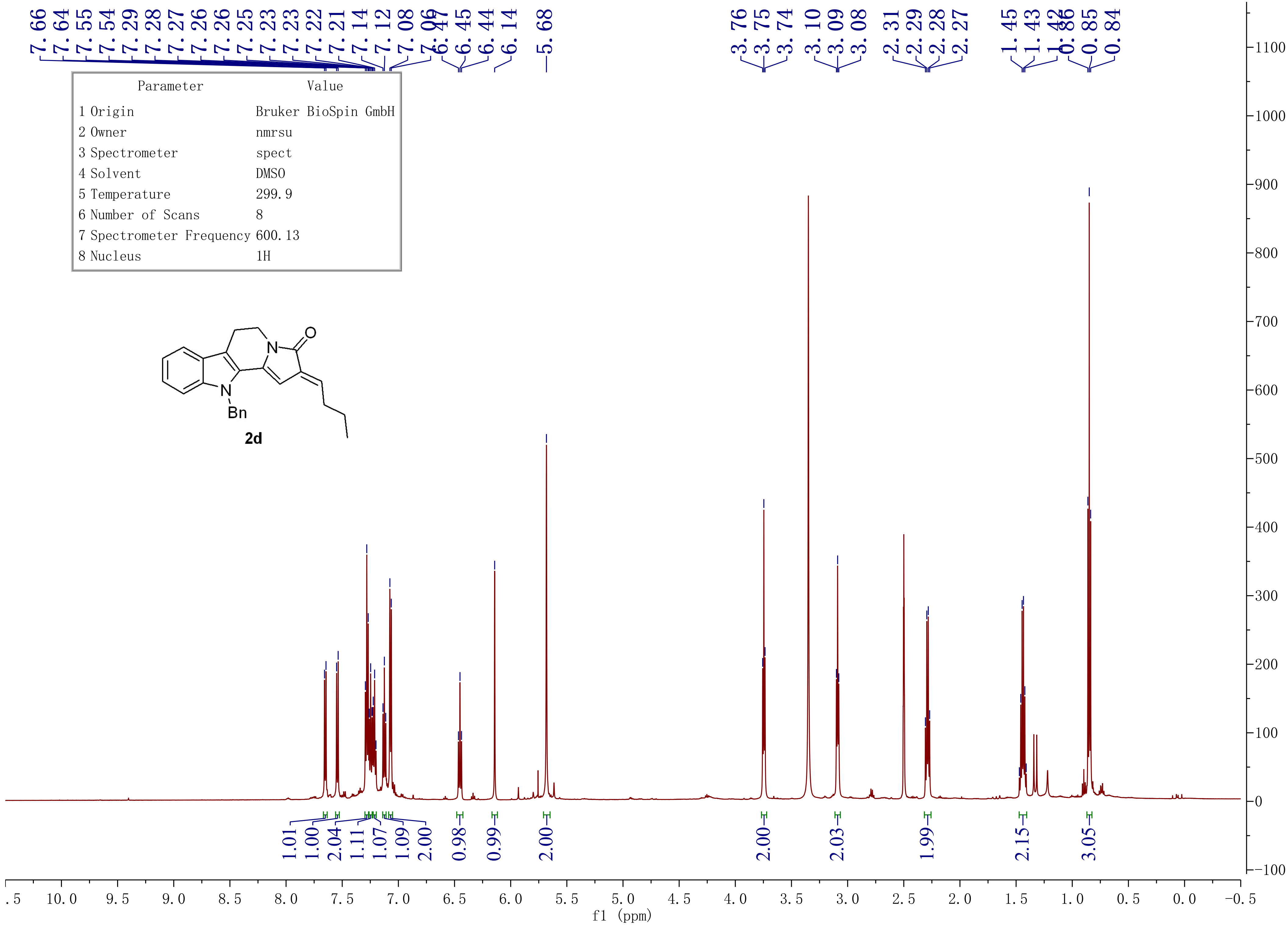
2b

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	241
7 Spectrometer Frequency	150.90
8 Nucleus	13C

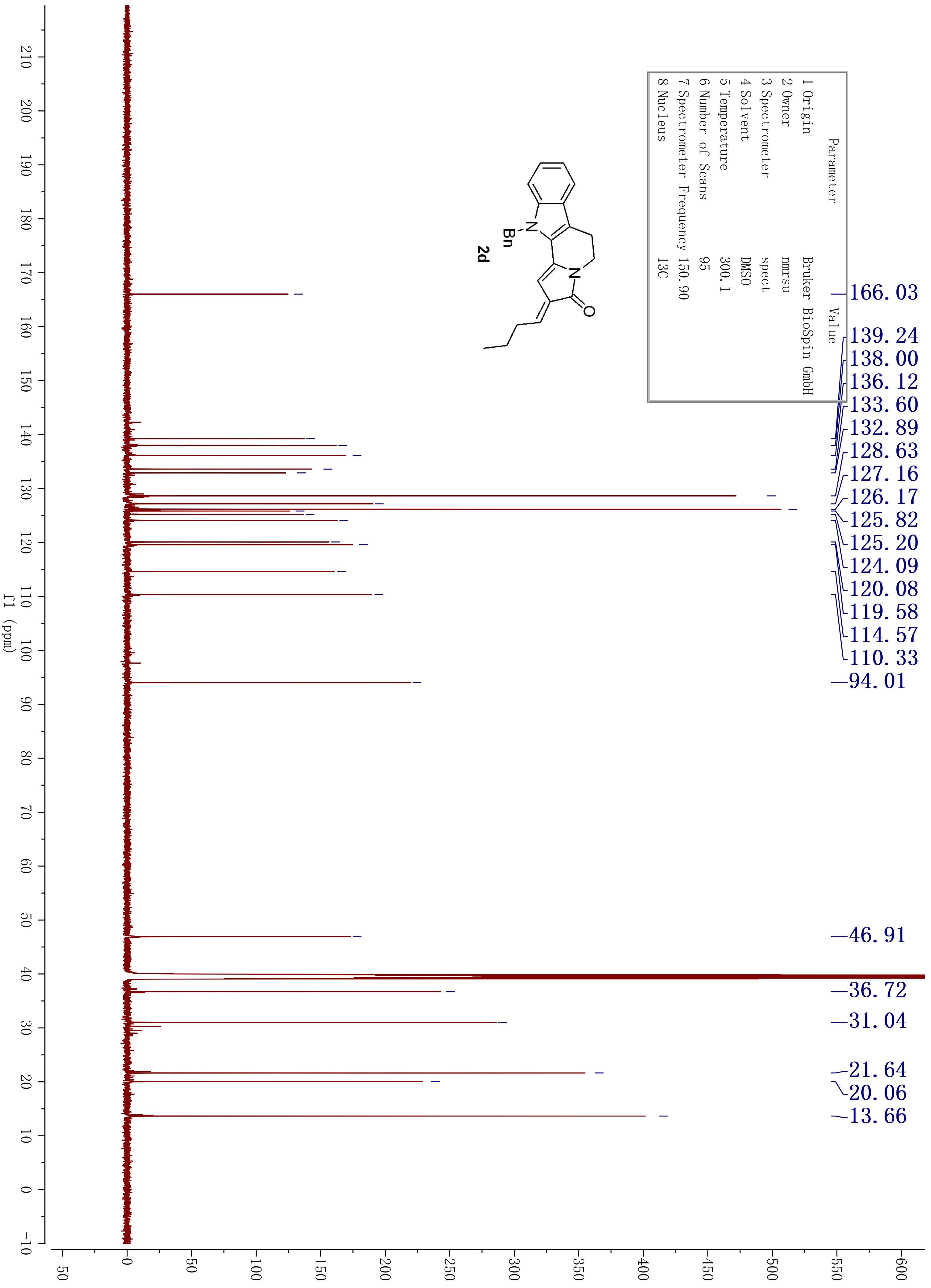


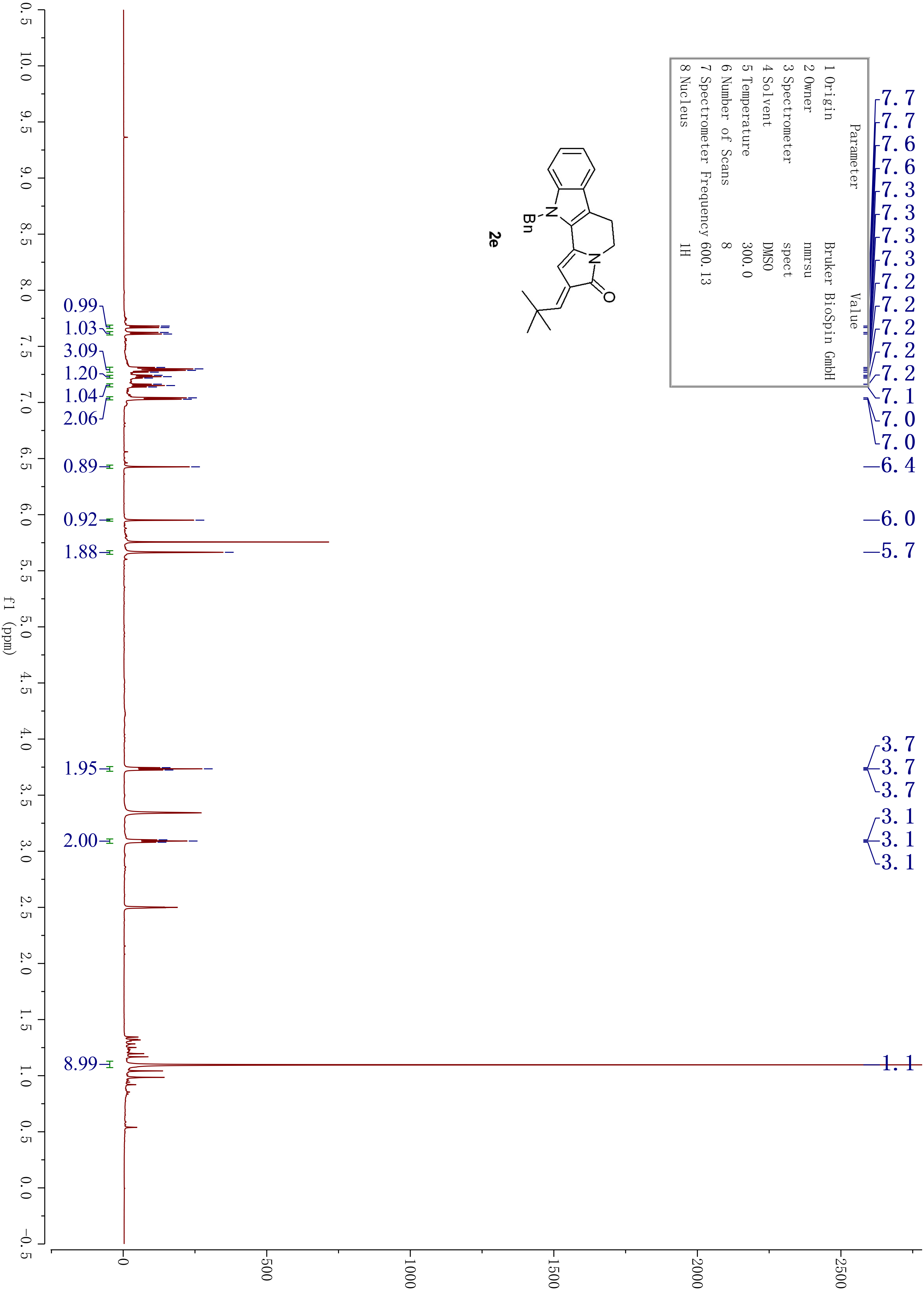

7.63
7.62
7.51
7.49
7.24
7.24
7.22
7.21
7.21
7.12
7.11
7.09
7.04
7.02
6.86
6.85
6.84
6.83
6.40
5.99
5.97
5.61
3.75
3.74
3.73
3.67
3.09
3.08
3.07
1.94
1.93
1.93
1.92
1.92
1.91
1.06
1.06
1.05
1.04
0.80
0.80
0.79
0.79
0.79
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
O
N
PMB
2c
1.04
1.01
1.12
1.19
2.00
2.00
0.97
0.97
1.96
2.05
3.04
2.00
1.09
2.09
2.00
f1 (ppm)

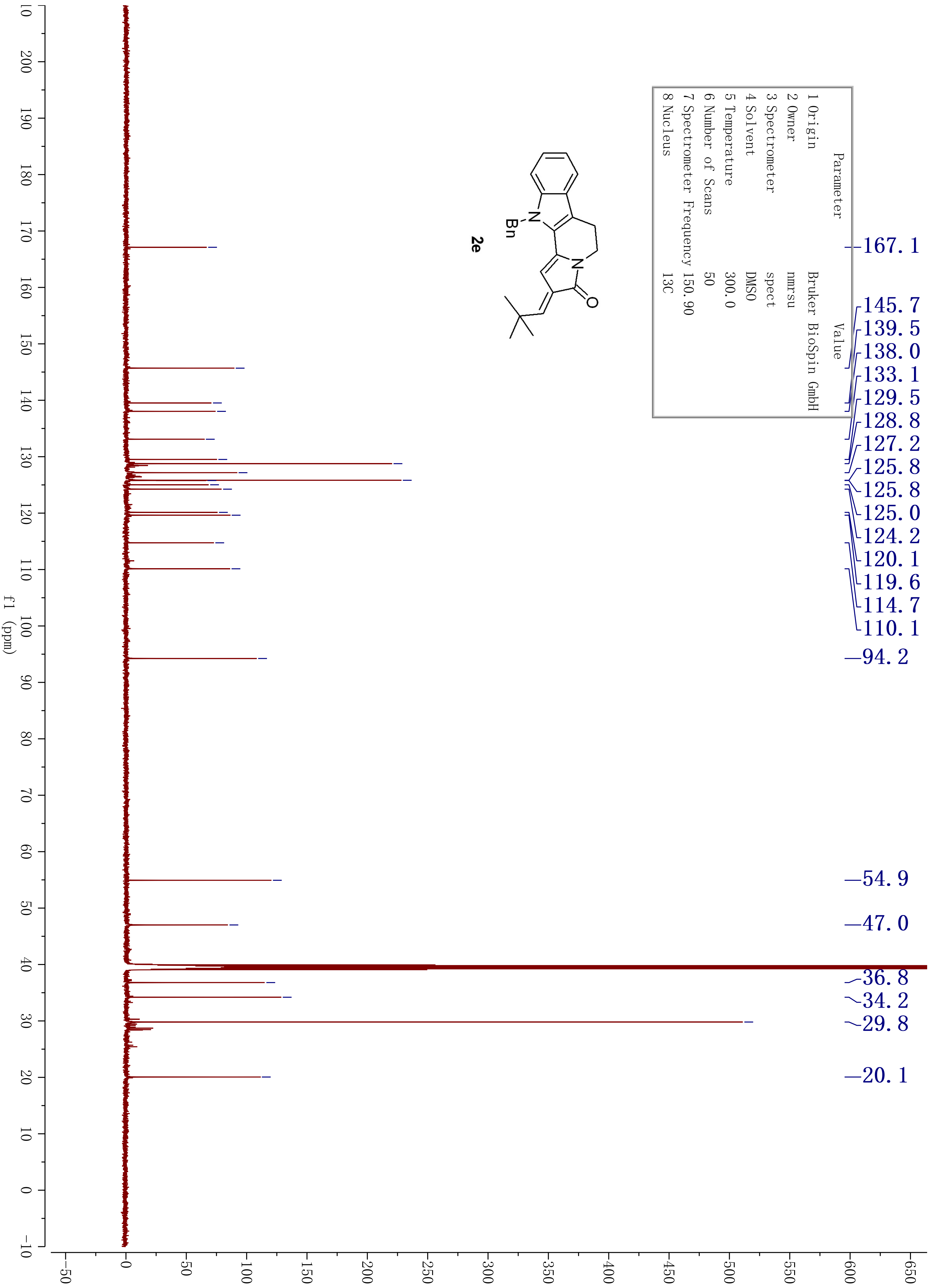

165.74
158.38
142.53
138.96
131.90
131.01
129.82
127.52
126.02
125.34
123.82
119.99
119.43
114.06
113.92
110.37
94.27
55.01
46.34
36.76
20.09
13.55
9.84
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 101
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
PMB
N
O
2c
f1 (ppm)



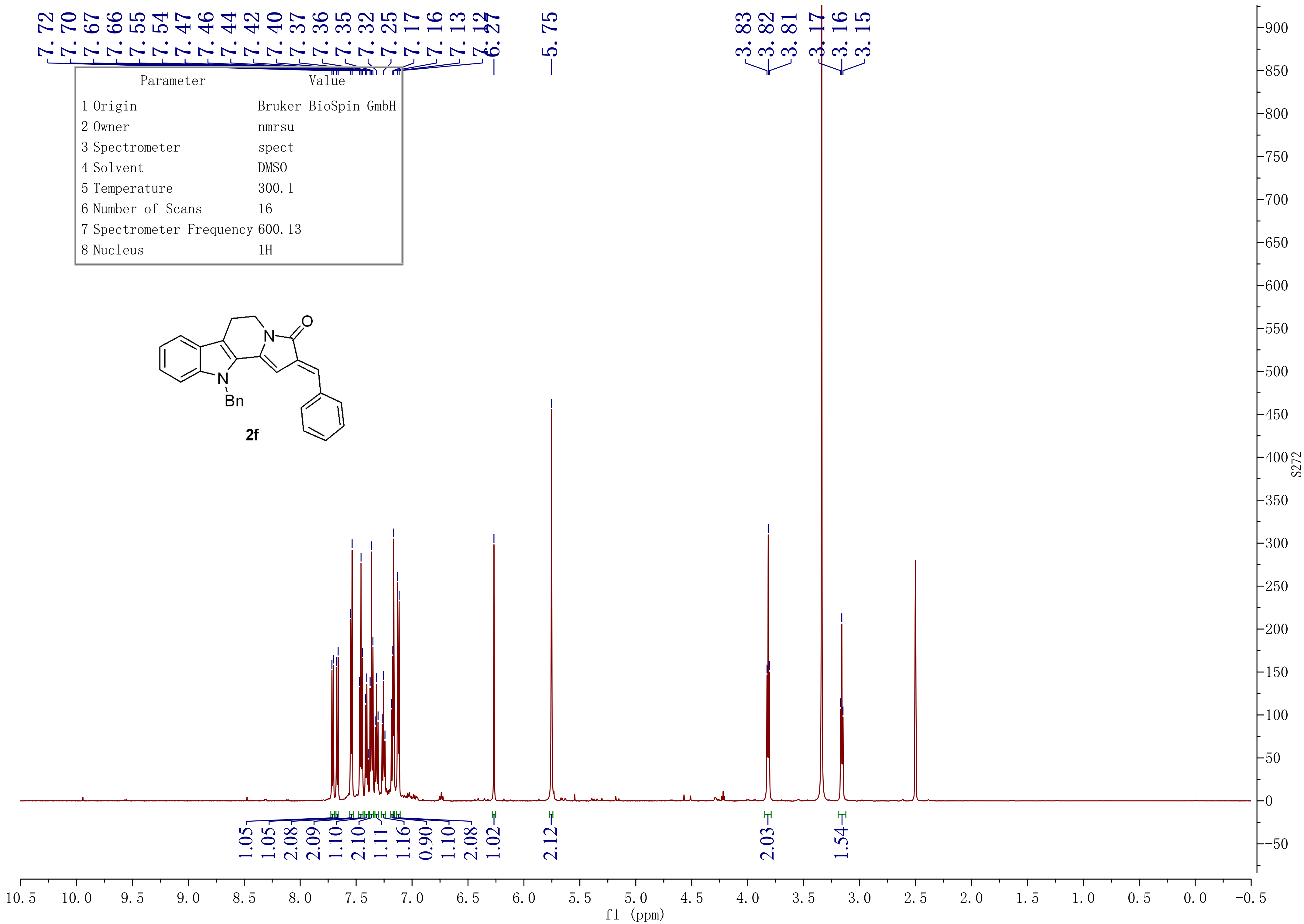
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	299.9
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H

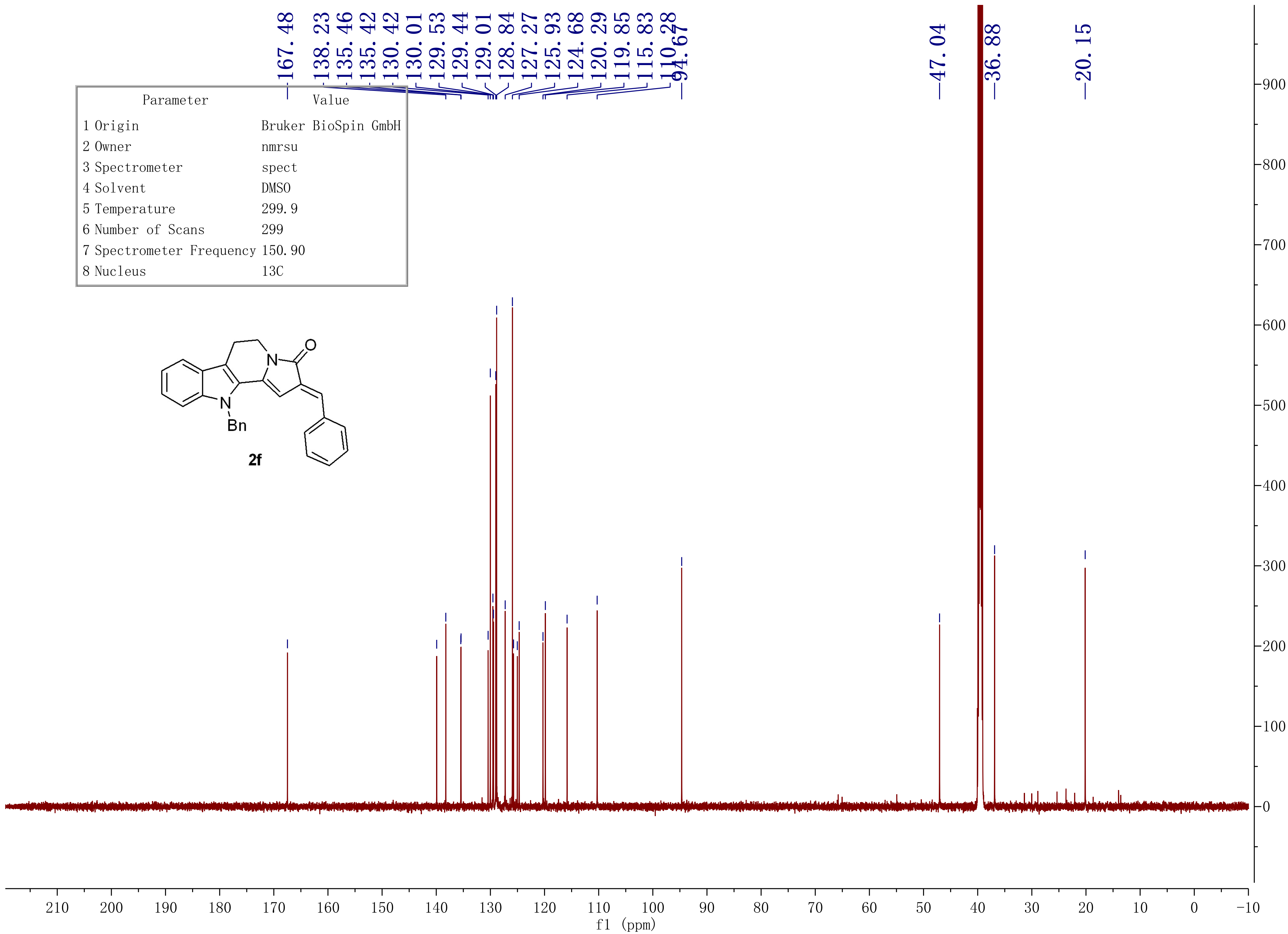

2d
Bn
N
N
O
Parameter | Value
1 Origin | Bruker BioSpin GmbH
2 Owner | nmrsu
3 Spectrometer | spect
4 Solvent | DMSO
5 Temperature | 300.1
6 Number of Scans | 95
7 Spectrometer Frequency | 150.90
8 Nucleus | 13C
166.03
139.24
138.00
136.12
133.60
132.89
128.63
127.16
126.17
125.82
125.20
124.09
120.08
119.58
114.57
110.33
94.01
46.91
36.72
31.04
21.64
20.06
13.66
f1 (ppm)

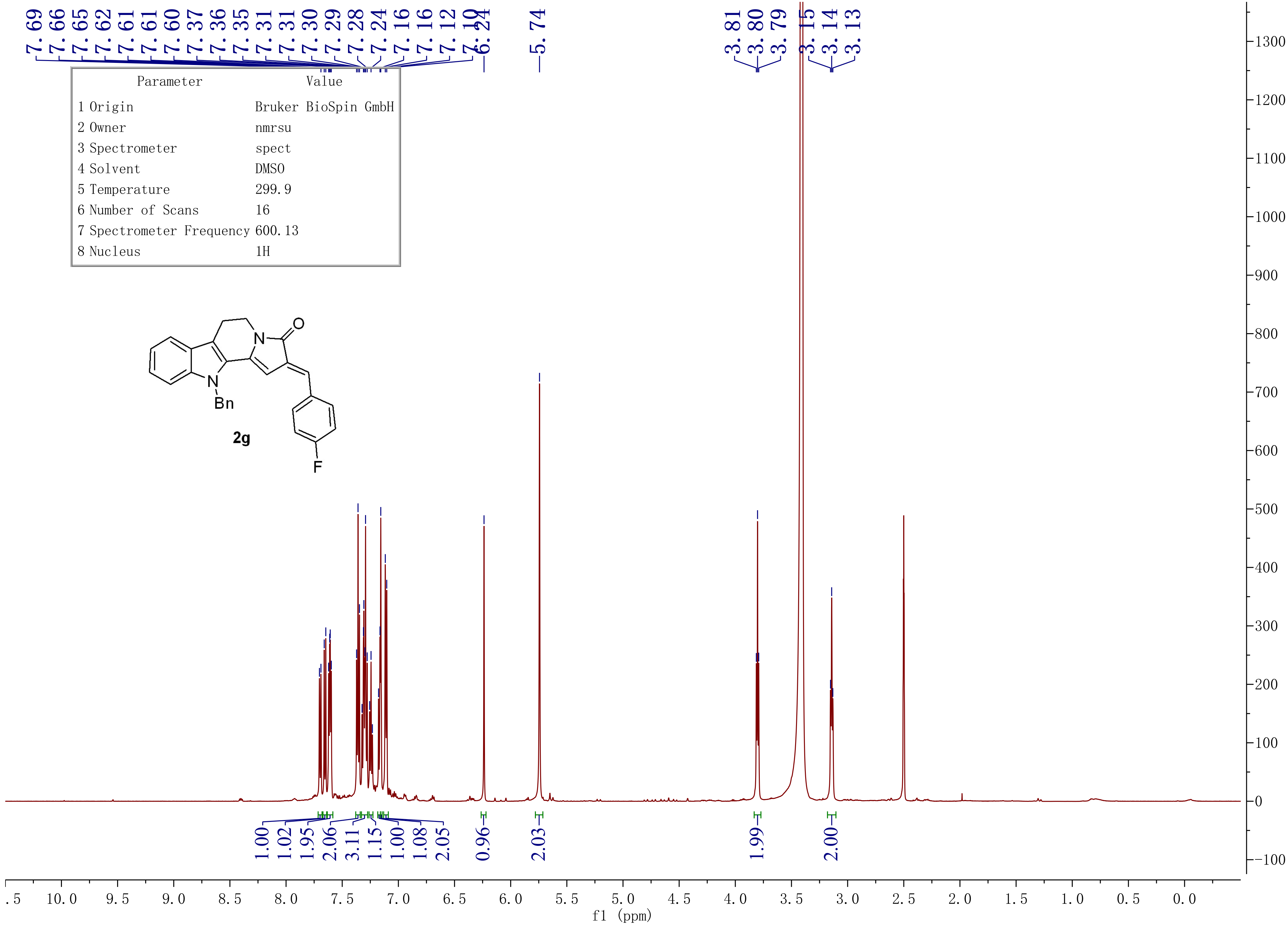

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
2e
f1 (ppm)

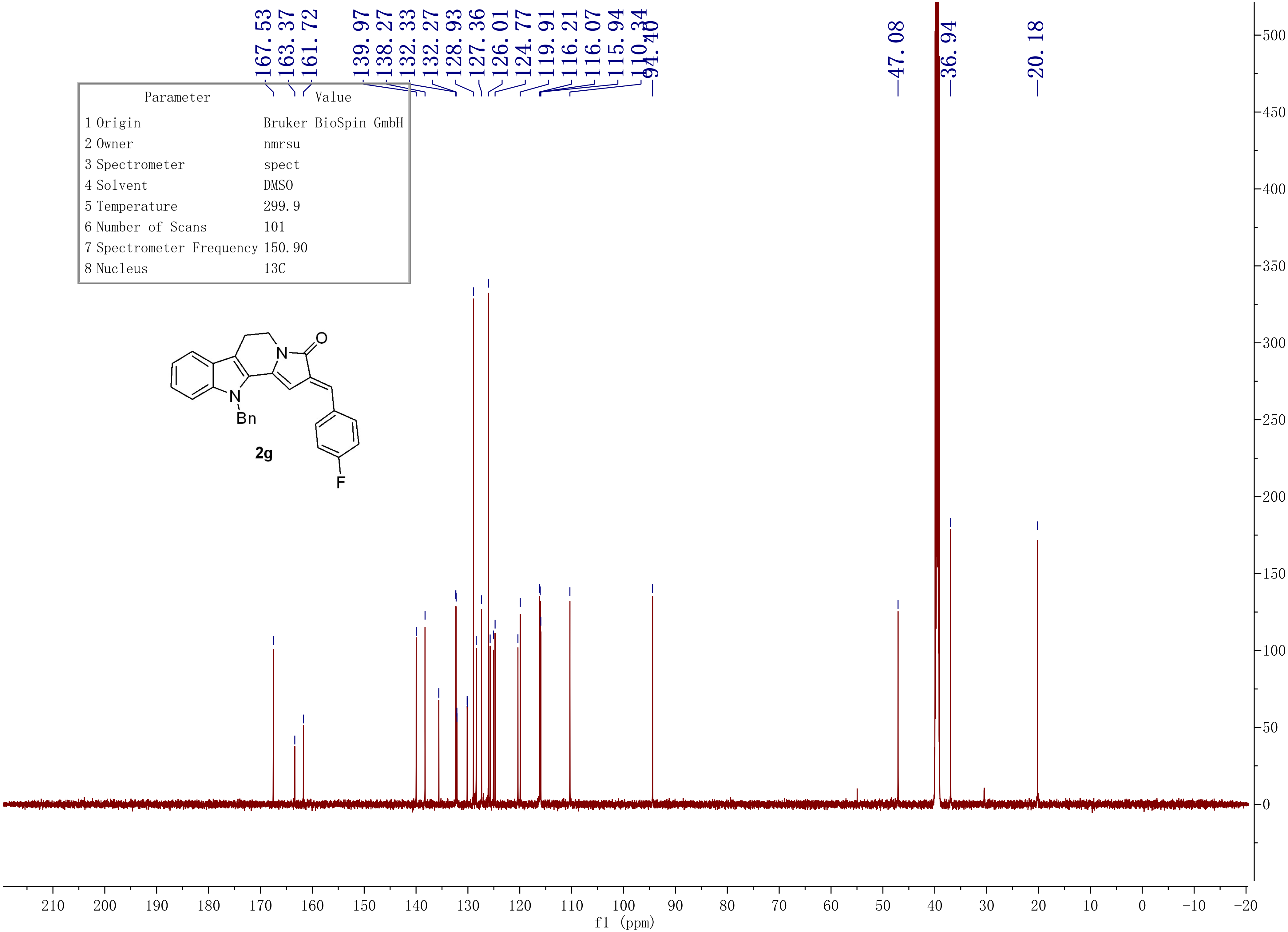


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 50
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Bn
N
N
O
2e
167.1
145.7
139.5
138.0
133.1
129.5
128.8
127.2
125.8
125.8
125.0
124.2
120.1
119.6
114.7
110.1
94.2
54.9
47.0
36.8
34.2
29.8
20.1
f1 (ppm)

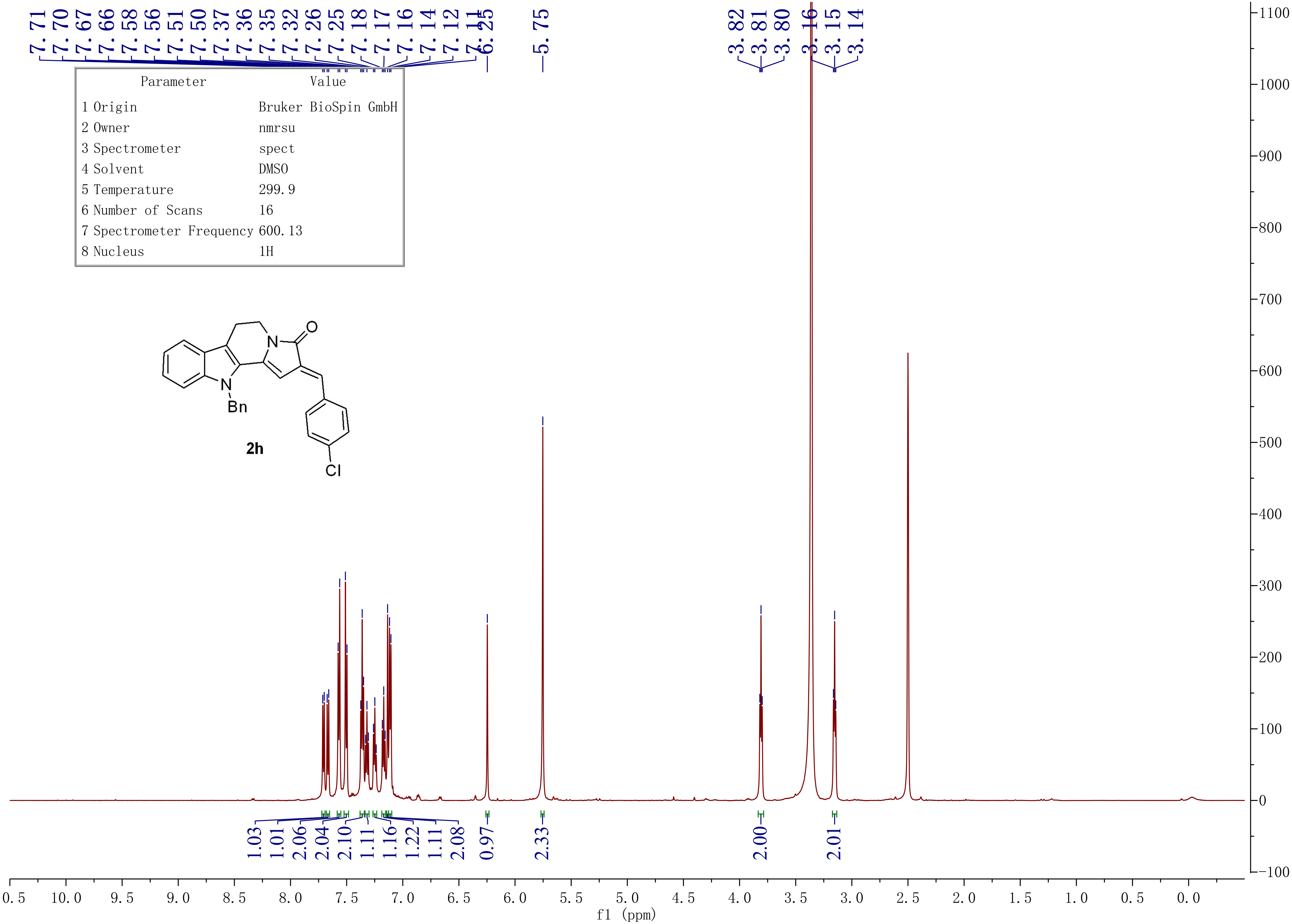

7.72 7.70 7.67 7.66 7.55 7.54 7.47 7.46 7.44 7.42 7.40 7.37 7.36 7.35 7.32 7.25 7.17 7.16 7.13 7.12 6.27
5.75
3.83 3.82 3.81 3.17 3.16 3.15
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Bn
N
O
2f
1.05 1.05 2.08 2.09 1.10 2.10 1.11 1.16 0.90 1.10 2.08 1.02 2.12 2.03 1.54
f1 (ppm)


167.48
138.23
135.46
135.42
130.42
130.01
129.53
129.44
129.01
128.84
127.27
125.93
124.68
120.29
119.85
115.83
110.28
94.67
47.04
36.88
20.15
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 299
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Bn
N
O
2f
f1 (ppm)

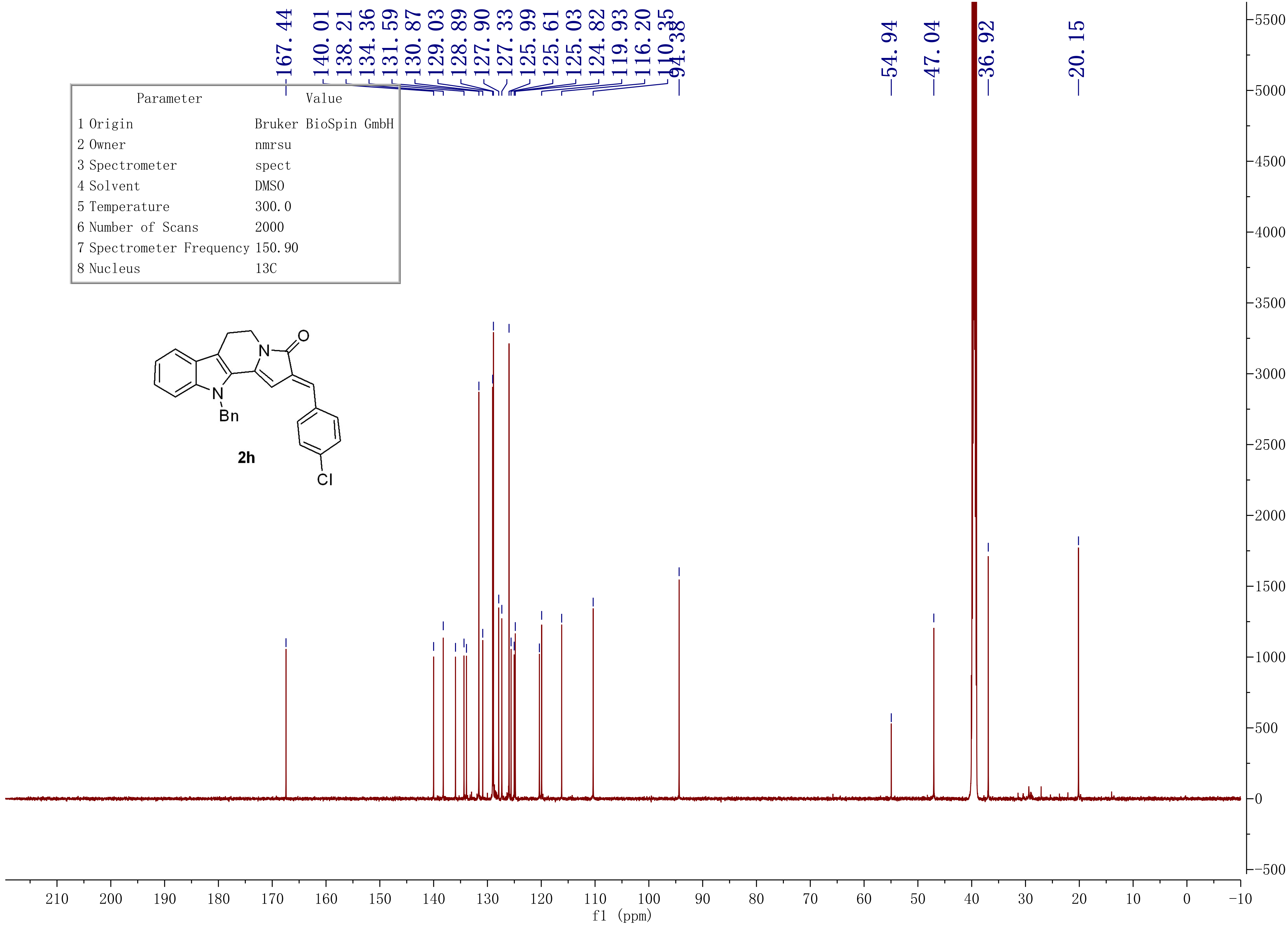

7.69 7.66 7.65 7.62 7.61 7.61 7.60 7.37 7.36 7.35 7.31 7.31 7.30 7.29 7.28 7.24 7.16 7.16 7.12 7.10 6.24 5.74 3.81 3.80 3.79 3.15 3.14 3.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Bn
N
O
F
2g
1.00 1.02 1.95 2.06 3.11 1.15 1.00 1.08 2.05 0.96 2.03 1.99 2.00
f1 (ppm)

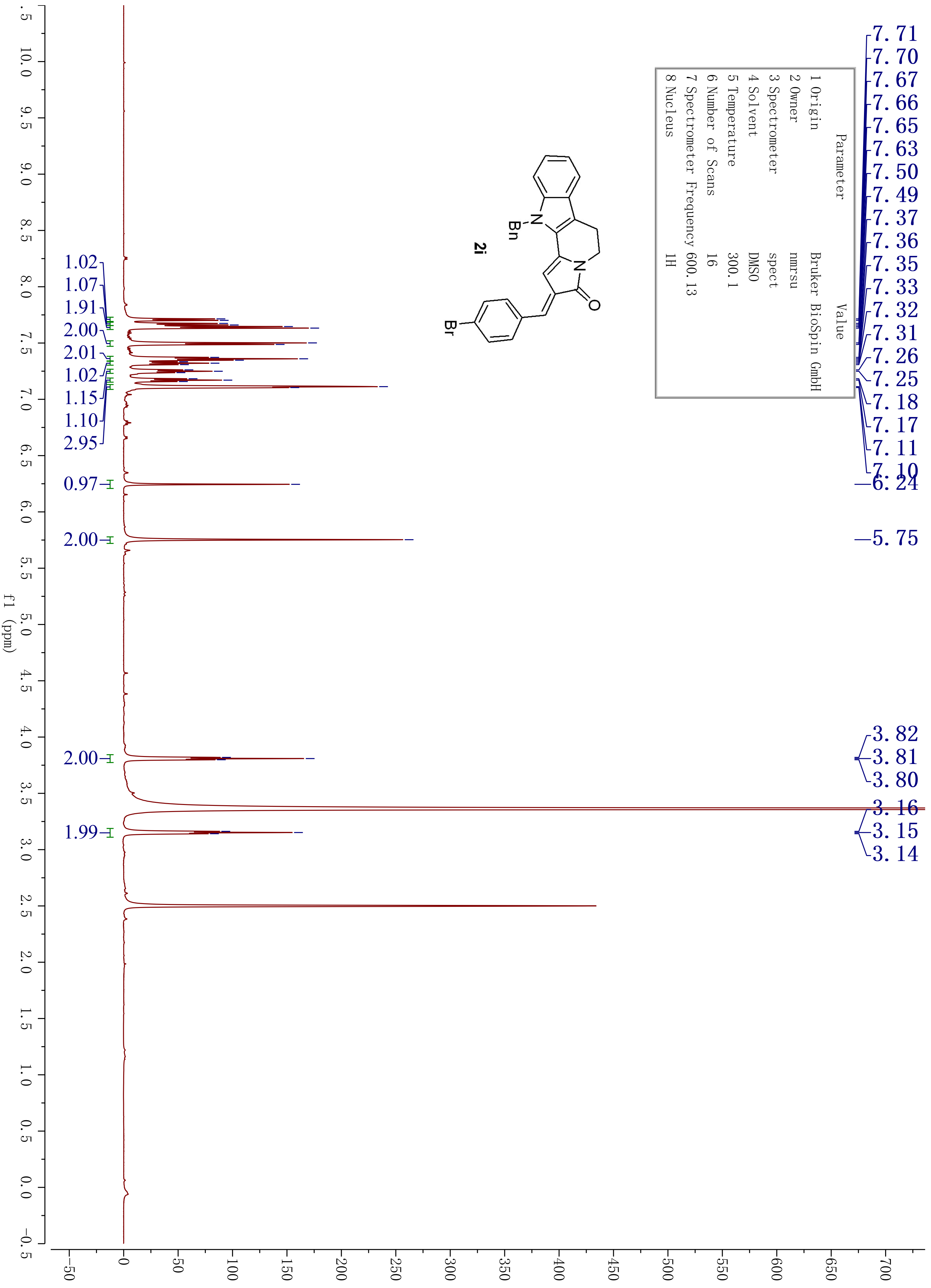

167.53
163.37
161.72
139.97
138.27
132.33
132.27
128.93
127.36
126.01
124.77
119.91
116.21
116.07
115.94
110.34
94.40
47.08
36.94
20.18
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 101
7 Spectrometer Frequency 150.90
8 Nucleus 13C
f1 (ppm)
N
Bn
N
O
F

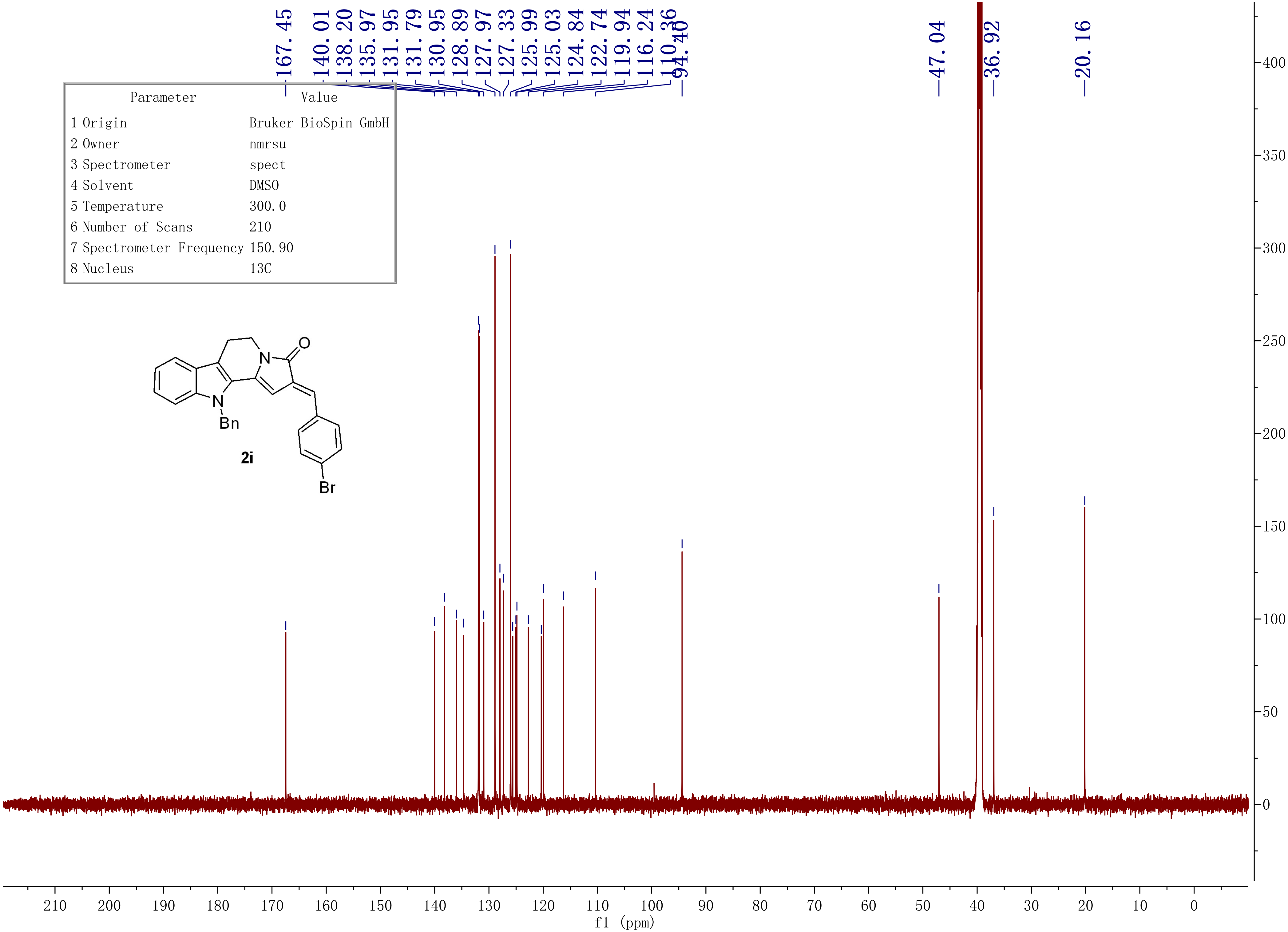
2g



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	299.9
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

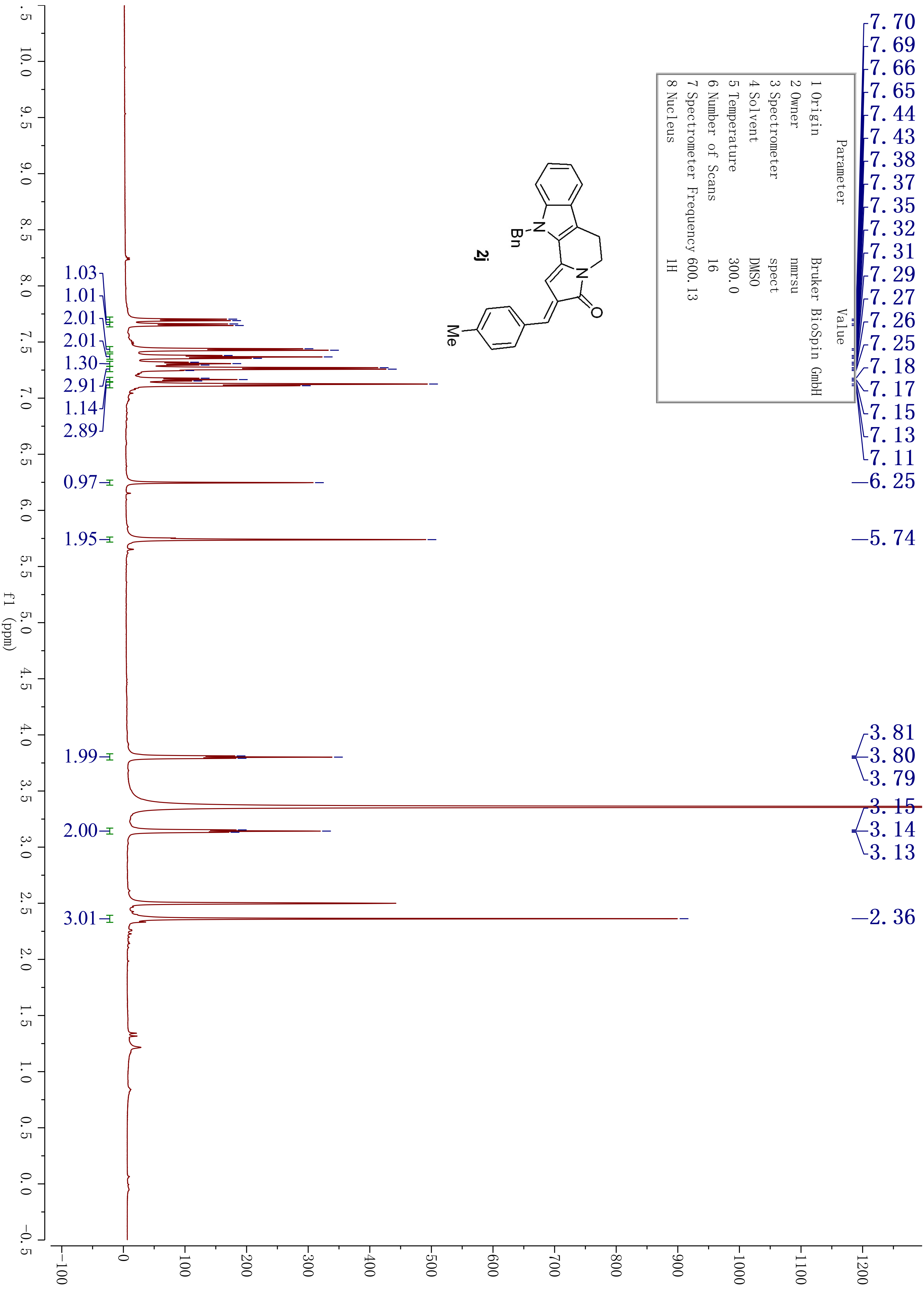

167.44
140.01
138.21
134.36
131.59
130.87
129.03
128.89
127.90
127.33
125.99
125.61
125.03
124.82
119.93
116.20
110.35
94.38
54.94
47.04
36.92
20.15
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 2000
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Bn
N
O
Cl
2h
f1 (ppm)

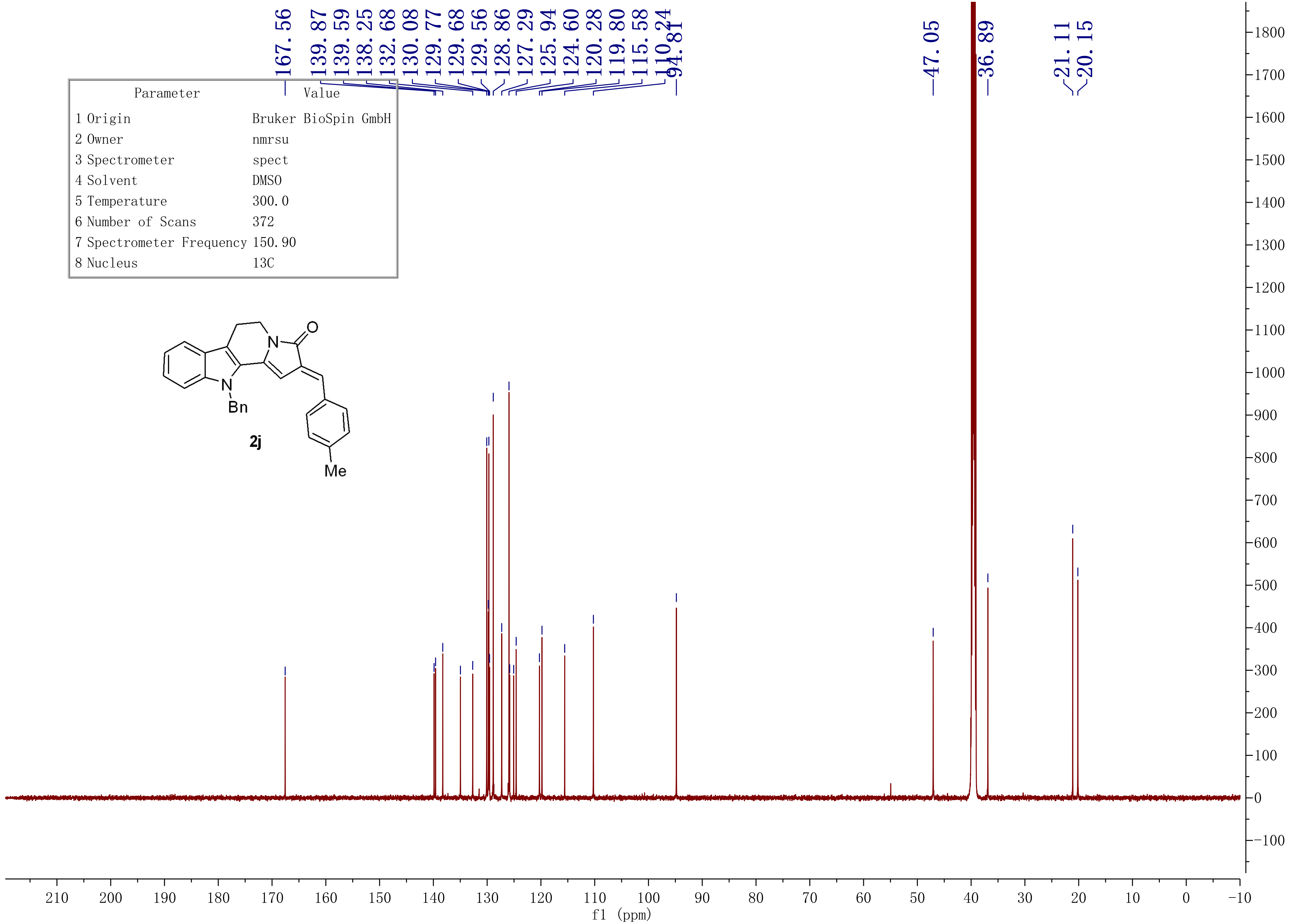

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
2i
Bn
Br
f1 (ppm)

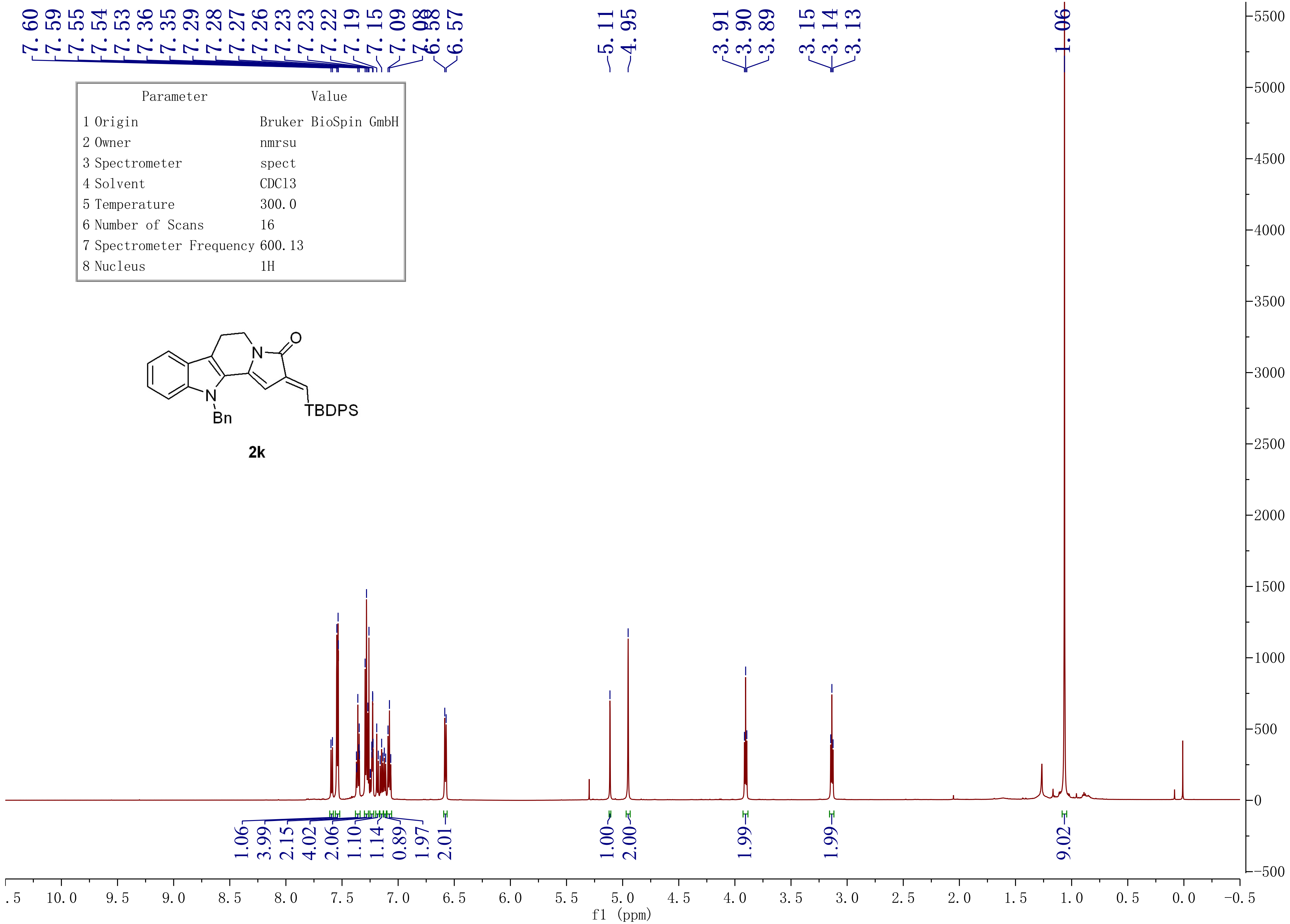


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	210
7 Spectrometer Frequency	150.90
8 Nucleus	13C

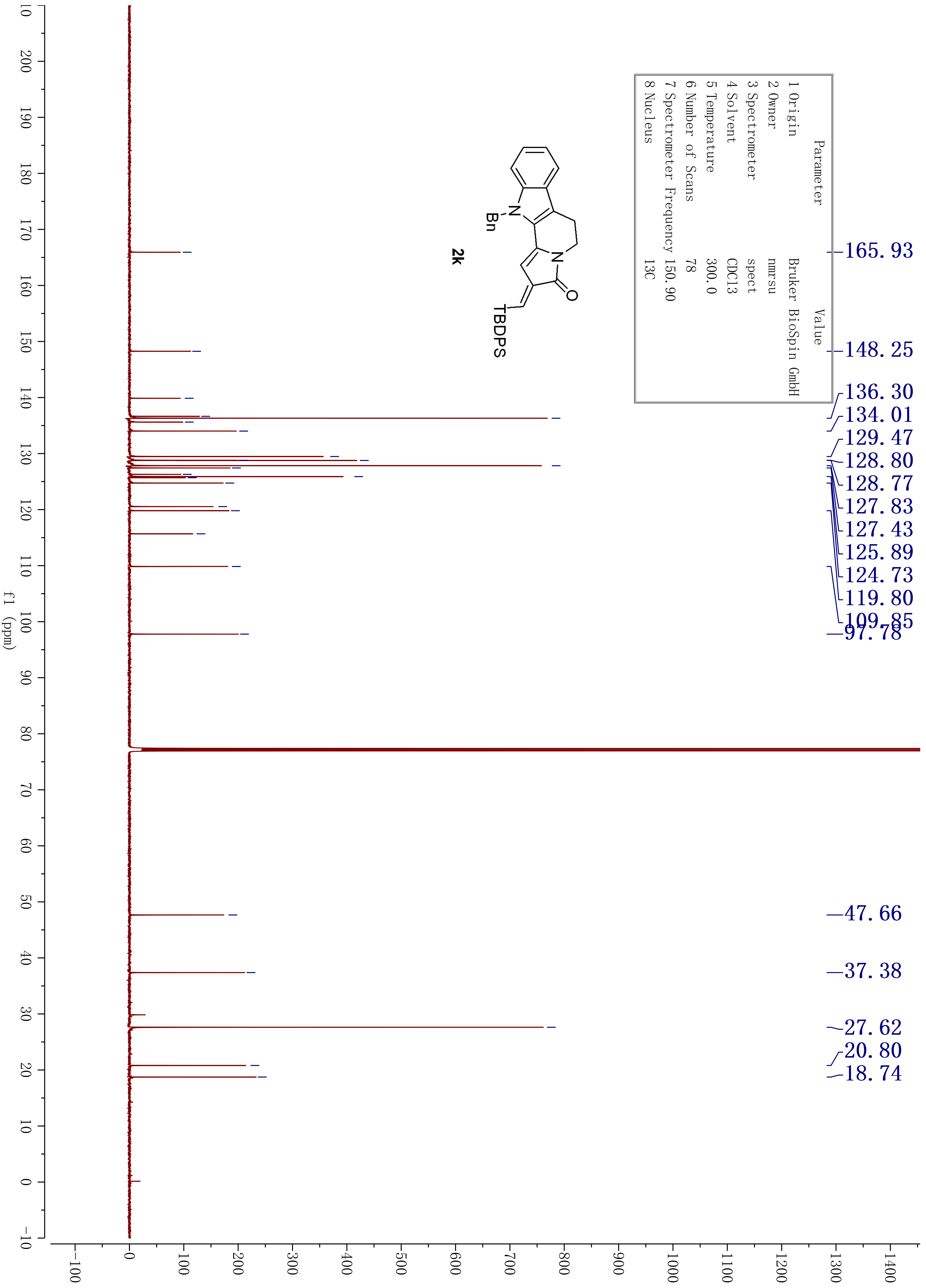
2i

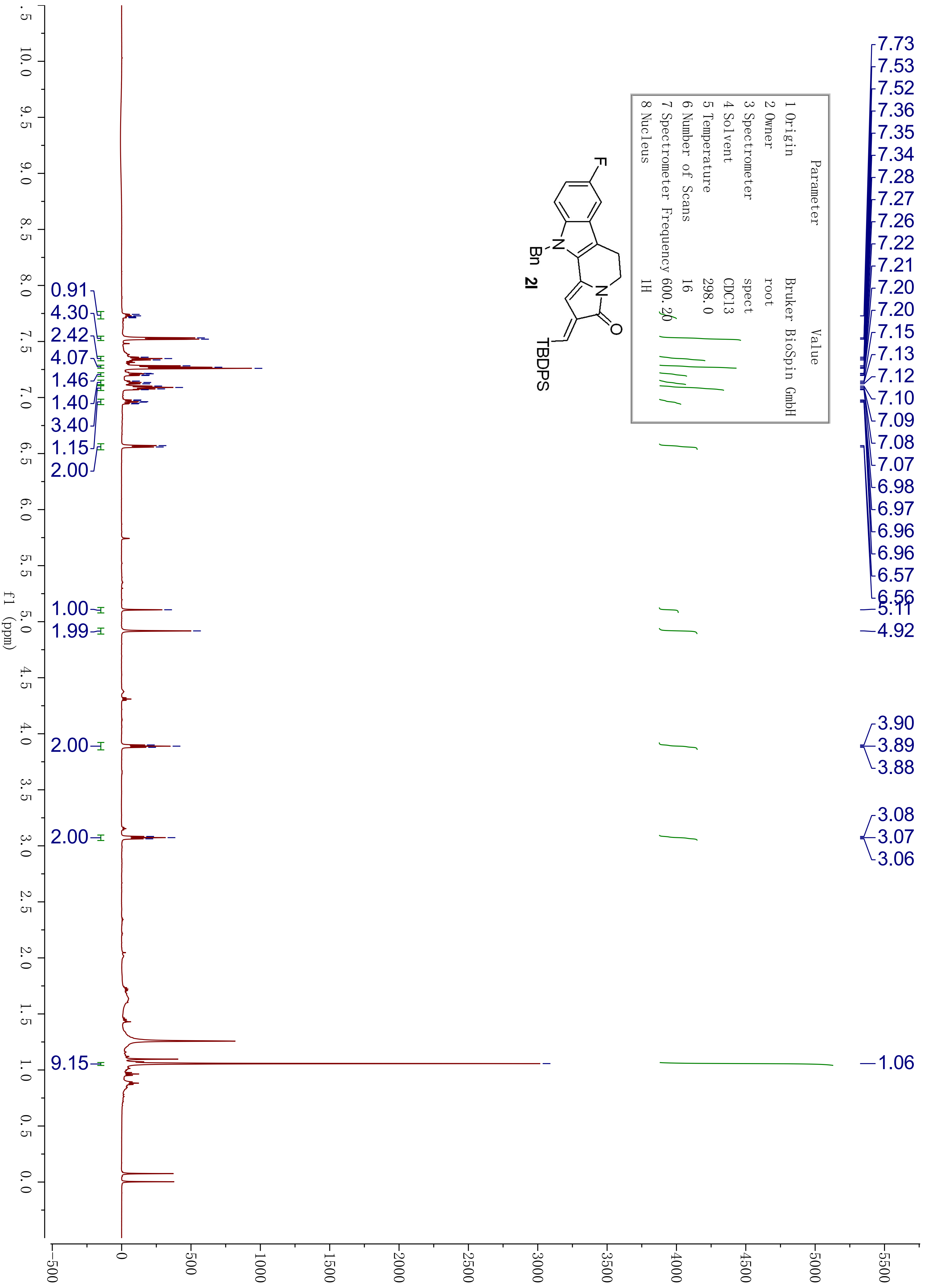

7.70
7.69
7.66
7.65
7.44
7.43
7.38
7.37
7.35
7.32
7.31
7.29
7.27
7.26
7.25
7.18
7.17
7.15
7.13
7.11
6.25
5.74
3.81
3.80
3.79
3.15
3.14
3.13
2.36
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
2j
Bn
N
O
Me
1.03
1.01
2.01
2.01
1.30
2.91
1.14
2.89
0.97
1.95
1.99
2.00
3.01
f1 (ppm)

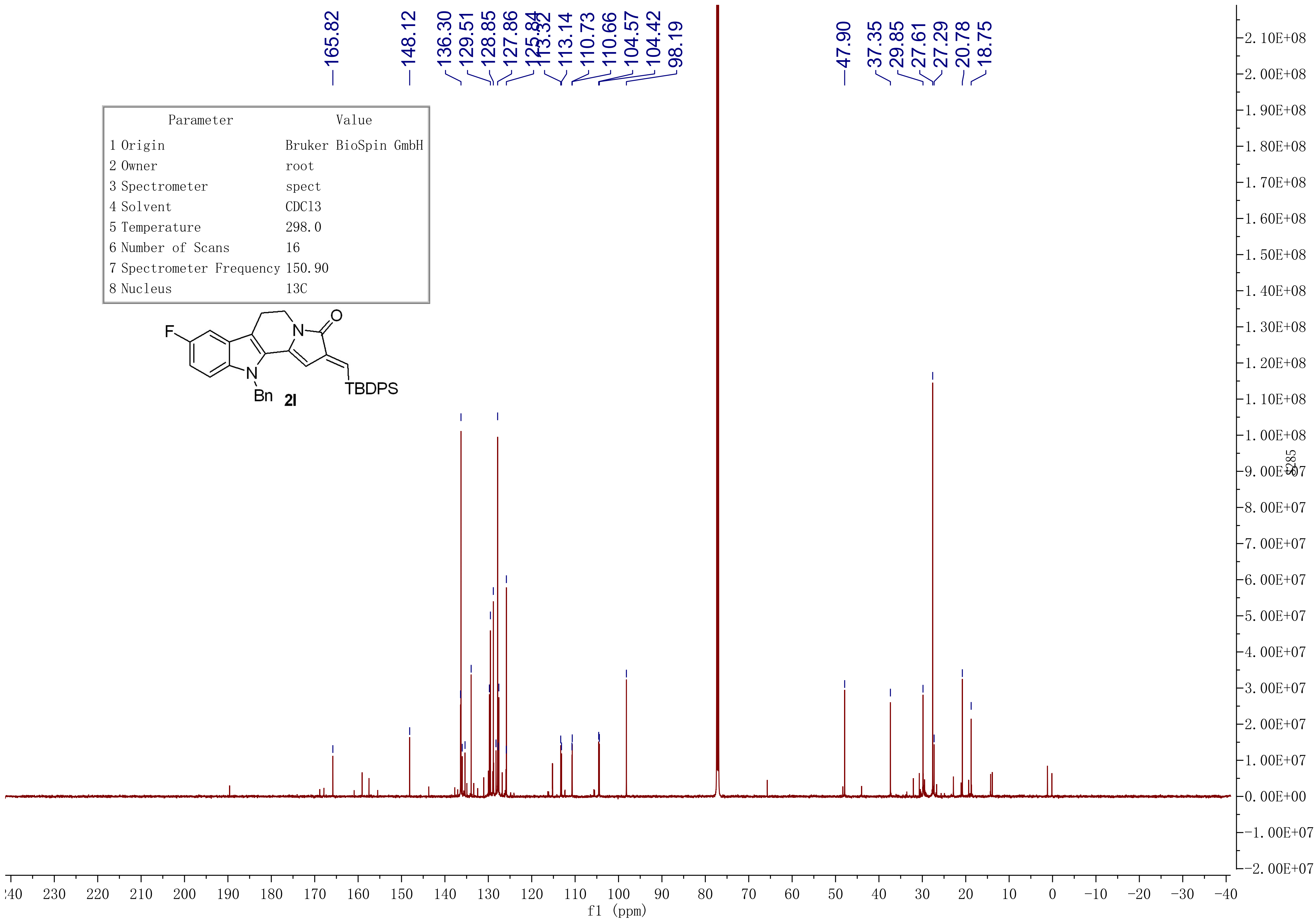

167.56
139.87
139.59
138.25
132.68
130.08
129.77
129.68
129.56
128.86
127.29
125.94
124.60
120.28
119.80
115.58
110.24
94.81
47.05
36.89
21.11
20.15
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 372
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Bn
N
O
Me
2j
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)
1800 1700 1600 1500 1400 1300 1200 1100 1000 900 800 700 600 500 400 300 200 100 0 −100



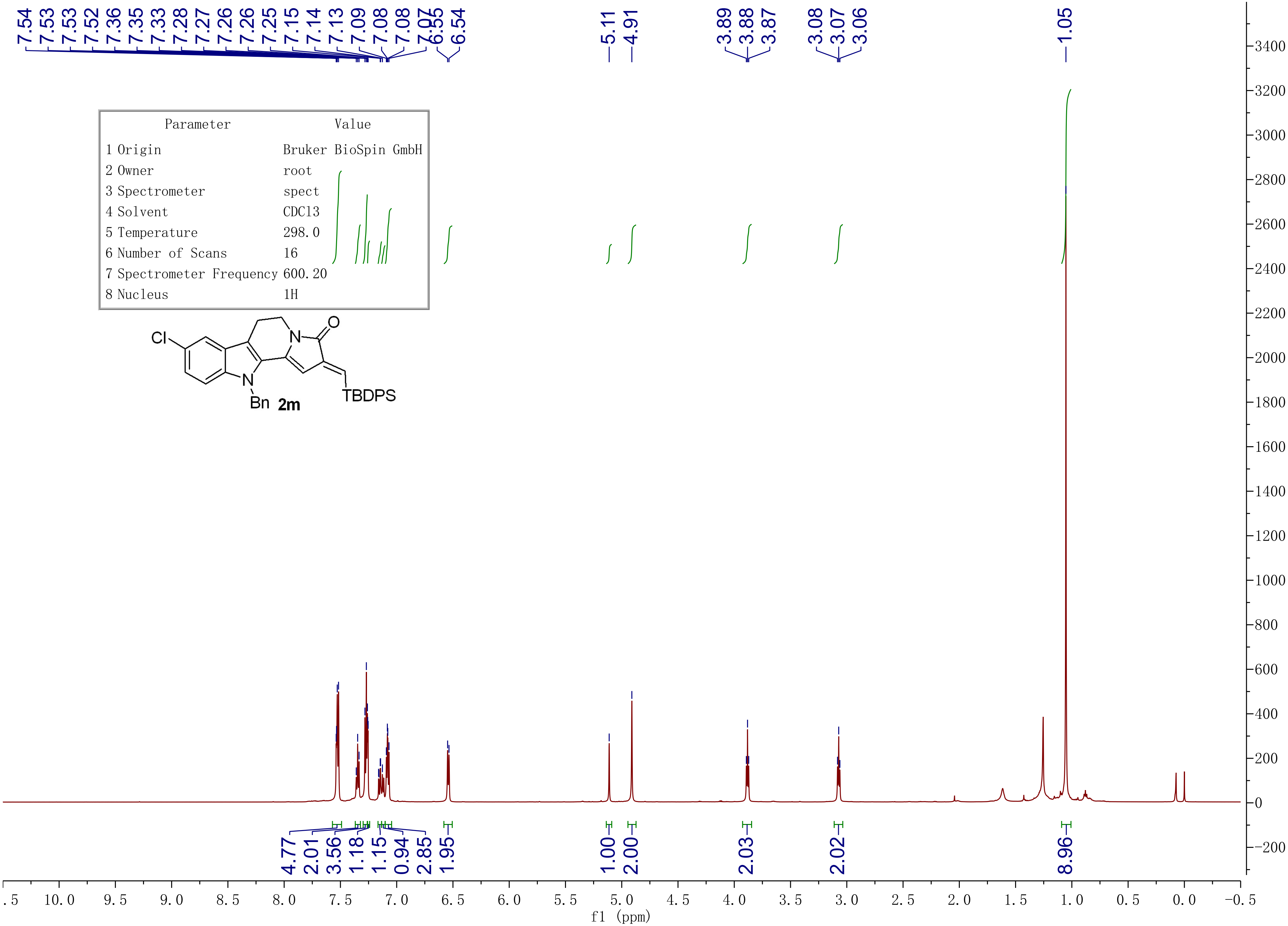
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

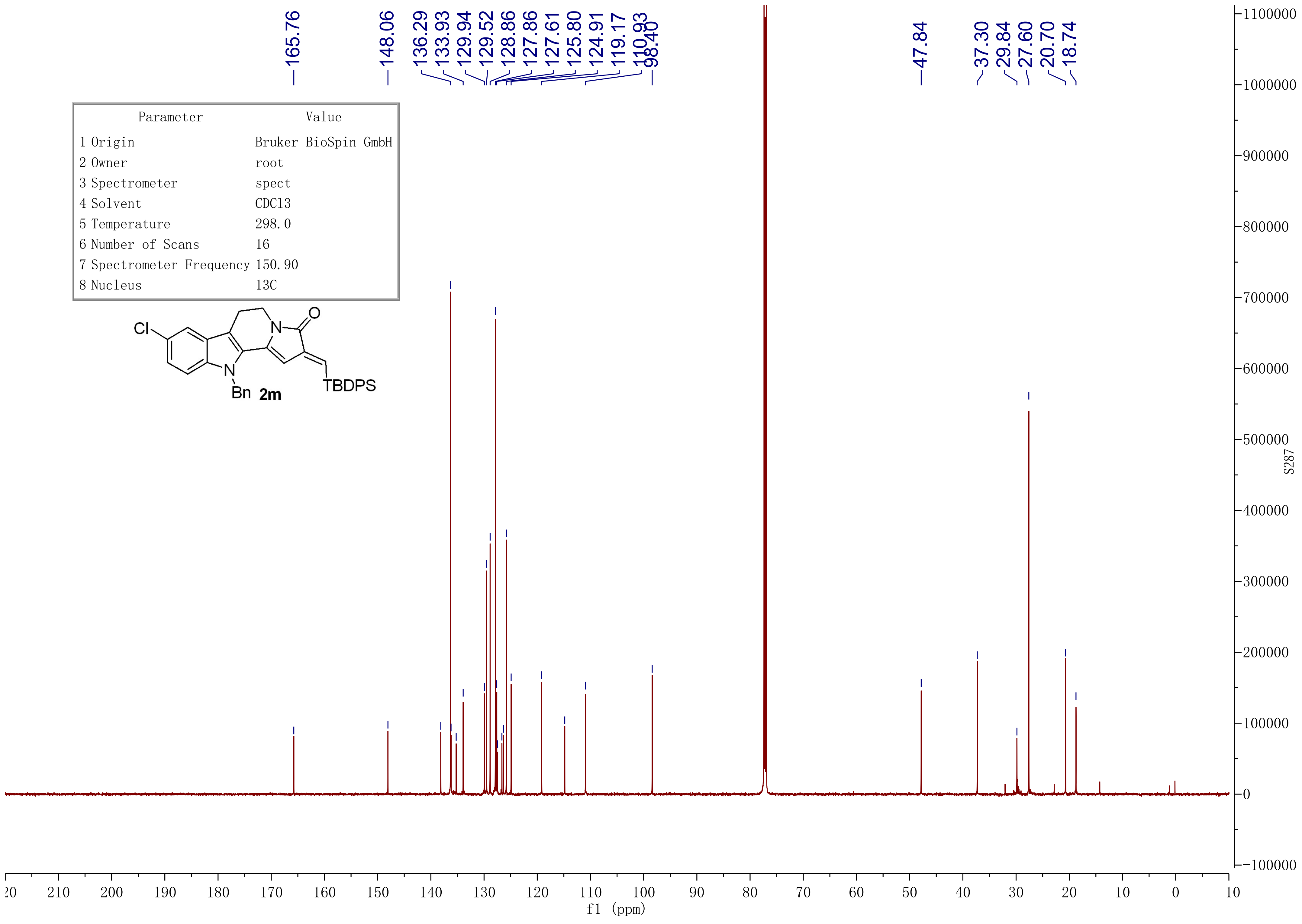

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 78
7 Spectrometer Frequency 150.90
8 Nucleus 13C
2k
TBDPS
Bn
N
N
O
165.93
148.25
136.30
134.01
129.47
128.80
128.77
127.83
127.43
125.89
124.73
119.80
109.85
97.78
47.66
37.38
27.62
20.80
18.74
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
2l
TBDPS
f1 (ppm)

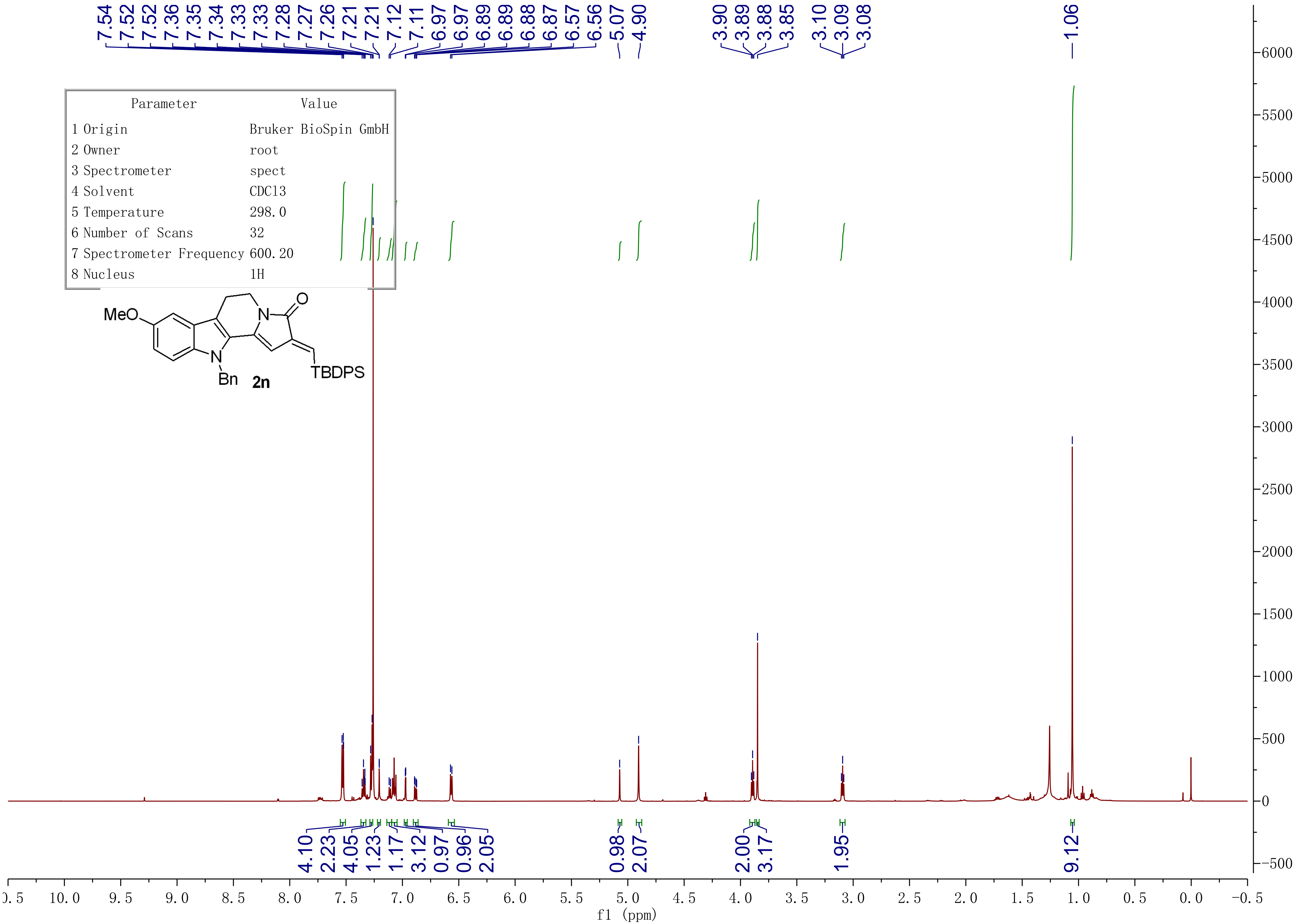


165.82
148.12
136.30
129.51
128.85
127.86
125.84
113.32
113.14
110.73
110.66
104.57
104.42
98.19
47.90
37.35
29.85
27.61
27.29
20.78
18.75
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 150.90
8 Nucleus 13C
F
N
O
N
Bn
TBDPS
2l
f1 (ppm)

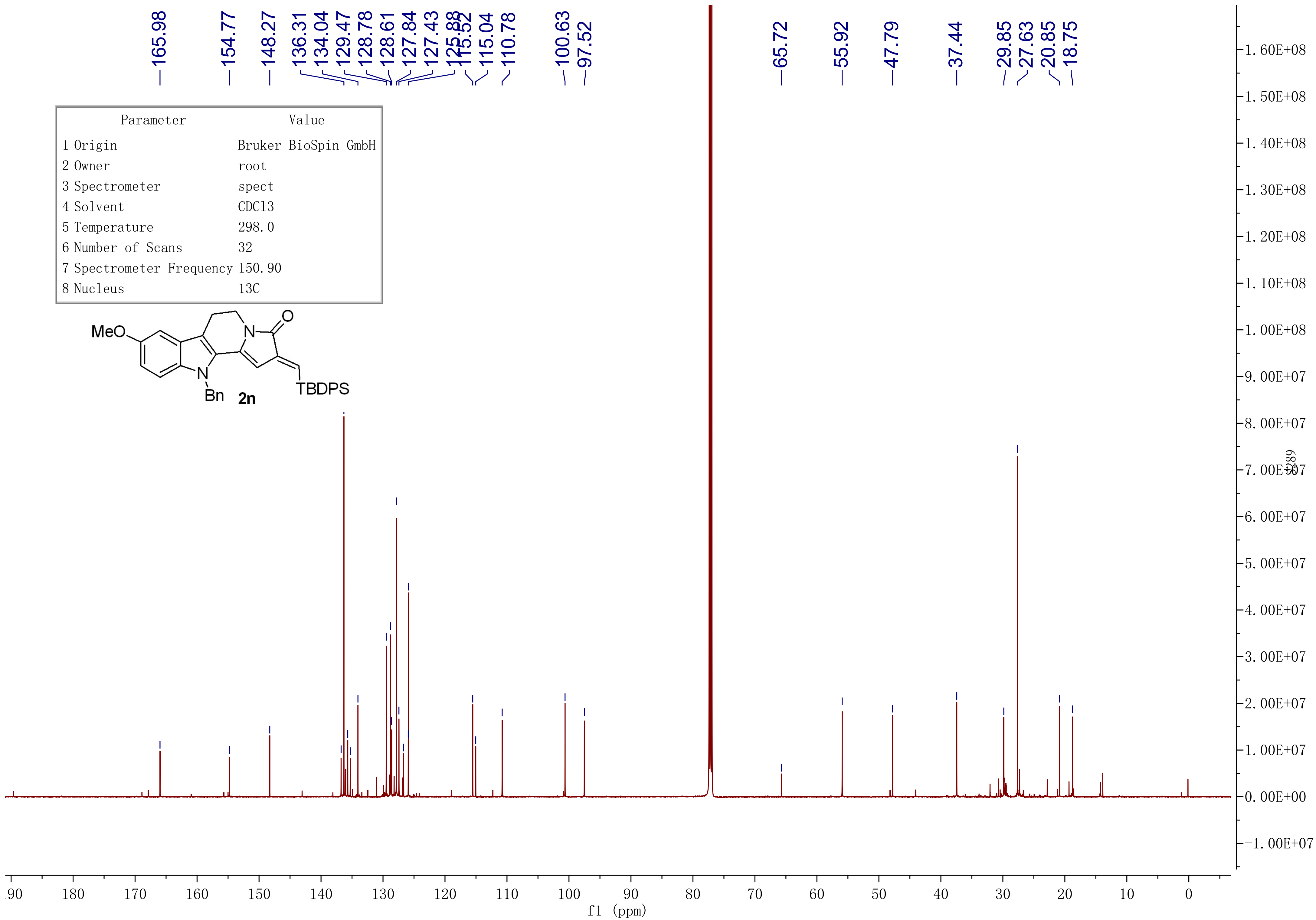

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
Cl
N
O
Bn
2m
TBDPS
7.54 7.53 7.53 7.52 7.36 7.35 7.33 7.28 7.27 7.26 7.26 7.25 7.15 7.14 7.13 7.09 7.08 7.08 7.07 6.55 6.54
5.11 4.91
3.89 3.88 3.87
3.08 3.07 3.06
1.05
4.77 2.01 3.56 1.18 1.15 0.94 2.85 1.95
1.00 2.00
2.03
2.02
8.96
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	298.0
6 Number of Scans	32
7 Spectrometer Frequency	600.20
8 Nucleus	1H



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154.77
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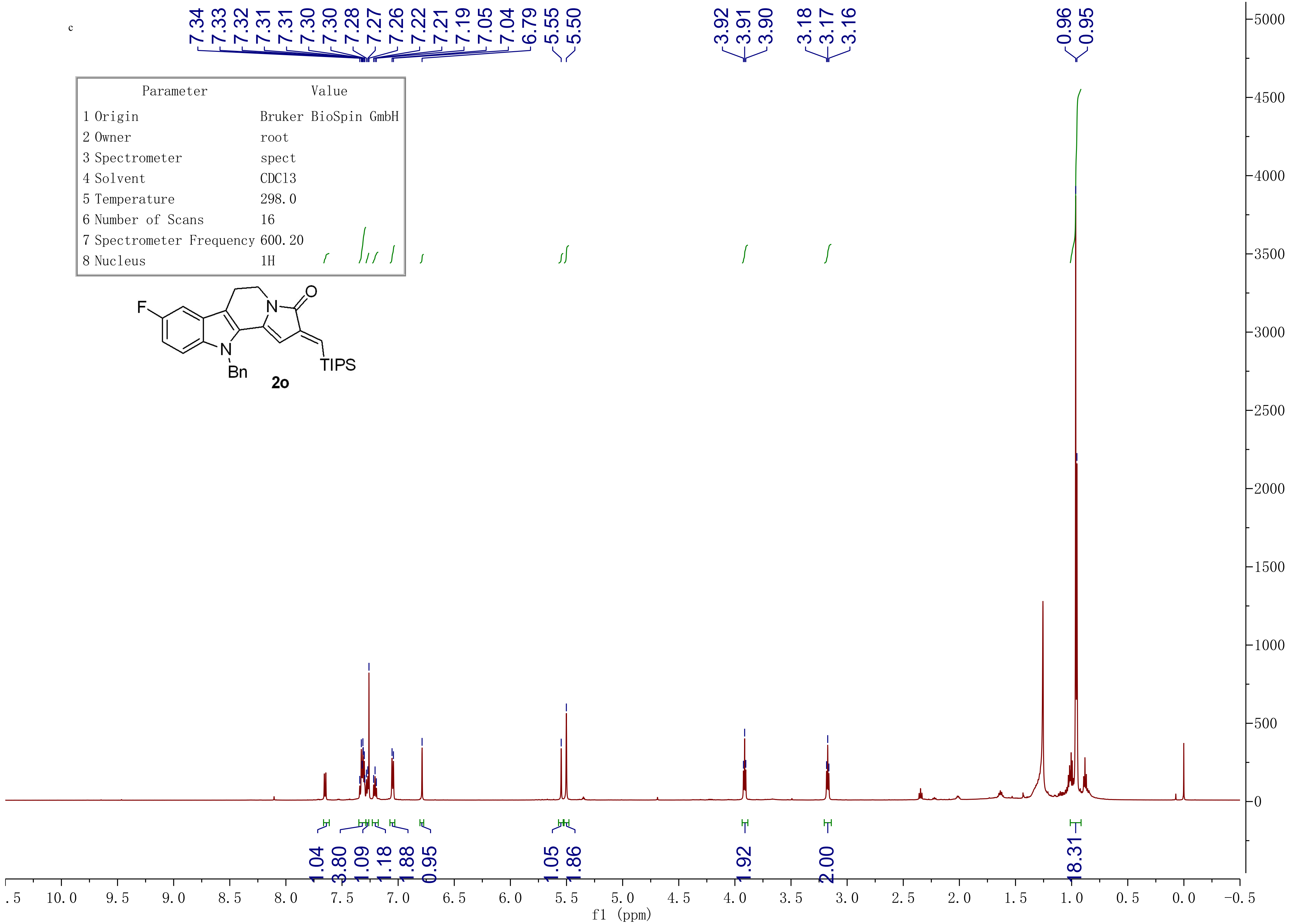
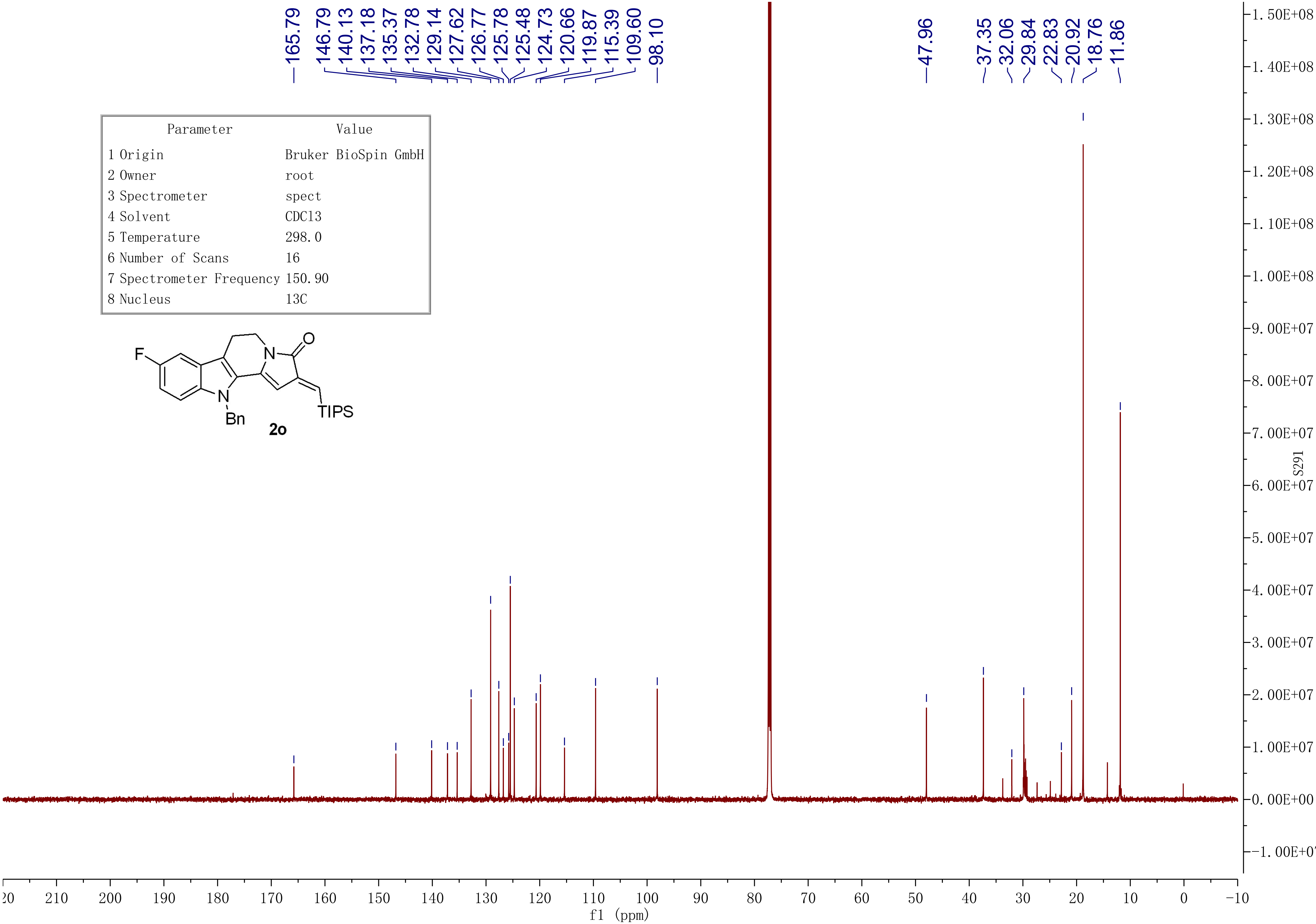
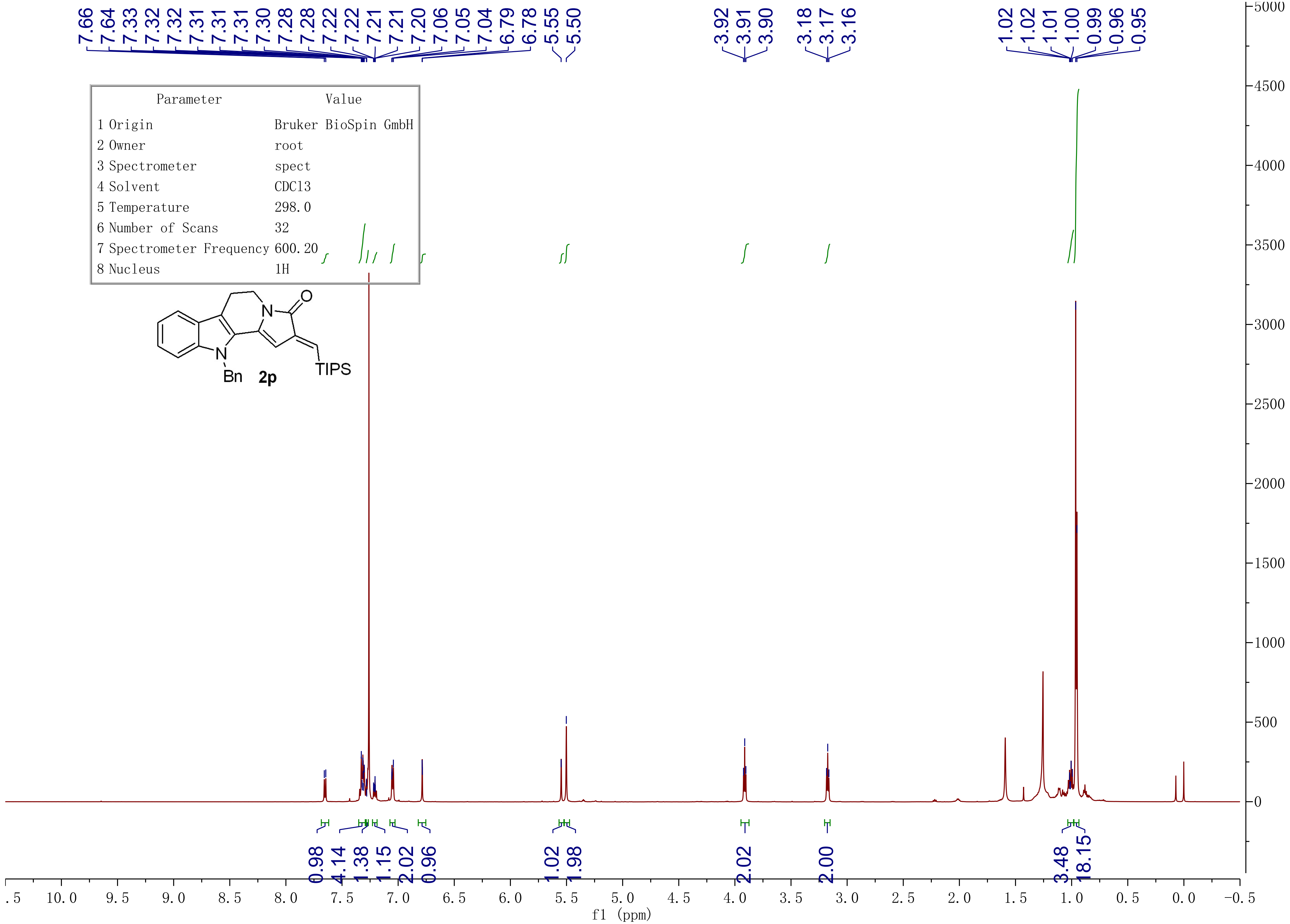
136.31
134.04
129.47
128.78
128.61
127.84
127.43
125.88
115.52
115.04
110.78
100.63
97.52
65.72
55.92
47.79
37.44
29.85
27.63
20.85
18.75
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 32
7 Spectrometer Frequency 150.90
8 Nucleus 13C
MeO
N
N
O
Bn
2n
TBDPS
f1 (ppm)


c
7.34 7.33 7.32 7.31 7.31 7.30 7.30 7.28 7.27 7.26 7.22 7.21 7.19 7.05 7.04 6.79 5.55 5.50
3.92 3.91 3.90 3.18 3.17 3.16 0.96 0.95
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
F
N
O
N
Bn
TIPS
2o
1.04 3.80 1.09 1.18 1.88 0.95 1.05 1.86 1.92 2.00 18.31
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	298.0
6 Number of Scans	16
7 Spectrometer Frequency	150.90
8 Nucleus	13C

2o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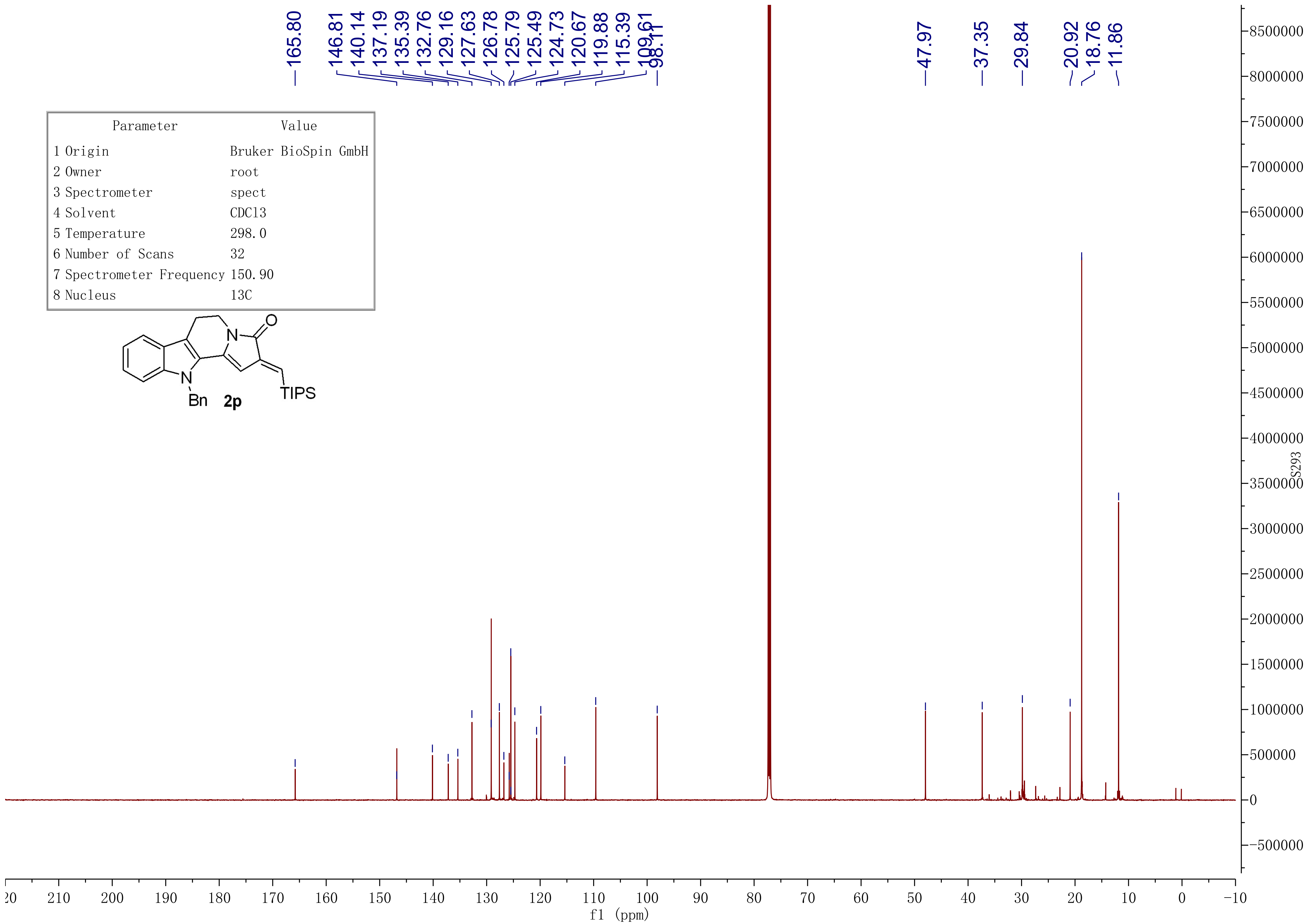
3.92 3.91 3.90
3.18 3.17 3.16
1.02 1.02 1.01 1.00 0.99 0.96 0.95
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 32
7 Spectrometer Frequency 600.20
8 Nucleus 1H
N
N
O
Bn
2p
TIPS
0.98 4.14 1.38 1.15 2.02 0.96 1.02 1.98 2.02 2.00 3.48 18.15
f1 (ppm)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146.81
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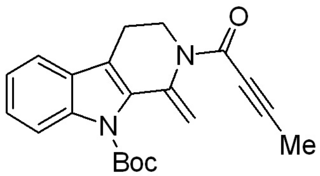
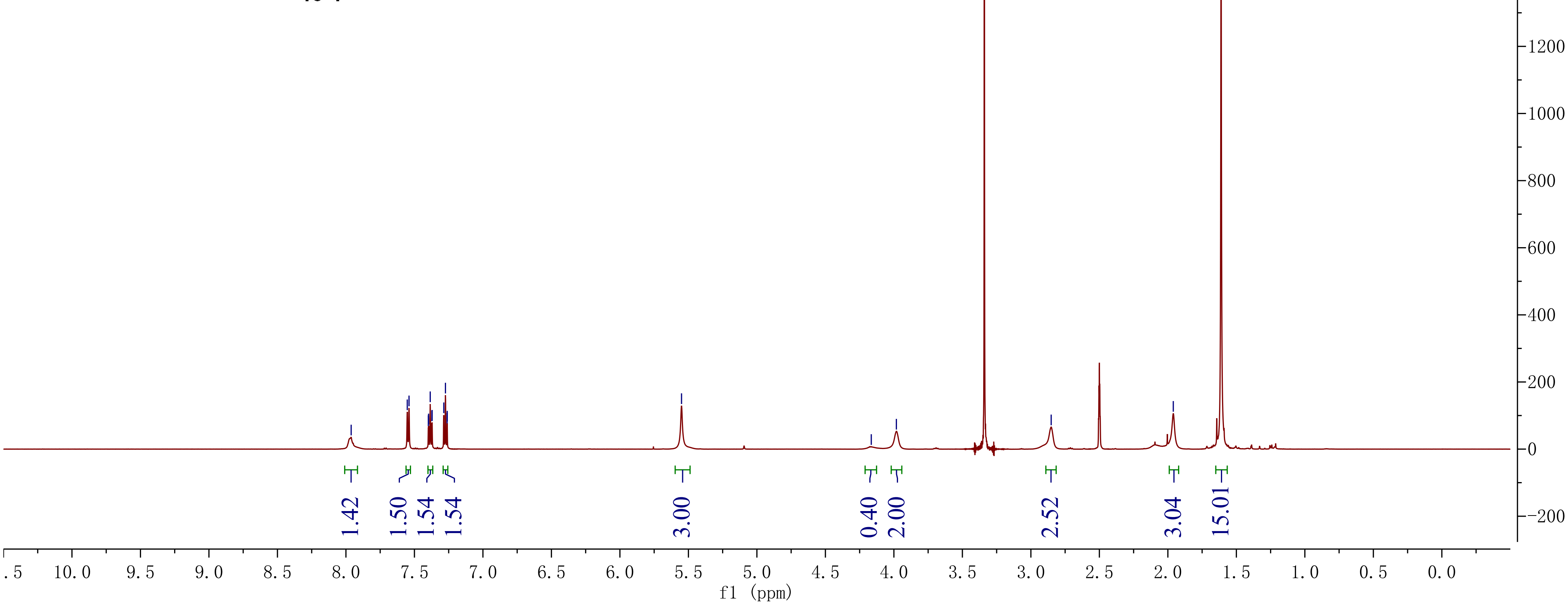
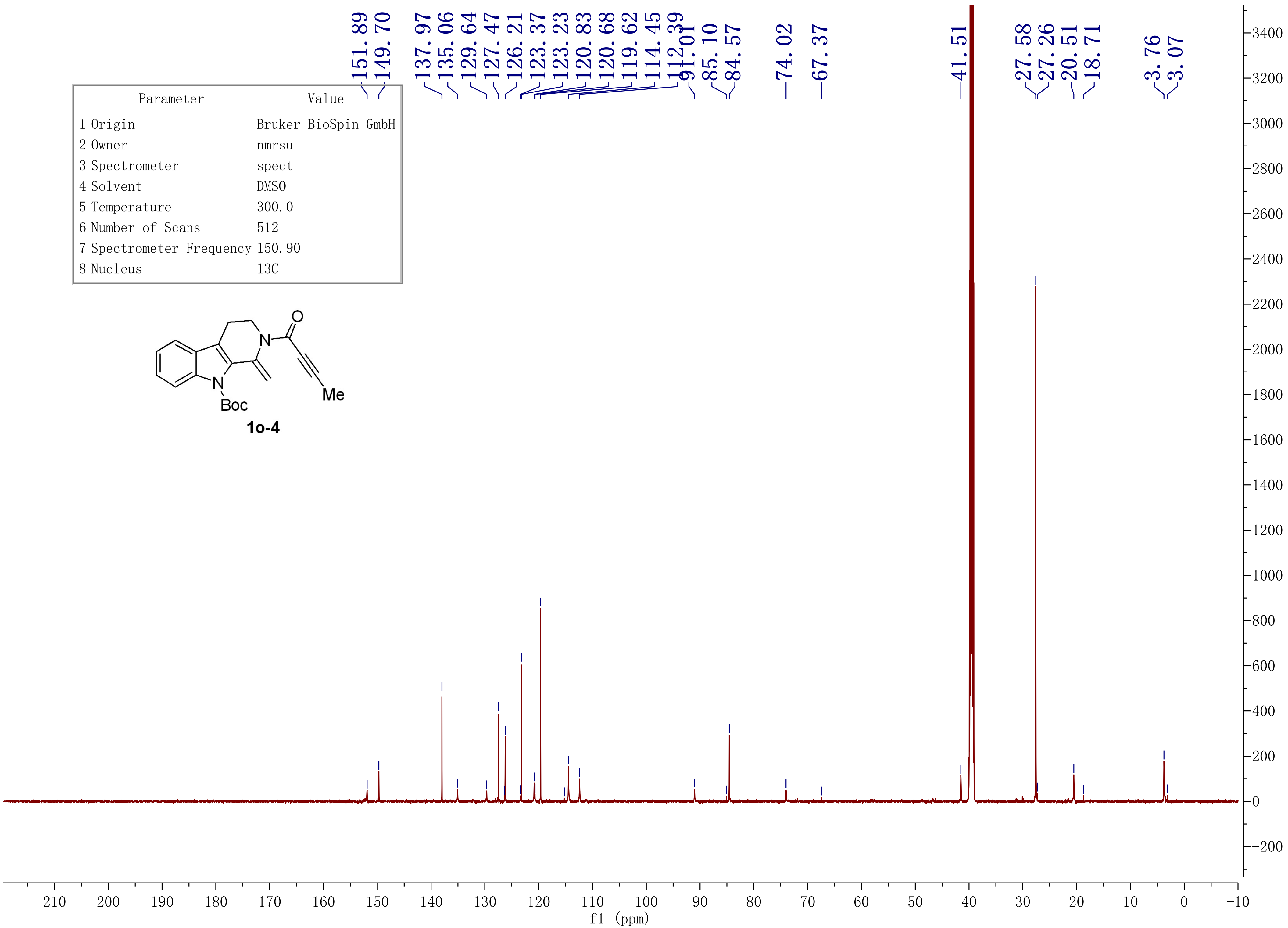
137.19
135.39
132.76
129.16
127.63
126.78
125.79
125.49
124.73
120.67
119.88
115.39
109.61
98.11
47.97
37.35
29.84
20.92
18.76
11.86
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 298.0
6 Number of Scans 32
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
N
O
Bn
2p
TIPS
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H



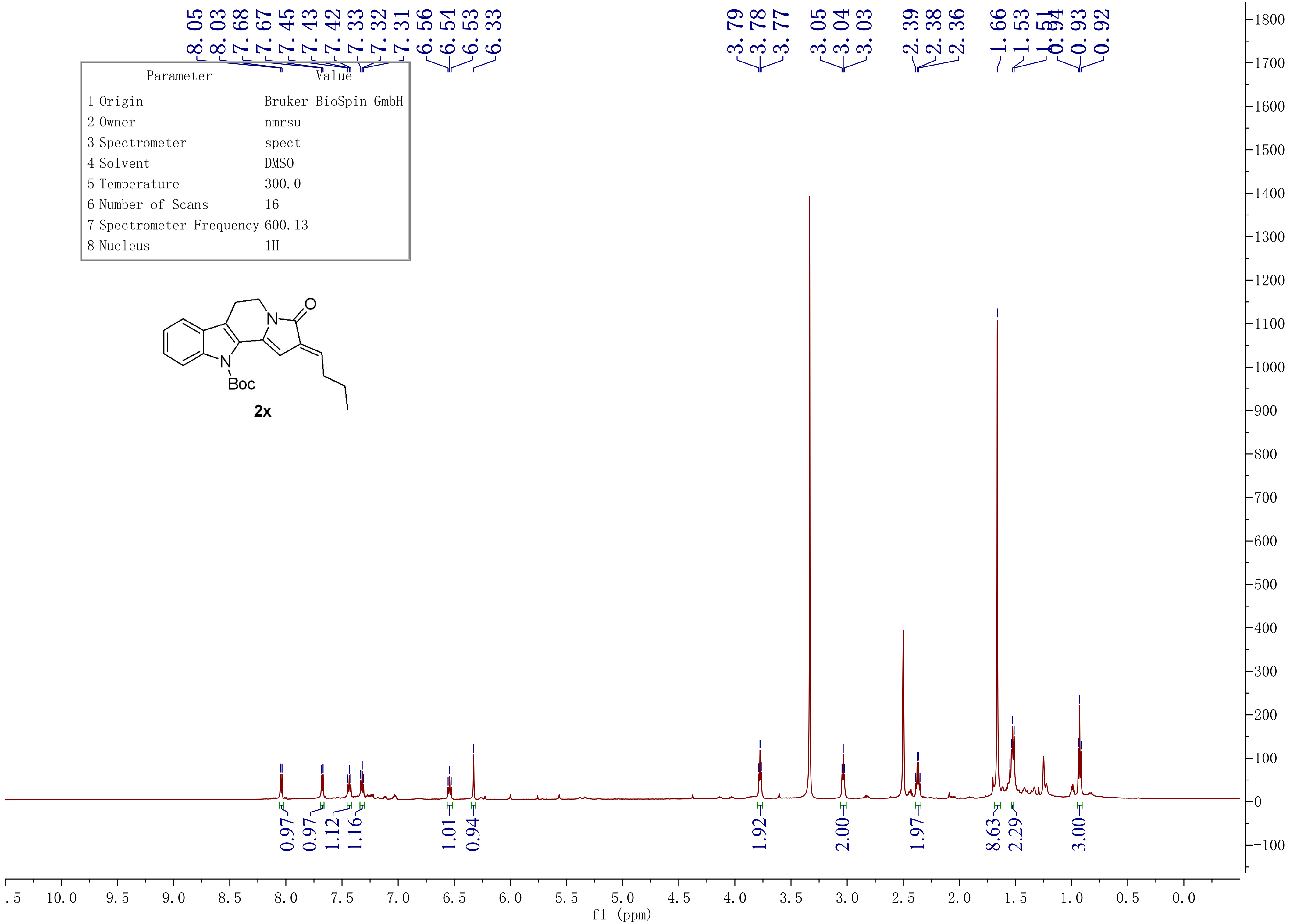
1o-4

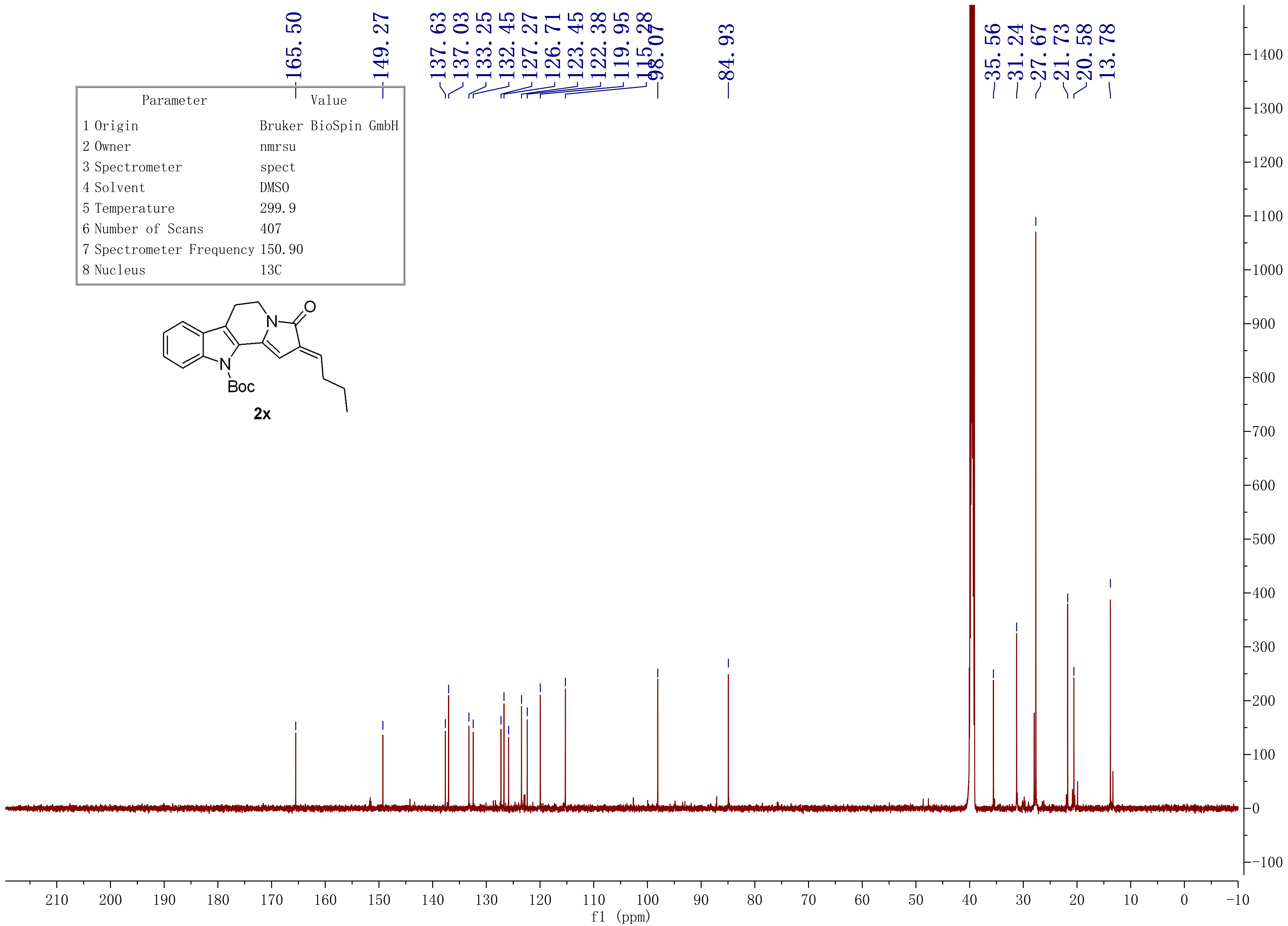


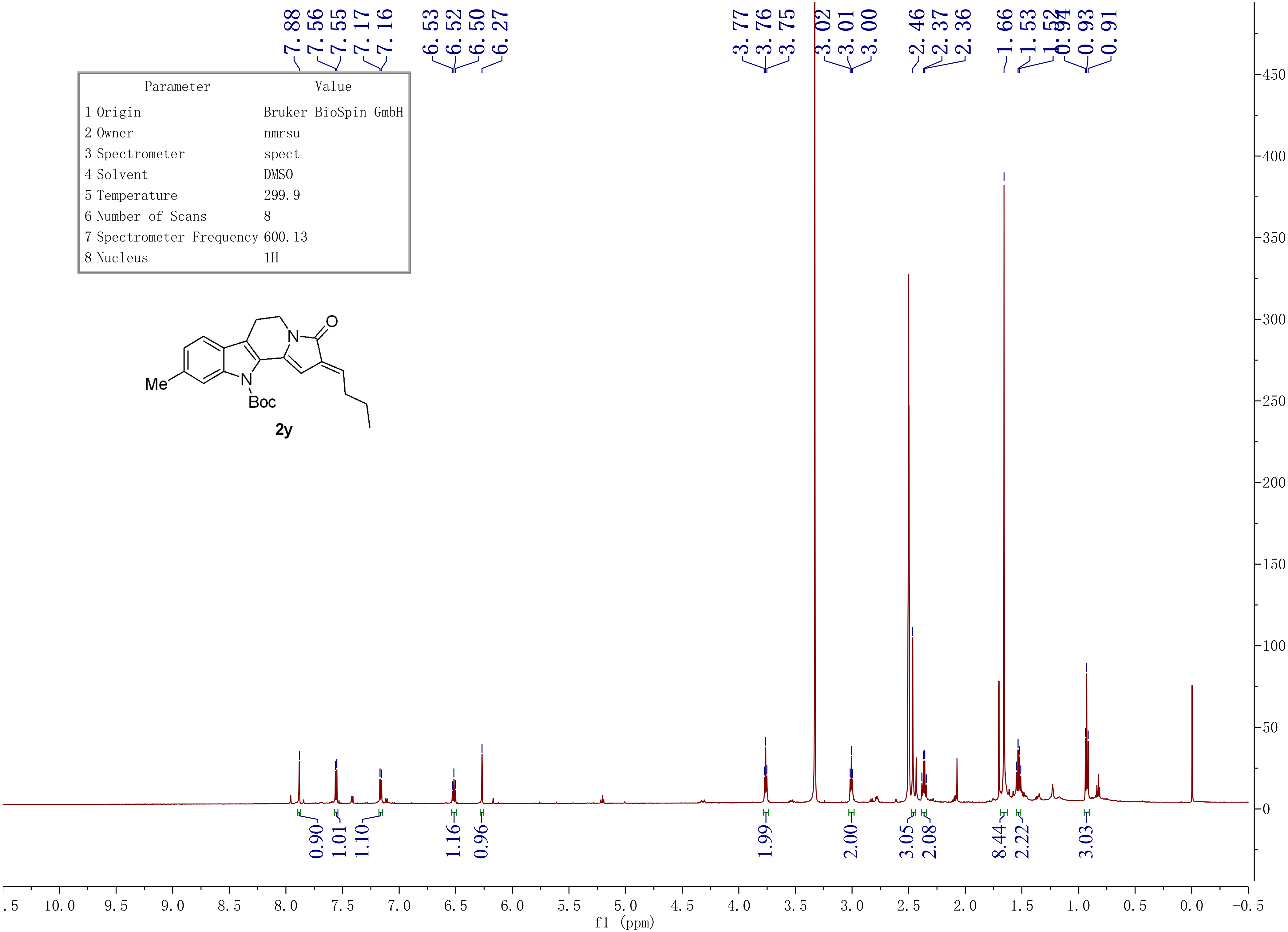


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	512
7 Spectrometer Frequency	150.90
8 Nucleus	13C

1o-4

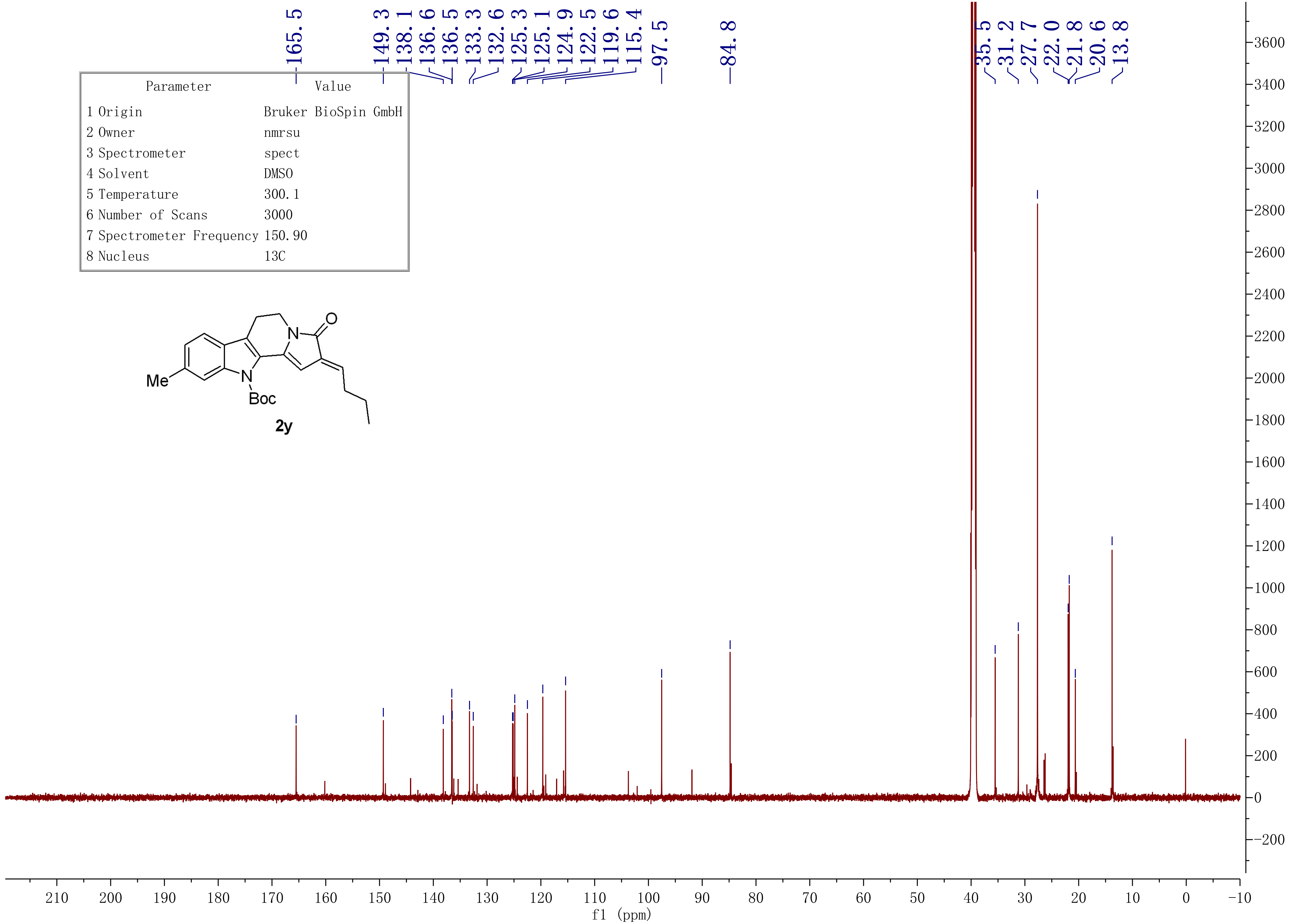

8.05
8.03
7.68
7.67
7.45
7.43
7.42
7.33
7.32
7.31
6.56
6.54
6.53
6.33
3.79
3.78
3.77
3.05
3.04
3.03
2.39
2.38
2.36
1.66
1.53
1.51
0.94
0.93
0.92
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
N
O
Boc
2x
0.97
0.97
1.12
1.16
1.01
0.94
1.92
2.00
1.97
8.63
2.29
3.00
f1 (ppm)

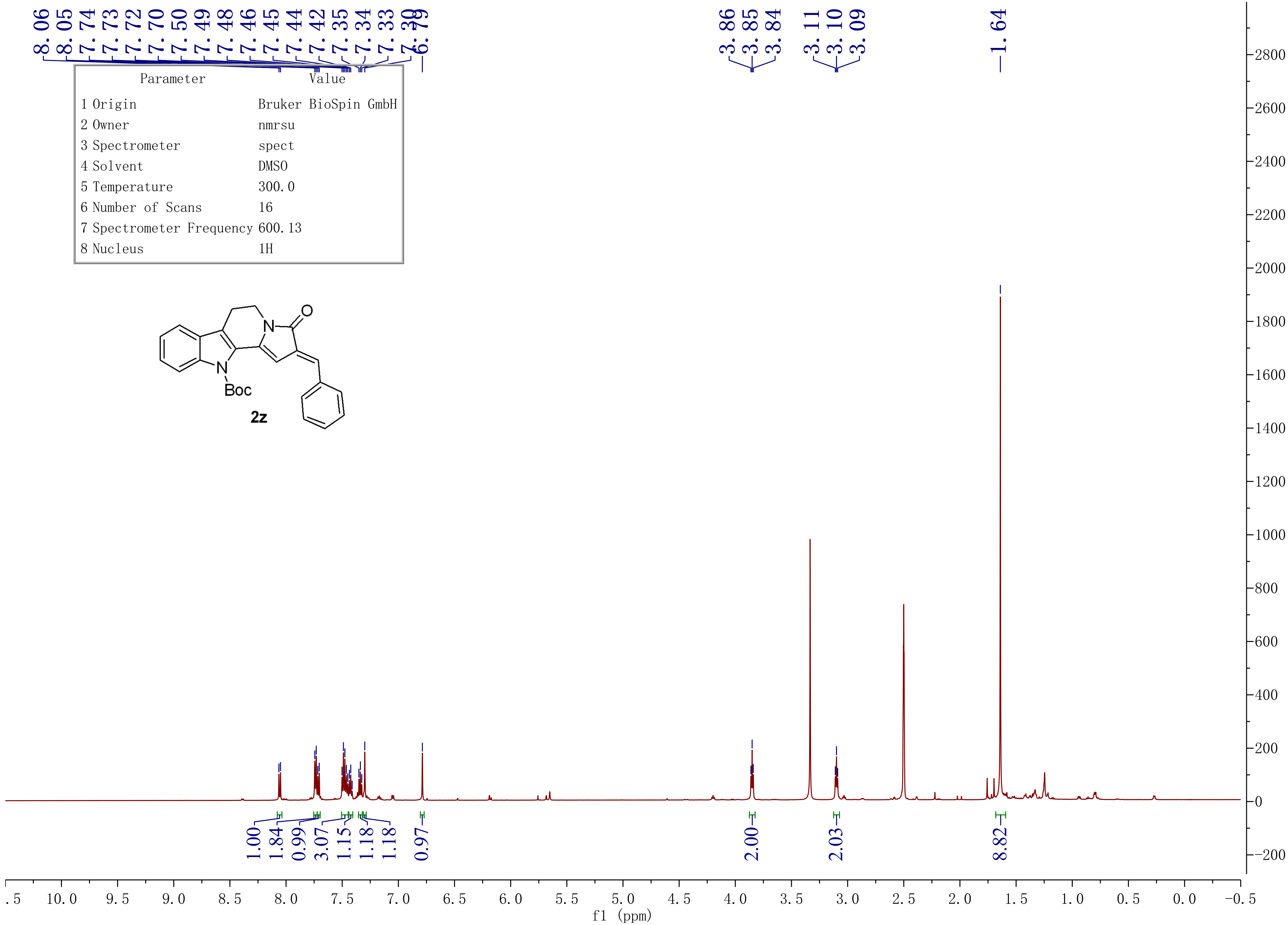

165.50
149.27
137.63
137.03
133.25
132.45
127.27
126.71
123.45
122.38
119.95
115.28
98.07
84.93
35.56
31.24
27.67
21.73
20.58
13.78
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 299.9
6 Number of Scans 407
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
Boc
N
O
2x
f1 (ppm)

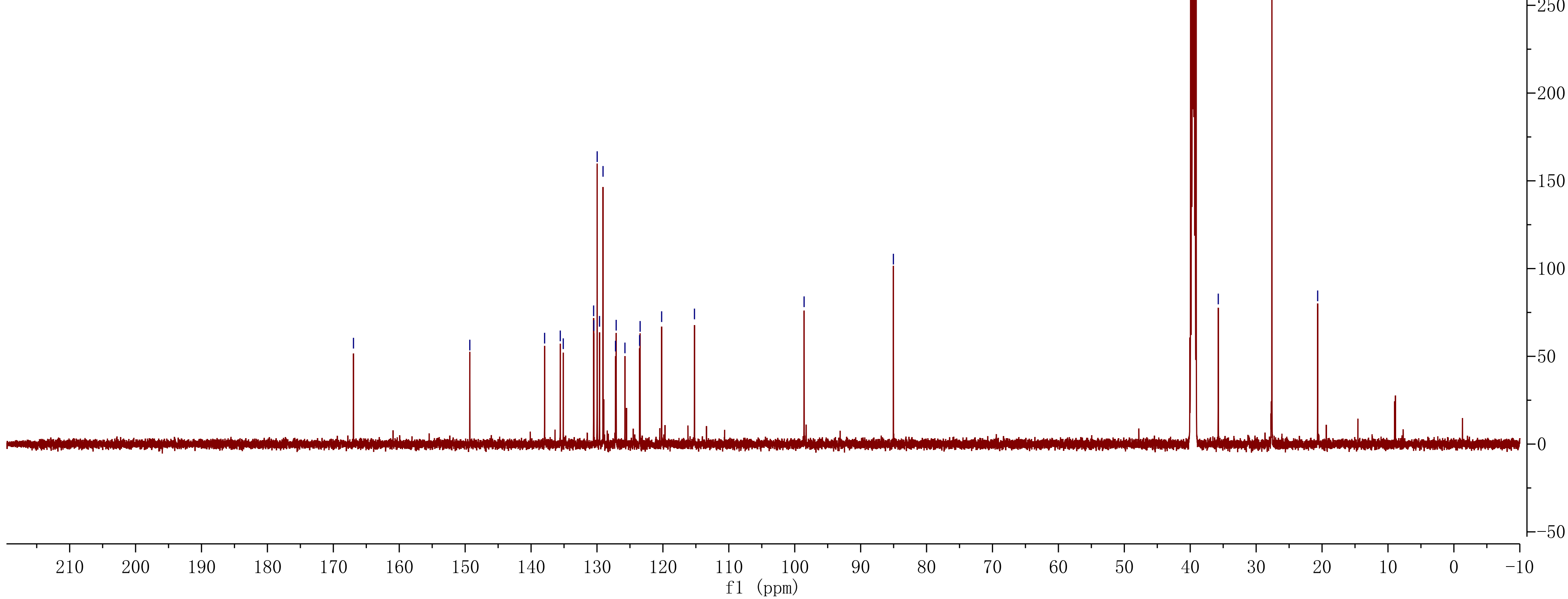


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	299.9
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H

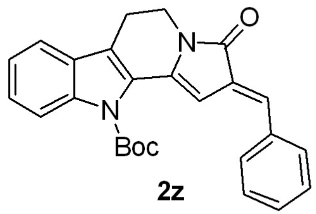
2y


165.5
149.3
138.1
136.6
136.5
133.3
132.6
125.3
125.1
124.9
122.5
119.6
115.4
97.5
84.8
35.5
31.2
27.7
22.0
21.8
20.6
13.8
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.1
6 Number of Scans 3000
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Me
N
Boc
N
O
2y
f1 (ppm)

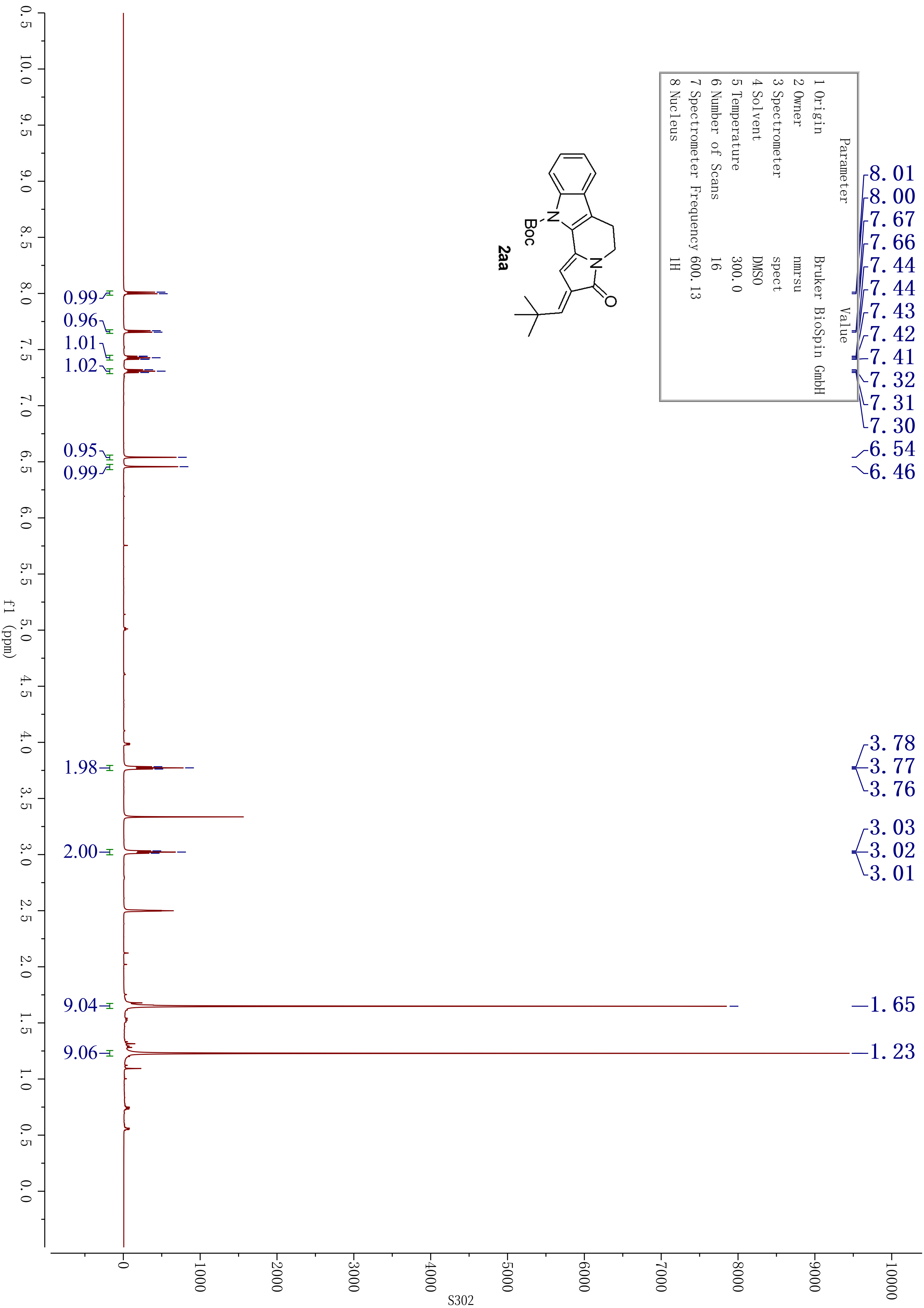

8.06
8.05
7.74
7.73
7.72
7.70
7.50
7.49
7.48
7.46
7.45
7.44
7.42
7.35
7.34
7.33
7.30
6.79
3.86
3.85
3.84
3.11
3.10
3.09
1.64
Parameter | Value
1 Origin | Bruker BioSpin GmbH
2 Owner | nmrsu
3 Spectrometer | spect
4 Solvent | DMSO
5 Temperature | 300.0
6 Number of Scans | 16
7 Spectrometer Frequency | 600.13
8 Nucleus | 1H
N
O
N
Boc
2z
1.00
1.84
0.99
3.07
1.15
1.18
1.18
0.97
2.00
2.03
8.82
f1 (ppm)



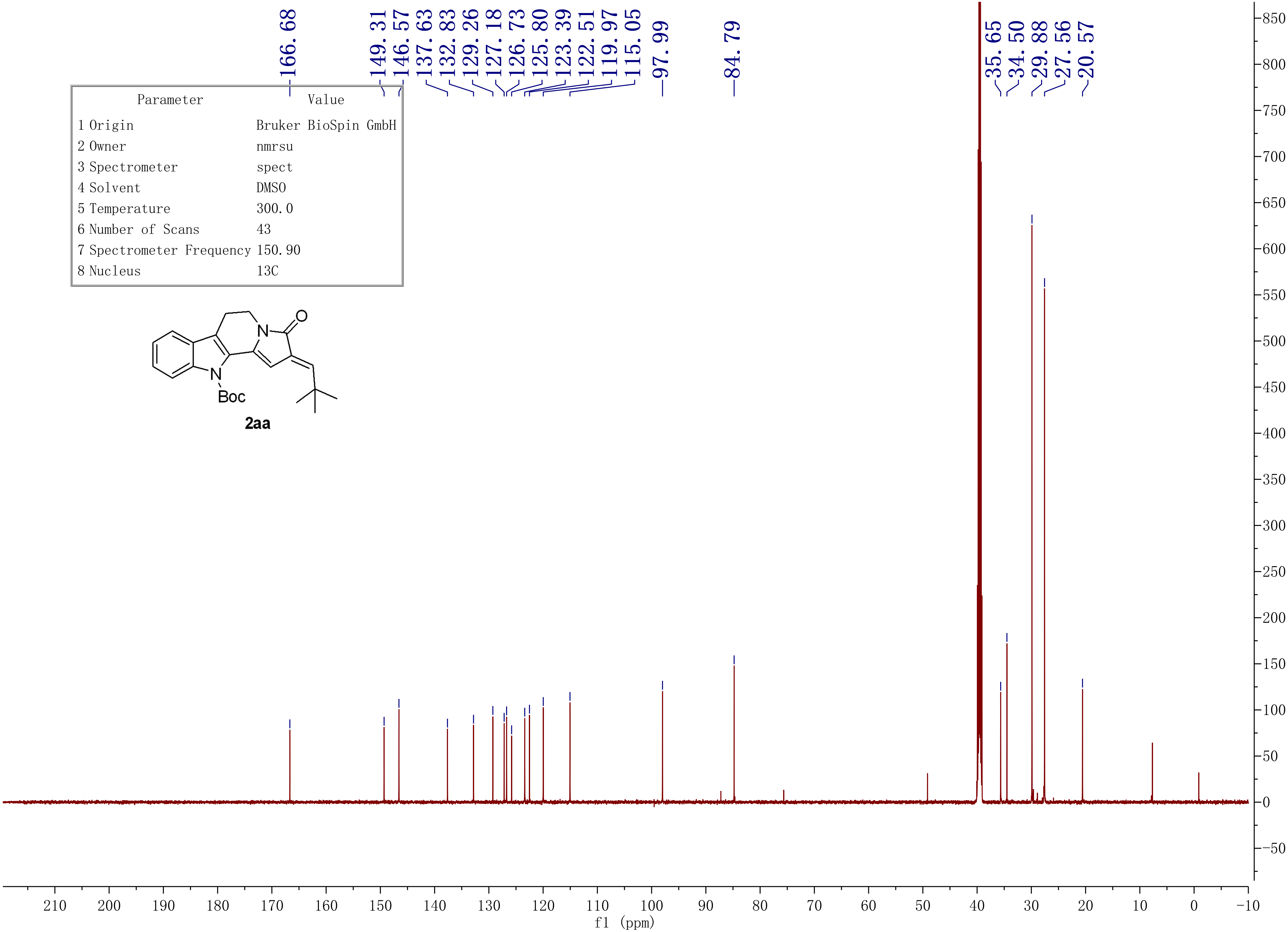
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	115
7 Spectrometer Frequency	150.90
8 Nucleus	13C

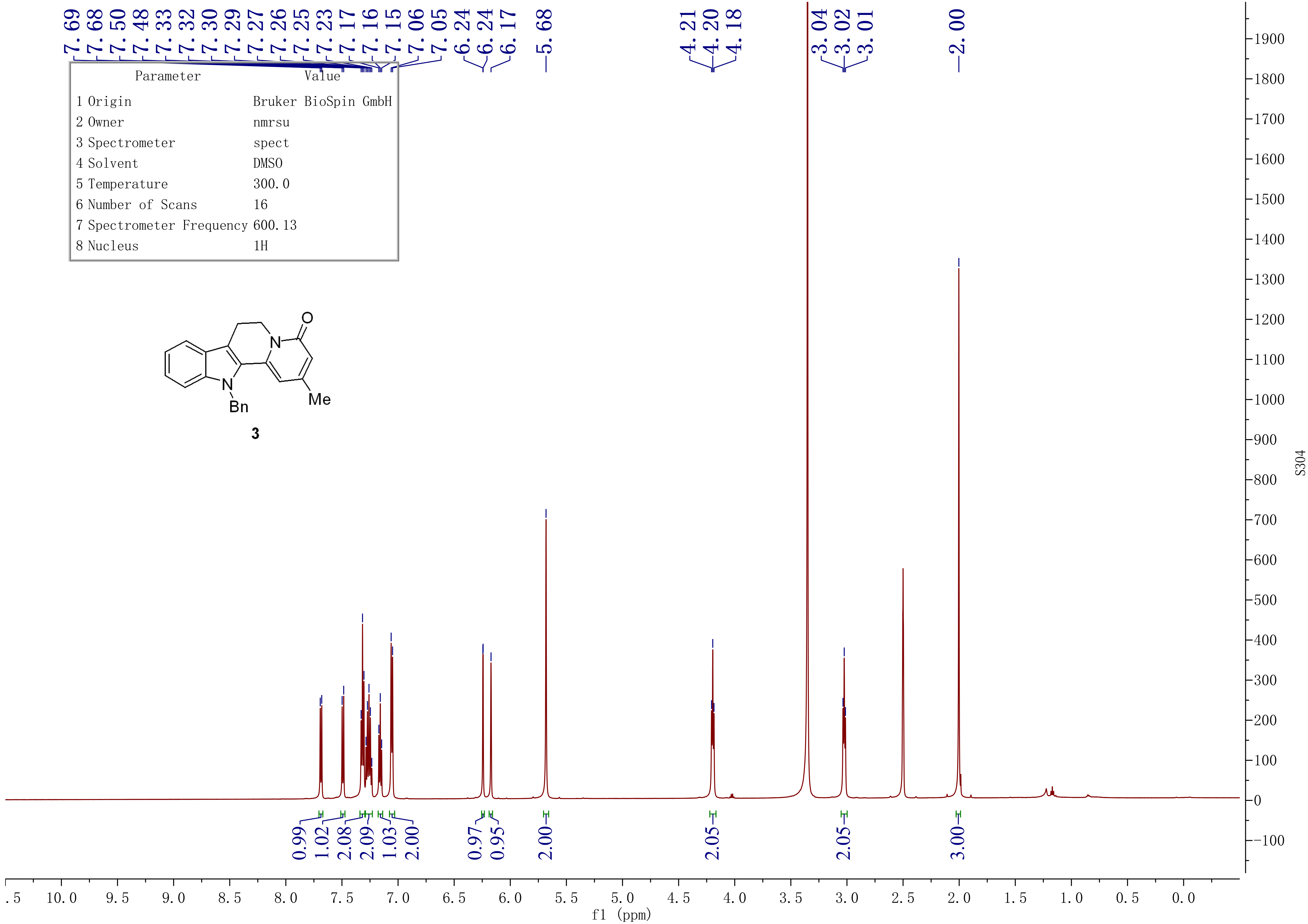


2z


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Boc
N
O
2aa
8.01
8.00
7.67
7.66
7.44
7.44
7.43
7.42
7.41
7.32
7.31
7.30
6.54
6.46
3.78
3.77
3.76
3.03
3.02
3.01
1.65
1.23
0.99
0.96
1.01
1.02
0.95
0.99
1.98
2.00
9.04
9.06
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.0
6 Number of Scans	43
7 Spectrometer Frequency	150.90
8 Nucleus	13C




7.69
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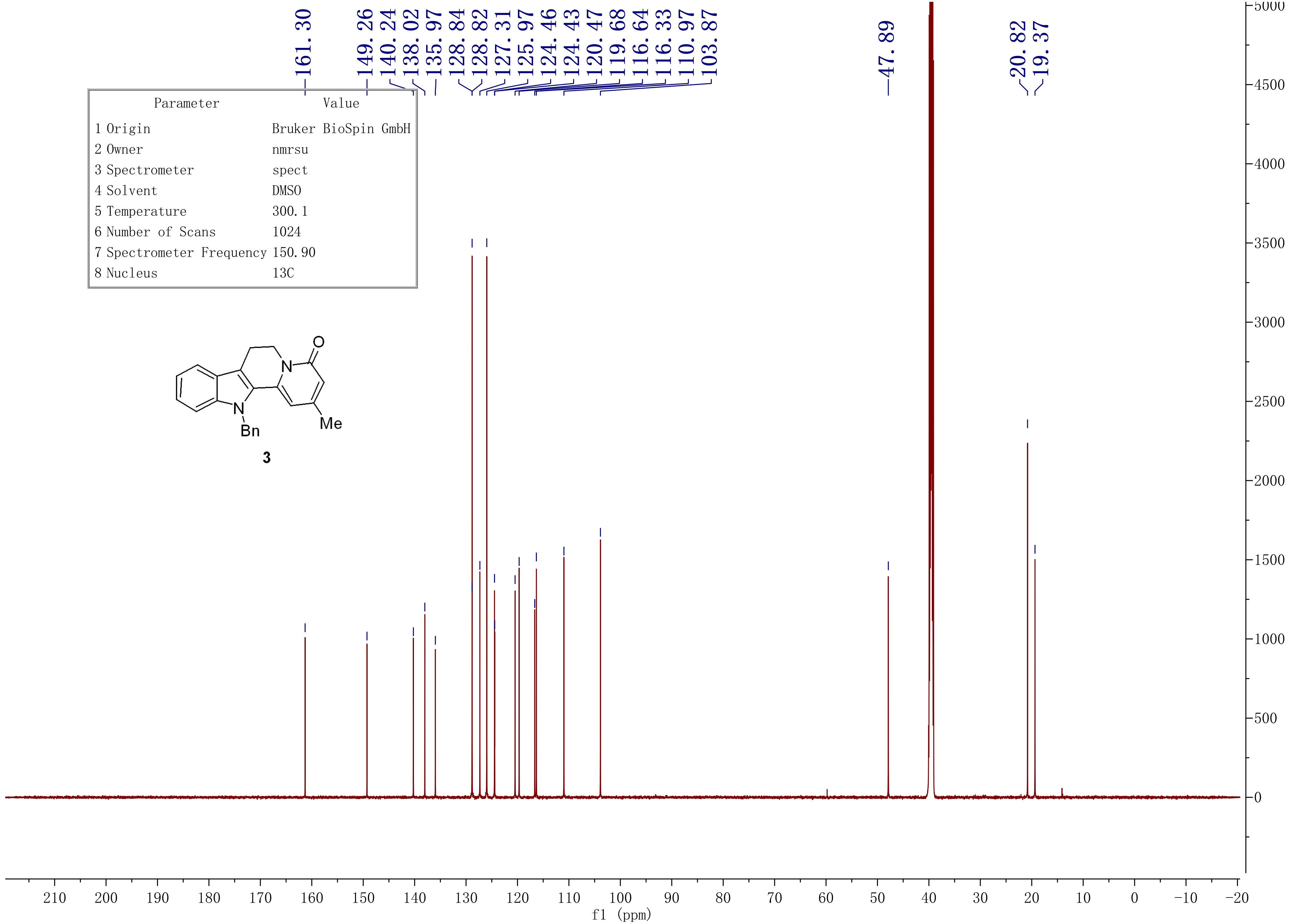
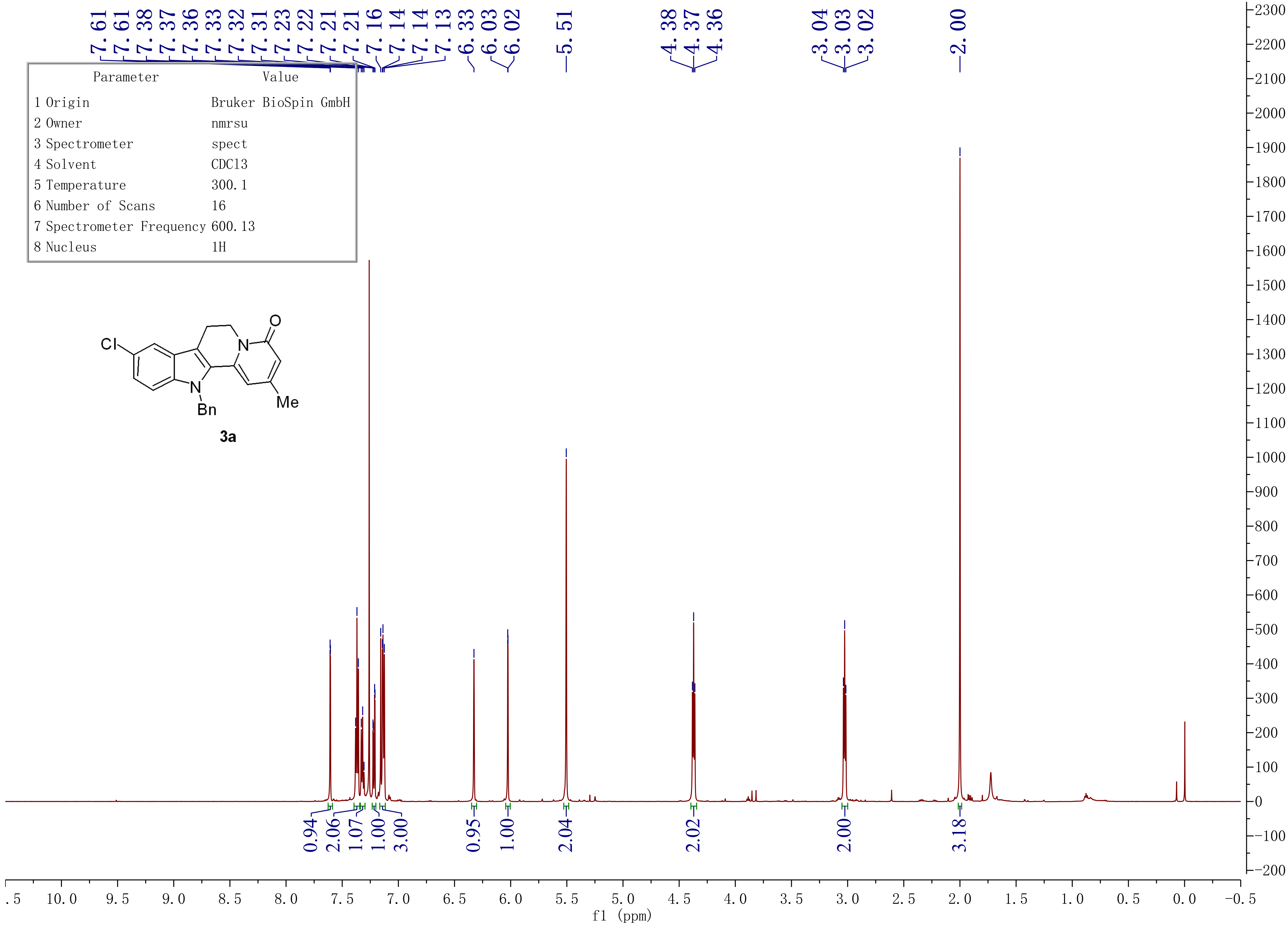
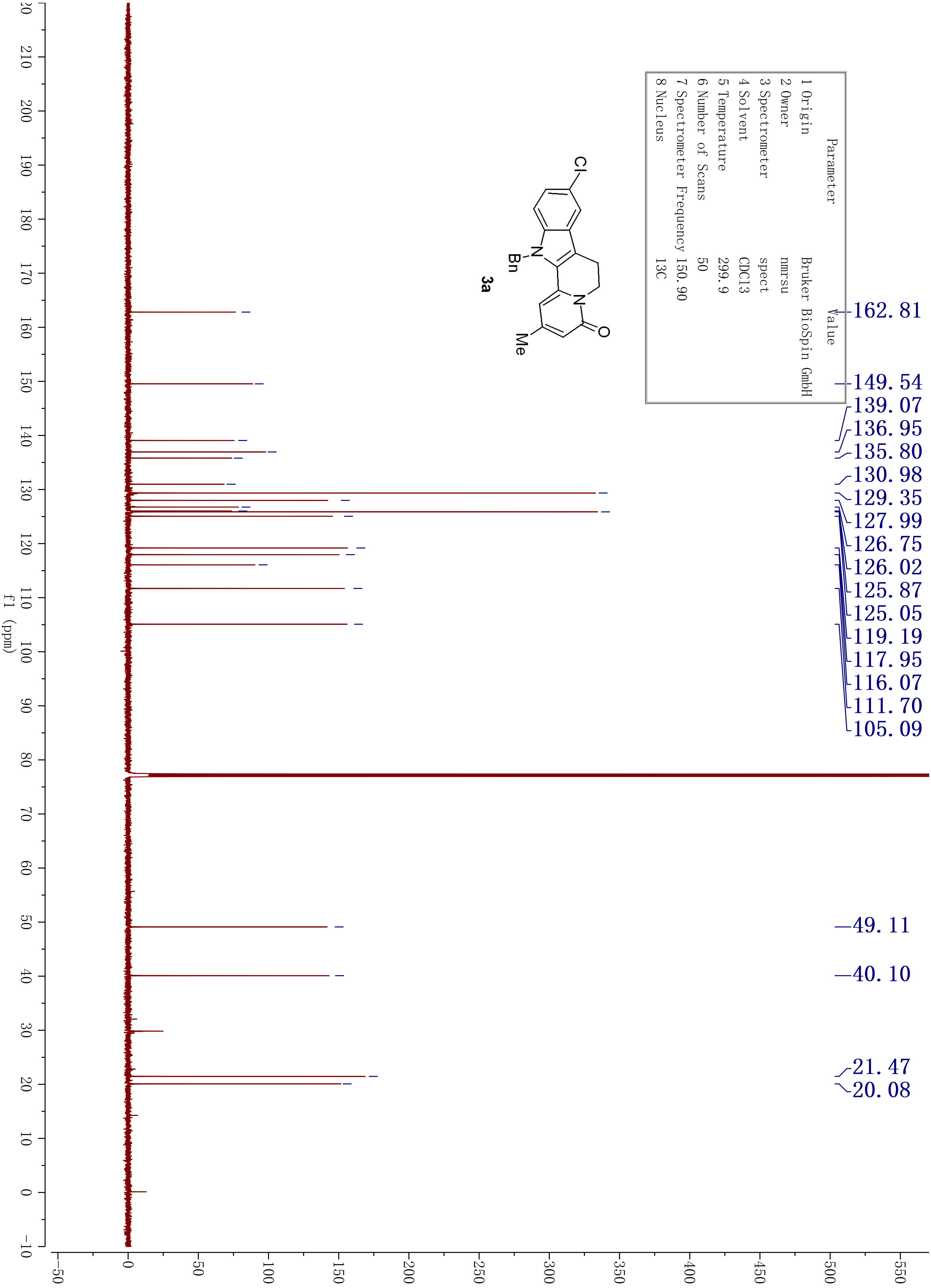
7.48
7.33
7.32
7.30
7.29
7.27
7.26
7.25
7.23
7.17
7.16
7.15
7.06
7.05
6.24
6.24
6.17
5.68
4.21
4.20
4.18
3.04
3.02
3.01
2.00
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
DMSO
5 Temperature
300.0
6 Number of Scans
16
7 Spectrometer Frequency
600.13
8 Nucleus
1H
N
N
O
Me
Bn
3
0.99
1.02
2.08
2.09
1.03
2.00
0.97
0.95
2.00
2.05
2.05
3.00
f1 (ppm)

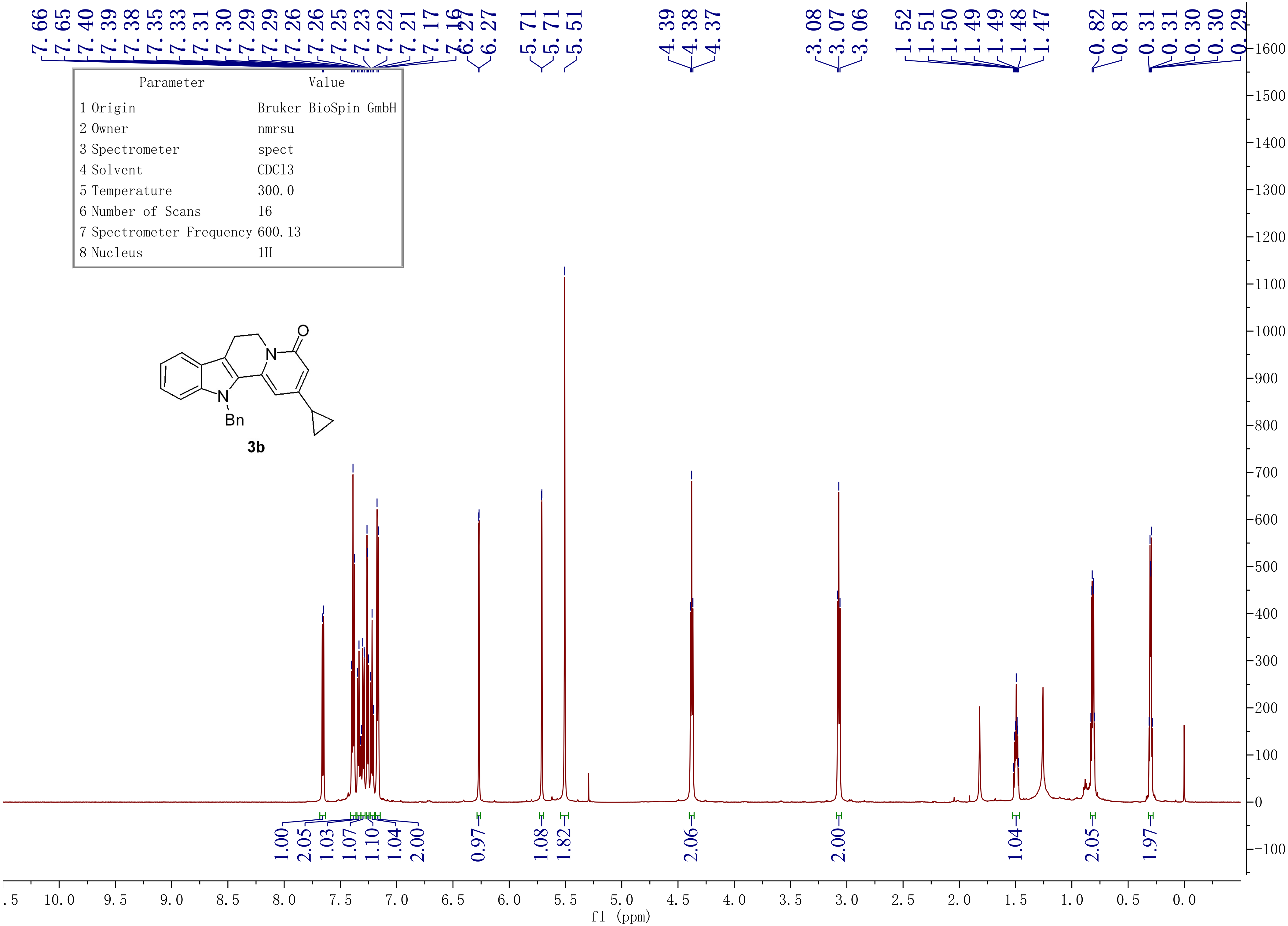


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	300.1
6 Number of Scans	1024
7 Spectrometer Frequency	150.90
8 Nucleus	13C



7.61 7.61 7.38 7.37 7.36 7.33 7.32 7.31 7.23 7.22 7.21 7.21 7.16 7.14 7.14 7.13 6.33 6.03 6.02 5.51 4.38 4.37 4.36 3.04 3.03 3.02 2.00
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Cl
N
O
N
Bn
Me
3a
0.94 2.06 1.07 1.00 3.00 0.95 1.00 2.04 2.02 2.00 3.18
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 50
7 Spectrometer Frequency 150.90
8 Nucleus 13C
3a
162.81
149.54
139.07
136.95
135.80
130.98
129.35
127.99
126.75
126.02
125.87
125.05
119.19
117.95
116.07
111.70
105.09
49.11
40.10
21.47
20.08
f1 (ppm)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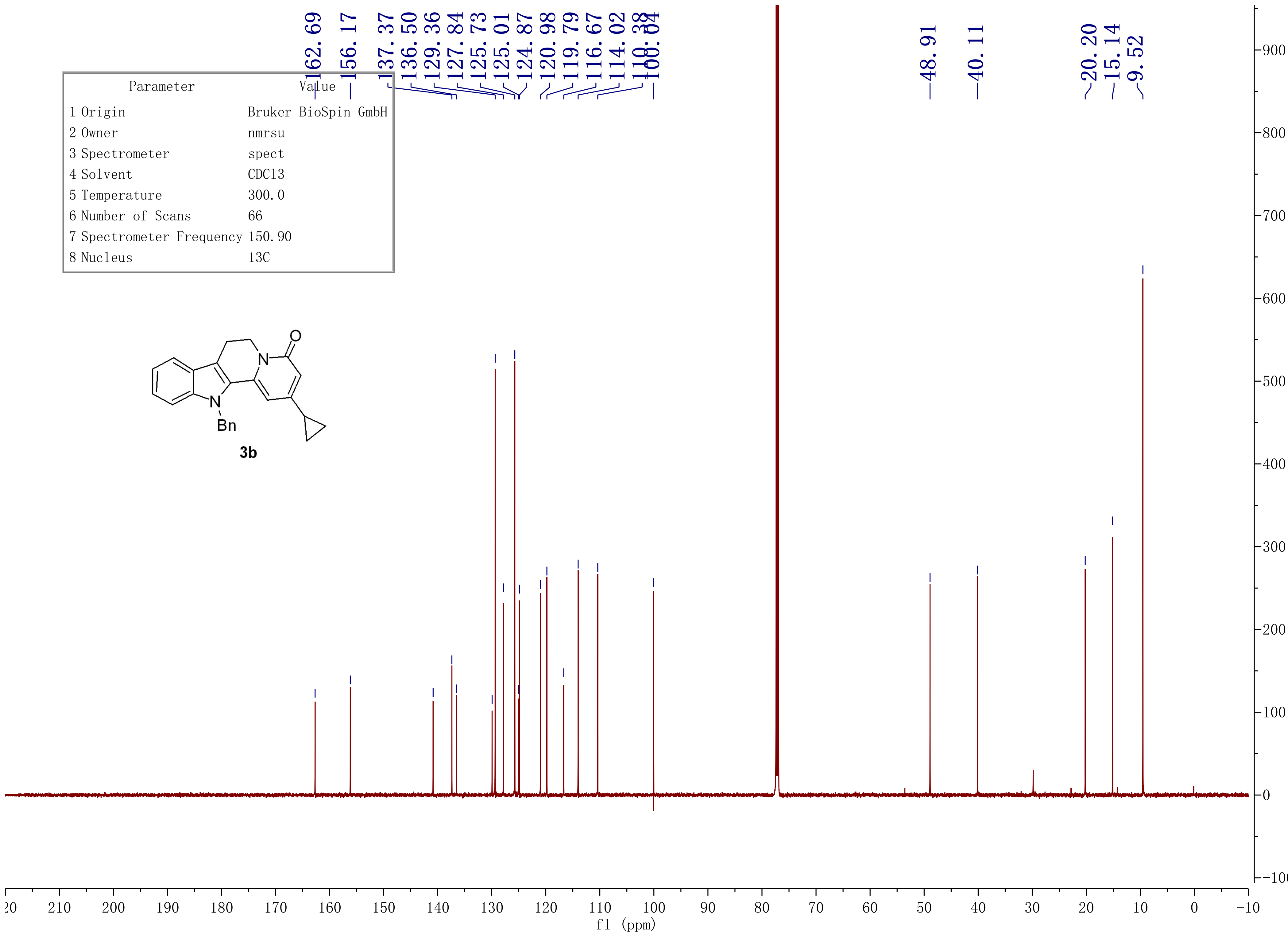
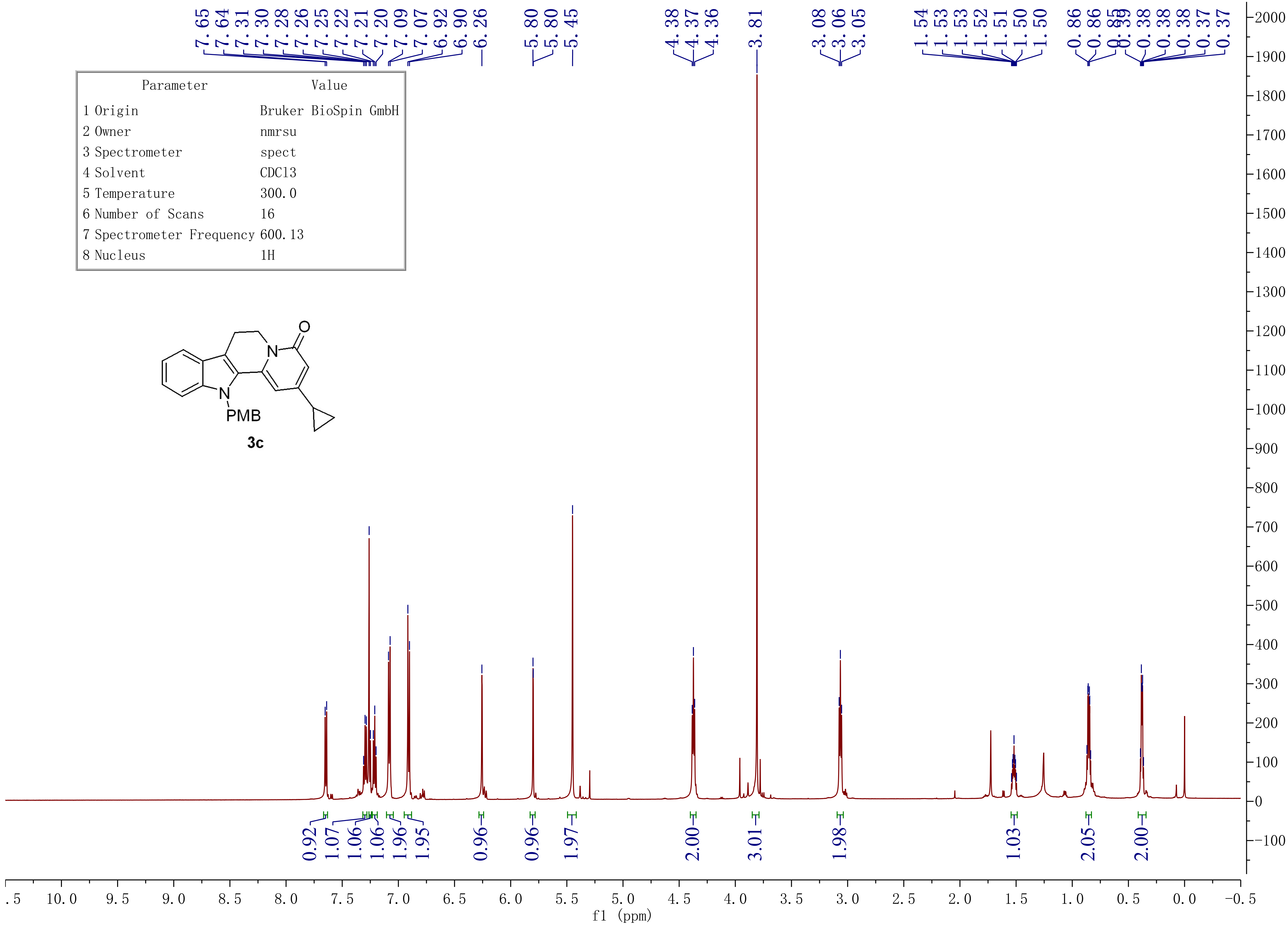
7.29
7.29
7.26
7.26
7.25
7.23
7.22
7.21
7.17
7.16
6.27
6.27
5.71
5.71
5.51
4.39
4.38
4.37
3.08
3.07
3.06
1.52
1.51
1.50
1.49
1.49
1.48
1.47
0.82
0.81
0.31
0.31
0.30
0.30
0.29
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
CDCl3
5 Temperature
300.0
6 Number of Scans
16
7 Spectrometer Frequency
600.13
8 Nucleus
1H
N
N
O
Bn
3b
1.00
2.05
1.03
1.07
1.10
1.04
2.00
0.97
1.08
1.82
2.06
2.00
1.04
2.05
1.97
f1 (ppm)



162.69
156.17
137.37
136.50
129.36
127.84
125.73
125.01
124.87
120.98
119.79
116.67
114.02
110.38
100.04
48.91
40.11
20.20
15.14
9.52
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 66
7 Spectrometer Frequency 150.90
8 Nucleus 13C
O
N
N
Bn
3b
f1 (ppm)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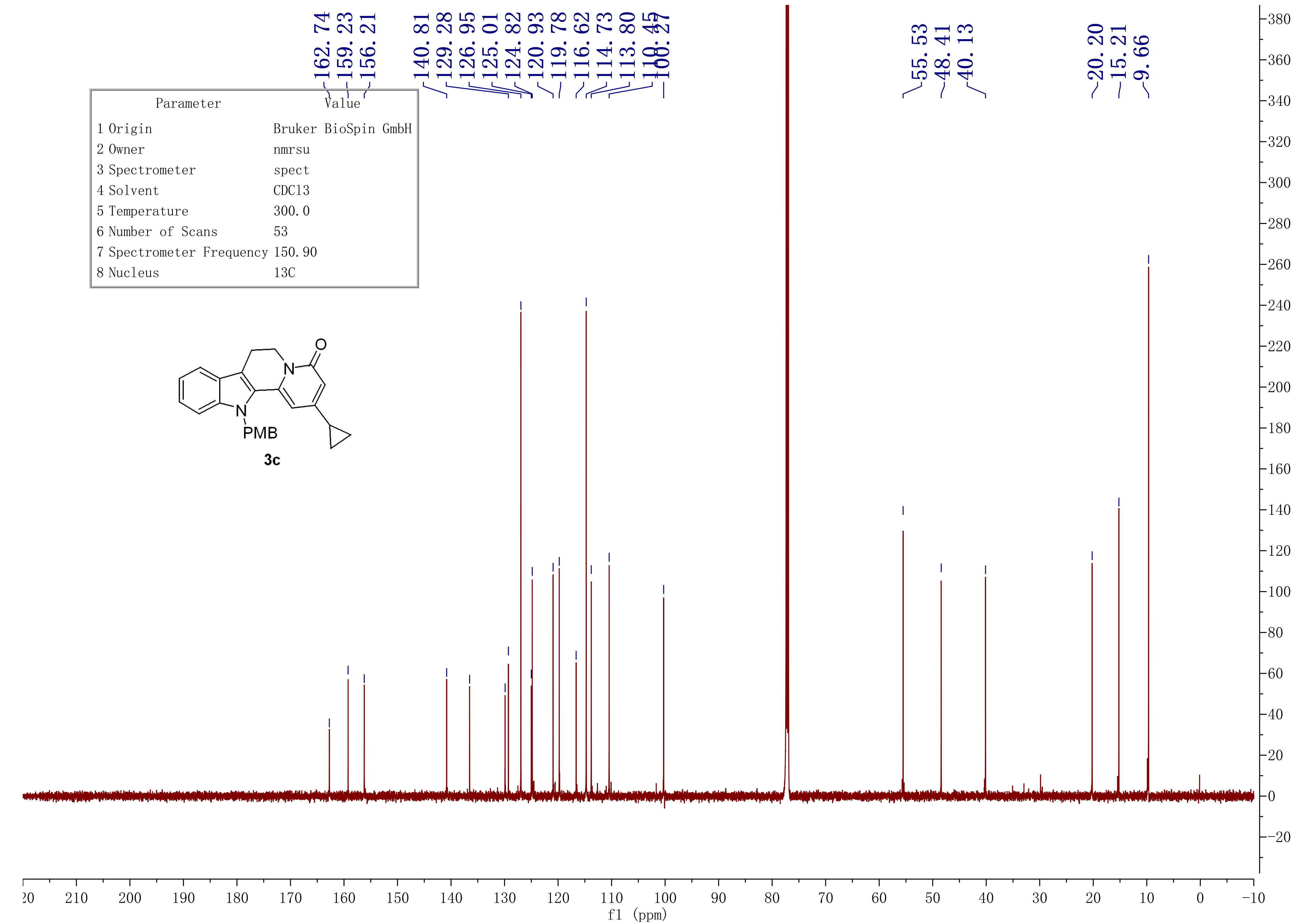
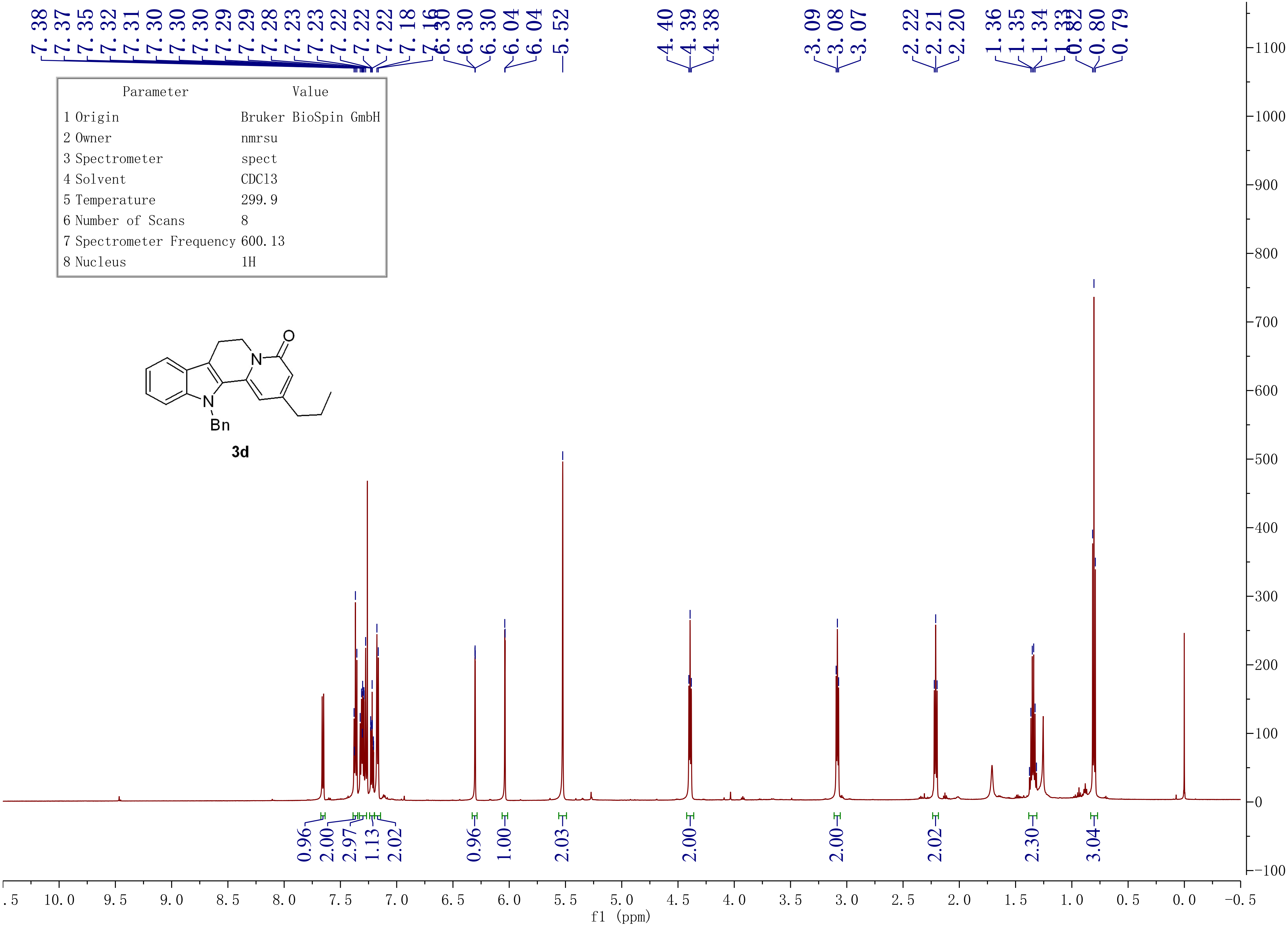
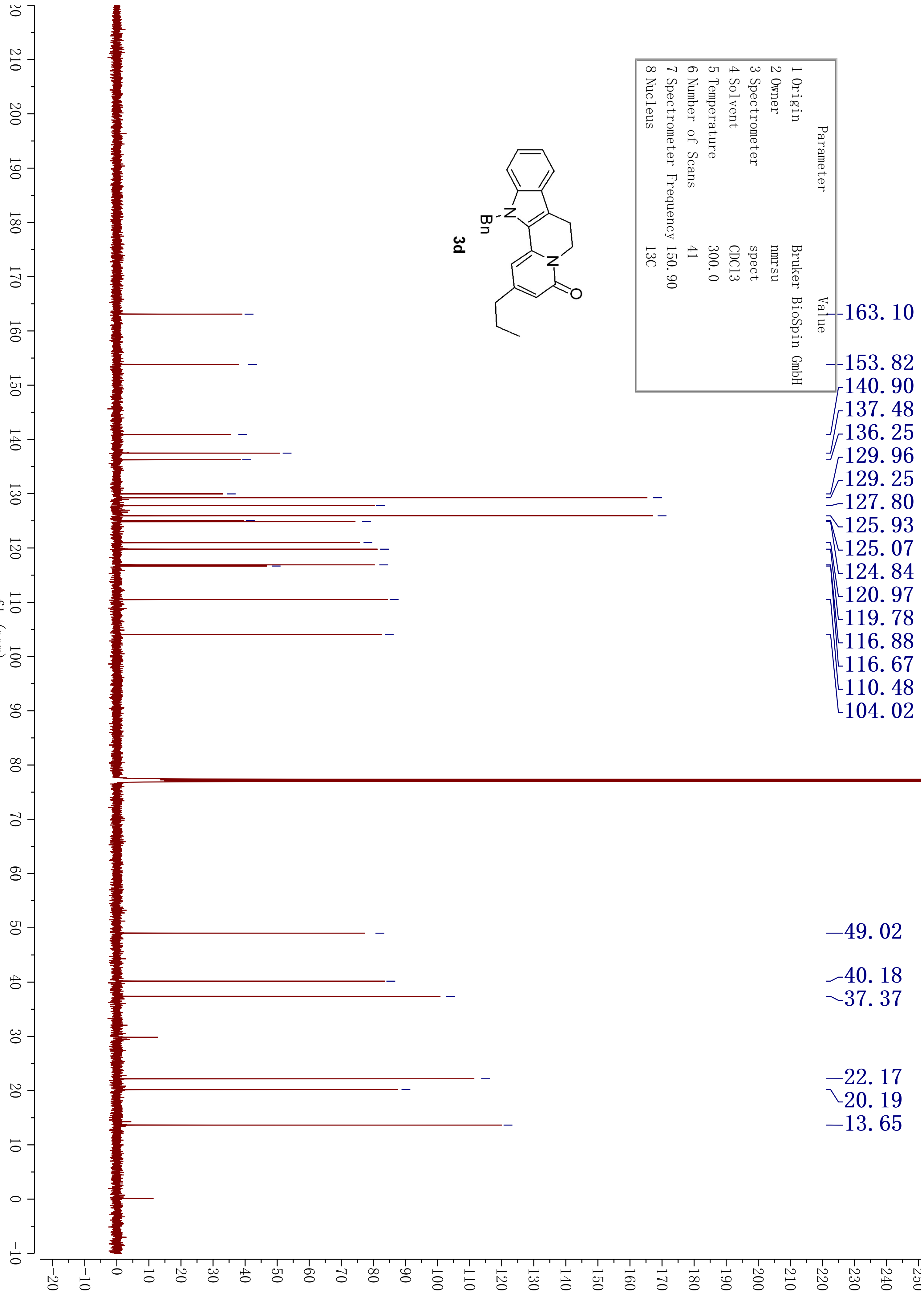
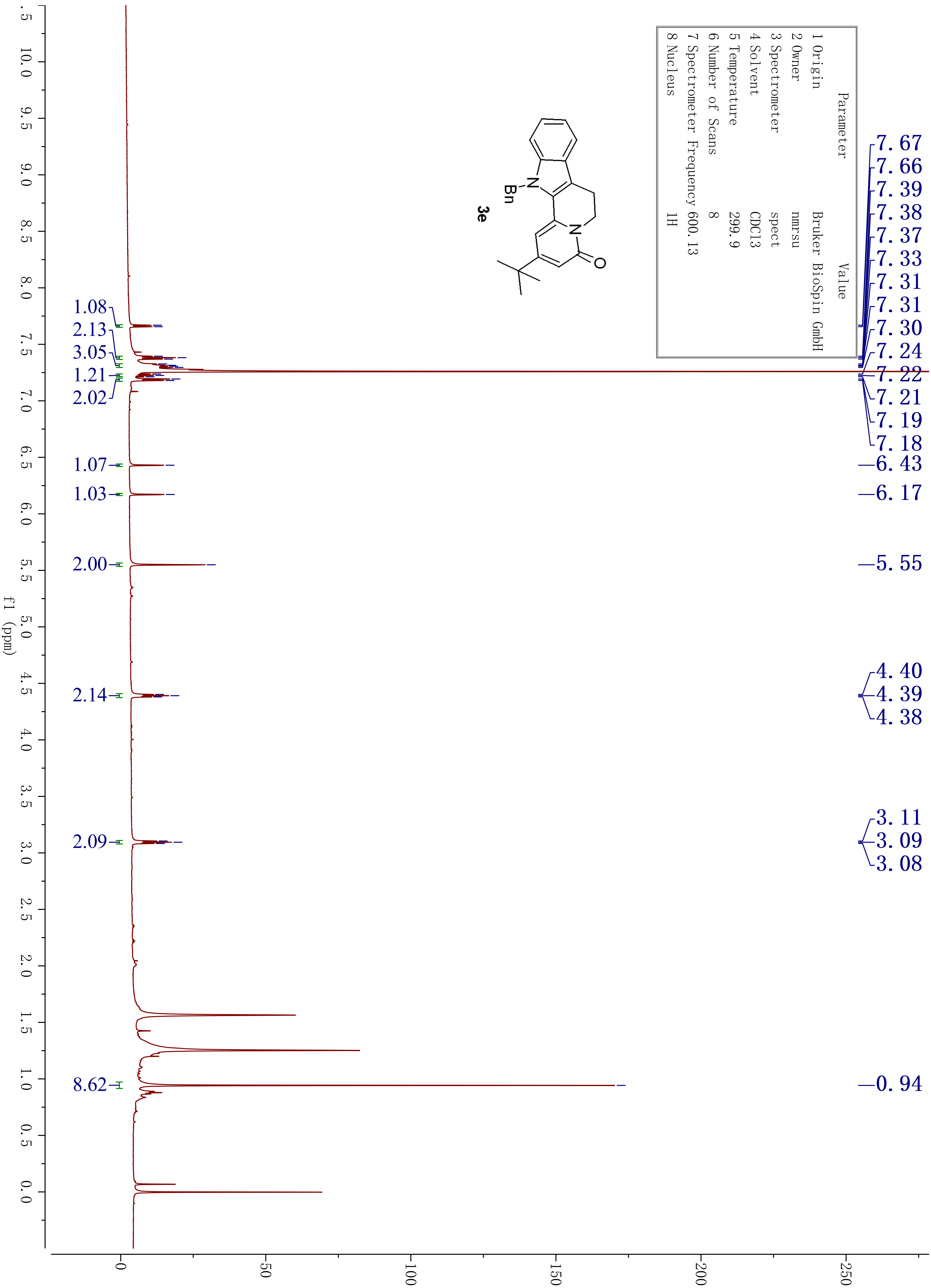
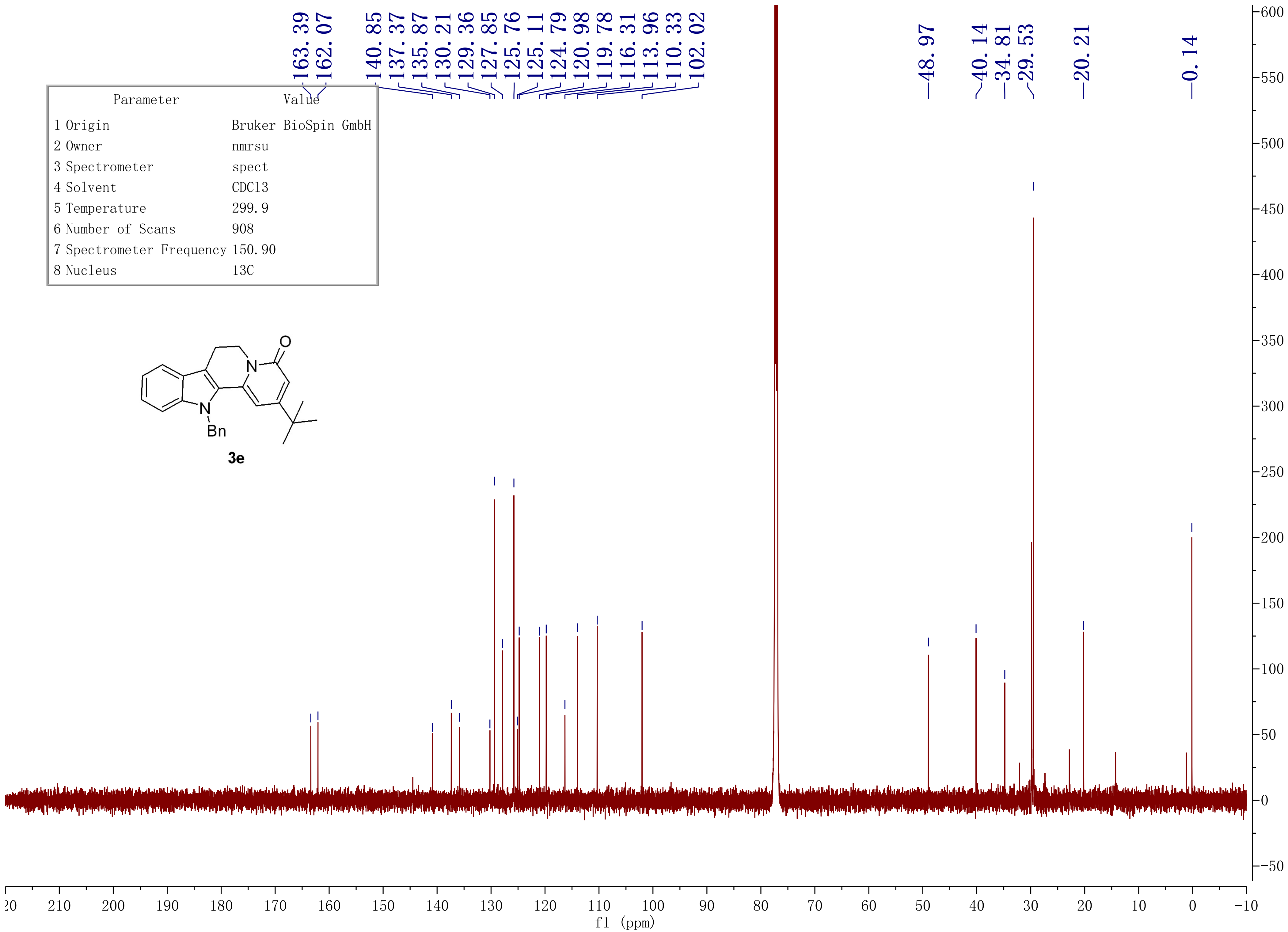
7.28
7.26
7.25
7.22
7.21
7.20
7.09
7.07
6.92
6.90
6.26
5.80
5.80
5.45
4.38
4.37
4.36
3.81
3.08
3.06
3.05
1.54
1.53
1.53
1.52
1.51
1.50
1.50
0.86
0.86
0.85
0.39
0.38
0.38
0.38
0.37
0.37
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
O
N
PMB
3c
0.92
1.07
1.06
1.06
1.96
1.95
0.96
0.96
1.97
2.00
3.01
1.98
1.03
2.05
2.00
f1 (ppm)

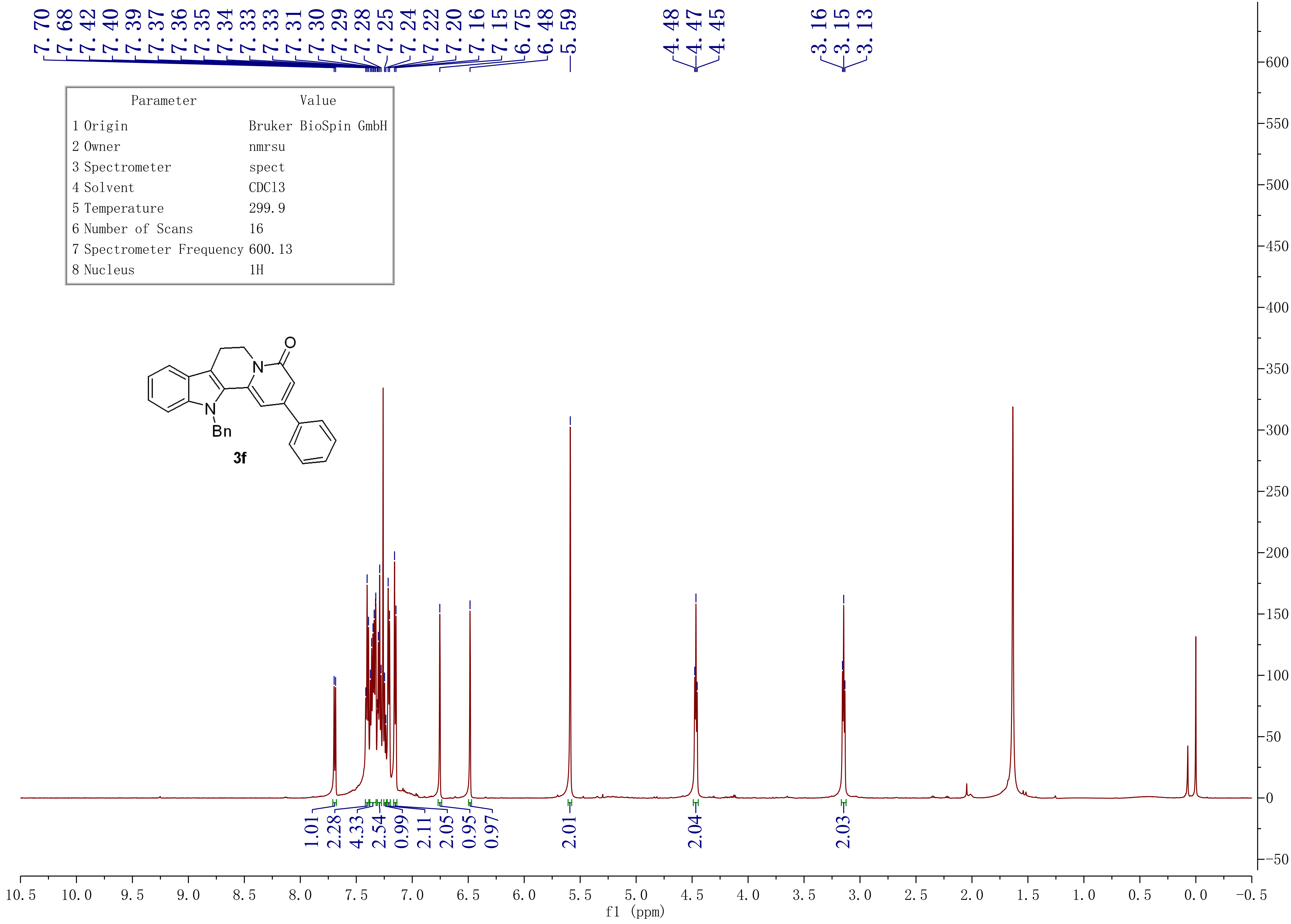

162.74
159.23
156.21
140.81
129.28
126.95
125.01
124.82
120.93
119.78
116.62
114.73
113.80
110.45
100.27
55.53
48.41
40.13
20.20
15.21
9.66
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 53
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
PMB
3c
O
f1 (ppm)

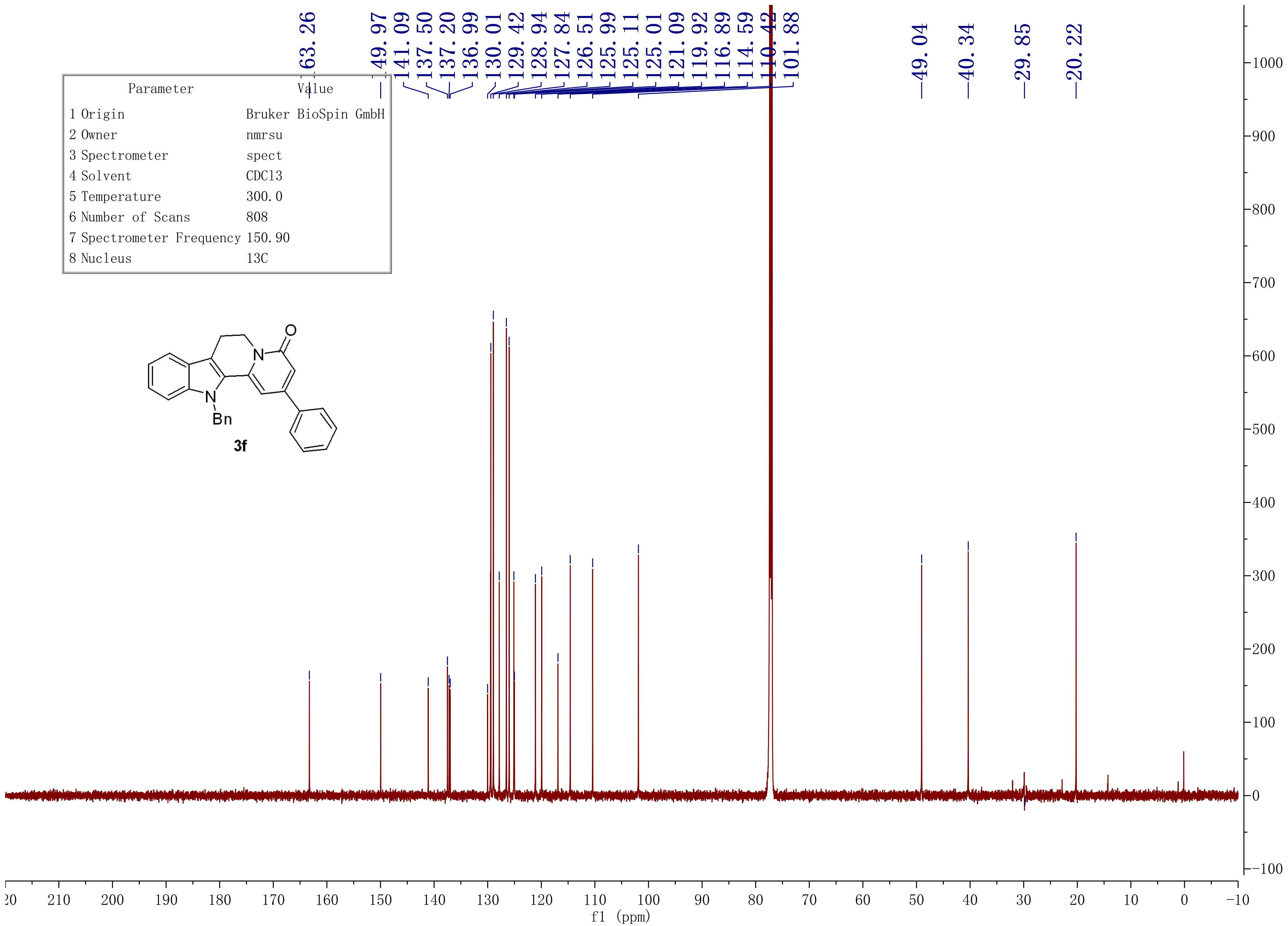

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
3d
f1 (ppm)

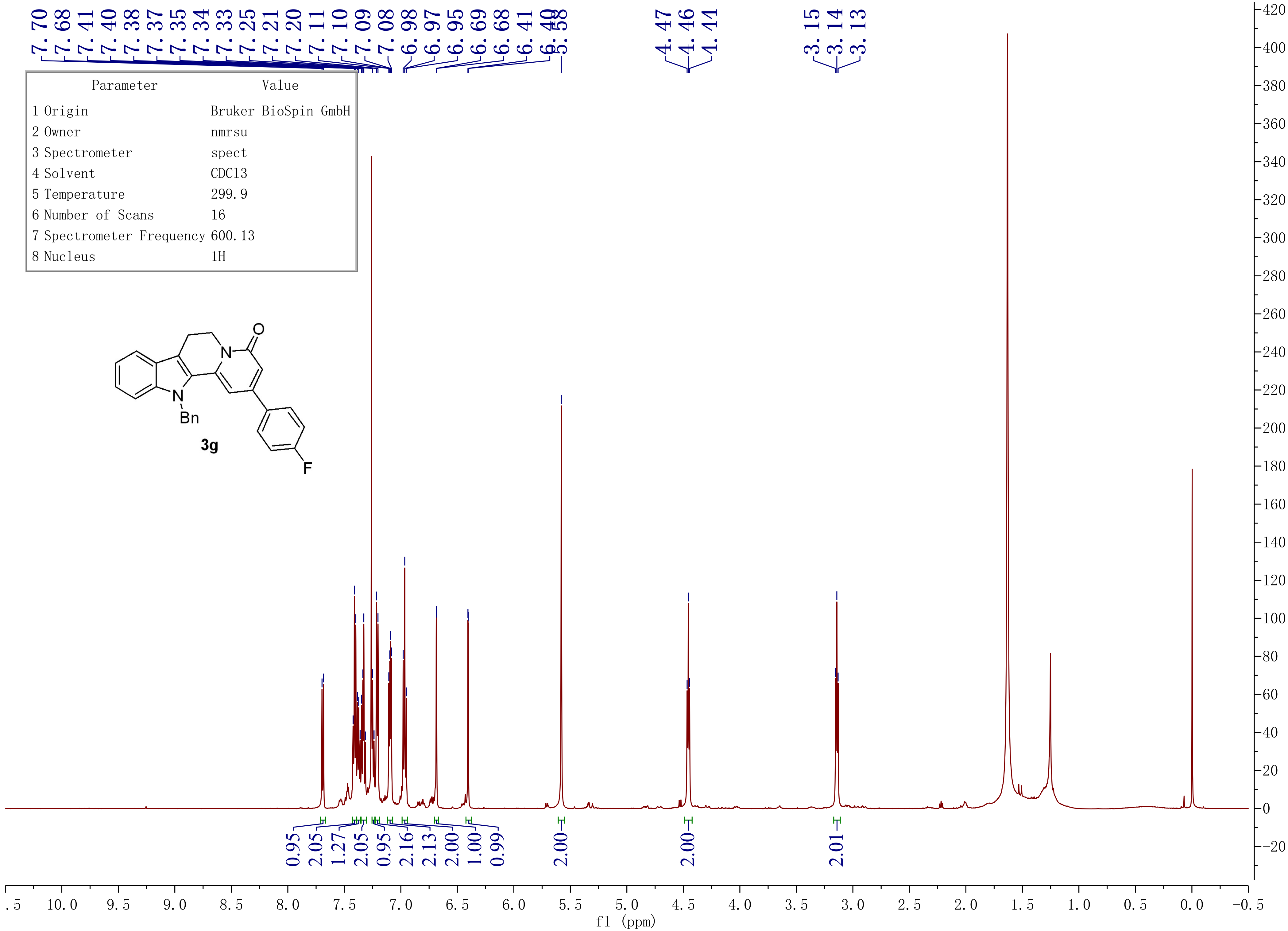

3d
Bn
N
N
O
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
CDCl3
5 Temperature
300.0
6 Number of Scans
41
7 Spectrometer Frequency
150.90
8 Nucleus
13C
163.10
153.82
140.90
137.48
136.25
129.96
129.25
127.80
125.93
125.07
124.84
120.97
119.78
116.88
116.67
110.48
104.02
49.02
40.18
37.37
22.17
20.19
13.65
f1 (ppm)

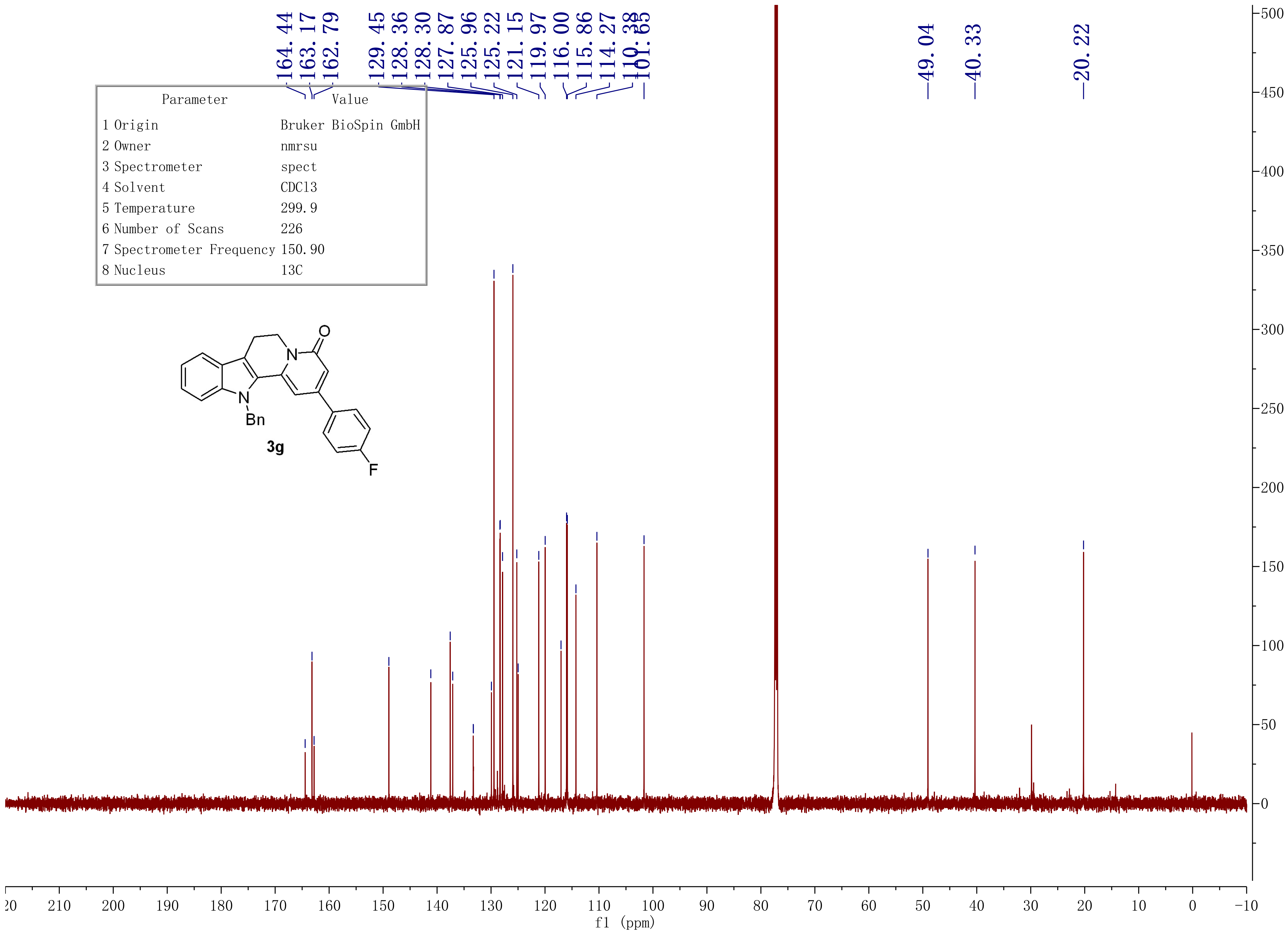

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Bn
3e
f1 (ppm)

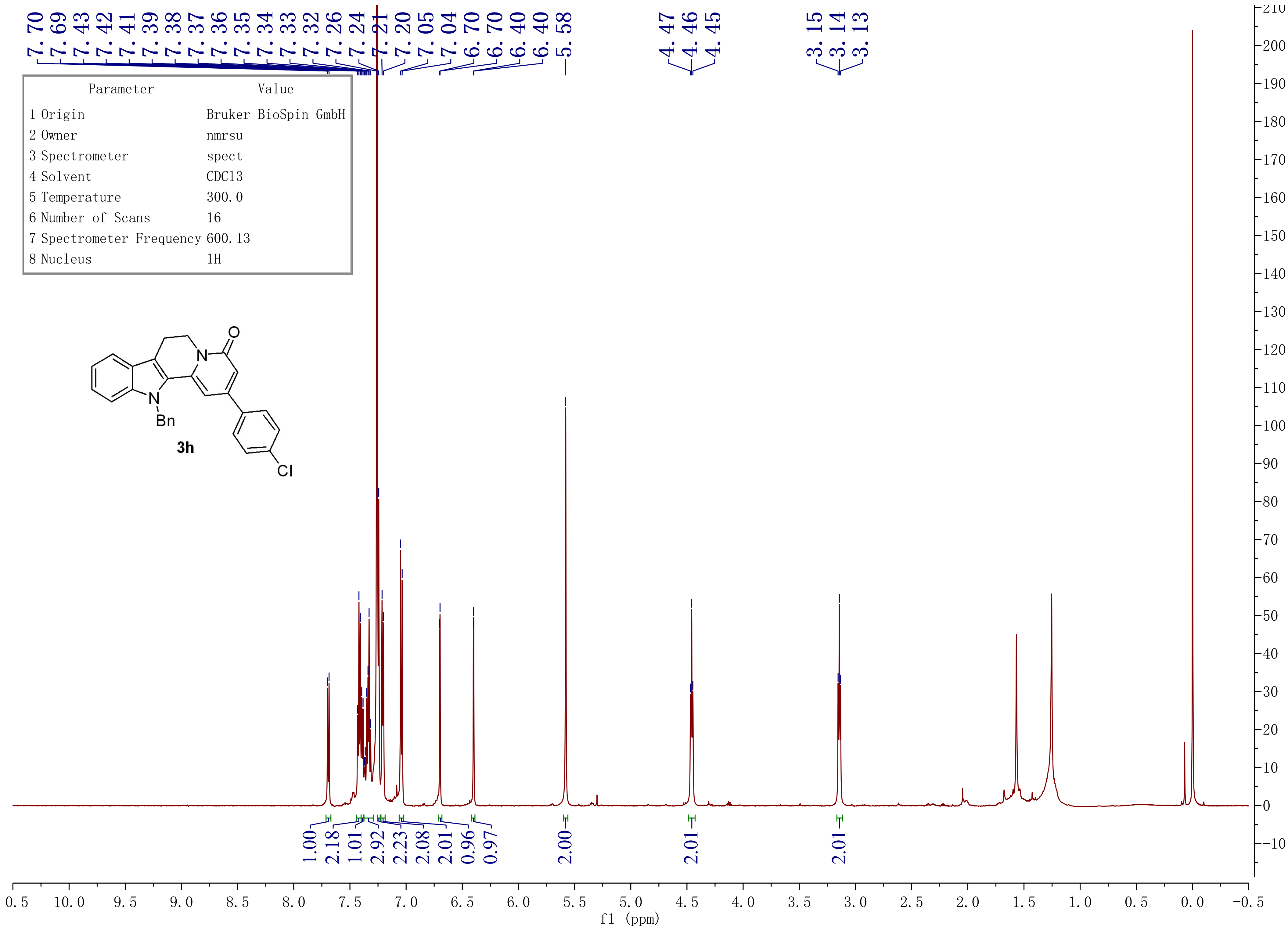

163.39
162.07
140.85
137.37
135.87
130.21
129.36
127.85
125.76
125.11
124.79
120.98
119.78
116.31
113.96
110.33
102.02
48.97
40.14
34.81
29.53
20.21
0.14
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 908
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
N
O
Bn
3e
f1 (ppm)

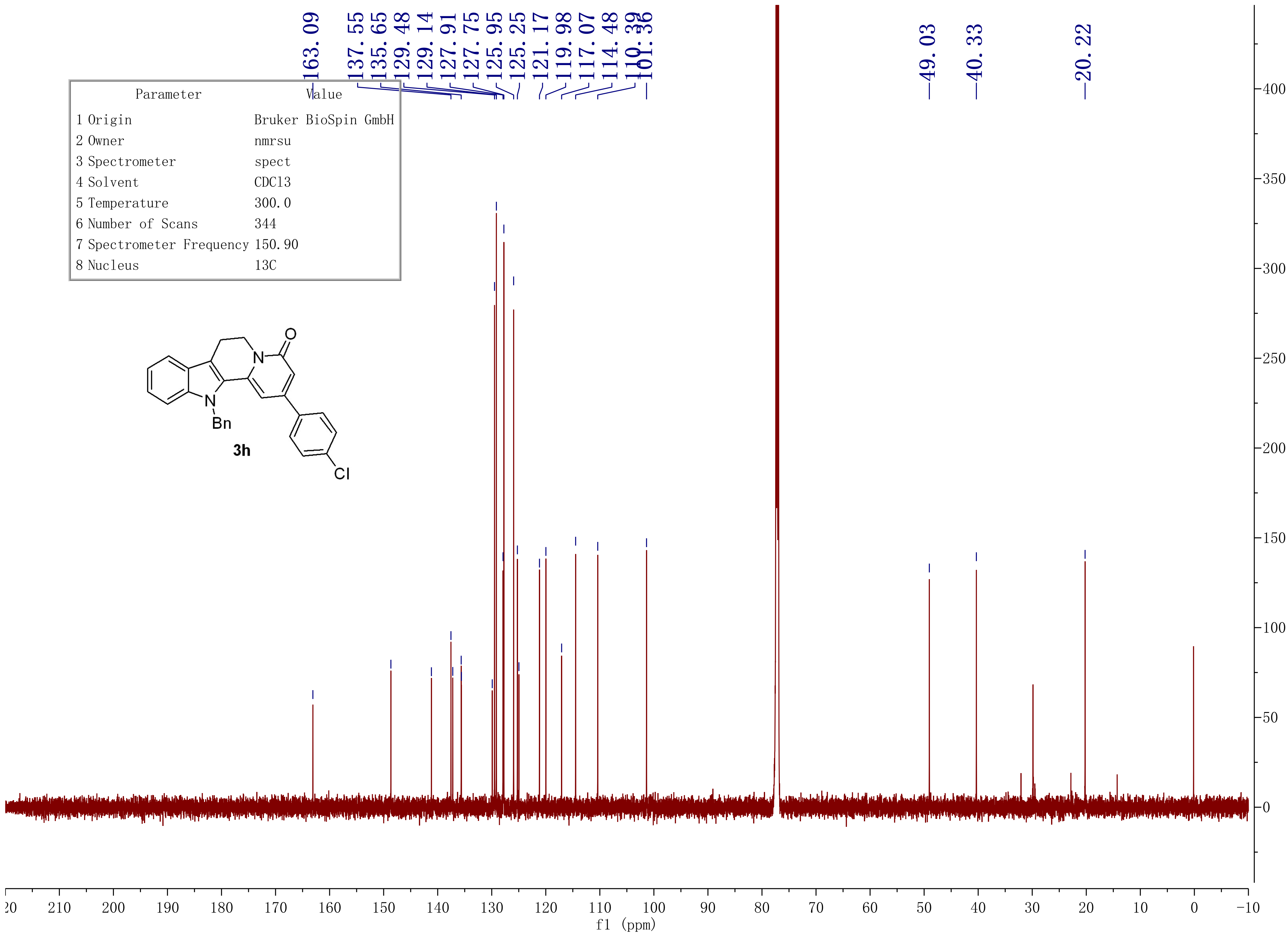

7.70 7.68 7.42 7.40 7.39 7.37 7.36 7.35 7.34 7.33 7.33 7.31 7.30 7.29 7.28 7.25 7.24 7.22 7.20 7.16 7.15 6.75 6.48
5.59
4.48 4.47 4.45
3.16 3.15 3.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
O
N
Bn
3f
1.01 2.28 4.33 2.54 0.99 2.11 2.05 0.95 0.97
2.01
2.04
2.03
f1 (ppm)

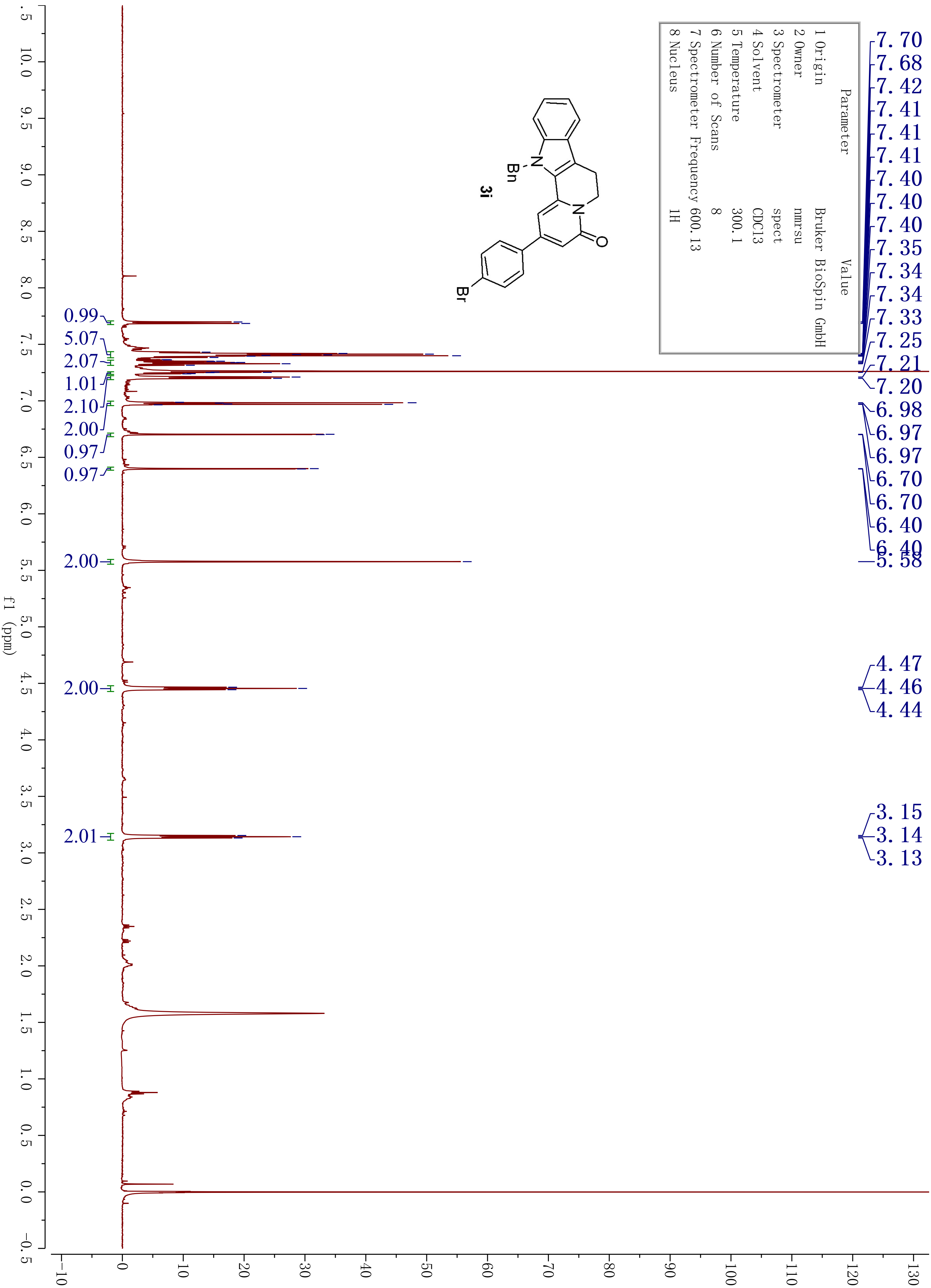

163.26
149.97
141.09
137.50
137.20
136.99
130.01
129.42
128.94
127.84
126.51
125.99
125.11
125.01
121.09
119.92
116.89
114.59
110.42
101.88
49.04
40.34
29.85
20.22
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 808
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
O
N
Bn
3f
f1 (ppm)

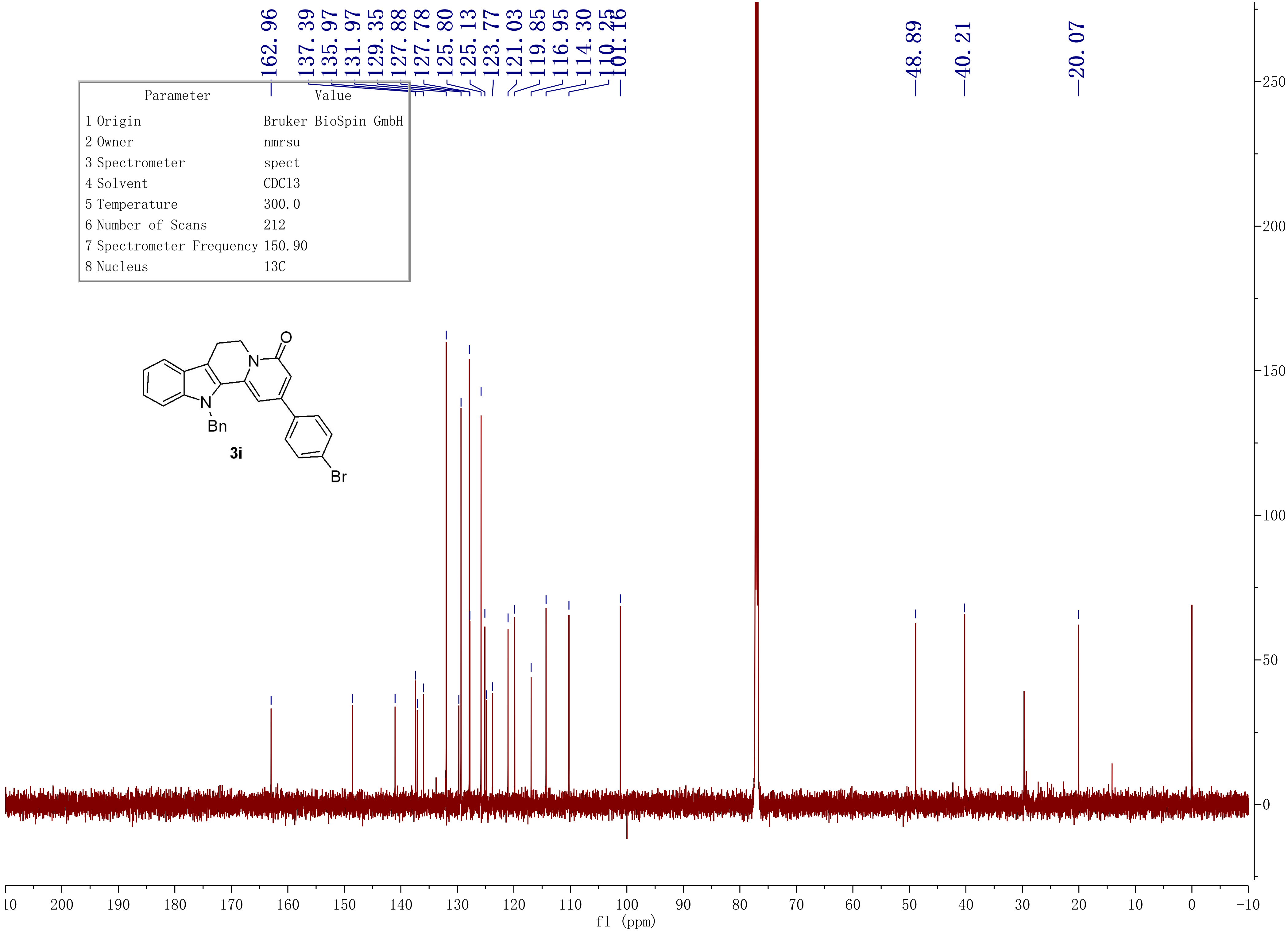

7.70
7.68
7.41
7.40
7.38
7.37
7.35
7.34
7.33
7.25
7.21
7.20
7.11
7.10
7.09
7.08
6.98
6.97
6.95
6.69
6.68
6.41
6.40
5.58
4.47
4.46
4.44
3.15
3.14
3.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Bn
N
O
F
3g
0.95
2.05
1.27
2.05
0.95
2.16
2.13
2.00
1.00
0.99
2.00
2.00
2.01
f1 (ppm)

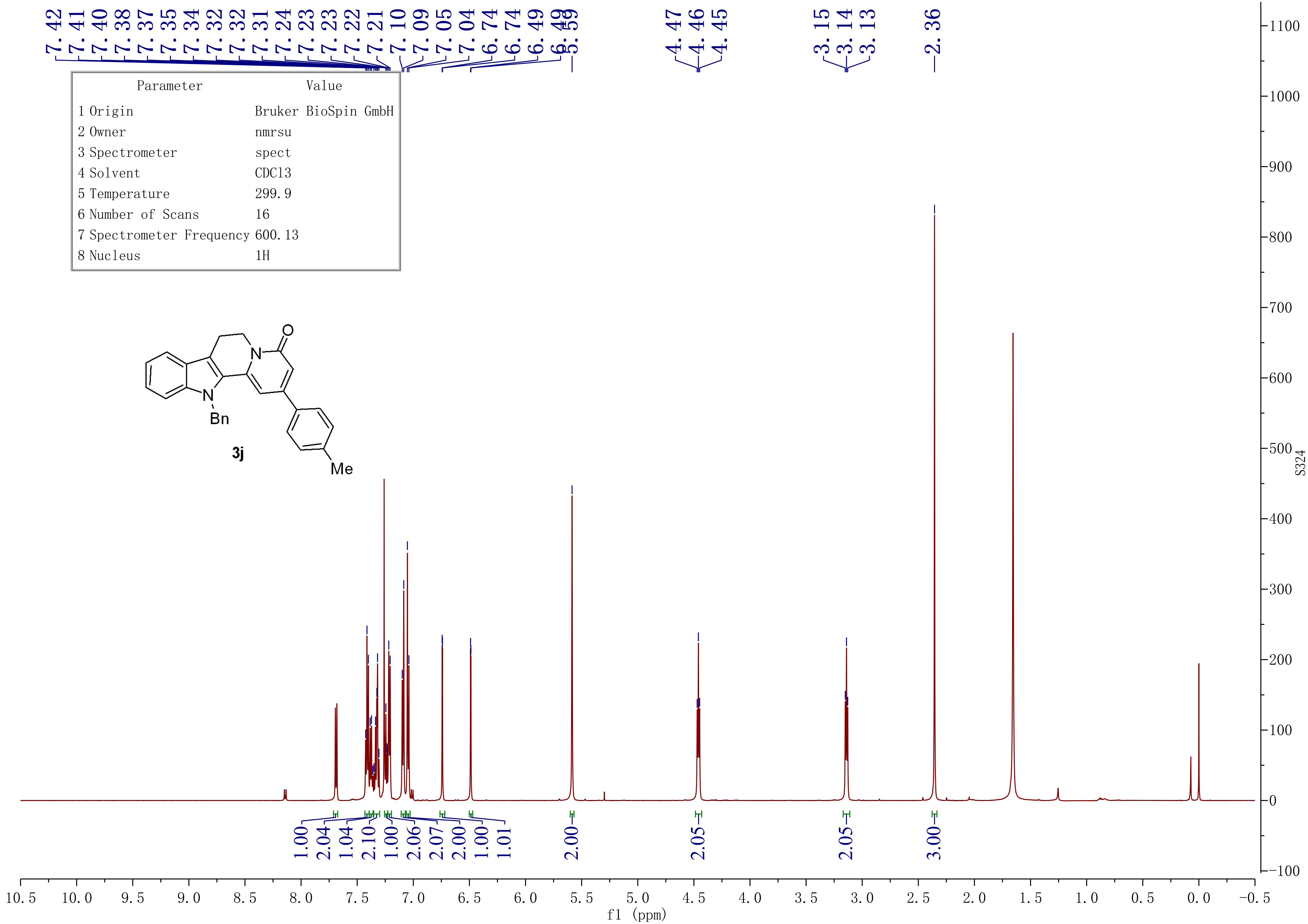

164.44
163.17
162.79
129.45
128.36
128.30
127.87
125.96
125.22
121.15
119.97
116.00
115.86
114.27
110.38
101.65
49.04
40.33
20.22
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 226
7 Spectrometer Frequency 150.90
8 Nucleus 13C
3g
f1 (ppm)

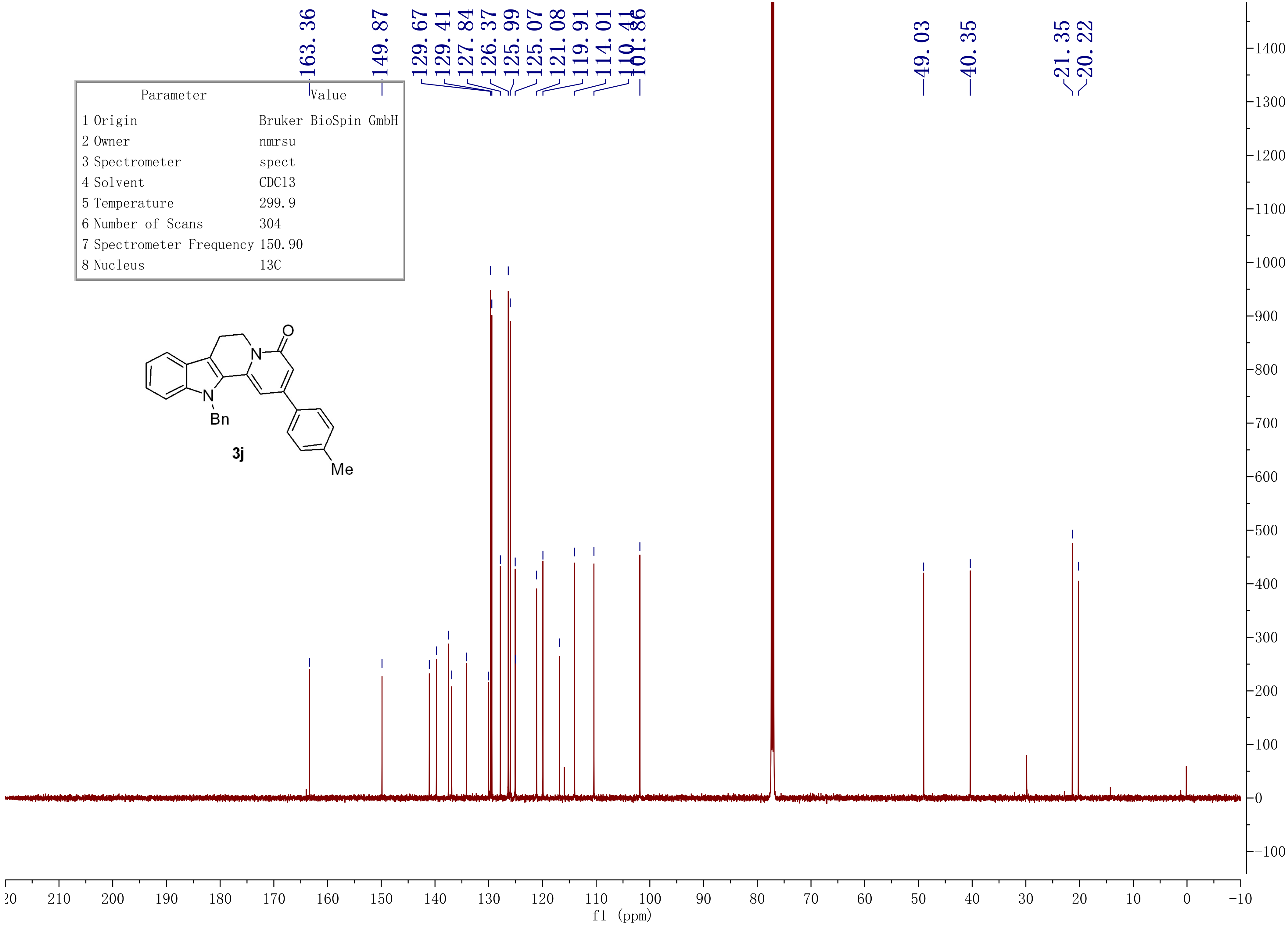

7.70
7.69
7.43
7.42
7.41
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.32
7.26
7.24
7.21
7.20
7.05
7.04
6.70
6.70
6.40
6.40
5.58
4.47
4.46
4.45
3.15
3.14
3.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
N
Bn
N
O
Cl
3h
1.00
2.18
1.01
2.92
2.23
2.08
2.01
0.96
0.97
2.00
2.01
2.01
f1 (ppm)

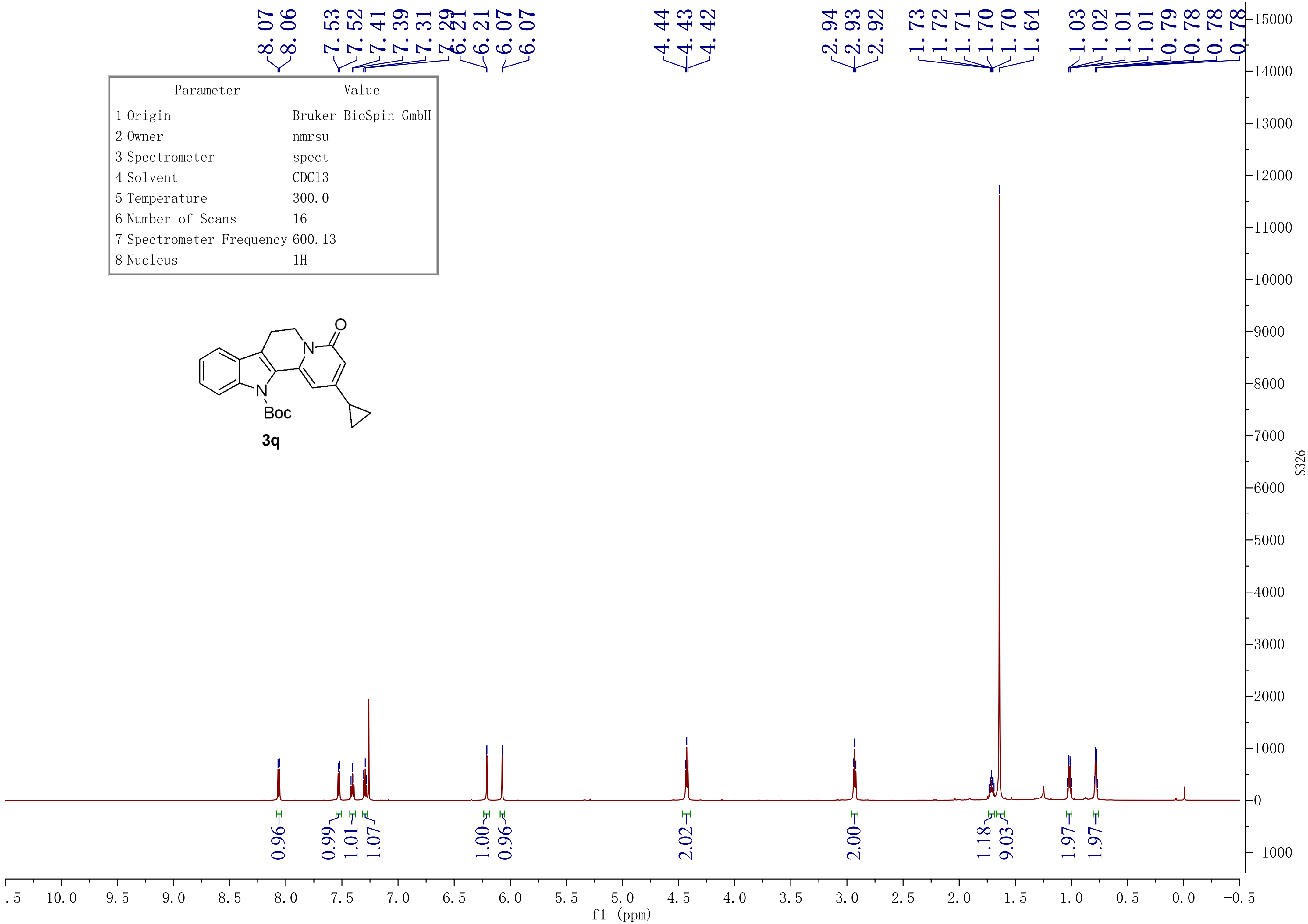

163.09
137.55
135.65
129.48
129.14
127.91
127.75
125.95
125.25
121.17
119.98
117.07
114.48
110.39
101.36
49.03
40.33
20.22
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 344
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
O
N
Bn
3h
Cl
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.1
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Bn
Br
O
N
3i
7.70
7.68
7.42
7.41
7.41
7.41
7.40
7.40
7.40
7.35
7.34
7.34
7.33
7.25
7.21
7.20
6.98
6.97
6.97
6.70
6.70
6.40
6.40
5.58
4.47
4.46
4.44
3.15
3.14
3.13
0.99
5.07
2.07
1.01
2.10
2.00
0.97
0.97
2.00
2.00
2.01
f1 (ppm)

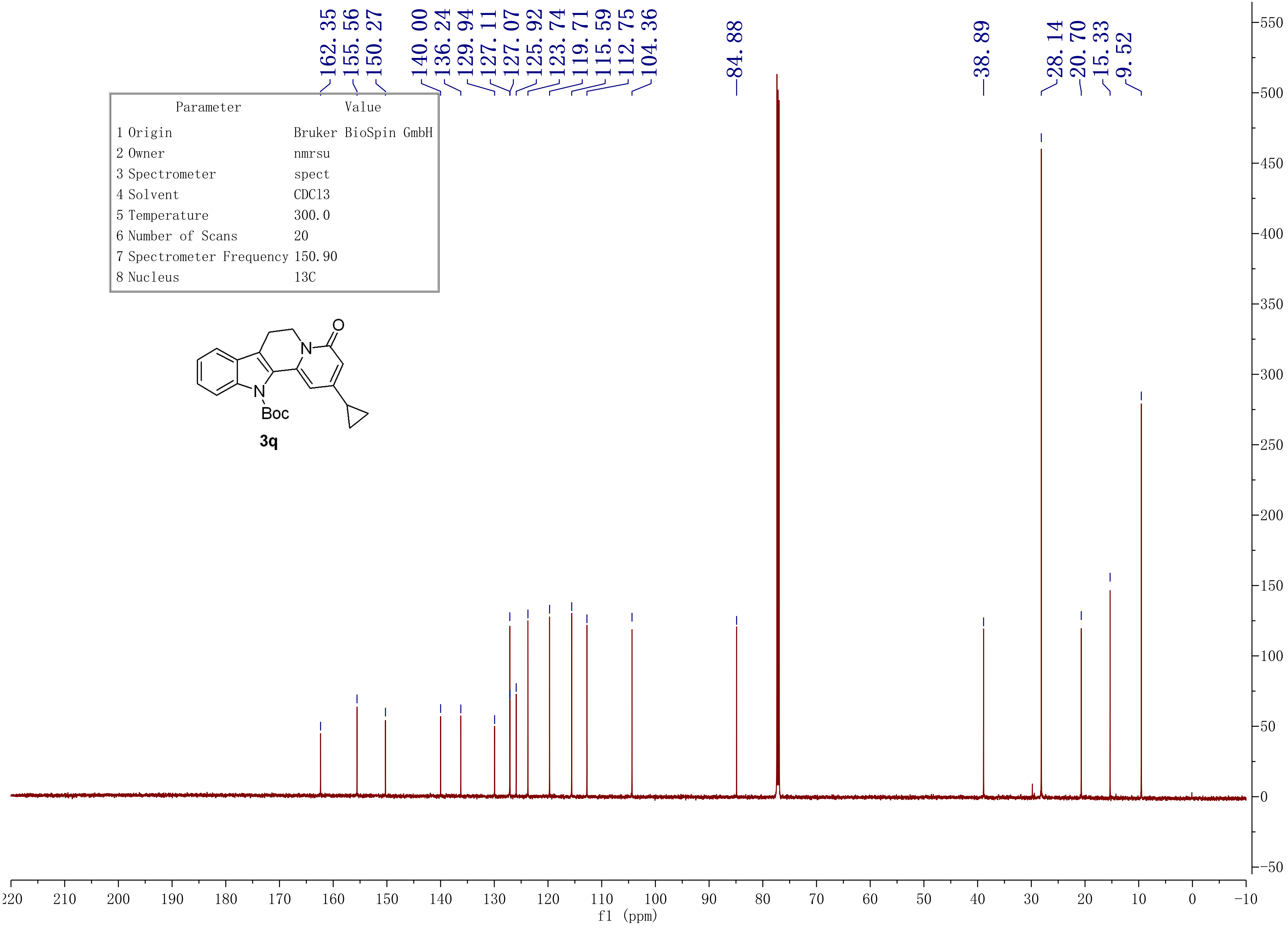

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 212
7 Spectrometer Frequency 150.90
8 Nucleus 13C
162.96
137.39
135.97
131.97
129.35
127.88
127.78
125.80
125.13
123.77
121.03
119.85
116.95
114.30
110.25
101.16
48.89
40.21
20.07
N
Bn
3i
N
O
Br
f1 (ppm)


Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
7.42 7.41 7.40 7.38 7.37 7.35 7.34 7.32 7.32 7.31 7.24 7.23 7.23 7.22 7.21 7.10 7.09 7.05 7.04 6.74 6.74 6.49 6.49 5.59
4.47 4.46 4.45
3.15 3.14 3.13
2.36
N
Bn
N
O
Me
3j
1.00 2.04 1.04 2.10 1.00 2.06 2.07 2.00 1.00 1.01
2.00
2.05
2.05
3.00
f1 (ppm)


163.36
149.87
129.67
129.41
127.84
126.37
125.99
125.07
121.08
119.91
114.01
110.41
101.86
49.03
40.35
21.35
20.22
Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
CDCl3
5 Temperature
299.9
6 Number of Scans
304
7 Spectrometer Frequency
150.90
8 Nucleus
13C
N
O
N
Bn
3j
Me
f1 (ppm)

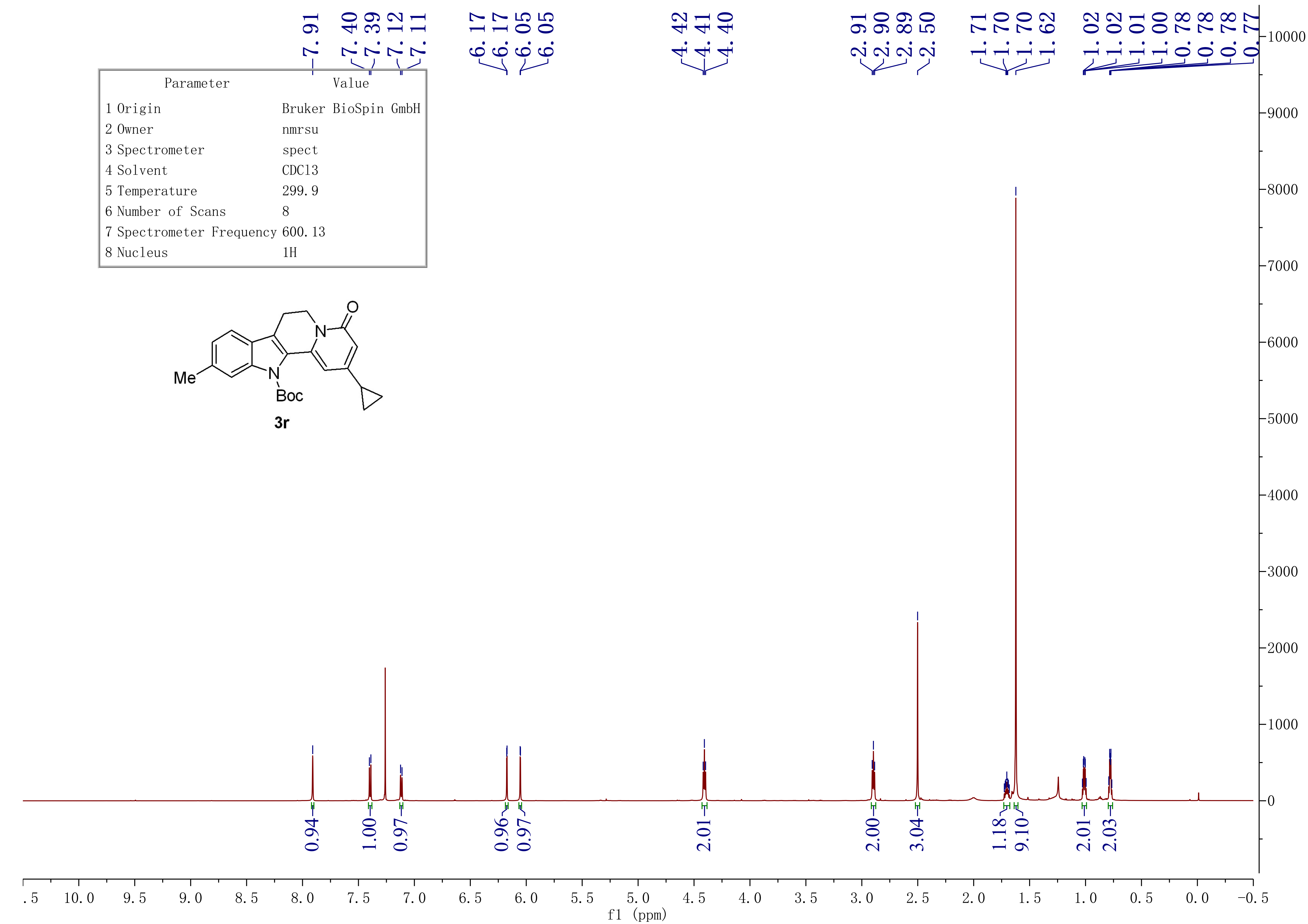


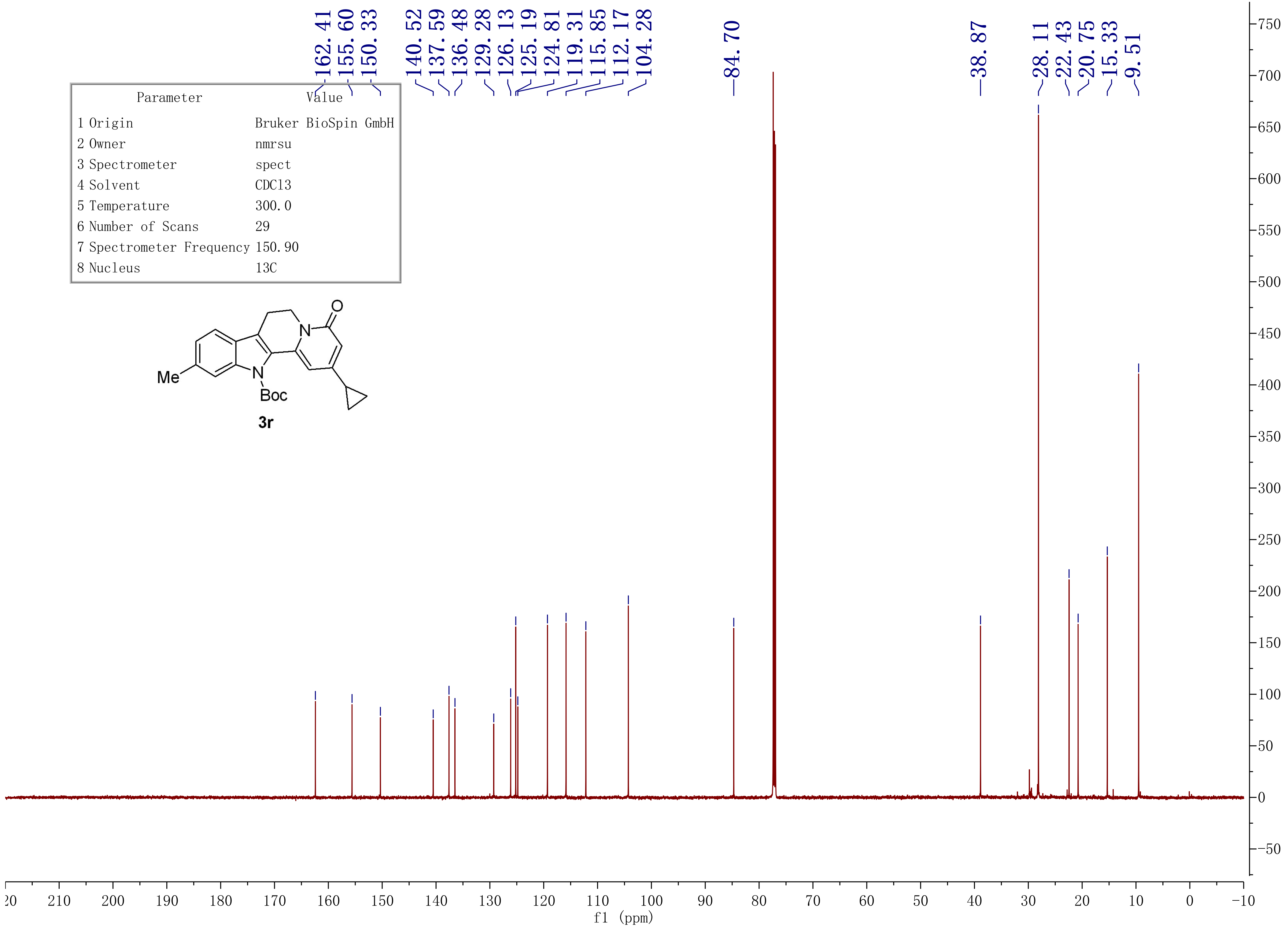
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	20
7 Spectrometer Frequency	150.90
8 Nucleus	13C

3q

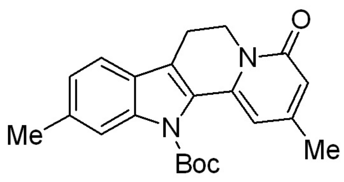

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 8
7 Spectrometer Frequency 600.13
8 Nucleus 1H
Me
N
Boc
N
O
3r
7.91 7.40 7.39 7.12 7.11 6.17 6.17 6.05 6.05 4.42 4.41 4.40 2.91 2.90 2.89 2.50 1.71 1.70 1.70 1.62 1.02 1.02 1.01 1.00 0.78 0.78 0.78 0.77
0.94 1.00 0.97 0.96 0.97 2.01 2.00 3.04 1.18 9.10 2.01 2.03
f1 (ppm)



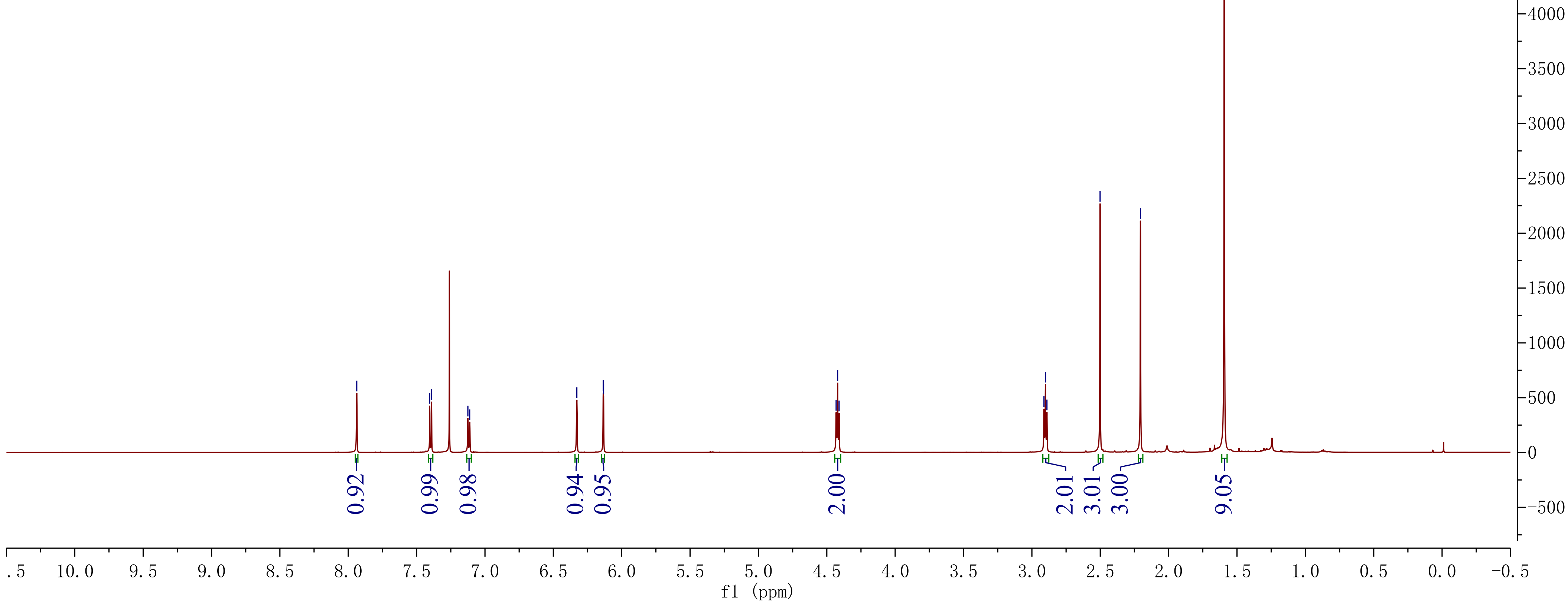
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 29
7 Spectrometer Frequency 150.90
8 Nucleus 13C
162.41
155.60
150.33
140.52
137.59
136.48
129.28
126.13
125.19
124.81
119.31
115.85
112.17
104.28
84.70
38.87
28.11
22.43
20.75
15.33
9.51
f1 (ppm)
Me
N
Boc
N
O

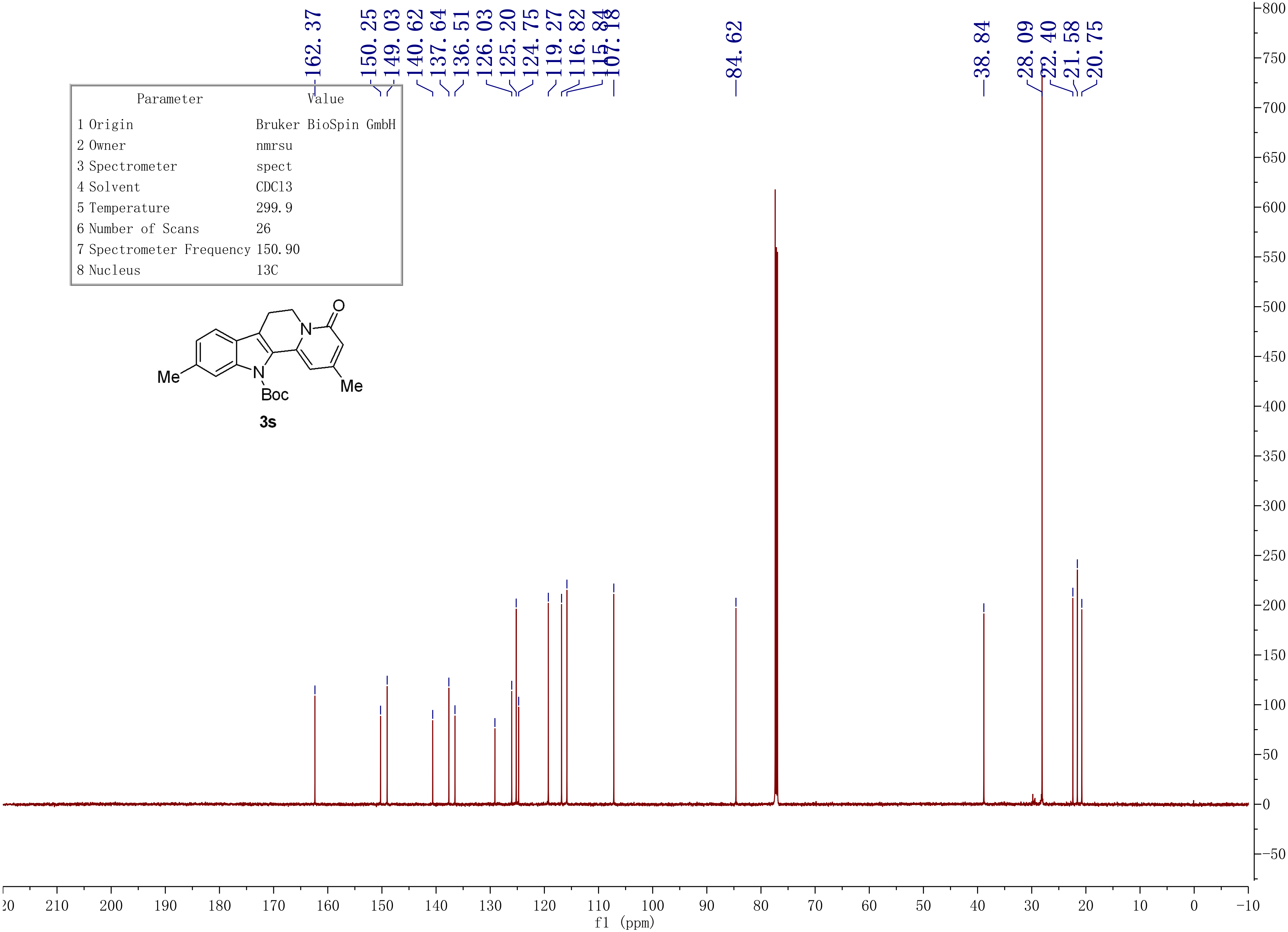
3r

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.1
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H

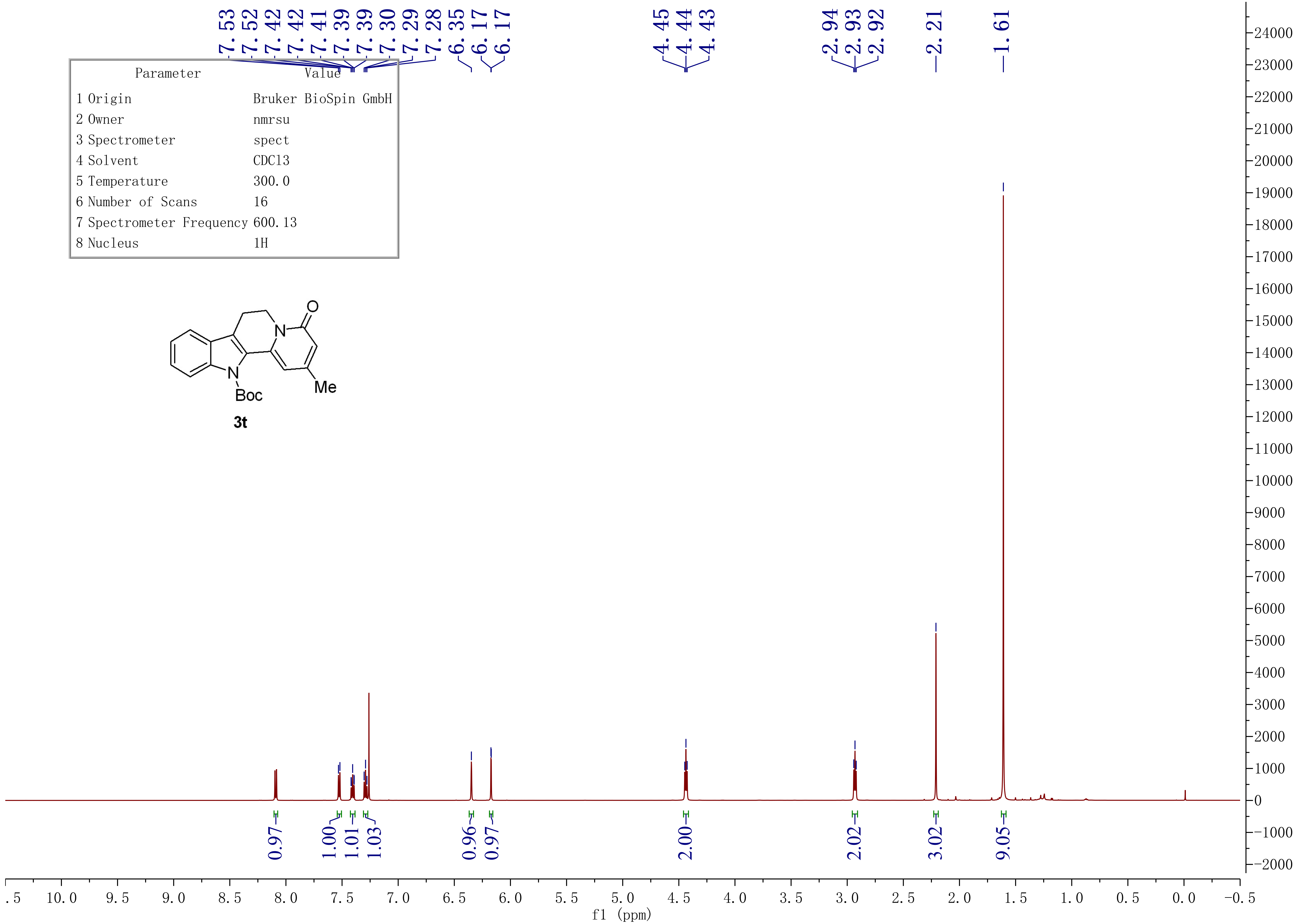


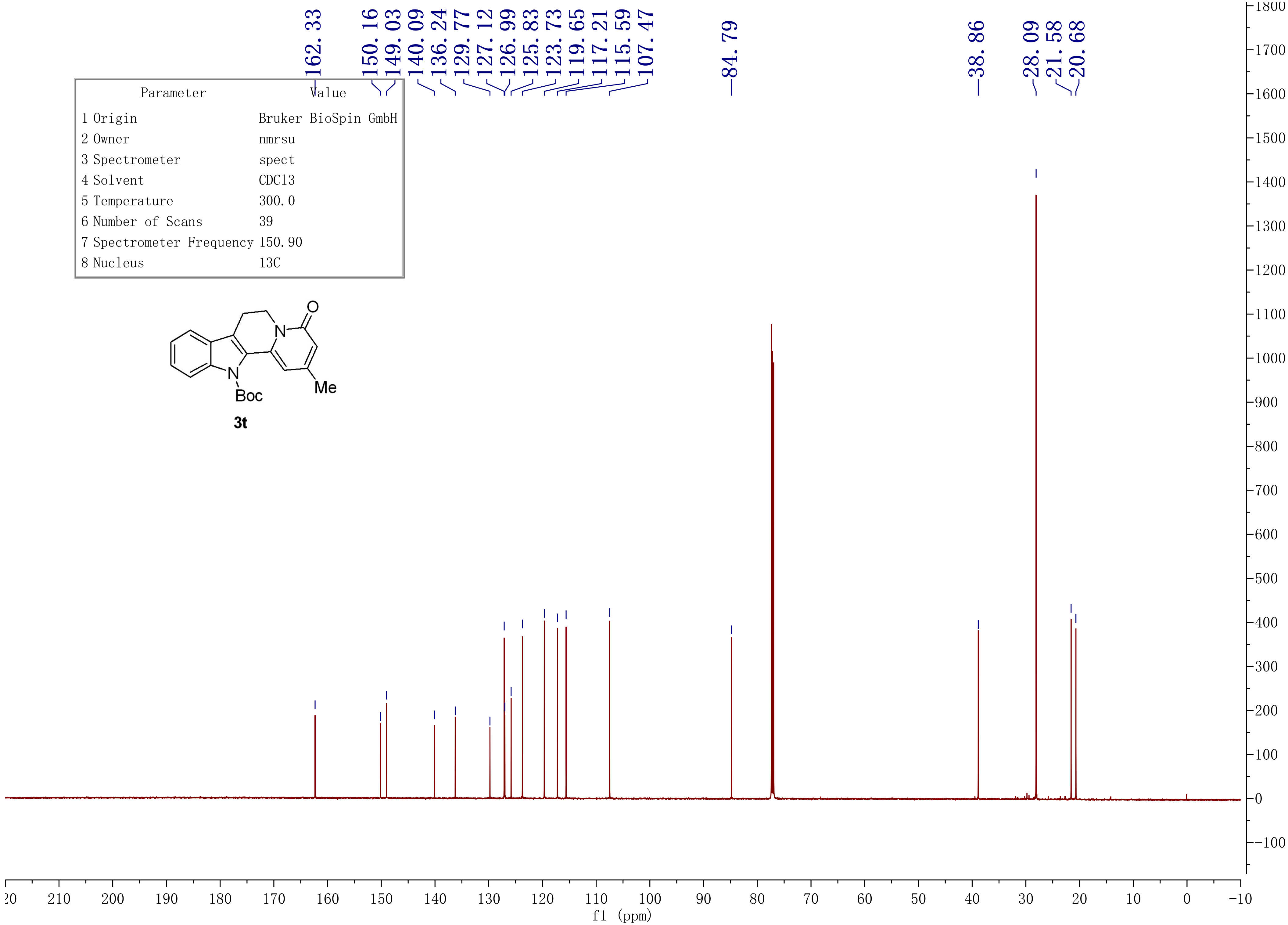
3s





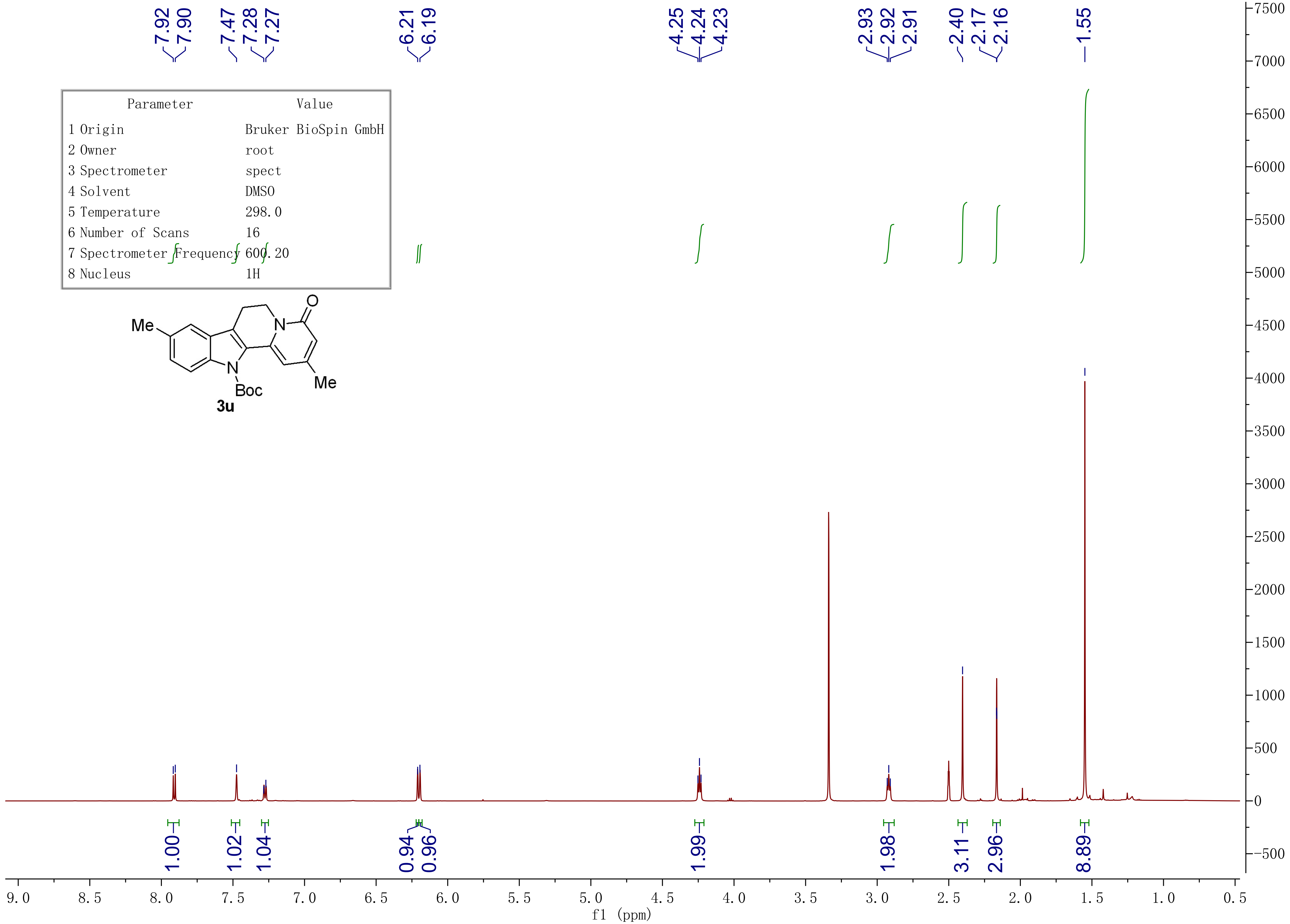
Parameter | Value
1 Origin | Bruker BioSpin GmbH
2 Owner | nmrsu
3 Spectrometer | spect
4 Solvent | CDCl3
5 Temperature | 299.9
6 Number of Scans | 26
7 Spectrometer Frequency | 150.90
8 Nucleus | 13C
Me
N
Boc
O
Me
3s
162.37
150.25
149.03
140.62
137.64
136.51
126.03
125.20
124.75
119.27
116.82
115.84
107.18
84.62
38.84
28.09
22.40
21.58
20.75
f1 (ppm)

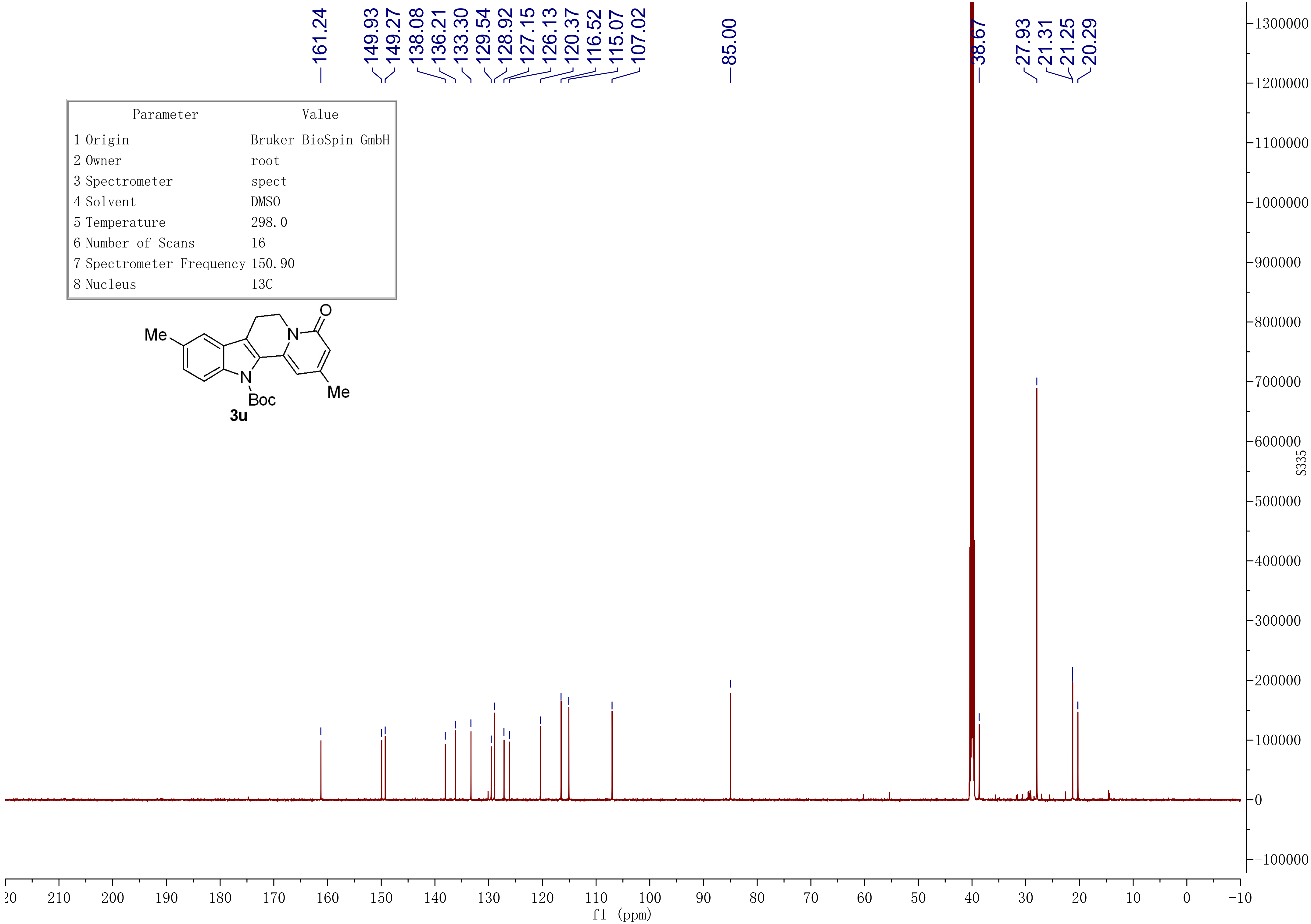

7.53
7.52
7.42
7.42
7.41
7.39
7.39
7.30
7.29
7.28
6.35
6.17
6.17
4.45
4.44
4.43
2.94
2.93
2.92
2.21
1.61
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 16
7 Spectrometer Frequency 600.13
8 Nucleus 1H
O
N
N
Boc
Me
3t
0.97
1.00
1.01
1.03
0.96
0.97
2.00
2.02
3.02
9.05
f1 (ppm)

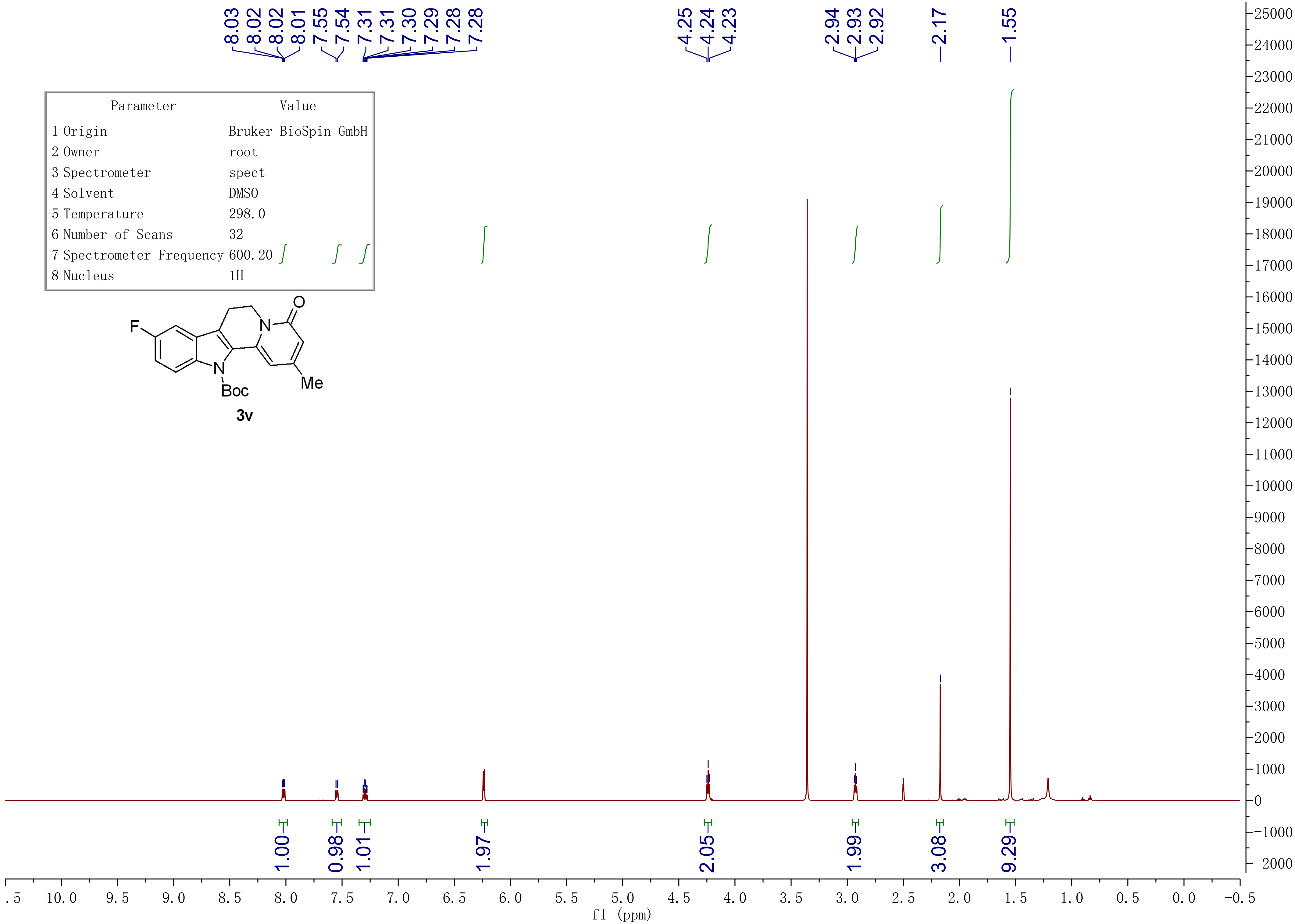


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	39
7 Spectrometer Frequency	150.90
8 Nucleus	13C

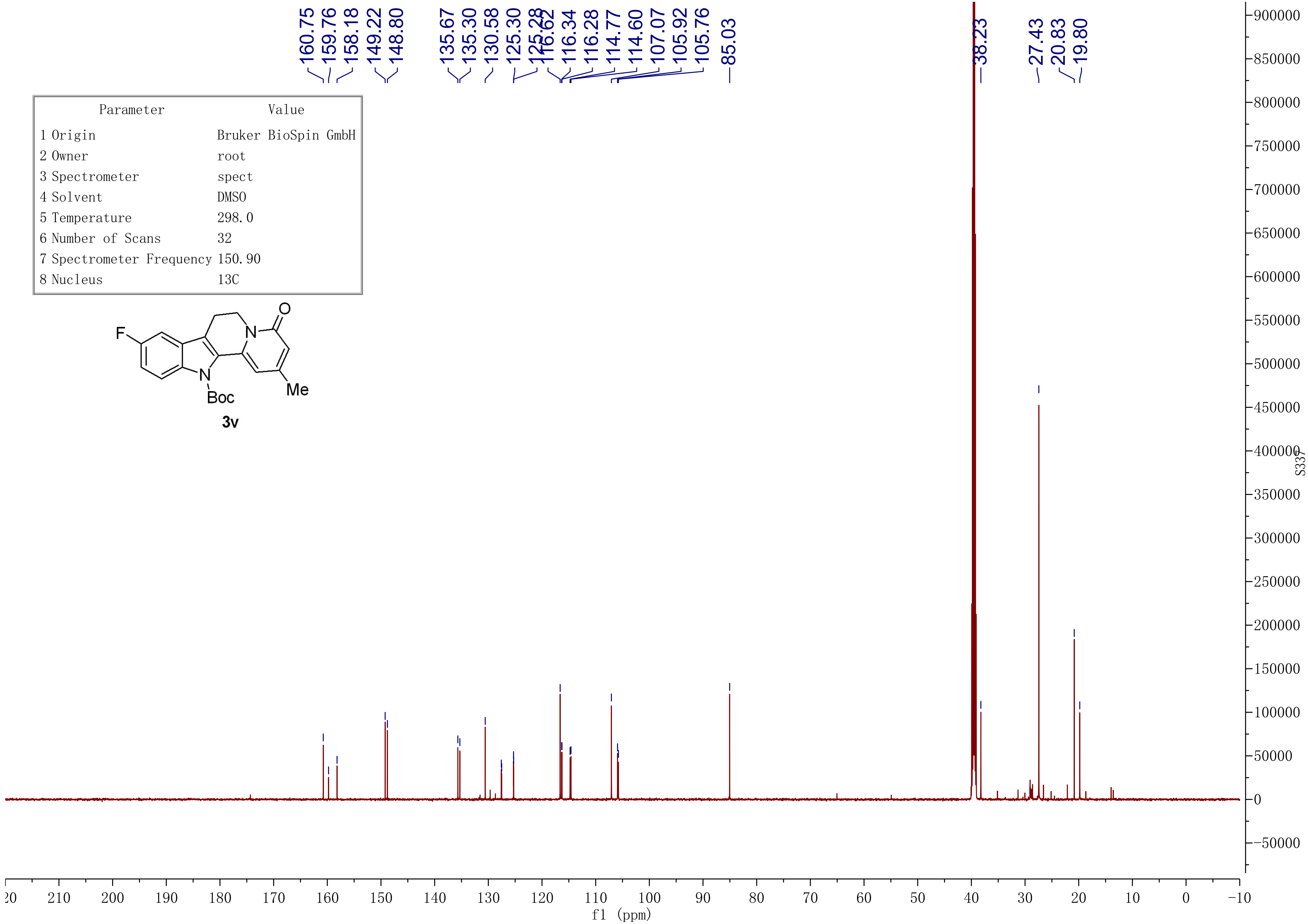
3t


7.92
7.90
7.47
7.28
7.27
6.21
6.19
4.25
4.24
4.23
2.93
2.92
2.91
2.40
2.17
2.16
1.55
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 600.20
8 Nucleus 1H
Me
N
O
N
Boc
Me
3u
1.00
1.02
1.04
0.94
0.96
1.99
1.98
3.11
2.96
8.89
f1 (ppm)

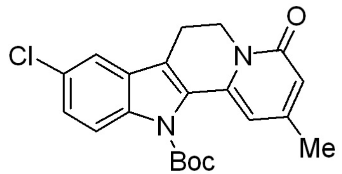

161.24
149.93
149.27
138.08
136.21
133.30
129.54
128.92
127.15
126.13
120.37
116.52
115.07
107.02
85.00
38.67
27.93
21.31
21.25
20.29
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 16
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Me
O
N
Me
N
Boc
3u
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	root
3 Spectrometer	spect
4 Solvent	DMSO
5 Temperature	298.0
6 Number of Scans	32
7 Spectrometer Frequency	600.20
8 Nucleus	1H


160.75
159.76
158.18
149.22
148.80
135.67
135.30
130.58
125.30
125.28
116.62
116.34
116.28
114.77
114.60
107.07
105.92
105.76
85.03
38.23
27.43
20.83
19.80
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner root
3 Spectrometer spect
4 Solvent DMSO
5 Temperature 298.0
6 Number of Scans 32
7 Spectrometer Frequency 150.90
8 Nucleus 13C
F
N
N
O
Boc
Me
3v
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H



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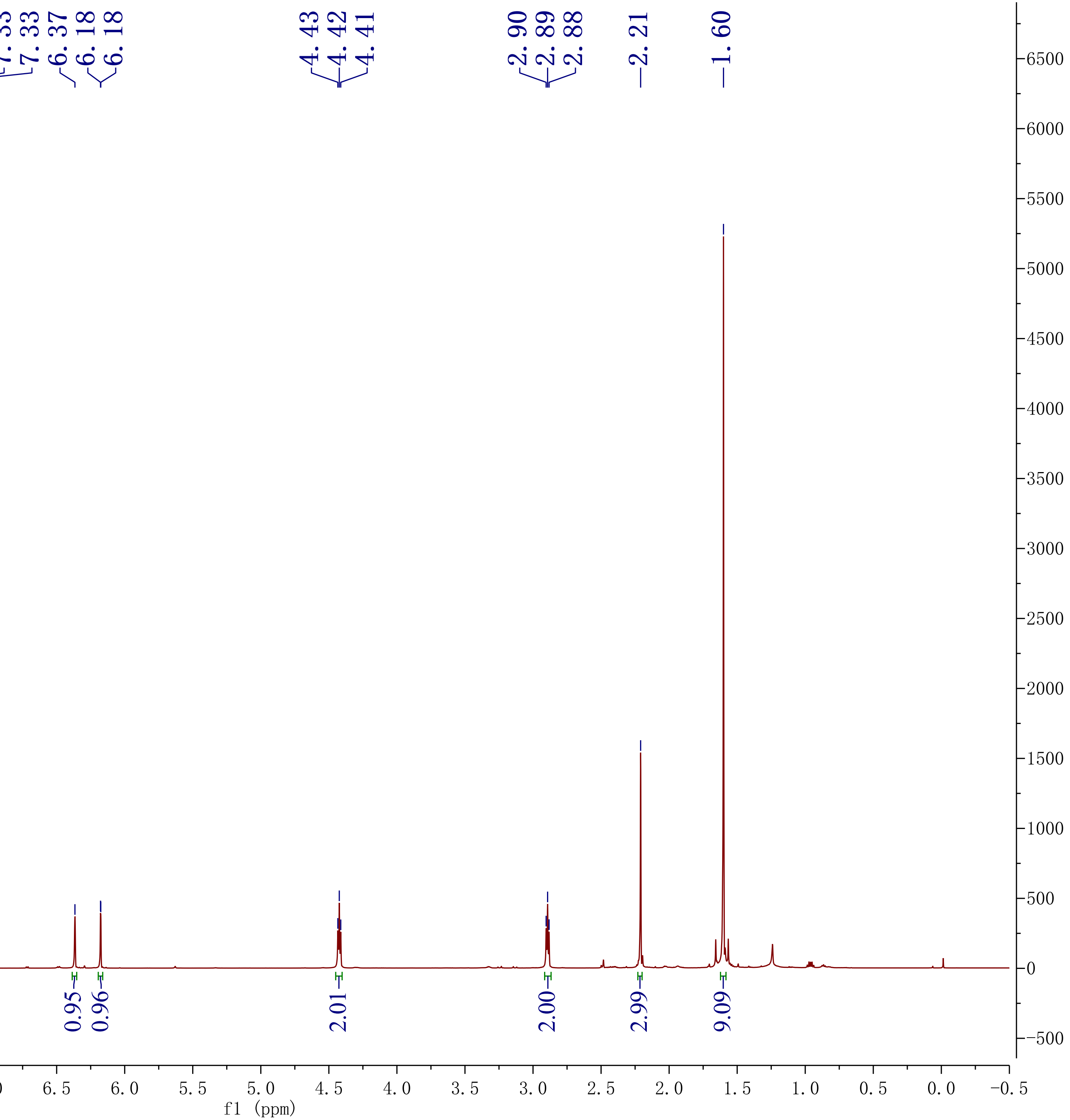
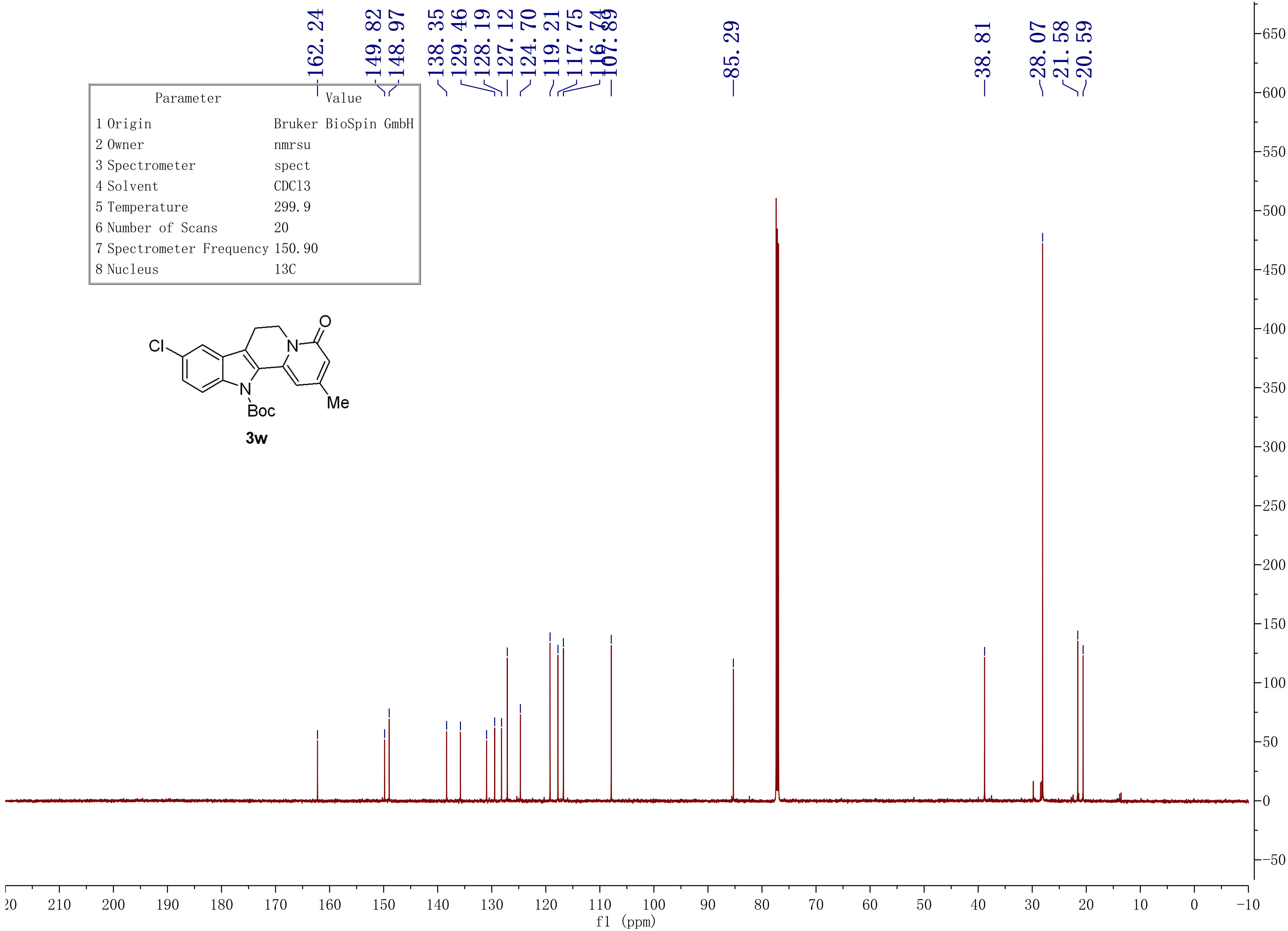
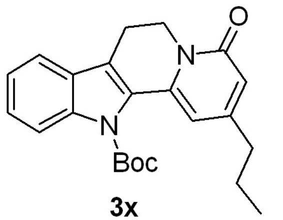




162.24
149.82
148.97
138.35
129.46
128.19
127.12
124.70
119.21
117.75
116.74
107.89
85.29
38.81
28.07
21.58
20.59
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 299.9
6 Number of Scans 20
7 Spectrometer Frequency 150.90
8 Nucleus 13C
Cl
N
O
N
Boc
Me
3w
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H



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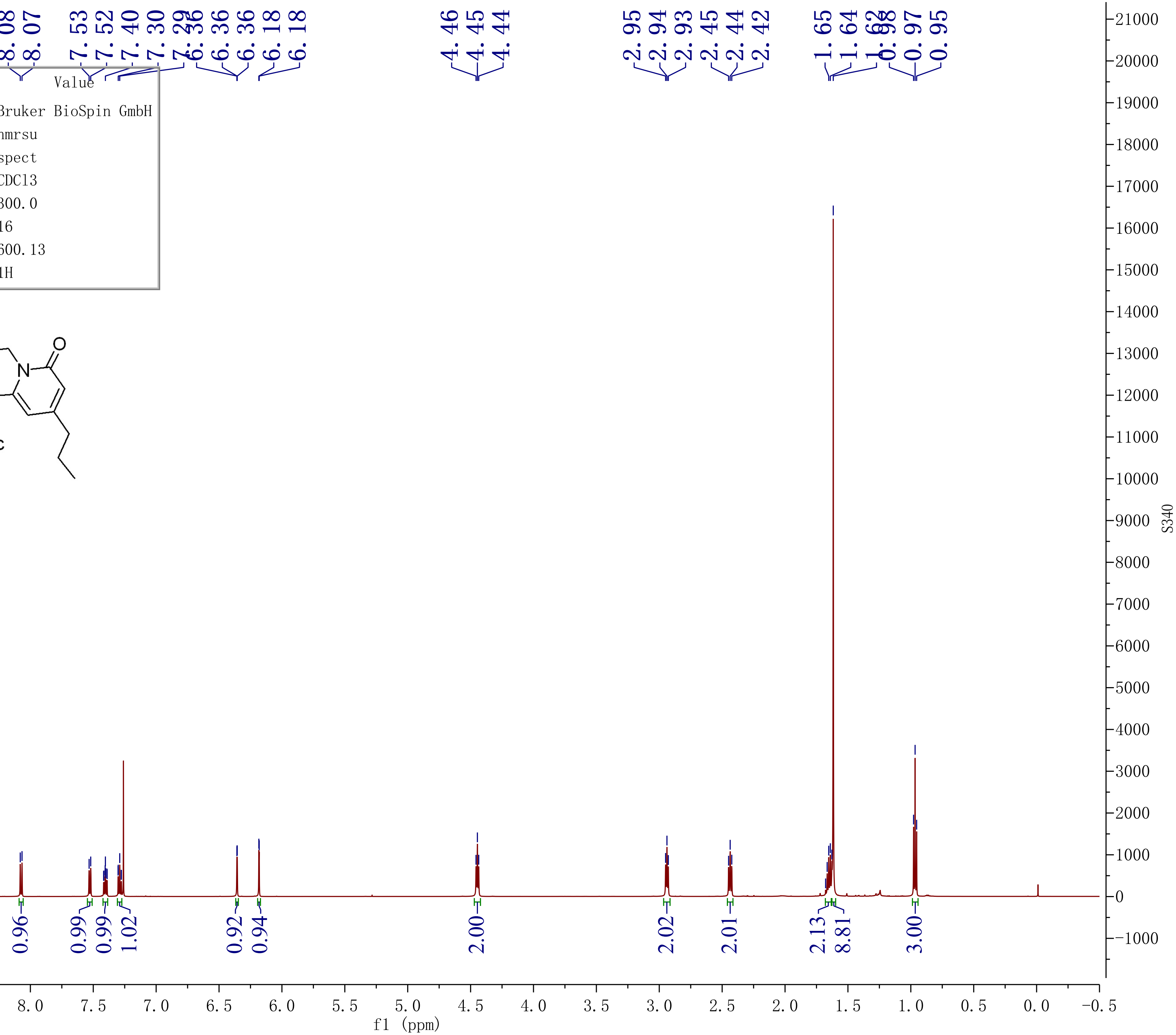
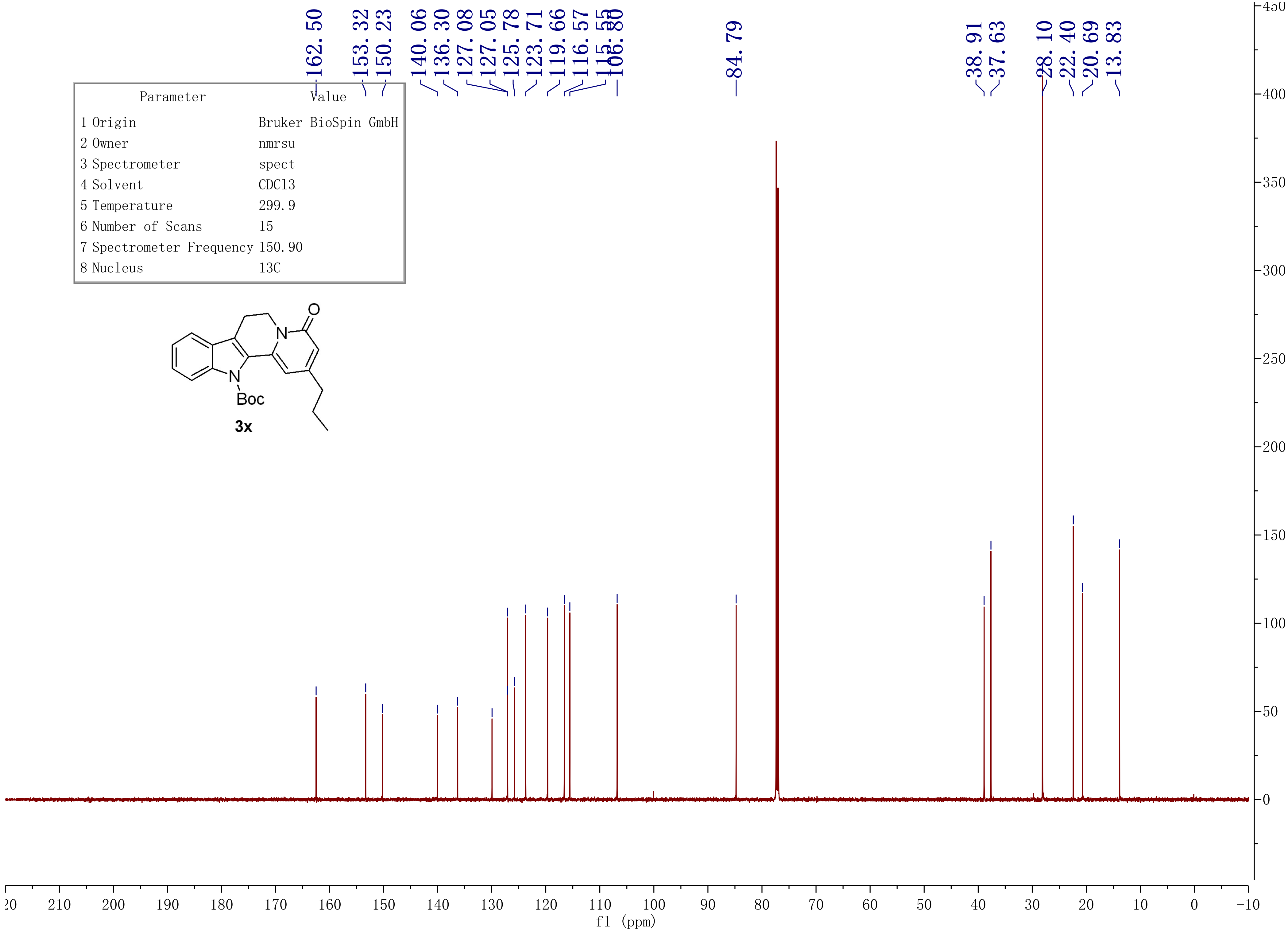
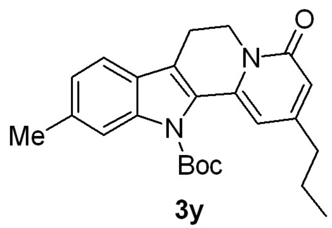


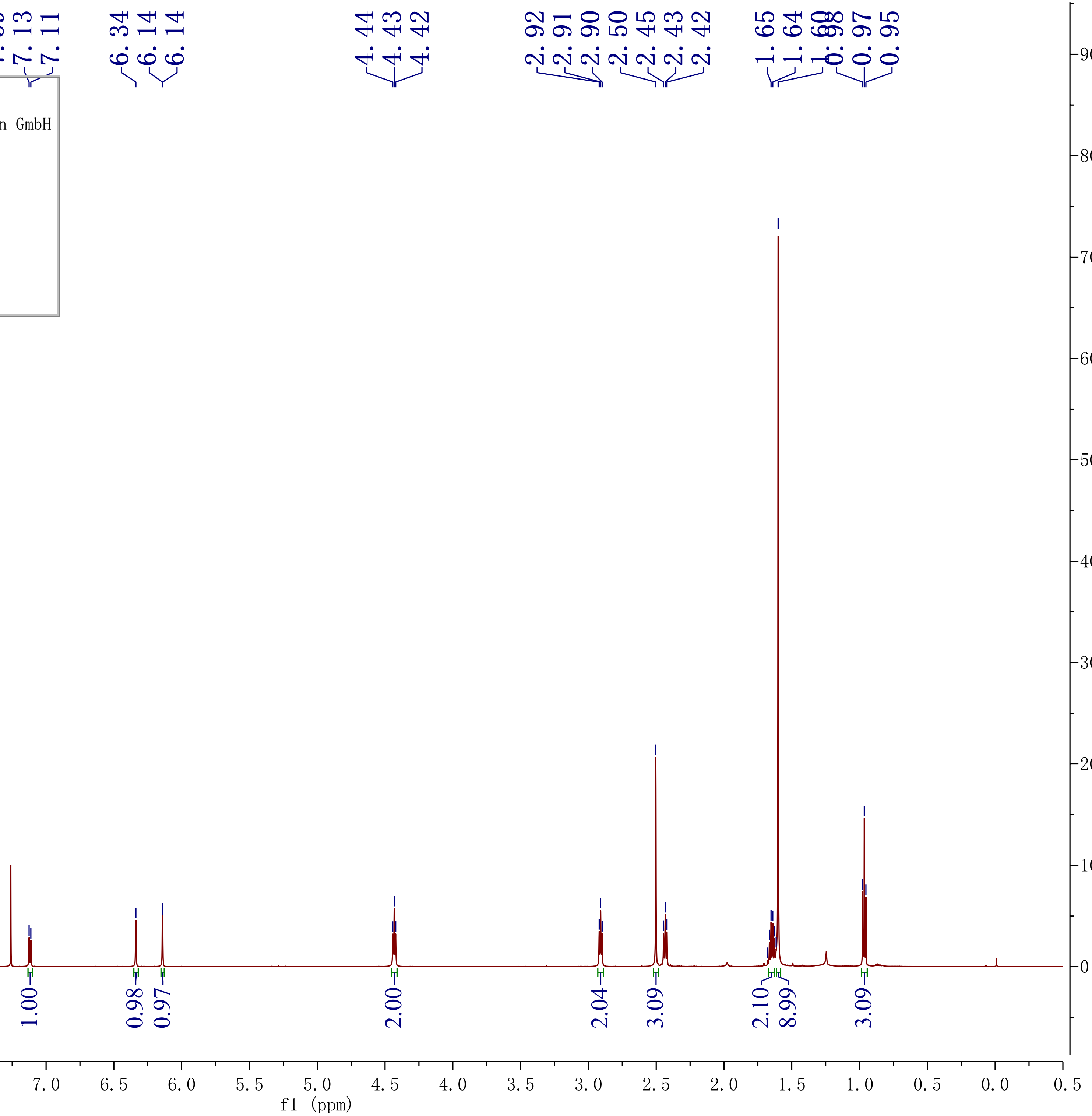


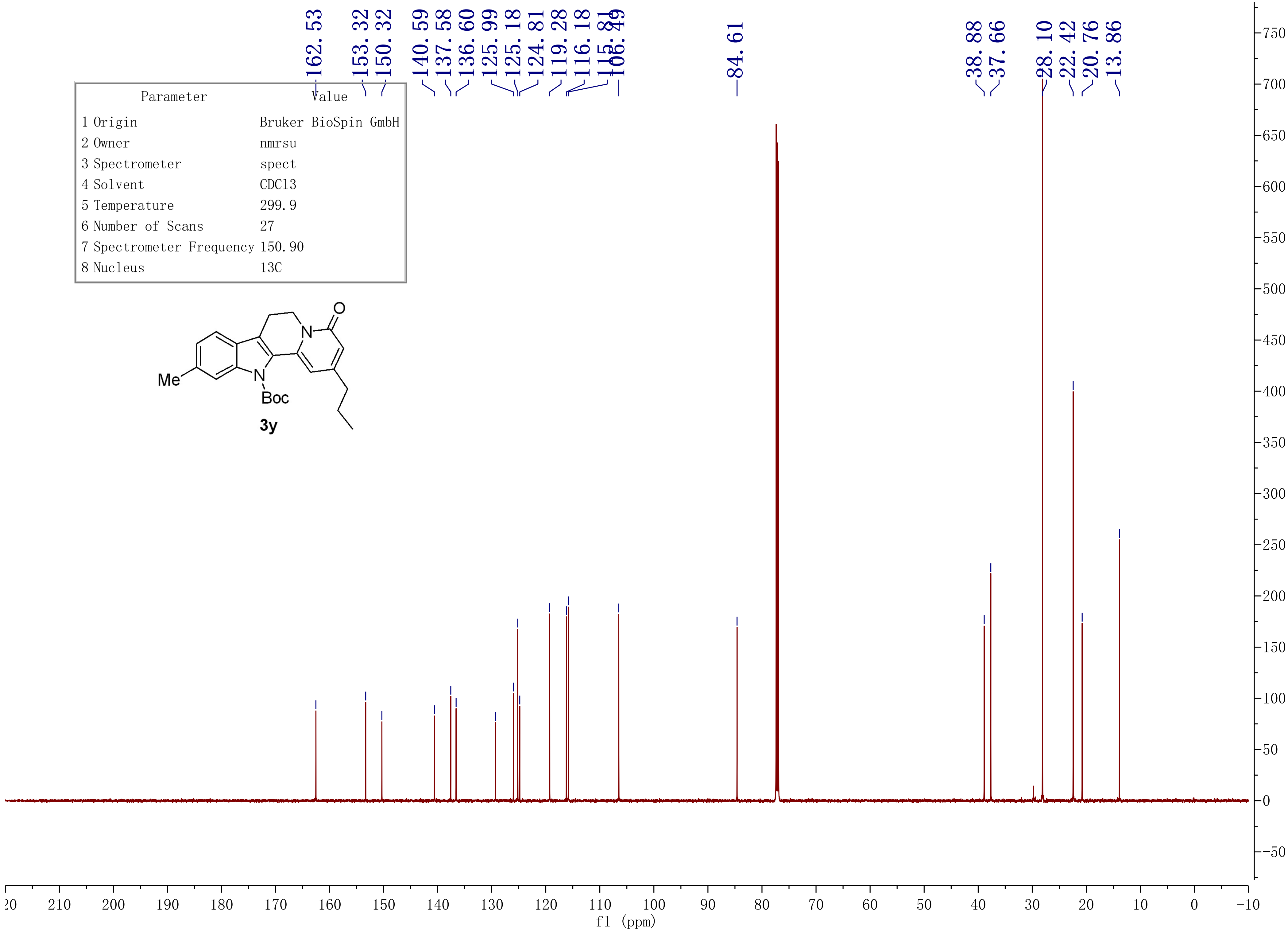
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	299.9
6 Number of Scans	15
7 Spectrometer Frequency	150.90
8 Nucleus	13C

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	299.9
6 Number of Scans	8
7 Spectrometer Frequency	600.13
8 Nucleus	1H

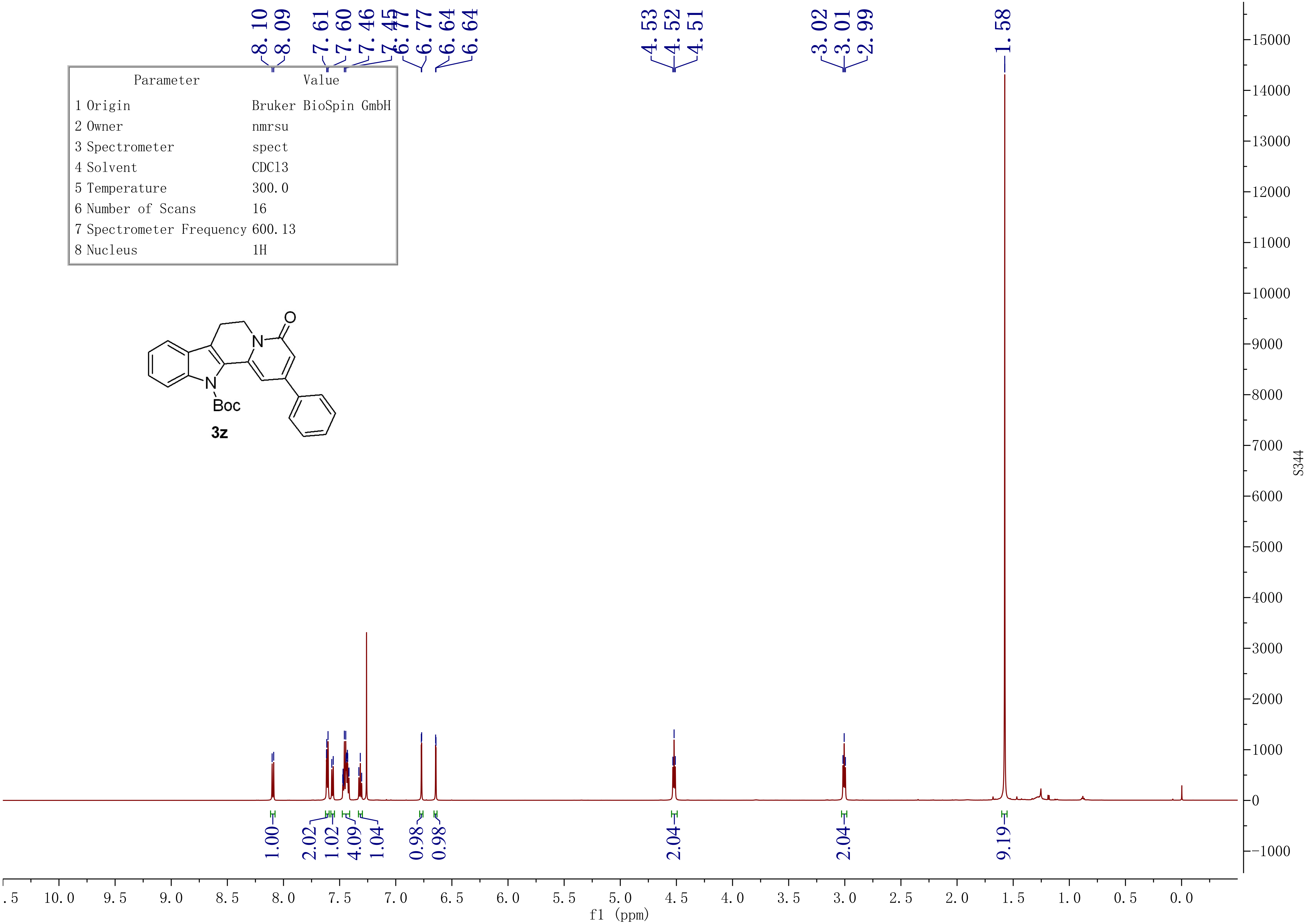


3y



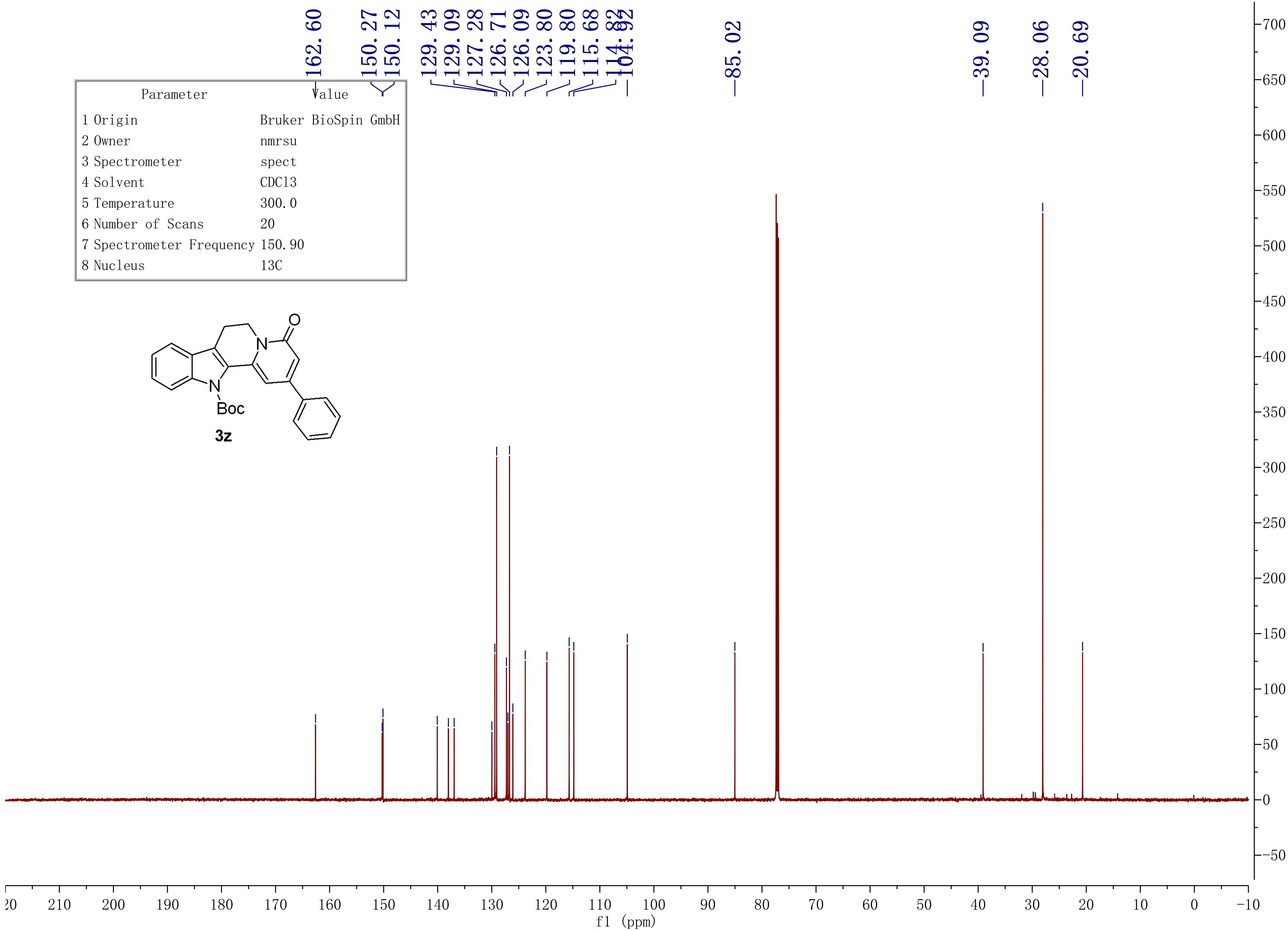


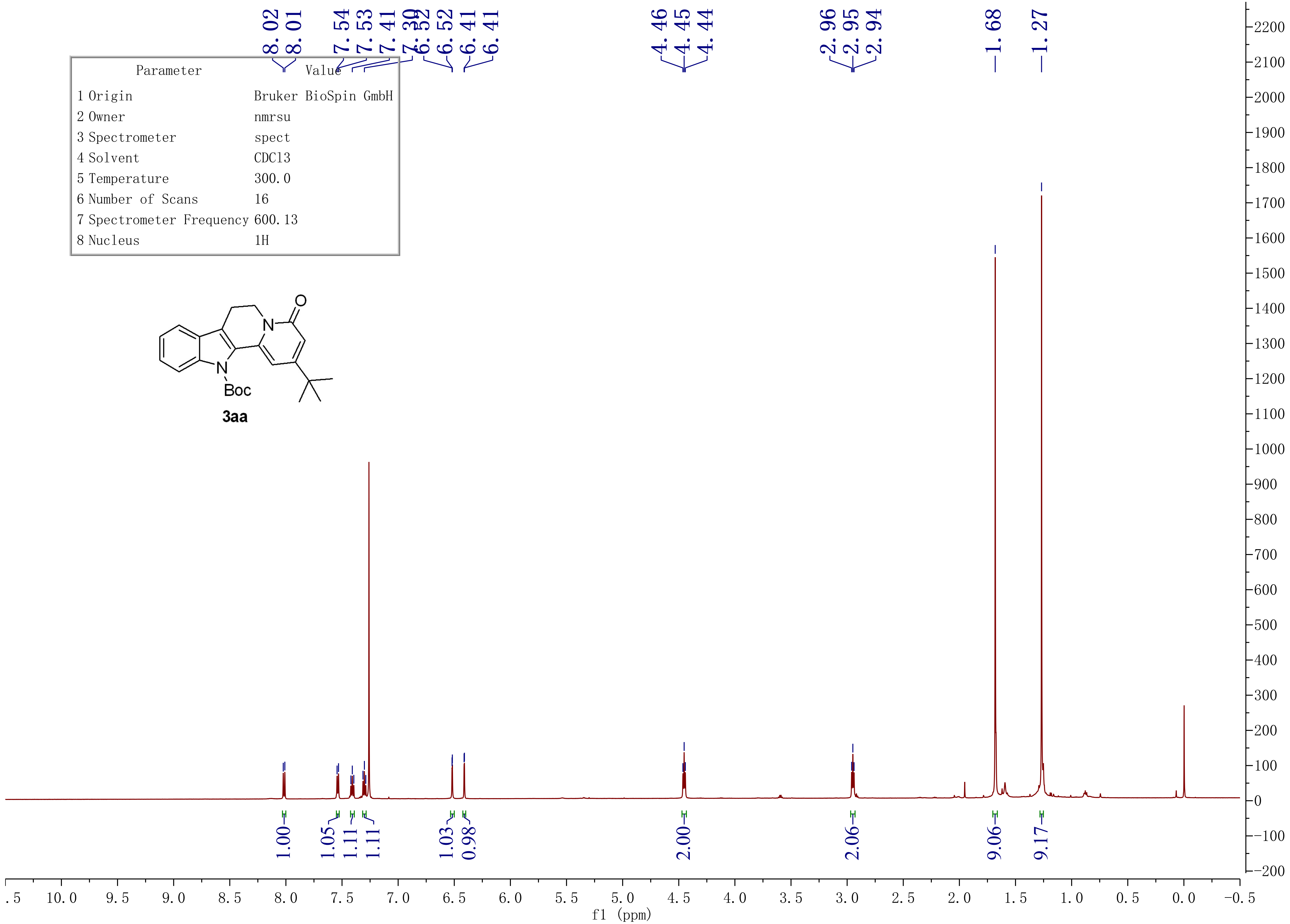
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	299.9
6 Number of Scans	27
7 Spectrometer Frequency	150.90
8 Nucleus	13C



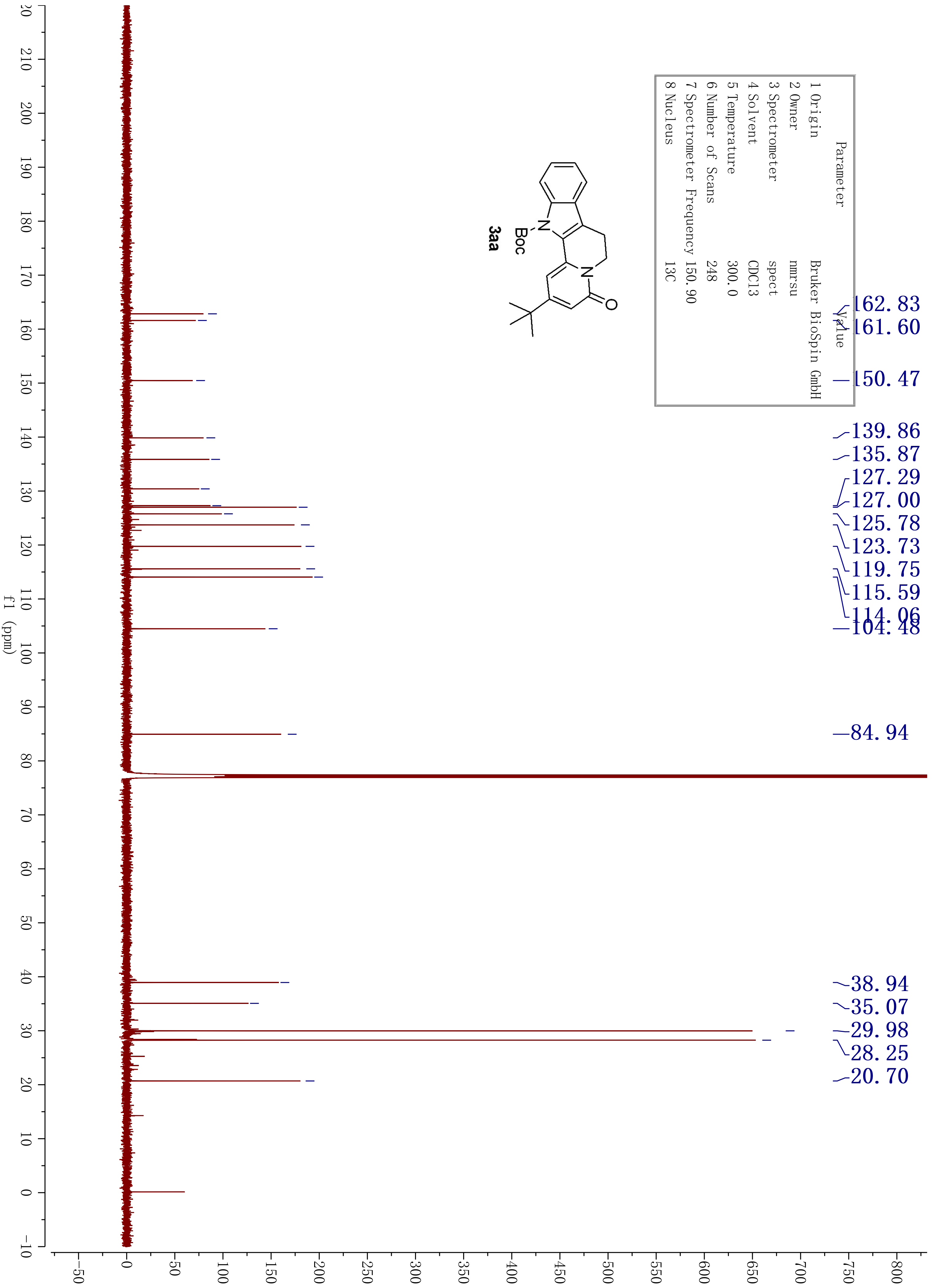
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H

3z


162.60
150.27
150.12
129.43
129.09
127.28
126.71
126.09
123.80
119.80
115.68
114.82
104.92
85.02
39.09
28.06
20.69
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Owner nmrsu
3 Spectrometer spect
4 Solvent CDCl3
5 Temperature 300.0
6 Number of Scans 20
7 Spectrometer Frequency 150.90
8 Nucleus 13C
N
N
O
Boc
3z
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	nmrsu
3 Spectrometer	spect
4 Solvent	CDCl3
5 Temperature	300.0
6 Number of Scans	16
7 Spectrometer Frequency	600.13
8 Nucleus	1H



Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
nmrsu
3 Spectrometer
spect
4 Solvent
CDCl3
5 Temperature
300.0
6 Number of Scans
248
7 Spectrometer Frequency
150.90
8 Nucleus
13C
Boc
3aa
162.83
161.60
150.47
139.86
135.87
127.29
127.00
125.78
123.73
119.75
115.59
114.06
104.48
84.94
38.94
35.07
29.98
28.25
20.70
f1 (ppm)