Electronic Supplementary Material (ESI) for ChemComm.

Synthesis and Study of Au(III)-Indolizine Derivatives: Turn-on Luminescence by Photo-induced Control Release.

Supporting information

Table of Content:

General Aspects:

Unless otherwise indicated, all reactions were performed under a nitrogen atmosphere from which oxygen and moisture were rigidly excluded from reagents and glassware, and all the metal salts were stored in a glovebox and used without further purification: $AuCl_3$, $AuBr_3$ and AuCl were purchased from Alfa, CuCl and CuBr were purchased from J&K or Alfa. Starting materials for cycloisomerization substrate synthesis such as n-Butyllithium, iodomethane, the pyridine and the acetylene derivatives were stored in a refrigerator and used without further purification. THF was dried over NaH before use. Extra Dry DCM was used directly and purchased from J&K.

Analytical thin layer chromatography (TLC) was performed using EM Science silica gel 60 F254 plates. The developed chromatogram was analyzed by UV lamp (254 nm). Purification of product was performed by using Silica Gel (230–400 mesh, 0.040-0.063 mm) coarse fritted glass column.

^{1}H and ^{13}C NMR spectra were recorded on Bruker spectrometers in deuteriated chloroform, acetone or DMSO (400 or 500 MHz for ^{1}H, and 100 or 125 MHz for ^{13}C). Chemical shifts in ^{1}H NMR spectra are reported in ppm on the δ scale from an internal standard of TMS. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant in hertz (Hz), and integration. Chemical shifts of ^{13}C NMR spectra are reported in ppm from the central peak of D6-DMSO (δ39.51 ppm), D6-Acetone, (δ206.68, 29.92 ppm) or $CDCl_3$ (δ77.13 ppm) on the δ scale.

Absorption spectra were recorded with a Cary 60 UV/Vis absorption spectrophotometer. Fluorescence spectra were recorded with an FS5 fluorescence spectrometer from Edinburgh Instrument™ at room temperature. Emission of singlet oxygen were recorded with an FLS 980 fluorescence spectrometer from Edinburgh Instrument™ equipped with an NIR-PMT detector and an 850 nm long pass filter in the emission arm. Quartz cuvettes (path length = 1 cm) were used for all spectrophotometric and fluorometric measurements.

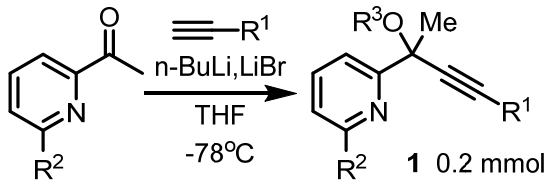
High resolution mass spectra (HRMS) were obtained on a Finnigan MAT 95XL GC Mass Spectrometer of the Southern University of Science and Technology.

All crystal data was collected from Bruker D8-Venture X-Ray Spectrometer by Dr. Xiaoyong Chang of the Southern University of Science and Technology.

Cell Cultures: Human A549 (lung), HCT116 (colon) and HepG2 (liver) cancer cells were obtained from American Type Culture Collection (ATCC) and cultured in Dulbecco's modification of Eagle medium (DMEM) supplemented with 10% fetal bovine serum, 100 units/ml penicillin, and 100 mg/ml streptomycin. Cells were cultured at 37^{o}C in an atmosphere of 5% CO_2 and 95% humidity.

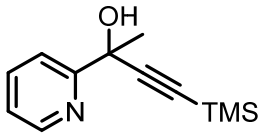
Cell proliferation was assessed by MTT [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide] assay. Briefly, cells were plated in 96-well plates (2x103cells/well) and then treated with indolizine derivatives ligated Au(III) complexes for 72 h. Afterward, cells were treated with MTT reagent and the absorbance at 570 nm was measured using a microplate reader. The viability of control (untreated cells) was regarded as 100%.

Procedure for the Cycloisomerization Substrate Preparation:



1a-c are known compounds and was prepared according to literature procedure.[1,2]

1a: *n*-Butyllithium (5.60 mL, 14.0 mmol, 2.5 M in hexanes) was added dropwise to trimethylsilyl acetylene (2.14 mL, 15.0 mmol) in Et_2O (10.0 mL) at 0 °C, and the resulting mixture was stirred for 30 min at this temperature. The lithium acetylide solution was added dropwise to a vigorously stirred mixture of 2-acetylpyridine (1.12 mL, 10.0 mmol) and lithium bromide (2.60 g, 30.0 mmol) in a 1:1 mixture of Et_2O and benzene (total volume = 60.0 mL). The reaction mixture was stirred at ambient temperature for 12 h at which point a saturated $NH_4Cl_{(aq)}$ solution (30 mL) was added to quench the reaction. The aqueous layer was extracted with EA (3 x 40 mL). The organic layers were combined, washed with brine, dried over $MgSO_4$ and concentrated under reduced pressure to afford the trimethylsilyl alkyne **1a**, which was purified by silica gel column chromatography.



1a

1a: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.74 (s, 1H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.26 (s, 1H), 5.49 (s, 1H), 1.75 (s, 3H), 0.16 (s, 9H)

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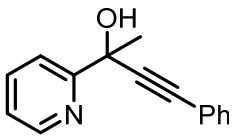
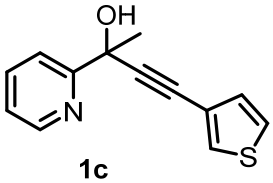
[1] Hardin Narayan, Alison R., Sarpong, Richmond, *Organic & Biomolecular Chemistry*, **2012**,10, 70

[2] Cho, Hanyang, Kim, Ikyon, *Tetrahedron*, **2012,** 68, 5464

1b-c are known compound and were prepared as below:



1b



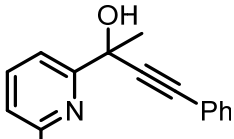
1c

To a stirred solution of terminal alkyne (1.2 equiv) in THF was added *n*-BuLi (1.1 equiv, 1.6 M solution in hexanes) at −78 °C. After 5 min, a solution of pyridinyl ketone (1.0 equiv) in THF was added to this mixture at −78 °C slowly. After 15 min at −78 °C, the reaction mixture was quenched with saturated $NH_4Cl_{(aq)}$. The reaction mixture was diluted with EA and washed with $NH_4Cl_{(aq)}$. The organic layer was dried over $MgSO_4$ and concentrated in vacuo to give a crude mixture, which was purified by silica gel column chromatography (hexane/EA/DCM) to afford the propargylic alcohol.

1b: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.5 Hz, 1H), 7.77 (td, *J* = 1.5, 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.49–7.44 (m, 2H), 7.31–7.24 (m, 4H), 5.62 (s, 1H), 1.87 (s, 3H)

1c: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.5 Hz, 1H), 7.77 (td, *J* = 1.0, 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.44 (dd, *J* = 1.0, 3.0 Hz, 1H), 7.27 (dd, *J* = 5.0, 7.0 Hz, 1H), 7.23 (dd, *J* = 3.0, 5.0 Hz, 1H), 7.10 (d, *J* = 5.0 Hz, 1H), 5.61 (s, 1H), 1.86 (s, 3H).

1d was prepared according to the above literature procedure for **1b-c** analogously:



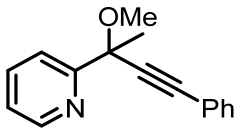
1d

1d: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (t, *J* = 7.7 Hz, 1H), 7.51 – 7.43 (m, 3H), 7.33 – 7.28 (m, 3H), 7.14 (d, *J* = 7.6 Hz, 1H), 6.09 (s, 1H), 2.60 (s, 3H), 1.87 (s, 3H).

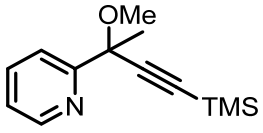
^{13}C NMR (126 MHz, $CDCl_3$) δ 160.91, 156.31, 137.80, 131.78, 128.31, 128.18, 122.75, 122.29, 117.08, 92.51, 83.39, 68.44, 32.34, 24.15.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{16}ON$: 238.12264; found 238.12209

1e-f were prepared by typical alcohol methylation procedure:



1f



1e

1e: A solution of propargylic alcohol **1a** (1.0 equiv) in THF was added NaH (60% in oil, 1.5 equiv) at 0 °C under nitrogen atmosphere. CH_3I (2.0 equiv) was added at 0 °C and stirred at 0 °C. After 40 mins, the mixture was quenched by $NH_4Cl_{(aq)}$ and extracted by EA. Organic layer was subjected to silica gel column chromatography (hexane/EA = 5:1) to afford the product.

1e: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.4 Hz, 1H), 7.77 – 7.66 (m, 2H), 7.25 (ddd, *J* = 7.1, 4.8, 1.4 Hz, 1H), 3.35 (s, 3H), 1.82 (s, 3H), 0.26 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.42, 149.49, 136.54, 122.70, 121.10, 105.05, 92.22, 52.51, 29.63, -0.02.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{13}H_{20}ONSi$: 234.13087; found 234.13043

1f: A solution of propargylic alcohol **1b** (1.0 equiv) in THF was added NaH (60% in oil, 1.5 equiv) at 0 °C under nitrogen atmosphere. CH_3I (3.0 equiv) was added at 0 °C and was allowed to stir at r.t.. After 2 hrs, the mixture was quenched by $NH_4Cl_{(aq)}$ and extracted by EA. Organic layer was subjected to silica gel column chromatography (hexane/EA = 5:1) to afford the product.

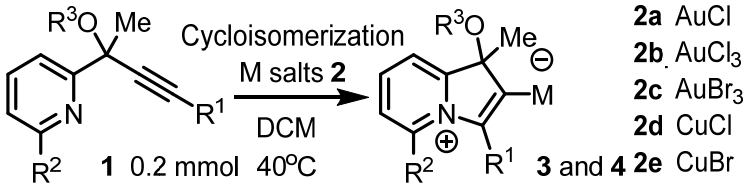
1f: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.0 Hz, 1H), 7.79 (d, *J* = 7.9 Hz, 1H), 7.72 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.57 – 7.49 (m, 2H), 7.36 – 7.30 (m, 3H), 7.23 (ddd, *J* = 7.4, 4.8, 1.1 Hz, 1H), 3.39 (s, 3H), 1.91 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.83, 149.47, 136.64, 131.87, 128.52, 128.29, 122.75, 122.59, 121.00, 88.95, 87.40, 77.49, 52.68, 29.68.

HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{16}ON$: 238.12264; found 238.12204

General Procedure for the Cycloisomerization Reactions:

a) General cycloisomerization procedure:

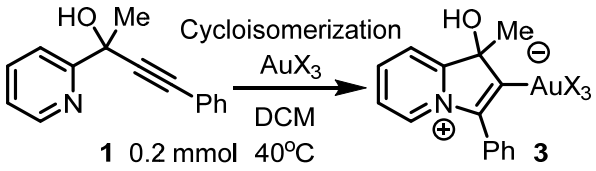


The M salts **2** (1.0 equiv) and **1** (1.0 equiv) were added to a test tube inside the glove box. After sealed with rubber septum and parafilm, the tube was taken out of the glovebox and 1 ml dried DCM was added at bench top under N_2 protection. The reaction was then heated to 40 °C and was stirred for 12 hrs. The desired product **3** and **4** showed low solubility in DCM and would precipitate out gradually during the process. Using a hot plate with effective stirring is therefore recommended.

b) General work up procedure

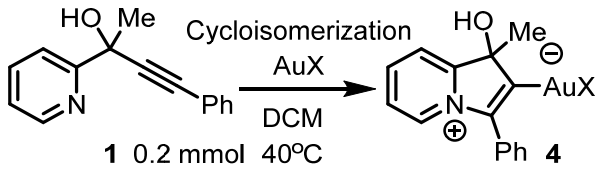
The desired product (ppt) was collected by filtration after cooling the reaction mixture to r.t.. It was rinsed further by DCM 5 times (4 mL) before vacuum dried. Preparative TLC was employed for further purification when necessary.

c) Representative procedure by using $AuCl_3$



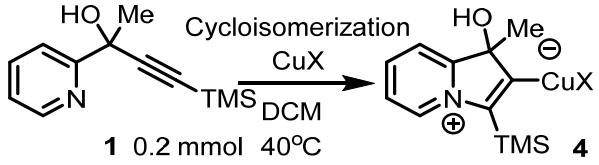
The cycloisomerization substrate **1b** and $AuCl_3$ **2b** (1.0 equiv, 0.2 mmol each) were added to a test tube inside the glove box. After sealed, 1 ml DCM was added at bench top under N_2 protection. The reaction was then heated to 40 °C and was stirred for 12 hrs. The desired product **3bb** was obtained by following the general work up procedure.

d) Representative procedure by using AuCl 2a



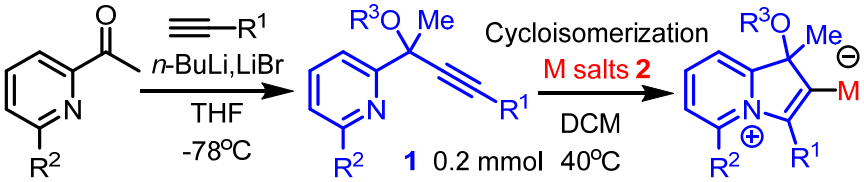
The cycloisomerization substrate **1b** and AuCl **2a** (1.0 equiv, 0.2 mmol each) were added to a test tube inside the glove box. After sealed, 1 ml DCM was added at bench top under N_2 protection. The reaction was then heated to 40 °C and was stirred for 12 hrs. The desired product **4ba** was obtained by following the general work up procedure. The crude product was purified by preparative TLC using 5% DCM in MeOH as eluent.

e) Representative procedure by using CuCl 2d



The cycloisomerization substrate **1a** and CuCl **2d** (1.0 equiv, 0.2 mmol each) were added to a test tube inside the glove box. After sealed, 1 ml DCM was added at bench top under N_2 protection. The reaction was then heated to 40 °C and was stirred for 12 hrs. The desired product **4ad** was obtained by following the general work up procedure, except the solvent was removed by trituration first followed by vacuum.

Table 1 Preparation of complex **3** and **4** by cycloisomerization of **1** and **2**.[a]



R^1 =	R^2 =	R^3 =	1	Yield %
TMS	H	H	1a	81
Ph	H	H	1b	72
3-thiophene	H	H	1c	83
Ph	Me	H	1d	62
TMS	H	Me	1e	89
Ph	H	Me	1f	95

NaH, MeI 0°C

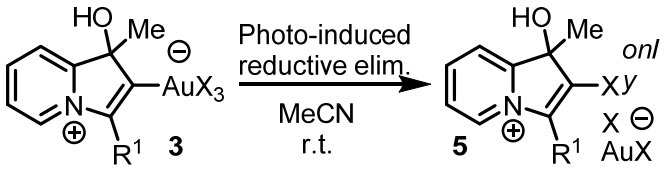
M salts 2	Complex 3, 4
2a AuCl	3 M = AuX_3
2b $AuCl_3$	4 M = AuCl
2c $AuBr_3$	4 M = CuX
2d CuCl	3xx 60-80% yield
2e CuBr	4xx 65-79% yield

entry	alkyne 1	M salt 2	complex 3, 4	Yield[b]
1	1a	2a	4aa	71%
2		2b	3ab	72%
3		2c	3ac	68%
4	1b	2a	4ba	73%
5		2b	3bb	75%
6		2c	3bc	70%
7	1c	2a	4ca	67%
8[c]		2b	3cb	80%
9	1d	2b	3db	63%
10	1e	2b	3eb	75%
11	1f		3fb	73%
12	1a	2d	4ad	79%
13		2e	4ae	65%

[a] see s7-8 for details of the experimental procedure. [b] Isolated yield via chromatography or recrystallization; characterized by NMR spectroscopy and HRMS. [c] conducted at rt.

Highly substituted **3** with different functional groups (R^1, R^2, and R^3), such as silyl, aryl, heteroaryl, methoxy, and alkyl, were obtained in good yield (entry 2, 5, and 8–11). The high generality of this approach is notable because it offers opportunities to both fine tune the photophysical properties of **3** and develop catalysts similar to NHC systems. Moreover, salts like **2a** and **c–e** were found to be compatible with the conditions (AuCl, $AuBr_3$, entry 1, 3, 4, 6, 7; CuCl, CuBr, entry 12 and 13), giving the corresponding Au(III) complexes **3**, Au(I) and Cu(I) complexes **4**. It allowed us to compare their properties as a function of M center, oxidation state, and counter ion later on.

General Procedure for Photo-induced Reductive Elimination Reactions:

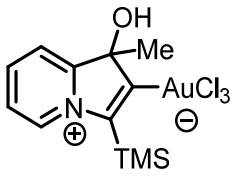


A stirring solution of **3bb** (5 mg in 10 ml MeCN, see maintext for structure) was exposed to photo-excitation (280-330 nm) for 5-10 mins. The desired reductive elimination product **5bb** was obtained in quantitative yield and no corresponding indolizine-AuCl product was observed. The product structure was determined and characterization by ^{1}H, ^{13}C NMR, HRMS. The characteristic vinyl halides C peaks were found in ^{13}C NMR.

5	Yield
5bc	quantitative
5ab	92%
5bb	quantitative
5cb	quantitative
5db	97%
5fb	quantitative
5ac	quantitative

Characterization Data:

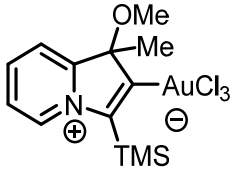
(a) NMR of Product **3**



^{1}H NMR (400 MHz, D6-Acetone) δ 9.10 (d, *J* = 6.1 Hz, 1H), 8.58 (ddd, *J* = 7.8, 7.8, 1.1 Hz, 1H), 8.36 (d, *J* = 7.8 Hz, 1H), 8.15 (dd, *J* = 6.9, 6.9 Hz, 1H), 4.79 (s, 1H), 1.82 (s, 3H), 0.70 (s, 9H).

^{13}C NMR (126 MHz, D6-Acetone) δ 162.34, 160.11, 143.29, 139.33, 137.01, 127.42, 122.76, 84.58, 25.44, -0.80.

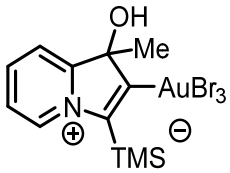
HRMS-ESI (m/z): $[M\text{-}Cl]^+$ calcd for $C_{12}H_{17}ONAuCl_2Si$: 486.01220; found 486.01022



^{1}H NMR (400 MHz, D6-Acetone) δ 9.20 (d, *J* = 6.1 Hz, 1H), 8.66 (ddd, *J* = 7.8, 7.8,1.0 Hz, 1H), 8.36 (d, *J* = 7.8 Hz, 1H), 8.24 (dd, *J* = 6.9, 6.9 Hz, 1H), 3.09 (s, 3H), 1.81 (s, 3H), 0.75 – 0.72 (m, 9H).

^{13}C NMR (101 MHz, D6-Acetone) δ 158.79, 158.32, 143.31, 142.37, 138.16, 128.16, 123.44, 90.77, 25.55, -0.60.

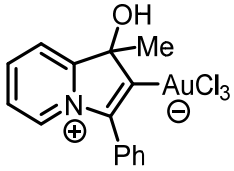
HRMS-ESI (m/z): $[M\text{-}Cl]^+$ calcd for $C_{13}H_{19}ONAuCl_2Si$: 500.02730; found 500.02662



^{1}H NMR (400 MHz, D6-Acetone) δ 9.08 (d, *J* = 6.1 Hz, 1H), 8.55 (ddd, *J* = 7.8, 7.8, 1.0 Hz, 1H), 8.36 (d, *J* = 7.8 Hz, 1H), 8.15 (dd, *J* = 6.9, 6.9 Hz, 1H), 4.67 (s, 1H), 1.84 (s, 3H), 0.68 (d, *J* = 3.3 Hz, 9H).

^{13}C NMR (126 MHz, D6-Acetone) δ 159.80, 143.07, 139.53, 136.81, 127.29, 122.73, 84.34, 26.74, -0.74.

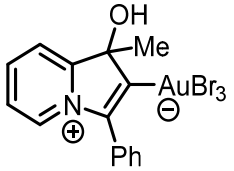
HRMS-ESI (m/z): $[M-Br]^+$ calcd for $C_{12}H_{17}ONAuBr_2Si$: 573.91117; found 573.90918



^{1}H NMR (500 MHz, D6-DMSO) δ 8.54 (d, *J* = 6.1 Hz, 1H), 8.50 (ddd, *J* = 7.8, 7.8, 1.2 Hz, 1H), 8.36 (d, *J* = 7.8 Hz, 1H), 7.93 (ddd, *J* = 7.6, 6.2, 1.4 Hz, 1H), 7.78 (d, *J* = 7.3 Hz, 2H), 7.71 – 7.61 (m, 3H), 6.40 (s, 1H), 1.79 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 161.51, 145.71, 144.31, 136.02, 135.21, 131.04, 130.87, 129.82, 127.56, 127.46, 122.96, 82.74, 26.16.

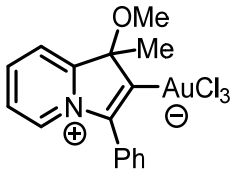
HRMS-ESI (m/z): $[M+NH_4]^+$ calcd for $C_{15}H_{17}ON_2AuCl_3$: 543.00665; found 543.00671



^{1}H NMR (400 MHz, D6-DMSO) δ 8.48 (m, 2H), 8.37 (d, *J* = 7.7 Hz, 1H), 7.92 (ddd, *J* = 7.6, 6.1, 1.4 Hz, 1H), 7.81 – 7.76 (m, 2H), 7.69 – 7.62 (m, 3H), 6.33 (s, 1H), 1.82 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 161.69, 145.52, 144.11, 135.82, 134.99, 130.96, 130.94, 129.73, 127.77, 127.38, 122.99, 82.59, 27.31.

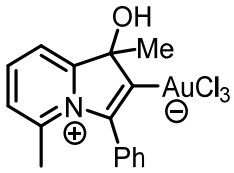
HRMS-ESI (m/z): $[M+Br]^-$ calcd for $C_{15}H_{13}ONAuBr_4$: 735.74061; found 735.74072



^{1}H NMR (400 MHz, D6-DMSO) δ 8.63 (d, *J* = 6.1 Hz, 1H), 8.57 (ddd, *J* = 7.8, 7.8, 1.2 Hz, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 8.00 (ddd, *J* = 7.6, 6.1, 1.3 Hz, 1H), 7.85 – 7.81 (m, 2H), 7.70 – 7.65 (m, 3H), 5.76 (s, 1H), 3.14 (s, 3H), 1.84 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 157.38, 144.53, 141.94, 139.45, 136.88, 131.24, 131.08, 129.77, 128.14, 127.43, 123.46, 88.87, 54.66, 25.63.

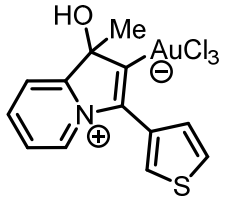
HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{16}ONAuCl_3$: 539.9968; found539.9971



^{1}H NMR (500 MHz, D6-DMSO) δ 8.33 (dd, *J* = 7.8, 7.8 Hz, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.68 (d, *J* = 7.0 Hz, 1H), 7.65 – 7.54 (m, 4H), 6.36 (s, 1H), 2.06 (s, 3H), 1.77 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 163.24, 150.22, 147.12, 143.47, 137.39, 132.24, 131.95, 131.76, 130.74, 130.51, 129.15, 129.00, 120.78, 81.70, 26.80, 21.94.

HRMS-ESI (m/z): $[M-H]^-$ calcd for $C_{16}H_{14}ONAuCl_3$: 537.98120; found 537.98181

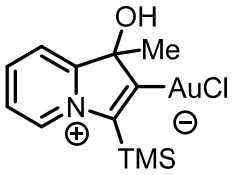


^{1}H NMR (400 MHz, D6-DMSO) δ 8.70 (d, *J* = 6.1 Hz, 1H), 8.51 (ddd, *J* = 7.7, 7.7, 1.1 Hz, 1H), 8.35 (d, *J* = 7.7 Hz, 1H), 8.16 (dd, *J* = 2.9, 1.2 Hz, 1H), 7.97 (ddd, *J* = 7.6, 6.1, 1.3 Hz, 1H), 7.92 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.58 (dd, *J* = 5.0, 1.2 Hz, 1H), 6.41 (s, 1H), 1.77 (s, 3H).

^{13}C NMR (101 MHz, D6-DMSO) δ 161.38, 145.82, 144.37, 135.39, 132.00, 130.33, 128.81, 128.76, 127.50, 127.46, 122.91, 82.54, 26.15.

HRMS-ESI (m/z): $[M-H]^-$ calcd for $C_{13}H_{10}ONAuCl_3S$: 529.9209; found 529.9205.

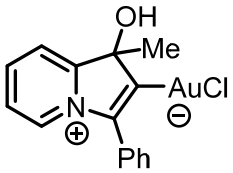
(b) NMR of Product 4



^{1}H NMR (500 MHz, D6-Acetone) δ 8.91 (d, *J* = 6.1 Hz, 1H), 8.42 (ddd, *J* = 7.7, 7.7, 1.2 Hz, 1H), 8.19 (d, *J* = 7.7 Hz, 1H), 8.01 (dd, *J* = 6.9, 6.9 Hz, 1H), 4.96 (s, 1H), 1.61 (s, 3H), 0.58 (s, 9H).

^{13}C NMR (126 MHz, D6-Acetone) δ 184.64, 163.43, 142.16, 140.83, 135.52 – 134.96, 126.79, 122.27, 87.80, 26.37, 0.02.

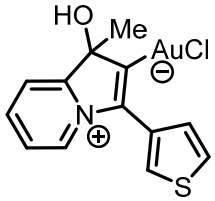
HRMS-ESI (m/z): $[M\text{-}Cl]^+$ calcd for $C_{12}H_{17}ONAuSi$: 416.07394; found 416.07223



^{1}H NMR (400 MHz, D6-DMSO) δ 8.53 (d, *J* = 6.1 Hz, 1H), 8.39 (dd, *J* = 7.7, 7.7 Hz, 1H), 8.24 (d, *J* = 7.7 Hz, 1H), 7.85 (dd, *J* = 6.9, 6.9 Hz, 1H), 7.76 – 7.69 (m, 2H), 7.60 – 7.52 (m, 3H), 6.08 (s, 1H), 1.59 (s, 3H).

^{13}C NMR (101 MHz, D6-DMSO) δ 168.63, 163.39, 142.11, 140.16, 133.52, 131.15, 130.41, 129.62, 129.35, 127.10, 122.53, 85.21, 26.58.

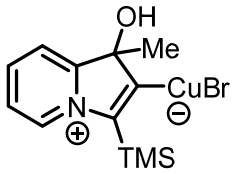
HRMS-ESI (m/z): $[M\text{-}H]^-$ calcd for $C_{15}H_{12}ONAuCl$: 454.02784; found 454.02795



^{1}H NMR (400 MHz, D6-DMSO) δ 8.68 (d, *J* = 6.1 Hz, 1H), 8.39 (dd, *J* = 7.7, 7.7 Hz, 1H), 8.22 (d, *J* = 7.7 Hz, 1H), 8.00 (d, *J* = 1.8 Hz, 1H), 7.89 (dd, *J* = 6.5, 6.5 Hz, 1H), 7.77 (dd, *J* = 4.9, 2.9 Hz, 1H), 7.56 – 7.52 (m, 1H), 6.04 (s, 1H), 1.58 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 168.71, 163.20, 142.17, 135.79, 133.70, 131.28, 129.29, 127.41, 127.15, 122.43, 85.00, 26.56.

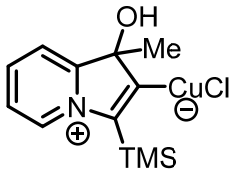
HRMS-ESI (m/z): $[M\text{-}H]^-$ calcd for $C_{13}H_{11}ONAuClS$: 459.9843 found 459.9842



^{1}H NMR (500 MHz, D6- Acetone) δ 8.55 (d, *J* = 4.8 Hz, 1H), 8.18 (ddd, *J* = 7.8, 7.8, 1.7 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.67 (ddd, *J* = 7.6, 5.2, 1.2 Hz, 1H), 6.12 (s, 1H), 1.90 (s, 3H), 0.37 (s, 9H).

^{13}C NMR (126 MHz, D6- Acetone) δ 167.29, 147.62, 140.19, 125.07, 121.82, 111.68, 96.04, 77.19, 31.44, -0.91.

HRMS-ESI (m/z): $[M-Br]^+$ calcd for $C_{12}H_{17}ONCuSi$: 282.03699; found 282.03650



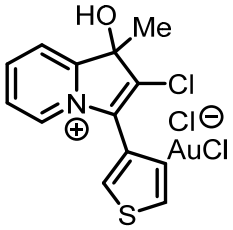
^{1}H NMR (500 MHz, D6-Acetone) δ 8.50 (d, *J* = 4.8 Hz, 1H), 8.15 (ddd, *J* = 7.8, 7.8, 1.4 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.63 (ddd, *J* = 7.5, 5.2, 1.2 Hz, 1H), 6.10 (s, 1H), 1.87 (s, 3H), 0.33 (s, 9H).

^{13}C NMR (126 MHz, D6-Acetone) δ 168.97, 149.17, 142.01, 126.83, 123.50, 112.90, 97.55, 78.85, 33.28, 0.90.

HRMS-ESI (m/z): $[M-Cl]^+$ calcd for $C_{12}H_{17}ONCuSi$: 282.03699; found 282.03641

(c) NMR of Product **5**

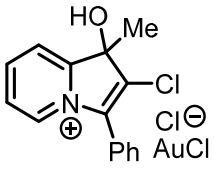
Structural assignment of **5** was done by NMR, HRMS and comparison of the relevant species reported in the literature: This included the spectroscopic comparison with the corresponding organometallic Au(I) species isolated as shown in the above, as well as non-organometallic species like the 2-halobenzimidazole[3], 2-haloindene[4] and conjugated indolizine[5] derivatives.



^{1}H NMR (500 MHz, D6-DMSO) δ 8.88 (d, *J* = 6.1 Hz, 1H), 8.70 (dd, *J* = 7.8, 7.8 Hz, 1H), 8.49 (d, *J* = 7.8 Hz, 1H), 8.26 (dd, *J* = 3.0, 1.5 Hz, 1H), 8.10 (dd, *J* = 7.0, 7.0 Hz, 1H), 7.98 (d, *J* = 3.3 Hz, 1H), 7.48 (d, *J* = 5.0 Hz, 1H), 7.07 (s, 1H), 1.75 (s, 3H).

13C NMR (126 MHz, D6-DMSO) δ 157.94, 146.31, 138.37, 137.24, 133.23, 132.39, 129.41, 128.29, 128.12, 123.34, 122.80, 79.33, 22.42.

HRMS-ESI (m/z): $[M\text{-}AuCl_2]^+$ calcd for $C_{13}H_{11}ONClS$: 264.0244; found 264.0243



^{1}H NMR (500 MHz, D6-DMSO) δ 8.75 (d, *J* = 6.1 Hz, 1H), 8.71 (dd, *J* = 7.8, 7.8 Hz, 1H), 8.51 (d, *J* = 7.9 Hz, 1H), 8.06 (t, *J* = 6.9 Hz, 1H), 7.71-7.64 (m, 5H), 7.03 (s, 1H), 1.77 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 158.10, 146.38, 138.65, 137.14, 137.07, 132.24, 130.91, 130.18, 128.18, 123.46, 123.36, 79.53, 22.33.

HRMS-ESI (m/z): $[M\text{-}AuCl_2]^+$ calcd for $C_{15}H_{13}ONCl$: 258.0680; found 258.0675.

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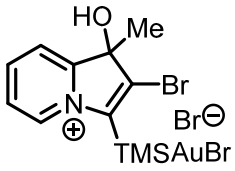
[3] Galy, J.-P.; Hanoun, J.-P.; Pique, V.; Jagerovic, N.; Eguero, J. *J. Heterocyclic Chem.* **1997**, *34*, 1781.

[4] a) Anke, L.; Weyerstahl, P. *Chemische Berichte* **1985**, *118*, 613; b) Schlegel, G.; Schaefer, H. J. *Chemische Berichte* **1983**, *116*, 960.

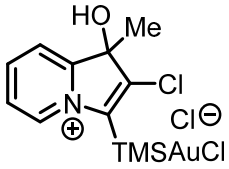
[5] For 1-haloindolizine: a) Yang, Y.; Kuang, C.; Jin, H.; Yang, Q. *Synthesis* **2011**, 3447; For simple indolizine: b) Chernyak, D.; Gadamsetty, S. B.; Gevorgyan, V. *Org. Letts.* **2008**, *10*, 2307.



^{1}H NMR (500 MHz, D6-Acetone) δ 9.27 (d, *J* = 6.1 Hz, 1H), 8.77 (dd, *J* = 7.8, 7.8 Hz, 1H), 8.52 (d, *J* = 7.8 Hz, 1H), 8.27 (dd, *J* = 7.1, 7.1 Hz, 1H), 6.01 (s, 1H), 1.78 (s, 3H), 0.68 (s, 10H).

^{13}C NMR (126 MHz, D6-Acetone) δ 159.56, 145.38, 145.14, 142.57, 139.06, 128.12, 123.51, 23.04, -1.19.

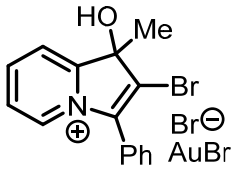
HRMS-ESI (m/z): $[M\text{-}AuBr_2]^+$ calcd for $C_{12}H_{17}ONBrSi$: 298.02573; found 298.02542



^{1}H NMR (500 MHz, D6-Acetone) δ 9.25 (d, *J* = 6.2 Hz, 1H), 8.77 (ddd, *J* = 7.9, 7.9, 1.2 Hz, 1H), 8.51 (d, *J* = 7.9 Hz, 1H), 8.28 (ddd, *J* = 7.7, 6.1, 1.4 Hz, 1H), 1.82 (d, *J* = 1.7 Hz, 3H), 0.66 (s, 9H).

^{13}C NMR (126 MHz, D6-Acetone) δ 158.93, 153.27, 145.28, 140.40, 139.29, 128.21, 123.39, 80.97, 22.14, -1.62.

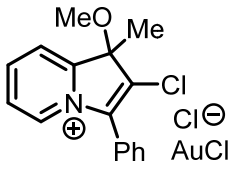
HRMS-ESI (m/z): $[M\text{-}AuCl_2]^+$ calcd for $C_{12}H_{17}ONClSi$: 254.07624; found 254.07584



^{1}H NMR (500 MHz, D6-DMSO) δ 8.72 – 8.67 (m, 2H), 8.51 (d, *J* = 7.8 Hz, 1H), 8.04 (dd, *J* = 7.7, 6.0 Hz, 1H), 7.71-7.64 (m, 5H), 1.74 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 158.92, 146.06, 139.04, 136.88, 132.10, 131.52, 130.90, 130.11, 128.11, 124.35, 123.53, 80.51, 23.12.

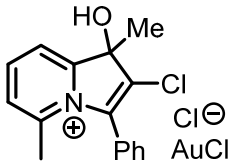
HRMS-ESI (m/z): $[M\text{-}AuBr_2]^+$ calcd for $C_{15}H_{13}ONBr$: 202.01750; found 202.01758.



^{1}H NMR (500 MHz, D6-DMSO) δ 8.86 (d, *J* = 6.1 Hz, 1H), 8.76 (dd, *J* = 7.8, 7.8 Hz, 1H), 8.55 (d, *J* = 7.8 Hz, 1H), 8.14 (dd, *J* = 7.0, 7.0 Hz, 1H), 7.83 – 7.78 (m, 2H), 7.77 – 7.71 (m, 3H), 3.08 (s, 3H), 1.80 (s, 3H).

^{13}C NMR (126 MHz, D6-DMSO) δ 154.26, 146.45, 139.98, 138.72, 134.76, 132.37, 131.13, 130.01, 128.72, 123.91, 123.12, 85.48, 53.80, 22.11.

HRMS-ESI (m/z): $[M\text{-}AuCl_2]^+$ calcd for $C_{16}H_{15}ONCl$: 272.08367; found 272.08267



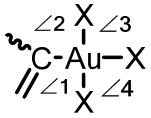
^{1}H NMR (500 MHz, D6-DMSO) δ 8.54 (dd, *J* = 7.9, 7.9 Hz, 1H), 8.32 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.72 – 7.59 (m, 5H), 7.04 (s, 1H), 2.15 (s, 3H), 1.75 (s, 3H).

^{13}C NMR (126 MHz, DMSO) δ 159.84, 151.96, 145.24, 140.84, 139.02, 131.80, 131.18, 131.07, 131.04, 129.85, 129.72, 127.97, 121.25, 78.27, 23.05, 22.14.

HRMS-ESI (m/z): $[M\text{-}AuCl_2]^+$ calcd for $C_{16}H_{15}ONCl$: 272.08367; found 272.08279

Selected Structural Information of Isolated Complexes

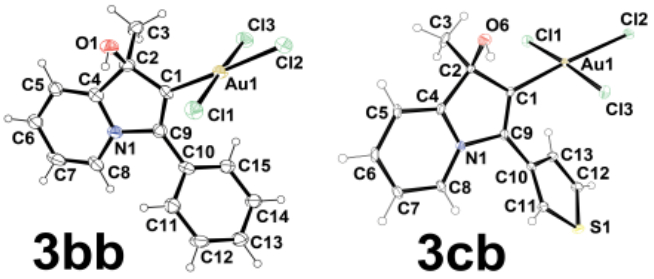
Selected bond lengths (A) and angles (deg) of **3ab**, **3bb**, **3cb**, **3fb** and **3bc**, and the ^{13}C NMR of the Au-C (ppm).

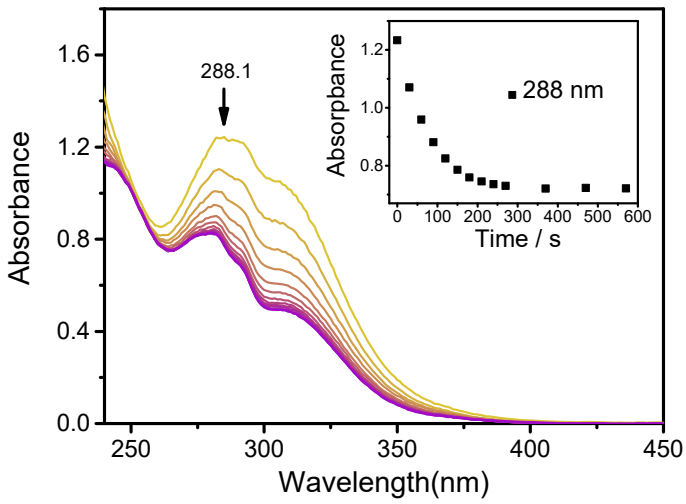
entry	1	2	3	4	5
Complex **3**	**3ab**	**3bb**	**3cb**	**3fb**	**3bc**
Dihedral angle of R^1 and core	n.a.	54.53	40.48	52.76	53.63
Au-C	2.0053	1.9949	1.9935	2.0017	2.030
Au-X_{trans}	2.3631	2.3565	2.3561	2.3372	2.4753
Au-X_{cis}	2.2871 2.2911	2.2802 2.2841	2.2961 2.2862	2.2932 2.2842	2.4084 2.4224
 ∠ 1, 2,3, 4	1 = 85.40 2 = 91.35 3 = 92.78 4 = 90.67	87.27 90.34 91.60 90.86	86.77 90.47 91.50 91.12	88.82 90.22 89.38 91.61	86.99 91.09 91.26 90.85
Length of C=C	1.337	1.329	1.329	1.329	1.270
^{13}C NMR at Au-C	160.11	145.70	145.82	144.53	145.52

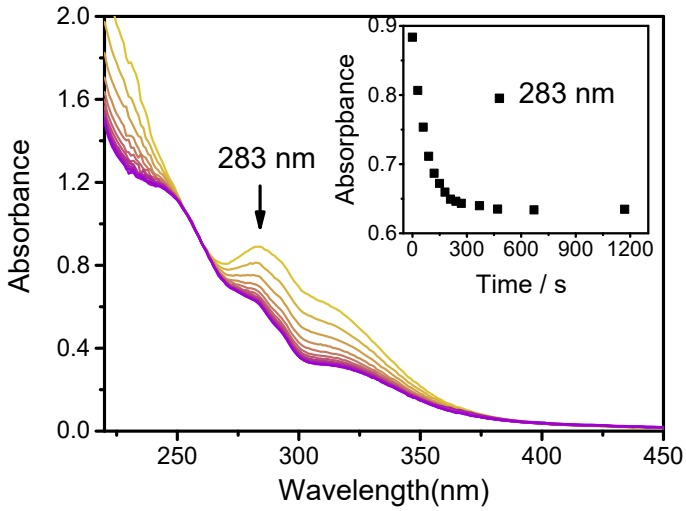
Absorption spectral changes of 3bb and 3cb

The absorption spectral changes of **3bb** (top, R^1 = Ph) and **3cb** (bottom, R^1 = thiophen) upon the irradiation of UV light (280 nm).

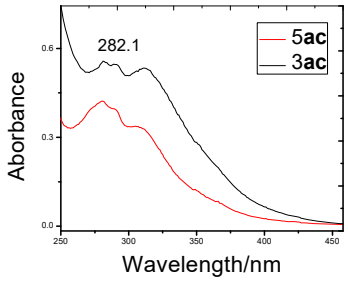
Inserts show the absorbance change of selected wavelength upon different irradiation duration.

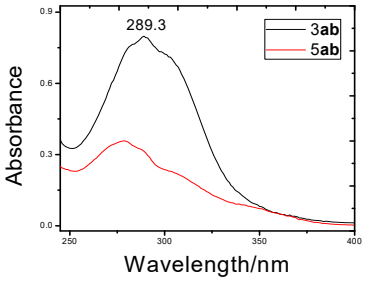


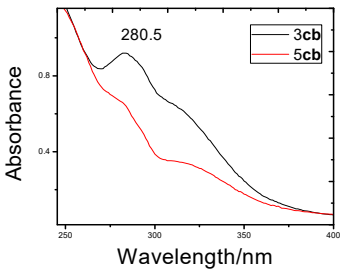


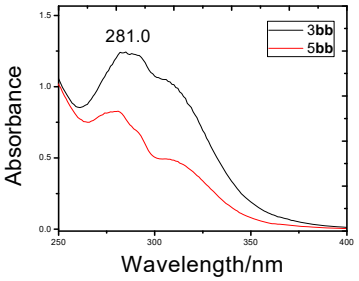


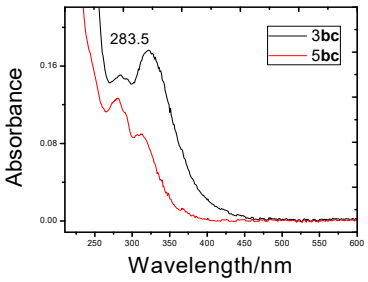
UV spectrum:

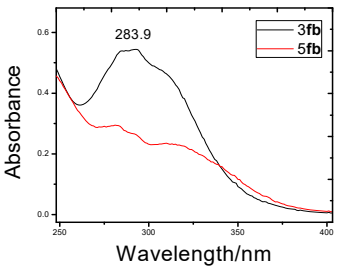


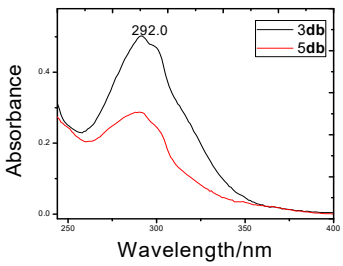












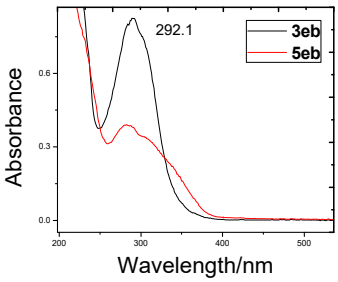


Figure 1: UV abs Comparisons of product **3** and product **5**

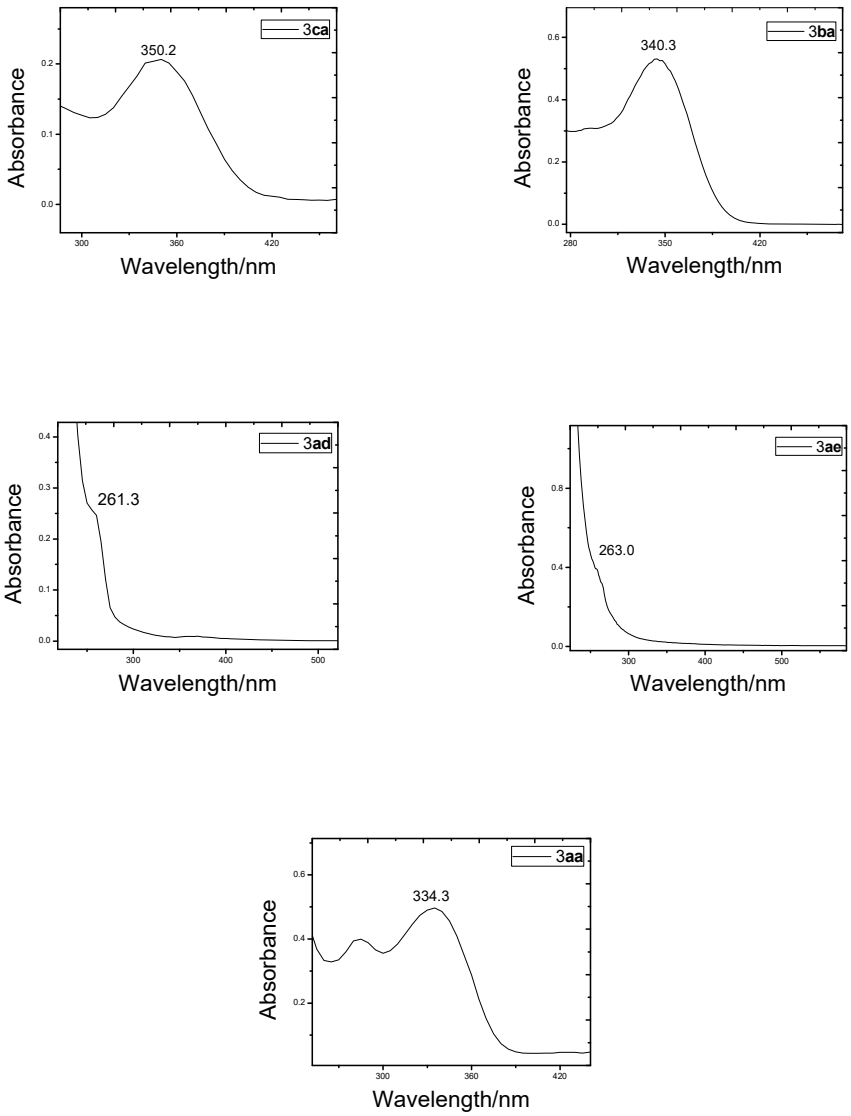


Figure 2: UV abs of other product **3**

Fluorescence spectrum:

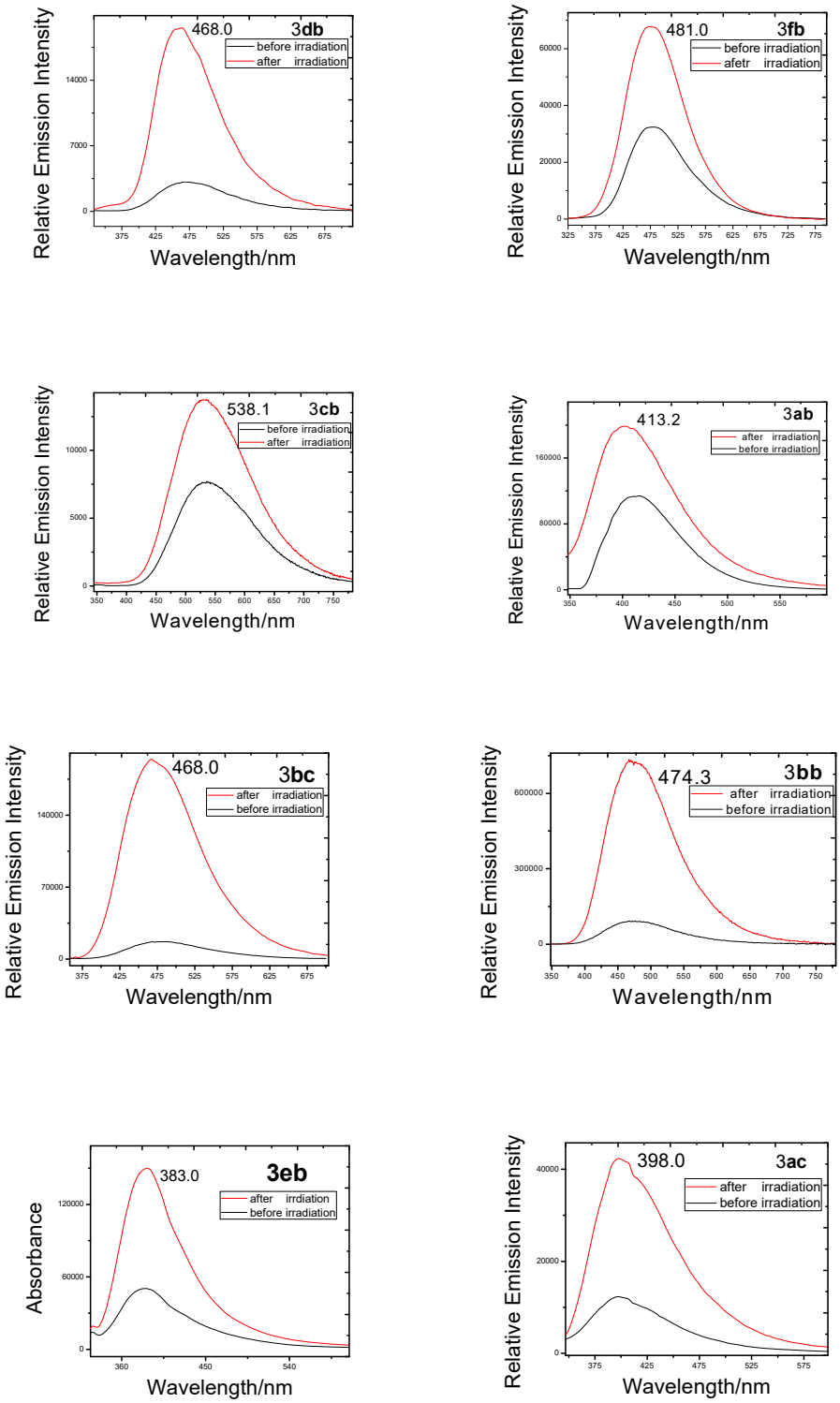


Figure 3: Emission scan of product **3** before and after irradiation comparisons **(photo induced R.E. reaction)**

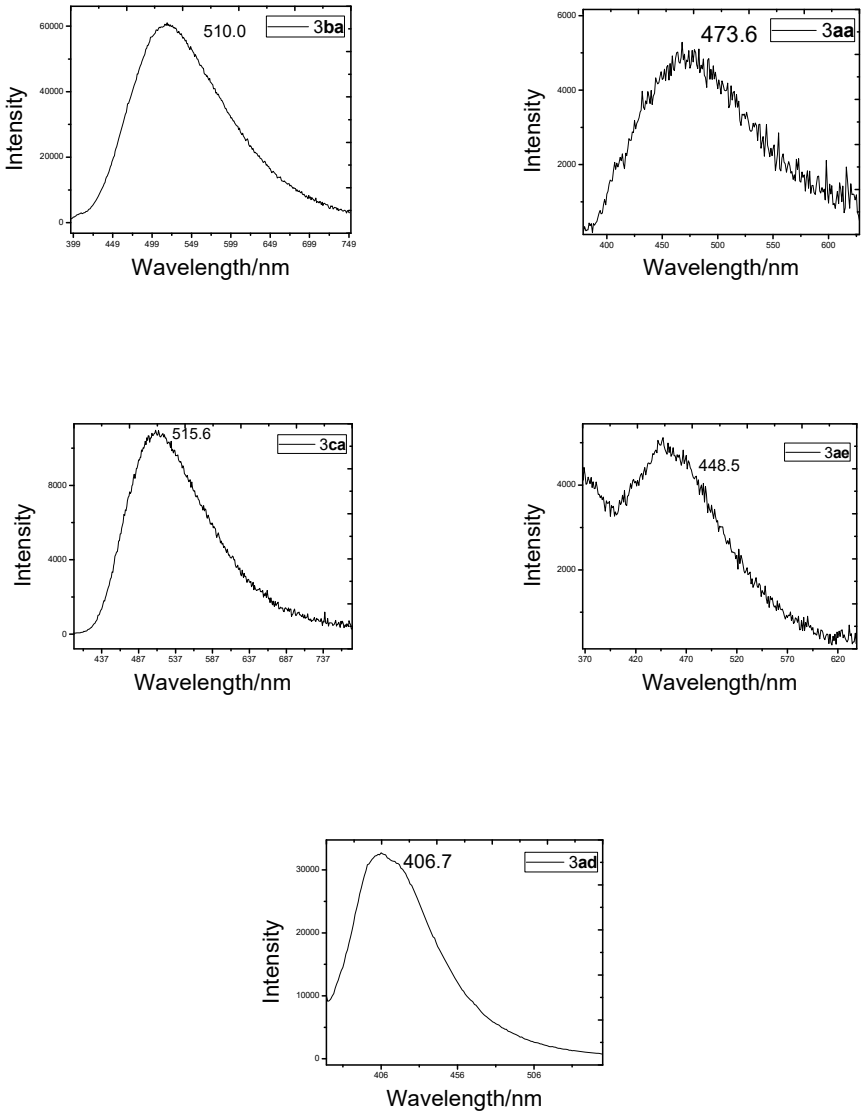
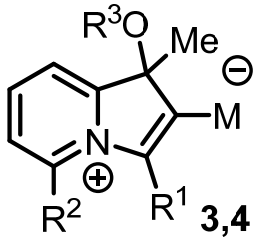
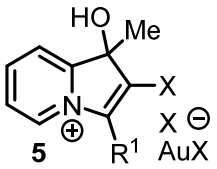


Figure 2: Emission scan of other product **3**

Absorption and Emission Wavelength Data of 3, 4 and 5



3,4



5

entry	M =	3 , 4	λ_{Abs} (nm)	λ_{Em} (nm)[b]
1	AuCl	4aa	334.3[c]	473.6
2	$AuCl_3$	3ab	289.3	413.2
3	$AuBr_3$	3ac	282.1	398.0
4	AuCl	4ba	340.3[c]	510.0
5	$AuCl_3$	3bb	281.0	474.3
6	$AuBr_3$	3bc	283.5	468.0
7	AuCl	4ca	350.2[c]	515.6
8	$AuCl_3$	3cb	280.5	538.1
9	$AuCl_3$	3db	292.0	468.0
10		3eb	292.1	383.0
11		3fb	283.9	481.0
12	CuCl	4ad	261.3[c]	406.7
13	CuBr	4ae	263.0[c]	448.5

All the studies were conducted in degassed CH_3CN at r.t.. [a] $\lambda_{Excitation}$ = 330 and 350 nm
[b] $\lambda_{Excitation}$ = 284 nm, λ_{em} before and after the photo-excitation are essentially the same (~ 5 nm differences).
[c] No obvious change in λ_{abs} (~ 5 nm differences) and intensity after photo-excitation.

Singlet Oxygen Emission Signal Study:

As mentioned in the maintext, we suspected that there was an intersystem crossing (ISC) of Au (III) and the indolizine derivatives at their excited states, which turned the emissive singlet to the dark triplet excited state. So, we conducted experiment to detect the singlet oxygen generation and the results were summarized as follow:

Table S1: singlet oxygen generation quantum yield

compound	Single oxygen quantum yield
3cb	26%
3bb	25%
3ac	14%

Emission of singlet oxygen was recorded with an FLS 980 fluorescence spectrometer from Edinburgh Instrument™ equiped with an NIR-PMT detector and an 850 nm long pass filter in the emission arm. Quartz cuvettes (path length = 1 cm).

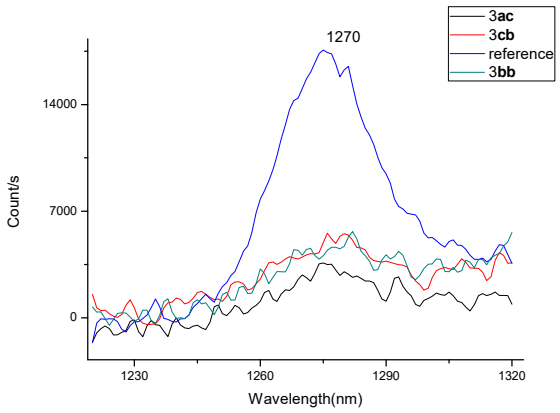


Figure 3: The NIR emission of $^1O_2$

Singlet oxygen quantum yields of the compounds were determined by measuring the peak areas of the NIR emission of $^1O_2$ centered at 1270 nm generated by these compounds and compared to that generated from the reference standard Rose Bengal (Qy = 76%) upon photo-excitation at 328 nm.

Cyctotoxicity evaluation of complex 3 on cancer cell lines

Cell Cultures

Human A549 (lung), HCT116 (colon) and HepG2 (liver) cancer cells were obtained from American Type Culture Collection (ATCC) and cultured in Dulbecco's modification of Eagle medium (DMEM) supplemented with 10% fetal bovine serum, 100 units/ml penicillin, and 100 mg/ml streptomycin. Cells were cultured at 37^{o}C in an atmosphere of 5% CO_2 and 95% humidity.

Cell proliferation assay

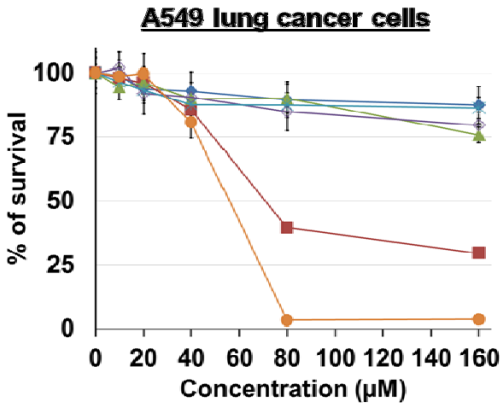
Cell proliferation was assessed by MTT [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide] assay. Briefly, cells were plated in 96-well plates ($2x10^3$cells/well) and then treated with indolizine derivatives ligated Au(III) complexes for 72 h. Afterward, cells were treated with MTT reagent and the absorbance at 570 nm was measured using a microplate reader. The viability of control (untreated cells) was regarded as 100%.

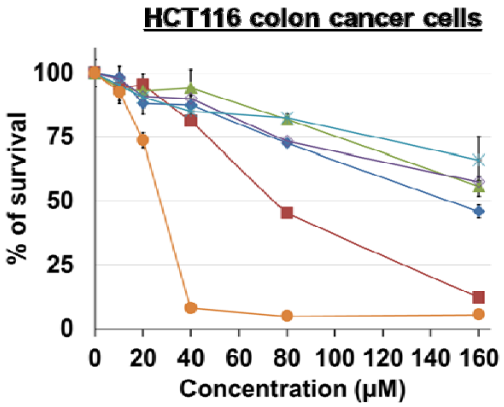
Cytotoxic effects of indolizine derivatives ligated Au(III) complexes.

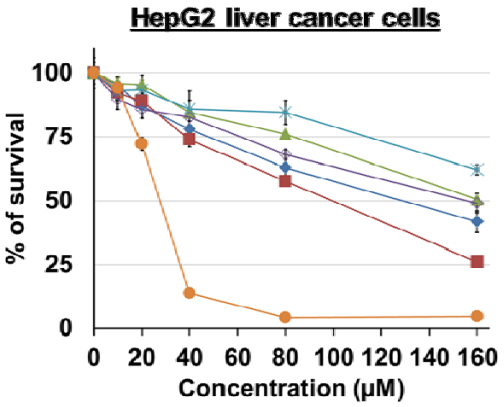
A549 (lung), HCT116 (colon) and HepG2 (liver) cancer cells were untreated or treated with different concentrations of indolizine derivatives ligated Au(III) complexes for 72 h. Cell viability was assessed by the MTT assay. IC50 represents the drug concentration required for 50% inhibition of cell proliferation. The data are presented as the mean ± SD of three replicates. Results are representative of 2 independent experiments.

Results

To determine the potential anticancer activity of indolizine derivatives ligated Au(III) complexes, three human cancer cell lines (A549, HCT116 and HepG2) were treated with different concentrations of Au(III) complexes and then assayed for cell viability. Conducted at 0.1% v/v DMSO in cell culture medium.







Au(III) complexes	IC50 (μM) A549	HCT116	HepG2
3cb	>160	148.1	129.1
3fb	71.4	75.3	99.5
3bc	>160	>160	>160
3ac	>160	>160	156.8
3db	>160	>160	>160
3ac	55.7	27.2	27.7

This preliminary study showed that the substituent effect is very critical, in which complex **3ac** exerted a good cytotoxic effects to those cell lines with IC50 values of 27.2 to 55.7μM, compared with other Au(III) complexes.

Raw data for the graphs above:

A549

% Survival

uM	3cb	3fb	3bc	3ac	3db	3ac
160	87.48	29.66	75.73	79.61	86.37	3.55
80	89.62	39.37	90.11	84.88	87.55	3.25
40	92.95	85.59	89.97	90.58	87.71	80.59
20	93.84	96.19	96.30	92.02	93.42	99.66
10	98.94	98.12	94.64	102.04	96.63	98.74
0	100.00	100.00	100.00	100.00	100.00	100.00

St. Dev.

uM	3cb	3fb	3bc	3ac	3db	3ac
160	7.38	0.25	3.07	5.14	4.16	0.10
80	7.09	0.74	5.74	7.42	0.60	0.16
40	7.72	2.92	6.47	9.65	4.16	6.11
20	4.55	6.13	2.15	8.12	5.11	7.76
10	9.18	4.16	1.65	6.23	2.90	6.22
0	6.11	8.01	5.77	0.90	3.31	2.02

H116

% Survival

uM	3cb	3fb	3bc	3ac	3db	3ac
160	45.82	12.13	55.72	57.45	65.97	5.36
80	72.49	45.12	81.85	73.35	82.41	4.76
40	87.49	81.21	94.30	90.05	85.02	7.97
20	88.18	95.50	93.12	90.84	90.58	73.70
10	98.43	94.14	94.07	97.79	95.29	92.63
0	100.00	100.00	100.00	100.00	100.00	100.00

St. Dev.

uM	3cb	3fb	3bc	3ac	3db	3ac
160	2.56	0.91	3.89	0.62	9.04	0.19
80	1.00	0.99	0.80	0.67	1.42	0.16
40	3.76	1.61	7.12	4.11	1.98	0.90
20	1.77	4.18	1.46	2.71	6.65	2.98
10	4.10	6.01	1.99	4.52	2.88	3.28
0	1.04	5.35	1.28	1.06	1.09	1.22

HepG2

% Survival

uM	3cb	3fb	3bc	3ac	3db	3ac
160	41.71	26.07	50.56	49.05	62.14	4.56
80	62.96	57.66	76.10	68.06	84.60	4.15
40	77.98	73.93	84.57	82.69	85.94	13.69
20	87.16	89.15	95.60	85.85	93.45	72.13
10	95.39	92.41	96.03	89.68	93.21	94.27
0	100.00	100.00	100.00	100.00	100.00	100.00

St. Dev.

uM	3cb	3fb	3bc	3ac	3db	3ac
160	4.21	1.44	2.32	3.89	1.99	0.12
80	4.91	1.64	0.72	1.94	4.75	0.12
40	6.93	0.81	4.84	1.54	7.12	1.56
20	4.79	3.04	1.64	3.37	5.58	2.46
10	2.96	3.09	2.34	3.90	3.30	1.43
0	4.17	0.71	5.81	2.40	5.87	1.53

Parameter	Value
1 Title	YJ-01-136
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	CDCl3
9 Temperature	296.2
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	12
13 Receiver Gain	95
14 Relaxation Delay	1.0000
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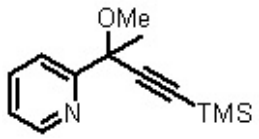
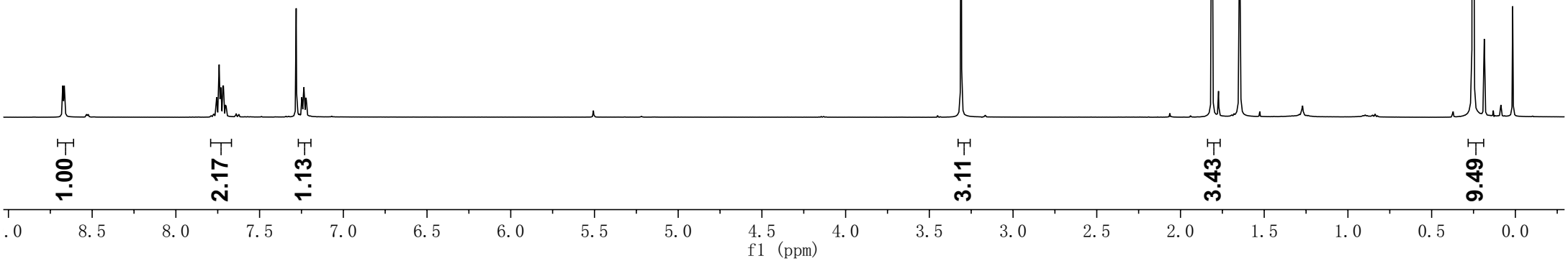
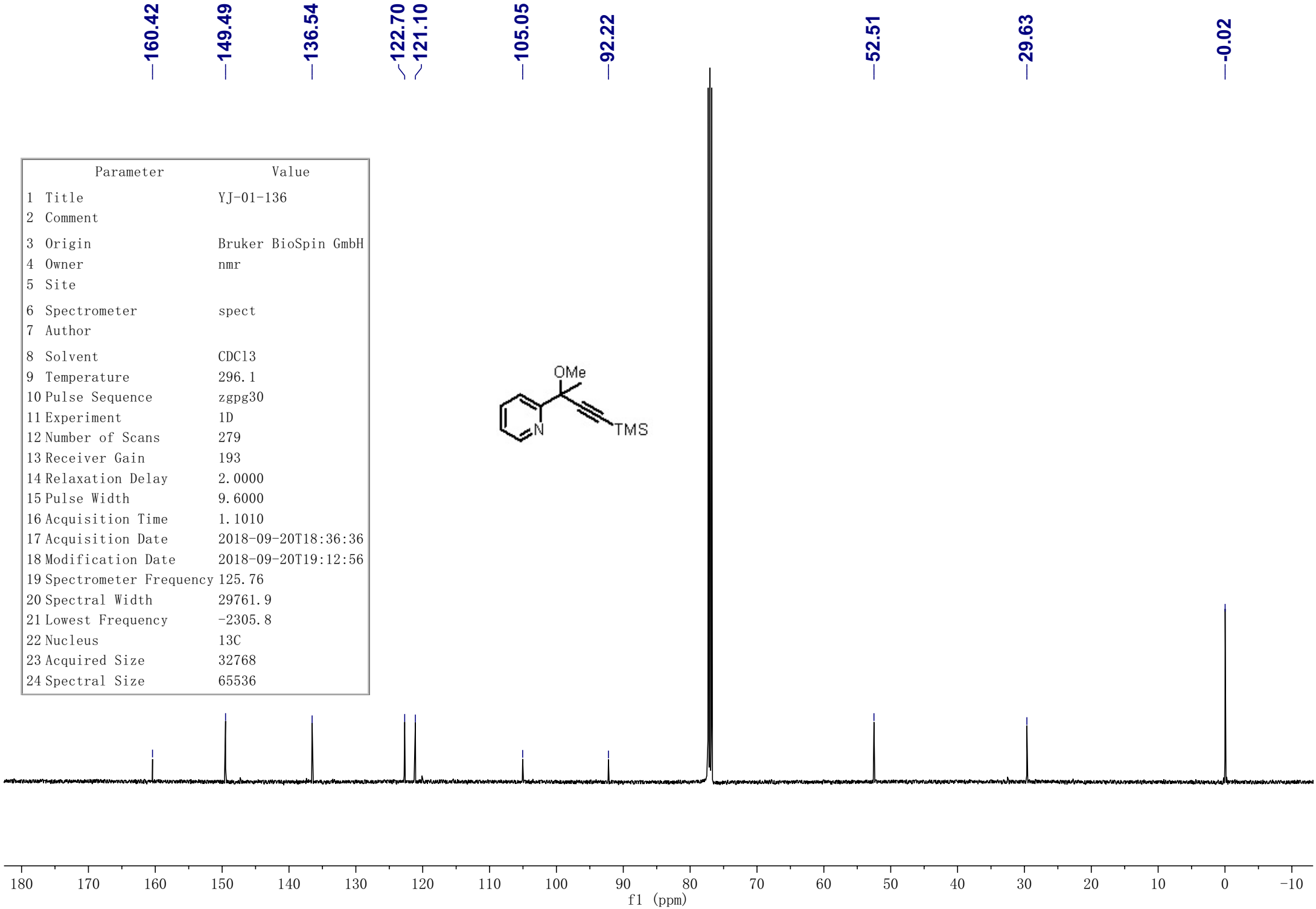
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536







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7 Author	
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9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	279
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
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22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

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8 Solvent	CDCl3
9 Temperature	296.2
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	6
13 Receiver Gain	78
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
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22 Nucleus	1H
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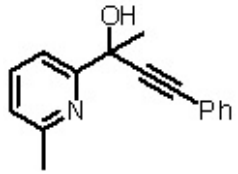

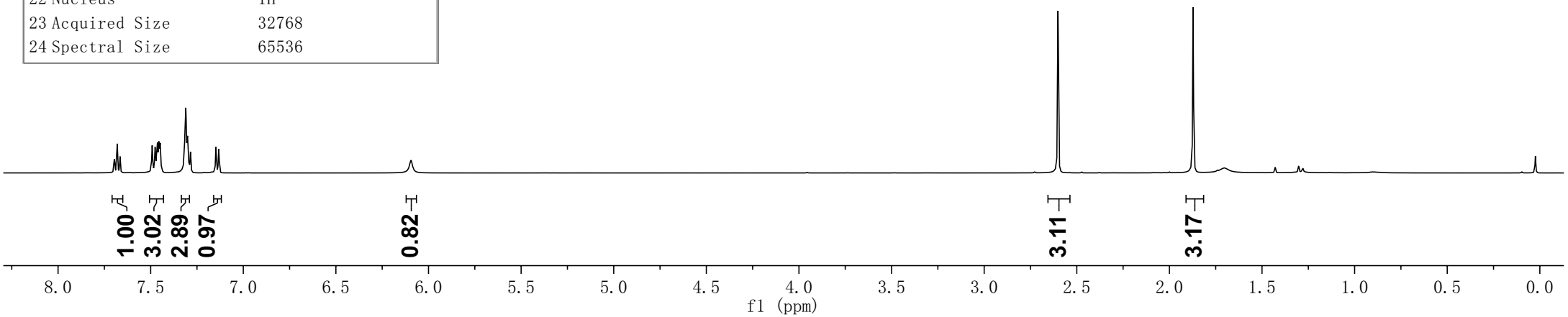

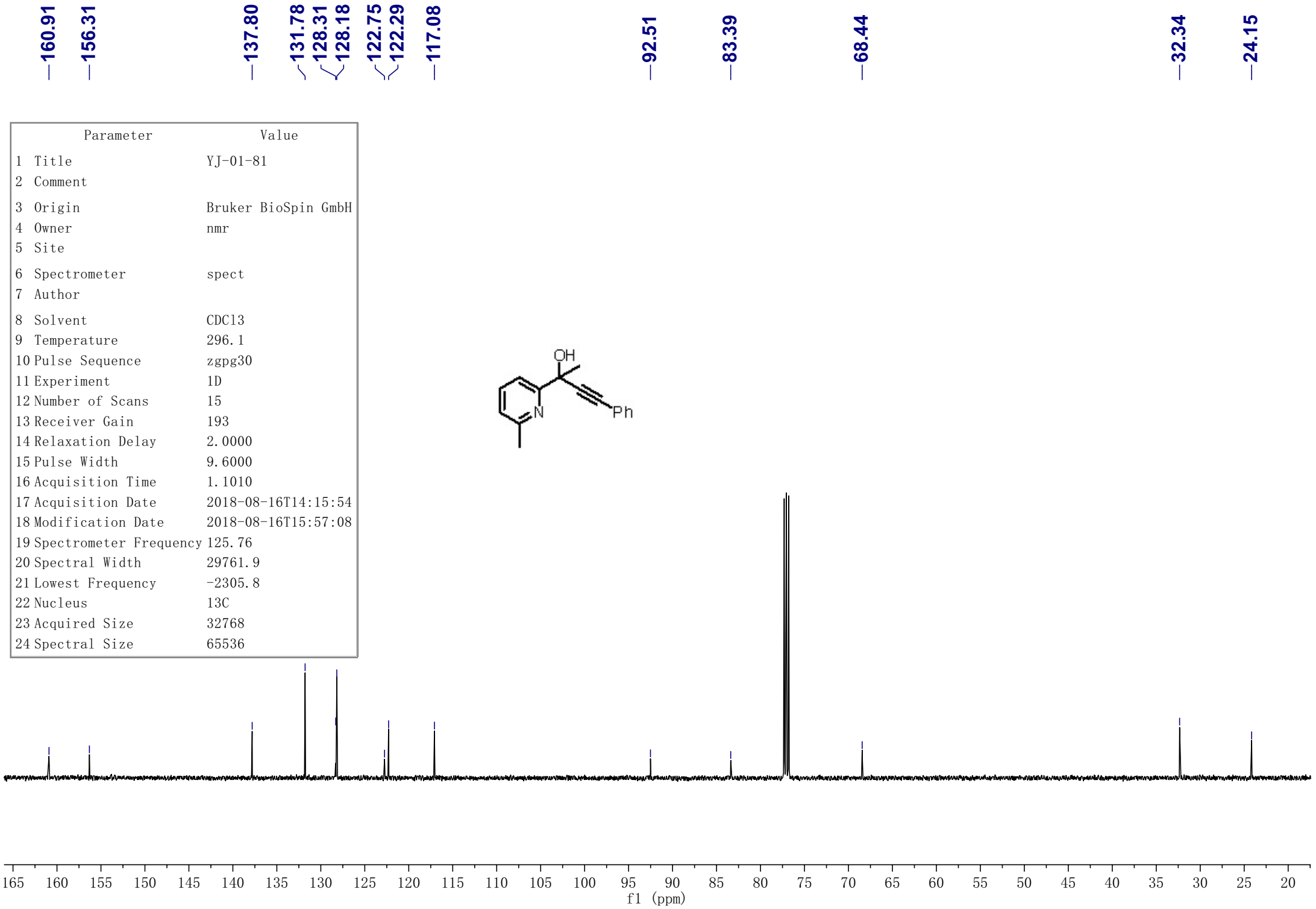

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4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	CDCl3
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	15
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
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20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

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4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	CDCl3
9	Temperature	295.7
10	Pulse Sequence	zg30
11	Experiment	1D
12	Number of Scans	8
13	Receiver Gain	22
14	Relaxation Delay	1.0000
15	Pulse Width	10.0000
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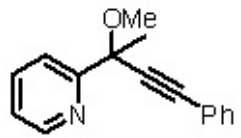

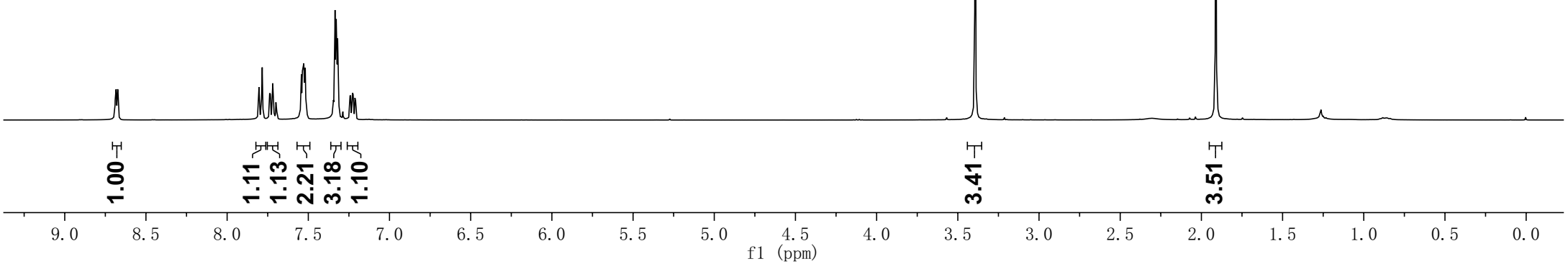

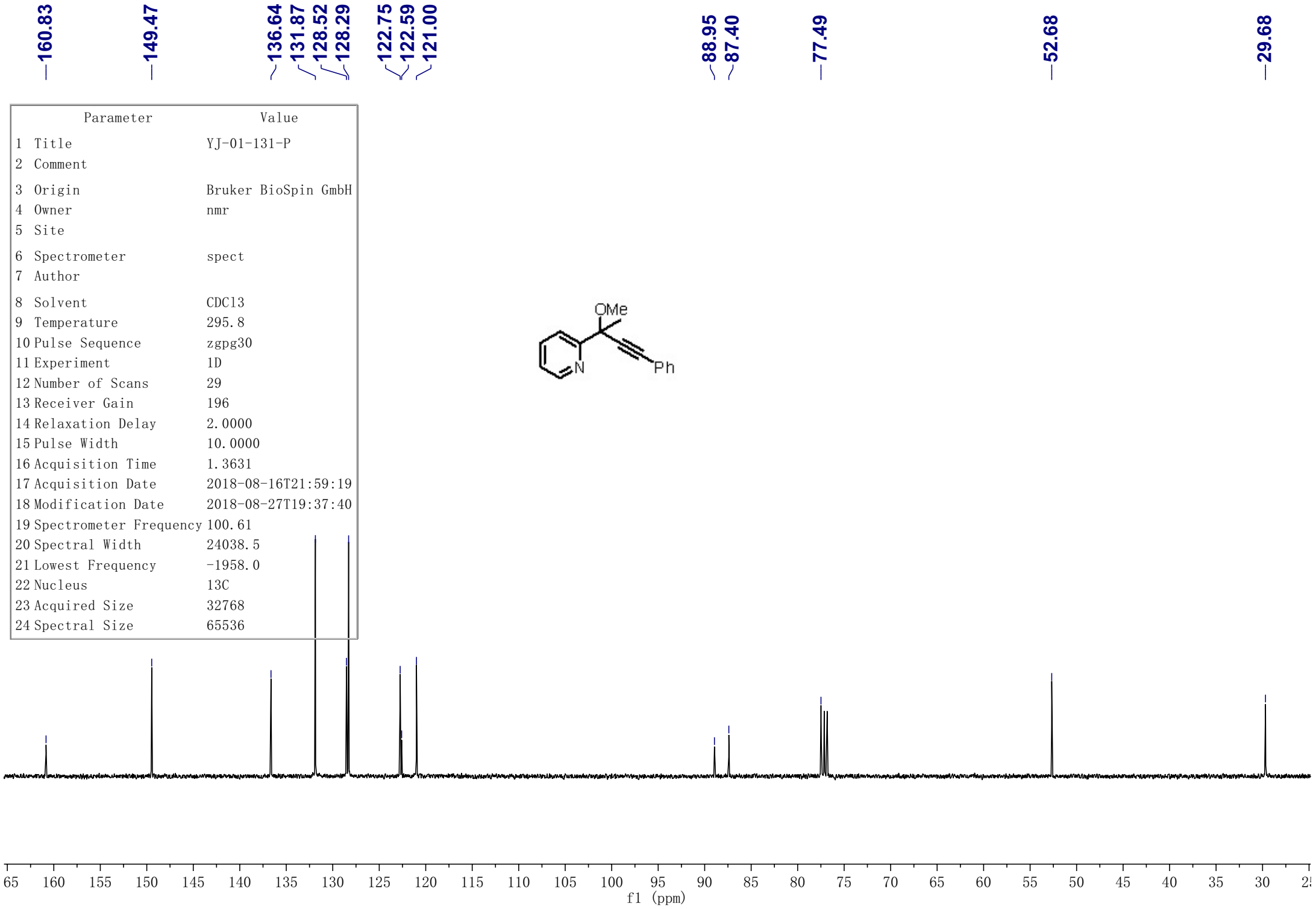

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3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	CDCl3
9 Temperature	295.8
10 Pulse Sequence	zgpg30
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21 Lowest Frequency	-1958.0
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

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6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	298.1
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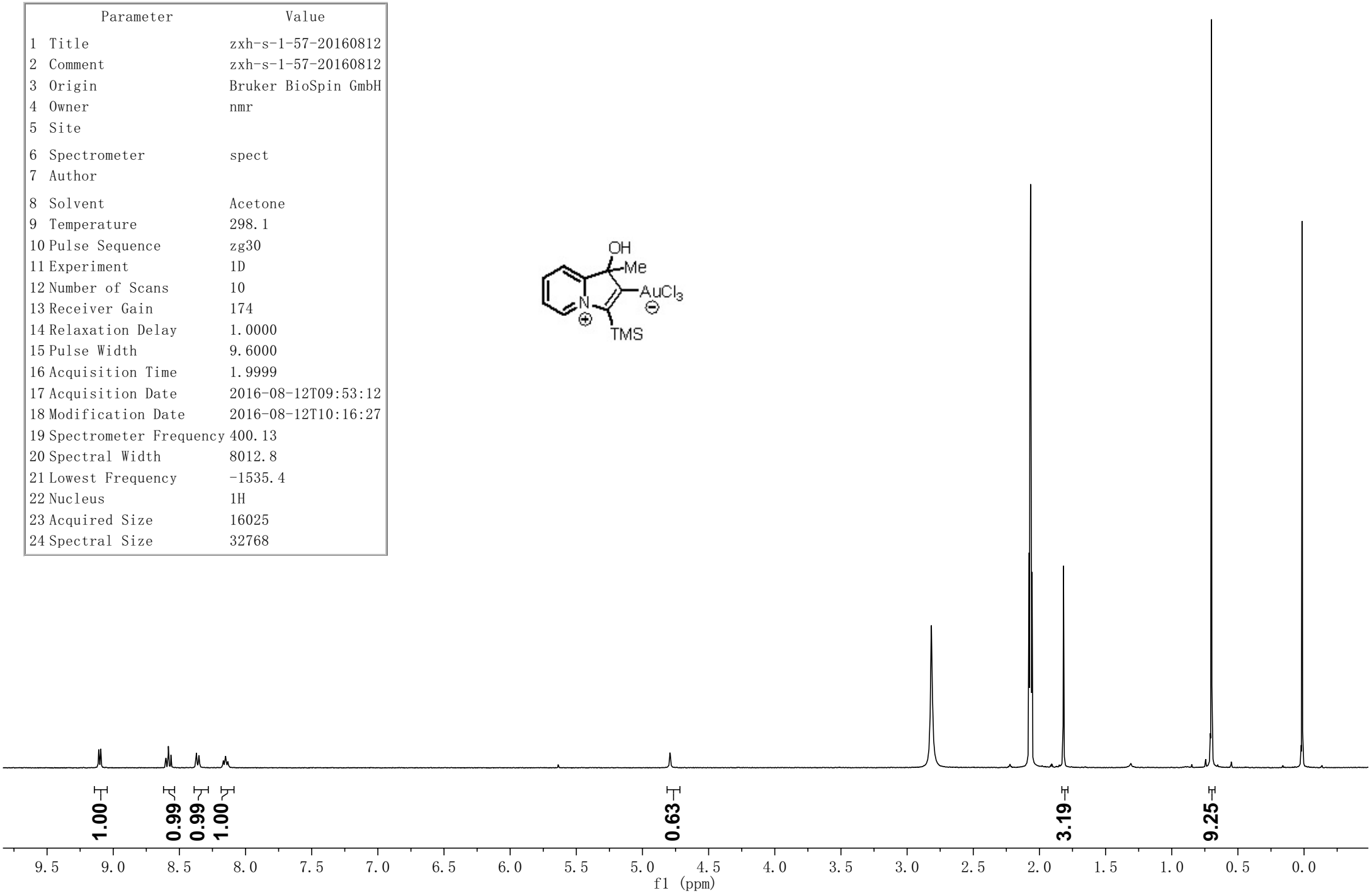
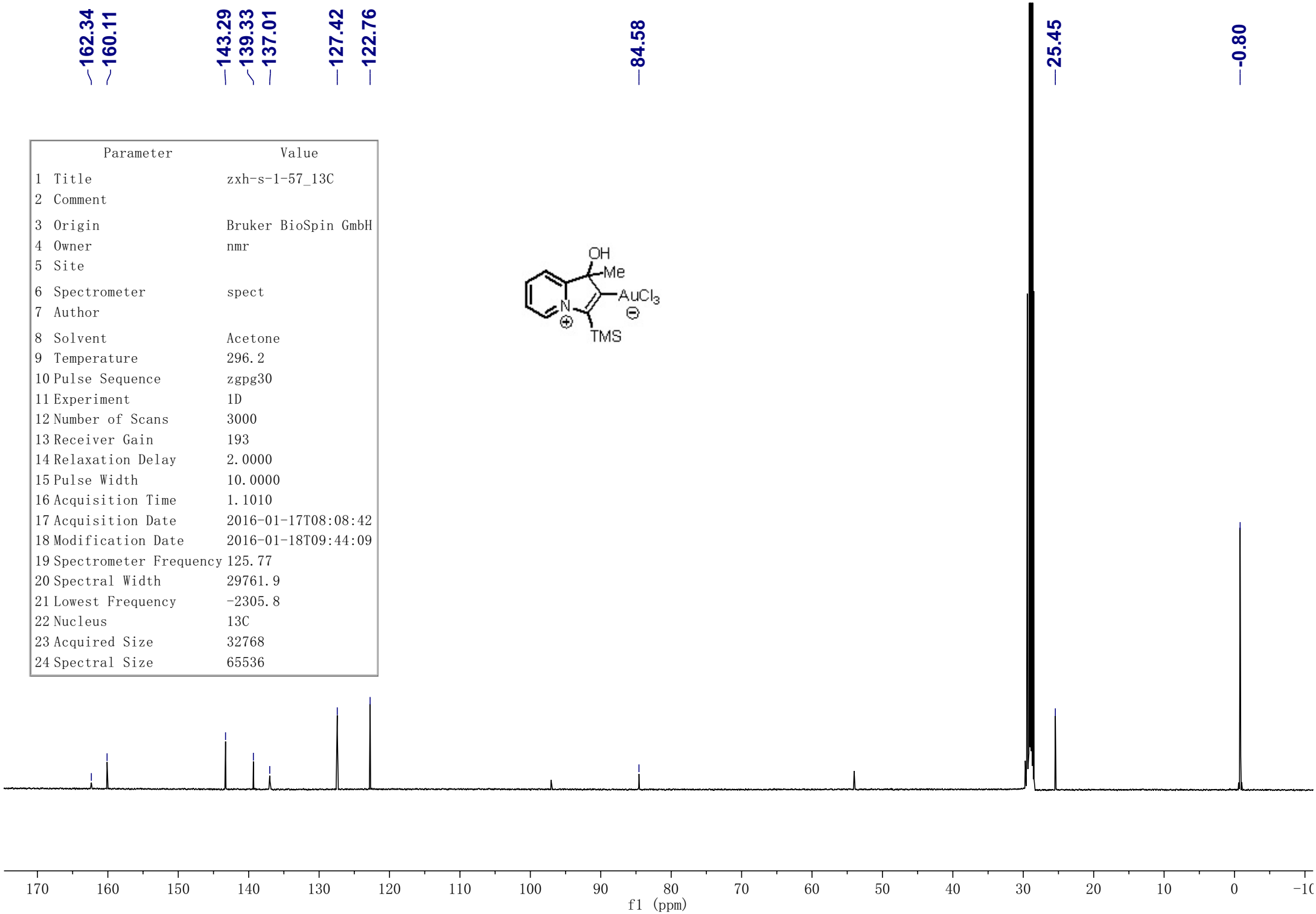
24 Spectral Size	32768





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4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
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22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

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4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
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11 Experiment	1D
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23 Acquired Size	16025
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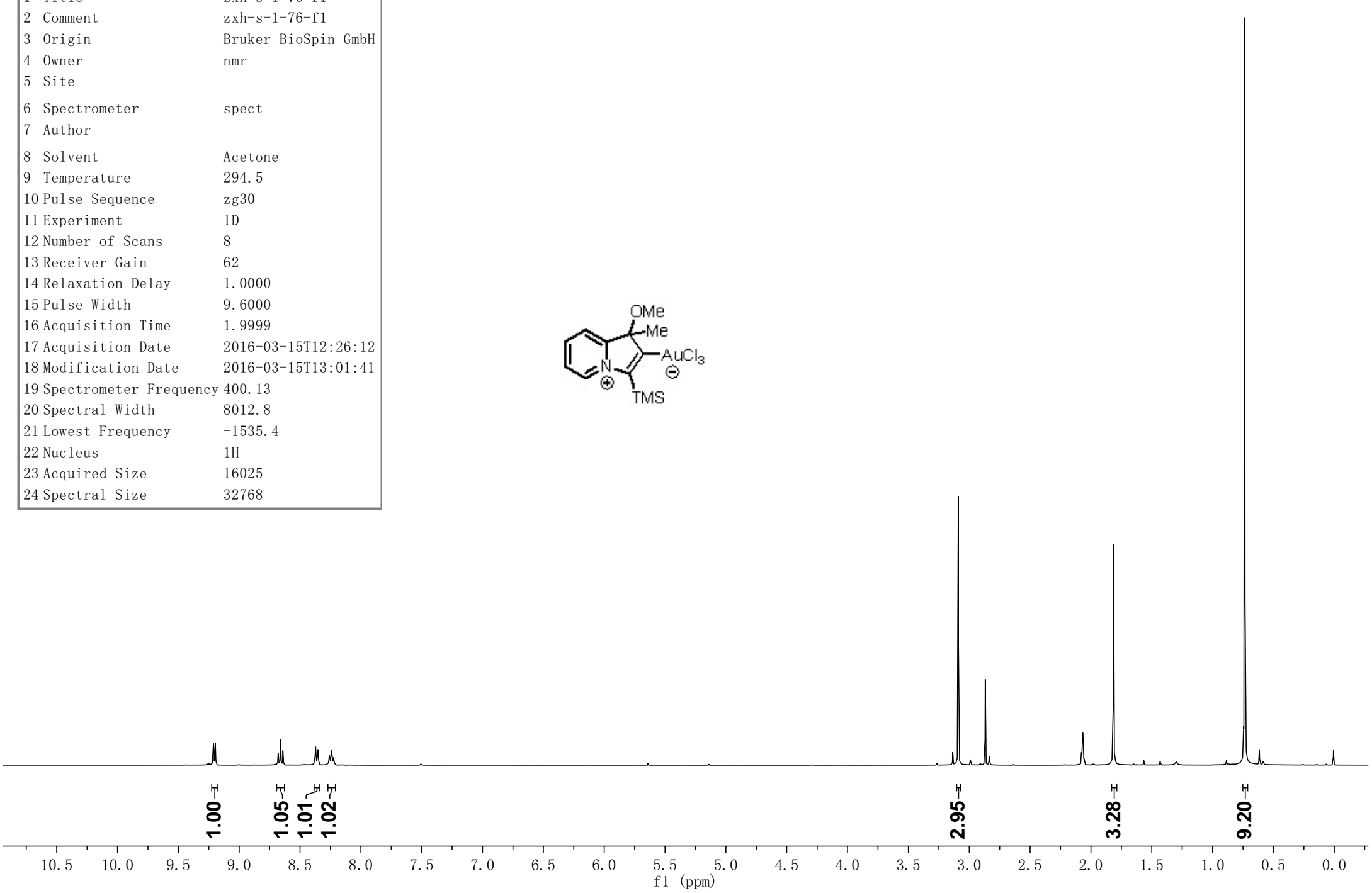

158.79
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142.37
138.16
128.16
123.44
90.77
25.55
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Parameter	Value
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3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	294.5
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	473
13 Receiver Gain	196
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
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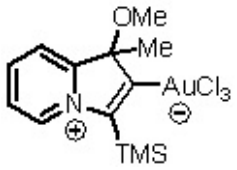
19 Spectrometer Frequency	100.61
20 Spectral Width	24038.5
21 Lowest Frequency	-1958.0
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

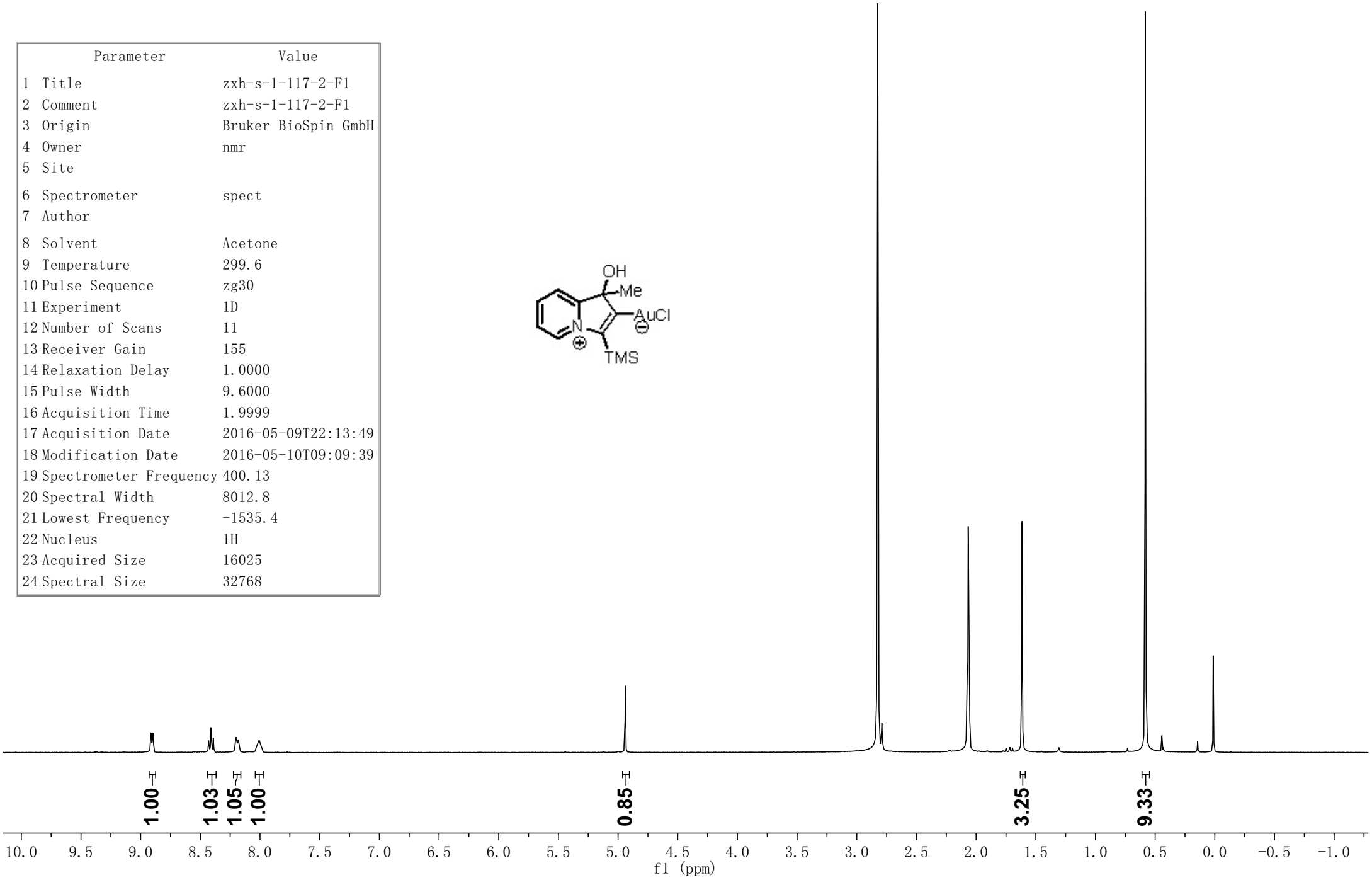


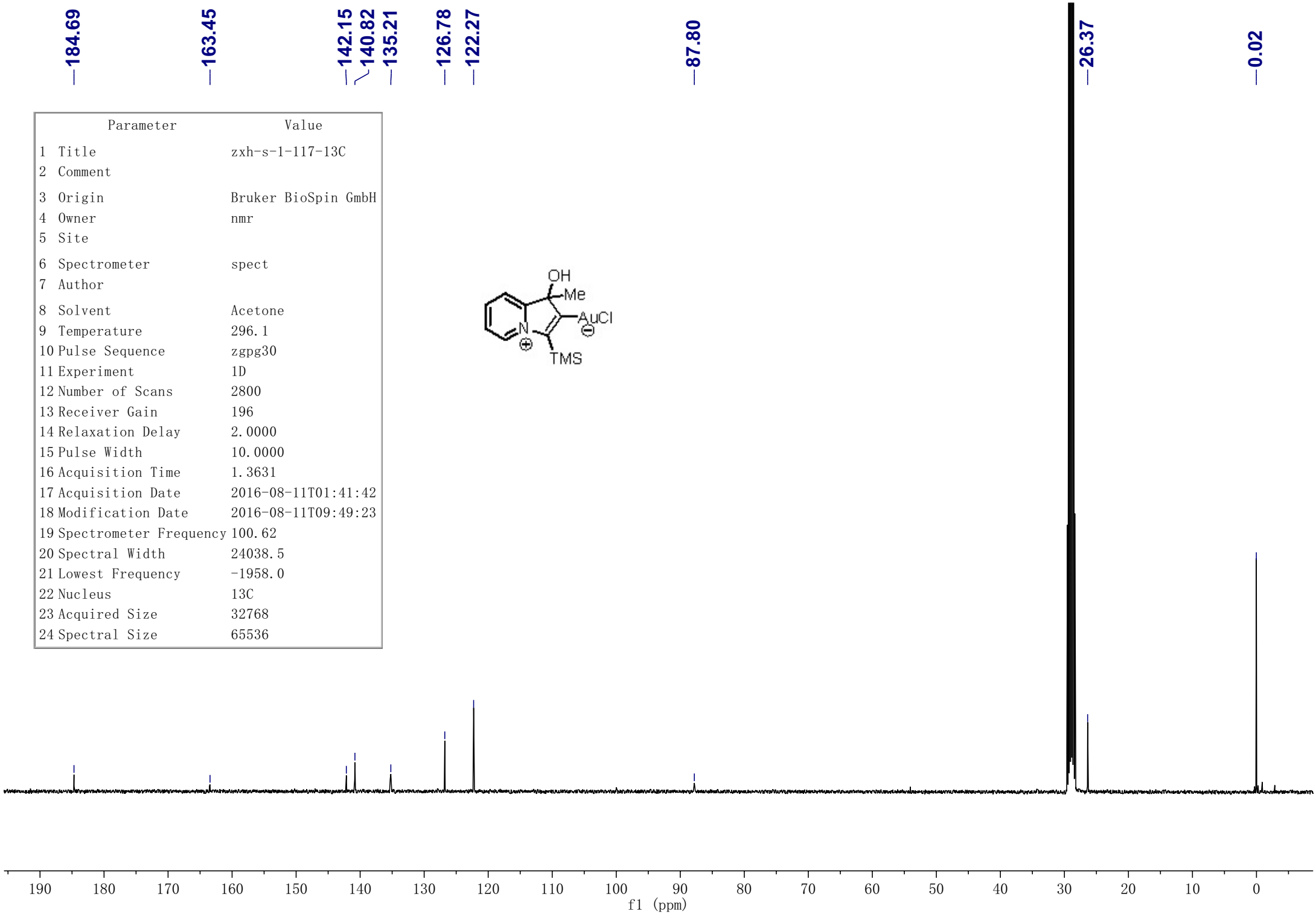
DCM

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

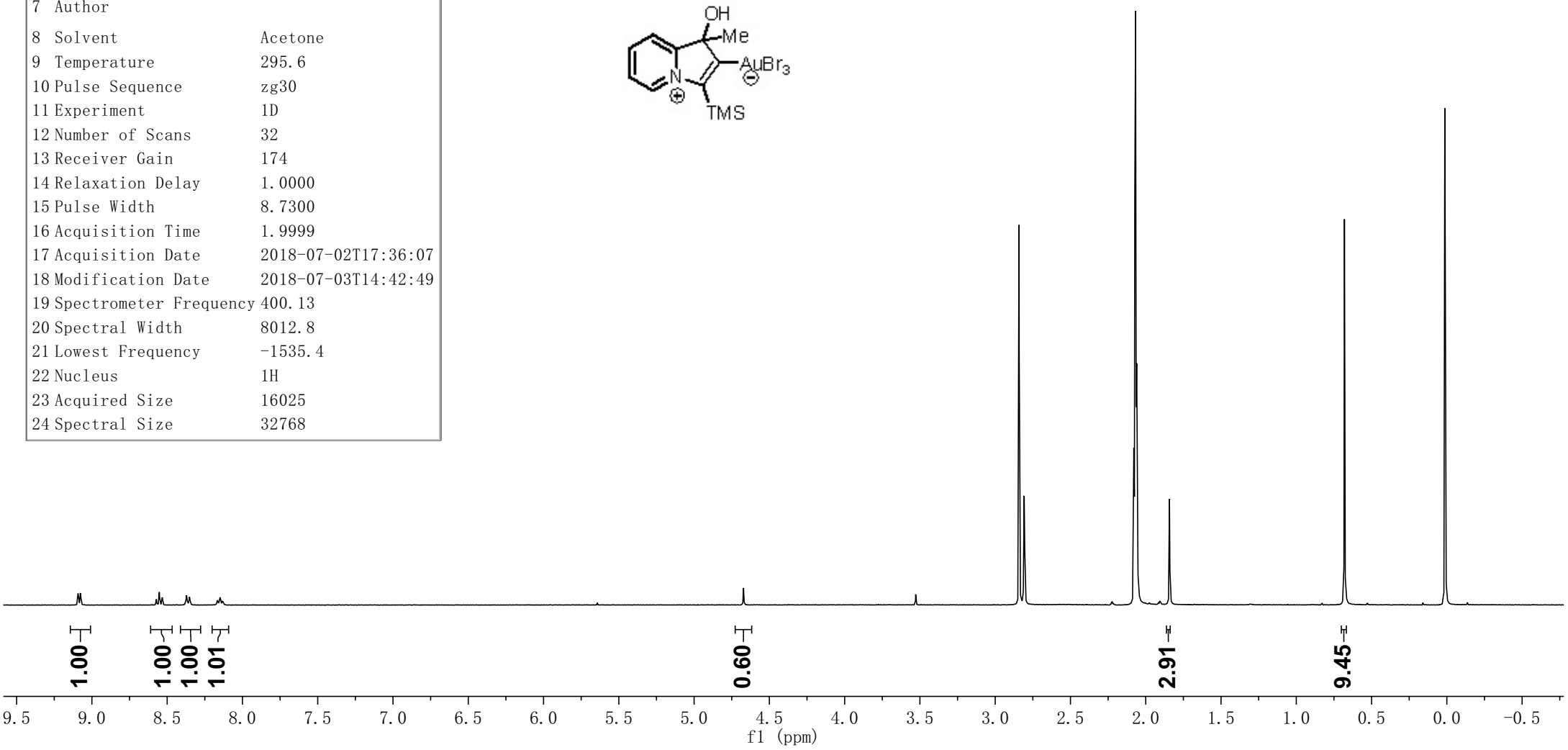
Parameter	Value
1 Title	zxh-s-1-117-2-F1
2 Comment	zxh-s-1-117-2-F1
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	299.6
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	11
13 Receiver Gain	155
14 Relaxation Delay	1.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.9999
17 Acquisition Date	2016-05-09T22:13:49
18 Modification Date	2016-05-10T09:09:39
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	16025
24 Spectral Size	32768

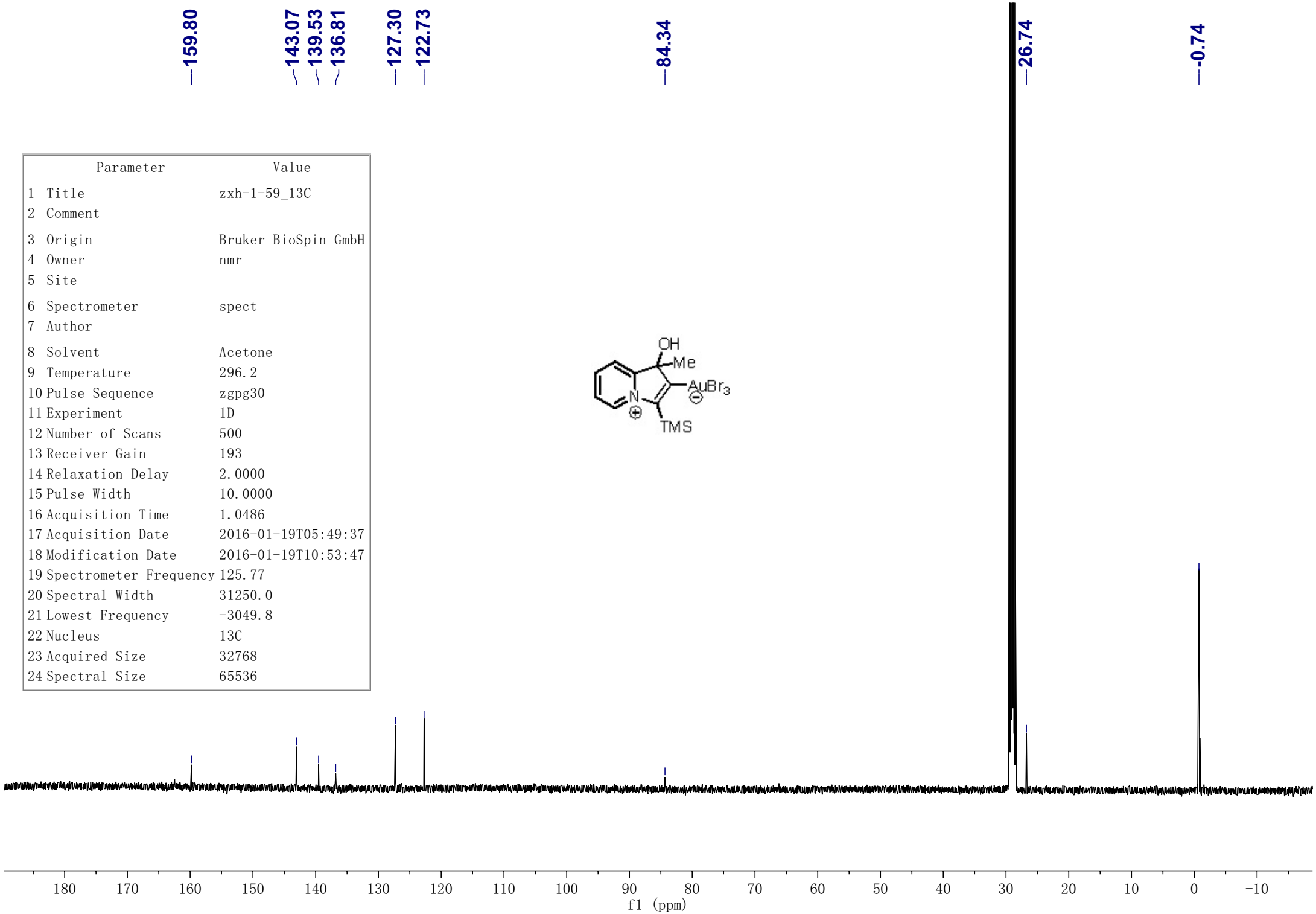




Parameter	Value
1 Title	zxh-s-1-117-13C
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	2800
13 Receiver Gain	196
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.3631
17 Acquisition Date	2016-08-11T01:41:42
18 Modification Date	2016-08-11T09:49:23
19 Spectrometer Frequency	100.62
20 Spectral Width	24038.5
21 Lowest Frequency	-1958.0
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

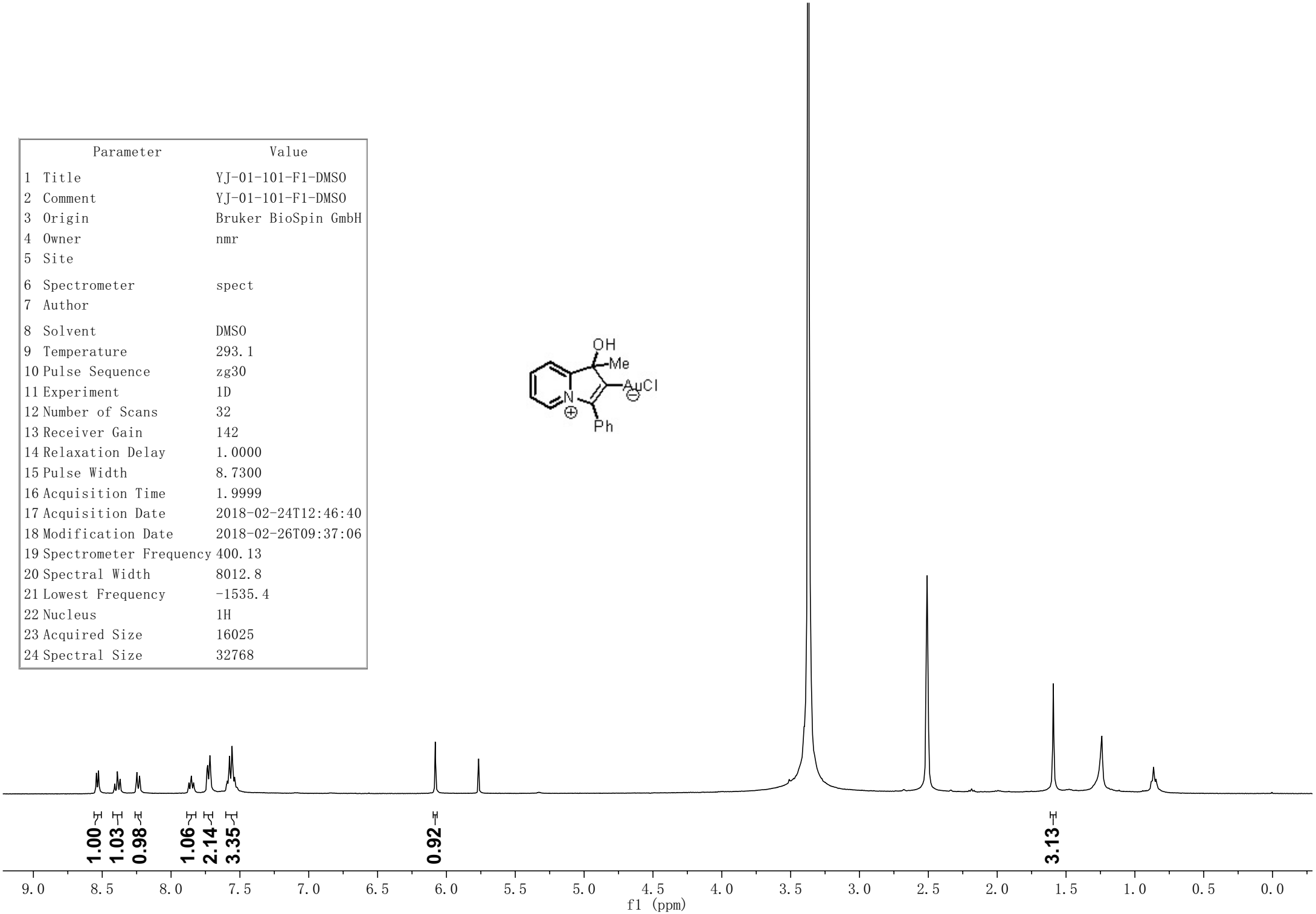
Parameter	Value
1 Title	YJ-01-130-ACETONE
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	295.6
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	32
13 Receiver Gain	174
14 Relaxation Delay	1.0000
15 Pulse Width	8.7300
16 Acquisition Time	1.9999
17 Acquisition Date	2018-07-02T17:36:07
18 Modification Date	2018-07-03T14:42:49
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	16025
24 Spectral Size	32768

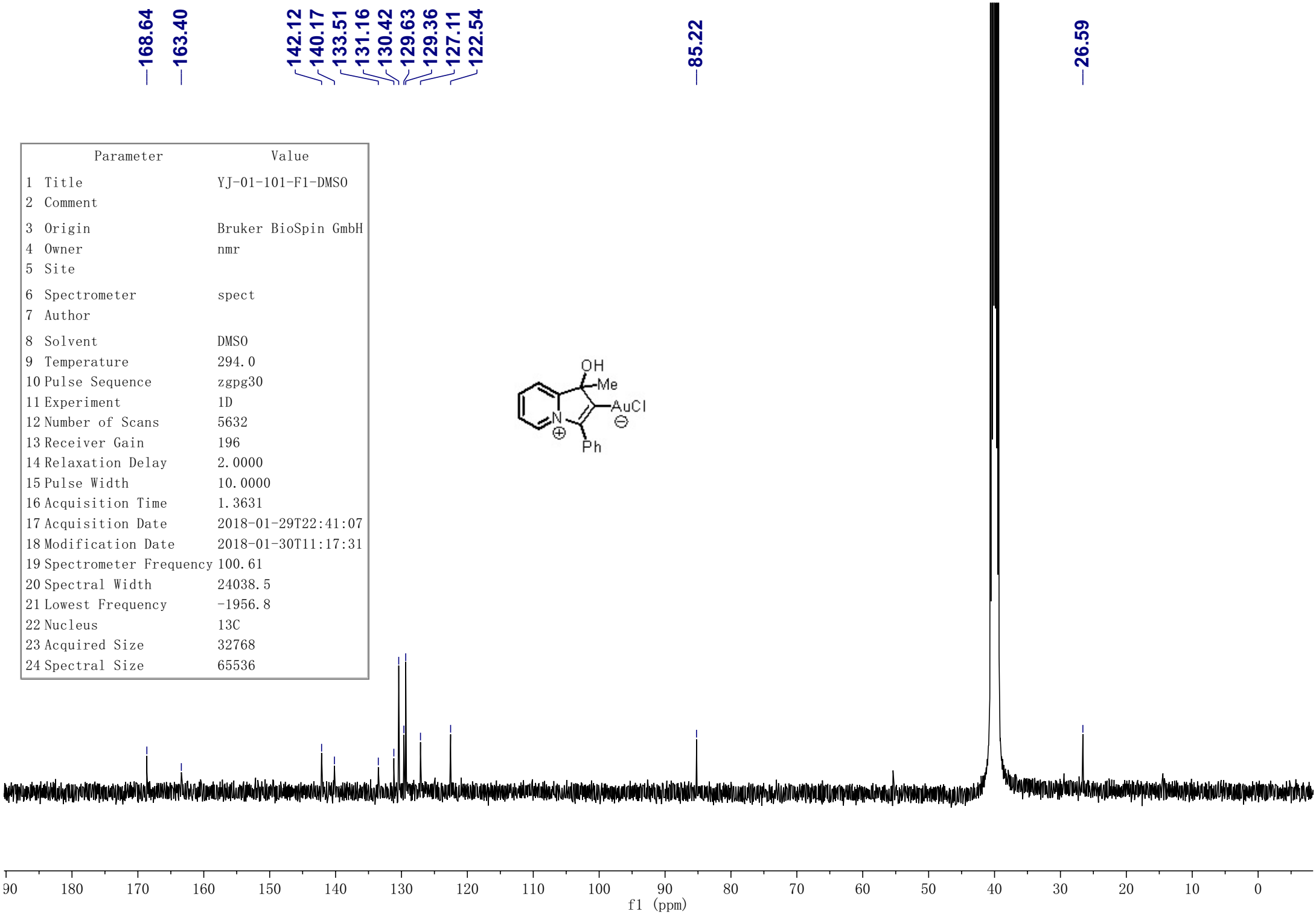




Parameter	Value
1 Title	zxh-1-59_13C
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	500
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.0486
17 Acquisition Date	2016-01-19T05:49:37
18 Modification Date	2016-01-19T10:53:47
19 Spectrometer Frequency	125.77
20 Spectral Width	31250.0
21 Lowest Frequency	-3049.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

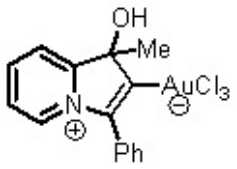
Parameter	Value
1 Title	YJ-01-101-F1-DMSO
2 Comment	YJ-01-101-F1-DMSO
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	293.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	32
13 Receiver Gain	142
14 Relaxation Delay	1.0000
15 Pulse Width	8.7300
16 Acquisition Time	1.9999
17 Acquisition Date	2018-02-24T12:46:40
18 Modification Date	2018-02-26T09:37:06
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	16025
24 Spectral Size	32768

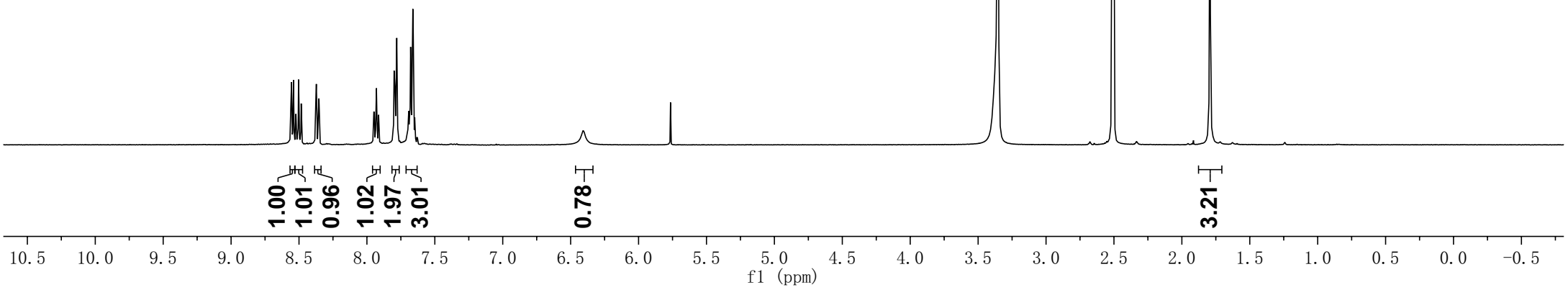


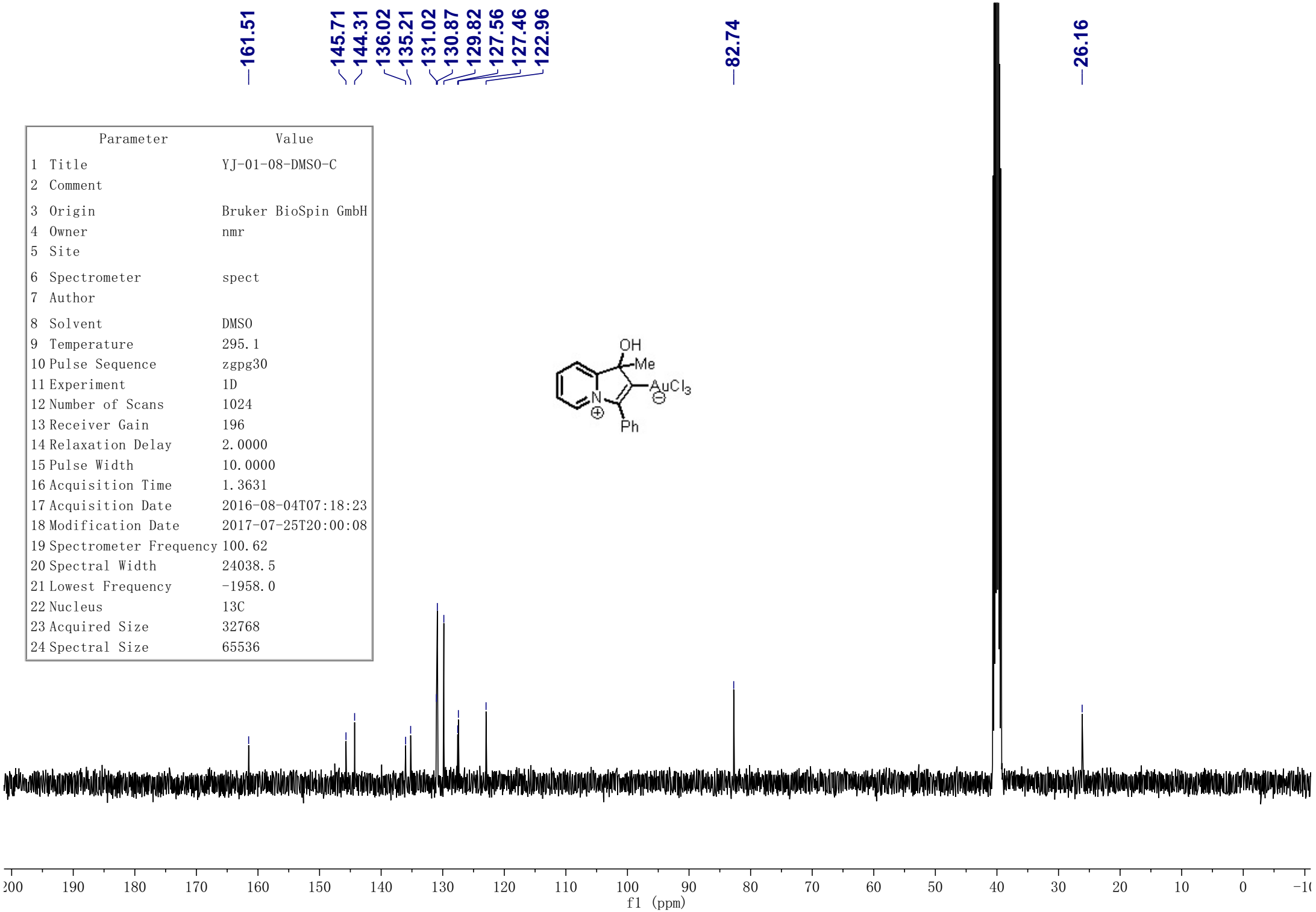


Parameter	Value
1 Title	YJ-01-101-F1-DMSO
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	294.0
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	5632
13 Receiver Gain	196
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.3631
17 Acquisition Date	2018-01-29T22:41:07
18 Modification Date	2018-01-30T11:17:31
19 Spectrometer Frequency	100.61
20 Spectral Width	24038.5
21 Lowest Frequency	-1956.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Parameter	Value
1 Title	YJ-01-08-DMSO
2 Comment	YJ-01-08-DMSO
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	295.3
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	32
13 Receiver Gain	155
14 Relaxation Delay	1.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.9999
17 Acquisition Date	2016-08-03T23:34:00
18 Modification Date	2017-07-25T20:00:07
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	16025
24 Spectral Size	32768

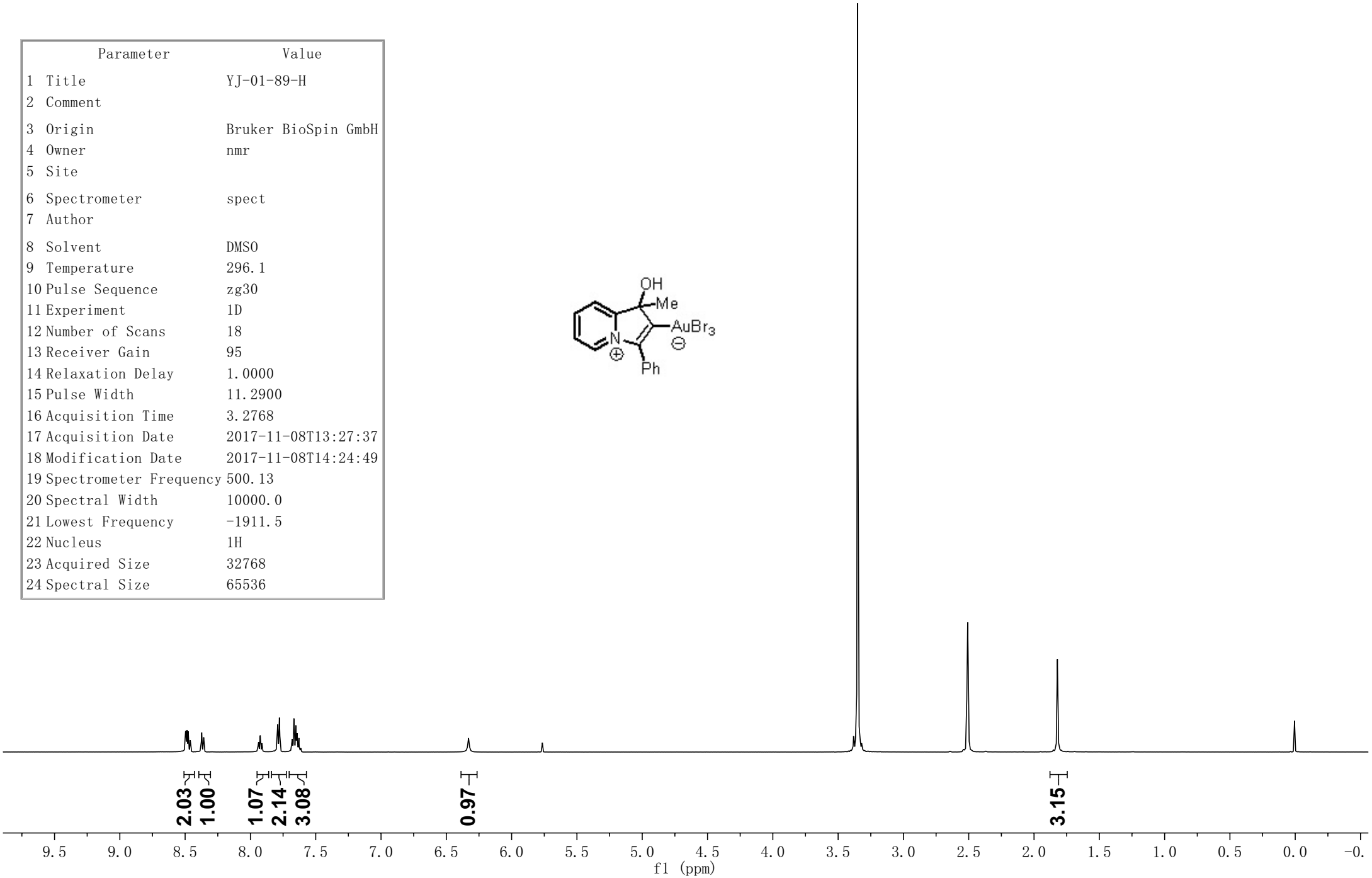


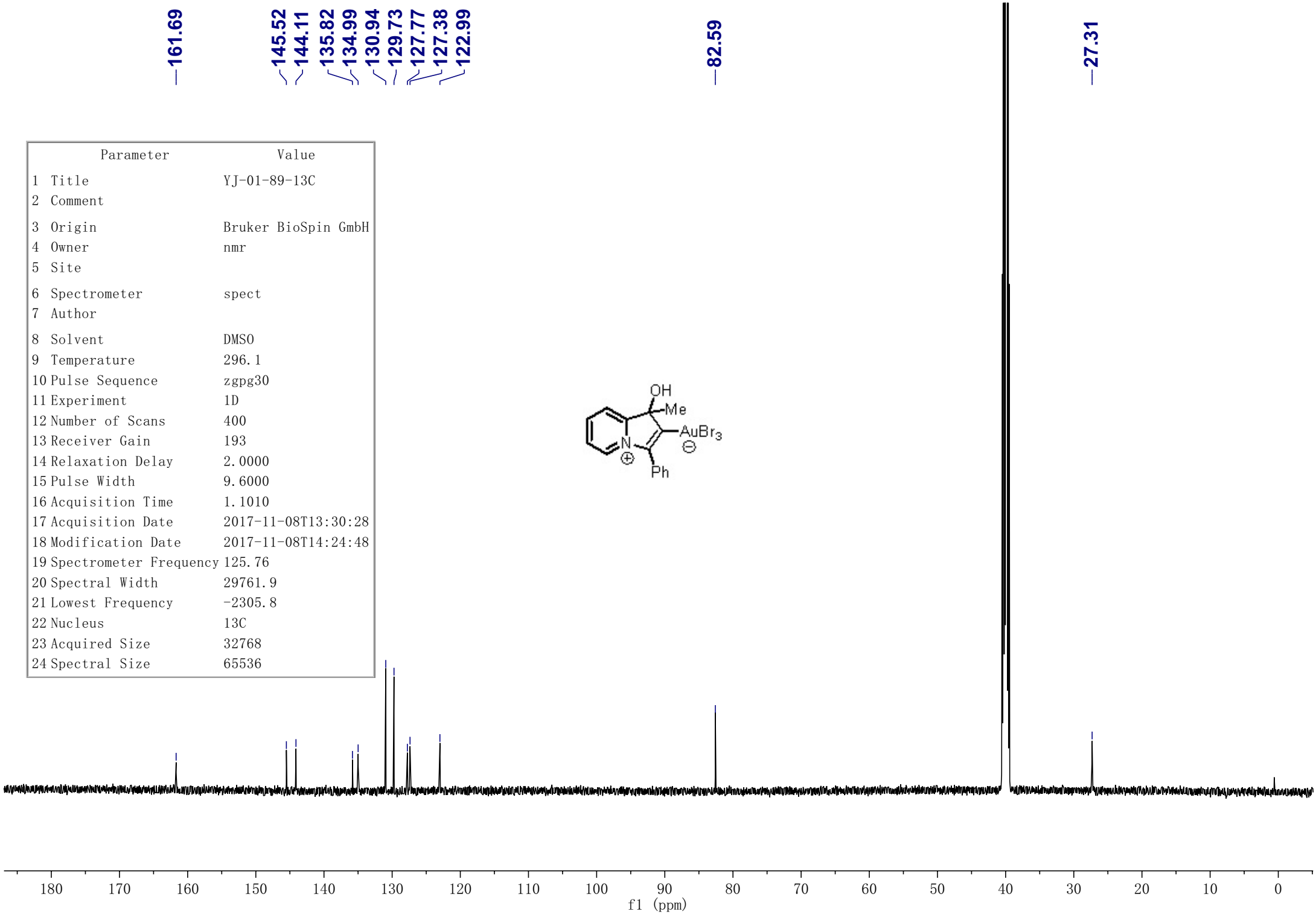




Parameter	Value
1 Title	YJ-01-08-DMSO-C
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	295.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	1024
13 Receiver Gain	196
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.3631
17 Acquisition Date	2016-08-04T07:18:23
18 Modification Date	2017-07-25T20:00:08
19 Spectrometer Frequency	100.62
20 Spectral Width	24038.5
21 Lowest Frequency	-1958.0
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

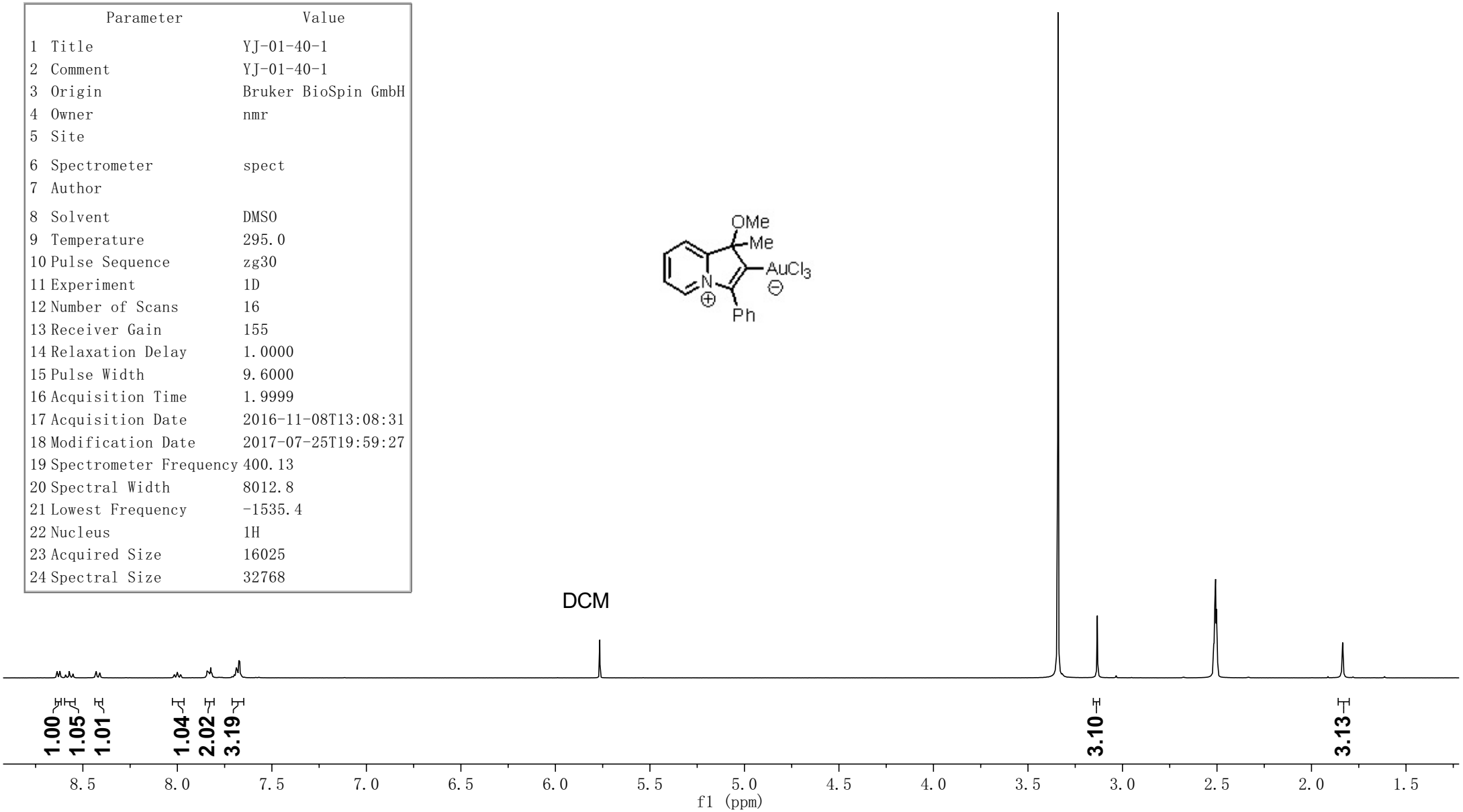
Parameter	Value
1 Title	YJ-01-89-H
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	18
13 Receiver Gain	95
14 Relaxation Delay	1.0000
15 Pulse Width	11.2900
16 Acquisition Time	3.2768
17 Acquisition Date	2017-11-08T13:27:37
18 Modification Date	2017-11-08T14:24:49
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

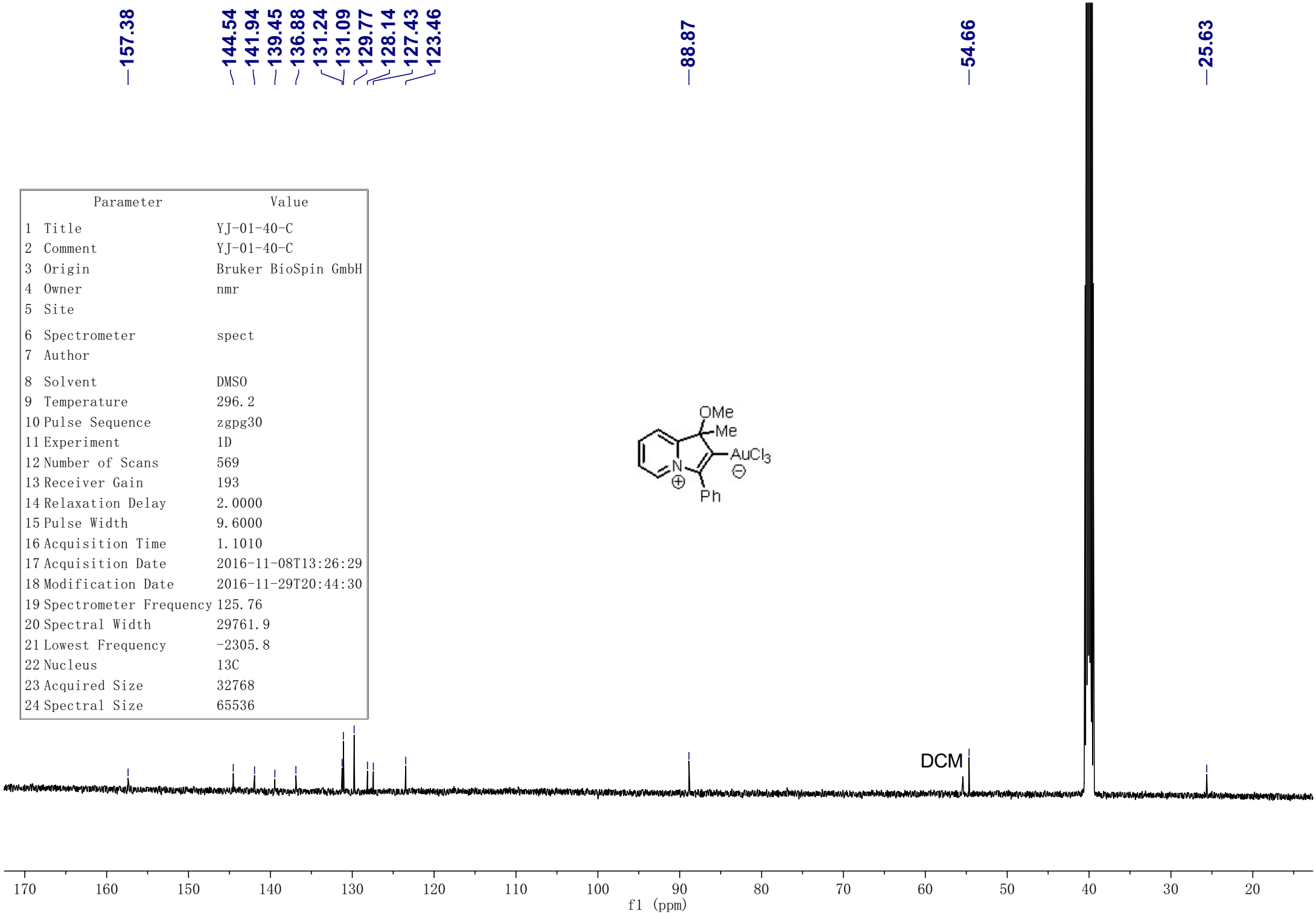




Parameter	Value
1 Title	YJ-01-89-13C
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	400
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2017-11-08T13:30:28
18 Modification Date	2017-11-08T14:24:48
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

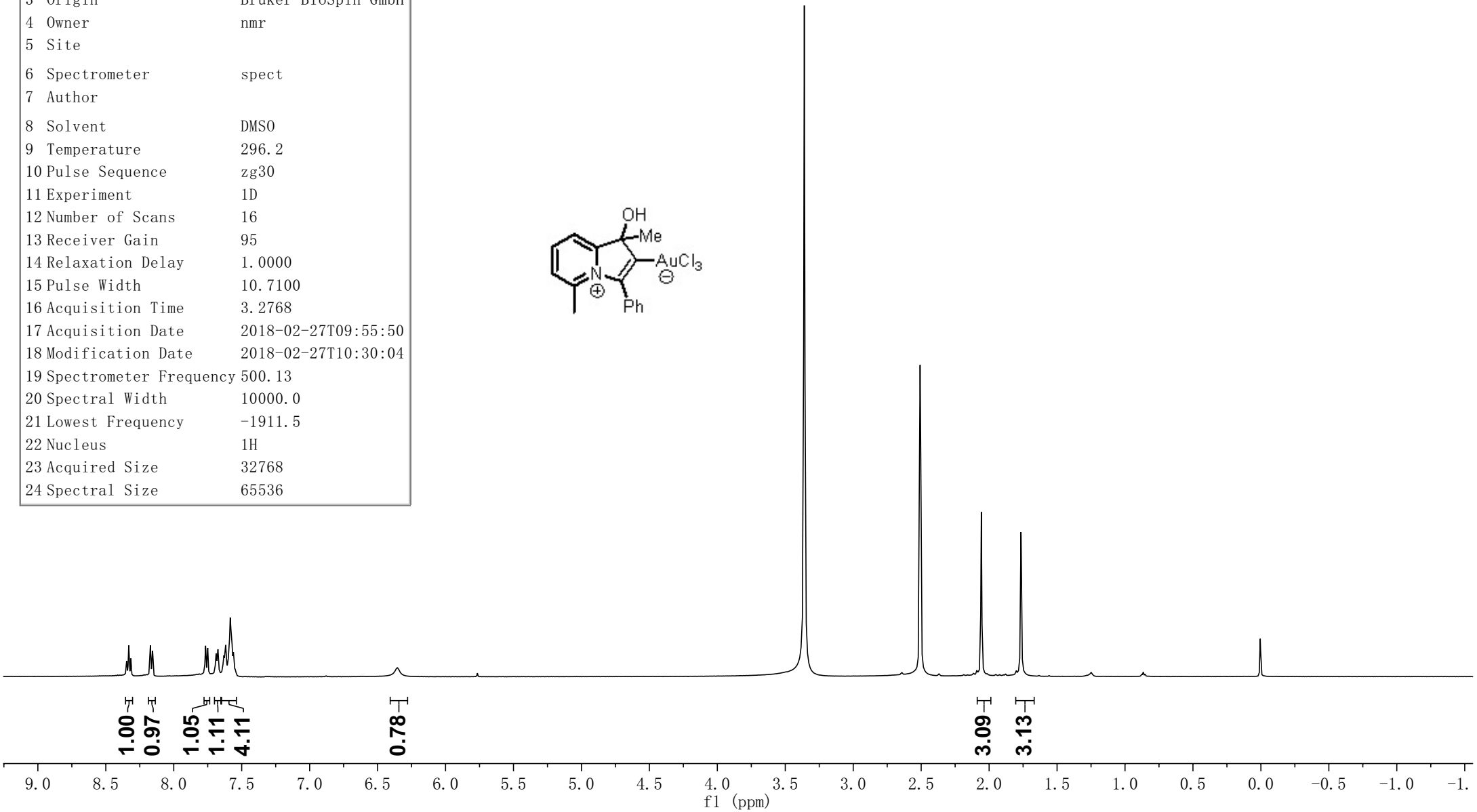
Parameter	Value
1 Title	YJ-01-40-1
2 Comment	YJ-01-40-1
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	295.0
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Receiver Gain	155
14 Relaxation Delay	1.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.9999
17 Acquisition Date	2016-11-08T13:08:31
18 Modification Date	2017-07-25T19:59:27
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	16025
24 Spectral Size	32768

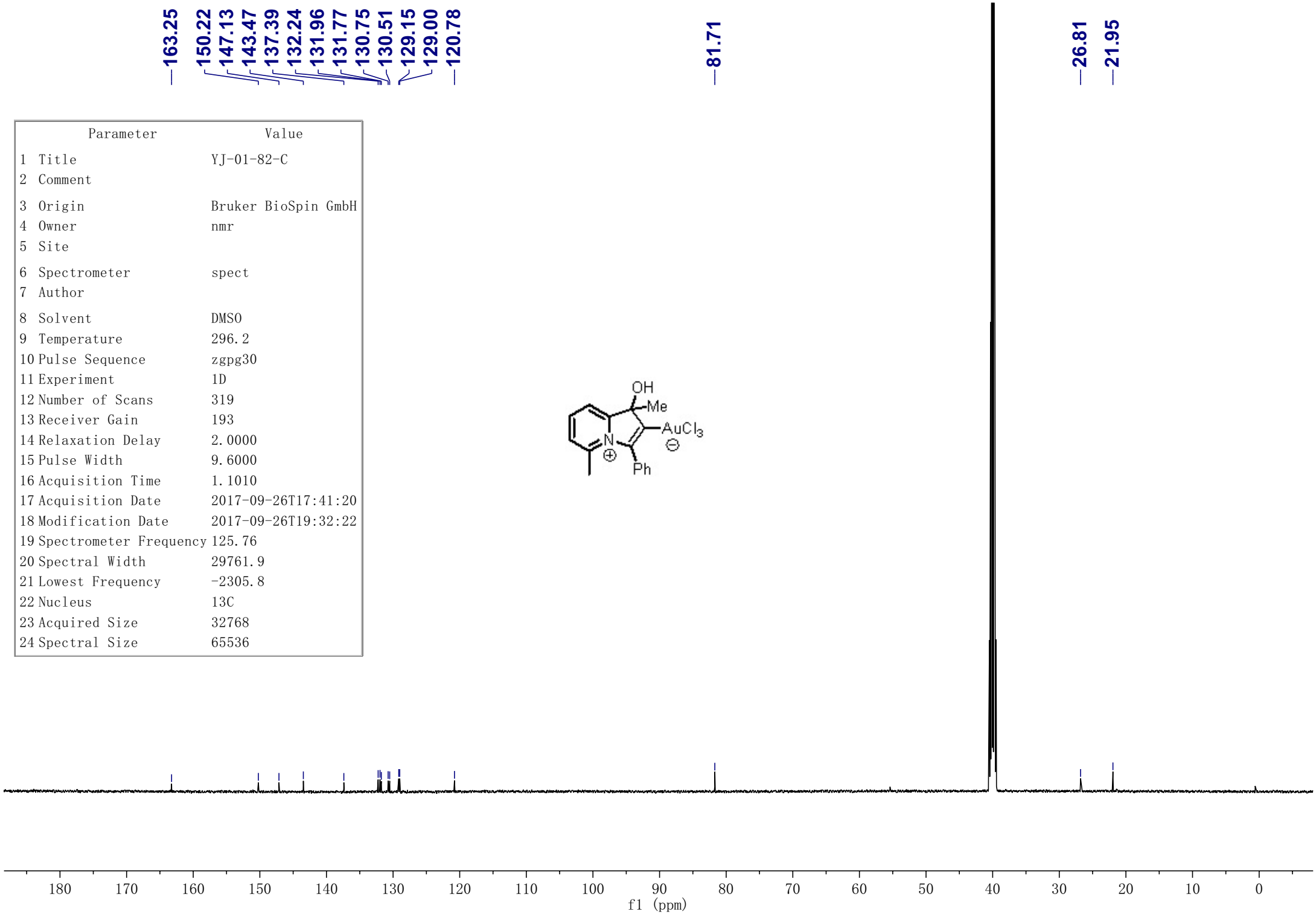




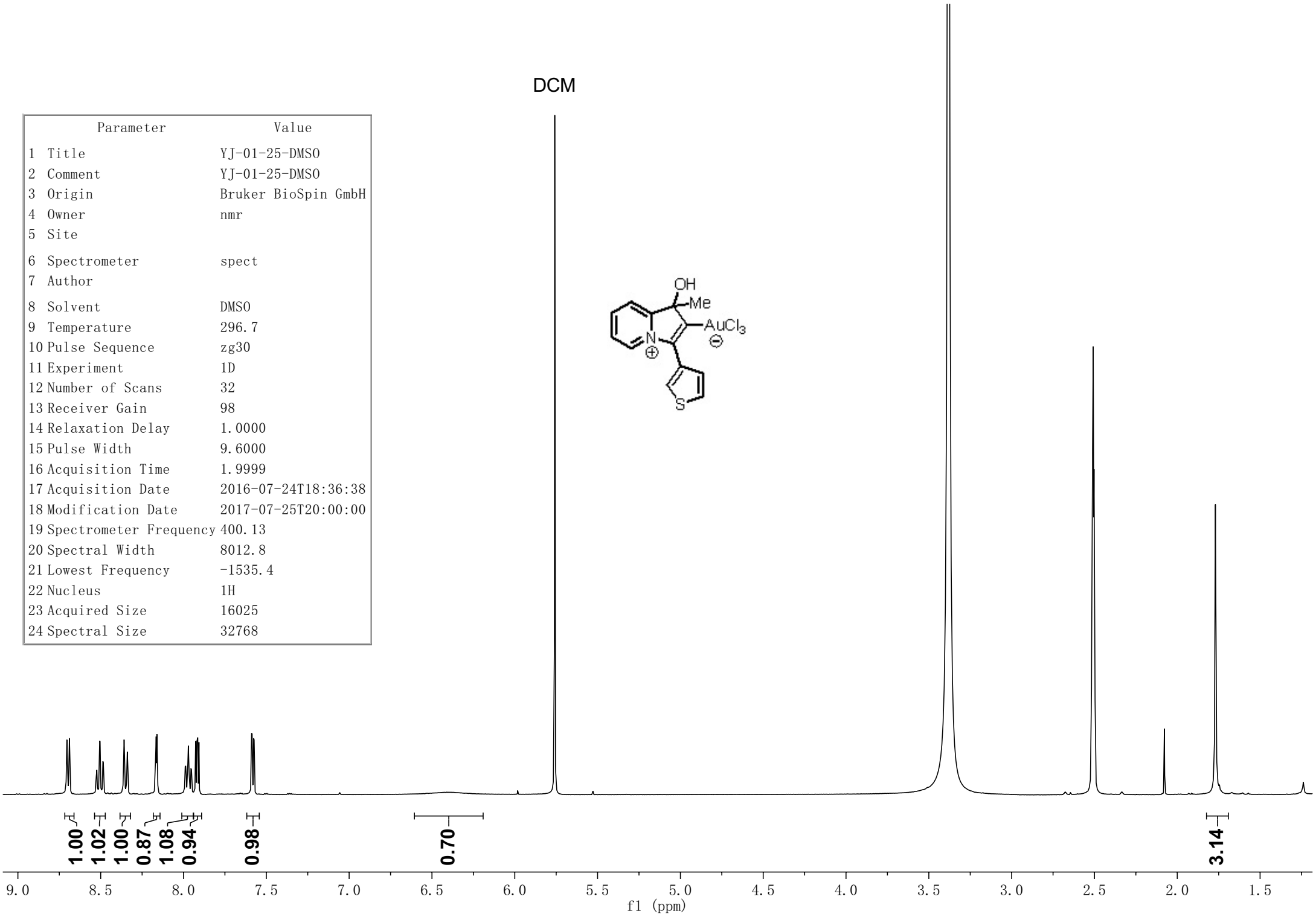
Parameter	Value
1 Title	YJ-01-40-C
2 Comment	YJ-01-40-C
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	569
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2016-11-08T13:26:29
18 Modification Date	2016-11-29T20:44:30
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Parameter	Value
1 Title	YJ-01-82-DMSO
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.2
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Receiver Gain	95
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-02-27T09:55:50
18 Modification Date	2018-02-27T10:30:04
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

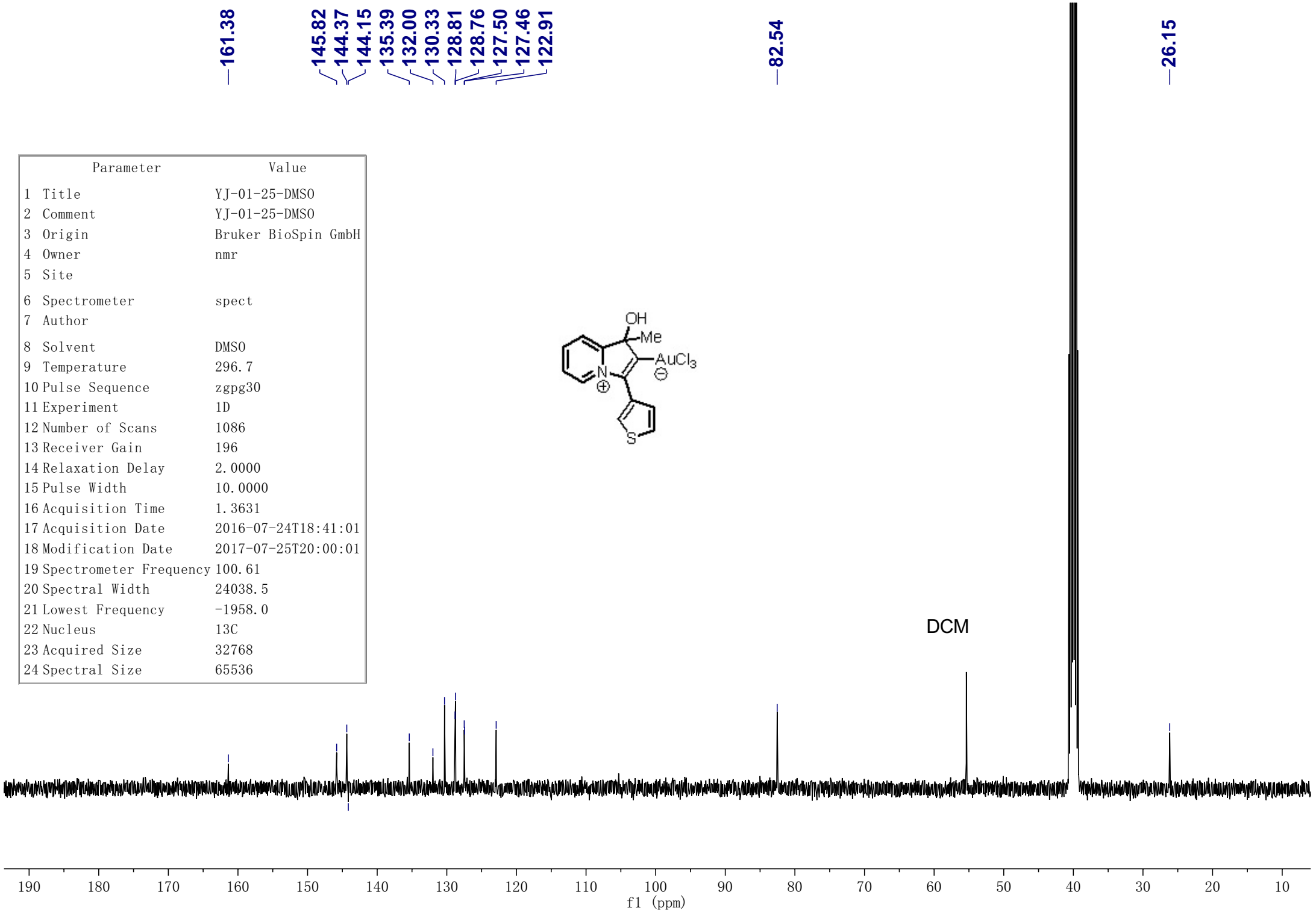




Parameter	Value
1 Title	YJ-01-82-C
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	319
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2017-09-26T17:41:20
18 Modification Date	2017-09-26T19:32:22
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

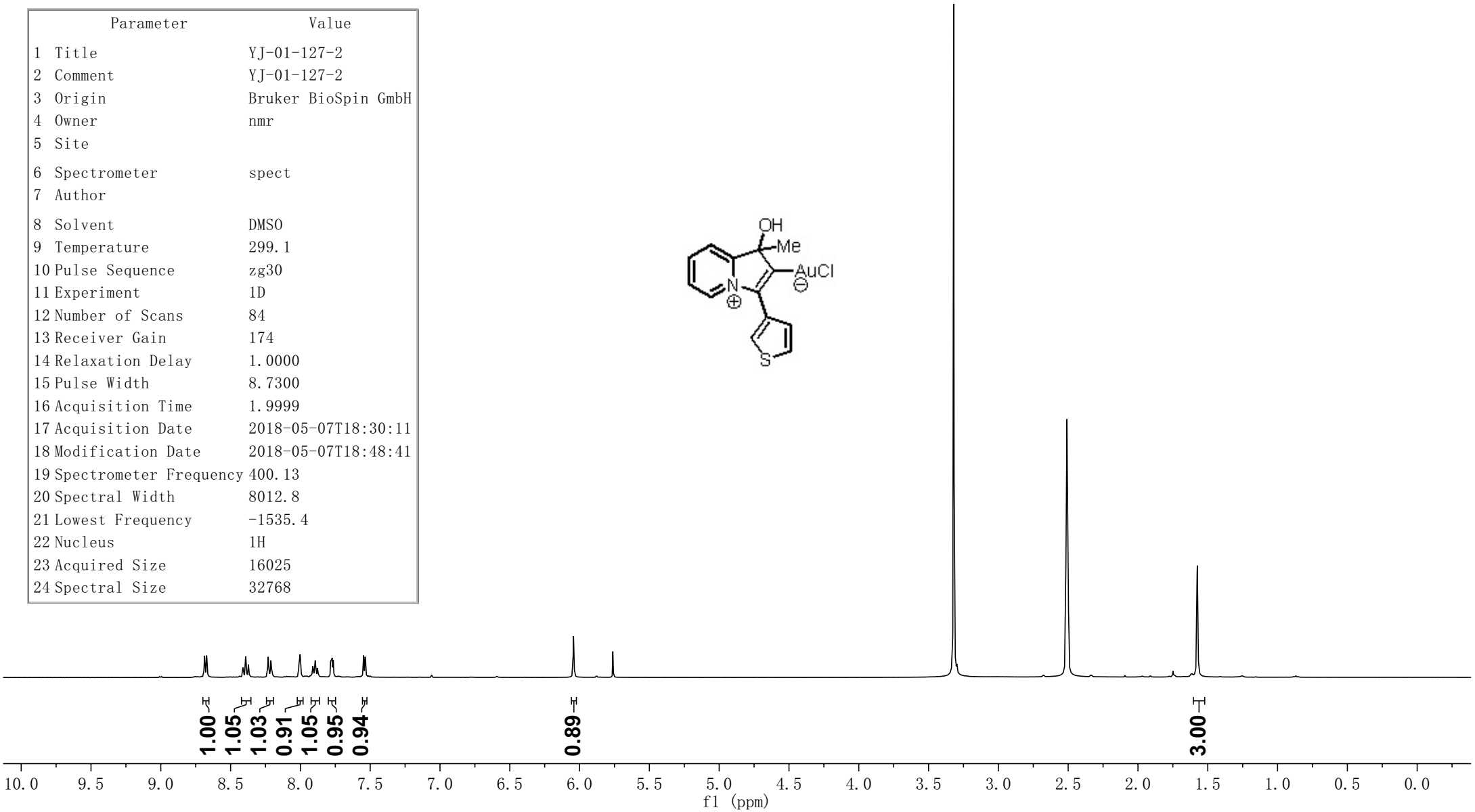


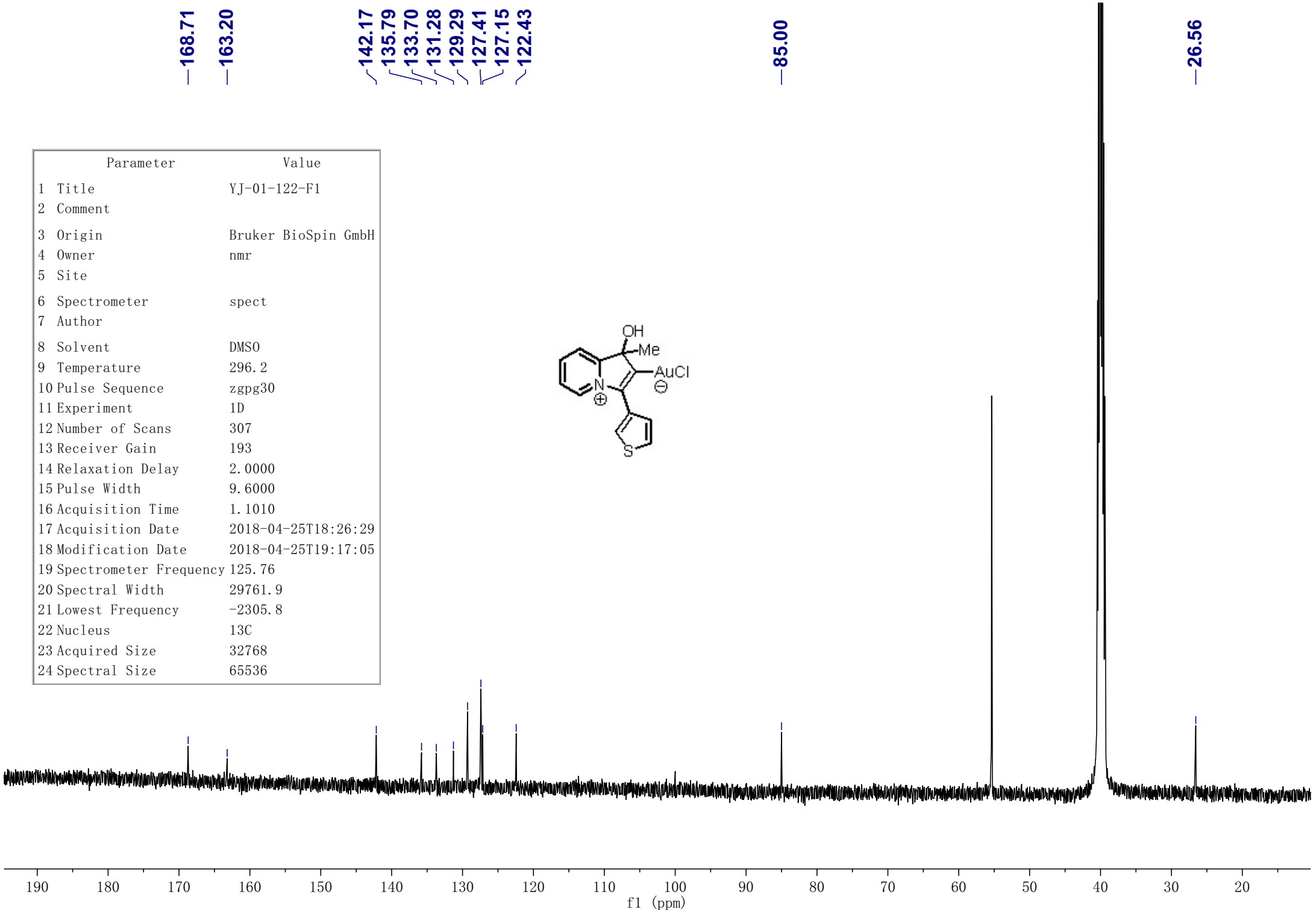
Parameter	Value
1 Title	YJ-01-25-DMSO
2 Comment	YJ-01-25-DMSO
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.7
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	32
13 Receiver Gain	98
14 Relaxation Delay	1.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.9999
17 Acquisition Date	2016-07-24T18:36:38
18 Modification Date	2017-07-25T20:00:00
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	16025
24 Spectral Size	32768



Parameter	Value
1 Title	YJ-01-25-DMSO
2 Comment	YJ-01-25-DMSO
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.7
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	1086
13 Receiver Gain	196
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.3631
17 Acquisition Date	2016-07-24T18:41:01
18 Modification Date	2017-07-25T20:00:01
19 Spectrometer Frequency	100.61
20 Spectral Width	24038.5
21 Lowest Frequency	-1958.0
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

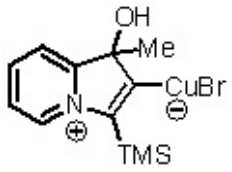
Parameter	Value
1 Title	YJ-01-127-2
2 Comment	YJ-01-127-2
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	299.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	84
13 Receiver Gain	174
14 Relaxation Delay	1.0000
15 Pulse Width	8.7300
16 Acquisition Time	1.9999
17 Acquisition Date	2018-05-07T18:30:11
18 Modification Date	2018-05-07T18:48:41
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.4
22 Nucleus	1H
23 Acquired Size	16025
24 Spectral Size	32768

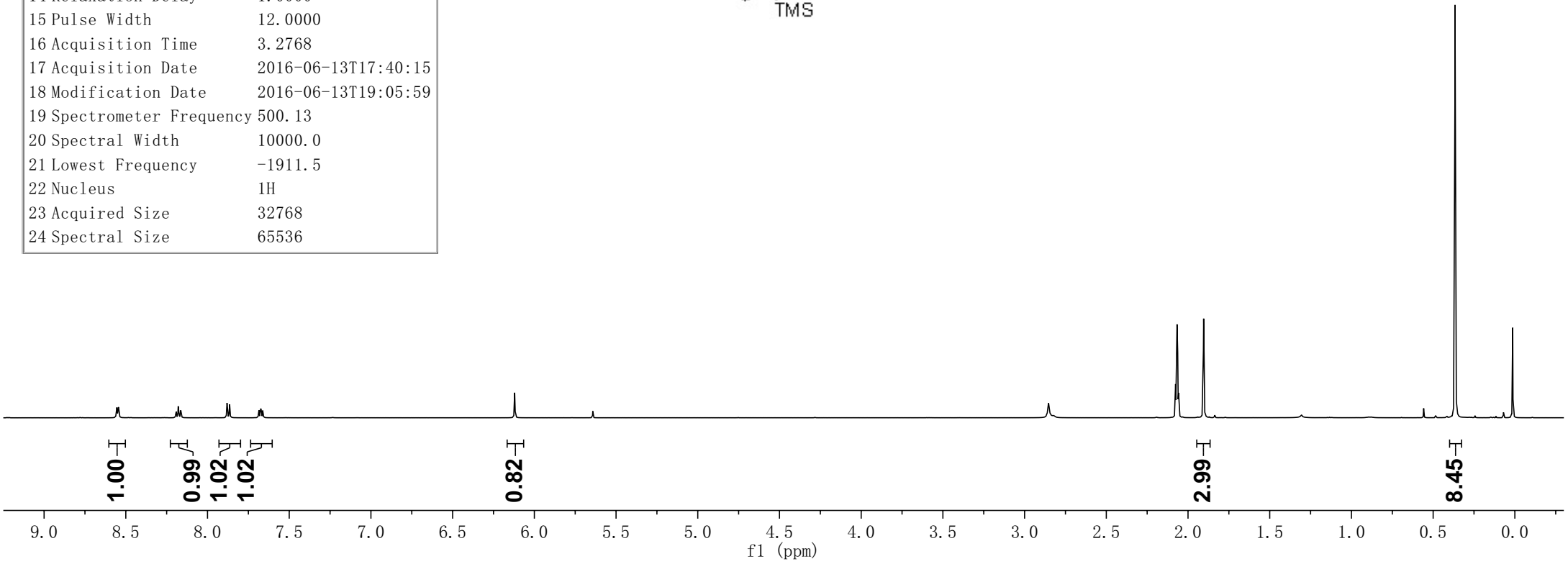


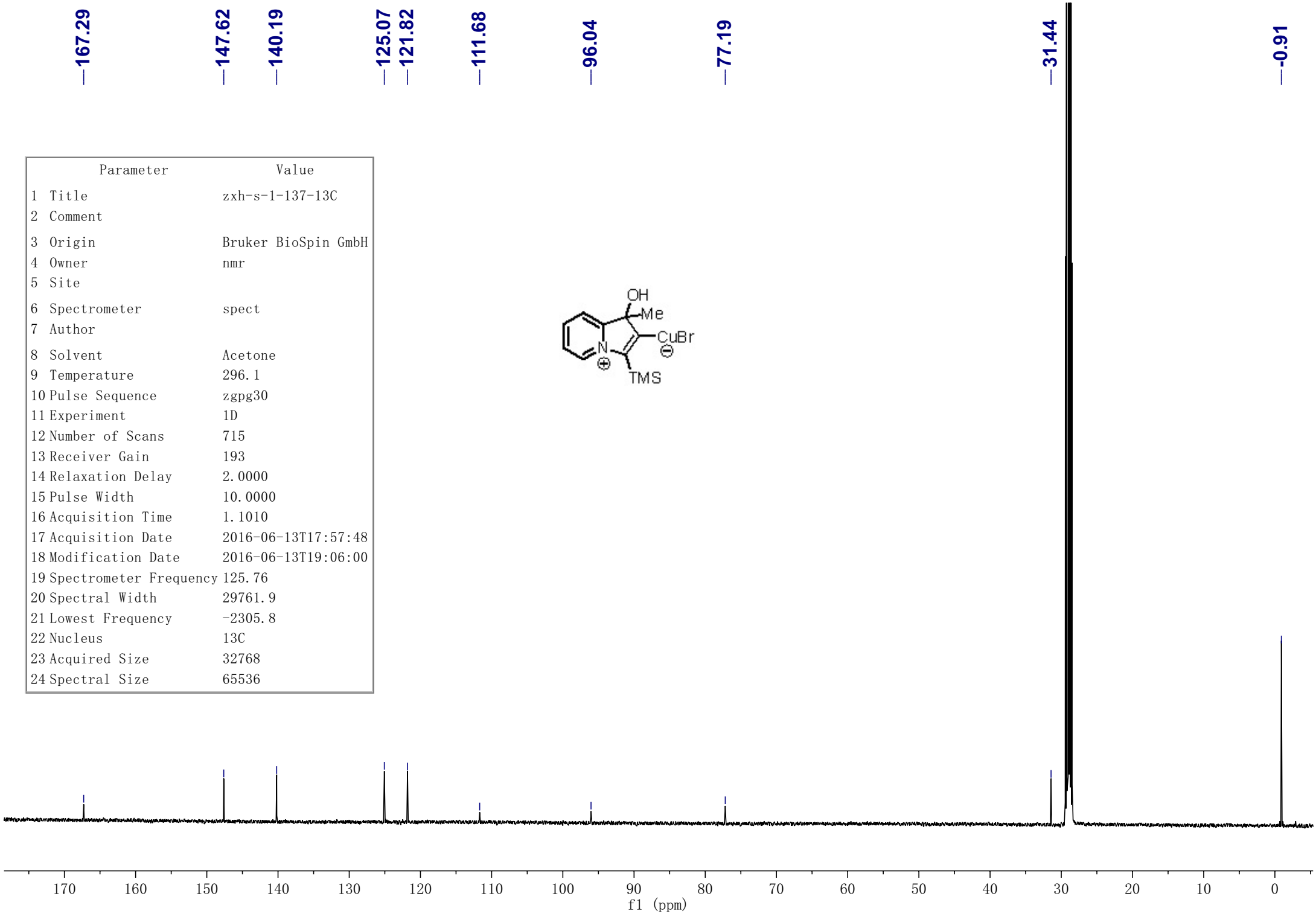


Parameter	Value
1 Title	YJ-01-122-F1
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	307
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-04-25T18:26:29
18 Modification Date	2018-04-25T19:17:05
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Parameter	Value
1 Title	zxh-s-1-137-H
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Receiver Gain	125
14 Relaxation Delay	1.0000
15 Pulse Width	12.0000
16 Acquisition Time	3.2768
17 Acquisition Date	2016-06-13T17:40:15
18 Modification Date	2016-06-13T19:05:59
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

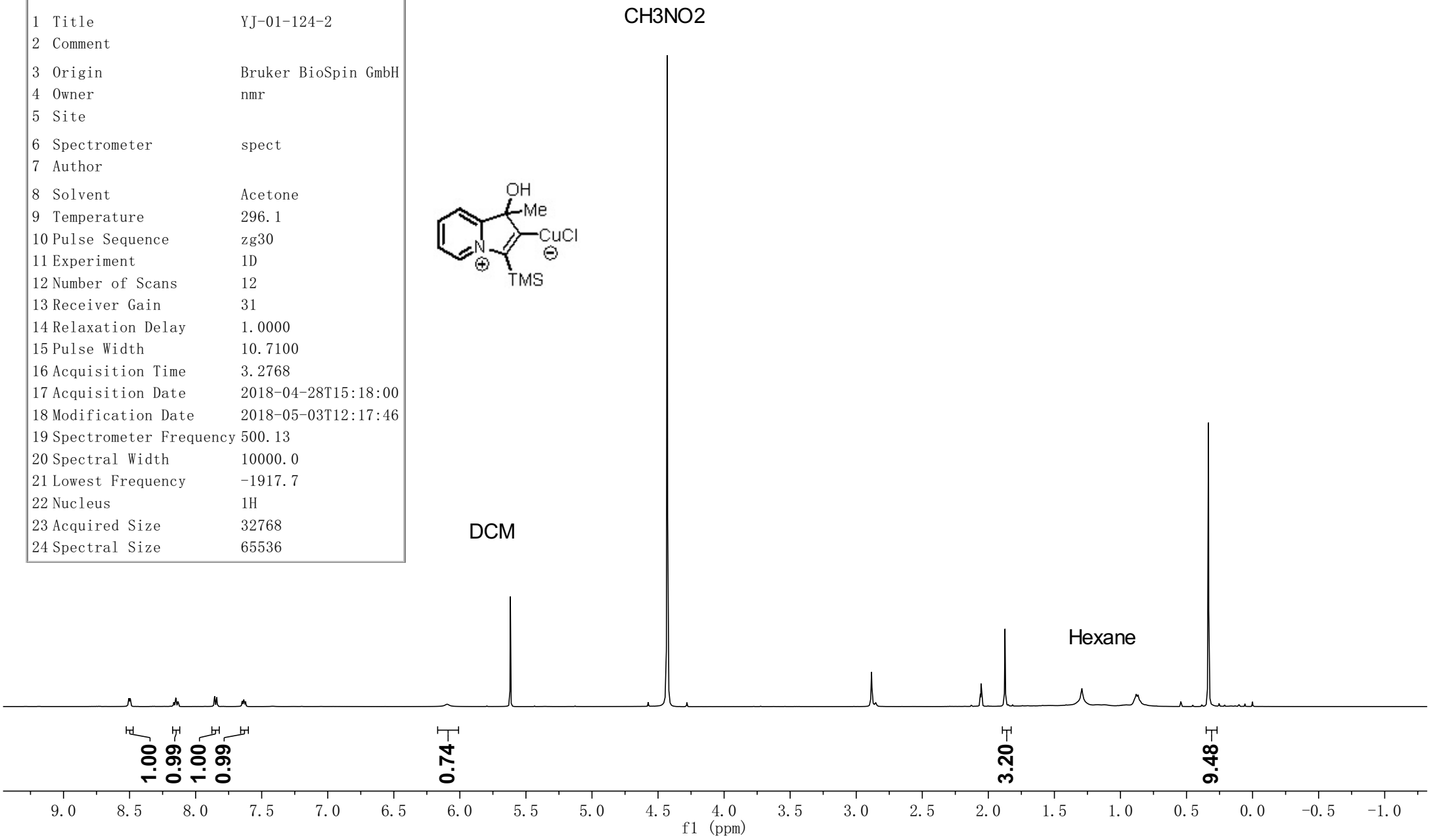


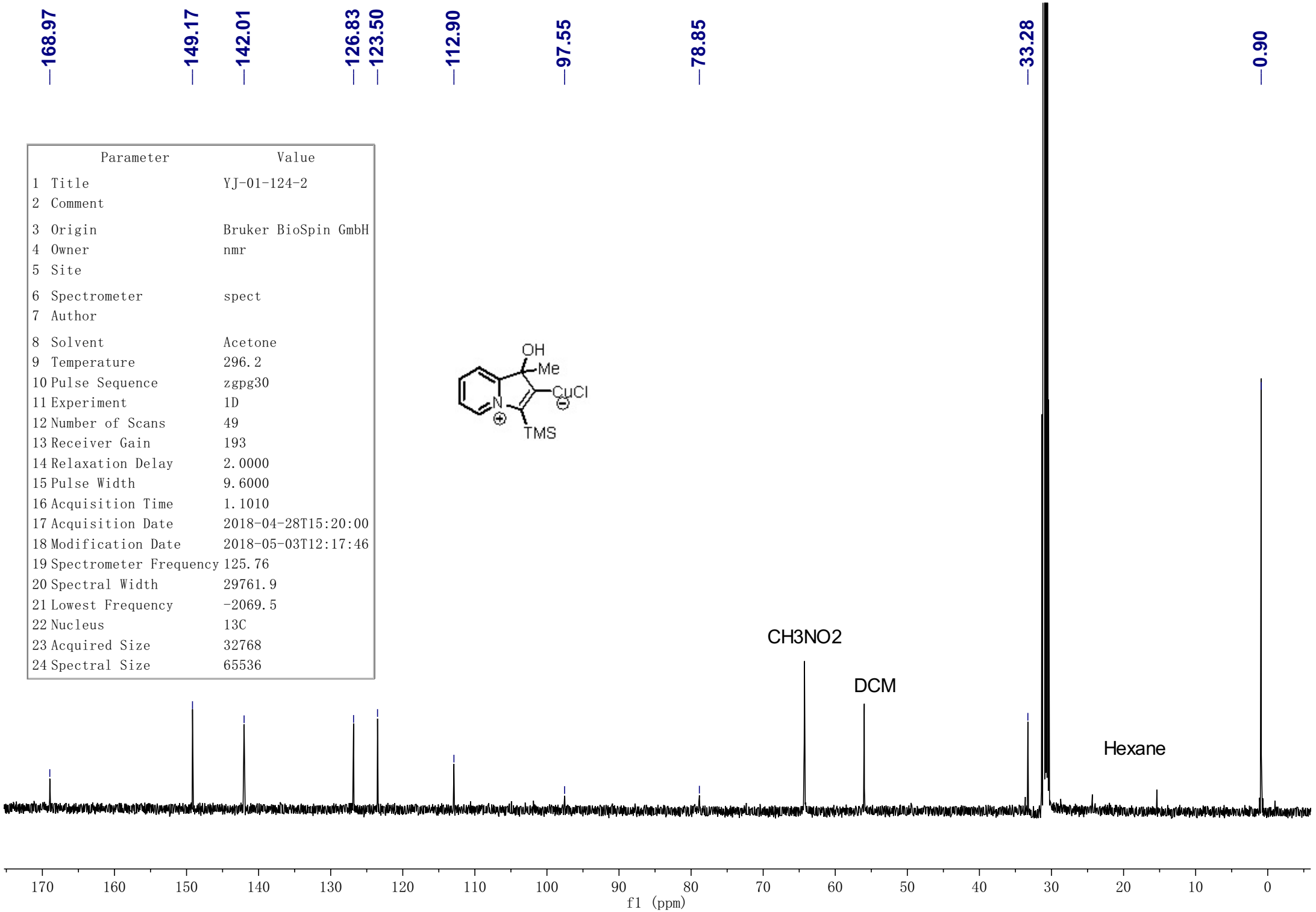




Parameter	Value
1 Title	zxh-s-1-137-13C
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	715
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.1010
17 Acquisition Date	2016-06-13T17:57:48
18 Modification Date	2016-06-13T19:06:00
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

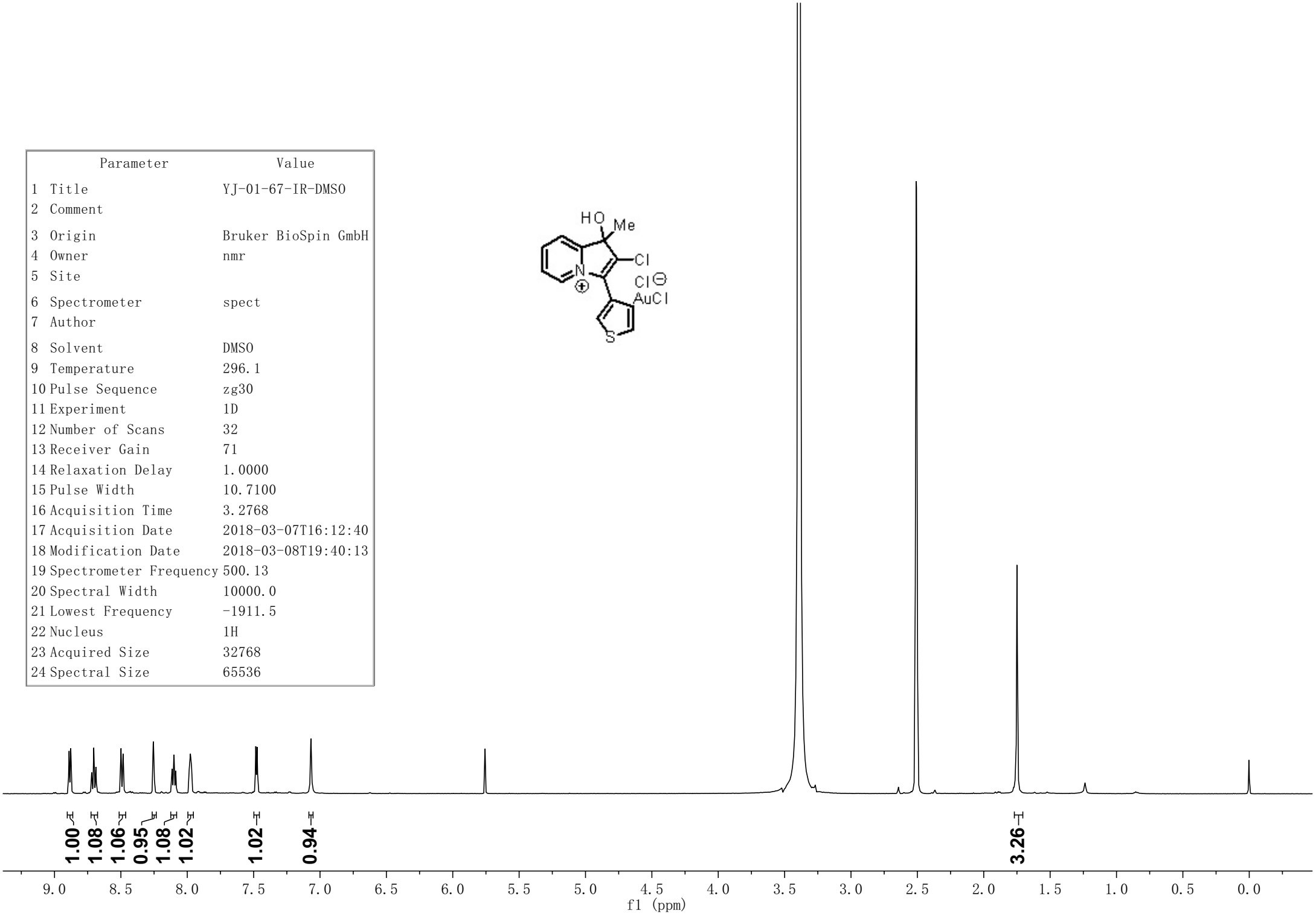
Parameter	Value
1 Title	YJ-01-124-2
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	12
13 Receiver Gain	31
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-04-28T15:18:00
18 Modification Date	2018-05-03T12:17:46
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1917.7
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

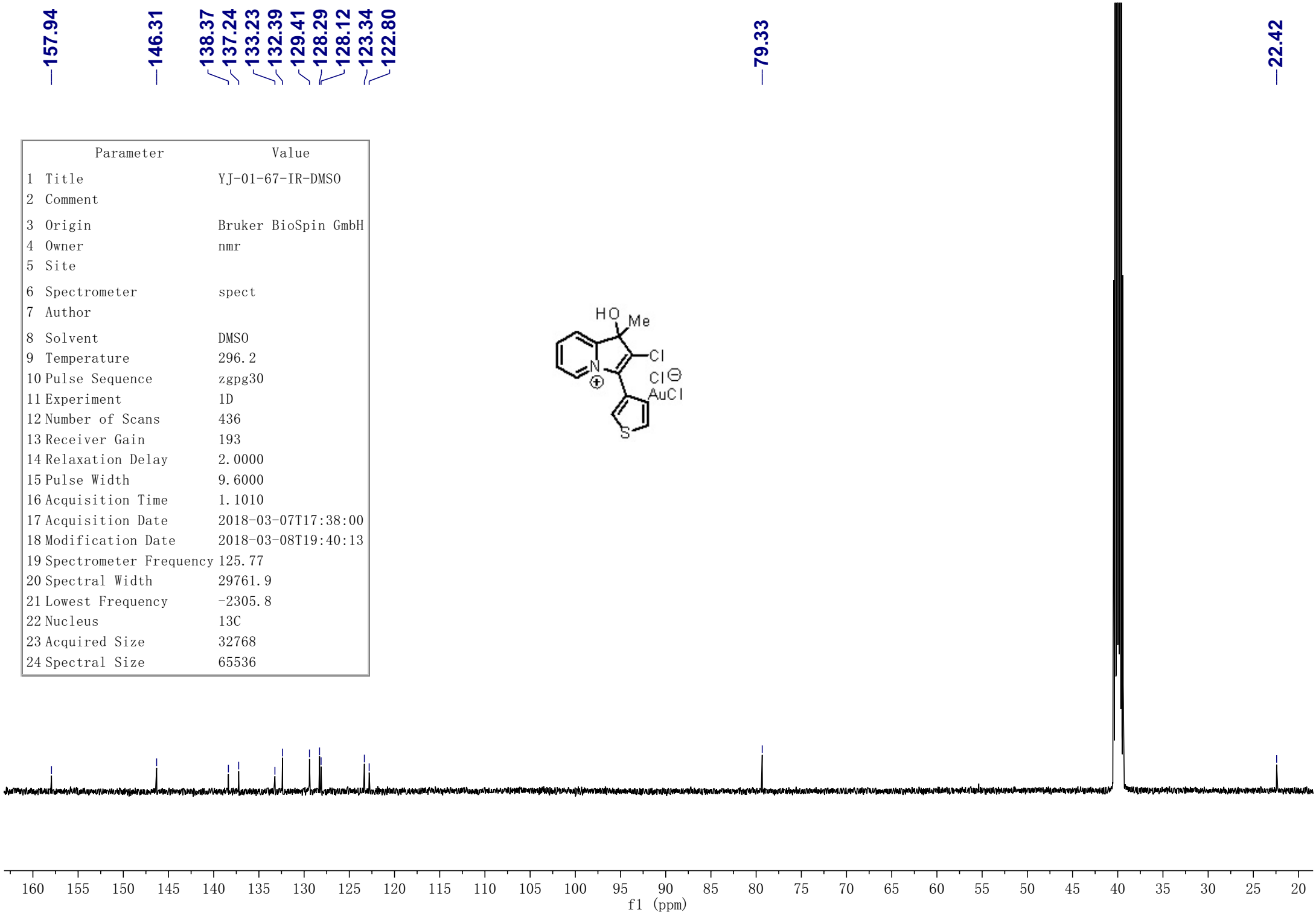




Parameter	Value
1 Title	YJ-01-124-2
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	49
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-04-28T15:20:00
18 Modification Date	2018-05-03T12:17:46
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2069.5
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

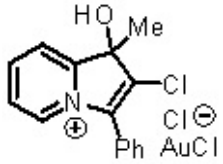
Parameter	Value
1 Title	YJ-01-67-IR-DMSO
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	32
13 Receiver Gain	71
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-03-07T16:12:40
18 Modification Date	2018-03-08T19:40:13
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

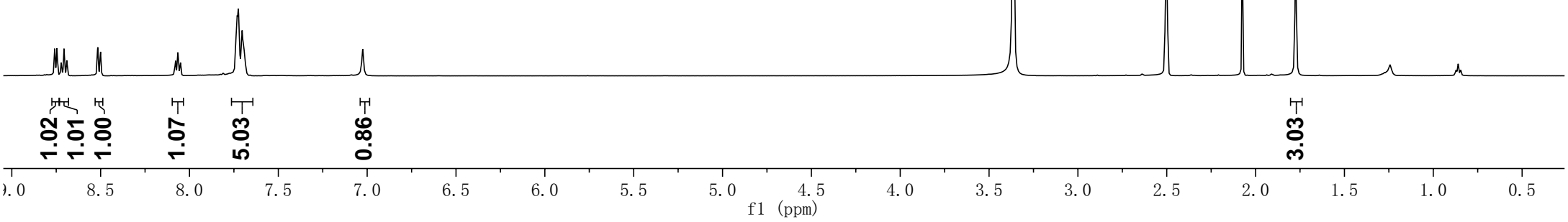


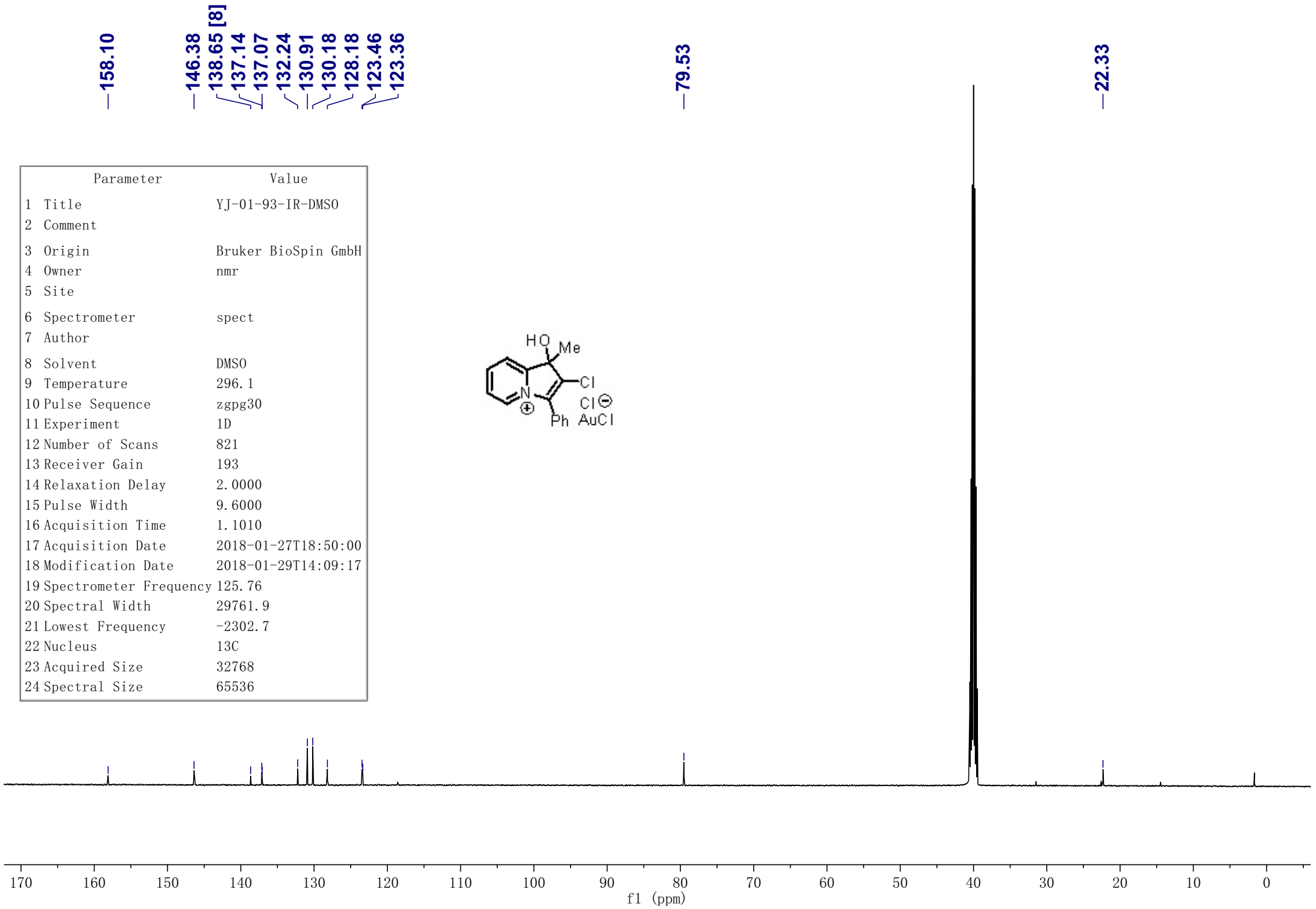


Parameter	Value
1 Title	YJ-01-67-IR-DMSO
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	436
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-03-07T17:38:00
18 Modification Date	2018-03-08T19:40:13
19 Spectrometer Frequency	125.77
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

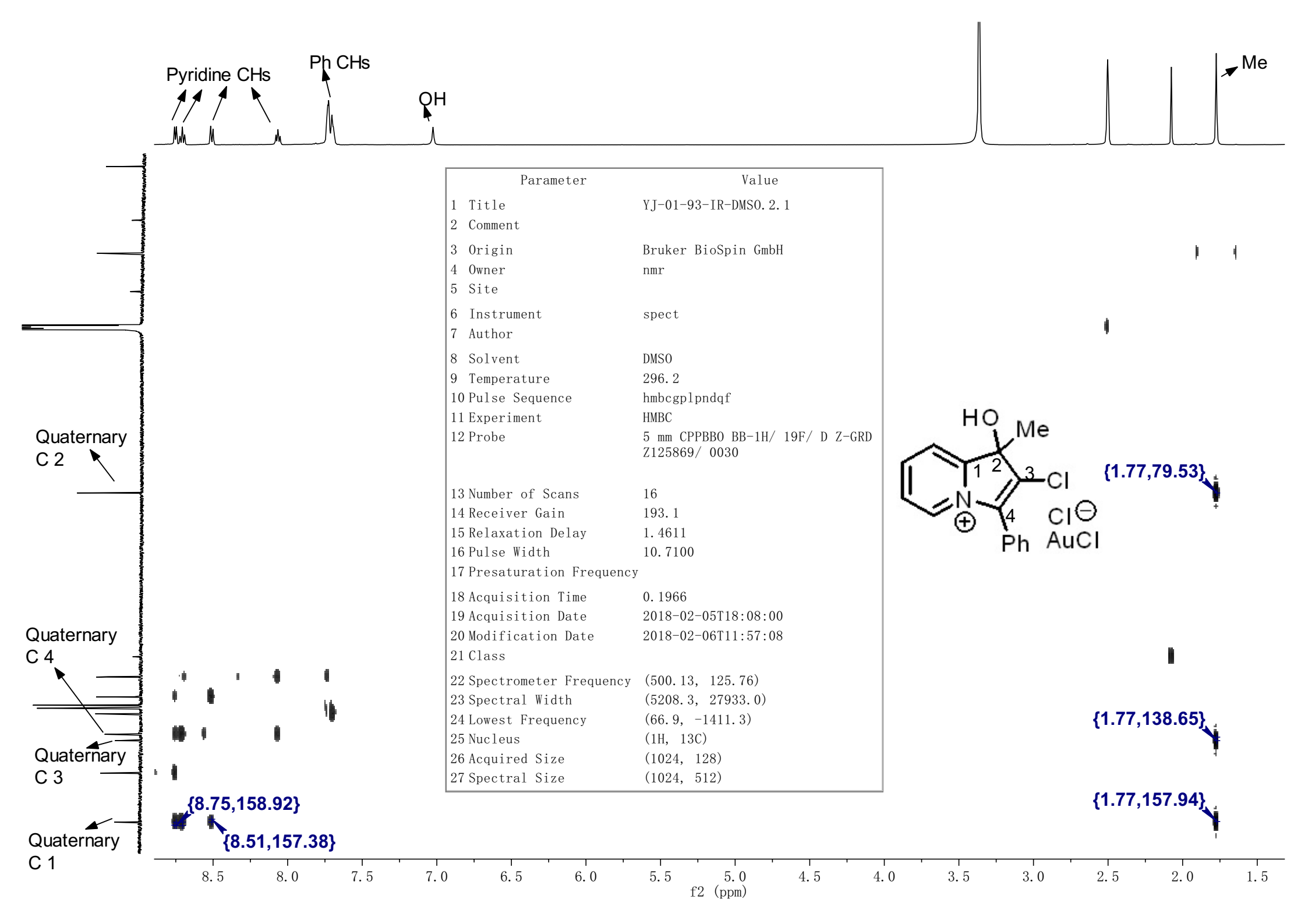
Parameter	Value
1 Title	YJ-01-93-IR-DMSO
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Receiver Gain	78
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-01-27T18:44:00
18 Modification Date	2018-01-29T14:09:16
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1914.6
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536





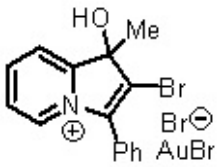


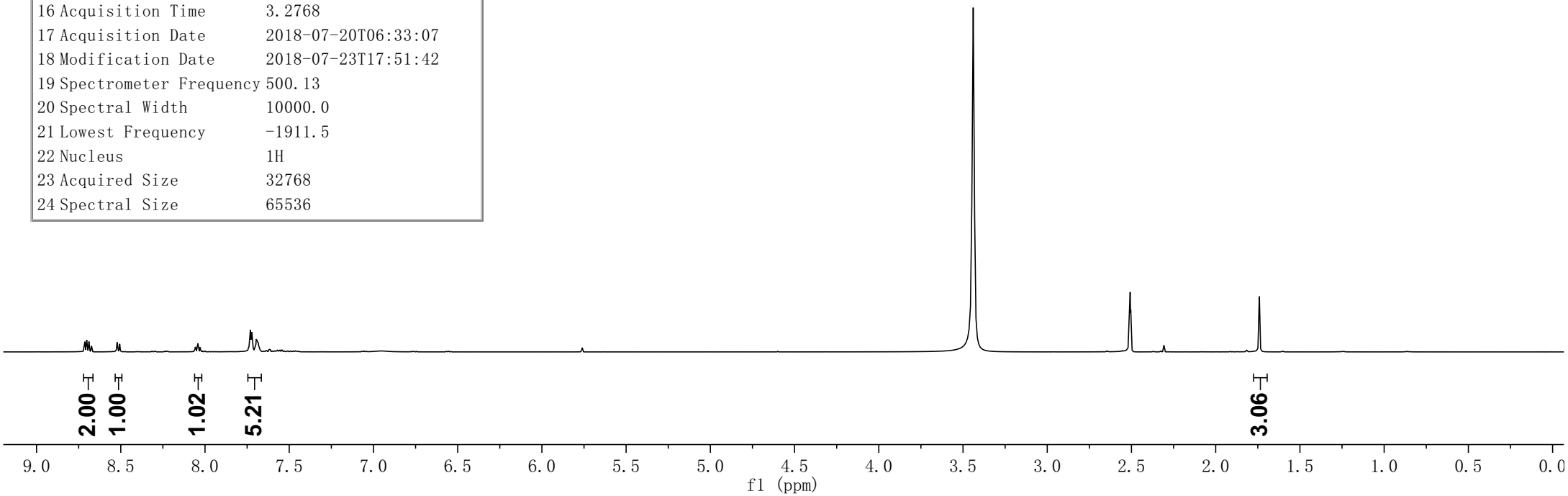
Parameter	Value
1 Title	YJ-01-93-IR-DMSO
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	821
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-01-27T18:50:00
18 Modification Date	2018-01-29T14:09:17
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2302.7
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

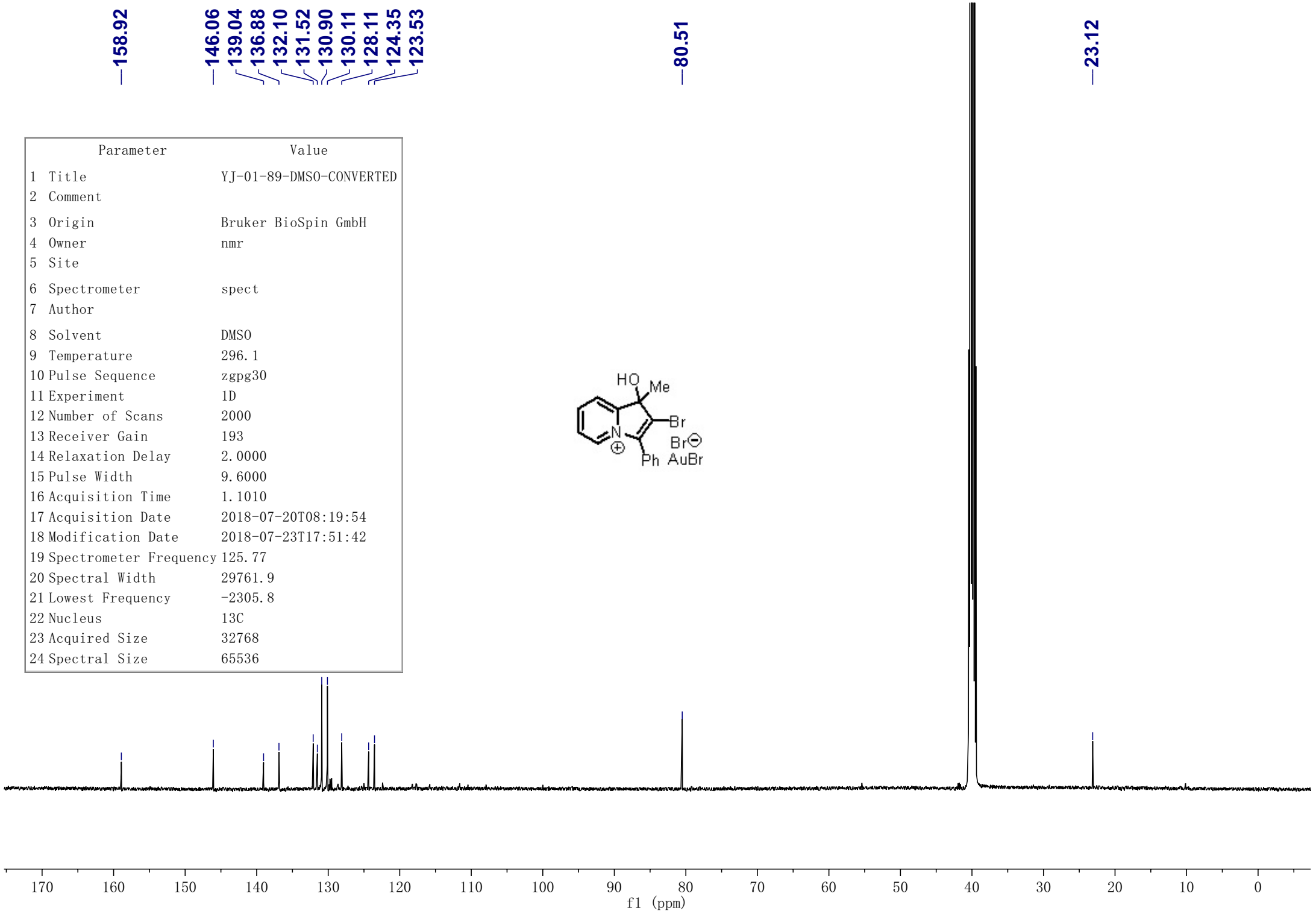


Parameter		Value
1	Title	YJ-01-93-IR-DMSO.2.1
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Instrument	spect
7	Author	
8	Solvent	DMSO
9	Temperature	296.2
10	Pulse Sequence	hmbcgplpndqf
11	Experiment	HMBC
12	Probe	5 mm CPPBBO BB-1H/ 19F/ D Z-GRD Z125869/ 0030
13	Number of Scans	16
14	Receiver Gain	193.1
15	Relaxation Delay	1.4611
16	Pulse Width	10.7100
17	Presaturation Frequency	
18	Acquisition Time	0.1966
19	Acquisition Date	2018-02-05T18:08:00
20	Modification Date	2018-02-06T11:57:08
21	Class	
22	Spectrometer Frequency	(500.13, 125.76)
23	Spectral Width	(5208.3, 27933.0)
24	Lowest Frequency	(66.9, -1411.3)
25	Nucleus	(1H, 13C)
26	Acquired Size	(1024, 128)
27	Spectral Size	(1024, 512)

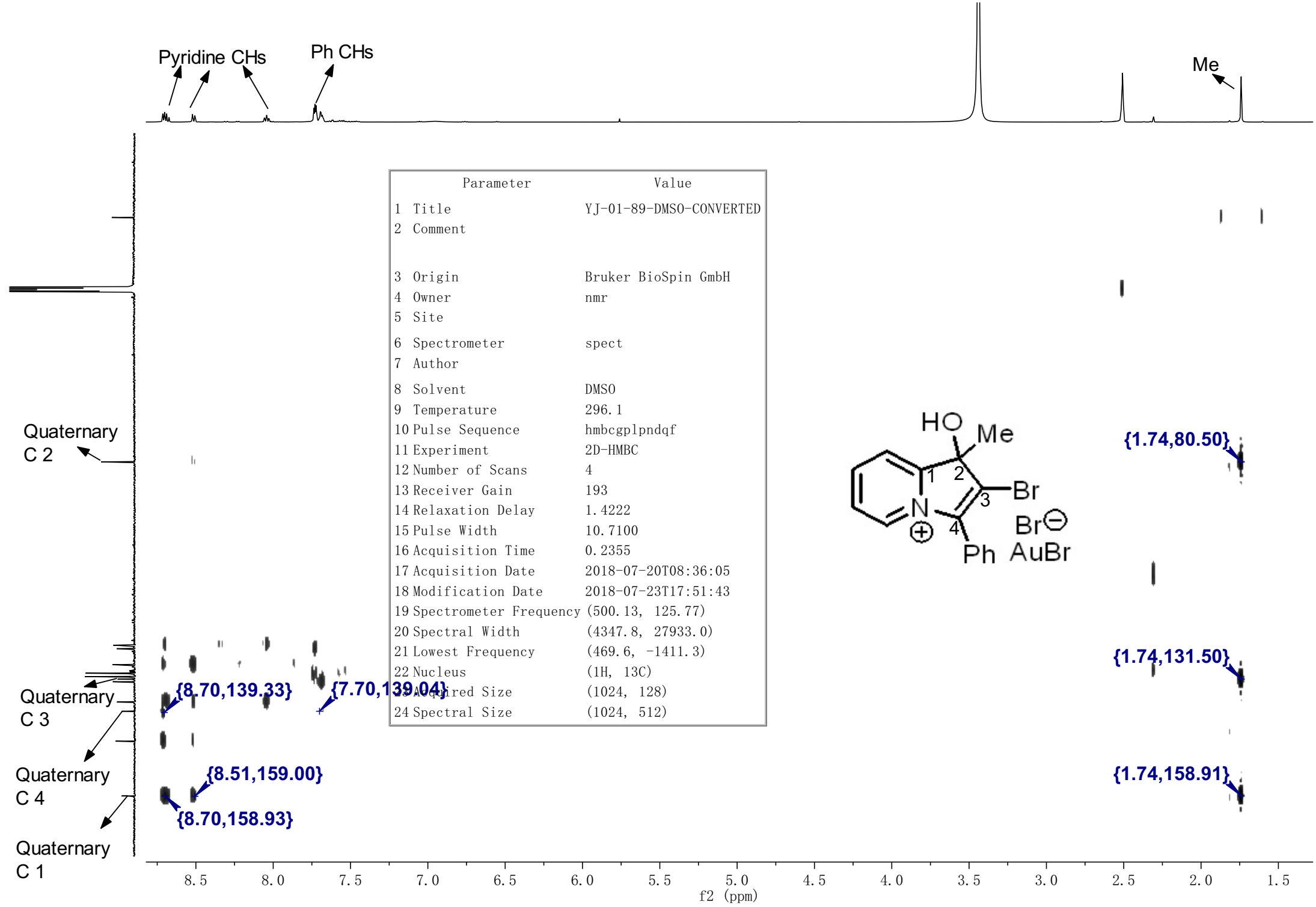
Parameter	Value
1 Title	YJ-01-89-DMSO-CONVERTED
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Receiver Gain	88
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-07-20T06:33:07
18 Modification Date	2018-07-23T17:51:42
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536





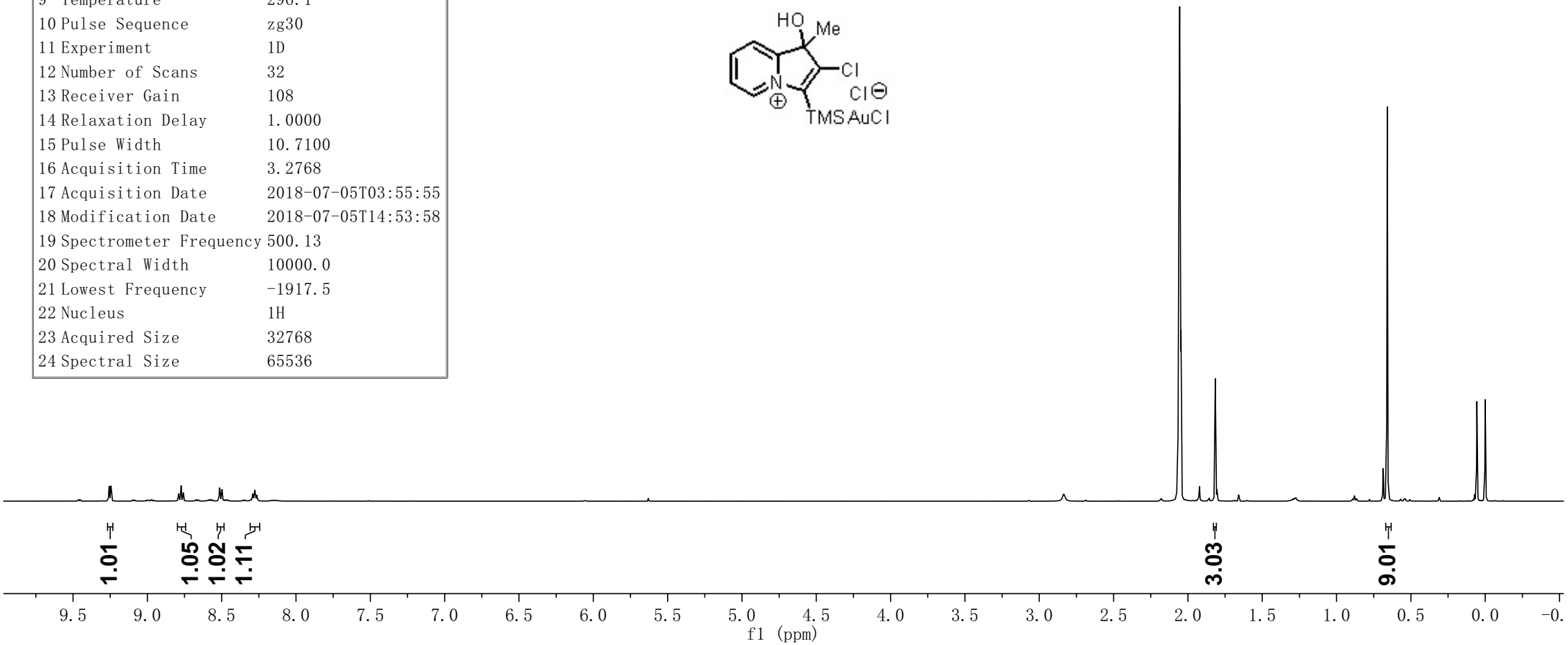


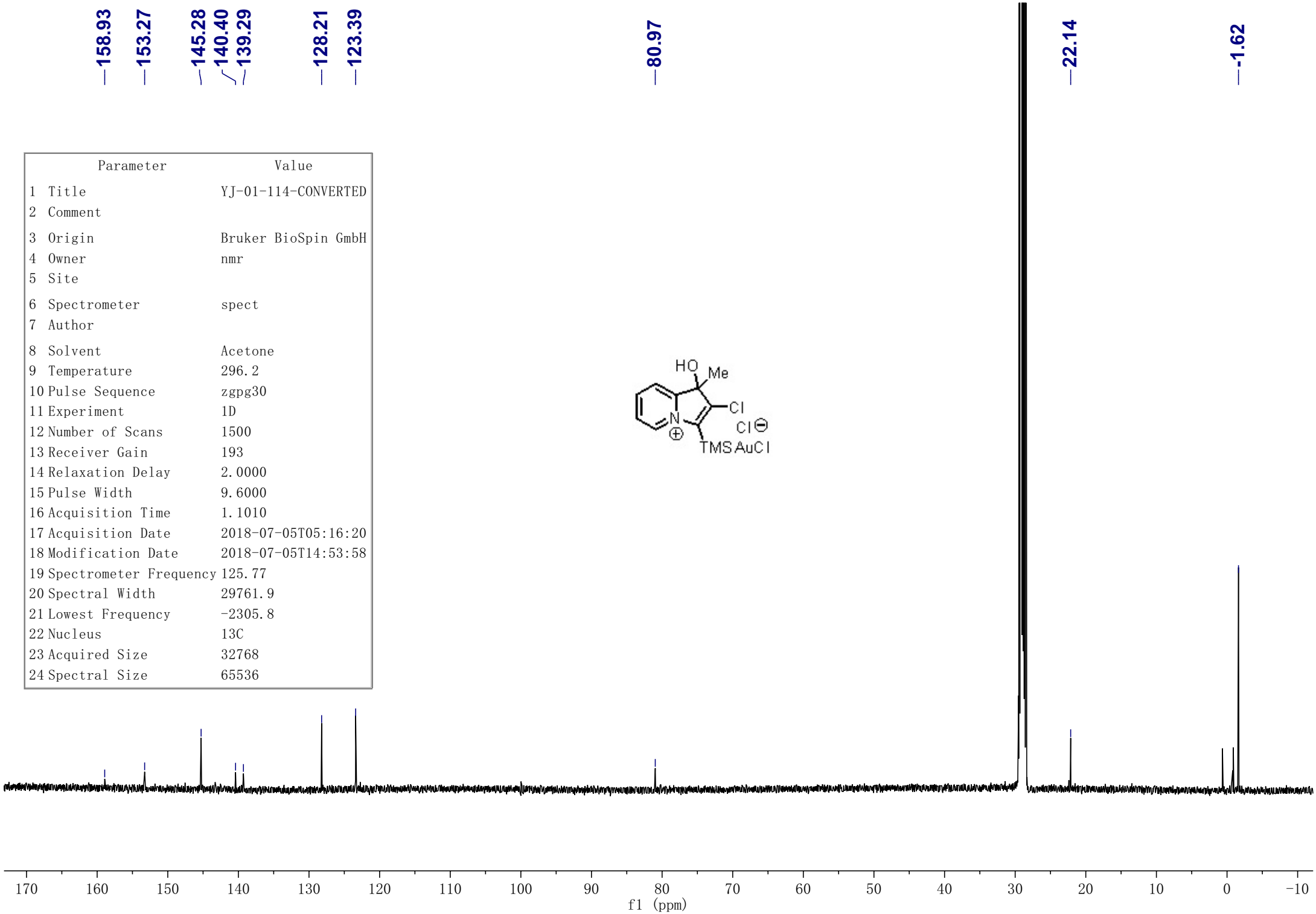
Parameter	Value
1 Title	YJ-01-89-DMSO-CONVERTED
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	2000
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-07-20T08:19:54
18 Modification Date	2018-07-23T17:51:42
19 Spectrometer Frequency	125.77
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536



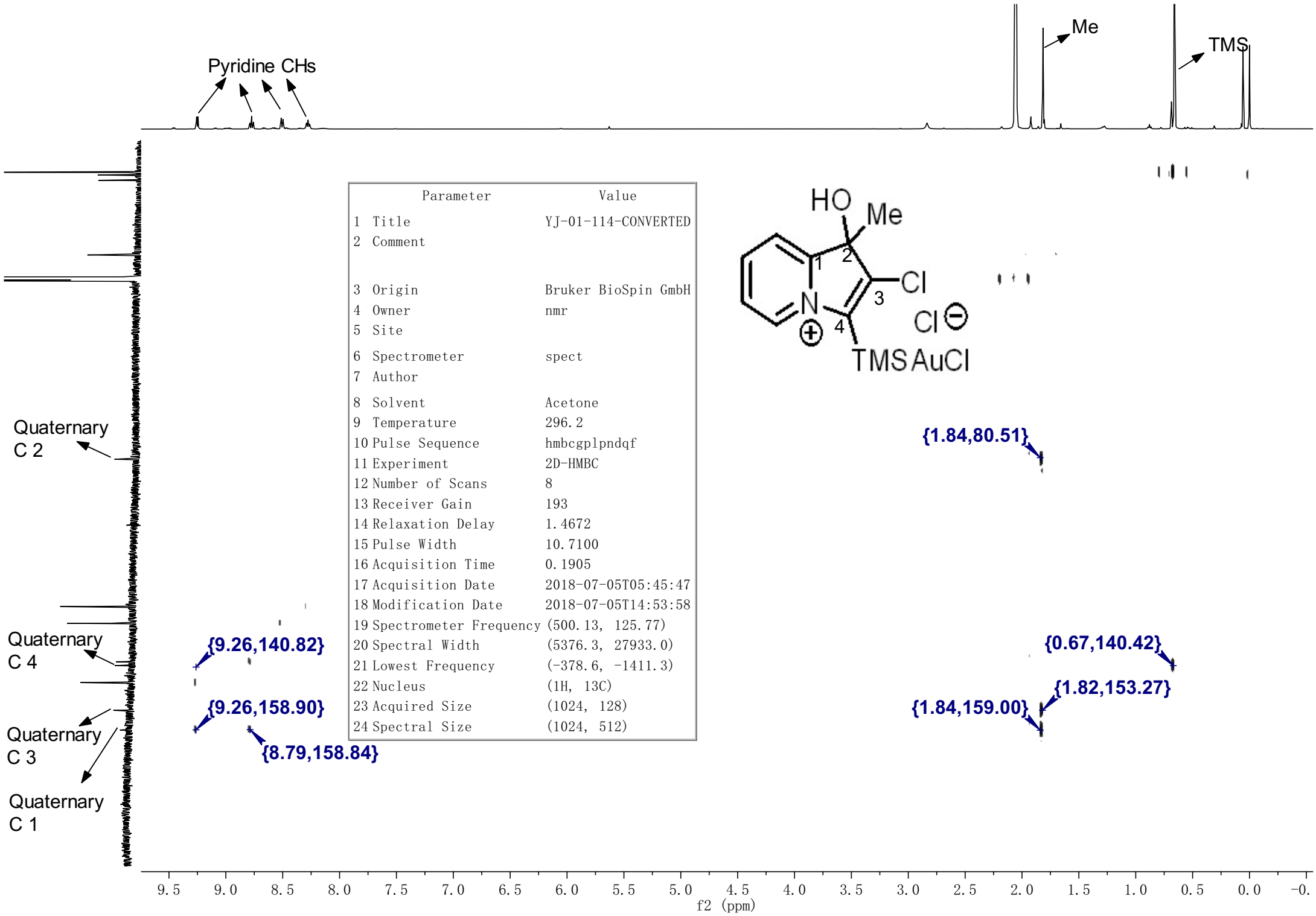
Parameter	Value
1 Title	YJ-01-89-DMSO-CONVERTED
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	hmbcgplpndqf
11 Experiment	2D-HMBC
12 Number of Scans	4
13 Receiver Gain	193
14 Relaxation Delay	1.4222
15 Pulse Width	10.7100
16 Acquisition Time	0.2355
17 Acquisition Date	2018-07-20T08:36:05
18 Modification Date	2018-07-23T17:51:43
19 Spectrometer Frequency	(500.13, 125.77)
20 Spectral Width	(4347.8, 27933.0)
21 Lowest Frequency	(469.6, -1411.3)
22 Nucleus	(1H, 13C)
23 Acquired Size	(1024, 128)
24 Spectral Size	(1024, 512)

Parameter	Value
1 Title	YJ-01-114-CONVERTED
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	32
13 Receiver Gain	108
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-07-05T03:55:55
18 Modification Date	2018-07-05T14:53:58
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1917.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



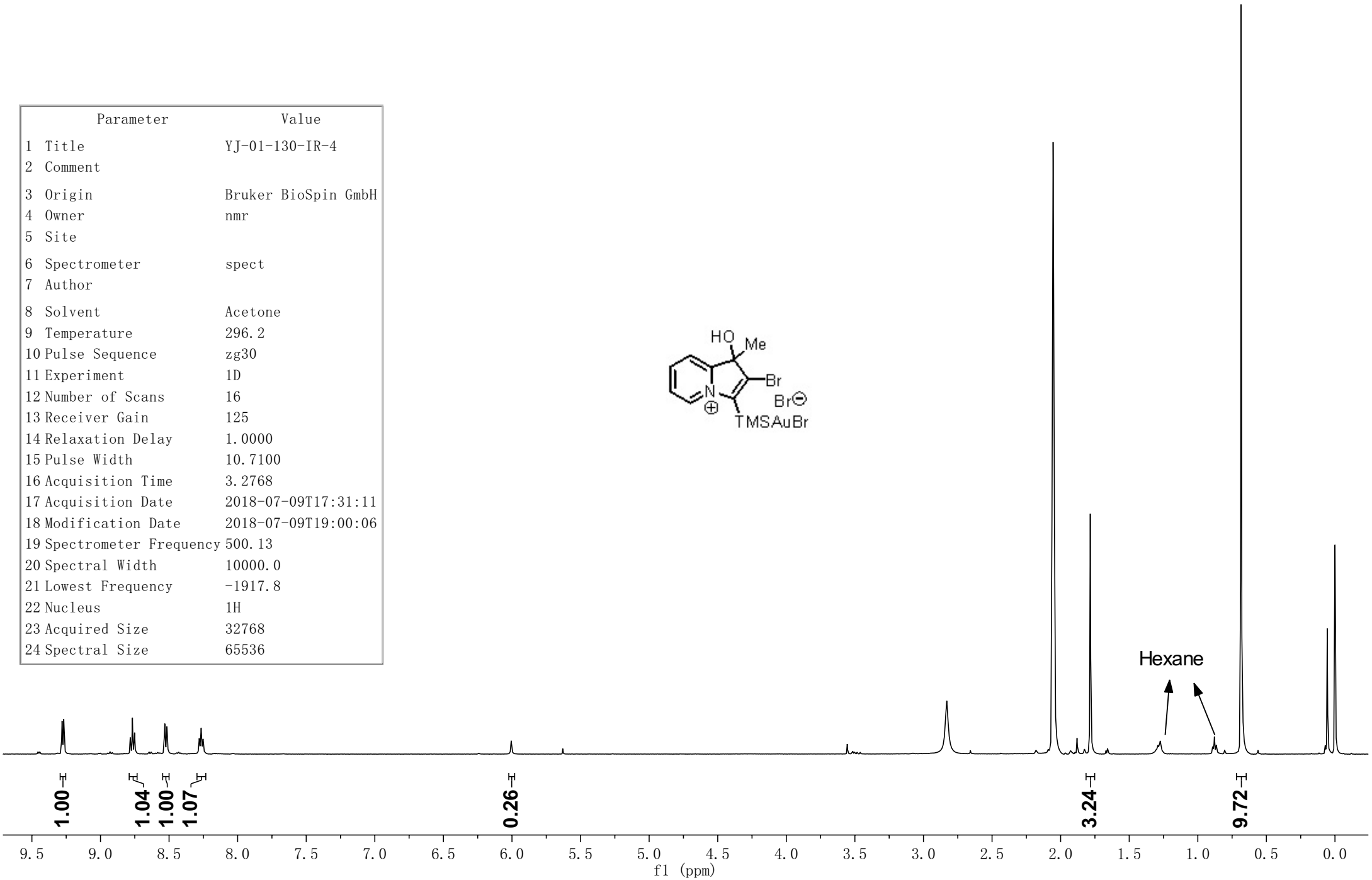


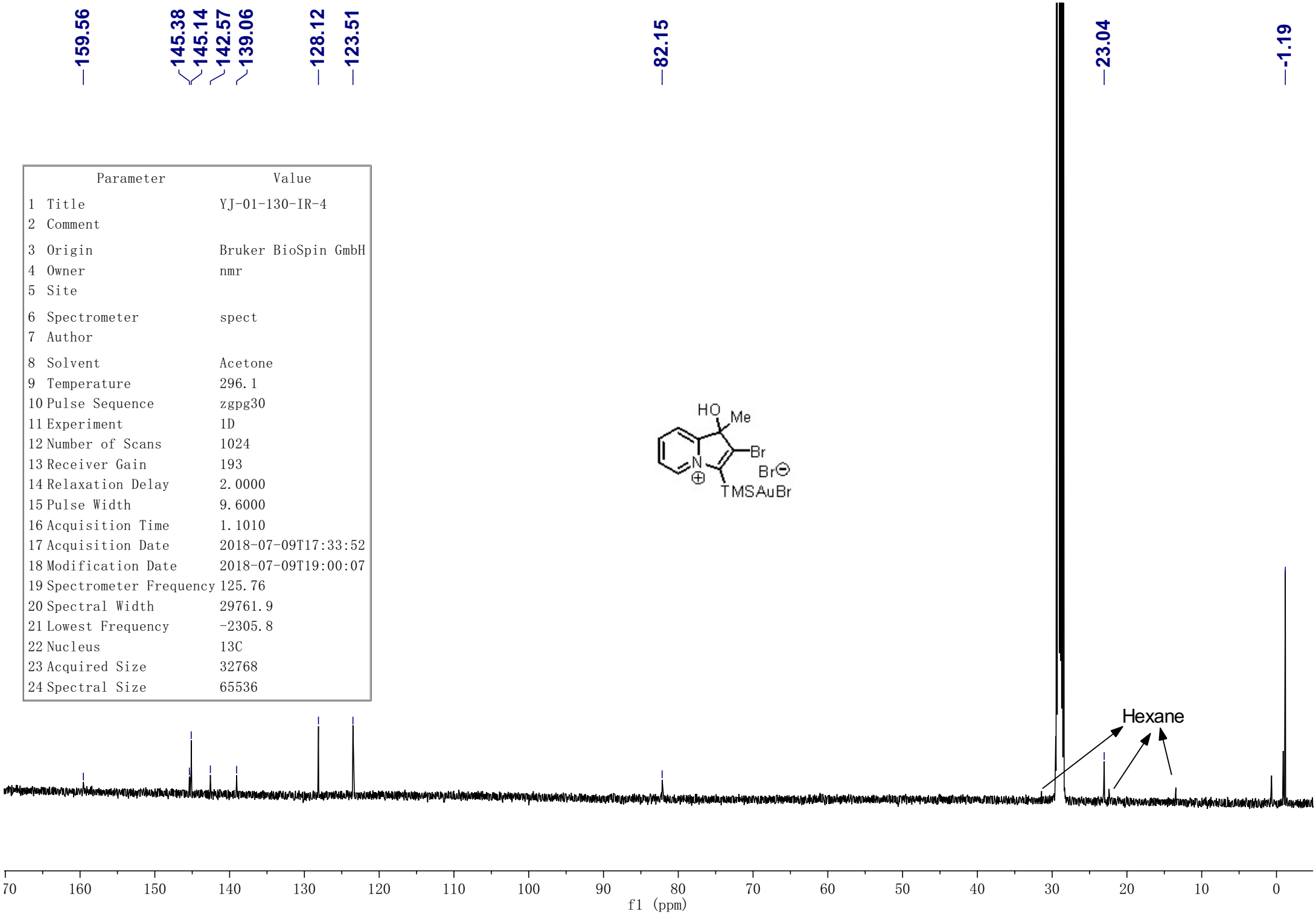
Parameter	Value
1 Title	YJ-01-114-CONVERTED
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	1500
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-07-05T05:16:20
18 Modification Date	2018-07-05T14:53:58
19 Spectrometer Frequency	125.77
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Title	YJ-01-114-CONVERTED
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.2
10 Pulse Sequence	hmbcgplpndqf
11 Experiment	2D-HMBC
12 Number of Scans	8
13 Receiver Gain	193
14 Relaxation Delay	1.4672
15 Pulse Width	10.7100
16 Acquisition Time	0.1905
17 Acquisition Date	2018-07-05T05:45:47
18 Modification Date	2018-07-05T14:53:58
19 Spectrometer Frequency	(500.13, 125.77)
20 Spectral Width	(5376.3, 27933.0)
21 Lowest Frequency	(-378.6, -1411.3)
22 Nucleus	(1H, 13C)
23 Acquired Size	(1024, 128)
24 Spectral Size	(1024, 512)

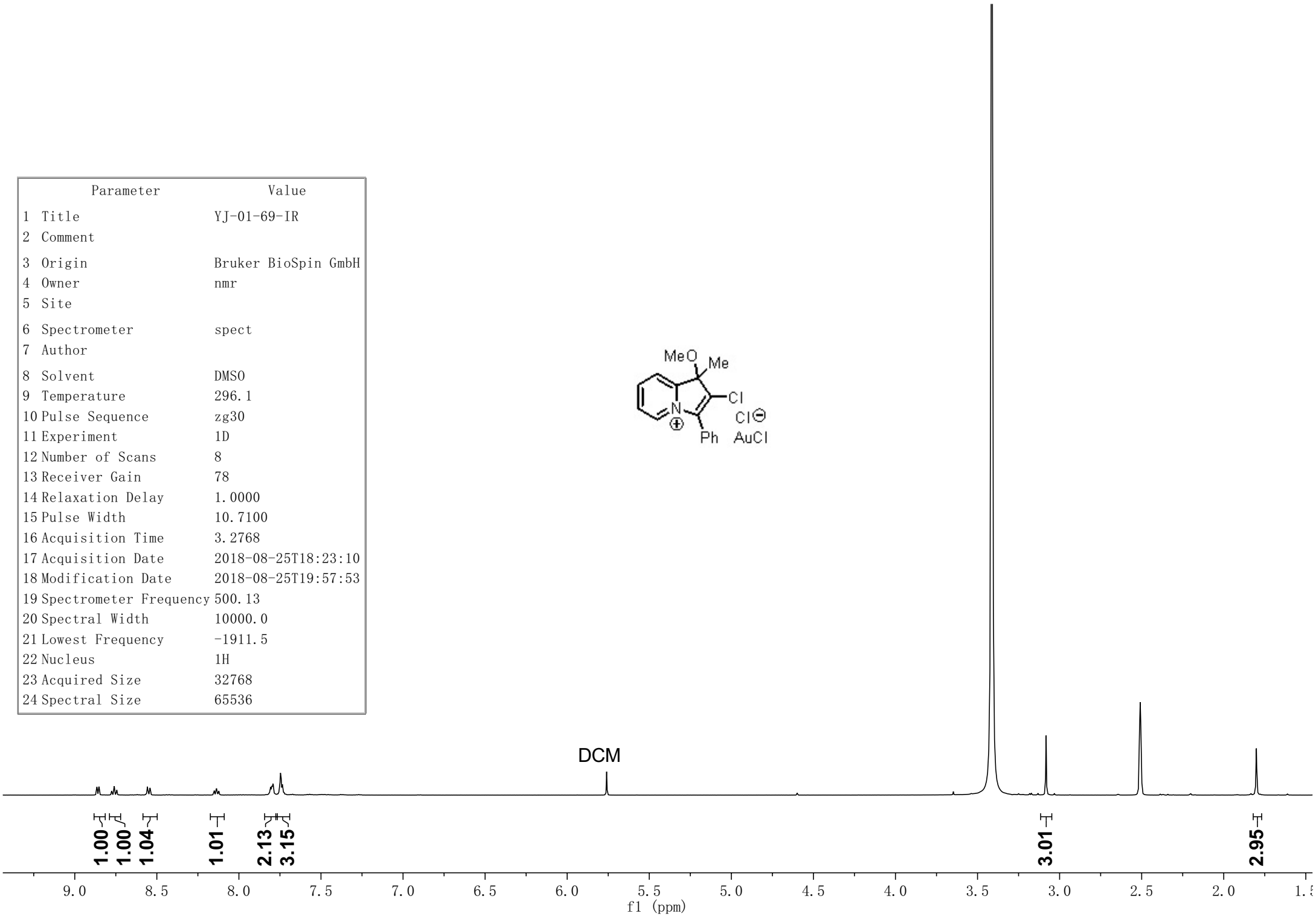
Parameter	Value
1 Title	YJ-01-130-IR-4
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.2
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Receiver Gain	125
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-07-09T17:31:11
18 Modification Date	2018-07-09T19:00:06
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1917.8
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

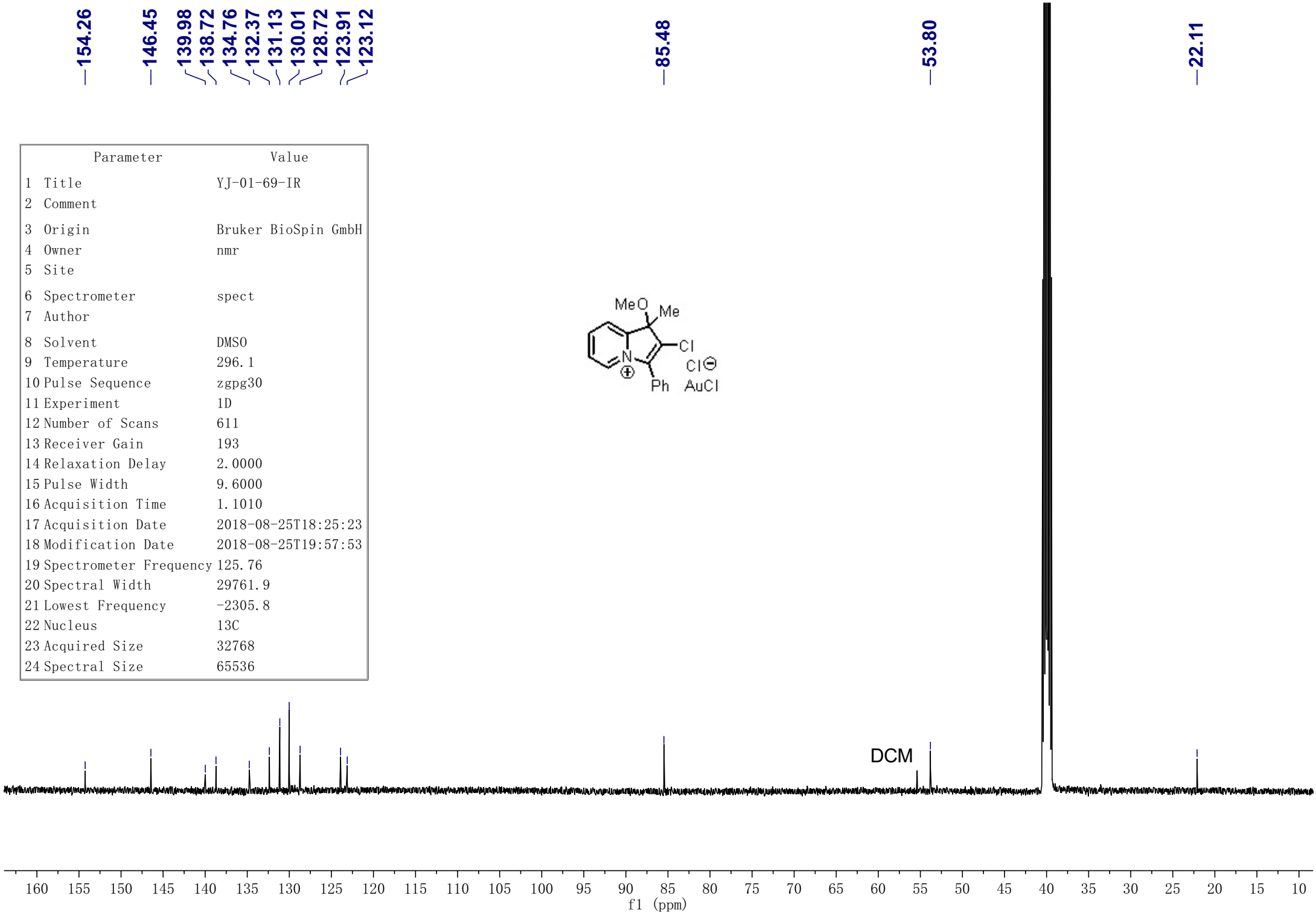




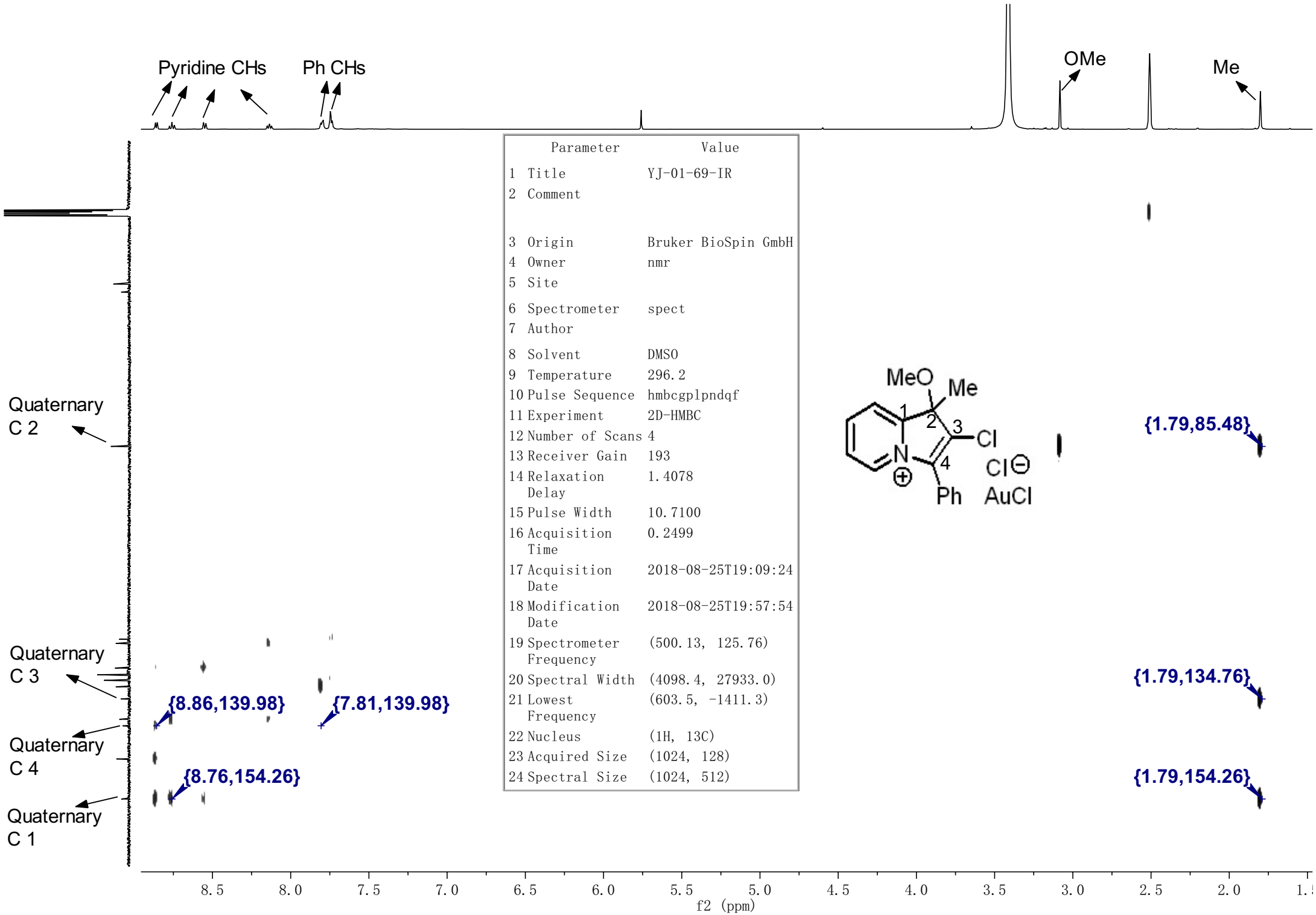
Parameter	Value
1 Title	YJ-01-130-IR-4
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	Acetone
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	1024
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-07-09T17:33:52
18 Modification Date	2018-07-09T19:00:07
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Parameter	Value
1 Title	YJ-01-69-IR
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	8
13 Receiver Gain	78
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-08-25T18:23:10
18 Modification Date	2018-08-25T19:57:53
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



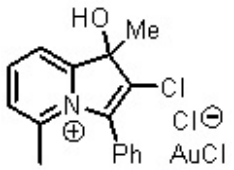


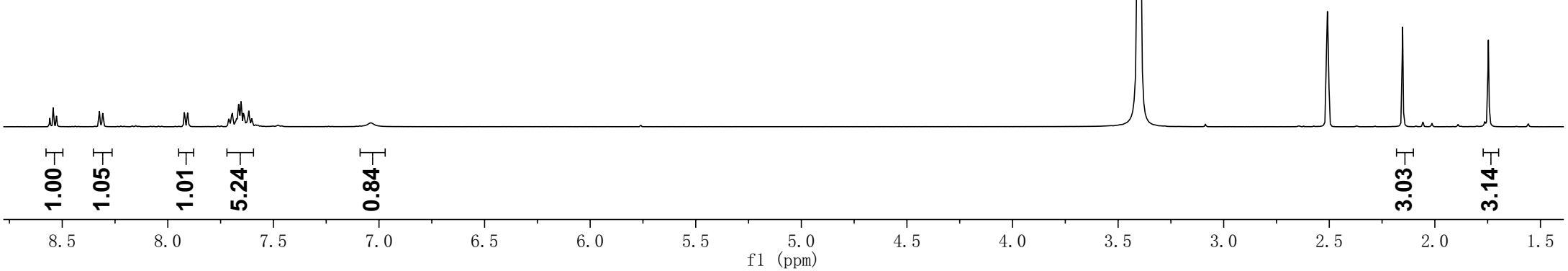
Parameter	Value
1 Title	YJ-01-69-IR
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	611
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-08-25T18:25:23
18 Modification Date	2018-08-25T19:57:53
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

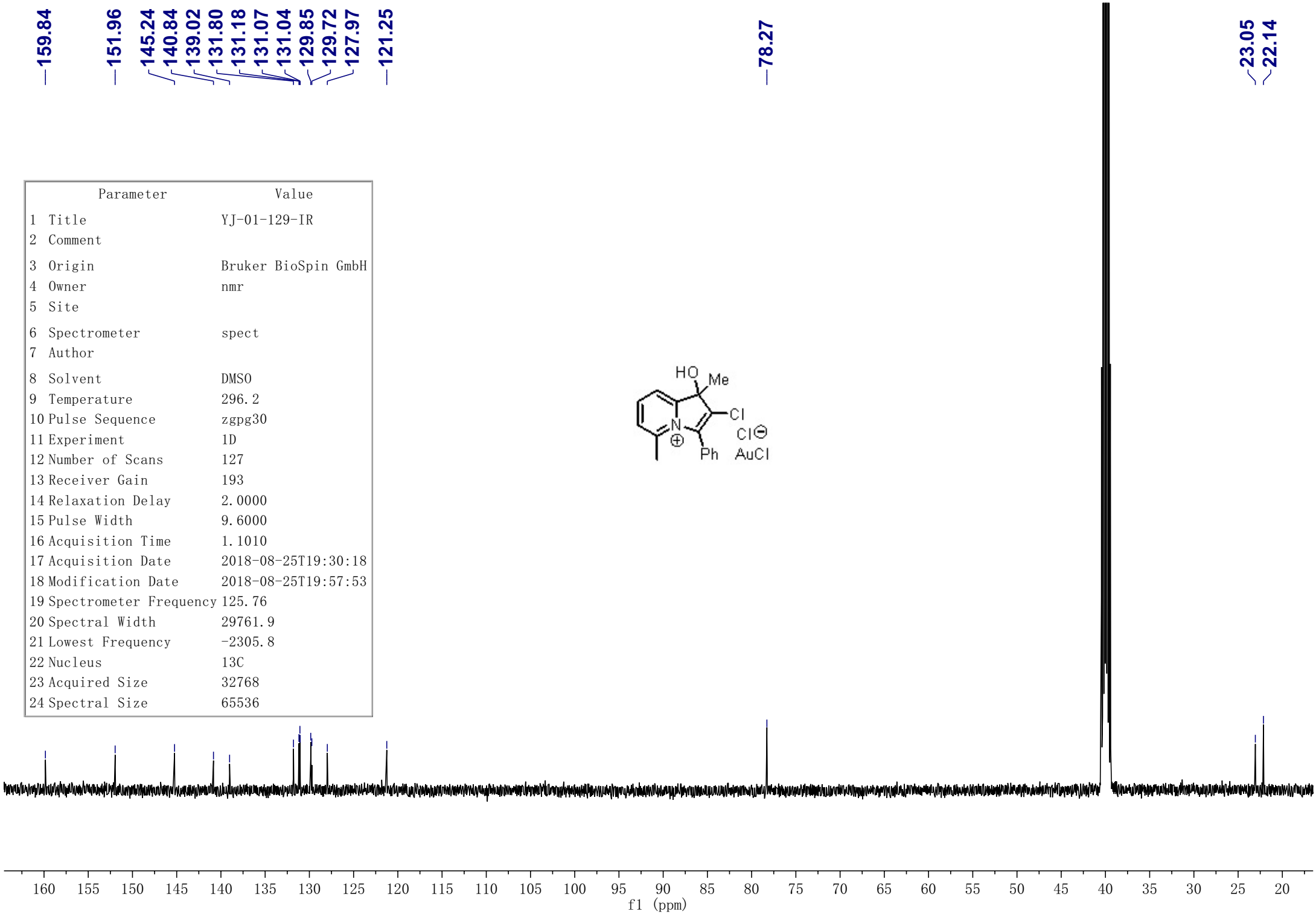


	Parameter	Value
1	Title	YJ-01-69-IR
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	DMSO
9	Temperature	296.2
10	Pulse Sequence	hmbcgplpndqf
11	Experiment	2D-HMBC
12	Number of Scans	4
13	Receiver Gain	193
14	Relaxation Delay	1.4078
15	Pulse Width	10.7100
16	Acquisition Time	0.2499
17	Acquisition Date	2018-08-25T19:09:24
18	Modification Date	2018-08-25T19:57:54
19	Spectrometer Frequency	(500.13, 125.76)
20	Spectral Width	(4098.4, 27933.0)
21	Lowest Frequency	(603.5, -1411.3)
22	Nucleus	(1H, 13C)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 512)

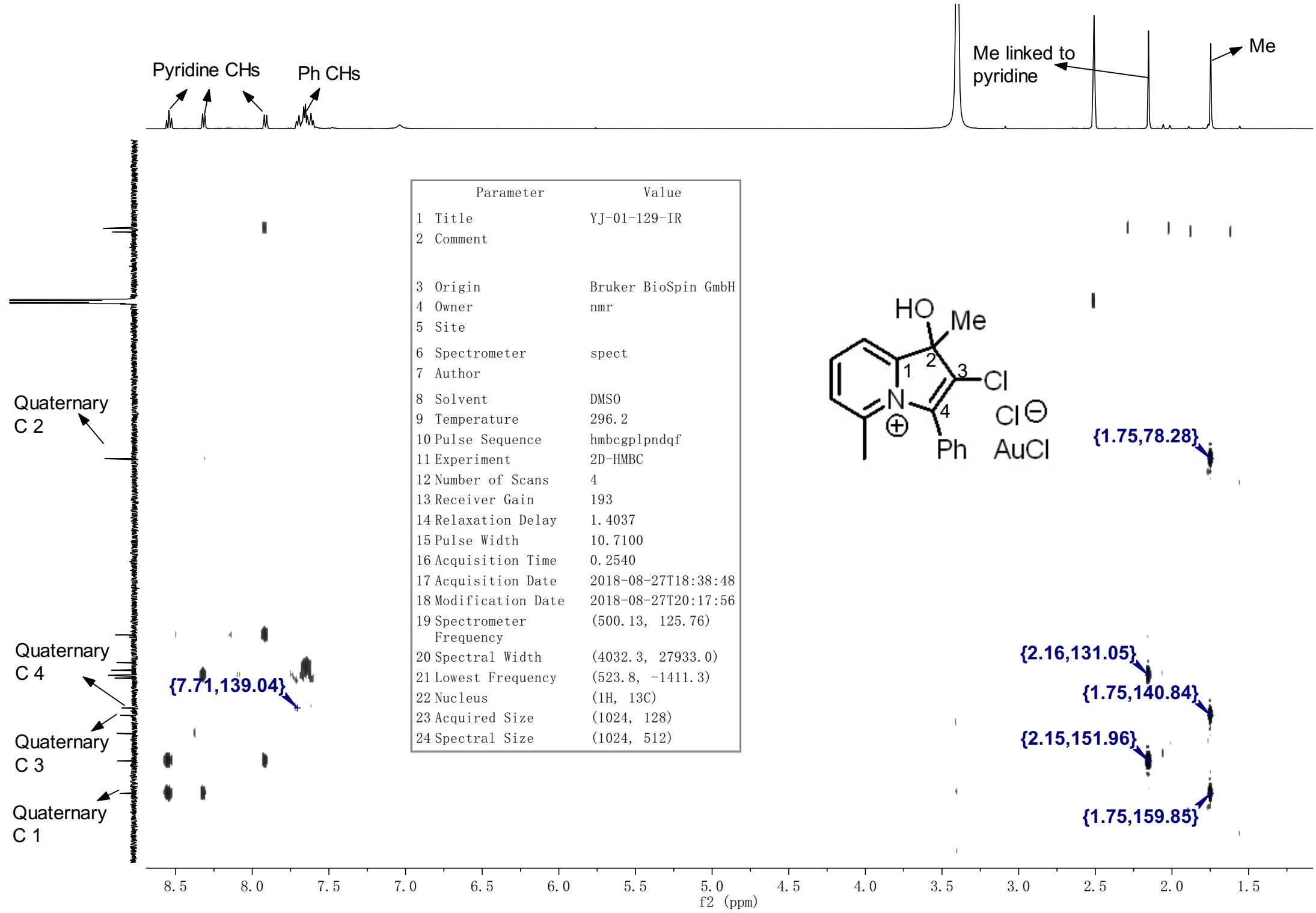
Parameter	Value
1 Title	YJ-01-129-IR
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	8
13 Receiver Gain	78
14 Relaxation Delay	1.0000
15 Pulse Width	10.7100
16 Acquisition Time	3.2768
17 Acquisition Date	2018-08-25T19:27:40
18 Modification Date	2018-08-25T19:57:53
19 Spectrometer Frequency	500.13
20 Spectral Width	10000.0
21 Lowest Frequency	-1911.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536







Parameter	Value
1 Title	YJ-01-129-IR
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmr
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	296.2
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	127
13 Receiver Gain	193
14 Relaxation Delay	2.0000
15 Pulse Width	9.6000
16 Acquisition Time	1.1010
17 Acquisition Date	2018-08-25T19:30:18
18 Modification Date	2018-08-25T19:57:53
19 Spectrometer Frequency	125.76
20 Spectral Width	29761.9
21 Lowest Frequency	-2305.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536



Parameter		Value
1	Title	YJ-01-129-IR
2	Comment	
3	Origin	Bruker BioSpin GmbH
4	Owner	nmr
5	Site	
6	Spectrometer	spect
7	Author	
8	Solvent	DMSO
9	Temperature	296.2
10	Pulse Sequence	hmbcgplpndqf
11	Experiment	2D-HMBC
12	Number of Scans	4
13	Receiver Gain	193
14	Relaxation Delay	1.4037
15	Pulse Width	10.7100
16	Acquisition Time	0.2540
17	Acquisition Date	2018-08-27T18:38:48
18	Modification Date	2018-08-27T20:17:56
19	Spectrometer Frequency	(500.13, 125.76)
20	Spectral Width	(4032.3, 27933.0)
21	Lowest Frequency	(523.8, -1411.3)
22	Nucleus	(1H, 13C)
23	Acquired Size	(1024, 128)
24	Spectral Size	(1024, 512)