Highly Active Platinum Catalysts for Nitrile and Cyanohydrin Hydration: Catalyst Design and Ligand Screening via High-Throughput Techniques

Xiangyou Xing[§†,‡], Chen Xu[§†,‡], Bo Chen[†], Chengcheng Li[†], Scott C. Virgil[‡]* and Robert H. Grubbs[‡]*

[†]Shenzhen Grubbs Institute, Southern University of Science and Technology (SUSTech), Shenzhen, 518055, China

[‡]The Warren and Katharine Schlinger Laboratory for Chemistry and PChemical Engineering, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, United States

rhg@caltech.edu and svirgil@caltech.edu

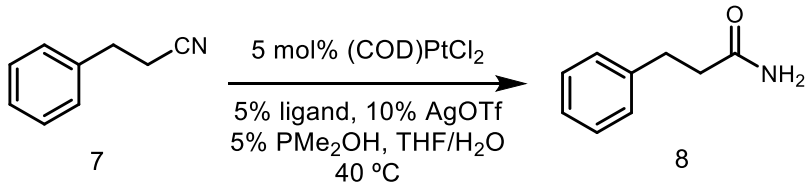
Supplementary Information

General Procedures

Unless otherwise stated, reactions were performed in brand-new Fisherbrand scintillation vials in a nitrogen filled glove box using dry, degassed. Organic solvents were dried by passage through an activated alumina column under argon and water was distilled under the protection of nitrogen. Commercial reagents (Sigma Aldrich or Alfa Aesar) were used as received with the exception of cyanohydrins which are purified by distillation before use. Dimethyl phosphine oxide was synthesized by following the known procedure[1] and it was kept in the nitrogen filled glovebox. Ligand screening was performed by using Freeslate Core Module 2 system which was enclosed in a nitrogen filled glovebox. Reaction progress was monitored by thin-layer chromatography (TLC) or Agilent 1290 UHPLC-LCMS analyses. TLC was performed using E. Merck silica gel 60 F254 precoated glass plates (0.25 mm) and visualized by UV fluorescence quenching or $KMnO_4$ staining. ^1H and ^{13}C NMR spectra were recorded on a Varian Inova 500 spectrometer (500 MHz and 126 MHz, respectively) or a Bruker AV III HD spectrometer equipped with a Prodigy liquid nitrogen temperature cryoprobe (400 MHz and 101 MHz, respectively), and are reported in terms of chemical shift relative to residual $CHCl_3$ (δ 7.26 and δ 77.16 ppm, respectively). Data for ^1H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Abbreviations are used as follows: s = singlet, bs = broad singlet, d = doublet, t = triplet, q = quartet, m = complex multiplet. High-resolution mass spectra (HRMS) were obtained from the Caltech Mass Spectral Facility using a JEOL JMS-600H High Resolution Mass Spectrometer with fast atom bombardment (FAB+) ionization mode or were acquired using an Agilent 6200 Series TOF with an Agilent G1978A Multimode source in electrospray ionization (ESI+) mode.

Reagents were purchased from commercial vendors as follows: Parkins catalyst was purchased from Strem Chemicals and stored in a nitrogen-filled glovebox. Dichloro(1,5-cyclooctadiene)Platinum, silver salts (silver trifluoromethanesulfonate *et al*) were purchased from Sigma-Aldrich and stored in a nitrogen-filled glovebox. Nitriles (*p*-tolunitrile *et al*) and cyanohydrins (mandelonitrile *et al*) were also purchased from Sigma-Aldrich.

1. Ligand screening by using high-throughput techniques



7 8

Hydrocinnamonitrile (**7**) was selected as our module substrate and the screening was performed by Freeslate core module 2 high-throughput screening system, which was enclosed in a nitrogen filled glovebox. 42 bidentate ligands were investigated at a time. All the materials were prepared as stock solution: $(COD)PtCl_2$, 0.02 M in CH_2Cl_2; PMe_2OH, 0.02 M in THF; AgOTf, 0.04 M in THF; bidentate ligands, 0.02 M in THF; hydrocinnamonitrile (**7**), 0.2 M in THF with 1 mmol% 4,4′-ditert-butylbiphenyl as internal standard. 2 mL vials (42) were arranged in a freeslate plate (7 rows × 6 column), and the screening was conducted in 20 μmol scale with the following procedure: 1) ligands (50 μL) were dispensed into each vial, and then $(COD)PtCl_2$ (50 μL) was dispensed. The reaction mixture was then stirred for 2 hours at room temperature; 2) PMe_2OH (50 μL) was dispensed into the above reaction mixture, and then AgOTf (50 μL) was dispensed; 3) water (150 μL) was dispensed to the above reaction mixture; 4) hydrocinnamonitrile (100 μL) was dispensed to the reaction mixture and the reaction was warmed up to 40 ℃. After stirred for 10 minutes, the plate was taken outside of the glovebox and cooled to room temperature. Then, the reaction was monitor by UHPLC-LCMS, and the conversion of each reaction was calculated based on the internal standard.

Table 1. Ligand screen and their corresponding conversions

Ligand	Conversion	Ligand	Conversion	Ligand	Conversion
DPEphos	25%	DTBPF	30%	(*S*)-C_3-TunePhos	57%
Xantphos	0%	$Ph_2P^tBu_2P$Ferroce	0%	(*R*)-SYNPHOS	57%
^{t}BuXantphos	0%	(2*S*,4*S*)-Et-FerroTANE	64%	BiPhePhos	0%
rac-BINAP	54%	(2*S*,5*S*)-Me-Ferrocelane	64%	Josiphos SL-J001-1	33%
(*S*)-BINAPINE	0%	(2*S*,5*S*)-iPr-Ferrocelane	5%	Josiphos SL-J008-2	0%
(*S*)-3,5-^{t}Bu-MeOBIPHEP	14%	(*S*)-CF_3-PHOX	31%	Josiphos SL-J009-1	4%
(*R*,*R*)-DIOP	66%	(*S*)- ^{t}Bu-PHOX	3%	Josiphos SL-J013-1	0%
(*R*)-Phanephos	32%	(4*S*)- ^{t}Bu-Me_2box	0%	Josiphos SL-J005-1	49%
(*R*)-SDP	72%	(4*S*)-Ph-H_2box	0%	Josiphos SL-J015-1	65%
(*R*,*R*)-Chiraphos	21%	2,2'-Bis[(4S)-4-benzyl-2-oxazoline]	22%	Josiphos SL-J505-1	25%
(*R*,*R*)-Norphos	42%	(*S*,*S*)-Me-BPE	31%	Walphos SL-W001-1	3%
(*S*,*S*)-BDPP	69%	(2*R*,5*R*)-Et-DUPHOS	20%	Walphos SL-W009-1	10%
DPPF	69%	(*R*)-QUINAP	22%	Walphos SL-W009-1	20%
DIPF	6%	(*R*)-SEGPHOS	63%	Walphos SL-W009-1	5%

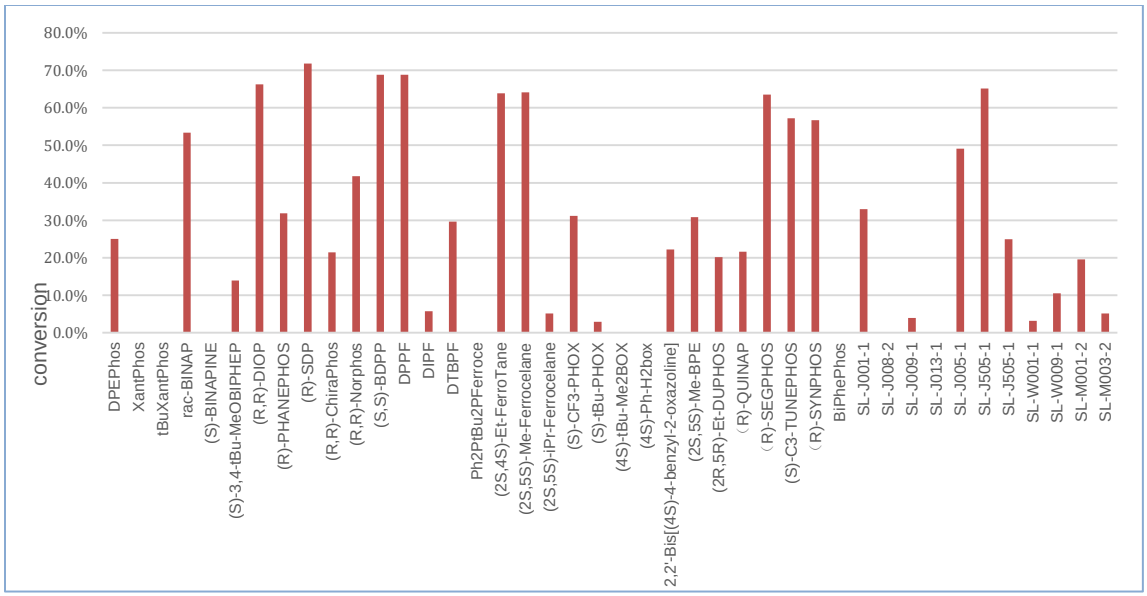


Figure 1. Ligand screen and their corresponding conversions

Note:

DPEphos: Bis[(2-diphenylphosphino)phenyl]ether;
Xantphos: 4,5-Bis(diphenylphosphino)-9,9-dimethylxanthene;
^{t}BuXantphos: 9,9-Dimethyl-4,5-bis(di-*tert*-butylphosphino)xanthene;
rac-BINAP: (±)-2,2′-Bis(diphenylphosphino)-1,1′-binaphthalene;
(*S*)-BINAPINE: (3S,3'S,4S,4'S,11bS,11'bS)-(+)-4,4′-Di-t-butyl-4,4′,5,5′-tetrahydro-3,3′-bi-3H-dinaphtho[2,1-c:1′,2′-e]phosphepin;
(S)-(3,5-*t*-Bu-MeOBIPHEP)**:** (*S*)-2,2′-Bis[bis(3,5-di-*tert*-butyl)phosphino]-6,6′-dimethoxy-1,1′-biphenyl ;
R,R)-DIOP: (−)-2,3-*O*-Isopropylidene-2,3-dihydroxy-1,4-bis(diphenylphosphino)butane;
(*R*)-PhanePhos: (*R*)-(–)-4,12-Bis(diphenylphosphino)-[2.2]-paracyclophane;
(*R*)-SDP: Spirobiindane-bis-PPh_2;
(*R,R*)-Chiraphos: Ph_2P-CH(Me)CH(Me)-PPh_2;
(*R,R*)-Norphos: Ph_2P-norbornene-PPh_2;
DPPF: 1,1′-Ferrocenediyl-bis(diphenylphosphine);
DIPF: 1,1′-Ferrocenediyl-bis(di-*iso*-propylphosphine);
(*S,S*)-BDPP: Ph_2P-CH(Me)CH_2CH(Me)-PPh_2;

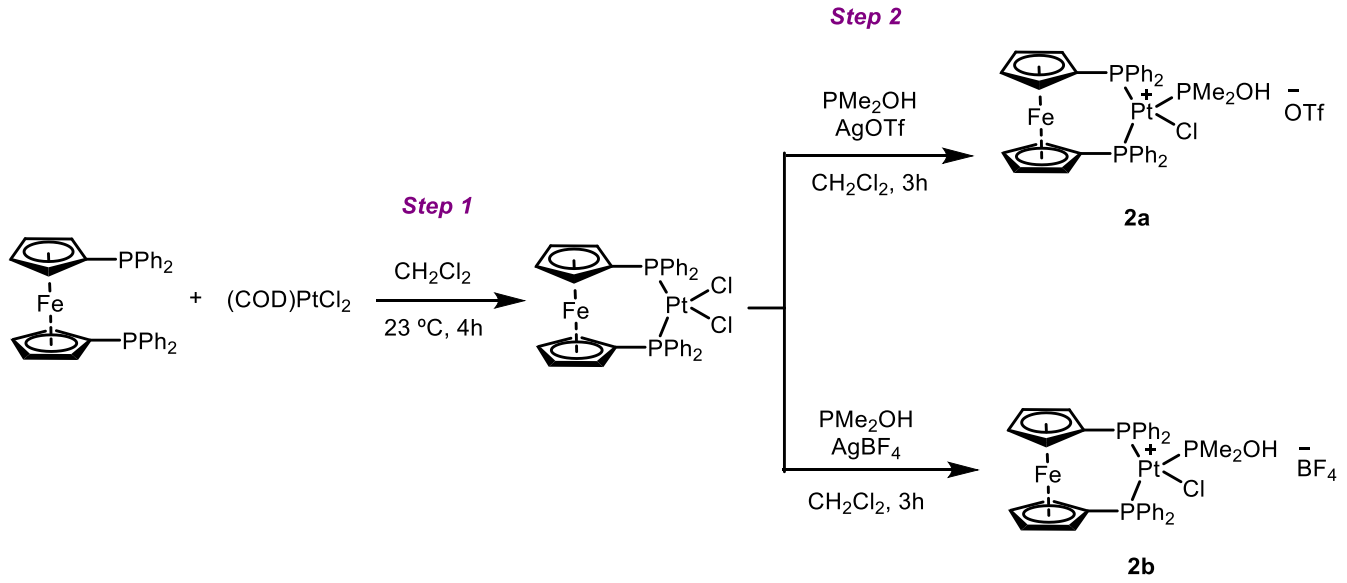
DTBPF: 1,1′-Ferrocenediyl-bis(di-*tert*-butyllphosphine);
$Ph_2P^tBu_2P$Ferroce: 1-Diphenylphosphino-1'-di-tert-butylphosphinoferrocene;
(*2S,4S*)-Et-FerroTANE: (-)-1,1'-Bis[(*2S,4S*)-2,4-Diethylphosphotano]Ferrocene;
(*2S,5S*)-Me-Ferrocelane: 1,1′-Bis[(2*S*,5*S*)-2,5-dimethylphospholano]Ferrocene;
(*2S,5S*)-^{i}Pr-Ferrocelane: 1,1′-Bis[(2*S*,5*S*)-2,5-diisopropylphospholano]Ferrocene;
(*S*)-CF_3-PHOX: (*S*)-4-tri-fluoro-2-[2-(diphenylphosphino)phenyl]-2-oxazoline;
(*S*)-^{t}Bu-PHOX: (*S*)-4-*tert*-Butyl-2-[2-(diphenylphosphino)phenyl]-2-oxazoline;
(4*S*)-^{t}Bu-Me_2box: 2,2′-Isopropylidenebis[(4*S*)-4-*tert*-butyl-2-oxazoline];
(4*S*)-Ph-H_2box: 2,2′-Methylenebis[(4*S*)-4-phenyl-2-oxazoline];
(*2S,5S*)-Me-BPE: (−)-1,2-Bis[(2*S*,5*S*)-2,5-dimethylphospholano]ethane;
(*2R,5R*)-Et-DUPHOS: (−)-1,2-Bis[(2*R*,5*R*)-2,5-diethylphospholano]benzene
(*R*)-QUINAP: (*R*)-(+)-1-(2-Diphenylphosphino-1-naphthyl)isoquinoline;

(*R*)-SEGPHOS: (*R*)-(+)-5,5′-Bis(diphenylphosphino)-4,4′-bi-1,3-benzodioxole, [4(*R*)-(4,4′-bi-1,3-benzodioxole)-5,5′-diyl]bis[diphenylphosphine;

(*S*)-C_3-TunePhos: (*R*)-1,13-Bis(diphenylphosphino)-7,8-dihydro-6*H*-dibenzo[f,h][1,5]dioxonin;
(*R*)-SYNPHOS: R-(+)-6,6'-Bis(diphenylphosphino)-2,2',3,3'-tetrahydro-5,5'-bi-1,4-benzodioxin;

SL-J001-1 : (*R*)-1-[(S_P)-2-(Diphenylphosphino)ferrocenyl]ethyldicyclohexylphosphine;
SL-J008-2: (*S*)-1-{(R_P)-2-[Bis[3,5-bis(trifluoromethyl)phenyl]phosphino]ferrocenyl}ethyldi(3,5-xylyl)phosphine
SL-J009-1: (*R*)-1-[(S_P)-2-(Dicyclohexylphosphino)ferrocenyl]ethyldi-*tert*-butylphosphine
SL-J013-1: (*R*)-1-{(S_P)-2-[Bis(4-methoxy-3,5-dimethylphenyl)phosphino]ferrocenyl}ethyldi-*tert*-butylphosphine
SL-J005-1: (*R*)-1-[(S_P)-2-(Diphenylphosphino)ferrocenyl]ethyldi(3,5-xylyl)phosphine
SL-J015-1: (*R*)-1-{(S_P)-2-[Di(2-furyl)phosphino]ferrocenyl}ethyldi(3,5-xylyl)phosphine
SL-J505-1: (*R*)-1-[(S_P)-2-(Di-*tert*-butylphosphino)ferrocenyl]ethylbis(2-methylphenyl)phosphine
SL-W001-1: (*R*)-1-{(R_P)-2-[2-(Diphenylphosphino)phenyl]ferrocenyl}ethylbis[3,5-bis-(trifluoromethyl)phenyl]phosphine
SL-W009-1: (*R*)-1-{(R_P)-2-[2-[Di(3,5-xylyl)phosphino]phenyl]ferrocenyl}ethyldi(3,5-xylyl)phosphine
SL-M001-2: (2S,2′S)-1,1′-Bis[(S)-(dimethylamino)phenylmethyl]-2,2′-bis(diphenylphosphino)ferrocene
SL-M003-2: (*R*)-1-{(R_P)-2-[2-[Di(3,5-xylyl)phosphino]phenyl]ferrocenyl}ethyldi(3,5-xylyl)phosphine

2. General procedure for synthesis of the catalysts 2a and 2b



Step 1: In a nitrogen filled glovebox, to a 20mL scintillation vial with a magnetic stir bar were added DPPF [1,1′-ferrocenediyl-bis(diphenylphosphine)] (832 mg, 1.5 mmol), $(COD)PtCl_2$ (561 mg, 1.5 mmol) and 4 mL CH_2Cl_2, then the vial was capped and taken outside of the dry box and stirred at room temperature for 4 hours. The yellow solution was filtered and concentrated to a yellow solid. The solid was recrystallized from CH_2Cl_2 and Hexane to give $(DPPF)PtCl_2$ (1.03 g, 85% yield).

Step 2: In a nitrogen filled glovebox, to a 10 mL vial with a magnetic stir bar were added $(DPPF)PtCl_2$ (205 mg, 0.25 mmol), silver salt (for AgOTf: 64 mg, 0.25 mmol; for $AgBF_4$: 49 mg, 0.25 mmol), dimethylphosphine oxide (20 mg, 0.26 mmol) and 2 mL CH_2Cl_2. The vial was taken outside of the dry box and stirred at room temperature for 3 hours. The yellow solution was filtered and concentrated to provide a yellow solid. The solid was recrystallized from CH_2Cl_2 and Hexane to give **2a** (185 mg, 73% yield) or **2b** (178 mg, 76% yield).

Catalyst 2a:

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.96 – 7.89 (m, 4H), 7.81 (ddd, *J* = 11.9, 8.3, 1.3 Hz, 4H), 7.69 – 7.64 (m, 2H), 7.63 – 7.56 (m, 6H), 7.51 (td, *J* = 7.7, 2.6 Hz, 4H), 4.51 (d, *J* = 1.8 Hz, 2H), 4.40 (d, *J* = 1.8 Hz, 2H), 4.39 (q, *J* = 1.9 Hz, 2H), 4.13 (q, *J* = 1.9 Hz, 2H), 1.72 (d, *J* = 2.5 Hz, 3H), 1.70 (d, *J* = 2.5 Hz, 3H) ppm

^{13}C NMR (126 MHz, CD_2Cl_2): δ 134.9 (dd, *J* = 11.1, 1.6 Hz), 134.2 (d, *J* = 11.9 Hz), 132.3 (d, *J* = 2.8 Hz), 131.5 (d, *J* = 2.7 Hz), 130.7, 130.2, 130.1, 129.5, 128.7 (d, *J* = 11.6 Hz), 128.3 (d, *J* = 11.0 Hz), 75.7 (d, *J* = 12.3 Hz), 75.5 (d, *J* = 10.8 Hz), 74.6 (d, *J* = 7.5 Hz), 73.9 (d, *J* = 8.2 Hz), 18.9 (d, *J* = 5.0 Hz), 18.6 (d, *J* = 3.8 Hz) ppm

^{31}P NMR (121 MHz, CD_2Cl_2): δ 105.0 (d, *J* = 24.4 Hz), 101.2 (d, *J* = 22.9 Hz), 93.5 (d, *J* = 20.0 Hz), 89.6 (d, *J* = 20.0 Hz), 82.0 (d, *J* = 19.2 Hz), 78.1 (d, *J* = 20.4 Hz), 34.6 (d, *J* = 15.5 Hz), 30.7 (d, *J* = 18.3 Hz), 25.5 (d, *J* = 15.8 Hz), 21.7 (d, *J* = 15.8 Hz), 16.43 (d, *J* = 15.3 Hz), 14.9 (dd, *J* = 20.0, 15.7 Hz), -0.97 ppm

^{19}F NMR (282 MHz, CD_2Cl_2): δ -79.1 ppm

HRMS (ESI+): $[C36H34P3OFePt]^+$: 826.0814, found 826.0816.

Catalyst 2b:

^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.01 (ddt, *J* = 12.8, 6.8, 1.5 Hz, 4H), 7.89-7.77 (m, 4H), 7.64-7.55 (m, 7H), 7.54-7.41 (m, 4H), 4.46 (dd, *J* = 2.1, 1.1 Hz, 2H), 4.44 (q, *J* = 1.9 Hz, 2H), 4.32 (q, *J* = 1.6 Hz, 2H), 4.05 (q, *J* = 1.9 Hz, 2H), 1.64 (d, *J* = 2.6 Hz, 3H), 1.61 (d, *J* = 2.6 Hz, 3H) ppm

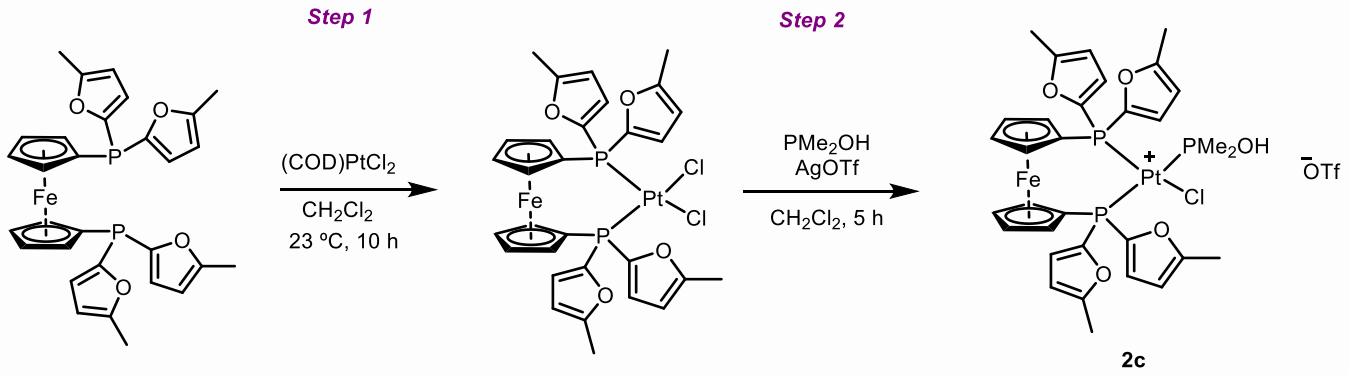
^{13}C NMR (101 MHz, CD_2Cl_2): δ 135.0 (dd, *J* = 11.1, 1.6 Hz), 134.6 (d, *J* = 11.8 Hz), 131.6 (d, *J* = 2.9 Hz), 131.4 (d, *J* = 2.3 Hz), 131.2 (d, *J* = 2.5 Hz), 130.9 (d, *J* = 2.5 Hz), 130.0, 129.3, 128.3 (d, *J* = 12.0 Hz), 128.2 (d, *J* = 12 Hz), 75.4 (dd, *J* = 10.5, 1.9 Hz), 75.2 (d, *J* = 10.3 Hz), 74.3 (d, *J* = 7.1 Hz), 73.5 (d, *J* = 7.7 Hz), 18.4 (d, *J* = 5.1 Hz), 18.0 (d, *J* = 5.3 Hz) ppm

^{31}P NMR (121 MHz, CD_2Cl_2): δ 95.8 (d, *J* = 20.0 Hz), 92.0 (d, *J* = 20.2 Hz), 25.6 (d, *J* = 15.4 Hz), 21.8 (d, *J* = 15.7 Hz), 14.5 (dd, *J* = 20.1, 15.5 Hz) ppm

^{19}F NMR (282 MHz, CD_2Cl_2): δ -150.8 ppm

HRMS (ESI+): $[C36H34P3OFePt]^+$: 826.0814, found 826.0814.

3. Synthesis of catalyst 2c



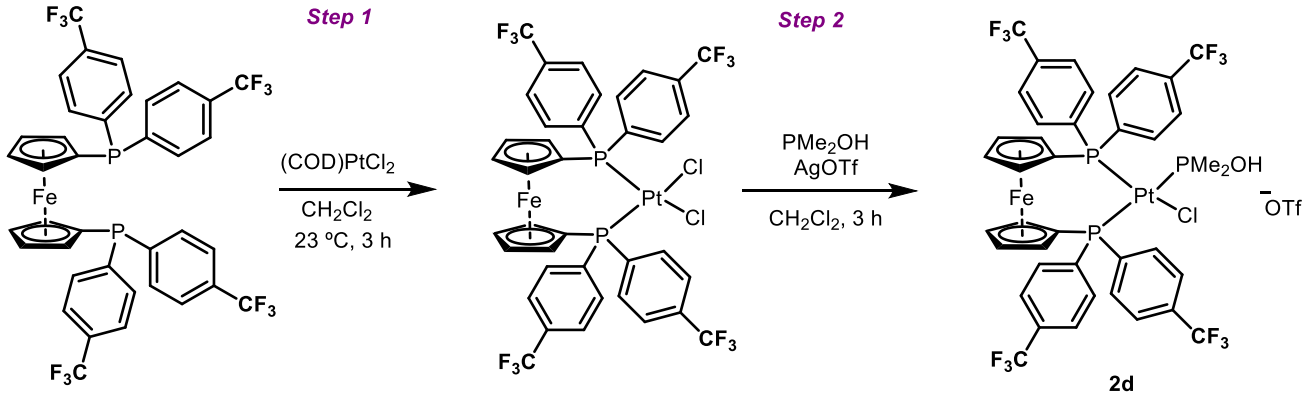
Step 1: In a nitrogen filled glovebox, to a 20 mL scintillation vial with a magnetic stir bar were added 1,1'-Bis[bis(5-methyl-2-furanyl)phosphino]ferrocene (182 mg, 0.32 mmol), $(COD)PtCl_2$ (120 mg, 0.32 mmol) and 3 mL CH_2Cl_2, then the vial was taken outside of the dry box and stirred at room temperature for 10 hours. The yellow solution was filtered and then evaporated to provide yellow solid, which was recrystallized through 1 mL CH_2Cl_2 and 1 mL hexane to give yellow precipitate. The solid was collected and dried in *vacuo* to yield $(dmfpf)PtCl_2$ (220 mg, 82% yield).

Step 2: In a nitrogen filled glovebox, to a 10 mL scintillation vial with a magnetic stir bar were added $(dmfpf)PtCl_2$ (209 mg, 0.25 mmol), silver trifluoromethanesulfonate (64 mg, 0.25 mmol), dimethylphosphine oxide (20 mg, 0.26 mmol) and 2 mL CH_2Cl_2. Then the vial was taken outside of the glovebox and was stirred at room temperature for 3 hours. The orange solution was filtered and CH_2Cl_2 was evaporated to provide orange solid, which was recrystallized through CH_2Cl_2 and Hexane to give yellow precipitate. The solid was collected and dried in vacuo to yield catalyst 2c (198 mg, 76% yield).

^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.01 (dt, *J* = 15.5, 2.9 Hz, 4H), 6.31 – 6.18 (m, 4H), 4.49 (dq, *J* = 5.8, 1.6 Hz, 4H), 4.41 (q, *J* = 2.1 Hz, 2H), 4.33 – 4.26 (m, 2H), 2.43 (dd, *J* = 15.3, 0.8 Hz, 12H), 2.08 – 1.74 (m, 6H) ppm

^{13}C NMR (101 MHz, CD_2Cl_2): δ 159.6 (d, *J* = 5.5 Hz), 159.5 (d, *J* = 6.6 Hz), 140.9, 140.7, 134.0, 139.6, 126.2 (d, *J* = 19.0 Hz), 125.0 (d, *J* = 19.3 Hz), 108.4 (d, *J* = 8.0 Hz), 107.8 (d, *J* = 8.0 Hz), 75.5– 75.00 (m), 74.34(d, *J* = 8.4 Hz), 74.0 (d, *J* = 9.4 Hz), 19.2 (d, *J* = 5.1 Hz), 18.8 (d, *J* = 5.1 Hz), 13.8, 13.8 ppm
^{31}P NMR (162 MHz, CD_2Cl_2): δ 102.40 (d, *J* = 17.8 Hz), 99.41 (d, *J* = 18.9 Hz), 93.75 (d, *J* = 18.6 Hz), 90.76 (d, *J* = 18.6 Hz), 85.10 (d, *J* = 18.8 Hz), 82.11 (d, *J* = 18.8 Hz), -2.95 (d, *J* = 19.5 Hz), -5.93 (d, *J* = 19.7 Hz), -9.63 (d, *J* = 19.6 Hz), -12.02 (t, *J* = 18.9 Hz), -12.62 (d, *J* = 19.5 Hz), -16.31 (d, *J* = 20.5 Hz), -19.30 (d, *J* = 19.4 Hz), -23.89 (t, *J* = 19.1 Hz), -35.76 (t, *J* = 19.1 Hz) ppm
^{19}F NMR (282 MHz, CD_2Cl_2): δ -79.0 (d, *J* = 3.2 Hz) ppm
HRMS (ESI+): $[C32H34P3O5FePt]^+$: 842.0611, found 842.0607.

4. Syntheses of catalysts 2d and 2e

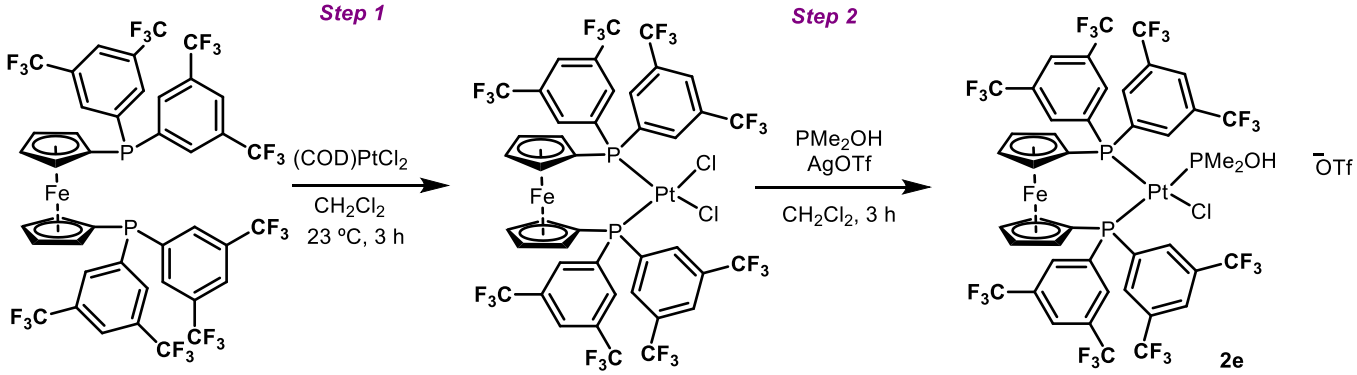


Step 1: In a nitrogen filled glovebox, to a 10 mL scintillation vial with a magnetic stir bar were added 1,1'-Bis[bis(4-(trifluoromethyl)phenyl)phosphino]ferrocene [2] (265 mg, 0.32 mmol), $(COD)PtCl_2$ (100 mg, 0.27 mmol) and 3 mL CH_2Cl_2, then the vial was taken outside of the dry box and stirred at room temperature for 3 hours. The yellow solution was filtered and then evaporated to provide yellow solid, which was recrystallized through 1 mL CH_2Cl_2 and 1 mL hexane to give yellow precipitate. The solid was collected and dried in *vacuo* to yield $[dp(4\text{-}CF_3)pf]PtCl_2$ (280 mg, 95% yield).
Step 2: In a nitrogen filled glovebox, to a 10 mL scintillation vial with a magnetic stir bar were added $[dp(4\text{-}CF_3)pf]PtCl_2$ (280 mg, 0.26 mmol), silver trifluoromethanesulfonate (65 mg, 0.26 mmol), dimethylphosphine oxide (21 mg, 0.27 mmol) and 2 mL CH_2Cl_2. Then the vial was taken outside of the glovebox and was stirred at room temperature for 3 hours. The orange solution was filtered and CH_2Cl_2 was evaporated to provide orange solid, which was recrystallized through CH_2Cl_2 and Hexane to give yellow precipitate. The solid was collected and dried in vacuo to yield catalyst 2c (270 mg, 82% yield).
^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.01 (dt, *J* = 15.5, 2.9 Hz, 4H), 6.31 – 6.18 (m, 4H), 4.49 (dq, *J* = 5.8, 1.6 Hz, 4H), 4.41 (q, *J* = 2.1 Hz, 2H), 4.33 – 4.26 (m, 2H), 2.43 (dd, *J* = 15.3, 0.8 Hz, 12H), 2.08 – 1.74 (m, 6H) ppm
^{13}C NMR (101 MHz, CD_2Cl_2): δ 159.6 (d, *J* = 5.5 Hz), 159.5 (d, *J* = 6.6 Hz), 140.9, 140.7, 134.0, 139.6, 126.2 (d, *J* = 19.0 Hz), 125.0 (d, *J* = 19.3 Hz), 108.4 (d, *J* = 8.0 Hz), 107.8 (d, *J* = 8.0 Hz), 75.5– 75.00 (m), 74.34 (d, *J* = 8.4 Hz), 74.0 (d, *J* = 9.4 Hz), 19.2 (d, *J* = 5.1 Hz), 18.8 (d, *J* = 5.1 Hz), 13.8, 13.8 ppm
^{31}P NMR (162 MHz, CD_2Cl_2): δ 102.40 (d, *J* = 17.8 Hz), 99.41 (d, *J* = 18.9 Hz), 93.75 (d, *J* = 18.6 Hz), 90.76 (d, *J* = 18.6 Hz), 85.10 (d, *J* = 18.8 Hz), 82.11 (d, *J* = 18.8 Hz), -2.95 (d, *J* = 19.5 Hz), -5.93 (d, *J*

= 19.7 Hz), -9.63 (d, *J* = 19.6 Hz), -12.02 (t, *J* = 18.9 Hz), -12.62 (d, *J* = 19.5 Hz), -16.31 (d, *J* = 20.5 Hz), -19.30 (d, *J* = 19.4 Hz), -23.89 (t, *J* = 19.1 Hz), -35.76 (t, *J* = 19.1 Hz) ppm

^{19}F NMR (282 MHz, CD_2Cl_2): δ -79.0 (d, *J* = 3.2 Hz) ppm

HRMS (ESI+): $[C40H31ClF12FeOP3Pt]^+$: 1134.0082, found 1134.0061.



Step 1: In a nitrogen filled glovebox, to a 10 mL scintillation vial with a magnetic stir bar were added 1,1'-Bis[bis(3,5-(trifluoromethyl)phenyl)phosphino]ferrocene [2](308 mg, 0.28 mmol), $(COD)PtCl_2$ (100 mg, 0.27 mmol) and 3 mL CH_2Cl_2, then the vial was taken outside of the dry box and stirred at room temperature for 3 hours. The yellow solution was filtered and then evaporated to provide yellow solid, which was recrystallized through 1 mL CH_2Cl_2 and 1 mL hexane to give yellow precipitate. The solid was collected and dried in *vacuo* to yield $[dp(3,5\text{-}CF_3)pf]PtCl_2$ (330 mg, 91% yield).

Step 2: In a nitrogen filled glovebox, to a 10 mL scintillation vial with a magnetic stir bar were added $[dp(4\text{-}CF_3)pf]PtCl_2$ (200 mg, 0.15 mmol), silver trifluoromethanesulfonate (39 mg, 0.15 mmol), dimethylphosphine oxide (12 mg, 0.15 mmol) and 2 mL CH_2Cl_2. Then the vial was taken outside of the glovebox and was stirred at room temperature for 3 hours. The orange solution was filtered and CH_2Cl_2 was evaporated to provide orange solid, which was recrystallized through CH_2Cl_2 and Hexane to give yellow precipitate. The solid was collected and dried in vacuo to yield catalyst **2e** (171 mg, 73% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (s, 4H), 8.16 (d, *J* = 13.5 Hz, 4H), 8.05 (d, *J* = 11.3 Hz, 4H), 4.74 (s, 2H), 4.61 (s, 2H), 4.35 (d, *J* = 1.7 Hz, 2H), 3.91 (d, *J* = 1.7 Hz, 2H), 1.86 (d, *J* = 9.6 Hz, 6H).

^{13}C NMR (101 MHz, CD_2Cl_2): δ 159.6 (d, *J* = 5.5 Hz), 159.5 (d, *J* = 6.6 Hz), 140.9, 140.7, 134.0, 139.6, 126.2 (d, *J* = 19.0 Hz), 125.0 (d, *J* = 19.3 Hz), 108.4 (d, *J* = 8.0 Hz), 107.8 (d, *J* = 8.0 Hz), 75.5– 75.00 (m), 74.34(d, *J* = 8.4 Hz), 74.0 (d, *J* = 9.4 Hz), 19.2 (d, *J* = 5.1 Hz), 18.8 (d, *J* = 5.1 Hz), 13.8, 13.8 ppm

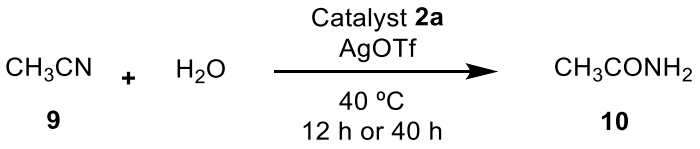
^{31}P NMR (162 MHz, CD_2Cl_2): δ 102.40 (d, *J* = 17.8 Hz), 99.41 (d, *J* = 18.9 Hz), 93.75 (d, *J* = 18.6 Hz), 90.76 (d, *J* = 18.6 Hz), 85.10 (d, *J* = 18.8 Hz), 82.11 (d, *J* = 18.8 Hz), -2.95 (d, *J* = 19.5 Hz), -5.93 (d, *J* = 19.7 Hz), -9.63 (d, *J* = 19.6 Hz), -12.02 (t, *J* = 18.9 Hz), -12.62 (d, *J* = 19.5 Hz), -16.31 (d, *J* = 20.5 Hz), -19.30 (d, *J* = 19.4 Hz), -23.89 (t, *J* = 19.1 Hz), -35.76 (t, *J* = 19.1 Hz) ppm

^{19}F NMR (282 MHz, CD_2Cl_2): δ -79.0 (d, *J* = 3.2 Hz) ppm

HRMS (ESI+): $[C44H27ClF24FeOP3Pt]^+$: 1405.9577, found 1405.9560.

5. Hydration of nitriles and cyanohydrins by catalyst 2a and 2c

5.1. Hydration of acetonitrile (9) with catalyst 2a and AgOTf at 40 °C

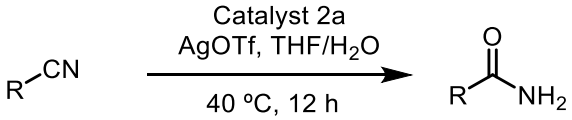


To a 20 mL scintillation vial with magnetic stir bar was added catalyst **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), acetonitrile (86.16 mmol, 4.50 mL) and water (2.1 mL). The reaction mixture was then warmed up to 40 ℃ and was stirred for 12 hours. After then, the solvent was evaporated by rotary evaporator under reduced pressure. The solid collected was washed by diethyl ether twice (5 mL for each) and amide **10** (59.30 mmol, 3.503 g, 69% yield, 5930 TON) was obtained.
To a 20 mL scintillation vial with magnetic stir bar was added catalyst **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), acetonitrile (162.75 mmol, 8.5 mL) and water (4 mL). The reaction mixture was then warmed up to 40 ℃ and was stirred for 40 hours. After then, the solvent was evaporated by rotary evaporator under reduced pressure. The solid collected was washed by diethyl ether twice (10 mL for each) and amide **10** (127.12 mmol, 7.508g, 78% yield, 12712 TON) was obtained.
^{1}H NMR (500 MHz, Deuterium Oxide): δ 6.01 (d, *J* = 39.7 Hz, 2H), 1.99 (d, *J* = 0.5 Hz, 3H).

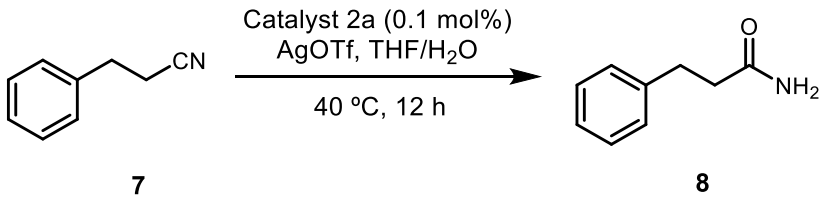
^{13}C NMR (126 MHz, $CDCl_3$): δ 173.3, 22.7 ppm

HRMS (ESI+): calc'd for C9H11NO $[M+H]^+$: 60.0474, found 60.0449.

5.2. General procedure I for hydration of nitriles with catalyst 2a and AgOTf at 40 °C

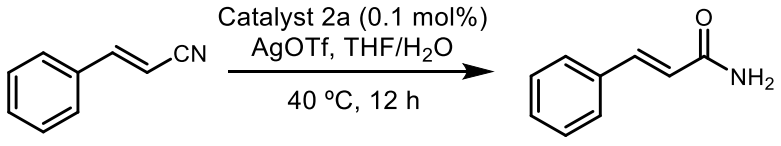


In a nitrogen filled glovebox, to an 8 mL vial with a magnetic stir bar were added catalyst 2a (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), THF (2 mL) and water (2 mL). The mixture was stirred for 2 minutes, then the vial was taken outside of the glovebox and nitriles (10 mmol or 4 mmol) were added. The reaction mixture was then warmed up to 40 ℃ and was stirred for 12 hours. After then, it was diluted with water (5 mL) and extracted by ethyl acetate twice (10 mL for each). The combined organic layer was washed with brine (10 mL), and then solvent was removed by rotary evaporator to produce the crude products, which were purified by recrystallization. The products were obtained in 52%-98% yields with TONs ranging from 207 to 981.



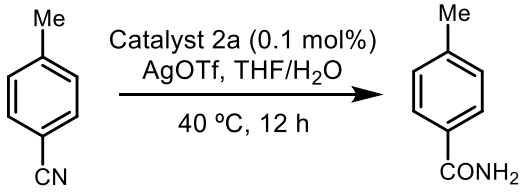
The general procedure I was followed. The desired product **8** (1.46 g, 98% yield, 980 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/3 mL).

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.31-9.21 (m, 2H), 9.22-9.09 (m, 3H), 7.92 (s, 1H), 7.62 (s, 1H), 4.93-4.89 (t, *J* = 7.6 Hz, 2H), 4.47 (t, *J* = 7.6 Hz, 2H) ppm
^{13}C NMR (126 MHz, $CDCl_3$): δ 176.5, 143.0, 130.3, 130.2, 128.0, 39.2, 33.2 ppm
HRMS (ESI+): calc'd for C9H11NO $[M+H]^+$: 150.0913, found 150.0911



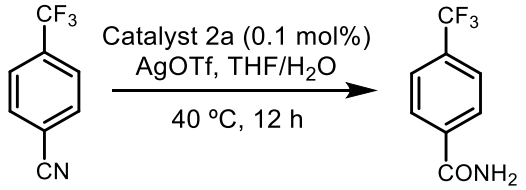
11 **11p**

The general procedure I was followed. The desired product **11p** (1.44 g, 98% yield, 981 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/4 mL).
^{1}H NMR (500 MHz, DMSO-d_6): δ 7.57-7.51 (m, 3H), 7.43-7.33 (m, 4H), 7.11 (s, 1H), 6.60 (d, *J* = 15.9 Hz, 1H) **ppm**
^{13}C NMR (126 MHz, DMSO-d_6): δ 167.1, 139.6, 135.3, 129.9, 129.4, 128.0, 122.8 ppm
HRMS (ESI+): calc'd for C9H9NO $[M+H]^+$: 148.0757, found 148.0760.



12 **12p**

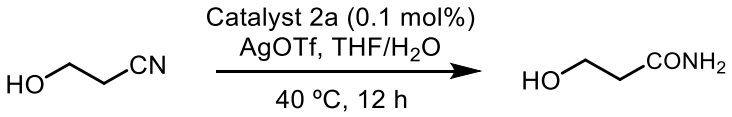
The general procedure I was followed. The desired product **12p** (1.25 g, 93% yield, 926 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/2 mL).
^{1}H NMR (500 MHz, DMSO-d_6): δ 7.91 (s, 1H), 7.79 (d, *J* = 8.2 Hz, 2H), 7.29 (s, 1H), 7.27-7.23 (m, 2H), 2.36 (s, 3H) ppm
^{13}C NMR (126 MHz, DMSO-d_6): δ 168.2, 141.5, 131.9, 129.2, 127.93, 21.4 ppm
HRMS (ESI+): calc'd for C8H9NO $[M+H]^+$: 136.0757, found 136.0757.



13 **13p**

The general procedure I was followed. The desired product **13p** (1.64 g, 96% yield, 960 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/4 mL).
^{1}H NMR (500 MHz, DMSO-d_6): δ 8.19 (s, 1H), 8.06-8.03 (m, 2H), 7.84-7.78 (m, 2H), 7.62 (s, 1H) ppm
^{13}C NMR (126 MHz, DMSO-d_6): δ 167.1, 138.5, 131.6 (q, *J* = 32.0 Hz), 128.75, 125.7 (q, *J* = 3.8 Hz), 124.4 (q, *J* = 273.4 Hz) ppm

HRMS (ESI+): calc'd for C8H7F3NO $[M+H]^+$: 190.0474, found 190.0470.



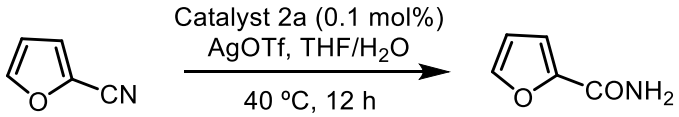
14 **14p**

The general procedure I was followed. The desired product **14p** (0.82 g, 92% yield, 921 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/4 mL).

^{1}H NMR (500 MHz, Deuterium Oxide): δ 3.72 (t, *J* = 6.1 Hz, 2H), 2.38 (t, *J* = 6.1 Hz, 2H) ppm

^{13}C NMR (126 MHz, Deuterium Oxide): δ 177.3, 57.7, 37.7 ppm

HRMS (ESI+): calc'd for C3H7NO2 $[M+H]^+$: 90.0555, found 90.0555.



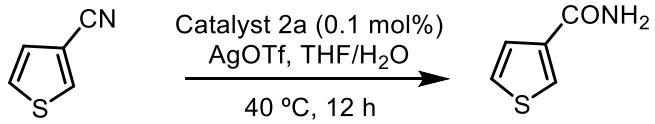
15 **15p**

The general procedure I was followed. The desired product **15p** (1.21 g, 96% yield, 960 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/3 mL).

^{1}H NMR (500 MHz, DMSO-d_6): δ 7.81 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.78 (bs, 1H), 7.38 (bs, 1H), 7.10 (dd, *J* = 3.4, 0.8 Hz, 1H), 6.60 (dd, *J* = 3.4, 1.7 Hz, 1H) ppm

^{13}C NMR (126 MHz, DMSO-d_6): δ 159.8, 148.5, 145.4, 114.0, 112.2 ppm

HRMS (ESI+): calc'd for C5H5NO2 $[M+H]^+$: 112.0399, found 112.0411



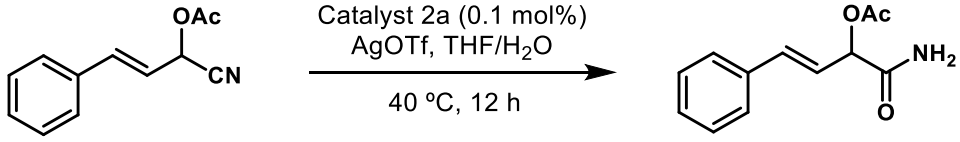
16 **16p**

The general procedure I was followed. The desired product **16p** (1.21 g, 96% yield, 960 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/3 mL).

^{1}H NMR (500 MHz, DMSO-d_6): δ 8.14 (dd, *J* = 3.0, 1.3 Hz, 1H), 7.80 (s, 1H), 7.56 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.49 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.25 (s, 1H) ppm.

^{13}C NMR (126 MHz, DMSO-d_6): δ 164.1, 138.4, 129.5, 127.6, 127.0 ppm

HRMS (ESI+): calc'd for C5H5NOS $[M+H]^+$: 128.0165, found 128.0168



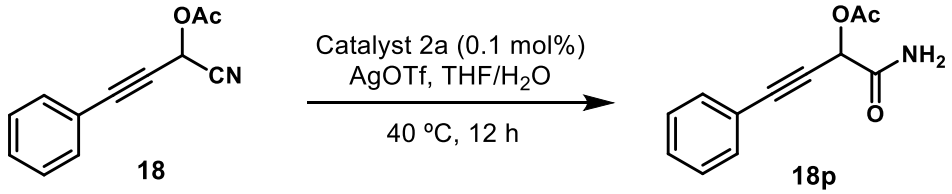
17 **17p**

The general procedure I was followed. The reaction was performed with catalyst **2a** (1 mg, 0.001 mmol), silver trifluoromethanesulfonate (0.26 mg, 0.001 mmol), (*E*)-1-cyano-3-phenylallyl acetate **17** (201 mg, 1 mmol). The desired product **17p** (188 mg, 86% yield, 860 TON) was obtained

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 – 7.27 (m, 5H), 6.78 (d, *J* = 15.9 Hz, 1H), 6.27 (dd, *J* = 15.9, 7.1 Hz, 1H), 6.10 (s, 1H), 5.76 (dd, *J* = 7.1, 1.2 Hz, 2H), 2.21 (s, 3H) ppm

^{13}C NMR (101 MHz, $CDCl_3$): δ 170.6, 169.3, 135.4, 128.7, 128.6, 126.9, 122.0, 74.2, 21.0 ppm.

HRMS (ESI+): calc'd for C12H13NNaO3 $[M+Na]^+$: 242.0788, found 242.0788



Preparation of substrate **18**: Phenylpropiolaldehyde (1.0 g, 7.69mmol), TMSCN (0.84g, 8.84mmol) were mixed neat, and LiCl (1 mg, cat.) was added. The resulting mixture was stirred at rt under Ar. After 1h, the reaction mixture was evaporated under vacuum, and the residue was dissolved in Ac_2O (1 mL). Scandium(III) trifluoromethanesulfonate (5 % mol) was added. After stirring for 1 h, the reaction mixture was purified by flash chromatography (EA/Hex = 1/10) to give **18** (1.22g, 82%).

1H NMR (400 MHz, CDCl3) δ 7.55 – 7.33 (m, 5H), 6.28 (s, 1H), 2.22 (s, 3H) ppm

13C NMR (101 MHz, CDCl3) δ 168.4, 132.2, 130.1, 128.6, 120.2, 113.5, 88.7, 51.0, 20.3 ppm

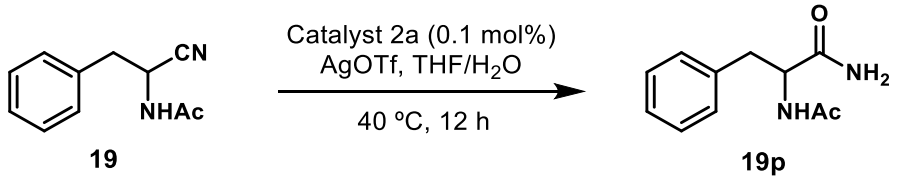
HRMS (ESI+): calc'd for C12H10NO2 $[M+H]^+$: 200.0706, found 200.0706.

Hydration of **18**: the general procedure I was followed. The reaction was performed with catalyst **2a** (1 mg, 0.001 mmol), silver trifluoromethanesulfonate (0.26 mg, 0.001 mmol) and **18** (199 mg, 1 mmol). The desired product **18p** (200 mg, 92% yield, 920 TON) was obtained.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 – 7.29 (m, 5H), 6.28 (d, *J* = 45.1 Hz, 2H), 2.22 (s, 3H) ppm

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.1, 167.5, 132.1, 129.4, 128.4, 121.2, 87.5, 81.5, 63.8, 20.8 ppm

HRMS (ESI+): calc'd for C12H11NNaO3 $[M+Na]^+$: 240.0631, found 240.0628

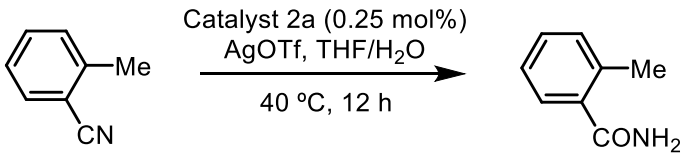


The general procedure I was followed. The reaction was performed with catalyst **2a** (0.3 mg, 0.0003 mmol), silver trifluoromethanesulfonate (0.07 mg, 0.0003 mmol), N-(1-cyano-2-phenylethyl)acetamide **19** (56 mg, 0.3 mmol). The desired product **19p** (38 mg, 61% yield, 610 TON) was obtained.

^{1}H NMR (400 MHz, DMSO): δ 8.03 (d, *J* = 8.5 Hz, 1H), 7.44 (s, 1H), 7.33 – 7.14 (m, 5H), 7.03 (s, 1H), 4.41 (td, *J* = 9.6, 4.7 Hz, 1H), 2.98 (dd, *J* = 13.7, 4.7 Hz, 1H), 2.71 (dt, *J* = 17.4, 8.7 Hz, 1H), 1.75 (s, 3H) ppm

^{13}C NMR (101 MHz, DMSO) δ 173.6, 169.5, 138.7, 129.6, 128.5, 126.6, 54.3, 38.1, 23.0 ppm

HRMS (ESI+): calc'd for C11H15N2O2 $[M+H]^+$: 207.1128, found 207.1128.



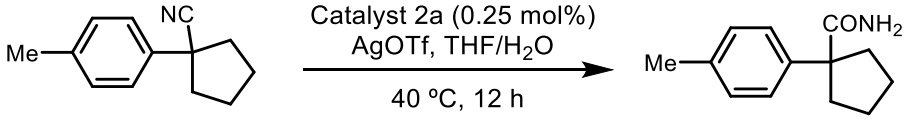
20 **20p**

The general procedure I was followed. The desired product **20p** (520 mg, 96% yield, 385 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (3 mL/3 mL).

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.48 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.38 (td, *J* = 7.5, 1.5 Hz, 1H), 7.30-7.23 (m, 2H), 6.17-5.19 (m, 2H), 2.51 (s, 3H) ppm

^{13}C NMR (126 MHz, CD_2Cl_2): δ 171.5, 136.3, 135.4, 131.1, 130.1, 126.8, 125.6, 19.7 ppm

HRMS (ESI+): calc'd for C8H9NO $[M+H]^+$: 136.0757, found 136.0753.



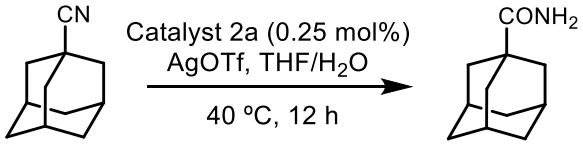
21 **21p**

The general procedure I was followed. The desired product **21p** (420 mg, 52% yield, 207 TON) was obtained after recrystallization by CH_2Cl_2/Hexane (2 mL/4 mL).

^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.32-7.28 (m, 2H), 7.22-7.18 (m, 2H), 5.52 (s, 1H), 5.28 (s, 1H), 2.52-2.42 (m, 2H), 2.37 (d, *J* = 0.6 Hz, 3H), 2.08-1.99 (m, 2H), 1.88-1.77 (m, 2H), 1.76-1.66 (m, 2H) ppm

^{13}C NMR (126 MHz, CD_2Cl_2): δ 178.7, 141.2, 136.5, 129.2, 126.5, 58.7, 36.6, 23.8, 20.6 ppm

HRMS (ESI+): calc'd for C13H17NO $[M+H]^+$: 204.1383, found 204.1386



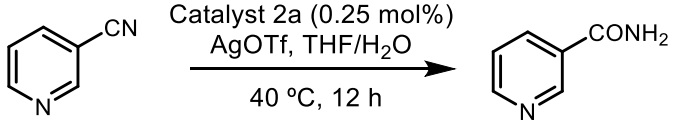
22 **22p**

The general procedure I was followed. The desired product **22p** (658 mg, 92% yield, 368 TON) was obtained after washing with Et_2O (5 mL) and recrystallization by CH_2Cl_2/Hexane (3 mL/4 mL).

^{1}H NMR (500 MHz, CD_2Cl_2): δ 5.67 (s, 2H), 2.07 (p, *J* = 3.3 Hz, 3H), 1.89 (d, *J* = 2.9 Hz, 6H), 1.87-1.71 (m, 6H) ppm

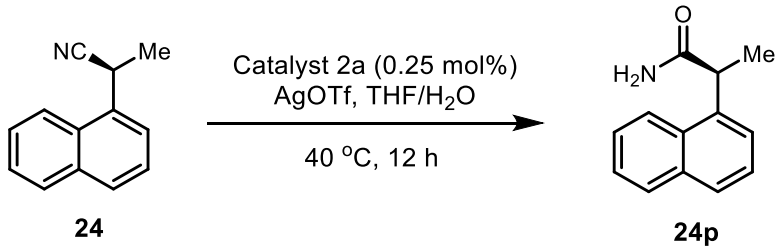
^{13}C NMR (126 MHz, CD_2Cl_2): δ 180.4, 40.5, 39.3, 36.4, 28.3 ppm

HRMS (ESI+): calc'd for C11H17NO $[M+H]^+$: 180.1383, found 180.1385



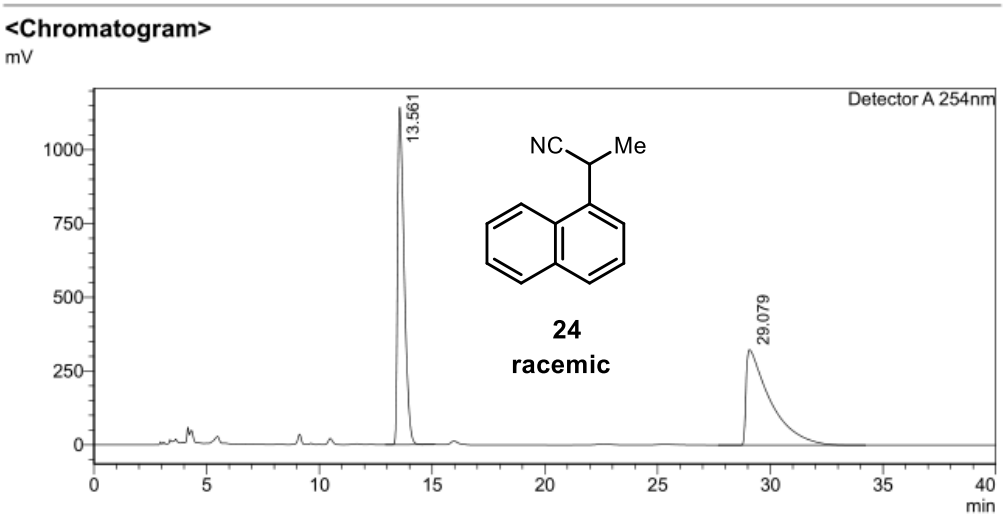
23 **23p**

The general procedure I was followed. The desired product **23p** (310 mg, 64% yield, 254 TON) was obtained after washing with Et_2O (5 mL) and recrystallization by CH_2Cl_2/Hexane (3 mL/3 mL).
^{1}H NMR (500 MHz, Deuterium Oxide): δ 8.72 (dd, *J* = 2.3, 0.9 Hz, 1H), 8.52 (dd, *J* = 5.0, 1.6 Hz, 1H), 8.04 (ddd, *J* = 8.0, 2.3, 1.6 Hz, 1H), 7.40 (ddd, *J* = 8.0, 5.0, 0.9 Hz, 1H) ppm
^{13}C NMR (126 MHz, Deuterium Oxide): δ 170.4, 151.7, 147.5, 136.3, 129.0, 124.1 ppm
HRMS (ESI+): calc'd for C6H6N2O $[M+H]^+$: 123.0553, found 123.0554.



24 **24p**

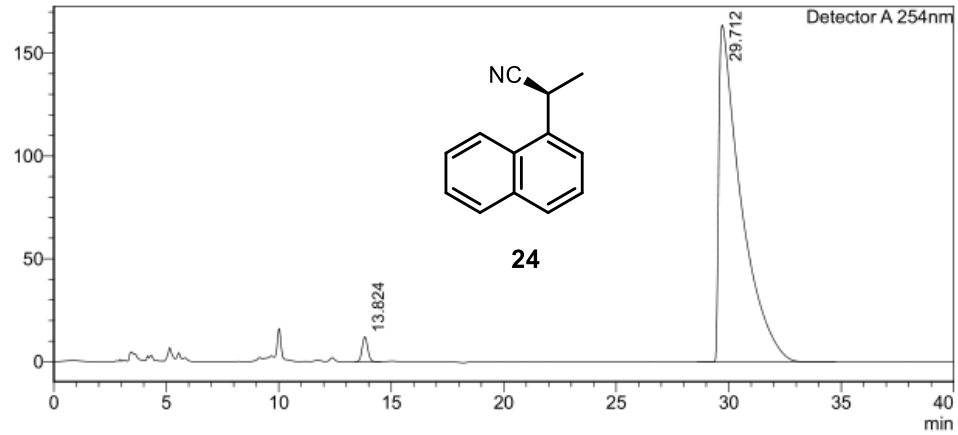
Chiral nitrile **24** (96% *ee*) was prepared following Stahl and Liu's procedure.[3]
HPLC (OD-H, 0.46*25 cm, 5μm, hexane / ethanol = 98/2, flow 1 mL/min, detection at 254 nm) retention time = 13.824 min (minor) and 29.712 min (major).



<Peak Table>
Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.561	23044349	1144191	49.117		M	
2	29.079	23873244	323152	50.883		M	
Total		46917593	1467343				

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.824	210319	12141	1.836		M	
2	29.712	11242468	163814	98.164		M	
Total		11452788	175955				

Hydration of **24**: the general procedure I was followed. The reaction was performed with catalyst 2a (1.7 mg, 0.0017mmol), silver trifluoromethanesulfonate (0.5 mg, 0.0017 mmol), (R)-2-(naphthalen-1-yl) propanenitrile **24** (120 mg, 0.662 mmol). The desired product **24p** (115 mg, 87% yield, 348 TON) was obtained with 97% *ee*.

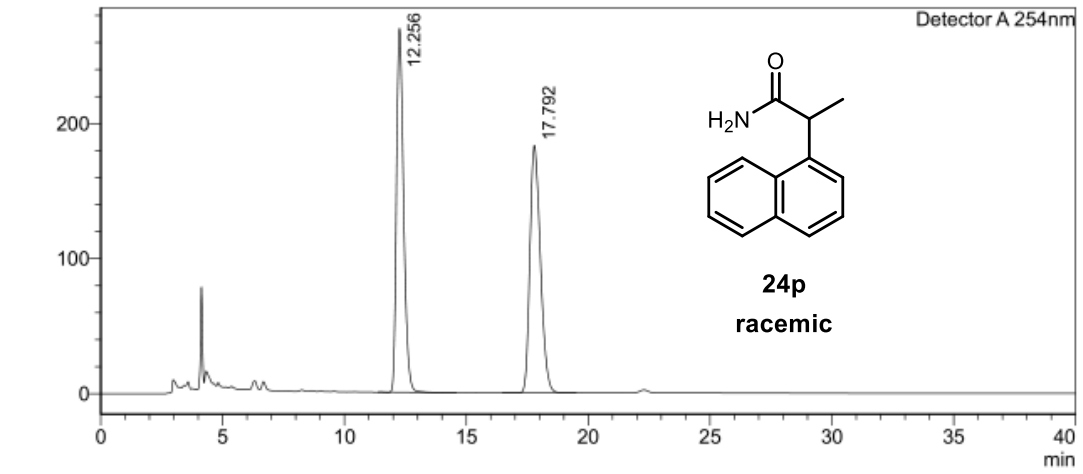
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 1H), 7.81 (d, *J* = 7.9 Hz, 1H), 7.64 – 7.42 (m, 4H), 5.29 (d, *J* = 44.6 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 1H), 1.72 (d, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 177.0, 137.0, 134.1, 131.5, 129.1, 128.3, 126.7, 126.02, 125.7, 124.9, 123.3, 43.4, 17.8 ppm.

HRMS (ESI+): calc'd for C13H13NO $[M+H]^+$200.1075, found 200.1066

HPLC (OD-H, 0.46*25 cm, 5μm, hexane / ethanol = 98/2, flow 1 mL/min, detection at 254 nm) retention time = 12.405 min (minor) and 17.702 min (major).

<Chromatogram>

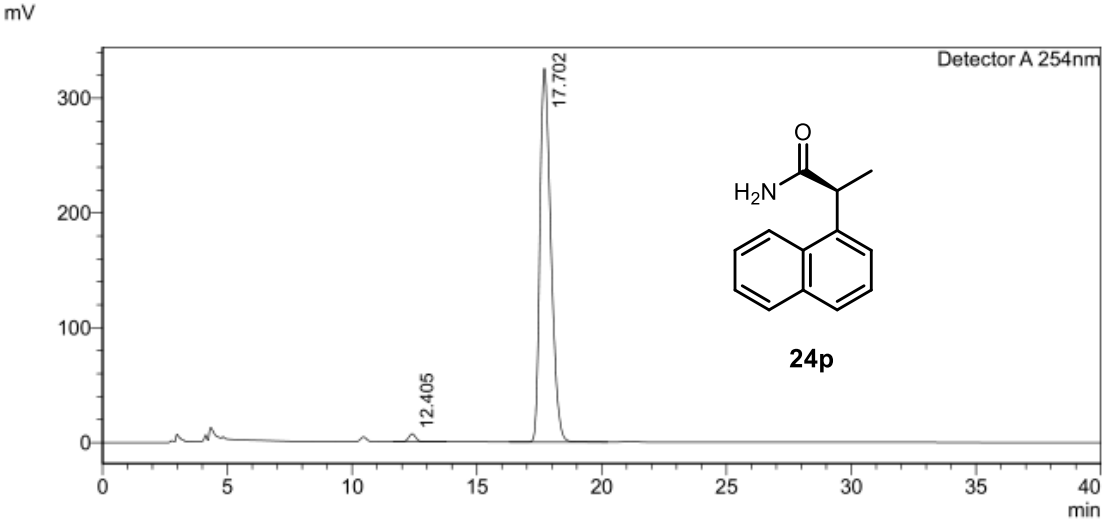


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.256	5484153	269608	49.957		M	
2	17.792	5493507	183224	50.043		M	
Total		10977660	452832				

<Chromatogram>

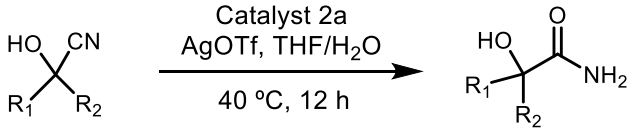


<Peak Table>

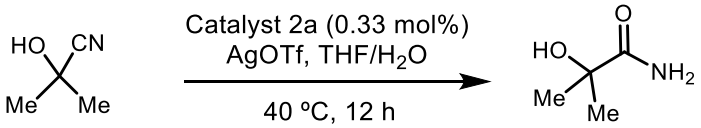
Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.405	139498	6952	1.383		M	
2	17.702	9950311	325807	98.617		M	
Total		10089809	332760				

5.3. General procedure II for hydration of cyanohydrins by catalyst 2a and AgOTf at 40 ^{o}C:



In a nitrogen filled glovebox, to a 8 mL vial with a magnetic stir bar were added **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), THF (2 mL) and water (2 mL), and the mixture was stirred for 2 minutes, then the vial was taken outside of the glovebox and cyanohydrin (2 mmol to 10 mmol) was added. The reaction mixture was then warm up to 40 ℃ and was stirred for 12 hours. After then, it was diluted with water (5 mL) and was extracted with Et_2O/CH_2Cl_2 (2:1) for twice (5 mL for each). Water was evaporated to produce crude product as white solid, which was washed with Et_2O/CH_2Cl_2 (1:1, 5 mL), and then dried in vacuo. The products were obtained in 22%-93% yield with TON ranging from 43 to 880.



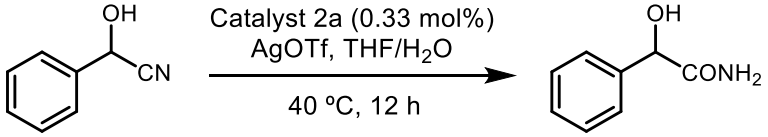
1 **1p**

The general procedure II was followed. The reaction was performed with catalyst **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), acetone cyanohydrin **1** (360 *u*L, 3 mmol). The desired product **1p** (115 mg, 37% yield, 112 TON) was obtained.

^{1}H NMR (500 MHz, DMSO-d_6): δ 7.06 (s, 1H), 6.96 (m, 1H), 1.21 (s, 6H) ppm

^{13}C NMR (126 MHz, DMSO-d_6): δ 179.5, 72.1, 28.1 ppm

HRMS (ESI+): calc'd for C4H10NO2 $[M+H]^+$: 104.0706, found 104.0705.



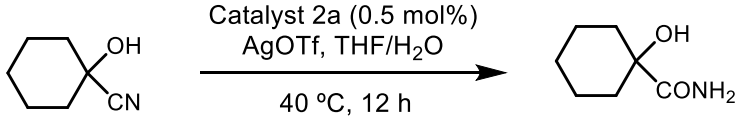
2 **2p**

The general procedure II was followed. The reaction was performed with catalyst **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), mandelonitrile (360 uL, 3 mmol). The desired product mandelamide **2p** (218 mg, 48% yield, 144 TON) was obtained.

^{1}H NMR (500 MHz, DMSO-d_6): δ 7.46-7.38 (m, 3H), 7.35-7.31 (m, 2H), 7.30-7.23 (m, 1H), 7.19 (s, 1H), 6.02 (d, *J* = 3.8 Hz, 1H), 4.85 (s, 1H) ppm

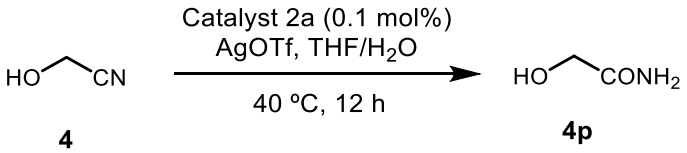
^{13}C NMR (126 MHz, DMSO-d_6): δ 175.0, 141.8, 128.3, 127.7, 126.9, 73.9 ppm

HRMS (ESI+): calc'd for C8H10NO2 $[M+H]^+$: 152.0706, found 152.0695.

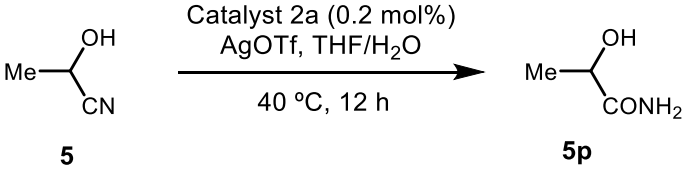


3 **3p**

The general procedure II was followed. The reaction was performed with catalyst **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), cyclohexanone cyanohydrin **3** (250 mg, 2 mmol). The desired product **3p** (61 mg, 22% yield, 43 TON) was obtained.
^{1}H NMR (500 MHz, Deuterium Oxide): δ 1.61 (td, *J* = 13.7, 4.6 Hz, 2H), 1.56-1.29 (m, 6H), 1.10 (qt, *J* = 12.7, 3.9 Hz, 1H) ppm
^{13}C NMR (126 MHz, Deuterium Oxide): δ 183.4, 75.0, 32.9, 24.5, 20.3 ppm
HRMS (ESI+): calc'd for C7H13NO2 $[M+H]^+$: 144.1019, found 144.1019.

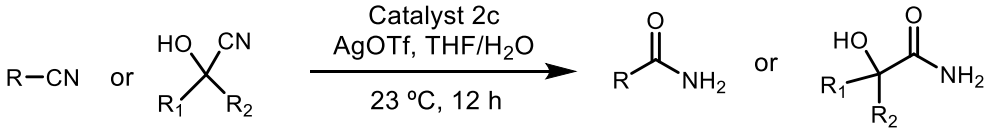


The general procedure II was followed. The reaction was performed with catalyst **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), and glycolic acid nitrile **4** (760 uL, 70% in water, 10 mmol). The desired product **4p** (660 mg, 88% yield, 880 TON) was obtained.
^{1}H NMR (500 MHz, Deuterium Oxide): δ 3.96 (s, 2H) ppm
^{13}C NMR (126 MHz, Deuterium Oxide): δ 178.0, 60.5 ppm
HRMS (ESI+): calc'd for C2H5NO2 $[M+H]^+$: 76.0399, found 76.0417.



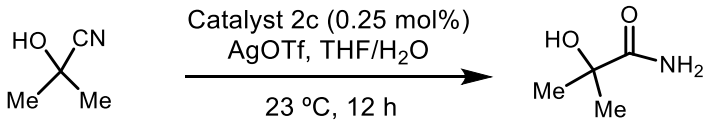
The general procedure II was followed. The reaction was performed with catalyst **2a** (10 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), and lactonitrile **5** (350 uL, 5 mmol). The desired product **5p** (412 mg, 93% yield, 463 TON) was obtained.
^{1}H NMR (500 MHz, DMSO-d_6): δ 7.12 (s, 1H), 7.06 (s, 1H), 5.32 (d, *J* = 4.9 Hz, 1H), 3.90 (qd, *J* = 6.8, 4.9 Hz, 1H), 1.21 (d, *J* = 6.8 Hz, 3H) ppm
^{13}C NMR (126 MHz, DMSO-d_6): δ 177.5, 67.5, 21.4 ppm
HRMS (ESI+): calc'd for C3H7NO2 $[M+H]^+$: 90.0555, found 90.0549.

5.4. General procedure III for hydration of nitriles and cyanohydrins by using catalyst 2c and AgOTf at room temperature:



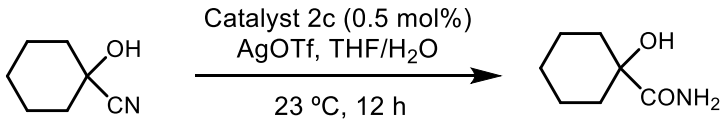
Hydration of nitriles and cyanohydrins with catalyst **2c** (catalyst loading 0.1%-0.5%) was following **general procedure I and II** respectively with exception of performing the reactions at room

temperature. For nitriles, the products were obtained in 45%-95% yields with TONs ranging from 156 to 950; for cyanohydrins, the products were obtained in 37%-98% yields with TONs ranging from 74 to 395.



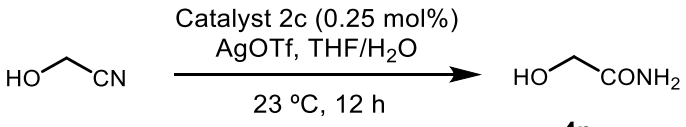
1 **1p**

The reaction was performed with catalyst **2c** (10.3 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), acetone cyanohydrin **1** (370 uL, 4 mmol). The desired product **1p** (223 mg, 54% yield, 216 TON) was obtained.



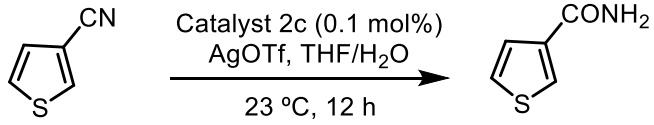
3 **3p**

The reaction was performed with catalyst 2c (10.3 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), cyclohexanone cyanohydrin **3** (250 mg, 2 mmol). The desired product **3p** (106 mg, 37% yield, 74 TON) was obtained.



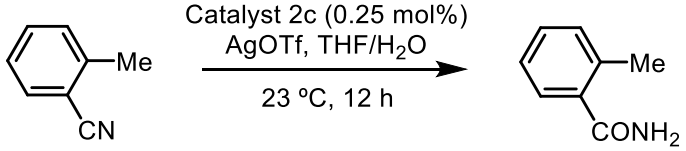
4 **4p**

The reaction was performed with catalyst 2c (10.3 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), glycolic acid nitrile **4** (300 uL, 4 mmol, 70% in water). The desired product **4p** (295 mg, 98% yield, 395 TON) was obtained.



16 **16p**

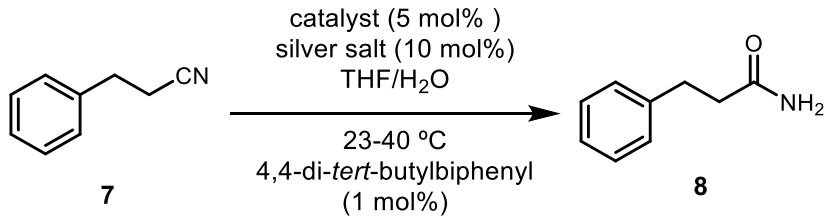
The reaction was performed with catalyst 2c (10.3 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), 3-thiophenecarbontrile **16** (900 *u*L, 10 mmol). The desired product **16p** (1.21 g, 95% yield, 950 TON) was obtained.



17 **17p**

The reaction was performed with catalyst **2c** (10.3 mg, 0.01 mmol), silver trifluoromethanesulfonate (2.6 mg, 0.01 mmol), *o*-tolunitrile **17** (480 uL, 4 mmol). The desired product **17p** (210 mg, 45% yield, 156 TON) was obtained.

6. Rate comparison experiments with different catalysts



In order to investigate the relative reaction rates with different hydration catalysts, hydrocinnamonitrile (**7)** was selected as our module substrate and it was prepared as 1 M solution in THF with 1% mmol 4,4′-di-*tert*-butylbiphenyl as internal standard. Six reactions were performed in parallel (generally in 0.5 mL THF and 0.5 mL H_2O, 0.2 mmol scale).

1) Parkins catalyst (**1a**) at 40 ℃ (0.5 mL EtOH, 0.5 mL H_2O);

2) catalyst **2a** without additives at 40 ℃;

3) catalyst **2b** and $AgBF_4$ at room temperature;

4) catalyst **2a** and AgOTf at 40 ℃;

5) catalyst **2b** and $AgBF_4$ at 40 ℃;

6) catalyst **2c** and AgOTf at room temperature.

Samples were taken at indicated times and they were monitored by UHPLC-LCMS, and the conversion was obtained by calculating relative peak area based on internal standard. The data was described below:

Table 2. Reaction conversions of the six hydration reactions of **7**

Entry	Catalyst	Temperature	additive	Time	Conversion
1	Parkins Catalyst	40 ºC	-	10 min 30 min 50 min 90 min 120 min 180 min 240 min 300 min	3.3% 8.3% 15.2% 34.0% 50.2% 72.3% 90.9% 100%
2	Catalyst 2a	40 ºC	-	10 min 20 min 30 min 40 min 50 min 60 min 90 min 120 min 180 min	10.2% 18.2% 28.4% 42.2% 53.7% 63.0% 84.2% 95.4% 100%
3	Catalyst 2a	40 ºC	AgOTf	5 min 10 min	75.5% 100%
4	Catalyst 2b	23 ºC	$AgBF_4$	10 min 20 min 30 min 40 min 50 min 60 min 70 min	16.4% 32.3% 49.3% 64.8% 75.1% 91.9% 100%
5	Catalyst 2b	40 ºC	$AgBF_4$	5 min 10 min	78.3% 100%
6	Catalyst 2c	23 ºC	AgOTf	5 min 10 min	85.5% 100%

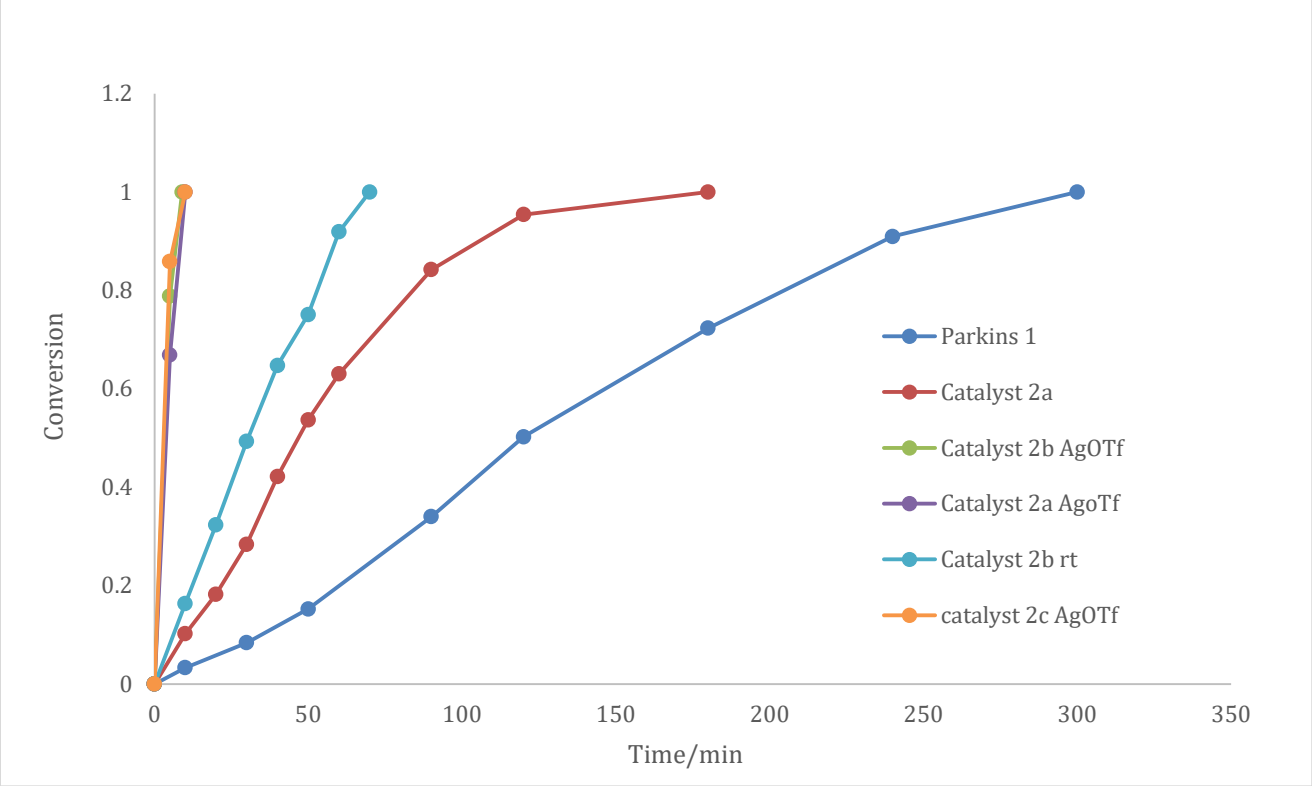


Figure 2. Comparison of the conversions of catalyst **1a** and **2a-c** in hydration of **7** within 5 h

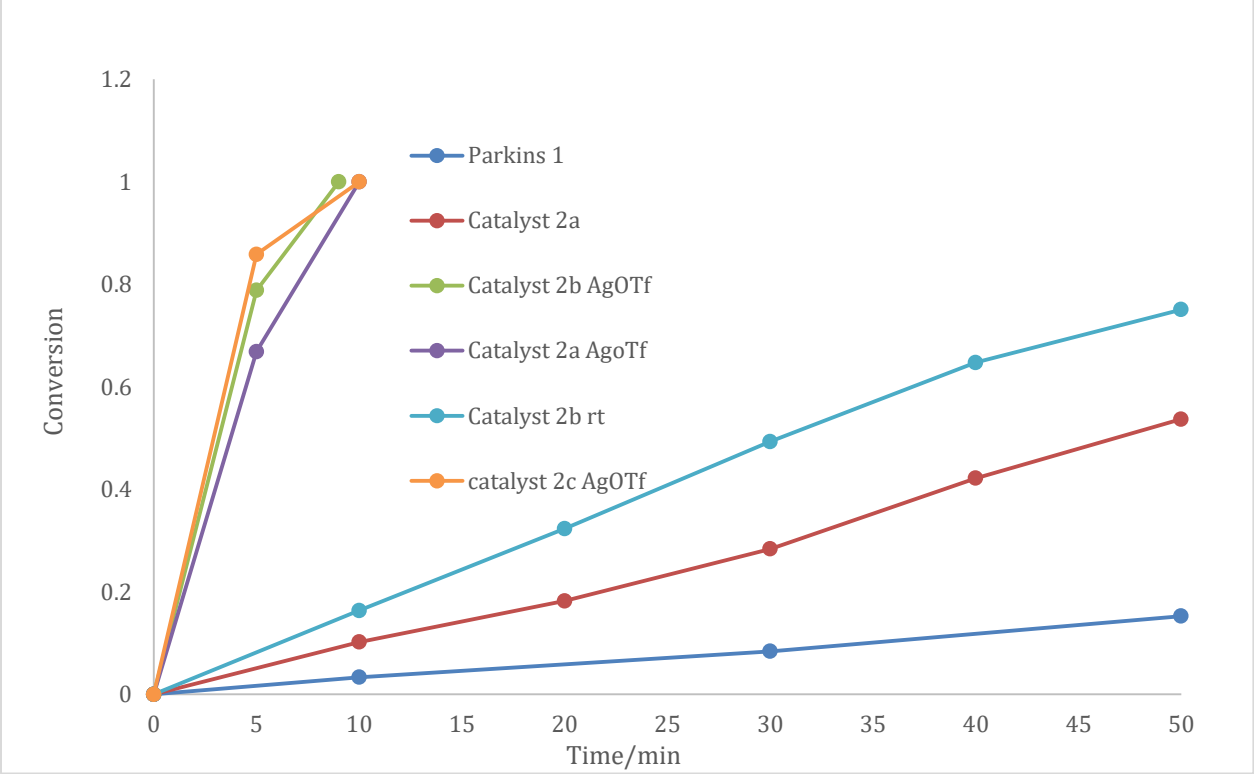
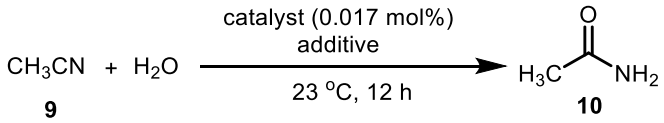


Figure 3. Comparison of the conversions of catalyst **1a** and **2a-c** in hydration of **7** within 50 min

7. Rate comparison on hydration of acetonitrile (9) at room temperature



Those reactions were performed in parallel. In a nitrogen filled glovebox, Parkins catalyst (4.3 mg, 0.01 mmol), catalyst 2a and AgOTf (10 mg, 0.01 mmol; 2.6mg, 0.01 mmol), catalyst 2c and AgOTf (10.3 mg, 0.01mmol; 2.6 mg, 0.01 mmol), catalyst 2c (10.3 mg, 0.01 mmol), were dispensed into 20 mL scintillation vials, respectively. Acetone nitrile (3.2 mL, 60 mmol) and water (1.1 mL, 60 mmol) were added to each of them. The reaction solution was taken outside of the glovebox and performed at room temperature for 12 hours. The solvent was removed by rotary evaporator to provide white solid, which was washed with CH_2Cl_2/Et_2O (1:1, 5 mL) and dried in *vacuo*. Accordingly, 48 mg, 1056 mg, 2630 mg and 410 mg of acetamides were obtained, respectively.

Table 3

Entry	Catalysts	Additives	Product (mg)	TON
1	Parkins	-	48	81
2	2a	-	1056	1790
3	2c	AgOTf	2630	4457
4	2c	-	410	695

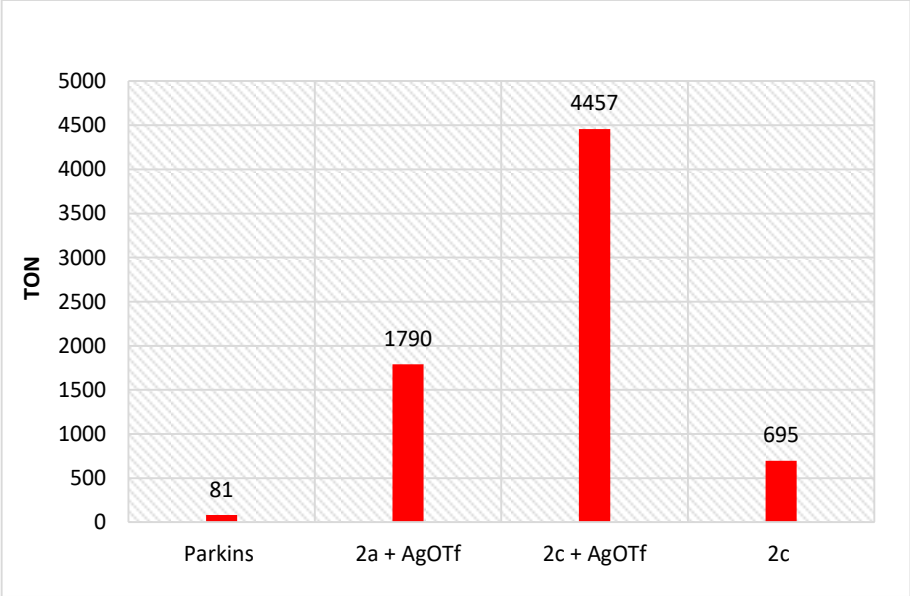
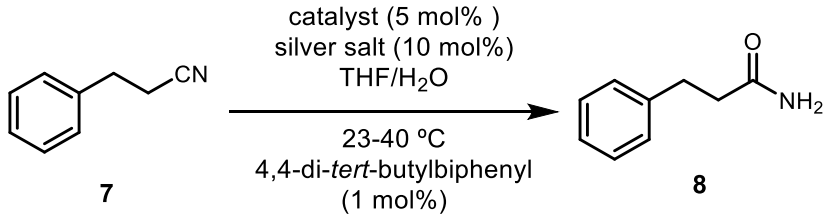


Figure 4 Comparison of TON of catalyst **1a**, **2a** and **2c** in hydration of acetonitrile at room temperature

8. Rate comparison experiments in hydration of nitrile 7 with catalysts 2a, 2c, 2d and 2e.



In order to investigate the relative reaction rates with different hydration catalysts, hydrocinnamonitrile (**7)** was selected as our module substrate and it was prepared as 1 M solution in THF with 1% mmol 4,4′-di-*tert*-butylbiphenyl as internal standard. Four reactions were performed in parallel (generally in 0.5 mL THF and 0.5 mL H_2O, 0.2 mmol scale).

1) catalyst **2a** and AgOTf at 40 ℃;

2) catalyst **2c** and AgOTf at room temperature;

3) catalyst **2d** and AgOTf at 40 ℃;

4) catalyst **2e** and AgOTf at 40 ℃.

Samples were taken at indicated times and they were monitored by UHPLC-LCMS, and the conversion was obtained by calculating relative peak area based on internal standard. The data was described below:

Table 4. Reaction conversions of the four hydration reactions of **7**

Entry	Catalyst	Temperature	additive	Time	Conversion
1	Catalyst 2a	40 ºC	AgOTf	5 min 10 min	75.5% 100%
2	Catalyst 2c	23 ºC	AgOTf	5 min 10 min	85.5% 100%
3	Catalyst 2d	40 ºC	AgOTf	10 min 20 min 30 min 40 min 50 min 60 min	37.4% 54.2% 70.4% 81.3% 91.8% 100%
4	Catalyst 2e	40 ºC	AgOTf	10 min 20 min 30 min 40 min 50 min 60 min 90 min 120 min 180 min 240 min 300 min 360min 15 h	11.3% 23.5% 33.0% 39.8% 45.4% 50.5% 57.1% 61.5% 65.5% 67.3% 68.2% 69.7% 72.6%*

*Note: after 15 hours, further conversion with catalyst **2e** is not observed.

9. X-Ray Structure Determination

Crystals were mounted on polyimide MiTeGen loops with STP Oil Treatment and placed under a nitrogen stream. Low temperature (100K) diffraction data for **2a** was collected on a Bruker AXS KAPPA APEX II diffractometer (50kV and 30mA) coupled to a APEX II CCD detector (equipped with a TRIUMPH graphite monochromator) with Mo-K_α radiation (λ = 0.71073 Å). High temperature (221K and 293K) diffraction data for **2a** was collected on a Bruker AXS D8 VENTURE KAPPA diffractometer (50 kV and 1mA) coupled to a PHOTON 100 CMOS detector (equipped with Helios focusing multilayer mirror optics) with Mo-K_α radiation (λ = 0.71073 Å). Low-temperature diffraction data (φ- and ω-scans) for **2b** and **2c** were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON 100 CMOS detector with Mo-K_α radiation (λ = 0.71073 Å) from an $I_\mu S$ micro-source. All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEXII software.[4] Absorption corrections were applied using SADABS.[5] Space groups were determined on the basis of systematic absences and intensity statistics. The structures were solved by direct methods using SHELXS or by intrinsic phasing using SHELXT[6], and were refined against F^5 on all data by full-matrix least squares with SHELXL-2014[6] using established refinement techniques.[7] All non-hydrogen atoms were refined anisotropically. Unless otherwise noted, all hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement paramet67ers of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Crystallographic data for **2a, 2b and 2c** can be obtained free of charge from The Cambridge Crystallographic Data Centre (CCDC) via www.ccdc.cam.ac.uk/data_request/cif under CCDC deposition numbers **1837963**-1**837974** Graphical representation of the structure with 50% probability thermal ellipsoids was generated using Mercury visualization software.[8]

Table 5. Crystal and refinement data for compounds 2a, 2b and 2c

	2a	**2b**	**2c**
CCDC Number	**1837963, 1837964, 1837965**	**1837973**	**1837974**
Empirical formula	$C_{37}H_{35}ClF_3FeO_4P_3PtS$	$C_{36}H_{35}BClF_4FeOP_3Pt$	$C_{33}H_{35}ClF_3FeO_8P_3PtS$
Formula weight	1012.01	949.75	1027.97
T (K)	100	100	100
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
a, Å	12.020(4)	10.6888(12)	9.1811(8)
b, Å	14.966(4)	11.6609(14)	12.1939(10)
c, Å	21.674(7)	14.5386(17)	16.6464(14)
α, °	74.877(11)	93.888(4)	87.574(4)
β, °	79.712(18)	102.803(4)	77.784(3)
γ, °	89.614(12)	97.548(4)	86.681(3)
Volume, $Å^3$	3700(2)	1742.9(4)	1817.5(3)
Z	4	2	2
d_{calc}, g/cm^3	1.817	1.810	1.878
Abs. coeff. (mm^{-1})	4.482	4.691	4.572
θ range, °	0.990 to 43.791	2.170 to 36.372	2.354 to 36.388
Abs. correction	Semi-empirical	Semi-empirical	Semi-empirical
GOF	1.007	1.181	1.020
R_1,[a] wR_2,[b] [I>2σ(I)]	0.0262, 0.0493	0.0222, 0.0510	0.0339, 0.0591

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

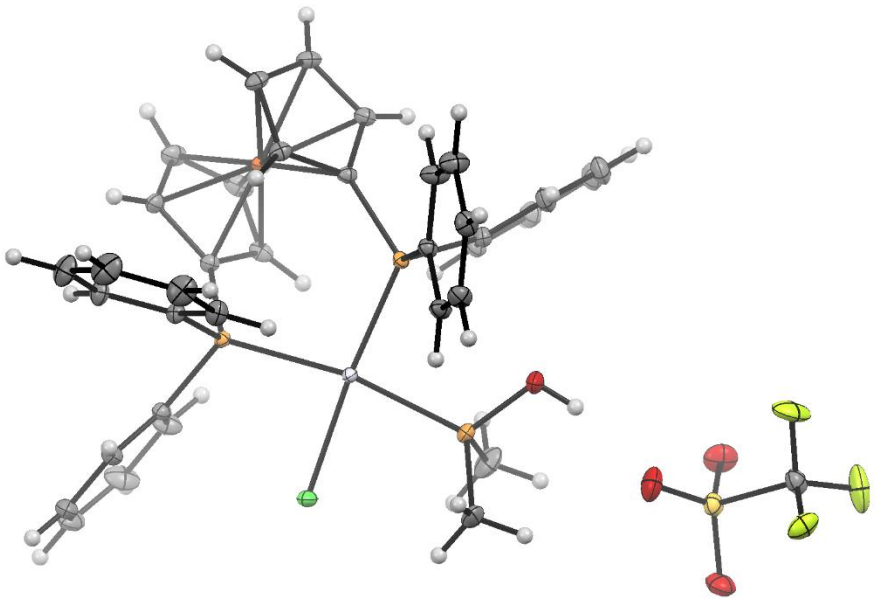


Figure 5. Structure of **2a** with 50% probability anisotropic displacement ellipsoids. The second molecule of **2a** and second triflate anion are not shown for clarity.

Special Refinement Details for 2a

Compound **2a** crystallizes in the triclinic space group *P*-1 with two complexes in the asymmetric unit. One triflate is disordered with a 78:22 ratio. The structure suggested a possible phase transition; after a variable temperature unit cell determination showed a doubling of the c-axis as the temperature decreases, additional data sets were collected at 221 and 293K on another crystal to see if the triflates would be ordered. The structure is still P-1 but with a Z' now of 1 instead of 2 as at 100K. However the sole triflate is still disordered, with a 56:44 ratio at 221K and a 54:46 ratio at 293K.

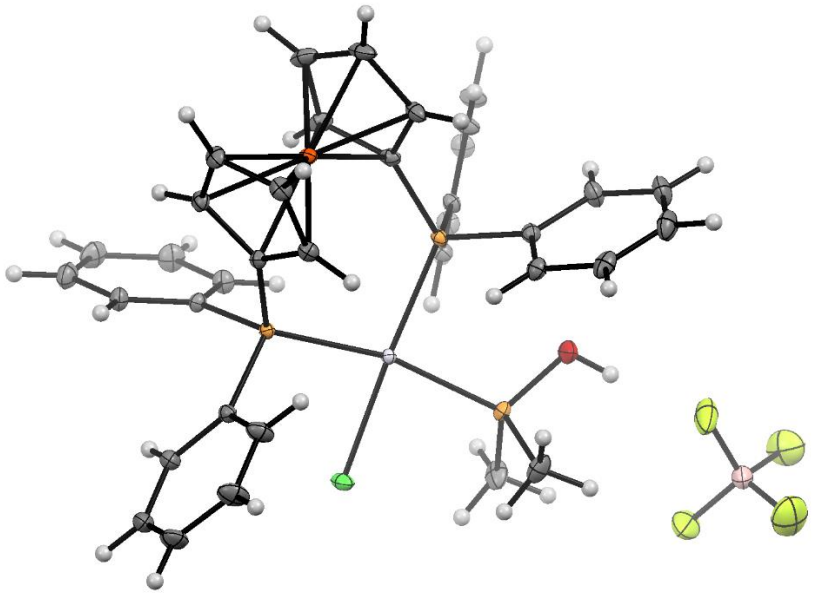


Figure 6. Structure of **2b** with 50% probability anisotropic displacement ellipsoids.

Special Refinement Details for 2b

Compound **2b** crystallizes in the triclinic space group *P*-1 with one molecule in the asymmetric unit. The hydrogen atom bound to O1 could not be located in the difference Fourier synthesis and was included into the model at geometrically calculated positions, and refined using a riding model.

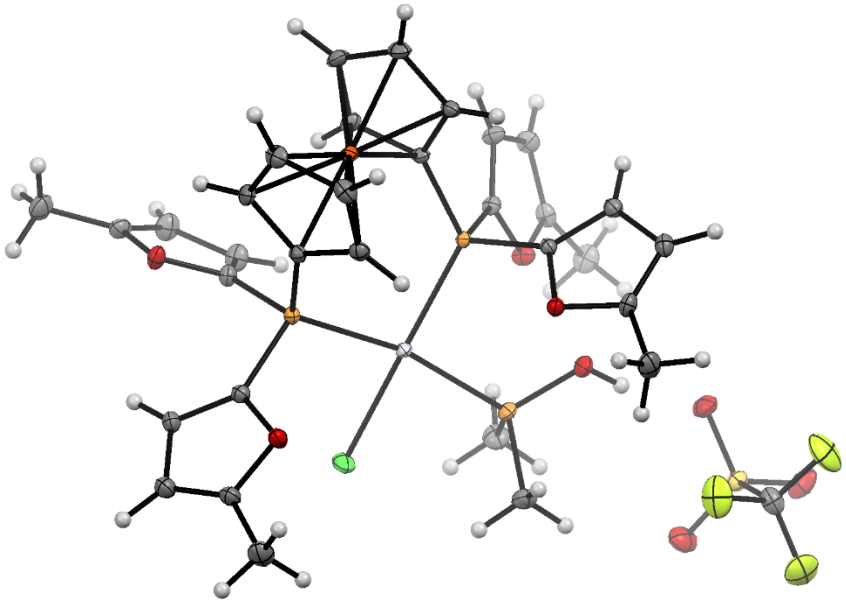


Figure 7. Structure of **2c** with 50% probability anisotropic displacement ellipsoids.

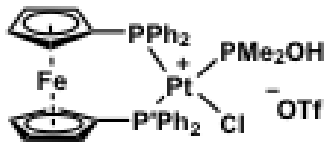
Special Refinement Details for 2c

Compound **2c** crystallizes in the triclinic space group *P*-1 with one molecule in the asymmetric unit. The coordinates for the hydrogen atom bound to O5 was located in the difference Fourier synthesis and refined semi-freely with the help of a restraint on the O-H distance (0.84(4) Å).

10. References:

[1] Collingwood, S. P.; Taylor, R. J. *Synlett*, **1998**, *3*, 283.
[2] These two ligands were made according to: Clark, J. S. K.; Voth, C. N.; Ferguson, M. J.; Stradiotto, M. *Organometallics* **2017**, *36*, 679.
[3] Zhang, W.; Wang, McCann, F. S. D.; Wang, D.; Chen, P.; Stahl, S. S.; Liu, G. *Science*, **2016**, *353*, 1014-1018.
[4] APEX2, Version 2 User Manual, M86-E01078, Bruker Analytical X-ray Systems, Madison, WI, **June 2006**.
[5] Sheldrick, G.M. *"SADABS (version 2008/1): Program for Absorption Correction for Data from Area Detector Frames"*, University of Göttingen, **2008**.
[6] Sheldrick, G. *Acta Crystallogr., Sect. A: Found. Crystallogr*. **2008**, *64*, 112.
[7] Müller, P. *Crystallogr. Rev.* **2009**, *15*, 57.
[8] Macrae, C. F.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Shields, G. P.; Taylor, R.; Towler M.; Van de Streek, J. *J. Appl. Cryst.* **2006**, *39*, 453.

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-dppfPtPMe2OH-OTf-1/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	16
Receiver Gain	48
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-09T14:31:25
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536

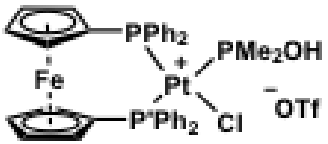


2a

CARBON01

xxy-vi-dppfPtPMe2OH-OTf-1

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-dppfPtPMe2OH-OTf-1/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1500
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-09T14:32:54
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



2a

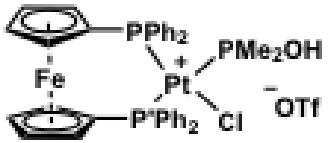
PHOSPHORUS01

xxy-vi-dppfptpme2oh

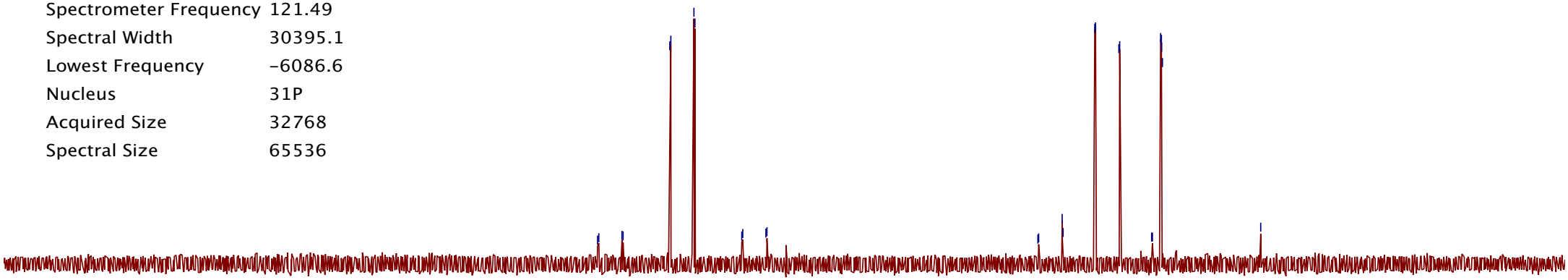
105.14 104.94 101.25 101.06 93.59 93.42 89.73 89.56 82.07 81.91 78.21 78.04

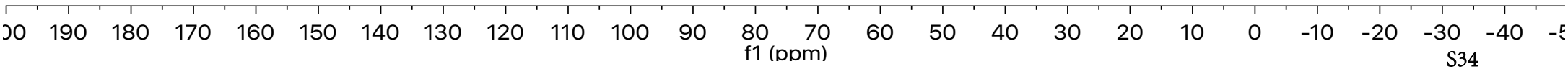
34.69 34.56 30.80 30.65 25.59 25.46 21.73 21.60 16.49 16.36 15.05 14.92 14.89 14.76 -0.97

Parameter	Value
Data File Name	/ Volumes/ nmrdata/ xiangyou/ vnmrsys/ data/ xxy-vi-dppfptpme2oh/ PHOSPHORUS01.fid/ fid
Title	PHOSPHORUS01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	ASW7284
Number of Scans	256
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	11.0000
Presaturation Frequency	
Acquisition Time	1.0781
Acquisition Date	2017-05-08T18:16:34
Spectrometer Frequency	121.49
Spectral Width	30395.1
Lowest Frequency	-6086.6
Nucleus	31P
Acquired Size	32768
Spectral Size	65536



2a





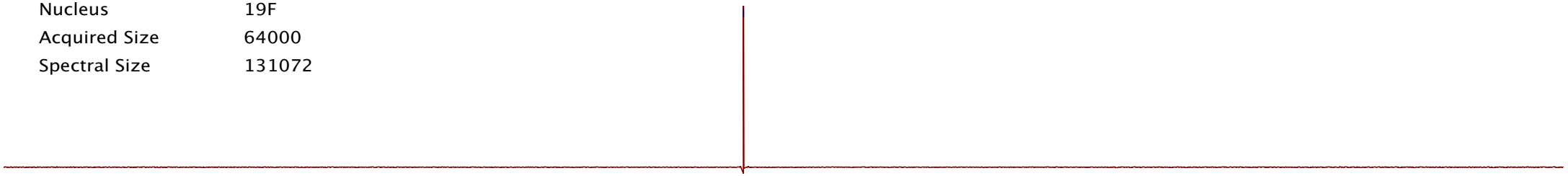
FLUORINE01

xxy-vi-dppfptpme2oh

-79.12

Parameter	Value
Data File Name	/ Volumes/ nmrdata/ xiangyou/ vnmrsys/ data/ xxy-vi-dppfptpme2oh/ FLUORINE01.fid/ fid
Title	FLUORINE01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	ASW7284
Number of Scans	256
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	6.3333
Presaturation Frequency	
Acquisition Time	0.9856
Acquisition Date	2017-05-08T18:25:38
Spectrometer Frequency	282.34
Spectral Width	64935.1
Lowest Frequency	-56468.8
Nucleus	19F
Acquired Size	64000
Spectral Size	131072

2a

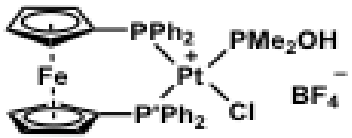


20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190

f1 (ppm)

xxy-vi-dppfPtPMe2OH-BF4.1.fid

Parameter	Value
Data File Name	/ Volumes/ nmrdata/ xiangyou/ nmr/ xxy-vi-dppfPtPMe2OH-BF4/ 1/ fid
Title	xxy-vi-dppfPtPMe2OH-BF4.1.fid
Origin	Bruker BioSpin GmbH
Solvent	CD2Cl2
Temperature	295.0
Pulse Sequence	zg30
Number of Scans	16
Receiver Gain	197.4
Relaxation Delay	1.0000
Pulse Width	11.7000
Acquisition Time	4.0894
Acquisition Date	2017-05-12T03:29:03
Spectrometer Frequency	400.13
Spectral Width	8012.8
Lowest Frequency	-1535.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



2b

xxy-vi-dppfPtPMe2OH-BF4.2.fid

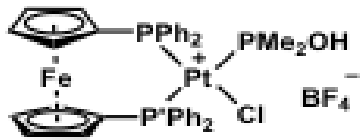
135.10 135.08 134.99 134.97 134.61 134.49 131.62 131.59 131.45 131.43 131.25 131.23 130.91 130.89 129.97 129.27 128.30 128.24 128.18 128.13

75.51 75.49 75.40 75.38 75.27 75.17 74.37 74.30 73.53 73.46

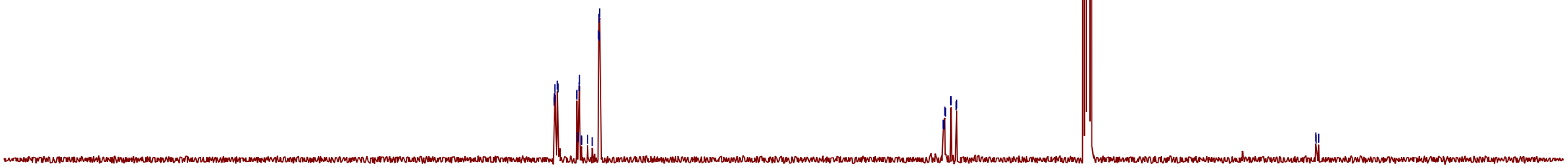
62.91

18.46 18.40 18.05 17.99

Parameter	Value
Data File Name	/ Volumes/ nmrdata/ xiangyou/ nmr/ xxy-vi-dppfPtPMe2OH-BF4/ 2/ fid
Title	xxy-vi-dppfPtPMe2OH-BF4.2.fid
Origin	Bruker BioSpin GmbH
Solvent	CD2Cl2
Temperature	294.9
Pulse Sequence	zgpg30
Number of Scans	3500
Receiver Gain	78.7
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Acquisition Date	2017-05-12T06:50:06
Spectrometer Frequency	100.62
Spectral Width	24038.5
Lowest Frequency	-1958.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



2b



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)

PHOSPHORUS01

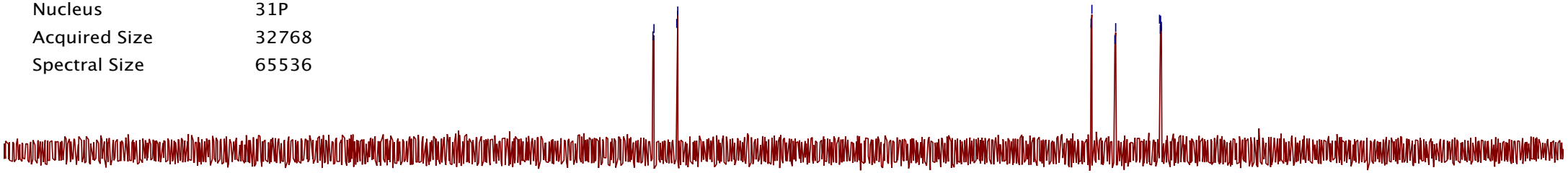
xxy-vi-dppfPt-PMe2OHBF4

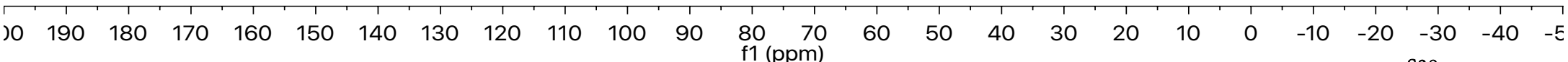
95.92
95.75
92.10
91.93

25.65
25.52
21.83
21.70
14.67
14.55
14.51
14.38

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-dppfPt-PMe2OHBF4/ PHOSPHORUS01.fid/ fid
Title	PHOSPHORUS01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	ASW7284
Number of Scans	256
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	11.0000
Presaturation Frequency	
Acquisition Time	1.0781
Acquisition Date	2017-05-08T11:01:11
Spectrometer Frequency	121.49
Spectral Width	30395.1
Lowest Frequency	-6086.6
Nucleus	31P
Acquired Size	32768
Spectral Size	65536

2b

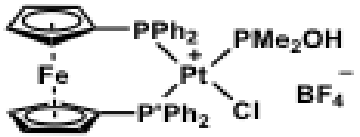




FLUORINE01

xxy-vi-dppfPt-PMe2OHBF4

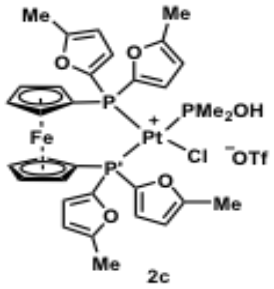
Parameter	Value
Comment	xxy-vi-dppfPt-PMe2OHBF4
Origin	Varian
Owner	
Site	
Spectrometer	mercury
Author	
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	ASW7284
Number of Scans	256
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	6.3333
Presaturation Frequency	
Acquisition Time	0.9856
Acquisition Date	2017-05-08T11:10:14
Modification Date	2017-05-08T11:18:48
Class	
Spectrometer Frequency	282.34
Spectral Width	64935.1
Lowest Frequency	-56468.8
Nucleus	19F
Acquired Size	64000
Spectral Size	131072



2b

xxy-vi-dmpfPtPMe2OH-Cl.1.fid

Parameter	Value
Title	xxy-vi-dmpfPtPMe2OH-Cl.1.fid
Origin	Bruker BioSpin GmbH
Spectrometer	spect
Solvent	CD2Cl2
Temperature	295.0
Pulse Sequence	zg30
Experiment	1D
Probe	Z122623_0045 (CPP BBO 400S1 BB-H&F-D-05 Z)
Number of Scans	32
Receiver Gain	197.4
Relaxation Delay	1.0000
Pulse Width	11.7000
Acquisition Time	4.0894
Acquisition Date	2017-07-30T23:53:11
Spectrometer Frequency	400.13
Spectral Width	8012.8
Lowest Frequency	-1535.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

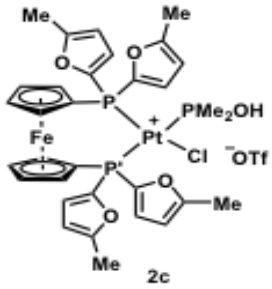


2c

XXY-VI-dmpfPtPme2OH-Cl-1.1.fid

159.66 159.61 159.49 159.42 140.86 140.68 139.99 139.64 126.29 126.10 125.09 124.89 108.46 108.38 107.81 107.73 75.42 75.32 75.19 74.38 74.30 74.05 73.95 19.24 19.19 18.83 18.78 13.79 13.76

Parameter	Value
Data File Name	/ florence/ xiangyou/ nmr/ XXY-VI-dmpfPtPme2OH-Cl-1/ 1/ fid
Title	XXY-VI-dmpfPtPme2OH-Cl-1.1.fid
Origin	Bruker BioSpin GmbH
Solvent	CD2Cl2
Temperature	295.0
Pulse Sequence	zgpg30
Number of Scans	5000
Receiver Gain	64.2
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Acquisition Date	2017-08-02T02:01:22
Spectrometer Frequency	100.62
Spectral Width	24038.5
Lowest Frequency	-1958.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

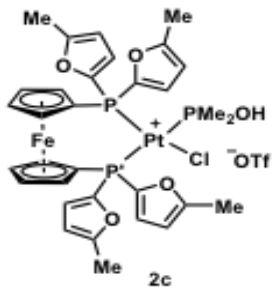


2c

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)

XXY-VI-dmpfPtPme2OH-Cl-1.2.fid



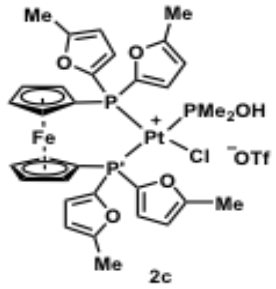
2c

Parameter	Value
Data File Name	/ florence/ xiangyou/ nmr/ XXY-VI-dmpfPtPme2OH-Cl-1/ 2/ fid
Title	XXY-VI-dmpfPtPme2OH-Cl-1.2.fid
Origin	Bruker BioSpin GmbH
Solvent	CD2Cl2
Temperature	294.9
Pulse Sequence	zgpg30
Number of Scans	256
Receiver Gain	197.4
Relaxation Delay	2.0000
Pulse Width	12.0000
Acquisition Time	0.5112
Acquisition Date	2017-08-02T02:13:40
Spectrometer Frequency	161.97
Spectral Width	64102.6
Lowest Frequency	-40150.1
Nucleus	31P
Acquired Size	32768
Spectral Size	65536

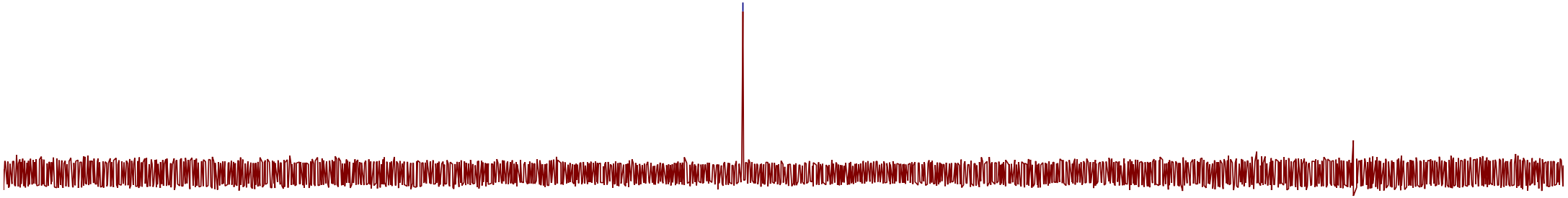
f1 (ppm)

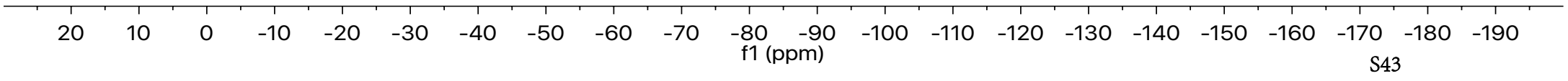
Parameter	Value
Title	FLUORINE01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	ASW7284
Number of Scans	128
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	6.3333
Presaturation Frequency	
Acquisition Time	0.9856
Acquisition Date	2017-07-31T13:35:02
Spectrometer Frequency	282.34
Spectral Width	64935.1
Lowest Frequency	-56468.8
Nucleus	19F
Acquired Size	64000
Spectral Size	131072

-79.04

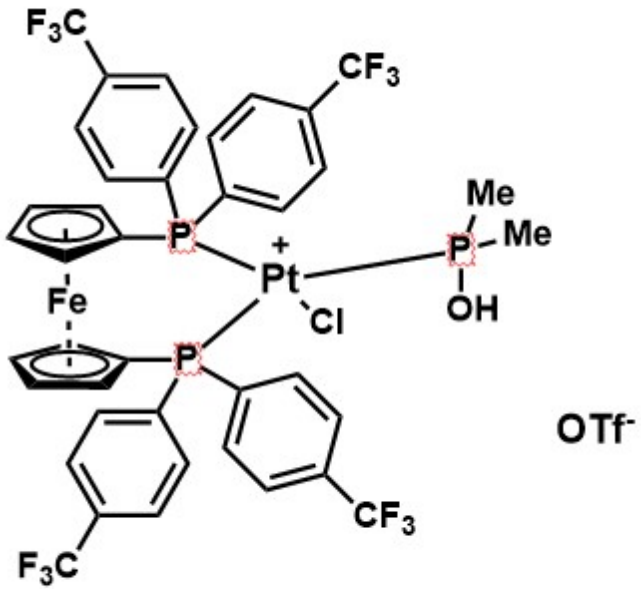


2c

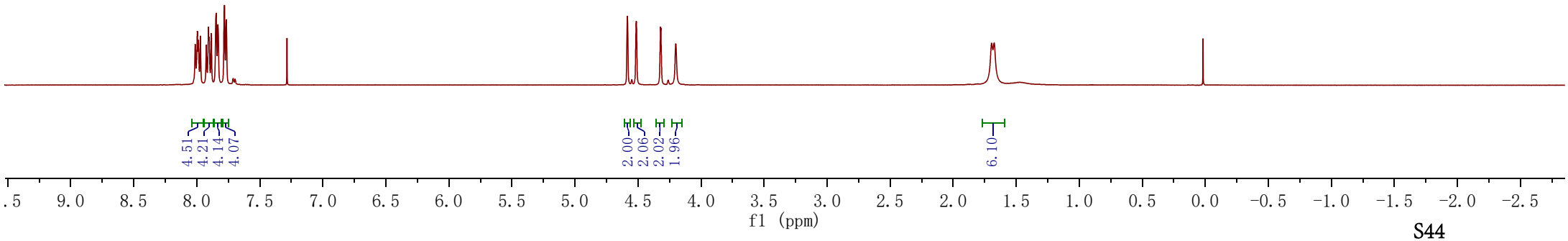




Parameter	Value
Title	chenbo-X-cat 13-0915
Comment	chenbo-X-cat 13-0915
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	296.1
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	63
Relaxation Delay	1.0000
Pulse Width	10.7100
Acquisition Time	3.2768
Acquisition Date	2018-09-15T22:20:00
Modification Date	2018-09-18T06:48:09
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-1911.5
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



2d

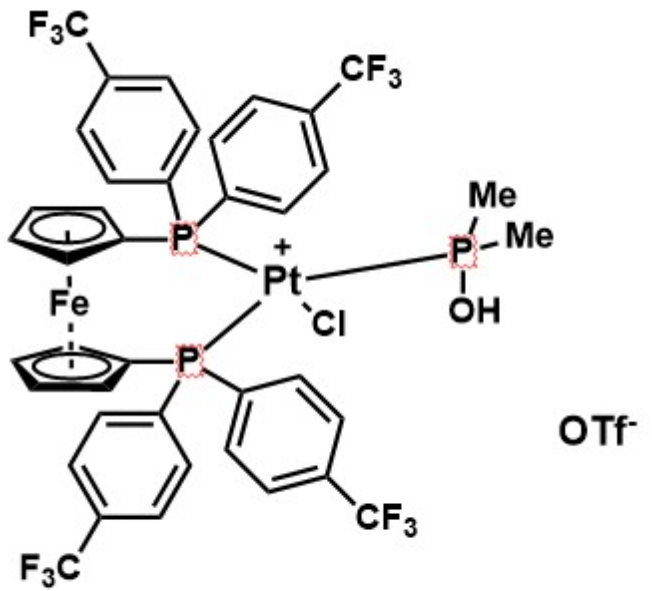


Parameter	Value
Title	chenbo-X-cat 13-0915
Comment	chenbo-X-cat 13-0915
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	296.2
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	4096
Receiver Gain	193
Relaxation Delay	2.0000
Pulse Width	9.6000
Acquisition Time	1.1010
Acquisition Date	2018-09-15T22:21:52
Modification Date	2018-09-18T06:48:09
Spectrometer Frequency	125.76
Spectral Width	29761.9
Lowest Frequency	-2305.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

135.36, 135.27, 134.52, 134.43, 134.35, 134.27, 133.91, 133.64, 133.62, 125.93, 125.90, 125.83, 125.80, 125.62, 125.59, 125.56, 125.53, 125.50, 124.40, 124.25, 122.23, 122.07

75.63, 75.54, 75.50, 75.44, 75.01, 74.95

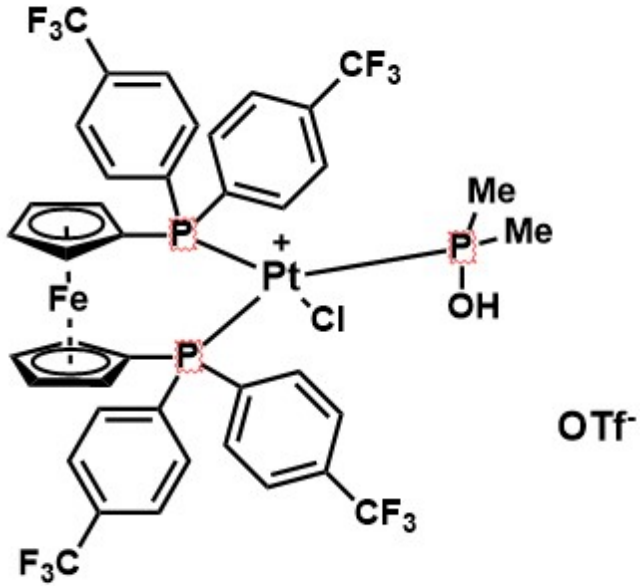
19.30, 19.26, 18.96, 18.93



2d

Parameter	Value
Title	chenbo-X-cat 13-0915
Comment	chenbo-X-cat 13-0915
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	296.2
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	3096
Receiver Gain	193
Relaxation Delay	2.0000
Pulse Width	12.0000
Acquisition Time	0.4020
Acquisition Date	2018-09-16T04:06:27
Modification Date	2018-09-18T06:48:09
Spectrometer Frequency	202.45
Spectral Width	81521.7
Lowest Frequency	-50883.7
Nucleus	31P
Acquired Size	32768
Spectral Size	65536

98.20 95.91 91.35 89.05 84.51 82.21 29.90 27.59 25.67 24.74 24.66 22.43 22.35 19.50 17.18 16.11 16.02 15.93 13.26 6.37

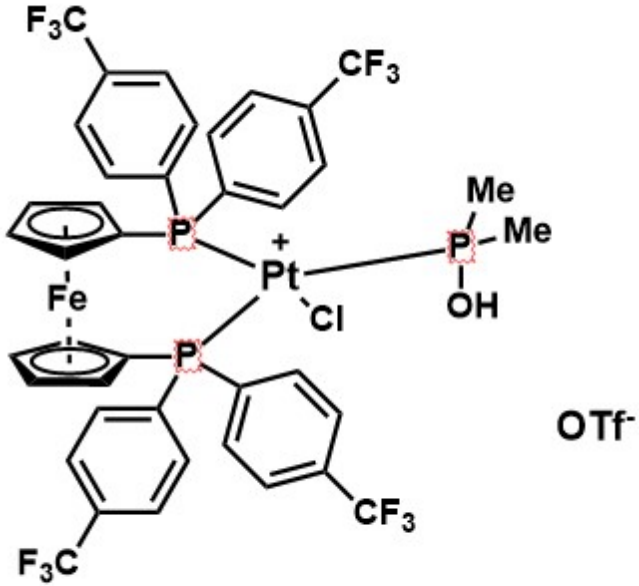


2d

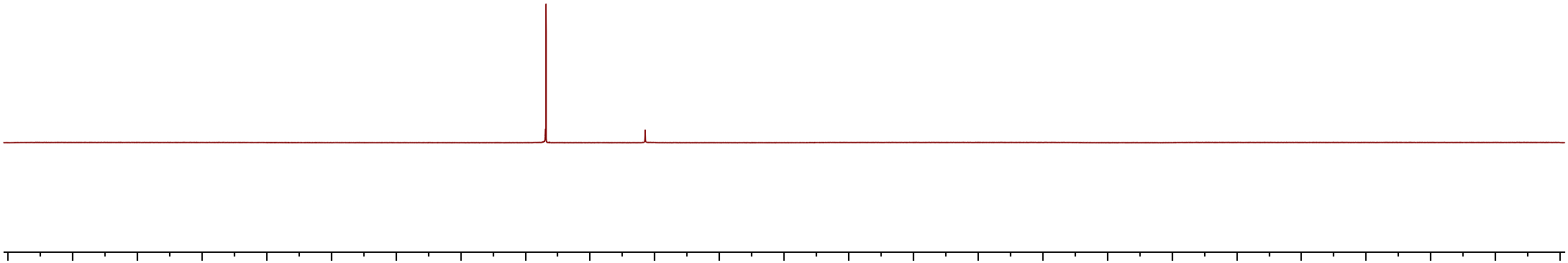
50 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240

f1 (ppm)

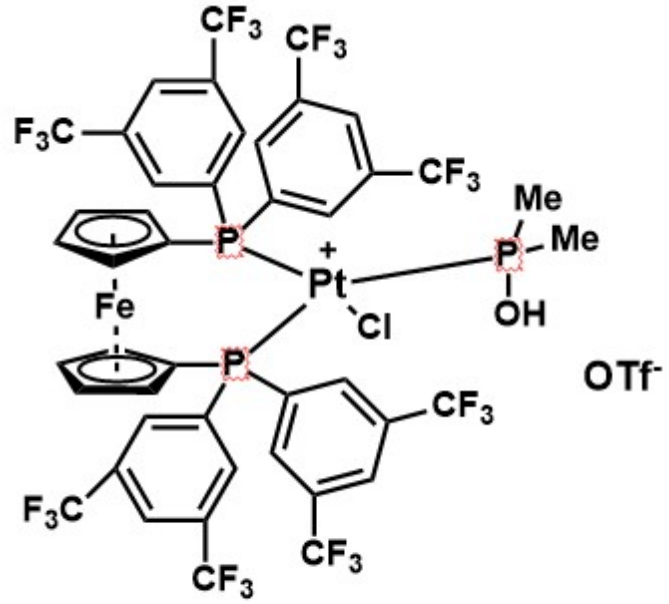
Parameter	Value
Title	chenbo-X-2-cat 13#-0911
Comment	chenbo-X-2-cat 13#-0911
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	296.6
Pulse Sequence	zgig
Experiment	1D
Number of Scans	256
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	18.0000
Acquisition Time	0.7209
Acquisition Date	2018-09-12T08:17:56
Modification Date	2018-09-12T11:25:26
Spectrometer Frequency	376.50
Spectral Width	90909.1
Lowest Frequency	-83104.4
Nucleus	19F
Acquired Size	65536
Spectral Size	65536



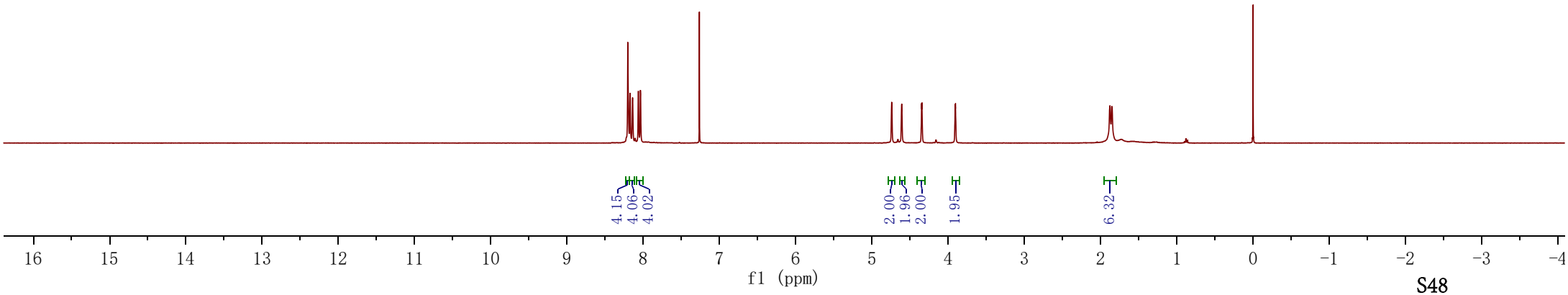
2d



Parameter	Value
Title	chenbo-X-2-cat 12#-R
Comment	chenbo-X-2-cat 12#
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	295.3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	3.9977
Acquisition Date	2018-09-06T12:54:19
Modification Date	2018-09-06T13:01:07
Spectrometer Frequency	400.13
Spectral Width	8196.7
Lowest Frequency	-1636.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



2e

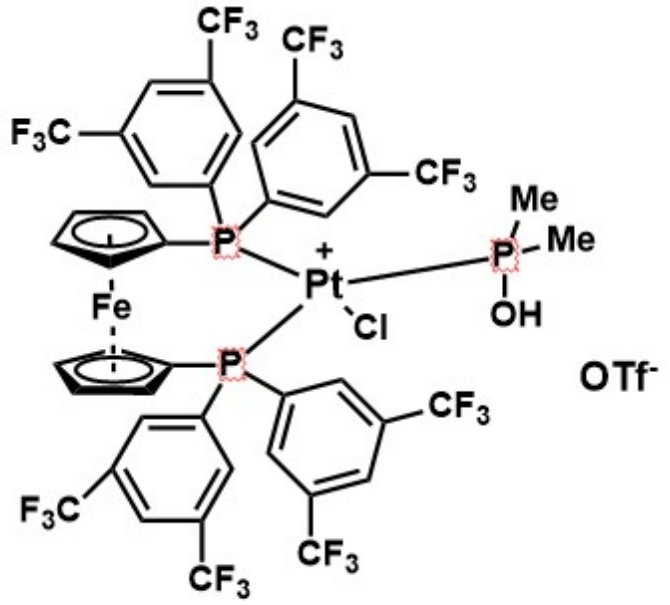


Parameter	Value
Title	chenbo-X-cat 12#-0915
Comment	chenbo-X-cat 12-0915
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	296.1
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	4096
Receiver Gain	193
Relaxation Delay	2.0000
Pulse Width	9.6000
Acquisition Time	1.1010
Acquisition Date	2018-09-16T07:48:19
Modification Date	2018-09-18T06:48:10
Spectrometer Frequency	125.77
Spectral Width	29761.9
Lowest Frequency	-2305.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

134.41 134.32 133.58 133.48 133.30 133.21 133.03 132.93 132.77 132.68 132.49 132.41 132.22 132.16 132.00 131.73 131.46 127.00 126.45 125.61 123.43 123.41 121.26 121.23

75.93 75.87 75.82 75.53 75.32 75.23

19.59 19.25



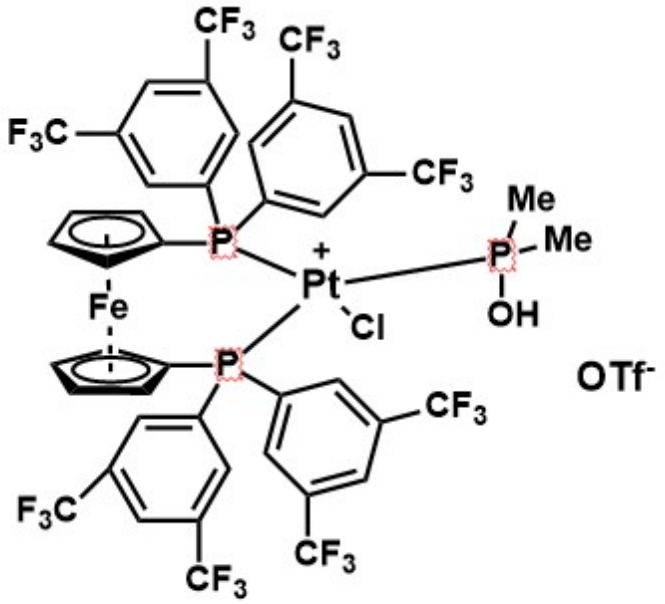
2e

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

Parameter	Value
Title	chenbo-X-cat 12#-0915
Comment	chenbo-X-cat 12-0915
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	296.2
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	3096
Receiver Gain	193
Relaxation Delay	2.0000
Pulse Width	12.0000
Acquisition Time	0.4020
Acquisition Date	2018-09-16T09:57:42
Modification Date	2018-09-18T06:48:10
Spectrometer Frequency	202.45
Spectral Width	81521.7
Lowest Frequency	-50883.7
Nucleus	31P
Acquired Size	32768
Spectral Size	65536

97.32 95.11 90.74 88.49 86.07 84.04 34.24 31.96 29.87 29.26 29.18 26.99 26.91 24.25 21.99 20.10 20.02 19.94 19.84 15.47 10.18

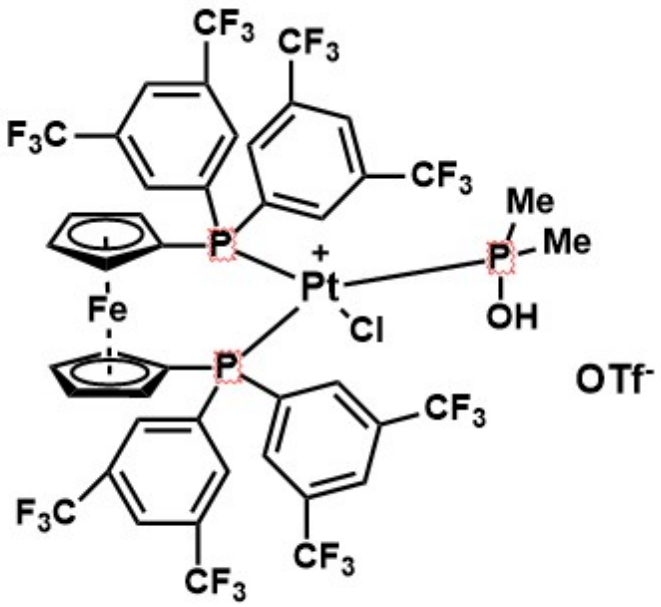


2e

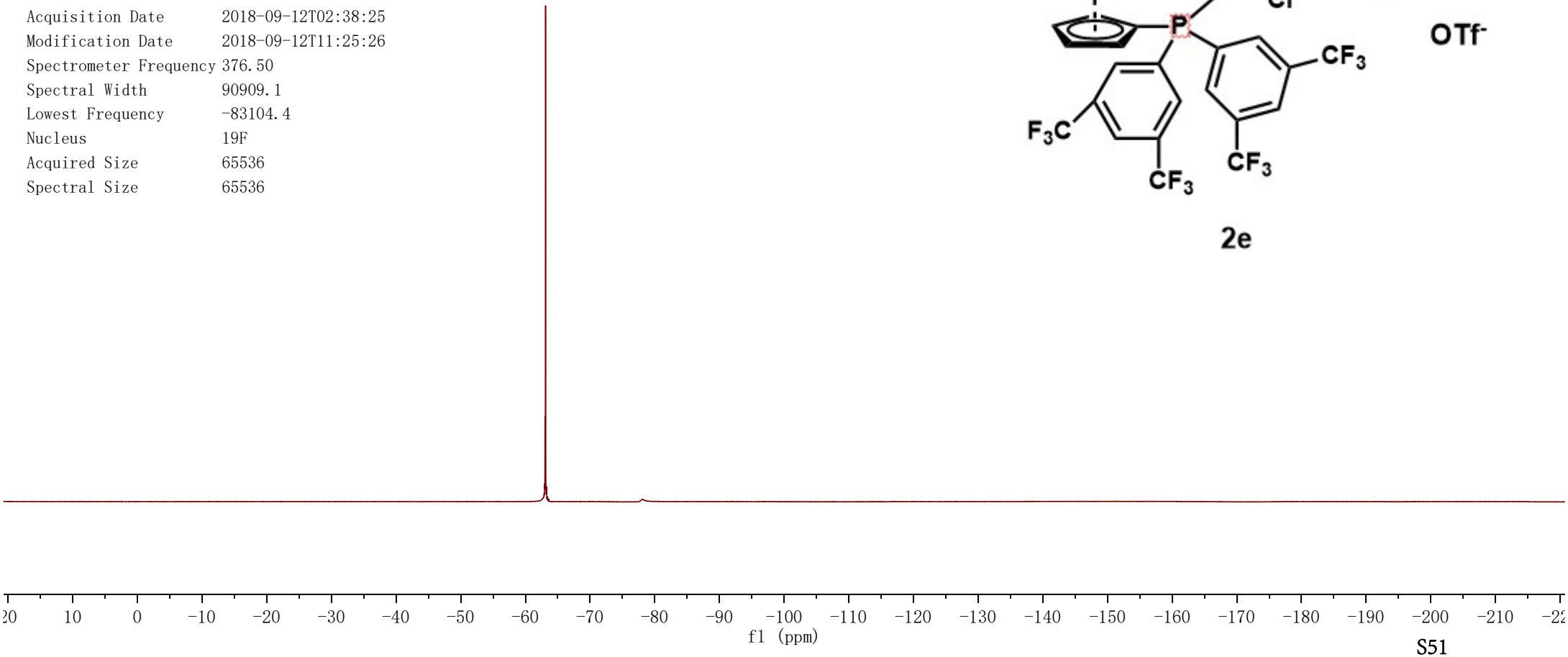
50 130 110 90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240

f1 (ppm)

Parameter	Value
Title	chenbo-X-2-cat 12#-0911
Comment	chenbo-X-2-cat 12#-0911
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	296.2
Pulse Sequence	zgig
Experiment	1D
Number of Scans	256
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	18.0000
Acquisition Time	0.7209
Acquisition Date	2018-09-12T02:38:25
Modification Date	2018-09-12T11:25:26
Spectrometer Frequency	376.50
Spectral Width	90909.1
Lowest Frequency	-83104.4
Nucleus	19F
Acquired Size	65536
Spectral Size	65536



2e



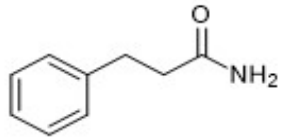
PROTON01

xxy-vi-164

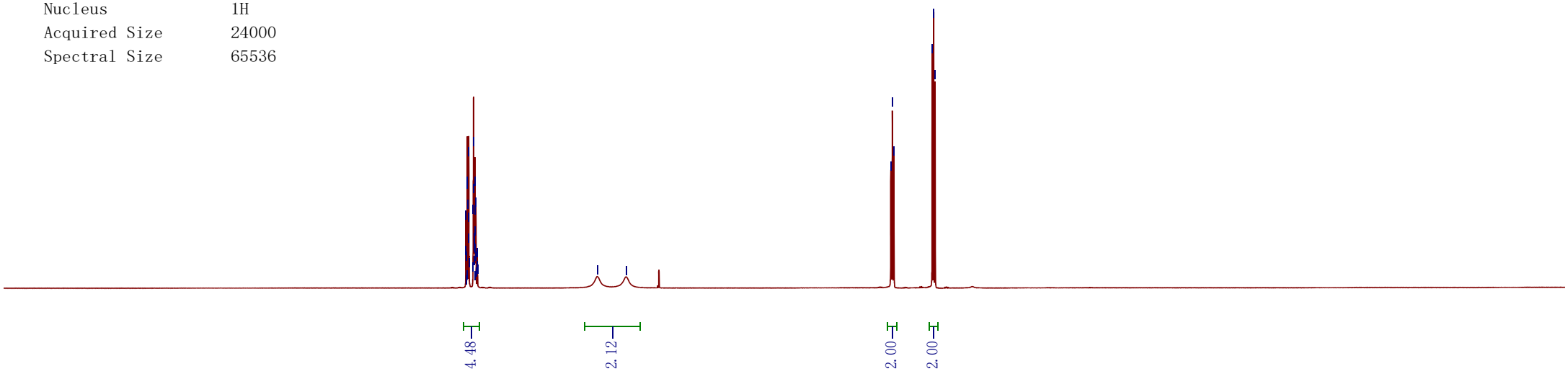
9.27 9.26 9.26 9.25 9.25 9.25 9.24 9.23 9.23 9.23 9.19 9.19 9.18 9.18 9.18 9.17 9.17 9.17 9.17 9.17 9.16 9.16 9.16 9.15 9.15 9.14 7.92 7.62

4.91 4.89 4.88 4.48 4.47 4.45

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-164/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	28
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-21T20:53:49
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



8

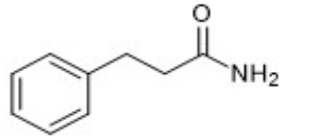


CARBON01

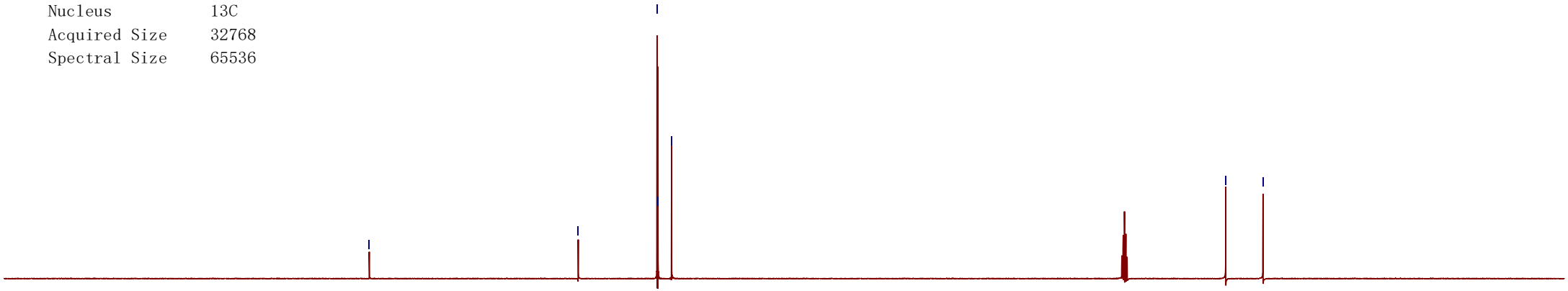
xxy-vi-164

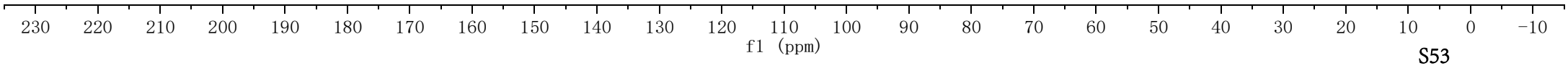
176.47 142.97 130.32 130.18 128.01 39.16 33.17

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-164/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1200
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-21T20:56:13
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



8

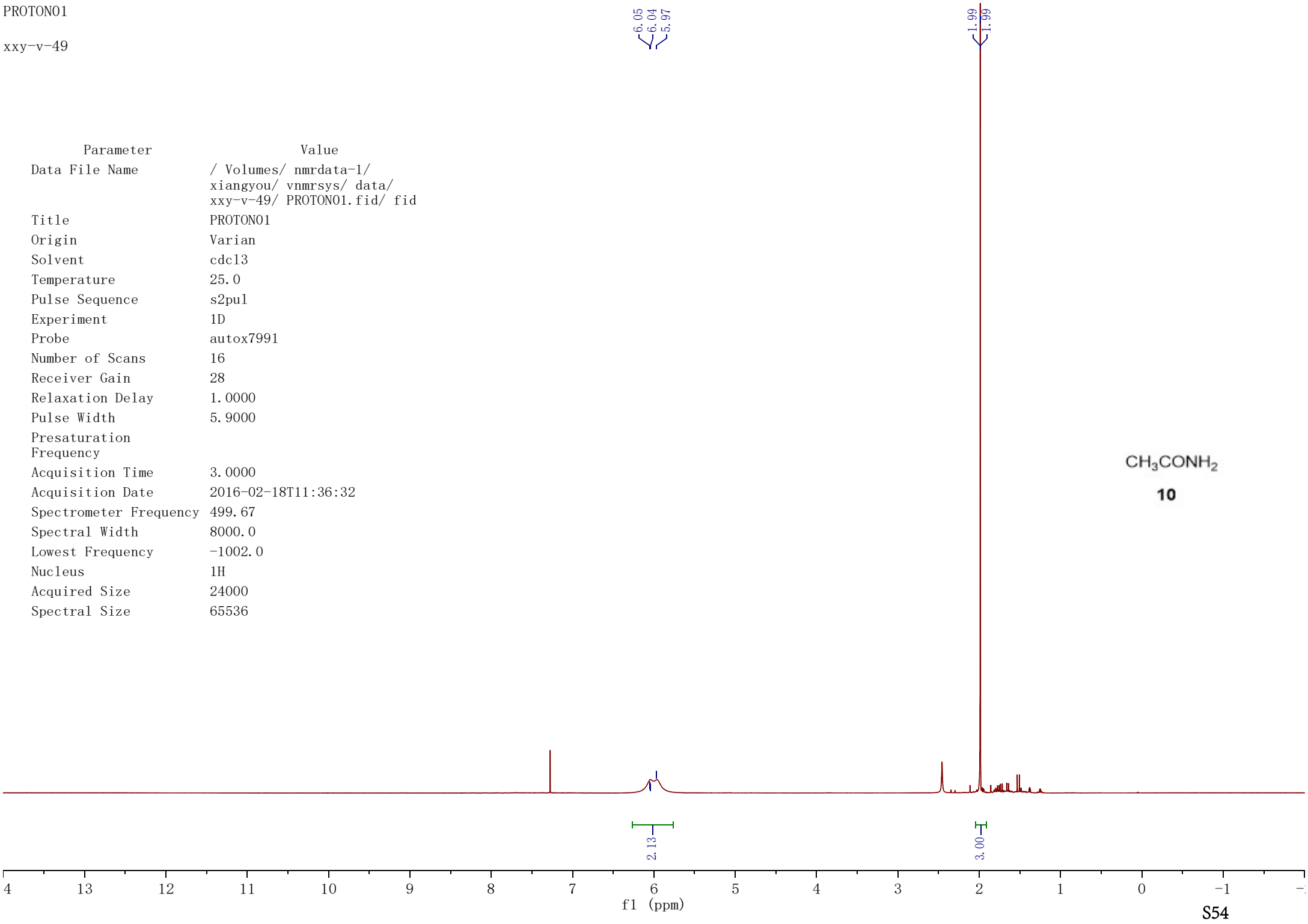




PROTON01

xxy-v-49

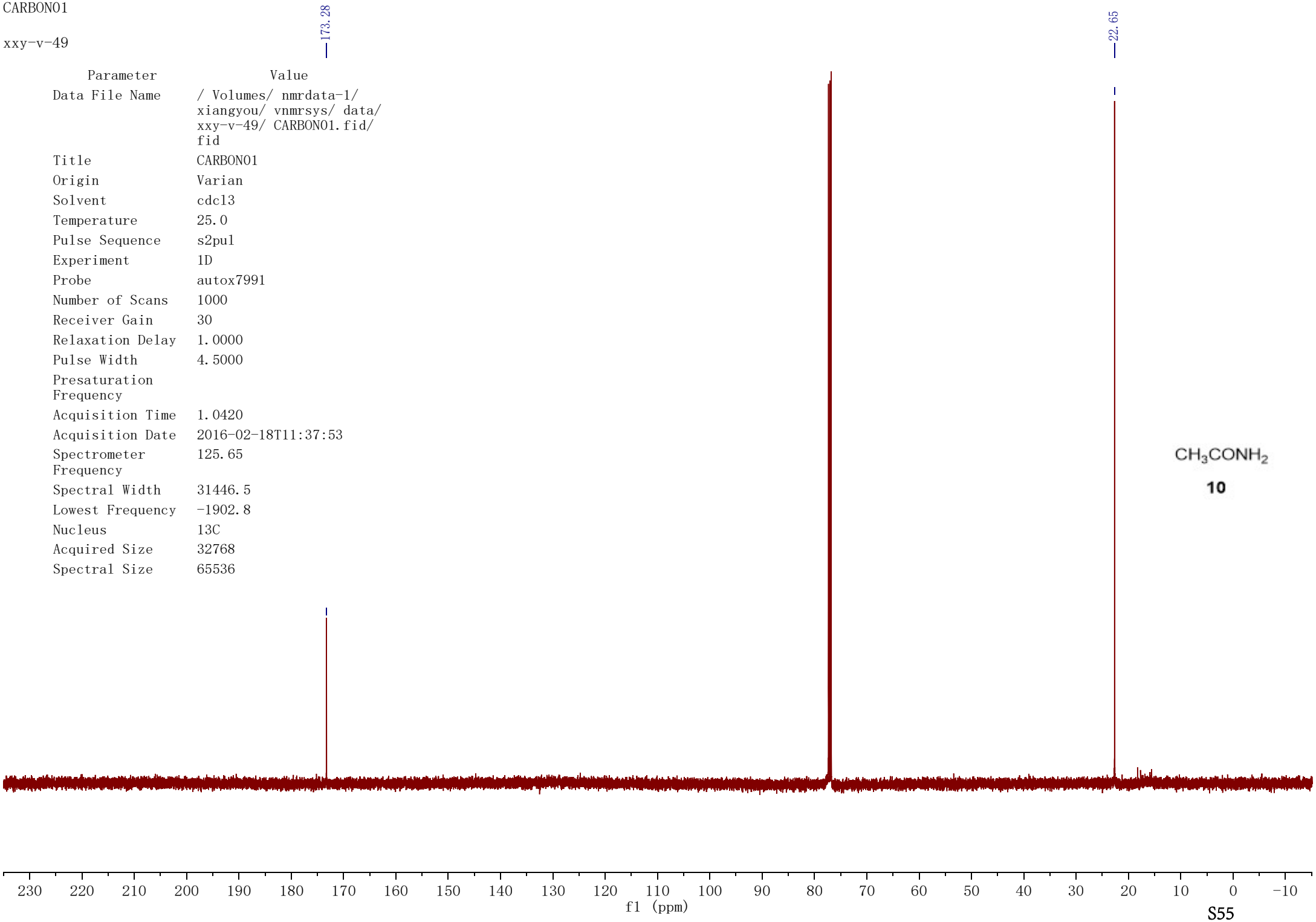
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-v-49/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	16
Receiver Gain	28
Relaxation Delay	1.0000
Pulse Width	5.9000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2016-02-18T11:36:32
Spectrometer Frequency	499.67
Spectral Width	8000.0
Lowest Frequency	-1002.0
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



CARBON01

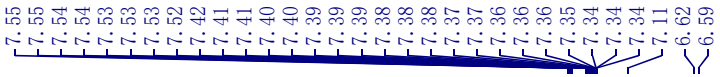
xxy-v-49

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-v-49/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1000
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.5000
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2016-02-18T11:37:53
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1902.8
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

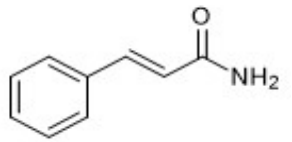


PROTON01

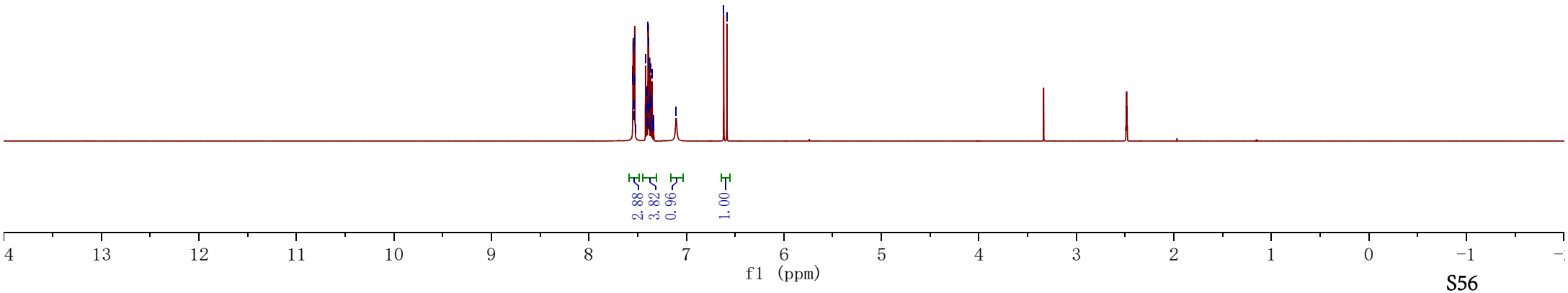
xy-vi-214



Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xy-vi-214/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	46
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-07-04T11:32:55
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



11p

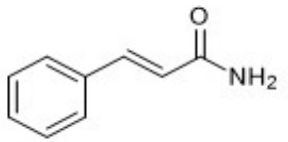


CARBON01

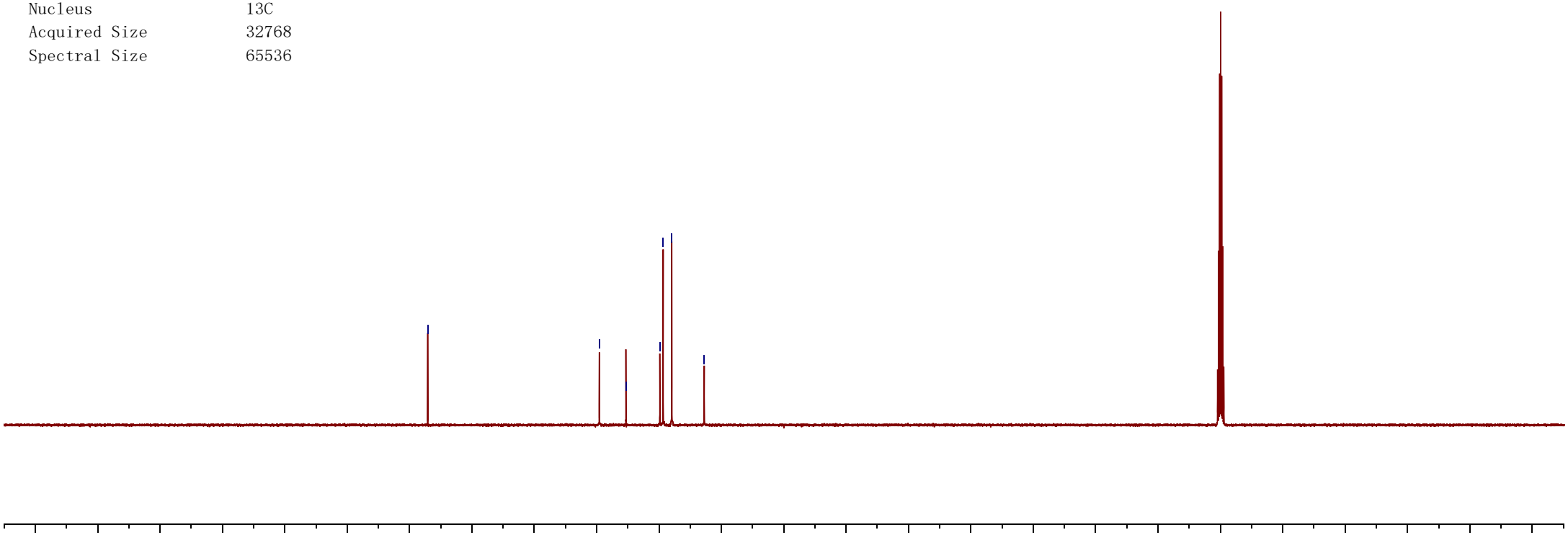
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xy-vi-214/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1500
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-07-04T11:35:19
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

xy-vi-214

167.09
139.58
135.31
129.88
129.36
127.97
122.77



11p



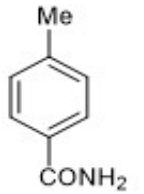
PROTON01

xxy-vi-177

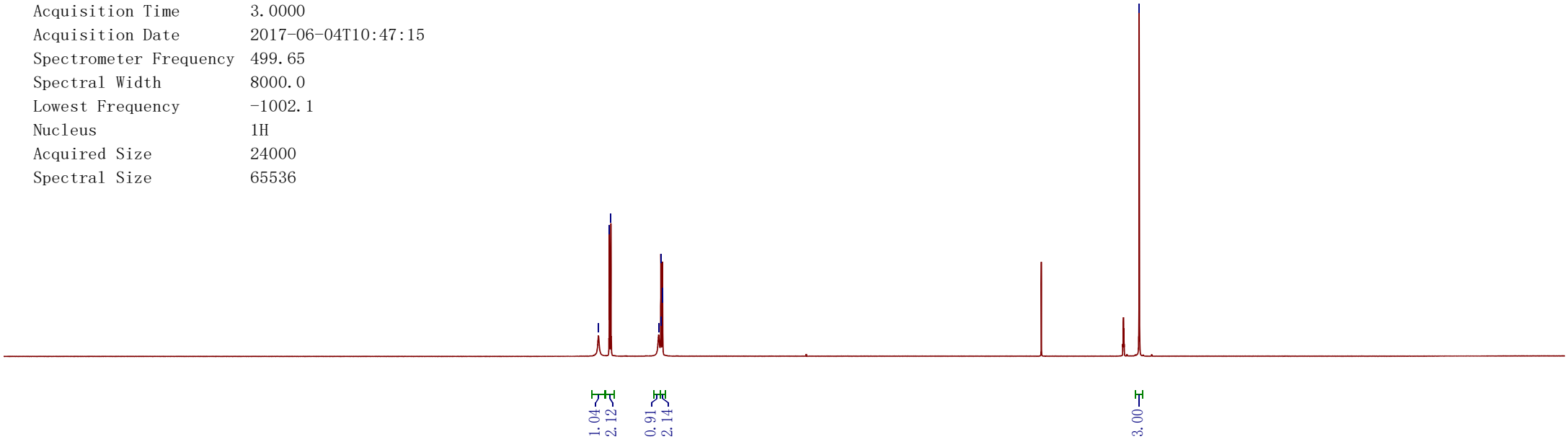
7.91 7.79 7.78 7.29 7.27 7.26 7.25 7.25

2.36

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-177/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-06-04T10:47:15
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



12p

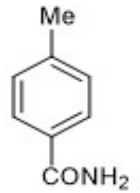


CARBON01

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-177/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1200
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-06-04T10:49:39
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

xxy-vi-177

168.20 141.47 131.90 129.16 127.93



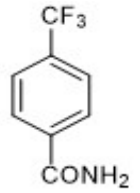
12p

PROTON01

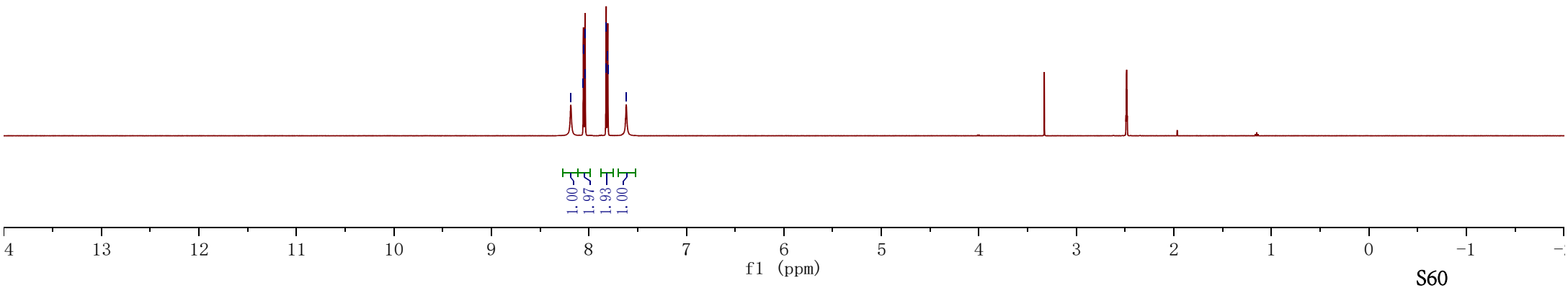
xxy-vi-199

8.19
8.06
8.06
8.04
8.04
7.82
7.82
7.81
7.81
7.62

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-199/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-07-21T15:36:34
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



13p



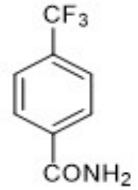
CARBON01

xxy-vi-199

167.10

138.51
131.96
131.70
131.45
131.19
128.75
127.65
125.70
125.67
125.48
123.31
121.14

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-199/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1200
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-07-21T15:38:58
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



13p

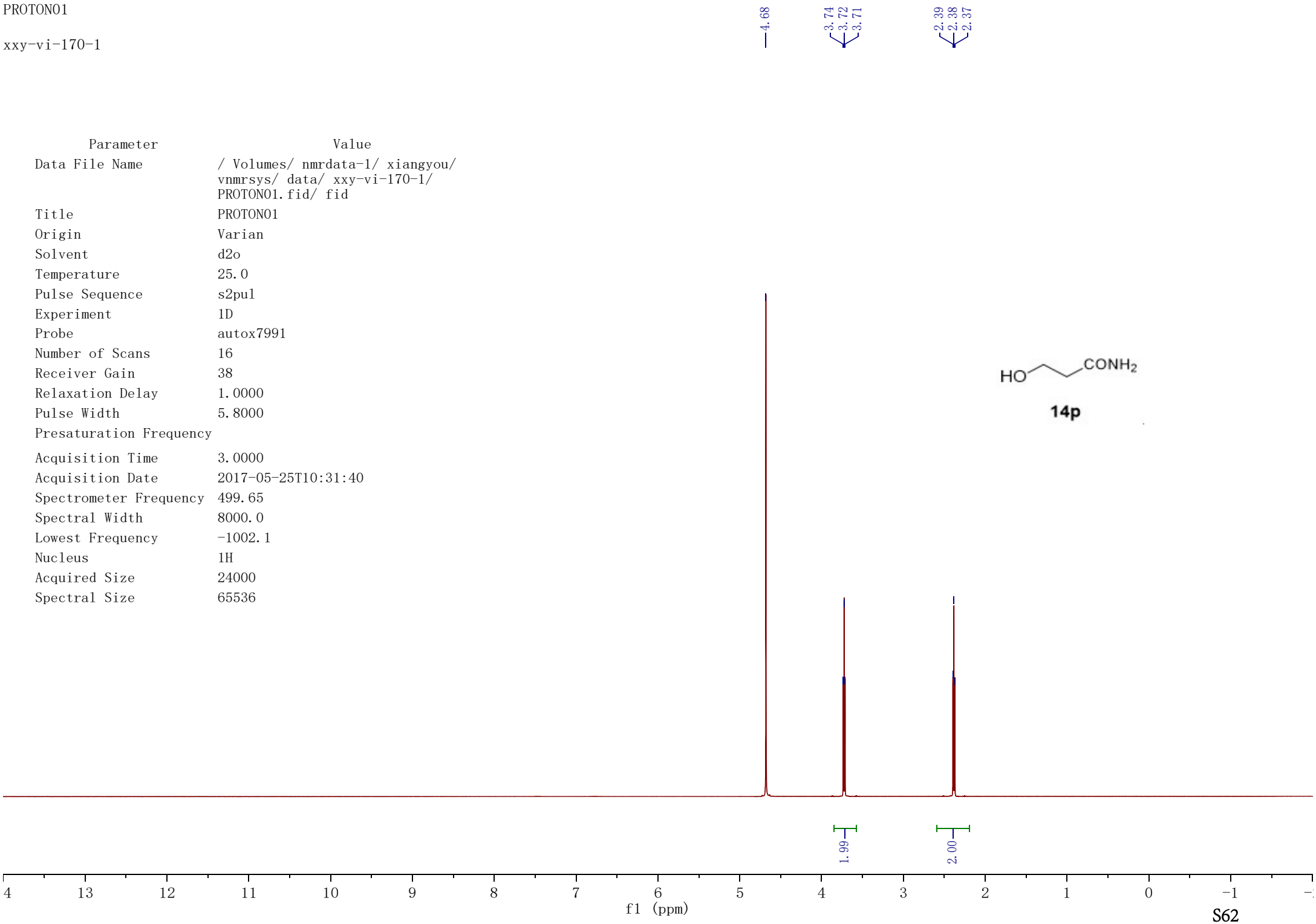
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

PROTON01

xxy-vi-170-1

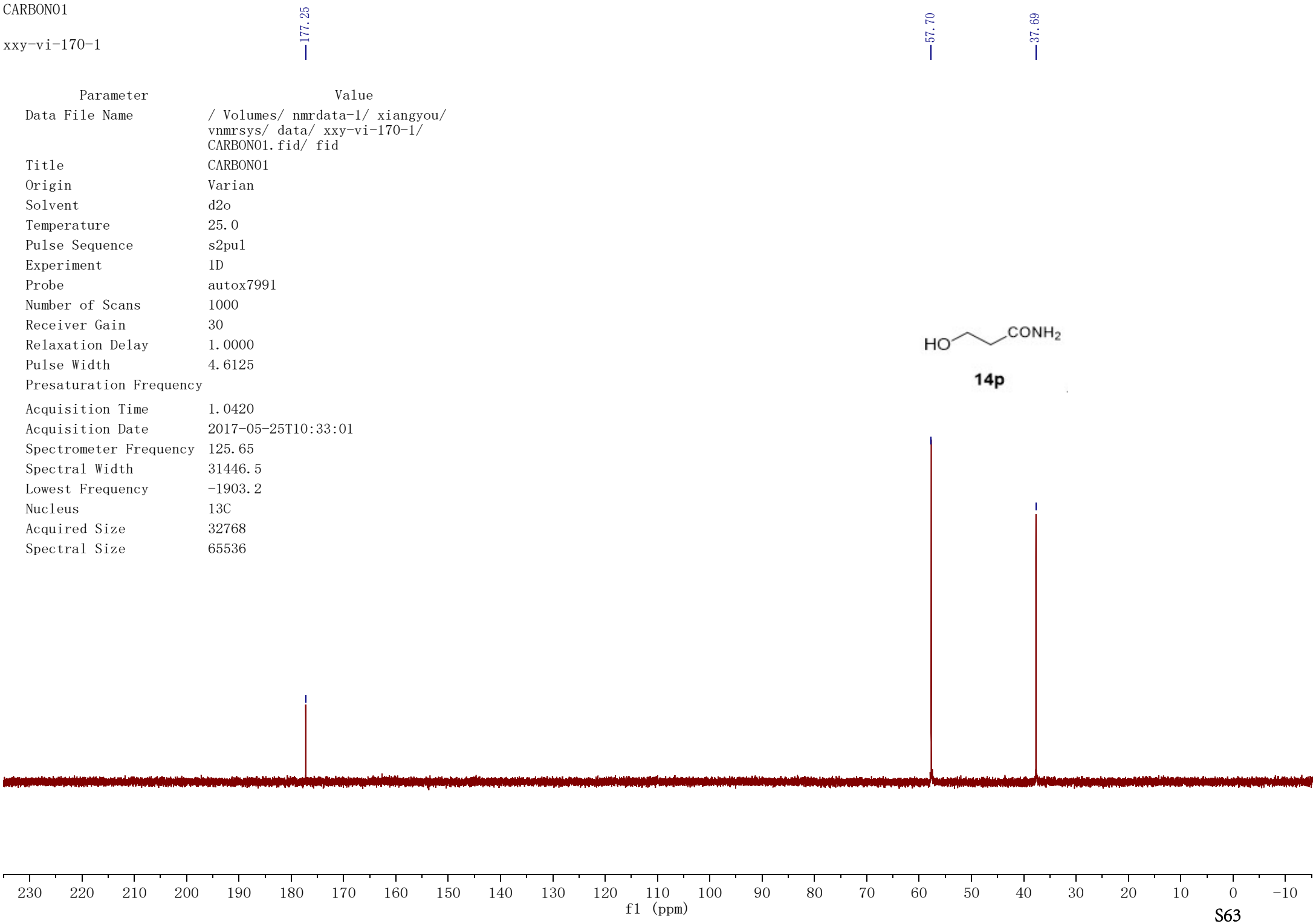
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-170-1/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	16
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-25T10:31:40
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



CARBON01

xxy-vi-170-1

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-170-1/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1000
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-25T10:33:01
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

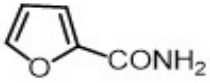


PROTON01

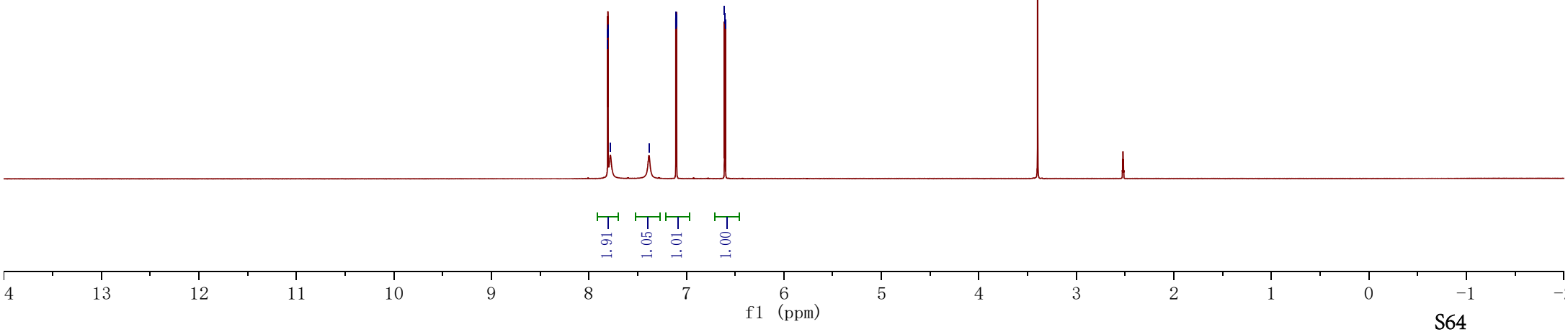
xxy-vi-162

7.81 7.81 7.81 7.80 7.78 7.11 7.11 7.10 7.10 6.61 6.60 6.60

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-162/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	16
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-20T11:03:28
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



15p

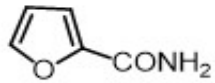


CARBON01

xxy-vi-162

159.84
148.45
145.43
114.04
112.21

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-162/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1500
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-20T11:04:48
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



15p

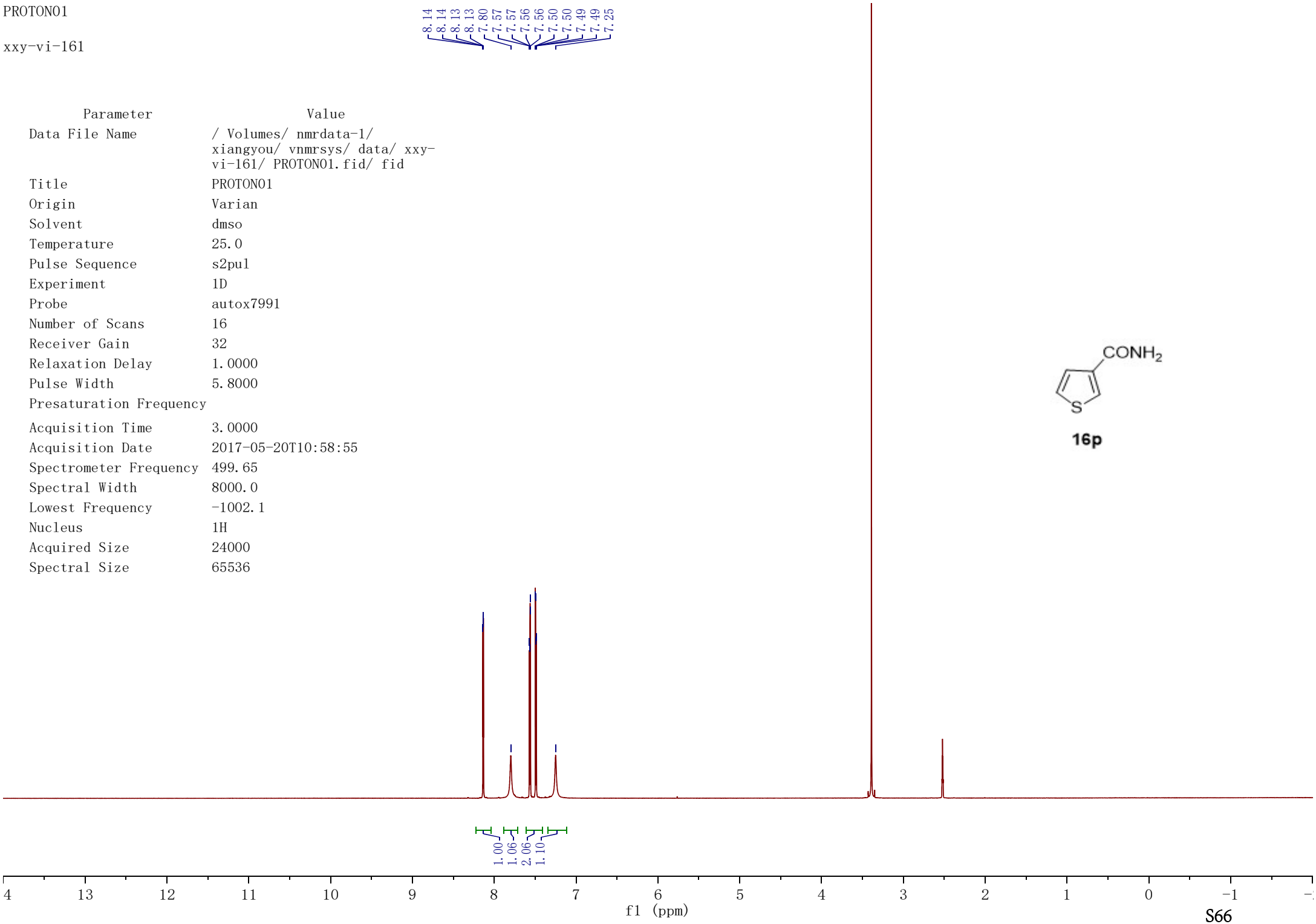
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

PROTON01

xxy-vi-161

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-161/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	16
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-20T10:58:55
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536

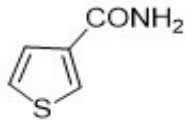


CARBON01

xxy-vi-161

164.14
138.41
129.46
127.58
127.00

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-161/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1500
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-20T10:07:06
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

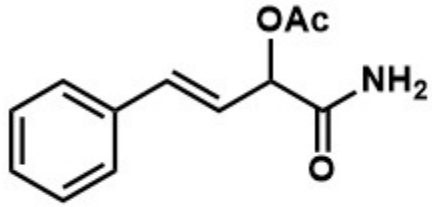


16p

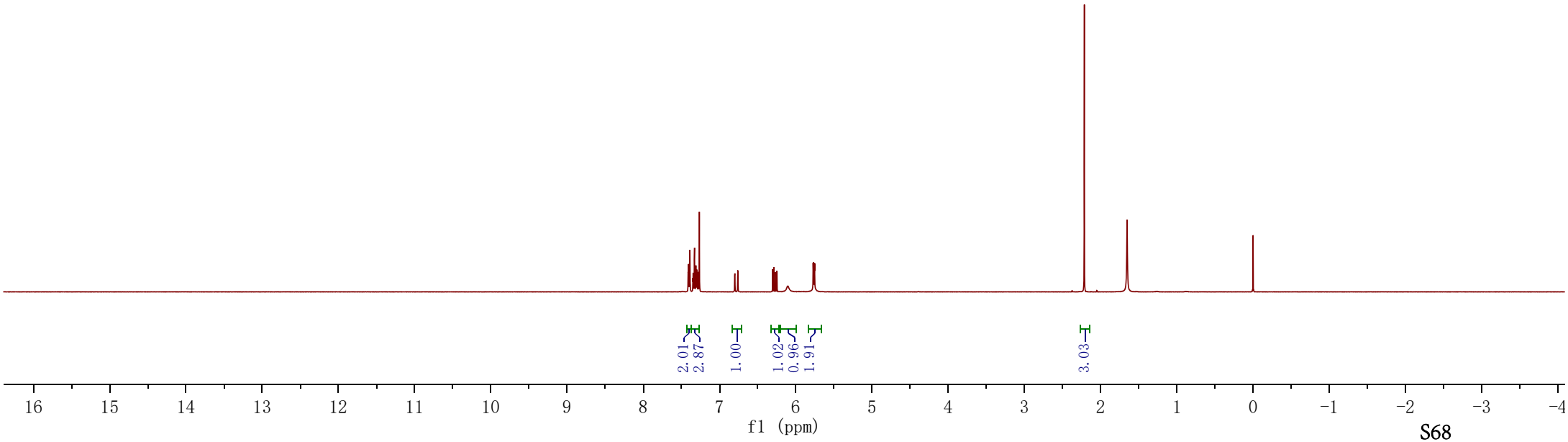
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

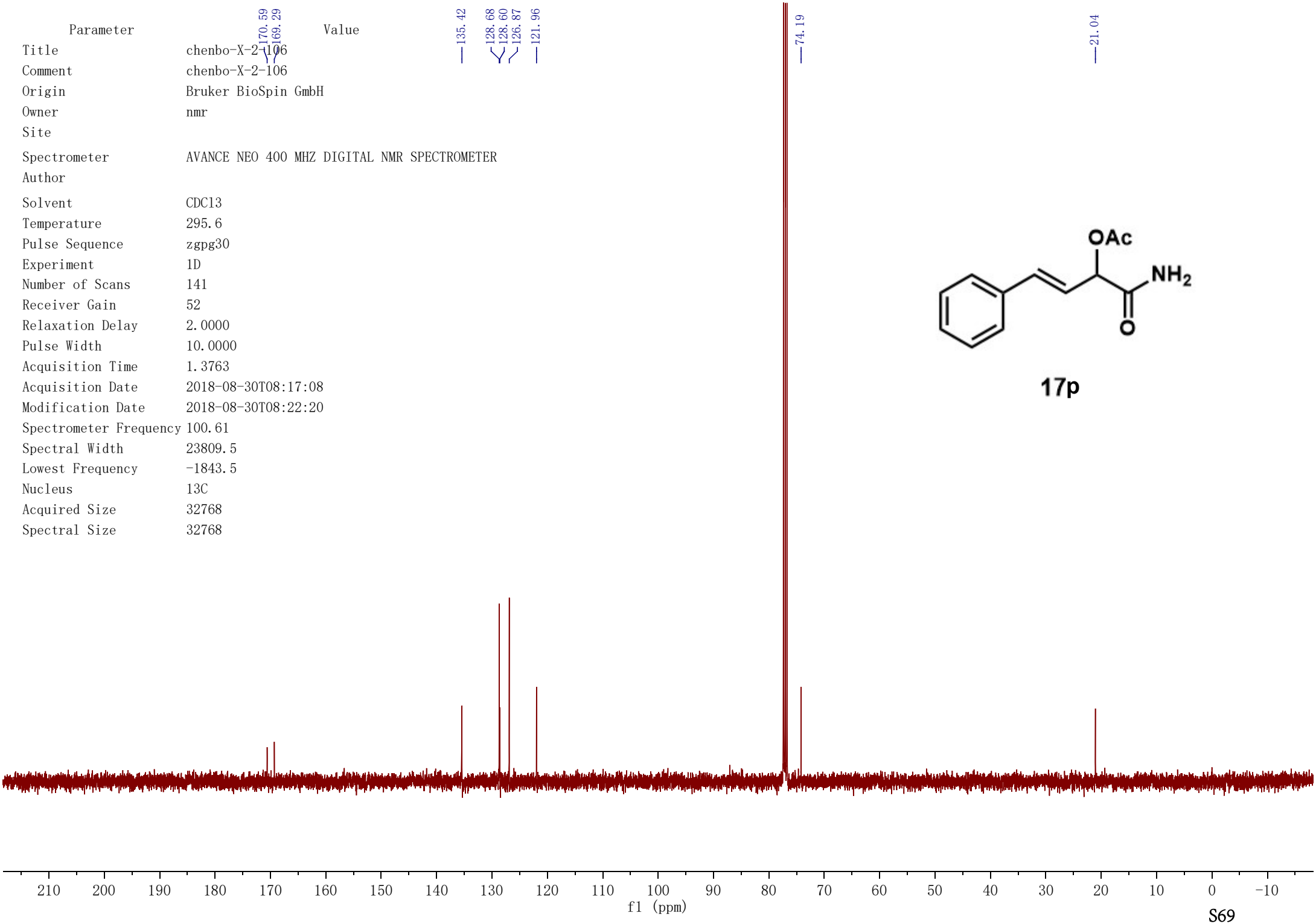
Parameter	Value
Title	chenbo-X-2-106
Comment	chenbo-X-2-106
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	294.9
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	3.9977
Acquisition Date	2018-08-30T08:08:02
Modification Date	2018-08-30T08:22:20
Spectrometer Frequency	400.13
Spectral Width	8196.7
Lowest Frequency	-1636.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



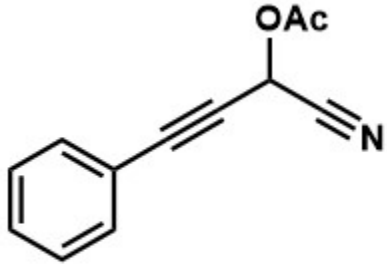
17p



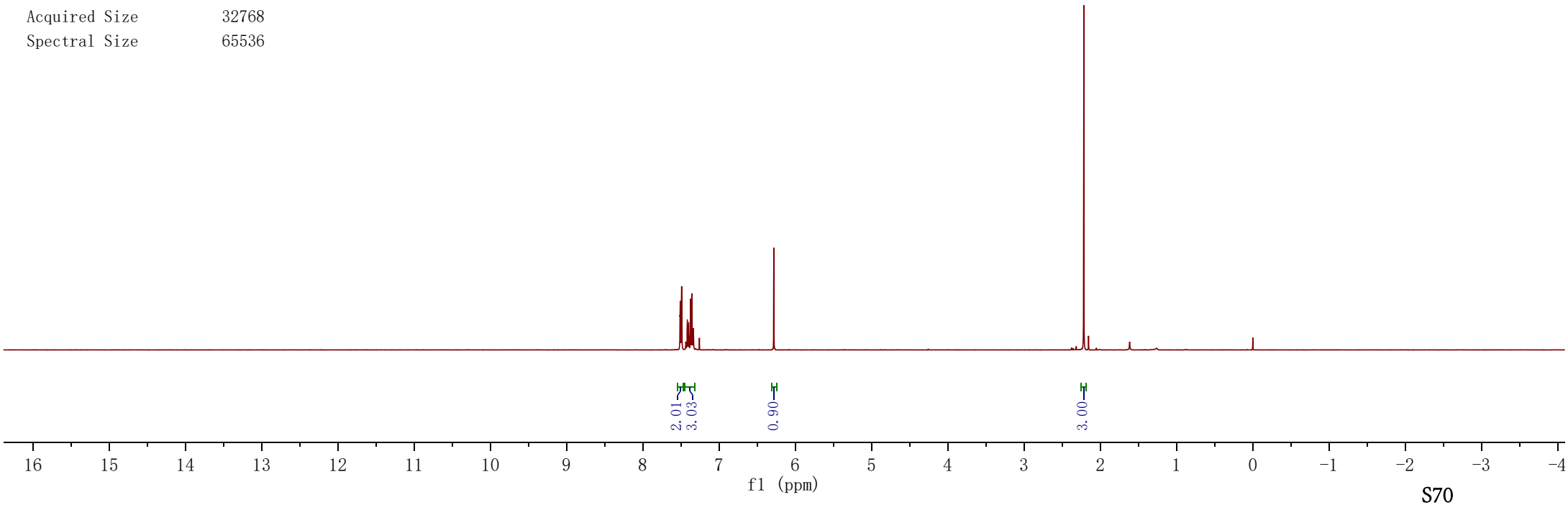
Parameter	Value
Title	chenbo-X-2-106
Comment	chenbo-X-2-106
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	295.6
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	141
Receiver Gain	52
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3763
Acquisition Date	2018-08-30T08:17:08
Modification Date	2018-08-30T08:22:20
Spectrometer Frequency	100.61
Spectral Width	23809.5
Lowest Frequency	-1843.5
Nucleus	13C
Acquired Size	32768
Spectral Size	32768



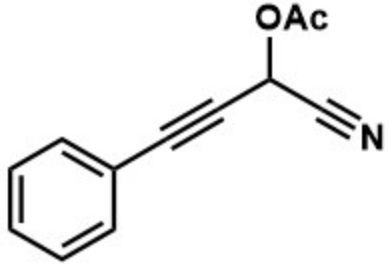
Parameter	Value
Title	lcc-080913-2
Comment	
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	295.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	8
Receiver Gain	80
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	3.9977
Acquisition Date	2018-09-13T20:42:27
Modification Date	2018-09-13T20:45:49
Spectrometer Frequency	400.13
Spectral Width	8196.7
Lowest Frequency	-1638.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



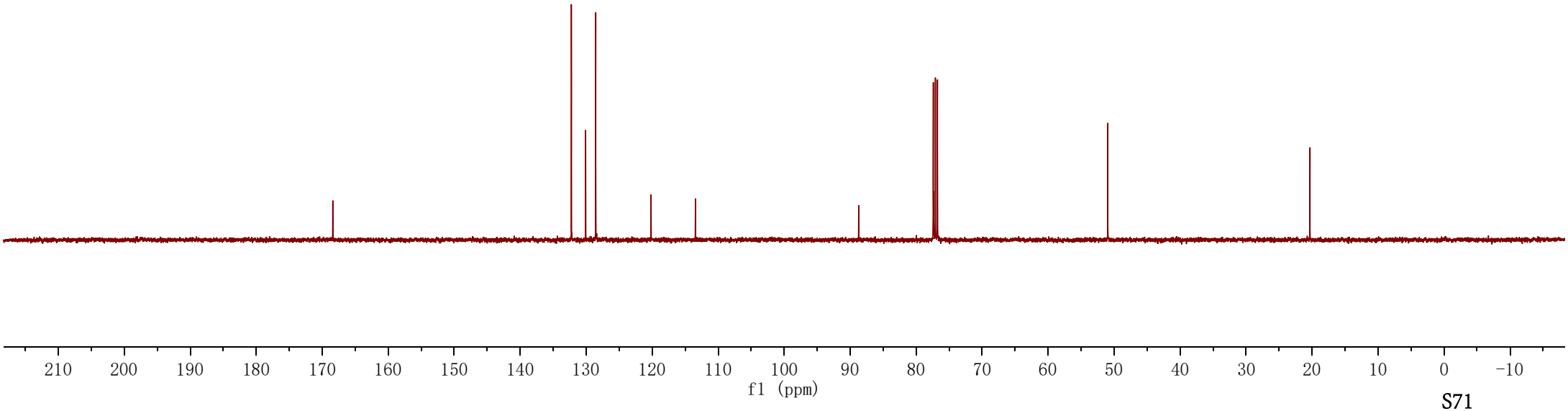
S-18



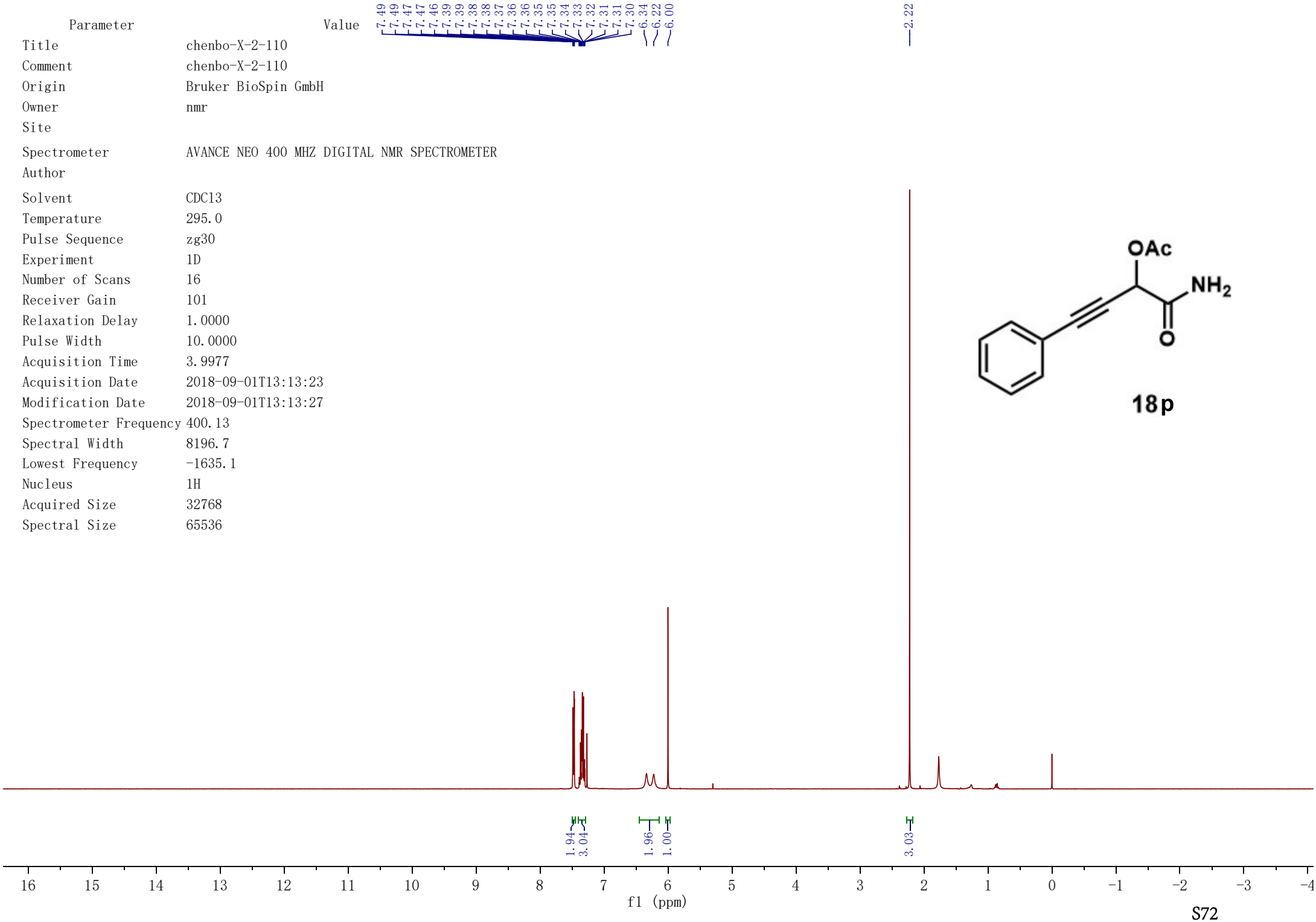
Parameter	Value
Title	lcc-080913-2
Comment	
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	295.7
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	84
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3763
Acquisition Date	2018-09-13T20:48:13
Modification Date	2018-09-13T20:45:49
Spectrometer Frequency	100.61
Spectral Width	23809.5
Lowest Frequency	-1843.5
Nucleus	13C
Acquired Size	32768
Spectral Size	32768



S-18

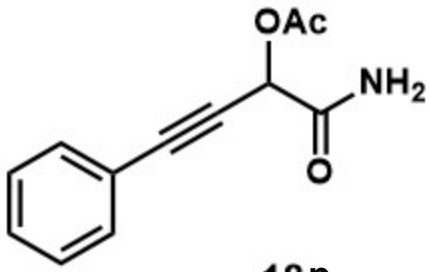


Parameter	Value
Title	chenbo-X-2-110
Comment	chenbo-X-2-110
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	295.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	3.9977
Acquisition Date	2018-09-01T13:13:23
Modification Date	2018-09-01T13:13:27
Spectrometer Frequency	400.13
Spectral Width	8196.7
Lowest Frequency	-1635.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

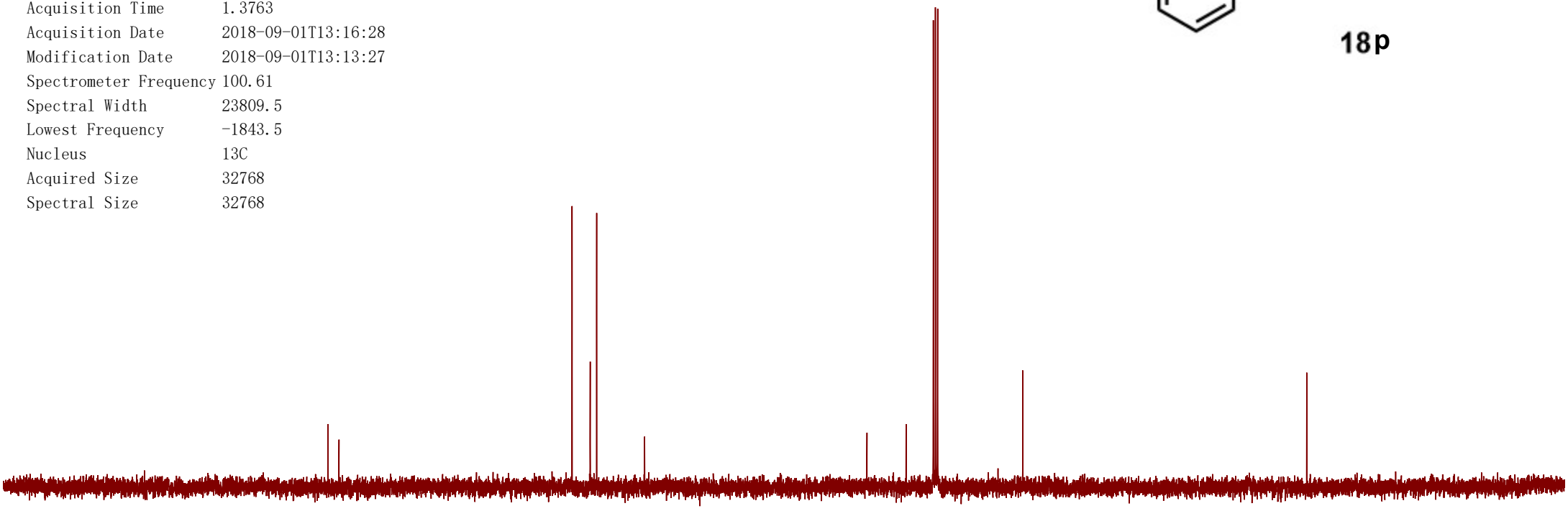


Parameter	Value
Title	chenbo-X-2-110
Comment	chenbo-X-2-110
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	CDCl3
Temperature	295.6
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	37
Receiver Gain	35
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3763
Acquisition Date	2018-09-01T13:16:28
Modification Date	2018-09-01T13:13:27
Spectrometer Frequency	100.61
Spectral Width	23809.5
Lowest Frequency	-1843.5
Nucleus	13C
Acquired Size	32768
Spectral Size	32768

169.12
167.46
132.13
129.39
128.40
121.16
87.46
81.50
63.84
20.79



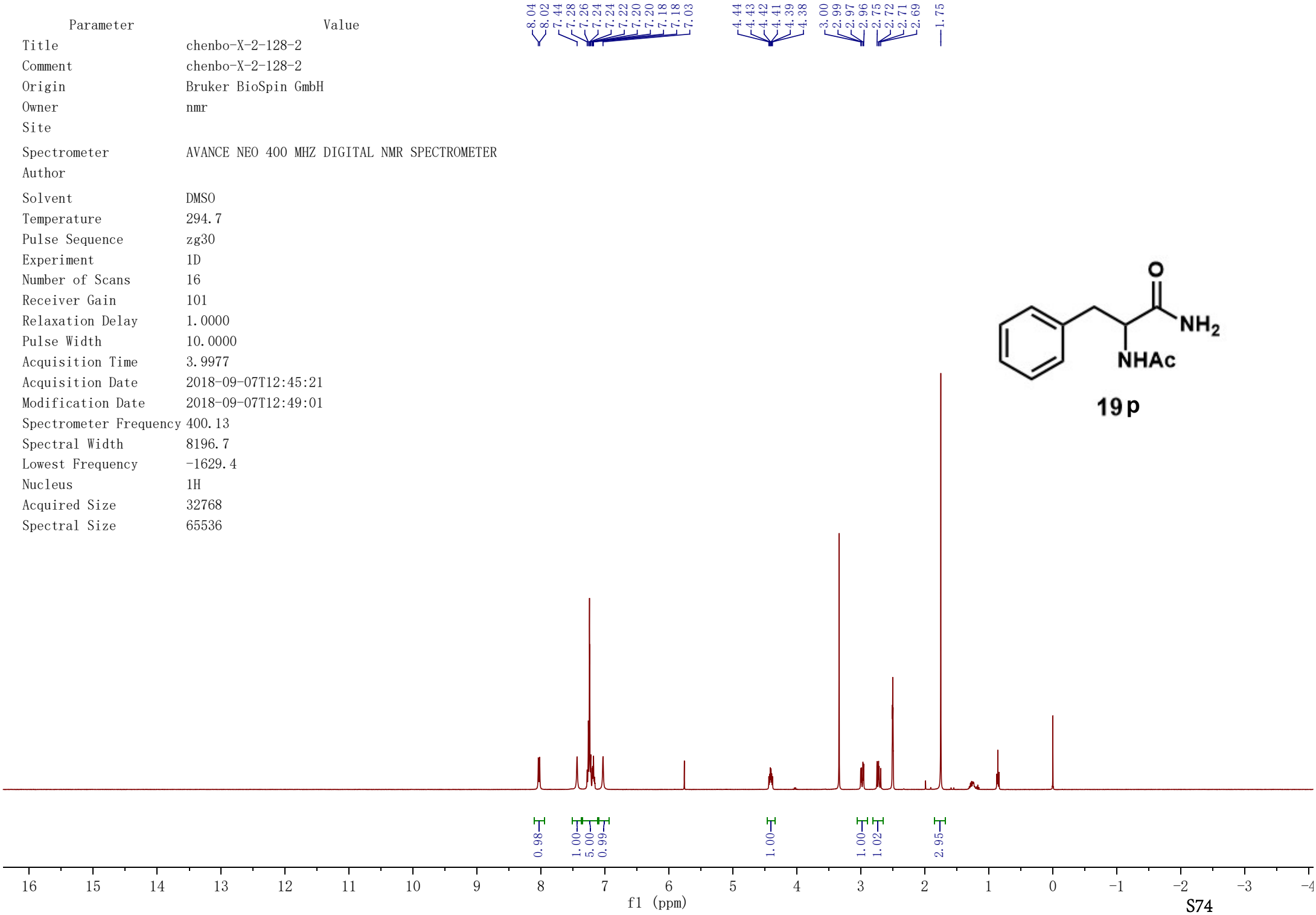
18p



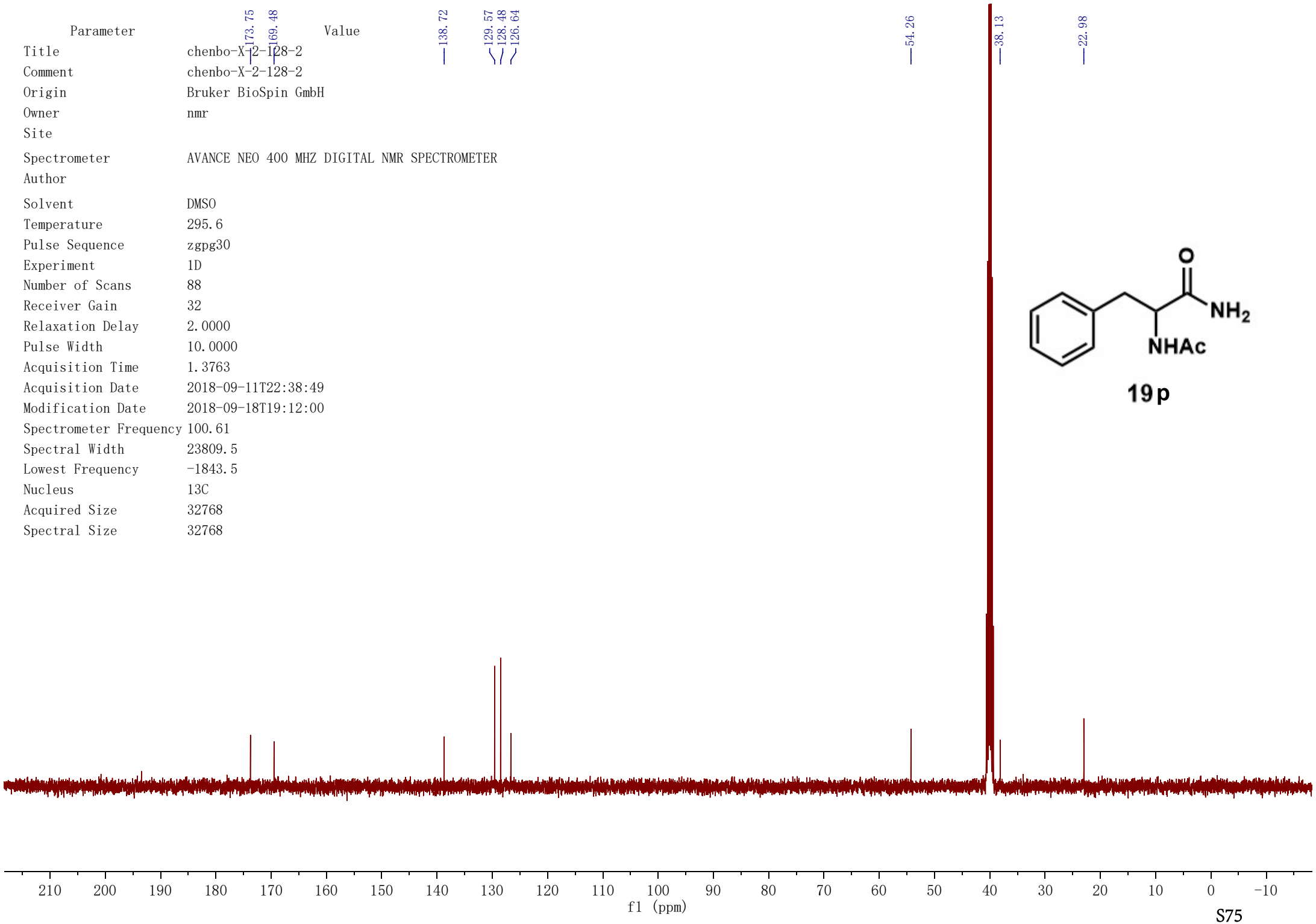
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

Parameter	Value
Title	chenbo-X-2-128-2
Comment	chenbo-X-2-128-2
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	DMSO
Temperature	294.7
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	101
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	3.9977
Acquisition Date	2018-09-07T12:45:21
Modification Date	2018-09-07T12:49:01
Spectrometer Frequency	400.13
Spectral Width	8196.7
Lowest Frequency	-1629.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

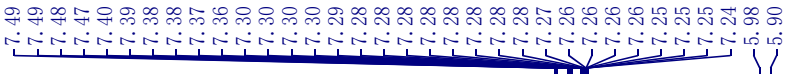


Parameter	Value
Title	chenbo-X-2-128-2
Comment	chenbo-X-2-128-2
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
Author	
Solvent	DMSO
Temperature	295.6
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	88
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3763
Acquisition Date	2018-09-11T22:38:49
Modification Date	2018-09-18T19:12:00
Spectrometer Frequency	100.61
Spectral Width	23809.5
Lowest Frequency	-1843.5
Nucleus	13C
Acquired Size	32768
Spectral Size	32768

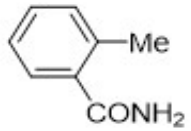


PROTON01

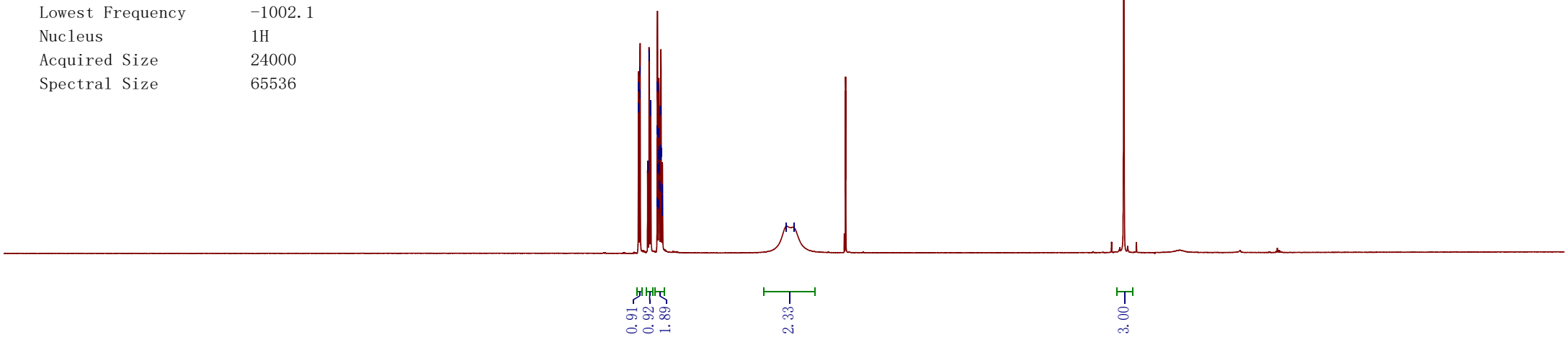
xxy-vi-175



Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-175/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	44
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-28T20:18:59
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



20p

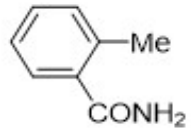


CARBON01

xxy-vi-175

171.53
136.29
135.38
131.06
130.07
126.84
125.61
19.67

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-175/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	cd2c12
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1200
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-28T20:21:24
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



20p

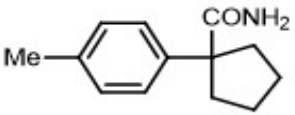
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

PROTON01

xxy-vi-165-1

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-165-1/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-22T21:53:24
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



21p

2.00 1.90 2.43 2.12 2.13 4.68

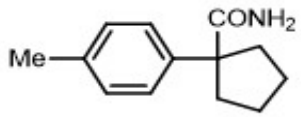
f1 (ppm)

CARBON01

xxy-vi-165-1

178.65 141.22 136.51 129.21 126.51 58.70 36.59 23.80 20.60

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-165-1/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1200
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-22T21:55:49
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



21p

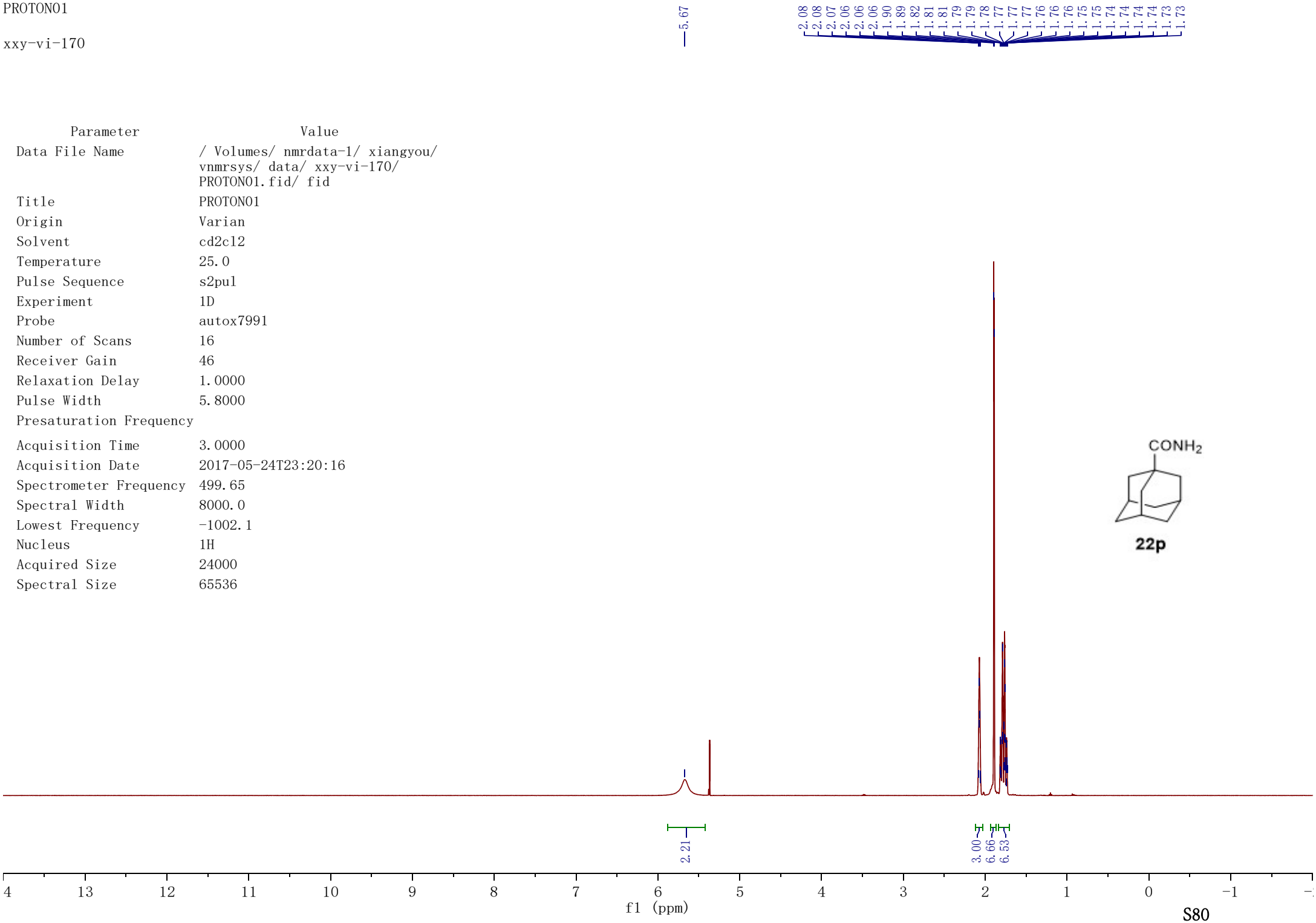
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

PROTON01

xxy-vi-170

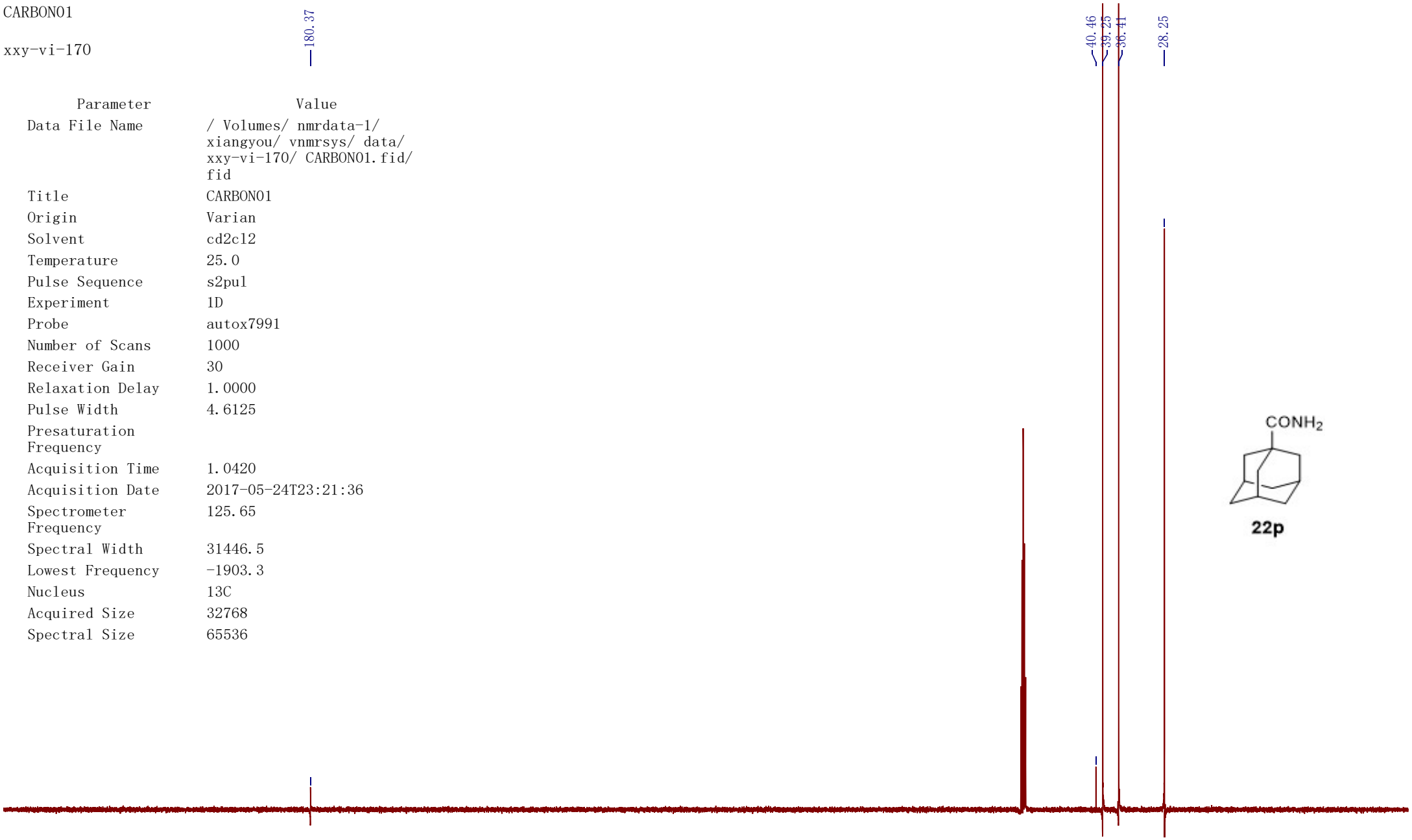
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-170/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	cd2cl2
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	16
Receiver Gain	46
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-24T23:20:16
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



CARBON01

xxy-vi-170

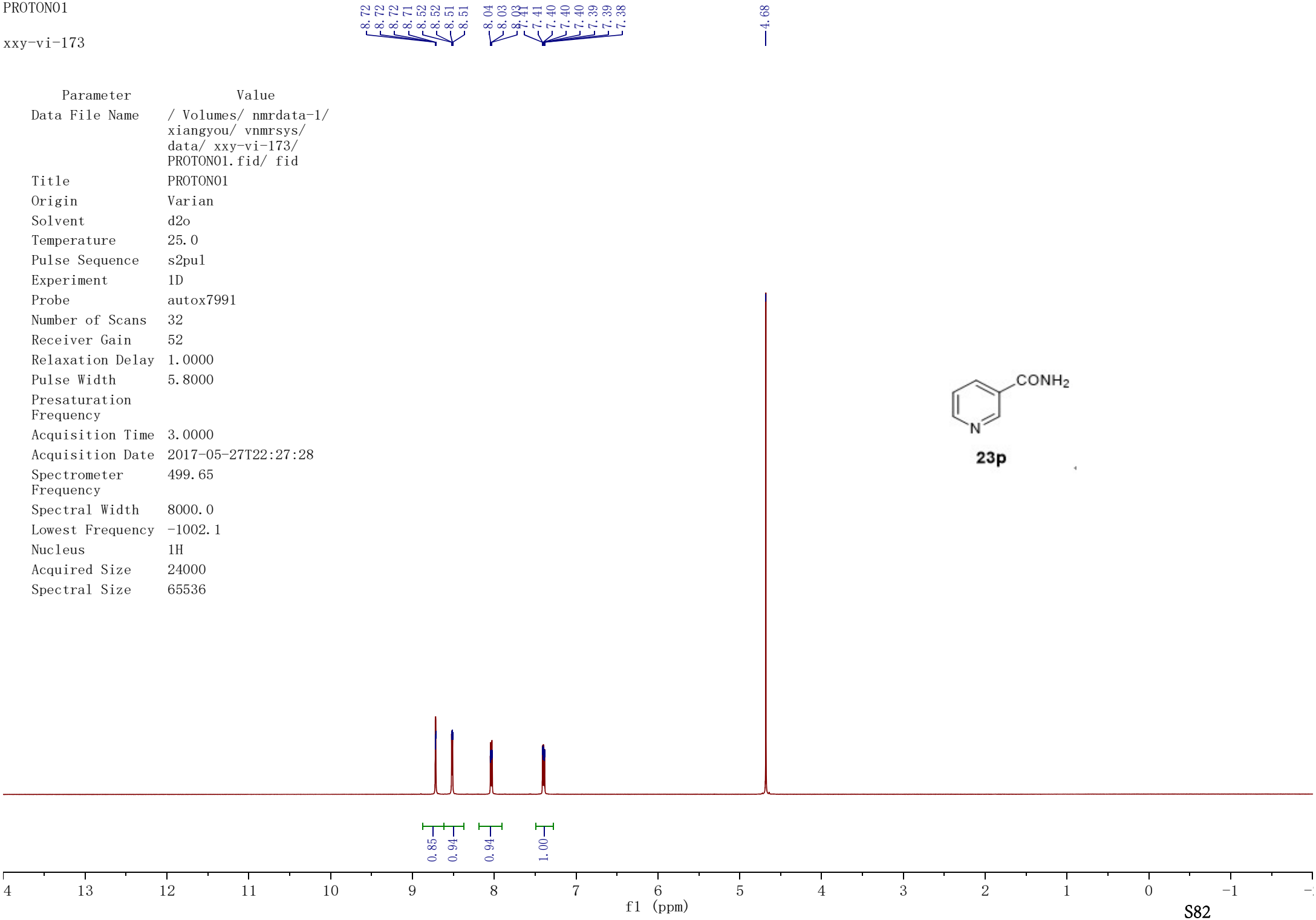
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-170/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	cd2c12
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1000
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-24T23:21:36
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



PROTON01

xxy-vi-173

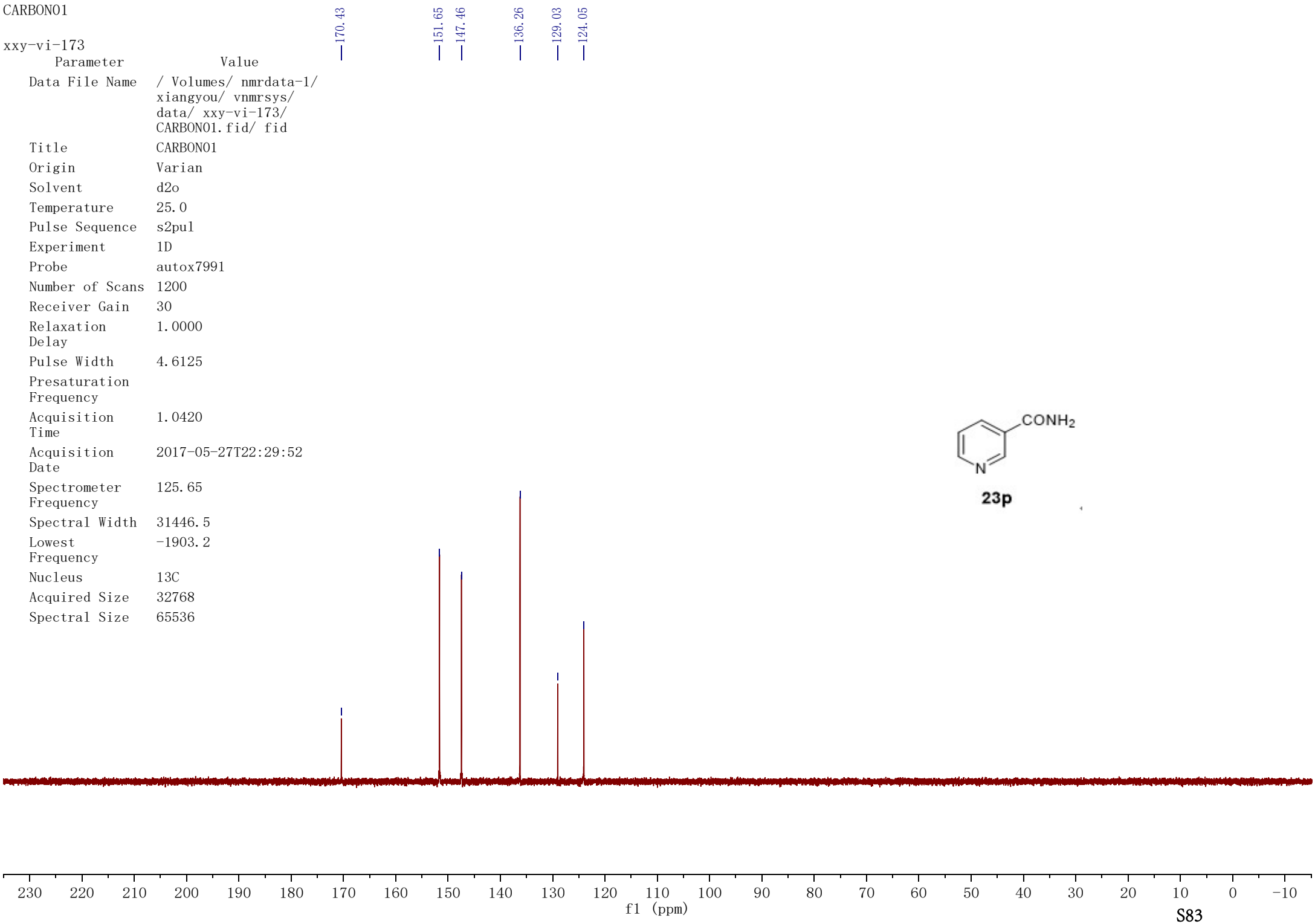
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-173/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	52
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-27T22:27:28
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



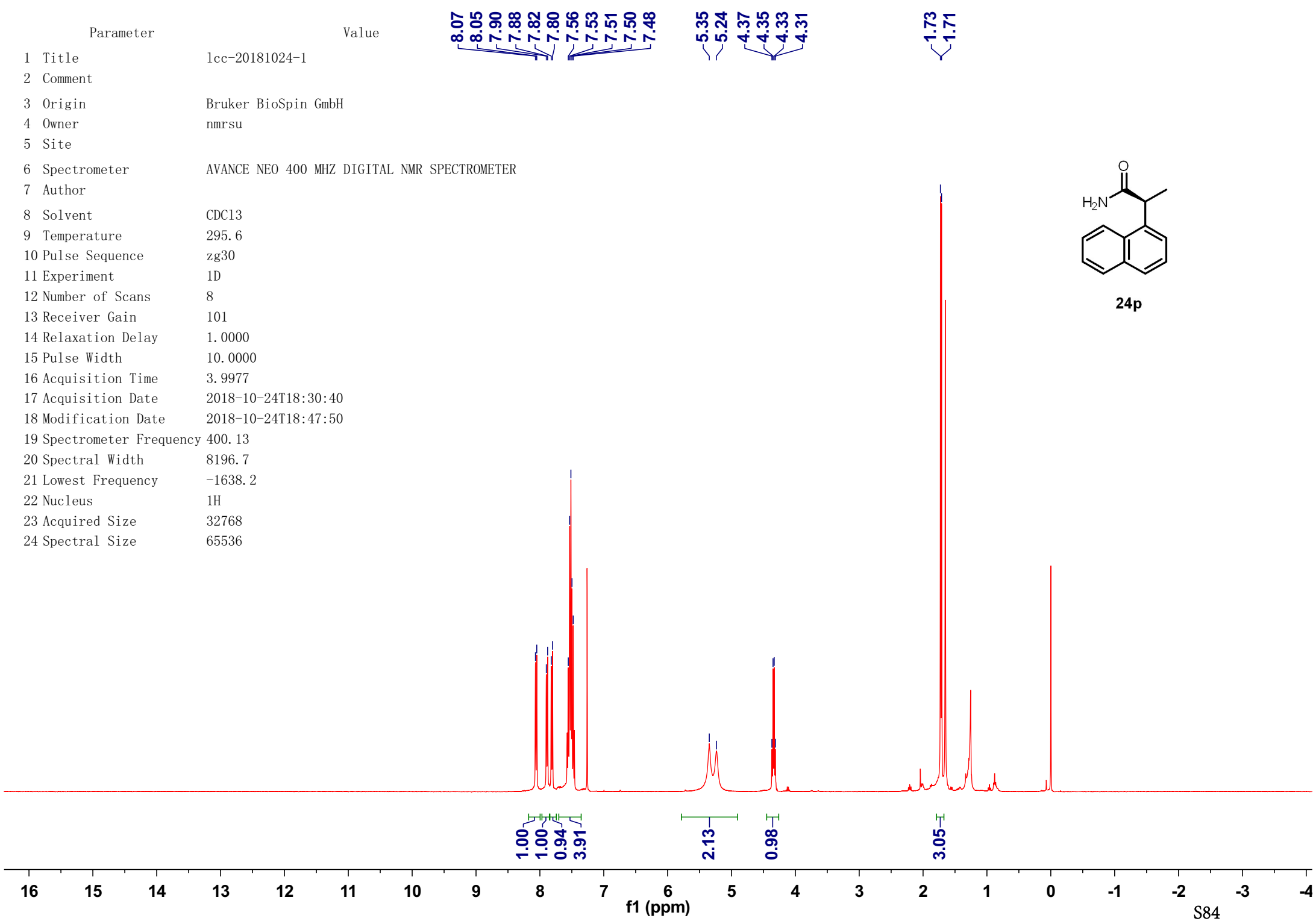
CARBON01

xxy-vi-173

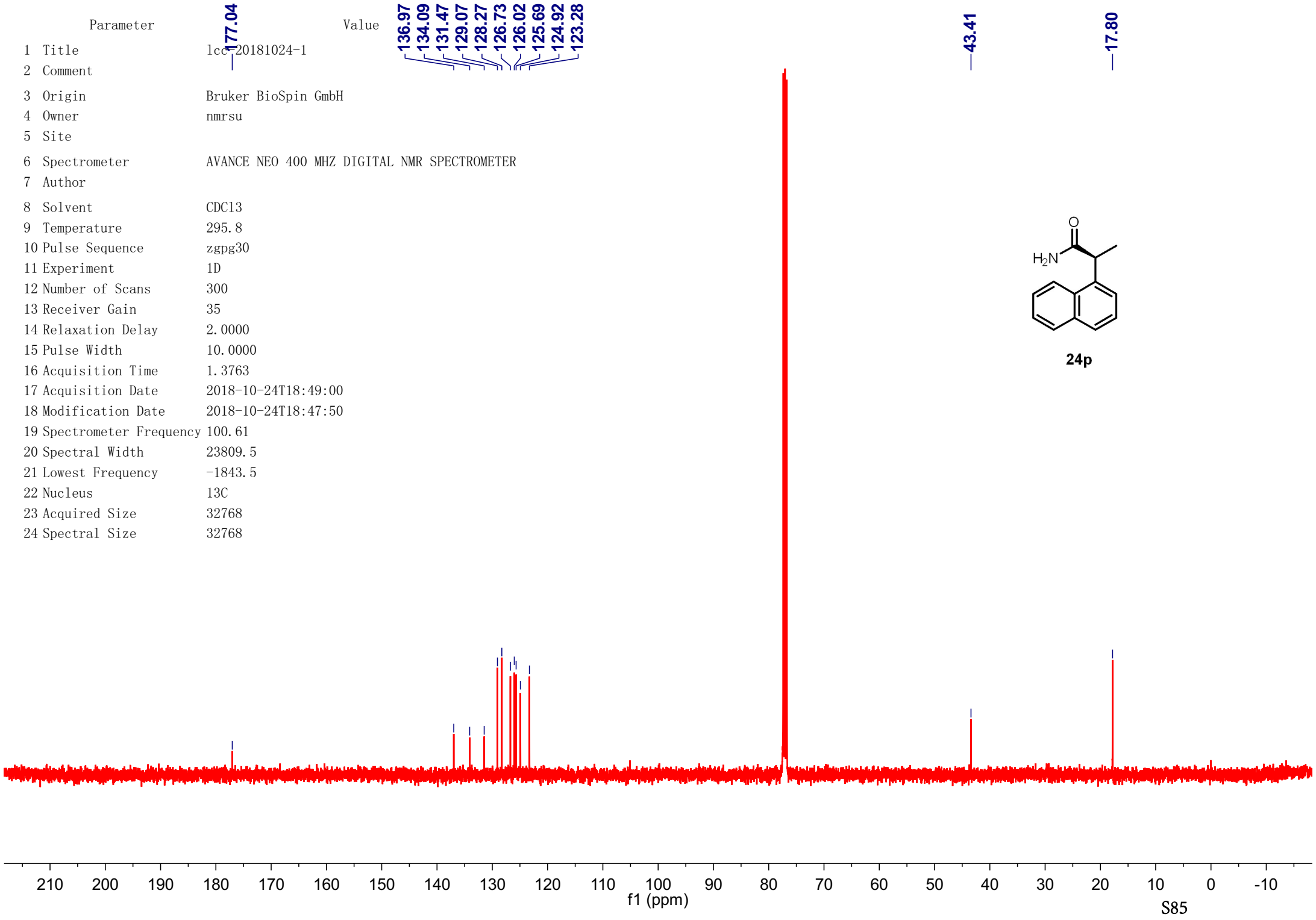
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-173/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1200
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-27T22:29:52
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



Parameter	Value
1 Title	lcc-20181024-1
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Site	
6 Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
7 Author	
8 Solvent	CDCl3
9 Temperature	295.6
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	8
13 Receiver Gain	101
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	3.9977
17 Acquisition Date	2018-10-24T18:30:40
18 Modification Date	2018-10-24T18:47:50
19 Spectrometer Frequency	400.13
20 Spectral Width	8196.7
21 Lowest Frequency	-1638.2
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



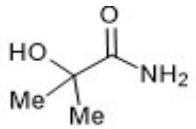
Parameter	Value
1 Title	lcc-20181024-1
2 Comment	
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Site	
6 Spectrometer	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
7 Author	
8 Solvent	CDCl3
9 Temperature	295.8
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	300
13 Receiver Gain	35
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.3763
17 Acquisition Date	2018-10-24T18:49:00
18 Modification Date	2018-10-24T18:47:50
19 Spectrometer Frequency	100.61
20 Spectral Width	23809.5
21 Lowest Frequency	-1843.5
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	32768



PROTON01

xxy-vi-153

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-153/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	38
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-07-18T17:42:28
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536

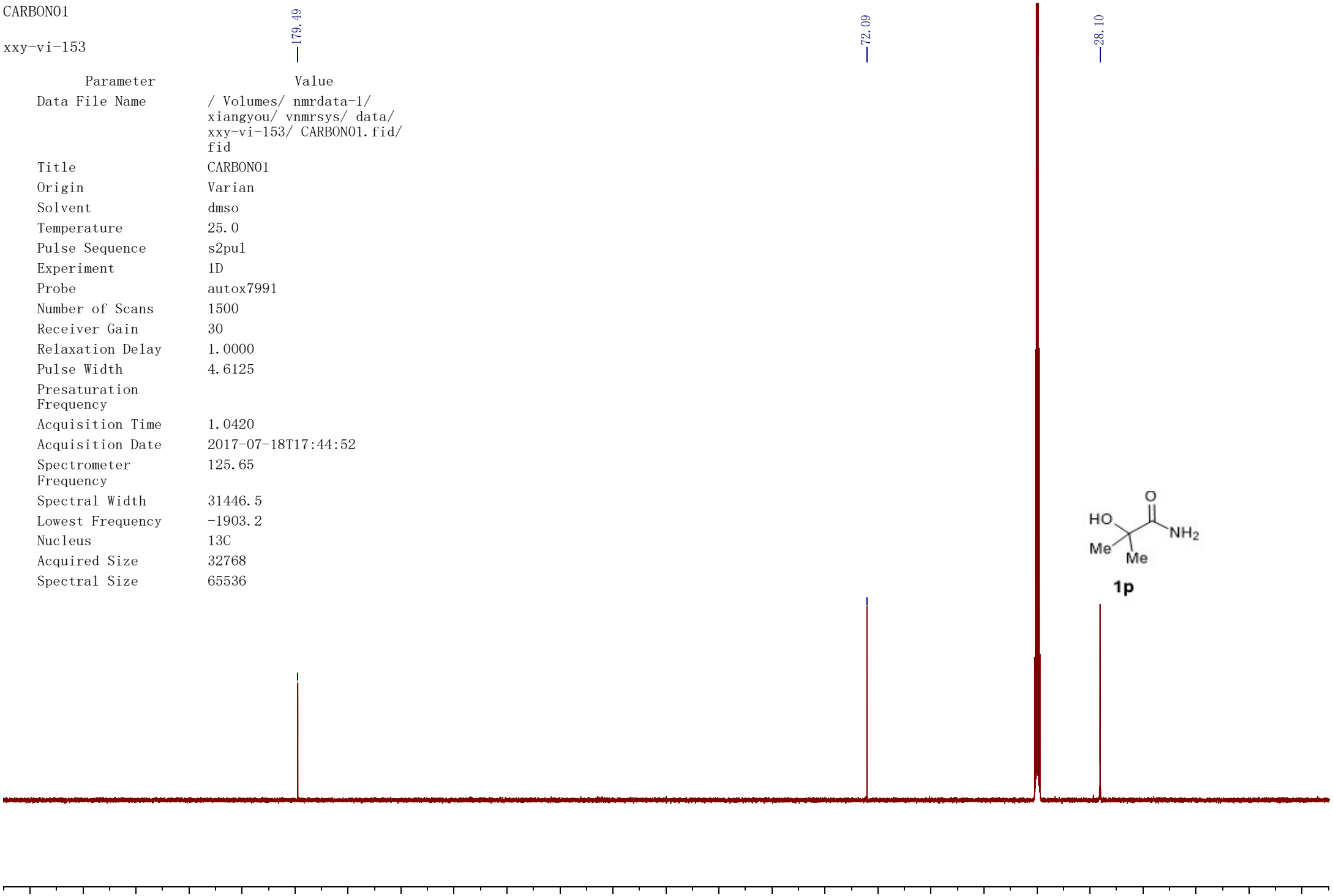


1p

CARBON01

xxy-vi-153

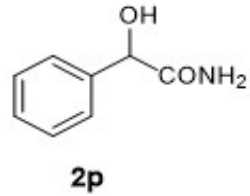
Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-153/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1500
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-07-18T17:44:52
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



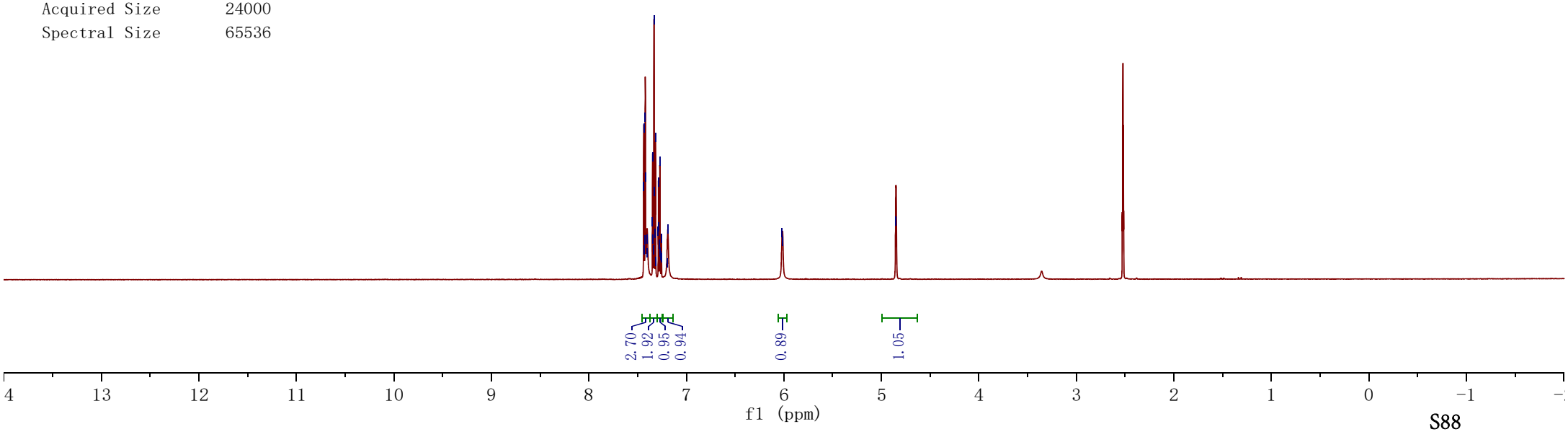
PROTON01

xxy-vi-mandeloamide

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-mandeloamide/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	16
Receiver Gain	50
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-08T18:49:21
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536

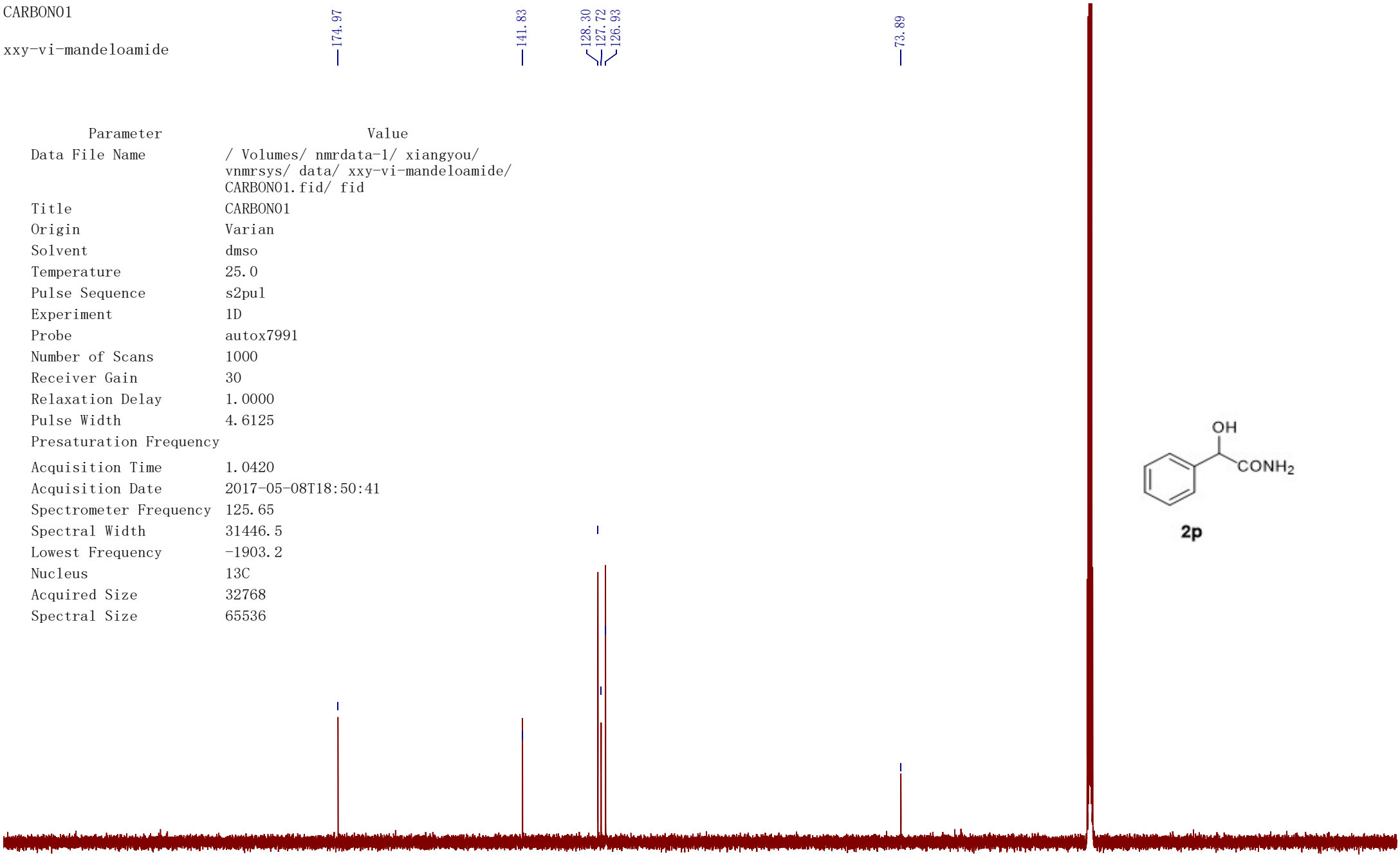


2p



CARBON01

xxy-vi-mandeloamide

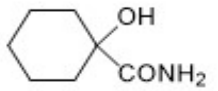


Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-mandeloamide/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1000
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-08T18:50:41
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

PROTON01

xxy-vi-197

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-197/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	48
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-07-04T10:36:03
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



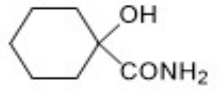
3p

CARBON01

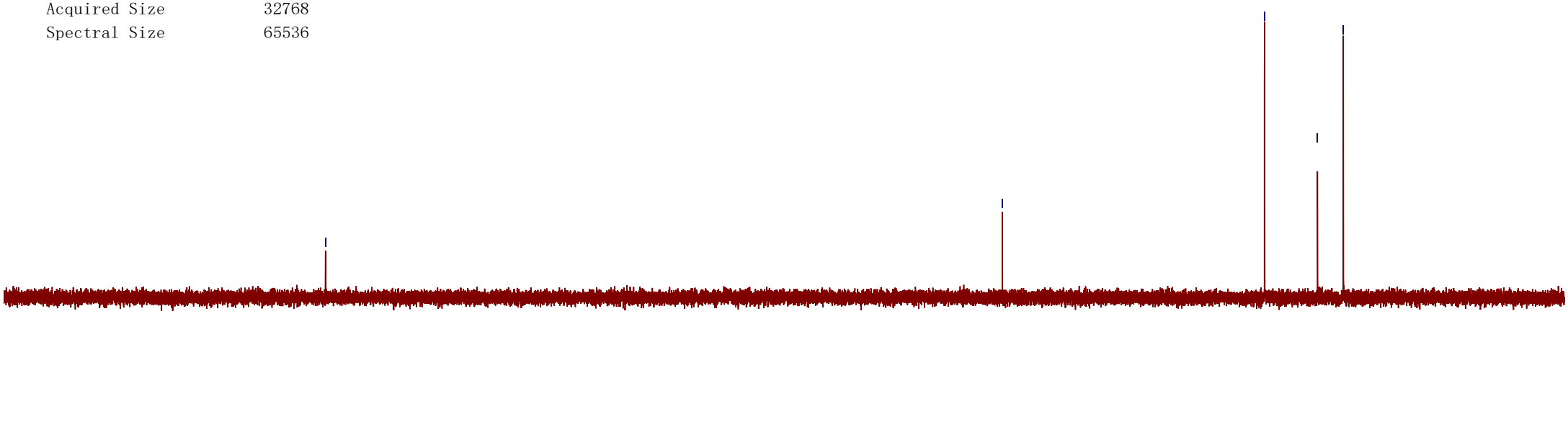
xxy-vi-197

183.48 74.96 32.92 24.43 20.30

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-197/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1500
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-07-04T10:38:28
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



3p



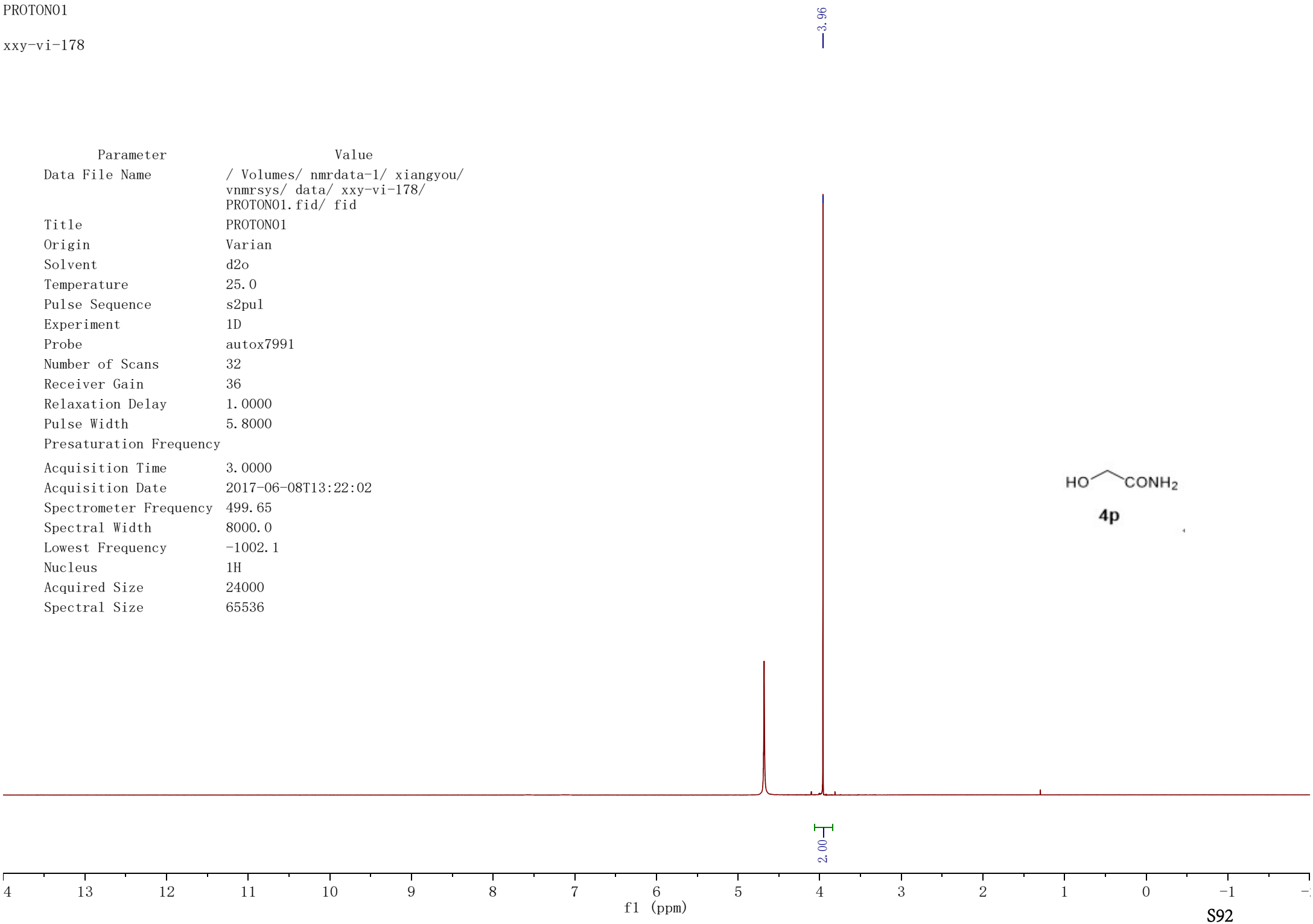
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

PROTON01

xxy-vi-178

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-178/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	36
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-06-08T13:22:02
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



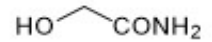
CARBON01

xxy-vi-178

178.02

60.51

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-178/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	d2o
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1200
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-06-08T13:24:27
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



4p

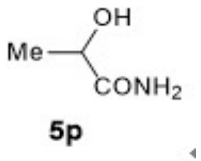
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

PROTON01

xxy-vi-160

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-160/ PROTON01.fid/ fid
Title	PROTON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	32
Receiver Gain	40
Relaxation Delay	1.0000
Pulse Width	5.8000
Presaturation Frequency	
Acquisition Time	3.0000
Acquisition Date	2017-05-20T09:10:24
Spectrometer Frequency	499.65
Spectral Width	8000.0
Lowest Frequency	-1002.1
Nucleus	1H
Acquired Size	24000
Spectral Size	65536



5p

CARBON01

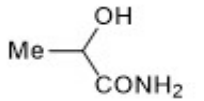
xxy-vi-160

177.48

67.54

21.42

Parameter	Value
Data File Name	/ Volumes/ nmrdata-1/ xiangyou/ vnmrsys/ data/ xxy-vi-160/ CARBON01.fid/ fid
Title	CARBON01
Origin	Varian
Solvent	dmso
Temperature	25.0
Pulse Sequence	s2pul
Experiment	1D
Probe	autox7991
Number of Scans	1500
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	4.6125
Presaturation Frequency	
Acquisition Time	1.0420
Acquisition Date	2017-05-20T09:12:52
Spectrometer Frequency	125.65
Spectral Width	31446.5
Lowest Frequency	-1903.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



5p

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)