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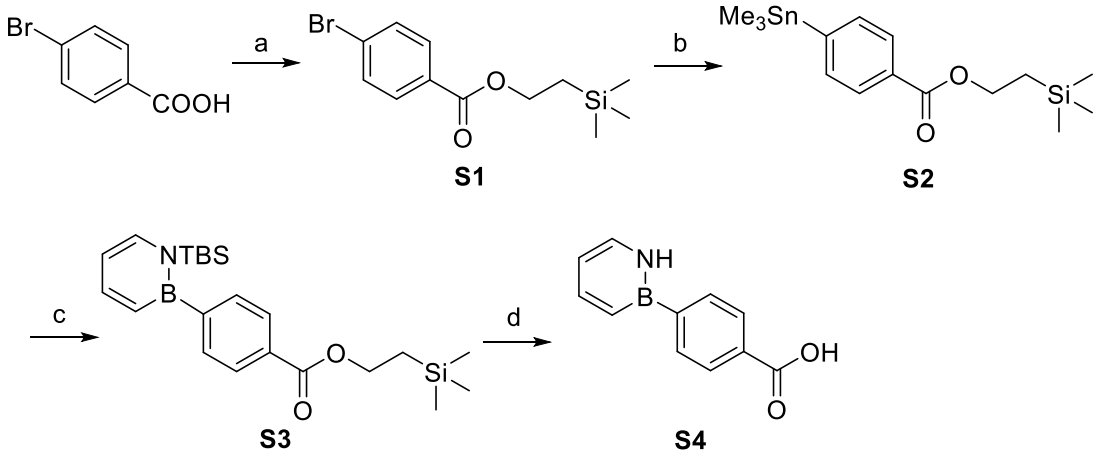
General Methods

Unless specifically stated otherwise, all the manipulations were carried in air in the fume hood in ambient environment. Oxygen- and moisture-sensitive manipulations were carried out under an inert atmosphere using either standard Schlenk techniques or a glove box. Chromatography for air-sensitive compounds was performed under an inert atmosphere using dry, degassed solvents and silica gel (240-300 mesh) which had been heated under vacuum in a 180 ˚C oil bath for 12 hours. Compound Febinac (4-biphenylacetic acid, CAS [5728-52-9]), **S6** (biphenyl-4-carboxylic acid, CAS [92-92-2]) and amine **S5** were purchased from Sigma-Aldrich. Reagents and catalyst were purchased from Sigma-Aldrich, TCI America, and Strem Chemicals and used without further purification. Anhydrous toluene, methylene chloride, pentane, THF, and ethyl ether were taken from a solvent purification system and used without further purification; the remaining solvents were dried over calcium hydride, distilled, and freeze-pump-thaw degassed before use. Additionally, all materials used under argon were either purged with argon (in the case of solids) or stirred over calcium hydride, distilled, then freeze-pump-thaw degassed (in the case of liquids). DMA solution for silica gel chromatography is a mixture of 80% CH_2Cl_2, 18% MeOH and 2% concentrated ammonium hydroxide.

^{1}H NMR, ^{13}C NMR and ^{11}B NMR spectra were recorded on a Varian Unity/Inova 300, Varian Unity/Inova 400, Varian Unity/Inova 500 or Varian Unity/Inova 600 spectrometer at ambient temperature. ^{11}B NMR were externally referenced to $BF_3 \bullet Et_2O$ ($\delta = 0$). IR spectra were recorded on a Nicolet Magna 550 FT-IR.

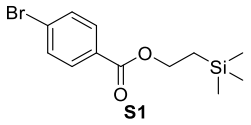
High-resolution mass spectrometry data were obtained at the following facilities: 1) Boston College mass spectrometry center on a JEOL AccuTOF instrument (JEOL USA, Peabody, MA), equipped with a Direct Analysis in Real Time (DART) ion source (IonSense, Inc., Danvers, MA) in positive ion mode. 2) Small Molecule Mass Spectrometry, FAS-Center for Systems Biology at Harvard University.

Scheme S1. Synthesis of BN-biphenyl carboxylic acid S4



Reagents and conditions: (a) 2-(trimethylsilyl)ethanol, DMAP, DCC, CH_2Cl_2, 98%; (b) $Pd(PPh_3)_4$, $(Me_3Sn)_2$, toluene, 100 ºC, N_2, 82%; (c) 1-(tert-butyldimethylsilyl)-2-chloro-1,2-dihydro-1,2-azaborinine, $[Rh(C_2H_4)_2Cl]_2$, BIPHEP, toluene, 100 ºC, N_2, 89%; (d) TBAF (1.0 M in THF), THF, –25 ºC to RT, N_2, 84%.

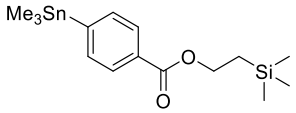
2-(Trimethylsilyl)ethyl-4-bromobenzoate **S1**



To a solution of 4-bromobenzoic acid (5.10 g, 24.9 mmol) in CH_2Cl_2 (150 mL) was added 4-dimethylaminopyridine (180 mg, 1.47 mmol), *N,N′*-dicyclohexylcarbodiimide (5.24 g, 25.4 mmol) and 2-(trimethylsilyl)ethanol (6.20 mL, 43.3 mmol) under ice-water bath. The reaction was stirred at room temperature for 14 hours. At the conclusion of the reaction, the mixture was passed through a glass frit, and the resulting filtrate was concentrated under reduced pressure. This crude material was purified by silica gel chromatography (5% EtOAc/hexane) (v/v) to provide the desired compound as colorless oil (7.52 g, yield 98%).

^{1}H NMR (300 MHz, CD_2Cl_2) δ 7.92 (d, J = 7.8 Hz, 2H), 7.62 (d, J = 7.8 Hz, 2H), 4.44 (t, J = 8.1 Hz, 2H), 1.16 (t, J = 4.8 Hz, 2H), 0.13 (s, 9H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 165.7, 131.6, 131.0, 129.8, 127.6, 63.4, 17.3, -1.77; FTIR (thin film): ῡ = 2953, 1708, 1588, 1483, 1398, 1274, 1247, 1174, 1103, 1064, 1009, 935, 829, 754, 681, 607, 459; HRMS (ESI) calcd for $C_{12}H_{17}BrO_2SiNa$ $(M+Na)^+$ 323.0073, found 323.0075.

2-(Trimethylsilyl)ethyl-4-(trimethylstannyl)benzoate **S2**

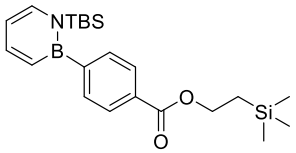


S2

In the glovebox, to a 20 mL a pressure vessel, compound **S1** (100 mg, 0.330 mmol), tetrakis(triphenylphosphine)palladium (20 mg, 0.017 mmol), hexamethylditin (140 mg, 0.427 mmol) and toluene (4.0 mL) was added. The solution was heated to 100 ºC for 15 hours, then allowed to cooled to room temperature. Volatiles were removed under reduced pressure, and the crude material was purified by silica gel chromatography (100% pentane then 10% EtOAc/hexane) (v/v) to afford the desired compound as a colorless oil (105 mg, yield 82 %).

^{1}H NMR (300 MHz, CD_2Cl_2) δ 7.99 (d, J = 4.5 Hz, 2H), 7.64 (d, J = 4.8 Hz, 2H), 4.44 (t, J = 5.1 Hz, 2H), 1.17 (t, J = 5.1 Hz, 2H), 0.36 (s, 9H), 0.13 (s, 9H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 166.8, 149.4, 135.8, 130.4, 128.2, 63.0, 17.2, -1.8, -9.9; FTIR (thin film): ϑ = 1715, 1273, 1110, 1064, 858, 836, 752, 694, 528; HRMS (ESI-TOF) calcd for $C_{15}H_{26}O_2SiSnNa$ $(M+Na)^+$ 409.0618, found 409.0618.

Compound **S3**



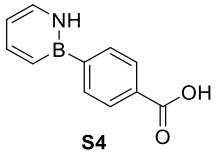
S3

In the glovebox, chlorobis(ethylene)rhodium dimer (52 mg, 0.13 mmol, 0.05 eq.), BIPHEP (140 mg, 0.26 mmol, 0.1 eq.) and toluene (5.0 mL) were added to a 20 mL vial. The solution was stirred for 30 min, then it was transferred to a pressure vessel containing 1-(tert-butyldimethylsilyl)-2-chloro-1,2-dihydro-1,2-azaborinine [CAS 1138164-75-6] (650 mg, 2.86 mmol, 1.1 eq.), compound **S2** (1.00 g, 2.59 mmol, 1.0 eq) and toluene (15 mL). The pressure vessel was sealed, and the reaction mixture was heated at 100 ºC for 15 hours. At the conclusion of the reaction, the reaction mixture was allowed to cool to room temperature. Volatiles were removed under reduced pressure, and the resulting crude material was purified in the glovebox

by silica gel chromatography (10% diethyl ether/pentane) to provide the desired product as white solid (951mg, yield 89%).

^{1}H NMR (300 MHz, CD_2Cl_2) δ 8.00 (d, J = 8.1 Hz, 2H), 7.66-7.71 (m, 1H), 7.51-7.55 (m, 3H), 6.68 (d, J = 10.5 Hz, 1H), 6.54 (m, 1H), 4.49 (t, J = 4.2, Hz, 2H), 1.23 (t, J = 4.5 Hz, 2H), 0.99 (s, 9H), 0.18 (s, 9H), 0.11 (s, 6H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 167.0, 143.2, 138.3, 132.0, 128.9, 127.5, 112.2, 62.9, 26.6, 18.8, 17.4, -1.7, -2.3 (the boron-bound carbono signals are not observed); ^{11}B NMR (96 MHz) δ 41.3; FTIR (thin film): ῡ = 3282, 2931, 1733, 1613, 1542, 1456, 1370, 1233, 1137, 813, 731, 676, 644, 504, 457; HRMS (ESI) calcd for $C_{22}H_{37}BNO_2Si_2$ $(M+H)^+$ 414.2456, found 414.2468.

Compound **S4**



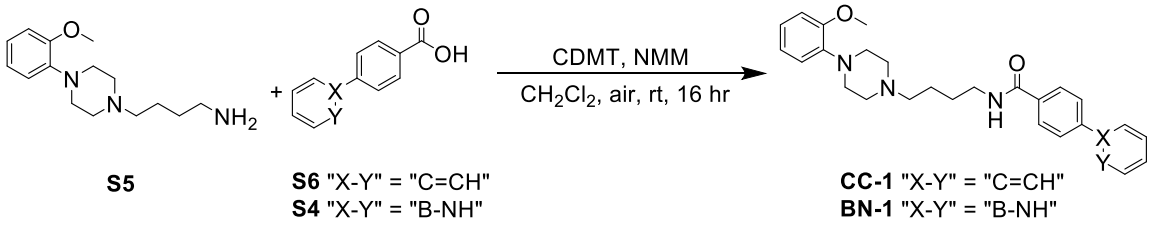
S4

In the glovebox, compound **S3** (850 mg, 2.06 mmol) was dissolved into THF (12.0 mL) in a round-bottom flask and cooled in a –25 ºC freezer for 30 min. The reaction flask was then taken out of the glovebox, and TBAF (5.0 mL, 1.0 M in THF, 5.0 mmol) was added slowly. The resulting yellow solution was stirred at room temperature for 3 hr. Volatiles were removed under reduced pressure, and the crude material was purified on silica gel chromatography using CH_2Cl_2/MeOH/AcOH 100:4:0.8 (v/v) as the eluent. The resulting off-white solid was recrystallized in CH_2Cl_2/hexane system to afford the desired compound (344 mg, yield 84%).

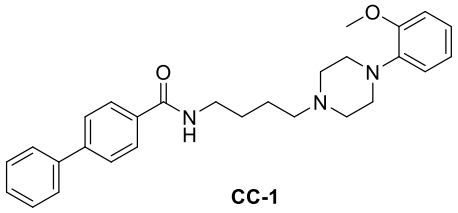
^{1}H NMR (300 MHz, acetone-d_6) δ 10.19 (br s, 1H), 7.89-8.07 (m, 4H), 7.81 (dd, J = 6.3, 11.1 Hz, 1H), 7.61 (t, J =6.6 Hz, 1H), 7.22 (d, J = 11.1 Hz, 1H), 6.47 (t, J = 6.6 Hz, 1H) (COOH peak is not observed); ^{13}C NMR (126 MHz, acetone-d_6) δ 167.2, 144.8, 135.2, 132.4, 130.6, 129.0, 111.2 (the boron-bound carbon signals are not observed); ^{11}B NMR (96 MHz) δ 33.6; FTIR (thin film): $\tilde{\upsilon}$ = 1733, 1716, 1684, 1635, 1557, 1540, 1521, 1473, 1374, 724, 671, 419; HRMS (DART) calcd for $C_{11}H_{11}BNO_2$ $(M+H)^+$ 200.08828, found 200.08758.

General experimental procedure to form BN-biarylcarboxamides

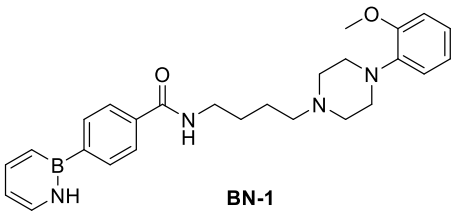
To the mixture of 2-chloro-4,6-dimethoxyl-1,3,5triazine (CDMT, 32.0 mg, 0.182 mmol) and BN Felbinac (38.0 mg, 0.176 mmol) or compound **S4** (35.0 mg, 0.176 mmol) in anhydrous CH_2Cl_2 (3.0 mL), *N*-methylmorpholine (NMM, 20.0 μL, 0.182 mmol) was added at 0 °C. The resulting clear solution was stirred at room temperature for 25 min. Then, the corresponding amine (1.1 equiv.) was added, and this mixture was stirred for 14 hours at room temperature (if this amine is in salt form, another 1 equiv. NMM is added). At the conclusion of the reaction, CH_2Cl_2 (50 mL) was added to the reaction mixture, and the resulting mixture was washed with saturated $NaHCO_3$. The organic phase was concentrated under reduced pressure. The resulting crude material was purified by silica gel chromatography to afford corresponding amide products. If necessary, recrystallization in CH_2Cl_2/hexane or MeOH/CH_2Cl_2/hexane can provide desired amide compounds as an off-white solid.



Amine **S5** [CAS 21103-33-3] was purchased from Aldrich, and the bioactive amide **CC-1** was prepared according to literature procedures.[1] ^{1}H NMR and mass spectra of **CC-1** match with those reported in the literature.



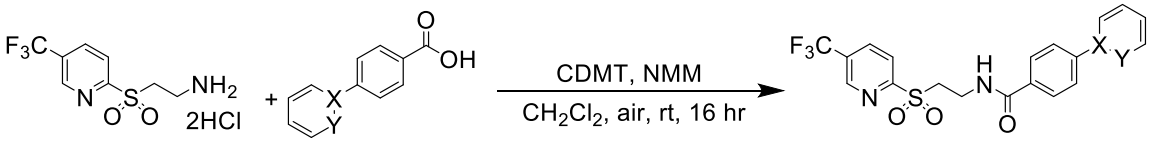
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84-7.86 (m, 2H), 7.56-7.63 (m, 4H), 7.34-7.45 (m, 3H), 6.93-7.00 (m, 2H), 6.83-6.87 (m, 3H), 3.83 (s, 3H), 3.49-3.51 (m, 2H), 3.08-3.11 (m, 4H), 2.69-2.75 (m, 3H), 2.54-2.58 (m, 3H), 1.67-1.73 (m, 4H); HRMS (DART) calcd for $C_{28}H_{34}N_3O_2$ $(M+H)^+$ 444.26510, found 444.26631.



BN-1

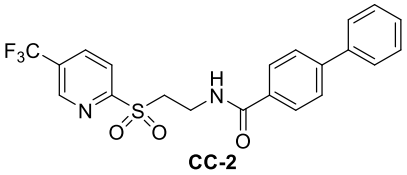
Silica gel chromatography condition (CH_2Cl_2/MeOH), off-white solid (110 mg, yield 82%).

^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.48 (br s, 1H), 7.79-7.86 (m, 5H), 7.47 (d, J = 6.5 Hz, 1H), 7.20 (d, J = 6.0 Hz, 1H), 6.86-6.97 (m, 5H), 6.46 (d, J = 6.0 Hz, 1H), 3.82 (s, 3H), 3.43-3.48 (m, 2H), 2.96-3.20 (m, 4H), 2.44-2.78 (m, 6H), 1.67-1.80 (m, br, 4H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ167.5, 152.4, 144.8, 141.5, 135.4, 128.4 (br), 126.5, 122.6, 120.9, 118.1, 111.4, 111.2, 57.9, 55.2, 50.2, 39.8, 31.6, 27.4, 24.2, 22.6, 13.9; ^{11}B NMR (160 MHz) δ 36.7; FTIR (thin film): ῡ = 3553, 1699, 1612, 1541, 1499, 1462, 1364, 1310, 1239, 1180, 1117, 1088, 1022, 979, 923, 736, 677, 534; HRMS (DART) calcd for $C_{26}H_{34}BN_4O_2$ $(M+H)^+$ 445.27748, found 445.27853.



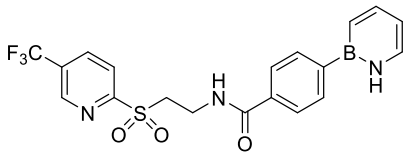
S7 | **S6** "X-Y" = "C=CH" / **S4** "X-Y" = "B-NH" | **CC-2** "X-Y" = "C=CH" / **BN-2** "X-Y" = "B-NH"

Amine **S7** [CAS 1850290-88-8] and the bioactive amide **CC-2** were prepared according to literature procedures.[2] ^{1}H NMR and mass spectra signals of **CC-2** match with those reported in the literature.



CC-2

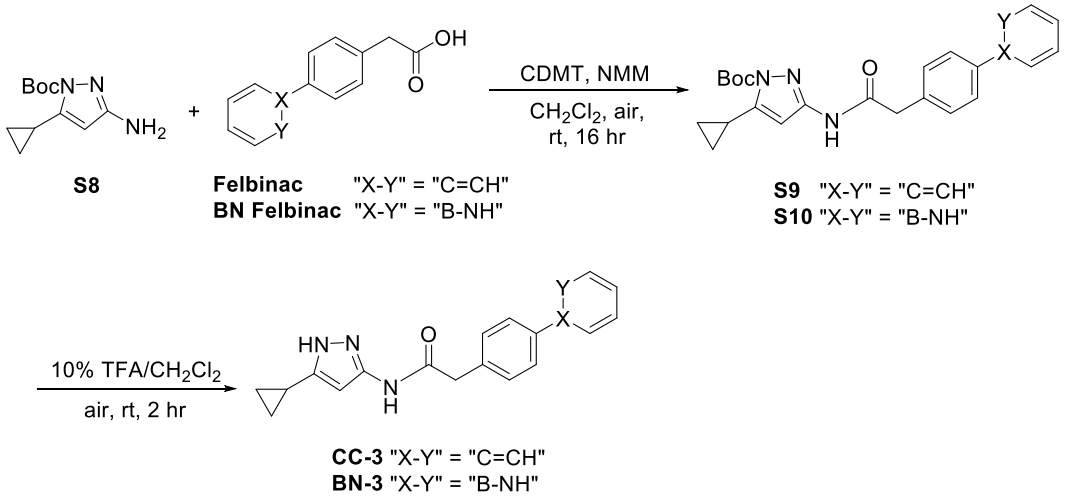
^{1}H NMR (500 MHz, Acetone-*d*6) δ 9.07 (s, 1H), 8.51-8.53 (m, 1H), 8.34-8.36 (m, 1H), 7.84-7.91 (m, 3H), 7.72-7.74 (m, 4H), 7.44-7.54 (m, 3H), 3.89-3.97 (m, 4H); HRMS (DART) calcd for $C_{21}H_{18}F_3N_2O_3S$ $(M+H)^+$ 435.09902, found 435.09851.



BN-2

After coupling reaction, the reaction mixture was directly purified by silica gel chromatography (DMA/CH_2Cl_2/hexane). Off-white solid (79 mg, yield 78%).

^{1}H NMR (500 MHz, DMSO-d_6) δ 10.67 (br s, 1H), 9.06 (s, 1H), 8.45-8.50 (m, 2H), 8.23 (d, J = 8.5 Hz, 1H), 7.85-7.90 (m, 2H), 7.63-7.72 (m, 1H), 7.58-7.60 (m, 2H), 7.48 (t, J = 7.5 Hz, 1H), 7.07 (d, J =11.0 Hz, 1H), 6.39 (t, J = 6.0 Hz, 1H), 3.84-3.93 (m, 2H), 3.60-3.78 (m, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 166.7, 160.5, 147.7, 145.1, 137.3, 136.0, 133.7, 132.6, 127.7, 126.7, 122.7, 111.3, 50.9, 34.2 (boron-bound carbon and the CF_3 signals are not observed) ^{11}B NMR (160 MHz) δ 34.3; FTIR (thin film): ῡ = 2924, 1734, 1642, 1540, 1463, 1361, 1300, 1141, 1097, 1072, 1012, 860, 814, 726, 612, 486; HRMS (DART) calcd for $C_{19}H_{18}BF_3N_3O_3S$ $(M+H)^+$ 436.11140, found 436.11278.

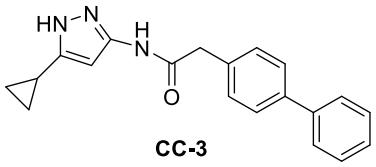


The synthesis of amine **S8** [CAS 326827-13-8][3a,3b] and the bioactive amide **CC-3**[3c] was reported in the reference. ^{1}H NMR and mass spectra signals of **CC-3** match with those reported in the literature.

Compound **BN-3** was prepared in a two-step procedure:

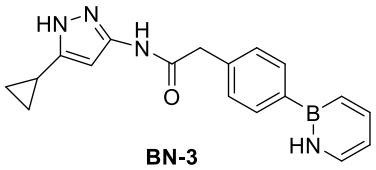
Amide coupling reaction: Amine **S8** (120 mg, 0.540 mmol) was dissovled in anhydrous CH_2Cl_2 (8.0 mL), then compound **BN Felbinac** (115mg, 0.54 mmol), 2-chloro-4,6-dimethoxyl-1,3,5-triazine (CDMT, 95 mg, 0.54 mmol), and N-methylmorpholine (NMM, 140 μL, 1.08 mmol) was added at 0 °C. The resulting solution was stirred at room temperature for 16 hours. At the conclusion of the reaction, CH_2Cl_2 (100 mL) was added to the reaction mixture, and the resulting mixture was washed with saturated $NaHCO_3$. The organic phase was concentrated under reduced pressure and the resulting crude material was purified by silica gel chromatography (DMA/CH_2Cl_2/hexane) to afford the desired amide **S10** as an yellow oil (^{1}H NMR purity >90%) which was used directly for the next step.

Boc-deprotection procedure: To the amide **S10** obtained in the previous step, 10% TFA/CH_2Cl_2 (5.0 mL) was added at 0 ^{o}C. The mixture was then allowed to stir at room temperature for 2 hours. At the conclusion of the reaction, CH_2Cl_2 (100 mL) was added to the reaction mixture, and the resulting mixture was washed with saturated $NaHCO_3$. The organic phase was concentrated under reduced pressure. The resulting crude material was purified by silica gel chromatography (hexane/CH_2Cl_2 to DMA/CH_2Cl_2) to afford a solid, which was further recystalized from CH_2Cl_2/hexane to yield pure product as off-white solid (104 mg, yield 61% for two steps).



CC-3

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.01 (s, 1H), 10.47 (s, 1H), 7.57-7.63 (m, 3H), 7.33-7.44 (m, 6H), 6.12 (s, 1H), 3.59 (s, 2H), 1.80-1.82 (m, 1H), 0.85-0.88 (m, 2H), 0.60-0.62 (m, 2H); HRMS (DART) calcd for $C_{20}H_{20}N_3O$ $(M+H)^+$ 318.16604, found 318.15979.



BN-3

^{1}H NMR (500 MHz, DMSO-d_6) δ 12.04 (s, 1H), 10.58 (bs, 1H), 10.47 (s, 1H), 7.82 (d, J = 8.0 Hz, 2H), 7.67-7.70 (m, 1H), 7.47 (t, J = 7.0 Hz, 1H), 7.34 (d, J = 8.0 Hz, 2H), 7.06 (d, J =11.0 Hz, 1H), 6.36 (t, J = 6.5 Hz, 1H), 6.15 (s, 1H), 3.59 (s, 2H), 1.76-1.83 (m, 1H), 0.88-0.90 (m, 2H), 0.62-0.65 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.5, 144.7, 137.1, 135.8, 132.9, 129.5, 129.1, 128.7, 127.7 (br), 126.9, 110.7, 43.0, 8.2, 7.3 (the exocyclic boron-bound carbon signal was not observed); ^{11}B NMR (160 MHz) δ 33.4; FTIR (thin film): $\tilde{\upsilon}$ = 3373, 1655, 1590, 1539, 1484, 994, 802, 731, 676, 597, 459; HRMS (DART) $C_{18}H_{20}BN_4O$ $(M+H)^+$ 319.17379, found 319.17413.

Air and water stability study of compound BN-1, BN-2 and BN-3

Air and water stability study procedures were adapted from a previously reported study with minor modifications.[4]

In the fume hood, a J-Young NMR tube was charged with compound **BN-1** (5.0 mg), $CDCl_3$ (0.5 mL), internal standard toluene (2 μL), and H_2O (2 μL). ^{1}H and ^{11}B NMR were taken at time 0 hr. Then the sample was vigorously shaken and immersed into a pre-heated 50 ^{o}C oil bath. ^{1}H and ^{11}B NMR were taken at indicated time points. ^{1}H and ^{11}B NMR analysis indicated no decomposition of **BN-1** after 24 hours.

In the fume hood, a J-Young NMR tube was charged with the individual compound **BN-2** or **BN-3** (5.0 mg), DMSO-d_6 (0.5 mL), internal standard toluene (2 μL), and H_2O (2 μL). ^{1}H and ^{11}B NMR were taken at time 0 hr. Then the sample was vigorously shaken and immersed into a pre-heated 50 ^{o}C oil bath. ^{1}H and ^{11}B NMR were taken at indicated time points. ^{1}H and ^{11}B NMR analysis indicated no decomposition of **BN-2** and **BN-3** after 24 hours.

Assays

Rat Liver Microsome assay

Performed according to standard literature methods (Obach, RS (1999) Drug Metab Dispos; 27:1350-1359). Liver microsomes from male Sprague-Dawley rats were obtained from BDGentest (catalog #452501), Briefly, test compound was dissolved in DMSO at 10 mM and diluted to 10 uM in 50 mM Pi, pH 7.4. 0.1 volume of this was added to a 0.5 mg/ml suspension of rat liver microsomes in 50 mM Pi, pH 7.4. Reaction is initiated by addition of 1 mM NADPH, 2 mM $MgCl_2$. Samples are withdrawn after 0, 5, 15, and 30 minutes incubation at 37 °C and mixed with 1 vol acetonitrile. Test compound remaining is determined by peak area in LC/MS chromatogram relative to t = 0 peak area. Clearance is calculated applying literature scaling factors to test compound elimination rate constant, which is determined by slope of ln[compound remaining] vs. time.

CYP3A4

Inhibition of CYP3A4 activity was performed according to literature methods (i.e. Kim, et al, (2005) Rapid Commun Mass Spectrom; 19:2650-2658 and Obach et al (2006) J Pharmacol Exp Ther; 316:336-348). Briefly, compounds at serially diluted concentrations between 0.1 and 20 uM (final) were included in incubations with human liver microsomes (0.05 mg/ml, BDGentest) at 37 °C. Midazolam was added at 1 uM as test substrate and reaction initiated by addition of 1 mM NADPH. Reaction was terminated after 10 minutes and amount of 1'-hydroxymidazolam (product formed from midazolam by CYP3A4) determined by LC/MS methods. Inhibition of 1'-hydroxymidazolam formation relative to buffer controls and calculation of IC50 was done by standard data analysis methods.

Rat in vivo PK

Male Sprague-Dawley rats, 9-11 weeks old and jugular vein cannulated, were obtained from Envigo. Test compound was dissolved in a formulation consisting of 15% PEG300, 7.5% Solutol and 7.5% CremophoreEL in water. **BN-3** was dosed to SD rat at 1 mg/kg by intravenous bolus injection (IV) through the jugular cannula. **CC-3** was dosed IV at 0.5 mg/kg. Blood samples were taken at times after dosing (up to 24 h). Similarly, **BN-3** and **CC-3** were dosed orally (PO, *per os*) at 5 mg/kg. Blood samples were taken up to 7 hours after dosing. Plasma was obtained by

centrifugation of the blood samples and analyzed for concentration of **BN-3** or **CC-3** by LC/MS methods. Non-compartmental analysis was performed on the concentration data according to standard methods to obtain area under the concentration-time curve (AUC), clearance (CL), bioavailability (F) and half-life (t ½) .

Concentration-time data (average of N=2):

Time (h)	CC-3 0.5 mg/kg IV (nM)	BN-3 1.0 mg/kg IV (nM)	CC-3 5 mg/kg PO (nM)	BN-3 5 mg/kg PO (nM)
0.083	1177.5	2761.7	--	--
0.25	552.1	2007.3	311.0	211.1
0.5	360.0	1066.4	691.6	239.7
1	90.7	514.0	448.6	485.6
2	11.1	69.4	341.8	685.4
4	9.1	30.4	75.8	546.8
7	4.2	16.2	31	117.4
24	4.8	7.6	--	--

hERG binding

Cell membranes were prepared from HEK-293 cells recombinantly expressing the KCNH2 (hERG) gene. Membranes (about 40 µg protein) were incubated for 60 min at 22 °C with 3 nM [^{3}H]dofetilide in the absence or presence of the test compound in a buffer containing 50 mM Tris-HCl (pH 7.4), 10 mM KCl and 1 mM $MgCl_2$, in an assay volume of 200 µl in a 96-well plate. Non-specific binding was determined in the presence of 25 µM terfenadine. Following the incubation, the samples were filtered rapidly under vacuum through glass fiber filters (GF/B) presoaked with 0.3% polyethyleneimine (PEI) and rinsed several times with ice-cold 50 mM Tris-HCl, 10 mM KCl and 1 mM $MgCl_2$ using a 96-sample cell harvester (Unifilter, Packard). The filters were then dried and counted for radioactivity in a scintillation counter (TopCount, PerkinElmer) using a scintillation cocktail (Microscint-O, PerkinElmer). Test compounds were dissolved in DMSO. The final concentration of DMSO in the assay was 1%.

PPAR (γ and δ) antagonist

LanthaScreen™ TR-FRET PR Coactivator Assay Kits were purchased from Life Technologies (e.g. Cat. #PV4685 for PPARdelta and PV4548 for PPARgamma). A terbium-labeled anti-GST

antibody is used to indirectly label a nuclear receptor by binding to its GST tag. When an agonist binds to the receptor, a conformational change takes place allowing a fluorescein-labeled co-activator to bind with high affinity. When the terbium label on the anti-GST antibody is excited at 340 nm, energy is transferred to the fluorescein label on the bound co-activator peptide and detected as emission at 520 nm.

The assays were performed in a final volume of 50 µL per well in a 384-well solid black plate (PerkinElmer, Cat. #6007279). The components of the PPAR δ assay were added in the following order: 0.25 µL test compound in 100% DMSO, 50 µL GST-PPARδ-LBD, Tb-antiGST antibody and Fluorescein-C33 Peptide (final concentrations of 5 nM, 10 nM, 100 nM respectively). For antagonist activity an additional 0.25 µL EC_{80} agonist (GW0742, 10 nM final concentration) was added. The plates were incubated in the dark at room temperature for 2 hours and then read in a PerkinElmer Envision. The signal measured was the fluorescence ratio 520 nm/495 nm.

The components of the PPAR γ assay were added in the following order: 0.25 µL test compounds in 100% DMSO, 50 µL GST-PPARγ-LBD, Tb-antiGST antibody and Fluorescein-TRAP220/DRIP-2 Peptide (final concentrations of 2.5 nM, 2.5 nM, 125 nM respectively). For antagonist activity an additional 0.25 µL EC_{80} agonist (rosiglitazone, 50 nM final concentration) was added. The plates were incubated in the dark at room temperature for 2 hours and then read in a PerkinElmer Envision. The signal measured is the fluorescence ratio 520 nm/495 nm.

Dopamine D3 binding

Wheatgerm agglutinin (WGA) scintillation proximity assay (SPA) beads (RPNQ0001) were purchased lyophilized from PerkinElmer (Boston, MA, USA). One vial (500 mg) was reconstituted using 5 mL of distilled water to give a final concentration of 100 mg/mL. Reconstituted SPA beads were stored at 4°C and not frozen. 384-well white, clear bottom plates (Cat. #3706) were purchased from Corning (Lowell, MA, USA). The incubations were performed in a final volume of 50 µL per well in 384-well white, clear bottom polystyrene plates. The components of the incubation were added to each well in the following order and volumes: 0.25 µL test compound / NSB / reference in 100 % DMSO; 9.75 µL distilled water; 20 µL radioligand; 20 µL SPA bead / membrane mixture.

The final concentration of WGA beads was 4 mg/mL and that of D3 membranes (PerkinElmer Cat. #ES-173) was 10 μg/mL. The final concentration of the radioligand [^{3}H]-Methylspiperone was 0.4 nM. Total binding was determined by adding DMSO and non-specific binding (NSB) was determined by the addition of (+)Butaclamol, final concentration 10 μM. The plates were then sealed and allowed to sit at room temperature for 5 hours of incubation time. Plates were counted in a PerkinElmer Microbeta Trilux reader for 90 seconds per well.

CDK2 kinase assay

Kinase reactions was performed in automated fashion for profiling with several kinases in parallel with higher throughput. All assays were performed in 384 well microtiter plates. Each assay plate contained 8-point serial dilutions for 40 test compounds, as well as two 16-point serial dilutions of staurosporine as reference compound, plus 16 high- and 16 low controls. Protocol: 0.1 μl Compound, 9 μl 2x peptide/ATP solution, 9 μl 2x enzyme solution, incubate for 60 min at 30 °C, 70 μl stop/run buffer. Independent of the kinase, all reactions were performed in 50 mM HEPES, pH 7.5, 1mM DTT, 0.02% (v/v) Tween20, 0.02% (w/v) BSA, 0.5-1% (v/v) DMSO, 10 mM beta-glycerophosphate, and 10μM sodium orthovanadate. CDK specific conditions: [CDK2] 8.2nM, [ATP] 25uM, [peptide] 2uM, [ATP KM] 25uM, [Mg] 8mM. Percent-inhibition values were calculated as the following: The relative amount of phosphorylated peptide r, was calculated using the heights of the substrate peak, s, and the product peak, p: $r = p/(p+s)$. Percent inhibition was then determined as : $\%inhibition = 100 \bullet (1-(r-r_{low\ control})/(r_{high\ control} - r_{low\ control}))$

Equilibrium solubility:

Equilibrium solubility was determined using a miniaturized shake flask approach as described in Zhou et al.[5] Aliquots of 10 mM DMSO compound solution were dispensed in triplicate in 96-well polypropylene plates. The DMSO was removed using a GeneVac HT4X evaporator for approximately one hour. Media (pH 4.0 buffer, pH 6.8 buffer, FaSSIF: Fasted State Simulated Intestinal Fluid) was added to each well to achieve a target concentration of 1 mM. The plate was sealed and shaken for a minimum of 16 hours, then centrifuged for phase separation. An aliquot of supernatant was transferred to a new plate, where it was further diluted for subsequent analysis. Quantification of solubility was performed using RapidFire/MS/MS and a four-point

calibration curve. Experimental variability was determined from approximately 300 duplicate measurements from different days and experimentalists, with a log standard deviation of 0.25.

HT logD:

Dried DMSO stock samples were incubated with buffer and 1-octanol and shaken for at least 4 hours. Sample preparation and phase separation were automated using centrifugation and liquid handling workstations. Both 1-octanol and buffer phases were quantified in triplicate and logD was derived from the ratio of peak area responses against an internal standard in a tandem mass spectrometer. To obtain logP, the buffer pH was selected where the compound was unionized, based on calculated pKa values.

PAMPA Assay:[6]

Permeation experiments were carried out in 96-well microtiter filter plates obtained from Millipore AG (Volketswil, Switzerland). Filter (isopore, polycarbonate) specifications were as follows: 3 *u*m pore size, 9-10 *u*m thickness, and 5-20% porosity. Each well of the filter plate was impregnated with 15 *u*L of 5% hexadecane dissolved in hexane (i.e., total amount of hexadecane: 0.75 *u*L) for at least 10 min to allow for complete evaporation of the hexane. Subsequently, the donor compartments were hydrated with 300 *u*L of 50 *u*g/ mL test compound in buffer, containing 5% DMSO and 100 mM KCl, and connected to a homemade Teflon acceptor plate which had been prefilled with buffer containing 5% DMSO. The resulting sandwich construct was incubated at room temperature under constant light shaking (50-100 rpm). After 5 h, the sandwich was disassembled and the solution in the acceptor was transferred to a disposable UV-transparent plate (Corning Costar, Corning, NY). UV absorption was measured with a SPECTRAmax190 microplate spectrophotometer (Molecular Devices Corp., Sunnyvale, CA) at absorption wavelengths between 260 and 290 nm. To ensure that the donor/acceptor fluxes were not due to porous or unstable hexadecane layers, the stability of the hexadecane membranes was tested at the end of the incubation period by electrical resistance measurements. Wells with barriers which displayed electrical resistance lower than 5 kΩ were discarded. Electrical resistance measurements were performed using a Keithley 6517A electrometer (Keithley Instruments S.A., Dubendorf, Switzerland) with Ag/AgCl electrodes from World Precision Instruments (Berlin, Germany). Ionization constants were measured by potentiometric titration in

0.15 M KCl at 25.0 °C using a GlpKa instrument (Sirius Analytical Instruments, Forest Row, U.K.). Partition and distribution coefficients were measured using the pH metric technique using a PCA101 automatic titrator (Sirius Analytical Instruments, Forest Row, U.K.).

At the end of the incubation period the sandwich was carefully disassembled, the acceptor plate measured with the UV microtiter plate spectrophotometer, and the donor plate submitted to current measurements to assess the integrity of the hexadecane membranes. The apparent permeability value *P*a is determined from the ratio *r* of the absorbance of compound found in the acceptor chamber divided by the theoretical equilibrium absorbance (determined independently):

$$P_a = -\frac{V_D \quad V_R}{(V_D + V_R)At} \cdot \ln(1 - r) \qquad (1)$$

In this equation, V_R is the volume of the acceptor compartment (0.4 cm^3), V_D is the donor volume (0.3 cm^3), A is the accessible filter area (total filter area, 0.24 cm^2, multiplied by a porosity ratio of 20%), and t is the incubation time. Equation 1 is obtained from the differential equation (2) with cD*(t)* being the compound concentration in the donor compartment and cR*(t)* being the concentration in the acceptor compartment. In absence of membrane retention *P*a is identical to *P*e, the effective membrane permeability. When membrane retention occurs *P*a can be converted to Pe using mass balance equations.

$$\frac{dc_R}{dt} = \frac{P_a A}{V_R}(c_D - c_R) \qquad (2)$$

Molecular modeling:

Docking poses were generated in a high resolution crystal structure of CDK2/cyclin A (PDB entry 1VYW) using Glide (version 6.6) from Schrödinger. The crystal structure was first prepared using the standard protein preparation wizard within the Maestro interface. Grid files were generated for docking after deleting the crystallographic water molecules. 3D-geometries of the ligands **BN-3** and **CC-3** were generated using ligprep. Compounds were docked in the pre-generated grid files in extra precision mode. Three docking poses were saved for each of the compounds and the docking results were analyzed visually. The robustness of the docking

protocol was confirmed by self-docking and cross-docking studies of the known CDK2 ligands from crystal structures. Geometry of the C-B bond in BN-3 was verified by comparing with the small molecule x-ray of 1,2-dihydro-2-phenyl-1,2-azaborine (CSD code WAJTEH).[7]

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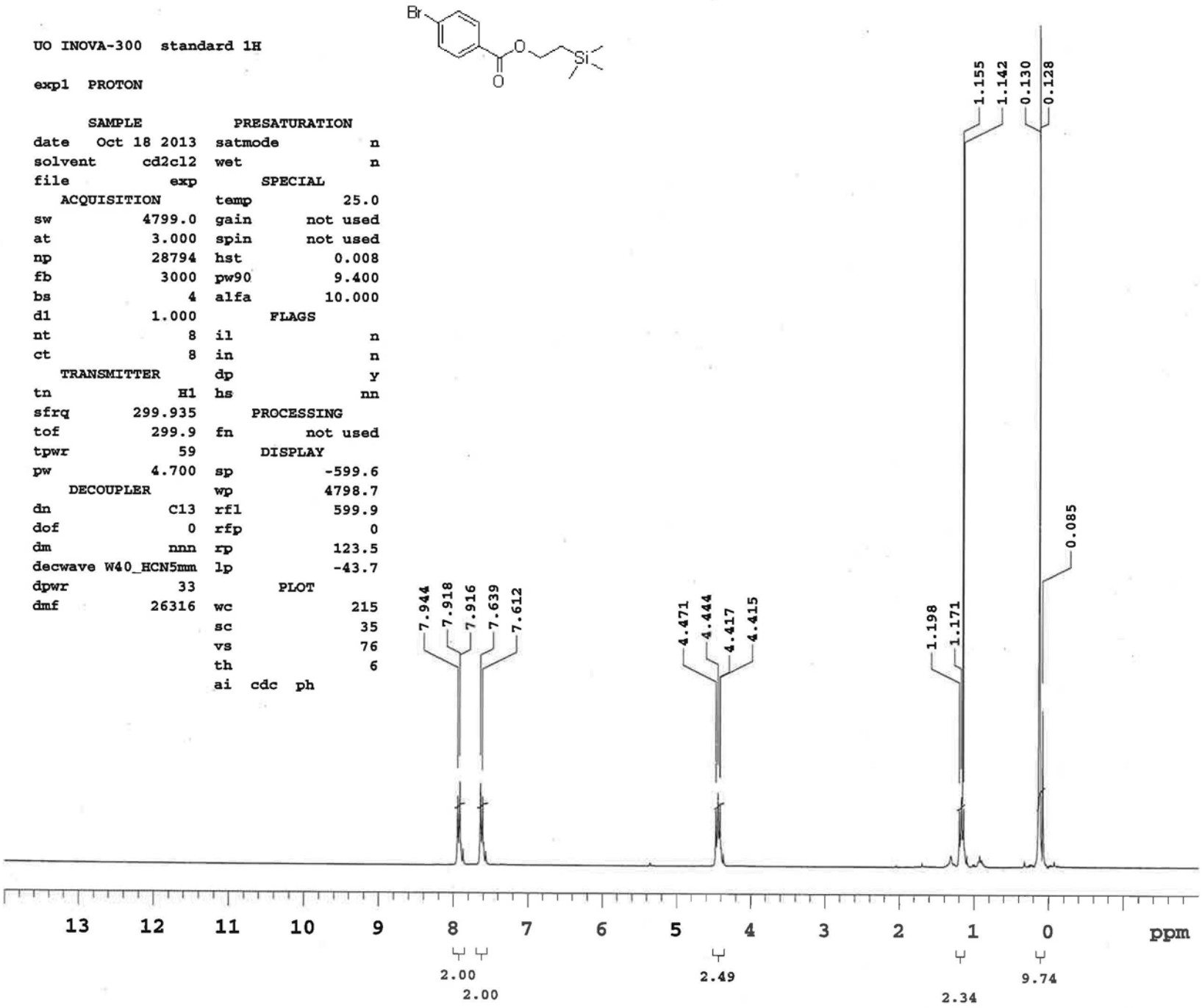
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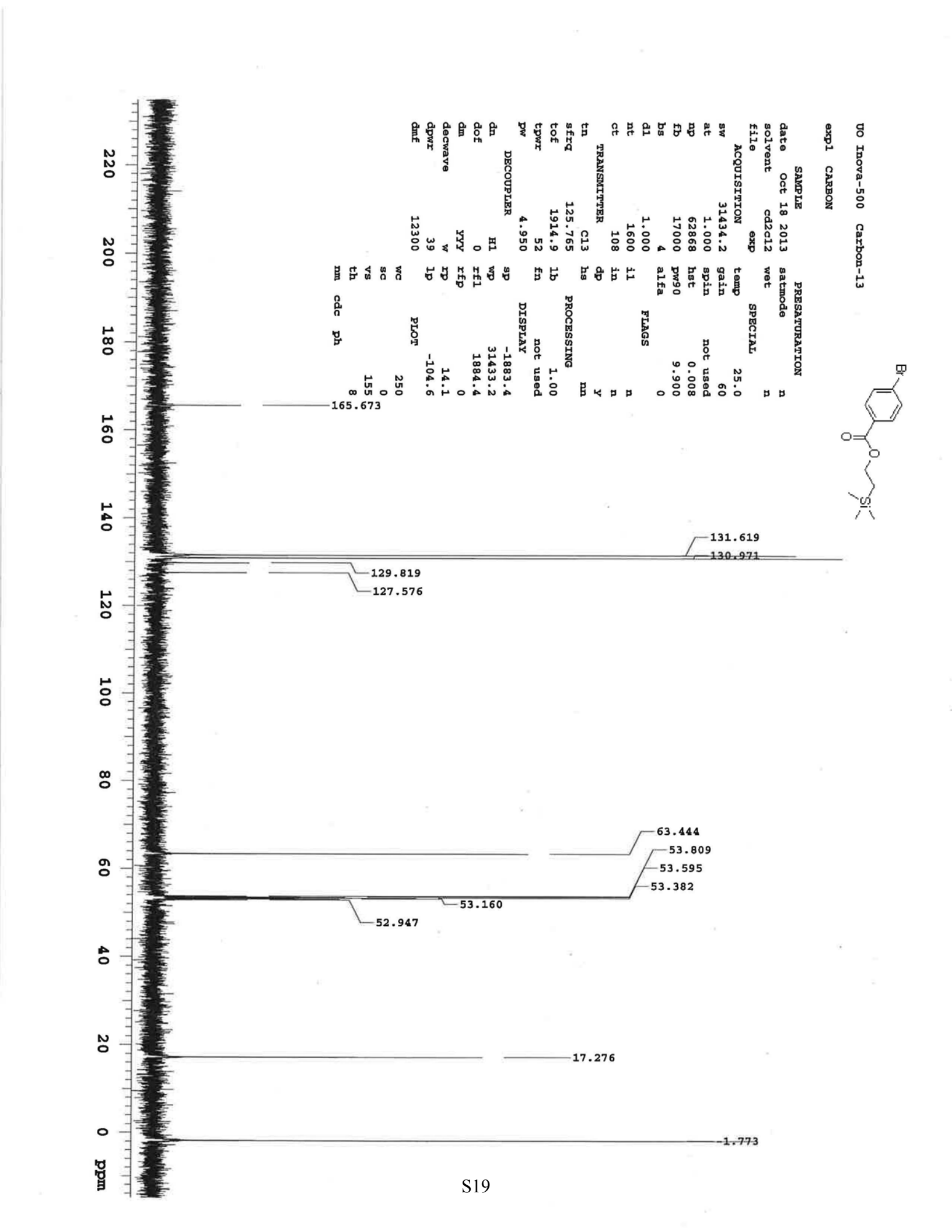
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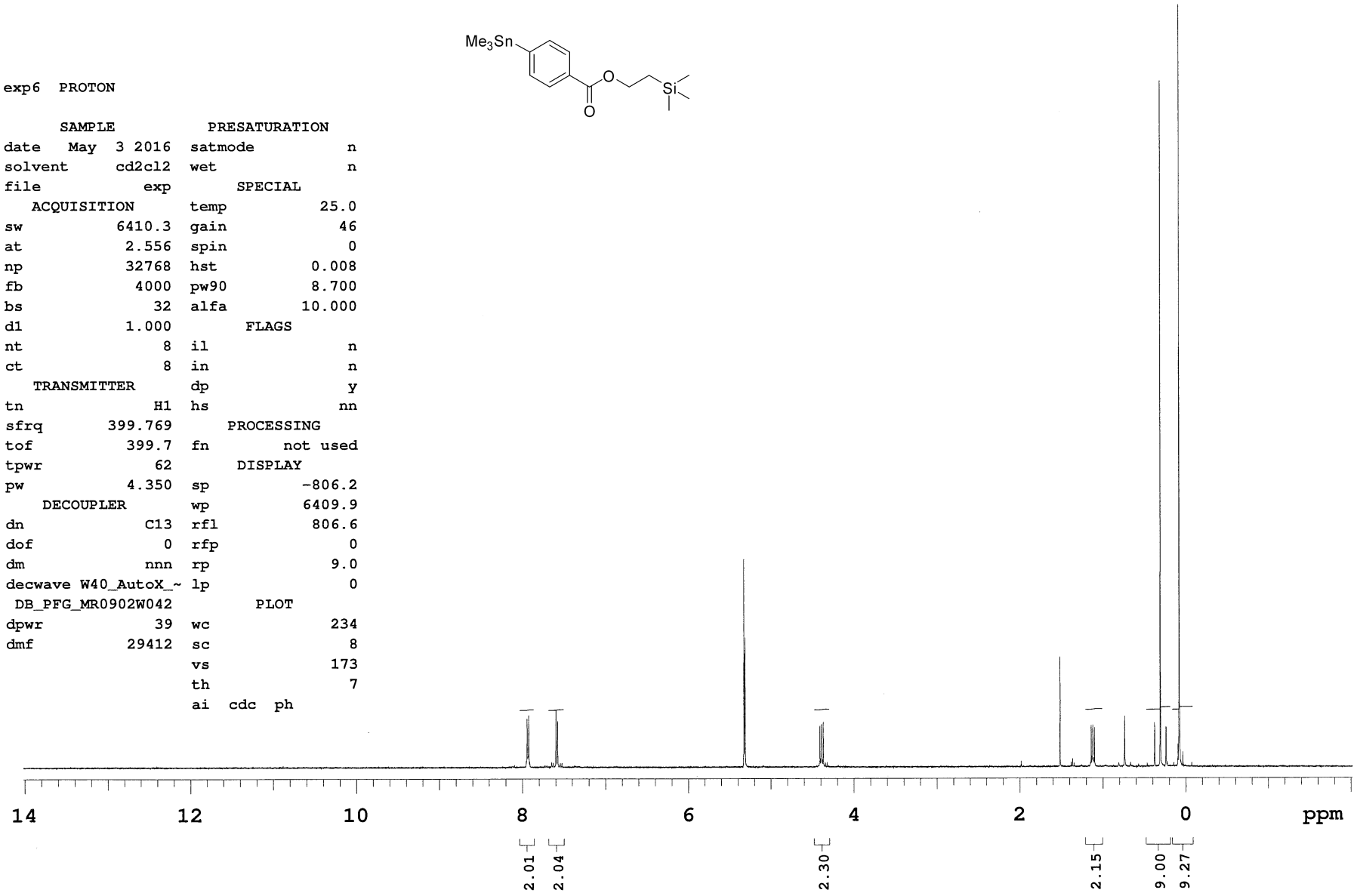
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UO Inova-500 Carbon-13

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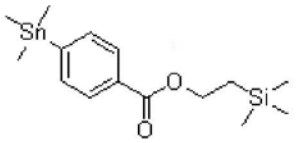

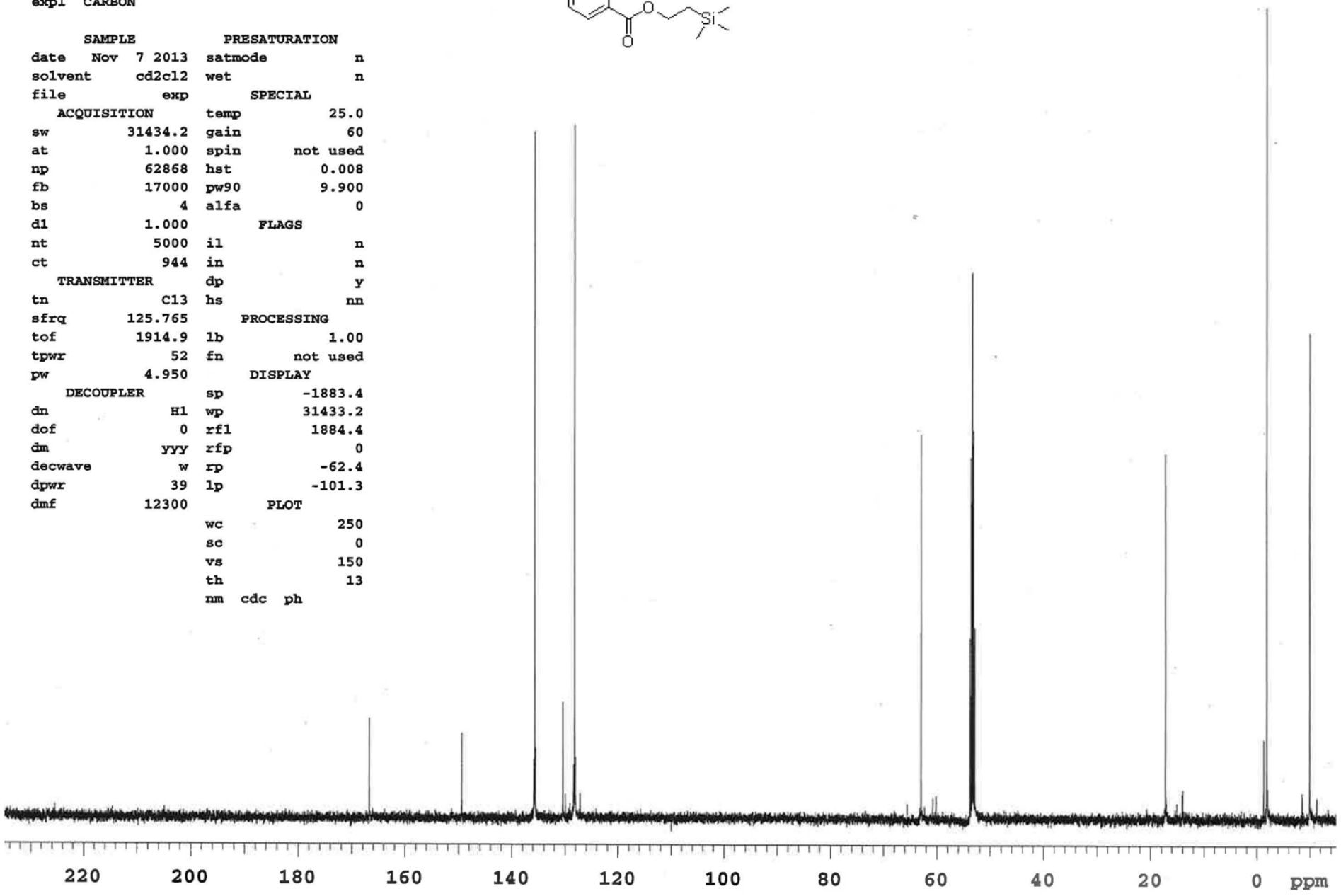

UO Inova-300-North standard 1H

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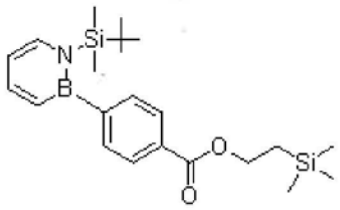

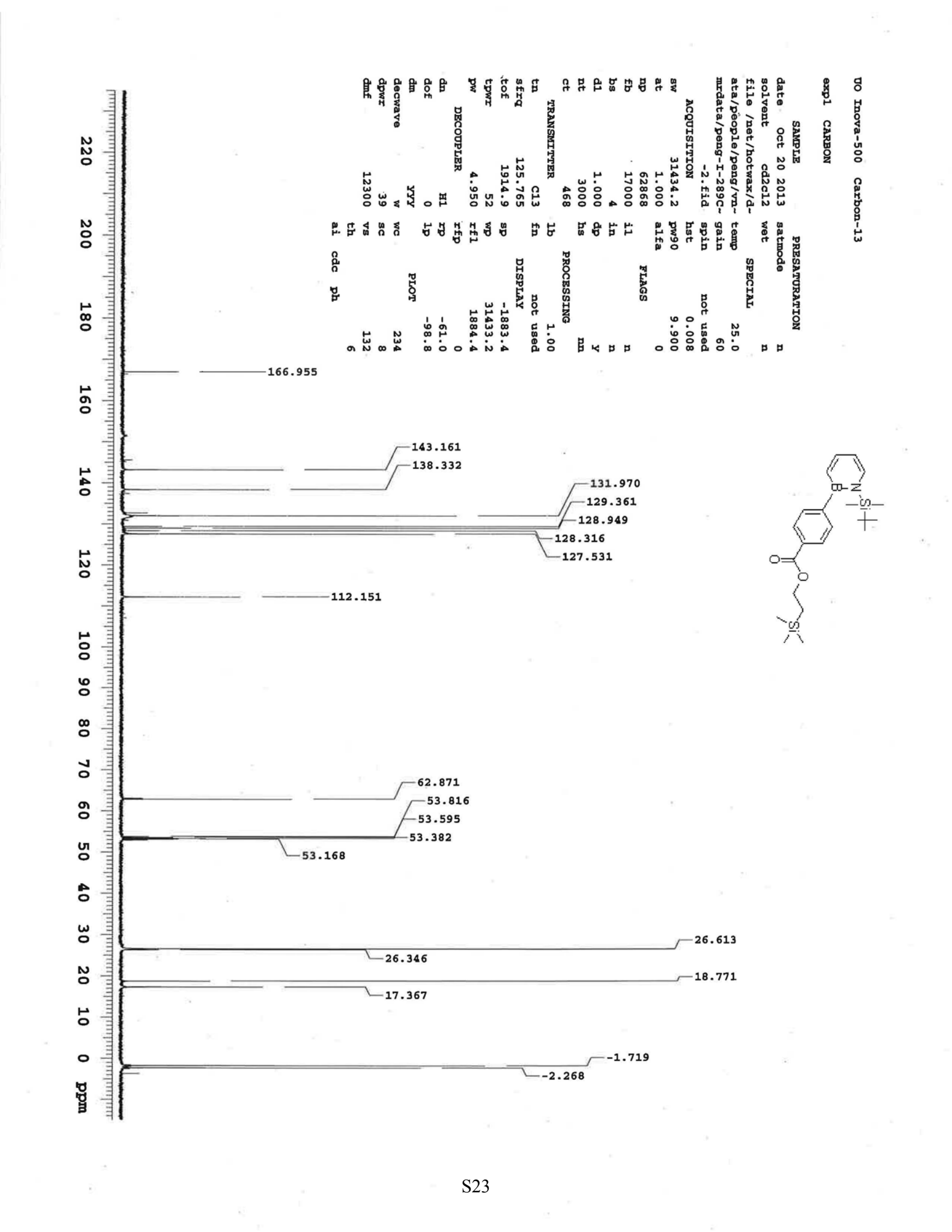
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UO Inova-300-North Boron-11

exp1 Boron-11

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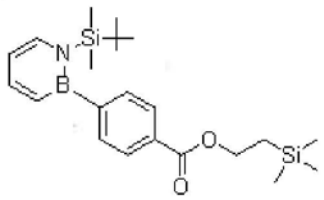
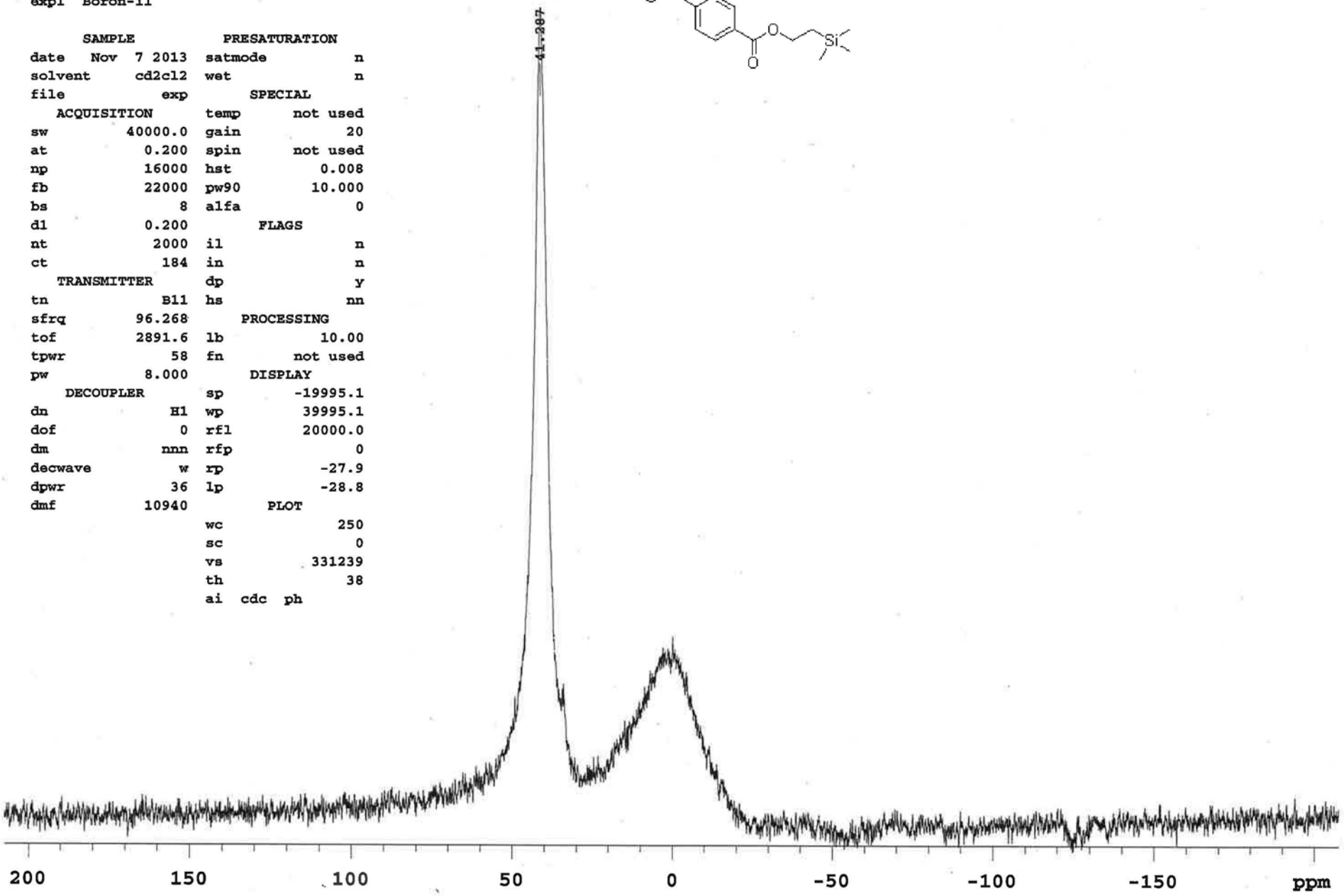
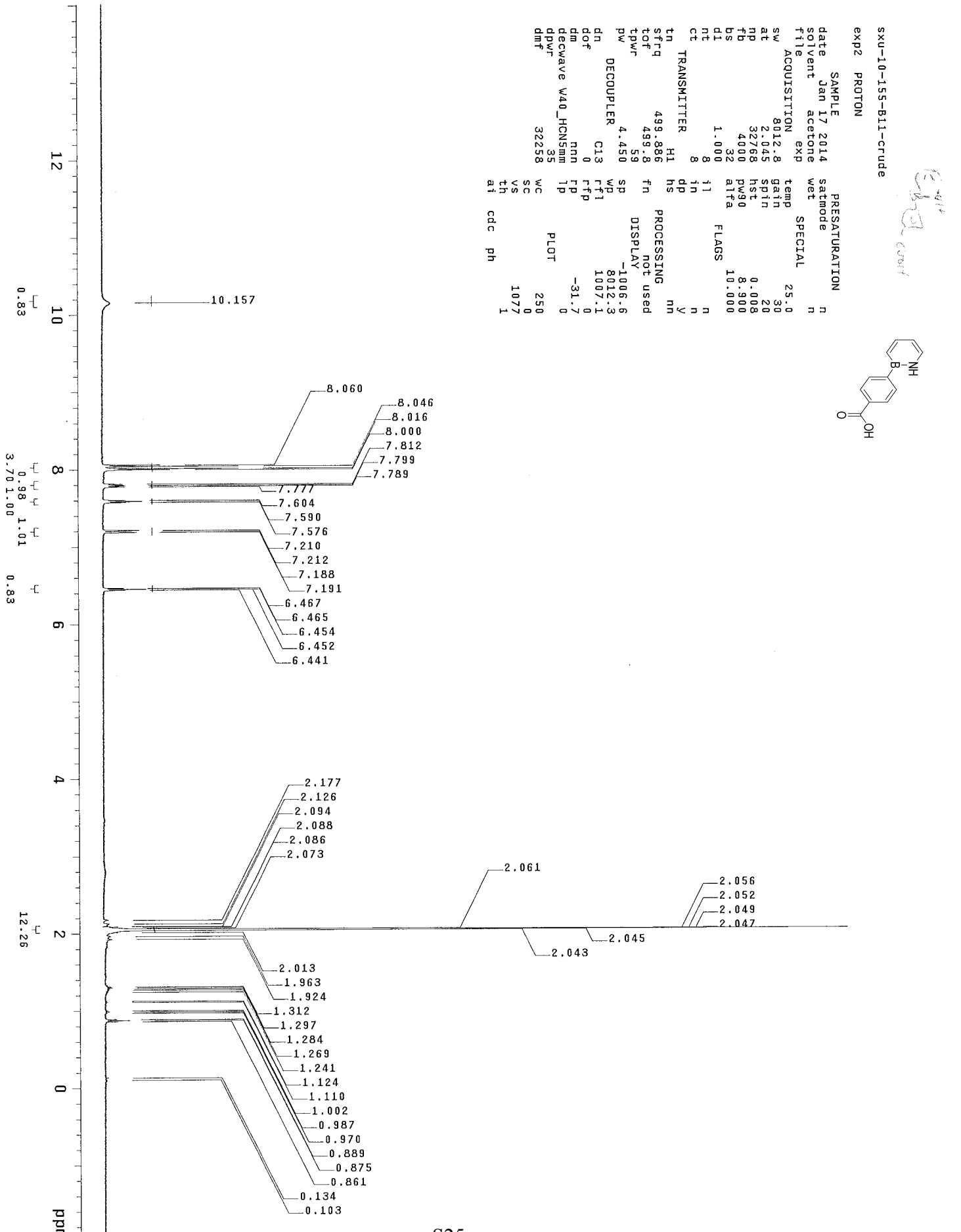
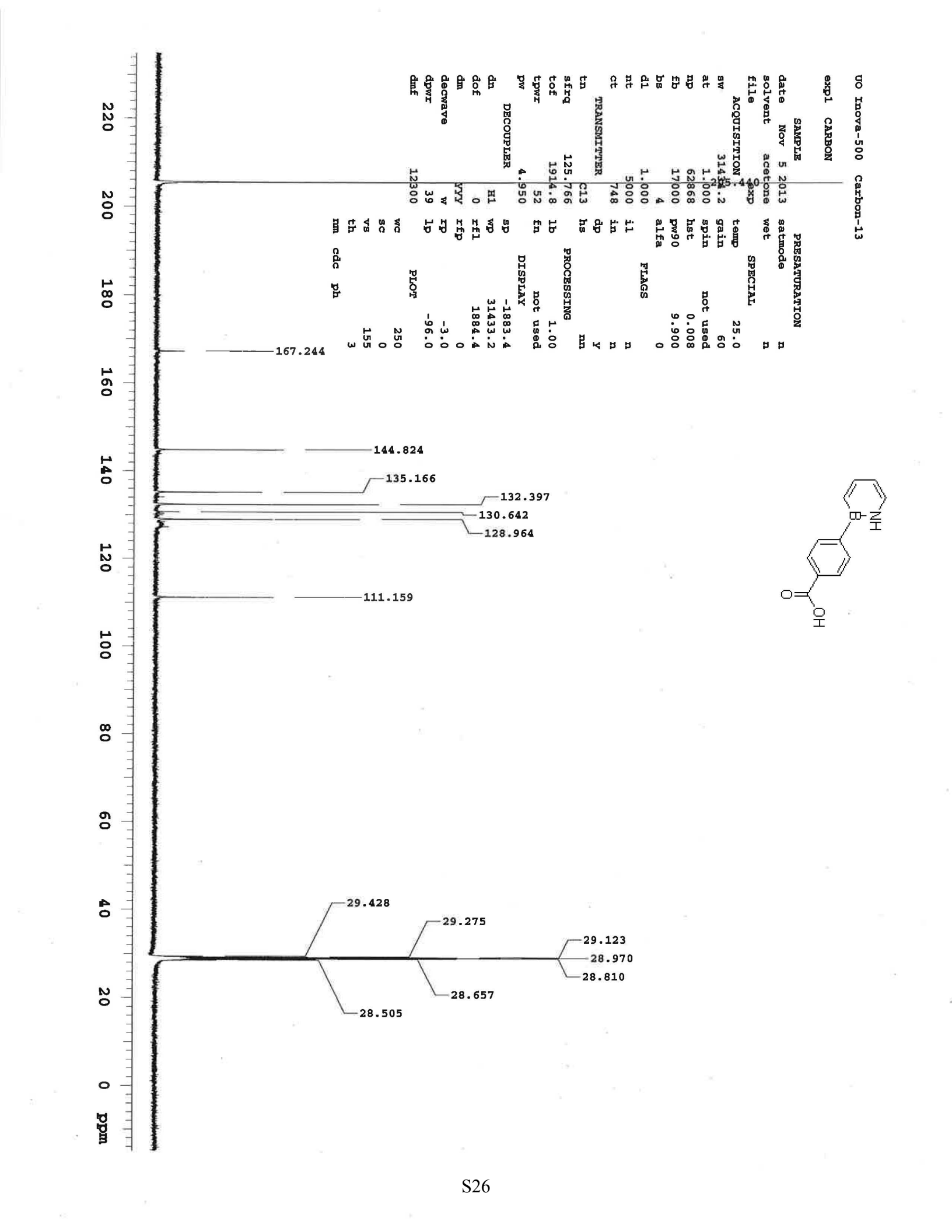




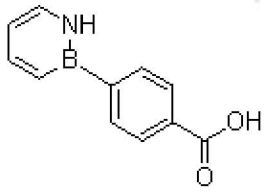

sxu-10-155-B11-crude
exp2 PROTON
SAMPLE
date Jan 17 2014
solvent acetone
file exp
ACQUISITION
sw 8012.8
at 2.045
np 32768
fb 4000
bs 32
d1 1.000
nt 8
ct 8
TRANSMITTER
tn H1
sfrq 499.886
tof 499.8
tpwr 59
pw 4.450
DECOUPLER
dn C13
dof 0
dm nnn
decwave W40_HCN5mm
dpwr 35
dmf 32258
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 30
spin 20
hst 0.008
pw90 8.900
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
not used
DISPLAY
-1006.6
8012.3
1007.1
0
-31.7
0
PLOT
wc 250
sc 0
vs 1077
th 1
ai cdc ph
NH
B
O
OH
10.157
8.060
8.046
8.016
8.000
7.812
7.799
7.789
7.777
7.604
7.590
7.576
7.210
7.212
7.188
7.191
6.467
6.465
6.454
6.452
6.441
2.177
2.126
2.094
2.088
2.086
2.073
2.061
2.056
2.052
2.049
2.047
2.045
2.043
2.013
1.963
1.924
1.312
1.297
1.284
1.269
1.241
1.124
1.110
1.002
0.987
0.970
0.889
0.875
0.861
0.134
0.103
0.83
3.70
0.98
1.00
1.01
0.83
12.26
12
10
8
6
4
2
0
ppm


UO Inova-500 Carbon-13
expl CARBON
SAMPLE
date Nov 5 2013
solvent acetone
file exp
ACQUISITION
sw 31445.4
at 1.000
np 62868
fb 17000
bs 4
d1 1.000
nt 5000
ct 748
TRANSMITTER
tn C13
sfrq 125.766
tof 1914.8
tpwr 52
pw 4.950
DECOUPLER
dn H1
dof 0
dm yyy
decwave w
dpwr 39
dmf 12300
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 60
spin not used
hst 0.008
pw90 9.900
alfa 0
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 1.00
fn not used
DISPLAY
sp -1883.4
wp 31433.2
rf1 1884.4
rfp 0
rp -3.0
lp -96.0
PLOT
wc 250
sc 0
vs 155
th 3
cdc ph
167.244
144.824
135.166
132.397
130.642
128.964
111.159
29.428
29.275
29.123
28.970
28.810
28.657
28.505
NH
B
OH
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm

UO Inova-300-North Boron-11

exp1 Boron-11

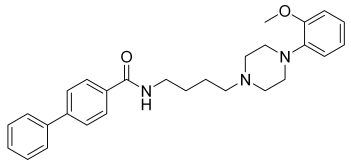
SAMPLE		PRESATURATION	
date	Nov 4 2013	satmode	n
solvent	cd2cl2	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	40000.0	gain	20
at	0.200	spin	not used
np	16000	hst	0.008
fb	22000	pw90	10.000
bs	8	alfa	0
d1	0.200	FLAGS	
nt	2000	il	n
ct	400	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	96.268	PROCESSING	
tof	2891.6	lb	10.00
tpwr	58	fn	not used
pw	8.000	DISPLAY	
DECOUPLER		sp	-19995.1
dn	H1	wp	39995.1
dof	0	rfl	20000.0
dm	nnn	rfp	0
decwave	w	rp	-28.3
dpwr	36	lp	-28.8
dmf	10940	PLOT	
		wc	250
		sc	0
		vs	345639
		th	60
		ai cdc ph	

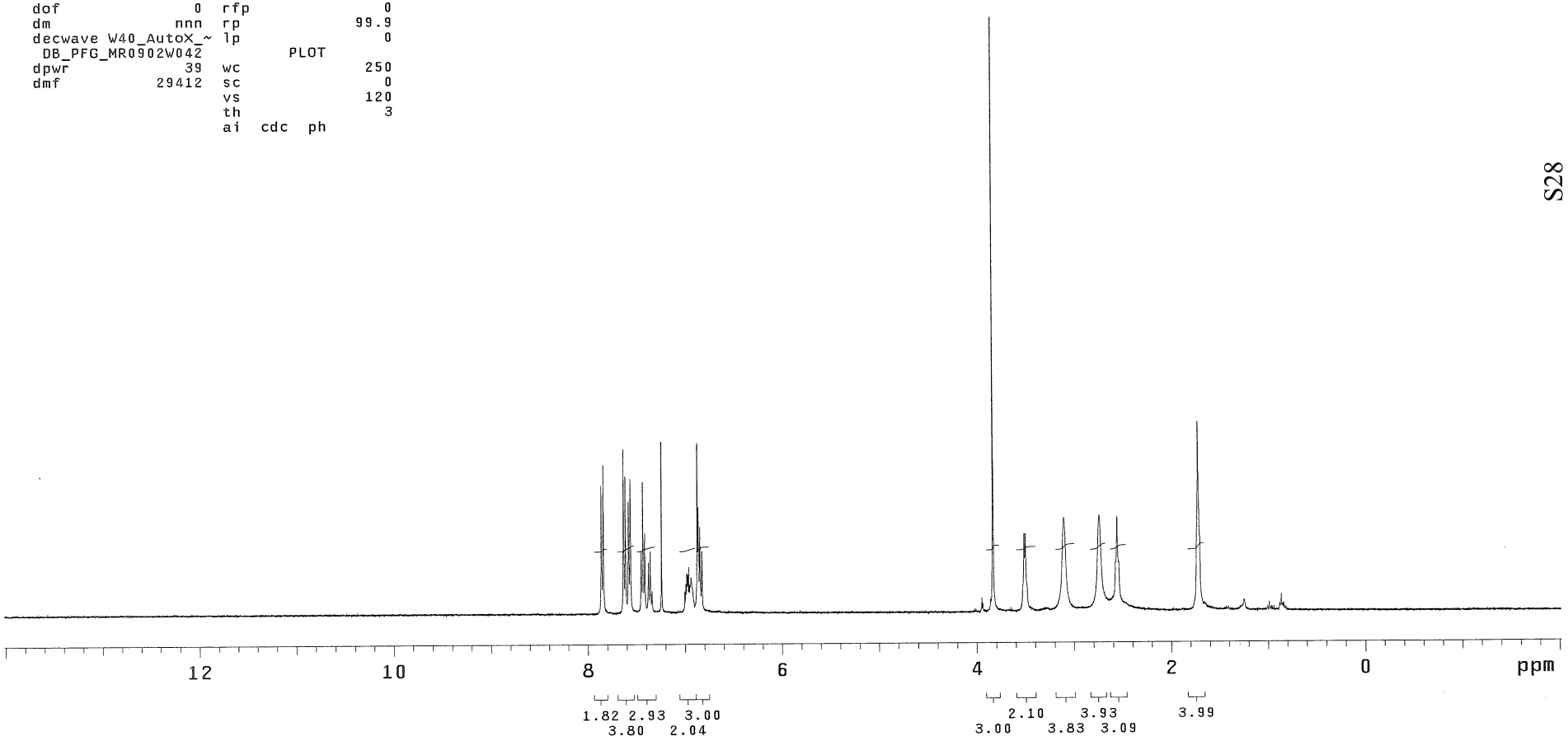


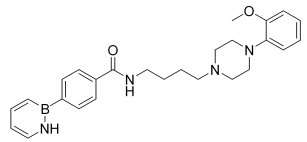
exp3 PROTON

SAMPLE	
date	May 5 2015
solvent	cdcl3
file	exp
ACQUISITION	
sw	6410.3
at	2.556
np	32768
fb	4000
bs	32
d1	1.000
nt	8
ct	8
TRANSMITTER	
tn	H1
sfrq	399.769
tof	399.8
tpwr	62
pw	4.350
DECOUPLER	
dn	C13
dof	0
dm	nnn
decwave	W40_AutoX_~ DB_PFG_MR0902W042
dpwr	39
dmf	29412

PRESATURATION	
satmode	n
wet	n
SPECIAL	
temp	25.0
gain	52
spin	not used
hst	0.008
pw90	8.700
alfa	10.000
FLAGS	
il	n
in	n
dp	y
hs	nn
PROCESSING	
fn	not used
DISPLAY	
sp	-806.1
wp	6409.9
rfl	806.5
rfp	0
rp	99.9
lp	0
PLOT	
wc	250
sc	0
vs	120
th	3
ai	cdc ph

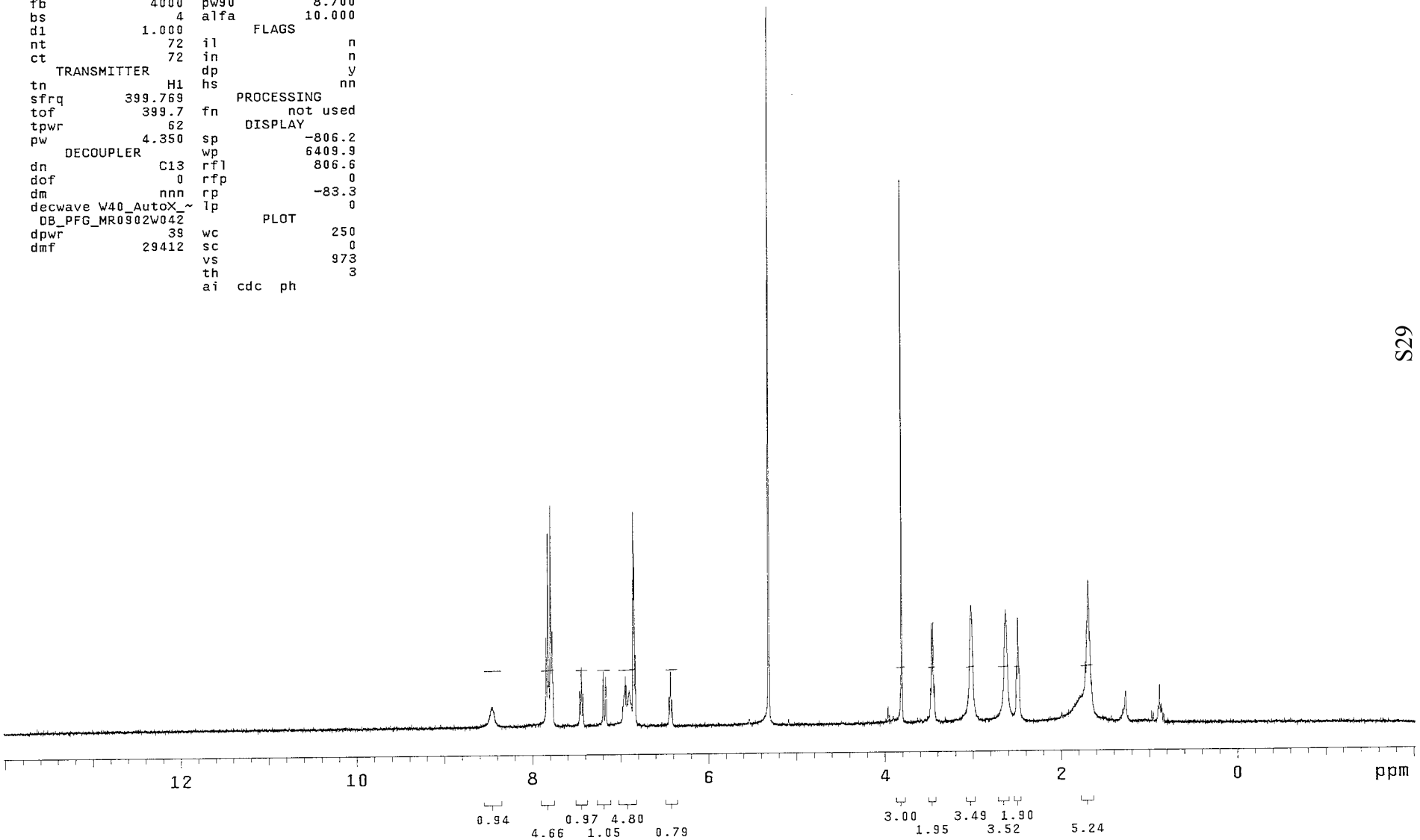






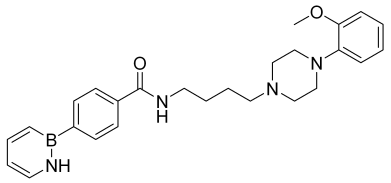
exp1 PROTON

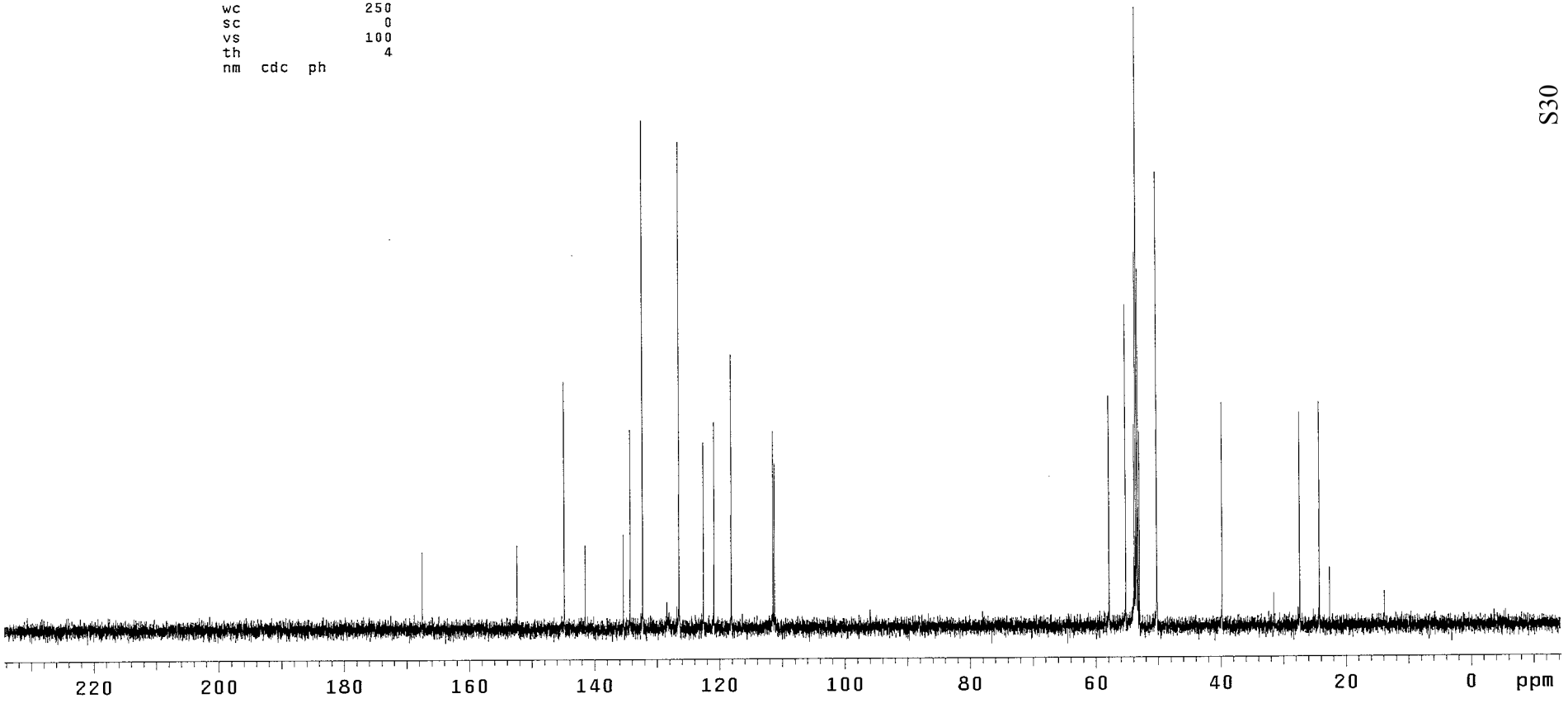
SAMPLE		PRESATURATION	
date	Nov 5 2015	satmode	n
solvent	cd2cl2	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	6410.3	gain	48
at	2.556	spin	not used
np	32768	hst	0.008
fb	4000	pw90	8.700
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	72	il	n
ct	72	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	399.769	PROCESSING	
tof	399.7	fn	not used
tpwr	62	DISPLAY	
pw	4.350	sp	-806.2
DECOUPLER		wp	6409.9
dn	C13	rfl	806.6
dof	0	rfp	0
dm	nnn	rp	-83.3
decwave	W40_AutoX_~ DB_PFG_MR0902W042	lp	0
dpwr	39	PLOT	
dmf	29412	wc	250
		sc	0
		vs	973
		th	3
		ai cdc ph	

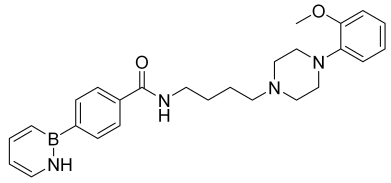


exp1 CARBON

SAMPLE		PRESATURATION	
date	Feb 12 2014	satmode	n
solvent	cd2cl2	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	31250.0	gain	30
at	1.049	spin	not used
np	65536	hst	0.008
fb	17000	pw90	10.000
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	2000	il	n
ct	332	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	125.709	PROCESSING	
tof	1914.0	lb	0.50
tpwr	55	fn	not used
pw	5.000	DISPLAY	
DECOUPLER		sp	-1797.5
dn	H1	wp	31249.0
dof	0	rfl	1798.5
dm	yyy	rfp	0
decwave	w	rp	-116.4
dpwr	40	lp	0
dmf	12361	PLOT	
		wc	250
		sc	0
		vs	100
		th	4
		nm	cdc ph



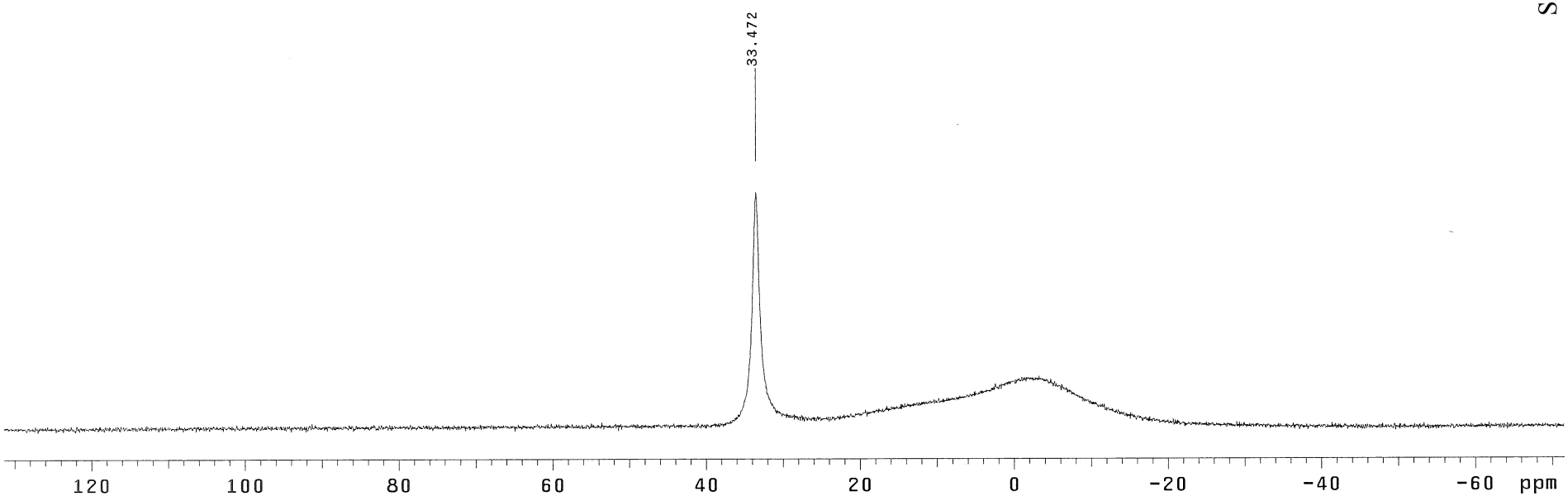


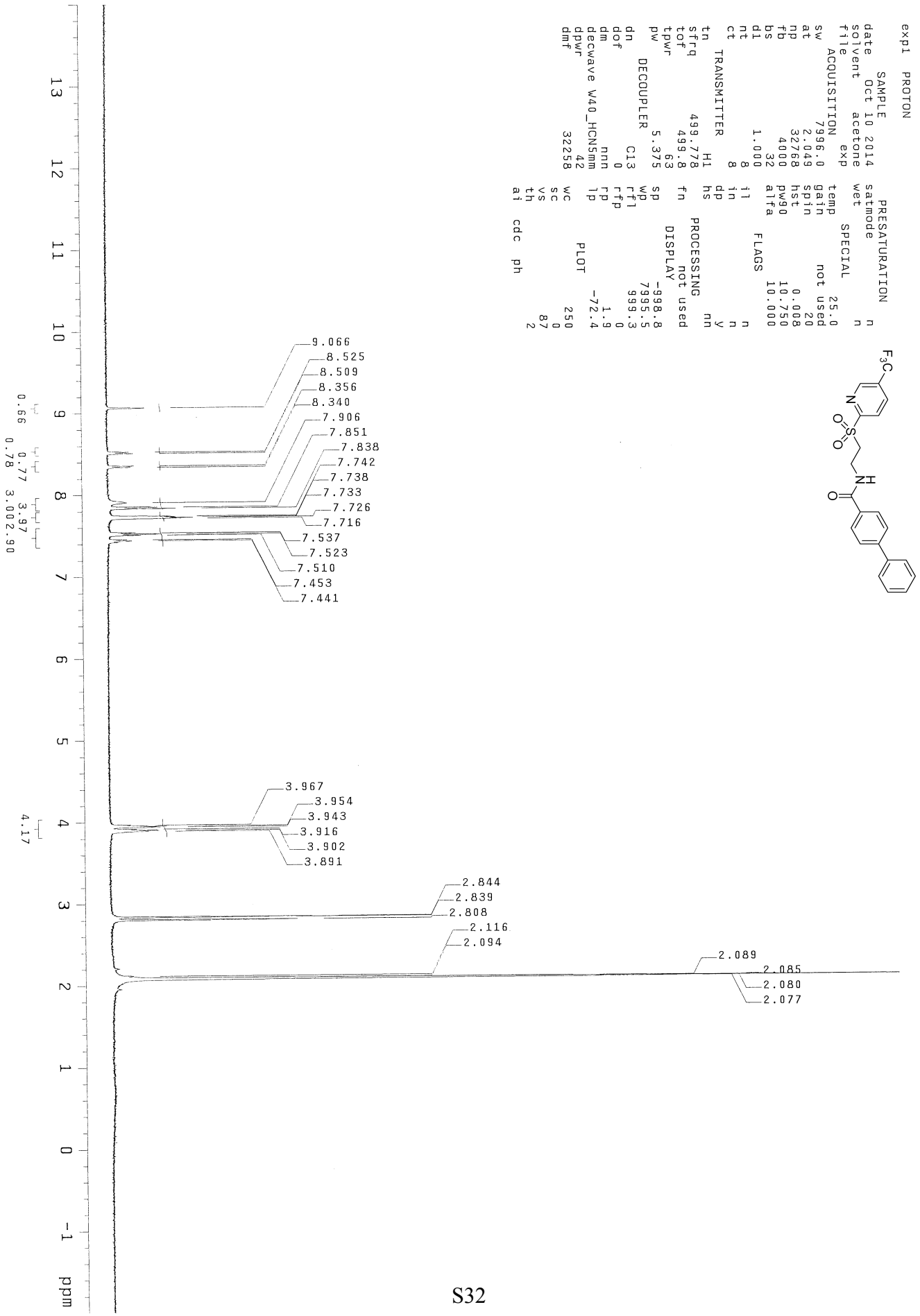


Automated Probe tuning parameter

exp1 s2pul

SAMPLE		PRESATURATION	
date	Apr 24 2015	satmode	n
solvent	cd2cl2	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	39062.5	gain	16
at	0.100	spin	not used
np	7812	hst	0.008
fb	17000	pw90	32.250
bs	4	alfa	10.000
d1	0.100	FLAGS	
nt	4000	il	n
ct	212	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	192.409	PROCESSING	
tof	11557.8	lb	0.50
tpwr	60	fn	not used
pw	32.250	DISPLAY	
DECOUPLER		sp	-13768.2
dn	H1	wp	39053.0
dof	0	rfl	13777.7
dm	nny	rfp	0
decwave	w	rp	104.6
dpwr	45	lp	0
dmf	15504	PLOT	
		wc	250
		sc	0
		vs	72489
		th	19
		ai cdc ph	

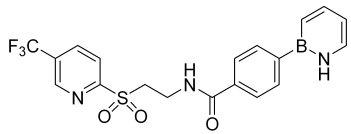


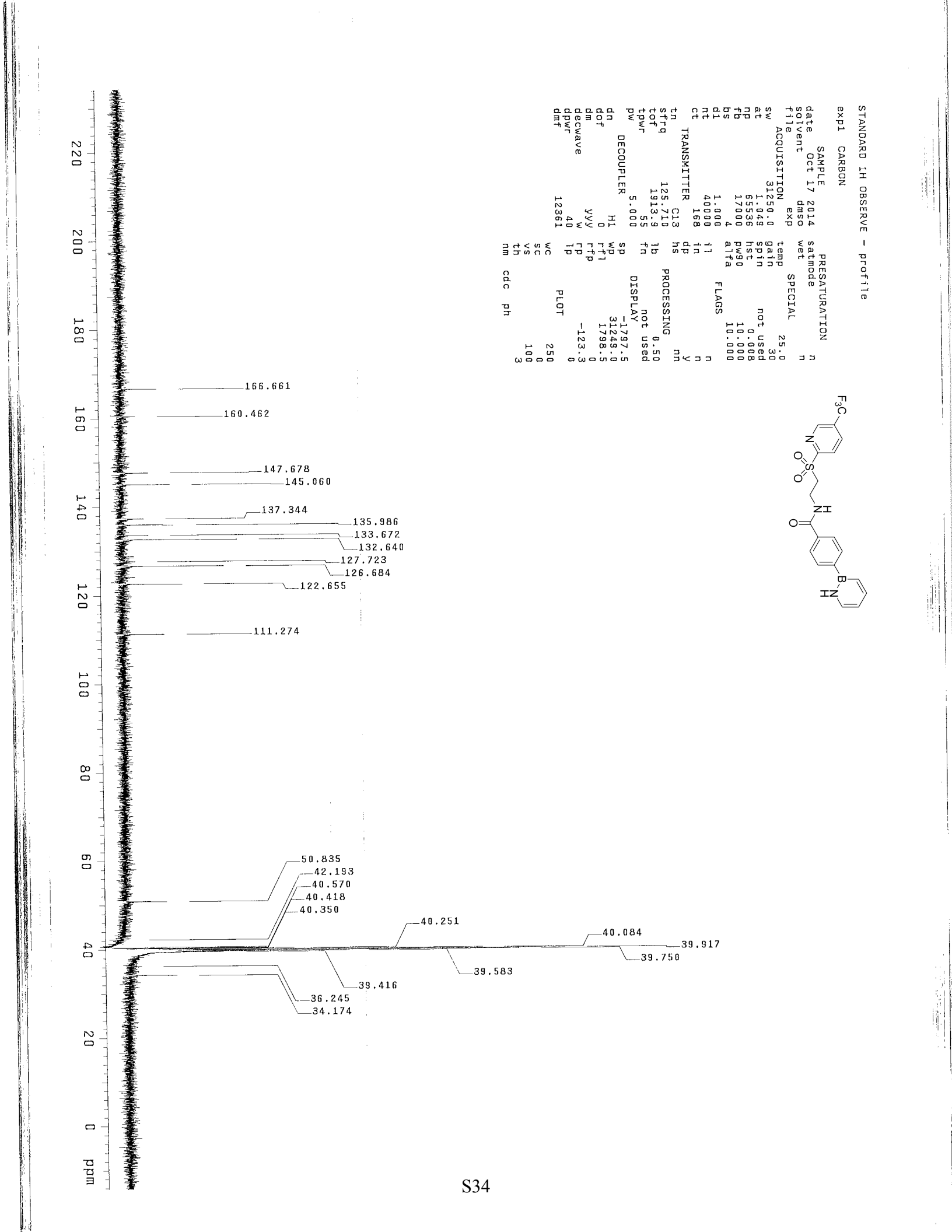

expl PROTON
SAMPLE
date Oct 10 2014
solvent acetone
file exp
ACQUISITION
sw 7996.0
at 2.049
np 32768
fb 4000
bs 32
d1 1.000
nt 8
ct 8
TRANSMITTER
tn H1
sfrq 499.778
tof 499.8
tpwr 63
pw 5.375
DECOUPLER
dn C13
dof 0
dm nnn
decwave W40_HCN5mm
dpwr 42
dmf 32258
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain not used
spin 20
hst 0.008
pw90 10.750
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
not used
fn DISPLAY
-998.8
7995.5
999.3
0
1.9
lp -72.4
PLOT
250
0
87
2
wc
sc
vs
th
ai cdc ph
F3C
N
O
S
O
N
H
O
9.066
8.525
8.509
8.356
8.340
7.906
7.851
7.838
7.742
7.738
7.733
7.726
7.716
7.537
7.523
7.510
7.453
7.441
3.967
3.954
3.943
3.916
3.902
3.891
2.844
2.839
2.808
2.116
2.094
2.089
2.085
2.080
2.077
0.66
0.77
3.97
0.78
3.00
2.90
4.17
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

STANDARD 1H OBSERVE - profile

exp1 PROTON

SAMPLE		PRESATURATION	
date	Oct 17 2014	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	8012.8	gain	30
at	2.045	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.125
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.886	PROCESSING	
tof	499.9	fn	not used
tpwr	59	DISPLAY	
pw	4.562	sp	-1006.6
DECOUPLER		wp	8012.3
dn	C13	rfl	1007.1
dof	0	rfp	0
dm	nnn	rp	130.3
decwave	W40_HCN5mm	lp	0
dpwr	35	PLOT	
dmf	32258	wc	250
		sc	0
		vs	75
		th	1
		ai cdc ph	

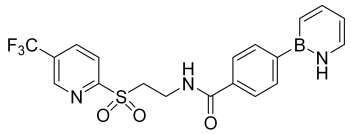


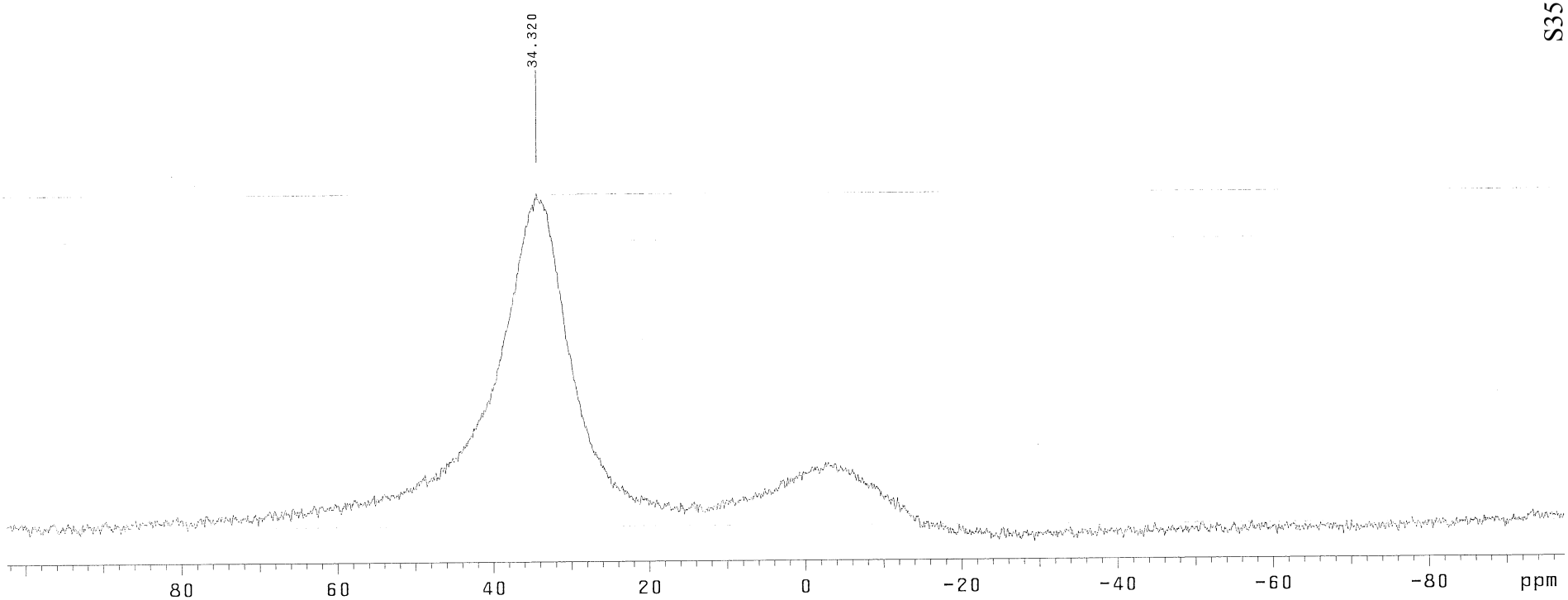

STANDARD 1H OBSERVE - profile
exp1 CARBON
SAMPLE
date Oct 17 2014
solvent dmso
file exp
ACQUISITION
sw 31250.0
at 1.049
np 65536
fb 17000
bs 4
d1 1.000
nt 40000
ct 168
TRANSMITTER
tn C13
sfrq 125.710
tof 1913.9
tpwr 55
pw 5.000
DECOUPLER
dn H1
dof 0
dm yyy
decwave w
dpwr 40
dmf 12361
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 30
spin not used
hst 0.008
pw90 10.000
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.50
fn not used
DISPLAY
sp -1797.5
wp 31249.0
rfl 1798.5
rfp 0
rp -123.3
lp 0
PLOT
wc 250
sc 0
vs 100
th 3
nm
cdc
ph
166.661
160.462
147.678
145.060
137.344
135.986
133.672
132.640
127.723
126.684
122.655
111.274
50.835
42.193
40.570
40.418
40.350
40.251
40.084
39.917
39.750
39.583
39.416
36.245
34.174
220
200
180
160
140
120
100
80
60
40
20
0
ppm

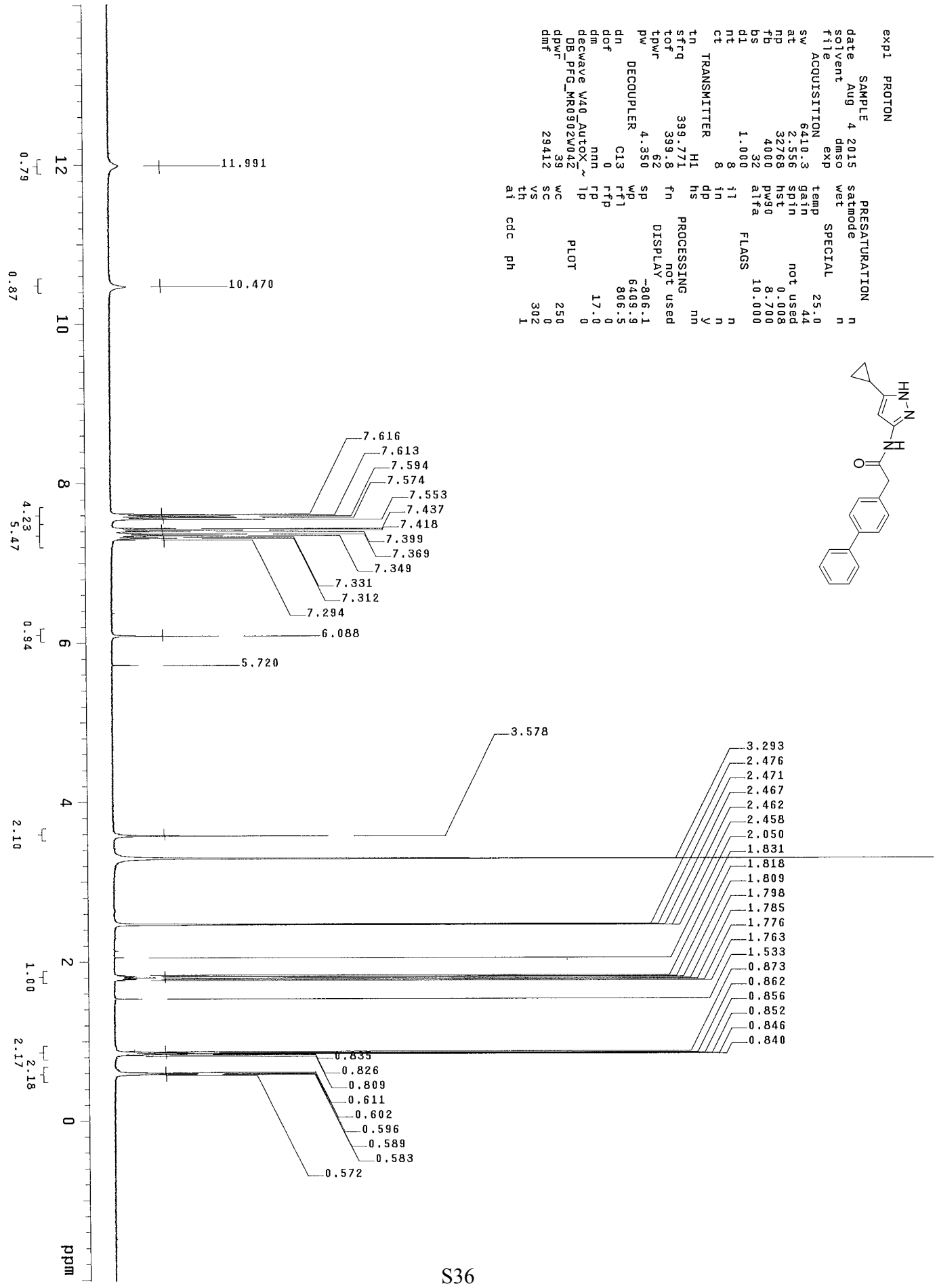
STANDARD 1H OBSERVE - profile

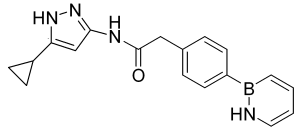
exp1 s2pul

SAMPLE		PRESATURATION	
date	Oct 17 2014	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	32051.3	gain	30
at	0.100	spin	not used
np	6410	hst	0.008
fb	17000	pw90	11.900
bs	4	alfa	10.000
d1	0.100	FLAGS	
nt	4000	il	n
ct	312	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	160.382	PROCESSING	
tof	4817.4	lb	15.00
tpwr	55	fn	not used
pw	11.750	DISPLAY	
DECOUPLER		sp	-15615.5
dn	H1	wp	32043.5
dof	0	rfl	15623.3
dm	nny	rfp	0
decwave	w	rp	152.1
dpwr	40	lp	0
dmf	12361	PLOT	
		wc	250
		sc	0
		vs	125748
		th	26
		ai cdc ph	






expl PROTON
SAMPLE
date Aug 4 2015
solvent dmso
file exp
ACQUISITION
sw 6410.3
at 2.556
np 32768
fb 4000
bs 32
d1 1.000
nt 8
ct 8
TRANSMITTER
tn H1
sfrq 399.771
tof 399.8
tpwr 62
pw 4.350
DECOUPLER
dn C13
dof 0
dm nnn
decwave W40_AutoX_~
DB_PFG_MR0902W042
dpwr 39
dmf 29412
PRESATURATION
satmode n
wet n
SPECIAL
temp 25.0
gain 44
spin not used
hst 0.008
pwg0 8.700
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
not used
DISPLAY
-806.1
6409.9
806.5
0
17.0
0
PLOT
250
0
302
1
cdc ph
wp
rfl
rfp
rp
lp
wc
sc
vs
th
ai
11.991
10.470
7.616
7.613
7.594
7.574
7.553
7.437
7.418
7.399
7.369
7.349
7.331
7.312
7.294
6.088
5.720
3.578
3.293
2.476
2.471
2.467
2.462
2.458
2.050
1.831
1.818
1.809
1.798
1.785
1.776
1.763
1.533
0.873
0.862
0.856
0.852
0.846
0.840
0.835
0.826
0.809
0.611
0.602
0.596
0.589
0.583
0.572
0.79
0.87
4.23
5.47
0.94
2.10
1.00
2.17
2.18
ppm

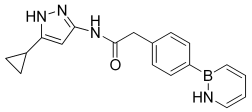


exp1 PROTON

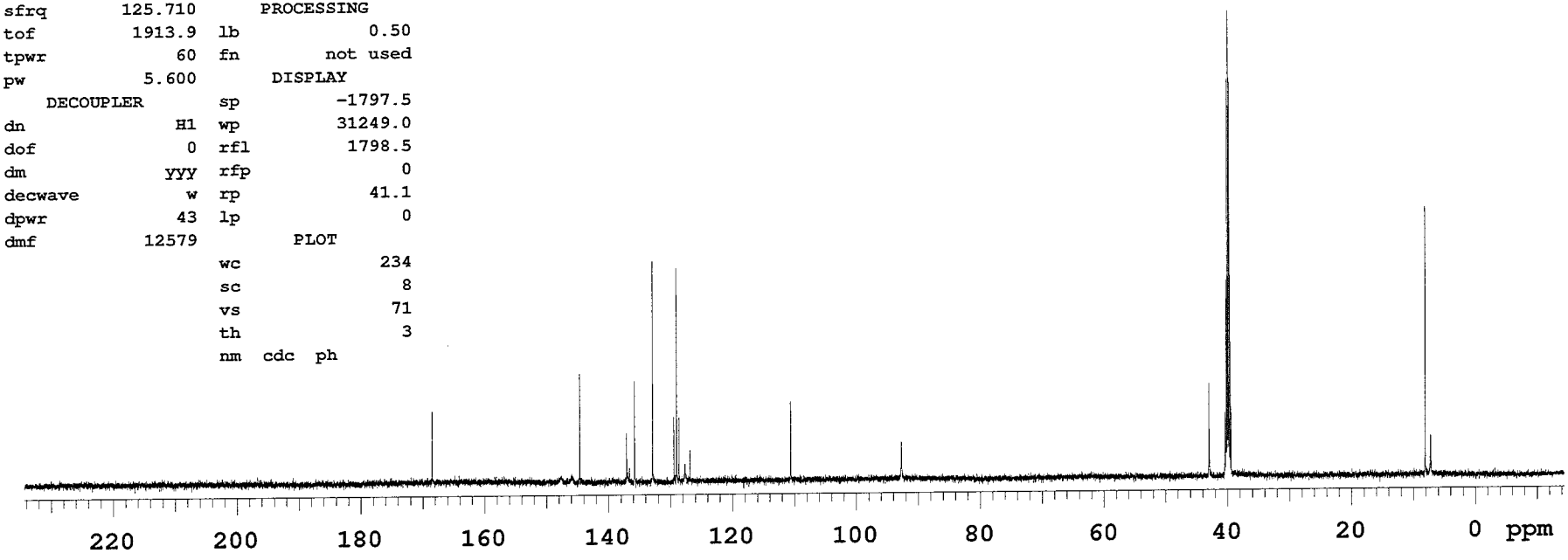
SAMPLE		PRESATURATION	
date	Aug 7 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	8012.8	gain	30
at	2.045	spin	not used
np	32768	hst	0.008
fb	4000	pw90	11.675
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.886	PROCESSING	
tof	499.9	fn	not used
tpwr	62	DISPLAY	
pw	5.838	sp	-1006.6
DECOUPLER		wp	8012.3
dn	C13	rfl	1007.1
dof	0	rfp	0
dm	nnn	rp	115.7
decwave	W40_Susan_~ Klein	lp	0
		PLOT	
dpwr	41	wc	250
dmf	32258	sc	0
		vs	312
		th	1
		ai cdc ph	

yz-2-271H-2

exp2 CARBON



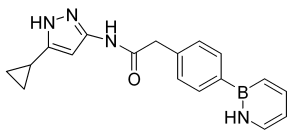
SAMPLE		PRESATURATION	
date	Oct 8 2016	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	31250.0	gain	30
at	1.049	spin	0
np	65536	hst	0.008
fb	17000	pw90	11.200
bs	4	alfa	10.000
d1	1.000	FLAGS	
nt	4000	il	n
ct	412	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfrq	125.710	PROCESSING	
tof	1913.9	lb	0.50
tpwr	60	fn	not used
pw	5.600	DISPLAY	
DECOUPLER		sp	-1797.5
dn	H1	wp	31249.0
dof	0	rfl	1798.5
dm	yyy	rfp	0
decwave	w	rp	41.1
dpwr	43	lp	0
dmf	12579	PLOT	
		wc	234
		sc	8
		vs	71
		th	3
		nm cdc ph	

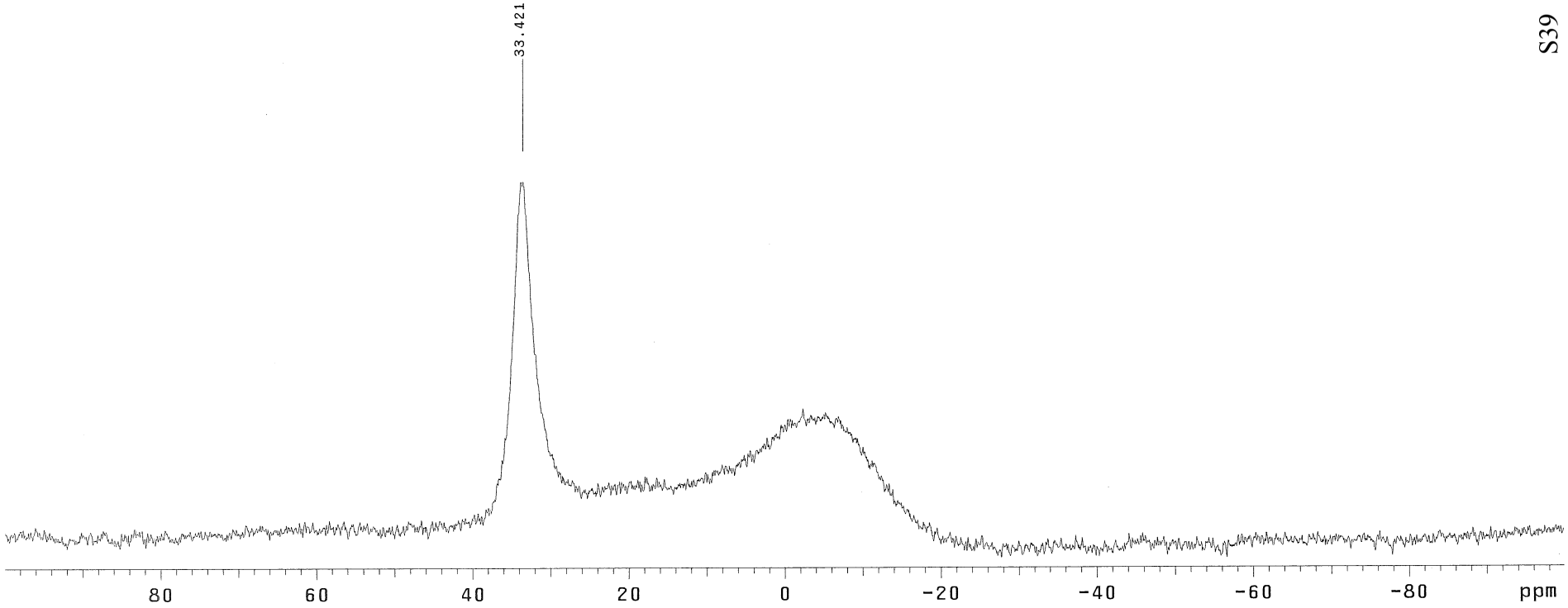


STANDARD 1H OBSERVE - profile

exp2 s2pul

SAMPLE		PRESATURATION	
date	May 20 2015	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	32051.3	gain	30
at	0.100	spin	not used
np	6410	hst	0.008
fb	17000	pw90	11.900
bs	4	alfa	10.000
d1	0.100	FLAGS	
nt	4000	il	n
ct	152	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	160.382	PROCESSING	
tof	4817.4	lb	15.00
tpwr	55	fn	not used
pw	11.750	DISPLAY	
DECOUPLER		sp	-16017.8
dn	H1	wp	32043.5
dof	0	rfl	16025.6
dm	nny	rfp	0
decwave	w	rp	94.0
dpwr	40	lp	0
dmf	12361	PLOT	
		wc	250
		sc	0
		vs	138848
		th	28
		ai cdc ph	

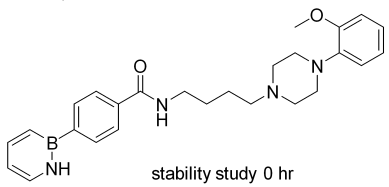




peng-34-2 stability time 0

exp1 PROTON

SAMPLE		PRESATURATION	
date	May 14 2015	satmode	n
solvent	cdcl3	wet	n
file	/home/Liu/vnm~	SPECIAL	
rsys/data/peng/V/5~	-159-0.fid	temp	25.0
ACQUISITION		gain	30
sw	7996.0	spin	not used
at	2.049	hst	0.008
np	32768	pw90	10.600
fb	4000	alfa	10.000
bs	32	FLAGS	
d1	1.000	il	n
nt	8	in	n
ct	8	dp	y
TRANSMITTER		hs	nn
tn	H1	PROCESSING	
sfrq	499.775	fn	not used
tof	499.8	DISPLAY	
tpwr	63	sp	-998.9
pw	5.300	wp	7995.5
DECOUPLER		rfl	999.4
dn		rfp	0
dof	0	rp	-78.7
dm	nnn	lp	-99.4
decwave	W40_HCN5mm	PLOT	
dpwr	42	wc	250
dmf	32258	sc	0
		vs	136
		th	50
		ai cdc ph	



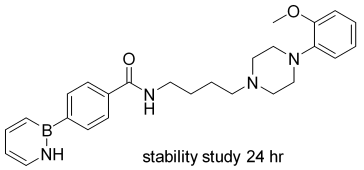
stability study 0 hr

peng-34-2 stability time 24hr

exp1 PROTON

SAMPLE	
date	May 15 2015
solvent	cdcl3
file	exp
ACQUISITION	
sw	8012.8
at	2.045
np	32768
fb	4000
bs	32
d1	1.000
nt	8
ct	8
TRANSMITTER	
tn	H1
sfrq	499.884
tof	499.8
tpwr	59
pw	4.562
DECOUPLER	
dn	C13
dof	0
dm	nnn
decwave	W40_HCN5mm
dpwr	35
dmf	32258

PRESATURATION	
satmode	n
wet	n
SPECIAL	
temp	25.0
gain	30
spin	not used
hst	0.008
pw90	9.125
alfa	10.000
FLAGS	
il	n
in	n
dp	y
hs	nn
PROCESSING	
fn	not used
DISPLAY	
sp	-1006.7
wp	8012.3
rfl	1007.2
rfp	0
rp	133.5
lp	0
PLOT	
wc	250
sc	0
vs	412
th	7
ai	cdc ph



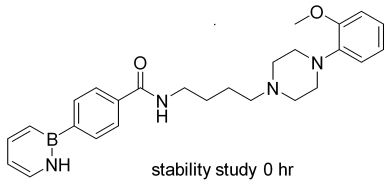
stability study 24 hr

peng-34-2 stability time 0

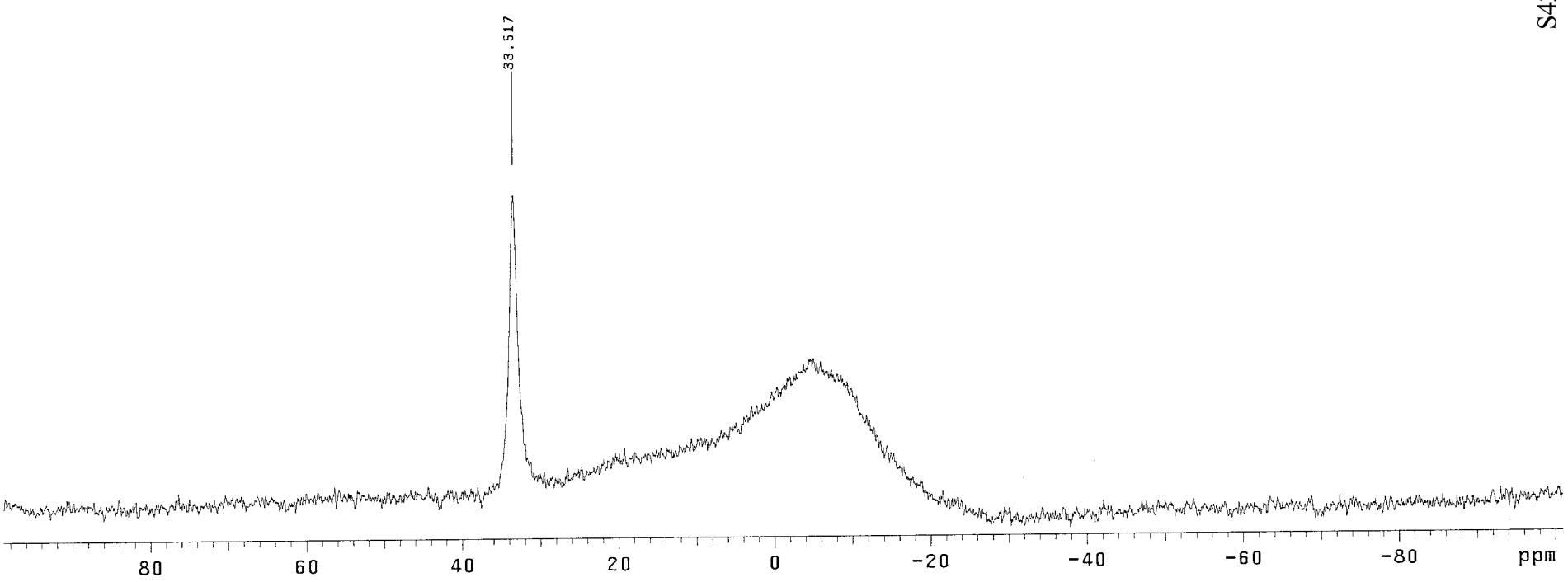
exp1 s2pul

SAMPLE	
date	May 14 2015
solvent	cdcl3
file	exp
ACQUISITION	
sw	32051.3
at	0.100
np	6410
fb	17000
bs	4
d1	0.100
nt	4000
ct	276
TRANSMITTER	
tn	B11
sfrq	160.382
tof	4817.4
tpwr	55
pw	11.750
DECOUPLER	
dn	H1
dof	0
dm	nny
decwave	w
dpwr	40
dmf	12361

PRESATURATION	
satmode	n
wet	n
SPECIAL	
temp	25.0
gain	30
spin	not used
hst	0.008
pw90	11.900
alfa	10.000
FLAGS	
il	n
in	n
dp	y
hs	nn
PROCESSING	
lb	15.00
fn	not used
DISPLAY	
sp	-16190.2
wp	32043.5
rfl	16198.0
rfp	0
rp	-149.0
lp	0
PLOT	
wc	250
sc	0
vs	211484
th	29
ai cdc ph	



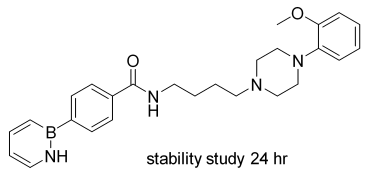
stability study 0 hr



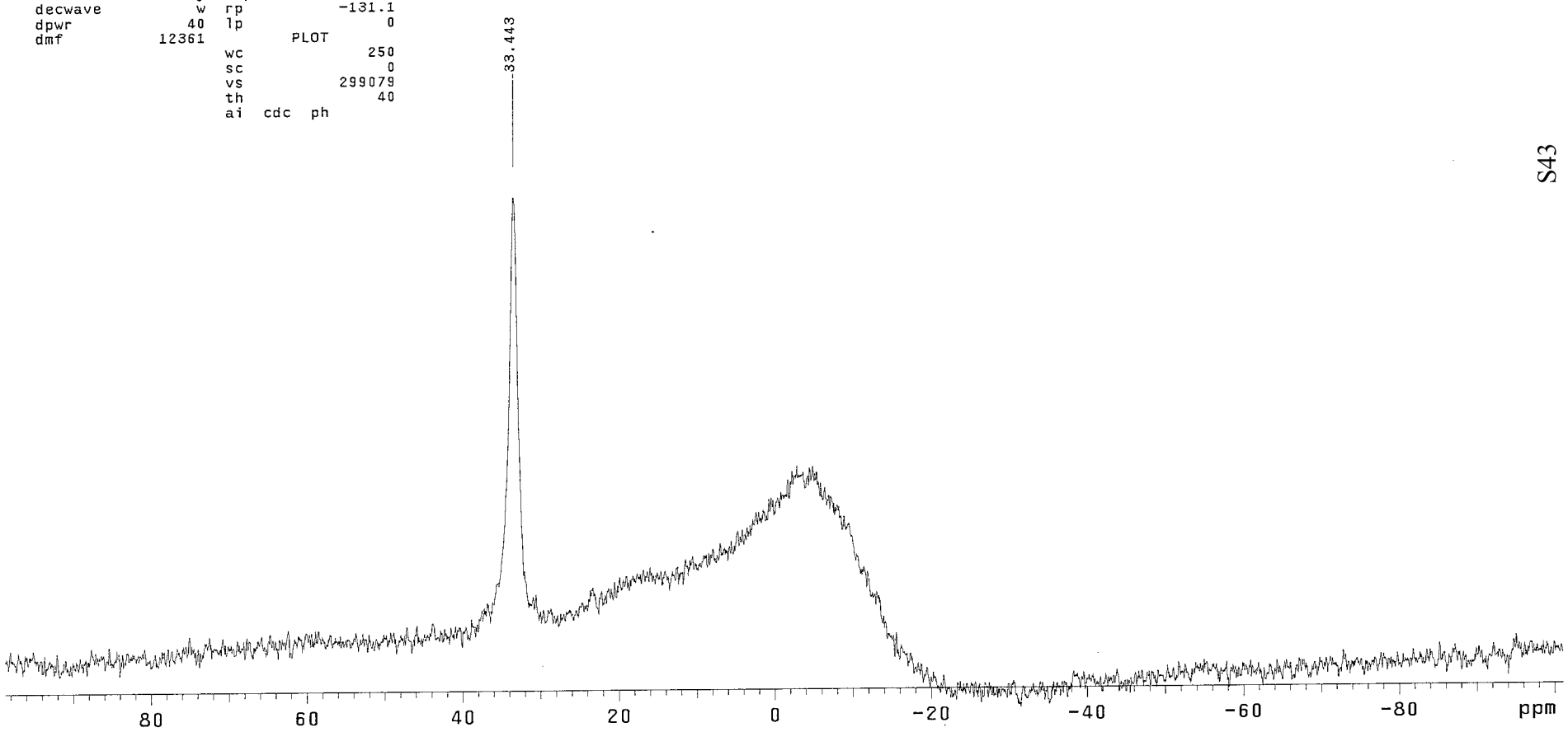
peng-34-2 stability time 24hr

exp1 s2pul

SAMPLE		PRESATURATION	
date	May 15 2015	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	32051.3	gain	30
at	0.100	spin	not used
np	6410	hst	0.008
fb	17000	pw90	11.900
bs	4	alfa	10.000
d1	0.100	FLAGS	
nt	4000	il	n
ct	288	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	160.382	PROCESSING	
tof	4817.4	lb	15.00
tpwr	55	fn	not used
pw	11.750	DISPLAY	
DECOUPLER		sp	-16210.0
dn	H1	wp	32043.5
dof	0	rfl	16217.8
dm	nny	rfp	0
decwave	w	rp	-131.1
dpwr	40	lp	0
dmf	12361	PLOT	
		wc	250
		sc	0
		vs	299079
		th	40
		ai cdc ph	



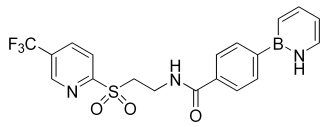
stability study 24 hr



peng-91-2 stability time0

exp3 PROTON

SAMPLE		PRESATURATION	
date	May 11 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	6410.3	gain	50
at	2.556	spin	not used
np	32768	hst	0.008
fb	4000	pw90	8.700
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	399.771	PROCESSING	
tof	399.8	fn	not used
tpwr	62	DISPLAY	
pw	4.350	sp	-806.1
DECOUPLER		wp	6409.9
dn	C13	rfl	806.5
dof	0	rfp	0
dm	nnn	rp	-160.1
decwave W40_AutoX_~ DB_PFG_MR0902W042		lp	0
		PLOT	
dpwr	39	wc	250
dmf	29412	sc	0
		vs	204
		th	2
		ai cdc ph	

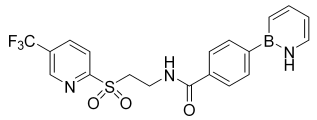


stability study 0 hr

peng-91-2 stability time24hr

exp2 PROTON

SAMPLE		PRESATURATION	
date	May 12 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	6410.3	gain	50
at	2.556	spin	not used
np	32768	hst	0.008
fb	4000	pw90	8.700
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	399.771	PROCESSING	
tof	399.8	fn	not used
tpwr	62	DISPLAY	
pw	4.350	sp	-806.1
DECOUPLER		wp	6409.9
dn	C13	rfl	806.5
dof	0	rfp	0
dm	nnn	rp	-161.7
decwave	W40_AutoX_~ DB_PFG_MR0902W042	lp	0
		PLOT	
dpwr	39	wc	250
dmf	29412	sc	0
		vs	171
		th	2
		ai cdc ph	

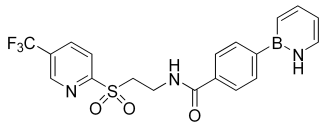


stability study 24 hr

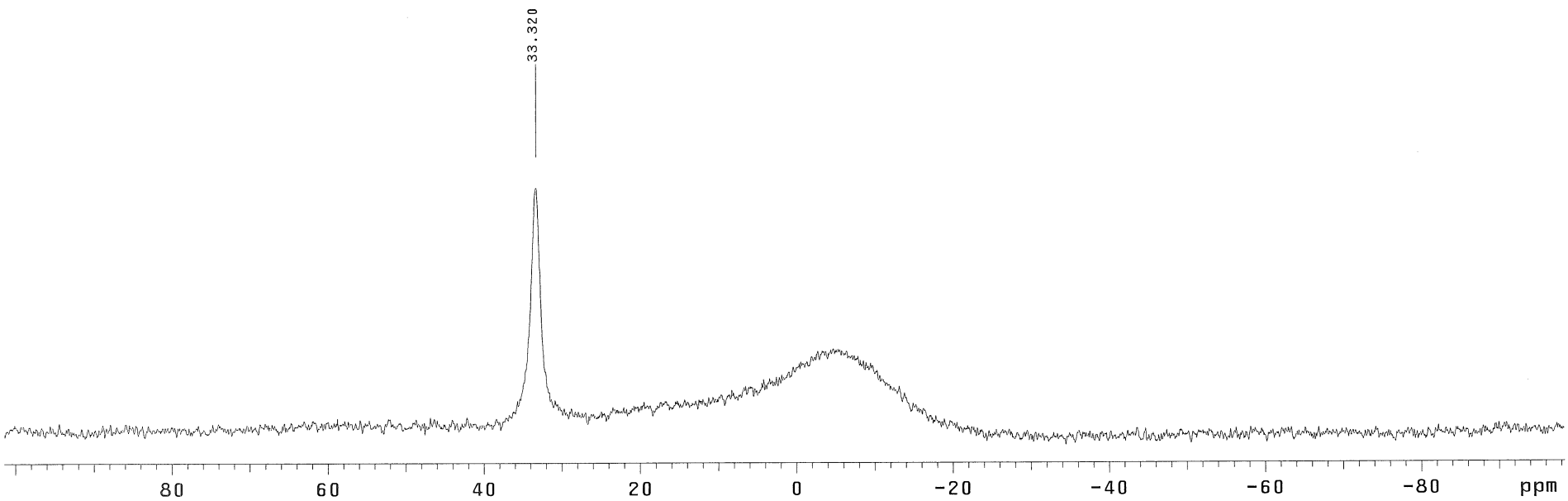
peng-91-2 stability time0

exp2 s2pul

SAMPLE		PRESATURATION	
date	May 11 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	32051.3	gain	30
at	0.100	spin	not used
np	6410	hst	0.008
fb	17000	pw90	11.900
bs	4	alfa	10.000
d1	0.100	FLAGS	
nt	4000	il	n
ct	164	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	160.382	PROCESSING	
tof	4817.4	lb	15.00
tpwr	55	fn	not used
pw	11.750	DISPLAY	
DECOUPLER		sp	-15775.9
dn	H1	wp	32043.5
dof	0	rfl	15783.7
dm	nny	rfp	0
decwave	w	rp	-149.4
dpwr	40	lp	0
dmf	12361	PLOT	
		wc	250
		sc	0
		vs	105741
		th	17
		ai cdc ph	



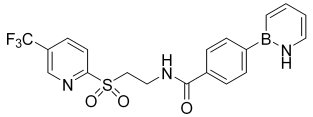
stability study 0 hr



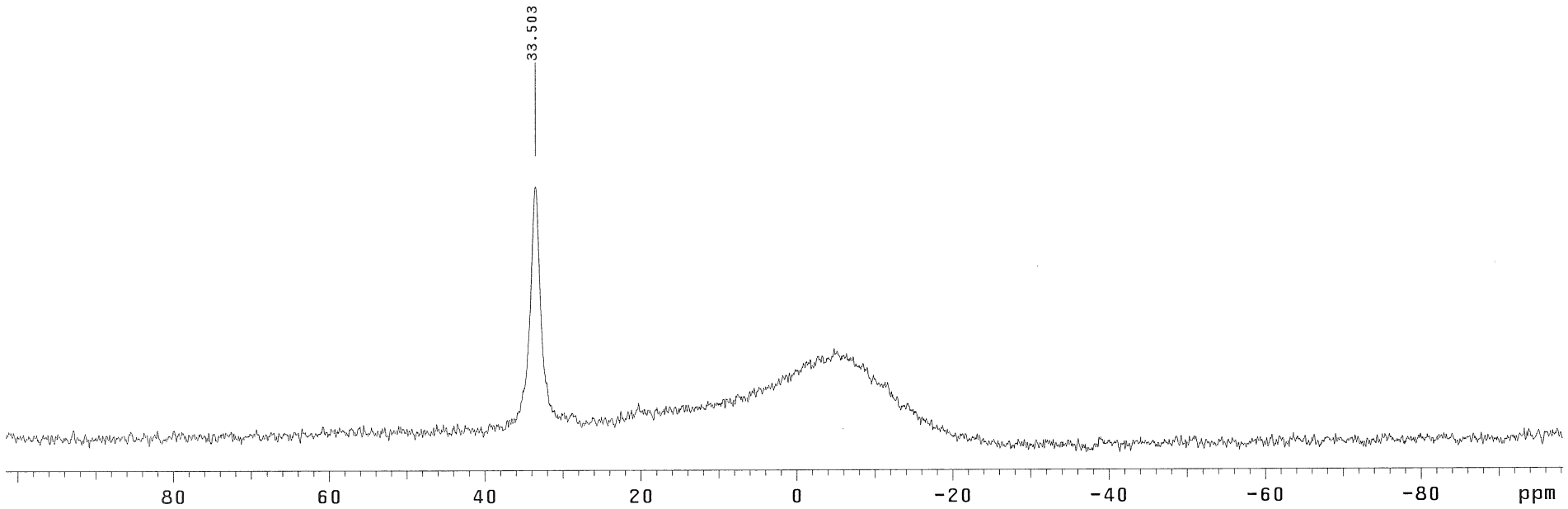
peng-91-2 stability time24hr

exp1 s2pul

SAMPLE		PRESATURATION	
date	May 12 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	32051.3	gain	30
at	0.100	spin	not used
np	6410	hst	0.008
fb	17000	pw90	11.900
bs	4	alfa	10.000
d1	0.100	FLAGS	
nt	4000	il	n
ct	284	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	160.382	PROCESSING	
tof	4817.4	lb	15.00
tpwr	55	fn	not used
pw	11.750	DISPLAY	
DECOUPLER		sp	-15754.2
dn	H1	wp	32043.5
dof	0	rfl	15762.0
dm	nny	rfp	0
decwave	w	rp	-136.2
dpwr	40	lp	0
dmf	12361	PLOT	
		wc	250
		sc	0
		vs	105741
		th	22
		ai cdc ph	



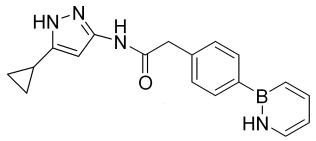
stability study 24 hr



peng-103 stability time 0

exp2 PROTON

SAMPLE		PRESATURATION	
date	May 20 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	6410.3	gain	46
at	2.556	spin	not used
np	32768	hst	0.008
fb	4000	pw90	8.700
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	399.771	PROCESSING	
tof	399.8	fn	not used
tpwr	62	DISPLAY	
pw	4.350	sp	-806.1
DECOUPLER		wp	6409.9
dn	C13	rfl	806.5
dof	0	rfp	0
dm	nnn	rp	-170.6
decwave	W40_AutoX_~ DB_PFG_MR0902W042	lp	0
		PLOT	
dpwr	39	wc	250
dmf	29412	sc	0
		vs	136
		th	7
		ai cdc ph	

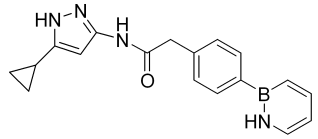


stability study 0 hr

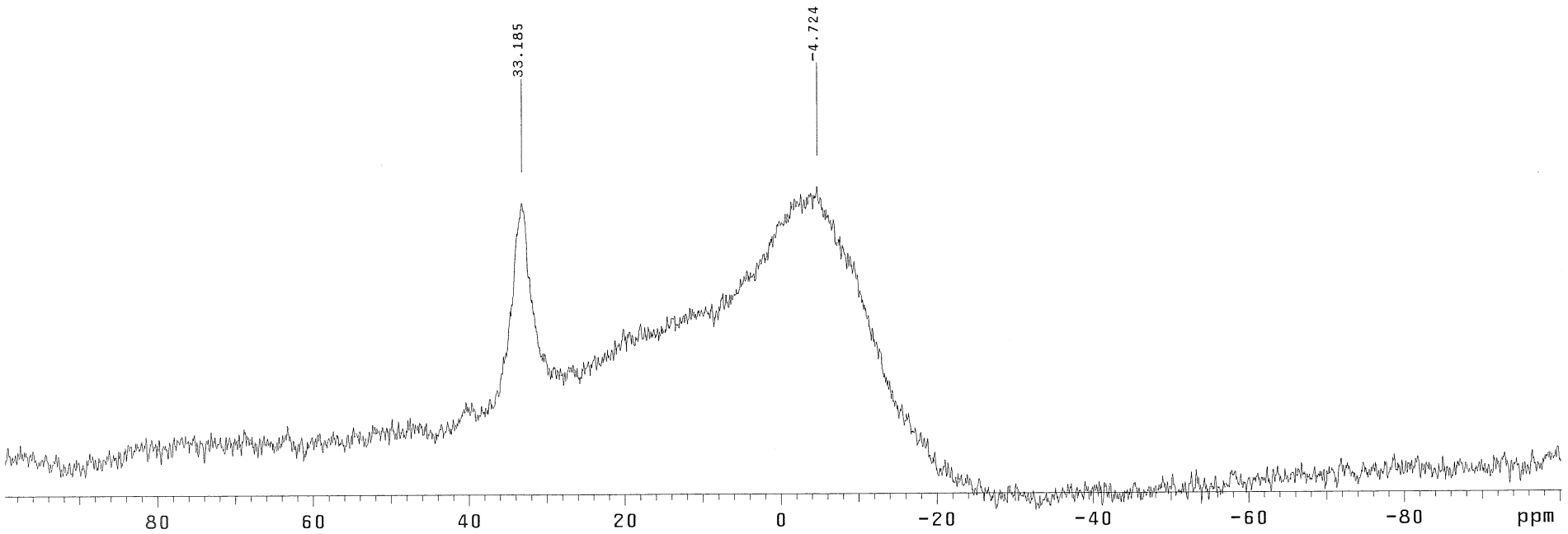
peng-103 stability time 0

exp1 s2pul

SAMPLE		PRESATURATION	
date	May 20 2015	satmode	n
solvent	cdcl3	wet	n
file	/home/Liu/vnm~	SPECIAL	
rsys/data/Peng/5-1~		temp	25.0
	71-2B.fid	gain	30
ACQUISITION		spin	not used
sw	32051.3	hst	0.008
at	0.100	pw90	11.900
np	6410	alfa	10.000
fb	17000	FLAGS	
bs	4	il	n
d1	0.100	in	n
nt	4000	dp	y
ct	372	hs	nn
TRANSMITTER		PROCESSING	
tn	B11	lb	15.00
sfrq	160.382	fn	not used
tof	4817.4	DISPLAY	
tpwr	55	sp	-16071.3
pw	11.750	wp	32043.5
DECOUPLER		rfl	16079.1
dn	H1	rfp	0
dof	0	rp	-266.9
dm	nny	lp	0
decwave	w	PLOT	
dpwr	40	wc	250
dmf	12361	sc	0
		vs	417150
		th	34
		ai	cdc ph



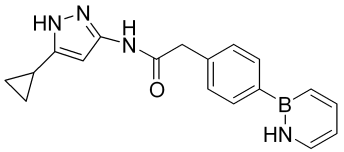
stability study 0 hr



peng-103 stabiity time 24hr

exp2 PROTON

SAMPLE		PRESATURATION	
date	May 21 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	6410.3	gain	46
at	2.556	spin	not used
np	32768	hst	0.008
fb	4000	pw90	8.700
bs	32	alfa	10.000
d1	1.000	FLAGS	
nt	8	il	n
ct	8	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	399.771	PROCESSING	
tof	399.8	fn	not used
tpwr	62	DISPLAY	
pw	4.350	sp	-806.1
DECOUPLER		wp	6409.9
dn	C13	rfl	806.5
dof	0	rfp	0
dm	nnn	rp	-170.9
decwave	W40_AutoX_~ DB_PFG_MR0902W042	lp	0
		PLOT	
dpwr	39	wc	250
dmf	29412	sc	0
		vs	181
		th	7
		ai cdc ph	

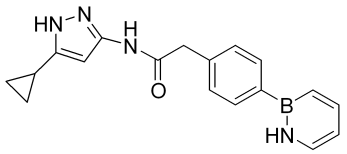


stability study 24 hr

peng-103 stability time 24hr

exp2 s2pul

SAMPLE		PRESATURATION	
date	May 21 2015	satmode	n
solvent	dmso	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	32051.3	gain	30
at	0.100	spin	not used
np	6410	hst	0.008
fb	17000	pw90	11.900
bs	4	alfa	10.000
d1	0.100	FLAGS	
nt	4000	il	n
ct	196	in	n
TRANSMITTER		dp	y
tn	B11	hs	nn
sfrq	160.382	PROCESSING	
tof	4817.4	lb	15.00
tpwr	55	fn	not used
pw	11.750	DISPLAY	
DECOUPLER		sp	-15615.5
dn	H1	wp	32043.5
dof	0	rfl	15623.3
dm	nny	rfp	0
decwave	w	rp	-128.5
dpwr	40	lp	0
dmf	12361	PLOT	
		wc	250
		sc	0
		vs	149540
		th	22
		ai cdc ph	



stability study 24 hr