Electronic Supplementary Material (ESI) for RSC Advances.

Development of subtype-selective estrogen receptor modulators using bis(4-hydroxyphenyl)silanol core as a stable isostere of bis(4-hydroxyphenyl)methanol

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Supplementary materials

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1. Supplementary Figure

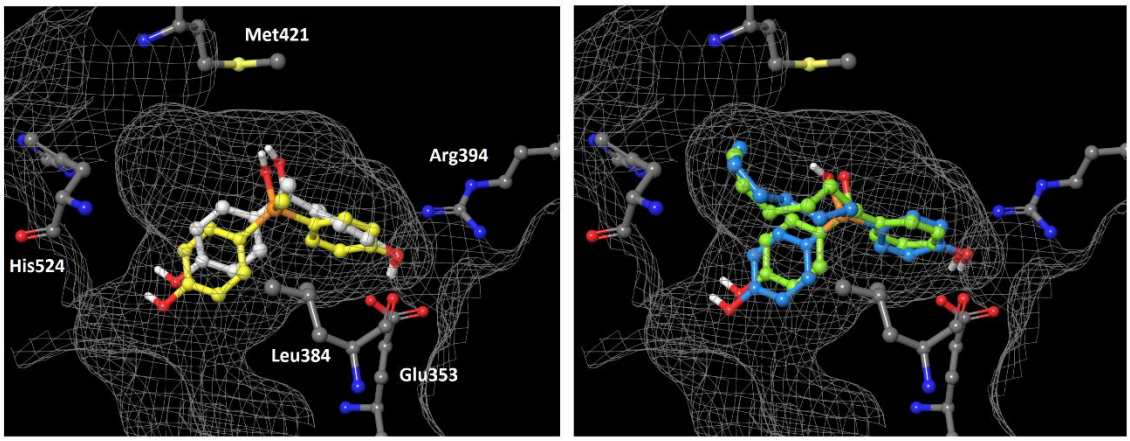
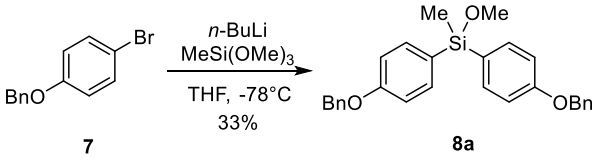


Fig. S1. Docking models of carbinols with hERα LBD (PDB ID: 3ERT) obtained with AutoDock 4.2. The protein surface is indicated as a gray mesh. Left: Superimposition of the docking models of methyl carbinol (grey) and methyl silanol **5a** (yellow). Right: Superimposition of the docking models of hexyl carbinol (green) and hexyl silanol **5f** (cyan).

2. Experimental Procedure for Synthesis of Compounds

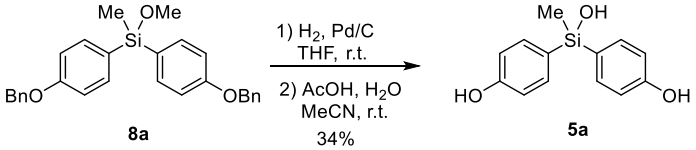
2.1. Synthesis of bis(4-(benzyloxy)phenyl)methoxymethylsilane (8a)



7 **8a**

To a solution of compound **7** (0.502 g, 1.91 mmol) in dry THF (15 mL) was added *n*-butyl lithium in *n*-hexane (1.6 M, 1.43 mL, 2.29 mmol) under an Ar atmosphere at –78 ˚C. The mixture was stirred at room temperature for 1 h. To this was added Trimethoxymethylsilane (0.19 mL, 1.34 mmol), and stirring at –78 ˚C for 3 h. The reaction was quenched with water, and the whole was extracted with ethyl acetate. The extract was successively washed with water and brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (hexane/ethyl acetate = 10:1) to give **8a** (0.137 g, 33%) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.51 (d, *J* = 8.6 Hz, 4H), 7.43 (d, *J* = 7.5 Hz, 4H), 7.40-7.37 (m, 4H), 7.34-7.31 (m, 2H), 7.00 (d, *J* = 8.6 Hz, 4H), 5.08 (s, 4H), 3.50 (s, 3H), 0.59 (s, 3H). MS (TOF, [M+Na]) m/z 463.

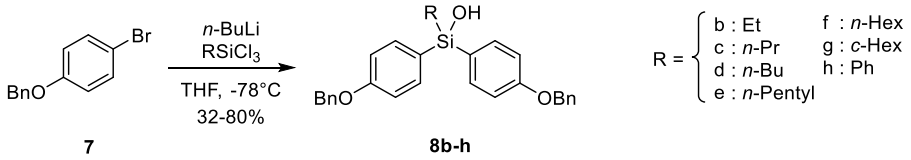
2.2. Synthesis of bis(4-(hydroxy)phenyl)methoxymethylsilane (5a)



8a **5a**

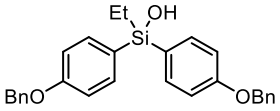
To a mixture of compound **8a** (0.137 g, 3.11 mmol), THF (5 mL) and ethyl acetate was added 10% Pd/C (14.3 mg) at room temperature, and the mixture was stirred under an H_2 atmosphere at the same temperature for 3 d. The reaction mixture was filtered through a Celite pad and the solvent was evaporated. The residue was purified by silica gel column chromatography (hexane/ethyl acetate =2:1) to give a mixture of the desired bisphenol **5a** and a mono-deprotected material (80 mg) as a white solid. Then, to a solution of the above obtained mixture (80 mg) in acetonitrile (10 mL) was added aqueous acetic acid (1.0 M, 10 mL) at room temperature. The mixture was stirred at room temperature for 2 h. The reaction was quenched with aqueous saturated $NaHCO_3$ solution, and the whole was extracted with ethyl acetate. The extract was successively washed with water and brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (hexane/ethyl acetate = 2:1) to give **5a** (25.6 mg, 34%) as a white soild. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.47 (s, 2H), 7.31 (d, *J* = 8.6 Hz, 4H), 6.74 (d, *J* = 8.6 Hz, 4H), 6.08 (s, 1H), 0.40 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) : δ 158.39, 135.21, 128.08, 114.77, - 0.41 ; HRMS (TOF) calcd for $C_{13}H_{13}O_3Si$ 245.0628; found: *m/z* 245.0612 (M–H).

2.3. Synthesis of bis(4-benzyloxyphenyl)lsilanols (8b-h)



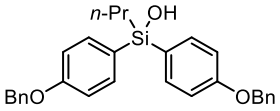
7 **8b-h**

2.3.1. Bis(4-benzyloxyphenyl)ethylsilanol (8b)



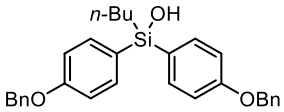
To a solution of compound **7** (0.203 g, 0.774 mmol) in dry THF (10 mL) was added *n*-butyl lithium in *n*-hexane (1.57 M, 0.592 mL, 0.929 mmol) under an Ar atmosphere at –78 ˚C. The mixture was stirred at the same temperature for 15 min. To this was added ethyltrichlorosilane (50.4 μL, 0.384 mmol), and stirring at –78 ˚C for 3 h. The reaction was quenched with saturated aqueous NH_4Cl solution, and the whole was extracted with ethyl acetate. The extract was successively washed with water and brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (hexane/ethyl acetate=4/1) to give **8b** (56.0 mg, 33%) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.6 Hz, 4H), 7.43 (d, *J* = 7.5 Hz, 4H), 7.39 (t, *J* = 7.5 Hz, 4H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 4H), 5.08 (s, 4H), 2.05 (br s, 1H), 1.12-1.02 (m, 5H). ^{13}C NMR (125 MHz, $CDCl_3$) : δ 160.37, 137.02, 135.99, 128.75, 128.15, 127.83, 127.65, 124.65, 69.90, 7.24, 6.91.

2.3.2. Bis(4-benzyloxyphenyl)*n*-propylsilanol (8c)



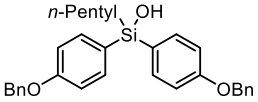
The title compound was prepared according to the procedure described for compound **8b**, by using *n*-propyltrichlorosilane as the starting material. Yield: 62%. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.0 Hz, 4H), 7.47 (d, *J* = 7.5 Hz, 4H), 7.40 (t, *J* = 7.5 Hz, 4H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 4H), 5.08 (s, 4H), 2.09 (br s, 1H), 1.48 (tq, *J* = 8.6 Hz, 7.5 Hz, 2H), 1.10 (t, *J* = 8.6 Hz, 2H), 0.99 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.33, 137.01, 135.94, 128.74, 128.14, 127.64, 114.61, 69.89, 18.32, 18.10, 16.88.

2.3.3. Bis(4-benzyloxyphenyl)-*n*-butylsilanol (8d)



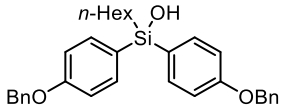
The title compound was prepared according to the procedure described for compound **8b**, by using *n*-butyltrichlorosilane as the starting material. Yield: 77%. Colorless oil. ^{1}H NMR (500 MHz, Acetone-d_6): δ 7.54 (d, *J* = 8.6 Hz, 4H), 7.48 (d, *J* = 7.5 Hz, 4H), 7.39 (t, *J* = 7.5 Hz, 4H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 4H), 5.17 (s, 1H), 5.13 (s, 4H), 1.45-1.31 (m, 4H), 1.07-1.04 (m, 2H), 0.85 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, Acetone-d_6): δ 160.88, 138.40, 136.48, 130.26, 129.29, 128.62, 128.44, 115.08, 70.14, 27.10, 26.26, 16.26, 14.07.

2.3.4. Bis(4-benzyloxyphenyl)-*n*-pentylsilanol (8e)



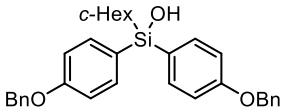
The title compound was prepared according to the procedure described for compound **8b**, by using *n*-pentyltrichlorosilane as the starting material. Yield: 66%. Colorless oil. ^{1}H NMR (500 MHz, Acetone-d_6): δ 7.54 (d, *J* = 8.6 Hz, 4H), 7.48 (d, *J* = 7.5 Hz, 4H), 7.39 (t, *J* = 6.9 Hz, 4H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 4H), 5.17 (s, 1H), 5.13 (s, 4H), 1.47-1.41 (m, 2H), 1.36-1.24 (m, 4H), 1.07-1.03 (m, 2H), 0.84 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (125 MHz, Acetone-d_6): δ 160.88, 138.40, 136.48, 130.27, 129.29, 128.62, 128.43, 115.09, 70.15, 36.44, 23.66, 22.97, 16.47, 14.28.

2.3.5. Bis(4-benzyloxyphenyl)-*n*-hexylsilanol (8f)



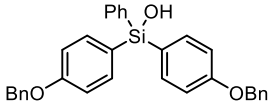
The title compound was prepared according to the procedure described for compound **8b**, by using *n*-hexyltrichlorosilane as the starting material. Yield: 80%. Colorless oil. ^{1}H NMR (500 MHz, Acetone-d_6): δ 7.54 (d, *J* = 8.6 Hz, 4H), 7.48 (d, *J* = 7.5 Hz, 4H), 7.39 (t, *J* = 6.9 Hz, 4H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 4H), 5.16 (s, 1H), 5.13 (s, 4H), 1.47-1.41 (m, 2H), 1.37-1.22 (m, 6H), 1.07-1.04 (m, 2H), 0.86 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (125 MHz, Acetone-d_6): δ 160.88, 138.40, 136.48, 130.27, 129.29, 128.62, 128.43, 115.08, 70.15, 33.89, 32.39, 23.97, 23.25, 16.53, 14.37.

2.3.6. Bis(4-benzyloxyphenyl)cyclohexylsilanol (8g)



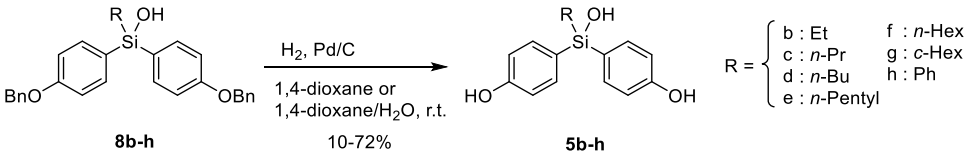
The title compound was prepared according to the procedure described for compound **8b**, by using cyclohexyltrichlorosilane as the starting material. Yield: 61%. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.53 (d, *J* = 8.0 Hz, 4H), 7.44 (d, *J* = 7.5 Hz, 4H), 7.39 (t, *J* = 7.5 Hz, 4H), 7.33 (t, *J* = 6.9 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 4H), 5.08 (s, 4H), 2.03 (br s, 1H), 1.84-1.78 (m, 2H), 1.77-1.66 (m, 3H), 1.30-1.18 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.29, 137.03, 136.27, 128.74, 128.14, 127.66, 127.07, 114.54, 69.88, 28.01, 27.06, 26.91, 25.83.

2.3.7. Bis(4-benzyloxyphenyl)phenylsilanol (8h)

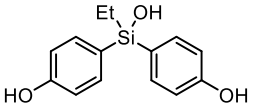


The title compound was prepared according to the procedure described for compound **8b**, by using phenyltrichlorosilane as the starting material. Yield: 32%. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.62 (dt, *J* = 6.3 Hz, 1.7 Hz, 2H), 7.55 (d, *J* = 8.6 Hz, 4H), 7.44-7.42 (m, 5H), 7.40-7.36 (m, 6H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 4H), 5.08 (s, 4H), 2.46 (br s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) : δ 160.58, 136.98, 136.78, 135.94, 135.06, 130.10, 128.76, 128.17, 128.02, 127.64, 126.89, 114.67, 69.92.

2.4. Synthesis of Bis(4-hydroxyphenyl)silanols (5b-h)



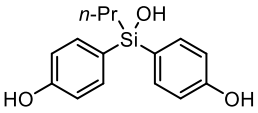
2.4.1. Bis(4-hydroxyphenyl)ethylsilanol (5b)



To a mixture of compound **8b (**60.0 mg, 0.136 mmol) and 1,4-dioxane (0.8 mL) was added 10% Pd/C (15.0 mg) at room temperature, and the mixture was stirred under an H_2 atmosphere at the same temperature for 3 d. The reaction mixture was filtered through a Celite pad and the solvent was evaporated. The residue was purified by means of silica gel column chromatography (hexane/ethyl

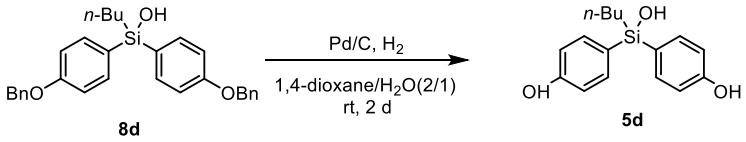
acetate = 1:1) to give **5b** (19.1 mg, 54%) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.47 (s, 2H), 7.31 (d, J = 8.6 Hz, 4H), 6.74 (d, J = 8.0 Hz, 4H), 6.06 (s, 1H), 0.92-0.85 (m, 5H). ^{13}C NMR (125 MHz, DMSO-d_6) : δ 158.38, 135.45, 126.96, 114.81, 7.25, 7.01 ; HRMS (TOF) calcd for $C_{14}H_{15}O_3Si$ 259.0796; found: *m/z* 259.0801 (M–H).

2.4.2. Bis(4-hydroxyphenyl)-*n*-propylsilanol (5c)



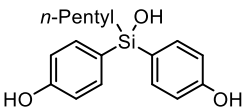
The title compound was prepared according to the procedure described for compound **5b**, by using **8c** as the starting material. Yield: 6.6 mg, 9.7%. Colorless crystal. ^{1}H NMR (500 MHz, Acetone-d_6): δ 8.38 (s, 2H), 7.44 (d, J = 8.6 Hz, 4H), 6.83 (d, J = 8.0 Hz, 4H), 5.02 (s, 1H), 1.45 (tq, J = 8.6 Hz, 7.5 Hz, 2H), 1.01 (t, J = 8.6 Hz, 2H), 0.95 (t, J = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, Acetone-d_6) : δ 159.41, 136.58, 128.73, 115.65, 19.35, 18.52, 17.59 ; HRMS (TOF) calcd for $C_{15}H_{17}O_3Si$ 273.0952; found: *m/z* 273.0946 (M–H).

2.4.3. Synthesis of Bis(4--hydroxyphenyl)*n*-butylsilanol (5d)



To a mixture of compound **8d** (0.138 g, 0.294 mmol), 1,4-dioxane (1.5 mL) and H_2O (0.75 mL) was added 10% Pd/C (22.8 mg) at room temperature, and the mixture was stirred under an H_2 atmosphere at the same temperature for 2 d. The reaction mixture was filtered through a Celite pad and the solvent was evaporated. The residue was purified by means of silica gel column chromatography (hexane/ethyl acetate = 3:2) to give **5d** (55.6 mg, 65%) as a white solid. ^{1}H NMR (500 MHz, Acetone-d_6): δ 8.39 (br s, 1H for phenolic OH), 7.44 (d, J = 8.6 Hz, 4H), 6.84 (d, J = 8.6 Hz, 4H), 5.02 (s, 1H), 1.45-1.31 (m, 4H), 1.03-1.00 (m, 2H), 0.85 (t, J = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, Acetone-d_6) : δ 159.34, 136.58, 128.71, 115.59, 27.14, 26.31, 16.42, 14.08 ; HRMS (TOF) calcd for $C_{16}H_{19}O_3Si$ 287.1109; found: *m/z* 287.1116 (M–H).

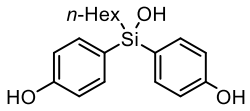
2.4.4. Bis(4--hydroxyphenyl)*n*-pentylsilanol (5e)



The title compound was prepared according to the procedure described for compound **5d**, by using

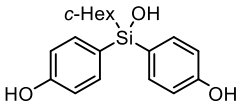
8e as the starting material. Yield: 29.0 mg, 33%. Colorless solid. ^{1}H NMR (500 MHz, Acetone-d_6): δ 8.39 (s, 1H for phenolic OH), 7.44 (d, J = 8.6 Hz, 4H), 6.84 (d, J = 8.0 Hz, 4H), 5.02 (s, 1H), 1.47-1.40 (m, 2H), 1.35-1.25 (m, 4H), 1.03-0.99 (m, 2H), 0.84 (t, J = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, Acetone-d_6): δ 159.40, 136.59, 128.75, 115.64, 36.49, 23.72, 22.98, 16.64, 14.28; HRMS (TOF) calcd for $C_{17}H_{21}O_3Si$ 301.1265; found: *m/z* 301.1263 (M–H).

2.4.5. Bis(4--hydroxyphenyl)*n*-hexylsilanol (5f)



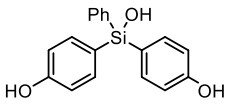
The title compound was prepared according to the procedure described for compound **5d**, by using **8f** as the starting material. Yield: 40%. Colorless solid. ^{1}H NMR (500 MHz, Acetone-d_6): δ 8.40 (br s, 1H for phenolic OH), 7.44 (d, J = 8.6 Hz, 4H), 6.84 (d, J = 8.6 Hz, 4H), 5.02 (br s, 1H), 1.46-1.40 (m, 2H), 1.37-1.22 (m, 6H), 1.03-1.00 (m, 2H), 0.85 (t, J = 6.9 Hz, 3H). ^{13}C NMR (125 MHz, Acetone-d_6): δ 159.34, 136.58, 128.70, 115.58, 33.93, 32.31, 24.01, 23.25, 16.70, 14.36; HRMS (TOF) calcd for $C_{18}H_{23}O_3Si$ 315.1422; found: *m/z* 315.1425 (M–H).

2.4.6. Bis(4--hydroxyphenyl)cyclohexylsilanol (5g)



The title compound was prepared according to the procedure described for compound **5d**, by using **8g** as the starting material. Yield: 72%. Colorless solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.46 (s, 2H), 7.33 (d, J = 8.0 Hz, 4H), 6.75 (d, J = 8.6 Hz, 4H), 6.02 (s, 1H), 1.68-1.60 (m, 5H), 1.19-1.10 (m, 5H), 1.00 (t, J = 11.5 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 158.30, 135.70, 126.09, 114.77, 27.48, 26.66, 26.58, 25.77; HRMS (TOF) calcd for $C_{18}H_{21}O_3Si$ 313.1265; found: *m/z* 313.1261 (M–H).

2.4.7. Bis(4--hydroxyphenyl)phenylsilanol (5h)



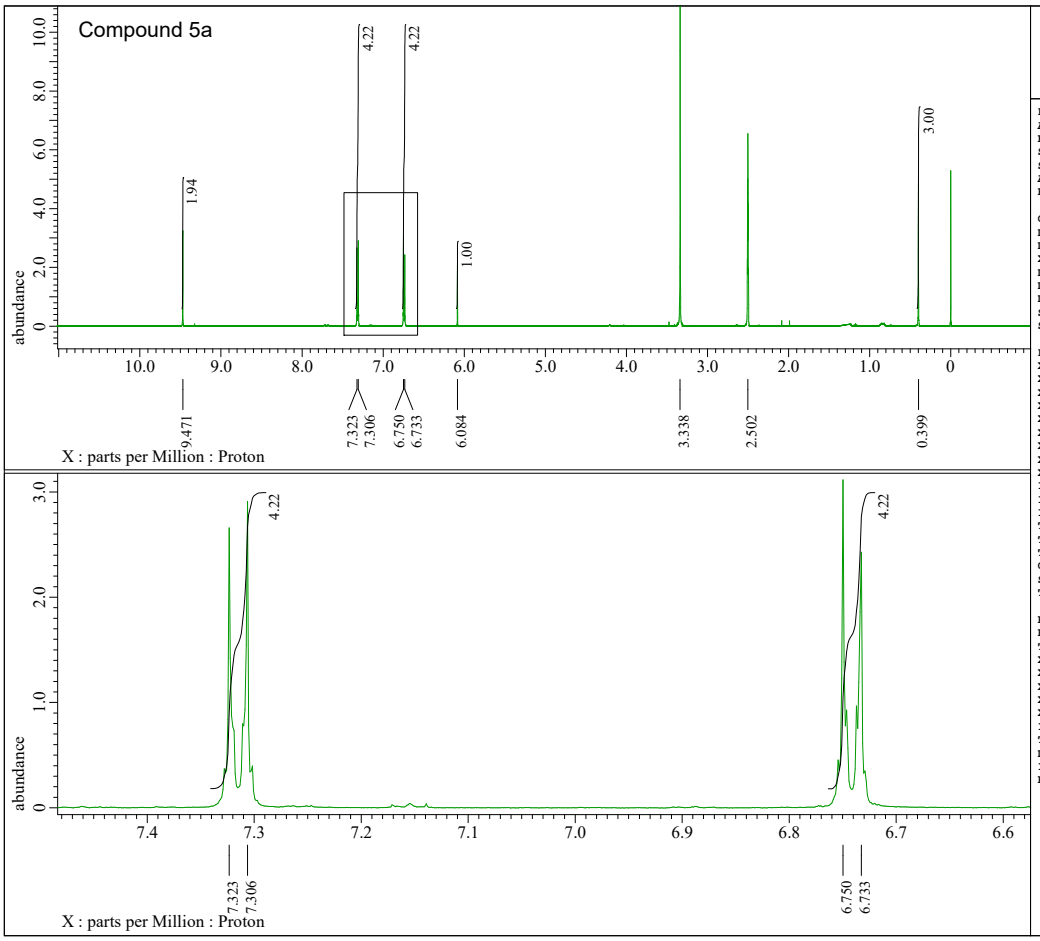
The title compound was prepared according to the procedure described for compound **5b**, by using **8h** as the starting material. Yield: 29%. Colorless solid. ^{1}H NMR (500 MHz, Acetone-d_6): δ 8.47 (br s, 2H), 7.61 (d, J = 6.9 Hz, 2H), 7.44 (d, J = 7.5 Hz, 4H), 7.41-7.34 (m, 3H), 6.85 (d, J = 8.6 Hz, 4H), 5.61 (br s, 1H). ^{13}C NMR (125 MHz, Acetone-d_6): δ 159.72, 138.78, 137.42, 135.66, 130.15, 128.38, 127.45, 115.72; HRMS (TOF) calcd for $C_{18}H_{15}O_3Si$ 307.0796; found: *m/z* 307.0795 (M–H).

3. Experimental Procedure for ER reporter gene assay

The ER-agonistic and antagonistic activities of compounds were evaluated by means of reporter gene assay using a Gal4-human ERα or ERβ reporter system. A fragment of human ERα/β was inserted into the pCMX-GAL4 vector to obtain pCMX-GAL4-hER (pCMX-flag vector to make pCMX-ERα/β). GAL4-responsive MH100 (USA)x4-tk-LUK reporter was used. Human embryonic kidney (HEK 293) cells were cultivated in Dulbecco's modified Eagle's medium (DMEM without Phenol Red) containing 5% fetal bovine serum (FBS) and antibiotic-antimycotic mixture (Nacalai) at 37°C in a humidified atmosphere of 5% CO_2 in air. Transfections were performed by the calcium phosphate coprecipitation method. Test compounds were added at 24 h after transfection. Cells were harvested 24 h after the treatment, and luciferase and β-galactosidase activities were assayed using a luminometer and a microplate reader. DNA cotransfection experiments were done with 50 ng of reporter plasmid, 15-20 ng pCMX-s-galactosidase, 10-15 ng of each receptor expression plasmid and pGEM carrier DNA to make a total of 150 ng DNA per well in a 96-well plate. Luciferase data were normalized to an internal β-galactosidase control, and reported values are means of triplicate assays. Antagonist activity was measured in the presence of 0.3 nM 17β-estradiol.

4. Experimental Procedure for Docking Simulation

The structure of the LBD of hERα and hERβ were prepared from the Protein Data Bank accession 3ERT and 3OLS, respectively. Polar hydrogens and partial atomic charges were assigned using AutoDockTools (ADT). Molecular docking was performed using AutoDock 4.2 with the Genetic Algorithm. AutoDock parameters for silicon atoms were Rii = 1.60 and εii = 0.875.

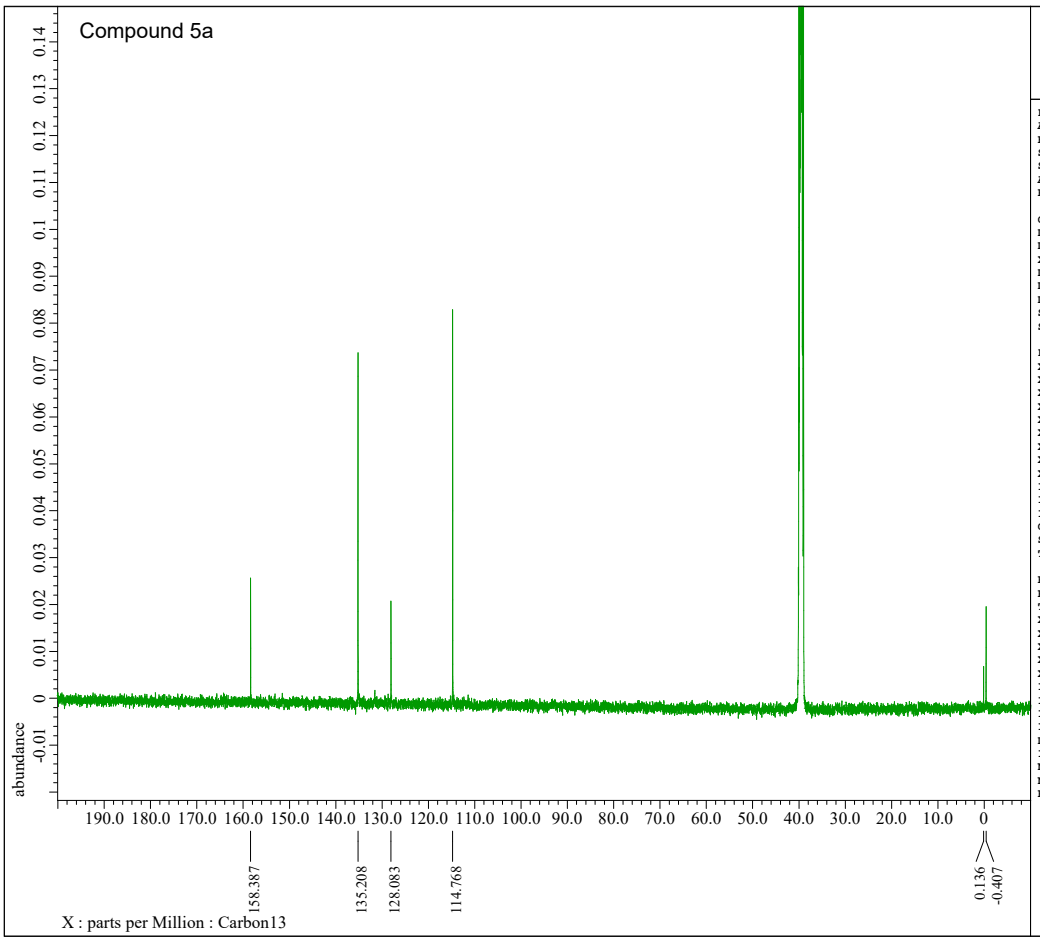



```
Filename          = silanol5_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = silanol5
Solvent           = DMSO-D6
Actual_Start_Time = 12-NOV-2017 16:31:35
Revision_Time     = 12-NOV-2017 16:19:53

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 52
Temp_Get          = 21.1[dC]
X_90_Width        = 6.04[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2[dB]
X_Pulse           = 3.02[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

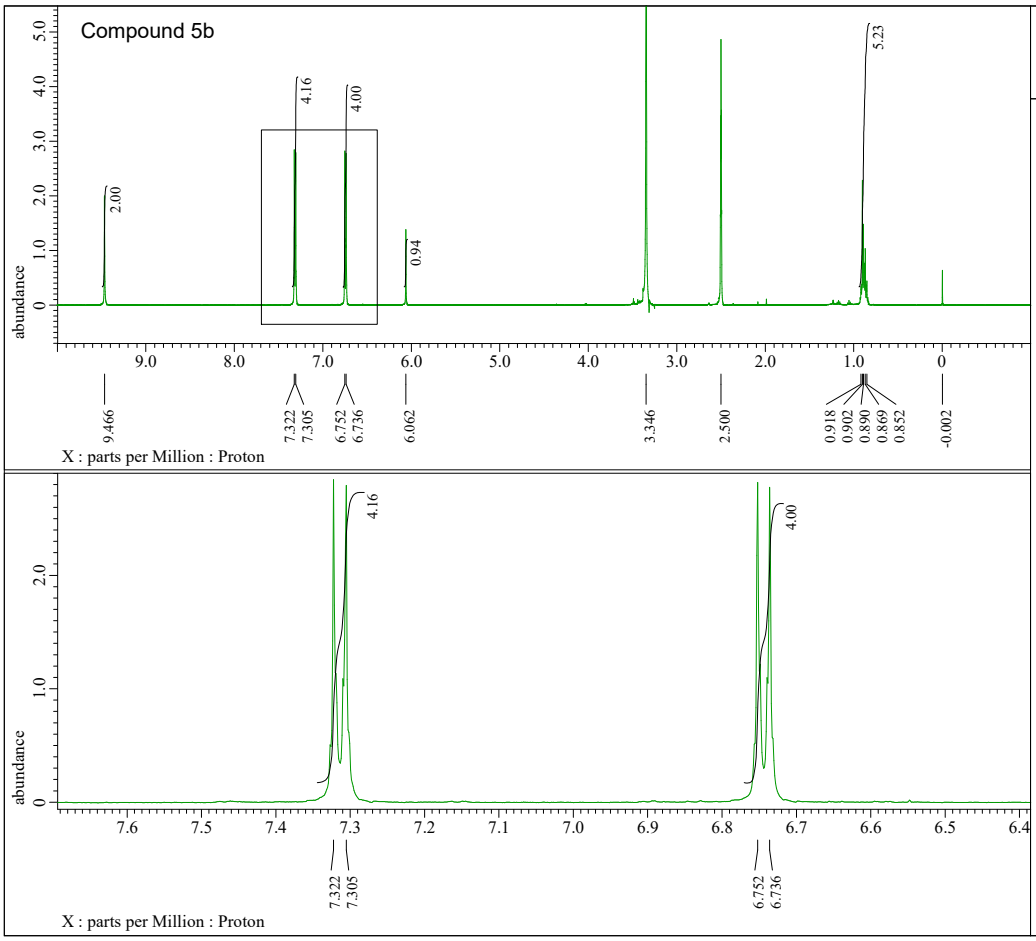



```
Filename          = silanol5_Carbon-1-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = silanol5
Solvent           = DMSO-D6
Actual_Start_Time = 13-NOV-2017 01:07:25
Revision_Time     = 13-NOV-2017 16:12:30

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 8192
Total_Scans       = 8192

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.2[dC]
X_90_Width        = 10.67[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 6.1[dB]
X_Pulse           = 3.55666667[us]
Irr_Atn_Dec       = 25.655[dB]
Irr_Atn_Noe       = 25.655[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

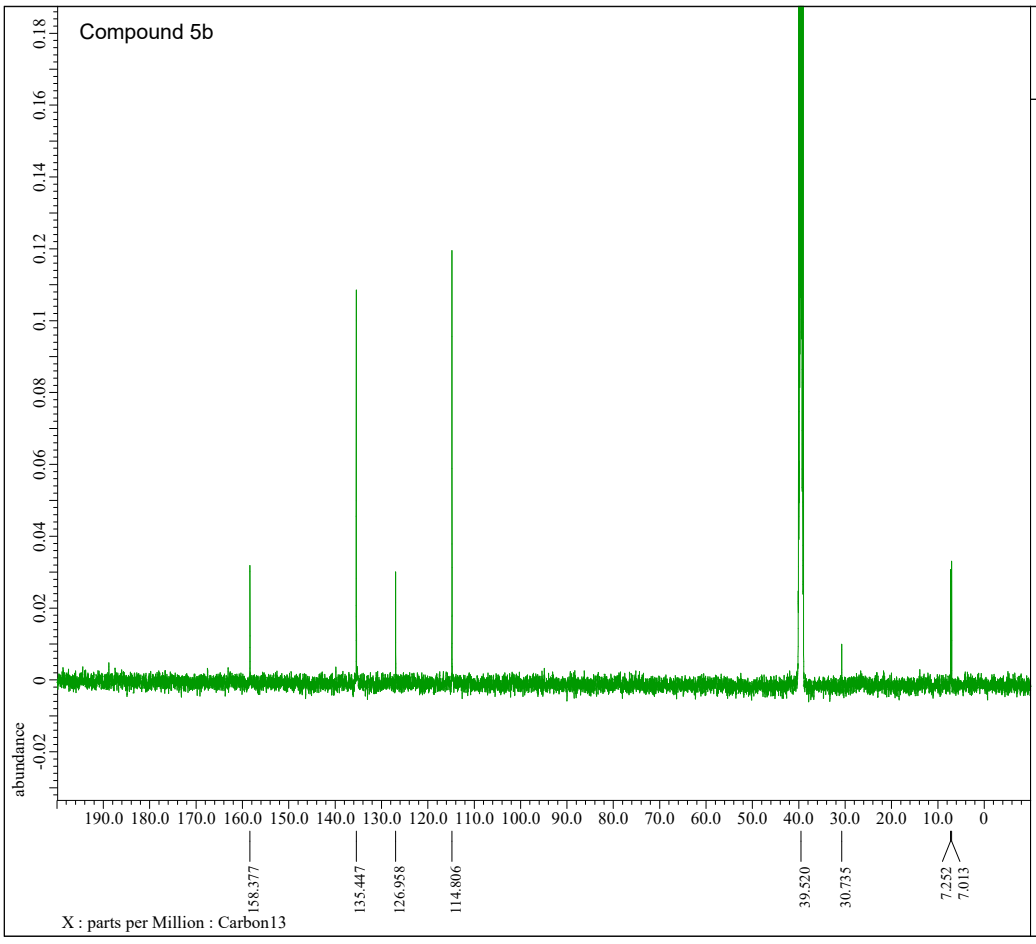



```
Filename          = YM146_2_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = YM146_2
Solvent           = DMSO-D6
Actual_Start_Time = 29-AUG-2018 17:52:06
Revision_Time     = 29-AUG-2018 17:39:48

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 50
Temp_Get          = 22.3[dC]
X_90_Width        = 6.04[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2[dB]
X_Pulse           = 3.02[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

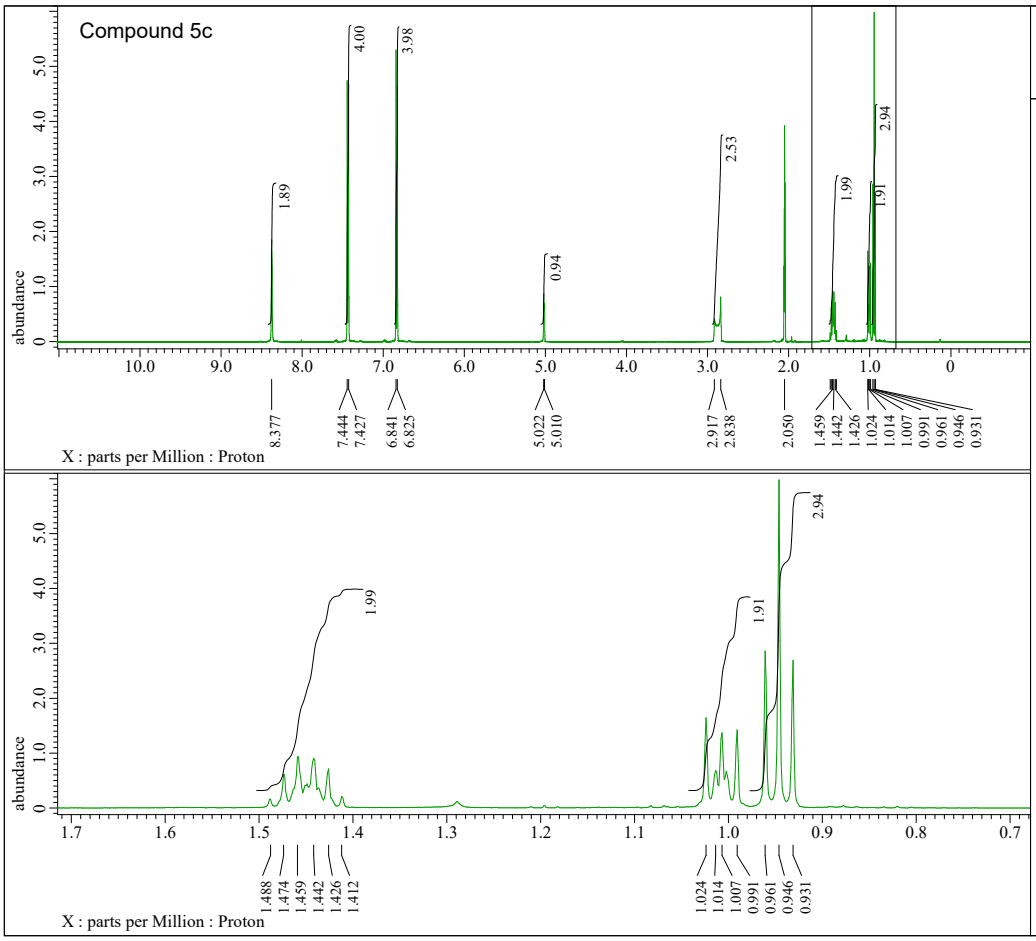



```
Filename          = YM146_2_Carbon-1-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = YM146_2
Solvent           = DMSO-D6
Actual_Start_Time = 30-AUG-2018 14:33:27
Revision_Time     = 30-AUG-2018 15:24:41

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.7[dC]
X_90_Width        = 10.67[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 6.1[dB]
X_Pulse           = 3.55666667[us]
Irr_Atn_Dec       = 25.655[dB]
Irr_Atn_Noe       = 25.655[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

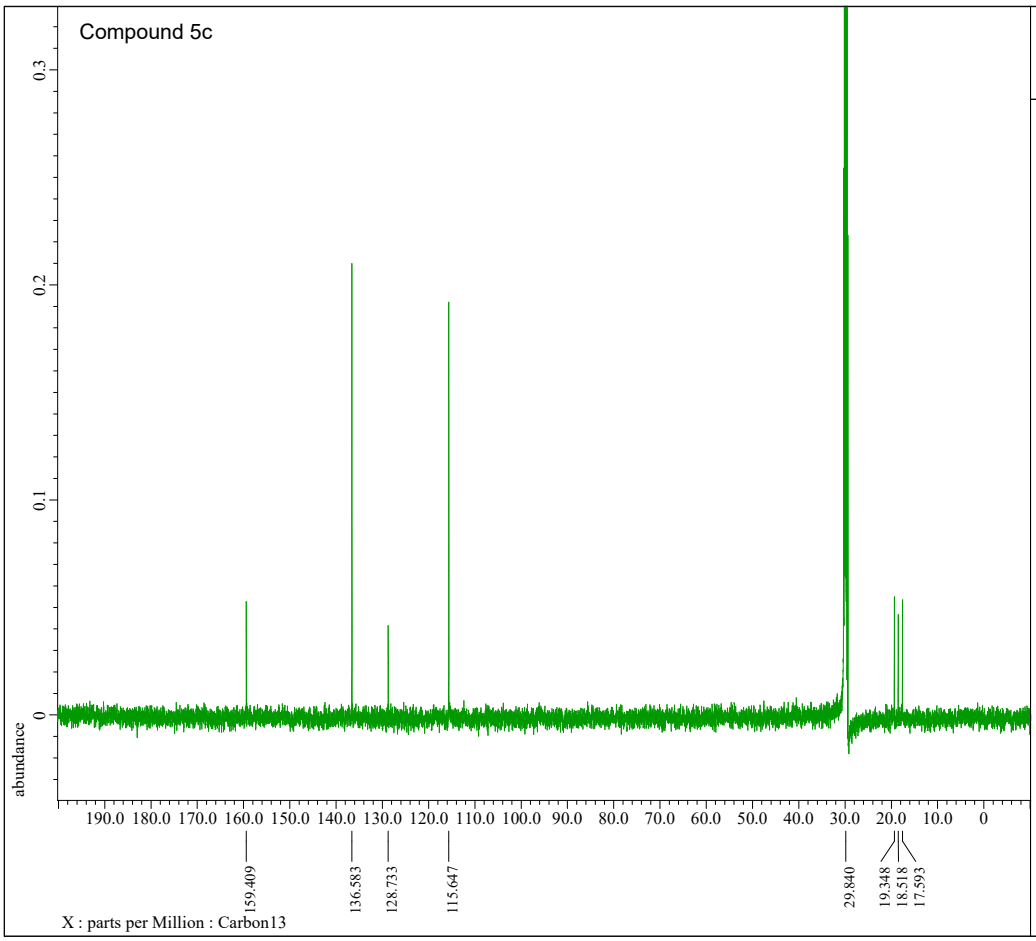



```
Filename            = YM153_3_Proton-1-4.jdf
Author              = delta
Experiment          = proton.jxp
Sample_Id           = YM153_3
Solvent             = ACETONE-D6
Actual_Start_Time   =  3-OCT-2018 11:50:38
Revision_Time       =  3-OCT-2018 11:38:01

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECA500
Spectrometer        = DELTA2_NMR

Field_Strength      = 11.7473579[T] (500[MHz])
X_Acq_Duration      = 1.74587904[s]
X_Domain            = 1H
X_Freq              = 500.15991521[MHz]
X_Offset            = 5.0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.57277737[Hz]
X_Sweep             = 9.38438438[kHz]
X_Sweep_Clipped     = 7.50750751[kHz]
Irr_Domain          = Proton
Irr_Freq            = 500.15991521[MHz]
Irr_Offset          = 5.0[ppm]
Tri_Domain          = Proton
Tri_Freq            = 500.15991521[MHz]
Tri_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 23[dC]
X_90_Width          = 6.04[us]
X_Acq_Time          = 1.74587904[s]
X_Angle             = 45[deg]
X_Atn               = 2[dB]
X_Pulse             = 3.02[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 6.74587904[s]
```

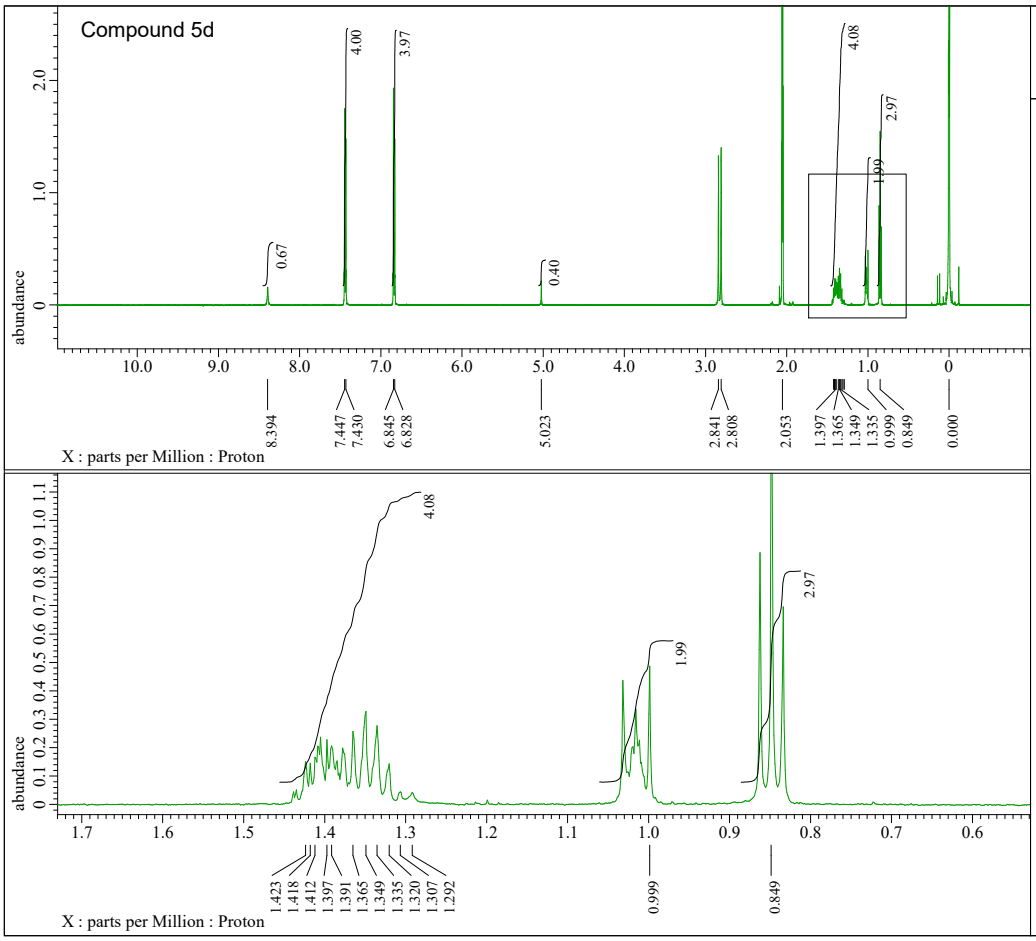



```
Filename            = YM153_3_Carbon-1-4.jdf
Author              = delta
Experiment          = carbon.jxp
Sample_Id           = YM153_3
Solvent             = ACETONE-D6
Actual_Start_Time   =  3-OCT-2018 11:54:05
Revision_Time       =  3-OCT-2018 11:51:00

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECA500
Spectrometer        = DELTA2_NMR

Field_Strength      = 11.7473579[T] (500[MHz])
X_Acq_Duration      = 0.83361792[s]
X_Domain            = 13C
X_Freq              = 125.76529768[MHz]
X_Offset            = 100[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.19959034[Hz]
X_Sweep             = 39.3081761[kHz]
X_Sweep_Clipped     = 31.44654088[kHz]
Irr_Domain          = Proton
Irr_Freq            = 500.15991521[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = TRUE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 23[dC]
X_90_Width          = 10.67[us]
X_Acq_Time          = 0.83361792[s]
X_Angle             = 30[deg]
X_Atn               = 6.1[dB]
X_Pulse             = 3.55666667[us]
Irr_Atn_Dec         = 25.655[dB]
Irr_Atn_Noe         = 25.655[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 92[us]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.83361792[s]
```

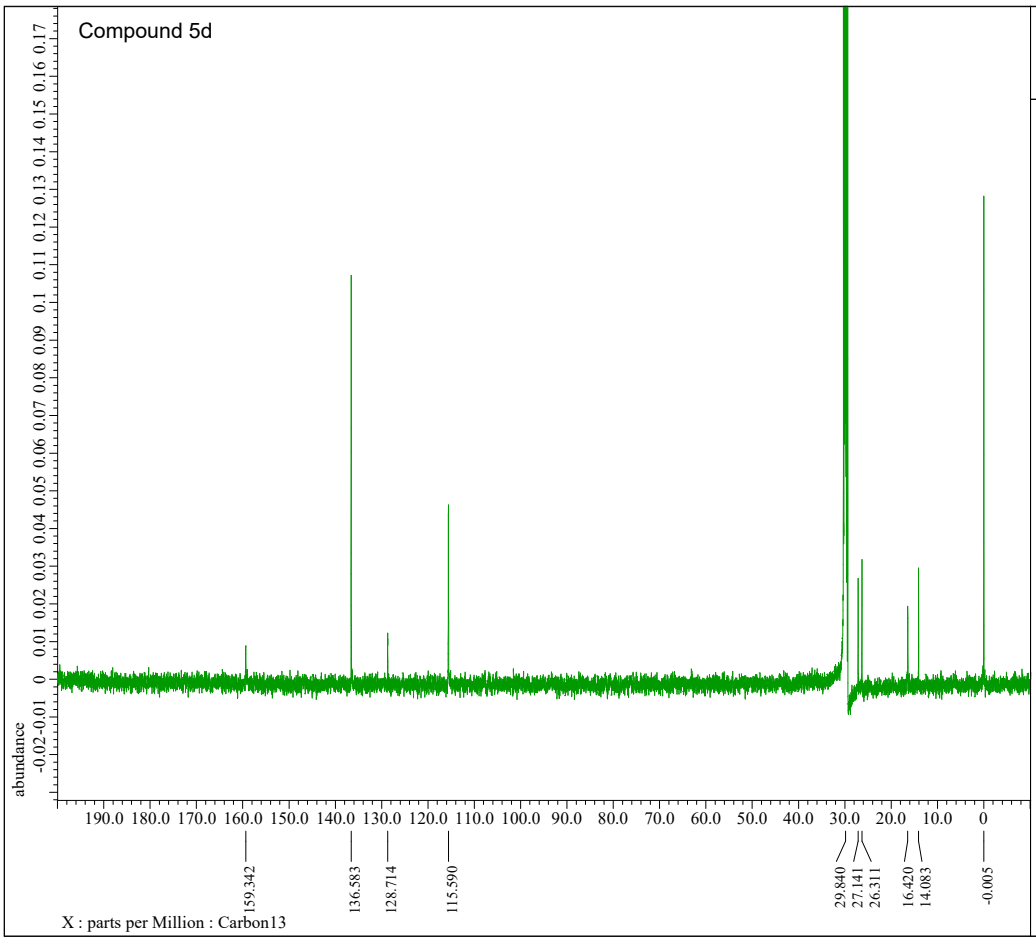



```
Filename          = YM168_3_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = YM168_3
Solvent           = ACETONE-D6
Actual_Start_Time =  9-JAN-2019 17:48:00
Revision_Time     =  9-JAN-2019 17:35:47

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 50
Temp_Get          = 22[dC]
X_90_Width        = 6.04[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2[dB]
X_Pulse           = 3.02[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

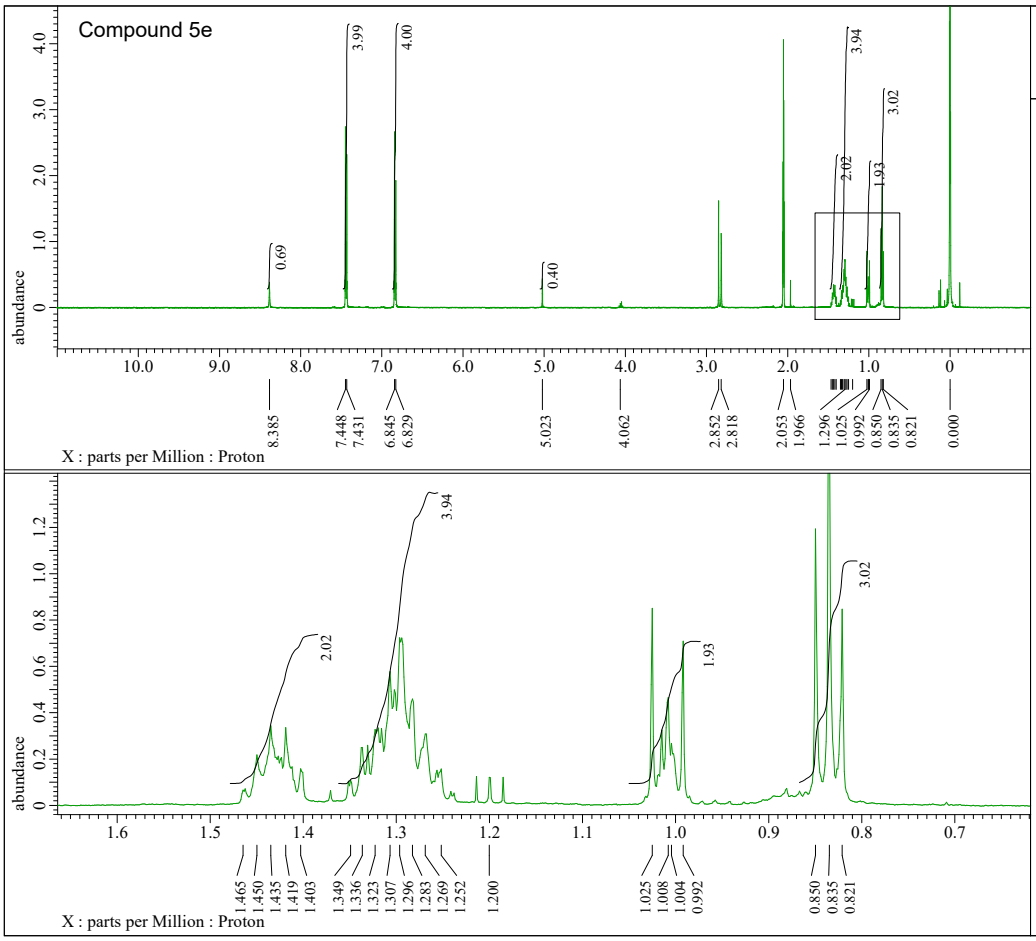



```
Filename          = YM168_3_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = YM168_3
Solvent           = ACETONE-D6
Actual_Start_Time = 10-JAN-2019 00:06:14
Revision_Time     = 18-JAN-2019 11:18:55

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.5[dC]
X_90_Width        = 10.67[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 6.1[dB]
X_Pulse           = 3.55666667[us]
Irr_Atn_Dec       = 25.655[dB]
Irr_Atn_Noe       = 25.655[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

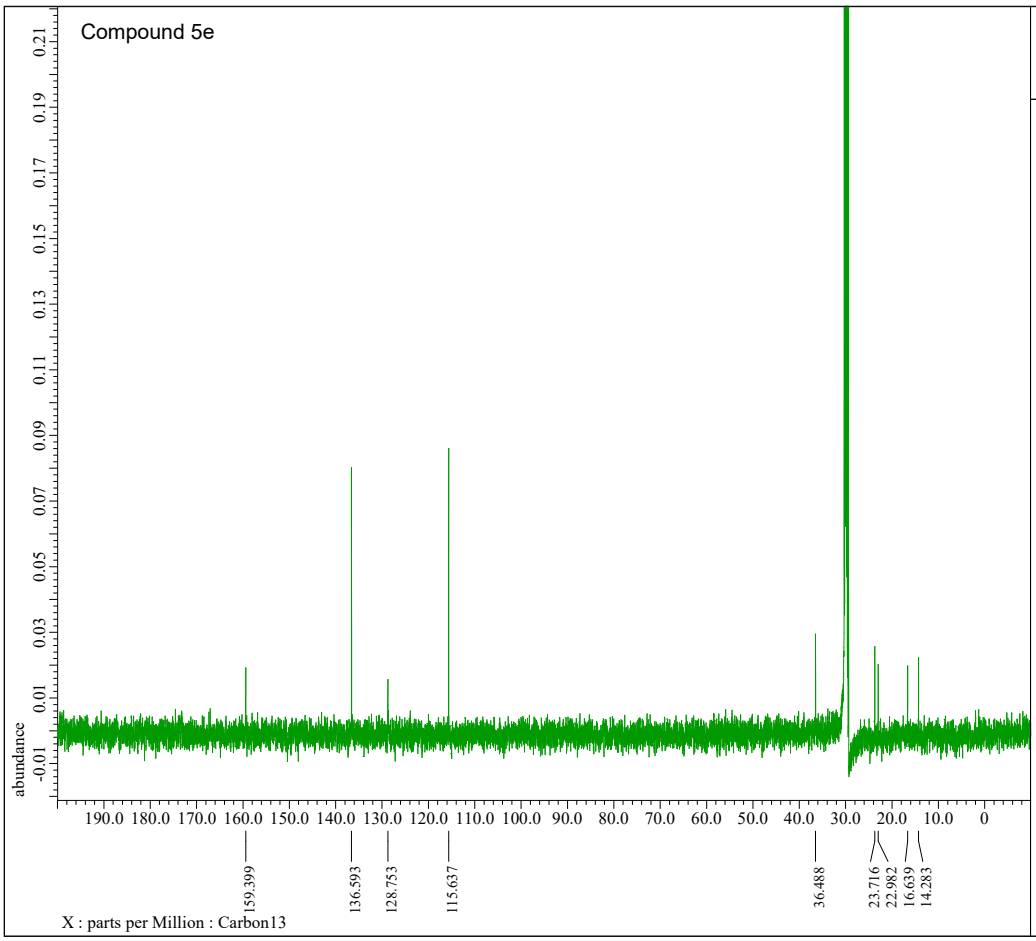



```
Filename          = YM164_2_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = YM164_2
Solvent           = ACETONE-D6
Actual_Start_Time =  9-JAN-2019 18:10:55
Revision_Time     =  9-JAN-2019 17:57:45

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 48
Temp_Get          = 22.2[dC]
X_90_Width        = 6.04[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2[dB]
X_Pulse           = 3.02[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

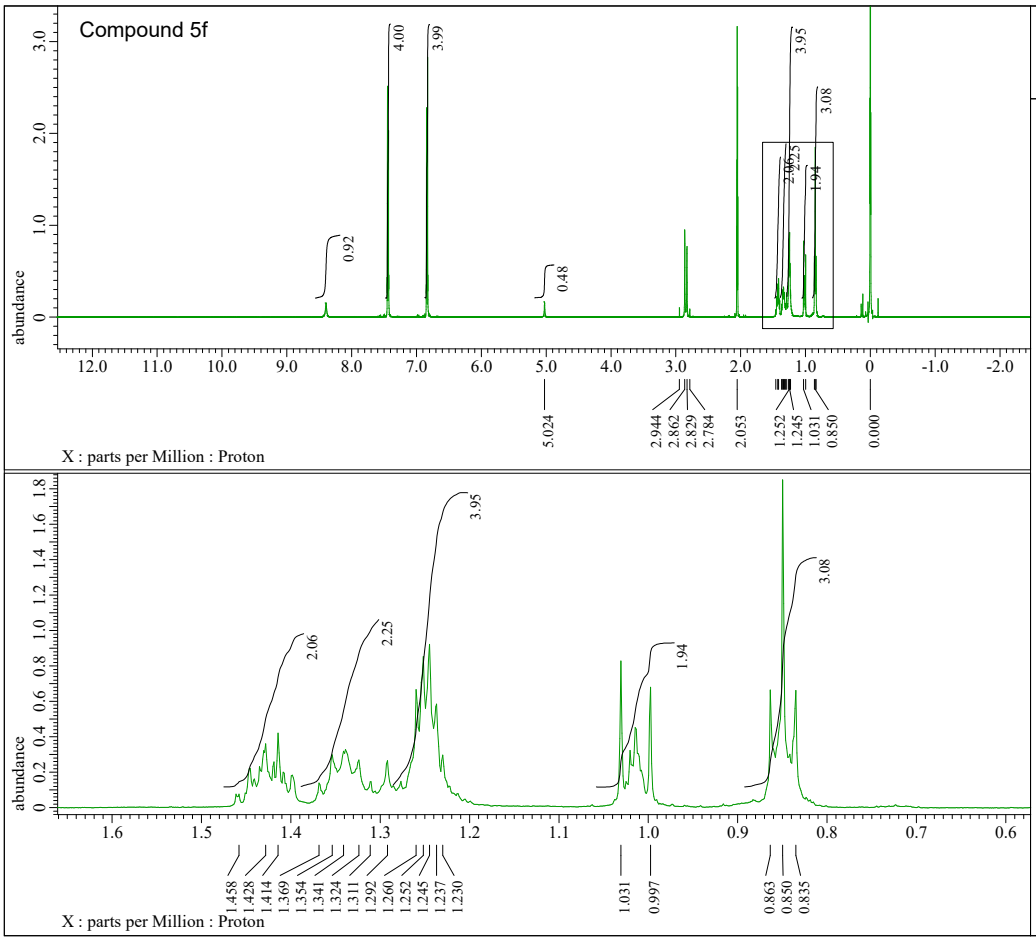



```
Filename          = YM164_1_Carbon-1-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = YM164_1
Solvent           = ACETONE-D6
Actual_Start_Time = 15-NOV-2018 16:01:27
Revision_Time     = 18-MAR-2019 15:14:59

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 22.1[dC]
X_90_Width        = 10.67[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 6.1[dB]
X_Pulse           = 3.55666667[us]
Irr_Atn_Dec       = 25.655[dB]
Irr_Atn_Noe       = 25.655[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

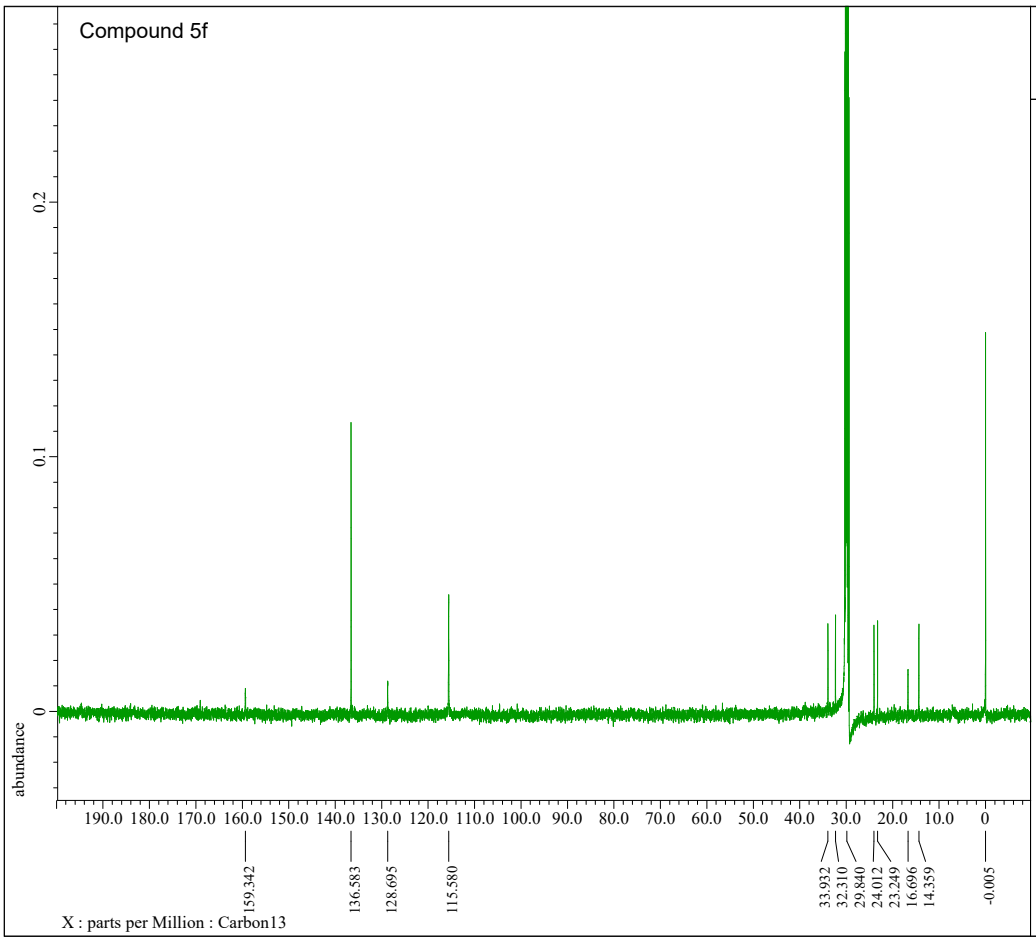



```
Filename          = YM172_5_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = YM172_5
Solvent           = ACETONE-D6
Actual_Start_Time =  9-JAN-2019 18:03:23
Revision_Time     =  9-JAN-2019 17:51:14

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 46
Temp_Get          = 22.2[dC]
X_90_Width        = 6.04[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2[dB]
X_Pulse           = 3.02[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

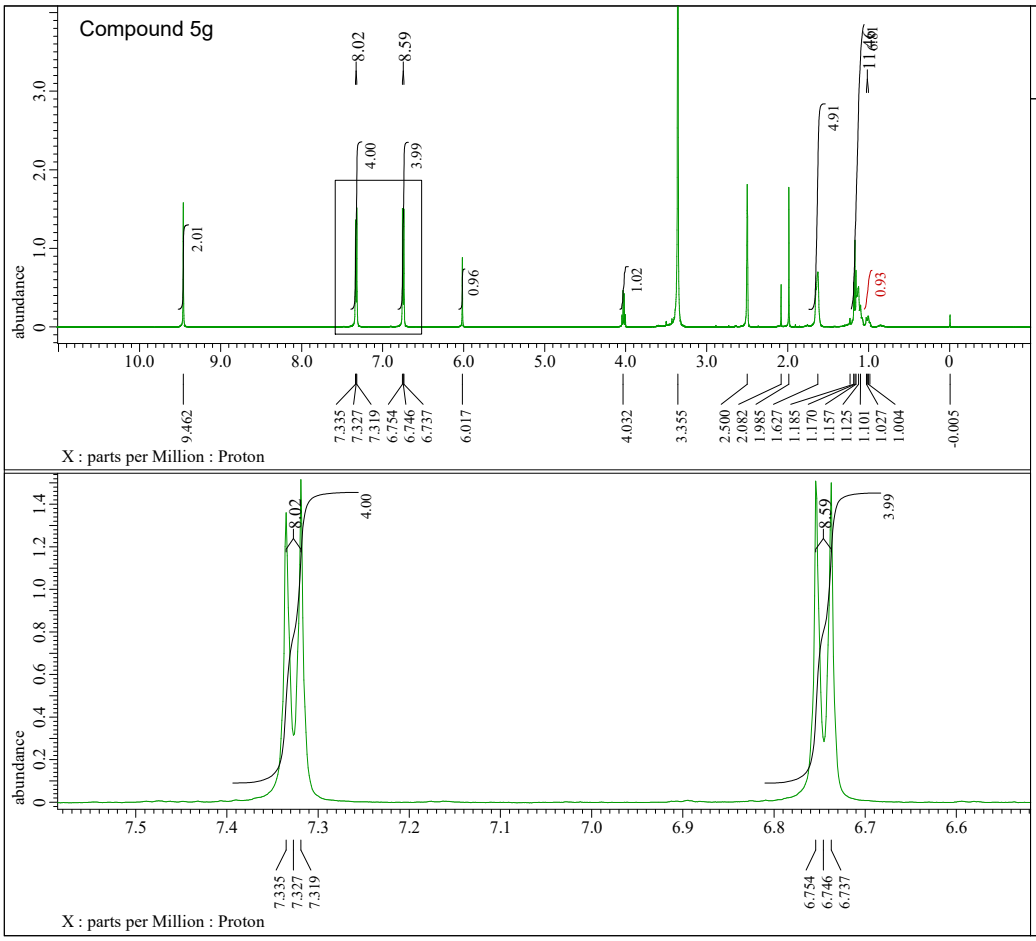



```
Filename          = YM172_5_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = YM172_5
Solvent           = ACETONE-D6
Actual_Start_Time = 10-JAN-2019 03:08:13
Revision_Time     = 18-JAN-2019 11:22:29

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.3[dC]
X_90_Width        = 10.67[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 6.1[dB]
X_Pulse           = 3.55666667[us]
Irr_Atn_Dec       = 25.655[dB]
Irr_Atn_Noe       = 25.655[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

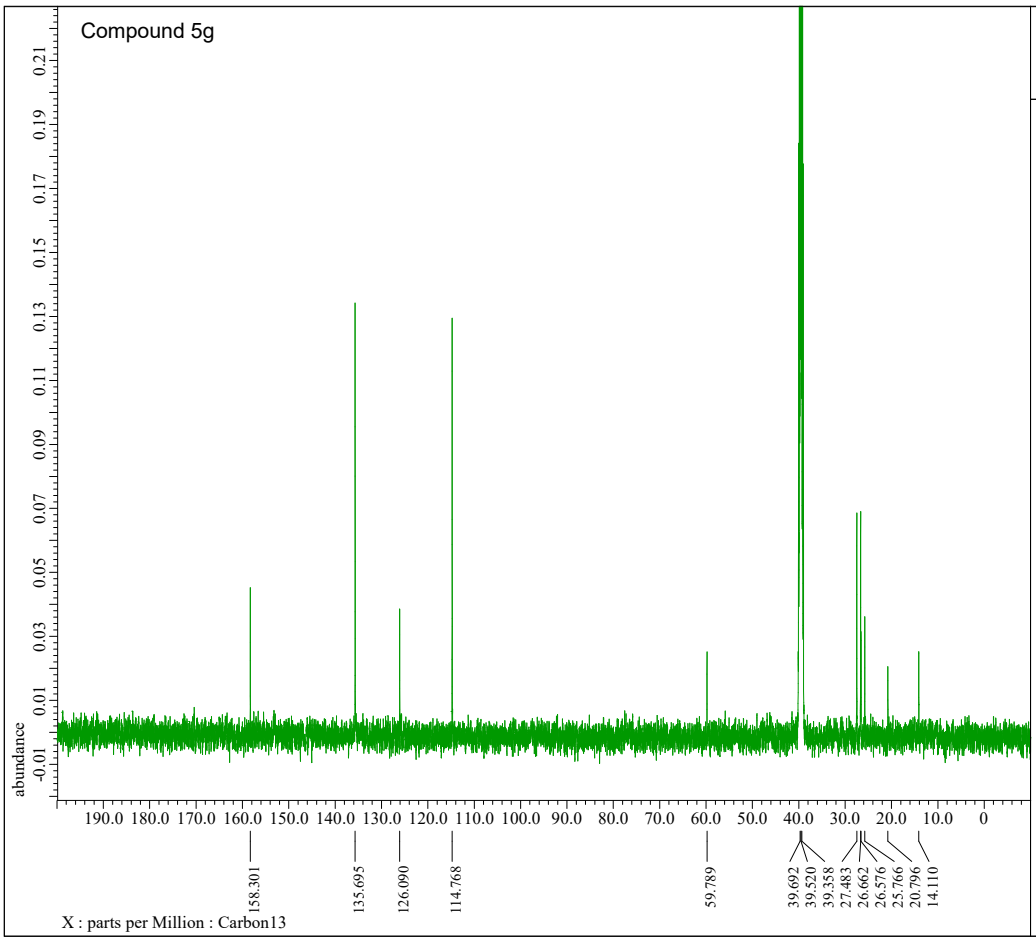



```
Filename            = YM161_4_Proton-1-4.jdf
Author              = delta
Experiment          = proton.jxp
Sample_Id           = YM161_4
Solvent             = DMSO-D6
Actual_Start_Time   =  9-NOV-2018 17:15:20
Revision_Time       =  7-FEB-2019 18:08:23

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECA500
Spectrometer        = DELTA2_NMR

Field_Strength      = 11.7473579[T]  (500[MHz])
X_Acq_Duration      = 1.74587904[s]
X_Domain            = 1H
X_Freq              = 500.15991521[MHz]
X_Offset            = 5.0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.57277737[Hz]
X_Sweep             = 9.38438438[kHz]
X_Sweep_Clipped     = 7.50750751[kHz]
Irr_Domain          = Proton
Irr_Freq            = 500.15991521[MHz]
Irr_Offset          = 5.0[ppm]
Tri_Domain          = Proton
Tri_Freq            = 500.15991521[MHz]
Tri_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 44
Temp_Get            = 22[dC]
X_90_Width          = 6.04[us]
X_Acq_Time          = 1.74587904[s]
X_Angle             = 45[deg]
X_Atn               = 2[dB]
X_Pulse             = 3.02[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 6.74587904[s]
```

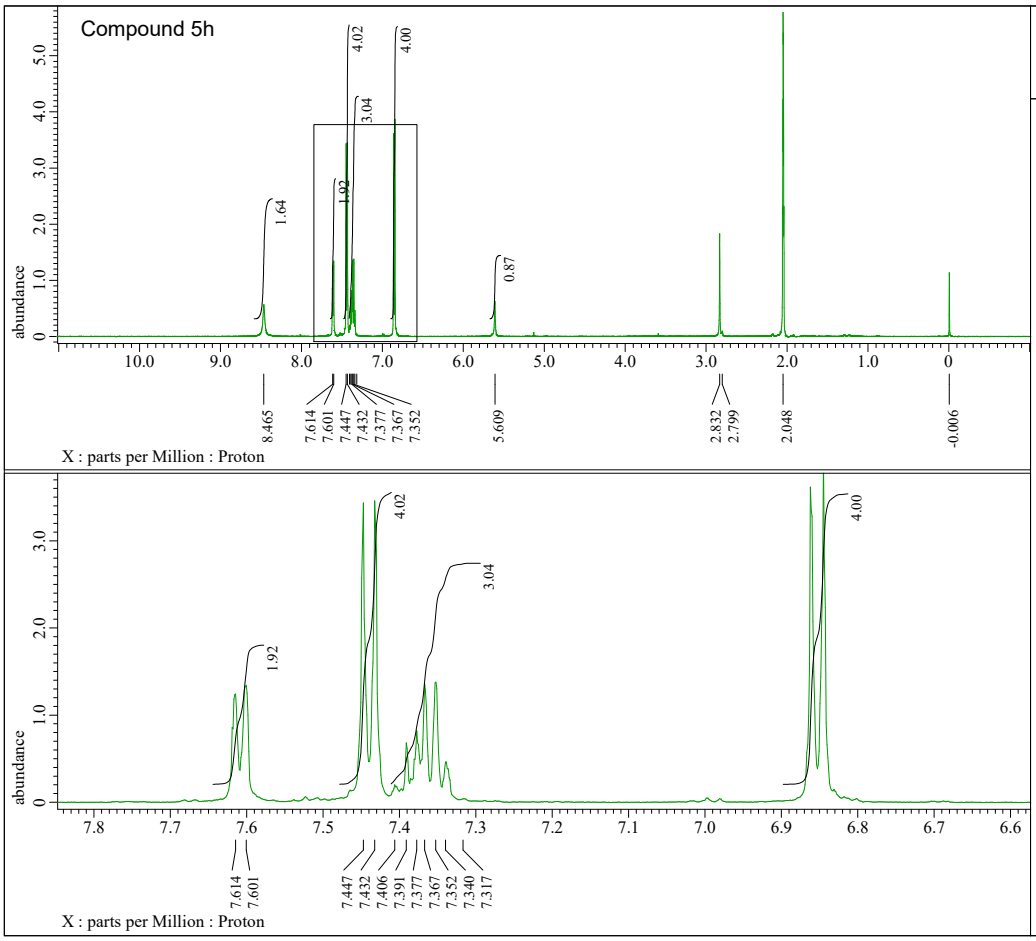



```
Filename            = YM161_4_Carbon-1-4.jdf
Author              = delta
Experiment          = carbon.jxp
Sample_Id           = YM161_4
Solvent             = DMSO-D6
Actual_Start_Time   =  9-NOV-2018 17:18:49
Revision_Time       =  9-NOV-2018 17:15:58

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECA500
Spectrometer        = DELTA2_NMR

Field_Strength      = 11.7473579[T]  (500[MHz])
X_Acq_Duration      = 0.83361792[s]
X_Domain            = 13C
X_Freq              = 125.76529768[MHz]
X_Offset            = 100[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.19959034[Hz]
X_Sweep             = 39.3081761[kHz]
X_Sweep_Clipped     = 31.44654088[kHz]
Irr_Domain          = Proton
Irr_Freq            = 500.15991521[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = TRUE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 22.3[dC]
X_90_Width          = 10.67[us]
X_Acq_Time          = 0.83361792[s]
X_Angle             = 30[deg]
X_Atn               = 6.1[dB]
X_Pulse             = 3.55666667[us]
Irr_Atn_Dec         = 25.655[dB]
Irr_Atn_Noe         = 25.655[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 92[us]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.83361792[s]
```



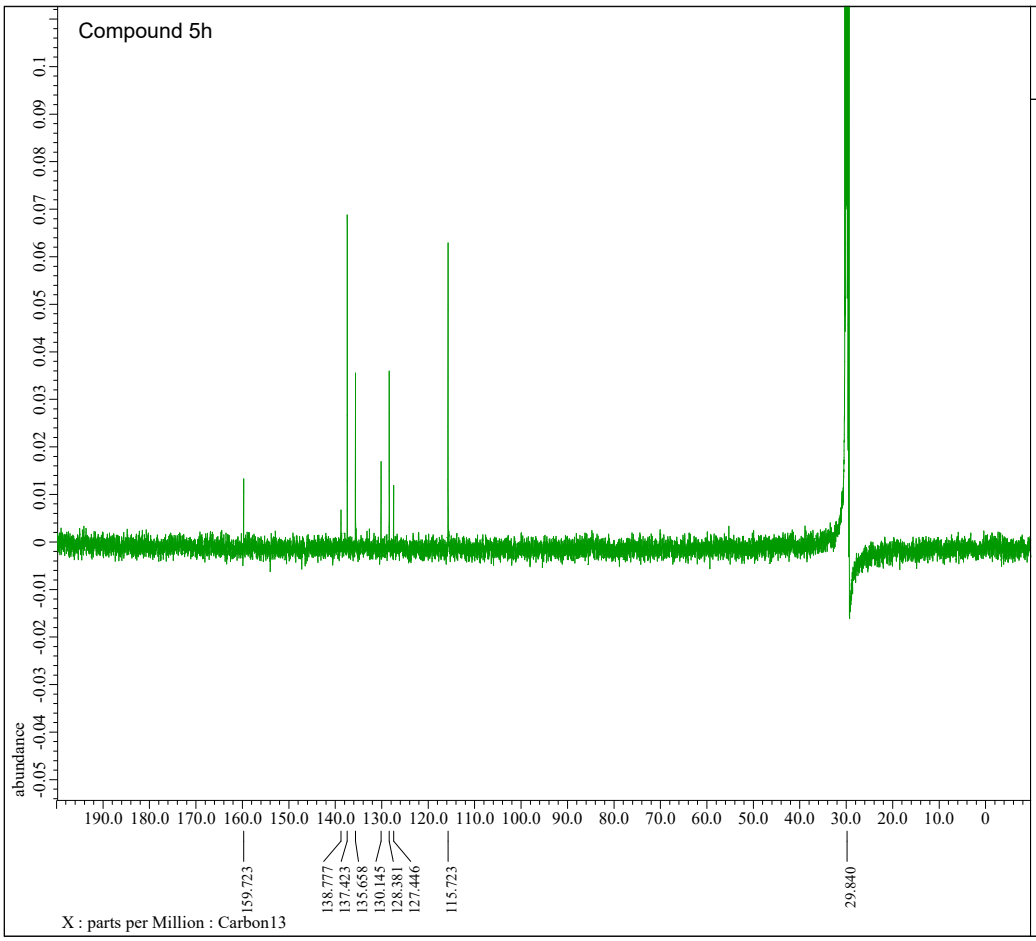
JEOL

```
Filename            = YM147_8_Proton-1-4.jdf
Author              = delta
Experiment          = proton.jxp
Sample_Id           = YM147_8
Solvent             = ACETONE-D6
Actual_Start_Time   = 19-JAN-2019 19:03:41
Revision_Time       = 19-JAN-2019 18:48:24

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECA500
Spectrometer        = DELTA2_NMR

Field_Strength      = 11.7473579[T] (500[MHz])
X_Acq_Duration      = 1.74587904[s]
X_Domain            = 1H
X_Freq              = 500.15991521[MHz]
X_Offset            = 5.0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.57277737[Hz]
X_Sweep             = 9.38438438[kHz]
X_Sweep_Clipped     = 7.50750751[kHz]
Irr_Domain          = Proton
Irr_Freq            = 500.15991521[MHz]
Irr_Offset          = 5.0[ppm]
Tri_Domain          = Proton
Tri_Freq            = 500.15991521[MHz]
Tri_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 58
Temp_Get            = 22.6[dC]
X_90_Width          = 6.04[us]
X_Acq_Time          = 1.74587904[s]
X_Angle             = 45[deg]
X_Atn               = 2[dB]
X_Pulse             = 3.02[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 6.74587904[s]
```



JEOL

```
Filename            = YM147_8_Carbon-1-2.jdf
Author              = delta
Experiment          = carbon.jxp
Sample_Id           = YM147_8
Solvent             = ACETONE-D6
Actual_Start_Time   = 19-JAN-2019 19:07:10
Revision_Time       =  7-FEB-2019 17:52:10

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECA500
Spectrometer        = DELTA2_NMR

Field_Strength      = 11.7473579[T] (500[MHz])
X_Acq_Duration      = 0.83361792[s]
X_Domain            = 13C
X_Freq              = 125.76529768[MHz]
X_Offset            = 100[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.19959034[Hz]
X_Sweep             = 39.3081761[kHz]
X_Sweep_Clipped     = 31.44654088[kHz]
Irr_Domain          = Proton
Irr_Freq            = 500.15991521[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 1024
Total_Scans         = 1024

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 22.8[dC]
X_90_Width          = 10.67[us]
X_Acq_Time          = 0.83361792[s]
X_Angle             = 30[deg]
X_Atn               = 6.1[dB]
X_Pulse             = 3.55666667[us]
Irr_Atn_Dec         = 25.655[dB]
Irr_Atn_Noe         = 25.655[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 92[us]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 2.83361792[s]
```