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Supporting Information

Visible-Light-Induced C(sp^3)-H Activation for a C–C Bond Forming Reaction of 3,4-Dihydroquinoxalin-2(1*H*)-one with Nucleophiles Using Oxygen with a Photoredox Catalyst or in Catalyst-Free Conditions

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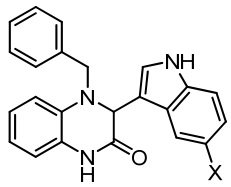
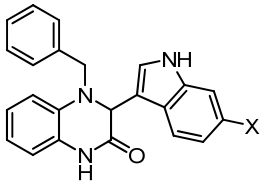
SUPPORTING INFORMATION:

Contents:

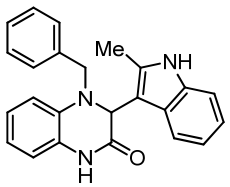
General Procedure. All solvents were reagent grade. Reactions were normally carried out under nitrogen atmosphere in glassware. Merck silica gel 60 (particle size 0.04-0.063 mm) was employed for flash chromatography. Melting points are uncorrected. ^{1}H NMR spectra were obtained in $CDCl_3$ unless otherwise noted at 400 MHz (Bruker DPX-400 or AVIII-400), or 500 MHz (Varian-Unity INOVA-500). ^{13}C NMR spectra were obtained at 125 MHz or 100 MHz. The melting point was recorded on a melting point apparatus (MPA100 – Automated melting point system, Stanford Research Systems, Inc.) and is uncorrected. The UV-vis spectra were recorded with a Varian Cary® 50 UV-Vis spectrophotometer.



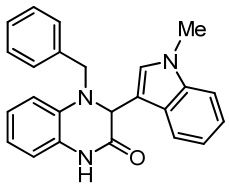
3ca X = H; 76%, 4 h (69%, 14 h)
3cd X = Br; 71%, 18 h (66%, 32 h)



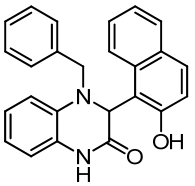
3ch X = F; 60%, 20 h (55%, 40 h)
3cj X = Br; 68%, 20 h (65%, 40 h)



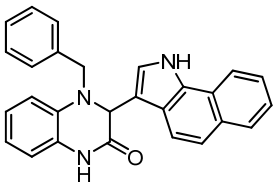
3cl 82%, 4 h (79%, 14 h)



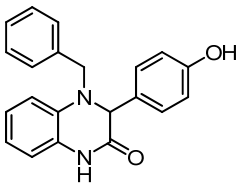
3co 73%, 10 h (72%, 24 h)



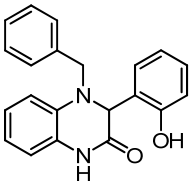
3cr 50%, 30 h (47%, 48 h)



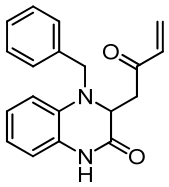
3cs 78%, 5 h (74%, 15 h)



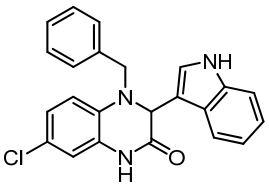
3cu-p 32%, 72 h (29%, 80 h)



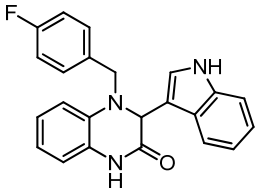
3cu-o 28%, 72 h (22%, 80 h)



3cw 79%, 4 h (70%, t = 12 h)



3ga 72%, 12 h (64%, 30 h)



3da 71%, 10 h (68%, 30 h)

Scheme S1. Unless otherwise noted, the reactions were performed with **1** (1 equiv) and **2** (2 equiv) with 2 mol % of $Ru(bpy)_3Cl_2•6H_2O$ in MeOH at ambient temperature. Percentage (%) for isolated yields after chromatography purification. Time (h) represented for the reaction to be completed. Yields in parenthesis for the reaction in the absence of $Ru(bpy)_3Cl_2•6H_2O$ (catalyst free condition).

The light on/off experiment:

1c (50 mg, 0.21 mmol), $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv), indole (48 mg, 0.40 mmol, 2.0 equiv) and CH_3OH (4.1 mL) were palced in a 10-mL two-neck flask with a magnetic stirring bar. The flask was equipped with a balloon of oxygen, and the solution was stirred at room temperature under irradiation with a 24 W white CFL (compact fluorescent light bulb, Philips, 24 W, white, Tornado, E27, 120 V, 60 Hz), located 10 cm away from the reaction vessel. After the indicated reaction time, ~50μL of the reaction mixture aliquot was collected, diluted with $CDCl_3$ and analyzed by ^1H NMR.

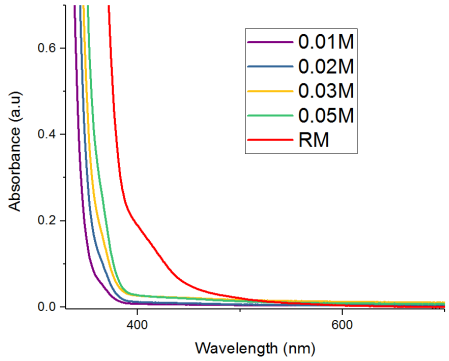


Fig S1. UV-visible absorption spectra of **1c** at different concentrations in MeOH, and the 1:2 mixture of **1c** and indole (**2a**) in MeOH (red line).

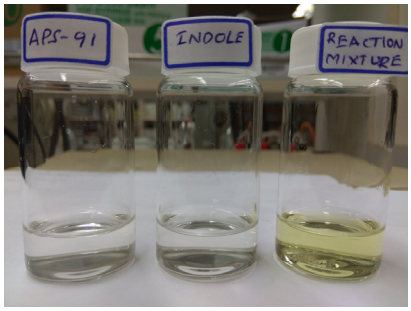


Fig S2. Pictures of the **1c**, indole (**2a**), and the mixture of **1c** and **2a**, after 30-min CFL irradiation.

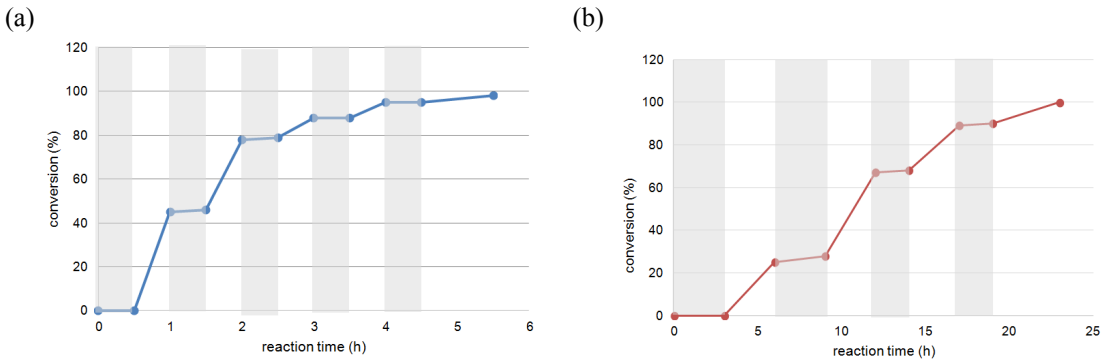


Fig S3. Conversion of **1c** to **3ca** in the light/dark sequence. Dark periods are shown in gray. (a) Reaction with ruthenium catalyst (blue), (b) reaction in the absence of catalyst (red)

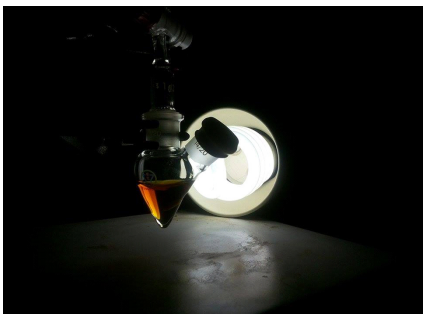
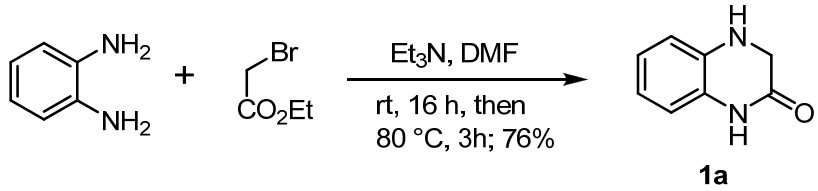


Fig S4. The reactions were irradiated by a PHILIPS 24 W white CFL (compact fluorescent light bulb)

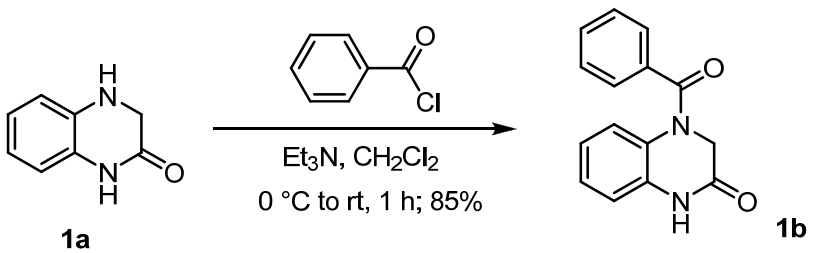
Preparation of 3,4-dihydroquinoxalin-2(1*H*)-one (1a):



1a

To a solution of *o*-phenylenediamine (5 g, 46.2 mmol) in DMF (50 mL) was sequentially added ethyl 2-bromoacetate (6.1 mL, 55.0 mmol, 1.2 equiv) and triethyl amine (12.9 mL, 92.5 mmol, 2.0 equiv) at 0 °C. The resulting solution was stirred at room temperature for 16 h, followed by heating to 80 °C for 3 h. Most of DMF was removed by rotary evaporator, and the residue was partitioned between H_2O (10 mL) and EtOAc (40 mL). The EtOAc layer was washed with saturated $NaHCO_3$ (10 mL), brine (10 mL), dried over Na_2SO_4, and concentrated in *vacuo* to give the crude residue. The residue was triturated with a mixture of CH_2Cl_2 and hexane (1:1 *v/v*). The precipitate was filtered and dried *in vacuo* to afford **1a** (5.2 g, 76% yield; R_f = 0.31 for **1a** in 50% EtOAc–hexane) as a beige powder. Mp: 136–138 °C. Lit. 136–138 °C.[1] Selected spectroscopic data for **1a**: IR (neat): 3369, 3197, 3069, 2976, 1678, 1508, 1185, 1304, 1258, 823, 748 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.62 (brs, 1 H), 6.89 – 6.85 (m, 1 H), 6.75 – 6.71 (m, 2 H), 6.65 (d, J = 7.5 Hz, 1 H), 3.97 (d, J = 1.5, 2 H), 3.84 (brs, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.9 (C), 133.7 (C), 125.4 (C), 123.9 (CH), 119.6 (CH), 115.7 (CH), 114.0 (CH), 47.1 (CH_2);[2] MS (*m/z*, relative intensity): 149 (M^++1, 4), 148 (M^+, 45), 119 (100), 118 (11), 92 (25), 91 (75), 65 (17); exact mass calculated for $C_8H_8N_2O$ (M^+): 148.0637, found: 148.0637.

Preparation of 4-benzoyl-3,4-dihydroquinoxalin-2(1*H*)-one (1b):



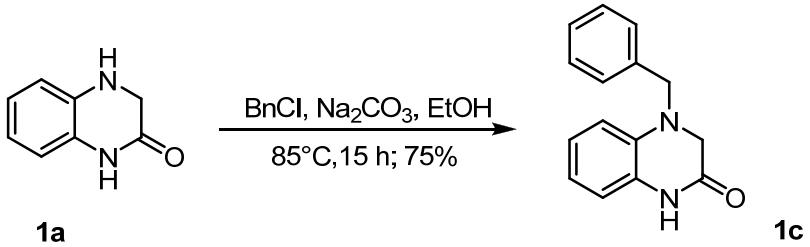
1a **1b**

To a solution of **1a** (200 mg, 1.35 mmol) in CH_2Cl_2 (4 mL) at 0 °C was added Et_3N (0.37 mL, 2.65 mmol, 2.0 equiv) and benzoyl chloride (0.23 mL, 1.98 mmol, 1.5 equiv). The resulting solution was stirred at room temperature for 1 h, and the reaction was quenched by the addition of water (10 ml), followed by the extraction with CH_2Cl_2 (2x10 mL). The combined organic solution was washed with saturated aqueous $NaHCO_3$ solution (5 mL), brine (5 mL), dried over anhydrous

[1] TenBrink, R. E.; Im, W. B.; Sethy, V. H.; Tang, A. H.; Carter, D. B. *J. Med. Chem.* **1994**, *37*, 758 – 768.
[2] Wang, S.-K.; Chen, M.-T.; Zhao, D.-Y.; You, X.; Luo, Q.-L. *Adv. Synth. Catal.* **2016**, *358*, 4093 – 4099.

Na_2SO_4, and concentrated *in vacuo* to give a crude residue. The crude product was purified by flash column chromatography with 40% EtOAc–hexane (R_f = 0.32 for **1b** in 50% EtOAc–hexane) to afford compound **1b** (289 mg, 85% yield) as brown color solids. Mp: 205–206 °C, lit. 208 °C.[3] Selected spectroscopic data for **1b:** ^{1}H NMR (400 MHz, acetone-d_6): δ 9.74 (brs, 1 H), 7.50 – 7.34 (m, 5 H), 7.15 – 7.05 (m, 2 H), 6.75 (brs, 1 H); ^{13}C NMR (100 MHz, acetone-d_6): δ 169.8 (C), 168.1 (C), 136.4 (C), 132.8 (C), 131.9 (CH), 129.9 (2CH), 129.5 (2CH), 129.0 (C), 127.0 (CH), 125.8 (CH), 123.1 (CH), 117.5 (CH), 48.7 (CH_2);

Preparation of 4-benzyl-3,4-dihydroquinoxalin-2(1*H*)-one (1c):



1a **1c**

To a solution of **1a** (1 g, 6.75 mmol) in EtOH (15 mL) was added Na_2CO_3 (1.43 g, 13.5 mmol, 2.0 equiv) and benzyl chloride (0.93 mL, 8.08 mmol, 1.2 equiv), and the solution was heated to reflux at 85 °C for 15 h until the completion of the reaction, as monitored by TLC. The reaction mixture was cooled to room temperature, concentrated in *vacuo* to give the crude residue. The crude product was dissolved in EtOAc (50 mL) and washed with water (2x20 mL). The aqueous layer was extracted with EtOAc (3x20 mL), and the combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated in *vacuo* to give a crude residue The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f = 0.49 for **1c** in 50% EtOAc–hexane) to afford **1c** (1.21 g, 75% yield) as off-white solids.[4] Mp: 152–154 °C, Selected spectroscopic data for **1c**: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (brs, 1 H), 7.35 – 7.25 (m, 5 H), 6.95 – 6.90 (m, 1 H), 6.75 – 6.72 (m, 3 H), 4.40 (s, 2 H), 3.80 (s, 2 H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 166.7 (C), 136.2 (C), 135.3 (C), 128.8 (2CH), 127.62 (2CH), 127.59 (CH), 126.0 (C), 124.2 (CH), 119.0 (CH), 115.5 (CH), 112.3 (CH), 53.6 (CH_2), 52.3 (CH_2); MS (*m/z*, relative intensity): 239 (M^++1, 11), 238 (M^+, 70), 194 (28), 147 (25), 119 (22), 91 (100), 65 (14); exact mass calculated for $C_{15}H_{14}N_2O$ (M^+): 238.1106; found: 238.1108.

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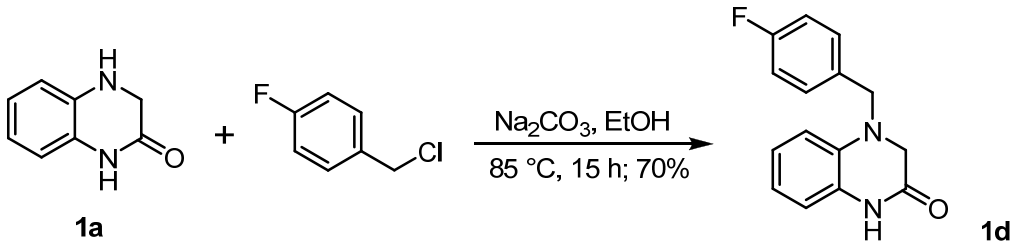
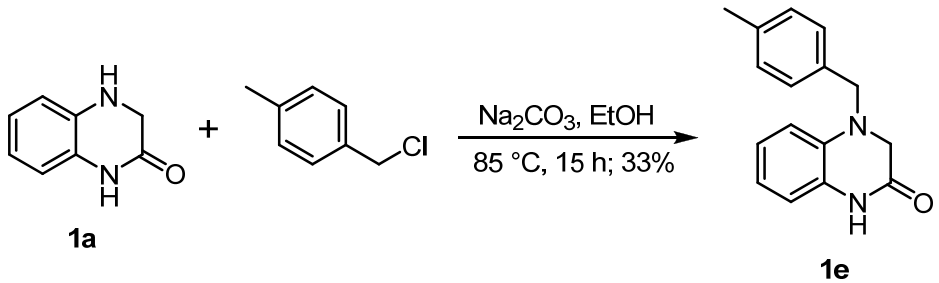
[3] TenBrink, R. E.; Im, W. B.; Sethy, V. H.; Tang, A. H.; Carter, D. B. *J. Med. Chem.*, **1994**, *37*, 758–768.
[4] Smith, R. F.; Rebel, W. J.; Beach, T. N. *J. Org. Chem.*, **1959**, *24*, 205–207.

Preparation of 4-(4-fluorobenzyl)-3,4-dihydroquinoxalin-2(1*H*)-one (1d):



To a solution of **1a** (500 mg, 3.37 mmol, 1.0 equiv) in EtOH (7.5 mL) was added Na_2CO_3 (714 mg, 6.74 mmol, 2.0 equiv) and 4-fluorobenzyl chloride (0.48 mL, 4.04 mmol, 1.2 equiv), and the solution was heated to reflux at 85 °C for 15 h until the completion of reaction, as monitored by TLC. The reaction mixture was cooled to room temperature and concentrated in *vacuo* to give a crude residue. The crude residue was dissolved in EtOAc (50 mL), washed with water (2x10 mL), and the aqueous layer was extracted with EtOAc (3x10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated in *vacuo* to give a crude residue. The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f = 0.52 for **1d** in 50% EtOAc–hexane) to afford **1d** (603 mg, 70% yield) as off-white solids. Mp: 182–184 °C, Selected spectroscopic data for **1d**: IR (KBr): 3208, 3071, 2918, 1685, 1510, 1402, 1221, 1154, 823, 744 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.51 (s, 1 H), 7.28 – 7.24 (m, 2 H), 7.03 – 6.99 (m, 2 H), 6.95 – 6.91 (m, 1 H), 6.77 – 6.75 (m, 2 H), 6.72 (d, J = 8.0 Hz, 1 H), 4.36 (s, 2 H), 3.77 (s, 2 H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.9 (C), 162.2 (d, J = 244 Hz, C), 135.1 (C), 131.9 (d, J = 3 Hz, C), 129.2 (d, J = 8 Hz, 2CH), 126.2 (C), 124.2 (CH), 119.3 (CH), 115.7 (d, J = 21 Hz, 2CH), 115.6 (CH), 112.3 (CH), 52.9 (CH_2), 52.2 (CH_2); MS (*m/z*, relative intensity): 257 (M^++1, 8), 256 (M^+, 54), 147 (17), 119 (16), 109 (100), 101 (10), 59 (20), 58 (22); exact mass calculated for $C_{15}H_{13}FN_2O$ (M^+): 256.1012; found: 256.1013.

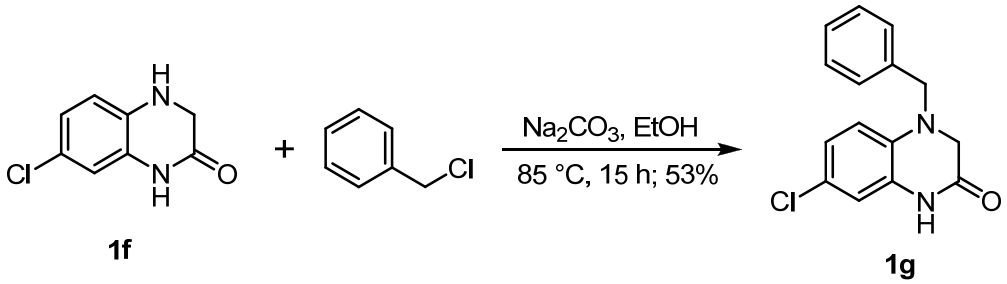
Preparation of 4-(4-methylbenzyl)-3,4-dihydroquinoxalin-2(1*H*)-one (1e):



To a solution of **1a** (200 mg, 1.35 mmol) in EtOH (3 mL) was added Na_2CO_3 (286 mg, 2.70

mmol, 2.0 equiv) and 4-methylbenzyl chloride (0.21 mL, 1.59 mmol, 1.2 equiv), and the solution was heated to reflux at 85 °C for 15 h until the completion of reaction, as monitored by TLC. The reaction mixture was cooled to room temperature and concentrated in *vacuo* to give a residue. The crude residue was dissolved in EtOAc (20 mL), and the solution was washed with water (2x10 mL). The aqueous layer was extracted with EtOAc (3x10 mL), and the combined organic layers were dried over anhydrous Na_2SO_4, concentrated in *vacuo* to give the crude compound. The crude product was purified by flash column chromatography with 20% EtOAc– hexane (R_f = 0.51 for **1e** in 50% EtOAc–hexane) to afford **1e** (112 mg, 33% yield) as off-white solids. Mp: 146–147 °C, Selected spectroscopic data for **1e**: IR (KBr): 3205, 3052, 2920, 1685, 1510, 1402, 1302, 743 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.12 (s, 1 H), 7.19 – 7.10 (m, 4 H), 6.95 – 6.90 (m, 1 H), 6.77 – 6.70 (m, 3 H), 4.35 (s, 2 H), 3.77 (s, 2 H), 2.31 (s, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.8 (C), 137.3 (C), 135.4 (C), 133.1 (C), 129.5 (2CH), 127.7 (2CH), 126.0 (C), 124.2 (CH), 119.0 (CH), 115.4 (CH), 112.3 (CH), 53.3 (CH_2), 52.1 (CH_2), 21.1 (CH_3); MS (*m/z*, relative intensity): 253 (M^++1, 6), 252 (M^+, 34), 147 (3), 146 (2), 119 (6), 106 (9), 105 (100), 92 (4), 77 (6); exact mass calculated for $C_{16}H_{16}N_2O$ (M^+): 252.1263; found: 252.1267.

Preparation of 4-benzyl-7-chloro-3,4-dihydroquinoxalin-2(1*H*)-one (1g):

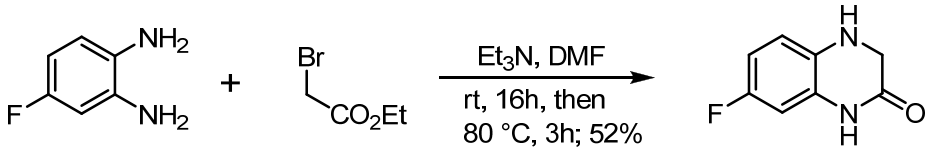


To a solution of **1f** (230 mg, 1.26 mmol)[5] in EtOH (7.5 mL) was added Na_2CO_3 (264.9 mg, 2.50 mmol, 2 equiv) and benzyl chloride (0.20 mL, 1.56 mmol, 1.2 equiv). The solution was heated to reflux at 80 °C for 15 h until the completion of reaction, as monitored by TLC. The reaction mixture was cooled to room temperature, concentrated in *vacuo* to give the crude residue. The crude residue was dissolved in EtOAc (20 mL), and the solution was washed with water (2 x 10 mL). The aqueous layer was extracted with EtOAc (3 x 10 mL), and the combined organic layers were dried over anhydrous Na_2SO_4, concentrated in *vacuo* to give the crude compound. The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f = 0.56 for **1g** in 50% EtOAc–hexane) to afford **1g** (182 mg, 53% yield) as off-white solid. Mp: 207-209 °C, Selected spectroscopic data for **1g**: IR (KBr): 3206, 3062, 2924, 2855, 1690, 1586, 1511, 1397, 1296, 703 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 9.12 (s, 1 H), 7.36 – 7.22 (m, 5 H), 6.86 (dd, J = 8.5, 2.0 Hz, 1 H), 6.77 (d, J = 2.0 Hz, 1 H), 6.62 (d, J = 8.5 Hz, 1 H), 4.37 (s, 2 H), 3.81 (s, 2 H), ^{13}C NMR (125

[5] For preparation, see: Baraldi, P. G.; Ruggiero, E.; Tabrizi, M. A. *J. Heterocyclic Chem.* **2014**, *51*, 101 – 105.

MHz, $CDCl_3$): δ 167.1 (C), 135.8 (C), 133.8 (C), 128.9 (two CH), 127.7 (CH), 127.5 (two CH), 127.1 (C), 123.77 (C), 123.73 (CH), 115.5 (CH), 113.1 (CH), 53.7 (CH_2), 52.1 (CH_2); MS (*m/z*, relative intensity): 274 (M^++2, 7), 273 (M^++1, 4), 272 (25), 181 (15), 153 (6), 92 (7), 91 (100), 65 (5); exact mass calculated for $C_{15}H_{13}ClN_2O$ (M^+): 272.0716; found: 272.0715.

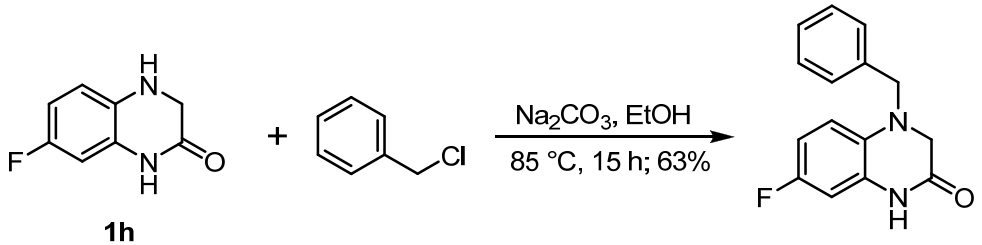
Preparation of 7-Fluoro-3,4-dihydroquinoxalin-2(1*H*)-one (1h):



1h

To a solution of 4-fluorobenzene-1,2-diamine (500 mg, 3.96 mmol) in DMF (5 mL) was added ethylbromoacetate (0.52 mL, 4.69 mmol, 1.2 equiv) and triethyl amine (1.1 mL, 7.9 mmol, 2.0 equiv) sequentially at 0 °C. The resulting solution was stirred at room temperature for 16 h, followed by heating to 80 °C for 3 h. Most of DMF was removed by rotary evaporator, and the residue was partitioned between H_2O (10 mL) and EtOAc (40 mL). The EtOAc layer was washed with saturated $NaHCO_3$ (10 ml), brine (10 mL), dried over Na_2SO_4, and concentrated in *vacuo* to give the crude residue. The crude product was purified by flash column chromatography with 40% EtOAc–hexane to afford **1h** (R_f = 0.29 for **1h** in 50% EtOAc-hexane) as brown color solids (341 mg, 52% yield). Mp: 245–246 °C, lit. 245–246 °C.[6] Selected spectroscopic data for **1h**: ^{1}H NMR (500 MHz, acetone-d_6): δ 9.35 (brs, 1 H), 6.72 (dd, J = 9.0, 5.5 Hz, 1 H), 6.66 (dd, J = 9.5, J = 2.5, 1 H), 6.59 – 6.54 (m, 1 H), 5.22 (brs, 1 H), 3.79 (s, 2 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 167.2 (C), 157.2 (d, J = 232 Hz, C), 132.4 (d, J = 1.9 Hz, C), 128.7 (d, J = 10 Hz, C), 115.1 (d, J = 9 Hz, CH), 109.3 (d, J = 22.5 Hz, CH), 103.2 (d, J = 27.5 Hz, CH), 47.8 (CH_2); MS (*m/z*, relative intensity): 166 (M^+, 61), 137 (100), 110 (13), 101 (7), 83 (13); exact mass calculated for $C_8H_7FN_2O$ (M^+): 166.0542; found: 166.0540.

Preparation of 4-benzyl-7-fluoro-3,4-dihydroquinoxalin-2(1*H*)-one (1i):

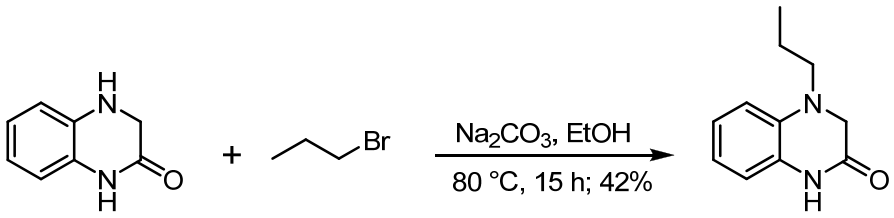


1h **1i**

[6] Baraldi, P. G.; Ruggiero, E.; Tabrizi, M. A. *J. Heterocyclic Chem.* **2014**, *51*, 101 – 105.

To a solution of **1h** (150 mg, 0.90 mmol) in EtOH (4 mL) was added Na_2CO_3 (191 mg, 1.8 mmol, 2.0 equiv) and benzyl chloride (0.14 mL, 1.1 mmol, 1.2 equiv). The solution was heated to reflux at 85 °C for 15 h until the completion of reaction, as monitored by TLC. The reaction mixture was cooled to room temperature, concentrated in *vacuo* to give the crude residue. The crude residue was dissolved in EtOAc (20 mL), and the solution was washed with water (2x10 mL). The aqueous layer was extracted with EtOAc (3x10 mL), and the combined organic layers were dried over anhydrous Na_2SO_4, concentrated in *vacuo* to give the crude compound. The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f = 0.54 for **1i** in 50% EtOAc–hexane) to afford **1i** (145 mg, 63% yield) as off-white solids. Mp: 131–132 °C. Selected spectroscopic data for **1i**: IR (KBr): 3338, 2982, 1691, 1524, 1399, 1269, 1144, 851, 782 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 9.28 (s, 1 H), 7.34 – 7.23 (m, 5 H), 6.63 – 6.56 (m, 3 H), 4.34 (s, 2H), 3.75 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.9 (C), 156.5 (d, J = 236.5 Hz, C), 136.1 (C), 131.7 (d, J = 2 Hz, C), 128.9 (two CH), 127.68 (CH), 127.66 (two CH), 127.31 (d, J = 10 Hz, C), 113.0 (d, J = 8.6 Hz, CH), 109.8 (d, J = 22 Hz, CH), 103.3 (d, J = 26.4 Hz, CH), 54.2 (CH_2), 52.3 (CH_2); MS (*m/z*, relative intensity): 257 (M^++1, 3), 256 (M^+, 16), 242 (9), 167 (11), 164 (18), 149 (25), 136 (19), 112 (18), 109 (13), 91 (100); exact mass calculated for $C_{15}H_{13}FN_2O$ (M^+): 256.1012; found: 256.1013.

Preparation of 4-propyl-3,4-dihydroquinoxalin-2(1*H*)-one (1j):



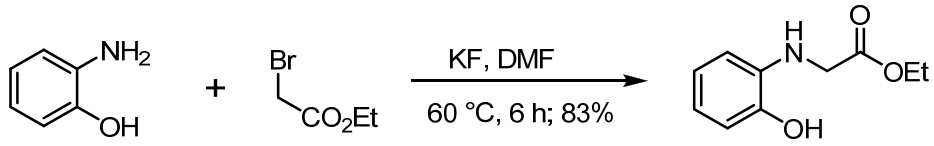
1a **1j**

To a solution of **1a** (200 mg, 1.35 mmol) in EtOH (4 mL) was added Na_2CO_3 (284 mg, 2.68 mmol, 2.0 equiv) and 1-bromo propane (0.17 mL, 1.6 mmol, 1.2 equiv). The solution was heated to reflux for 15 h until the completion of reaction, as monitored by TLC. The reaction mixture was cooled to room temperature, concentrated in *vacuo* to give the crude residue. The crude residue was dissolved in EtOAc (20 mL), and the solution was washed with water (2x10 mL). The aqueous layer was extracted with EtOAc (3x10 mL) and the combined organic layers were dried over anhydrous Na_2SO_4, concentrated in *vacuo* to give the crude compound. The crude product was purified by flash column chromatography with 15% EtOAc–hexane (R_f = 0.59 for **1j** in 50% EtOAc–hexane) to afford **1j** (109 mg, 42% yield) as off-white solids.[7] Mp: 98–99 °C. Selected

[7] For other preaparation in literature, but without spectra data, see: Smith, R. F.; Rebel, W. J.; Beach, T. S. *J. Org.*

spectroscopic data for **1j**: IR (KBr): 3369, 3199, 3069, 2972, 2892, 1675, 1600, 1508, 1385, 1303, 1256, 919, 823, 746 cm^{-1};^{1}H NMR (500 MHz, $CDCl_3$): δ 8.51 (s, 1 H), 6.97 – 6.93 (m, 1 H), 6.74 – 6.68 (m, 2 H), 6.66 (d, J = 8.0 Hz, 1 H), 3.84 (s, 2 H), 3.16 (t, J = 7.5 Hz, 2 H), 1.68 – 1.61 (m, 2 H), 0.97 (t, J = 7.5 Hz, 3 H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.9 (C), 135.1 (C), 125.9 (C), 124.2 (CH), 118.3 (CH), 115.5 (CH), 111.6 (CH), 52.2 (CH_2), 51.4 (CH_2), 18.3 (CH_2), 11.4 (CH_3);[8] MS (*m/z*, relative intensity): 191 (M^++1, 9), 190 (M^+, 66), 162 (30), 161 (100), 147 (25), 133 (64), 131 (32), 119 (37), 106 (8), 92 (20), 77 (12); exact mass calculated for $C_{11}H_{14}N_2O$ (M^+): 190.1106; found: 190.1105.

Preparation of ethyl 2-(2-hydroxyphenylamino)acetate (APS-135):



APS-135

To a solution of 2-aminophenol (1 g, 9.16 mmol) and potassium fluoride (1.33 g, 22.9 mmol, 2.5 equiv) in DMF (50 mL) was added ethyl bromo acetate (6.1 mL, 55.0 mmol, 2.4 equiv). The resulting mixture was heated to 60 °C and stirred for 6 h, followed by the concentration in *vacuo* to give a resisdue. The residue was partitioned between H_2O (10 mL) and EtOAc (25 mL). The EtOAc layer was washed with saturated $NaHCO_3$ (2x10 ml), brine (10 mL), dried over Na_2SO_4, filtered and concentrated in *vacuo* to give the crude residue. The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f = 0.46 for **APS-135** in 40% EtOAc–hexane) to afford **APS-135** (1.48 g, 83% yield) as brown solid. Mp: 91–93 °C, lit. 91–93 °C,[9] lit. 90–94 °C.[10] Selected spectroscopic data for **APS-135**: IR (KBr): 3419, 3051, 2981, 2903, 1721, 1612, 1530, 1439, 1381, 1222, 1030, 893, 737 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.81 (t, J = 7.5 Hz, 1 H), 6.71 (d, J = 7.5 Hz, 1H), 6.65 (dd, J = 7.5, 7.5 Hz, 1 H), 6.57 (d, J = 7.5 Hz, 1 H), 4.23 (q, J = 7.0 Hz, 2 H), 3.91 (s, 2 H), 1.28 (t, J = 7.0 Hz, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 172.0 (C), 144.5 (C), 136.0 (C), 121.4 (CH), 119.1 (CH), 114.9 (CH), 113.1 (CH), 61.4 (CH_2), 46.6 (CH_2), 14.2 (CH_3).

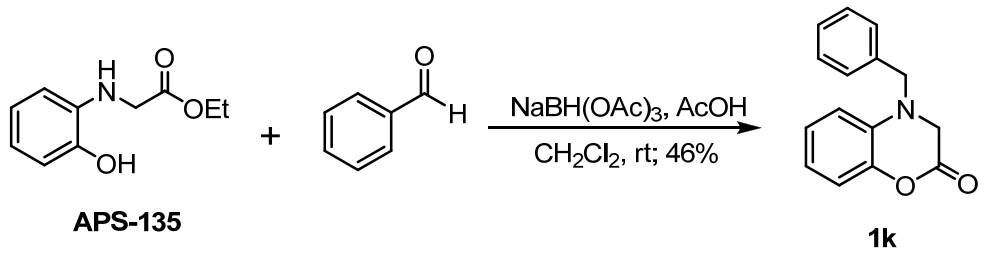
Chem. **1959**, *24*, 205–207.

[8] (a) Zidar, N,; Kikelj, D. *Tetrahedron* **2008**, *64*, 5756 – 5761. (b) Mbuvi, H. M.; Klobukowski, E. R.; Roberts, G. M.; Woo, L. K. J. *Porphyrins Phthalocyanines* **2010**, *14*, 284–292.

[9] D. S. Kemp, D. S.; Vellaccio, F. *J. Org. Chem.* **1975**, *40*, 3464 – 3464.

[10] Zidar, N,; Kikelj, D. *Tetrahedron* **2008**, *64*, 5756 – 5761.

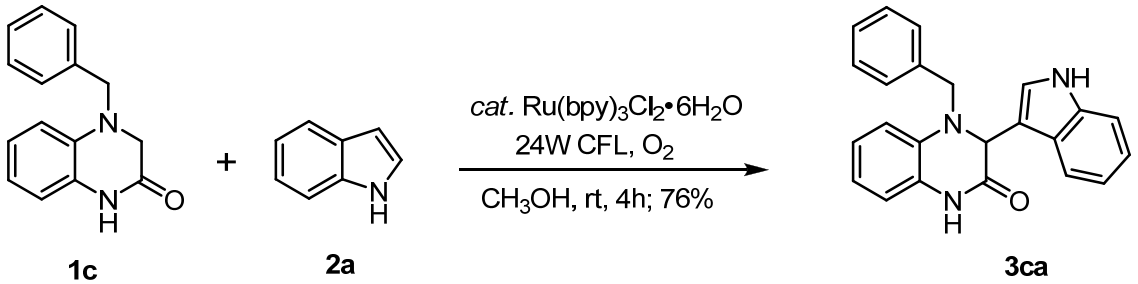
Preparation of 4-benzyl-3,4-dihydro-2H-benzo[*b*][1,4]oxazin-2-one (1k):



APS-135 **1k**

A solution of **APS-135** (200 mg, 1.02 mmol), benzaldehyde (0.12 mL, 1.2 mmol, 1.2 equiv) and glacial acetic acid (0.08 mL, 1.4 mmol, 1.4 equiv) in CH_2Cl_2 (6.3 mL) was stirred with ice bath cooling for 30 min. To this solution was added in portion of sodium triacetoxyborohydride (324 mg, 1.5 mmol, 1.5 equiv), and the reaction mixture was stirred at room temperature for 15 h. The reaction mixture was diluted with CH_2Cl_2 (10 mL), washed with saturated aqueous $NaHCO_3$ (10 mL), brine (10 mL), dried over Na_2SO_4, filtered and concentrated in *vacuo* to give the crude residue. The crude product was purified by flash column chromatography with 15% EtOAc–hexane (R_f = 0.45 for **1k** in 25% EtOAc/hexane) to afford **1k** (112 mg, 46% yield) as colorless oil; Selected spectroscopic data for **1k**: IR (neat): 3064, 3030, 2923, 2816, 1777, 1612, 1503, 1341, 1292, 1212, 919, 746, 700 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 7.38 – 7.27 (m, 5 H), 7.08 – 7.01 (m, 2 H), 6.88 – 6.83 (m, 2 H), 4.36 (s, 2 H), 3.77 (s, 2 H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.8 (C), 141.7 (C), 135.6 (C), 134.8 (C), 128.9 (2CH), 127.9 (CH), 127.8 (2CH), 125.2 (CH), 120.1 (CH), 117.0 (CH), 113.2 (CH), 53.5 (CH_2), 49.8 (CH_2);[11] MS (*m/z*, relative intensity): 240 (M^++1, 10), 239 (67), 211 (14), 120 (54), 91 (100); exact mass calculated for $C_{15}H_{13}NO_2$ (M^+): 239.0946; found: 239.0947.

Preparation of 4-benzyl-3-(1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ca)

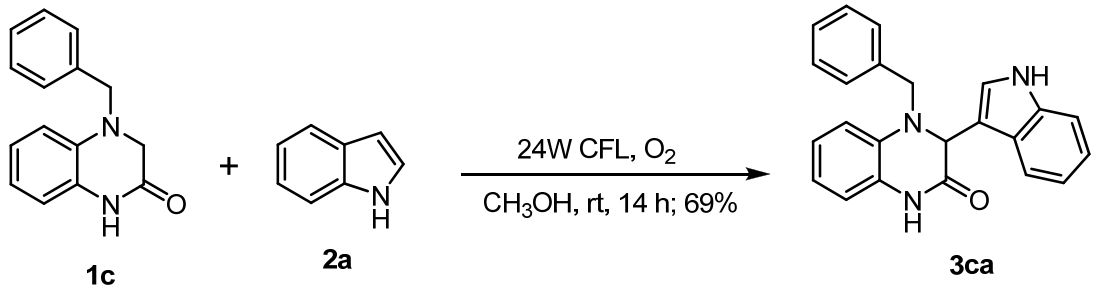


1c **2a** **3ca**

[11] (a) Zidar, N.; Kikelj, D. *Tetrahedron* **2008**, *64*, 5756 – 5761. (b) Huo, C.; Dong, J.; Su, Y.; Tang, J.; Chen, F. *Chem. Commun.* **2016**, *52*, 13341 – 13344.

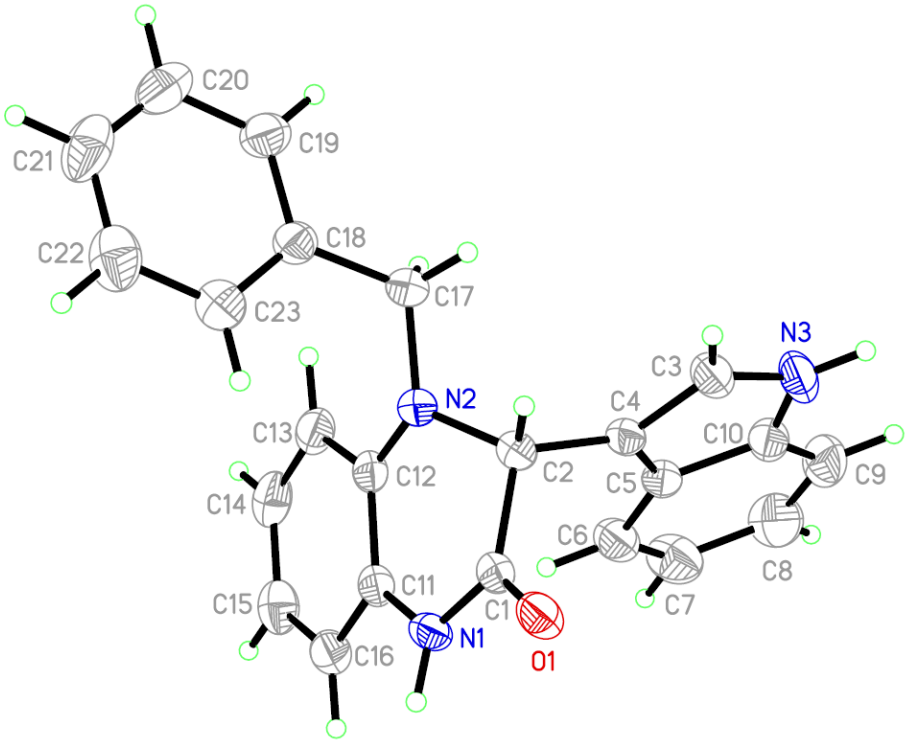
To a solution of **1c** (50 mg, 0.21 mmol) and indole (48 mg, 0.4 mmol, 2.0 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 4 h. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.4 for **3ca** in 50% EtOAc–hexane) to afford product **3ca** (56.6 mg, 76% yield) as white solids; Mp: 220–222 °C. Selected spectroscopic data for **3ca**: IR (KBr): 3317, 3029, 2981, 2894, 1667, 1506, 1408, 1245, 1112, 741 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.14 (brs, 1 H), 9.53 (s, 1 H), 7.55 (d, J = 8.0 Hz, 1 H), 7.40 – 7.30 (m, 5 H), 7.29 – 7.24 (m, 1 H), 7.11 – 7.07 (m, 1 H), 7.03 – 6.95 (m, 3 H), 6.90 – 6.85 (m, 1 H), 6.80 – 6.75 (m, 2 H), 5.27 (s, 1 H), 4.66 (d, J = 15.0 Hz, 1 H), 4.33 (d, J = 15.0 Hz, 1 H), ^{13}C NMR (125 MHz, acetone-d_6): δ 166.9 (C), 138.9 (C), 137.6 (C), 135.9 (C), 129.5 (two CH), 128.7 (C), 128.6 (two CH), 128.1 (CH), 127.6 (C), 124.2 (CH), 124.1 (CH), 122.6 (CH), 120.5 (CH), 120.2 (CH), 119.7 (CH), 115.9 (CH), 114.0 (CH), 112.3 (CH), 112.1 (C), 60.1 (CH), 52.7 (CH_2) ; MS (*m/z*, relative intensity): 354 (M^++1, 24), 353 (M^+, 100), 324 (36), 262 (34), 233 (22), 196 (27), 169 (11), 149 (22), 119 (45), 91 (52); exact mass calculated for $C_{23}H_{19}N_3O$ (M^+): 353.1528; found: 353.1526.

Preparation of 3ca via catalyst-free condition:



1c **2a** **3ca**

A solution of **1c** (50 mg, 0.21 mmol) and indole (48 mg, 0.4 mmol, 2.0 equiv) in CH_3OH was stirred under oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 14 h until the completion of reaction, as monitored by TLC and crude ^1H NMR. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.4 for **3ca** in 50% EtOAc–hexane) to afford product **3ca** (51.2 mg, 69% yield) as white solids.



Thermal ellipsoids draw at the 50% probability level

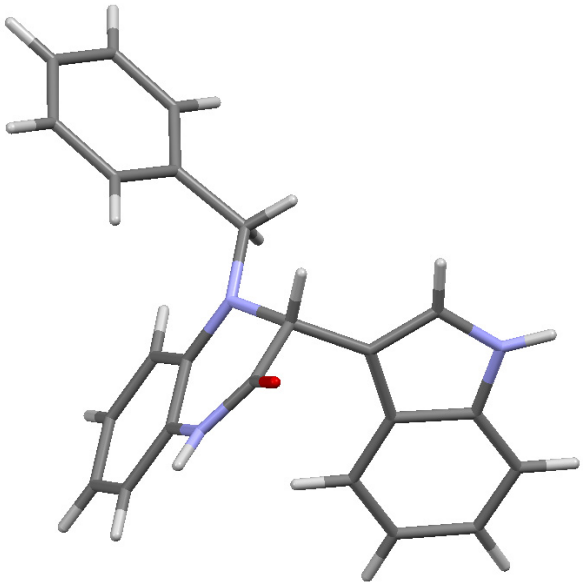


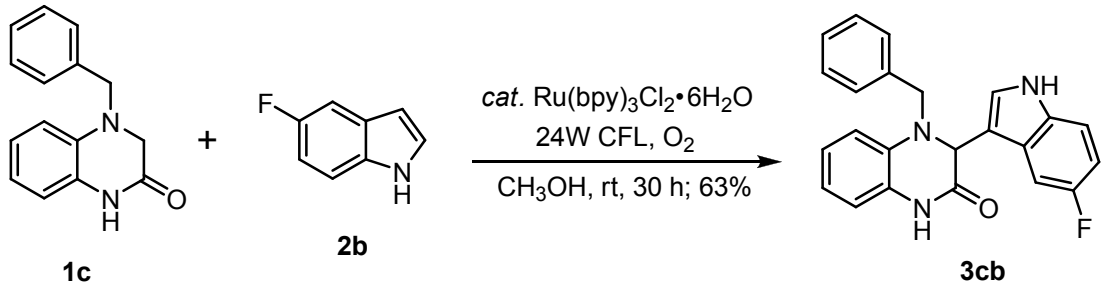
Figure S1. ORTEP and Stereo plots for X-ray crystal structures of **3ca** (**ic18907**).

CCDC 1816891 contains the supplementary crystallographic data for **3ca** (**ic18907**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S1. Crystal data and structure refinement for **3ca** (**ic18907**).

Identification code	ic18907	
Empirical formula	C23 H19 N3 O	
Formula weight	353.41	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 10.21340(10) Å	α= 90°.
	b = 18.2798(2) Å	β= 90°.
	c = 19.5856(3) Å	γ = 90°.
Volume	3656.61(8) $Å^3$	
Z	8	
Density (calculated)	1.284 Mg/m^3	
Absorption coefficient	0.635 mm^{-1}	
F(000)	1488	
Crystal size	0.244 x 0.244 x 0.045 mm^3	
Theta range for data collection	4.515 to 74.989°.	
Index ranges	-12<=h<=12, -22<=k<=22, -24<=l<=24	
Reflections collected	19042	
Independent reflections	3764 [R(int) = 0.0212]	
Completeness to theta = 67.679°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7539 and 0.6382	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3764 / 0 / 252	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0845	
R indices (all data)	R1 = 0.0386, wR2 = 0.0891	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.256 and -0.160 $e.Å^{-3}$	

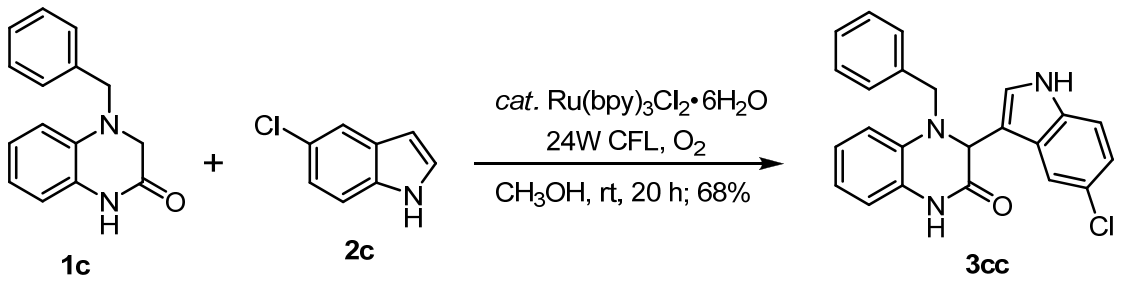
Preparation of 4-benzyl-3-(5-fluoro-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cb):



1c **2b** **3cb**

To a solution of **1c** (50 mg, 0.21 mmol) and 5-fluoroindole (54 mg, 0.4 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 30 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.39 for **3cb** in 50% EtOAc–hexane) to afford product **3cb** (49.3 mg, 63% yield) as white solids, Mp: 240–242 °C. Selected spectroscopic data for **3cb**: IR (KBr): 3300, 3172, 3029, 2983, 1668, 1505, 1406, 1245, 1175, 1110, 929, 854, 744 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 11.1 (brs, 1 H), 10.6 (s, 1 H), 7.36 – 7.30 (m, 5 H), 7.27 – 7.22 (m, 1 H), 7.09 (dd, J = 2.5, 2.5 Hz, 1 H), 6.99 (d, J = 2.5 Hz, 1 H), 6.94 – 6.88 (m, 2 H), 6.83 – 6.79 (m, 1 H), 6.74 – 6.70 (m, 1 H), 6.62 (d, J = 8.0 Hz, 1 H), 5.20 (s, 1 H), 4.50 (d, J = 15.5 Hz, 1 H), 4.32 (d, J = 15.5 Hz, 1 H), ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.8 (C), 156.9 (d, J = 230 Hz, C), 137.8 (C), 134.0 (C), 132.8 (C), 128.4 (two CH), 127.25 (two CH), 127.16 (C), 127.0 (CH), 126.0 (d, J = 10.3 Hz, C), 125.5 (CH), 123.1 (CH), 118.4 (CH), 114.8 (CH), 112.8 (CH), 112.5 (d, J = 9.8 Hz, CH), 110.8 (d, J = 4.5 Hz, C), 109.5 (d, J = 26 Hz, CH), 103.9 (d, J = 24 Hz, CH), 59.0 (CH), 51.3 (CH_2); MS (*m/z*, relative intensity): 373 (M^++2, 4), 372 (M^++1, 33), 371 (M^+, 100), 342 (40), 280 (42), 252 (28), 195 (33), 148 (19), 119 (43), 91 (53); exact mass calculated for $C_{23}H_{18}FN_3O$ (M^+): 371.1434; found: 371.1436.

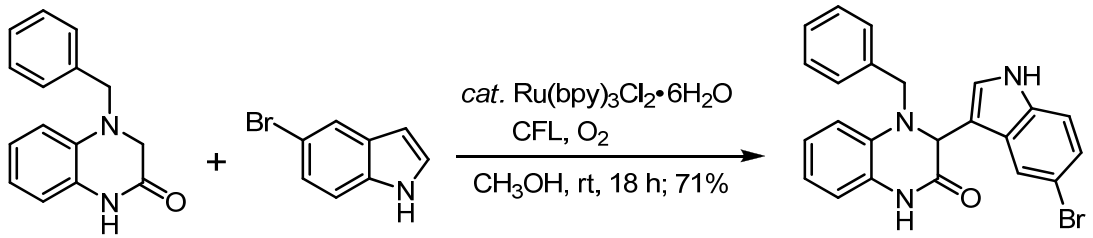
Preparation of 4-benzyl-3-(5-chloro-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cc)



1c **2c** **3cc**

To a solution of **1c** (50 mg, 0.21 mmol) and 5-chloroindole (61 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 20 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.37 for **3cc** in 50% EtOAc–hexane) to afford product **3cc** (55.2 mg; 68% yield) as white solids. Mp: 239–241 °C. Selected spectroscopic data for **3cc**: IR (KBr): 3477, 3290, 3172, 3029, 2982, 2898, 1668, 1504, 1408, 1112, 892, 796, 734 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 11.20 (s, 1 H), 10.60 (s, 1 H), 7.41 (d, J = 2.0 Hz, 1 H), 7.36 (d, J = 9.0 Hz, 1 H), 7.33 – 7.29 (m, 4 H), 7.28 – 7.22 (m, 1 H), 7.06 (dd, J = 8.5, 2.0 Hz, 1 H), 6.98 (s, 1 H), 6.90 (d, J = 7.5 Hz, 1 H), 6.82 (dd, J = 8.0, 7.5 Hz, 1 H), 6.73 (dd, J = 8.0, 7.5 Hz, 1 H), 6.64 (d, J = 8.0, 1 H), 5.22 (s, 1 H), 4.51 (d, J = 15.5 Hz, 1 H), 4.31 (d, J = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.8 (C), 137.8 (C), 134.6 (C), 134.0 (C), 128.4 (two CH), 127.3 (two CH), 127.1 (C), 127.0 (CH), 126.9 (C), 125.2 (CH), 123.7 (C), 123.1 (CH), 121.3 (CH), 118.6 (CH), 118.5 (CH), 114.9 (CH), 113.1 (CH), 112.8 (CH), 110.4 (C), 58.8 (CH), 51.3 (CH_2); MS (m/z, relative intensity): 389 (M^++2, 36), 388 (M^++1, 45), 387 (M^+, 100), 358 (29), 296 (39), 268 (17), 233 (15), 226 (15), 196 (35), 195 (36), 119 (52), 91 (66). Exact mass calculated for $C_{23}H_{18}ClN_3O$ (M^+): 387.1138; found: 387.1135.

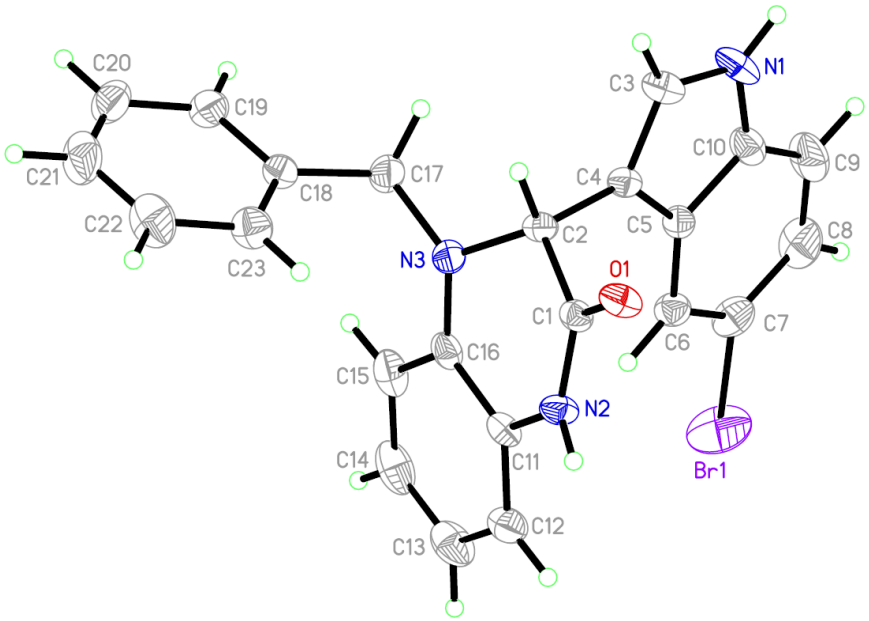
Preparation of 4-benzyl-3-(5-bromo-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cd)



1c **2d** **3cd**

To a solution of **1c** (50 mg, 0.21 mmol) and 5-bromoindole (78.4 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 18 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.38 for **3cd** in 50% EtOAc–hexane) to afford product **3cd** (64.1 mg; 71% yield) as white solids. Mp: 236–238 °C. Selected spectroscopic data for **3cd:** IR (KBr): 3279, 3177, 3056, 3028, 2981, 2898, 2868, 1670, 1504, 1457, 1409, 1112, 884, 795, 734 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.35 (brs, 1 H), 9.54 (s, 1 H), 7.72 (d, J = 1.5 Hz, 1

H), 7.40 – 7.31 (m, 5 H), 7.30 – 7.25 (m, 1 H), 7.20 (dd, J = 8.5, 2.0 Hz, 1 H), 7.05 – 6.98 (m, 2 H), 6.93 – 6.88 (m, 1 H), 6.83 – 6.77 (m, 2 H), 5.25 (s, 1 H), 4.70 (d, J = 15.5 Hz, 1 H), 4.34 (d, J = 15.5, 1 H), ^{13}C NMR (125 MHz, acetone-d_6): δ 166.6 (C), 138.8 (C), 136.3 (C), 135.7 (C), 129.5 (two CH), 129.3 (C), 128.63 (two CH), 128.58 (C), 128.2 (CH), 125.6 (CH), 125.4 (CH), 124.3 (CH), 123.2 (CH), 119.9 (CH), 116.0 (CH), 114.2 (CH), 114.1 (CH), 113.2 (C), 112.0 (C), 60.0 (CH), 52.8 (CH_2) ; MS (*m/z*, relative intensity): 434 (M^++3, 23), 433 (M^++2, 100), 432 (M^++1, 25), 431 (M^+, 98), 404 (25), 402 (24), 342 (29), 340 (30), 261 (11), 233 (39), 208 (12), 196 (42), 195 (44), 119 (56), 91 (81); exact mass calculated for $C_{23}H_{18}BrN_3O$ (M^+): 431.0633; found: 431.0633.



Thermal ellipsoids draw at the 50% probability level

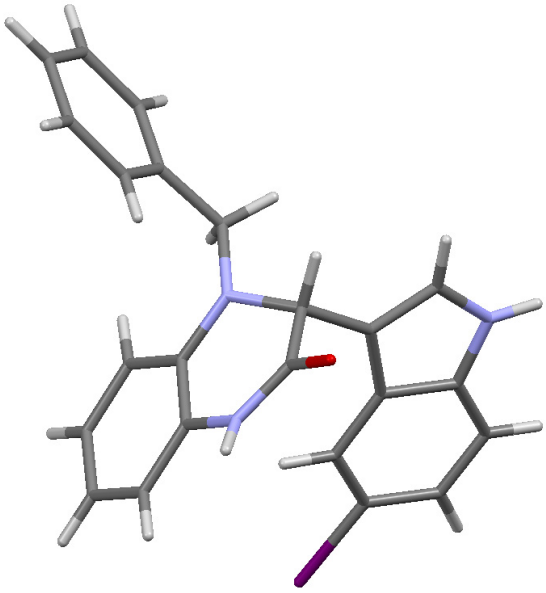


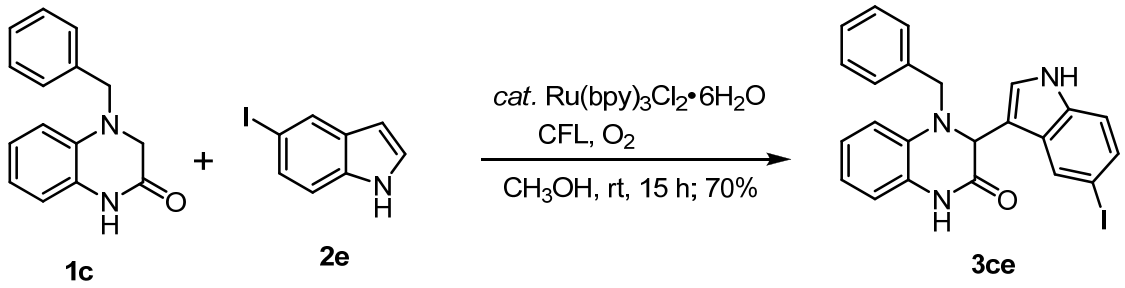
Figure S1. ORTEP and Stereo plots for X-ray crystal structures of **3cd** (**ic18196**).

CCDC 1816892 contains the supplementary crystallographic data for **3cd** (**ic18196**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S1. Crystal data and structure refinement for **3cd** (**ic18196**).

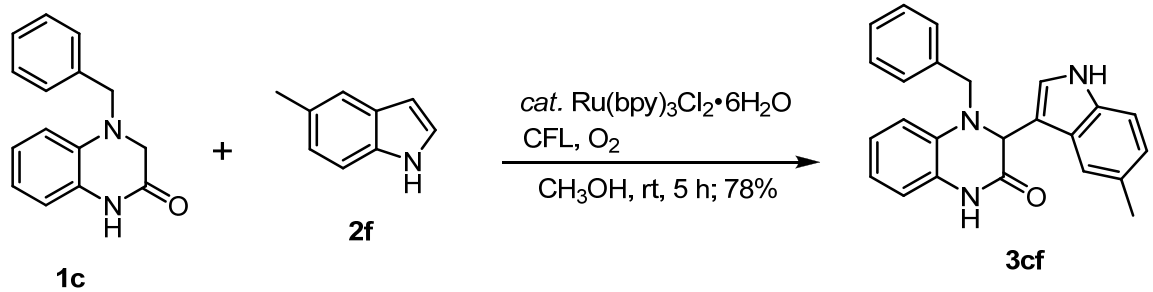
Identification code	ic18196	
Empirical formula	C23 H18 Br N3 O	
Formula weight	432.31	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 19.2070(5) Å	α= 90°.
	b = 10.1247(3) Å	β= 90°.
	c = 19.7884(5) Å	γ = 90°.
Volume	3848.15(18) $Å^3$	
Z	8	
Density (calculated)	1.492 Mg/m^3	
Absorption coefficient	3.057 mm^{-1}	
F(000)	1760	
Crystal size	0.271 x 0.244 x 0.113 mm^3	
Theta range for data collection	4.604 to 69.962°.	
Index ranges	-23<=h<=20, -12<=k<=12, -24<=l<=24	
Reflections collected	22356	
Independent reflections	3624 [R(int) = 0.0169]	
Completeness to theta = 67.679°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.5463	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3624 / 0 / 261	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0365, wR2 = 0.0939	
R indices (all data)	R1 = 0.0371, wR2 = 0.0945	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.095 and -1.036 $e.Å^{-3}$	

Preparation of 4-benzyl-3-(5-iodo-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ce):



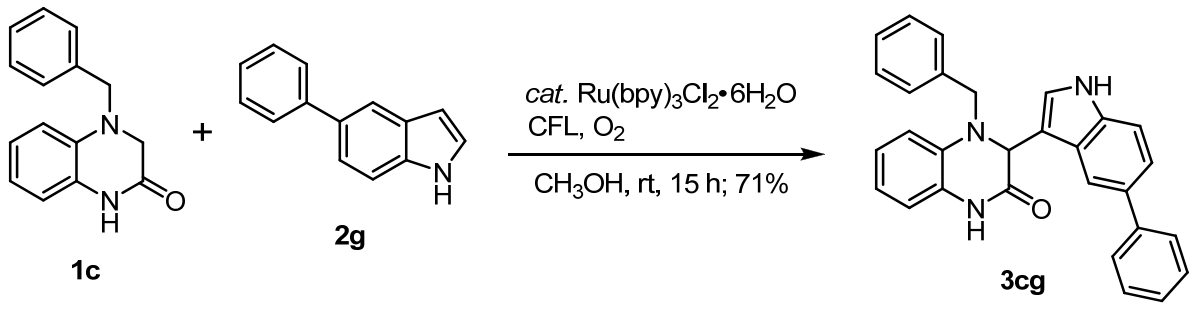
To a solution of **1c** (50 mg, 0.21 mmol) and 5-iodoindole (97.2 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 15 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.38 for **3ce** in 50% EtOAc–hexane) to afford product **3ce** (70 mg; 70% yield) as off-white solids. Mp: 238–240 °C. Selected spectroscopic data for **3ce :** IR (KBr): 3304, 3271, 3028, 2980, 2899, 2868, 1667, 1501, 1416, 1108, 881, 797, 739 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.34 (brs, 1 H), 9.54 (s, 1 H), 7.89 (d, J = 1.5 Hz, 1 H), 7.40 – 7.32 (m, 5 H), 7.31 – 7.22 (m, 2 H), 7.04 – 6.97 (m, 2 H), 6.93 – 6.88 (m, 1 H), 6.83 – 6.77 (m, 2 H), 5.23 (s, 1 H), 4.69 (d, J = 15.5 Hz, 1 H), 4.32 (d, J = 15.5, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.7 (C), 138.8 (C), 136.7 (C), 135.7 (C), 130.9 (CH), 130.1 (C), 129.6 (two CH), 128.7 (two CH), 128.2 (CH), 125.2 (CH), 125.1 (C), 124.3 (CH), 119.9 (CH), 116.0 (CH), 115.9 (CH), 114.6 (CH), 114.1 (CH), 111.6 (C), 83.4 (C), 59.9 (CH), 52.8 (CH_2) ; MS (*m/z*, relative intensity): 480 (M^++1, 51), 479 (M^+, 100), 450 (33), 388 (46), 387 (30), 261 (10), 233 (37), 196 (36), 195 (35), 119 (47), 91 (75); exact mass calculated for $C_{23}H_{18}IN_3O$ (M^+): 479.0495; found: 479.0493.

Preparation of 4-benzyl-3-(5-methyl-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cf):



To a solution of **1c** (50 mg, 0.21 mmol) and 5-methylindole (53 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 5 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.39 for **3cf** in 50% EtOAc–hexane) to afford product **3cf** (60.2 mg; 78% yield) as white solids. Mp: 245–247 °C. Selected spectroscopic data for **3cf:** IR (KBr): 3317, 3170, 3029, 2981, 2916, 1668, 1504, 1412, 1350, 1112, 738 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 10.84 (s, 1 H), 10.54 (s, 1 H), 7.36 – 7.29 (m, 4 H), 7.28 – 7.23 (m, 1 H), 7.22 (d, J = 8.5 Hz, 1 H), 7.13 (s, 1 H), 6.93 – 6.86 (m, 2 H), 6.84 – 6.79 (m, 2 H), 6.76 – 6.70 (m, 1 H), 6.63 (d, J = 8.0 Hz, 1 H), 5.13 (s, 1 H), 4.49 (d, J = 15.5 Hz, 1 H), 4.24 (d, J = 15.5 Hz, 1 H), 2.27 (s, 3 H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 166.1 (C), 137.8 (C), 134.4 (C), 133.3 (C), 128.4 (two CH), 127.4 (two CH and one C), 127.2 (C), 127.0 (CH), 126.1 (C), 123.3 (CH), 123.0 (CH), 122.9 (CH), 118.8 (CH), 118.3 (CH), 114.8 (CH), 112.8 (CH), 111.1 (CH), 109.8 (C), 58.7 (CH), 51.2 (CH_2), 21.2 (CH_3); MS (*m/z*, relative intensity): 368 (M^++1, 32), 367 (M^+, 100), 338 (44), 276 (40), 247 (25), 233 (13), 196 (43), 144 (30), 119 (53), 91 (45); exact mass calculated for $C_{24}H_{21}N_3O$: 367.1685; found: 367.1684.

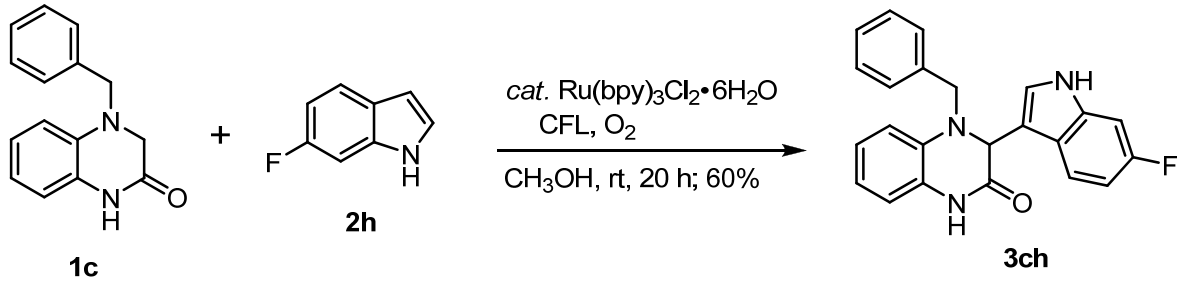
Preparation of 4-benzyl-3-(5-phenyl-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cg):



To a solution of **1c** (50 mg, 0.21 mmol) and 5-phenylindole (77.2 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 15 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.41 for **3cg** in 50% EtOAc–hexane) to afford product **3cg** (64.3 mg; 71% yield) as white solids. Mp: 209–211 °C. Selected spectroscopic data for **3cg**: IR (KBr): 3412, 3290, 3029, 2899, 1667, 1505, 1421, 1112, 749 cm^{-1}; ^1H NMR (500 MHz,

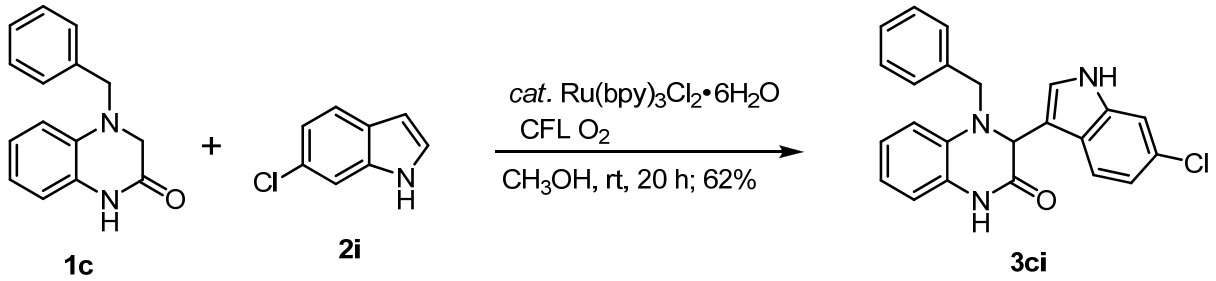
acetone-d_6): δ 10.26 (brs, 1 H), 9.57 (s, 1 H), 7.72 (s, 1 H), 7.52 (d, J = 8.0 Hz, 2 H), 7.48 – 7.37 (m, 6 H), 7.36 – 7.32 (m, 2 H), 7.30 – 7.24 (m, 2 H), 7.10 (d, J = 2.0 Hz, 1 H), 7.04 (dd, J = 7.5, 1.5 Hz, 1 H), 6.93 – 6.88 (m, 1 H), 6.85 – 6.81 (m, 1 H), 6.78 (d, J = 8.0 Hz, 1 H), 5.34 (s, 1 H), 4.65 (d, J = 15.5 Hz, 1 H), 4.36 (d, J = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.9 (C), 143.3 (C), 139.0 (C), 137.3 (C), 135.9 (C), 133.4 (C), 129.5 (four CH), 128.7 (C), 128.6 (two CH), 128.1 (CH), 127.9 (two CH), 127.1 (CH), 125.5 (CH), 124.3 (CH), 122.1 (CH), 119.7 (CH), 119.1 (CH), 116.0 (CH), 113.9 (CH), 112.9 (C), 112.7 (CH), 111.0 (C), 60.4 (CH), 52.6 (CH_2); MS (*m/z*, relative intensity): 430 (M^++1, 35), 429 (M^+, 100), 400 (32), 338 (33), 337 (16), 310 (21), 309 (22), 206 (27), 195 (24), 149 (18), 119 (27), 91 (38); exact mass calculated for $C_{29}H_{23}N_3O$: 429.1841; found: 429.1843.

Preparation of 4-benzyl-3-(6-fluoro-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ch):



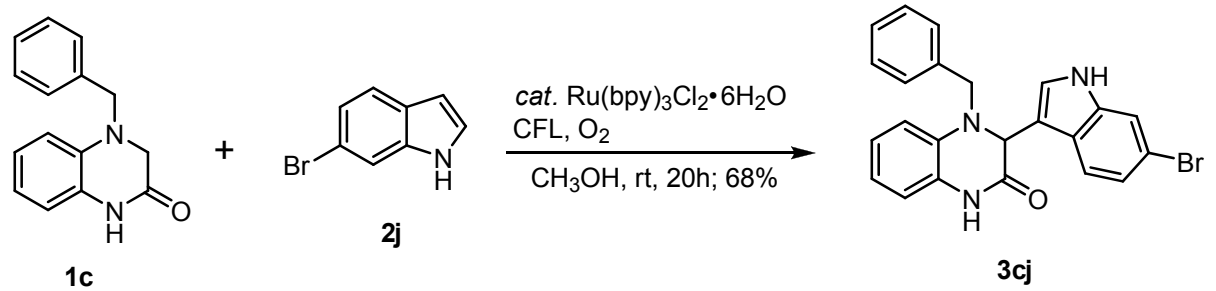
To a solution of **1c** (50 mg, 0.21 mmol) and 6-fluoroindole (54 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 20 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.38 for **3ch** in 50% EtOAc–hexane) to afford product **3ch** (47.1 mg; 60% yield) as white solids. Mp: 218–220 °C , Selected spectroscopic data for **3ch**: IR (KBr): 3280, 3197, 3055, 2990, 2908, 1674, 1620, 1507, 1409, 1110, 836, 803, 739 cm^{-1}; ^{1}H NMR (500 MHz, acetone-d_6): δ 10.22 (brs, 1 H), 9.52 (s, 1 H), 7.52 (dd, J = 9.0, 5.5 Hz, 1 H), 7.39 – 7.30 (m, 4 H), 7.29 – 7.24 (m, 1 H), 7.11 (dd, J = 10.0, 2.0 Hz, 1 H), 7.02 – 6.98 (m, 2 H), 6.92 – 6.87 (m, 1 H), 6.82 – 6.76 (m, 3 H), 5.25 (s, 1 H), 4.69 (d, J = 15.5, 1 H), 4.34 (d, J = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz,acetone-d_6): δ 166.7 (C), 160.7 (d, J = 235 Hz, C), 138.9 (C), 137.6 (d, J = 12.8 Hz, C), 135.7 (C), 129.5 (two CH), 128.6 (two CH), 128.2 (CH), 124.7 (d, J = 3.4 Hz, CH), 124.5 (two C), 124.3 (CH), 121.6 (d, J = 10 Hz, CH), 119.8 (CH), 115.9 (CH), 114.0 (CH), 112.4 (C), 108.6 (d, J = 24.6 Hz, CH), 98.3 (d, J = 26 Hz, CH), 60.1 (CH), 52.8 (CH_2); MS (*m/z*, relative intensity): 372 (M^++1, 23), 371 (M^+, 100), 342 (29), 280 (31), 252 (19), 195 (24), 148 (13), 119 (30), 91 (37); exact mass calculated for $C_{23}H_{18}FN_3O$ (M^+): 371.1434; found: 371.1434.

Preparation of 4-benzyl-3-(6-chloro-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ci):



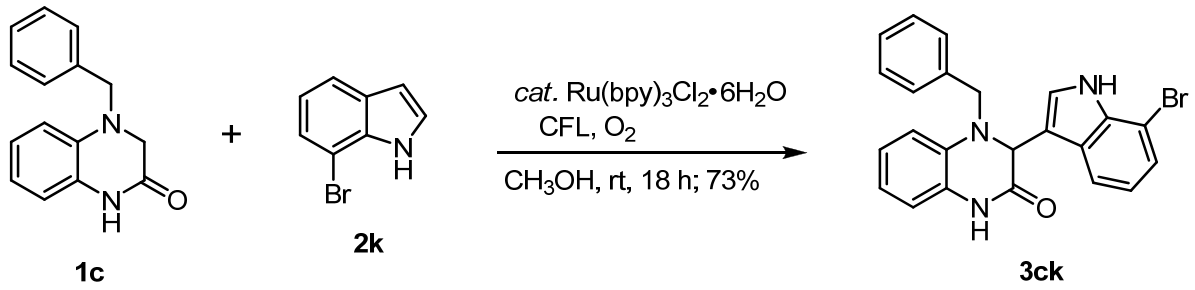
To a solution of **1c** (50 mg, 0.21 mmol) and 6-chloroindole (61 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 20 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.38 for **3ci** in 50% EtOAc–hexane) to afford product **3ci** (50.4 mg; 62% yield) as white solids. Mp: 239–241 °C. Selected spectroscopic data for **3ci**: IR (KBr): 3272, 3175, 3029, 2981, 2898, 1664, 1504, 1415, 1113, 1066, 803, 739 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.30 (brs, 1 H), 9.53 (s, 1H), 7.53 (d, J = 9.0 Hz, 1 H), 7.42 (d, J = 1.5 Hz, 1 H), 7.41 – 7.33 (m, 4 H), 7.32 – 7.28 (m, 1 H), 7.02 – 6.96 (m, 3 H), 6.92 – 6.87 (m, 1 H), 6.81 – 6.76 (m, 2 H), 5.25 (s, 1 H), 4.68 (d, J = 15.0 Hz, 1 H), 4.33 (d, J = 15.0 Hz, 1 H); ^{13}C NMR (125 MHz,acetone-d_6): δ 166.6 (C), 138.8 (C), 138.0 (C), 135.7 (C), 129.5 (two CH), 128.6 (two CH), 128.2 (CH), 128.1 (C), 126.3 (C), 125.1 (CH), 124.3 (CH), 121.8 (CH), 120.6 (CH), 119.8 (CH), 116.0 (CH), 115.9 (C), 114.0 (CH), 112.4 (C), 112.15 (CH), 60.0 (CH), 52.8 (CH_2); MS (*m/z*, relative intensity): 389 (M^++2, 42), 388 (M^++1, 32), 387 (M^+, 100), 358 (36), 296 (42), 268 (18), 233 (12), 195 (41), 164 (17), 119 (52), 91 (57); exact mass calculated for $C_{23}H_{18}ClN_3O$ (M^+): 387.1138; found: 387.1136.

Preparation of 4-benzyl-3-(6-bromo-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cj)



To a solution of **1c** (50 mg, 0.21 mmol) and 6-bromoindole (78.4 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 20 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.38 for **3cj** in 50% EtOAc–hexane) to afford product **3cj** (61.2 mg; 68% yield) as white solids. Mp: 251–253 °C. Selected spectroscopic data for **3cj:** IR (KBr): 3279, 3171, 3114, 3028, 2980, 2901, 1663, 1610, 1504, 1418, 1350, 1255, 1113, 802, 739 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 11.12 (brs, 1 H), 10.60 (s, 1 H), 7.54 (d, J = 2.0 Hz, 1 H), 7.38 (d, J = 8.5 Hz, 1 H), 7.34 – 7.28 (m, 4 H), 7.27 – 7.21 (m, 1 H), 7.07 (dd, J = 8.5, 1.5 Hz, 1 H), 6.92 (d, J = 2.0 Hz, 1 H), 6.89 (dd, J = 7.5, 1.5 Hz, 1 H), 6.84 – 6.78 (m, 1 H), 6.74 – 6.69 (m, 1 H), 6.63 (d, J = 8.0 Hz, 1 H), 5.21 (s, 1 H), 4.52 (d, J = 16.0 Hz, 1 H), 4.30 (d, J = 16.0 Hz, 1 H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.7 (C), 137.8 (C), 136.9 (C), 134.0 (C), 128.4 (two CH), 127.3 (two CH), 127.1 (C), 127.0 (CH), 124.9 (C), 124.3 (CH), 123.1 (CH), 121.8 (CH), 120.9 (CH), 118.4 (CH), 114.9 (CH), 114.12 (C), 114.08 (CH), 112.8 (CH), 110.7 (C), 58.7 (CH), 51.3 (CH_2); MS (*m/z*, relative intensity): 434 (M^++3, 51), 433 (M^++2, 100), 432 (M^++1, 53), 431 (M^+, 100), 404 (46), 402 (43), 196 (4), 195 (4) 119 (6), 91 (7); exact mass calculated for $C_{23}H_{18}BrN_3O$ (M^+): 431.0633; found: 431.0631.

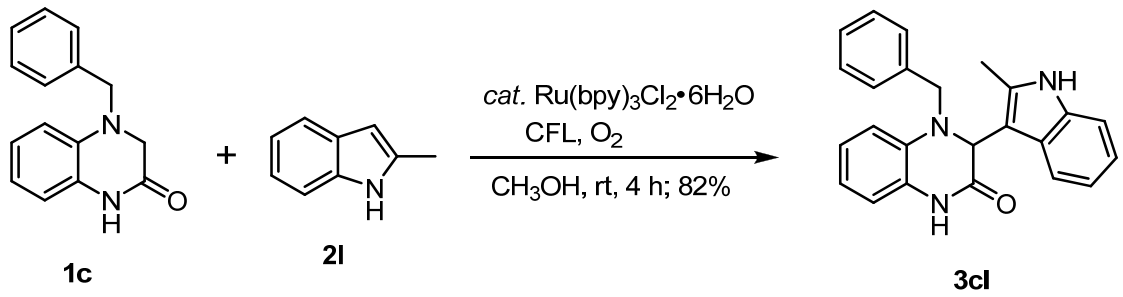
Preparation of 4-benzyl-3-(7-bromo-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ck):



To a solution of **1c** (50 mg, 0.21 mmol) and 7-bromoindole (78.4 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 18 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.39 for **3ck** in 50% EtOAc–hexane) to afford product **3ck** (66.1 mg; 73% yield) as off-white solids. Mp: 228–230 °C. Selected spectroscopic data for **3ck**: IR (KBr): 3267, 3065, 3034, 2910, 2852, 1668, 1500, 1430, 1253, 1110, 745, 700 cm^{-1}; ^1H

NMR (500 MHz, acetone-d_6): δ 10.30 (brs, 1 H), 9.54 (s, 1 H), 7.57 (d, J = 8.0 Hz, 1 H), 7.39 – 7.24 (m, 6 H), 7.06 (d, J = 2.0 Hz, 1 H), 7.01 (dd, J = 8.5, 1.5 Hz, 1 H), 6.97 – 6.87 (m, 2 H), 6.83 – 6.77 (m, 2 H), 5.27 (s, 1 H), 4.69 (d, J = 15.5 Hz, 1 H), 4.34 (d, J = 15.5, 1 H), ^{13}C NMR (125 MHz, acetone-d_6): δ 166.5 (C), 138.8 (C), 135.9 (C), 135.7 (C), 129.5 (two CH), 129.1 (C), 128.6 (two CH), 128.2 (CH), 125.3 (CH), 125.1 (CH), 124.3 (CH), 121.6 (CH), 120.2 (CH), 119.9 (CH), 116.0 (CH), 115.9 (C), 114.1 (CH), 113.7 (C), 105.2 (C), 60.1 (CH), 52.8 (CH_2); MS (*m/z*, relative intensity): 434 (M^++3, 23), 433 (M^++2, 100), 432 (M^++1, 25), 431 (M^+, 99), 404 (31), 402 (30), 342 (28), 340 (29), 312 (10), 233 (24), 208 (15), 195 (45), 119 (52), 91 (58); exact mass calculated for $C_{23}H_{18}BrN_3O$: 431.0633; found: 431.0632.

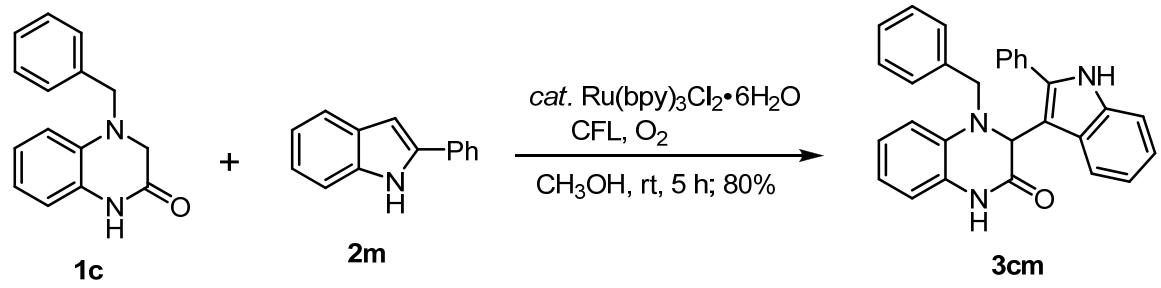
Preparation of 4-benzyl-3-(2-methyl-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cl)



1c + **2l** → **3cl**

To a solution of **1c** (50 mg, 0.21 mmol) and 2-methylindole (52.4 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 4 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.39 for **3cl** in 50% EtOAc–hexane) to afford product **3cl** (63.1 mg; 82% yield) as light yellow solids; Mp: 234–236 °C. Selected spectroscopic data for **3cl:** IR (KBr): 3283, 3194, 3059, 2977, 2892, 1656, 1507, 1426, 1302, 1252, 1228, 1154, 738, 698, 676 cm^{-1}; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.99 (s, 1 H), 10.65 (s, 1 H), 7.30 – 7.25 (m, 2 H), 7.24 – 7.18 (m, 4 H), 6.95 – 6.90 (m, 2 H), 6.82 – 6.76 (m, 2 H), 6.72 – 6.66 (m, 2 H), 6.54 (d, J = 8.0 Hz, 1 H), 5.28 (s, 1 H), 4.45 (d, J = 16.5 Hz, 1 H), 4.03 (d, J = 16.5 Hz, 1 H), 2.18 (s, 3 H), ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.8 (C), 137.7 (C), 135.2 (C), 135.0 (C), 134.3 (C), 128.4 (two CH), 127.0 (two CH), 126.8 (CH), 126.3 (C), 126.1 (C), 123.2 (CH), 120.2 (CH), 118.6 (CH), 118.3 (CH), 117.4 (CH), 114.8 (CH), 111.4 (CH), 110.5 (CH), 107.9 (C), 58.0 (CH), 50.1 (CH_2), 11.3 (CH_3); MS (*m/z*, relative intensity): 368 (M^++1, 66), 367 (M^+, 100), 338 (42), 276 (65), 275 (44), 247 (60), 236 (77), 219 (38), 196 (70), 195 (63), 144 (82), 119 (100), 91 (89); exact mass calculated for $C_{24}H_{21}N_3O$ (M^+): 367.1685; found: 367.1682.

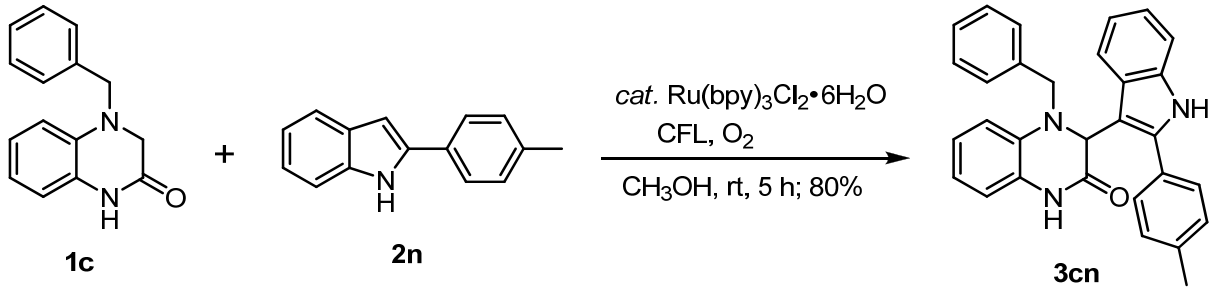
Preparation of 4-benzyl-3-(2-phenyl-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cm)



1c 2m 3cm

To a solution of **1c** (50 mg, 0.21 mmol) and 2-phenylindole (77.2 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 5 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.4 for **3cm** in 50% EtOAc–hexane) to afford product **3cm** (71.8 mg; 80% yield) as white solid; Mp: 240–242 °C. Selected spectroscopic data for **3cm:** IR (KBr): 3386, 3189, 3053, 2985, 2900, 1673, 1506, 1397, 1447, 1307, 1231, 743, 701 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.53 (brs, 1 H), 9.76 (s, 1 H), 7.87 (d, J = 6.5 Hz, 2 H), 7.47 – 7.36 (m, 4 H), 7.11 – 7.00 (m, 6 H), 6.99 – 6.95 (m, 2 H), 6.89 – 6.83 (m, 1 H), 6.82 – 6.72 (m, 2 H), 6.63 (d, J = 8.0 Hz, 1 H), 5.59 (s, 1 H), 4.41 (d, J = 16.0 Hz, 1 H), 3.82 (d, J = 16.0 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.9 (C), 139.9 (C), 138.5 (C), 137.6 (C), 135.6 (C), 133.3 (C), 130.4 (two CH), 129.5 (two CH), 129.19 (CH), 129.17 (two CH), 128.0 (two CH), 127.64 (CH), 127.56 (C), 126.8 (C), 124.6 (CH), 122.9 (CH), 121.1 (CH), 120.4 (CH), 118.5 (CH), 116.0 (CH), 112.24 (CH), 112.21 (CH), 111.0 (C), 58.9 (CH), 51.0 (CH_2).; MS (*m/z*, relative intensity): 430 (M^++1, 31), 429 (M^+, 100), 400 (38), 338 (48), 308 (30), 236 (37), 206 (63), 204 (78), 196 (37), 119 (39), 91 (50); exact mass calculated for $C_{29}H_{23}N_3O$ (M^+): 429.1841; found: 429.1840.

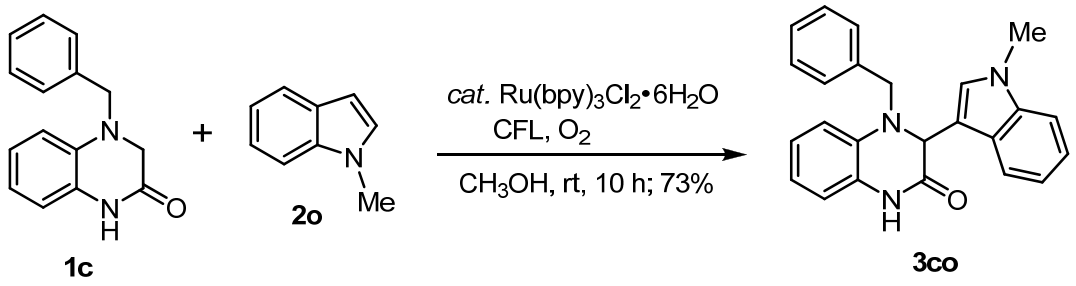
Preparation of 4-benzyl-3-(2-(p-tolyl)-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cn):



1c 2n 3cn

To a solution of **1c** (50 mg, 0.21 mmol) and 2-(*p*-tolyl)-1*H*-indole (82.9 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 5 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f= 0.39 for **3cn** in 50% EtOAc–hexane) to afford product **3cn** (74.2 mg; 80% yield) as white solid; Mp: 215–217 °C. Selected spectroscopic data for **3cn:** IR (KBr): 3424, 3187, 3055, 2978, 2891, 1674, 1507, 1428, 1307, 824, 738 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.46 (brs, 1 H), 9.74 (s, 1 H), 7.75 (d, J = 8.0 Hz, 2 H), 7.40 (d, J = 8.0 Hz, 1 H), 7.24 (d, J = 7.5 Hz, 2 H), 7.11 – 7.03 (m, 5 H), 7.02 – 6.96 (m, 3 H), 6.88 – 6.82 (m, 1 H), 6.81 – 6.72 (m, 2 H), 6.60 (d, J = 8.0 Hz, 1 H), 5.59 (s, 1 H), 4.38 (d, J = 16.5 Hz, 1 H), 3.82 (d, J = 16.5 Hz, 1 H), 2.38 (s, 3 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.9 (C), 140.1 (C), 139.0 (C), 138.5 (C), 137.5 (C), 135.6 (C), 130.4 (C), 130.3 (two CH), 130.1 (two CH), 129.2 (two CH), 127.9 (two CH), 127.61 (C), 127.58 (CH), 126.9 (C), 124.6 (CH), 122.7 (CH), 121.0 (CH), 120.4 (CH), 118.5 (CH), 116.0 (CH), 112.2 (CH), 112.1 (CH), 110.8 (C), 59.0 (CH), 51.0 (CH_2), 21.4 (CH_3); MS (*m/z*, relative intensity): 444 (M^++1, 32), 443 (M^+, 100), 414 (41), 352 (57), 322 (31), 247 (13), 236 (47), 220 (70), 218 (49), 204 (41), 196 (33), 119 (35), 91 (51); exact mass calculated for $C_{30}H_{25}N_3O$ (M^+): 443.1998; found: 443.1998.

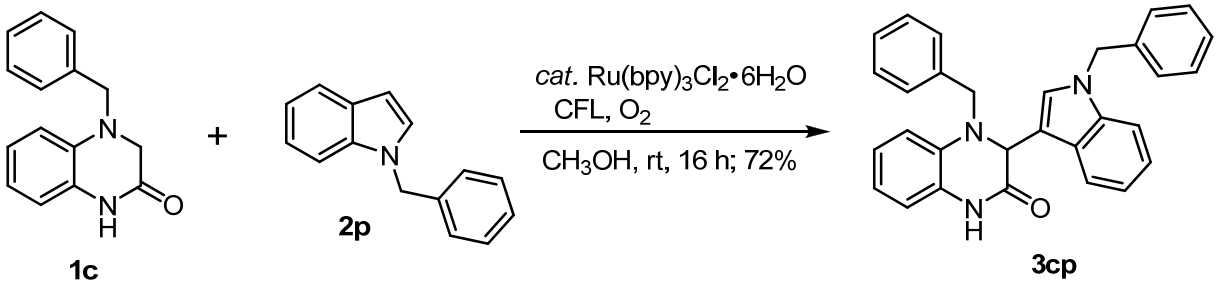
Preparation of 4-benzyl-3-(1-methyl-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3co):



To a solution of **1c** (50 mg, 0.21 mmol) and *N*-methylindole (52.4 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 10 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.47 for **3co** in 50% EtOAc–hexane) to afford product **3co** (56.1 mg; 73% yield) as white solids; Mp: 224–226 °C. Selected spectroscopic data for **3co**: IR (KBr): 3182, 3045, 2976, 2913, 1678, 1501, 1391, 1225, 1147, 857, 742 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 10.60 (s, 1 H), 7.39 (dd, J = 16.5, 8.0 Hz, 2 H), 7.33 – 7.29 (m, 4 H),

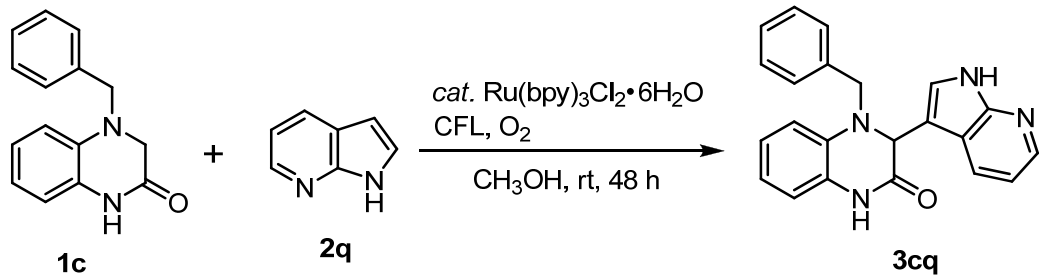
7.27 – 7.22 (m, 1 H), 7.15 – 7.10 (m, 1 H), 6.98 – 6.94 (m, 1 H), 6.93 – 6.89 (m, 2 H), 6.83 – 6.78 (m, 1 H), 6.74 – 6.69 (m, 1 H), 6.61 (d, J = 8.0 Hz, 1 H), 5.22 (s, 1 H), 4.51 (d, J = 15.5 Hz, 1 H), 4.30 (d, J = 15.5 Hz, 1 H), 3.67 (s, 3 H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.8 (C), 137.8 (C), 136.5 (C), 133.9 (C), 128.4 (two CH), 127.6 (CH), 127.3 (two CH), 127.1 (two C), 127.0 (CH), 126.2 (C), 123.0 (CH), 121.4 (CH), 119.4 (CH), 119.1 (CH), 118.3 (CH), 114.9 (CH), 112.7 (CH), 109.7 (CH), 58.8 (CH), 51.2 (CH_2), 32.4 (CH_3); MS (*m/z*, relative intensity): 368 (M^++1, 14), 367 (M^+, 58), 338 (25), 276 (28), 247 (23), 236 (21), 233 (15), 219 (10), 144 (100), 91 (52); exact mass calculated for $C_{24}H_{21}N_3O$ (M^+): 367.1685; found: 367.1685.

Preparation of 4-benzyl-3-(1-benzyl-1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cp):



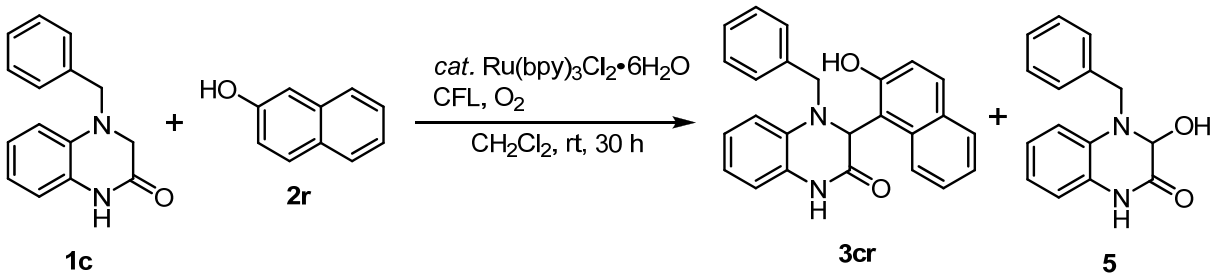
To a solution of **1c** (50 mg, 0.21 mmol) and *N*-benzylindole (83 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 16 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.52 for **3cp** in 50% EtOAc–hexane) to afford product **3cp** (66.8 mg; 72% yield) as white solids; Mp: 151–153 °C. Selected spectroscopic data for **3cp**: IR (KBr): 3191, 3131, 3062, 3029, 2916, 2859, 1668, 1501, 1382, 1156, 738 cm^{-1}; ^{1}H NMR (500 MHz, acetone-d_6): δ 9.55 (s, 1 H), 7.54 (d, J = 8.0 Hz, 1 H), 7.37 – 7.29 (m, 5 H), 7.28 – 7.20 (m, 4 H), 7.11 – 7.05 (m, 4 H), 7.02 – 6.95 (m, 2 H), 6.90 – 6.85 (m, 1 H), 6.80 – 6.72 (m, 2 H), 5.31 (s, 2 H), 5.28 (s, 1 H), 4.65 (d, J = 15.5 Hz, 1 H), 4.34 (d, J = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.8 (C), 139.0 (C), 138.9 (C), 137.6 (C), 135.7 (C), 129.50 (two CH), 129.48 (two CH), 128.63 (C), 128.59 (two CH), 128.31 (CH), 128.27 (C), 128.20 (CH), 128.1 (CH), 127.8 (two CH), 124.2 (CH), 122.7 (CH), 120.9 (CH), 120.4 (CH), 119.7 (CH), 115.9 (CH), 114.1 (CH), 111.7 (C), 111.0 (CH), 60.1 (CH), 52.8 (CH_2), 50.4 (CH_2); MS (*m/z*, relative intensity): 443 (M^+, 4), 414 (2), 352 (2), 220 (6), 153 (38), 136 (42), 107 (46), 89 (58), 77 (100); exact mass calculated for $C_{30}H_{25}N_3O$ (M^+): 443.1998; found: 443.1994.

Preparation of 4-benzyl-3-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one



To a solution of **1c** (50 mg, 0.21 mmol) and 7-azaindole (47.2 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 16 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 40% EtOAc–hexane (R_f = 0.23 for **3cq** in 50% EtOAc–hexane) to afford product **3cq** (16.1 mg; 22% yield) as gummy compound; Selected spectroscopic data for **3cq**: IR (KBr): 3059, 2922, 2851, 1683, 1387, 1258, 884, 768 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.61 (brs, 1 H), 9.58 (s, 1 H), 8.20 (dd, J = 4.5, 1.5 Hz, 1 H), 7.80 (dd, J = 8.0, 1.5 Hz, 1 H), 7.39 – 7.31 (m, 4 H), 7.29 – 7.24 (m, 1 H), 7.16 (d, J = 2.0 Hz, 1 H), 7.03 – 6.96 (m, 2 H), 6.92 – 6.88 (m, 1 H), 6.80 (d, J = 7.5 Hz, 2 H), 5.25 (s, 1 H), 4.70 (d, J = 15.5 Hz, 1 H), 4.36 (d, J = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.6 (C), 149.6 (C), 144.3 (CH), 138.8 (C), 135.7 (C), 129.5 (two CH), 128.7 (CH), 128.6 (two CH), 128.5 (C), 128.2 (CH), 124.7 (CH), 124.4 (CH), 119.9 (CH), 119.4 (C), 116.6 (CH), 116.0 (CH), 114.0 (CH), 111.1 (C), 60.4 (CH), 52.8 (CH_2); MS (*m/z*, relative intensity): 355 (M^++1, 12), 354 (M^+, 47), 325 (16), 263 (30), 235 (24), 195 (35), 131 (41), 119 (93), 91 (100); exact mass calculated for $C_{22}H_{18}N_4O$: 354.1481; found: 354.1480.

Preparation of 4-benzyl-3-(2-hydroxynaphthalen-1-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cr):

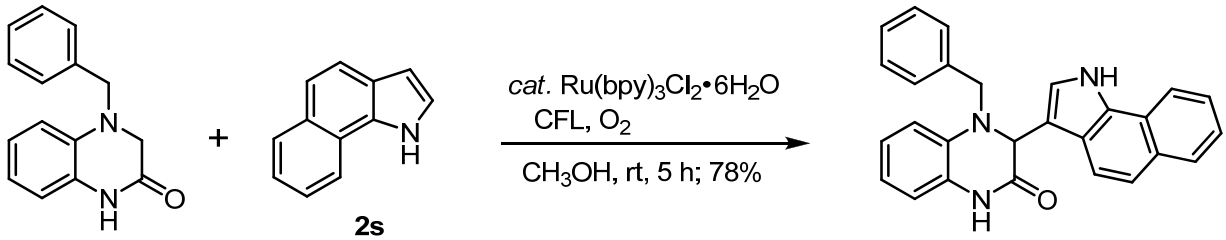


To a solution of **1c** (50 mg, 0.21 mmol) and naphthalen-2-ol (288.3 mg, 2.0 mmol, 9.5 equiv)

in CH_2Cl_2 (3.9 mL) was added $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with with a household compact florescence lamp (24 W) for 48 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 40% EtOAc–hexane (R_f = 0.37 for **3cr** in 50% EtOAc–hexane) to afford product **3cr** (40.2 mg; 50% yield) as white solids and **5** (R_f = 0.30 for **5** in 50% EtOAc–hexane, 12.1 mg, 23% yield). For **3cr**: mp, 202–203 ^oC; elected spectroscopic data for **3cr:** IR (KBr): 3299, 3191, 3114, 3027, 2918, 1651, 1507, 1433, 1273, 973, 814, 745 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 10.63 (s, 1 H), 10.01 (s, 1 H), 8.05 (d, J = 8.5 Hz, 1 H), 7.78 (d, J = 8.5 Hz, 1 H), 7.73 (d, J = 8.5 Hz, 1 H), 7.38 – 7.33 (m, 1 H), 7.27 – 7.22 (m, 1 H), 7.16 – 7.06 (m, 6 H), 6.87 (d, J = 7.5 Hz, 1 H), 6.70 (dd, J = 7.5, 7.5 Hz 1 H), 6.61 (dd, J = 7.5, 7.0 Hz, 1 H), 6.38 (d, J = 8.0 Hz, 1 H), 6.23 (s, 1 H), 4.32 (d, J = 17.0 Hz, 1 H), 4.06 (d, J = 17.0 Hz, 1 H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 166.5 (C), 154.7 (C), 138.2 (C), 134.4 (C), 129.8 (CH), 128.6 (CH), 128.1 (four CH), 126.35 (CH), 126.32 (four CH), 125.7 (C), 122.9 (CH), 122.3 (CH), 117.9 (CH), 114.6 (CH), 57.5 (CH), 50.6 (CH_2), *few aryl carbons are broadened and disappeared due to the slow rotation and coalescence phenomenon; MS (*m/z*, relative intensity): 380 (M^+, 10), 378 (M^+–2, 6), 361 (5), 289 (10), 252 (10), 224 (28), 205 (23), 144 (22), 115 (15), 91 (100); exact mass calculated for $C_{25}H_{20}N_2O_2$: 380.1525; found: 380.1527.

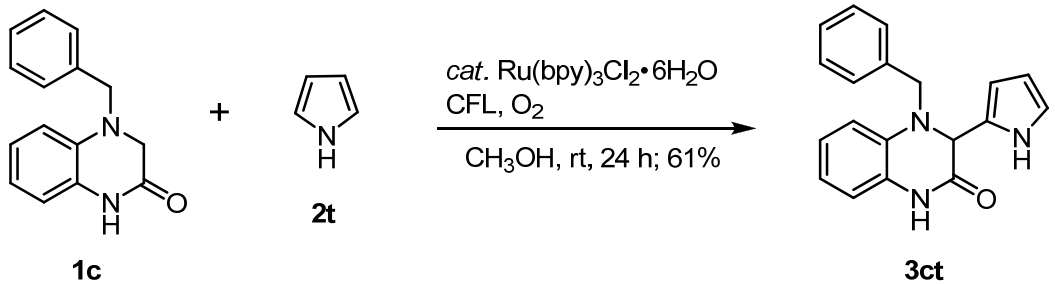
For **5**: mp, 137–138 ^oC; IR (KBr): 3304, 3187, 3039, 2922, 1664, 1510, 1385, 1312, 994, 965, 746, 700 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 9.60 (brs, 1 H), 7.41 (d, J = 8.0 Hz, 2 H), 7.33 (dd, J = 7.5, 7.5 Hz, 2 H), 7.26 (dd, J = 7.5, 7.5 Hz, 1 H), 7.00 (dd, J = 8.0, 1.5 Hz, 1 H), 6.89 – 6.84 (m, 1 H), 6.82 – 6.77 (m, 2 H), 5.53 (d, J = 6.5 Hz, 1 H), 5.16 (d, J = 6.5 Hz, 1 H), 4.81 (d, J = 15.0 Hz, 1 H), 4.59 (d, J = 15.0 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 164.4 (C), 138.7 (C), 133.0 (C), 129.4, (two CH), 128.6 (two CH), 128.1 (CH), 127.8 (C), 123.7 (CH), 120.3 (CH), 115.9 (CH), 114.9 (CH), 82.1 (CH), 52.5 (CH_2); MS (*m/z*, relative intensity): 253 (M^+-1, 1), 238 (1), 221 (2), 208 (2), 178 (3), 167 (4), 153 (10), 149 (15), 136 (14), 105 (41), 101 (28), 89 (27), 77 (62), 58 (100); exact mass calculated for $C_{15}H_{14}N_2O_2$: 254.1055; found: 254.1058.

Preparation of 3-(1*H*-benzo[*g*]indol-3-yl)-4-benzyl-3,4-dihydroquinoxalin-2(1*H*)-one (3cs):



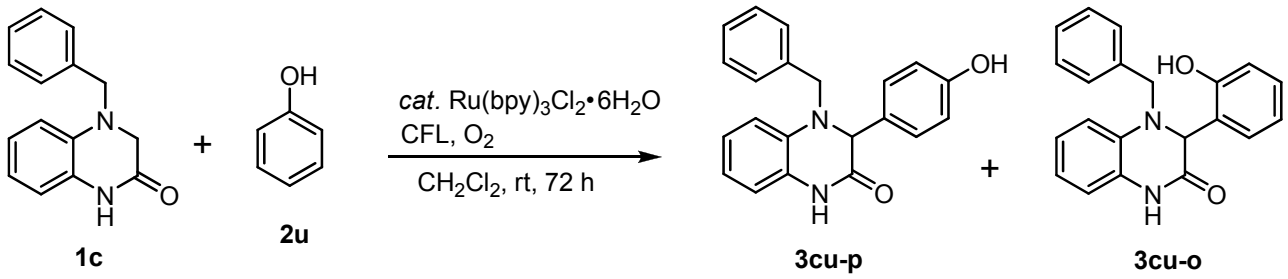
To a solution of **1c** (50 mg, 0.21 mmol) and 1*H*-benzo[*g*]indole (66.8 mg, 0.40 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 5 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.4 for **3cs** in 50% EtOAc–hexane) to afford product **3cs** (66.4 mg; 78% yield) as off-white solids. Mp: 241–243 °C. Selected spectroscopic data for **3cs**: IR (KBr): 3306, 3061, 2952, 2920, 2851, 1667, 1506, 1392, 1252, 1222, 1109, 800, 746, 697 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 11.93 (s, 1 H), 10.62 (s, 1 H), 8.28 (d, J = 8.5 Hz, 1 H), 7.89 (d, J = 8.5 Hz, 1 H), 7.58 – 7.49 (m, 2 H), 7.43 – 7.37 (m, 2 H), 7.34 – 7.30 (m, 4 H), 7.28 – 7.22 (1 H), 6.95 – 6.92 (m, 2 H), 6.85 – 6.80 (m, 1 H), 6.78 – 6.72 (m, 1 H), 6.65 (d, J = 8.0 Hz, 1 H), 5.30 (s, 1 H), 4.53 (d, J = 15.0 Hz, 1 H), 4.33 (d, J = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 166.1 (C), 137.8 (C), 134.2 (C), 130.6 (C), 129.6 (C), 128.4 (two CH), 128.2 (CH), 127.36 (two CH), 127.33 (C), 127.0 (CH), 125.3 (CH), 123.7 (CH), 123.1 (CH), 121.8 (CH), 121.7 (C), 121.3 (C), 120.4 (CH), 119.7 (CH), 119.4 (CH), 118.5 (CH), 114.8 (CH), 112.9 (CH), 112.4 (C), 58.8 (CH), 51.3 (CH_2); MS (*m/z*, relative intensity): 404 (M^++1, 29), 403 (M^+, 100), 374 (38), 312 (35), 283 (21), 196 (28), 180 (29), 119 (30), 97 (32), 91 (29); exact mass calculated for $C_{27}H_{21}N_3O$ (M^+): 403.1685; found: 403.1685.

Preparation of 4-benzyl-3-(1*H*-pyrrol-2-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ct):



To a solution of **1c** (50 mg, 0.21 mmol) and pyrrole (28 mg, 0.42 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 24 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.47 for **3ct** in 50% EtOAc–hexane) to afford product **3ct** (39.1 mg; 61% yield) as yellow solids. Mp: 213–214 °C. Selected spectroscopic data for **3ct**: IR (KBr): 3335, 3059, 2910, 1674, 1504, 1397, 1225, 1111, 1026, 975, 885, 739, 702 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 9.83 (brs, 1 H), 9.54 (s, 1 H), 7.39 – 7.30 (m, 4 H), 7.29 – 7.23 (m, 1 H), 6.96 (dd, J = 8.0, 1.5 Hz, 1 H), 6.89 – 6.85 (m, 1 H), 6.78 – 6.74 (m, 2 H), 6.70 – 6.67 (m, 1 H), 5.93 (dd, J = 6.0, 2.5 Hz, 1 H), 5.74 (m, 1 H), 4.93 (s, 1 H), 4.66 (d, J = 15.5 Hz, 1 H), 4.27 (d, J = 15.5, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.3 (C), 138.7 (C), 135.4 (C), 129.5 (two CH), 128.6 (two CH), 128.3 (C), 128.2 (CH), 127.3 (C), 124.2 (CH), 119.9 (CH), 119.0 (CH), 116.0 (CH), 114.2 (CH), 108.8 (CH), 107.4 (CH), 61.1 (CH), 52.8 (CH_2); MS (*m/z*, relative intensity): 304 (M^++1, 20), 303 (M^+, 100), 275 (10), 274 (15), 212 (47), 196 (34), 195 (43), 184 (15), 169 (16), 119 (62), 91 (76); exact mass calculated for $C_{19}H_{17}N_3O$: 303.1372; found: 303.1369.

Preparation of 3cu-p and 3cu-o.

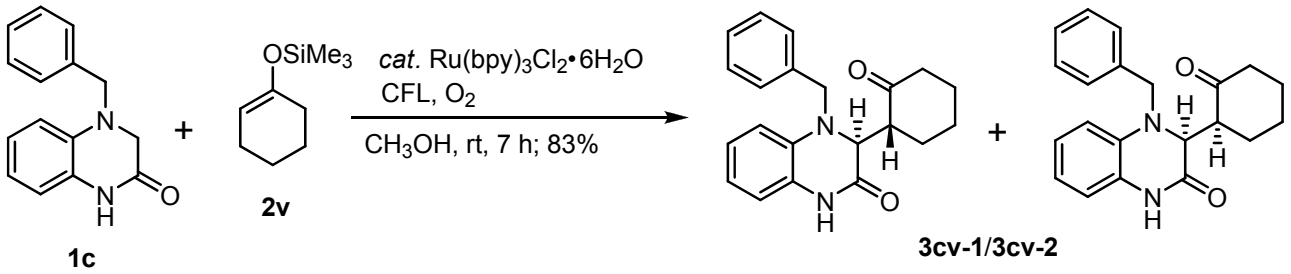


To a solution of **1c** (50 mg, 0.21 mmol) and phenol (190 mg, 2.02 mmol, 10 equiv) in CH_2Cl_2 (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 72 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 20% to 40% EtOAc–hexane (R_f= 0.54 for **3cu-o** in 50% EtOAc–hexane) to afford product **3cu-o** (19.2 mg; 28% yield) as white solids and **3cu-p** (R_f = 0.27 for **3cu-p** in 50% EtOAc–hexane, 22.1 mg, 32% yield) as white solids. For **3cu-p**: mp: 205–207 °C; IR (KBr): 3266, 3174, 3028, 2980, 2913, 1661, 1504, 1423, 1384, 1256, 739 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ 10.60 (s, 1 H), 9.47 (s, 1 H), 7.35 – 7.21 (m, 5 H), 6.92 (d, J = 8.5 Hz, 2 H), 6.84 (dd, J = 8.0, 1.5 Hz, 1 H), 6.81 – 6.76 (m, 1 H), 6.69 – 6.64 (m, 3 H), 6.62 (d, J = 8.0 Hz, 1 H), 4.84 (s, 1 H), 4.52 (d,

J = 16.0 Hz, 1 H), 4.20 (d, *J* = 16.0 Hz, 1 H), ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.9 (C), 157.3 (C), 137.6 (C), 133.5 (C), 128.5 (two CH), 128.0 (two CH), 127.8 (C), 127.3 (two CH), 127.0 (CH), 126.5 (C), 123.1 (CH), 118.1 (CH), 115.3 (two CH), 114.8 (CH), 112.3 (CH), 64.7 (CH), 51.1 (CH_2); MS (*m/z*, relative intensity): 331 (M^++1, 42), 330 (M^+, 100), 301 (10), 239 (49), 209 (62), 195 (18), 91 (5); exact mass calculated for $C_{21}H_{18}N_2O_2$: 330.1368; found: 330.1369.

For **3cu-o**: mp, 183–184 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.83 (s, 1 H), 8.51 (s, 1 H), 7.33 – 7.13 (m, 6 H), 7.04 – 6.91 (m, 3 H), 6.85 (d, *J* = 8.5 Hz, 1 H), 6.80 – 6.70 (m, 3 H), 5.36 (s, 1 H), 4.83 (d, *J* = 15.5 Hz, 1 H), 4.17 (d, *J* = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.0 (C), 154.9 (C), 135.9 (C), 134.2 (C), 129.7 (CH), 128.9 (two CH), 127.8 (CH), 127.4 (two CH), 126.0 (CH), 125.5 (CH), 124.0 (C), 123.5 (C), 120.5 (CH), 119.0 (CH), 118.7 (CH), 116.0 (CH), 112.2 (CH), 60.7 (CH), 52.1 (CH_2); MS (*m/z*, relative intensity): 331 (M^++1, 15), 330 (M^+, 69), 301 (5), 239 (65), 209 (33), 195 (6), 119 (19), 91 (100), 65 (20); exact mass calculated for $C_{21}H_{18}N_2O_2$: 330.1368; found: 330.1366.

Preparation of 3cv-1 and 3cv-2:



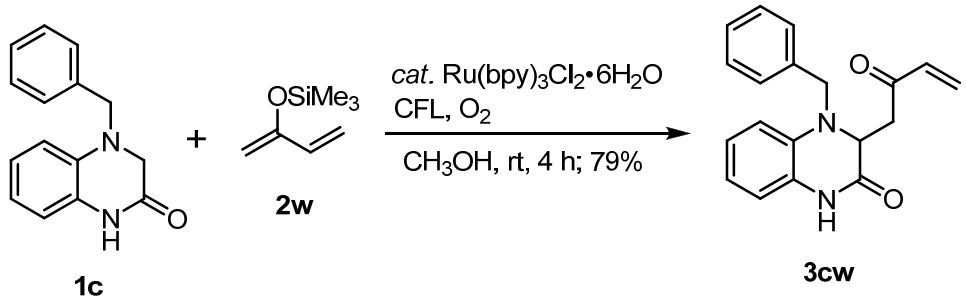
To a solution of **1c** (50 mg, 0.21 mmol) and (cyclohex-1-en-1-yloxy)trimethylsilane (70 mg, 0.41 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 7 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f= 0.45 for **3cv-1**; R_f= 0.44 for **3cv-2** in 40% EtOAc–hexane, developed twice) to afford pure product **3cv-1** and **3cv-2** mixtures (58.2 mg; 83% yield, in a ratio of 80:20, determined by ^{1}H NMR). The mixture was further purified by flash column chromatography to give the pure **3cv-1** and pure **3cv-2** for spectra analysis. Both of them are colorless gummy compounds.

Selected spectroscopic data for **3cv-1**: IR (neat): 3208, 3062, 2937, 2864, 1680, 1507, 1379, 1260, 1126, 1027, 744, 700 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.87(s, 1 H), 7.26 – 7.14 (m, 5 H), 6.92 – 6.85 (m, 1 H), 6.77 (d, *J* = 4.0 Hz, 2 H), 6.70 (d, *J* = 8.0 Hz, 1 H), 4.60 – 4.48 (m, 3 H), 2.54 – 2.46 (m, 1 H), 2.42 – 2.35 (m, 1 H), 2.28 – 2.17 (m, 1 H), 1.99 – 1.84 (m, 2 H), 1.83 – 1.74

(m, 1 H), 1.68 – 1.44 (m, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 210.3 (C), 165.8 (C), 137.7 (C), 133.4 (C), 128.5 (two CH), 127.4 (two CH), 127.3 (CH), 126.9 (C), 124.1 (CH), 119.5 (CH), 115.9 (CH), 115.6 (CH), 61.1 (CH), 55.1 (CH_2), 50.9 (CH), 42.1 (CH_2), 30.5 (CH_2), 27.7 (CH_2), 24.5 (CH_2); MS (*m/z*, relative intensity): 334 (M^+, 8), 244 (10), 243 (71), 237 (30), 194 (15), 129 (5), 92 (14), 91 (100); exact mass calculated for $C_{21}H_{22}N_2O_2$: 334.1681; found: 334.1678.

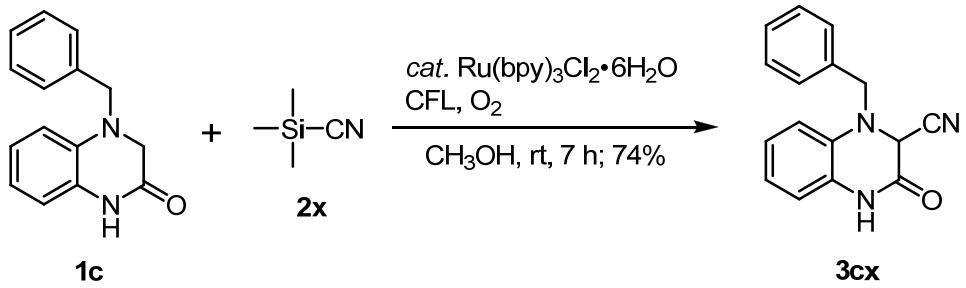
Selected spectroscopic data for **3cv-2**: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (s, 1 H), 7.28 – 7.16 (m, 5 H), 6.88 – 6.82 (m, 1 H), 6.70 – 6.63 (m, 3 H), 4.78 (d, J = 3.0 Hz, 1 H), 4.61 (s, 2 H), 2.83 – 2.77 (m, 1 H), 2.47 – 2.40 (m, 1 H), 2.27 – 2.18 (m, 1 H), 1.98 – 1.91 (m, 1 H), 1.89 – 1.82 (m, 1 H), 1.78 – 1.71 (m, 1 H), 1.67 – 1.47 (m, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 209.6 (C), 168.1 (C), 137.8 (C), 134.5 (C), 128.6 (two CH), 127.4 (CH), 127.2 (two CH), 126.1 (C), 124.3 (CH), 118.9 (CH), 115.2 (CH), 114.5 (CH), 60.4 (CH), 55.9 (CH), 55.2 (CH_2), 41.7 (CH_2), 28.9 (CH_2), 26.7 (CH_2), 24.4 (CH_2).

Preparation of 4-benzyl-3-(2-oxobut-3-en-1-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3cw):



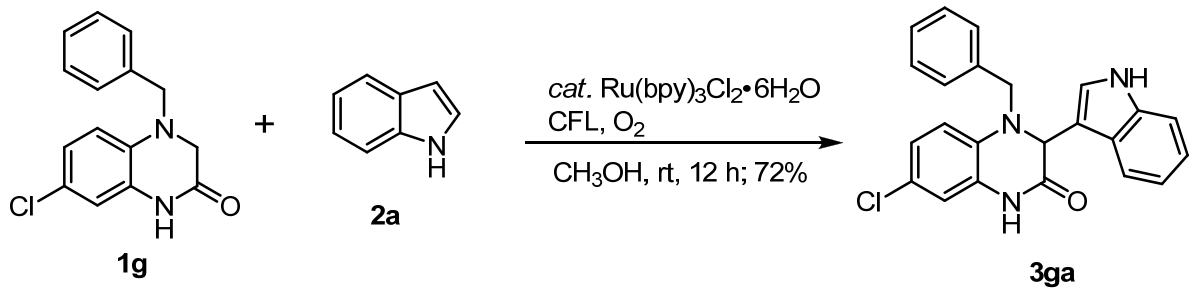
To a solution of **1c** (50 mg, 0.21 mmol) and 2-trimethylsilyloxy-1,3-butadiene (65 mg, 0.46 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 4 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f= 0.48 for **3cw** in 50% EtOAc–hexane) to afford product **3cw** (51 mg; 79% yield) as colorless gummy compound. Selected spectroscopic data for **3cw**: IR (neat): 3208, 3062, 2964, 2922, 1684, 1507, 1401, 1261, 1092, 1027, 800, 744, 700 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.05 (s, 1 H), 7.37 – 7.11 (m, 5 H), 6.93 – 6.86 (m, 1 H), 6.82 – 6.71 (m, 2 H), 6.64 (d, *J* = 8.0 Hz, 1 H), 6.32 – 6.20 (m, 1 H), 6.05 (d, *J* = 17.6 Hz, 1 H), 5,77 (*d*, J = 10.4 Hz, 1 H), 4.58 – 4.46 (m, 2 H), 4.36 (d, *J* = 15.6 Hz, 2 H), 2.98 – 2.87 (m, 1 H), 2.82 – 2.74 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.3 (C), 167.8 (C), 137.0 (C), 136.2 (CH), 133.1 (C), 129.2 (CH_2), 128.7 (two CH), 127.4 (CH), 127.3 (two CH), 126.2 (C), 124.3 (CH), 119.6 (CH), 115.6 (CH), 114.7 (CH), 58.7 (CH), 53.6 (CH_2), 39.7 (CH_2); MS (*m/z*, relative intensity): 306 (M^+, 8), 237 (6), 215 (85), 187 (37), 161 (9), 131 (5), 91 (100); exact mass calculated for $C_{19}H_{18}N_2O_2$: 306.1368; found: 306.1377.

Preparation of 1-benzyl-3-oxo-1,2,3,4-tetrahydroquinoxaline-2-carbonitrile (3cx)



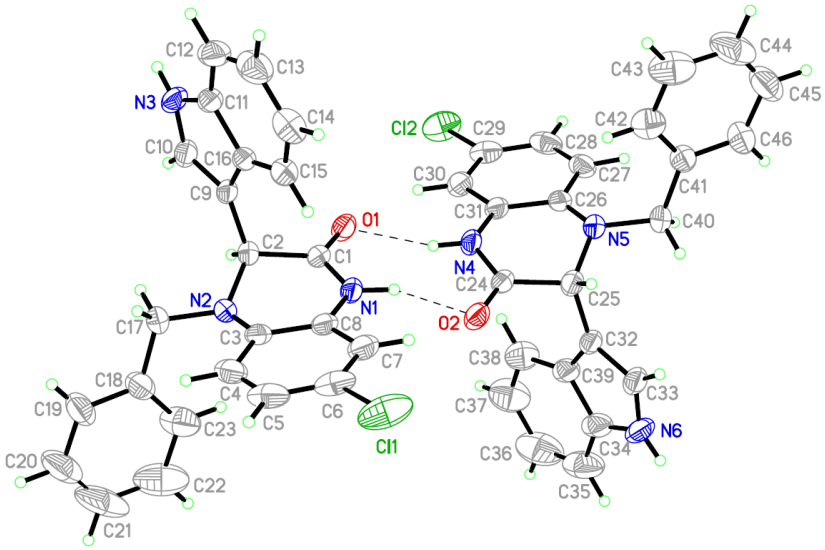
To a solution of **1c** (50 mg, 0.21 mmol) and trimethylsilyl cyanide (42 mg, 0.42 mmol, 2 equiv) in CH_3OH (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 7 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f = 0.52 for **3cx** in 50% EtOAc–hexane) to afford product **3cx** (41 mg; 74% yield) as white solids. Mp: 161–162 °C. Selected spectroscopic data for **3cx**: IR (neat): 3206, 3066, 2961, 2923, 2855, 1702, 1504, 1260, 1021, 802, 746, 701 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.40 (s, 1 H), 7.43 – 7.34 (m, 5 H), 7.14 – 7.07 (m, 1 H), 7.02 – 6.89 (m, 3 H), 4.80 (d, J = 13.5 Hz, 1 H), 4.56 (s, 1 H), 4.07 (d, J = 13.5 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7 (C), 133.8 (C), 132.4 (C), 129.3 (two CH), 128.8 (three CH), 125.8 (C), 125.2 (CH), 122.10 (CH), 116.5 (CH), 114.4 (CH), 112.8 (C), 52.1 (CH_2), 51.9 (CH); MS (*m/z*, relative intensity): 264 (M^++1, 3), 263 (M^+, 20), 172 (1), 146 (19), 118 (3), 91 (100); exact mass calculated for $C_{16}H_{13}N_3O$: 263.1059; found: 263.1059.

Preparation of 4-benzyl-7-chloro-3-(1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ga):



To a solution of **1g** (50 mg, 0.18 mmol) and indole (42.1 mg, 0.36 mmol, 2 equiv) in CH_3OH (3.6 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact

florescence lamp (24 W) for 12 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.48 for **3ga** in 50% EtOAc–hexane) to afford product **3ga** (51.5 mg; 72% yield) as white solids. Mp: 200–201 °C. Selected spectroscopic data for **3ga**: IR (KBr): 3292, 3066, 2960, 1662, 1582, 1504, 1393, 1227, 948, 804, 740, 709 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.20 (brs, 1 H), 9.66 (s, 1 H), 7.57 (d, J = 8.0 Hz, 1 H), 7.40 – 7.25 (m, 6 H), 7.13 – 7.08 (m, 1 H), 7.06 – 6.97 (m, 3 H), 6.88 (dd, J = 8.5, 2.5 Hz, 1 H), 6.73 (d, J = 8.5 Hz, 1 H), 5.31 (s, 1 H), 4.64 (d, J = 15.5 Hz, 1 H), 4.38 (d, J = 15.5 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.7 (C), 138.5 (C), 137.6 (C), 134.7 (C), 129.9 (C), 129.5 (two CH), 128.5 (two CH), 128.2 (CH), 127.5 (C), 124.1 (CH), 123.8 (C), 123.5 (CH), 122.8 (CH), 120.4 (CH), 120.3 (CH), 115.5 (CH), 115.1 (CH), 112.4 (CH), 111.8 (C), 60.0 (CH), 52.9 (CH_2); MS (*m/z*, relative intensity): 389 (M^++2, 34), 388 (M^++1, 25), 387 (100), 358 (26), 296 (35), 268 (19), 230 (39), 153 (36), 130 (40), 91 (59); exact mass calculated for $C_{23}H_{18}ClN_3O$: 387.1138; found: 387.1136.



Thermal ellipsoids draw at the 50% probability level

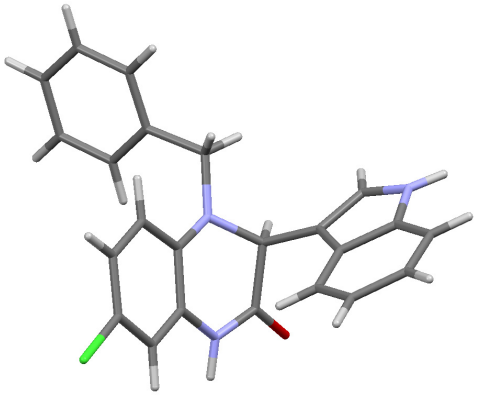


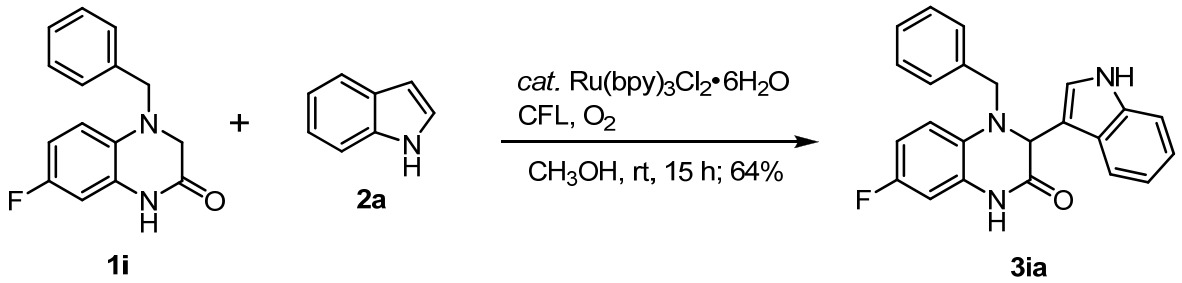
Figure S1. ORTEP and Stereo plots for X-ray crystal structures of **3ga** (**ic18529_sq**).

CCDC 1816893 contains the supplementary crystallographic data for **3ga** (**ic18529_sq**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S1. Crystal data and structure refinement for **3ga** (**ic 18529_sq**).

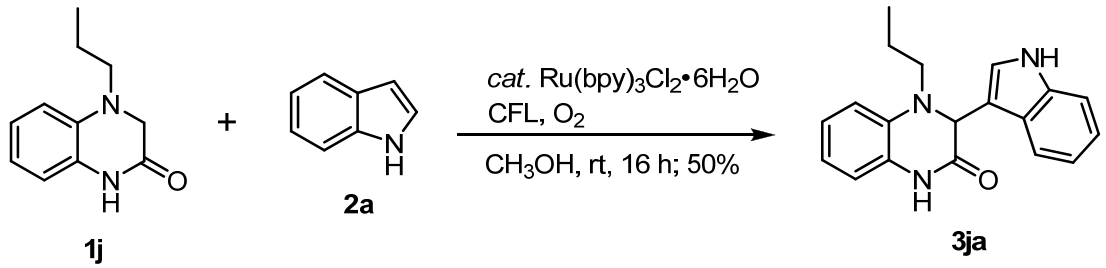
Identification code	ic18529_sq	
Empirical formula	C49 H42 Cl2 N6 O3	
Formula weight	833.78	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.3326(2) Å	α= 90°.
	b = 20.1095(4) Å	β= 95.5803(8)°.
	c = 22.0811(4) Å	γ = 90°.
Volume	4566.34(15) $Å^3$	
Z	4	
Density (calculated)	1.213 Mg/m^3	
Absorption coefficient	1.652 mm^{-1}	
F(000)	1744	
Crystal size	0.223 x 0.196 x 0.038 mm^3	
Theta range for data collection	2.979 to 69.977°.	
Index ranges	-12<=h<=12, -23<=k<=24, -26<=l<=26	
Reflections collected	30022	
Independent reflections	8662 [R(int) = 0.0218]	
Completeness to theta = 67.679°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.6652	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8662 / 6 / 559	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0453, wR2 = 0.1194	
R indices (all data)	R1 = 0.0539, wR2 = 0.1311	
Extinction coefficient	n/a	

Preparation of 4-benzyl-7-fluoro-3-(1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ia):



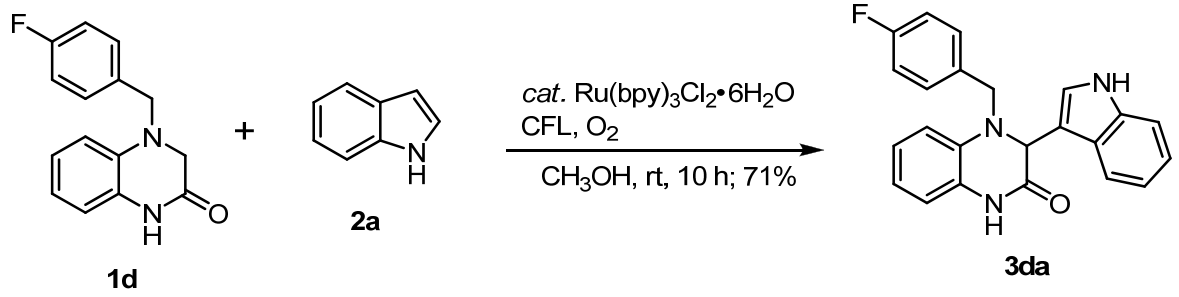
To a solution of **1i** (50 mg, 0.19 mmol) and indole (44.5 mg, 0.38 mmol, 2 equiv) in CH_3OH (3.8 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 15 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.46 for **3ia** in 50% EtOAc–hexane) to afford product **3ia** (46.2 mg; 64% yield) as white solids. Mp: 211–212 °C. Selected spectroscopic data for **3ia:** IR (KBr): 3287, 3189, 3059, 3027, 2977, 2925, 2885, 1661, 1603, 1521, 1408, 1225, 1153, 963, 844, 790, 736, 697 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.18 (brs, 1 H), 9.64 (s, 1 H), 7.56 (d, J = 8.0 Hz, 1 H), 7.40 – 7.31 (m, 5 H), 7.30 – 7.24 (m, 1 H), 7.12 – 7.08 (m, 1 H), 7.02 – 6.97 (m, 2 H), 6.84 (dd, J = 9.5, 3.0 Hz, 1 H), 6.73 – 6.69 (m, 1 H), 6.67 – 6.62 (m, 1 H), 5.27 (s, 1 H), 4.60 (d, J = 15.0 Hz, 1 H), 4.35 (d, J = 15.0 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 167.2 (C), 157.5 (d, J = 234.4 Hz, C), 138.7 (C), 137.5 (C), 132.3 (d, J = 2.3 Hz, C), 130.0 (d, J = 10.5 Hz, C), 129.5 (two CH), 128.6 (two CH), 128.2 (CH), 127.6 (C), 124.0 (CH), 122.7 (CH), 120.3 (CH), 120.2 (CH), 114.8 (d, J = 8.8 Hz, CH), 112.4 (CH), 111.6 (C), 109.4 (d, J = 22.1 Hz, CH), 103.3 (d, J = 26.3 Hz, CH), 60.0 (CH), 53.3 (CH_2); MS (*m/z*, relative intensity): 372 (M^++1, 35), 371 (M^+, 100), 343 (15), 342 (35), 280 (44), 252 (36), 251 (28), 214 (42), 213 (32), 137 (50), 130 (46), 91 (76); exact mass calculated for $C_{23}H_{18}FN_3O$: 371.1434; found: 371.1437.

Preparation of 3-(1*H*-indol-3-yl)-4-propyl-3,4-dihydroquinoxalin-2(1*H*)-one (3ja):



To a solution of **1i** (50 mg, 0.26 mmol) and indole (60.9 mg, 0.52 mmol, 2 equiv) in CH_3OH (5.2 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 16 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 20% EtOAc–hexane (R_f = 0.46 for **3ja** in 40% EtOAc–hexane) to afford product **3ja** (40.5 mg; 50% yield) as pale yellow solids. Mp: 189–190 °C. Selected spectroscopic data for **3ja**: IR (KBr): 3290, 3184, 3056, 2960, 2926, 2869, 1660, 1507, 1430, 1245, 1099, 739 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.09 (brs, 1 H), 9.42 (s, 1 H), 7.68 (d, J = 8.0 Hz, 1 H), 7.35 (d, J = 8.0 Hz, 1 H), 7.08 (dd, J = 8.0, 7.0 Hz, 1 H), 7.01 – 6.93 (m, 4 H), 6.81 (d, J = 8.0 Hz, 1 H), 6.77 – 6.72 (m, 1 H), 5.27 (s, 1 H), 3.50 – 3.42 (m, 1 H), 3.16 – 3.08 (m, 1 H), 1.76 – 1.56 (m, 2 H), 0.94 (t, J = 7.5 Hz, 3 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.6 (C), 137.6 (C), 135.9 (C), 128.3 (C), 127.5 (C), 124.3 (CH), 123.9 (CH), 123.7 (C), 122.6 (CH), 120.6 (CH), 120.1 (CH), 118.9 (CH), 115.9 (CH), 112.9 (CH), 112.2 (CH), 60.4 (CH), 51.0 (CH_2), 21.1 (CH_2), 11.7 (CH_3); MS (m/z, relative intensity): 306 (M^++1, 23), 305 (M^+, 100), 277 (29), 276 (87), 262 (17), 248 (24), 234 (16), 161 (13), 130 (52), 119 (64); exact mass calculated for $C_{19}H_{19}N_3O$: 305.1528; found: 305.1526.

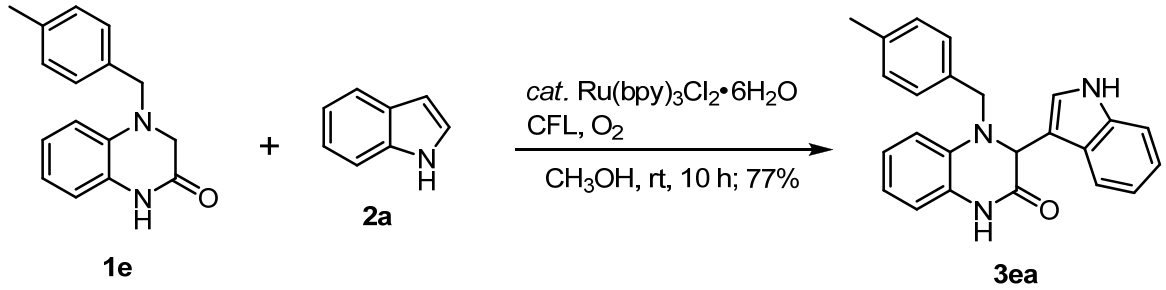
Preparation of 4-(4-fluorobenzyl)-3-(1*H*-indol-3-yl)-3,4-dihydroquinoxalin-2(1*H*)-one (3da):



To a solution of **1d** (50 mg, 0.19 mmol) and indole (46.8 mg, 0.4 mmol, 2 equiv) in CH_3OH (3.9 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 10 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.44 for **3da** in 50% EtOAc–hexane) to afford product **3da** (51.5 mg; 71% yield) as white solids. Mp: 227–228 °C. Selected spectroscopic data for **3da**: IR (KBr): 3441, 3331, 3185, 3066, 2987, 2922, 2828, 1683, 1507, 1374, 1224, 1151, 1102, 828, 742 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 10.15 (brs, 1 H), 9.53 (s, 1 H), 7.56 (d, J = 8.0

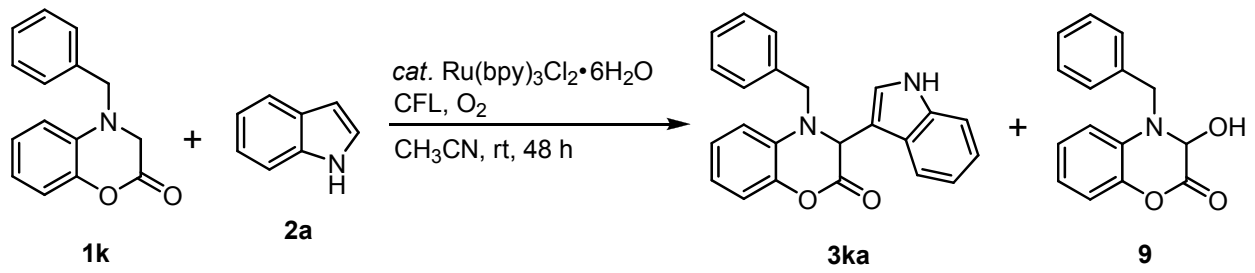
Hz, 1 H), 7.43 – 7.36 (m, 3 H), 7.12 – 7.06 (m, 3 H), 7.02 – 6.95 (m, 3 H), 6.91 – 6.86 (m, 1 H), 6.81 – 6.77 (m, 1 H), 6.74 (d, J = 8.0 Hz, 1 H), 5.27 (s, 1 H), 4.64 (d, J = 15.0 Hz, 1 H), 4.34 (d, J = 15.0 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ166.9 (C), 163.0 (d, J = 243.2 Hz, C), 137.6 (C), 135.6 (C), 135.0 (d, J = 3.1 Hz, C), 130.4 (d, J = 8.1 Hz, two CH), 128.8 (C), 127.6 (C), 124.2 (CH), 124.1 (CH), 122.7 (CH), 120.5 (CH), 120.2 (CH), 119.8 (CH), 116.1 (d, J = 21.5 Hz, two CH), 115.9 (CH), 114.0 (CH), 112.3 (CH), 112.0 (C), 60.2 (CH), 52.1 (CH_2); MS (*m/z*, relative intensity): 373 (M^++2, 5), 372 (M^++1, 37), 371 (M^+, 100), 342 (47), 262 (53), 234 (31), 233 (25), 214 (50), 213 (39), 130 (41), 119 (46), 109 (82), 92 (16); exact mass calculated for $C_{23}H_{18}FN_3O$: 371.1434; found: 371.1434.

Preparation of 3-(1*H*-indol-3-yl)-4-(4-methylbenzyl)-3,4-dihydroquinoxalin-2(1*H*)-one (3ea):



To a solution of **1e** (50 mg, 0.20 mmol) and indole (44.5 mg, 0.4 mmol, 2 equiv) in CH_3OH (3.8 mL) was added $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 10 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 25% EtOAc–hexane (R_f = 0.40 for **3ea** in 50% EtOAc–hexane) to afford product **3ea** (56.2 mg; 77% yield) as white solids. Mp: 218–220 °C. Selected spectroscopic data for **3ea:** IR (KBr): 3254, 3179, 3038, 2974, 2897, 2851, 1655, 1503, 1415, 1219, 1150, 1109, 738 cm^{-1}; ^{1}H NMR (500 MHz, acetone-d_6): δ 10.14 (brs, 1 H), 9.51 (s, 1 H), 7.55 (d, J = 8.0 Hz, 1 H), 7.37 (d, J = 8.0 Hz, 1 H), 7.24 (d, J = 7.5 Hz, 2 H), 7.14 (d, J = 8.0 Hz, 2 H), 7.11 – 7.07 (m, 1 H), 7.01 – 6.95 (m, 3 H), 6.91 – 6.87 (m, 1 H), 6.80 – 6.75 (m, 2 H), 5.25 (s, 1 H), 4.62 (d, J = 15.5, 1 H), 4.27 (d, J = 15.5, 1 H), 2.31 (s, 3 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 166.9 (C), 137.6 (C), 137.5 (C), 136.0 (C), 135.7 (C), 130.1 (two CH), 128.7 (C), 128.6 (two CH), 127.6 (C), 124.2 (CH), 124.0 (CH), 122.6 (CH), 120.5 (CH), 120.1 (CH), 119.6 (CH), 115.9 (CH), 114.0 (CH), 112.3 (CH), 112.1 (C), 59.9 (CH), 52.4 (CH_2), 21.2 (CH_3); MS (*m/z*, relative intensity): 368 (M^++1, 7), 367 (M^+, 26), 338 (6), 262 (10), 234 (8), 210 (8), 209 (9), 171 (43), 170 (100), 169 (55), 168 (23), 144 (22), 105 (24), 85 (19); exact mass calculated for $C_{24}H_{21}N_3O$: 367.1685; found: 367.1685.

Preparation of 4-benzyl-3-(1*H*-indol-3-yl)-3,4-dihydro-2*H*-benzo[*b*] [1,4]oxazin-2-one (3ka) and 9



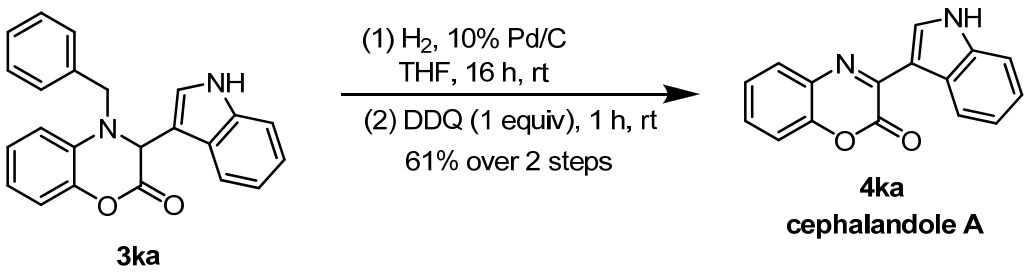
To a solution of **1k** (50 mg, 0.209 mmol) and indole (48 mg, 0.4 mmol, 2 equiv) in CH_3CN (4.1 mL) was added $Ru(bpy)_3Cl_2•6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv). The solution was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 48 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 15% EtOAc–hexane (R_f = 0.38 for **3ka** in 25% EtOAc–hexane) to afford product **3ka** (32.6 mg; 44% yield) as gummy compound and **9** (10.5 mg; 20% yield; R_f= 0.26 for **9** in 25% EtOAc–hexane) as brown color gummy compound.

Selected spectroscopic data for **3ka**: IR (neat): 3416, 2963, 1748, 1613, 1501, 1260, 1095, 1020, 800, 744 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 8.08 (s, 1 H), 7.48 (d, J = 8.0 Hz, 1 H), 7.36 – 7.24 (m, 6 H), 7.18 (dd, J = 7.5, 7.5 Hz, 1 H), 7.10 (dd, J = 7.5, 7.5 Hz, 2 H), 7.05 (dd, J = 8.0, 7.5 Hz, 1 H), 6.89 (dd, J = 8.0, 7.5 Hz, 1 H), 6.80 (d, J = 8.0 Hz, 1 H), 6.71 (d, J = 2.5, 1 H), 5.38 (s, 1 H), 4.60 (d, J = 14.5 Hz, 1 H), 4.14 (d, J = 14.5 Hz, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.5 (C), 141.9 (C), 136.1 (C), 135.8 (C), 134.2 (C), 128.8 (two CH), 127.80 (two CH), 127.78 (CH), 126.1 (C), 125.4 (CH), 122.8 (two CH), 120.5 (CH), 119.9 (CH), 119.2 (CH), 116.6 (CH), 113.9 (CH), 111.2 (CH), 108.8 (C), 55.9 (CH), 51.6 (CH_2);[12] MS (*m/z*, relative intensity): 355 (M^++1, 9), 354 (M^+, 34), 338 (19), 326 (51), 276 (17), 235 (100), 196 (28), 157 (19), 129 (30), 119 (25), 91 (61); exact mass calculated for $C_{23}H_{18}N_2O_2$: 354.1368; found: 354.1371.

Selected spectroscopic data for **9**: IR (neat): 3323, 2925, 2854, 1671, 1500, 1242, 1035, 753 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 7.34 – 7.27 (m, 2 H), 7.26 – 7.21 (m, 3 H), 7.07 (dd, J = 8.0, 1.0 Hz, 1 H), 7.04 – 6.98 (m, 1 H), 6.97 – 6.89 (m, 2 H), 5.73 (s, 1 H), 5.27 (d, J = 16.0 Hz, 1 H), 5.06 (d, J = 16.0 Hz, 1 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.0 (C), 142.0 (C), 135.4 (C), 128.9 (two CH), 128.0 (C), 127.6 (CH), 126.5 (two CH), 124.5 (CH), 123.3 (CH), 118.2 (CH), 115.7 (CH), 90.6 (CH), 45.6 (CH_2); MS (*m/z*, relative intensity): 255 (M^+, 7), 226 (19), 148 (3), 136 (2), 111 (2), 91 (100); exact mass calculated for $C_{15}H_{13}NO_3$: 255.0895; found: 255.0893.

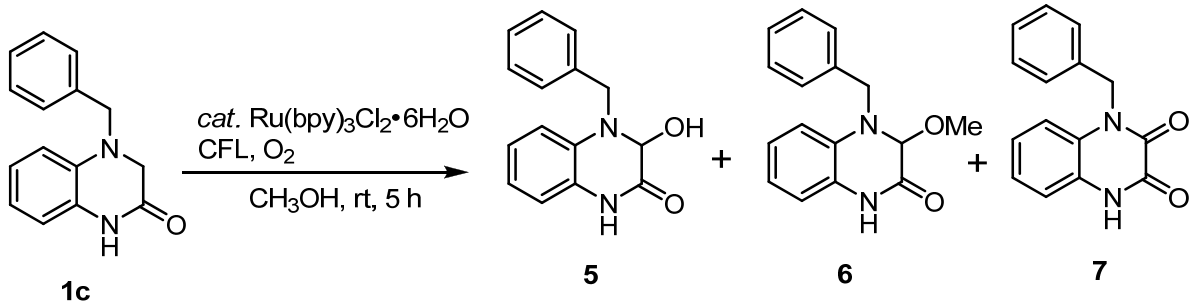
[12] Huo, C.; Dong, J.; Su, Y.; Tang, J.; Chen, F. *Chem. Commun.* **2016**, *52*, 13341 – 13344.

Preparation of natural product cephalandole A (4ka):



To a solution of **3ka** (50 mg, 0.14 mmol) in dry THF (1 mL) 10% Pd/C (10 mg) was added and the reaction mixture was stirred under hydrogen atmosphere for 16 h, diluted with THF (1 mL) added DDQ (32 mg, 0.14 mmol, 1.0 equiv) and stirred for 1 h under nitrogen atmosphere. The reaction mixture was filtered through celite. The organic layer was concentrated in vacuo to give the crude residue. The crude product was purified by flash column chromatography with 10% EtOAc–hexane (R_f= 0.45 for **4ka** in 25% EtOAc–hexane) to afford compound **4ka** (22.5 mg, 61% yield) as yellow solid; Mp: 247–248 °C. Selected spectroscopic data for **4ka**: IR (neat): 3297, 3052, 2959, 2923, 1718, 1605, 1531, 1429, 1238, 1103, 940, 742 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 11.04 (brs, 1 H), 8.91 – 8.87 (m, 1 H), 8.82 (d, J = 3.5 Hz, 1 H), 7.88 (dd, J = 8.0, 1.5 Hz, 1 H), 7.59 – 7.55 (m, 1 H), 7.51 – 7.46 (m, 1 H), 7.45 – 7.40 (m, 1 H), 7.35 – 7.33 (m, 1 H), 7.31 – 7.25 (m, 2 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 153.1 (C), 149.1 (C), 146.3 (C), 138.0 (C), 134.7 (CH), 133.3 (C), 129.7 (CH), 129.0 (CH), 127.5 (C), 126.2 (CH), 124.3 (CH), 124.2 (CH), 122.6 (CH), 116.8 (CH), 112.8 (CH), 112.5 (C);[13] MS (*m/z*, relative intensity): 263 (M^++1, 9), 262 (M^+, 52), 235 (17), 234 (100), 205 (13), 142 (15), 117 (7), 115 (11), 103 (4); exact mass calculated for $C_{16}H_{10}N_2O_2$: 262.0742; found: 262.0745.

Preparation of 5, 6 and 7

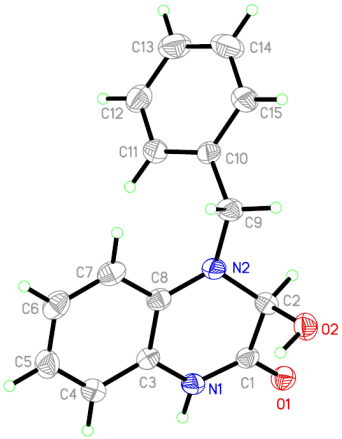


A solution of **1c** (50 mg, 0.21 mmol) and $Ru(bpy)_3Cl_2$•$6H_2O$ (2.9 mg, 0.004 mmol, 0.02 equiv) in CH_3OH (4.1 mL) was stirred under an oxygen atmosphere at room temperature and irradiated

[13] (a) Huo, C.; Dong, J.; Su, Y.; Tang, J.; Chen, F. *Chem. Commun.* **2016**, *52*, 13341–13344. (b) Mason, J. J.; Bergman, J.; Janosik, T. *J. Nat. Prod.* **2008**, *71*, 1447–1450.

with a household compact florescence lamp (24 W) for 5 h until the completion of the reaction. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f= 0.30 for **5**, and R_f= 0.32 for **6** in 50% EtOAc–hexane) to afford mixture of compounds **5** (14.1 mg; 26% yield) and **6** (30.1 mg, 53% yield) and **7** (7.1 mg, 13% yield; R_f = 0.23 in 50% EtOAc–hexane) as white solids.

For **5**: mp, 137–138 °C; IR (KBr): 3304, 3187, 3039, 2922, 2854, 1664, 1510, 1385, 1312, 994, 964, 746, 700 cm^{-1}; ^1H NMR (500 MHz, acetone-d_6): δ 9.60 (brs, 1 H), 7.41 (d, J = 8.0 Hz, 2 H), 7.33 (dd, J = 7.5, 7.5 Hz, 2 H), 7.26 (dd, J = 7.5, 7.5 Hz, 1 H), 7.00 (dd, J = 8.0, 1.5 Hz, 1 H), 6.89 – 6.84 (m, 1 H), 6.82 – 6.77 (m, 2 H), 5.53 (d, J = 6.5 Hz, 1 H), 5.16 (d, J = 6.5 Hz, 1 H), 4.81 (d, J = 15.0 Hz, 1 H), 4.59 (d, J = 15.0 Hz, 1 H); ^{13}C NMR (125 MHz, acetone-d_6): δ 164.4 (C), 138.7 (C), 133.0 (C), 129.4, (two CH), 128.6 (two CH), 128.1 (CH), 127.8 (C), 123.7 (CH), 120.3 (CH), 115.9 (CH), 114.9 (CH), 82.1 (CH), 52.5 (CH_2); MS (*m/z*, relative intensity): 253 (M^+–1, 1), 238 (1), 208 (2), 178 (3), 167 (4), 149 (15), 136 (14), 105 (41), 101 (28), 77 (62), 58 (100); exact mass calculated for $C_{15}H_{14}N_2O_2$: 254.1055; found: 254.1058.



Thermal ellipsoids draw at the 50% probability level

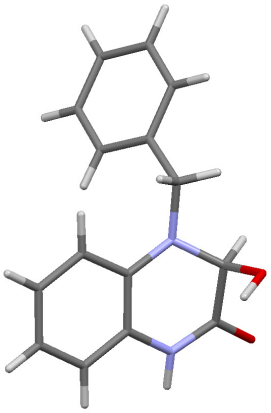


Figure S1. ORTEP and Stereo plots for X-ray crystal structures of **5** (**ic18595**).

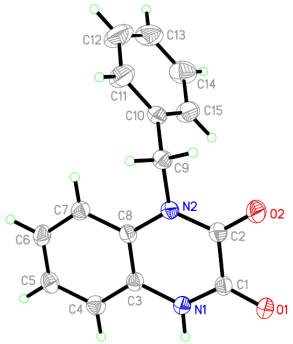
CCDC 1816894 contains the supplementary crystallographic data for **5** (**ic18595**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S1. Crystal data and structure refinement for **5** (**ic18595**).

Identification code	ic18595	
Empirical formula	C15 H14 N2 O2	
Formula weight	254.28	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 28.8295(7) Å	α= 90°.
	b = 4.67620(10) Å	β= 117.3759(6)°.
	c = 20.3019(5) Å	γ = 90°.
Volume	2430.43(10) $Å^3$	
Z	8	
Density (calculated)	1.390 Mg/m^3	
Absorption coefficient	0.761 mm^{-1}	
F(000)	1072	
Crystal size	0.362 x 0.109 x 0.064 mm^3	
Theta range for data collection	4.518 to 69.965°.	
Index ranges	-34<=h<=34, -5<=k<=5, -24<=l<=24	
Reflections collected	7758	
Independent reflections	2301 [R(int) = 0.0196]	
Completeness to theta = 67.679°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.6290	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2301 / 0 / 178	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0365, wR2 = 0.0927	
R indices (all data)	R1 = 0.0374, wR2 = 0.0935	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.349 and -0.194 $e.Å^{-3}$	

For **6**: yellow gummy compound; IR (neat): 3211, 3062, 2924, 2855, 1687, 1508, 1384, 1054, 922, 742, 697 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.76 (brs, 1 H), 7.37 – 7.21 (m, 5 H), 6.98 – 6.91 (m, 1 H), 6.87 – 6.77 (m, 3 H), 4.80 (d, J = 15.0 Hz, 1 H), 4.74 (s, 1 H), 4.52 (d, J = 14.5 Hz, 1 H), 3.37 (s, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.2 (C), 136.1 (C), 131.7 (C), 128.8 (two CH), 127.8 (two CH), 127.7 (CH), 124.9 (C), 124.1 (CH), 120.1 (CH), 115.5 (CH), 113.5 (CH), 87.9 (CH_3), 56.5 (CH), 52.6 (CH_2); MS (*m/z*, relative intensity): 269 (M^++1, 3), 268 (M^+, 13), 237 (9), 209 (24), 208 (16), 146 (11), 118 (11), 91 (100); exact mass calculated for $C_{16}H_{16}N_2O_2$: 268.1212; found: 268.1212.

For **7**: mp: 268–269 °C; IR (neat): 3189, 3052, 2997, 2913, 2869, 2776, 1684, 1503, 1387, 1259, 882, 766 cm^{-1}; ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.10 (brs, 1 H), 7.34 – 7.23 (m, 5 H), 7.21 – 7.16 (m, 2 H), 7.15 – 7.10 (m, 1 H), 7.08 – 7.04 (m, 1 H), 5.38 (s, 2 H);[14] ^{13}C NMR (125 MHz, DMSO-d_6): δ 155.7 (C), 153.6 (C), 135.7 (C), 128.6 (two CH), 127.2 (CH), 126.6 (two CH), 126.3 (C), 125.9 (C), 123.6 (CH), 123.0 (CH), 115.7 (CH), 115.4 (CH), 45.5 (CH_2); MS (*m/z*, relative intensity): 253 (M^++1, 8), 252 (M^+, 47), 235 (2), 224 (2), 195 (2), 161 (2), 146 (3), 133 (6), 119 (3), 106 (3), 92 (10), 91 (100); exact mass calculated for $C_{15}H_{12}N_2O_2$: 252.0899; found: 252.0898.



Thermal ellipsoids draw at the 50% probability level

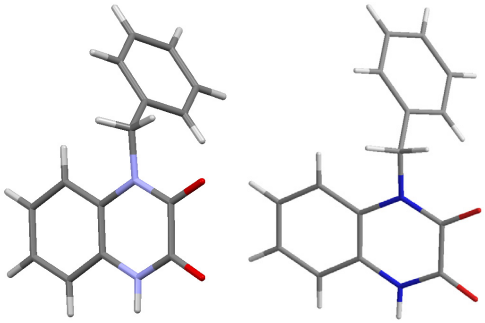


Figure S1. ORTEP and Stereo plots for X-ray crystal structures of **7** (**ic18614**).

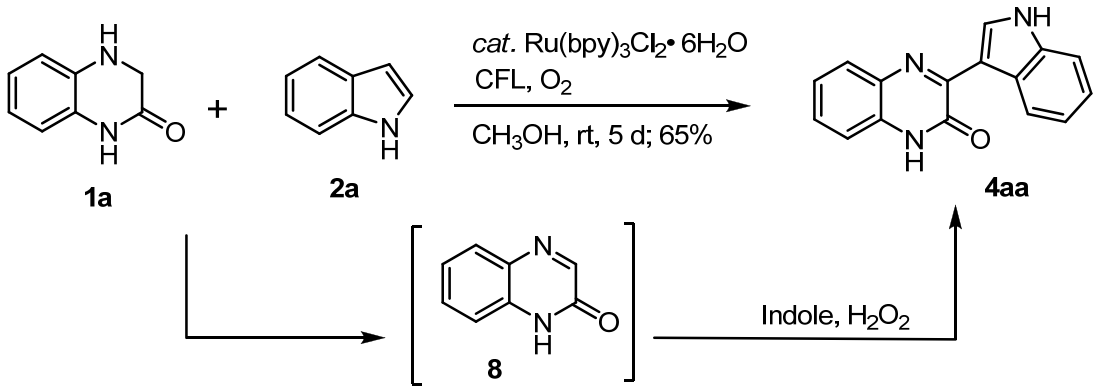
CCDC 1816895 contains the supplementary crystallographic data for **7** (**ic18614**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

[14] Jarrar, A. A.; Fataftah, Z. A. *Tetrahedron* **1977**, *33*, 2127–2129.

Table S1. Crystal data and structure refinement for **7** (**ic18614**)..

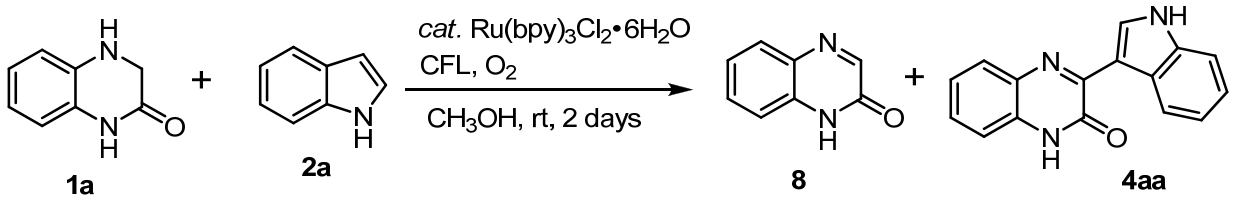
Identification code	ic18614	
Empirical formula	C15 H12 N2 O2	
Formula weight	252.27	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.6642(2) Å	α= 86.2570(7)°.
	b = 7.5948(2) Å	β= 87.5435(7)°.
	c = 12.0893(3) Å	γ = 79.1977(7)°.
Volume	599.46(3) $Å^3$	
Z	2	
Density (calculated)	1.398 Mg/m^3	
Absorption coefficient	0.771 mm^{-1}	
F(000)	264	
Crystal size	0.241 x 0.164 x 0.061 mm^3	
Theta range for data collection	7.169 to 69.988°.	
Index ranges	-8<=h<=8, -9<=k<=9, -14<=l<=14	
Reflections collected	4360	
Independent reflections	2256 [R(int) = 0.0128]	
Completeness to theta = 67.679°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.6296	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2256 / 0 / 176	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0925	
R indices (all data)	R1 = 0.0366, wR2 = 0.0936	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.193 and -0.173 $e.Å^{-3}$	

Preparation of 3-(1*H*-indol-3-yl)quinoxalin-2(1*H*)-one



A solution of **1a** (50 mg, 0.338 mmol), indole (77.3 mg, 0.66 mmol, 2 equiv) and $Ru(bpy)_3Cl_2$•$6H_2O$ (4.5 mg, 0.007 mmol, 0.02 equiv) in CH_3OH (6.7 mL) was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp (24 W) for 2 until the completion of the reaction, as monitored by TLC. **1a** was completely converted into **8** with trace amounts of **4aa**, determined by crude ^{1}H-NMR of reaction mixture. The reaction was continued to for 5 days until **8** was converted into **4aa** monitored by the TLC. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f= 0.33 for **4aa** in 50% EtOAc–hexane) to afford compound **4aa** (57.3 mg, 65% yield) as yellow solids. Mp: 332–334 °C. Selected spectroscopic data for **4aa:** ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.39 (brs, 1 H), 11.77 (brs, 1 H), 8.94 (s, 1 H), 8.89 – 8.85 (m, 1 H), 7.86 (d, J = 8.0 Hz, 1 H), 7.53 – 7.49 (m, 1 H), 7.45 – 7.40 (m, 1 H), 7.34 – 7.28 (m, 2H), 7.26 – 7.20 (m, 2 H), ^{13}C NMR (125 MHz, DMSO-d_6): δ 154.4 (C), 151.9 (C), 136.2 (C), 133.0 (CH), 132.6 (C), 130.1 (C), 127.9 (CH), 127.5 (CH), 126.1 (C), 123.2 (CH), 122.9 (CH), 122.5 (CH), 120.9 (CH), 114.9 (CH), 111.8 (CH), 111.3 (C).[15]

Preparation of quinoxalin-2(1*H*)-one (8)



A solution of **1a** (50 mg, 0.338 mmol), indole (77.3 mg, 0.66 mmol, 2 equiv) and $Ru(bpy)_3Cl_2$•$6H_2O$ (4.5 mg, 0.007 mmol, 0.02 equiv) in CH_3OH (6.7 mL) was stirred under an oxygen atmosphere at room temperature and irradiated with a household compact florescence lamp

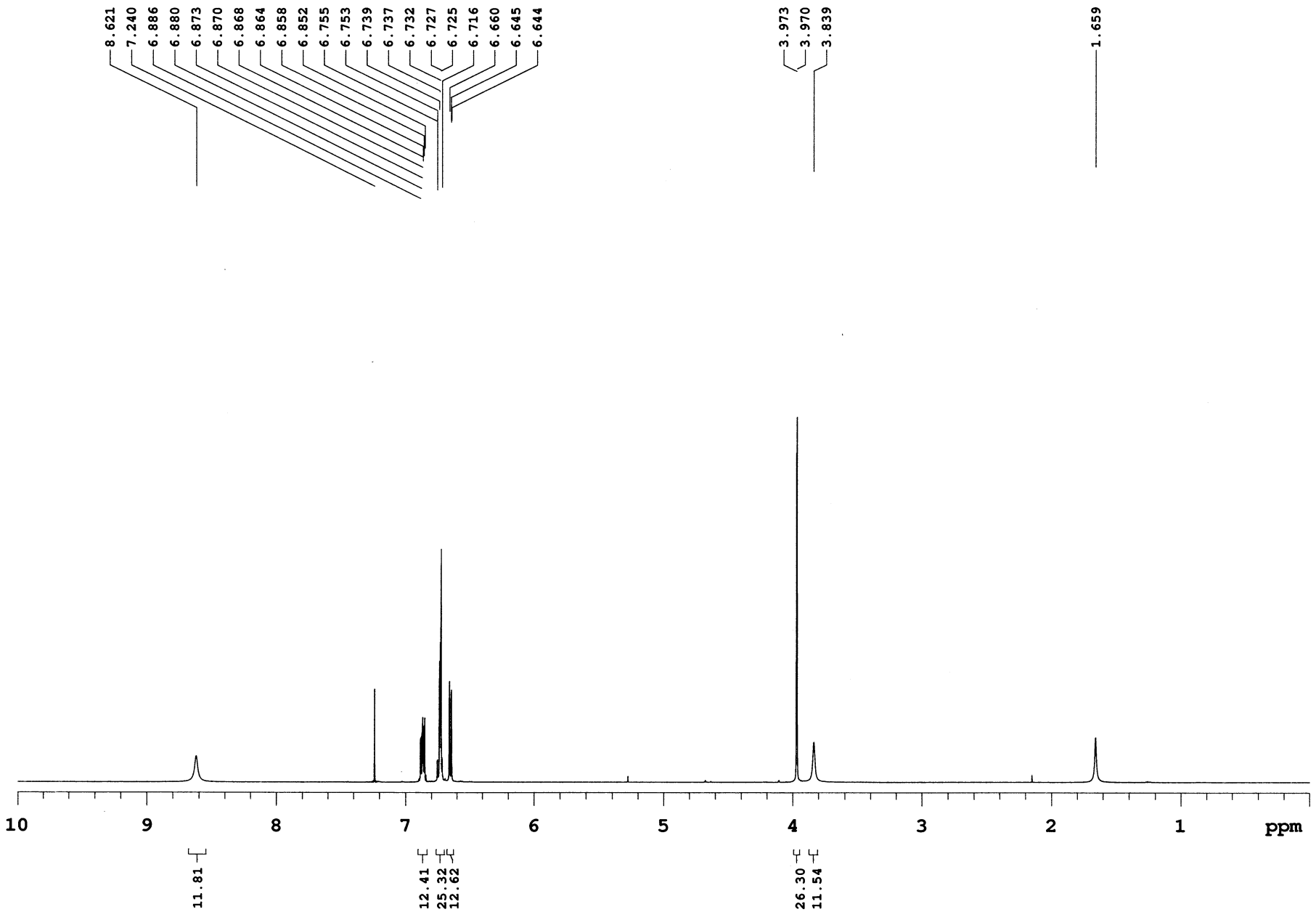
[15] (a) Han, Y.-Y.; Wu, Z.-J.; Zhang, X.-M.; Yuan, W.-C. *Tetrahedron Lett.* **2010**, *51*, 2023 – 2028. (b) Aoki, K.; Koseki, J.-I.; Takeda, S.; Aburada, M.; Miyamoto, K.-I. *Chem. Pharm. Bull.* **2007**, *55*, 922 – 925.

(24 W) for 2 until the completion of the reaction, as monitored by TLC. The reaction mixture was concentrated in *vacuo* to give a residue. The crude product was purified by flash column chromatography with 30% EtOAc–hexane (R_f = 0.31 for **8** in 50% EtOAc–hexane) to afford compound **8** (34.9 mg, 71% yield) as yellow solids and trace amount of **4aa** (around 1 mg). For **8**: mp, 261–263 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.41 (brs, 1 H), 8.16 (s, 1 H), 7.77 (d, J = 7.5 Hz, 1 H), 7.56 – 7.52 (m, 1 H), 7.32 – 7.27 (m, 2 H), ^{13}C NMR (125 MHz, DMSO-d_6): δ 154.9 (C), 151.6 (CH), 132.0 (C), 131.8 (C), 130.7 (CH), 128.7 (CH), 123.2 (CH), 115.7 (CH).[16]

[16] Han, Y.-Y.; Wu, Z.-J.; Zhang, X.-M.; Yuan, W.-C. *Tetrahedron Lett.* **2010**, *51*, 2023 – 2028.

APS-01-128

Sample Name **APS-01-128**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-128/PROTON_19

Fig S48. 1H NMR (CDCl3, 500 MHz) of compound 1a

Plot date 2017-05-31

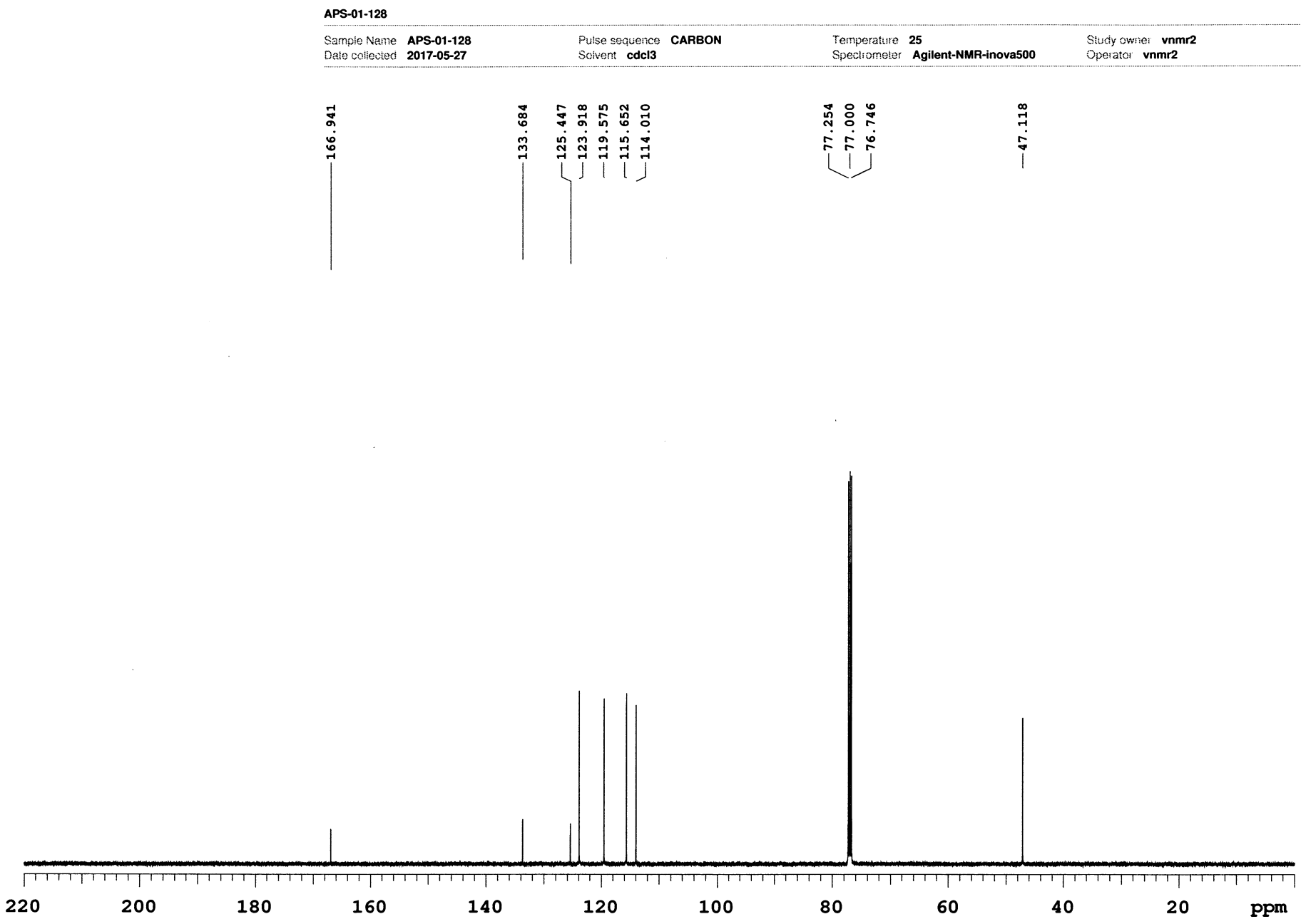


Fig S49. 13C NMR (CDCl3, 125 MHz) of compound 1a

APS-01-128

Sample Name **APS-01-128**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-27**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

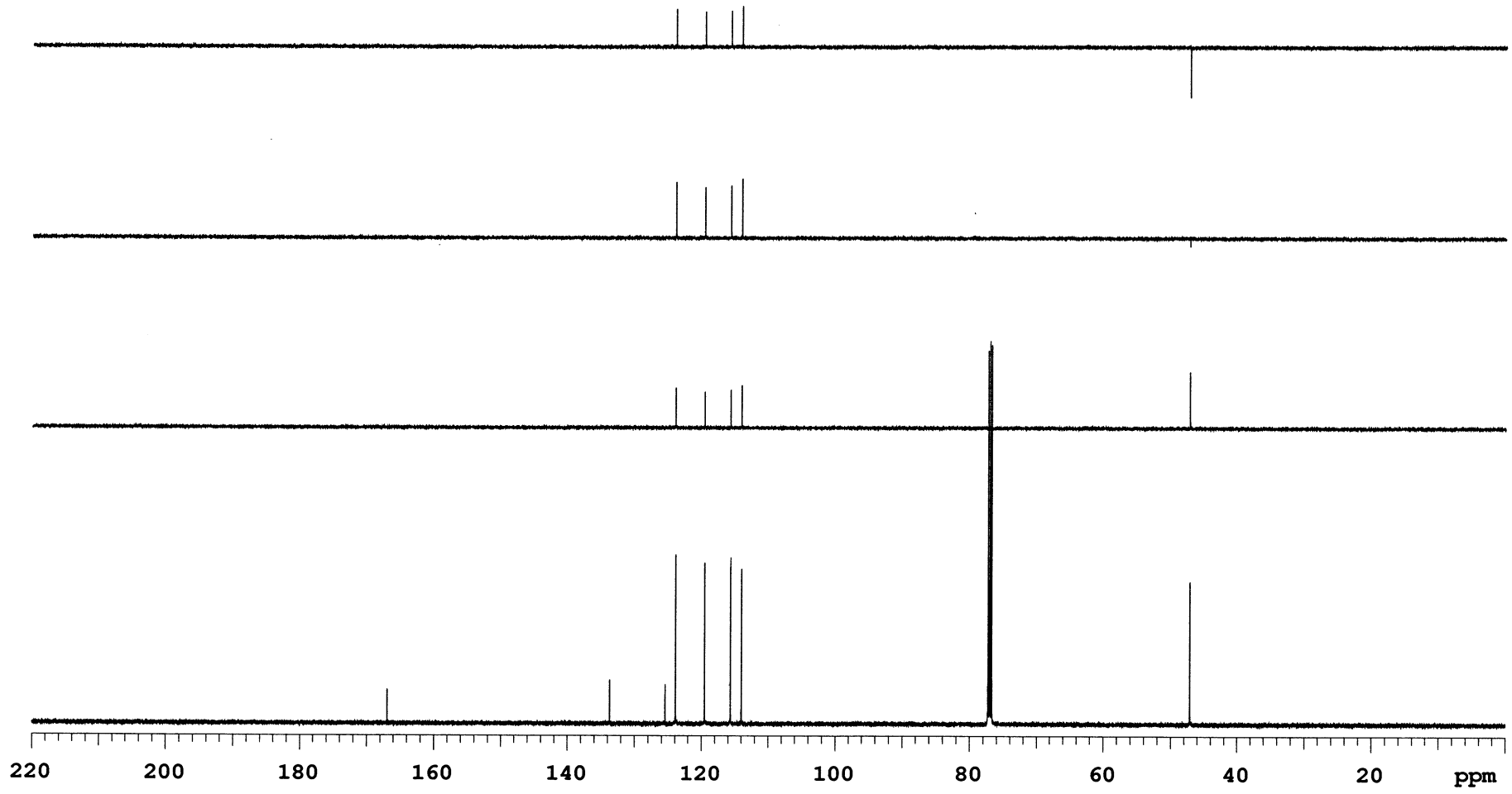
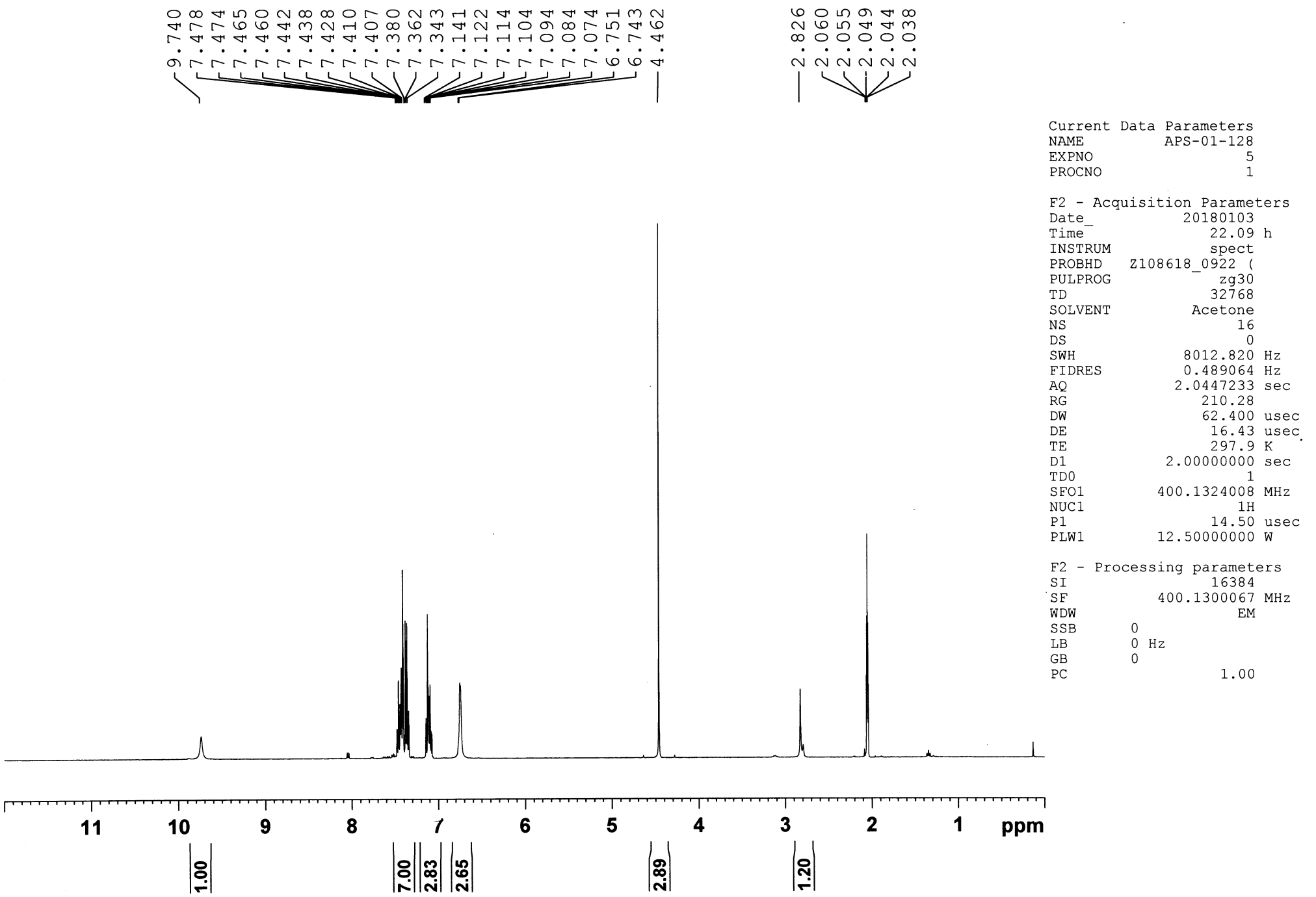


Fig S50. DEPT of compound 1a

Fig S51. 1H NMR (acetone-d6, 400 MHz) of compound 1b

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PROCNO                 1

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PULPROG             zg30
TD                 32768
SOLVENT          Acetone
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES             0.489064 Hz
AQ              2.0447233 sec
RG                 210.28
DW                 62.400 usec
DE                 16.43 usec
TE                 297.9 K
D1              2.00000000 sec
TD0                    1
SFO1          400.1324008 MHz
NUC1                  1H
P1                 14.50 usec
PLW1          12.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300067 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
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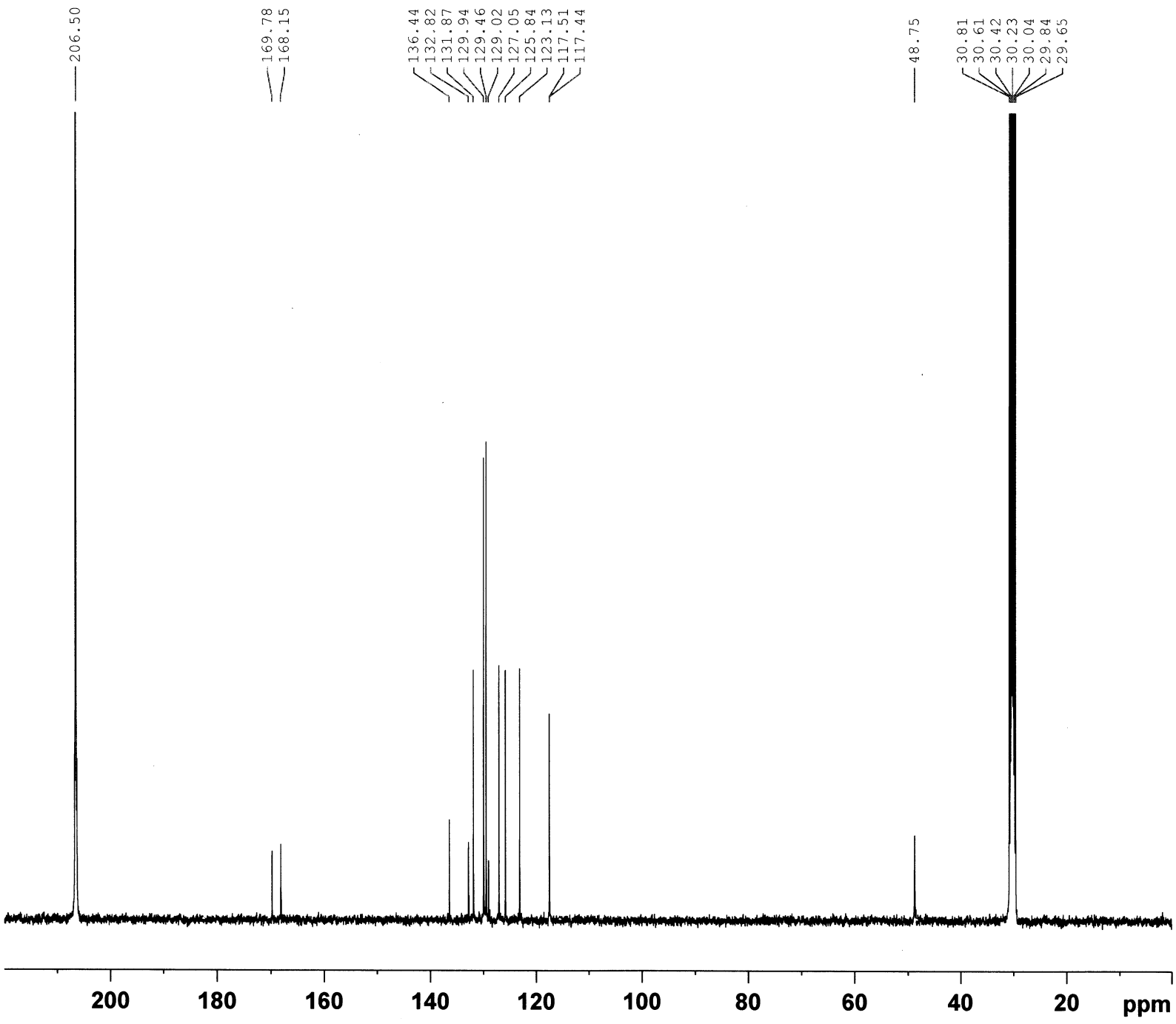
Fig S52. 13C NMR (acetone-d6, 100 MHz) of compound 1b

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EXPNO                  6
PROCNO                 1

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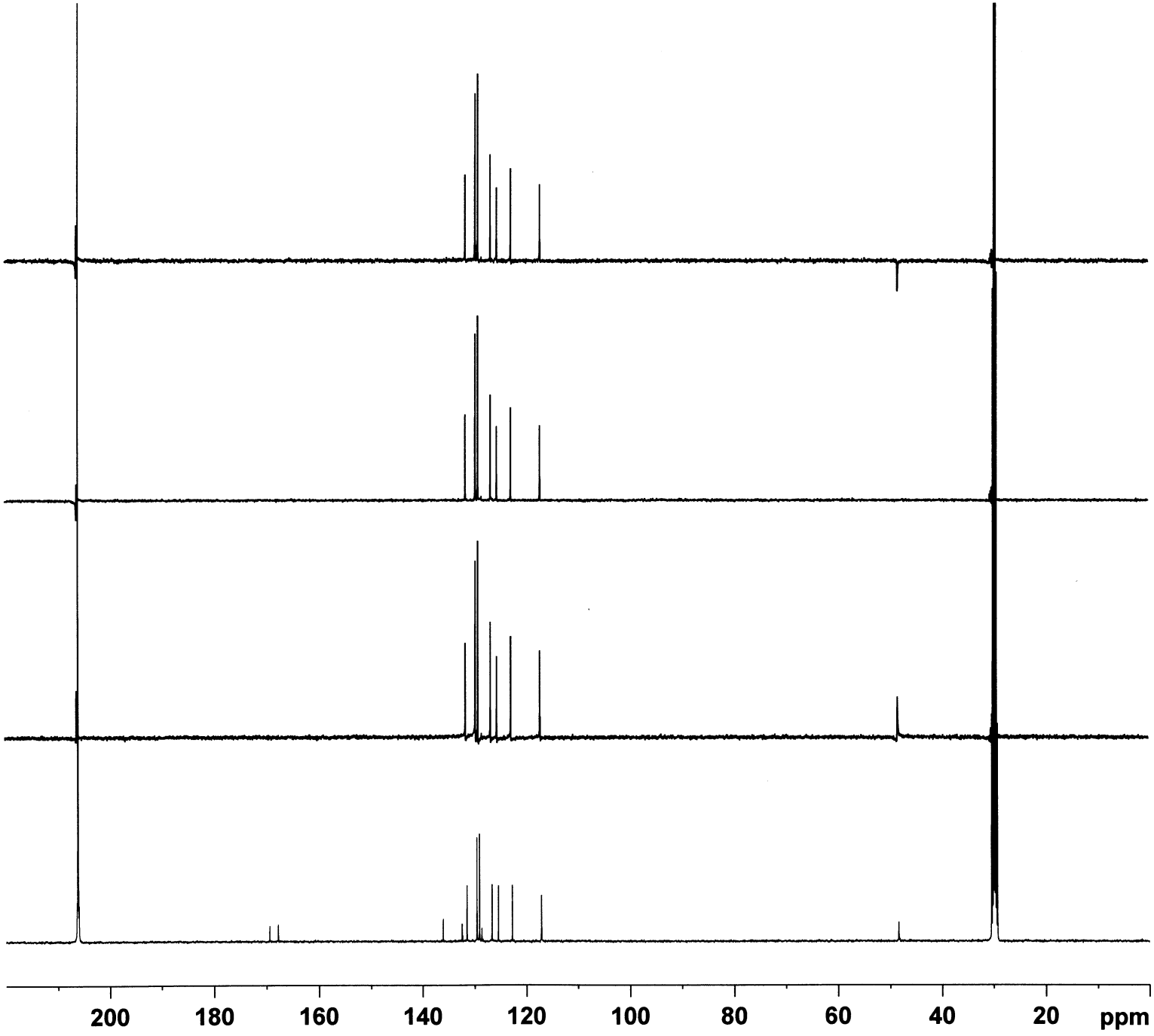
PULPROG          zgpg30
TD                32768
SOLVENT         Acetone
NS                 4096
DS                    0
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               299.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6233329 MHz
NUC1               13C
P1                9.90 usec
PLW1        43.00000000 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2        13.00000000 W
PLW12        0.33744001 W
PLW13        0.16946000 W

F2 - Processing parameters
SI                32768
SF          100.6126374 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
```

Fig S53. DEPT of compound 1b

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EXPNO                  7
PROCNO                 1

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PULPROG          dept45
TD                32768
SOLVENT         Acetone
NS                 2048
DS                    8
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               210.28
DW               20.800 usec
DE                6.50 usec
TE               298.9 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1
SFO1         100.6233300 MHz
NUC1                 13C
P1                9.90 usec
P2               19.80 usec
PLW1         43.00000000 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
P3               14.50 usec
P4               29.00 usec
PCPD2            90.00 usec
PLW2         13.00000000 W
PLW12         0.33744001 W

F2 - Processing parameters
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WDW                  EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
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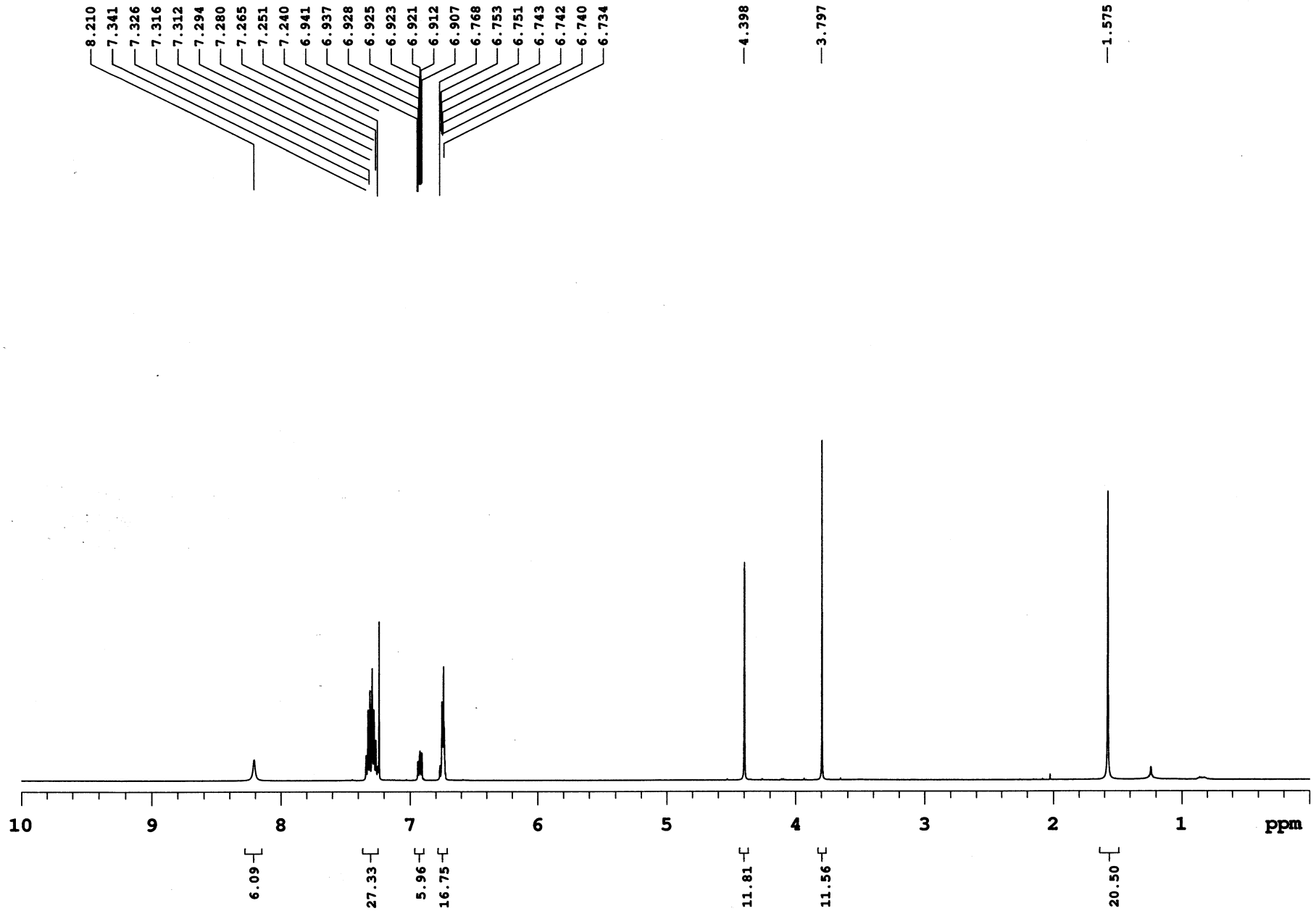
APS-01-129

Sample Name	**APS-01-129**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-10-18**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-129/PROTON_02

Fig S54. 1H NMR (CDCl3, 500 MHz) of compound 1c

Plot date 2016-10-18

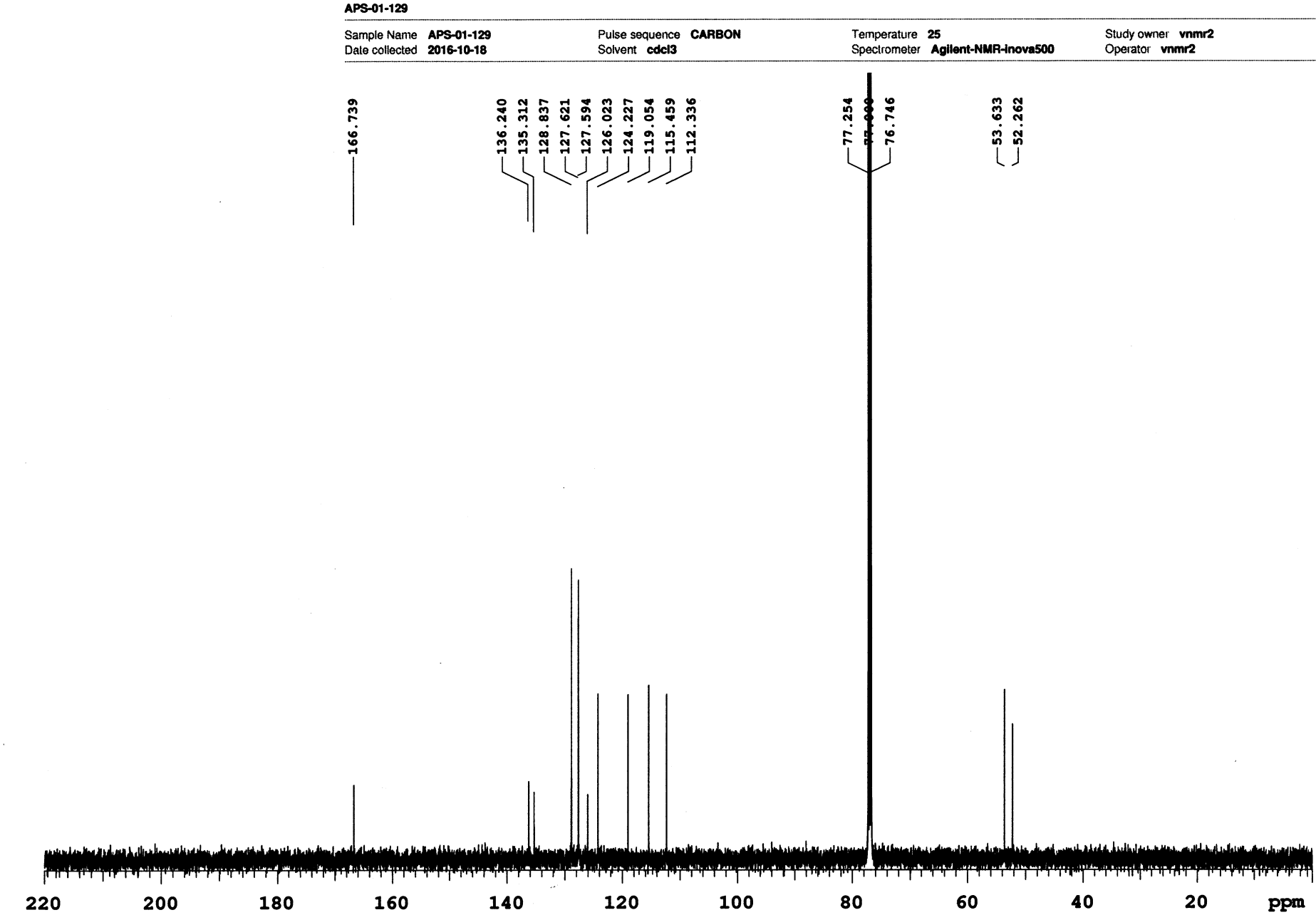


Fig S55. 13C NMR (CDCl3, 125 MHz) of compound 1c

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-129/CARBON_03

Plot date 2016-10-18

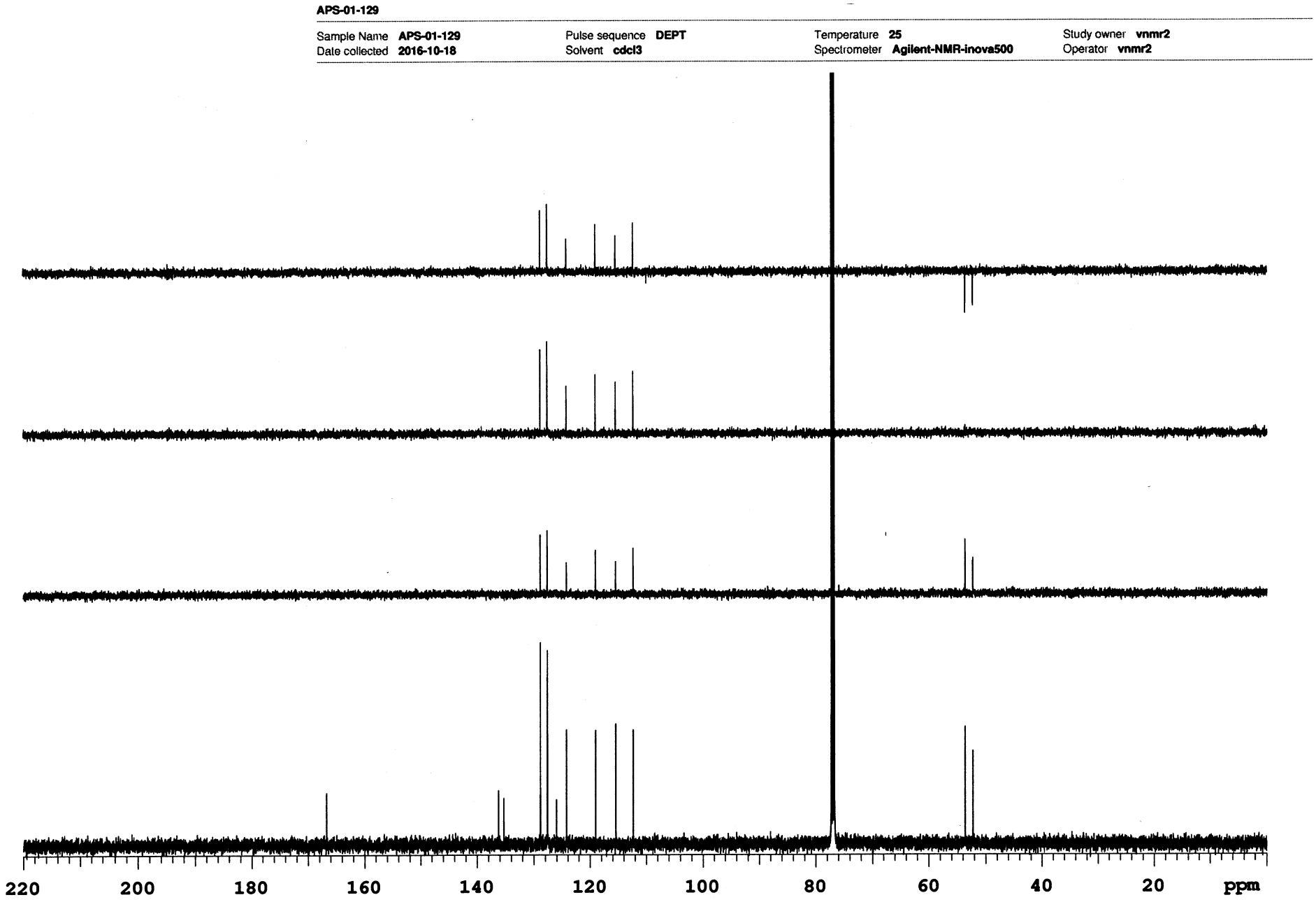
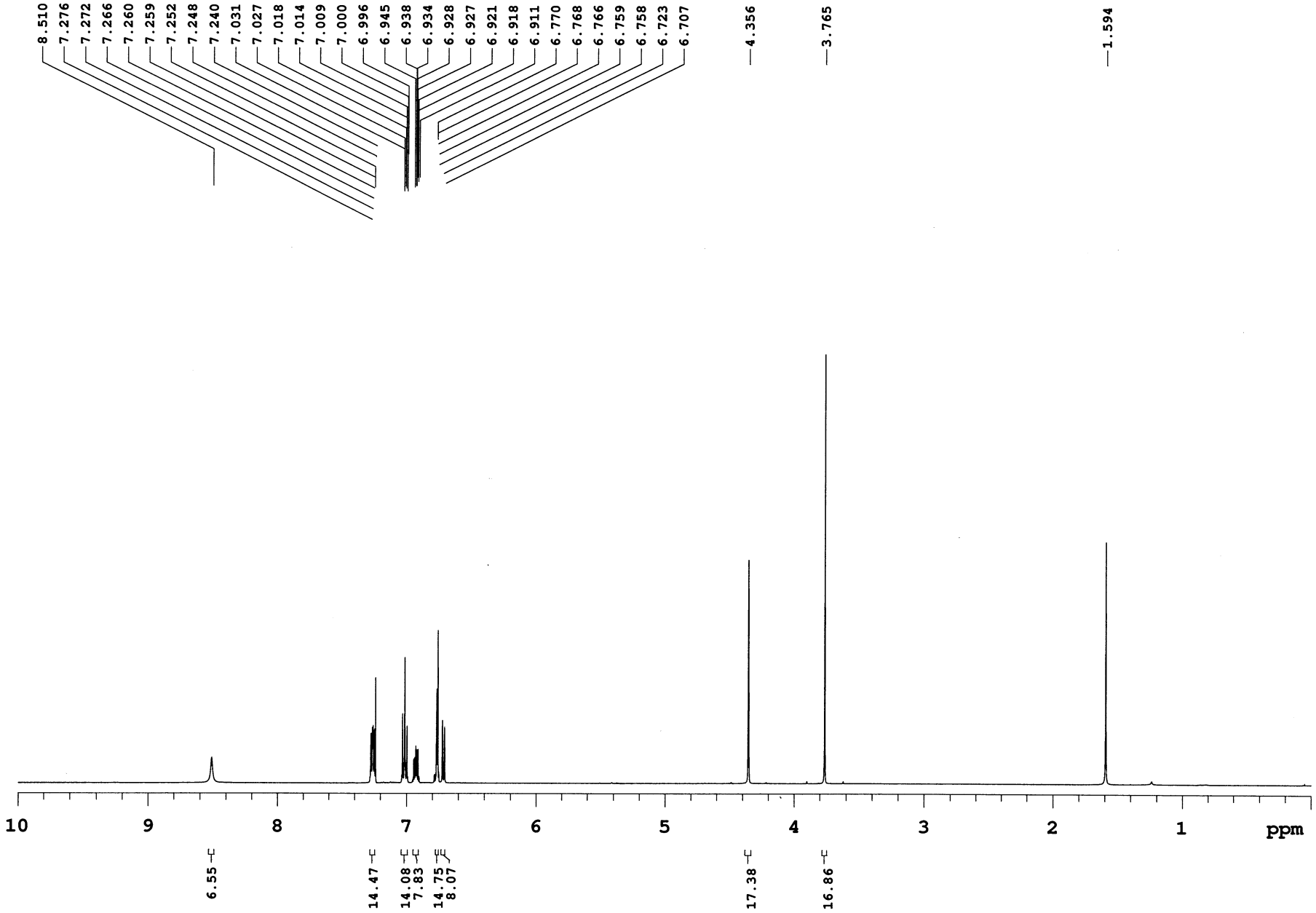


Fig S56. DEPT of compound 1c

APS-133

Sample Name	**APS-133**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2018-01-08**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-133/PROTON_05

Plot date 2018-01-08

Fig S57. 1H NMR (CDCl3, 500 MHz) of compound 1d

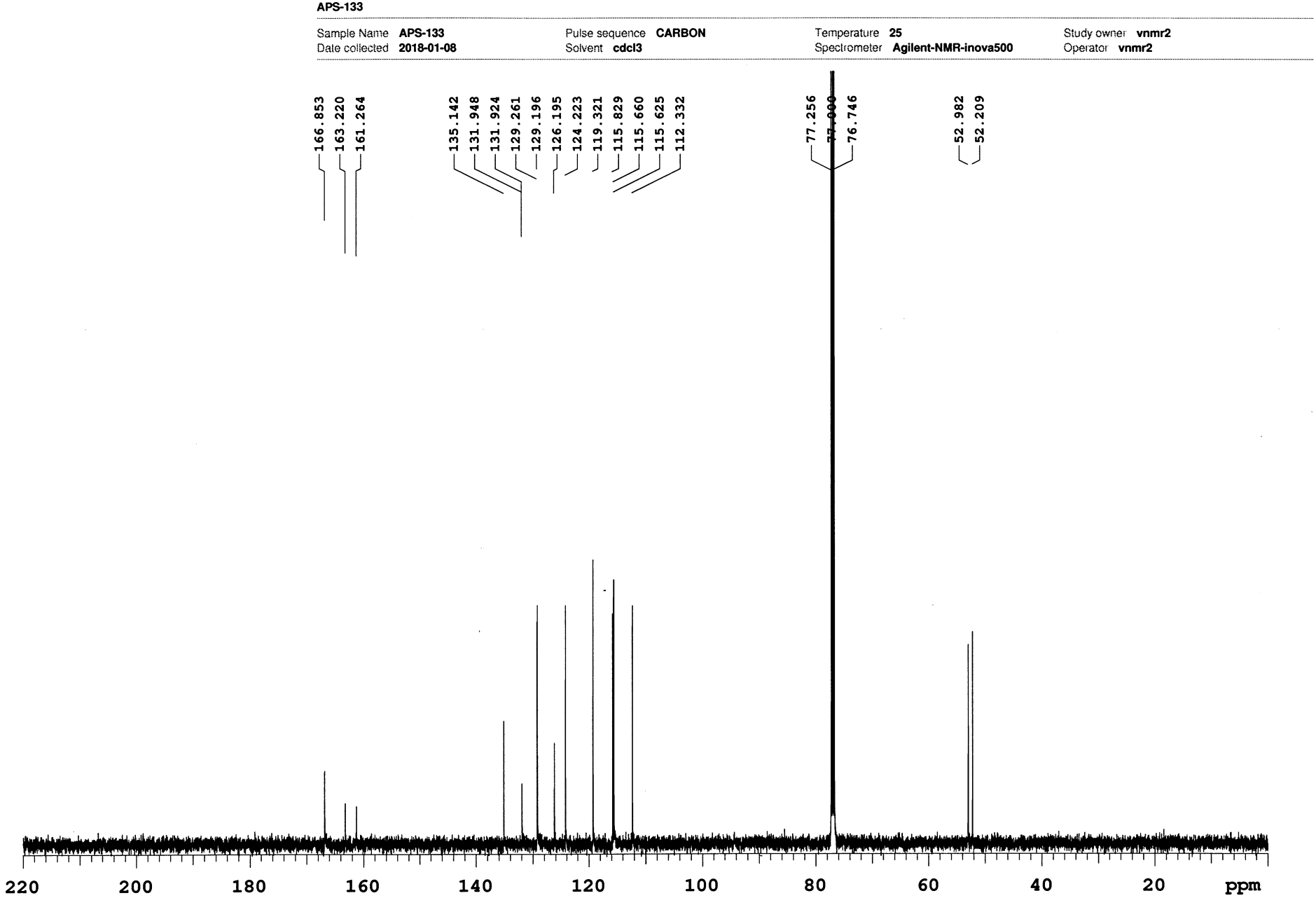


Fig S58. 1H NMR (CDCl3, 125 MHz) of compound 1d

APS-133

Sample Name **APS-133** | Pulse sequence **DEPT** | Temperature **25** | Study owner **vnmr2**
Date collected **2018-01-08** | Solvent **cdcl3** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**

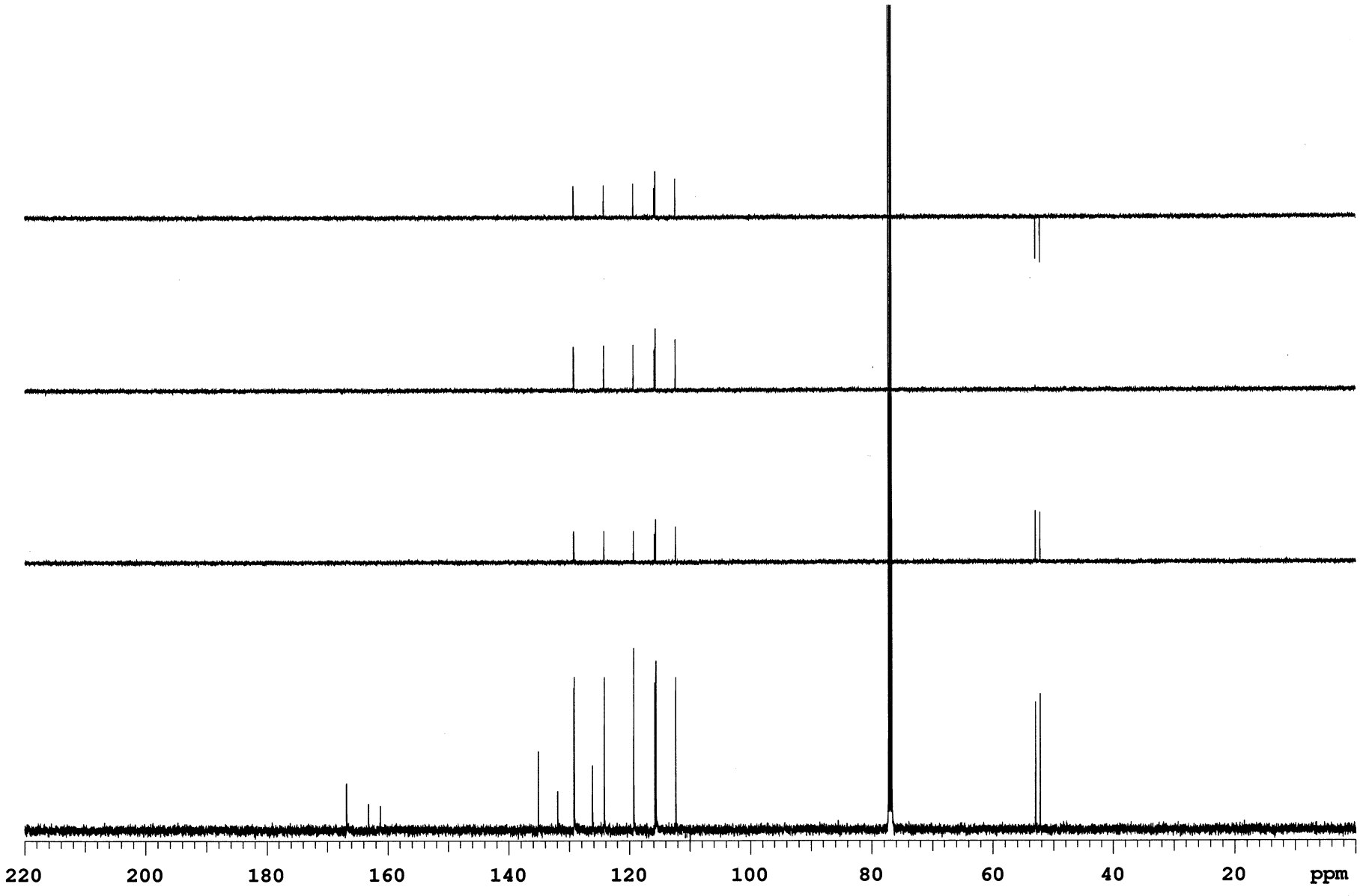


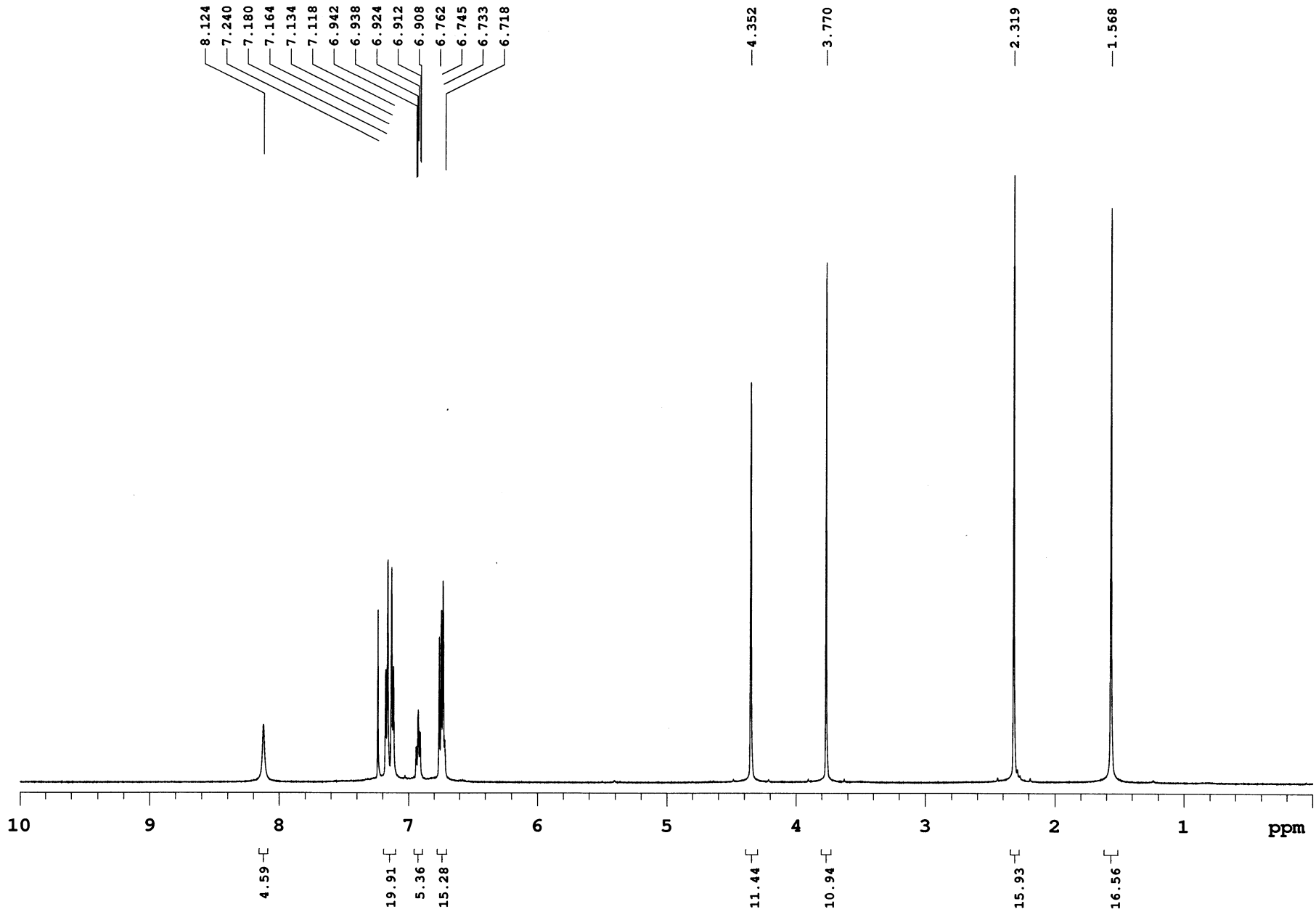
Fig S59. DEPT of compound 1d

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-133/DEPT_01

Plot date 2018-01-08

APS-01-191

Sample Name **APS-01-191**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-20**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-191/PROTON_10

Plot date 2017-06-21

Fig S60. 1H NMR (CDCl3, 500 MHz) of compound 1e

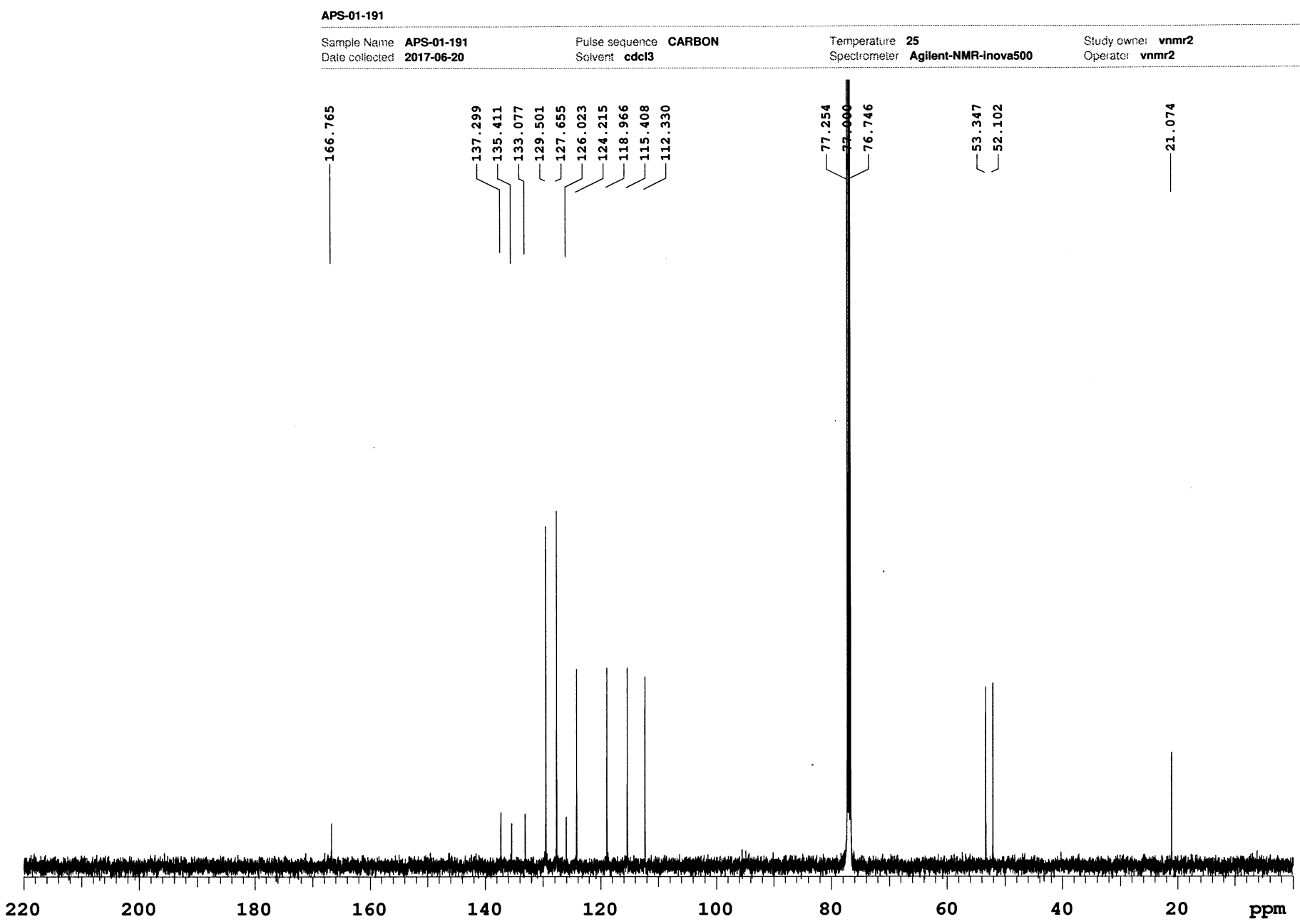


Fig S61. 13C NMR (CDCl3, 500 MHz) of compound 1e

APS-01-191

Sample Name **APS-01-191**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-20**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

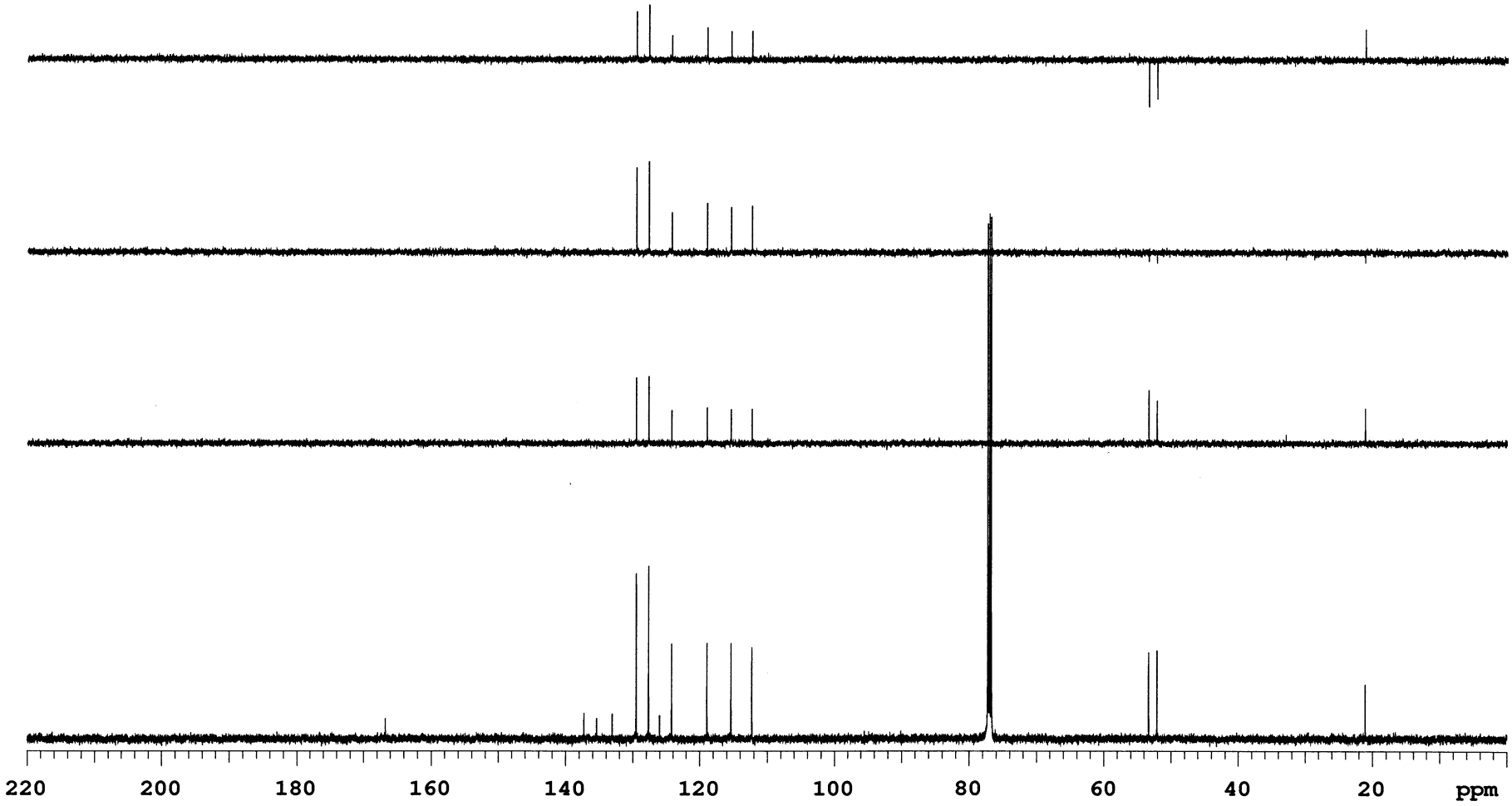
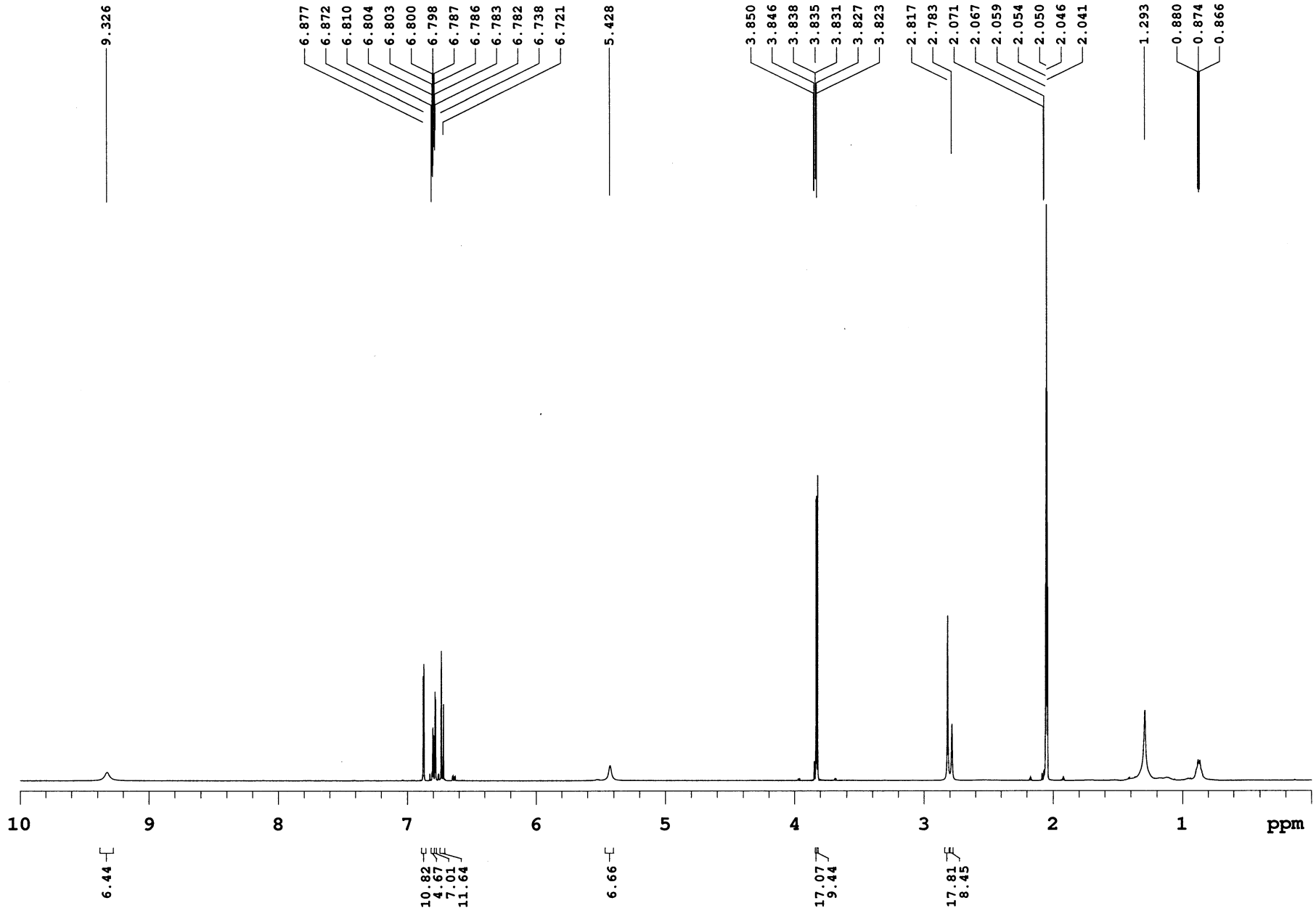


Fig S62. DEPT of compound 1e

APS-140

Sample Name	**APS-140**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2018-01-19**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



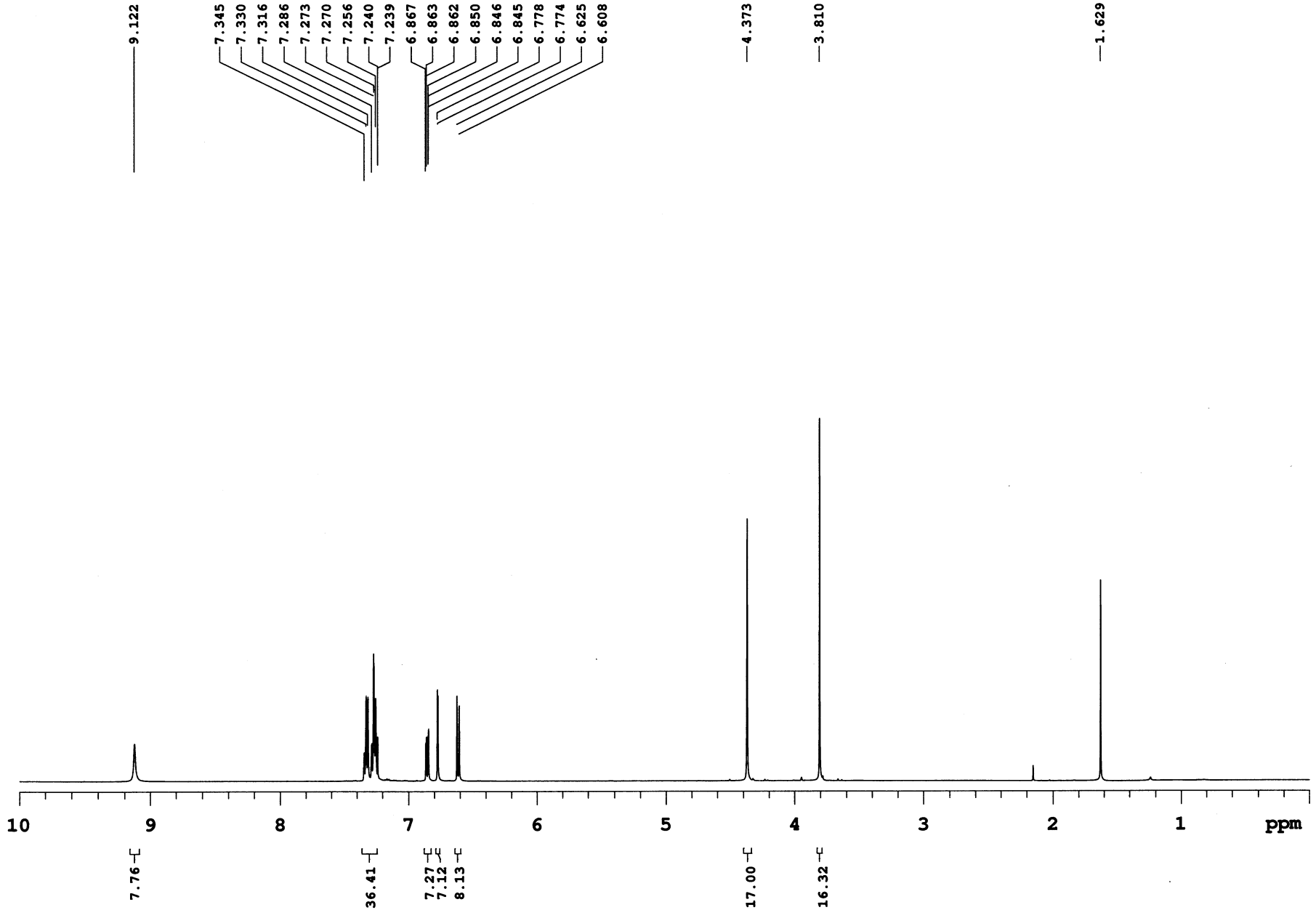
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-140/PROTON_05

Fig S63. 1H NMR (acetone-d6, 500 MHz) of compound 1f

Plot date 2018-01-19

APS-01-219

Sample Name	**APS-01-219**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-04-17**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-219/PROTON_06

Plot date 2017-04-17

Fig S64. 1H NMR (CDCl3, 500 MHz) of compound 1g

APS-01-219

Sample Name	**APS-01-219**	Pulse sequence	**CARBON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-04-17**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

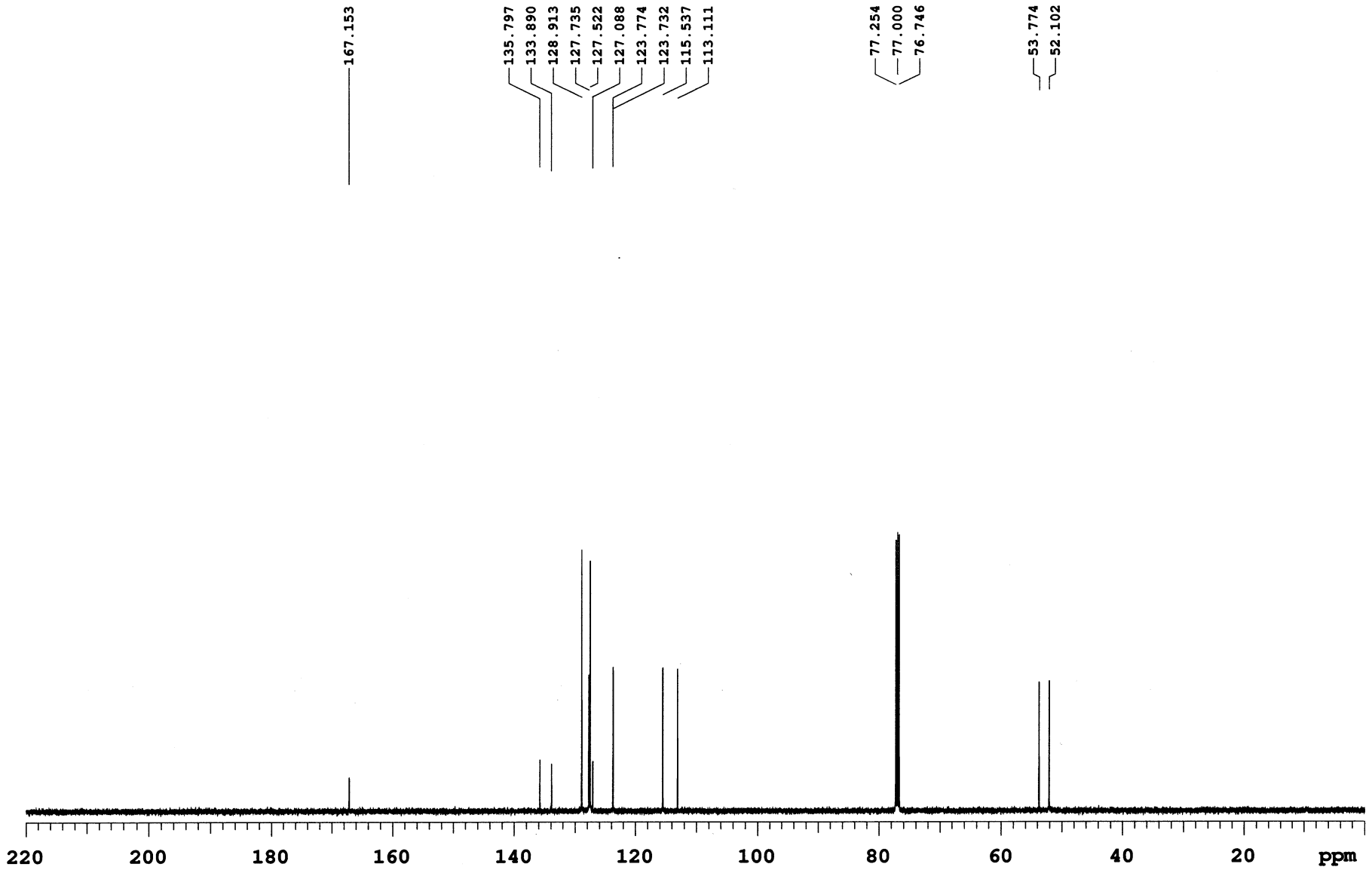


Fig S65. 13C NMR (CDCl3, 125 MHz) of compound 1g

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-219/CARBON_02

Plot date 2017-04-19

APS-01-219

Sample Name **APS-01-219**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-17**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

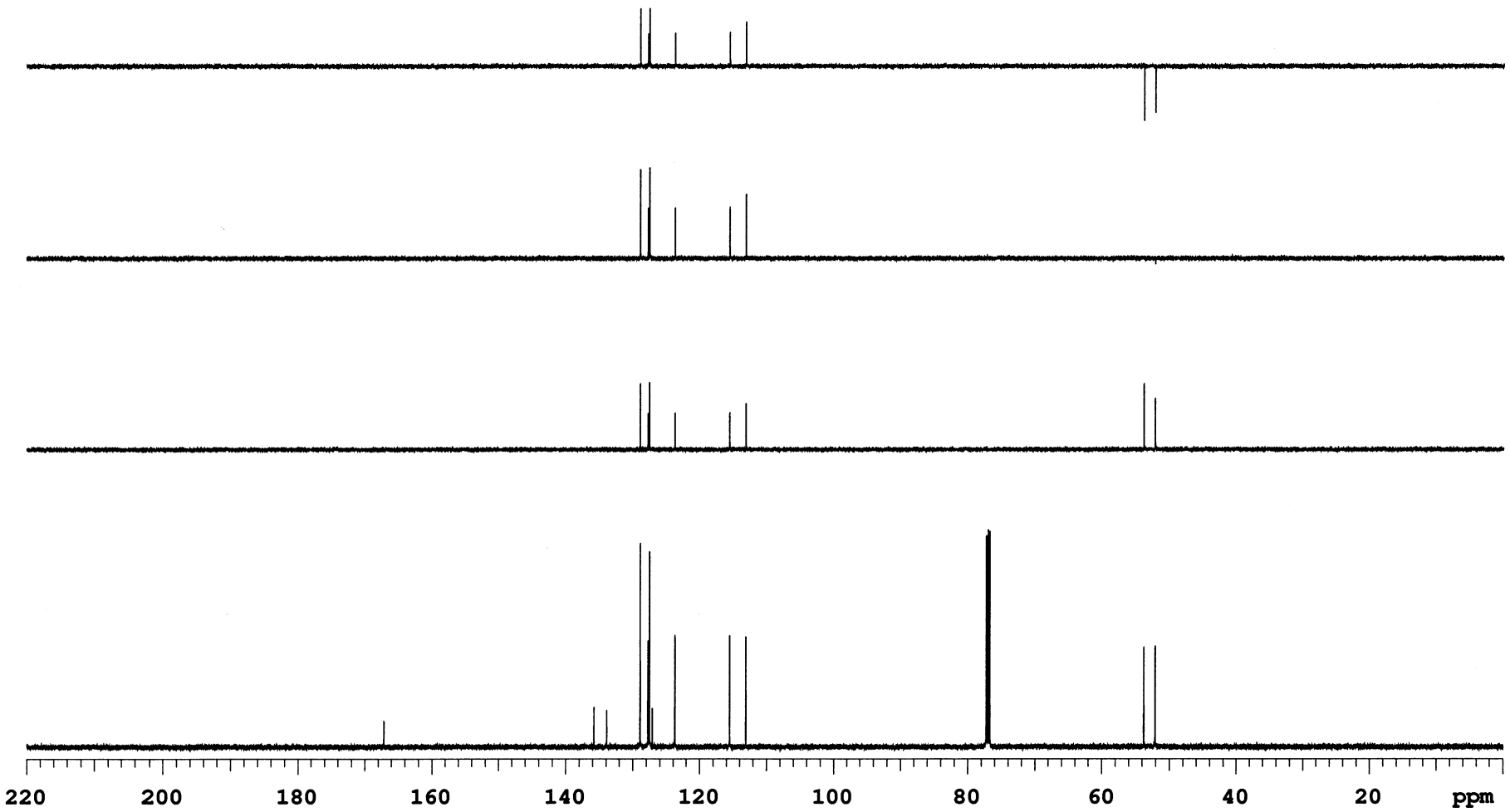


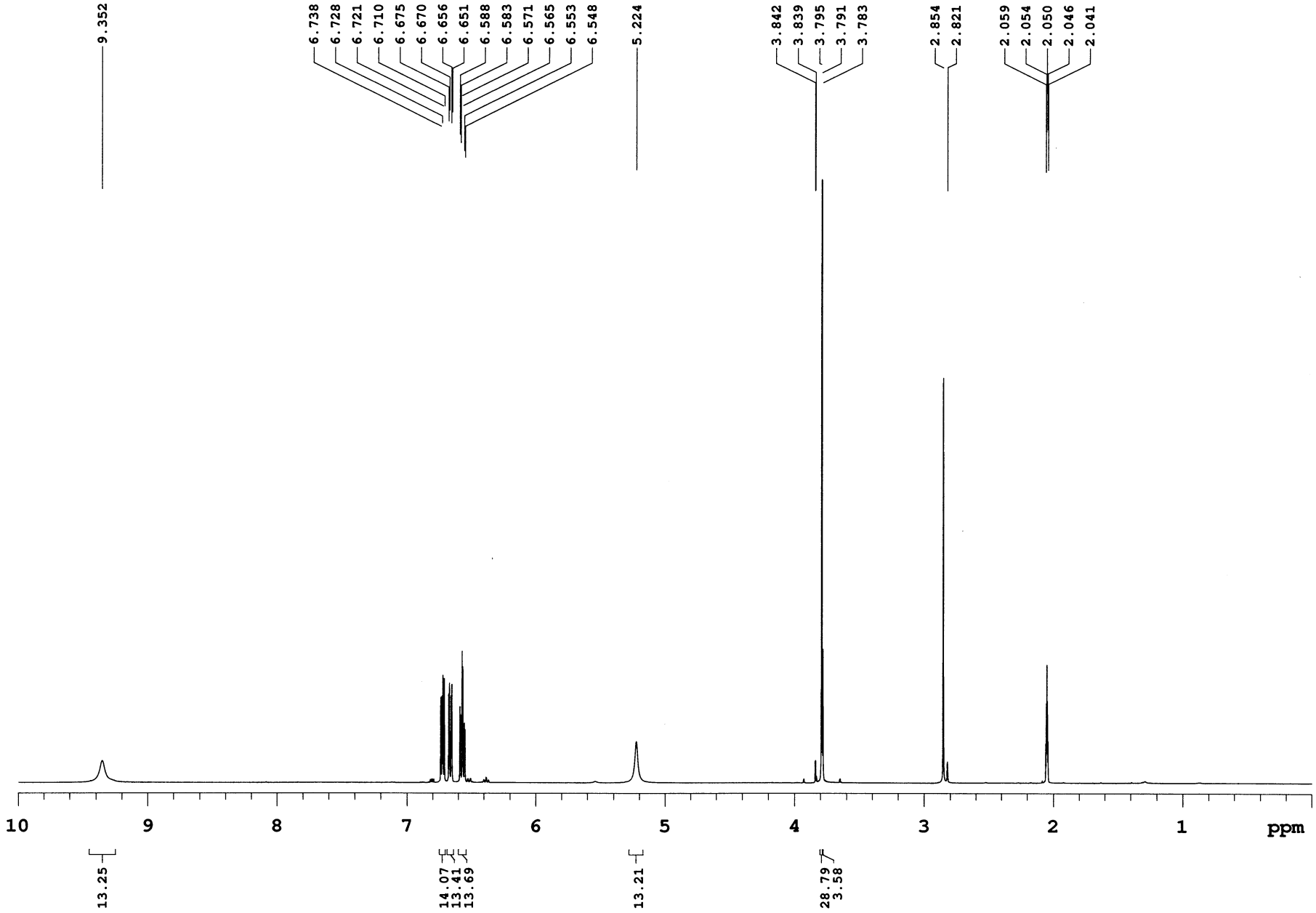
Fig S66. DEPT of compound 1g

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-219/DEPT_01

Plot date 2017-04-19

APS-01-223

Sample Name **APS-01-223**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-22**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-223/PROTON_05

Plot date 2017-06-23

Fig S67. 1H NMR (acetone-d6, 500 MHz) of compound 1h

APS-01-223

Sample Name **APS-01-223**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-22**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

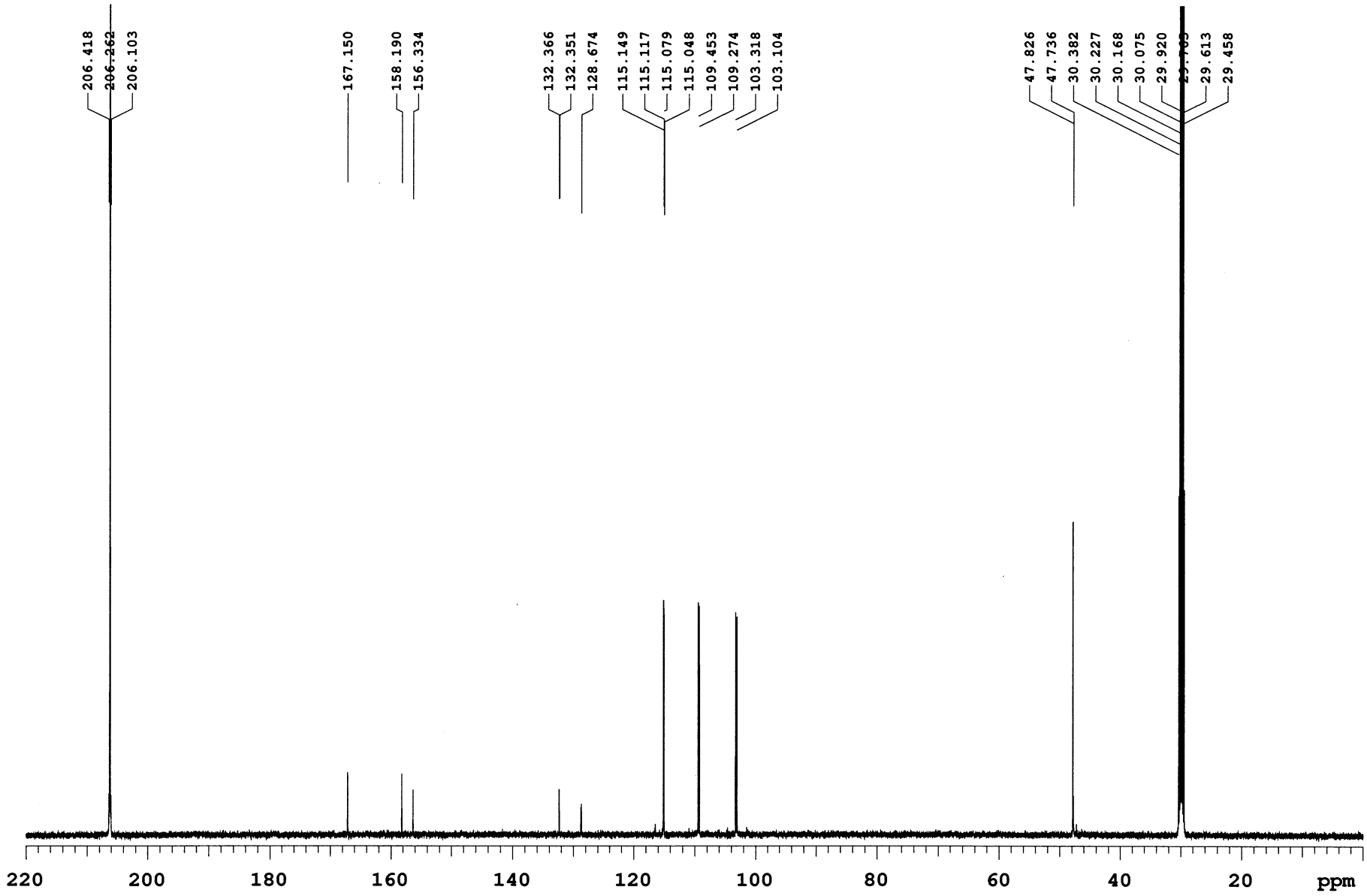


Fig S68. 13C NMR (acetone-d6, 125 MHz) of compound 1h

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-223/CARBON_02

Plot date 2017-06-23

APS-01-223

Sample Name **APS-01-223**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-22**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

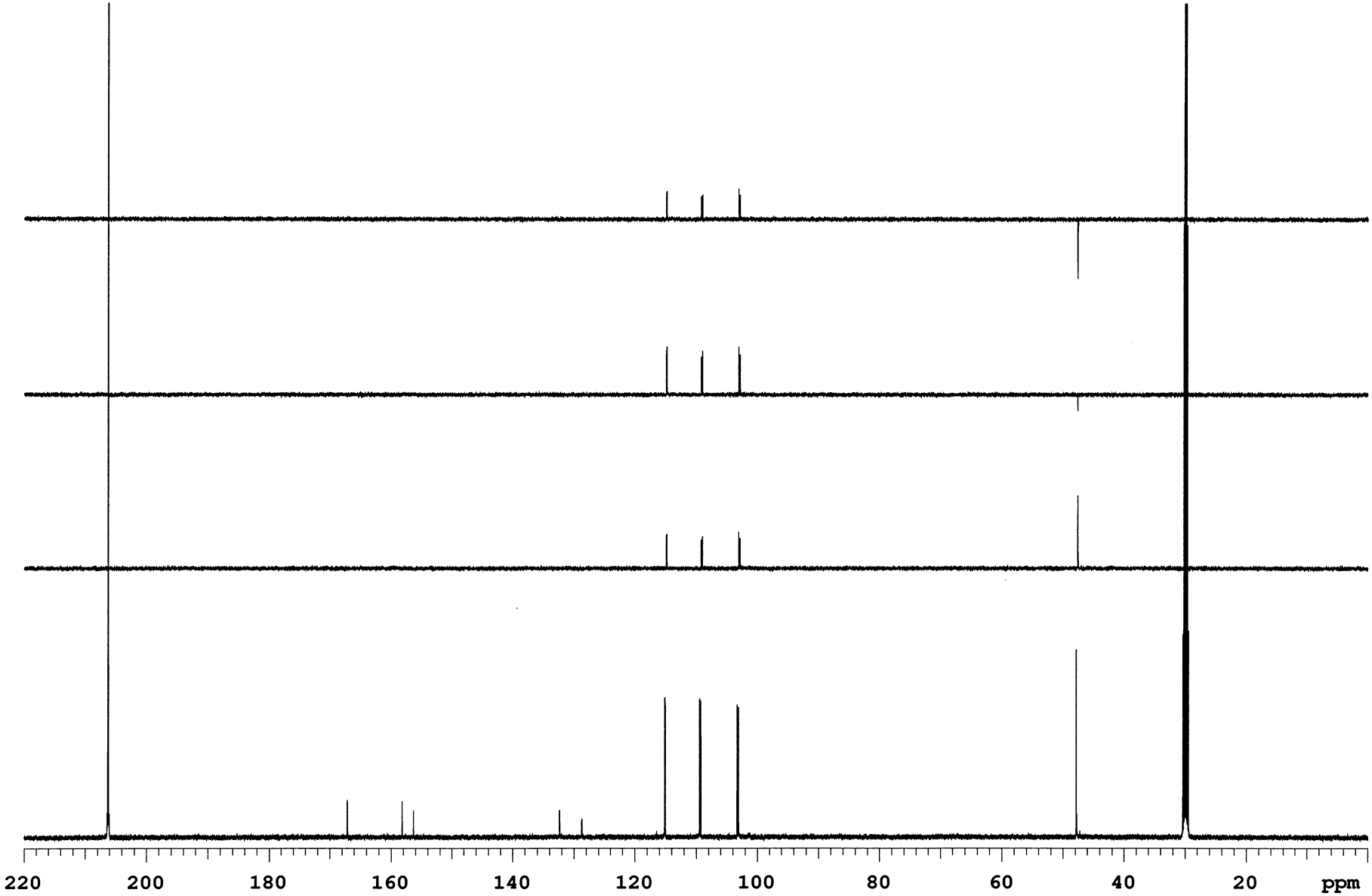


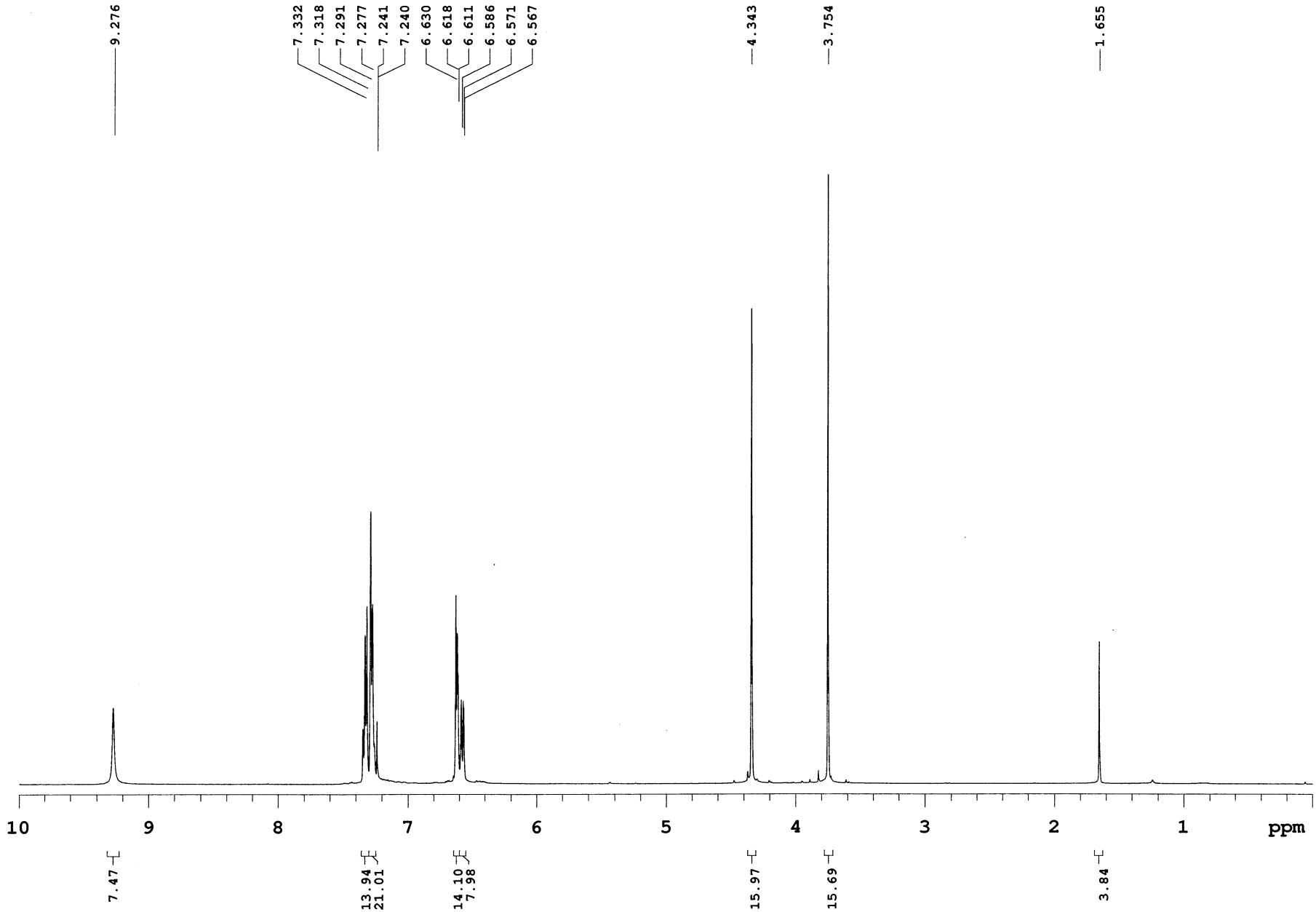
Fig S69. DEPT of compound 1h

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-223/DEPT_01

Plot date 2017-06-23

APS-01-224

Sample Name **APS-01-224**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-29**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-224/PROTON_08

Plot date 2017-05-02

Fig S70. 1H NMR (CDCl3, 500 MHz) of compound 1i

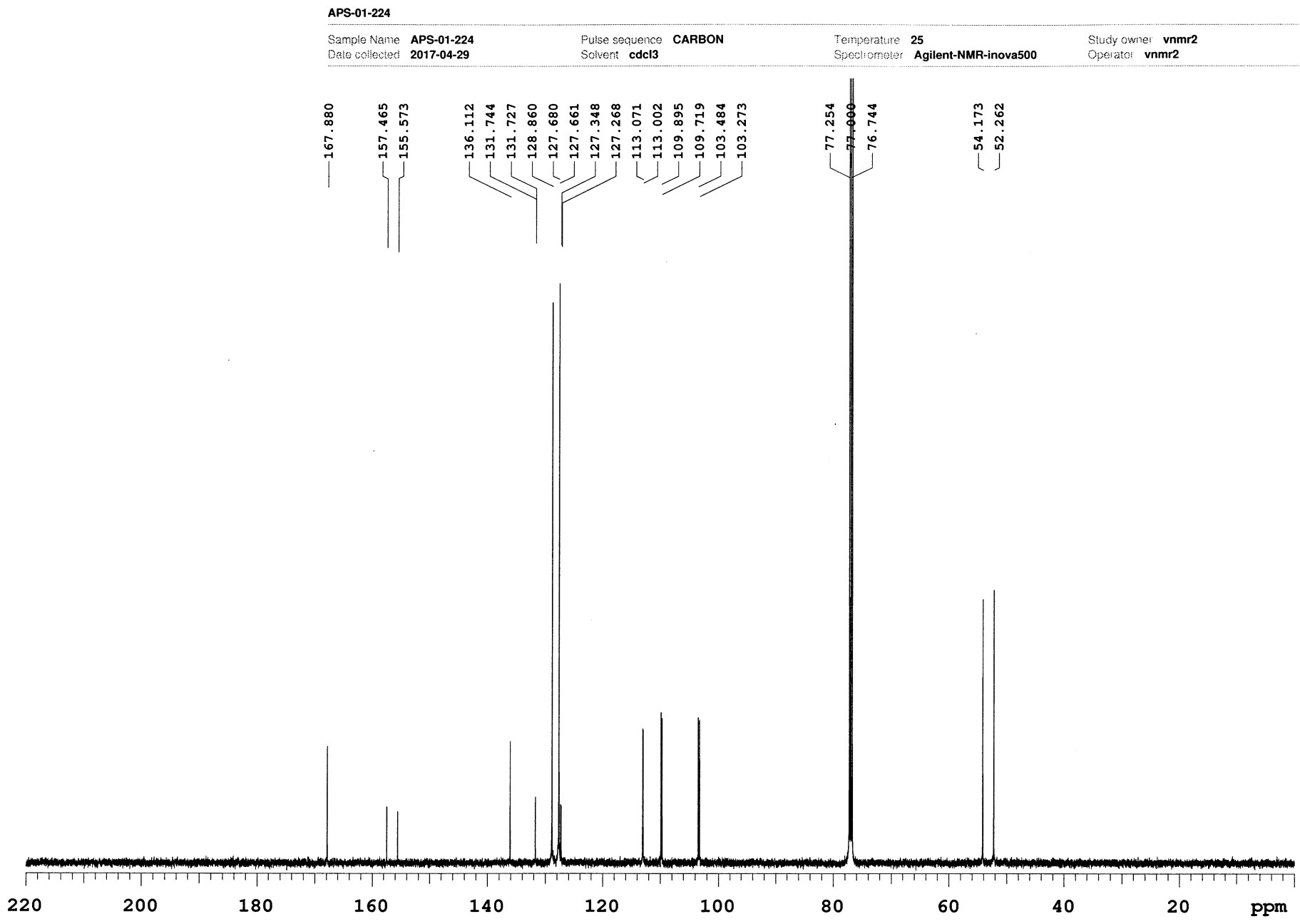


Fig S71. 13C NMR (CDCl3, 125 MHz) of compound 1i

APS-01-224

Sample Name **APS-01-224**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-29**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

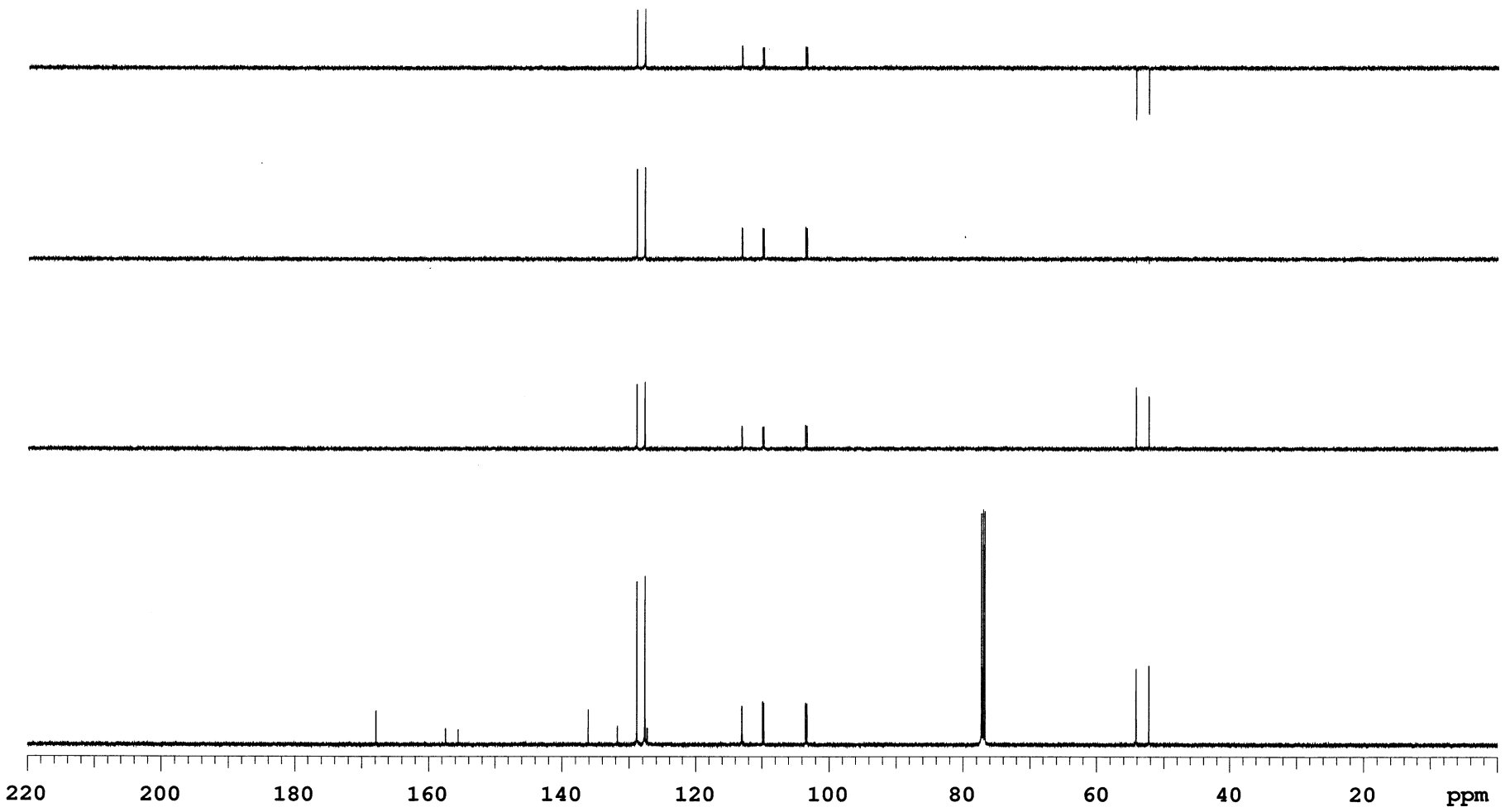


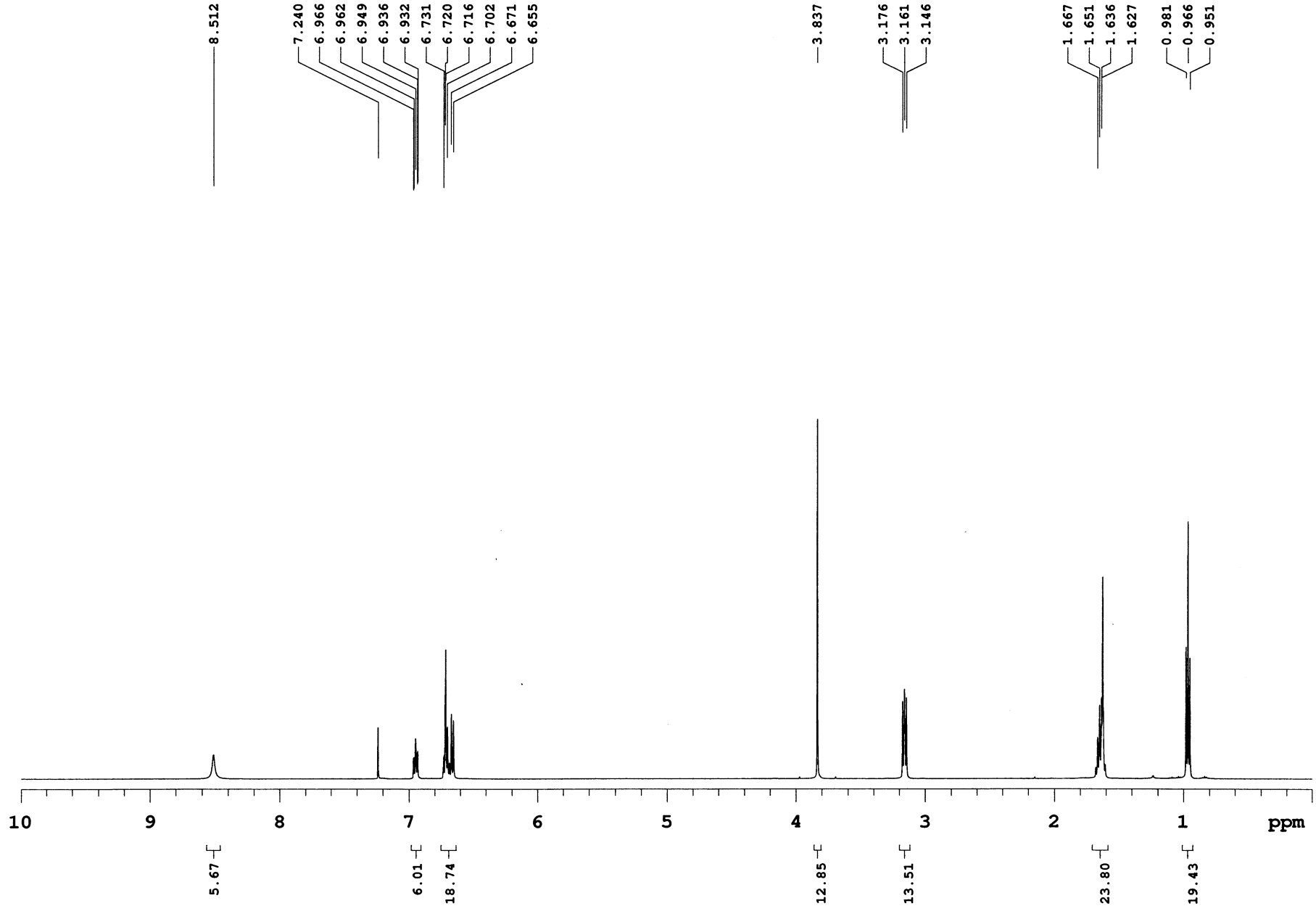
Fig S72. DEPT of compound 1i

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-224/DEPT_01

Plot date 2017-05-02

APS-01-179

Sample Name **APS-01-179**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-31**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-179/PROTON_07

Fig S73. 1H NMR (CDCl3, 500 MHz) of compound 1j

Plot date 2017-06-01

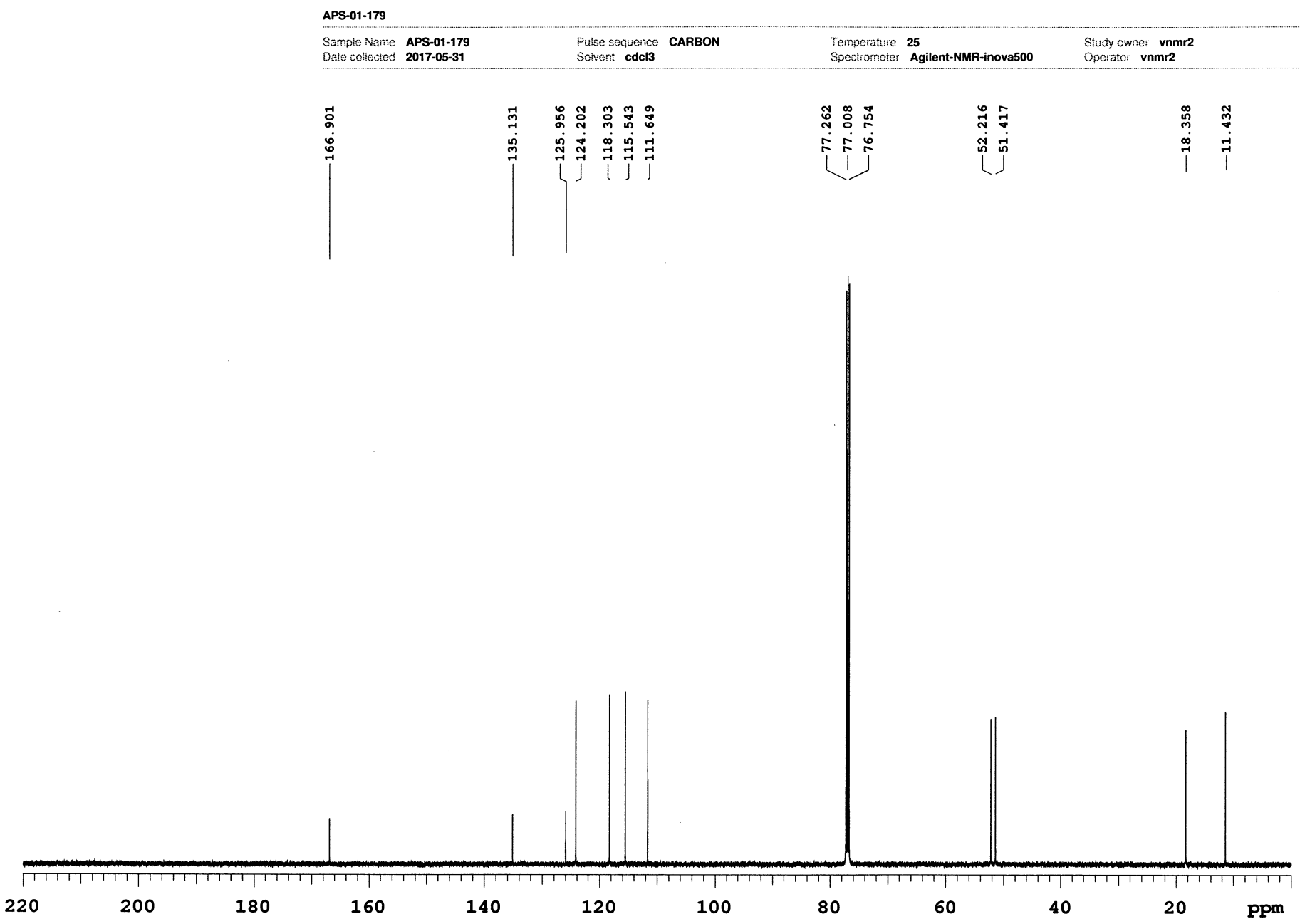


Fig S74. 13C NMR (CDCl3, 125 MHz) of compound 1j

APS-01-179

Sample Name **APS-01-179**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-01**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

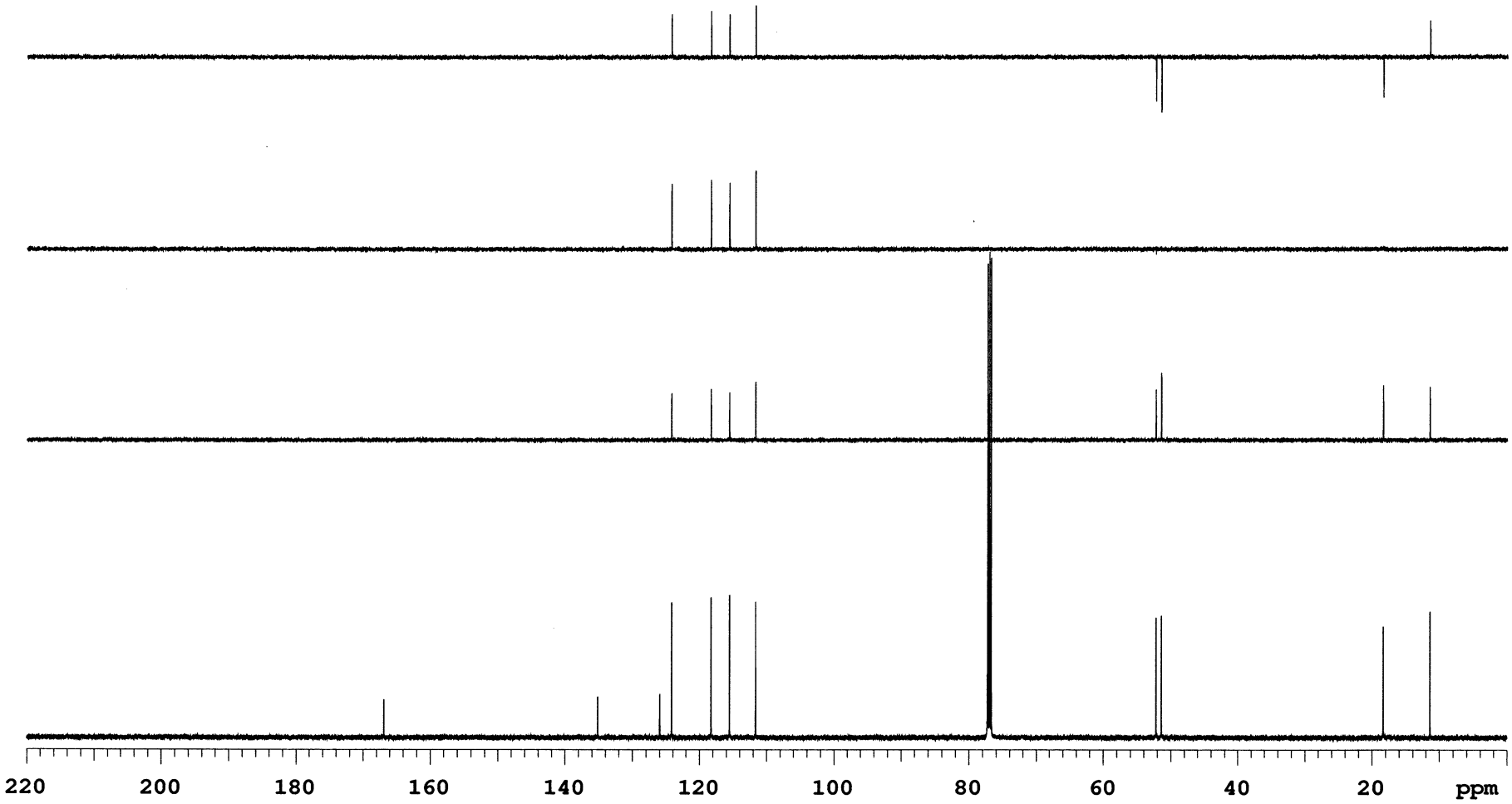


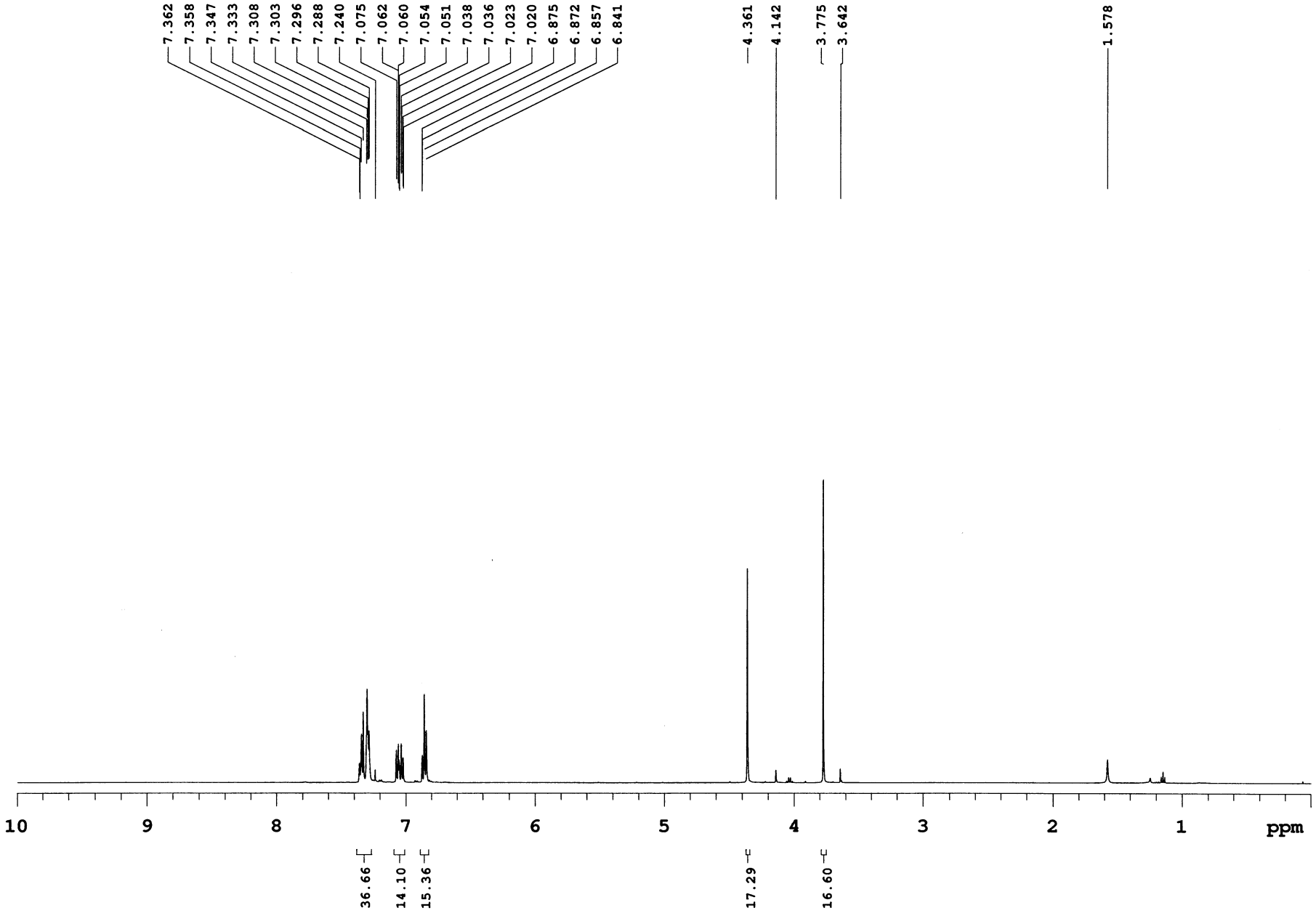
Fig S75. DEPT of compound 1j

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-179/DEPT_02

Plot date 2017-06-01

APS-01-196

Sample Name **APS-01-196**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-12**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-196/PROTON_03

Fig S76. 1H NMR (CDCl3, 500 MHz) of compound 1k

Plot date 2017-06-12

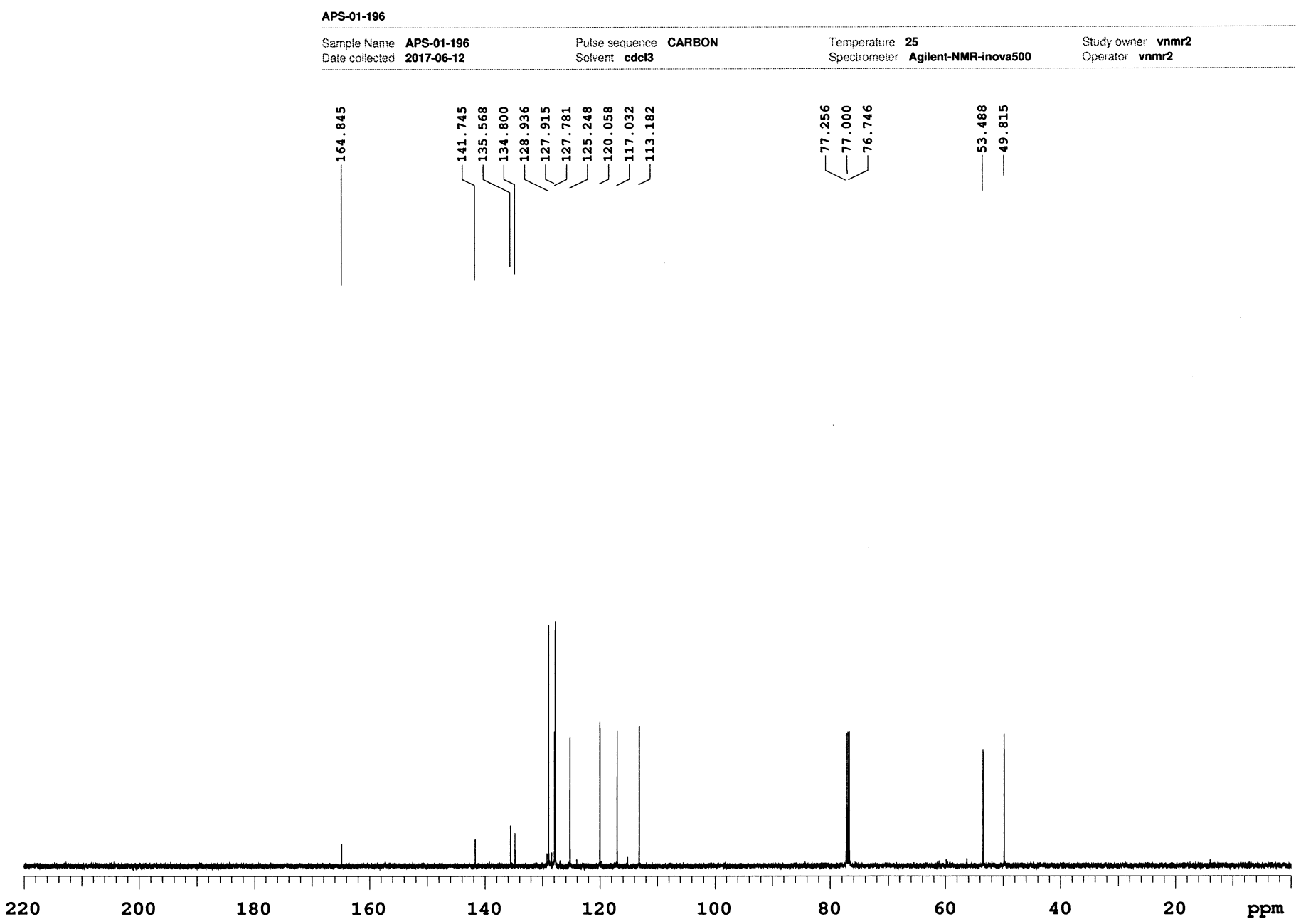


Fig S77. 13C NMR (CDCl3, 125 MHz) of compound 1k

APS-01-196

Sample Name **APS-01-196**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-12**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

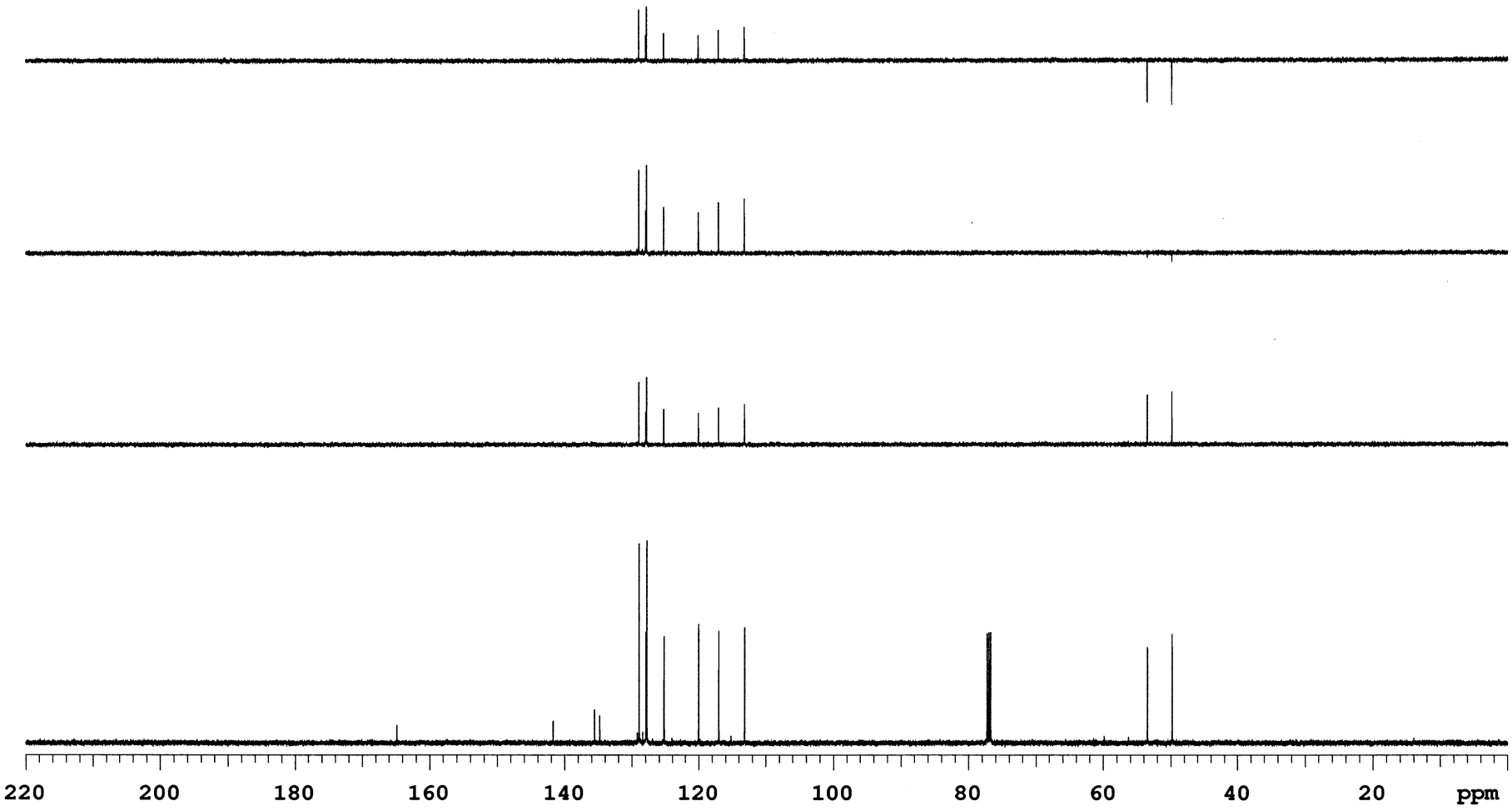
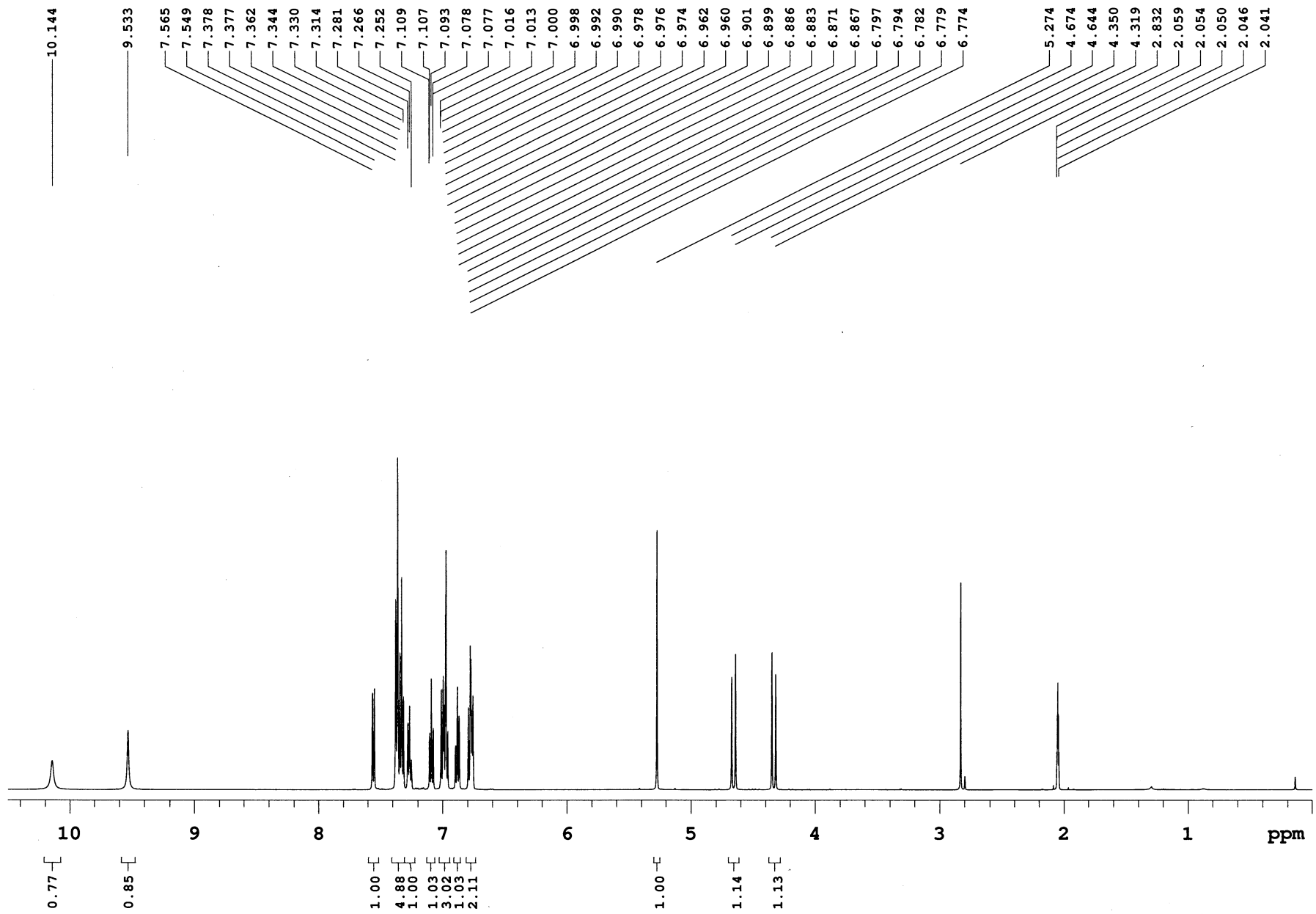


Fig S78. DEPT of compound 1k

APS-01-141

Sample Name **APS-01-141**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-11**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



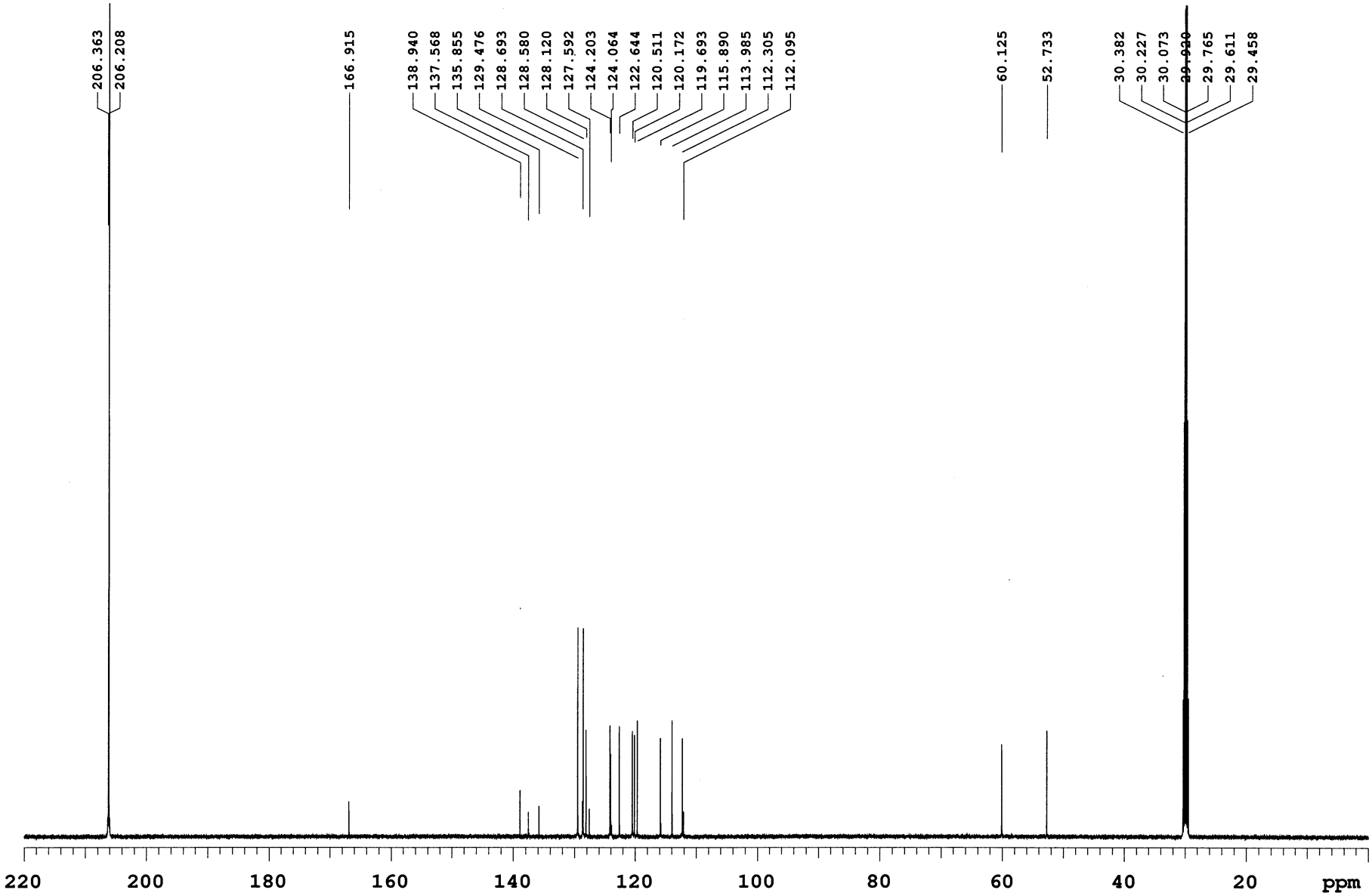
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-141/PROTON_02

Fig S79. 1H NMR (acetone-d6, 500 MHz) of compound 3ca

Plot date 2017-01-12

APS-01-141

Sample Name **APS-01-141**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-12**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



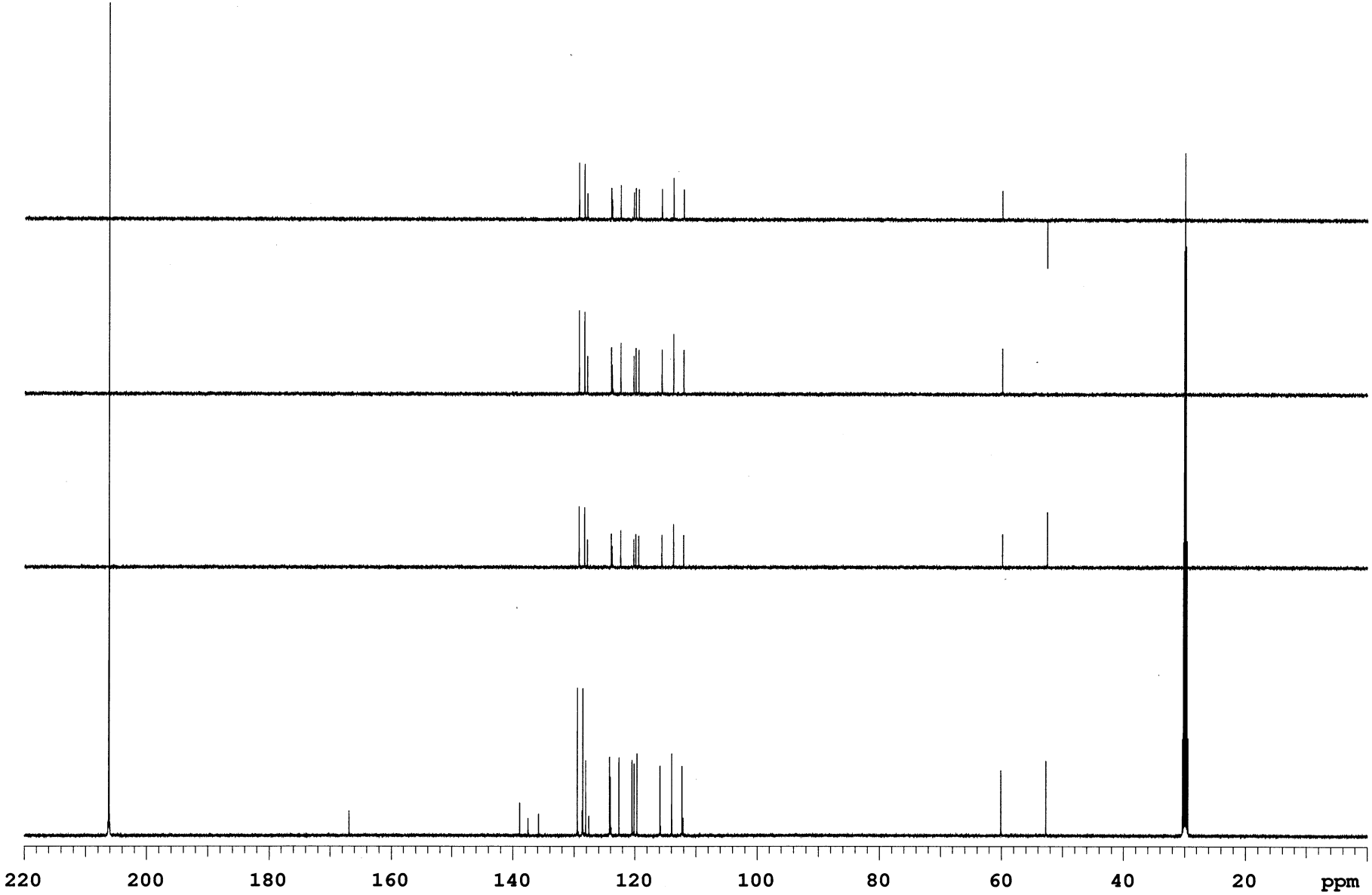
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-141/CARBON_02

Fig S80. 13C NMR (acetone-d6, 125 MHz) of compound 3ca

Plot date 2017-01-12

APS-01-141

Sample Name **APS-01-141**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-12**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



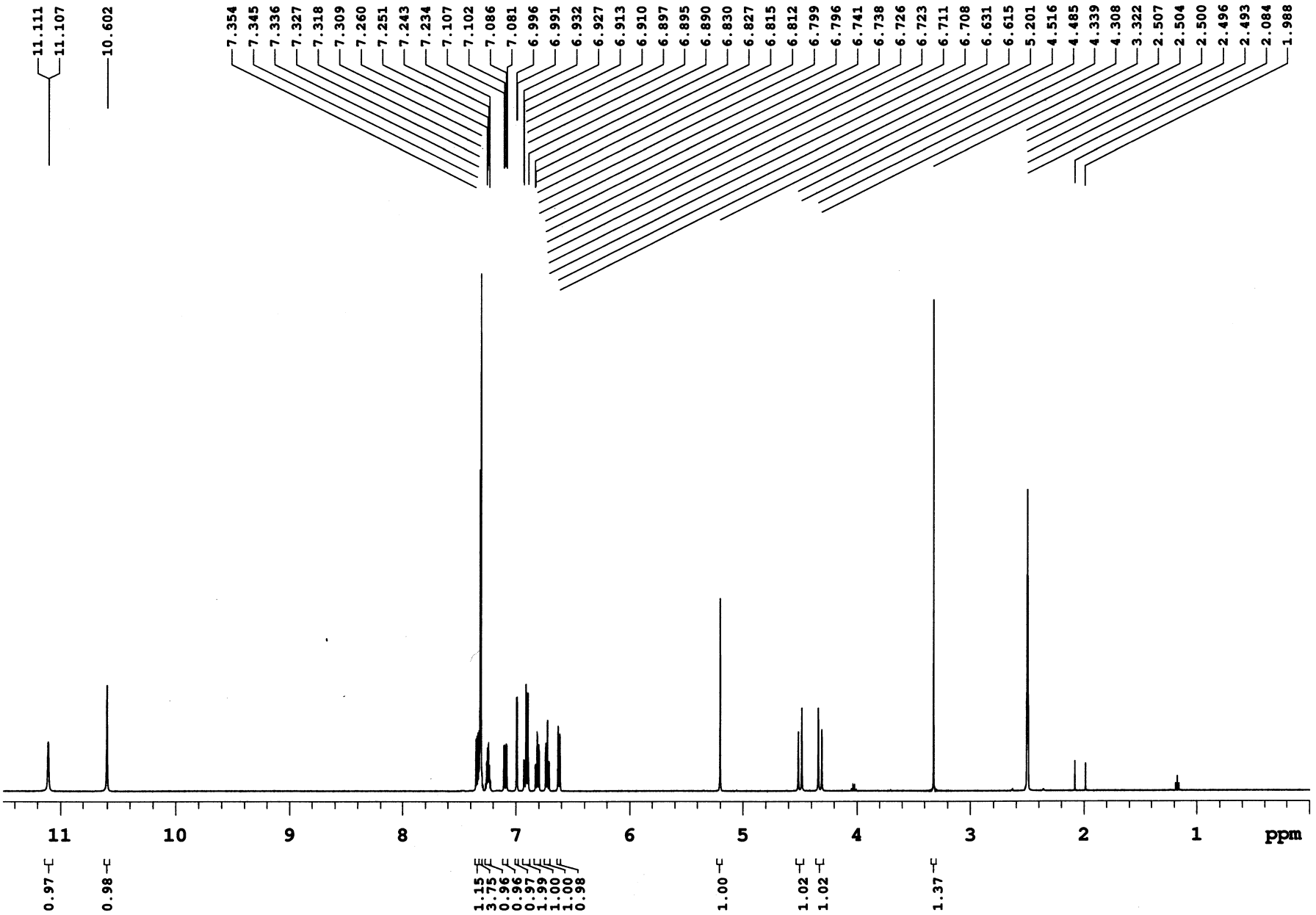
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-141/DEPT_01

Fig S81. DEPT of compound 3ca

Plot date 2017-01-12

APS-01-183

Sample Name	**APS-01-183**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-12-26**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-183/PROTON_04

Fig S82. 1H NMR (DMSO-d6, 500 MHz) of compound 3cb

Plot date 2016-12-29

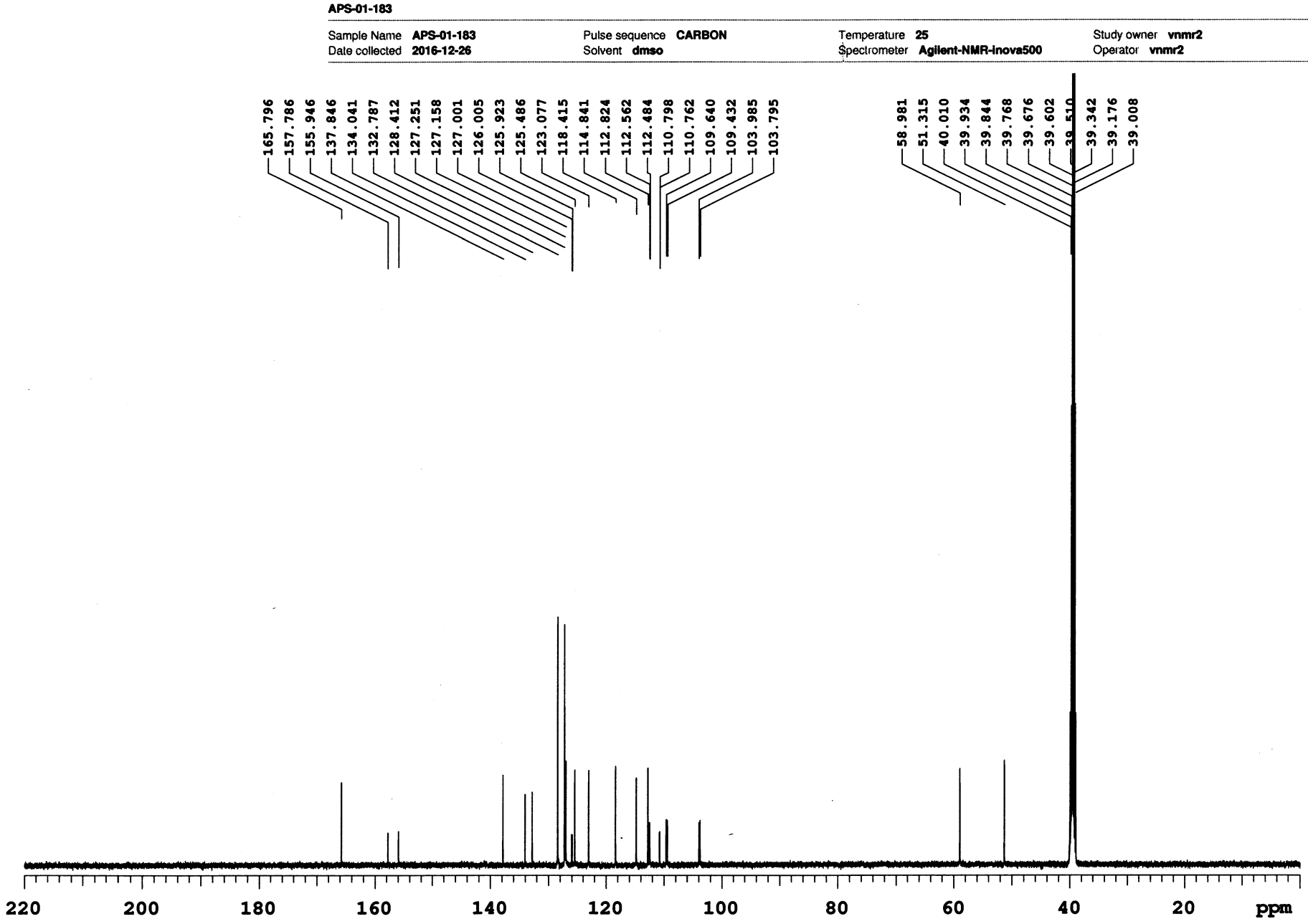


Fig S83. 13C NMR (DMSO-d6, 125 MHz) of compound 3cb

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-183/CARBON_02

Plot date 2016-12-29

APS-01-183

Sample Name	**APS-01-183**	Pulse sequence	**DEPT**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-12-27**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

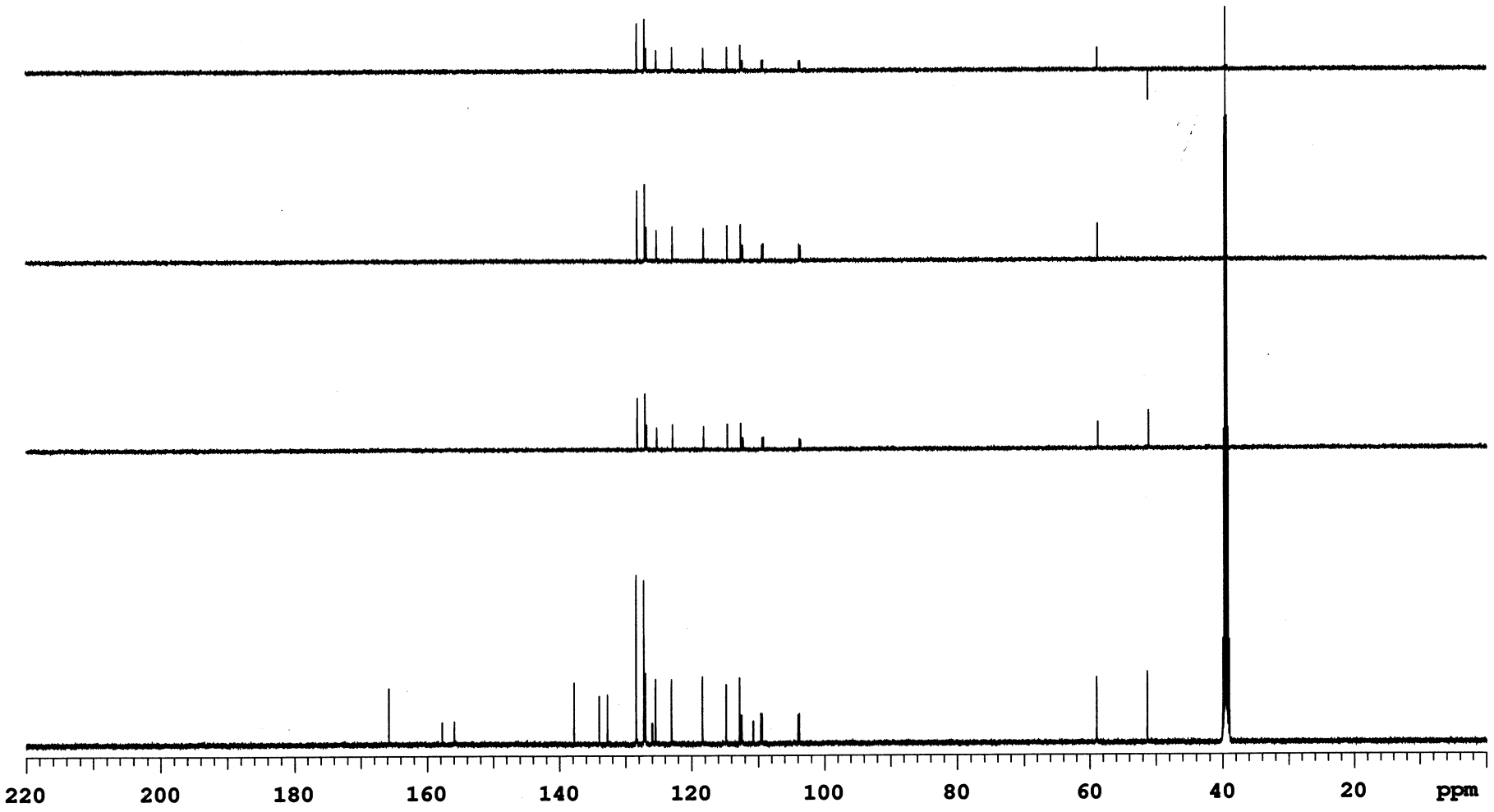


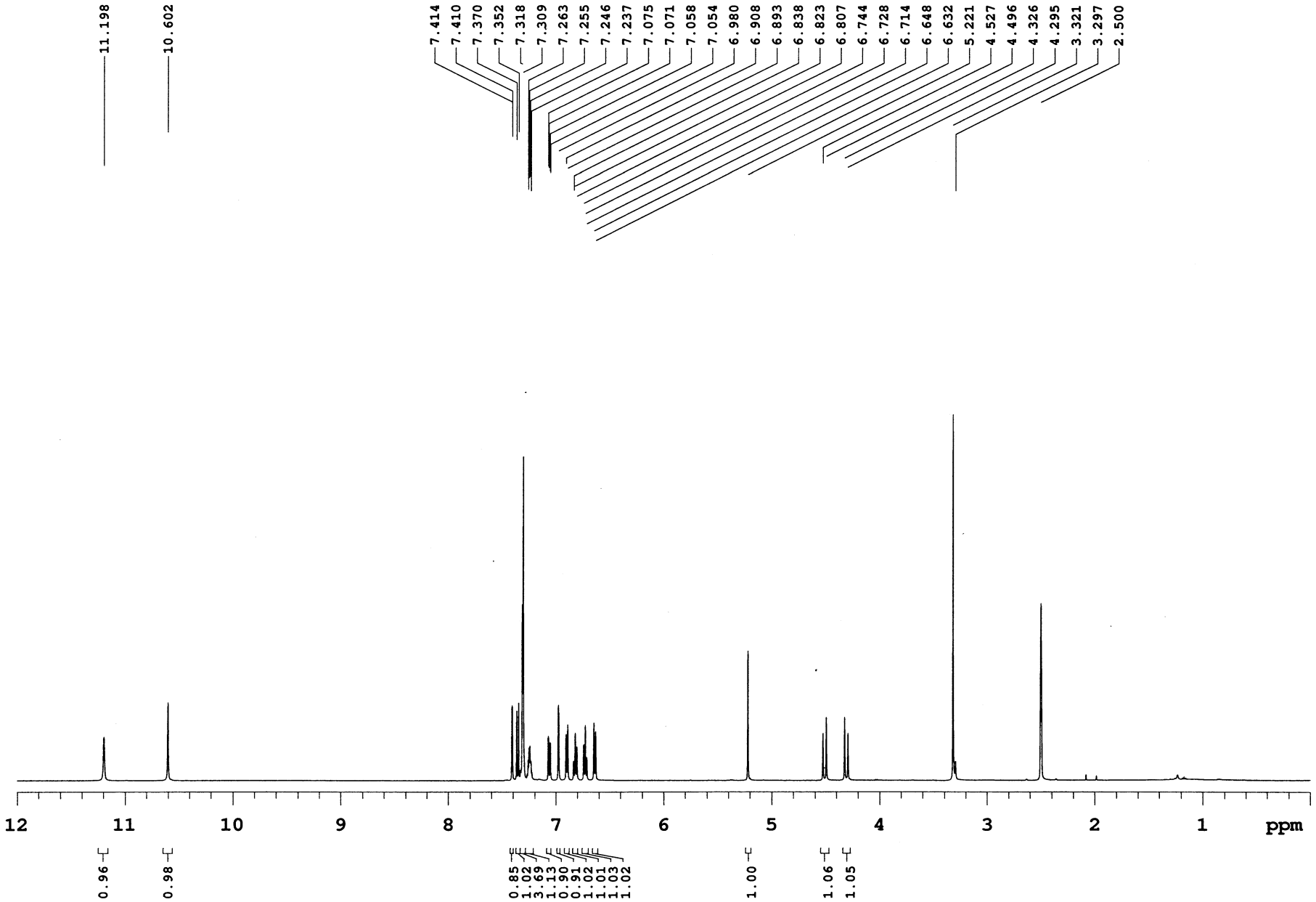
Fig S84. DEPT of compound 3cb

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-183/DEPT_01

Plot date 2016-12-29

APS-01-167-A

Sample Name	**APS-01-167-A**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-05-06**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-167-A/PROTON_03

Fig S85. 1H NMR (DMSO-d6, 500 MHz) of compound 3cc

Plot date 2017-05-15

APS-01-167

Sample Name **APS-01-167**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-02-13**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

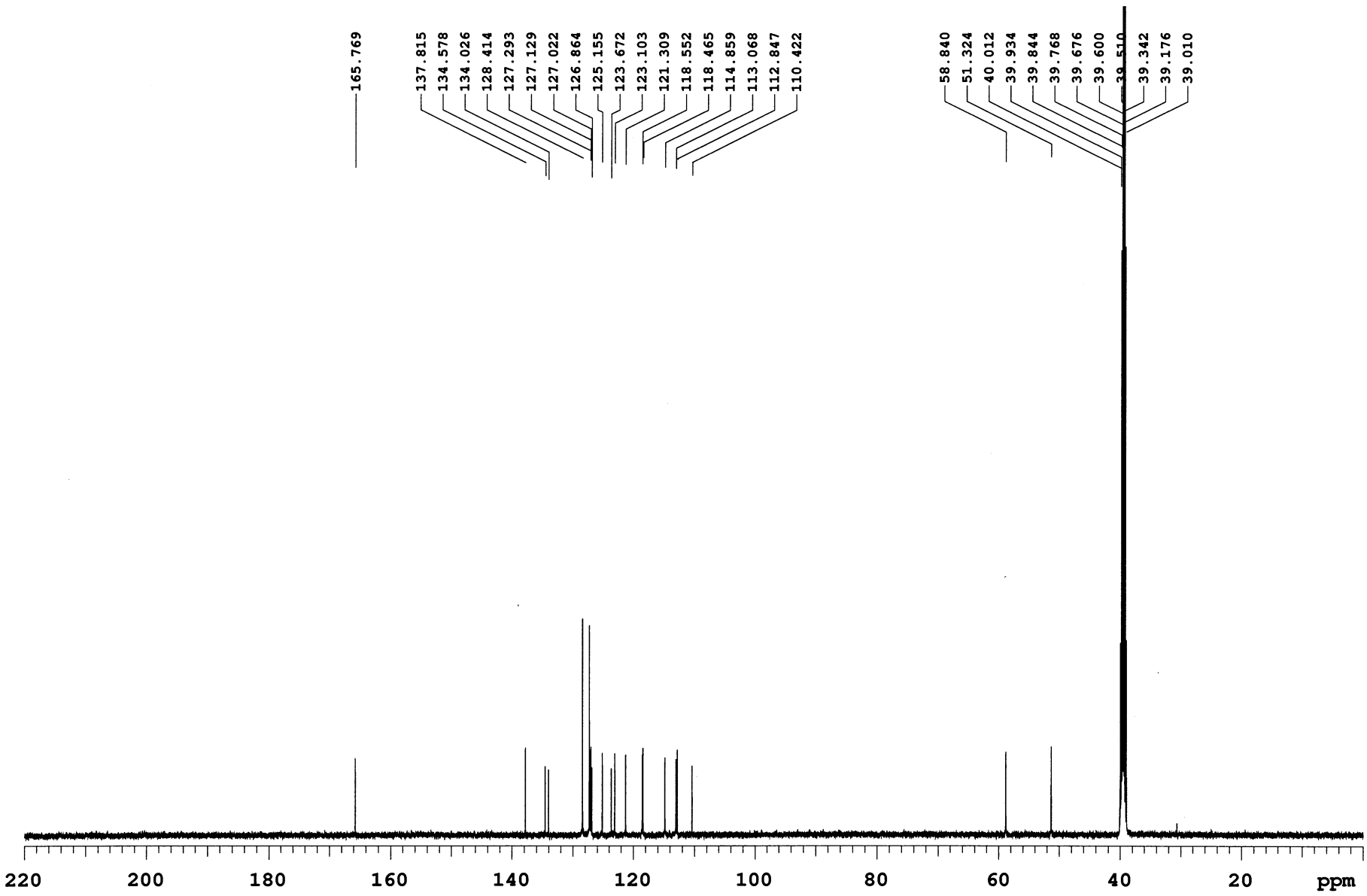


Fig S86. 13C NMR (DMSO-d6, 125 MHz) of compound 3cc

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-167/CARBON_08

Plot date 2017-02-15

APS-01-167

Sample Name **APS-01-167**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-02-13**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

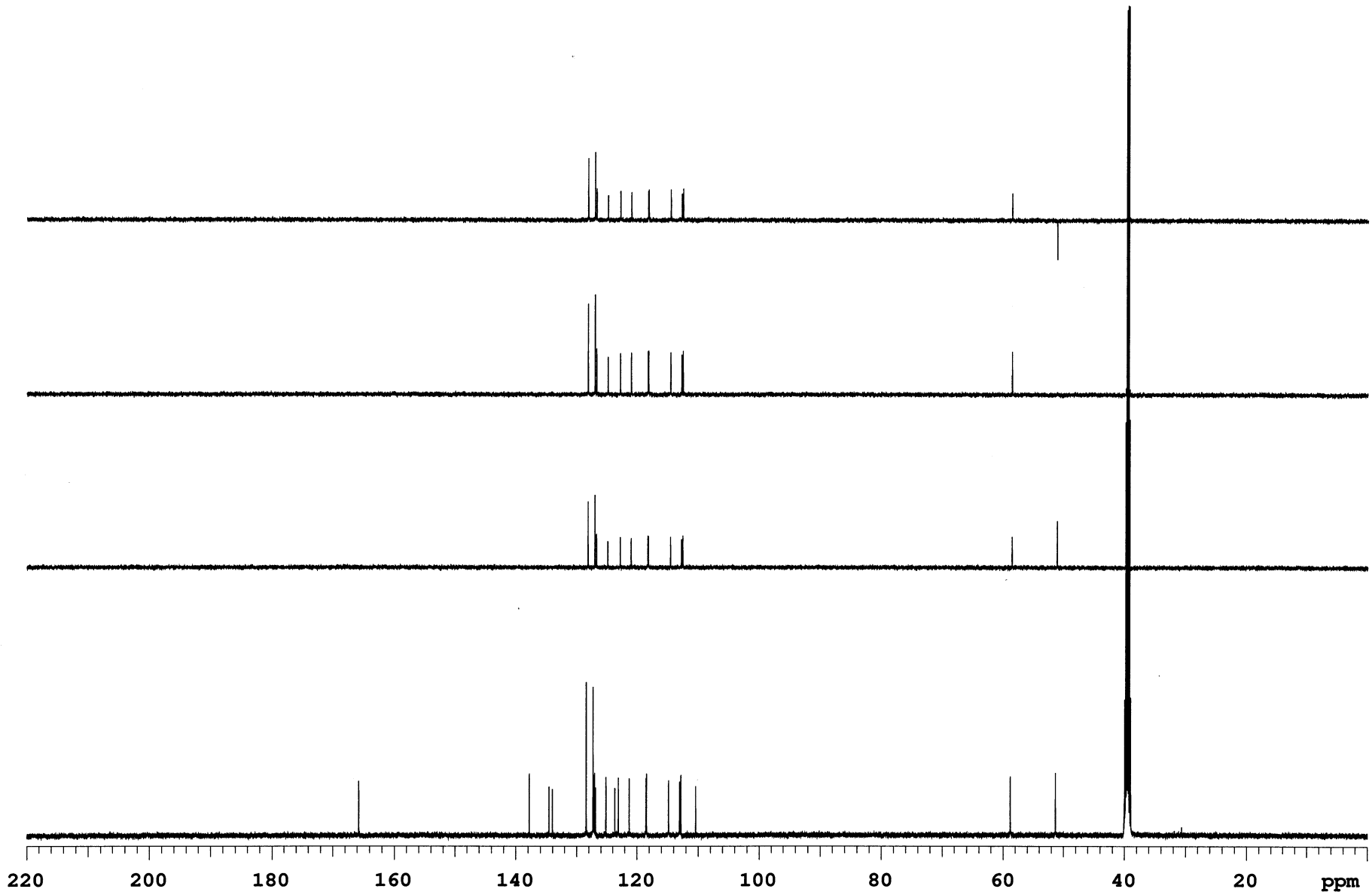


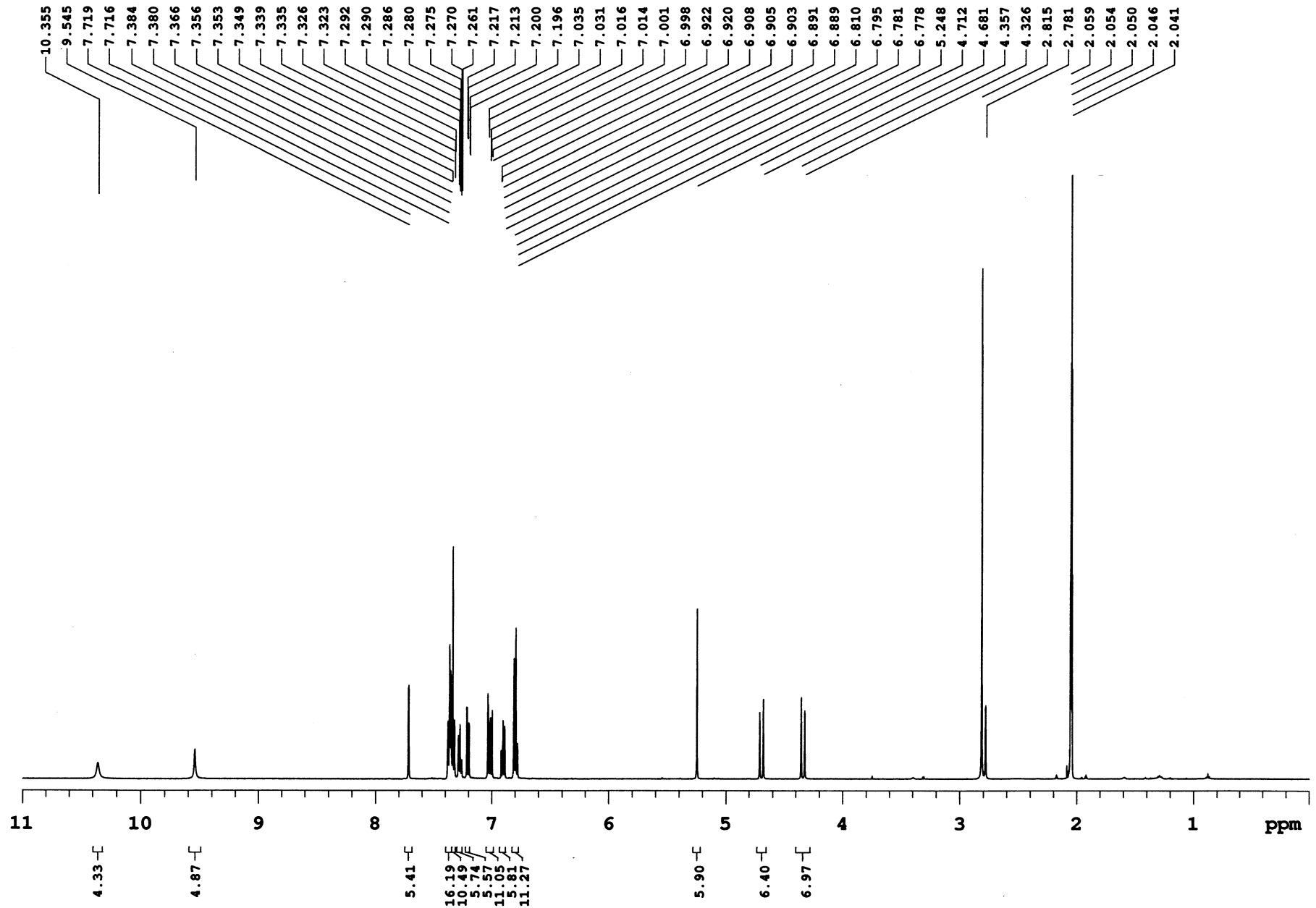
Fig S87. DEPT of compound 3cc

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-167/DEPT_03

Plot date 2017-02-15

APS-01-146-A

Sample Name	**APS-01-146-A**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-11-12**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



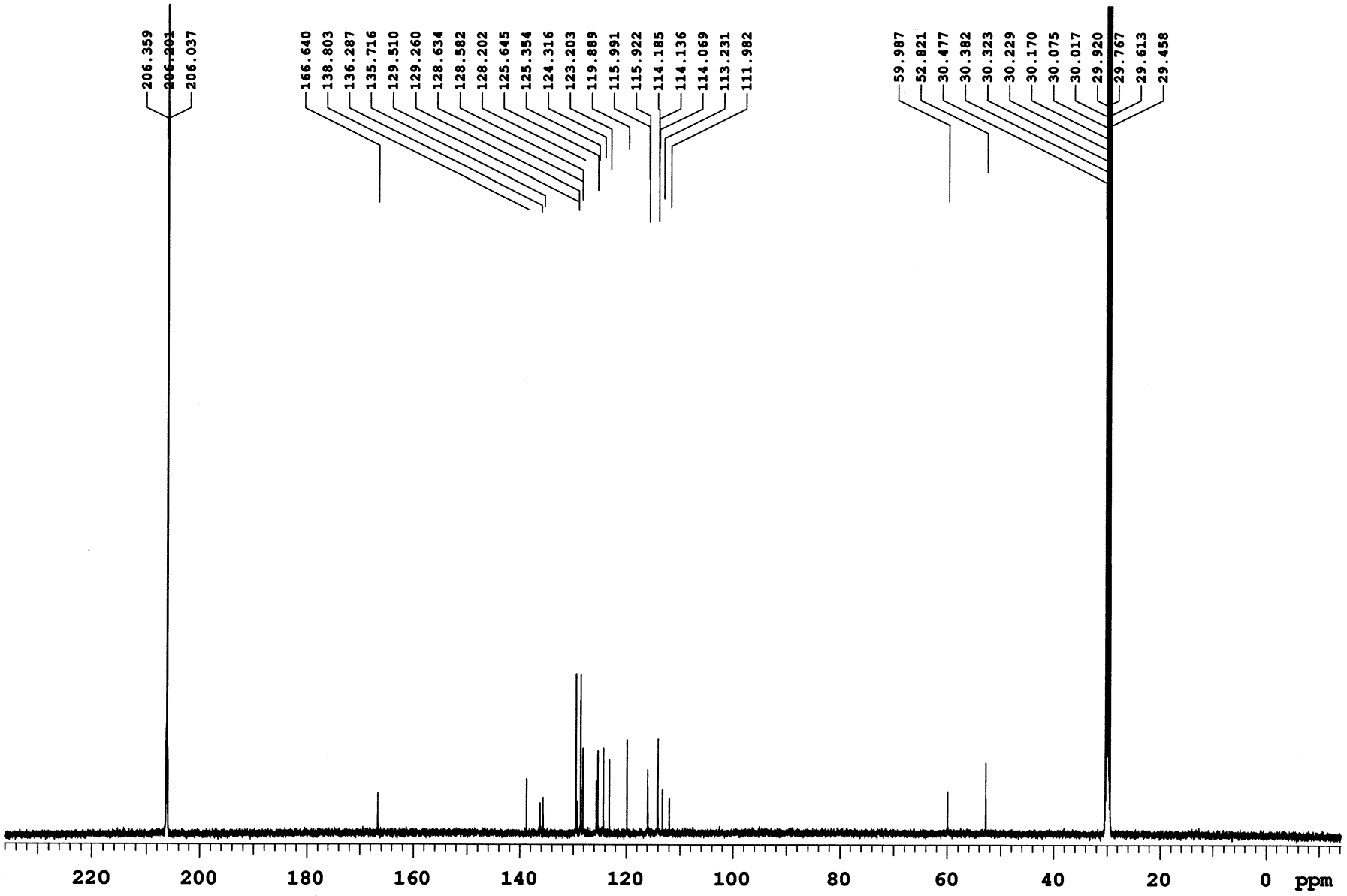
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-146-A/PROTON_02

Fig S88. 1H NMR (acetone-d6, 500 MHz) of compound 3cd

Plot date 2016-11-18

APS-01-146-A

Sample Name **APS-01-146-A**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2016-11-12**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-146-A/CARBON_02

Fig S89. 13C NMR (acetone-d6, 125 MHz) of compound 3cd

Plot date 2016-11-16

APS-01-146-A

Sample Name **APS-01-146-A**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2016-11-12**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

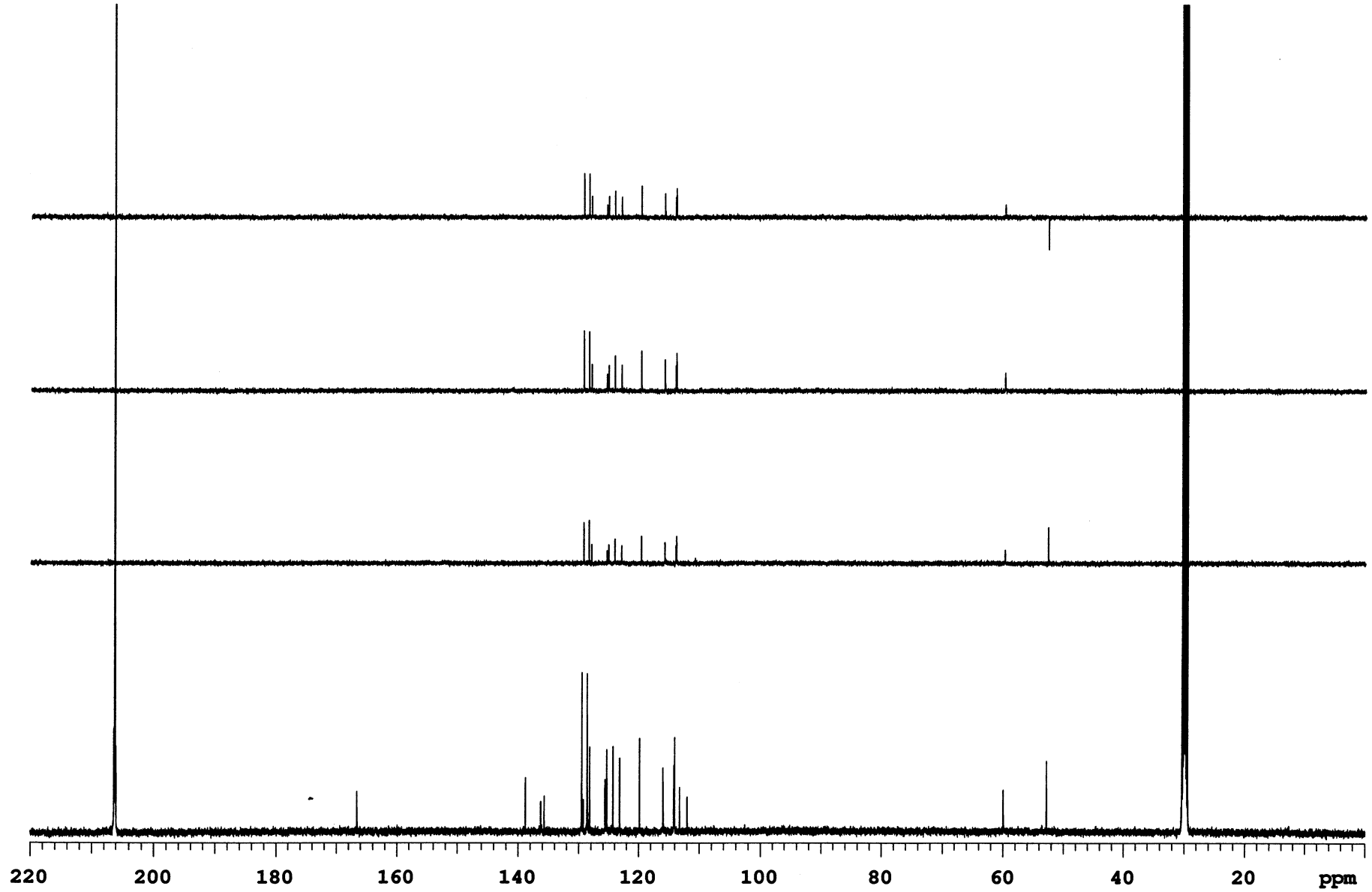


Fig S90. DEPT of compound 3cd

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-146-A/DEPT_01

Plot date 2016-11-16

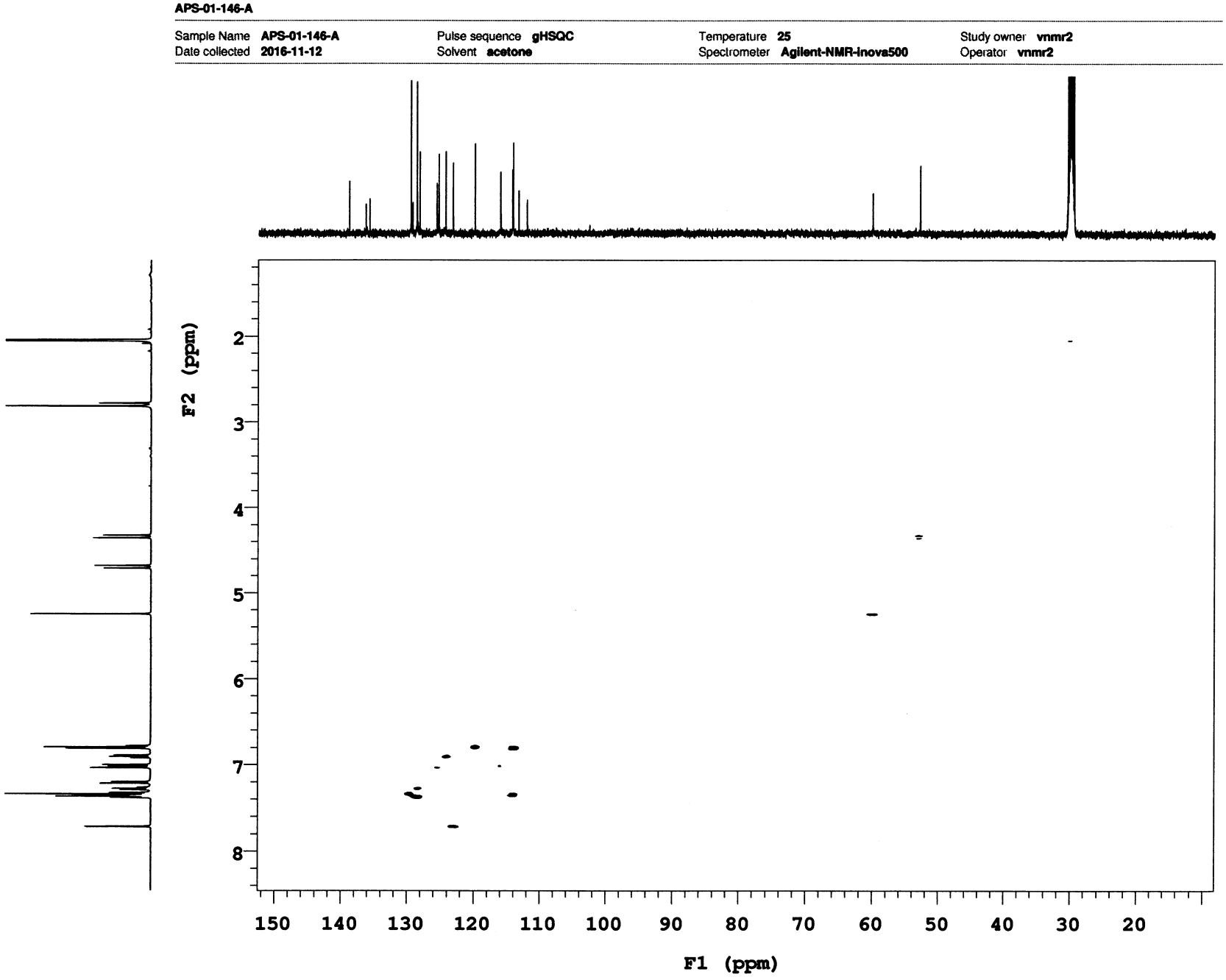


Fig S91. HSQC of compound 3cd

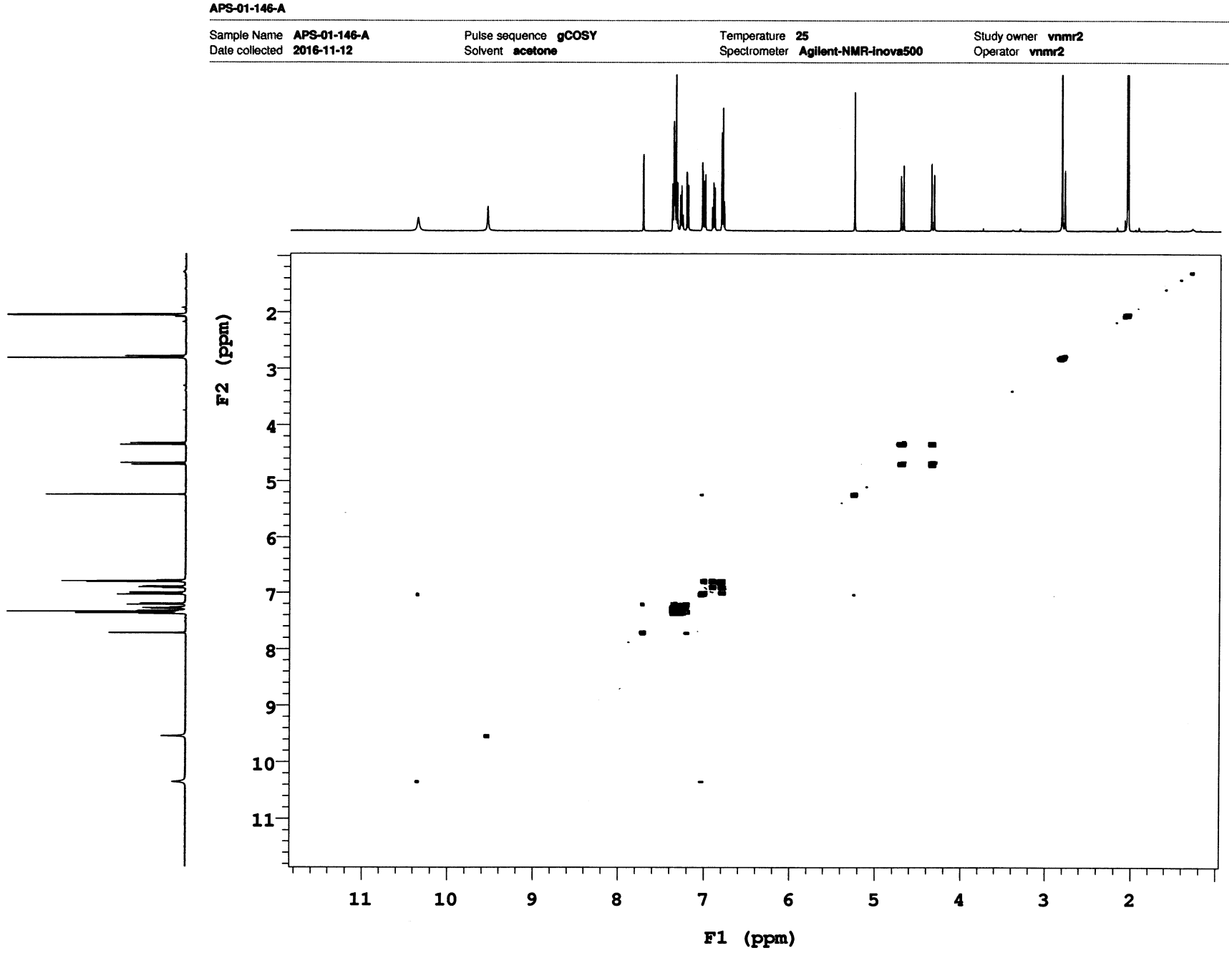


Fig S92. COSY of compound 3cd

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-146-A/gCOSY_01

Plot date 2016-11-16

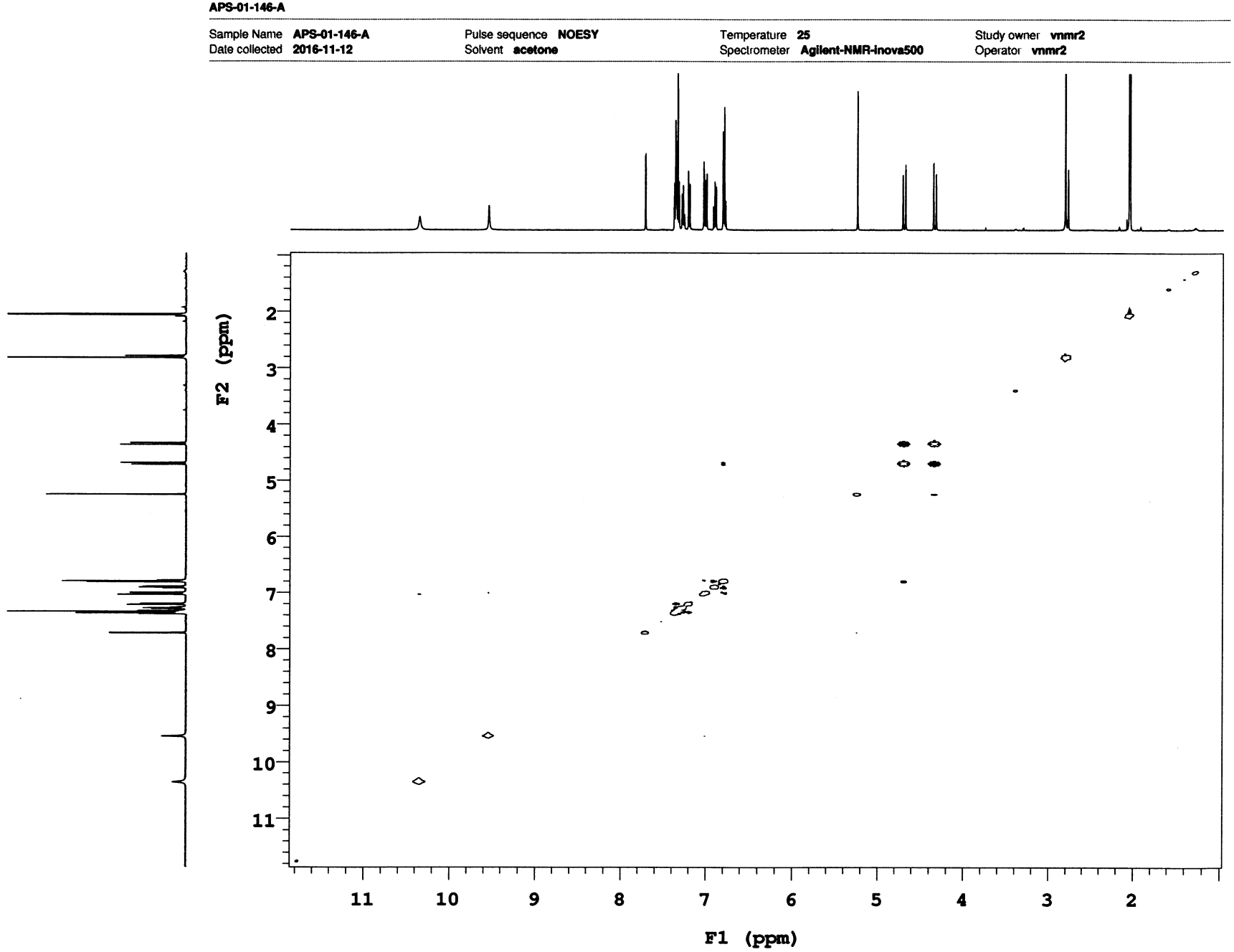


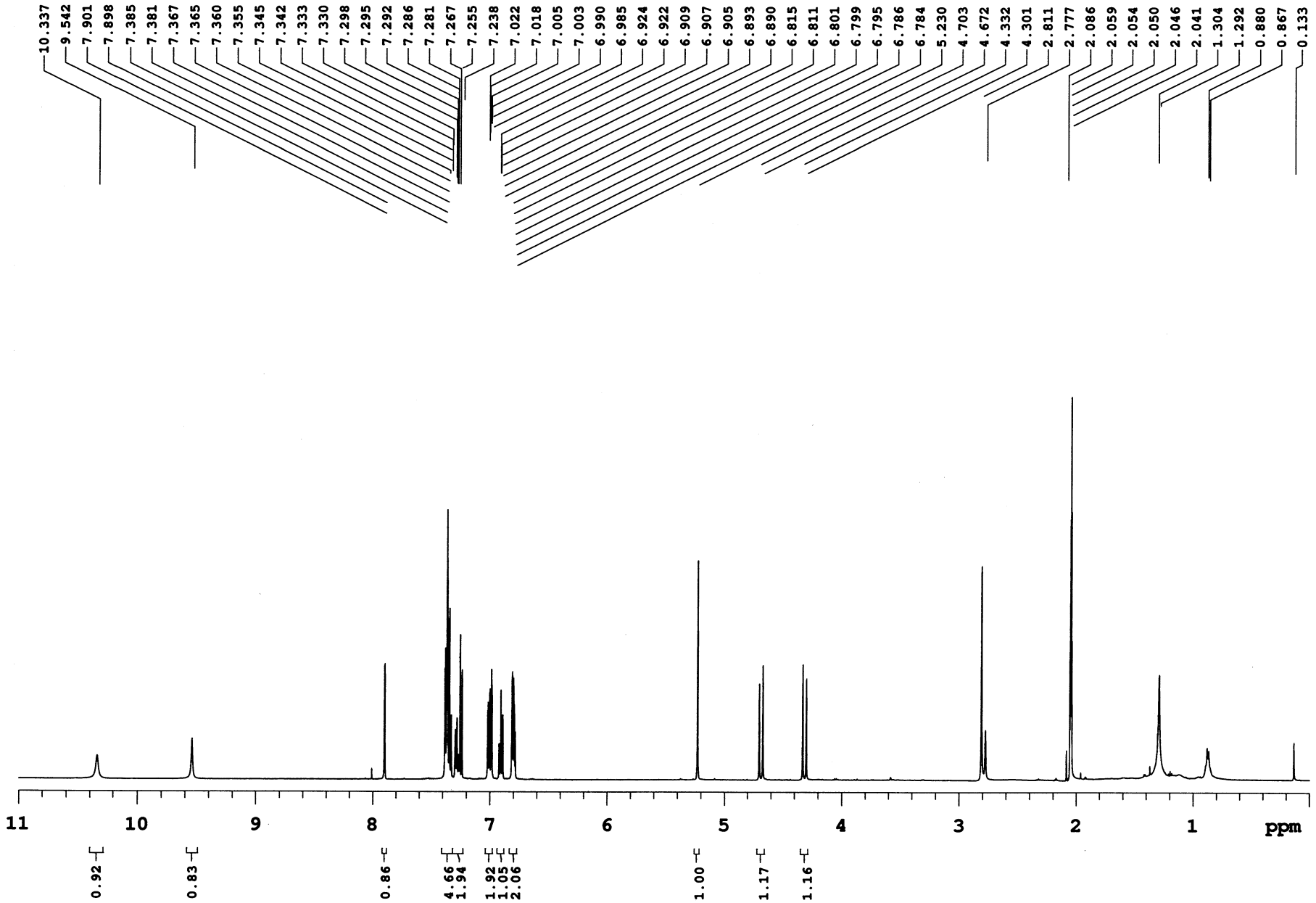
Fig S93. NOESY of compound 3cd

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-146-A/NOESY_01

Plot date 2016-11-16

APS-01-156

Sample Name	**APS-01-156**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-02-10**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-156/PROTON_03

Fig S94. 1H NMR (acetone-d6, 500 MHz) of compound 3ce

Plot date 2017-02-10

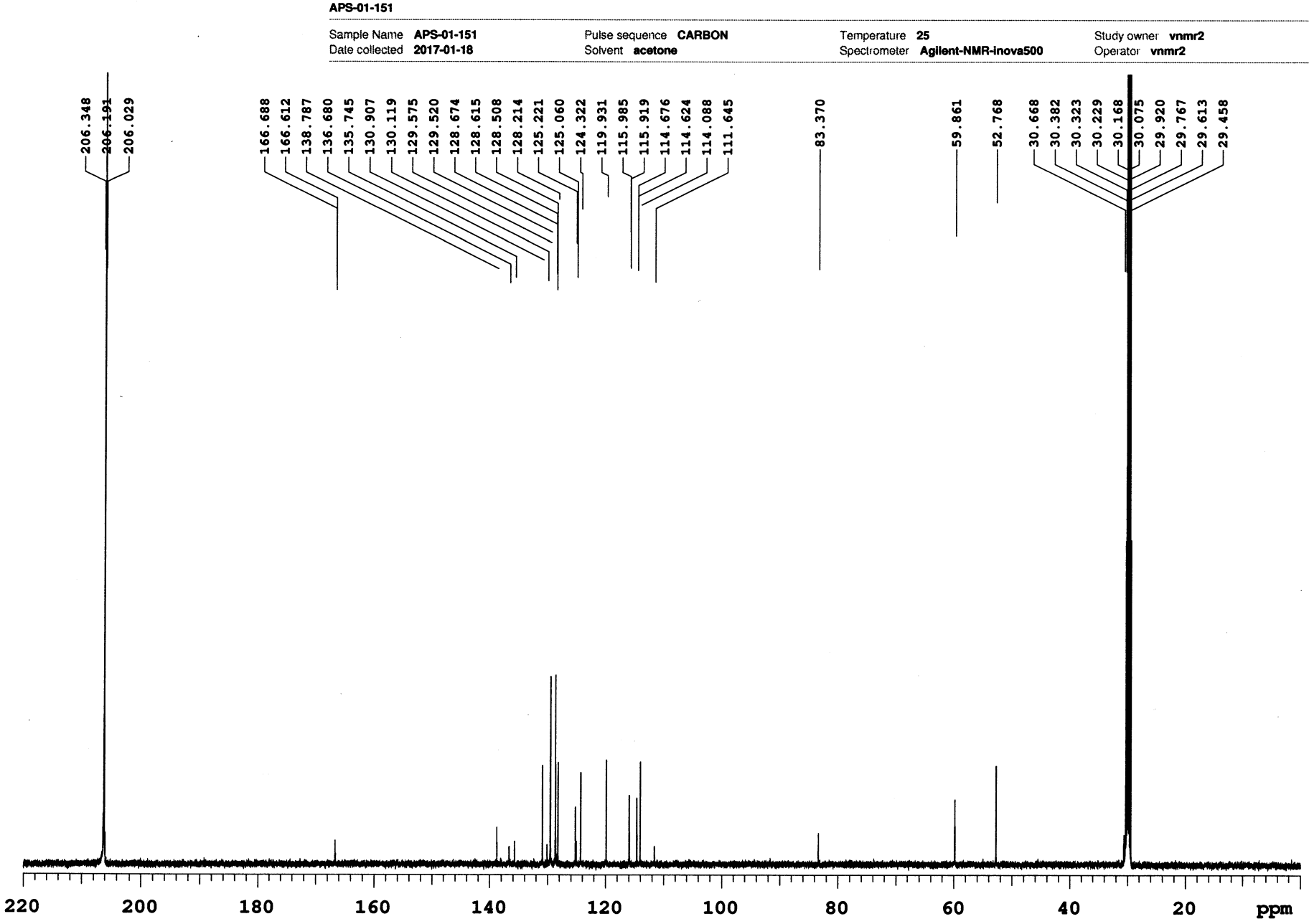


Fig S95. 13C NMR (acetone-d6 125 MHz) of compound 3ce

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-151/CARBON_04

Plot date 2017-01-18

APS-01-151

Sample Name **APS-01-151**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-18**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

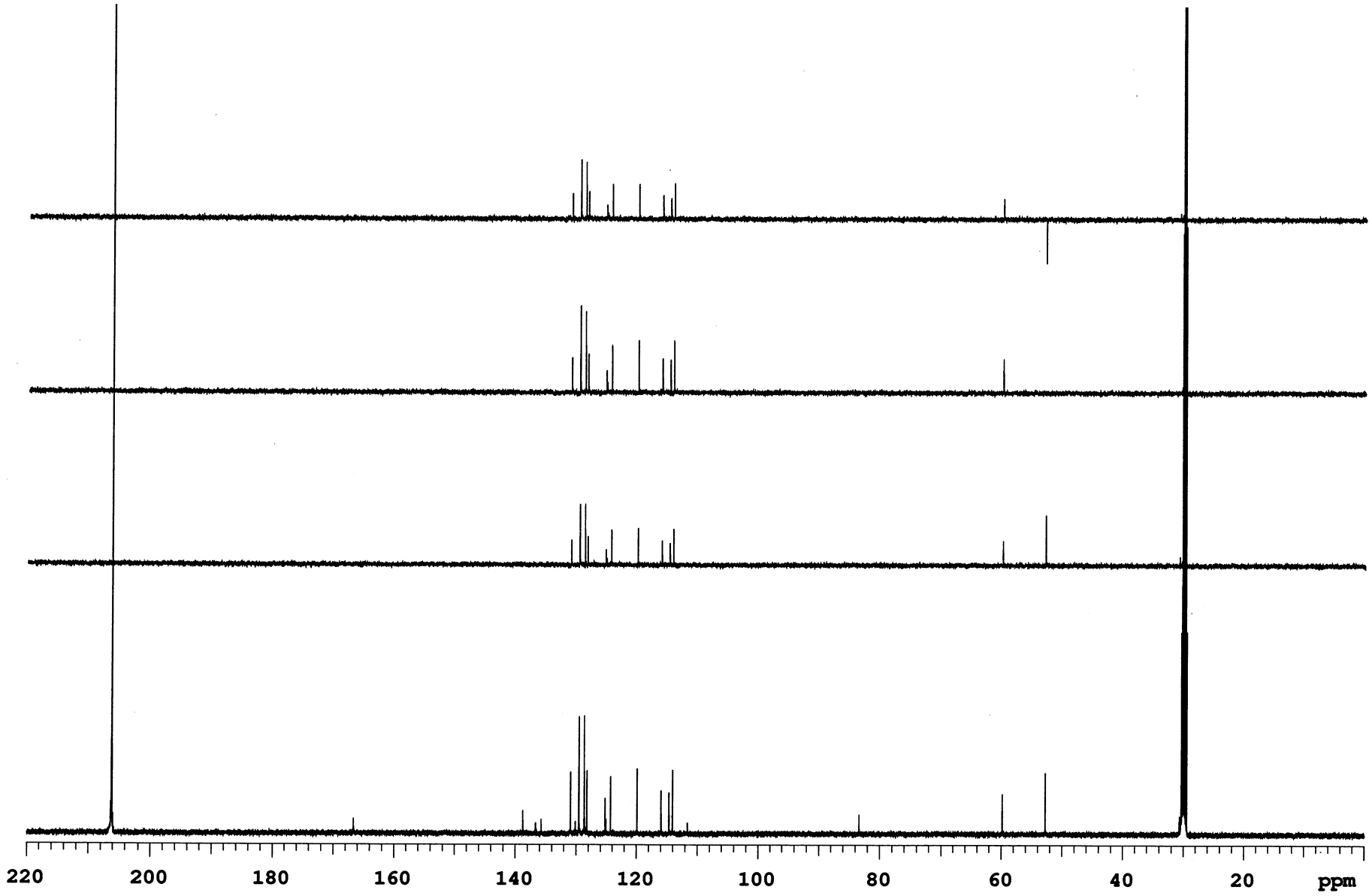


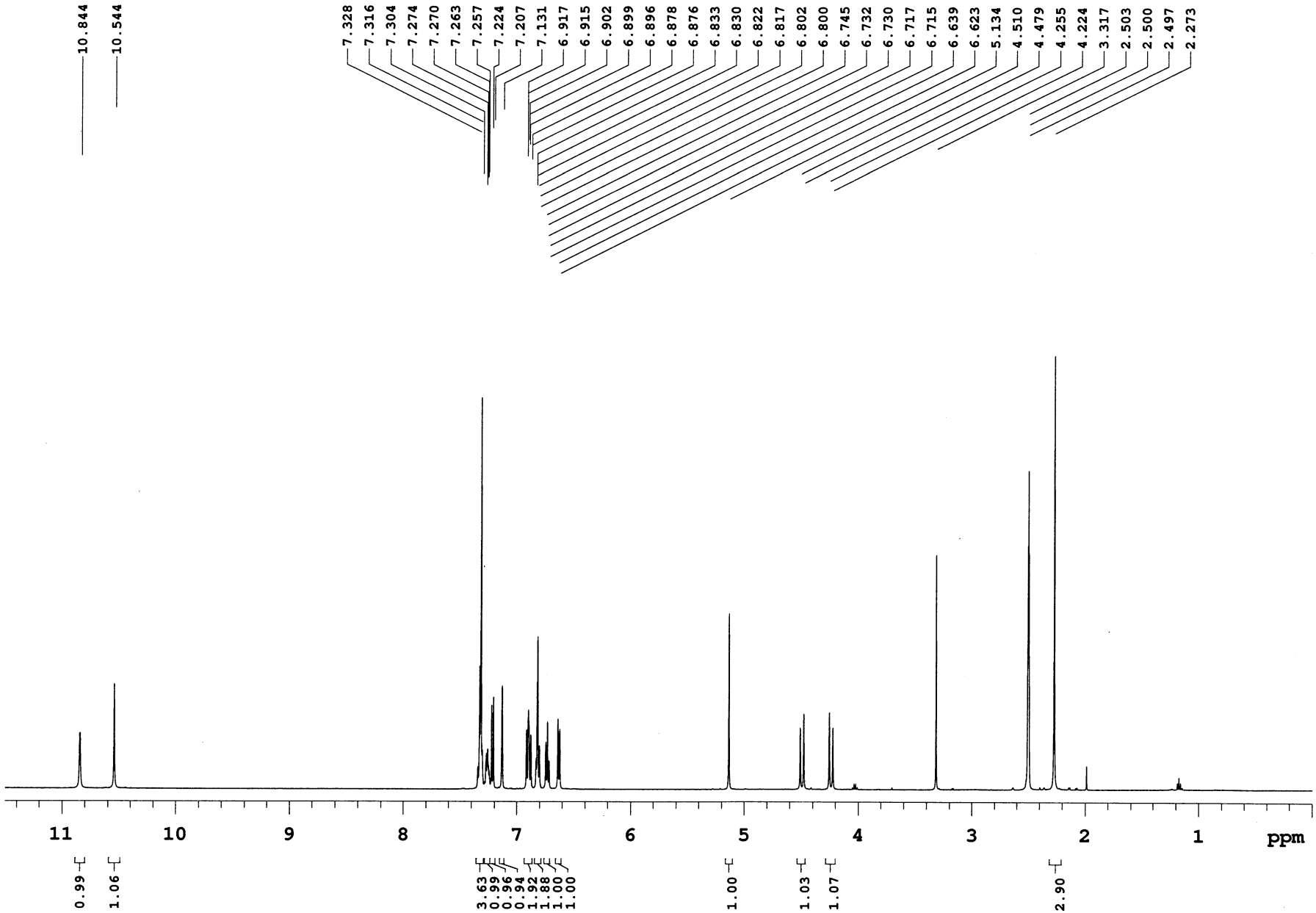
Fig S96. DEPT of compound 3ce

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-151/DEPT_02

Plot date 2017-01-18

APS-01-194

Sample Name	**APS-01-194**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-02-06**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



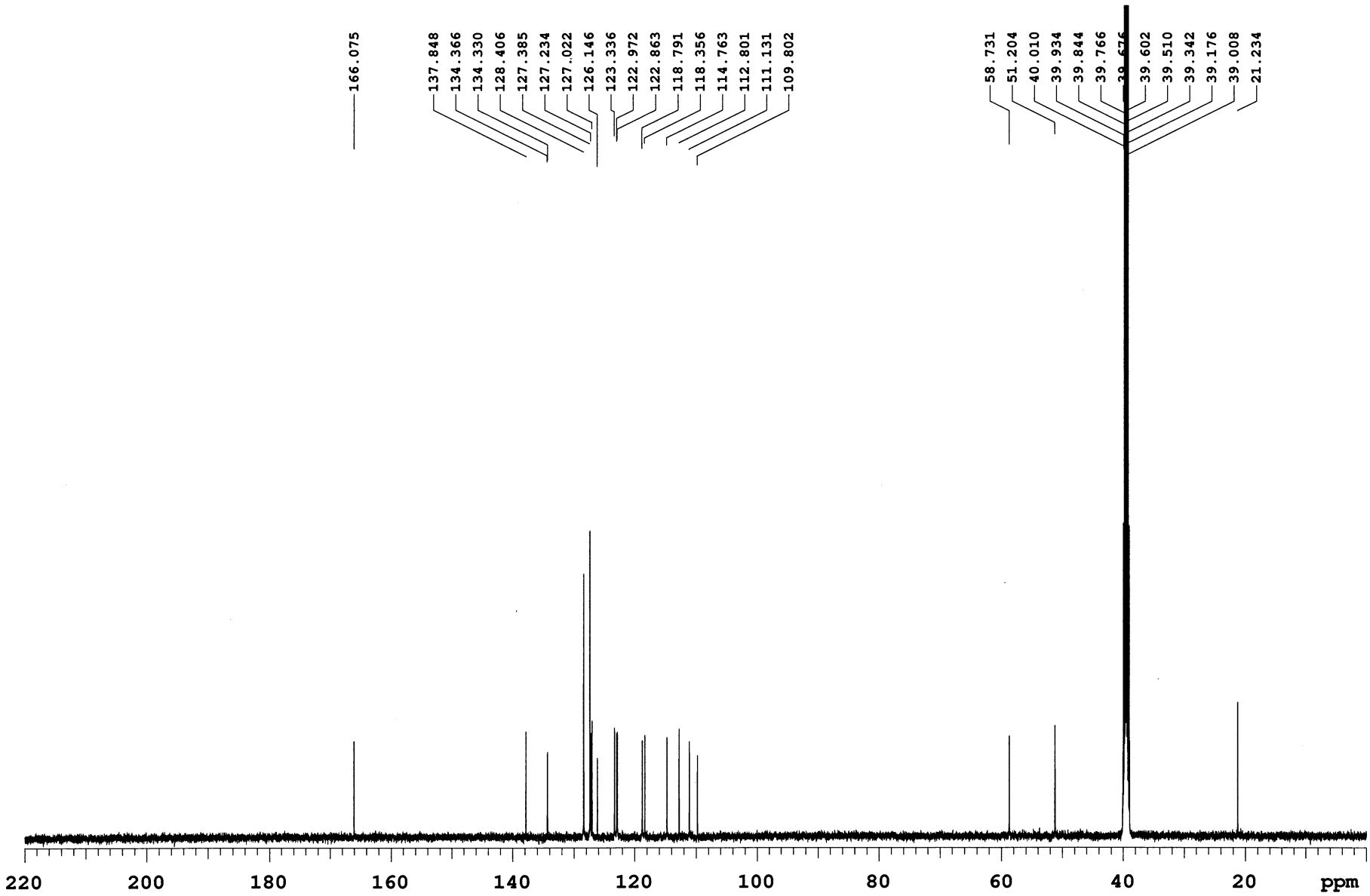
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-194/PROTON_04

Fig S97. 1H NMR (DMSO-d6, 500 MHz) of compound 3cf

Plot date 2017-03-01

APS-01-194

Sample Name **APS-01-194**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-02-06**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-194/CARBON_02

Fig S98. 13C NMR (DMSO-d6, 125 MHz) of compound 3cf

Plot date 2017-02-08

APS-01-194

Sample Name **APS-01-194**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-02-06**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

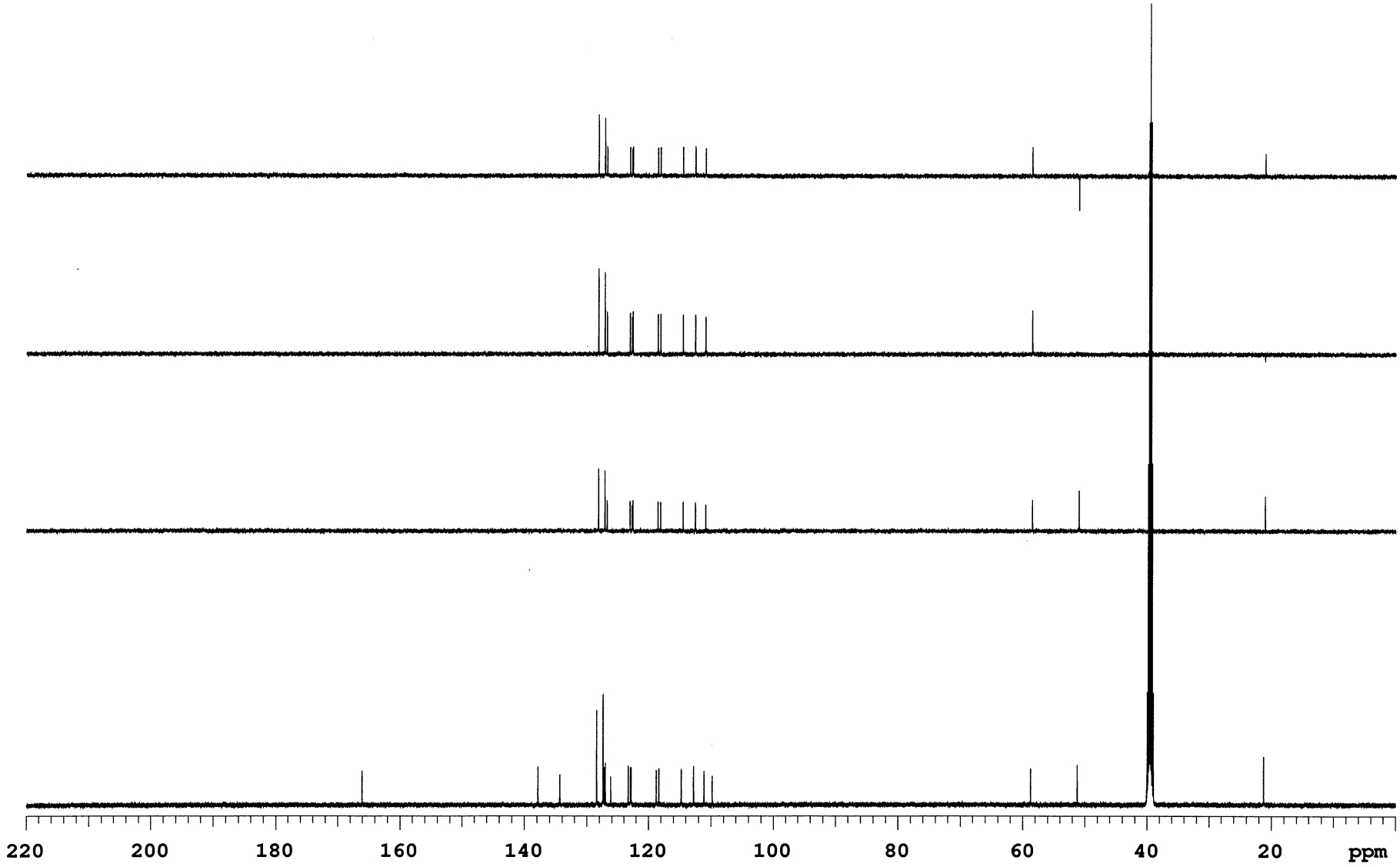
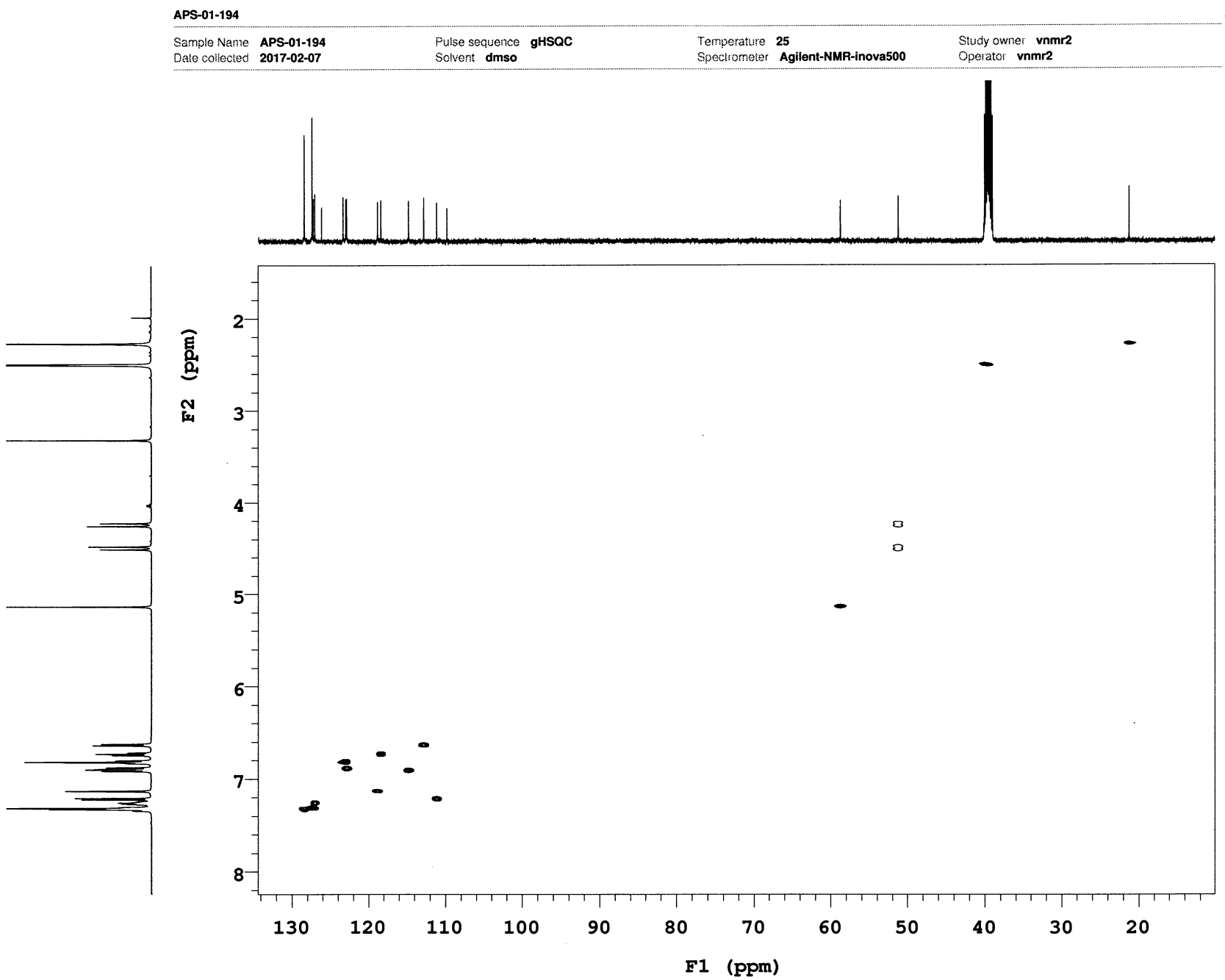


Fig S99. DEPT of compound 3cf

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-194/DEPT_01

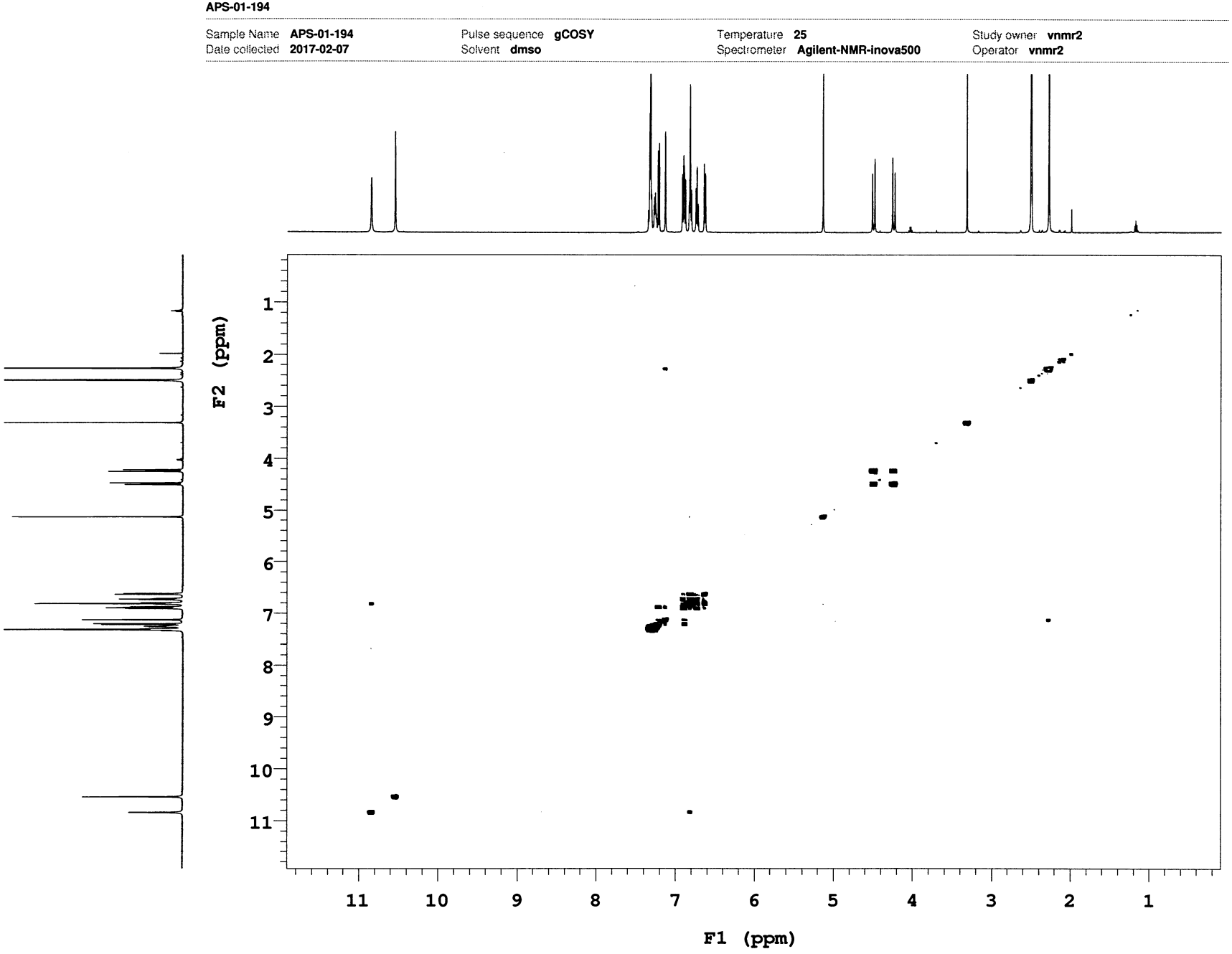
Plot date 2017-02-08



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-194/gHSQC_01

Fig S100. HSQC of compound 3cf

Plot date 2017-02-08



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-194/gCOSY_01

Fig S101. COSY of compound 3cf

Plot date 2017-02-08

APS-01-194

Sample Name	**APS-01-194**	Pulse sequence	**NOESY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-02-07**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

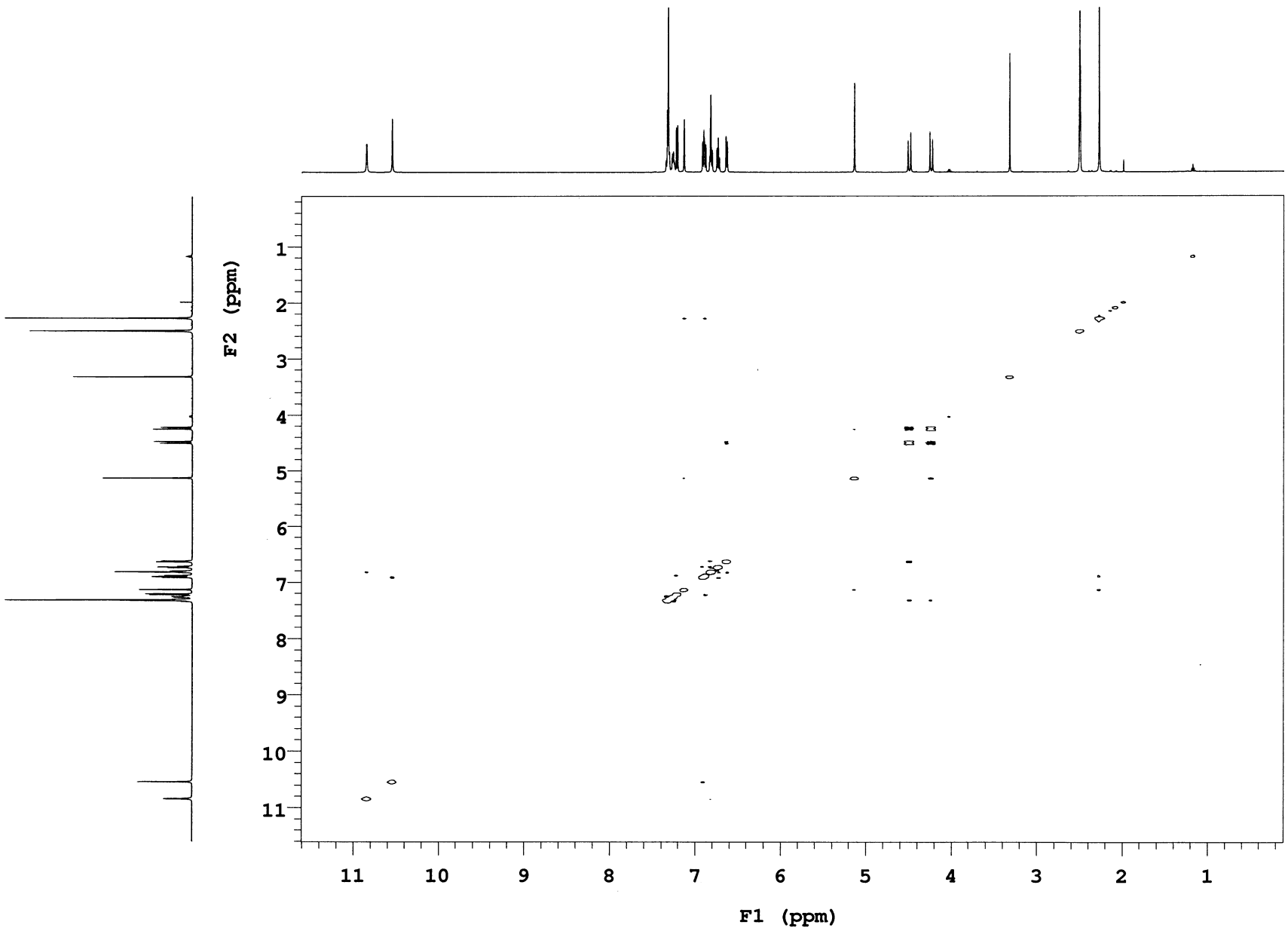


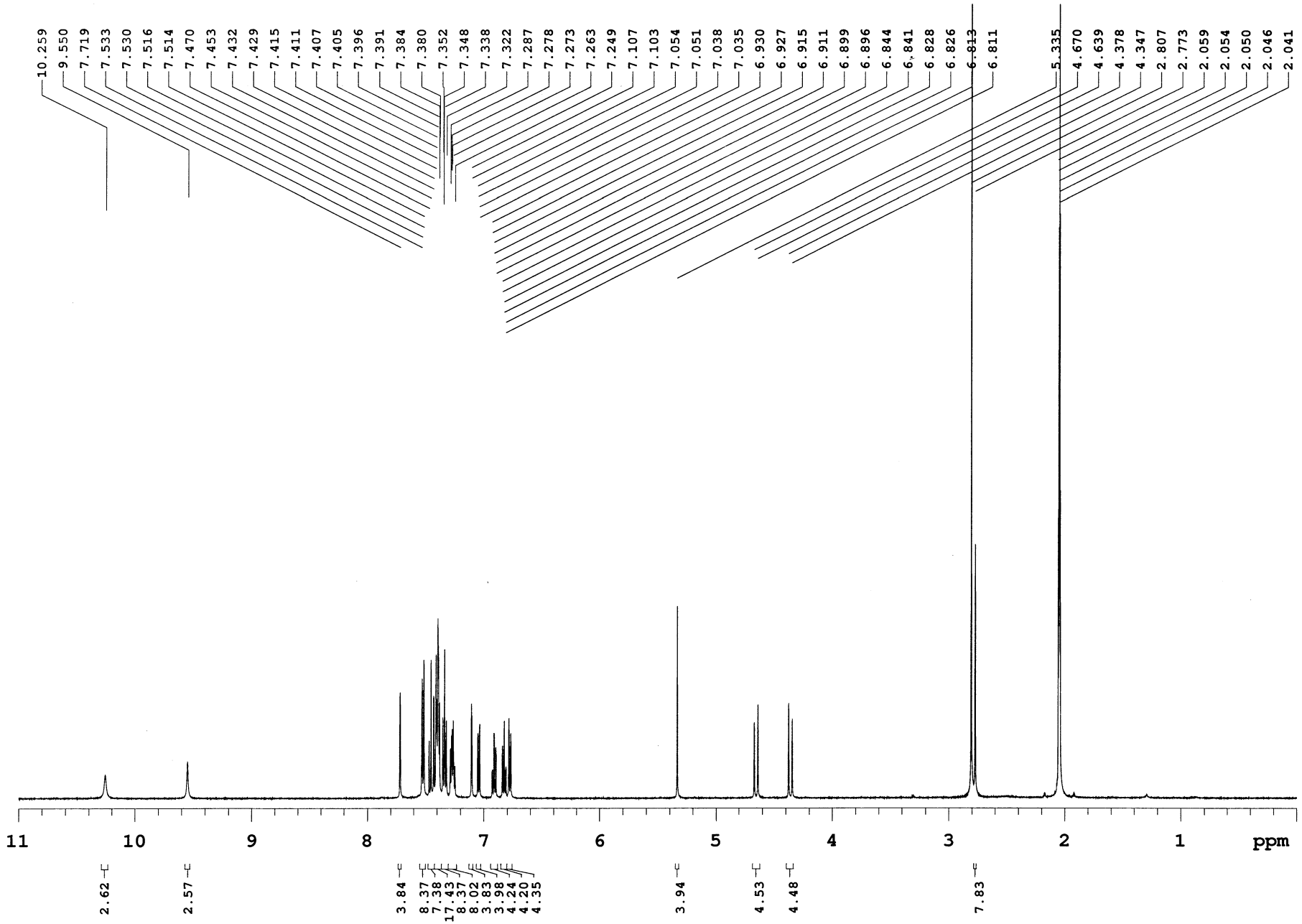
Fig S102. NOESY of compound 3cf

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-194/NOESY_01

Plot date 2017-02-09

APS-01-189

Sample Name	APS-01-189	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr2
Date collected	2017-05-04	Solvent	acetone	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-189/PROTON_03

Plot date 2017-05-04

Fig S103. 1H NMR (acetone-d6, 500 MHz) of compound 3cg

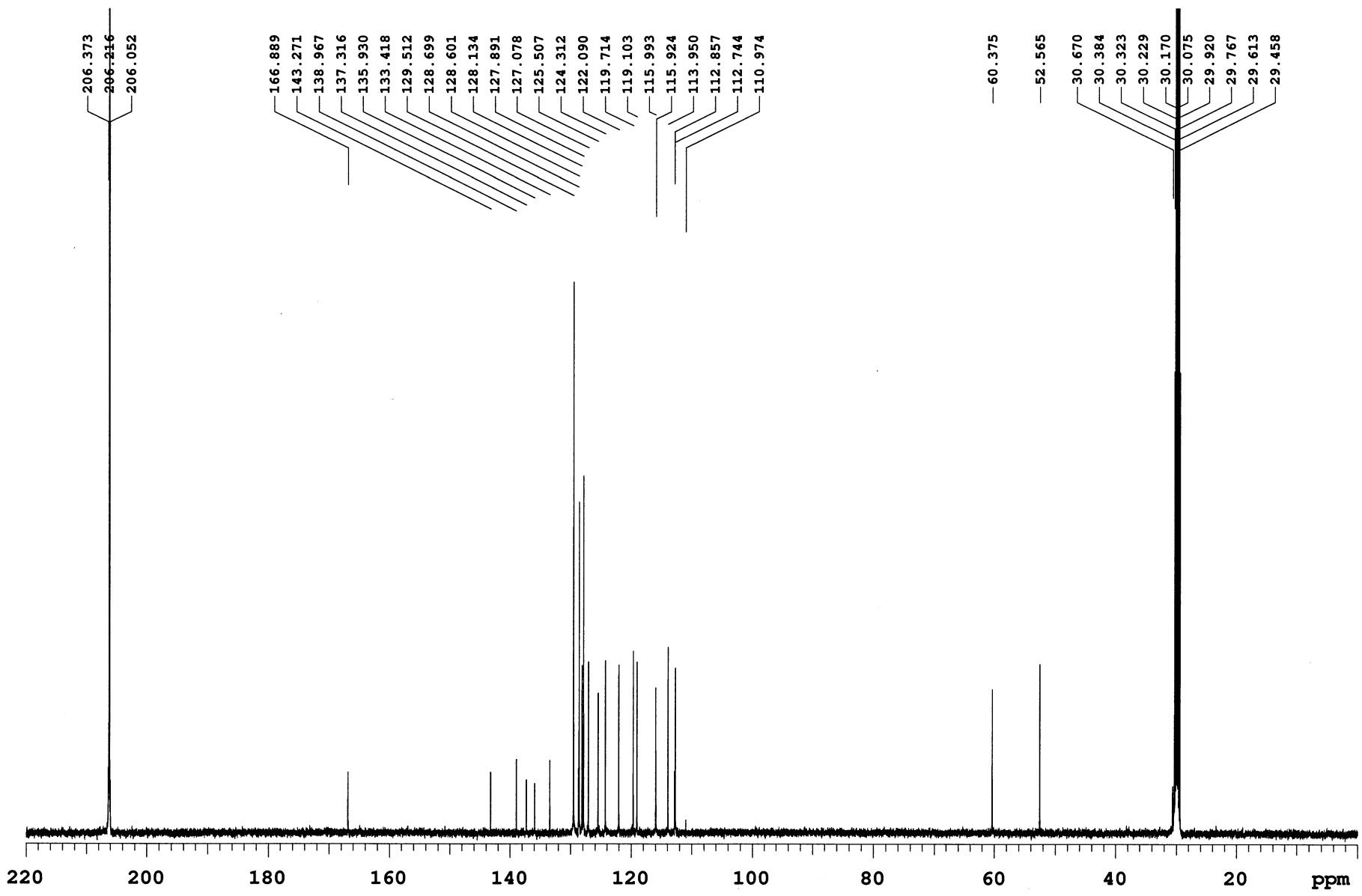


Fig S104. 13C NMR (acetone-d6, 125 MHz) of compound 3cg

APS-01-189

Sample Name **APS-01-189**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-02-15**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

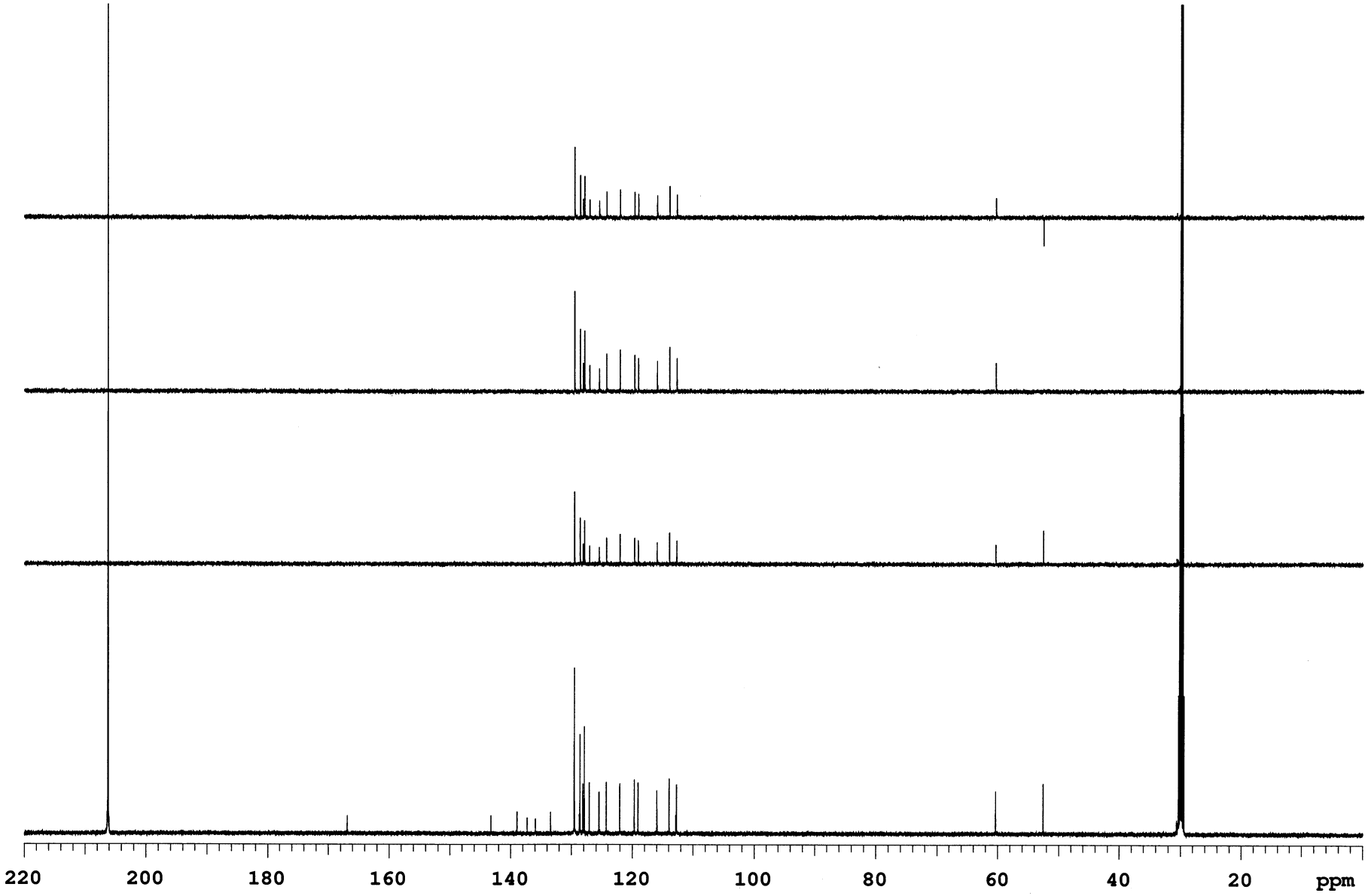


Fig S105. DEPT of compound 3cg

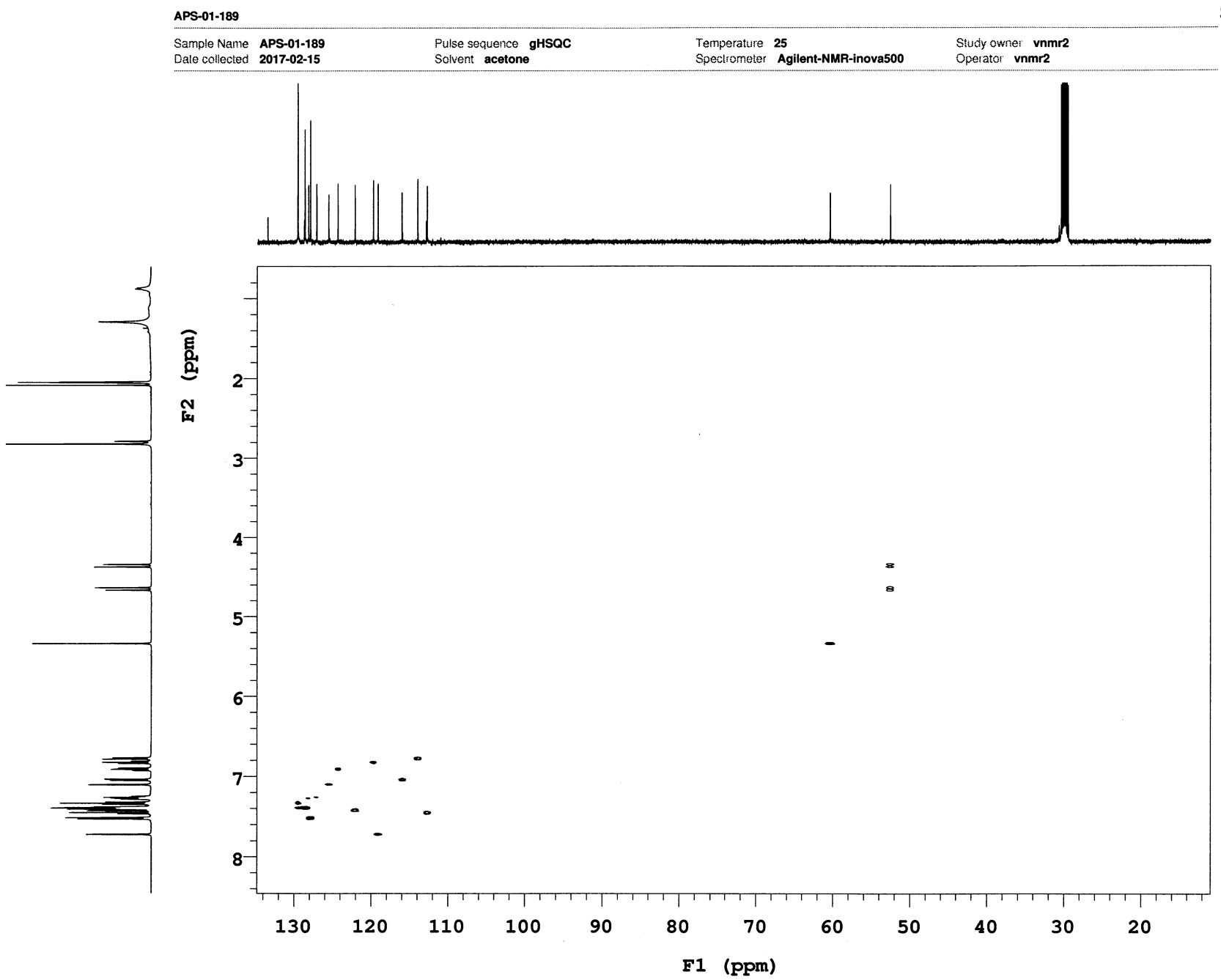
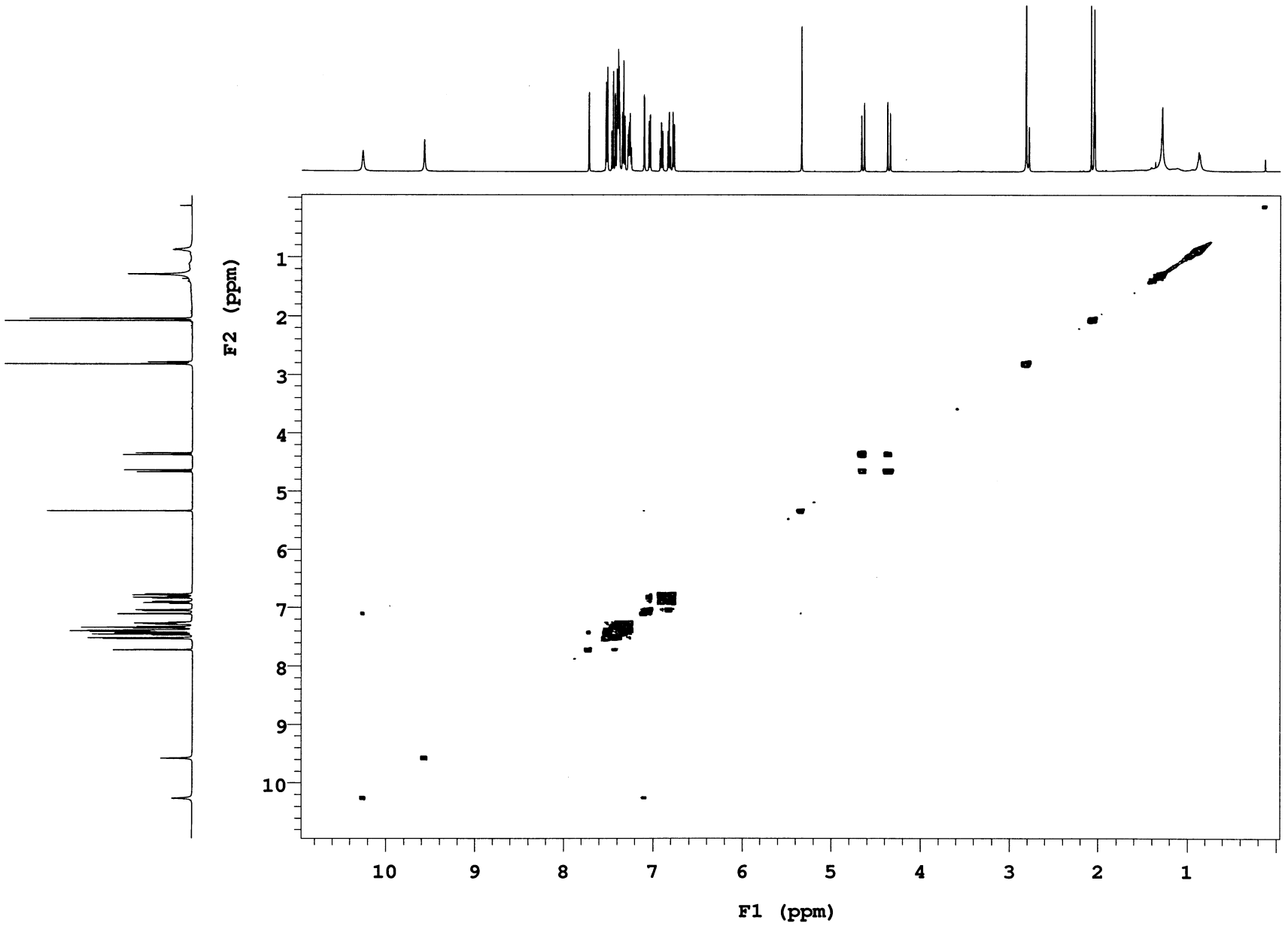


Fig S106. HSQC of compound 3cg

APS-01-189

Sample Name **APS-01-189**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-02-15**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-189/gCOSY_01

Fig S107. COSY of compound 3cg

Plot date 2017-02-15

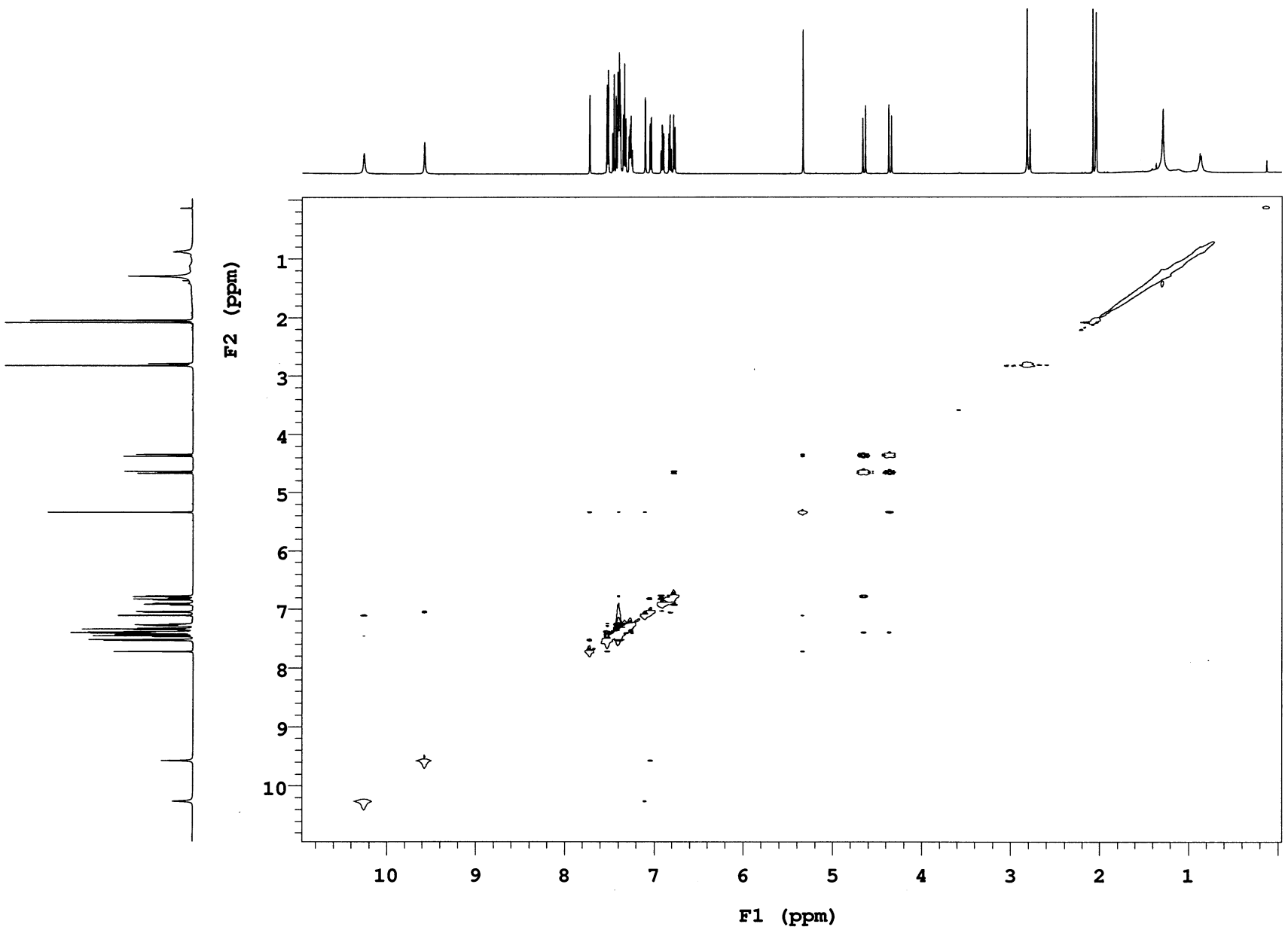


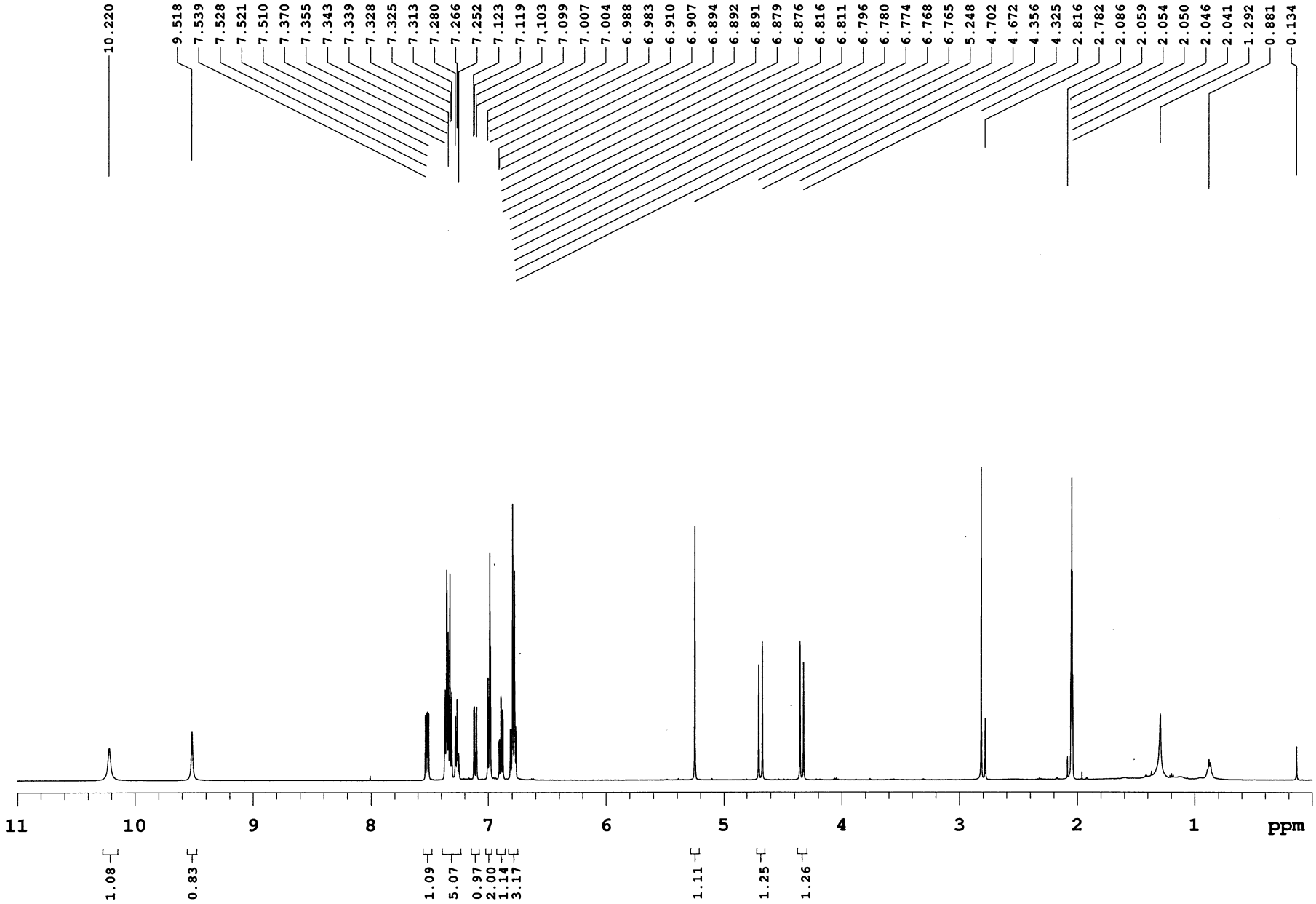
Fig S108. NOESY of compound 3cg

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-189/NOESY_01

Plot date 2017-02-15

APS-01-186

Sample Name	**APS-01-186**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-02-10**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



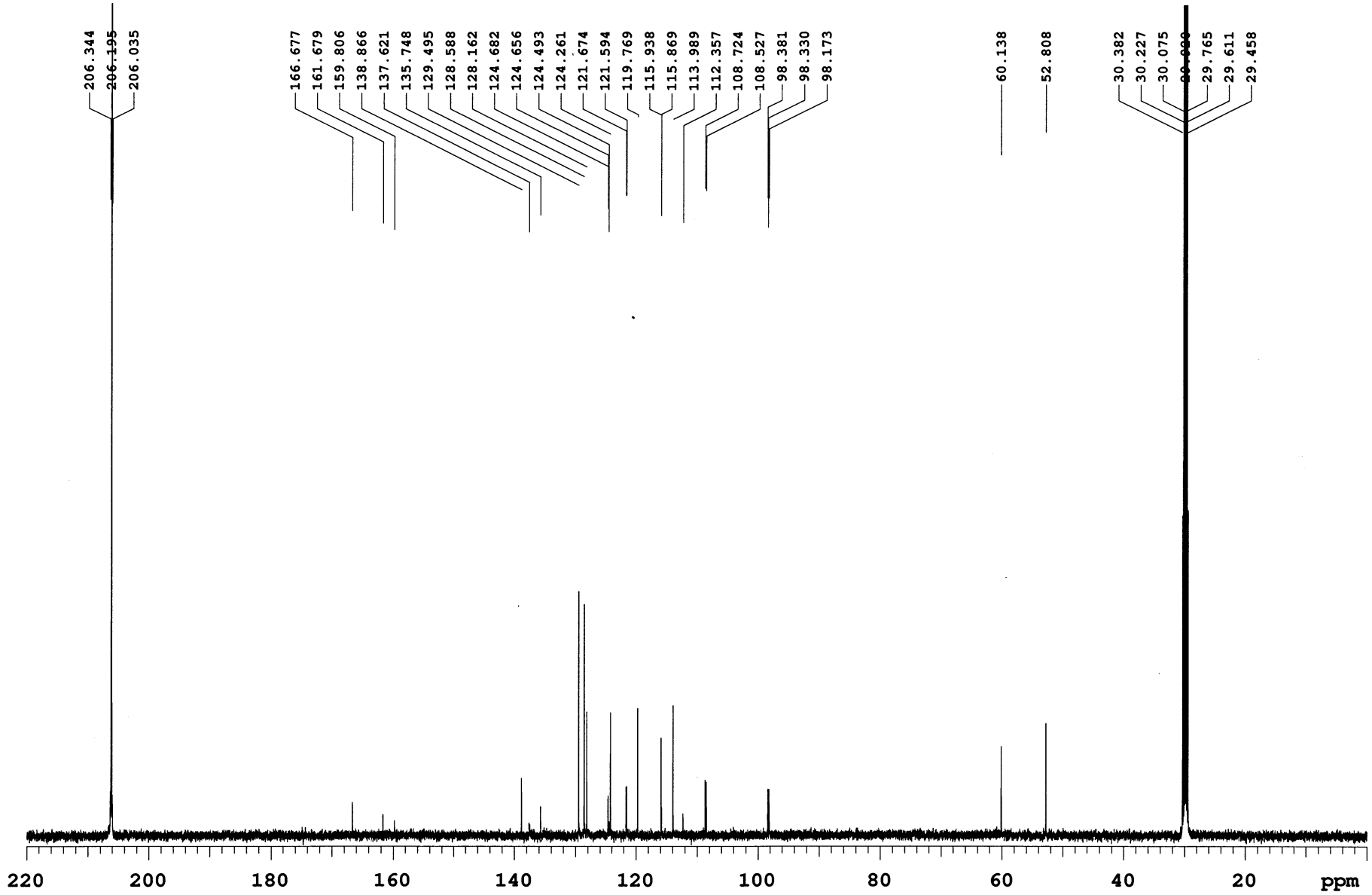
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-186/PROTON_06

Plot date 2017-02-10

Fig S109. 1H NMR (acetone-d6, 500 MHz) of compound 3ch

APS-01-186

Sample Name	**APS-01-186**	Pulse sequence	**CARBON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-01-20**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-186/CARBON_02

Fig S110. 13C NMR (acetone-d6, 125 MHz) of compound 3ch

Plot date 2017-01-24

APS-01-186

Sample Name **APS-01-186**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-20**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

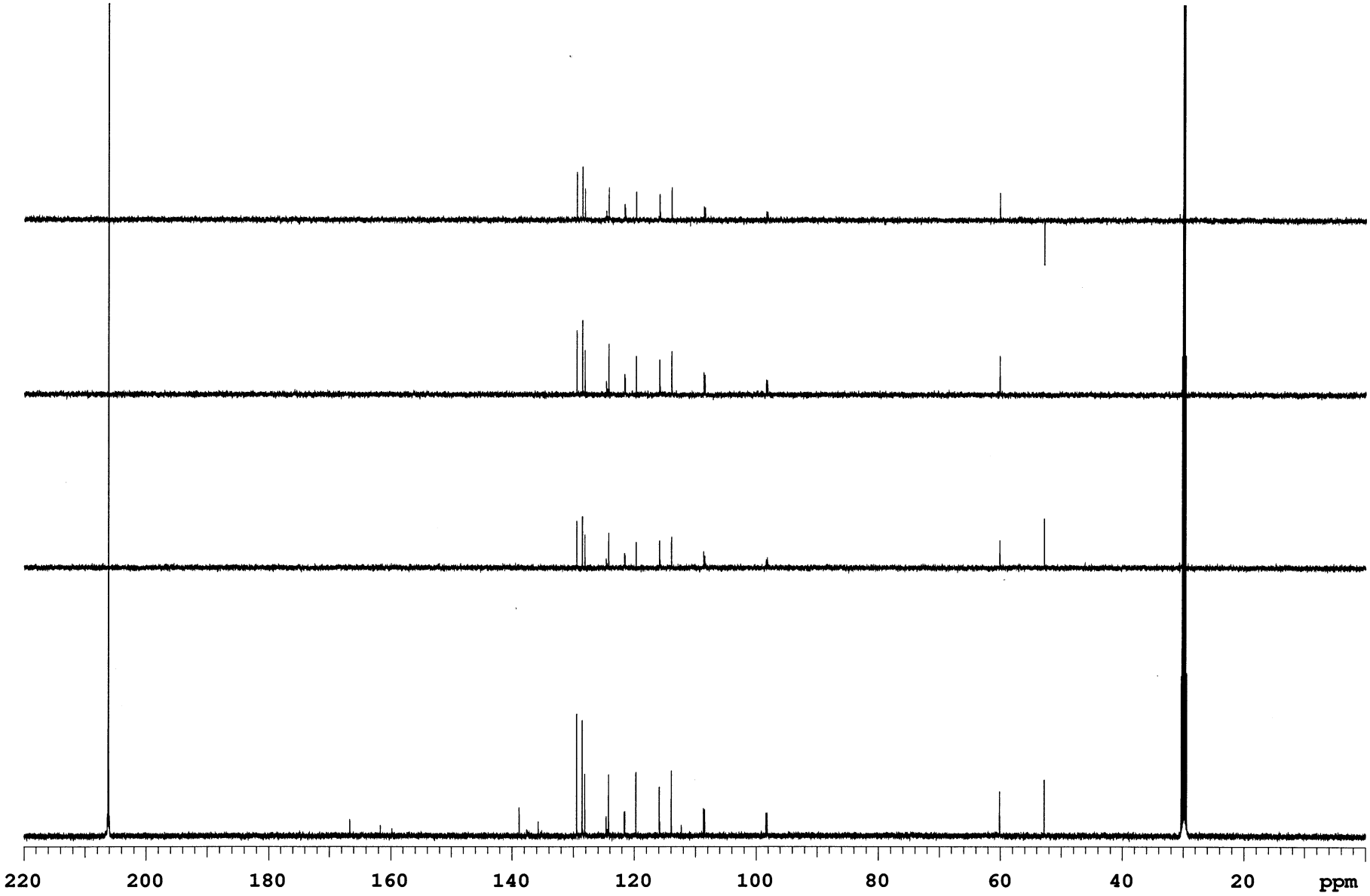
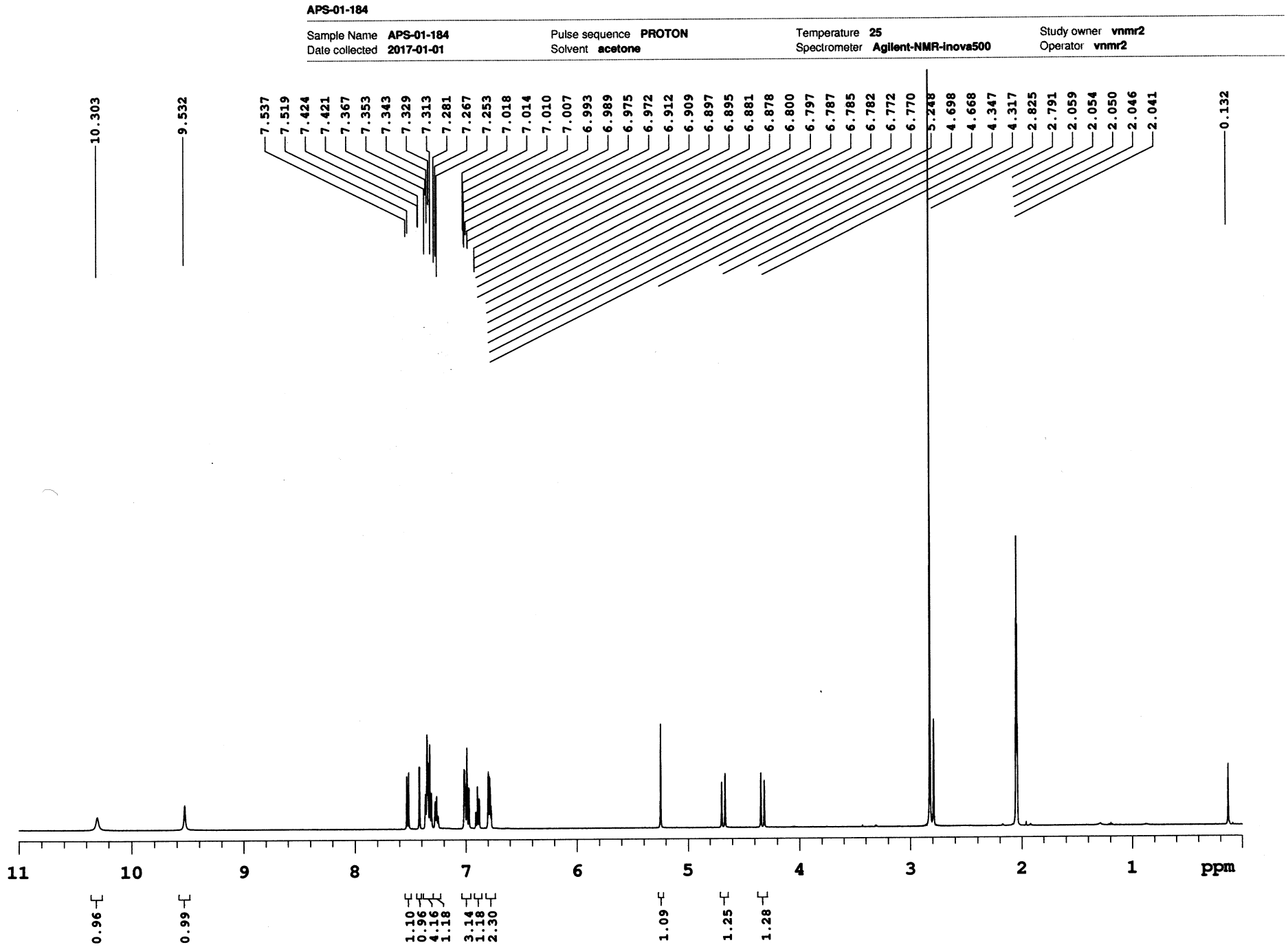


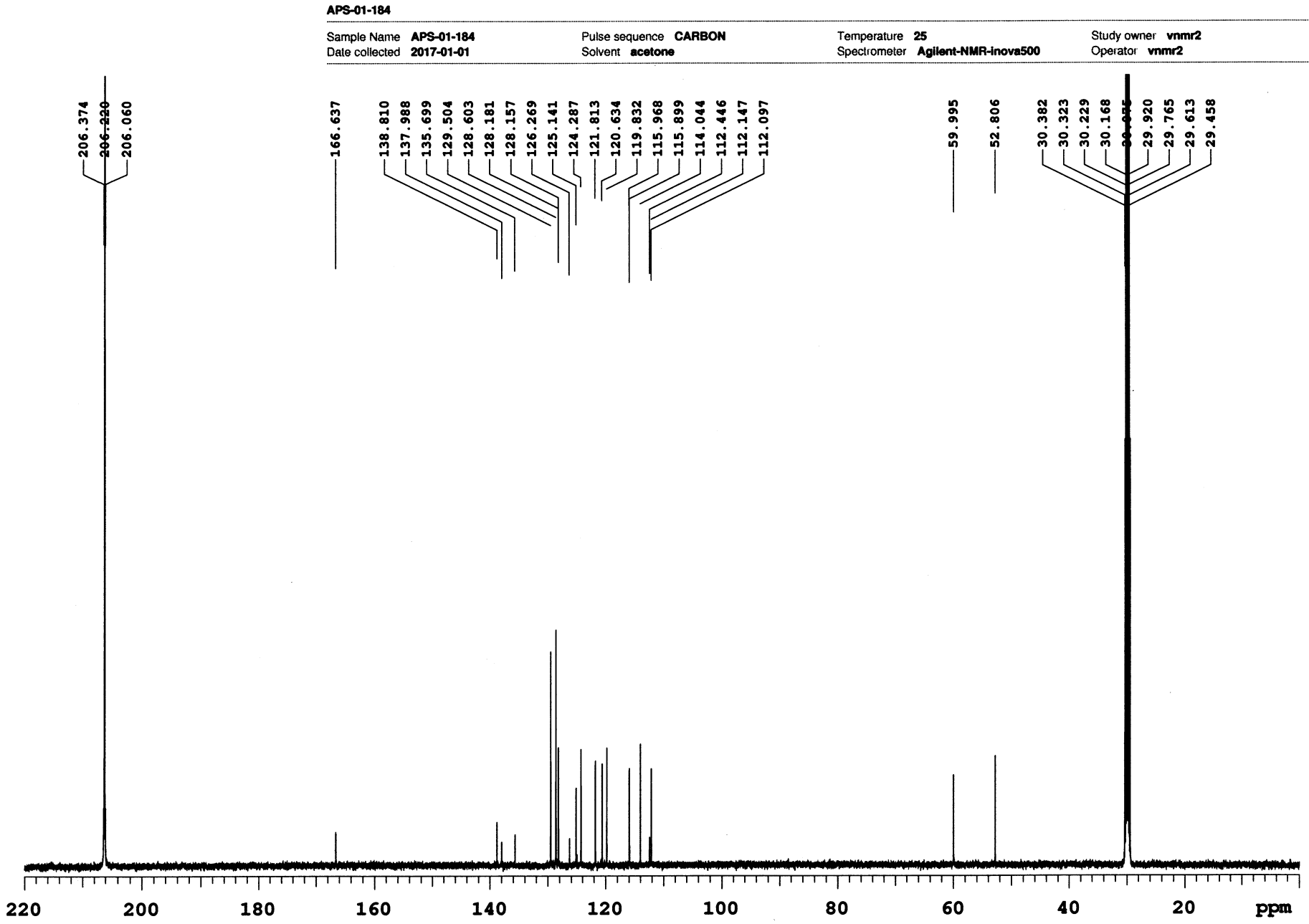
Fig S111. DEPT of compound 3ch



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-184/PROTON_02

Fig S112. 1H NMR (acetone-d6, 500 MHz) of compound 3ci

Plot date 2017-01-04



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-184/CARBON_02

Fig S113. 13C NMR (acetone-d6, 125 MHz) of compound 3ci

Plot date 2017-01-03

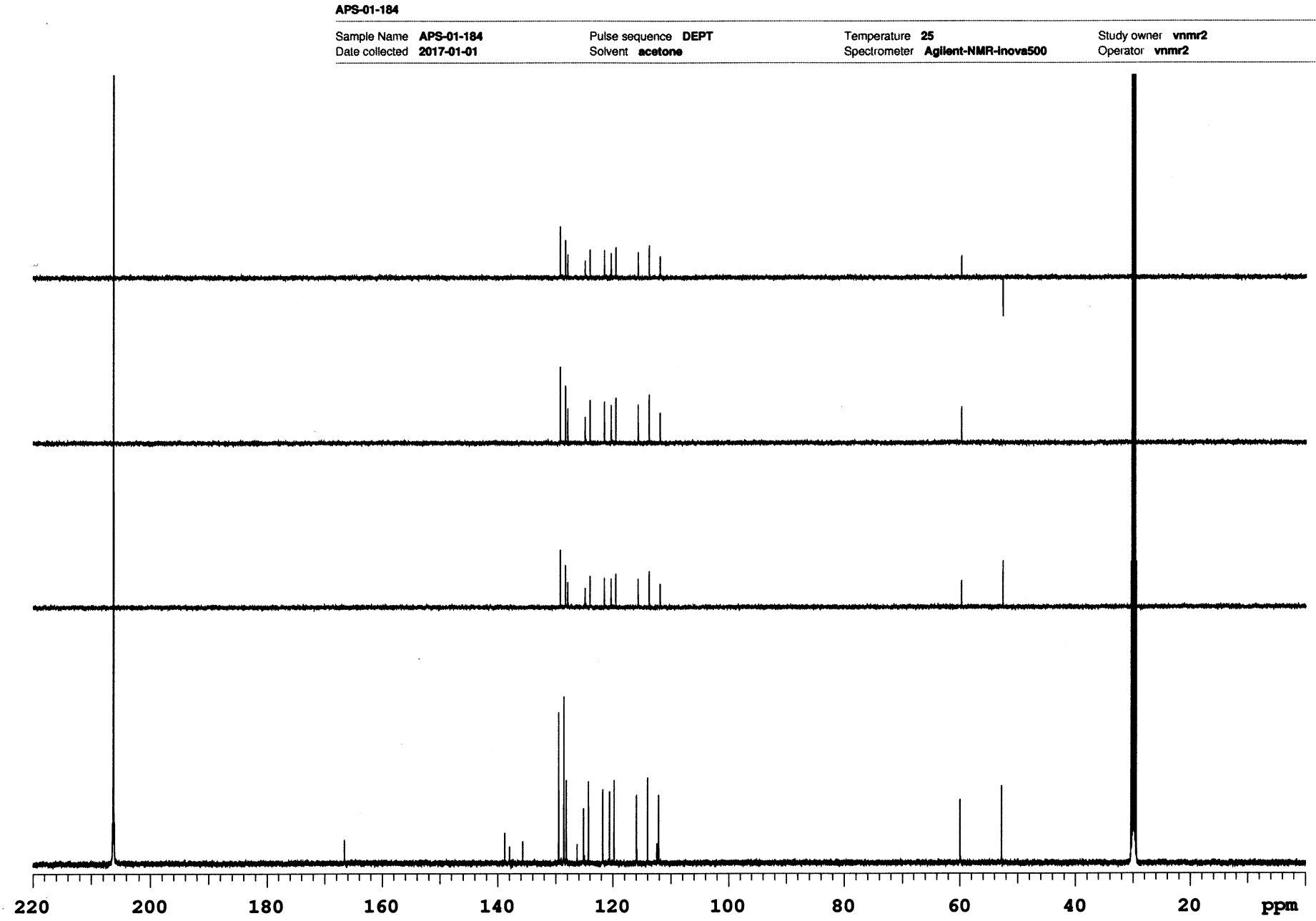


Fig S114. DEPT of compound 3ci

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-184/DEPT_01.fid

Plot date 2017-01-03

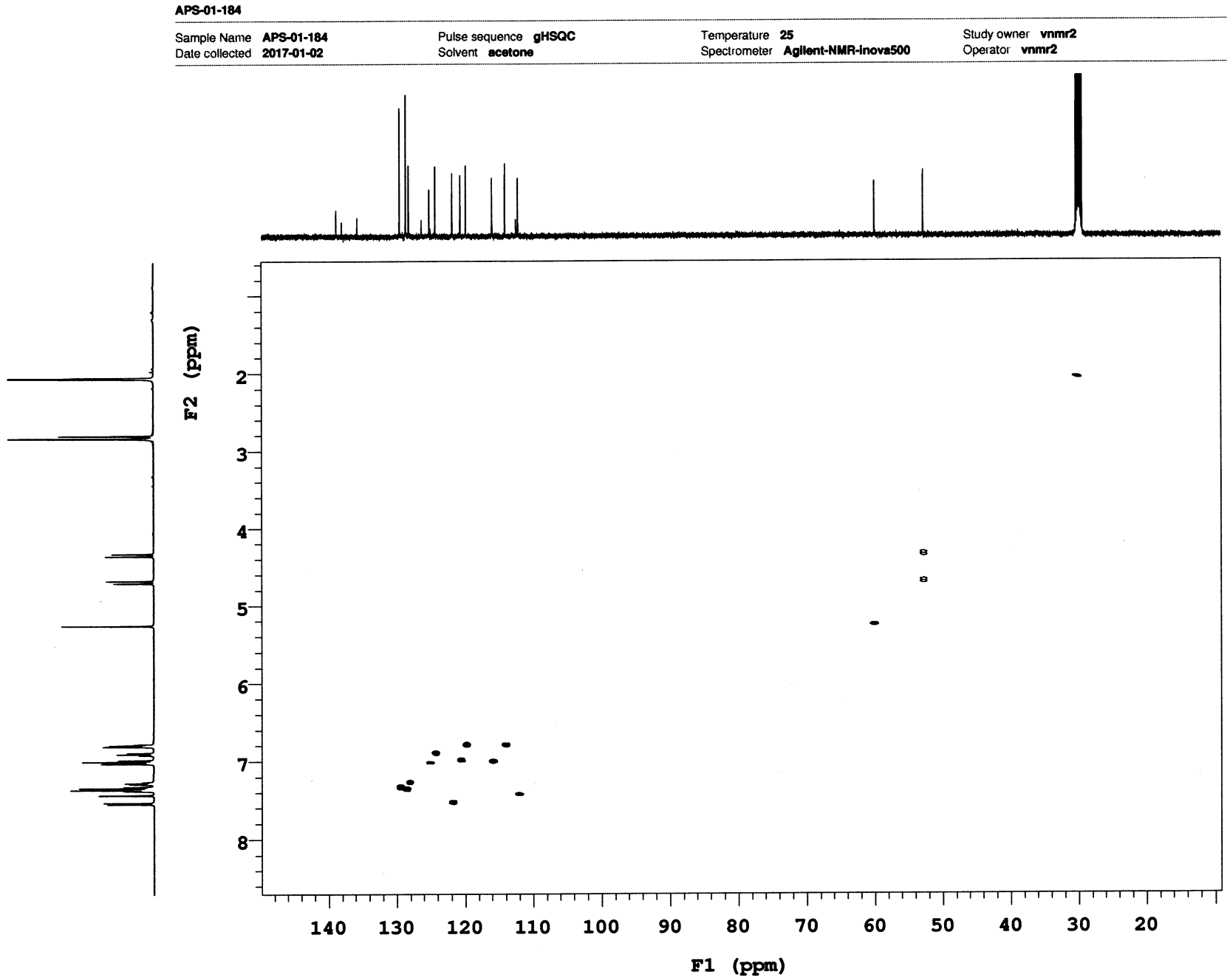


Fig S115. HSQC of compound 3ci

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-184/gHSQC_01

Plot date 2017-01-04

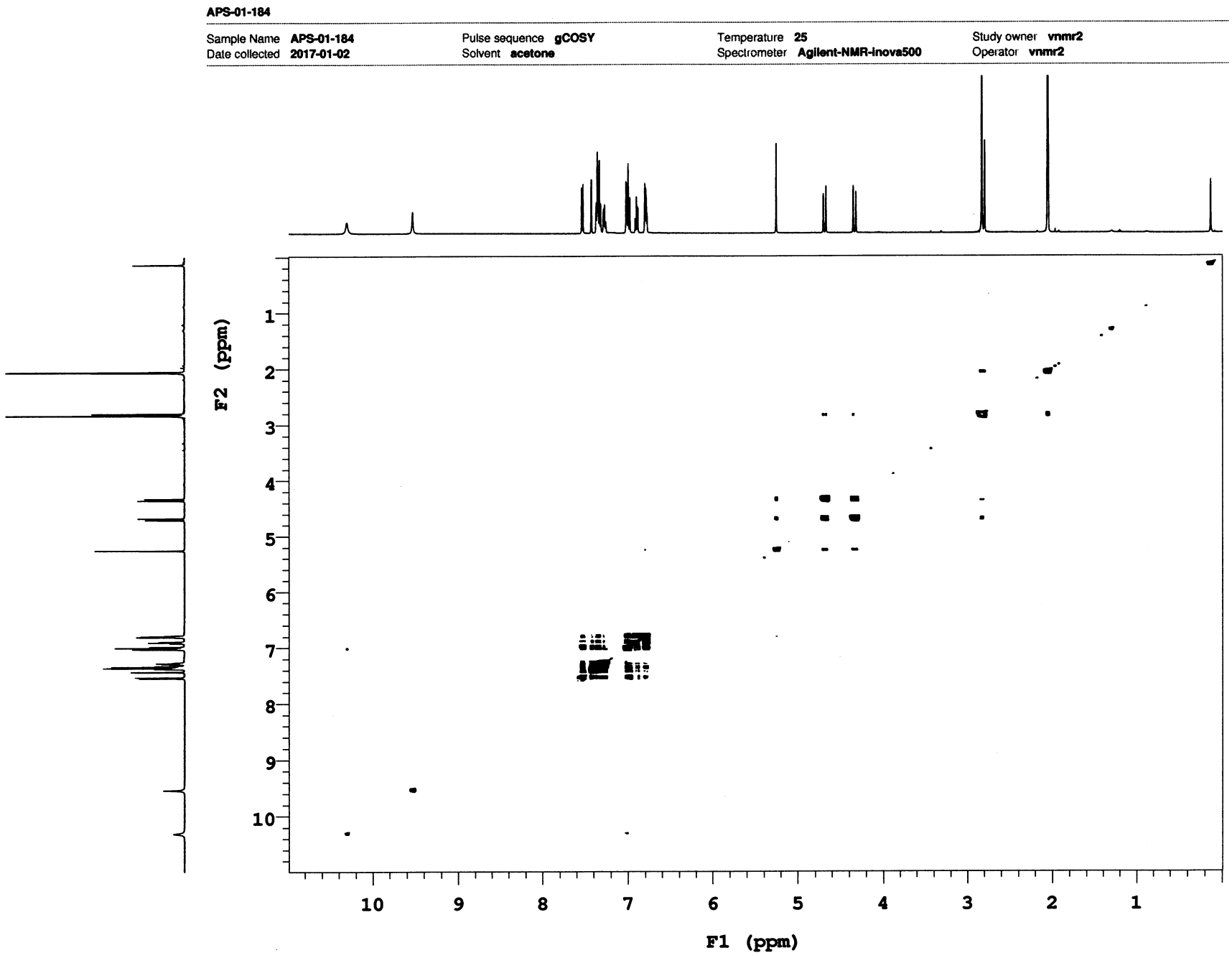


Fig S116. COSY of compound 3ci

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-184/gCOSY_01

Plot date 2017-01-04

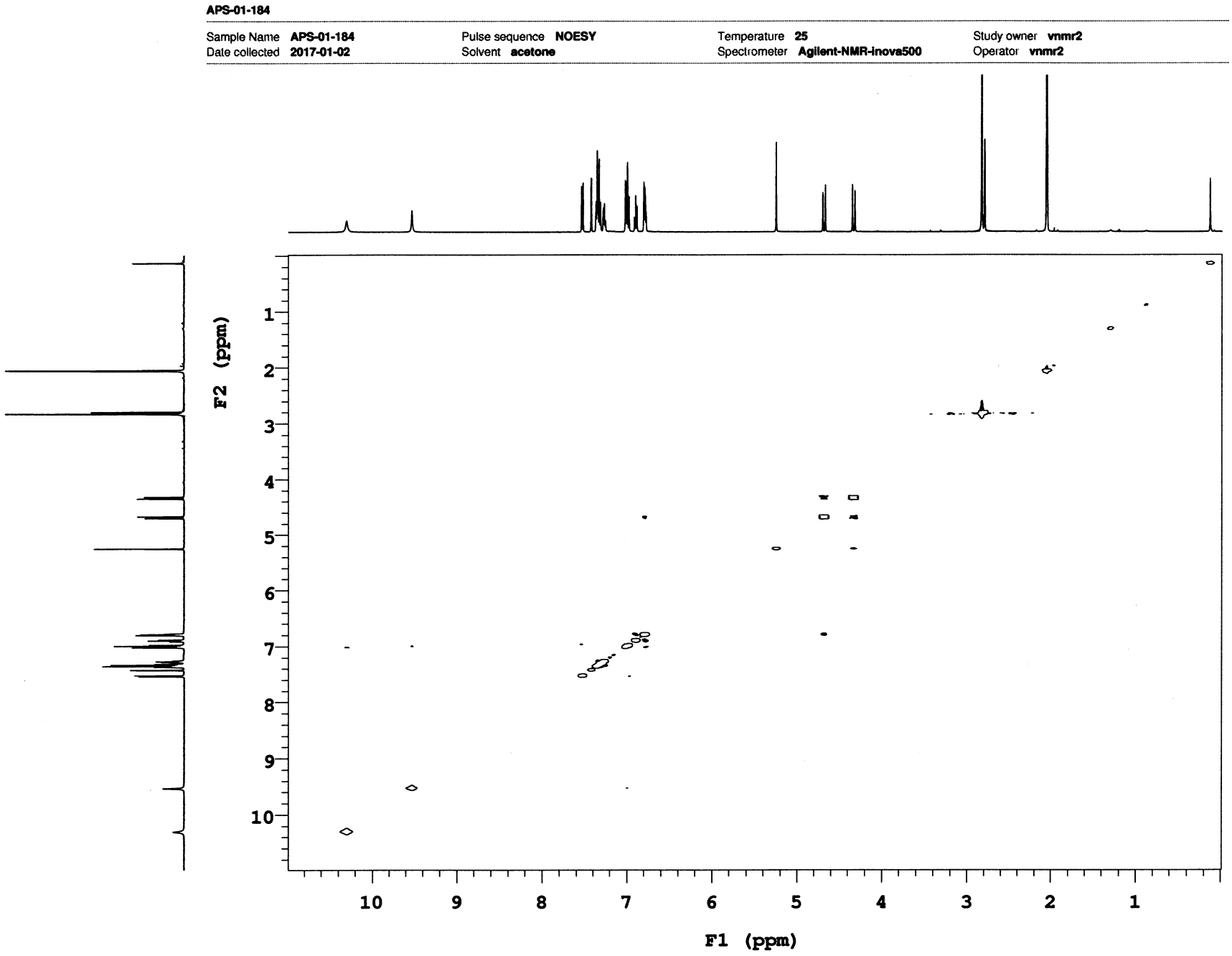


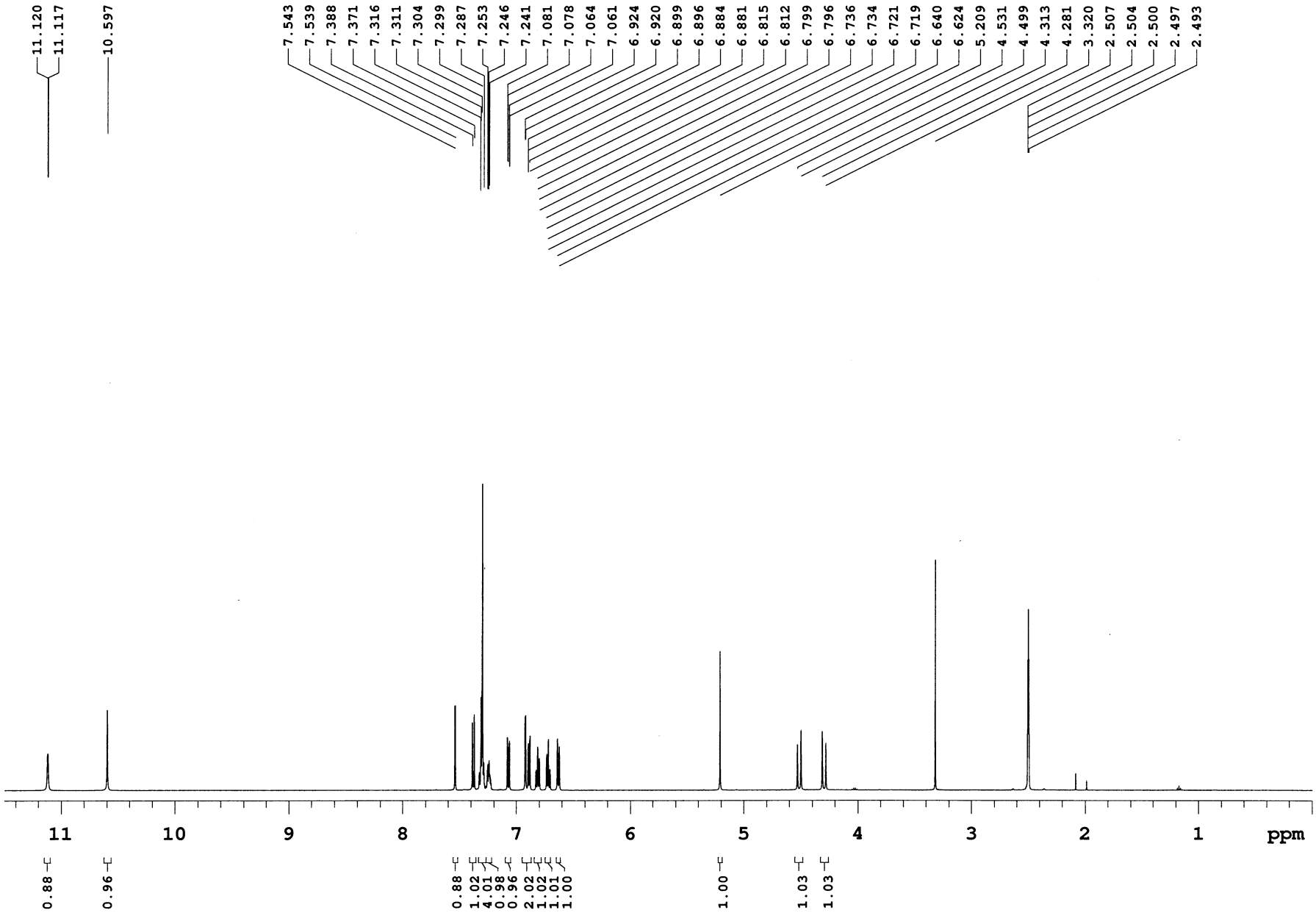
Fig S117. NOESY of compound 3ci

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-184/NOESY_01

Plot date 2017-01-04

APS-01-164

Sample Name	**APS-01-164**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-01-19**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



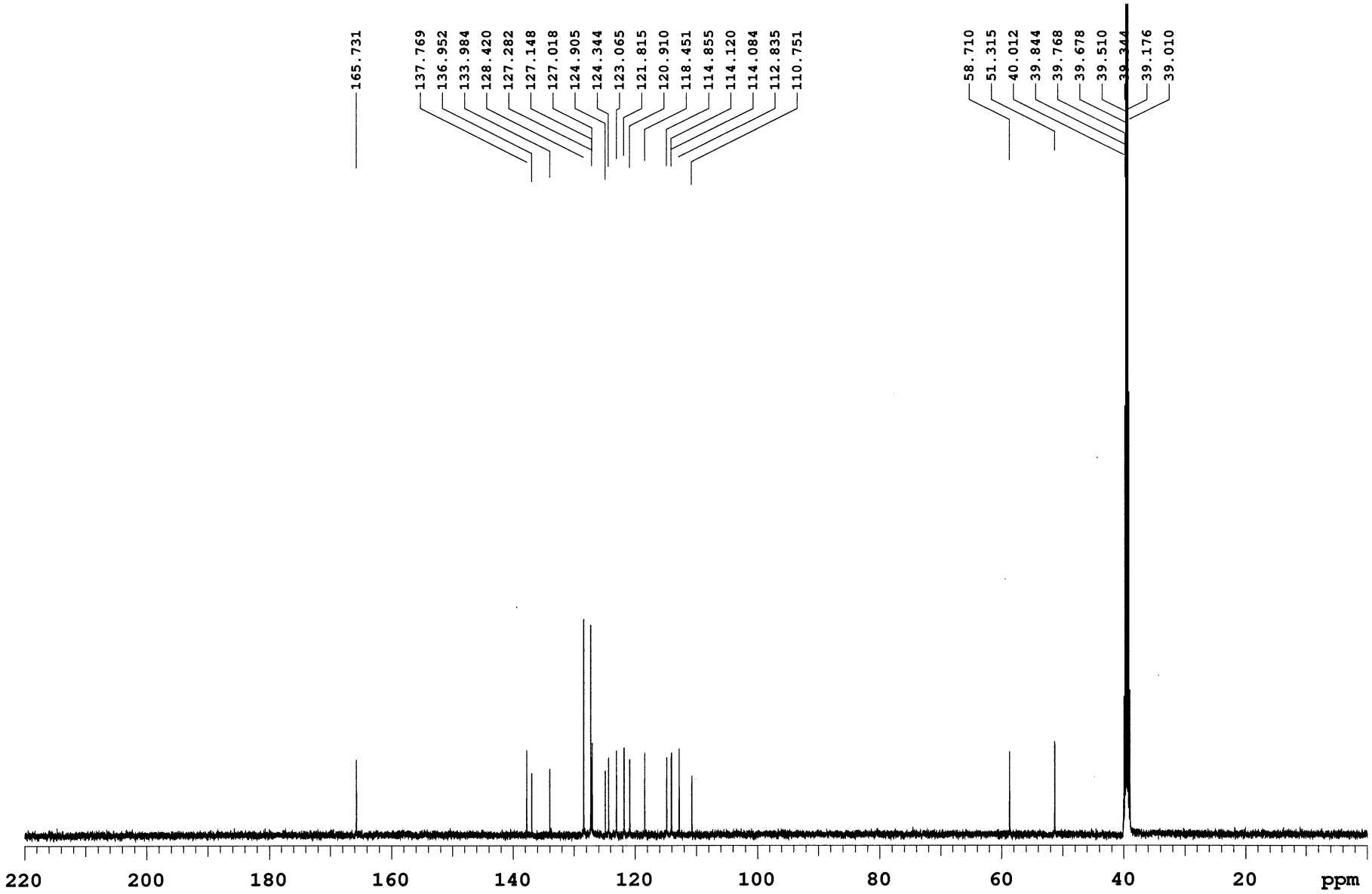
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-164/PROTON_05

Plot date 2017-01-20

Fig S118. 1H NMR (DMSO-d6, 500 MHz) of compound 3cj

APS-01-164

Sample Name	**APS-01-164**	Pulse sequence	**CARBON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-01-19**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-164/CARBON_01

Plot date 2017-01-20

Fig S119. 13C NMR (DMSO-d6, 125 MHz) of compound 3cj

APS-01-164

Sample Name **APS-01-164**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-19**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

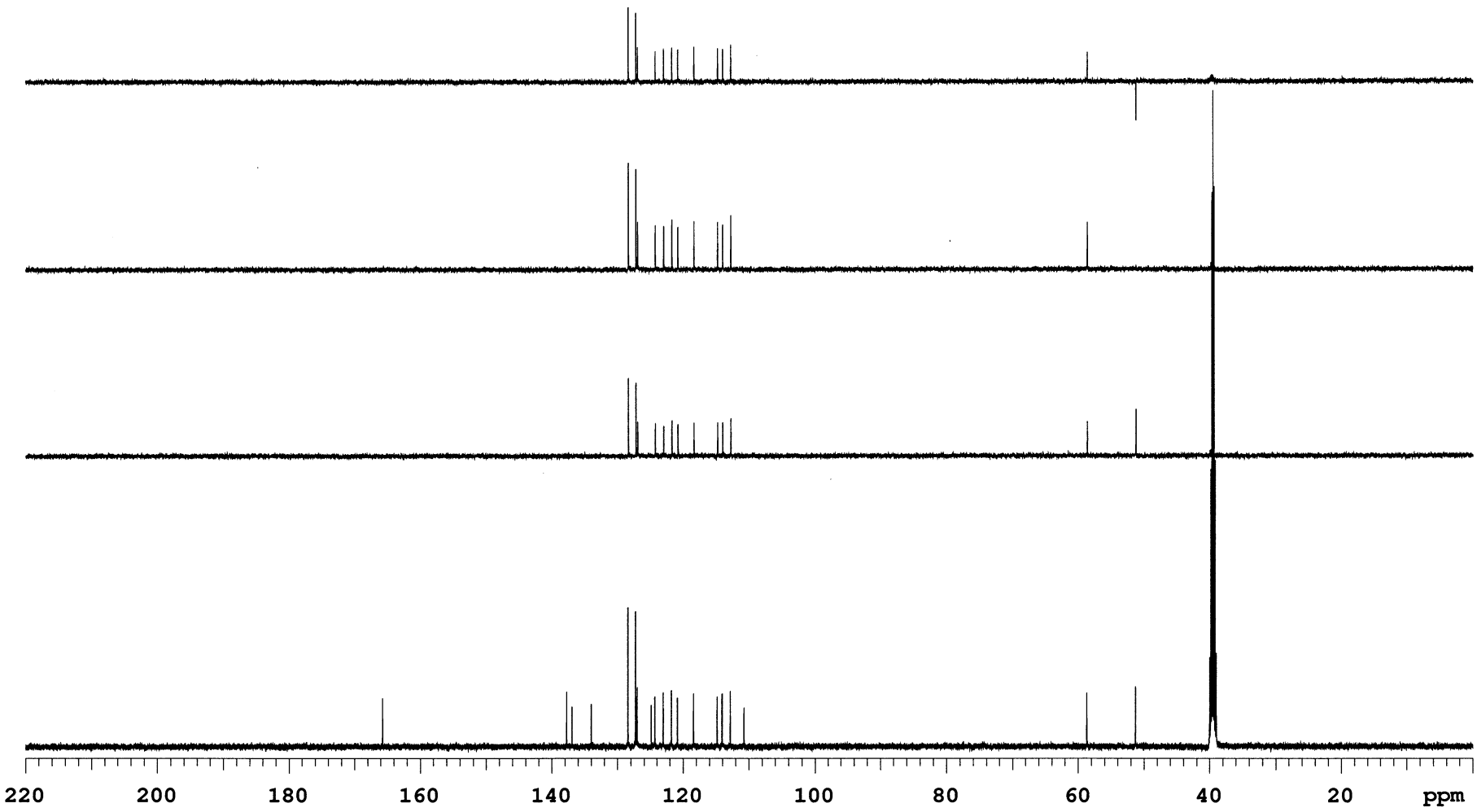


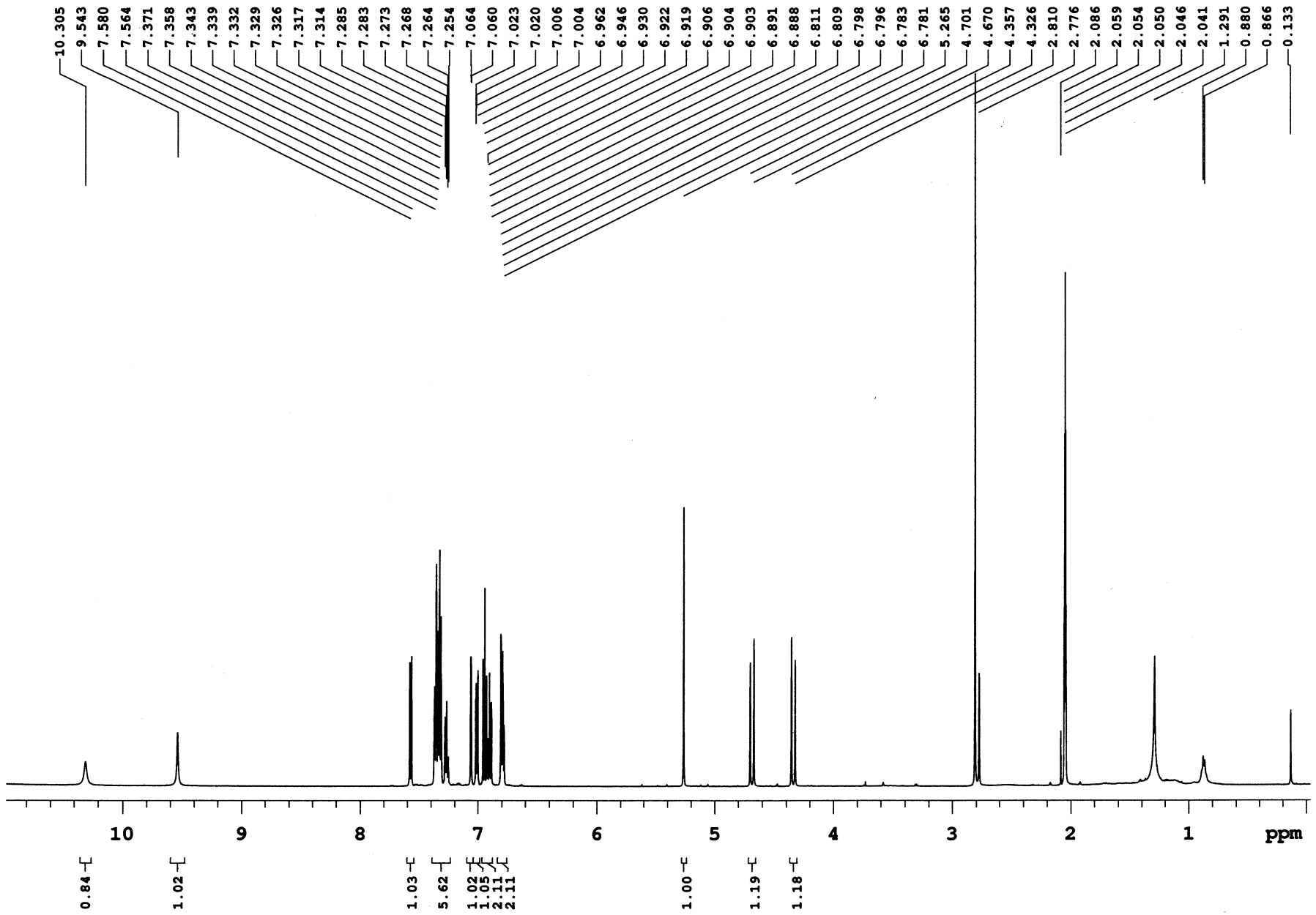
Fig S120. DEPT of compound 3cj

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-164/DEPT_01

Plot date 2017-01-20

APS-01-187

Sample Name	**APS-01-187**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-02-11**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-187/PROTON_07

Fig S121. 1H NMR (acetone-d6, 500 MHz) of compound 3ck

Plot date 2017-02-11

APS-01-187

Sample Name **APS-01-187**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-23**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

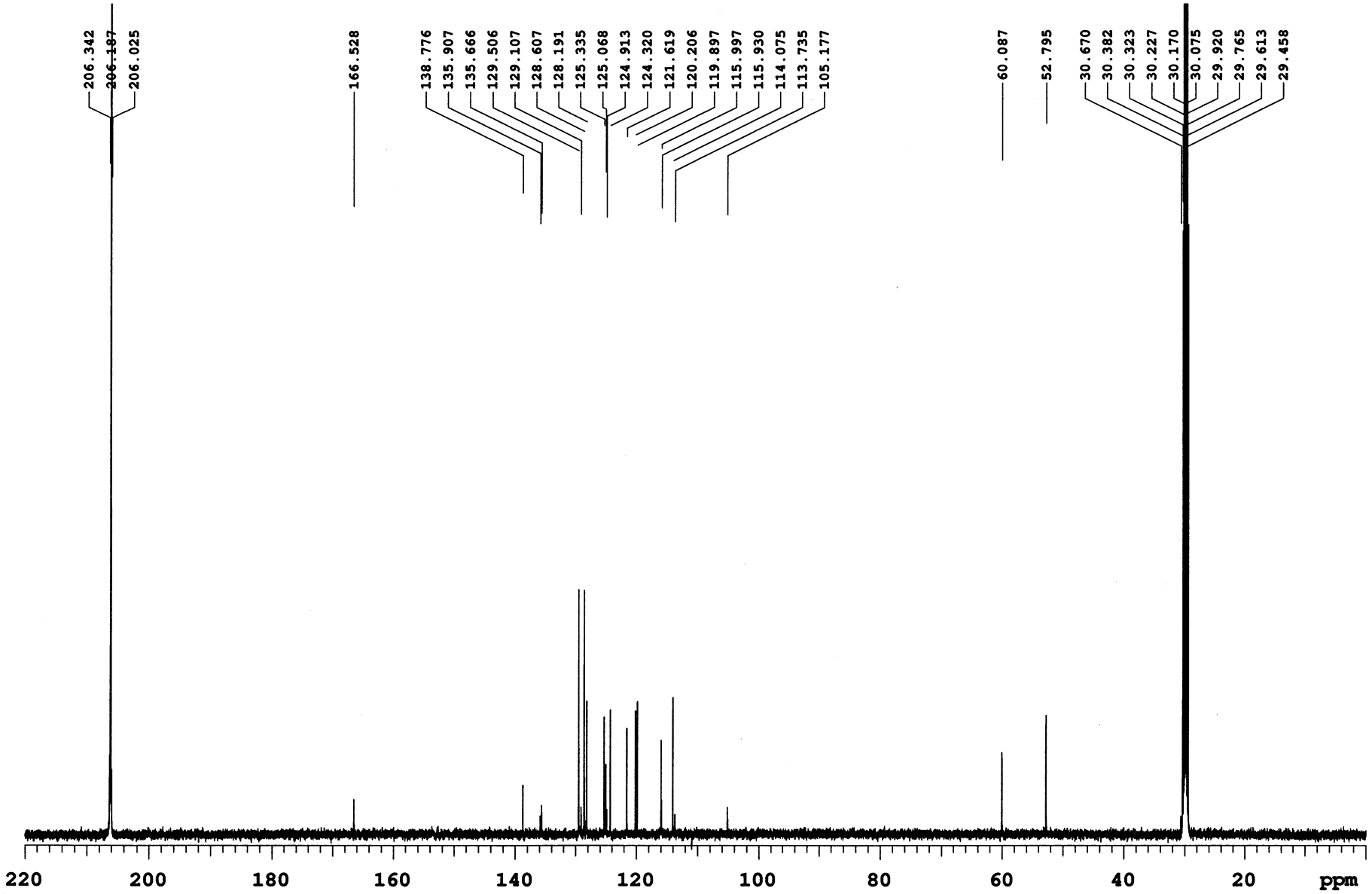


Fig S122. 13C NMR (acetone-d6, 125 MHz) of compound 3ck

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-187/CARBON_02

Plot date 2017-01-24

APS-01-187

Sample Name **APS-01-187**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-23**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

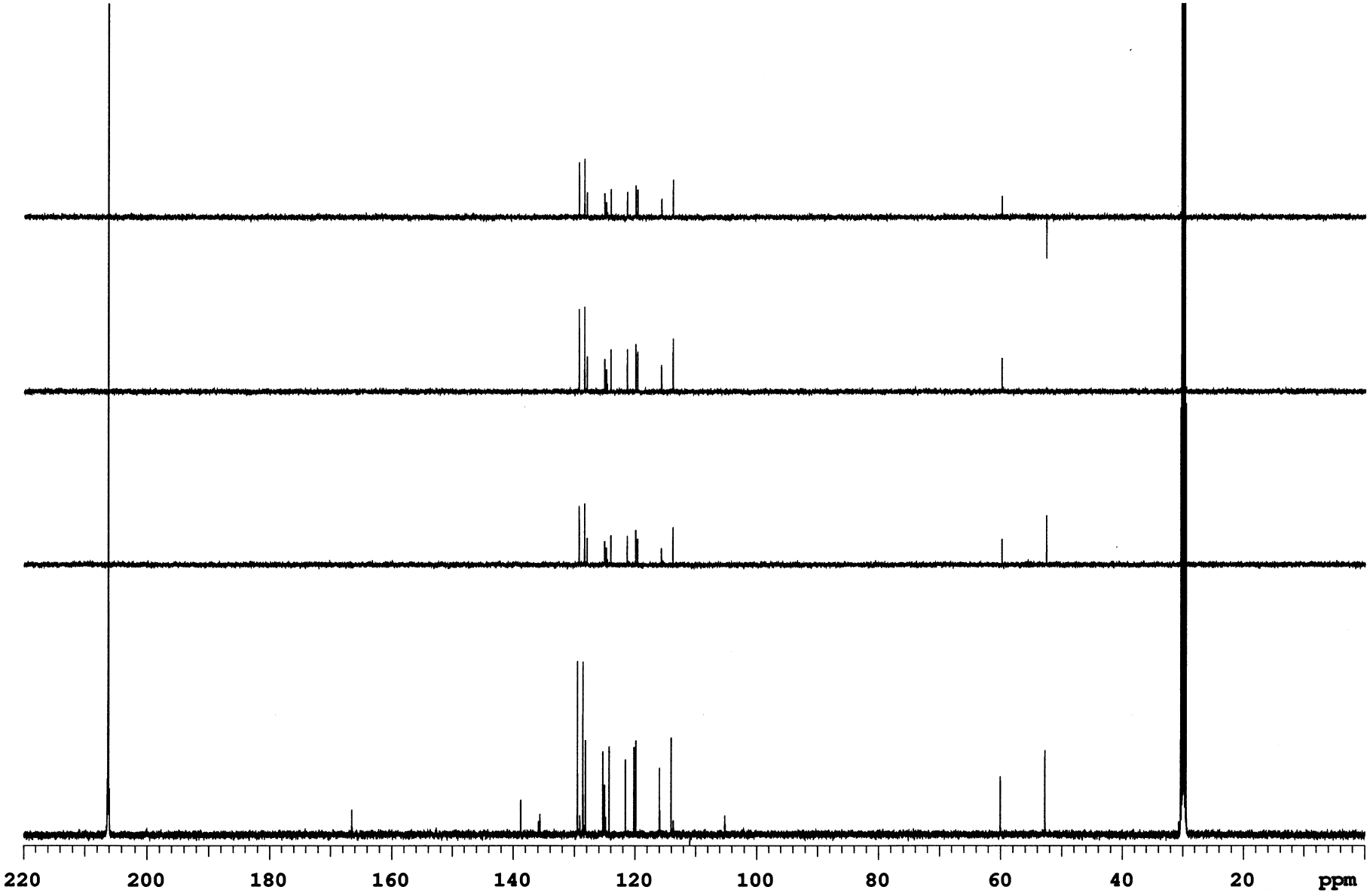


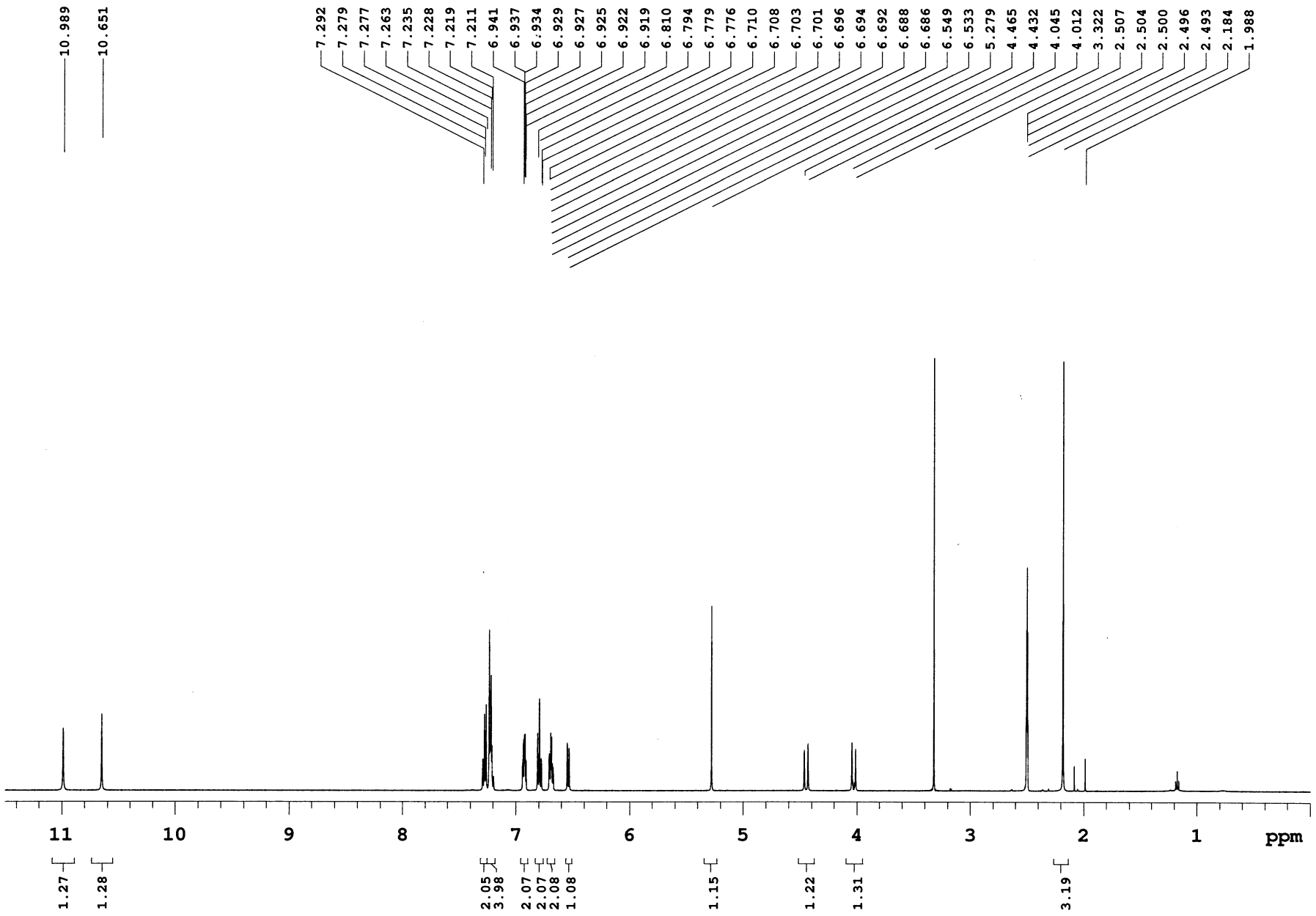
Fig S123. DEPT of compound 3ck

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-187/DEPT_01

Plot date 2017-01-24

APS-01-149

Sample Name	**APS-01-149**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-12-20**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-149/PROTON_03

Fig S124. 1H NMR (DMSO-d6, 500 MHz) of compound 3cl

Plot date 2017-03-01

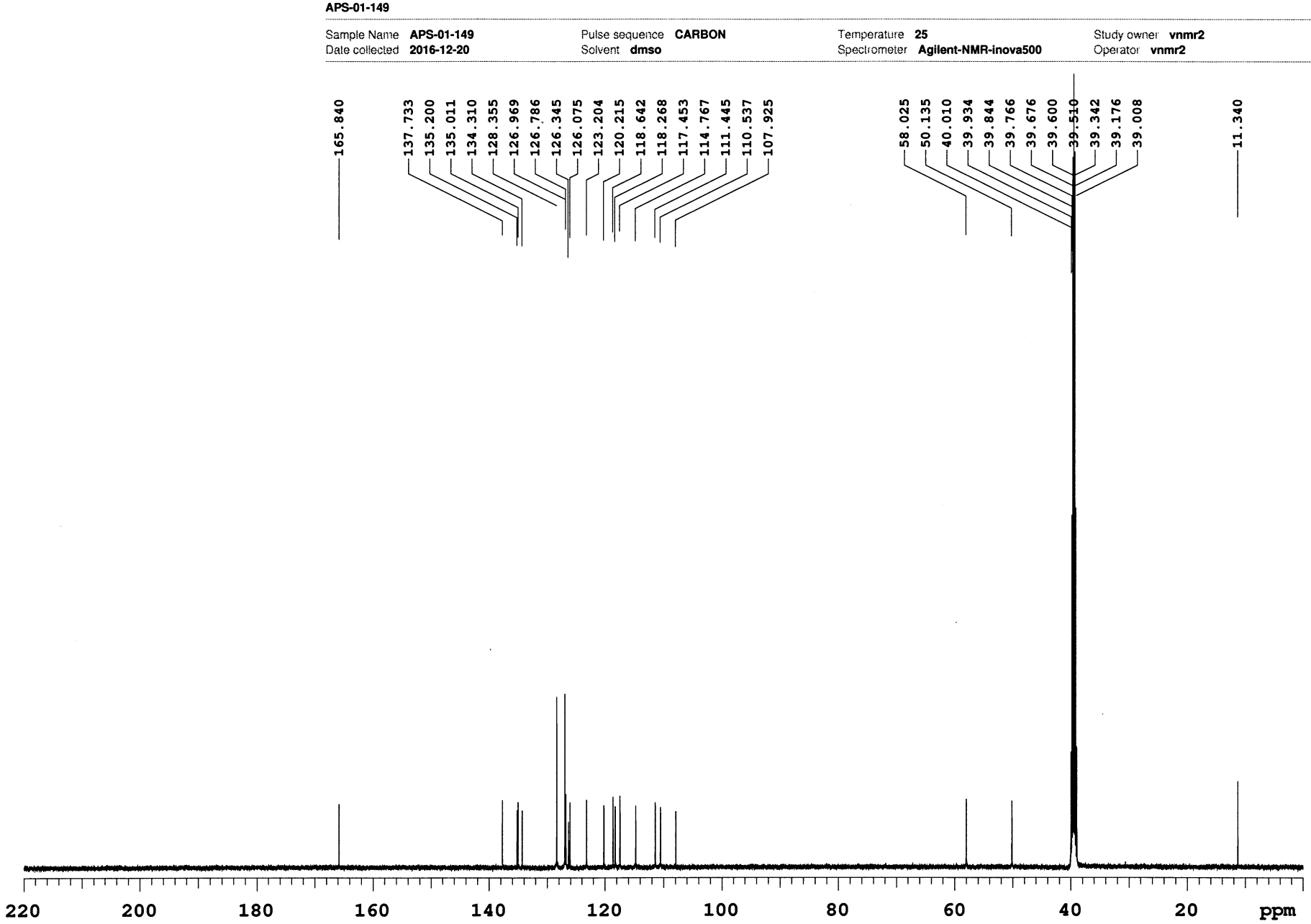


Fig S125. 13C NMR (DMSO-d6, 125 MHz) of compound 3cl

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-149/CARBON_02

Plot date 2016-12-21

APS-01-149

Sample Name **APS-01-149**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2016-12-21**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

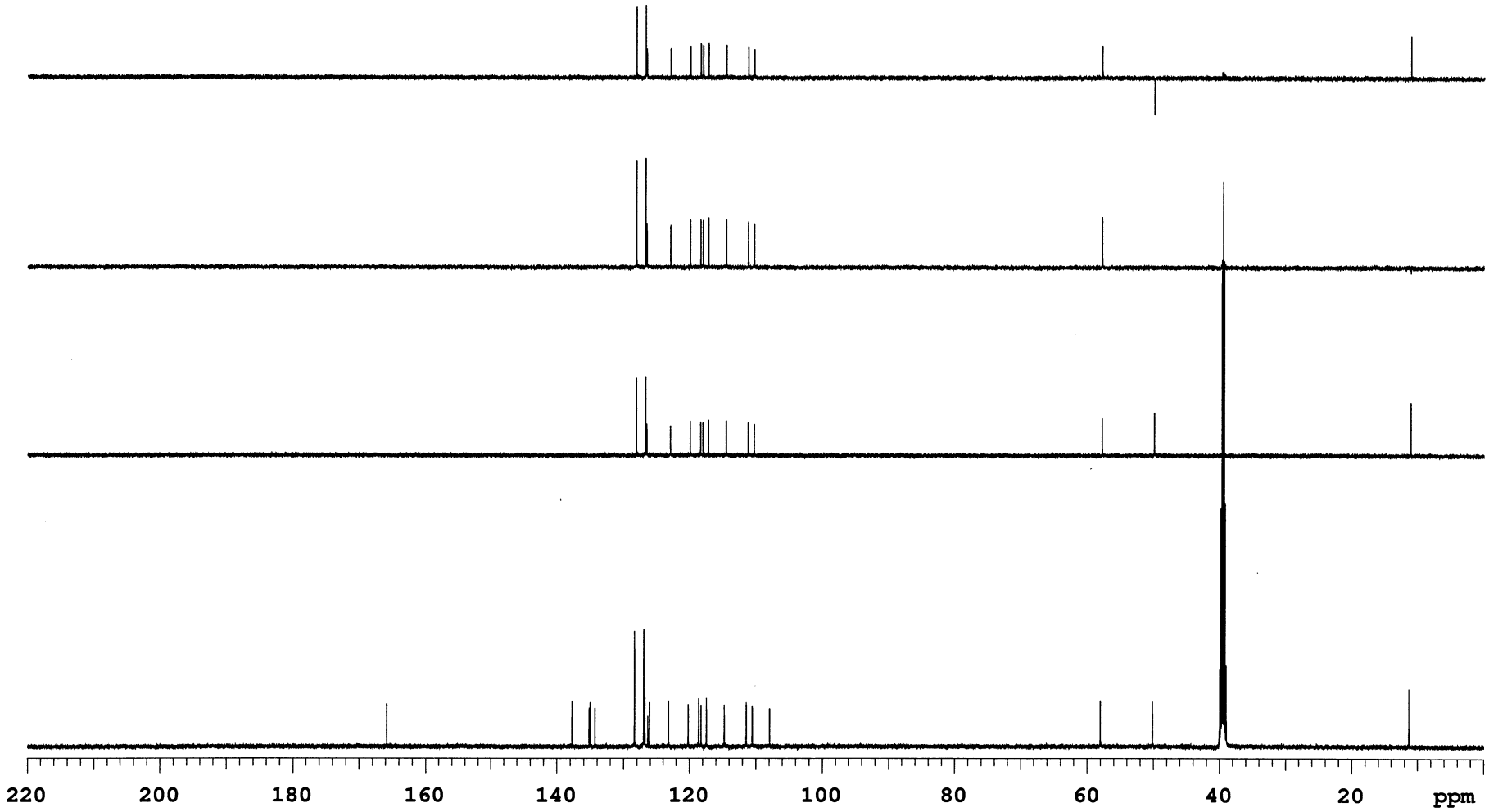


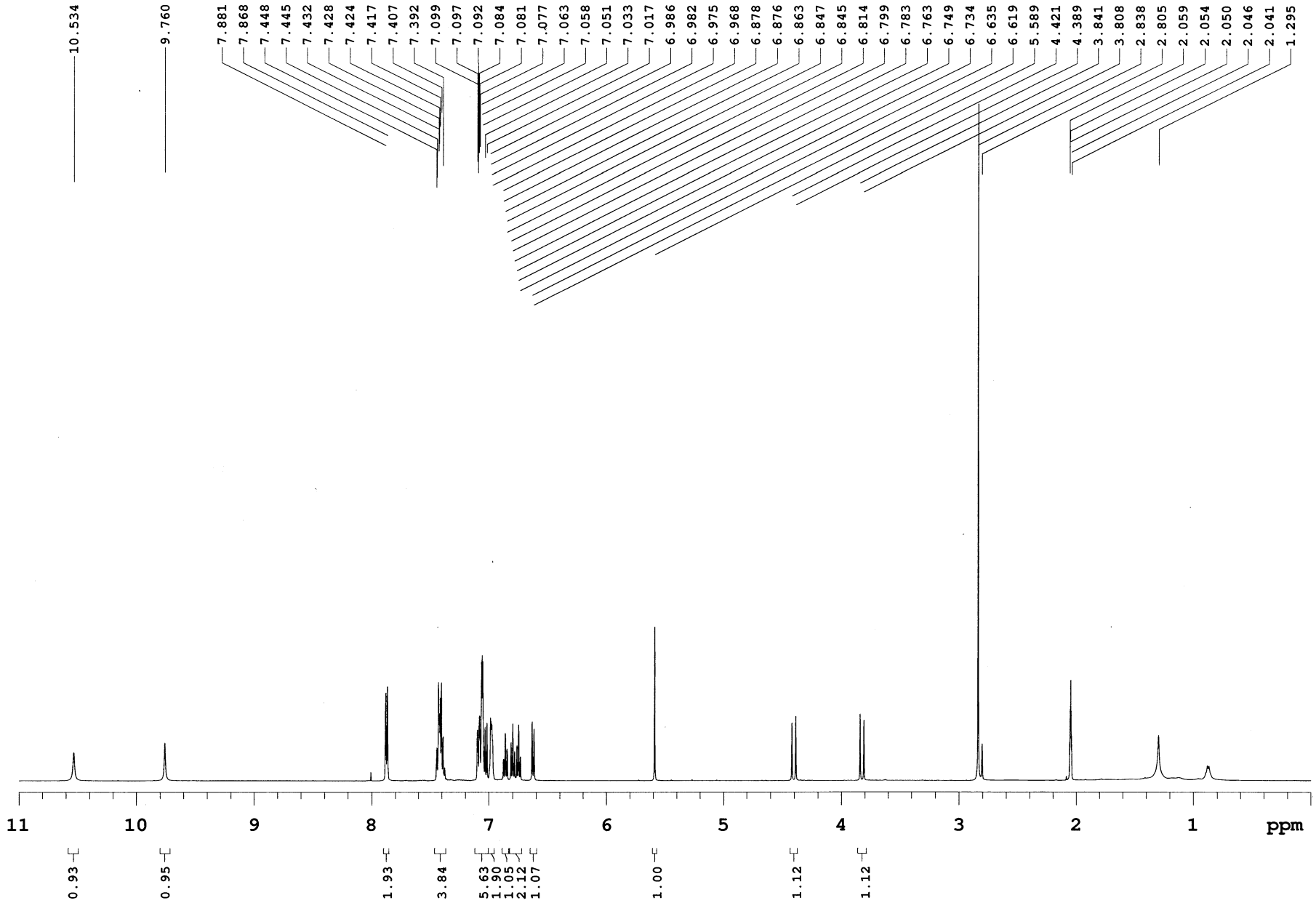
Fig S126. DEPT of compound 3cl

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-149/DEPT_01

Plot date 2016-12-21

APS-01-170

Sample Name	APS-01-170	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr2
Date collected	2017-04-27	Solvent	acetone	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-170/PROTON_04

Plot date 2017-04-27

Fig S127. 1H NMR (acetone-d6, 500 MHz) of compound 3cm

APS-01-170

Sample Name	APS-01-170	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2017-04-27	Solvent	acetone	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

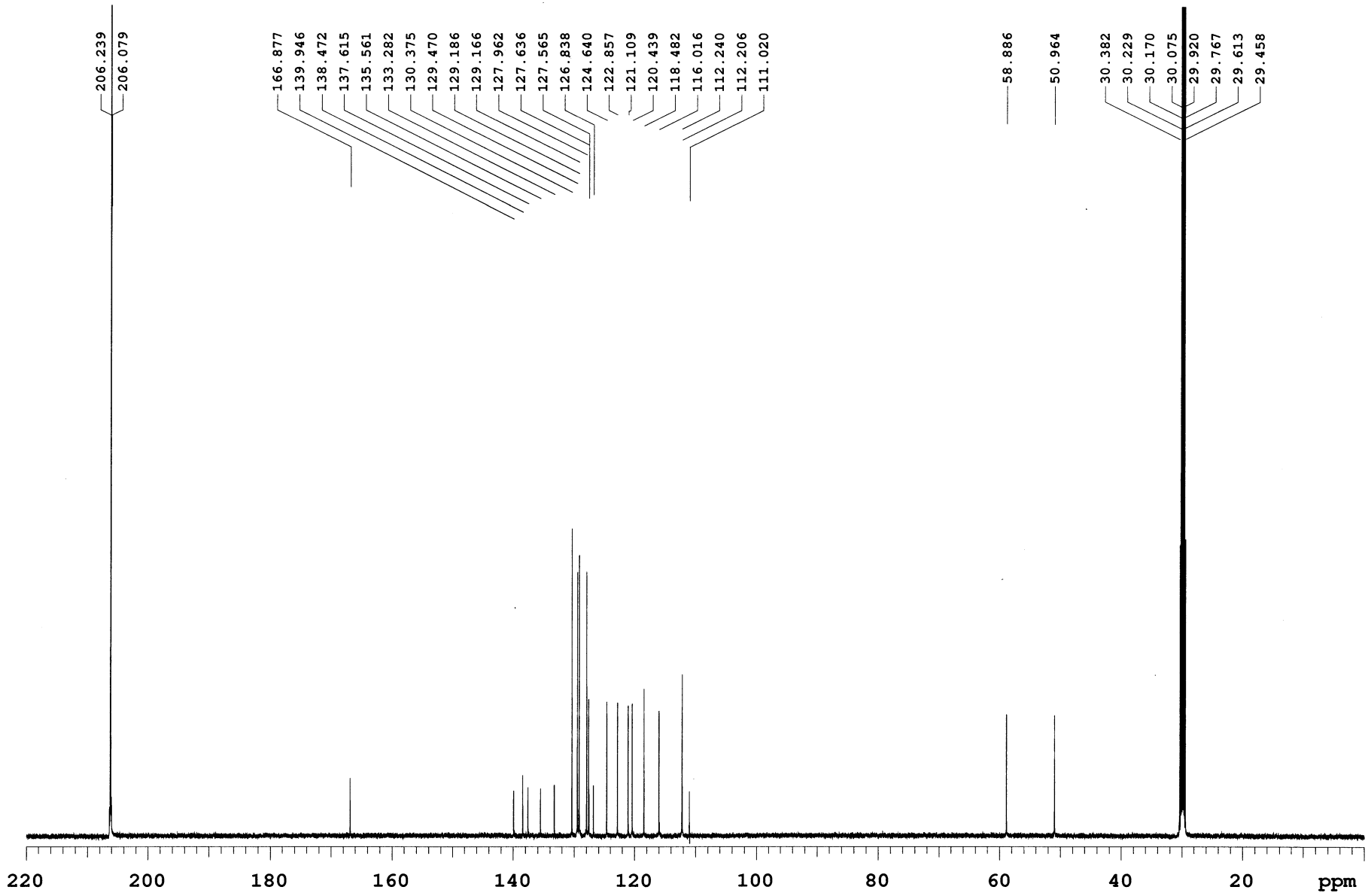


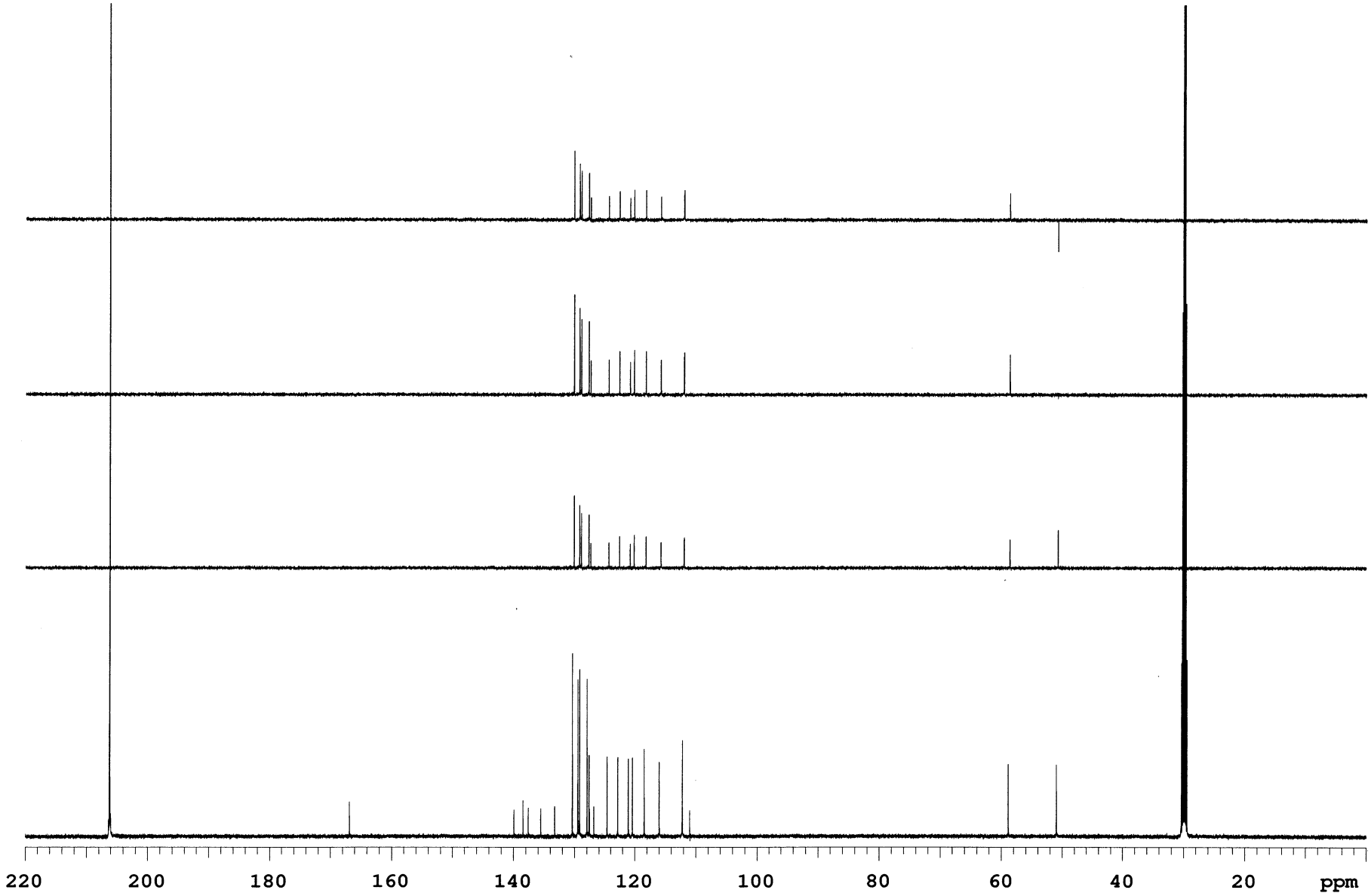
Fig S128. 13C NMR (acetone-d6, 125 MHz) of compound 3cm

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-170/CARBON_02

Plot date 2017-04-27

APS-01-170

Sample Name **APS-01-170**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-27**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



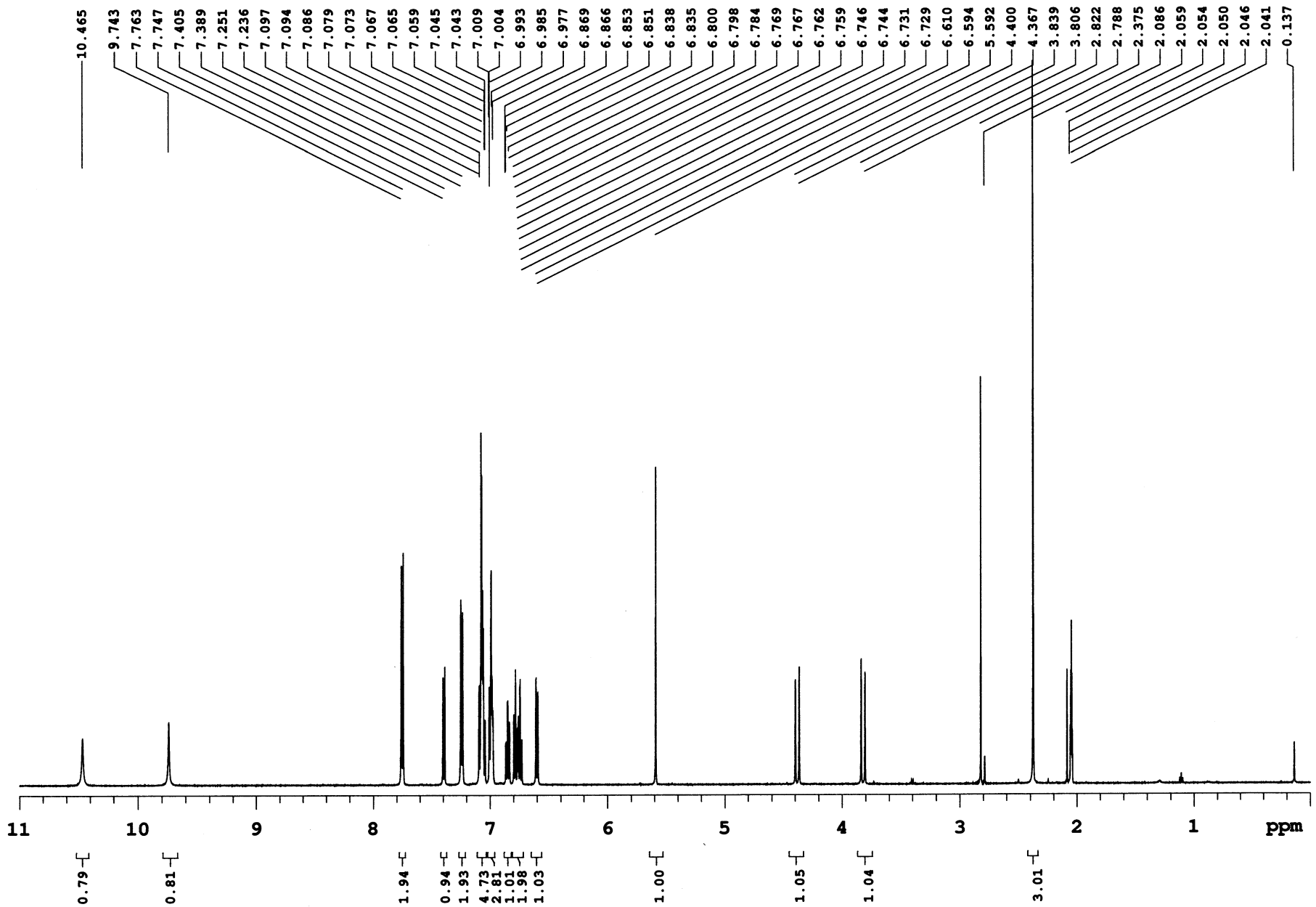
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-170/DEPT_01

Fig S129. DEPT of compound 3cm

Plot date 2017-04-27

APS-01-171

Sample Name	**APS-01-171**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-12-07**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-171/PROTON_02

Plot date 2016-12-07

Fig S130. 1H NMR (acetone-d6, 500 MHz) of compound 3cn

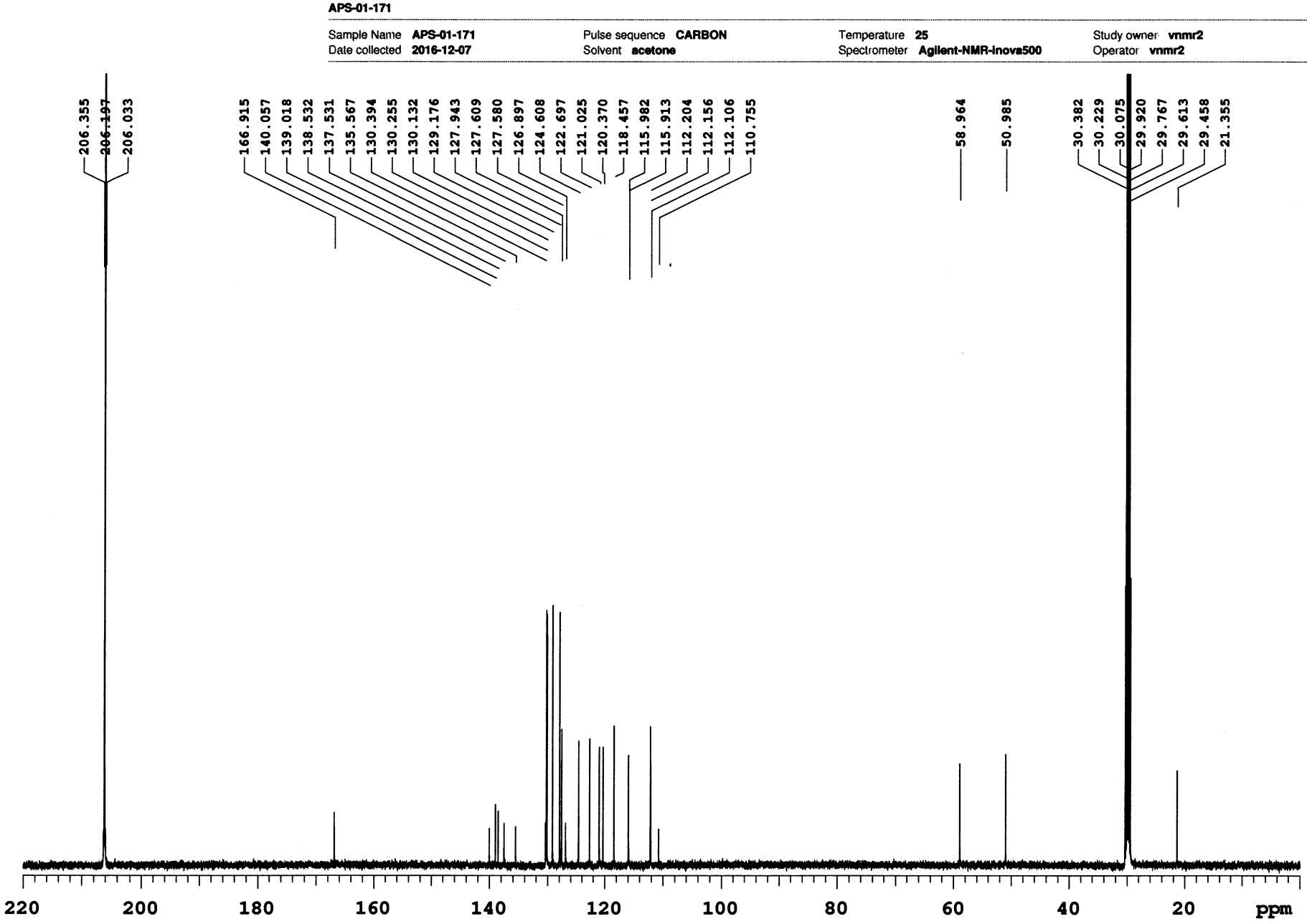


Fig S131. 13C NMR (acetone-d6, 125 MHz) of compound 3cn

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-171/CARBON_02

Plot date 2016-12-07

APS-01-171

Sample Name **APS-01-171**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2016-12-07**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

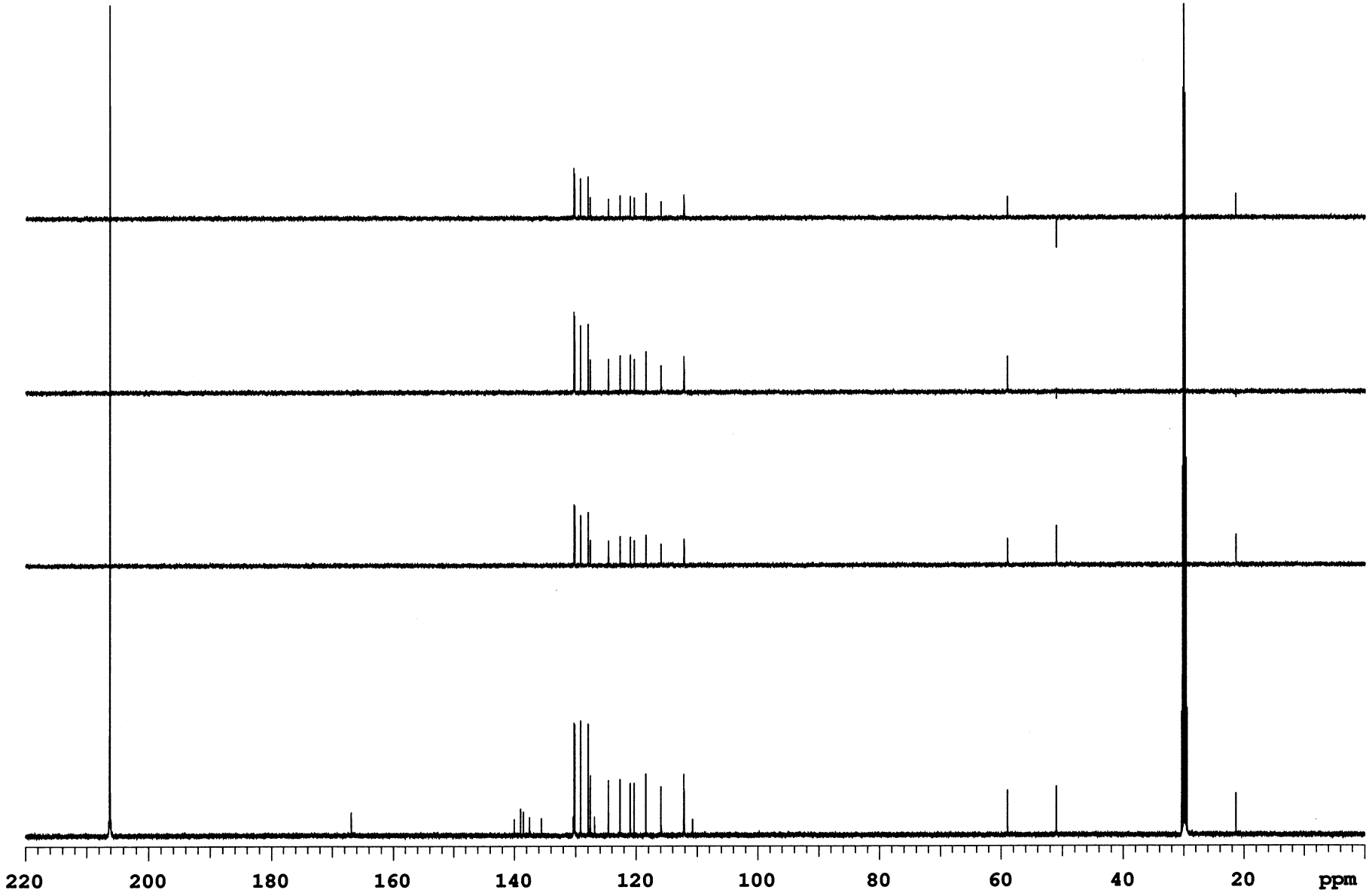


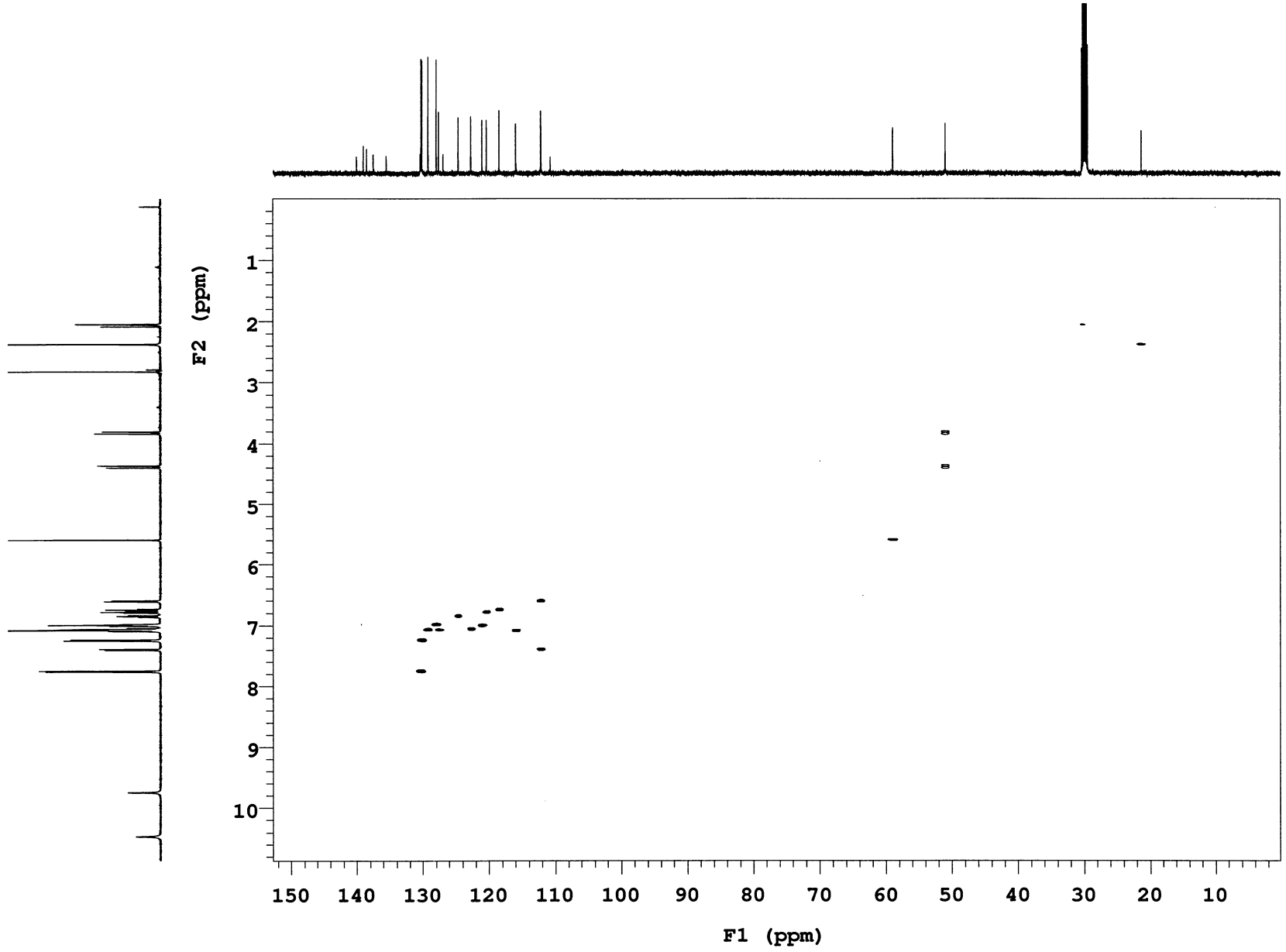
Fig S132. DEPT of compound 3cn

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-171/DEPT_01

Plot date 2016-12-07

APS-01-171

Sample Name **APS-01-171**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2016-12-07**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-171/gHSQC_01

Fig S133. HSQC of compound 3cn

Plot date 2016-12-07

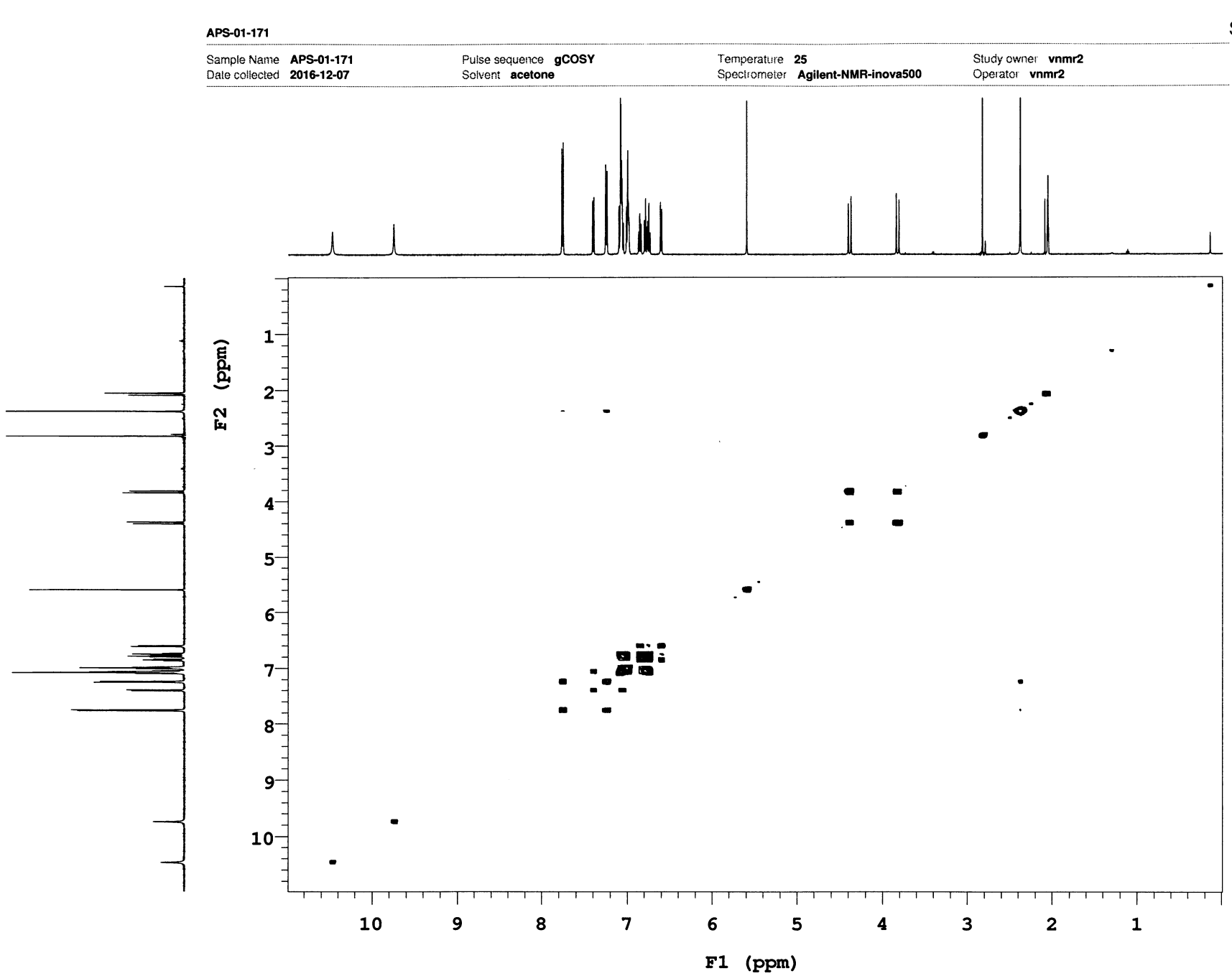


Fig S134. COSY of compound 3cn

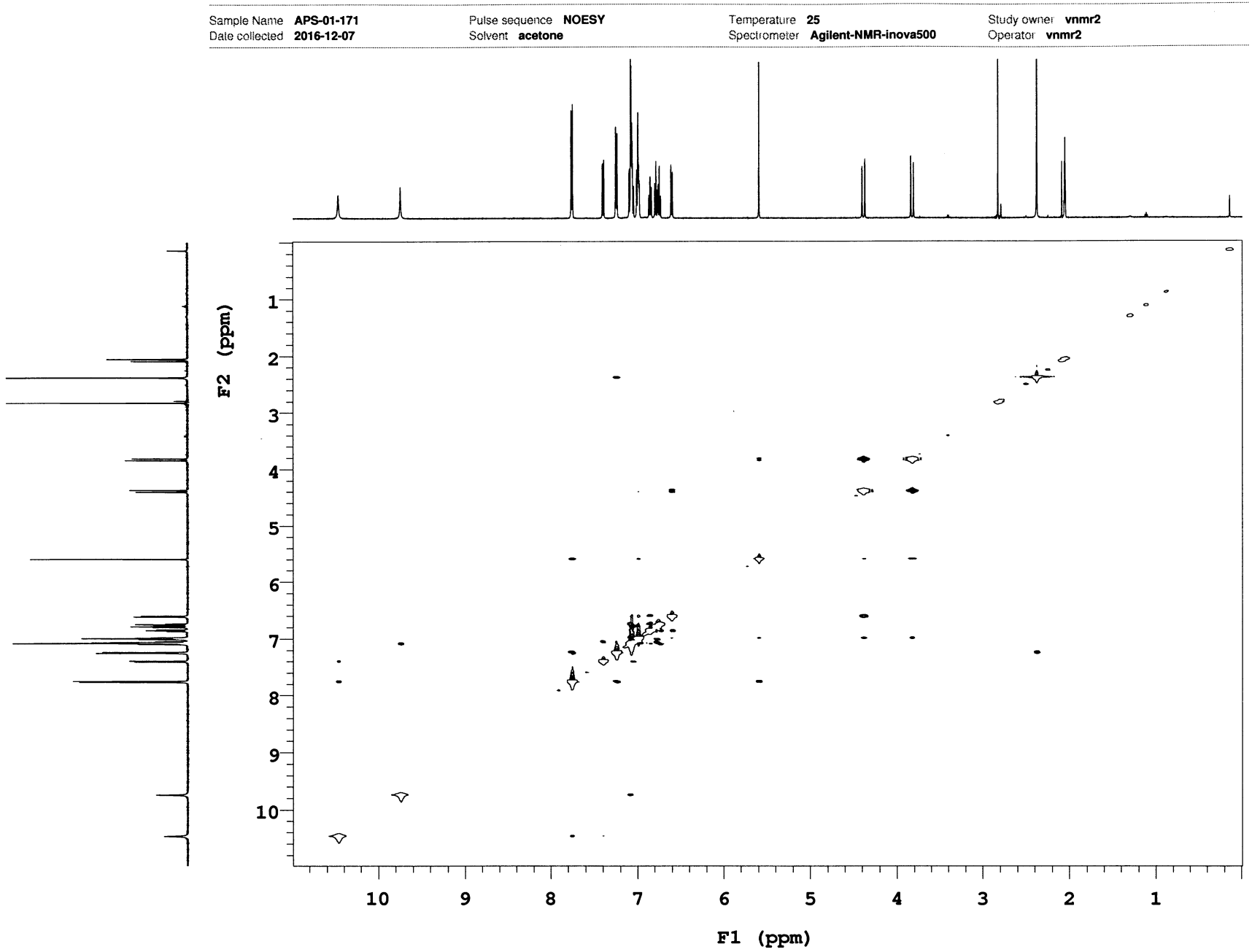


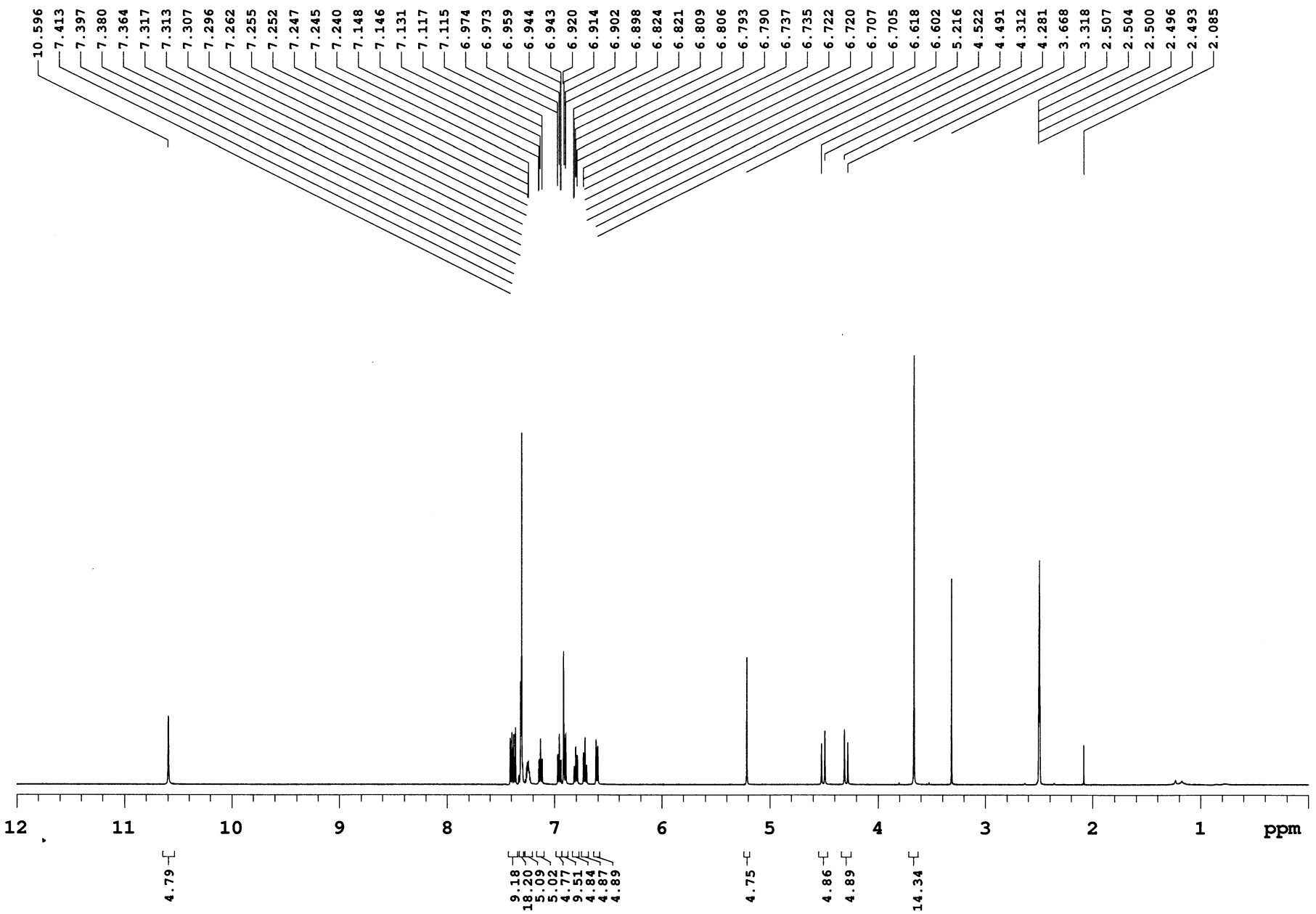
Fig S135. NOESY of compound 3cn

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-171/NOESY_01

Plot date 2016-12-07

APS-01-174

Sample Name **APS-01-174**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2016-12-14**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-174/PROTON_05.fid

Fig S136. 1H NMR (DMSO-d6, 500 MHz) of compound 3co

Plot date 2016-12-14

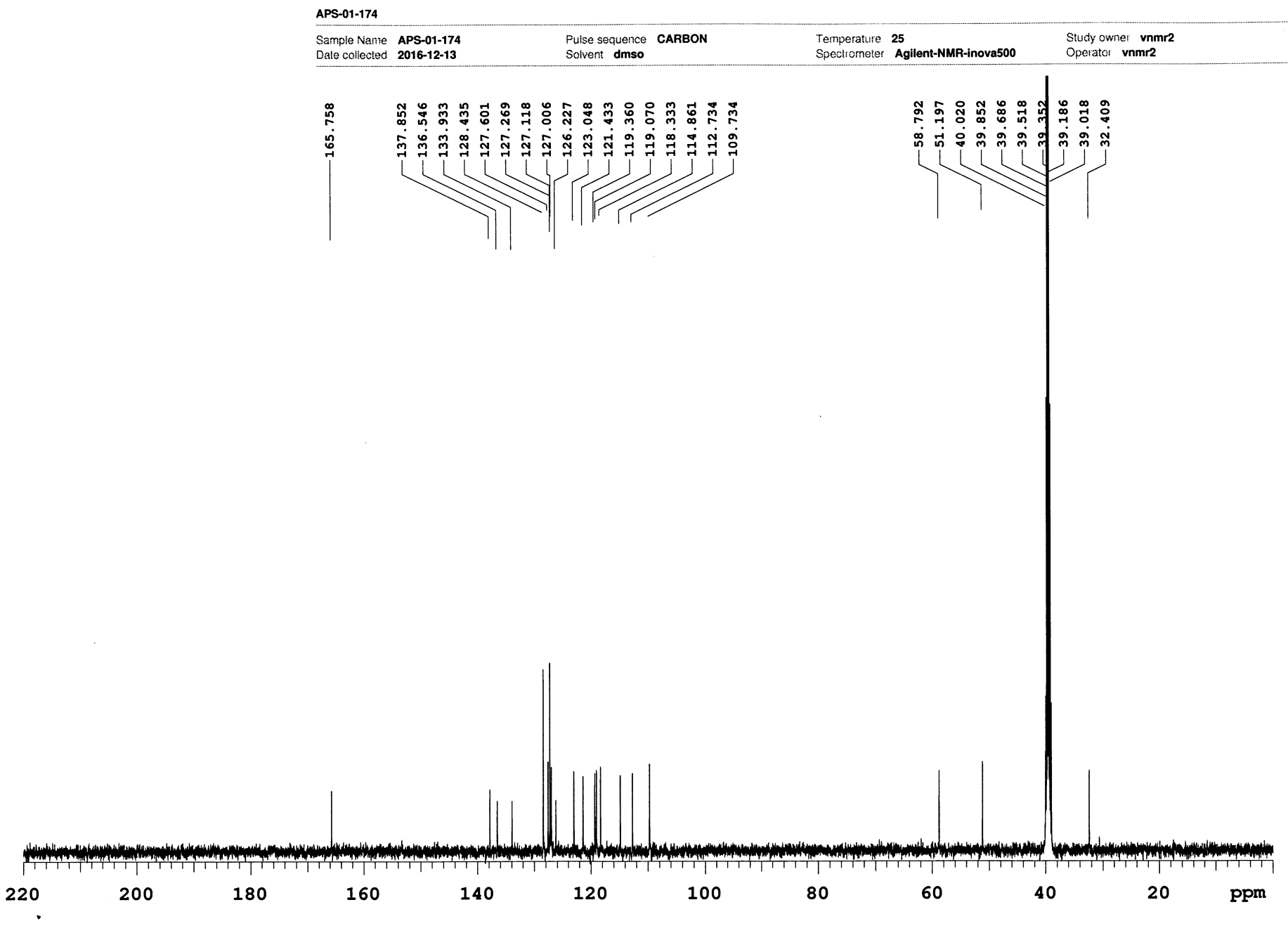


Fig S137. 13C NMR (DMSO-d6, 125 MHz) of compound 3co

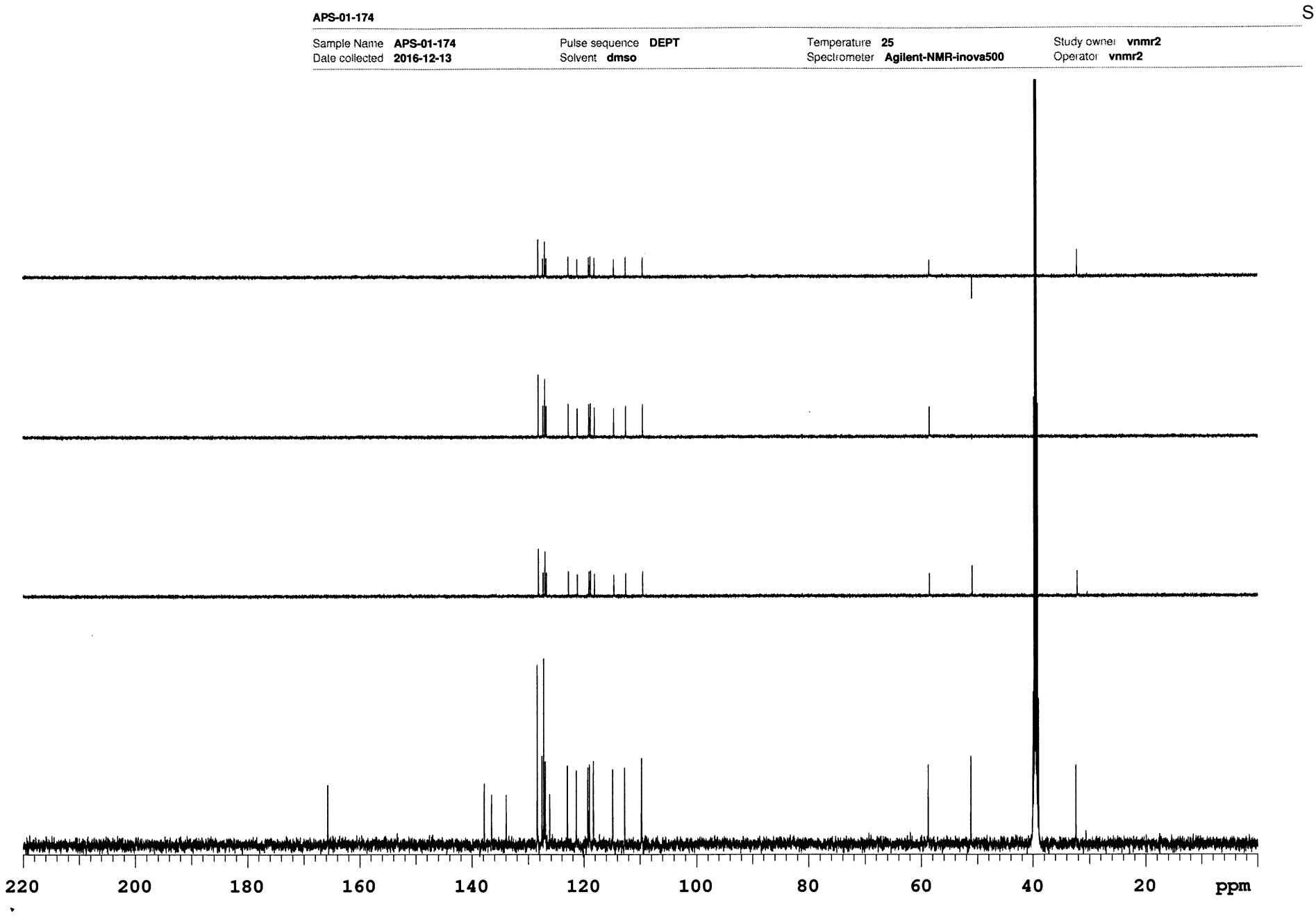


Fig S138. DEPT of compound 3co

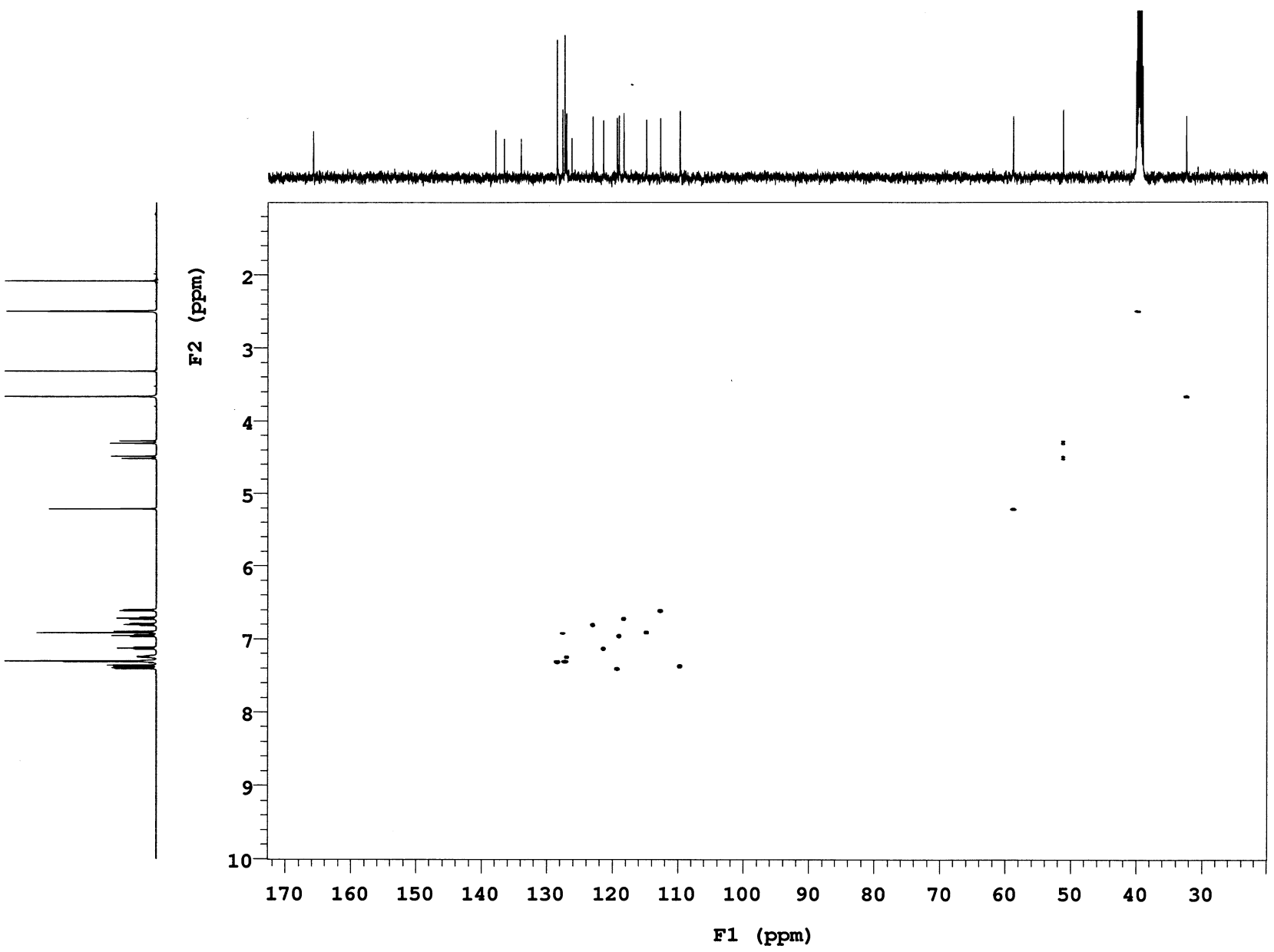


Fig S139. HSQC of compound 3co

APS-01-174

Sample Name **APS-01-174**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2016-12-13**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

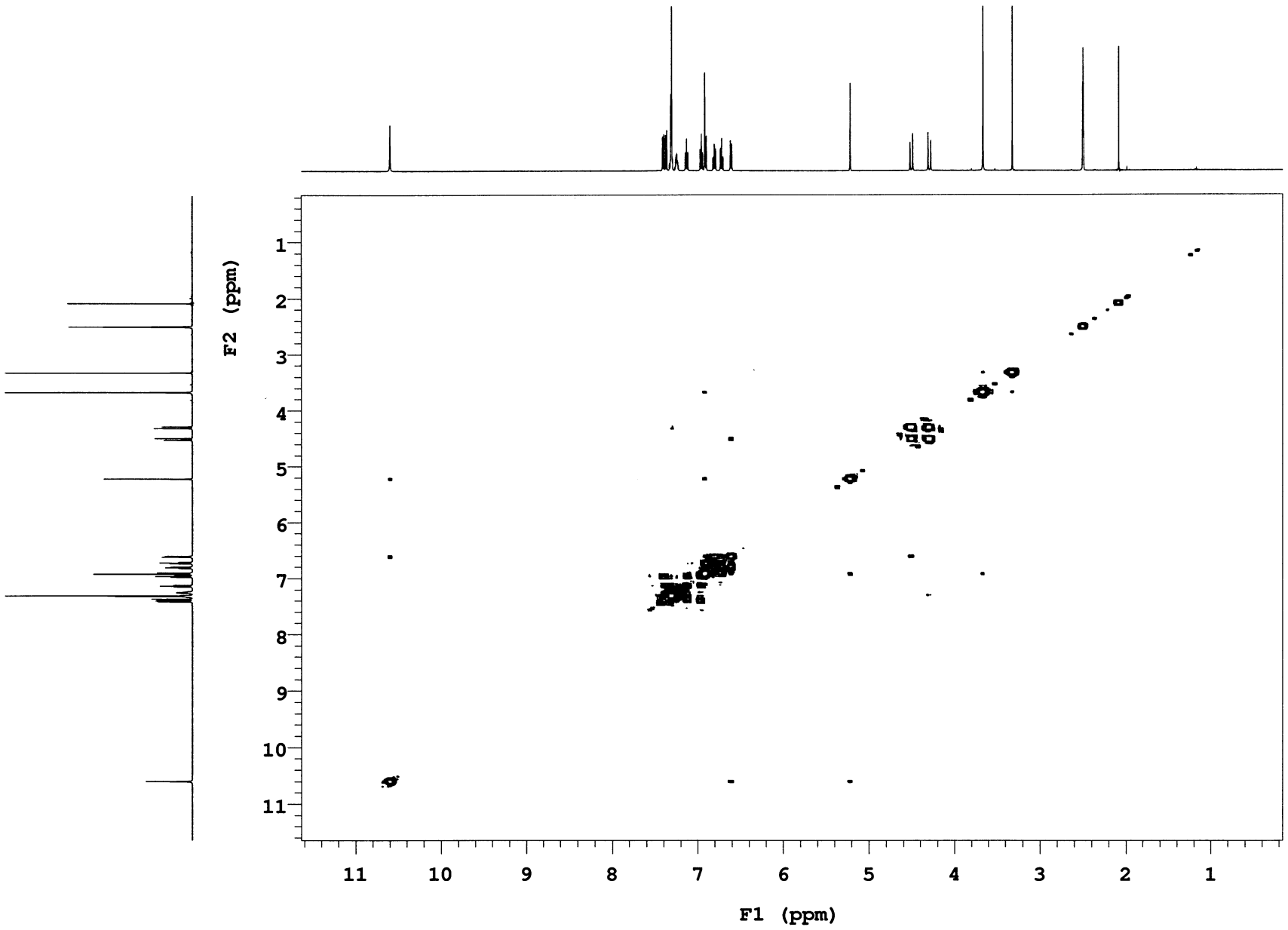


Fig S140. COSY of compound 3co

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-174/gCOSY_01

Plot date 2016-12-13

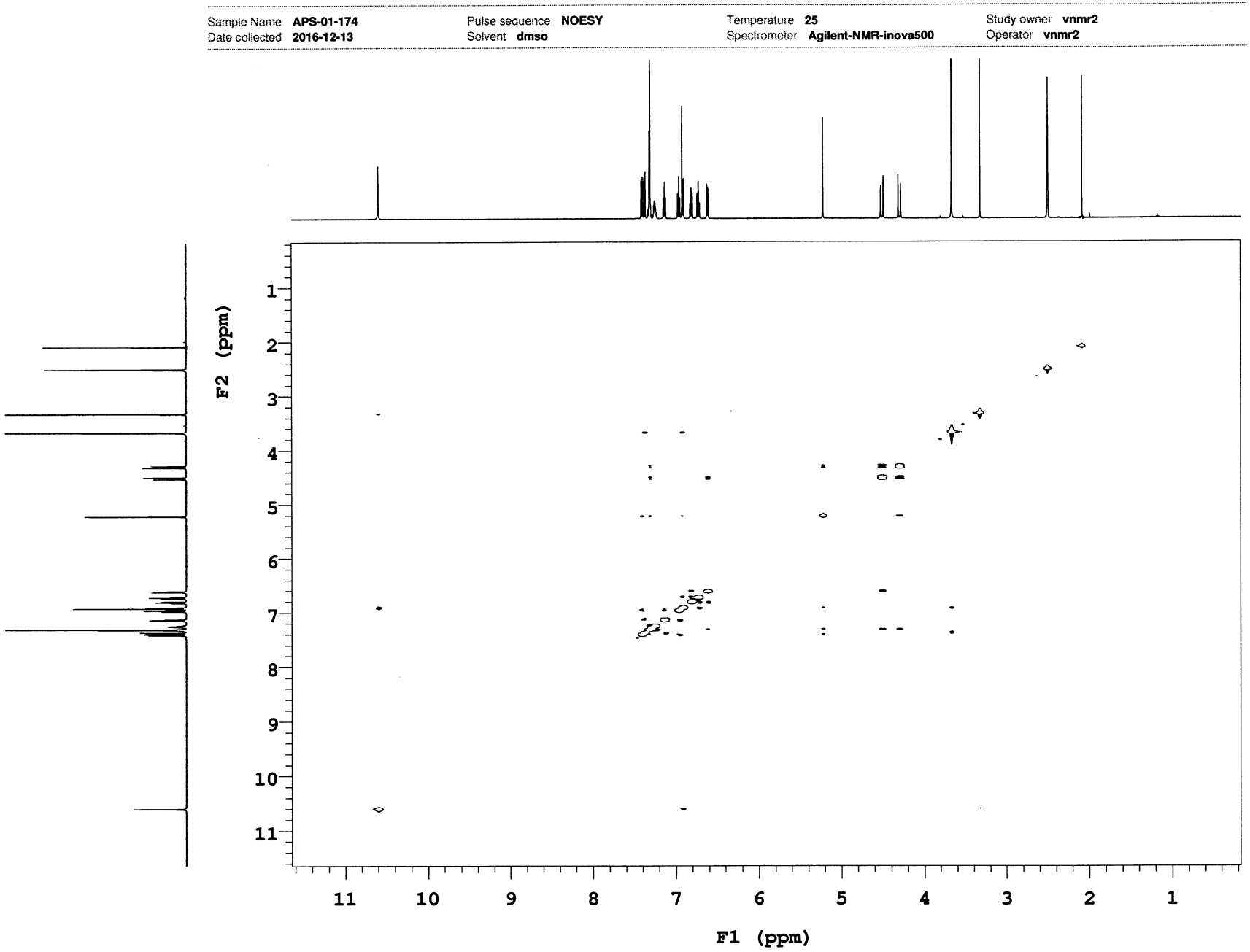


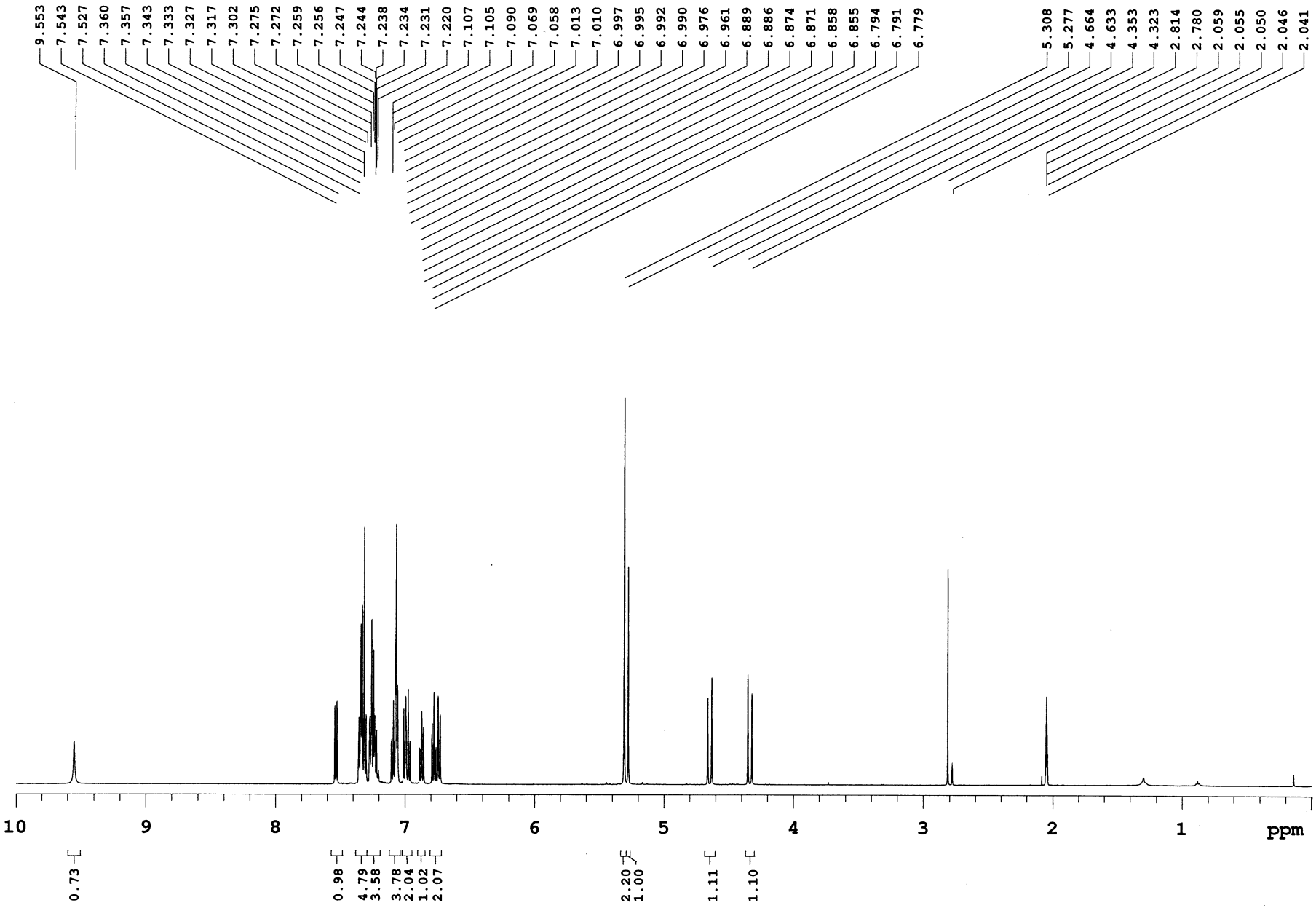
Fig S141. NOESY of compound 3co

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-174/NOESY_01

Plot date 2016-12-13

APS-01-181

Sample Name **APS-01-181**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-09**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



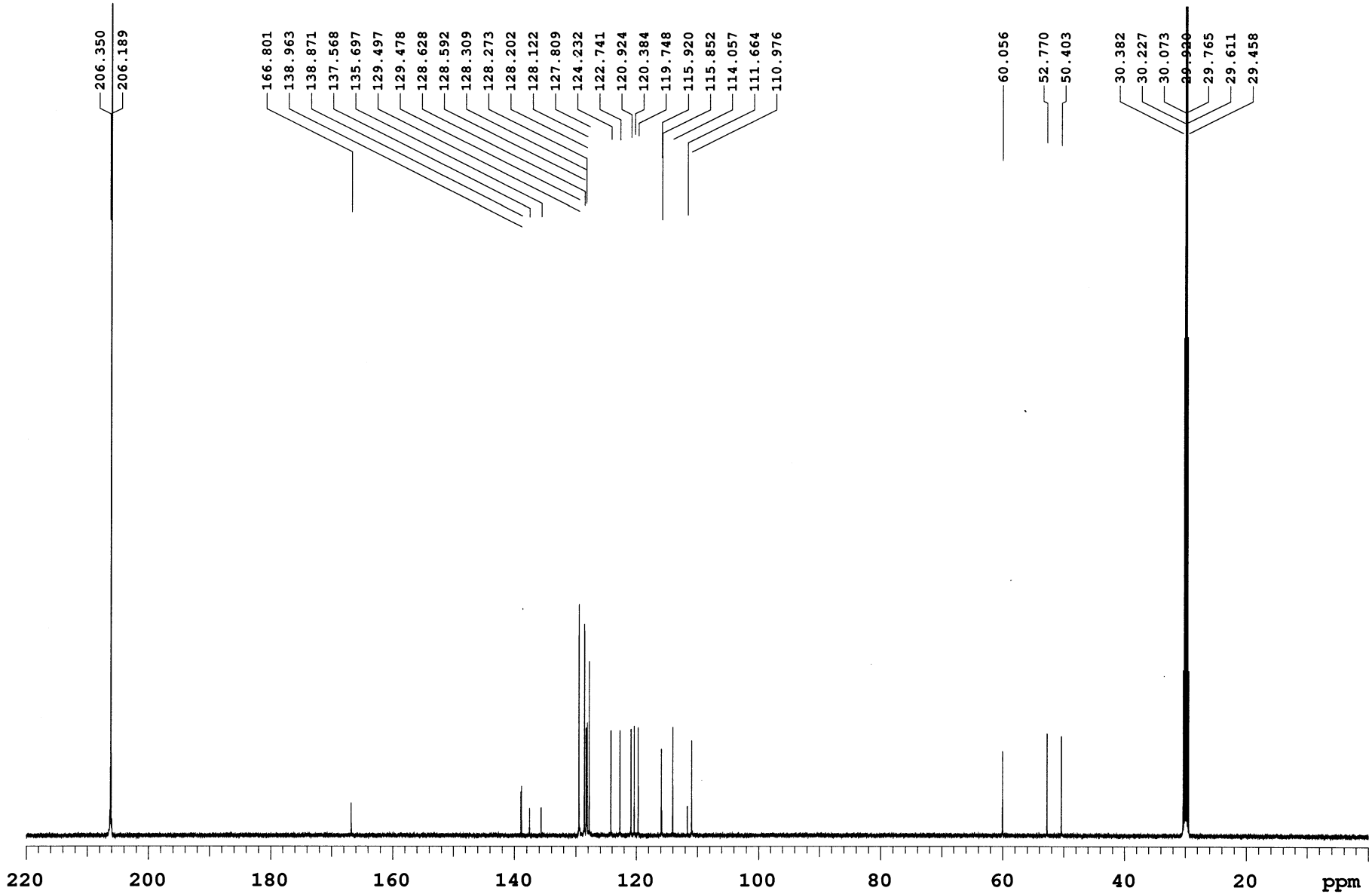
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-181/PROTON_03

Plot date 2017-01-11

Fig S142. 1H NMR (acetone-d6, 500 MHz) of compound 3cp

APS-01-181

Sample Name **APS-01-181**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-09**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



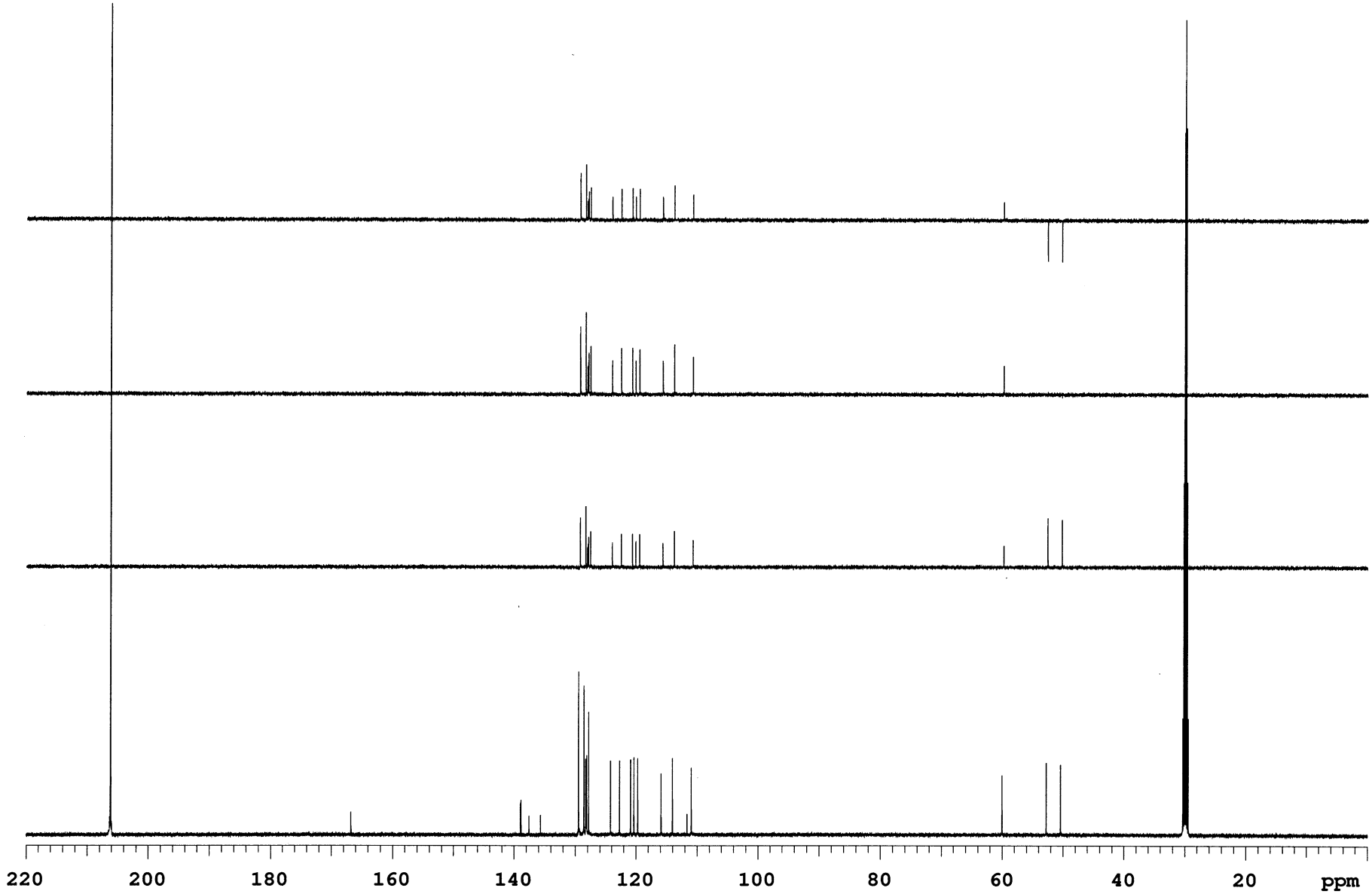
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-181/CARBON_02

Fig S143. 13C NMR (acetone-d6, 125 MHz) of compound 3cp

Plot date 2017-01-11

APS-01-181

Sample Name **APS-01-181**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-10**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-181/DEPT_01

Fig S144. DEPT of compound 3cp

Plot date 2017-01-11

APS-01-181

Sample Name **APS-01-181**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-10**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

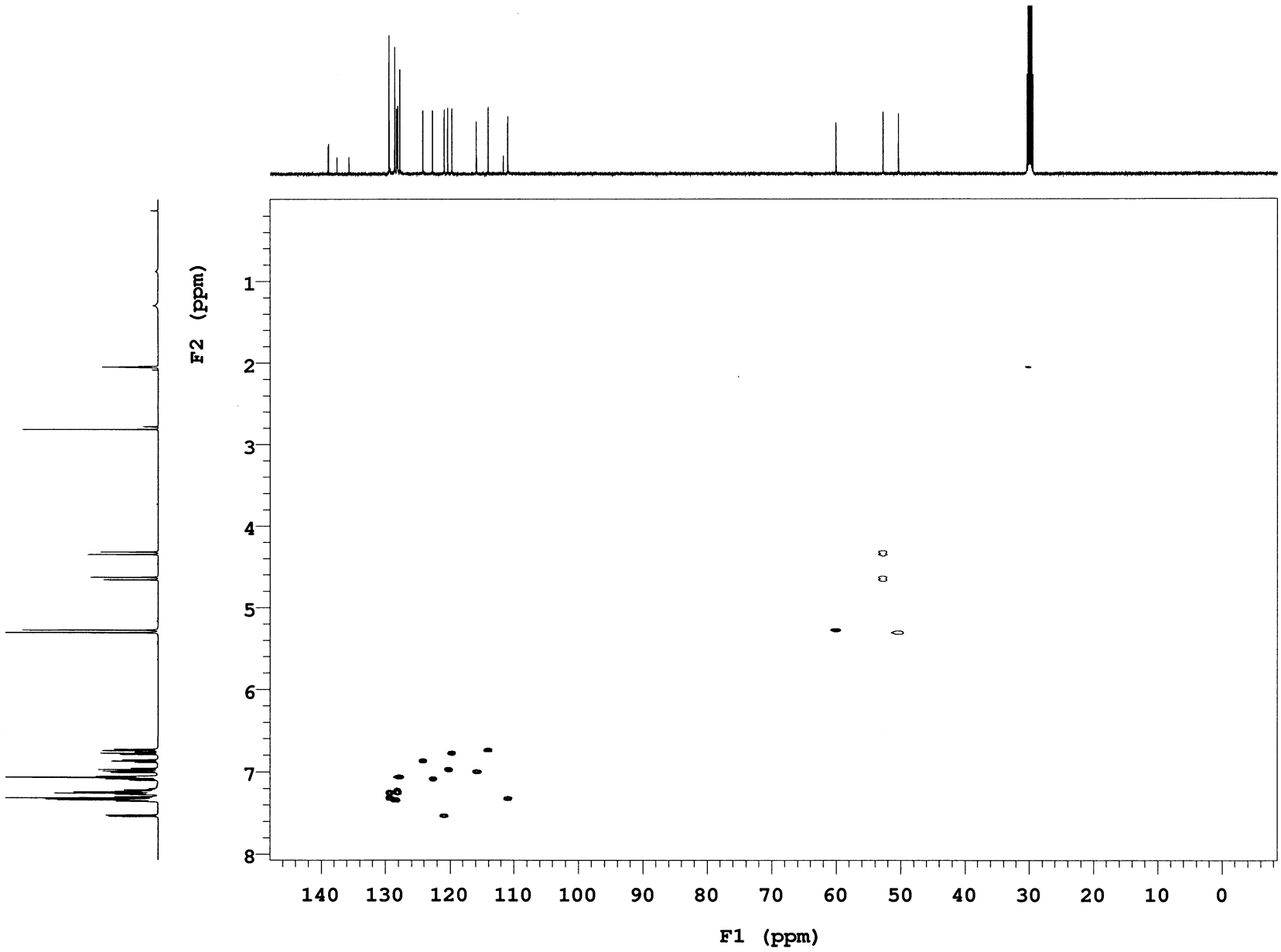


Fig S145. HSQC of compound 3cp

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-181/gHSQC_01

Plot date 2017-01-11

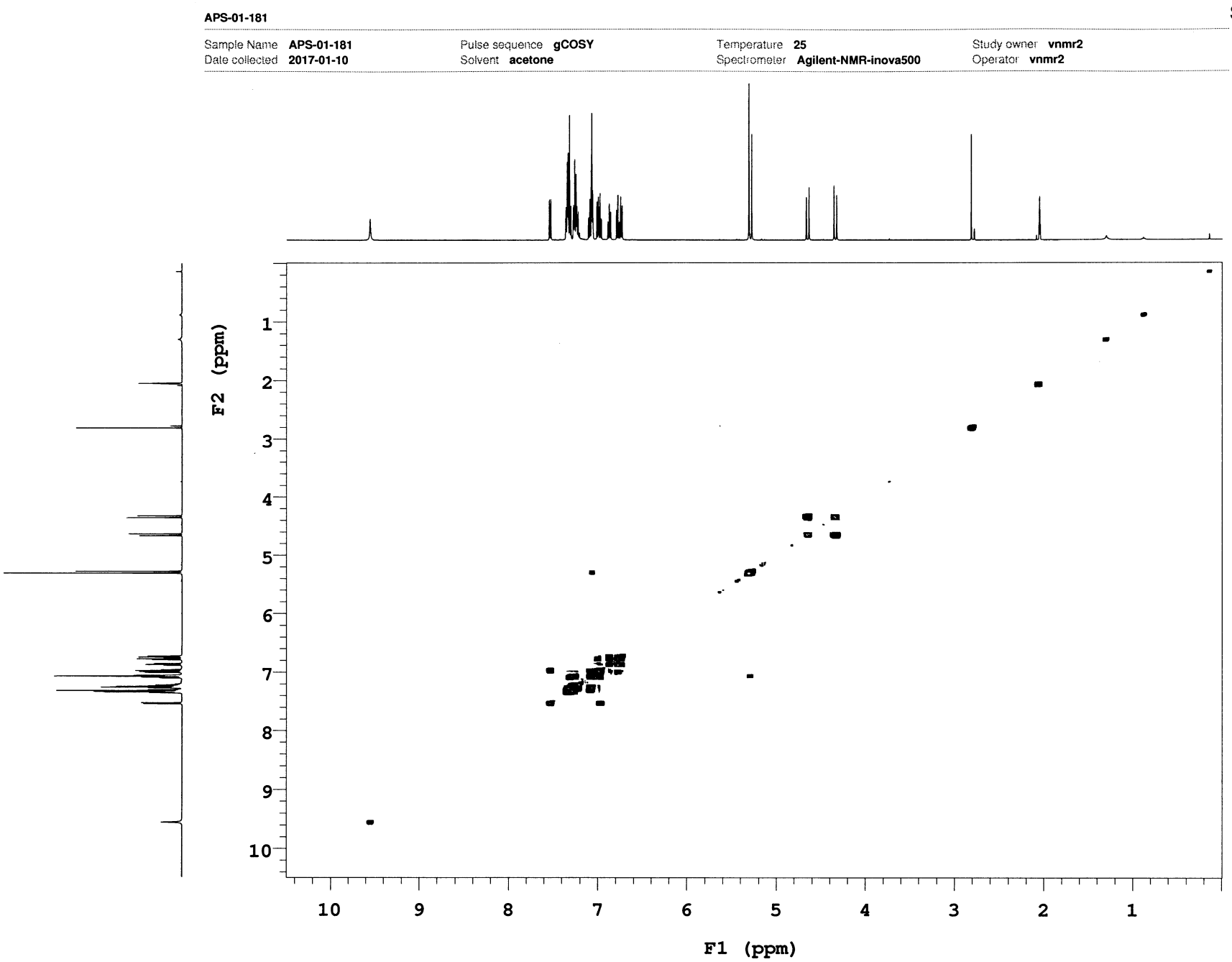


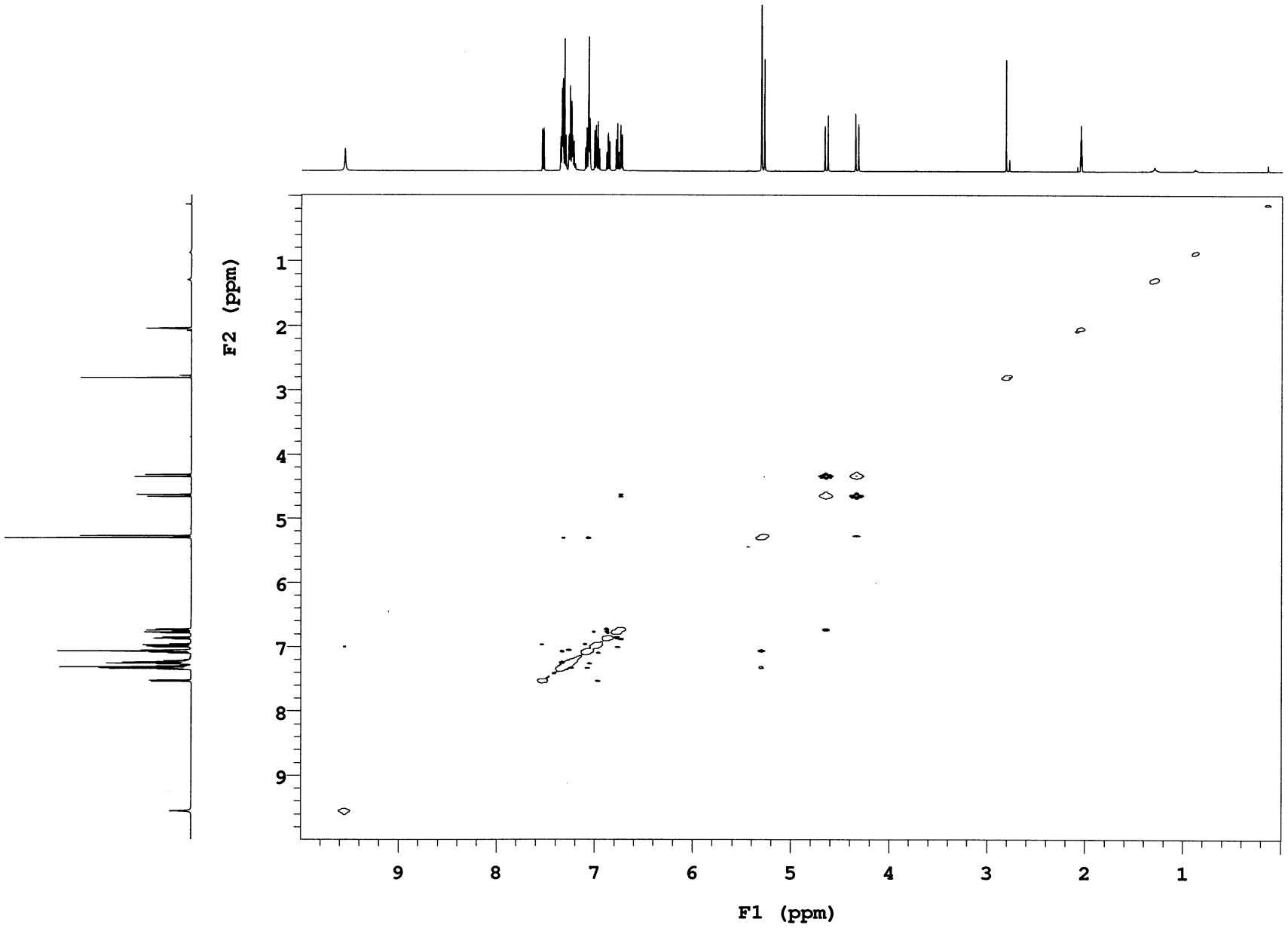
Fig S146. COSY of compound 3cp

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-181/gCOSY_01

Plot date 2017-01-11

APS-01-181

Sample Name	**APS-01-181**	Pulse sequence	**NOESY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-01-10**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



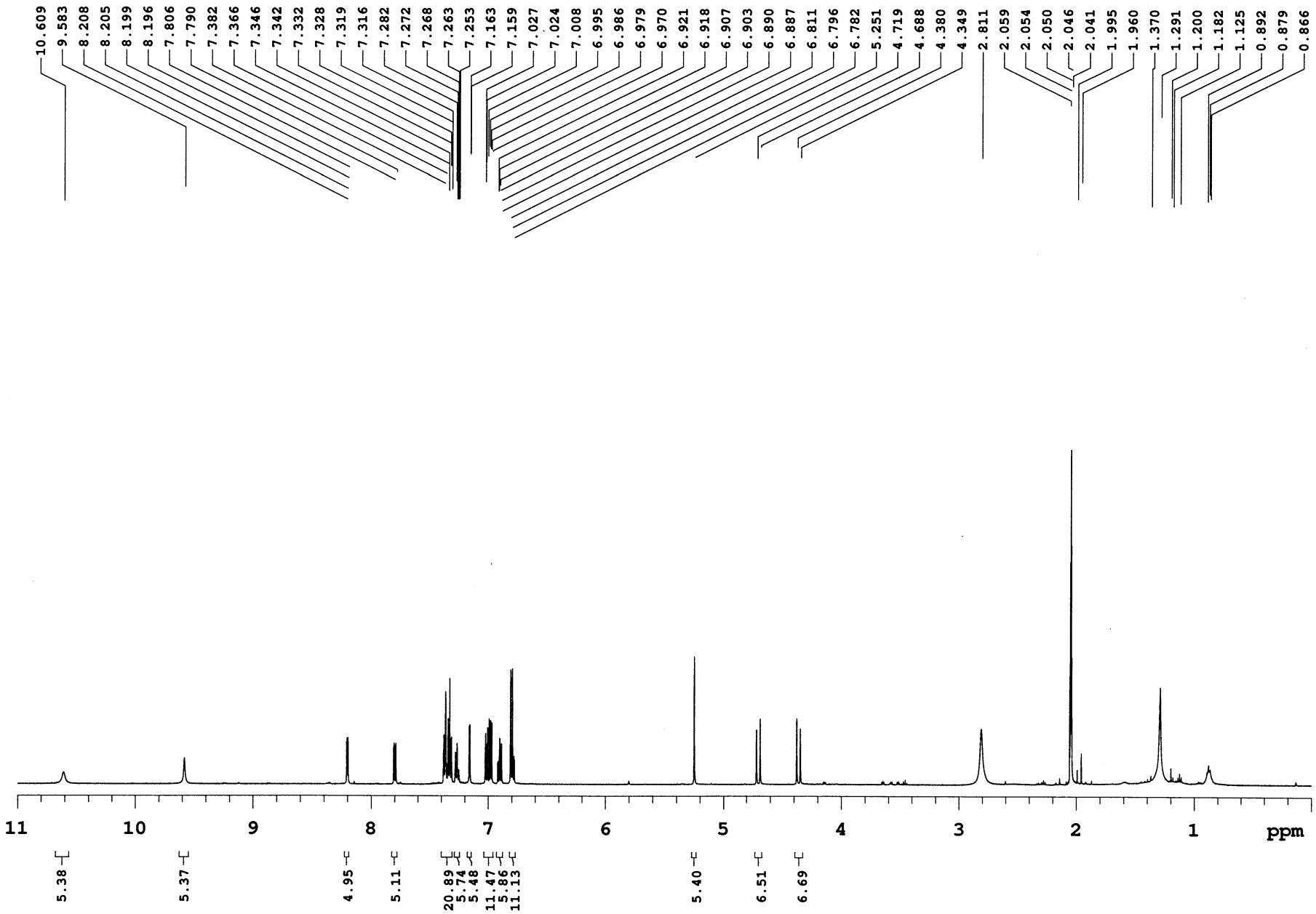
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-181/NOESY_01.fid

Fig S147. NOESY of compound 3cp

Plot date 2017-03-01

APS-1-235

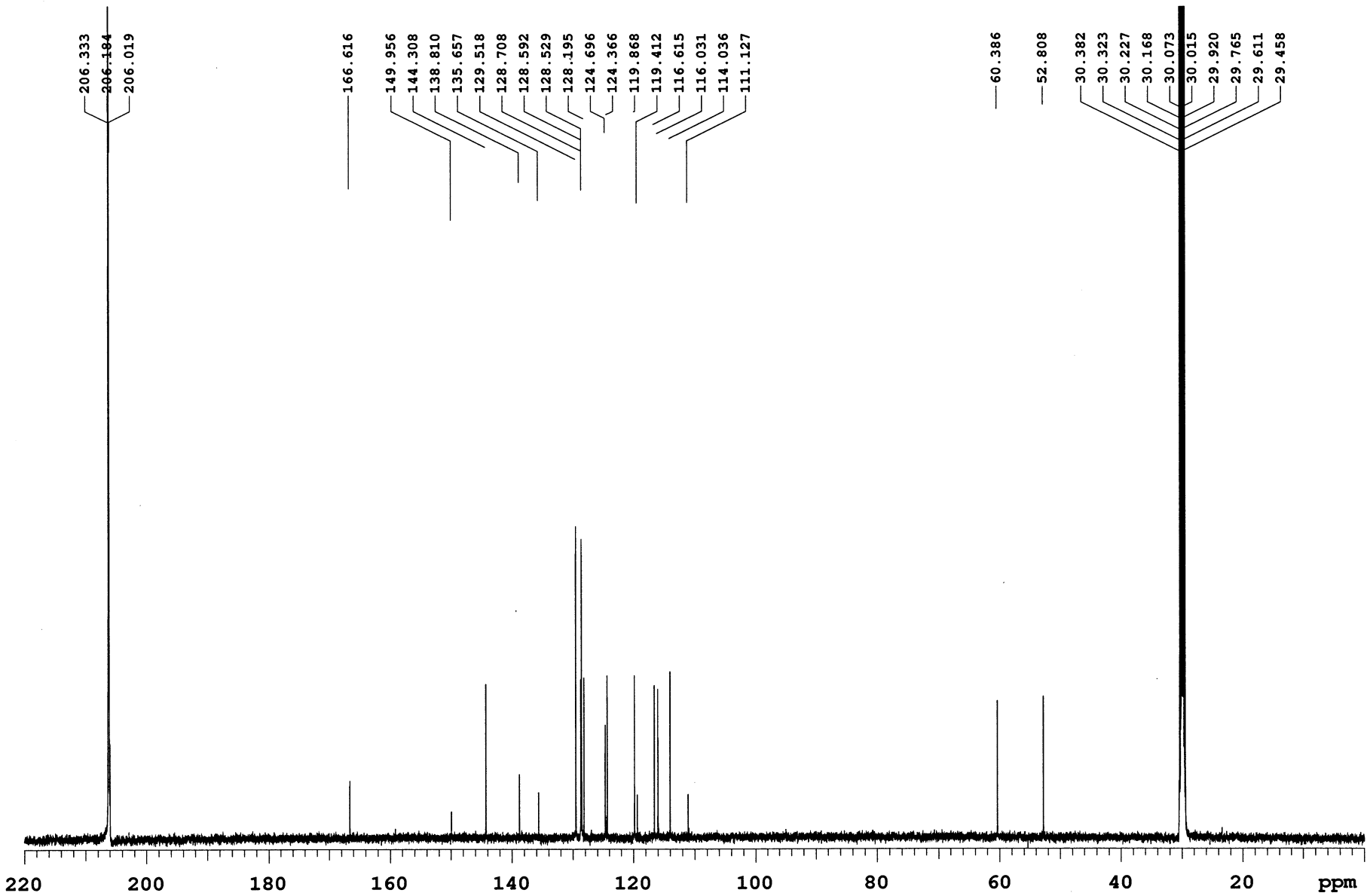
Sample Name **APS-1-235**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-10-10**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-1-235/PROTON_03

Plot date 2017-10-12

Fig S148. 1H NMR (acetone-d6, 500 MHz) of compound 3cq



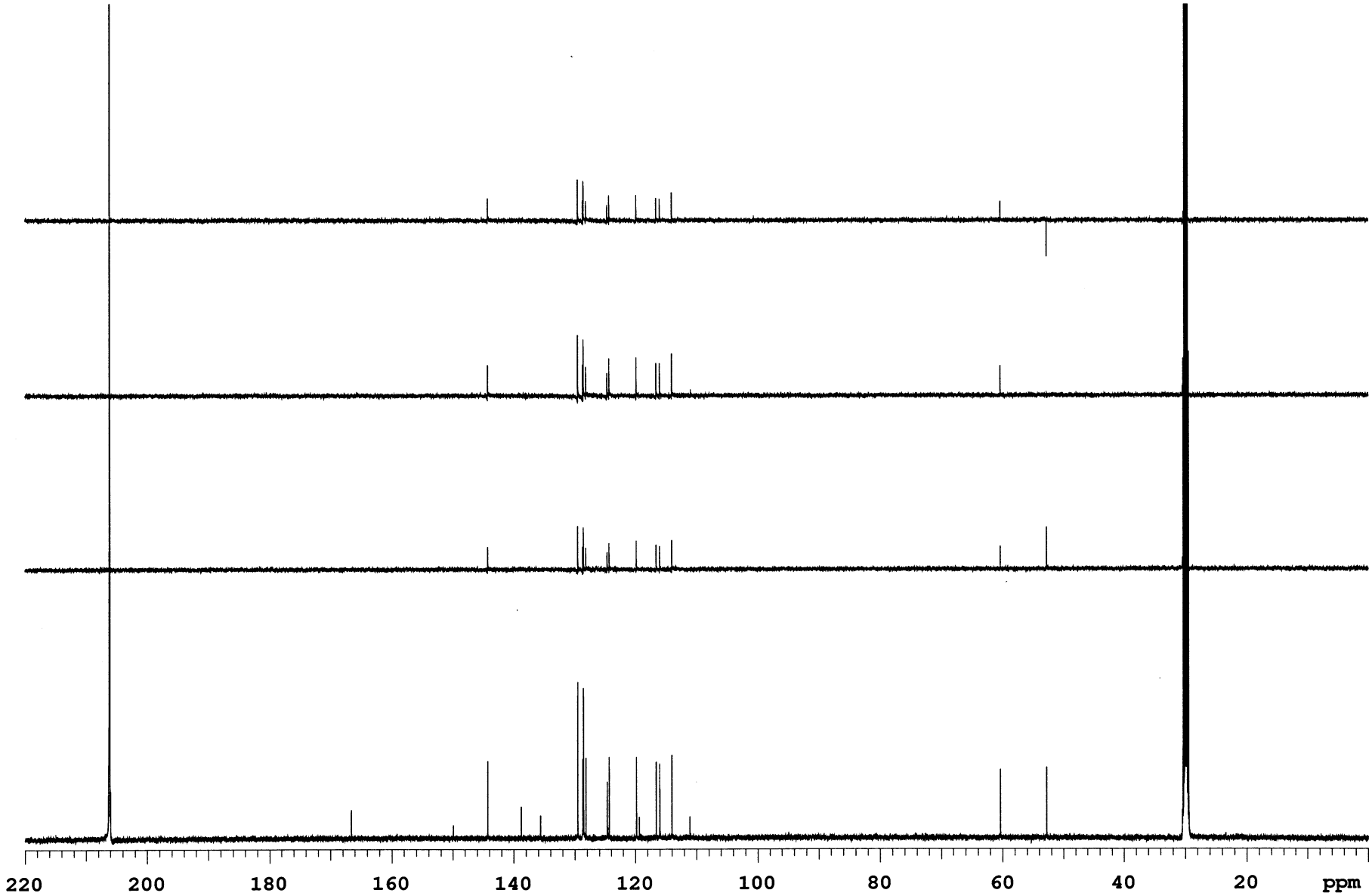
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-1-235/CARBON_02

Plot date 2017-10-11

Fig S149. 13C NMR (acetone-d6, 125 MHz) of compound 3cq

APS-1-235

Sample Name **APS-1-235**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-10-10**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



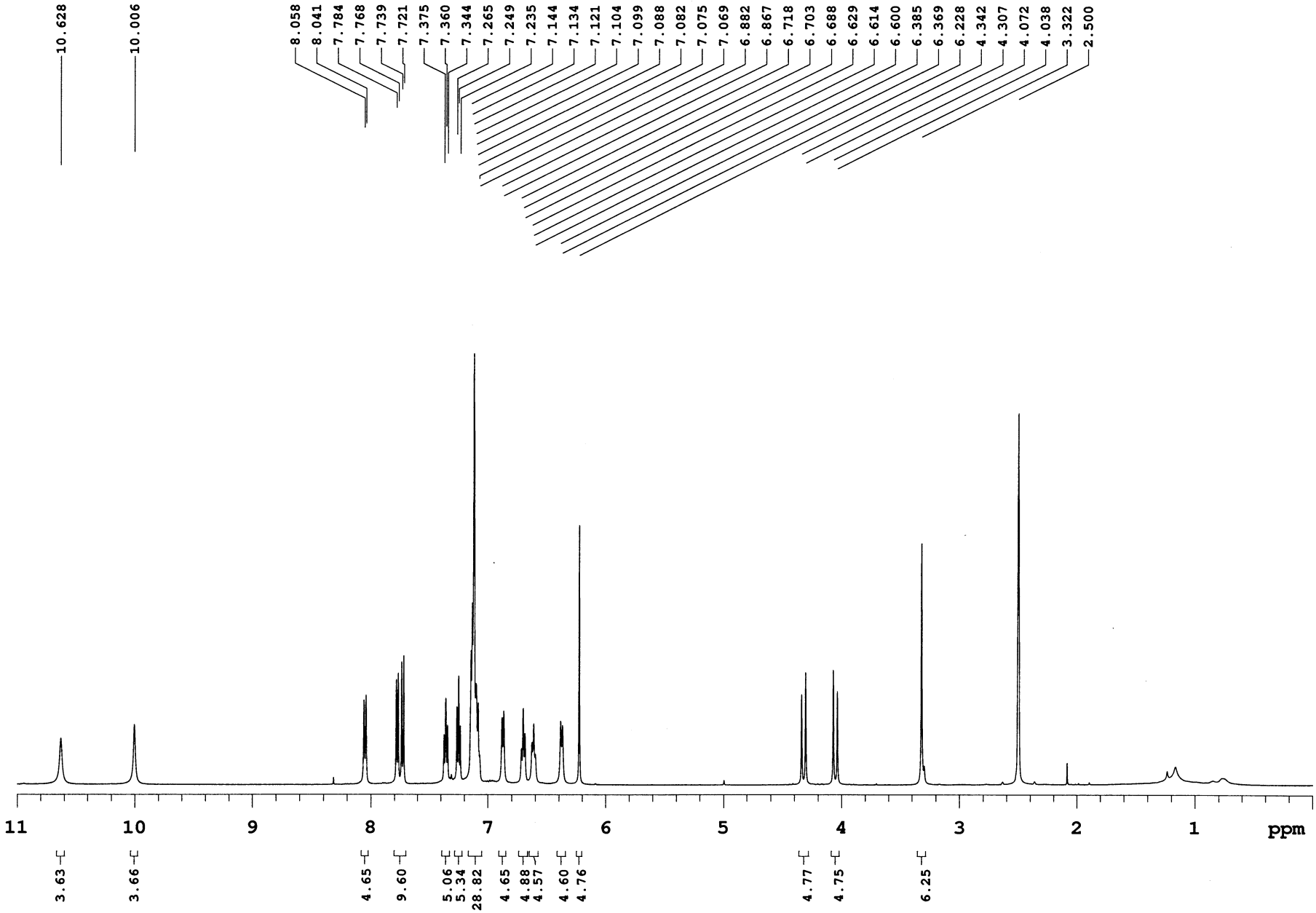
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-1-235/DEPT_01

Fig S150. DEPT of compound 3cq

Plot date 2017-10-11

APS-1-217

Sample Name **APS-1-217**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-10-30**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-1-217/PROTON_23

Fig S151. 1H NMR (DMSO-d6, 500 MHz) of compound 3cr

Plot date 2017-10-31

APS-1-217

Sample Name **APS-1-217** | Pulse sequence **CARBON** | Temperature **25** | Study owner **vnmr2**
Date collected **2017-10-31** | Solvent **dmso** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**

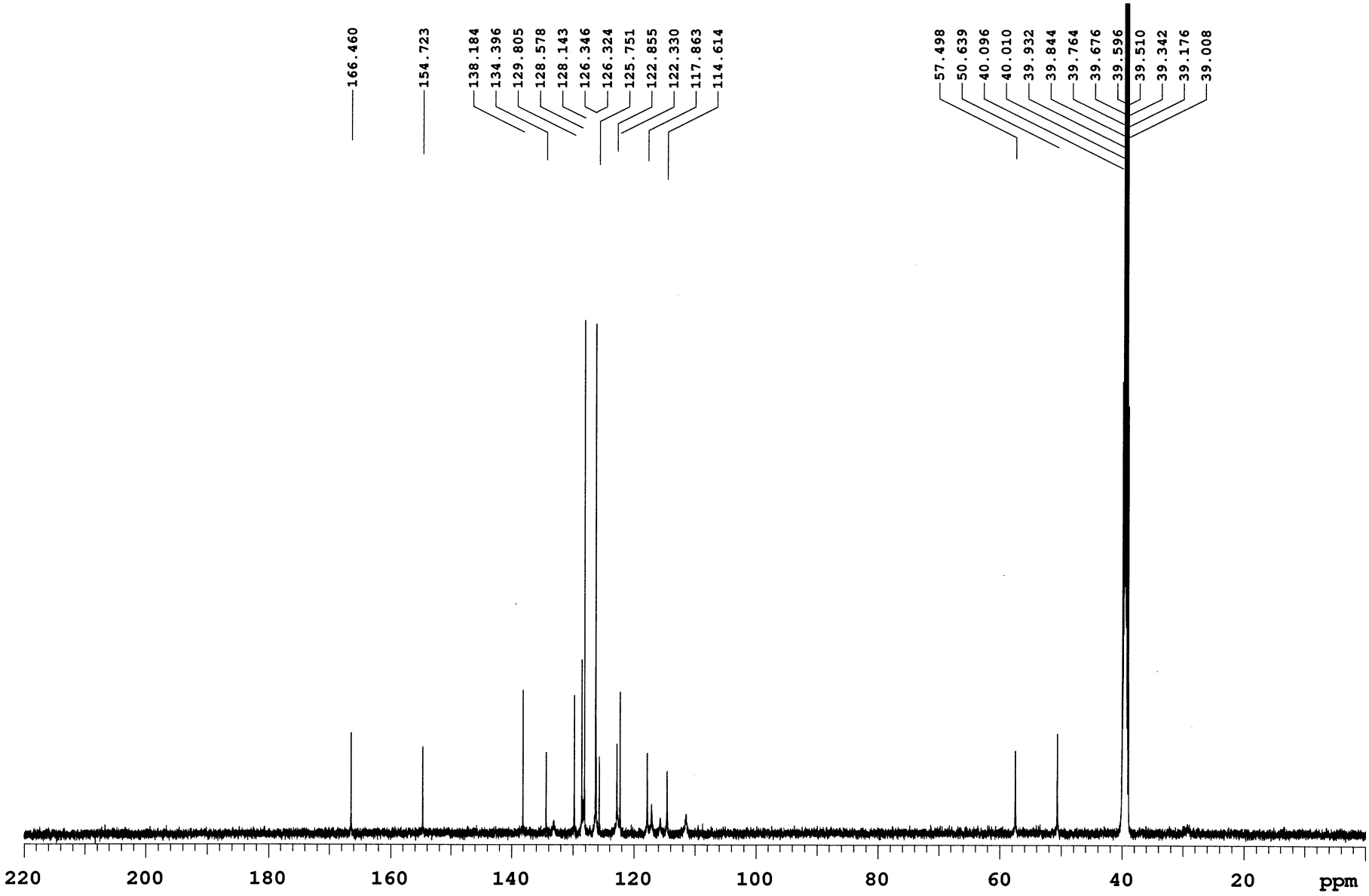


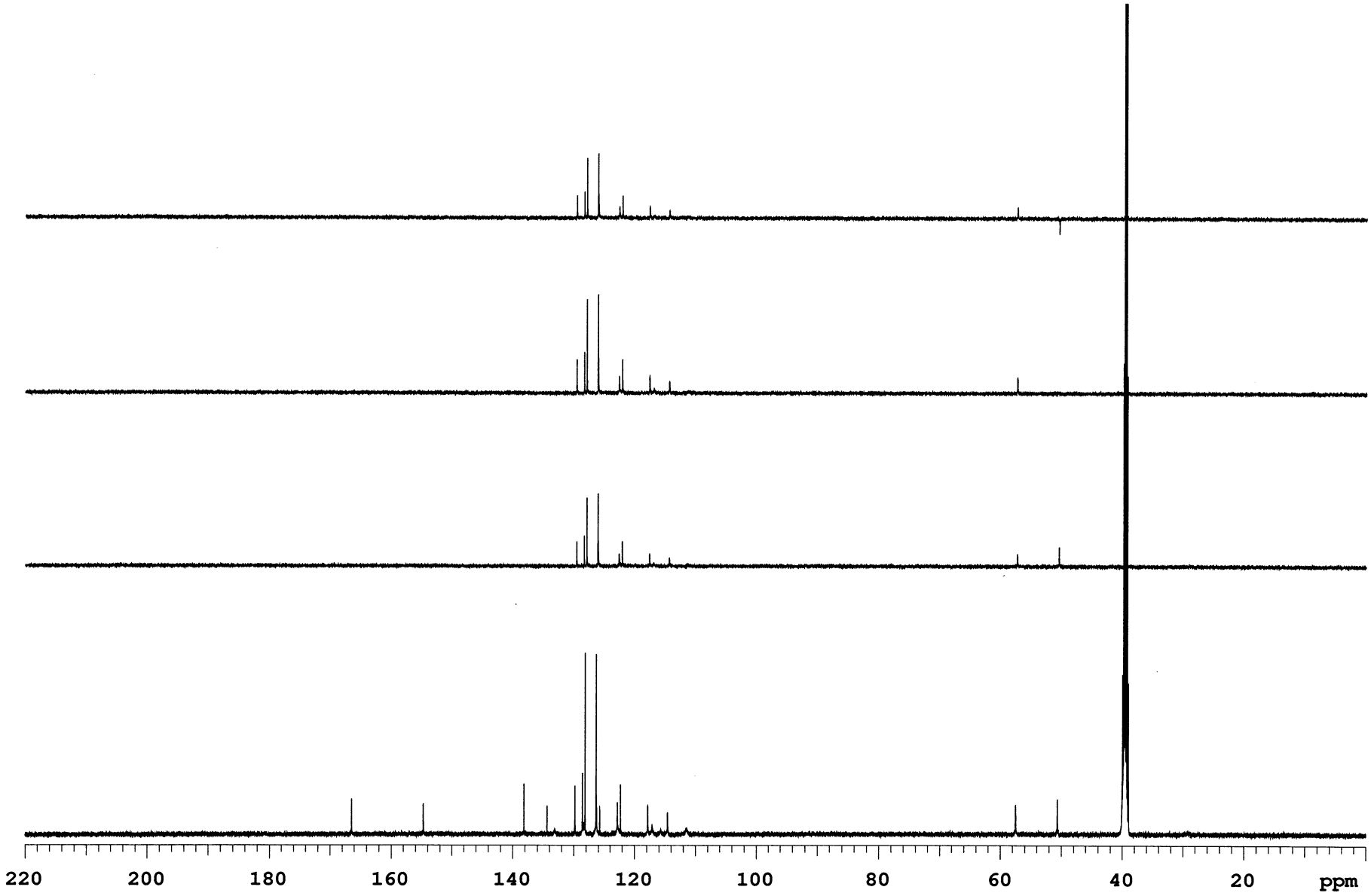
Fig S152. 13C NMR (DMSO-d6, 125 MHz) of compound 3cr

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-1-217/CARBON_02

Plot date 2017-10-31

APS-1-217

Sample Name **APS-1-217**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-10-31**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



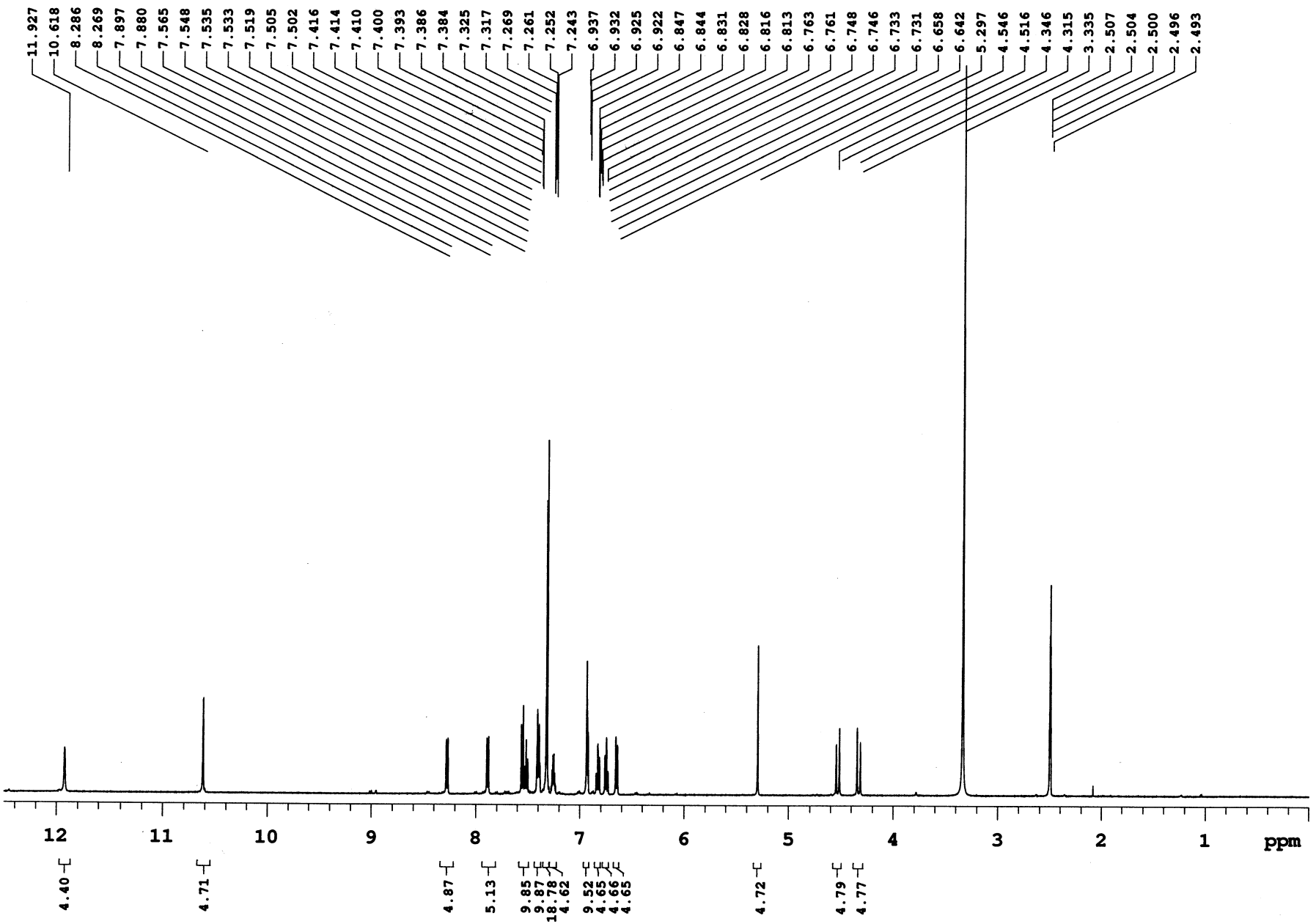
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-1-217/DEPT_01

Fig S153. DEPT of compound 3cr

Plot date 2017-10-31

APS-01-162

Sample Name	**APS-01-162**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-11-27**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-162/PROTON_03

Fig S154. 1H NMR (DMSO-d6, 500 MHz) of compound 3cs

Plot date 2016-11-29

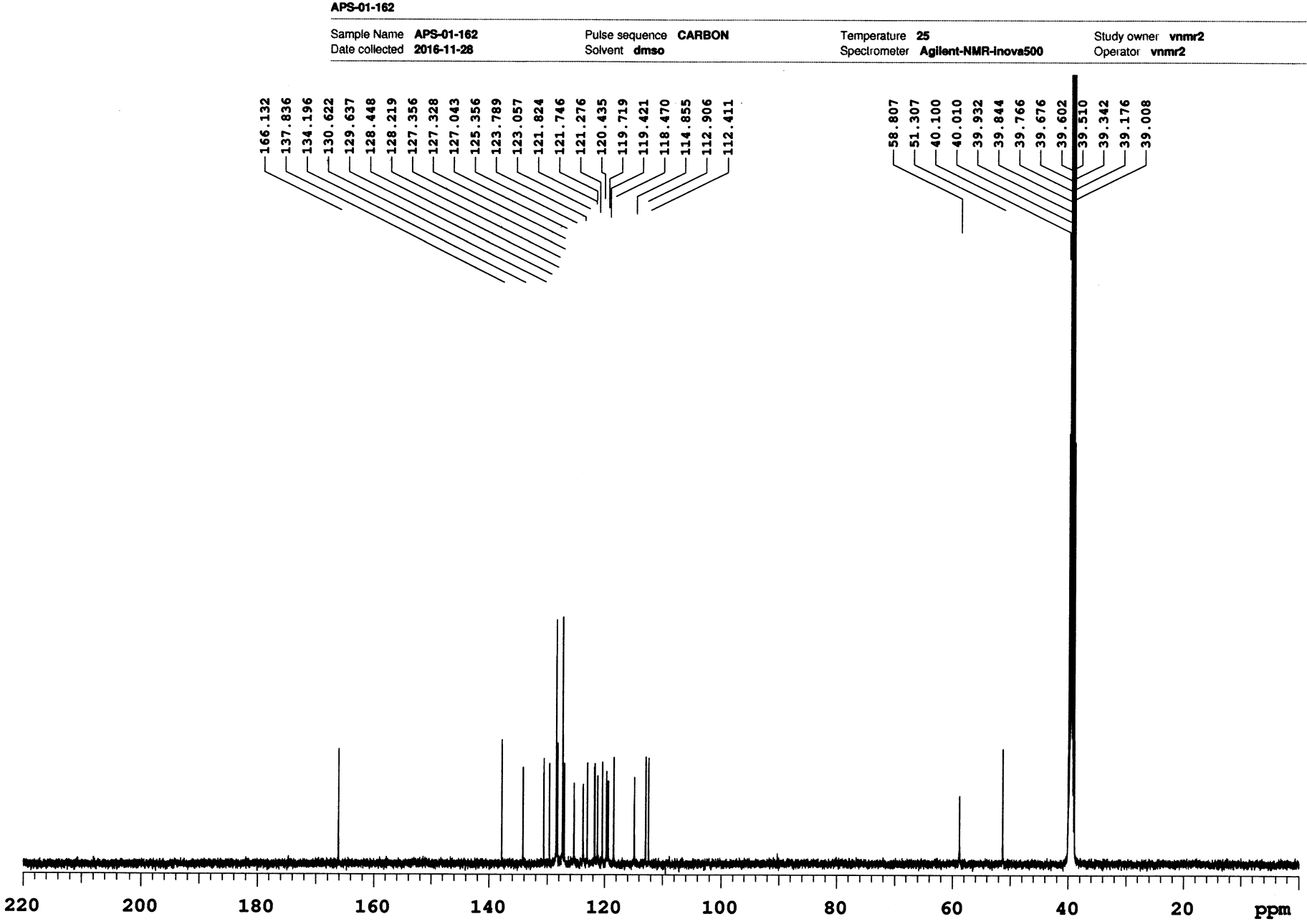


Fig S155. 13C NMR (DMSO-d6, 125 MHz) of compound 3cs

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-162/CARBON_02

Plot date 2016-11-29

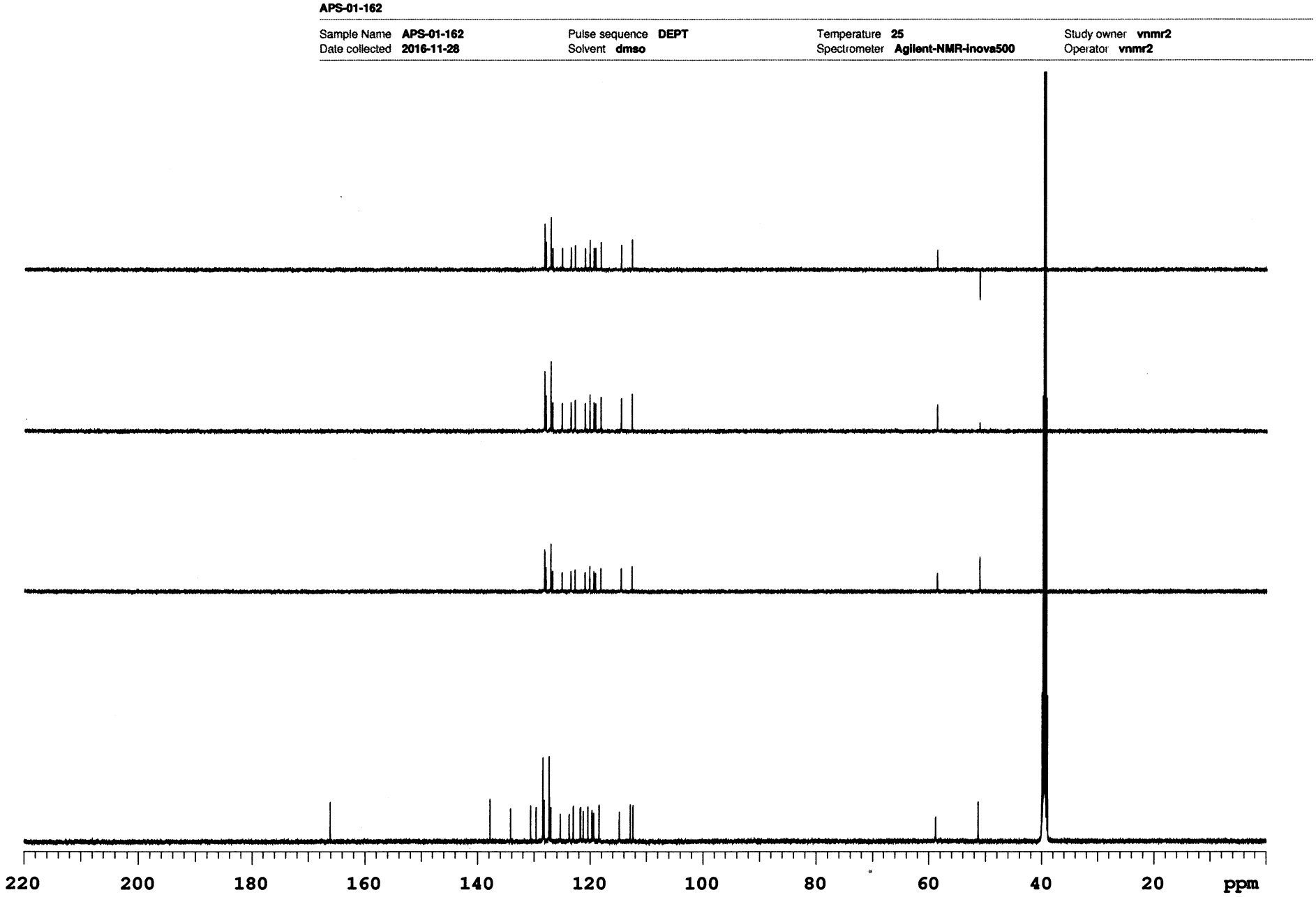


Fig S156. DEPT of compound 3cs

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-162/DEPT_01

Plot date 2016-11-29

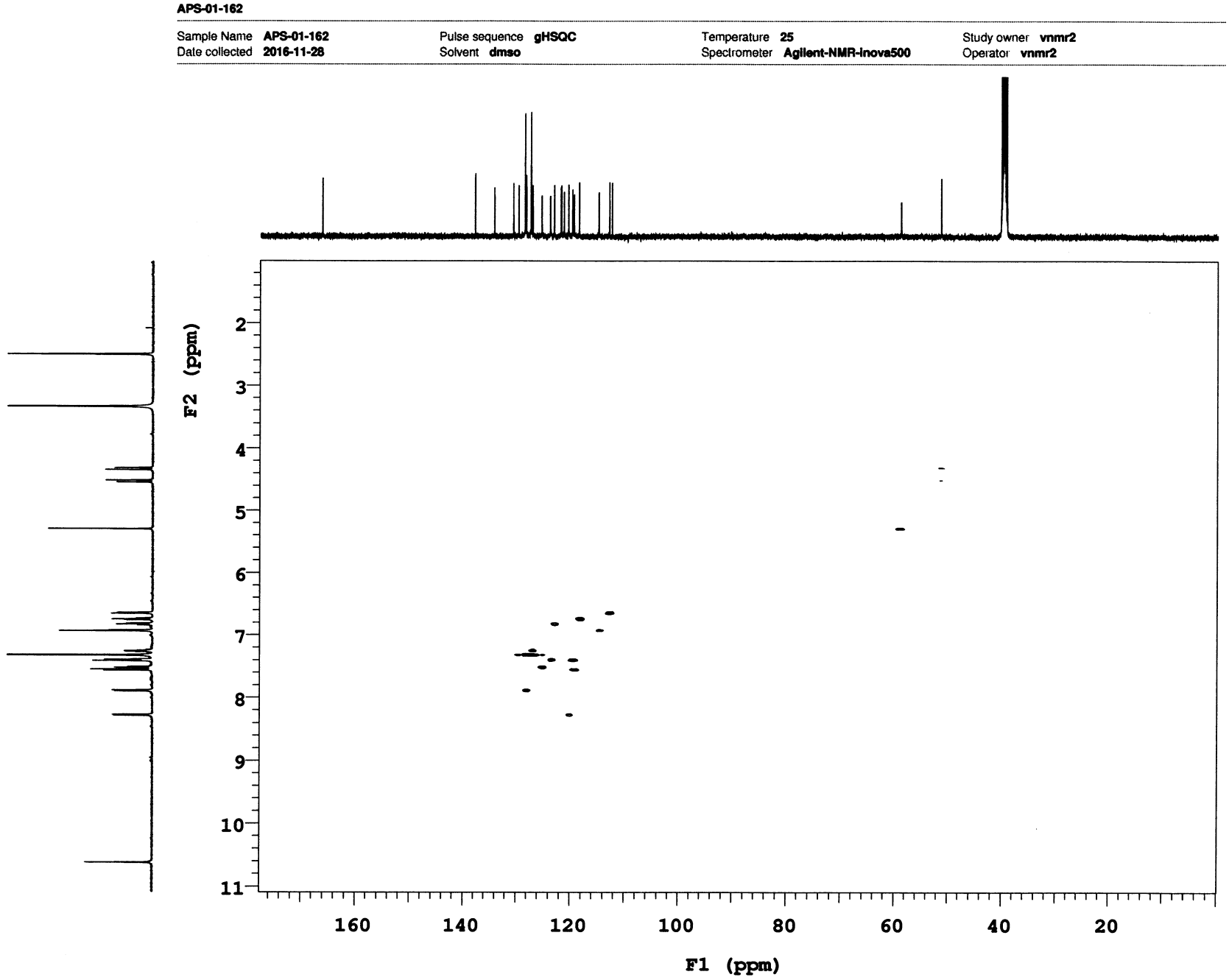


Fig S157. HSQC of compound 3cs

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-162/gHSQC_01

Plot date 2016-11-30

APS-01-162

Sample Name	**APS-01-162**	Pulse sequence	**gCOSY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2016-11-28**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

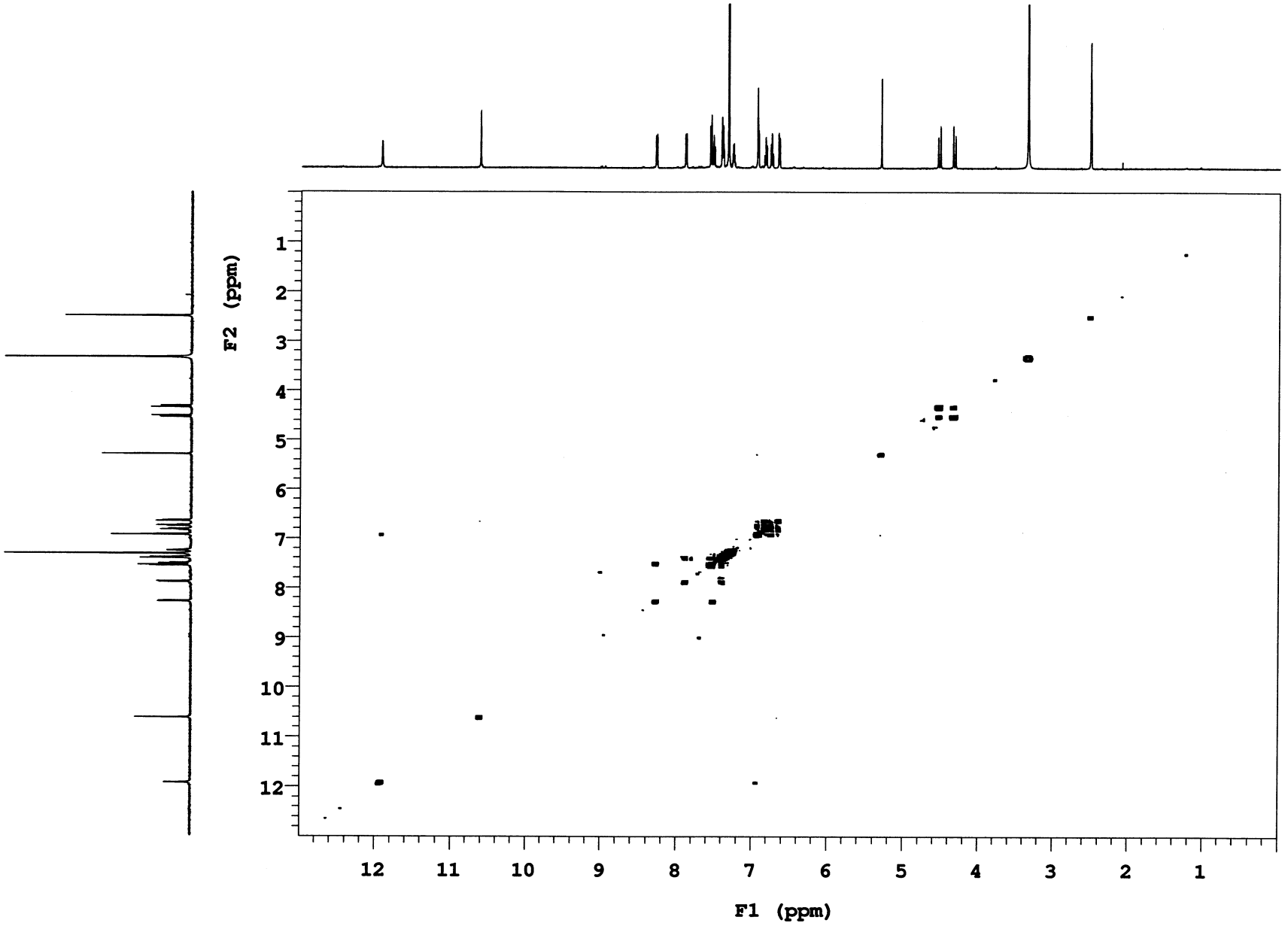


Fig S158. COSY of compound 3cs

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-162/gCOSY_01

Plot date 2016-11-30

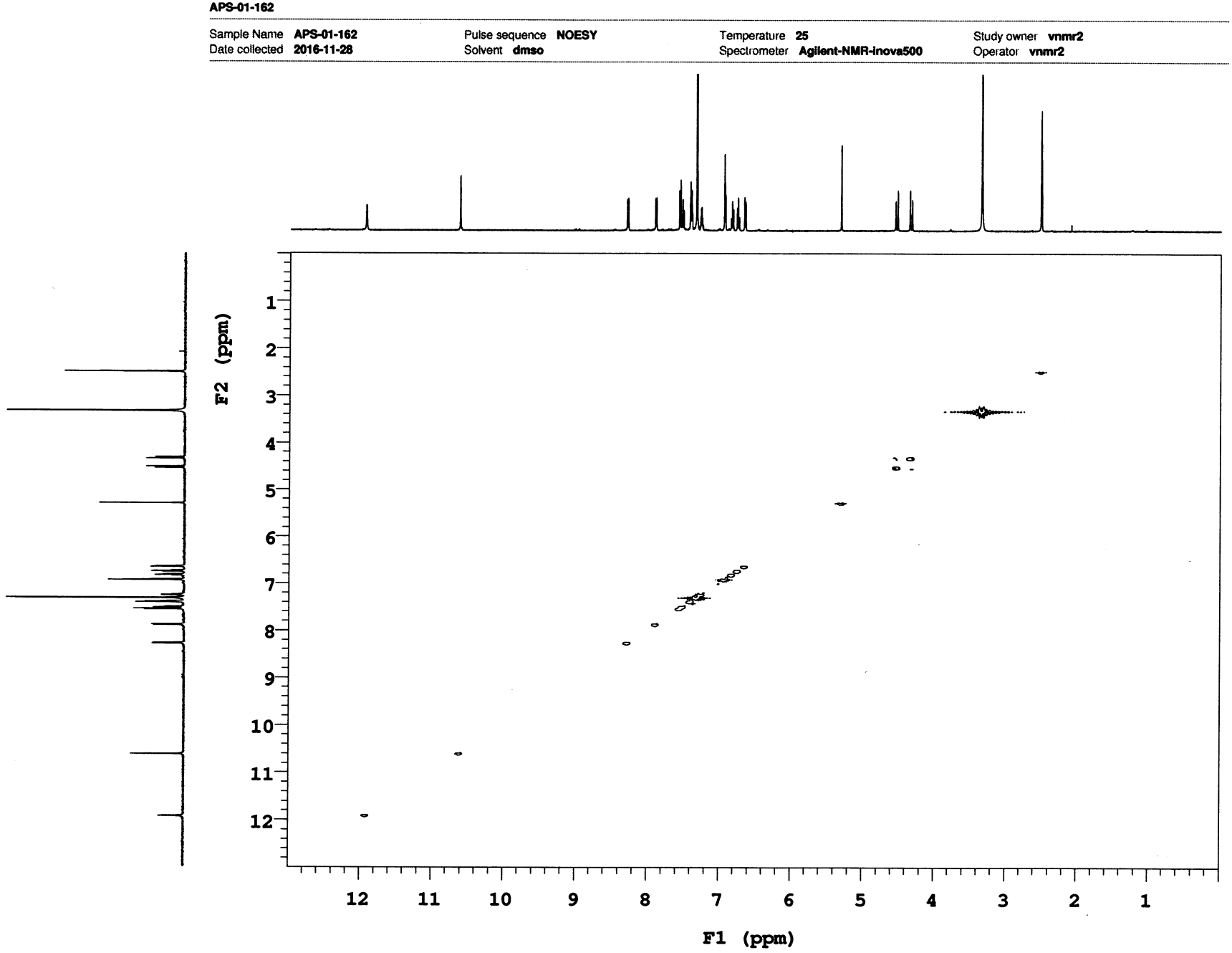


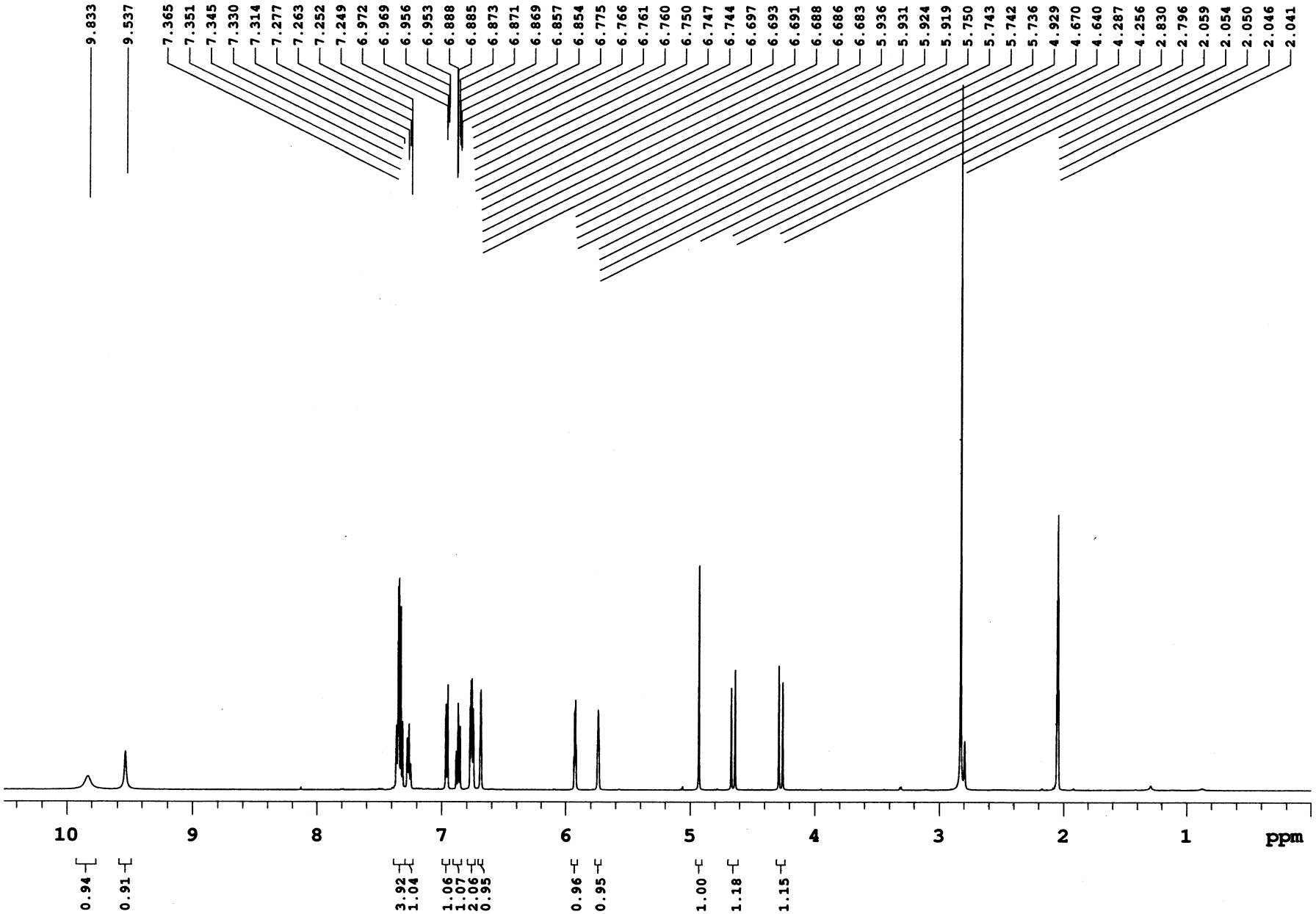
Fig S159. NOESY of compound 3cs

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-162/NOESY_01

Plot date 2016-11-30

APS-01-193

Sample Name **APS-01-193**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-31**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-193/PROTON_03

Fig S160. 1H NMR (acetone-d6, 500 MHz) of compound 3ct

Plot date 2017-06-02

APS-01-193

Sample Name **APS-01-193**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-31**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

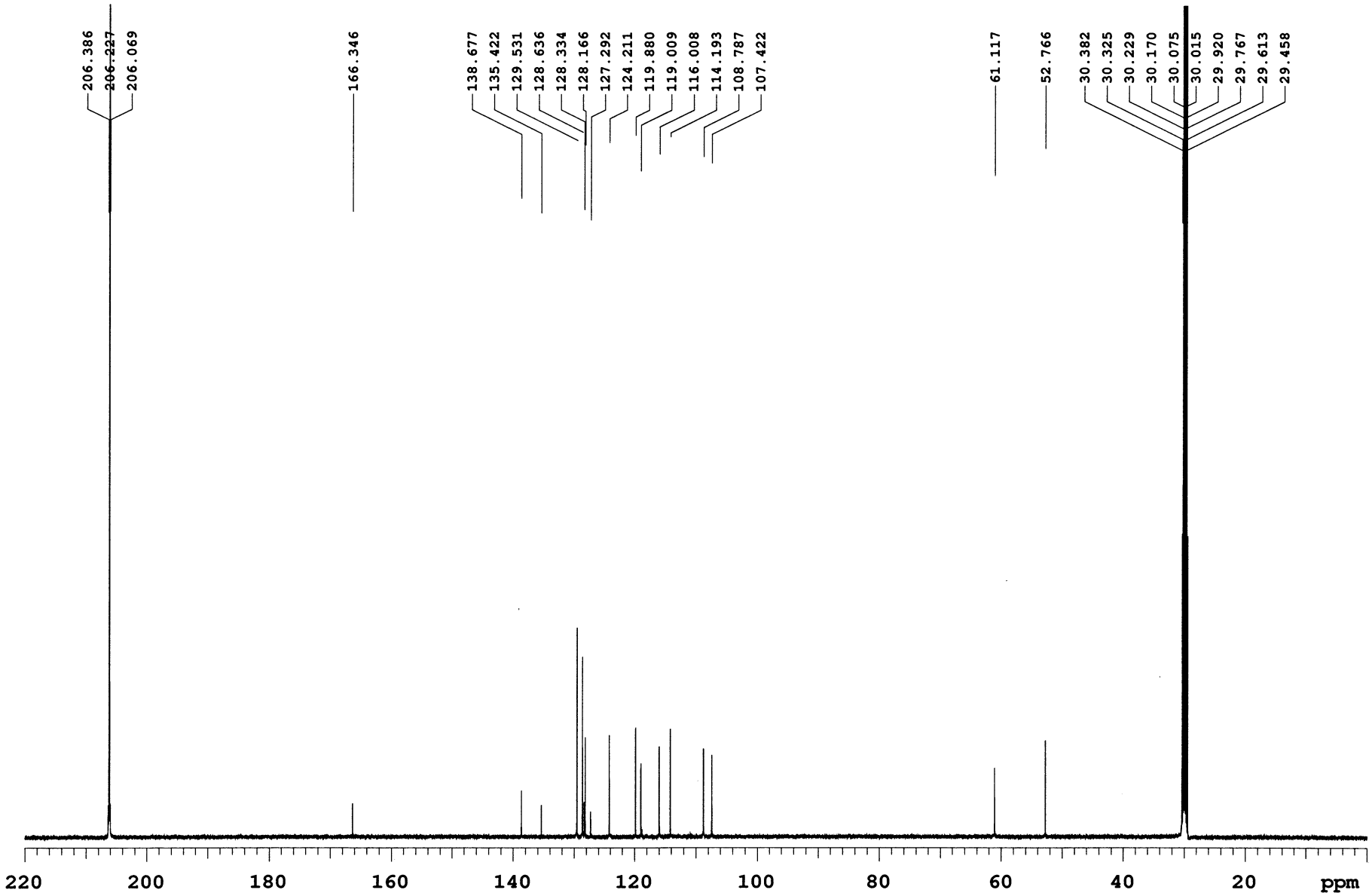


Fig S161. 13C NMR (acetone-d6, 125 MHz) of compound 3ct

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-193/CARBON_02

Plot date 2017-06-02

APS-01-193

Sample Name **APS-01-193**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-31**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

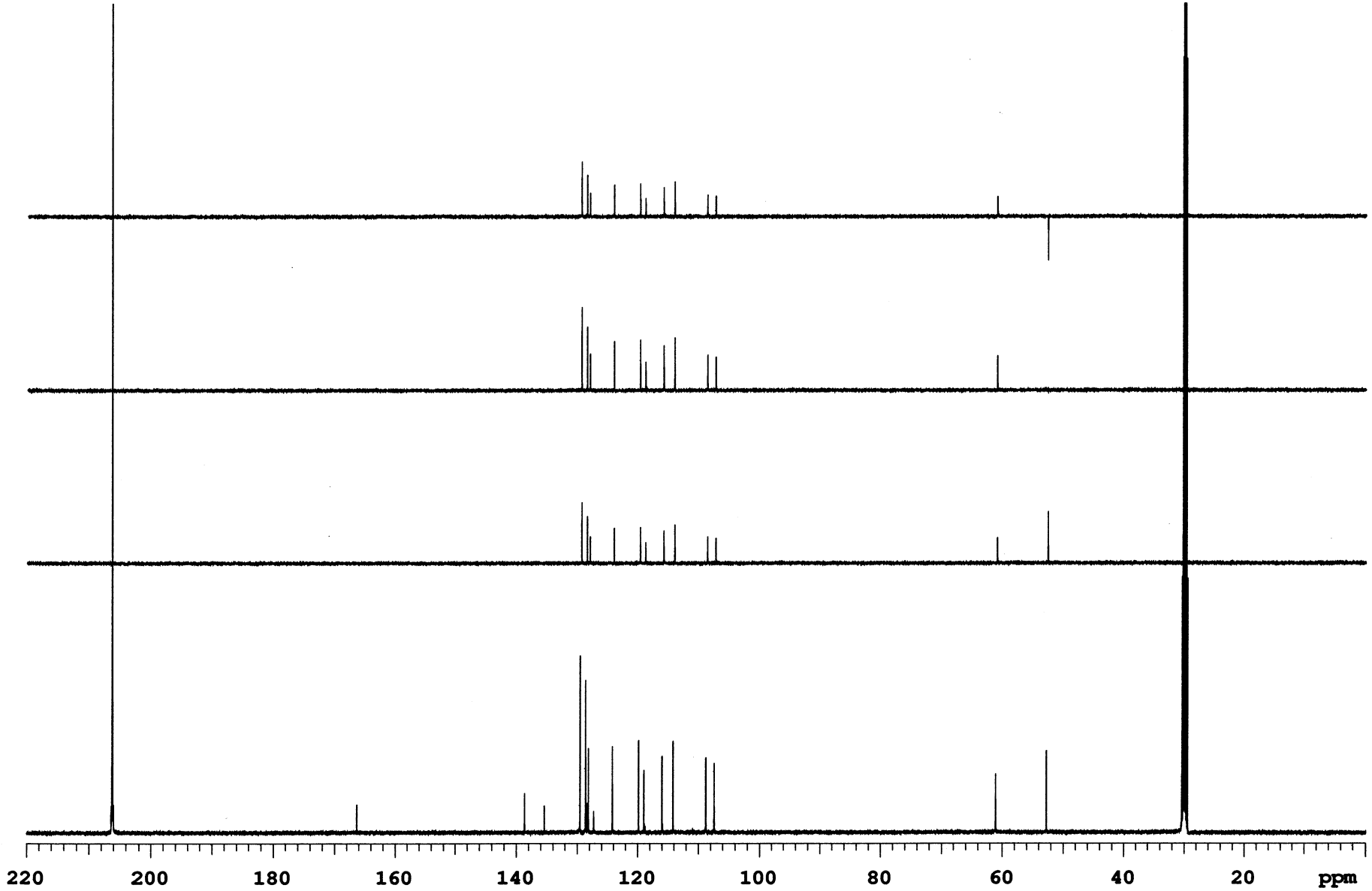


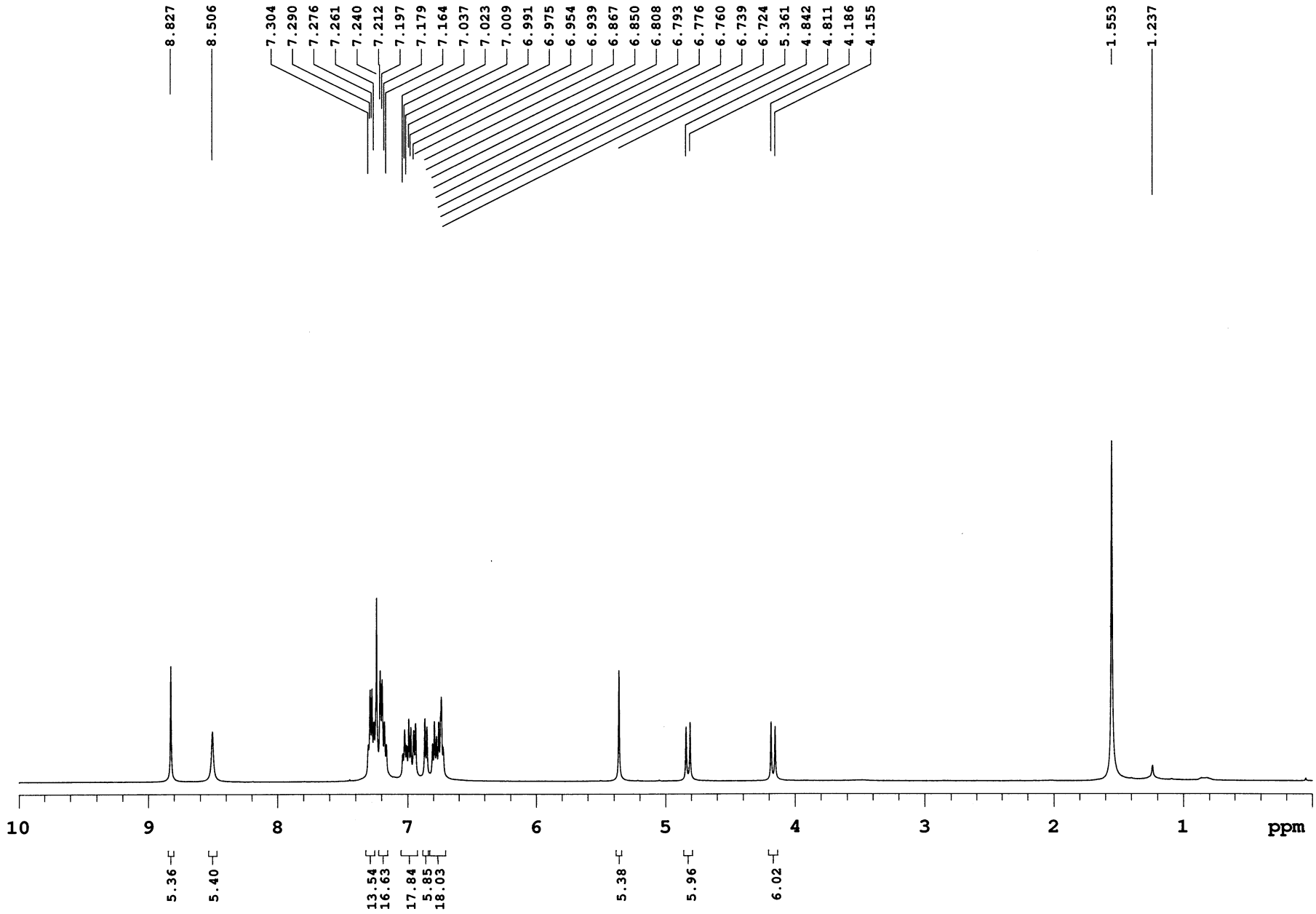
Fig S162. DEPT of compound 3ct

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-193/DEPT_01

Plot date 2017-06-02

APS-01-210-f1

Sample Name	**APS-01-210-f1**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-10-16**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-210-f1/PROTON_03

Fig S163. 1H NMR (CDCl3, 500 MHz) of compound 3cu-o

Plot date 2017-10-17

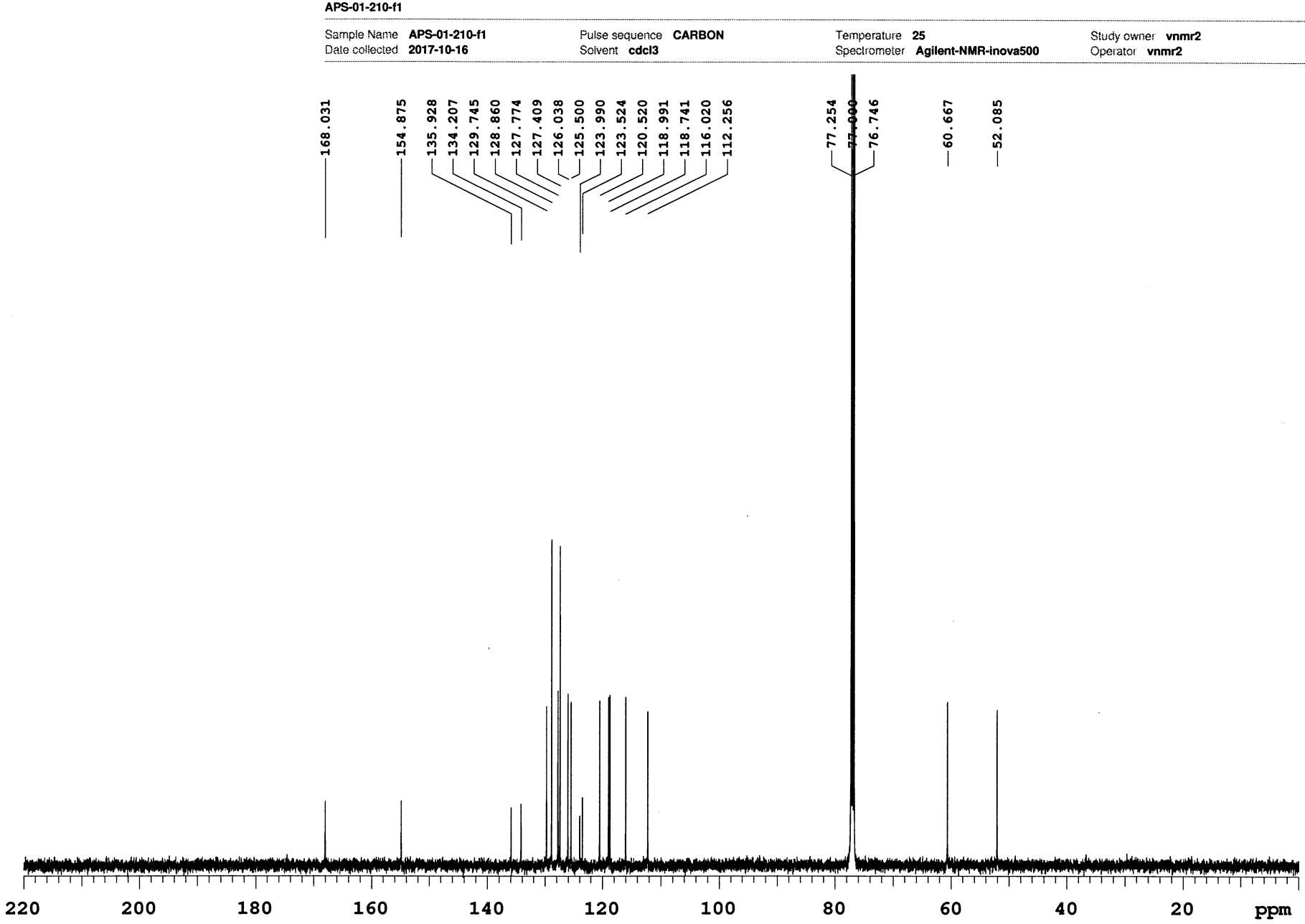


Fig S164. 13C NMR (CDCl3, 125 MHz) of compound 3cu-o

APS-01-210-f1

Sample Name **APS-01-210-f1**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-10-17**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

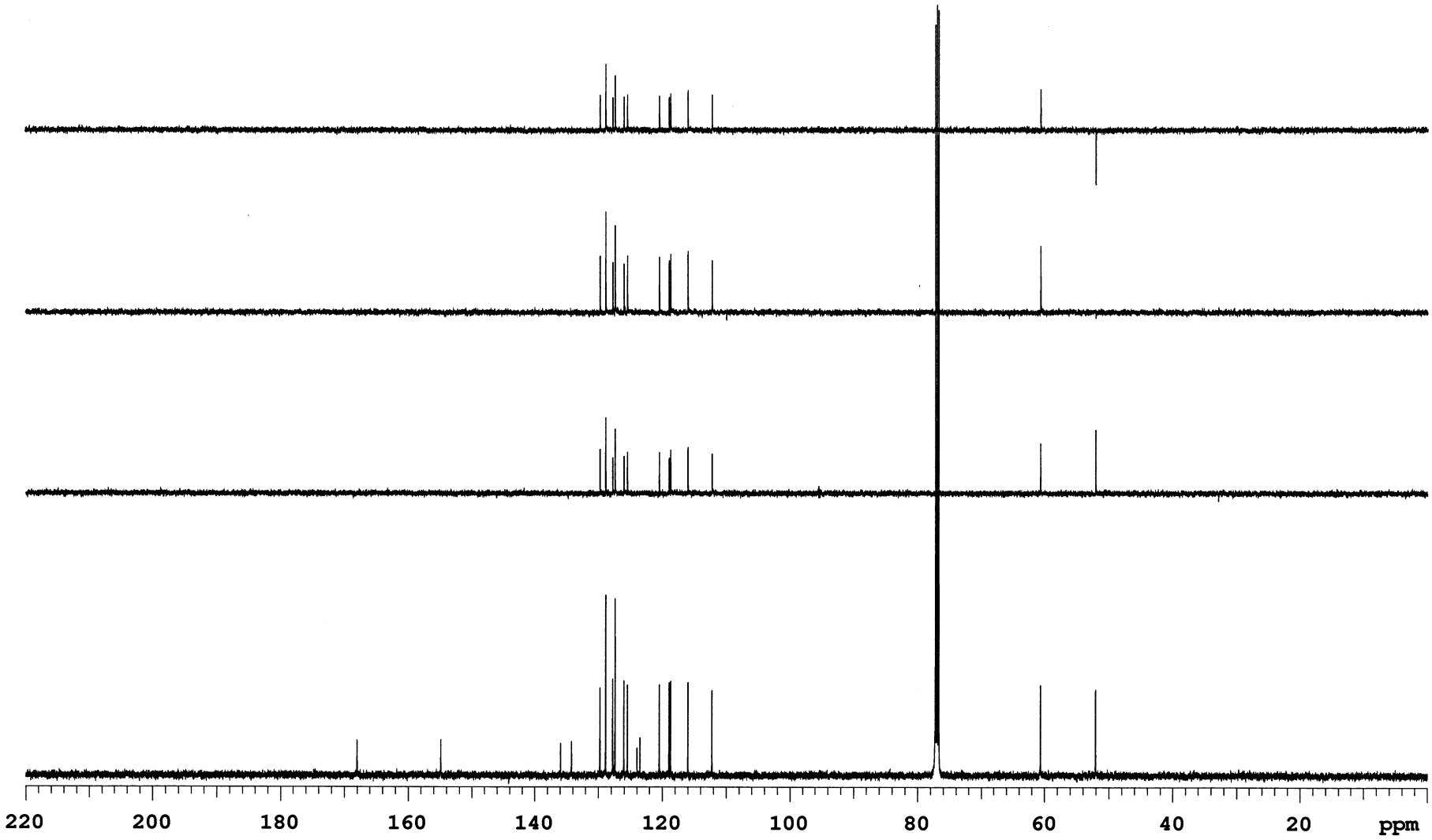
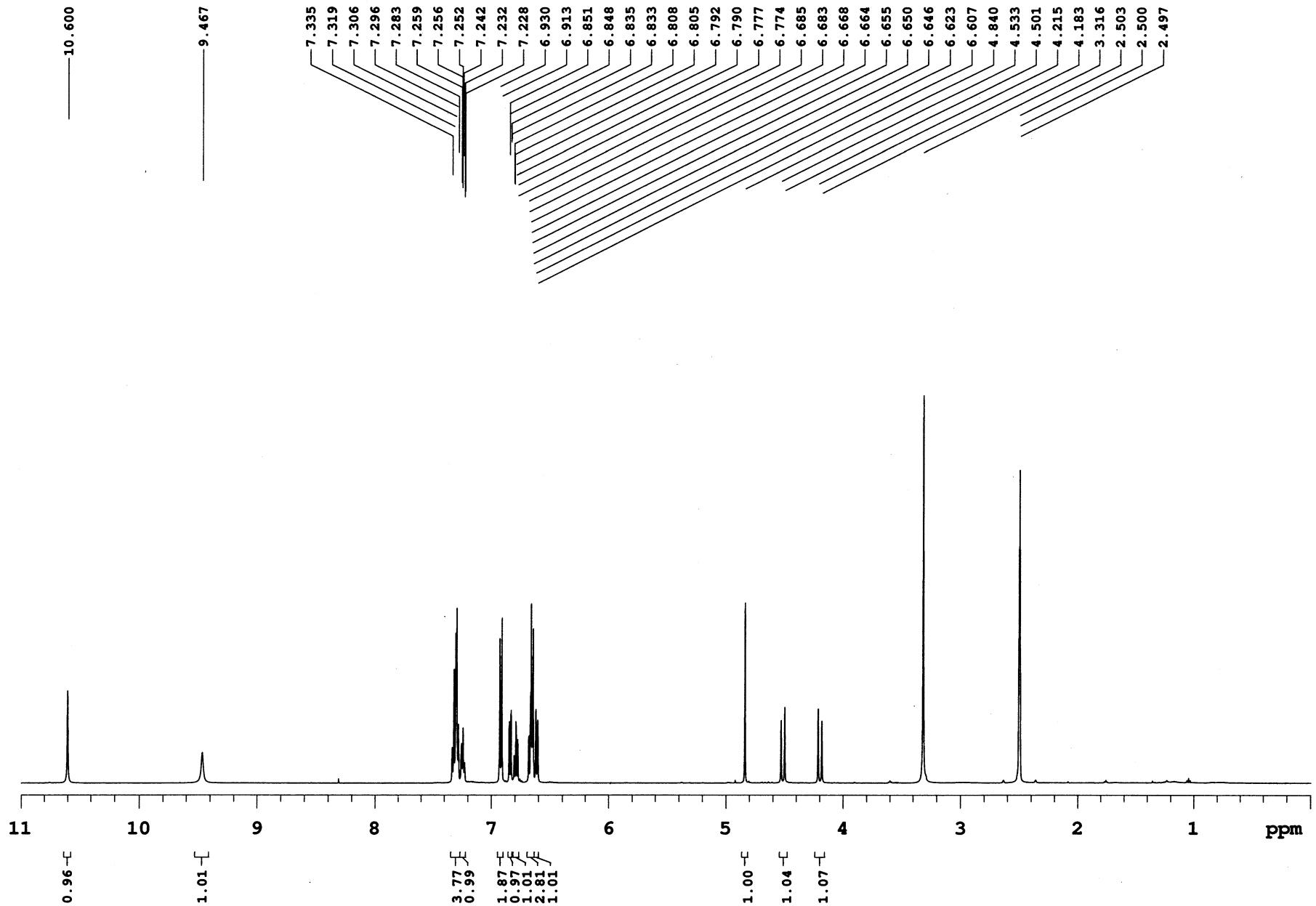


Fig S165. DEPT of compound 3cu-o

APS-01-210

Sample Name	**APS-01-210**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-04-03**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-210/PROTON_04

Plot date 2017-04-07

Fig S166. 1H NMR (DMSO-d6, 500 MHz) of compound 3cu-p

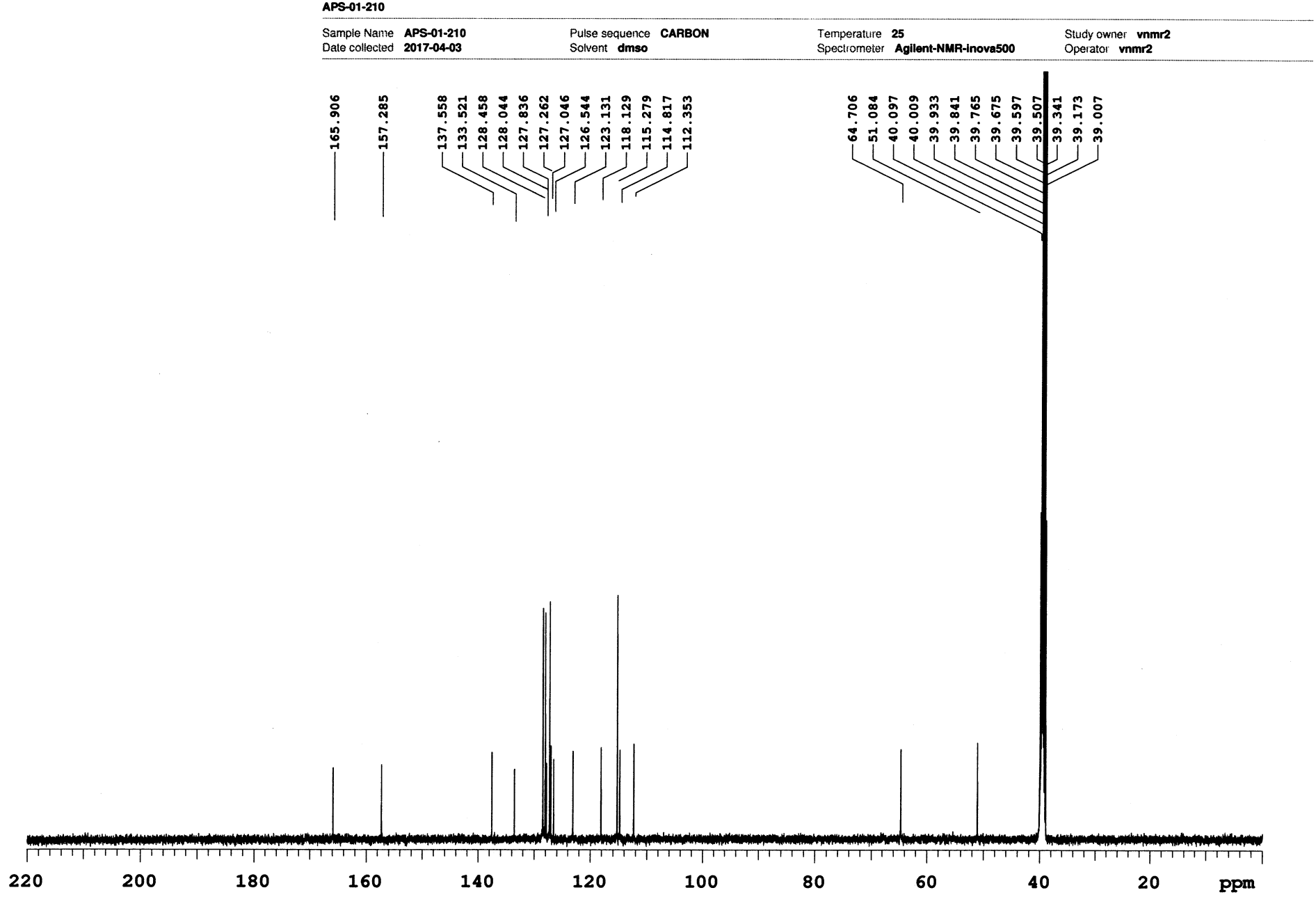


Fig S167. 13C NMR (DMSO-d6, 125 MHz) of compound 3cu-p

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-210/CARBON_02

Plot date 2017-04-07

APS-01-210

Sample Name **APS-01-210**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-03**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

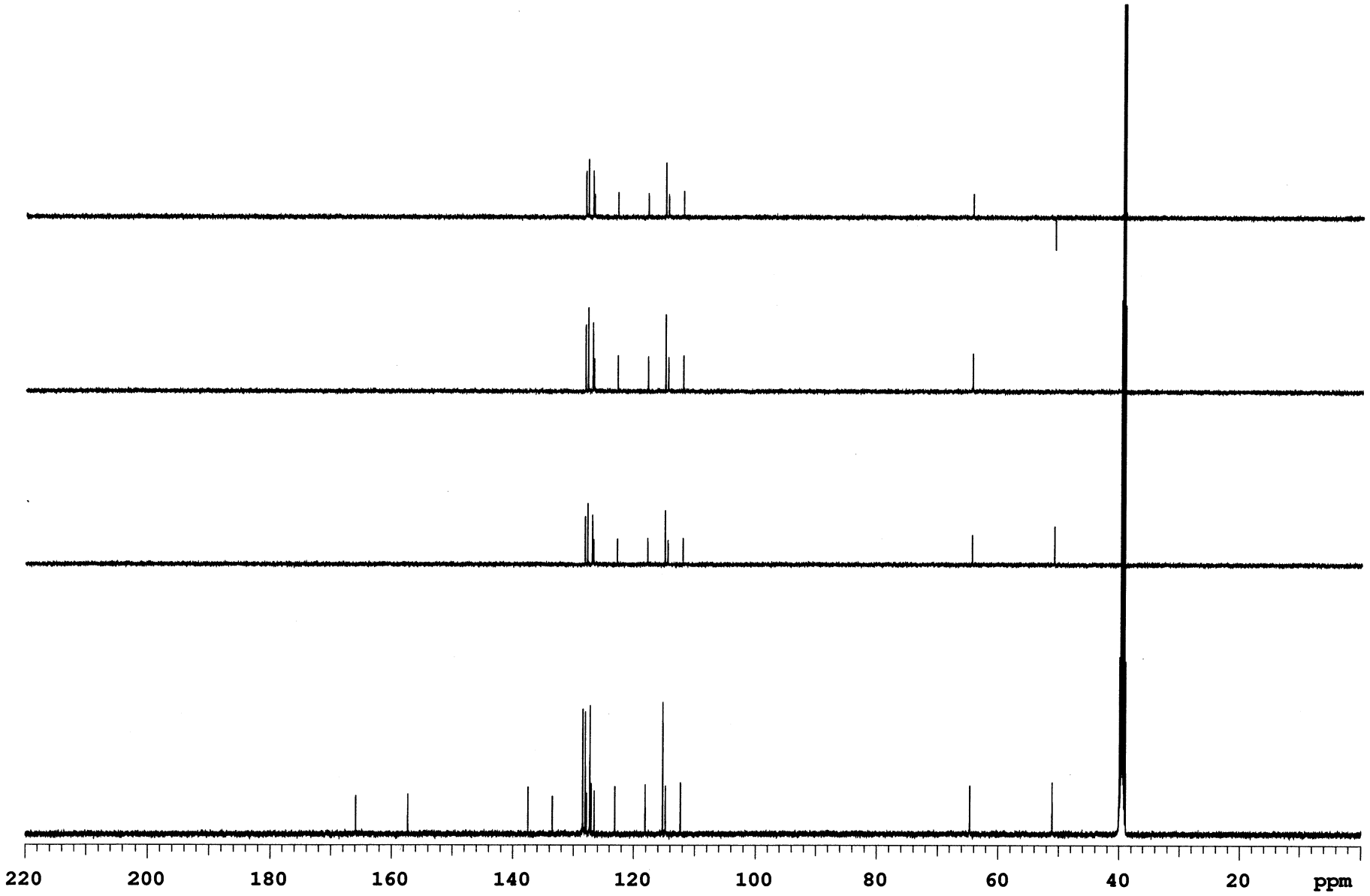


Fig S168. DEPT of compound 3cu-p

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-210/DEPT_01

Plot date 2017-04-07

APS-01-210

Sample Name	**APS-01-210**	Pulse sequence	**gHSQC**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-04-03**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

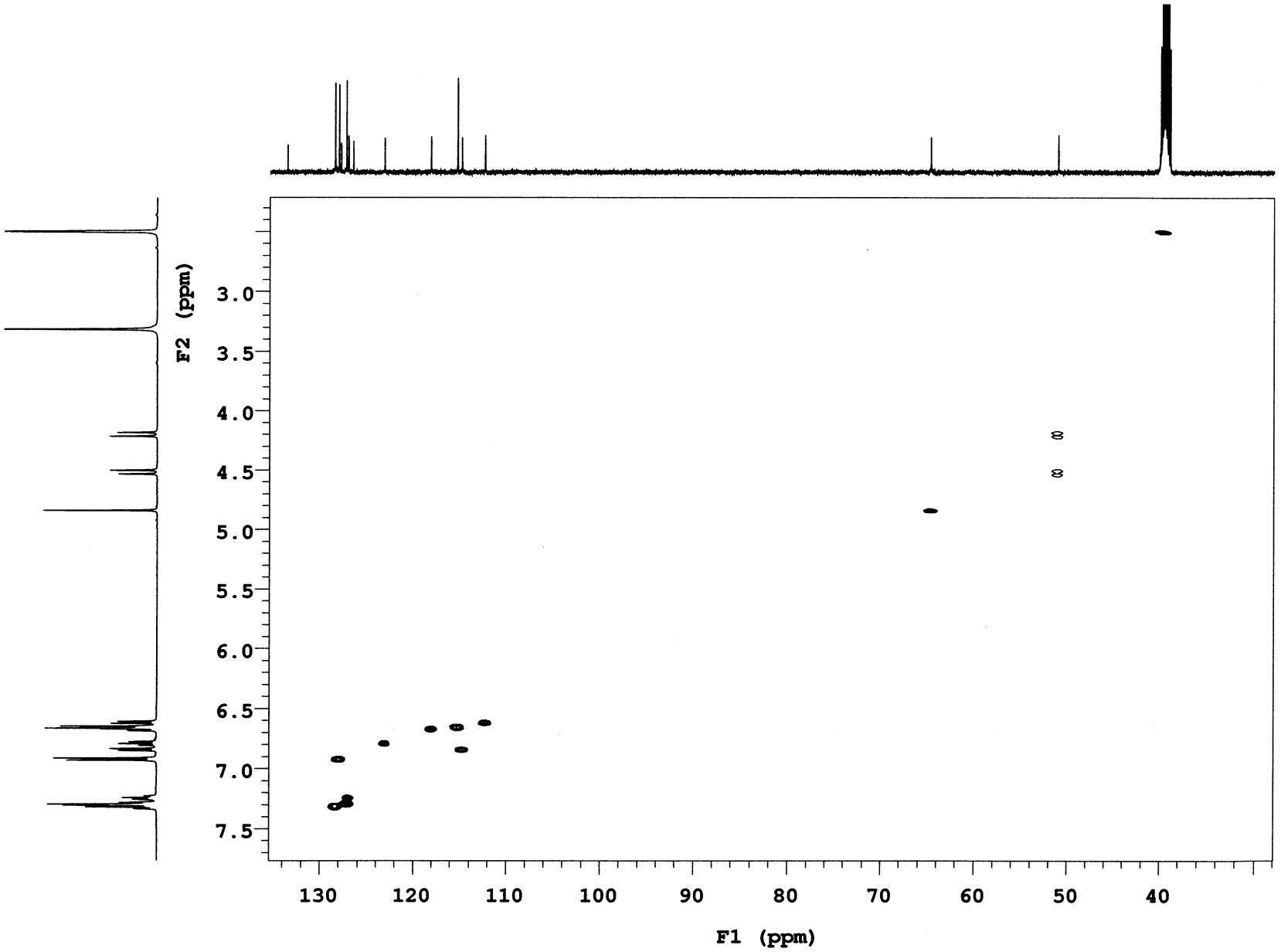


Fig S169. HSQC of compound 3cu-p

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-210/gHSQC_01

Plot date 2017-04-07

APS-01-210

Sample Name	**APS-01-210**	Pulse sequence	**gCOSY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-04-03**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

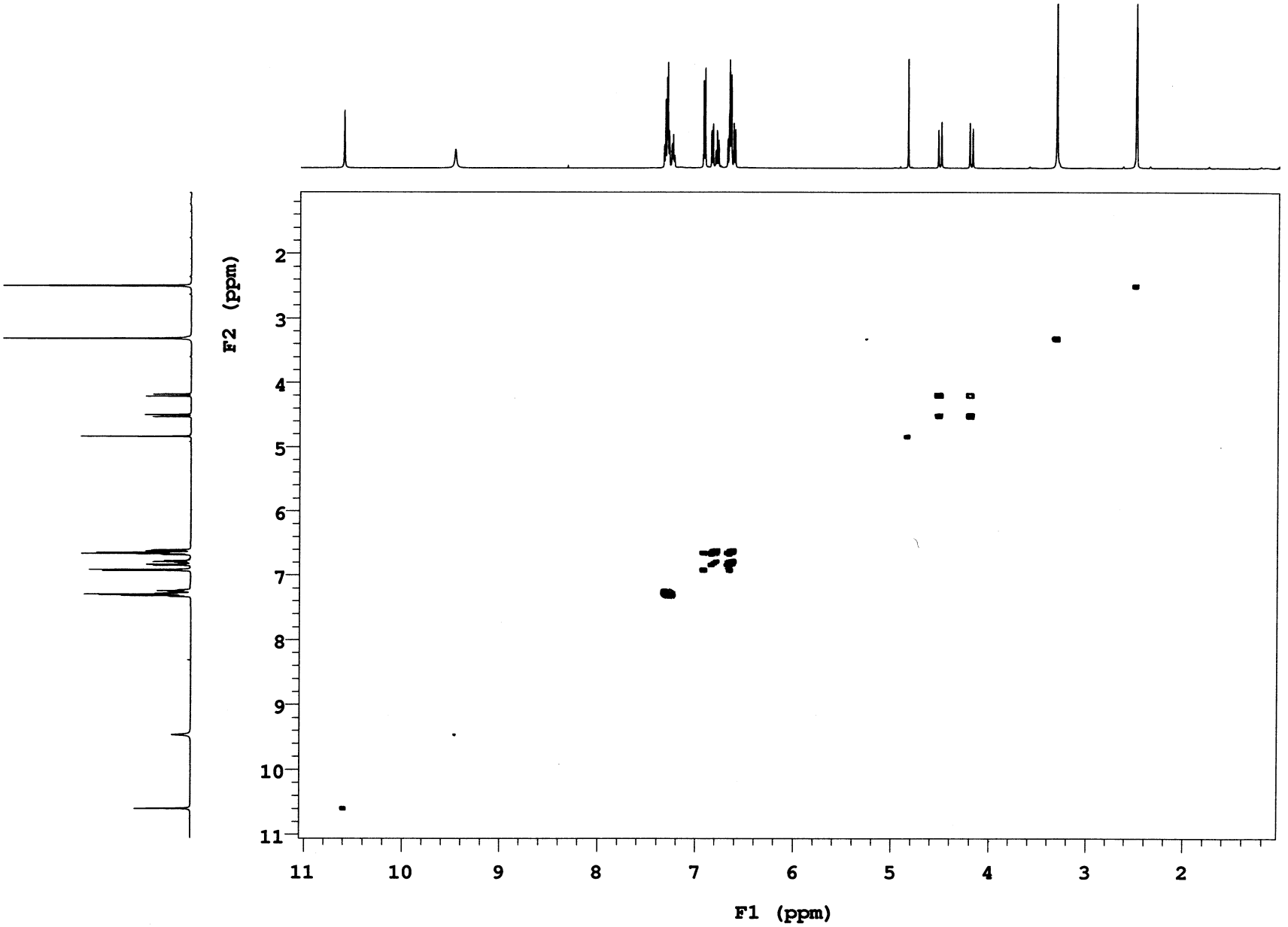


Fig S170. COSY of compound 3cu-p

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-210/gCOSY_01

Plot date 2017-04-07

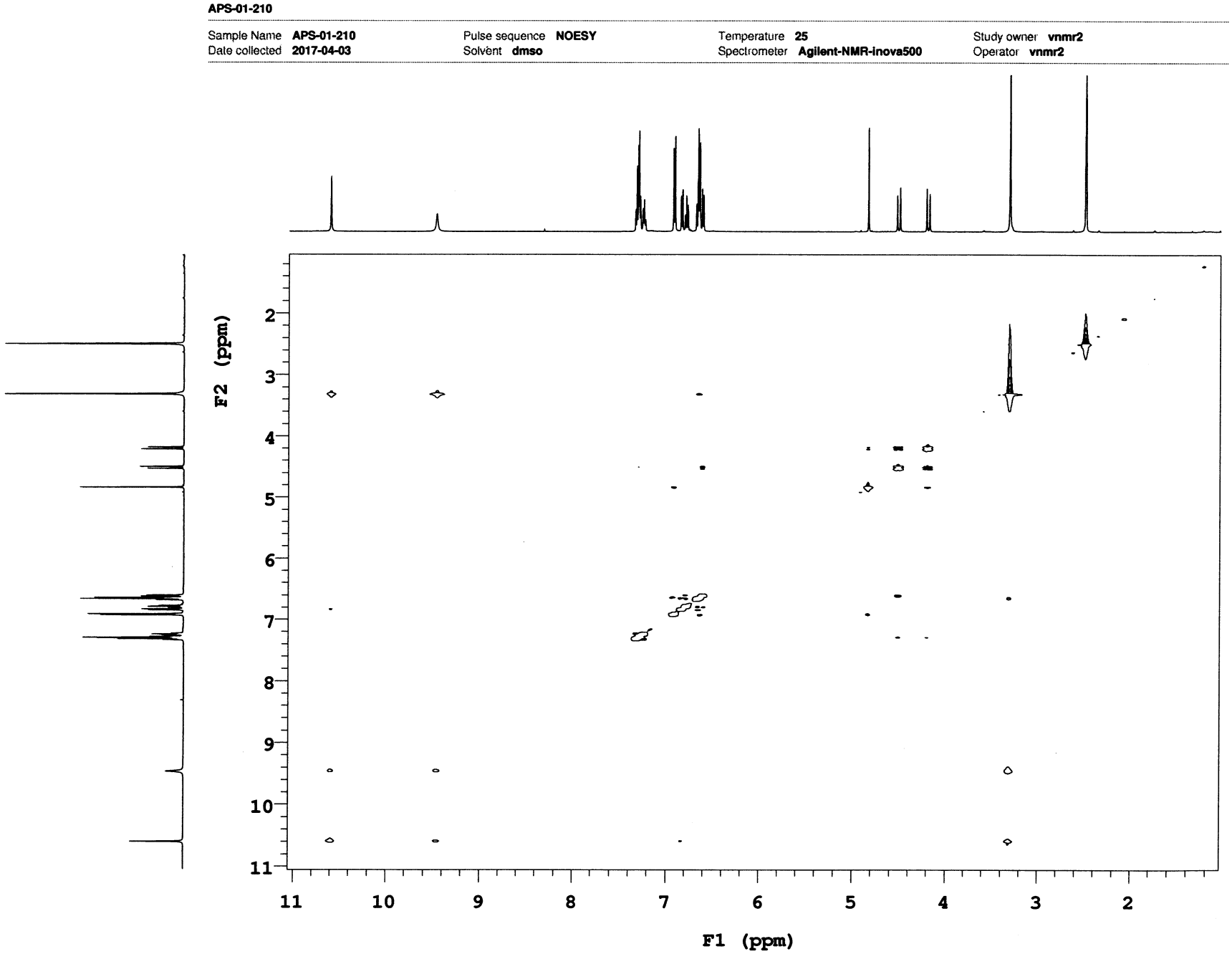


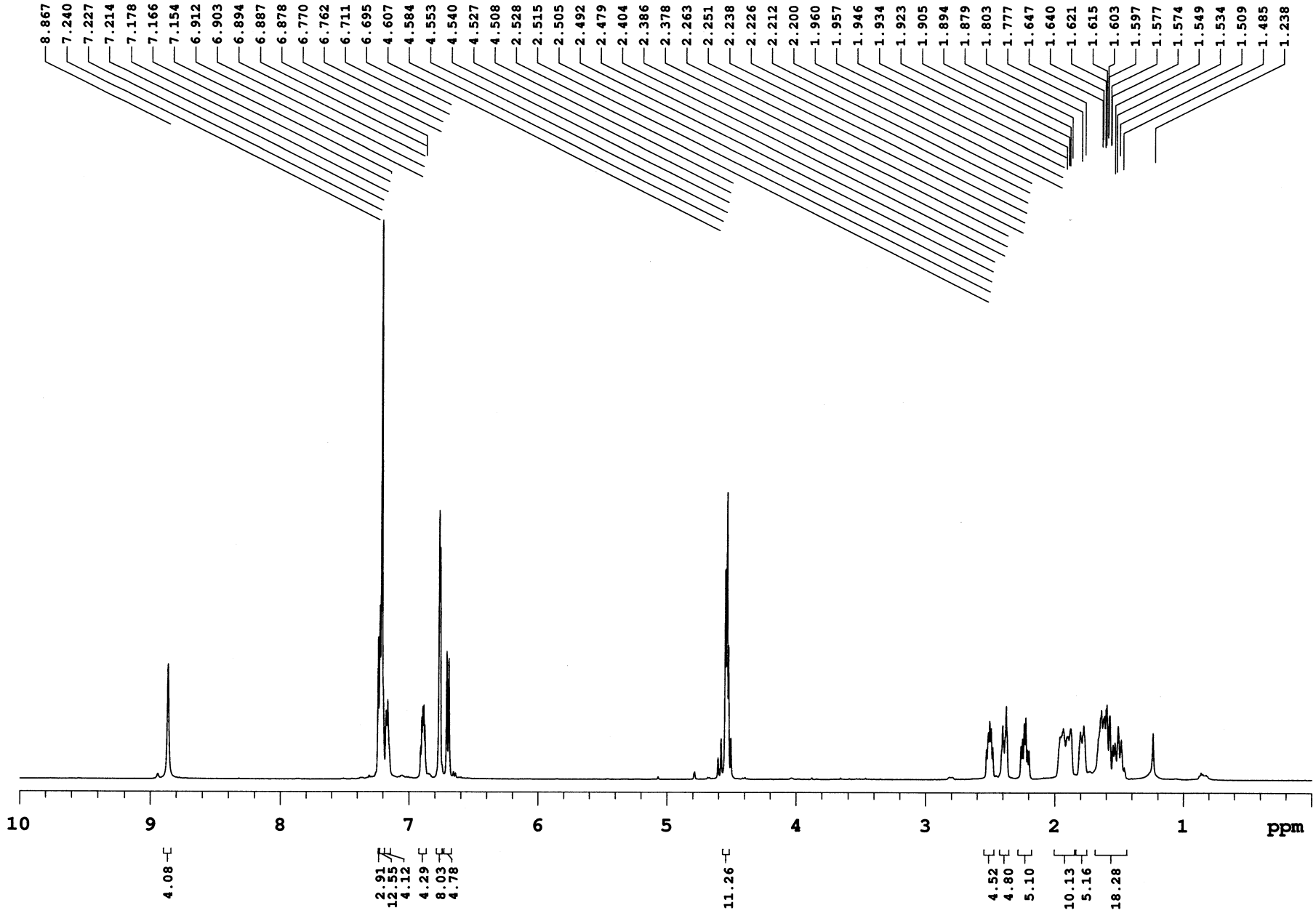
Fig S171. NOESY of compound 3cu-p

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-210/NOESY_01

Plot date 2017-04-07

APS-01-292-NP

Sample Name	**APS-01-292-NP**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-24**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-292-NP/PROTON_01

Fig S172. 1H NMR (CDCl3, 500 MHz) of compound 3cv-1

Plot date 2017-03-24

APS-01-202NP

Sample Name	**APS-01-202NP**	Pulse sequence	**CARBON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-14**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

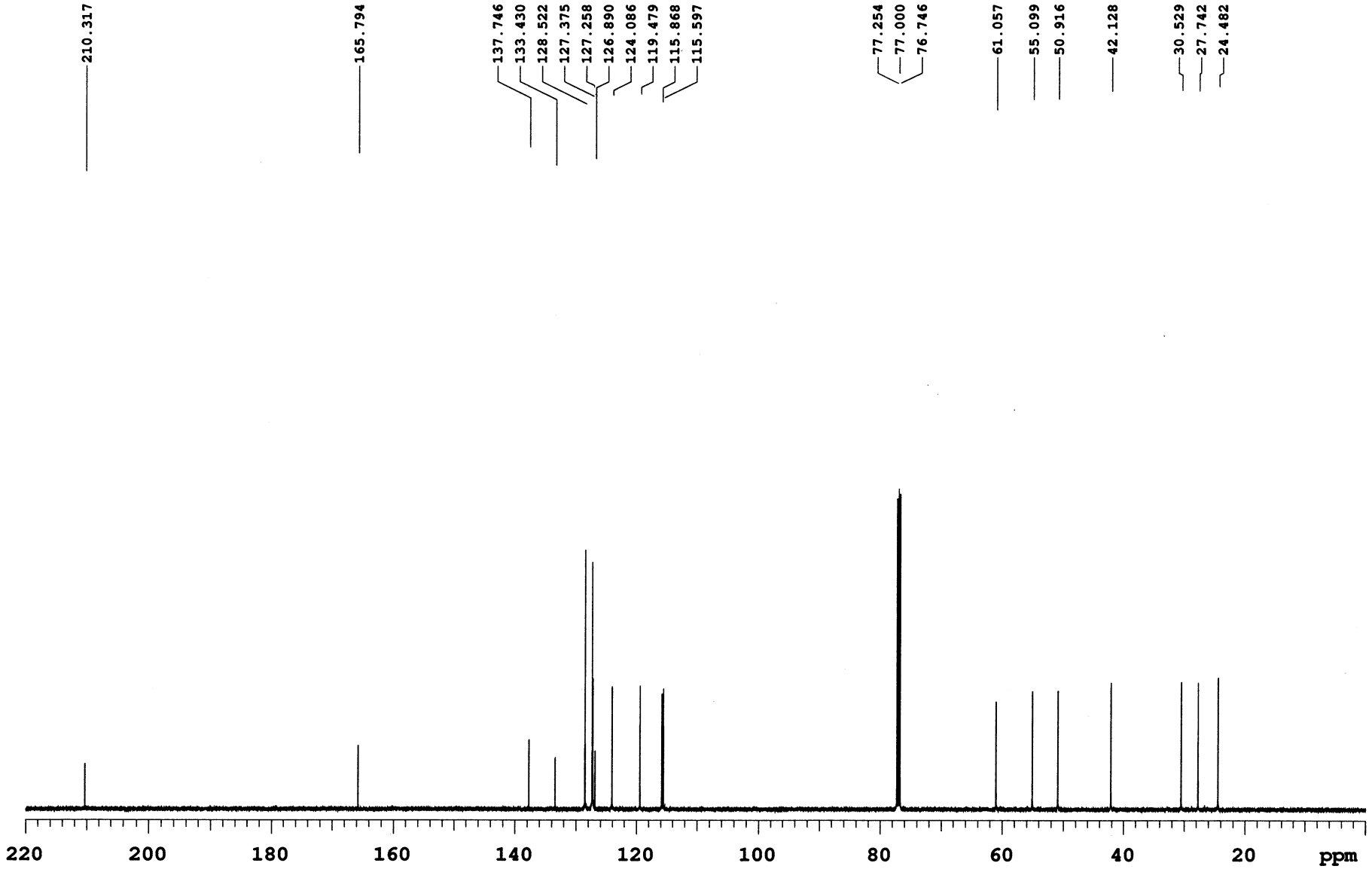


Fig S173. 13C NMR (CDCl3, 125 MHz) of compound 3cv-1

APS-01-202NP

Sample Name	**APS-01-202NP**	Pulse sequence	**DEPT**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-14**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

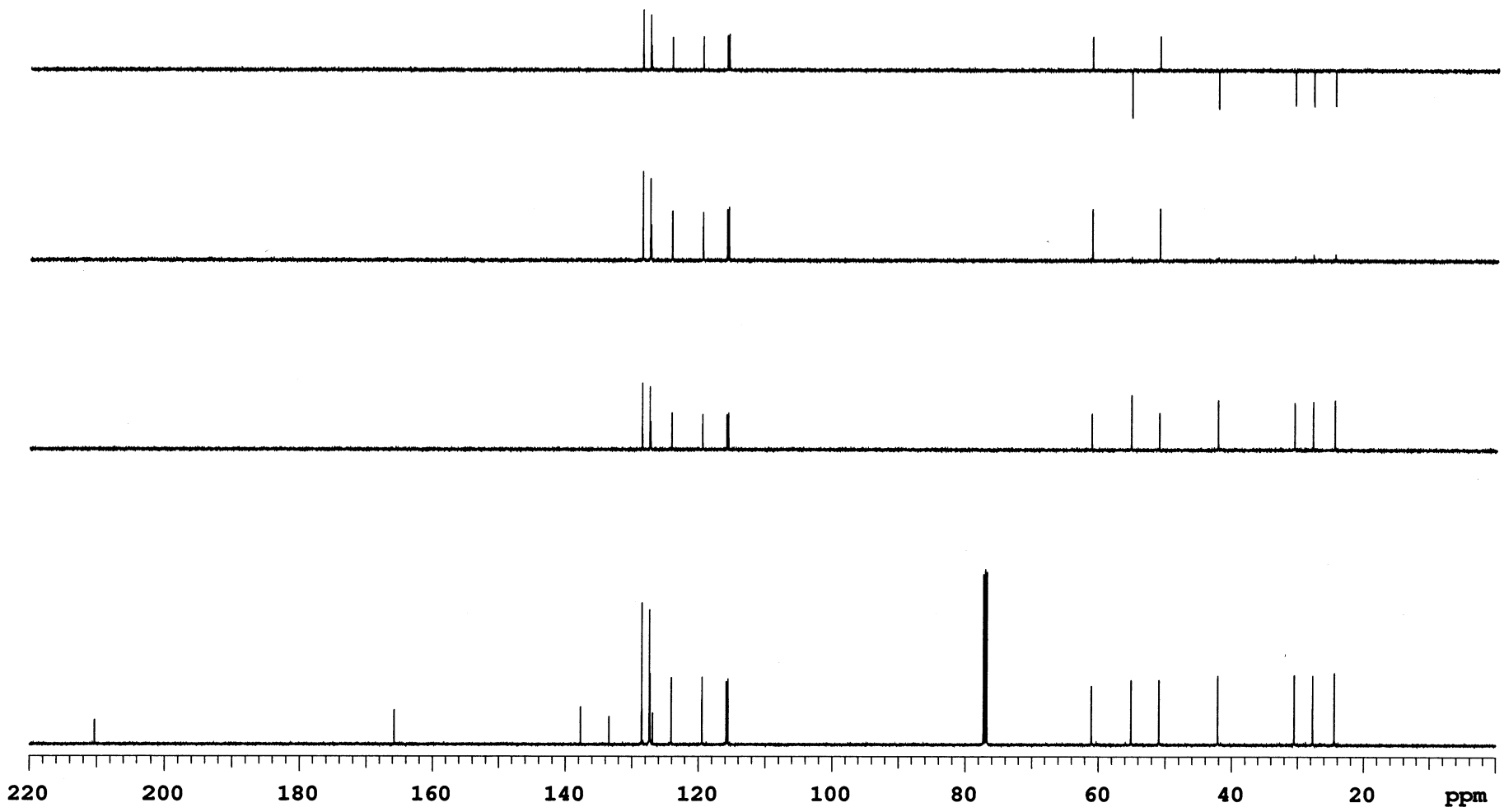


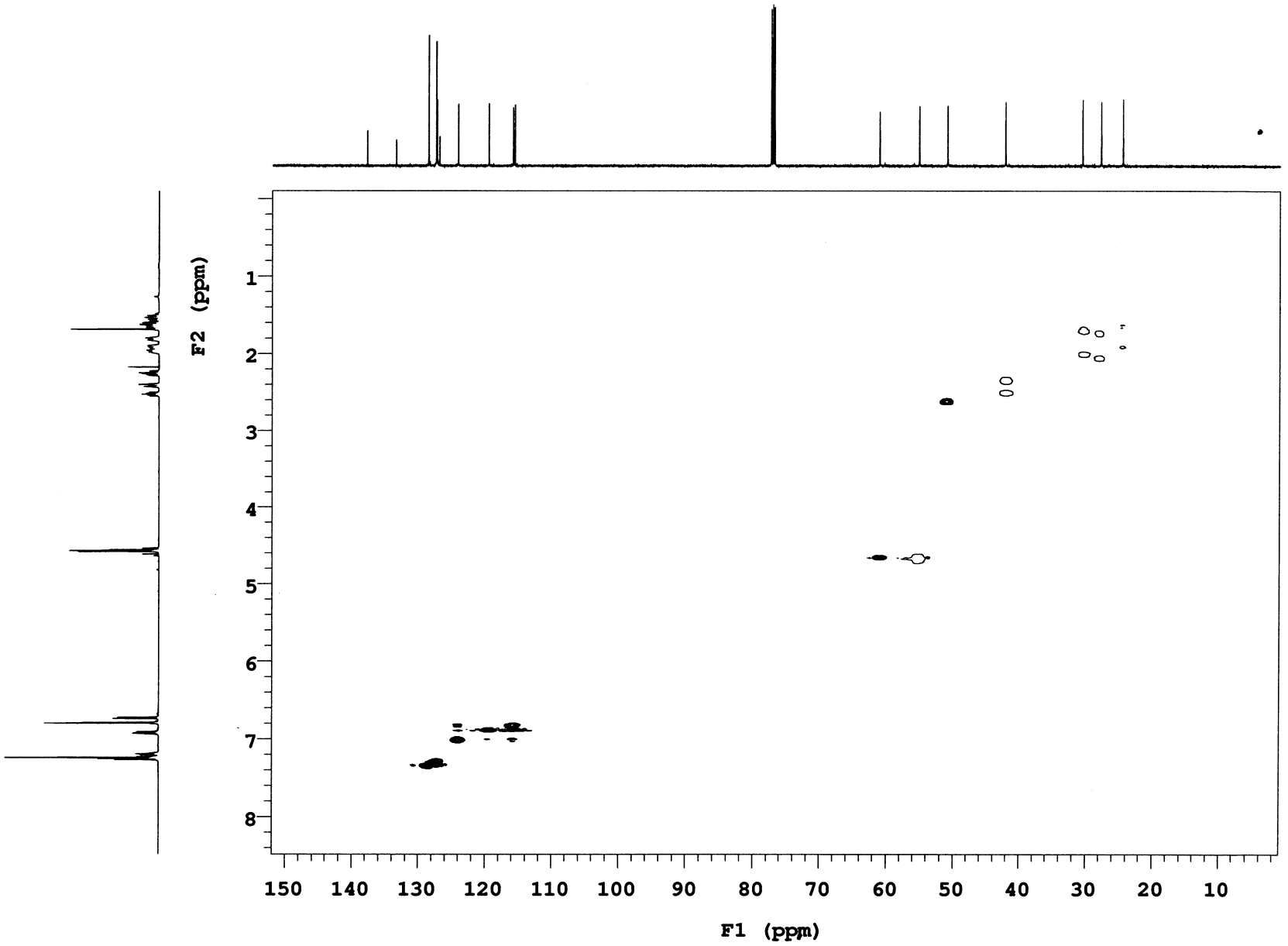
Fig S174. DEPT of compound 3cv-1

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202NP/DEPT_01.fid

Plot date 2017-03-15

APS-01-202NP

Sample Name	**APS-01-202NP**	Pulse sequence	**gHSQC**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-15**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202NP/gHSQC_01

Fig S175. HSQC of compound 3cv-1

Plot date 2017-03-17

APS-01-202NP

Sample Name	**APS-01-202NP**	Pulse sequence	**gCOSY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-15**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

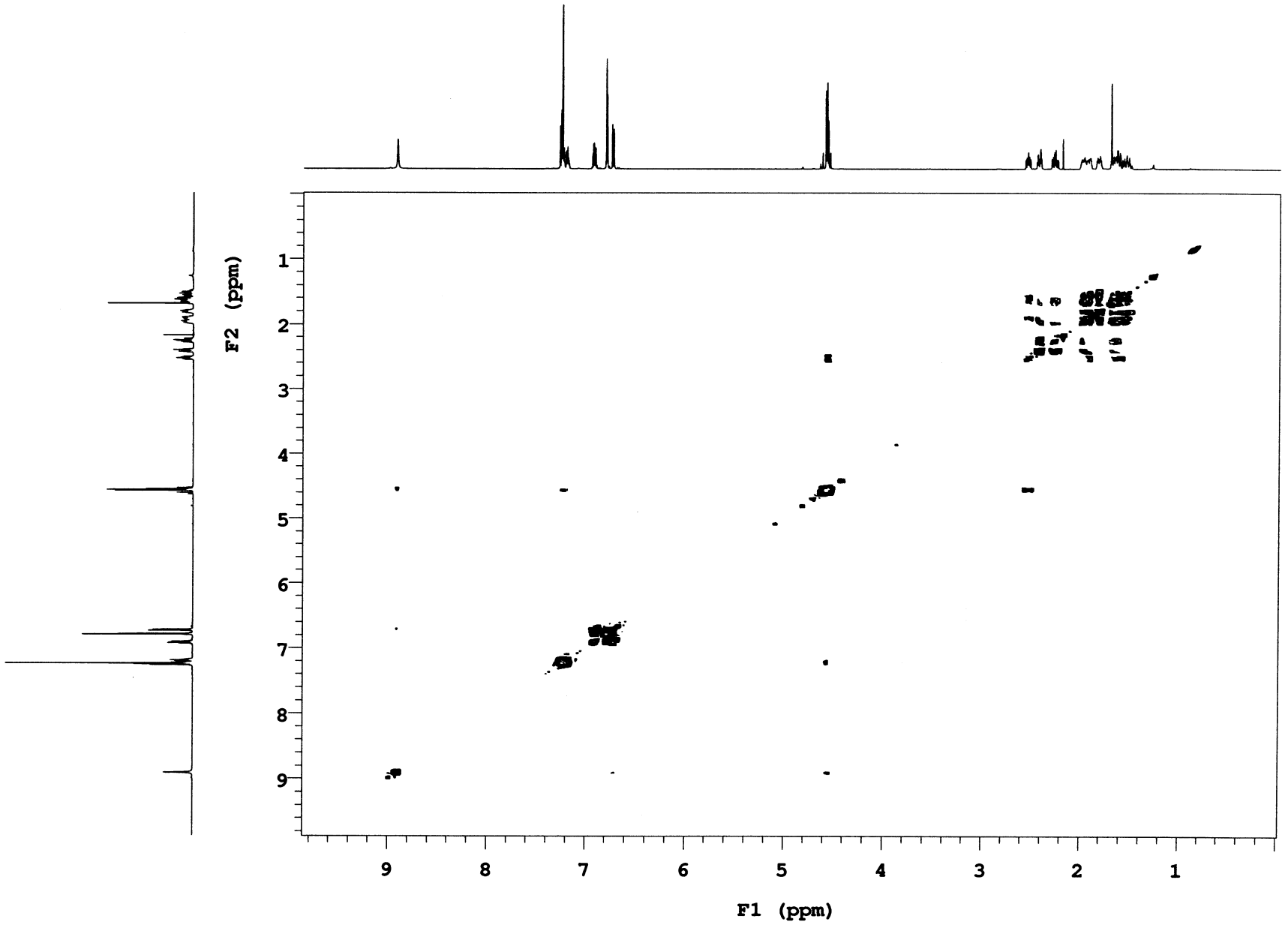


Fig S176. COSY of compound 3cv-1

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202NP/gCOSY_01

Plot date 2017-03-17

APS-01-202NP

Sample Name	**APS-01-202NP**	Pulse sequence	**NOESY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-15**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

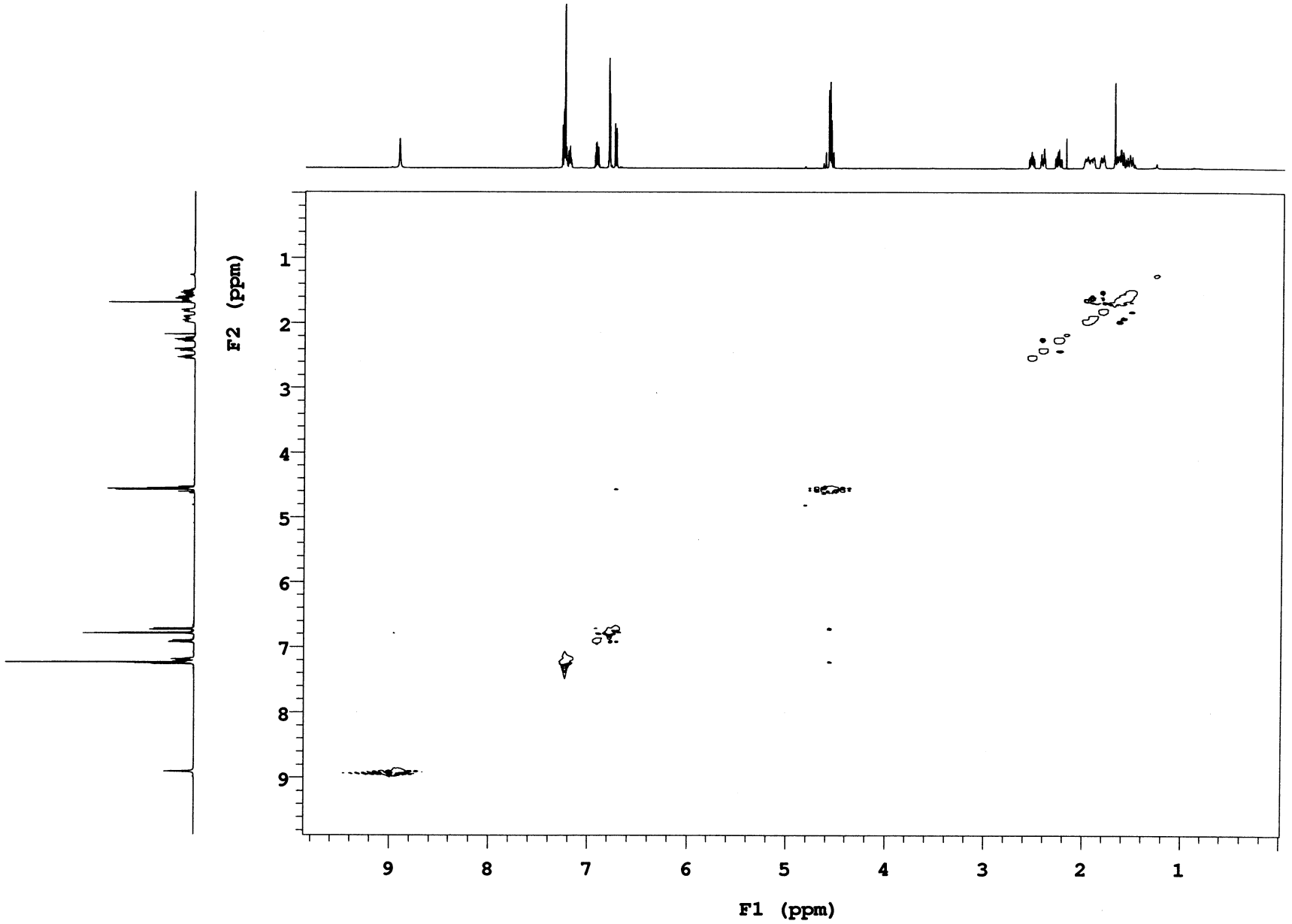


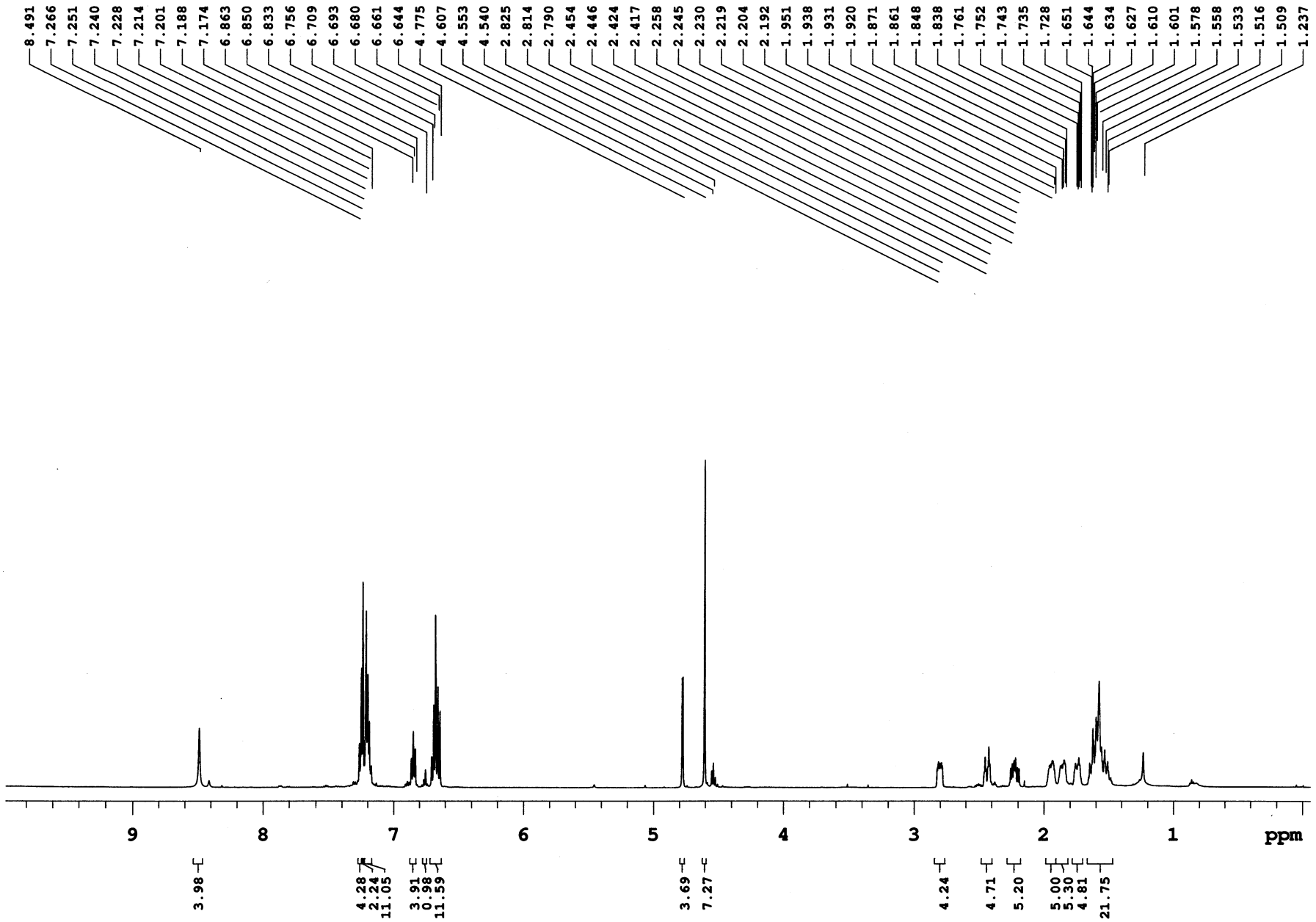
Fig S177. NOESY of compound 3cv-1

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202NP/NOESY_01

Plot date 2017-03-17

APS-01-202-P

Sample Name	**APS-01-202-P**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-22**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202-P/PROTON_06

Fig S178. 1H NMR (CDCl3, 500 MHz) of compound 3cv-2

Plot date 2017-03-24

APS-01-202-P

Sample Name **APS-01-202-P**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-22**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

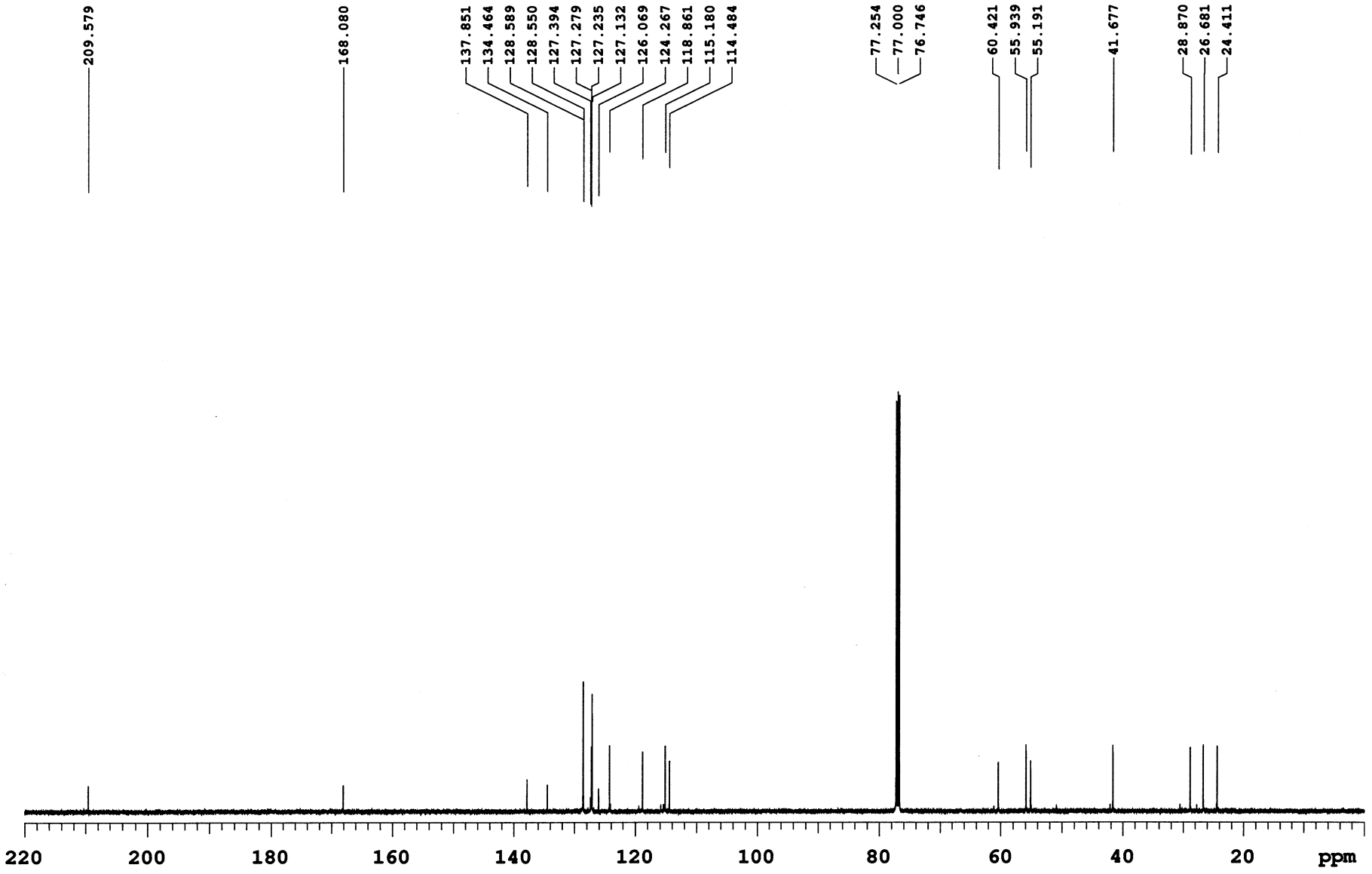


Fig S179. 13C NMR (CDCl3, 125 MHz) of compound 3cv-2

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202-P/CARBON_02

Plot date 2017-03-24

APS-01-202-P

Sample Name **APS-01-202-P**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-23**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

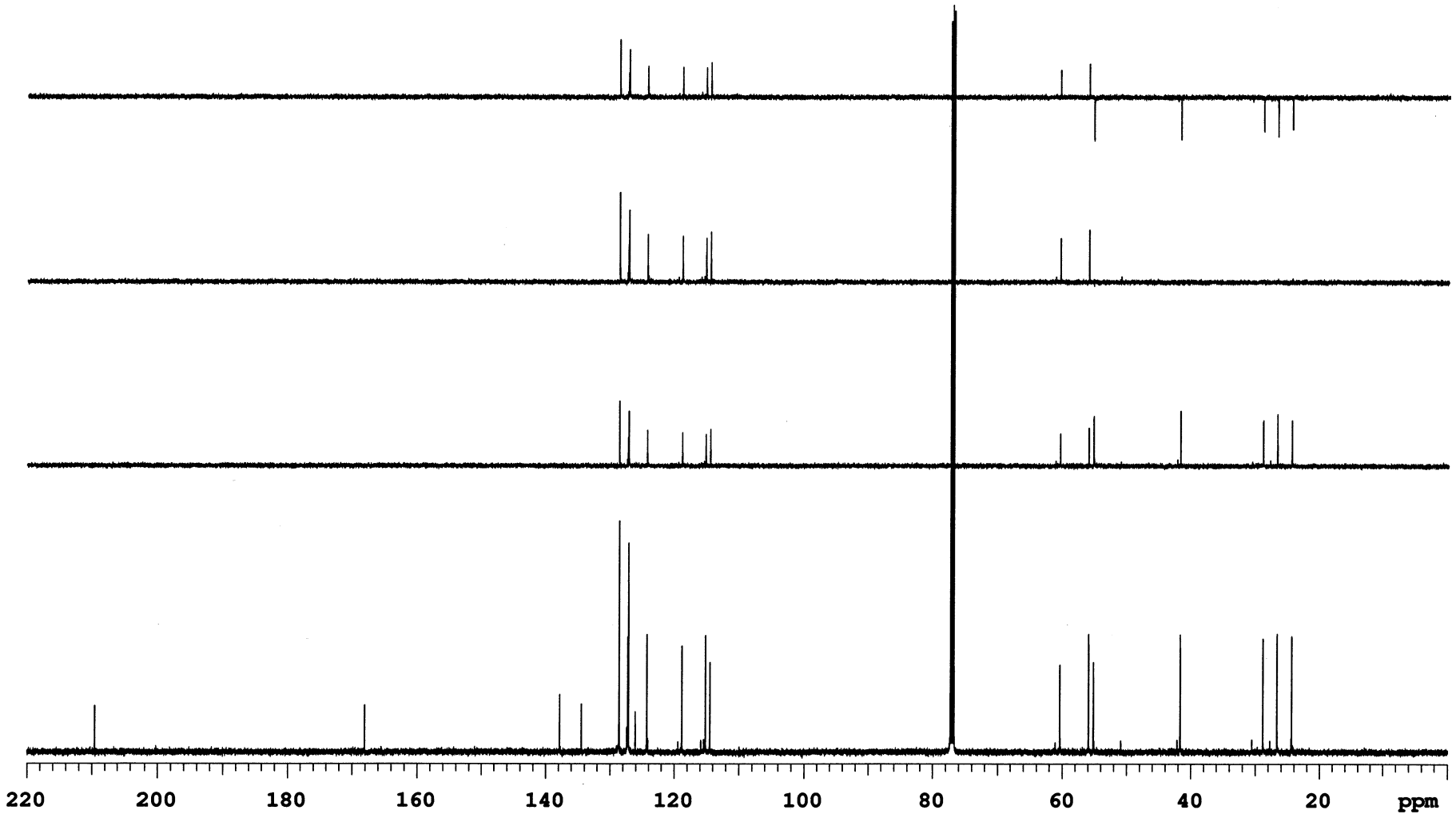


Fig S180. DEPT of compound 3cv-2

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202-P/DEPT_01.fid

Plot date 2017-03-24

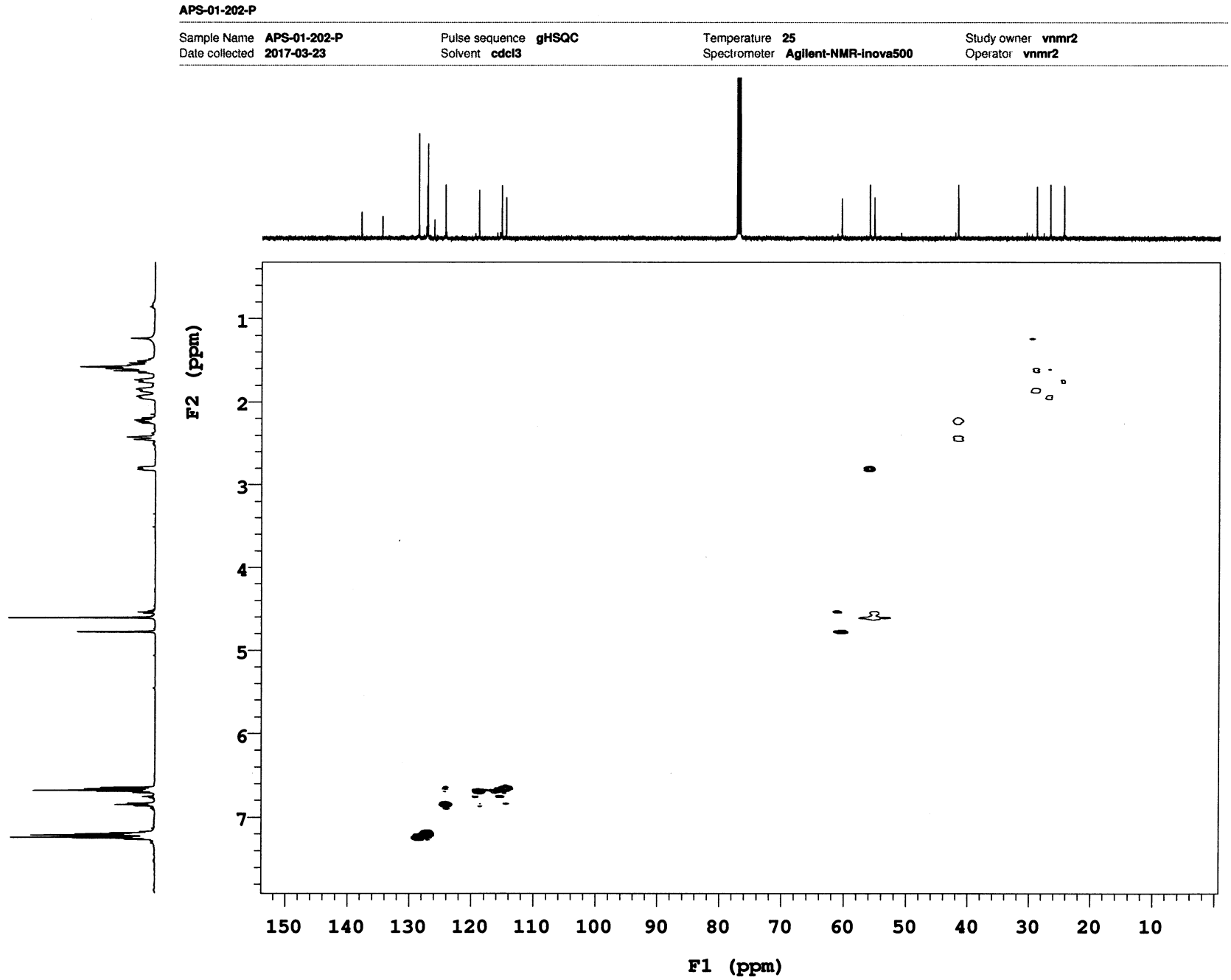


Fig S181. HSQC of compound 3cv-2

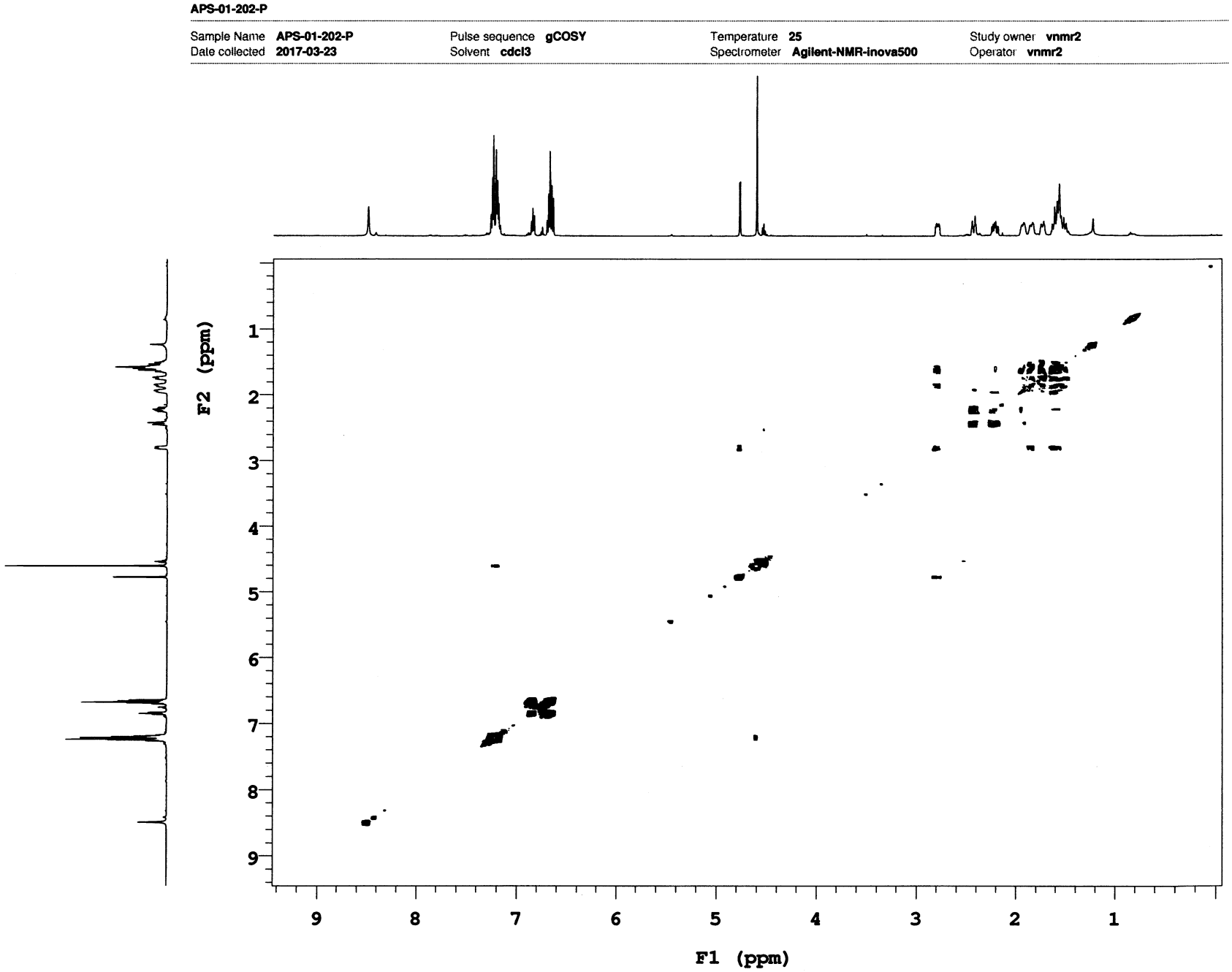


Fig S182. COSY of compound 3cv-2

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202-P/gCOSY_01

Plot date 2017-03-24

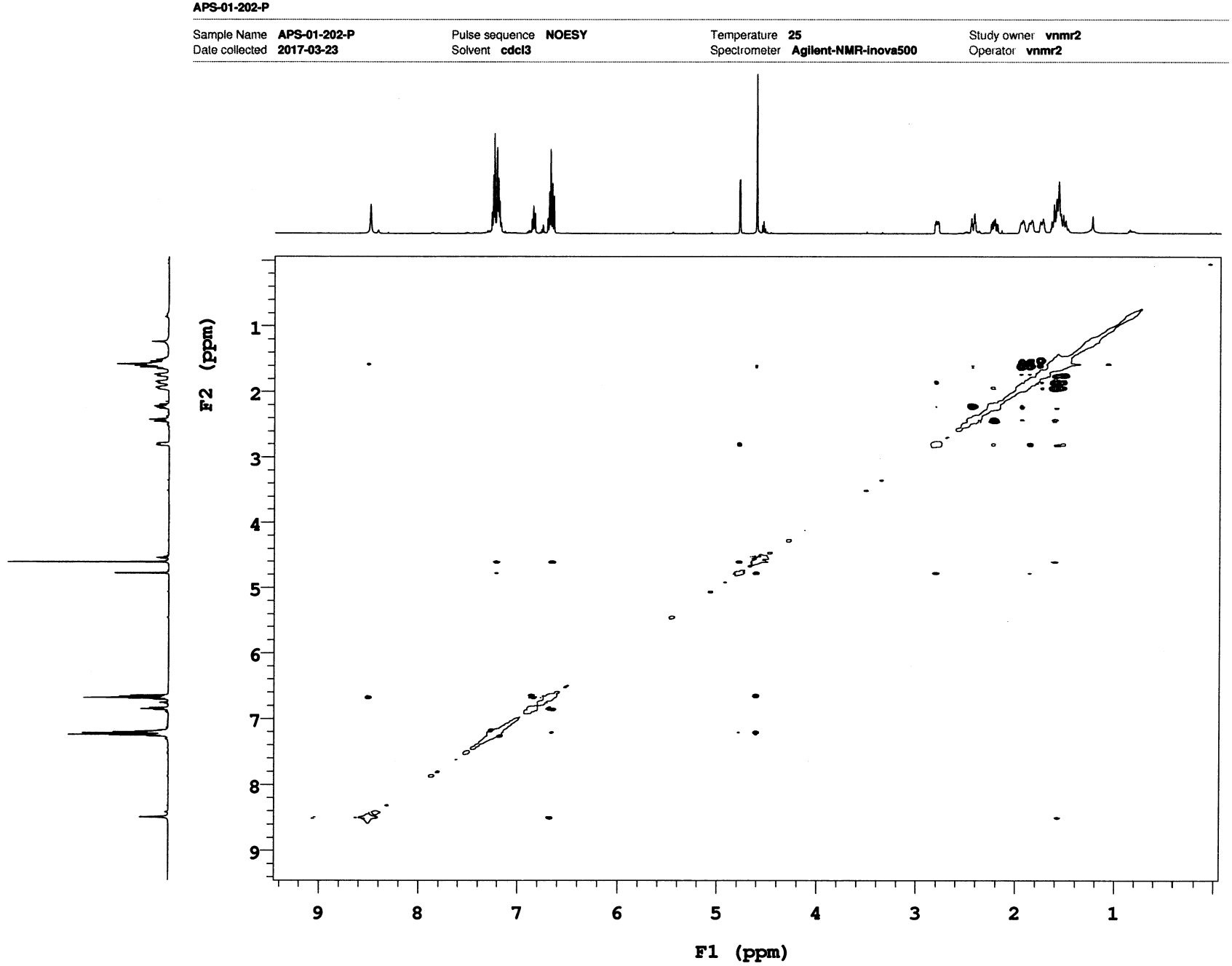
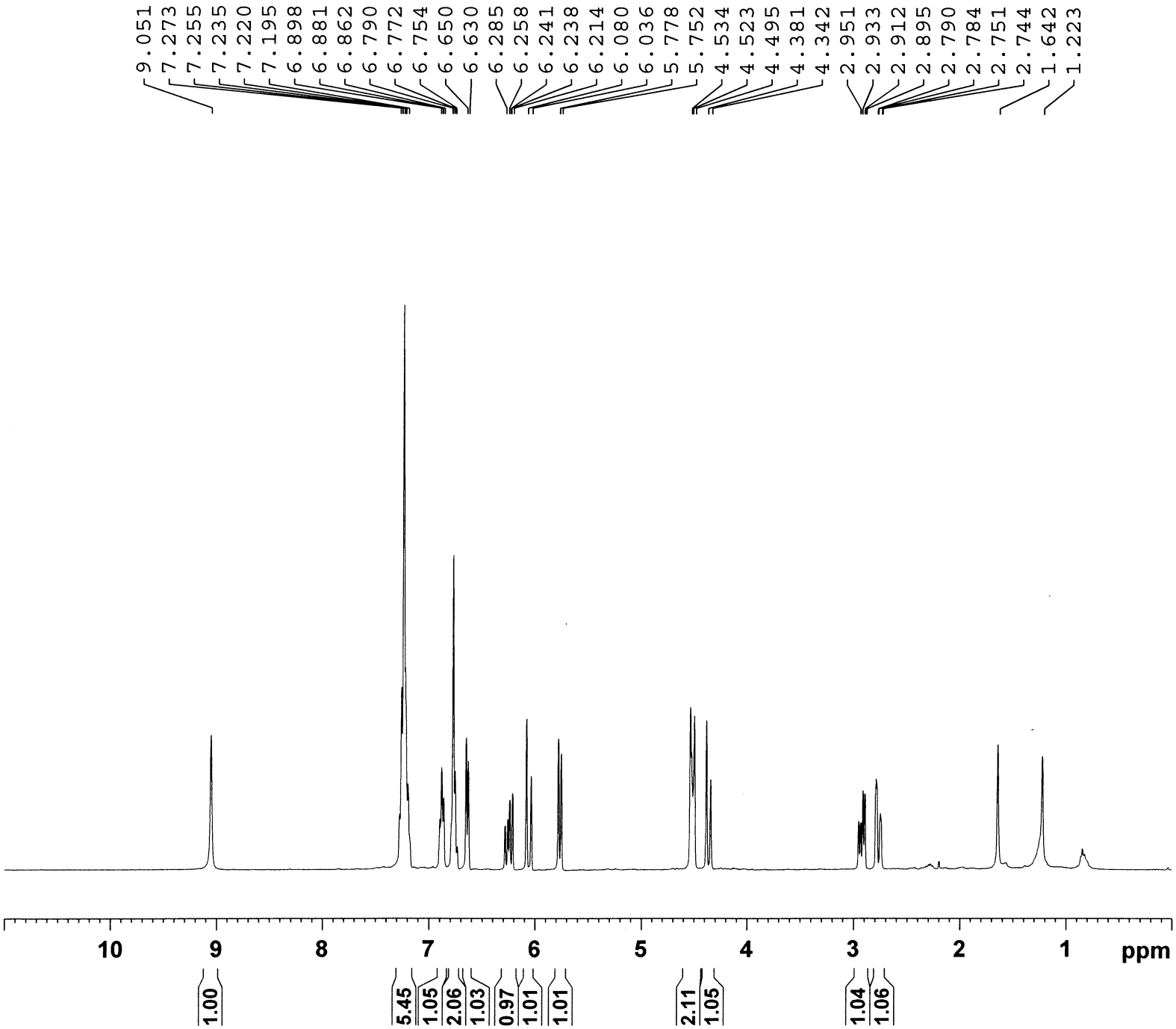


Fig S183. NOESY of compound 3cv-2

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-202-P/NOESY_01

Plot date 2017-03-24

Fig S184. 1H NMR (CDCl3, 400 MHz) of compound 3cw

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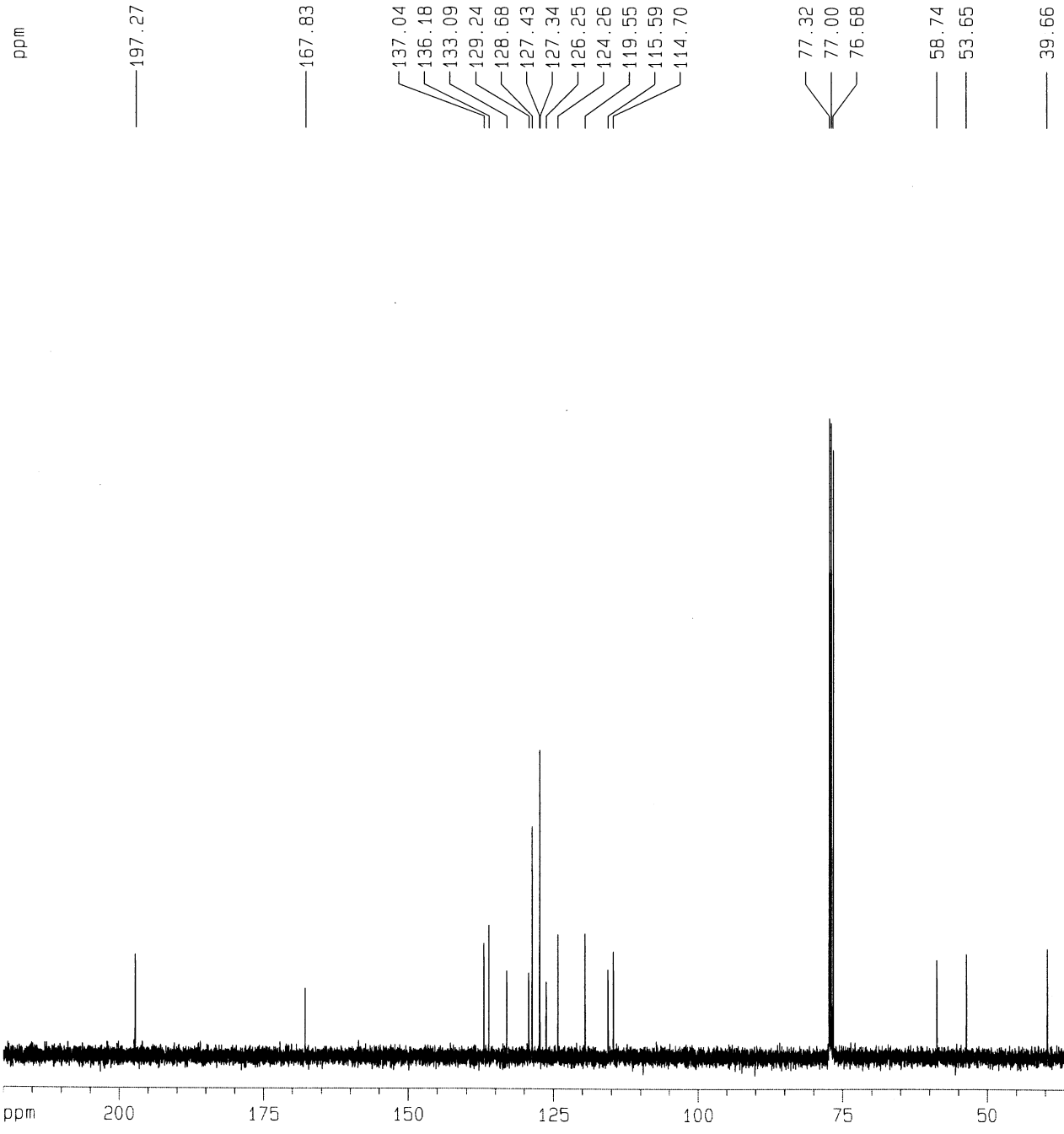
Current Data Parameters
NAME          APS-01-201
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170313
Time              18.54 h
INSTRUM             spect
PROBHD   Z108618_0922 (
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             2.0447233 sec
RG                210.28
DW                62.400 usec
DE                16.43 usec
TE                299.3 K
D1             2.00000000 sec
TD0                    1
SFO1         400.1324008 MHz
NUC1                  1H
P1                14.50 usec
PLW1         12.50000000 W

F2 - Processing parameters
SI                 16384
SF           400.1300241 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

Fig S185. 13C NMR (CDCl3, 100 MHz) of compound 3cw

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Current Data Parameters
NAME          APS-01-201
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170315
Time               16.16
INSTRUM            spect
PROBHD     5 mm QNP  1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  376
DS                    4
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ             1.3042164 sec
RG                  256
DW               19.900 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

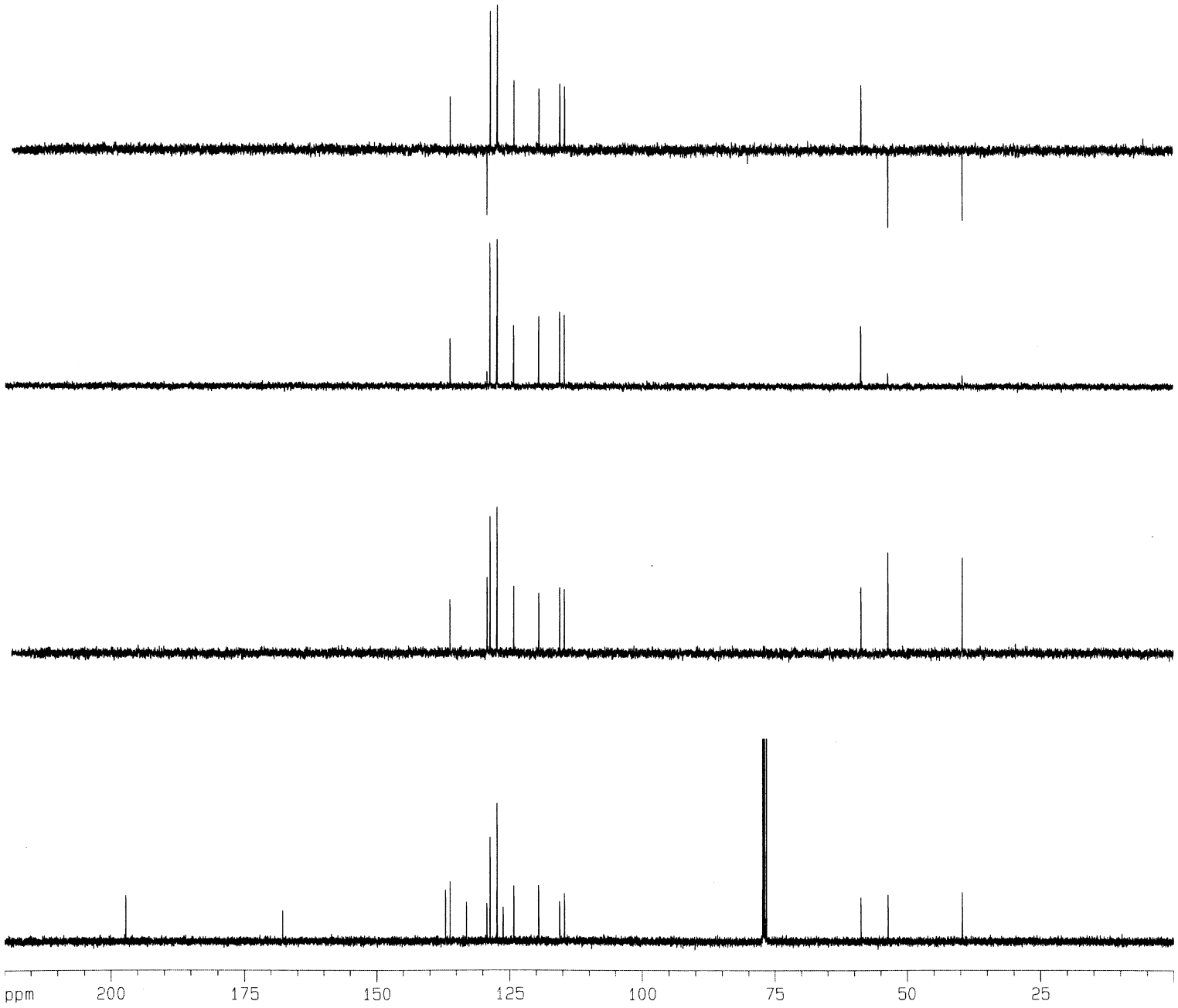
============ CHANNEL f1 =============
NUC1                13C
P1               10.20 usec
PL1               0.00 dB
SFO1         100.6237959 MHz

============ CHANNEL f2 =============
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2              -3.00 dB
PL12             14.50 dB
PL13             17.50 dB
SFO2         400.1326008 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127723 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.40

1D NMR plot parameters
CX               20.00 cm
F1P             220.000 ppm
F1            22134.81 Hz
F2P             0.000 ppm
F2              0.00 Hz
PPMCM         11.00000 ppm/cm
HZCM          1106.74048 Hz/cm
```

Fig S186. DEPT of compound 3cw




```
Current Data Parameters
NAME          APS-01-201
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170315
Time               16.16
INSTRUM            spect
PROBHD     5 mm QNP  1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  376
DS                    4
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ             1.3042164 sec
RG                  256
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

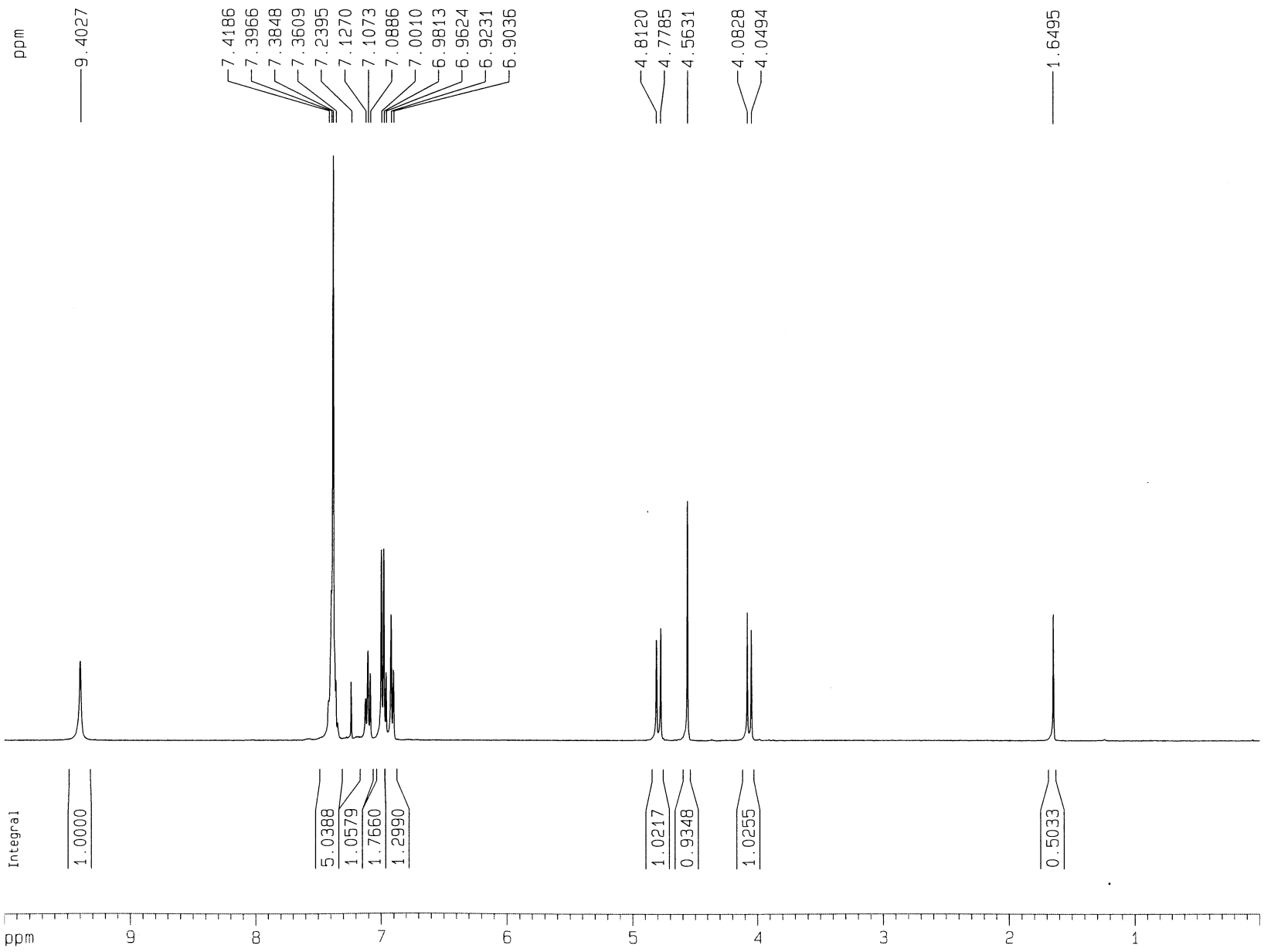
============ CHANNEL f1 =============
NUC1                13C
P1                10.20 usec
PL1                0.00 dB
SFO1         100.6237959 MHz

============ CHANNEL f2 =============
CPDPRG2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -3.00 dB
PL12              14.50 dB
PL13              17.50 dB
SFO2         400.1326008 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127723 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                20.00 cm
F1P              220.000 ppm
F1             22134.81 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM          11.00000 ppm/cm
HZCM         1106.74048 Hz/cm
```

Fig S187. 1H NMR (CDCl3, 400 MHz) of compound 3cx



Current Data Parameters
NAME APS-01-205
EXPNO 1
PROCNO 1

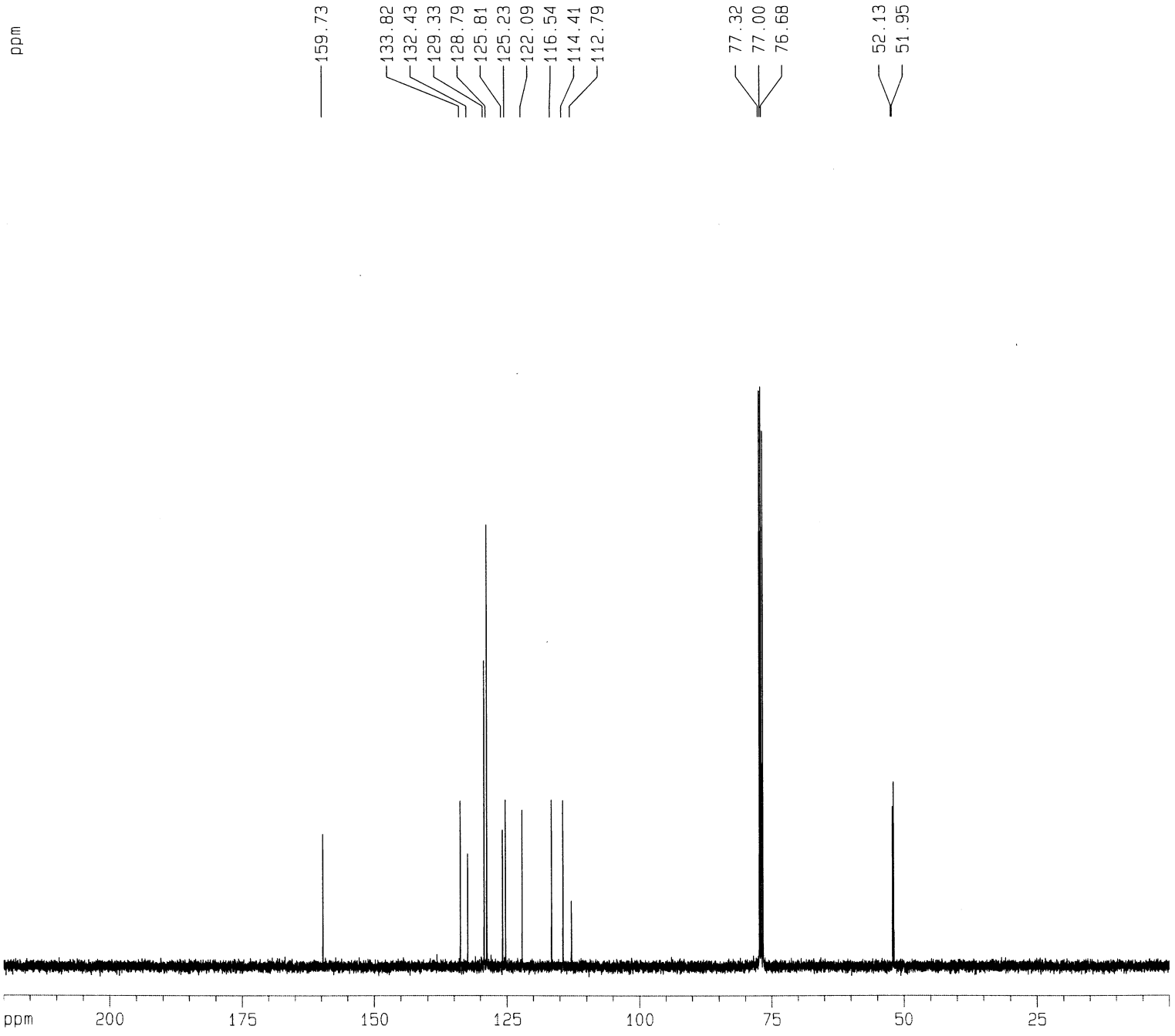
F2 - Acquisition Parameters
Date_ 20170318
Time 13.35
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 6502
DW 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec

========== CHANNEL f1 ==========
NUC1 1H
P1 14.30 usec
PL1 -0.30 dB
SFO1 400.1326008 MHz

F2 - Processing parameters
SI 8192
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 21.50 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.46512 ppm/cm
HZCM 186.10699 Hz/cm

Fig S188. 13C NMR (CDCl3, 100 MHz) of compound 3cx




```
Current Data Parameters
NAME          APS-01-205
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20170318
Time              14.34
INSTRUM           spect
PROBHD     5 mm QNP  1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ             1.3042164 sec
RG                  256
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
d12          0.00002000 sec

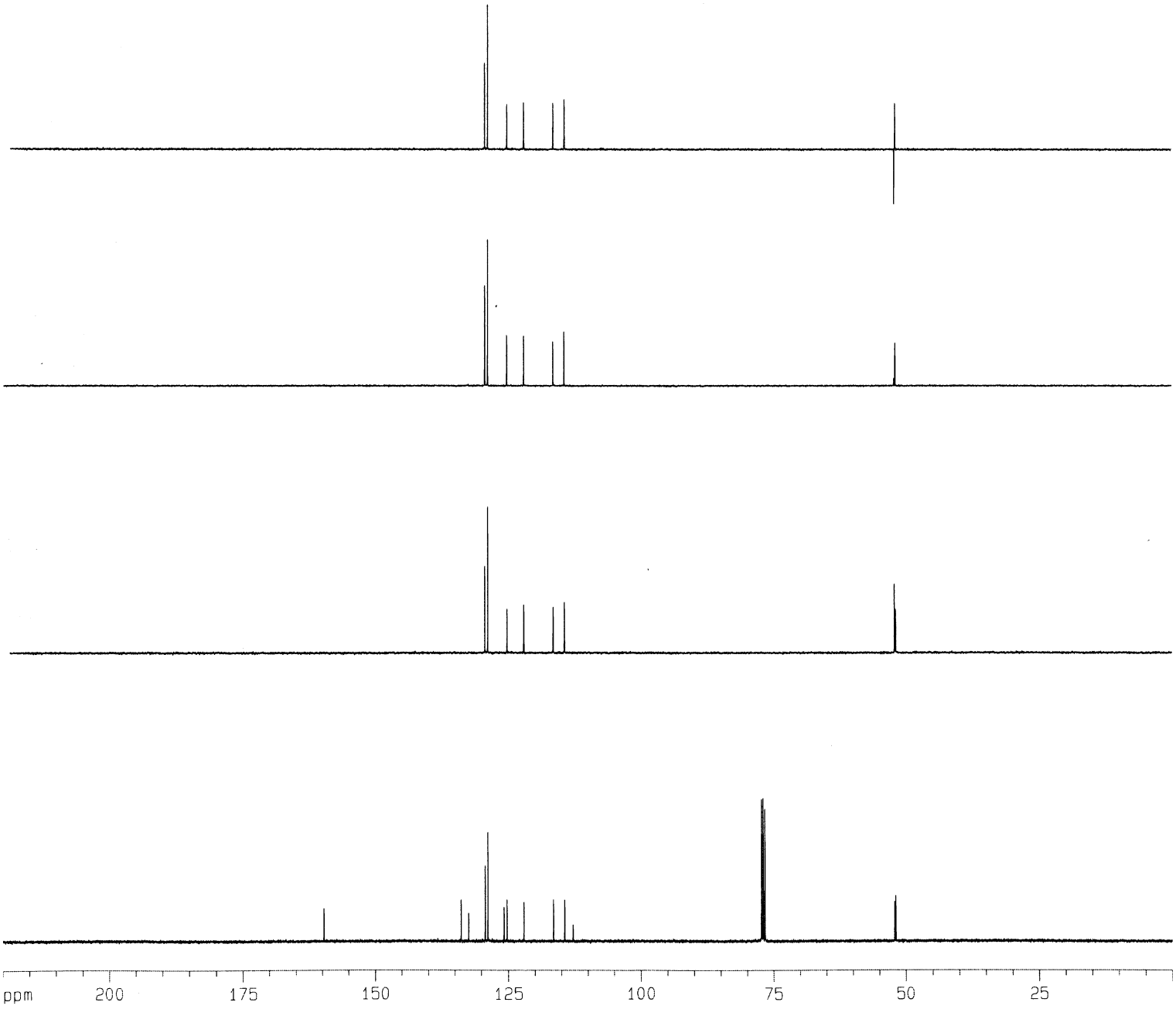
============ CHANNEL f1 =============
NUC1                13C
P1                10.20 usec
PL1                0.00 dB
SFO1         100.6237959 MHz

============ CHANNEL f2 =============
CPDPRG2         waltz16
NUC2                1H
PCPD2           90.00 usec
PL2             -3.00 dB
PL12            14.50 dB
PL13            17.50 dB
SFO2         400.1326008 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127723 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                20.00 cm
F1P              220.000 ppm
F1             22134.81 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM         11.00000 ppm/cm
HZCM        1106.74048 Hz/cm
```

Fig S189. DEPT of compound 3cx




```
Current Data Parameters
NAME          APS-01-205
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170318
Time               14.34
INSTRUM            spect
PROBHD     5 mm QNP  1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           25125.629 Hz
FIDRES         0.383387 Hz
AQ             1.3042164 sec
RG                  256
DW                19.900 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

============ CHANNEL f1 =============
NUC1                13C
P1                10.20 usec
PL1                0.00 dB
SFO1         100.6237959 MHz

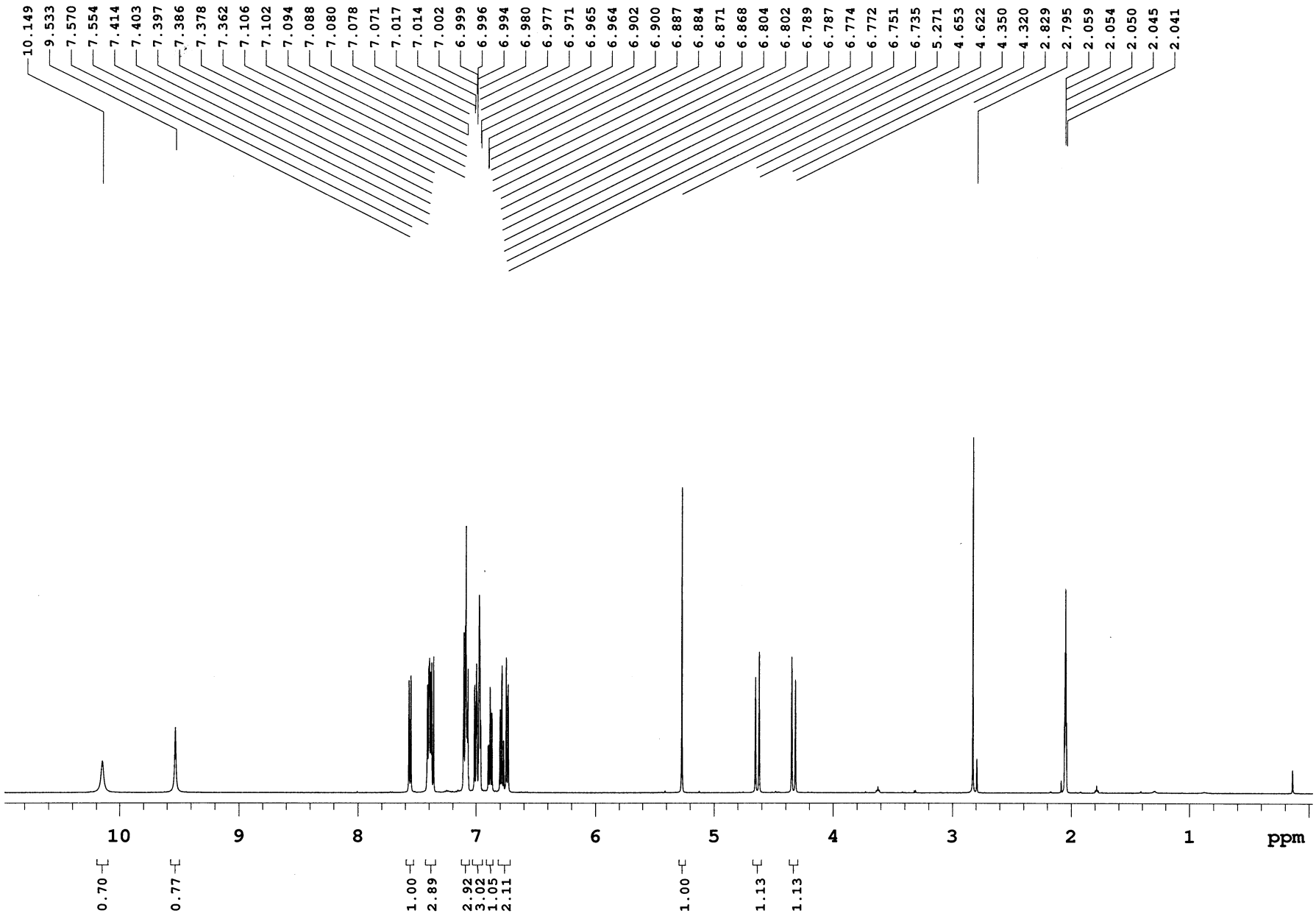
============ CHANNEL f2 =============
CPDPRG2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2               -3.00 dB
PL12              14.50 dB
PL13              17.50 dB
SFO2         400.1326008 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127723 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P               220.000 ppm
F1              22134.81 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          11.00000 ppm/cm
HZCM         1106.74048 Hz/cm
```

APS-01-207

Sample Name **APS-01-207**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-17**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-207/PROTON_03

Plot date 2017-03-22

Fig S190. 1H NMR (acetone-d6, 500 MHz) of compound 3da

APS-01-207

Sample Name **APS-01-207**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-17**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

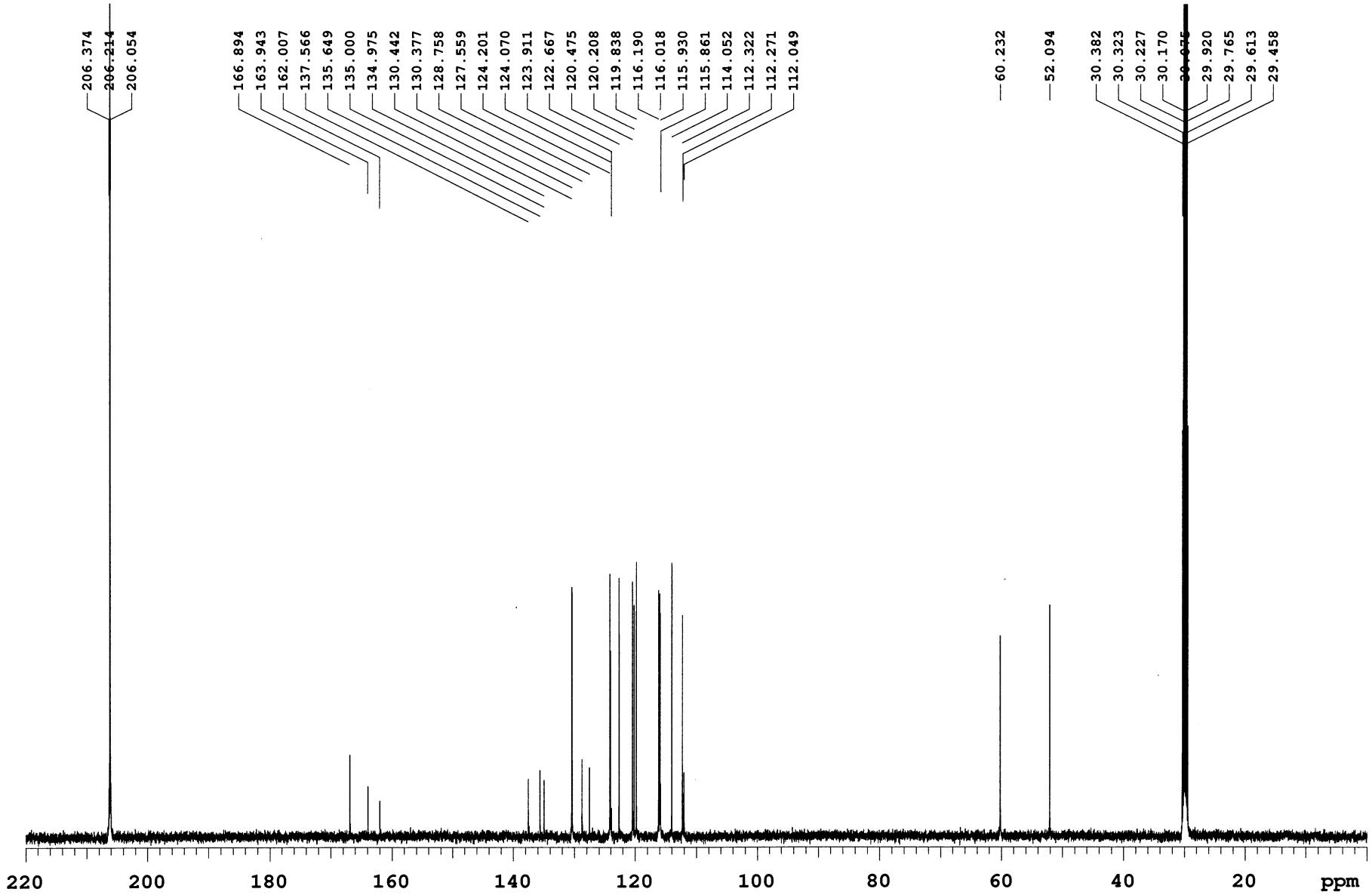


Fig S191. 13C NMR (acetone-d6, 125 MHz) of compound 3da

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-207/CARBON_02

Plot date 2017-03-22

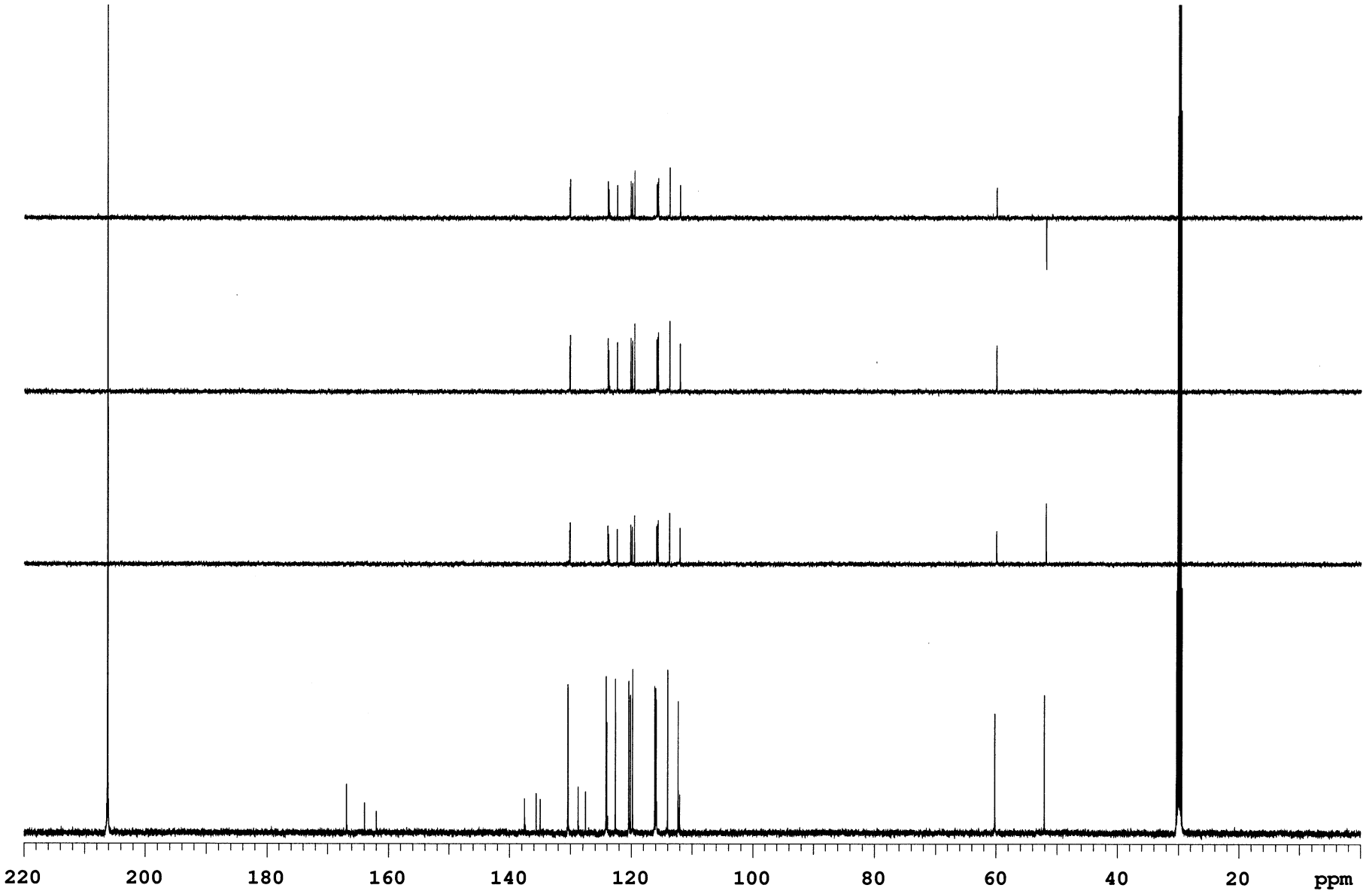
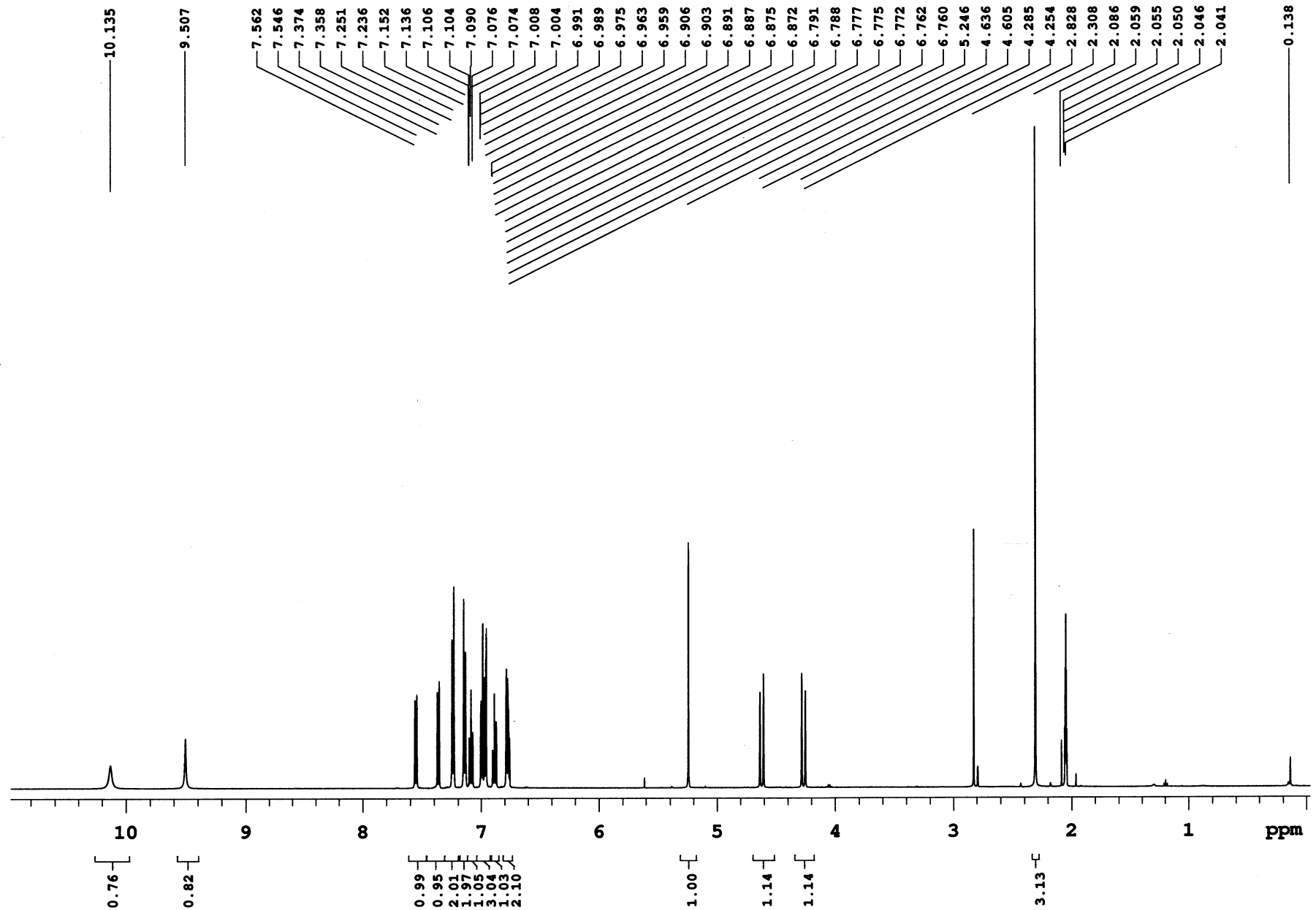


Fig S192. DEPT of compound 3da

APS-01-192

Sample Name	**APS-01-192**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-01-04**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-192/PROTON_03

Plot date 2017-01-04

Fig S193. 1H NMR (acetone-d6, 500 MHz) of compound 3ea

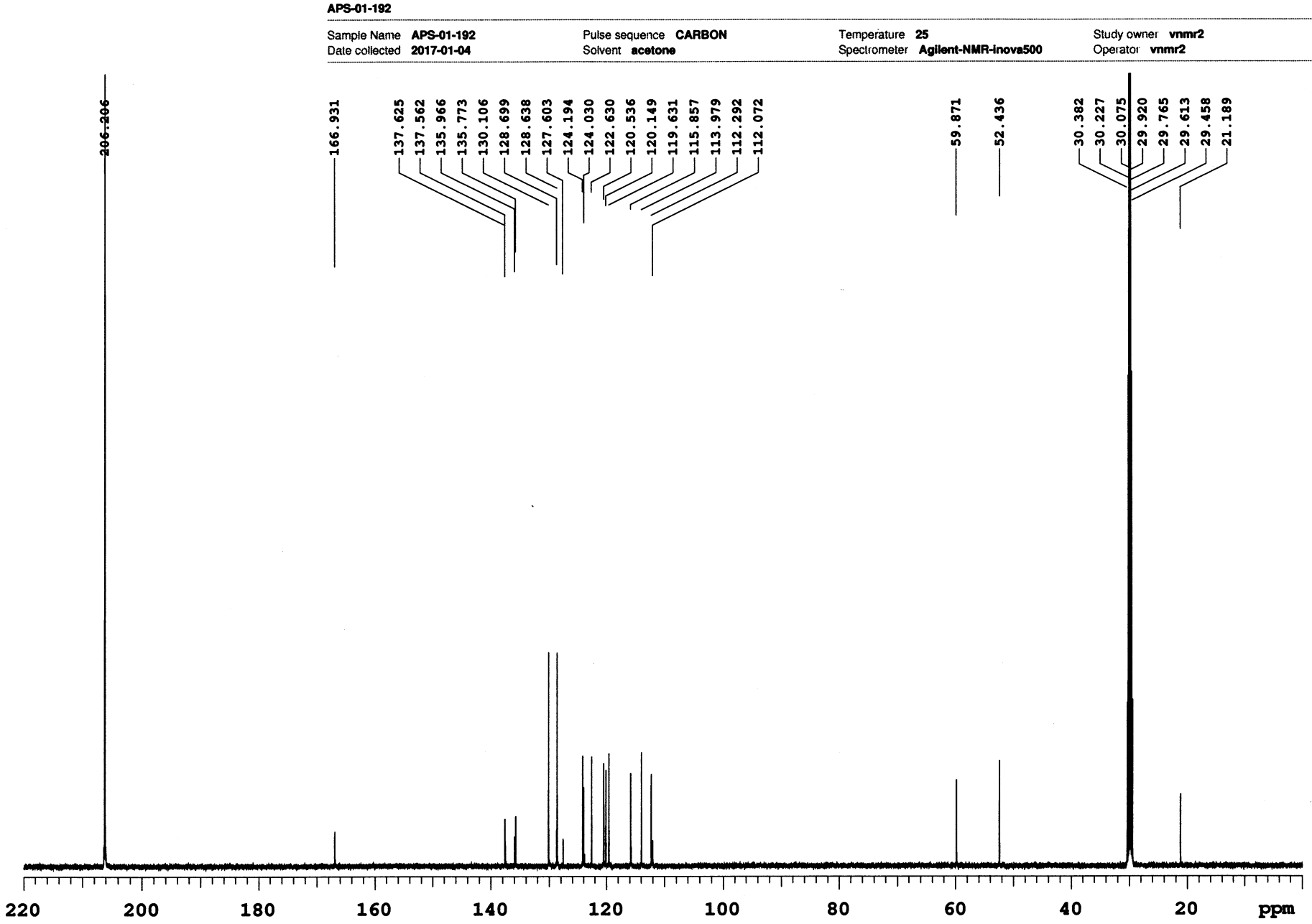


Fig S194. 13C NMR (acetone-d6, 125 MHz) of compound 3ea

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-192/CARBON_02

Plot date 2017-01-04

APS-01-192

Sample Name **APS-01-192**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-01-04**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

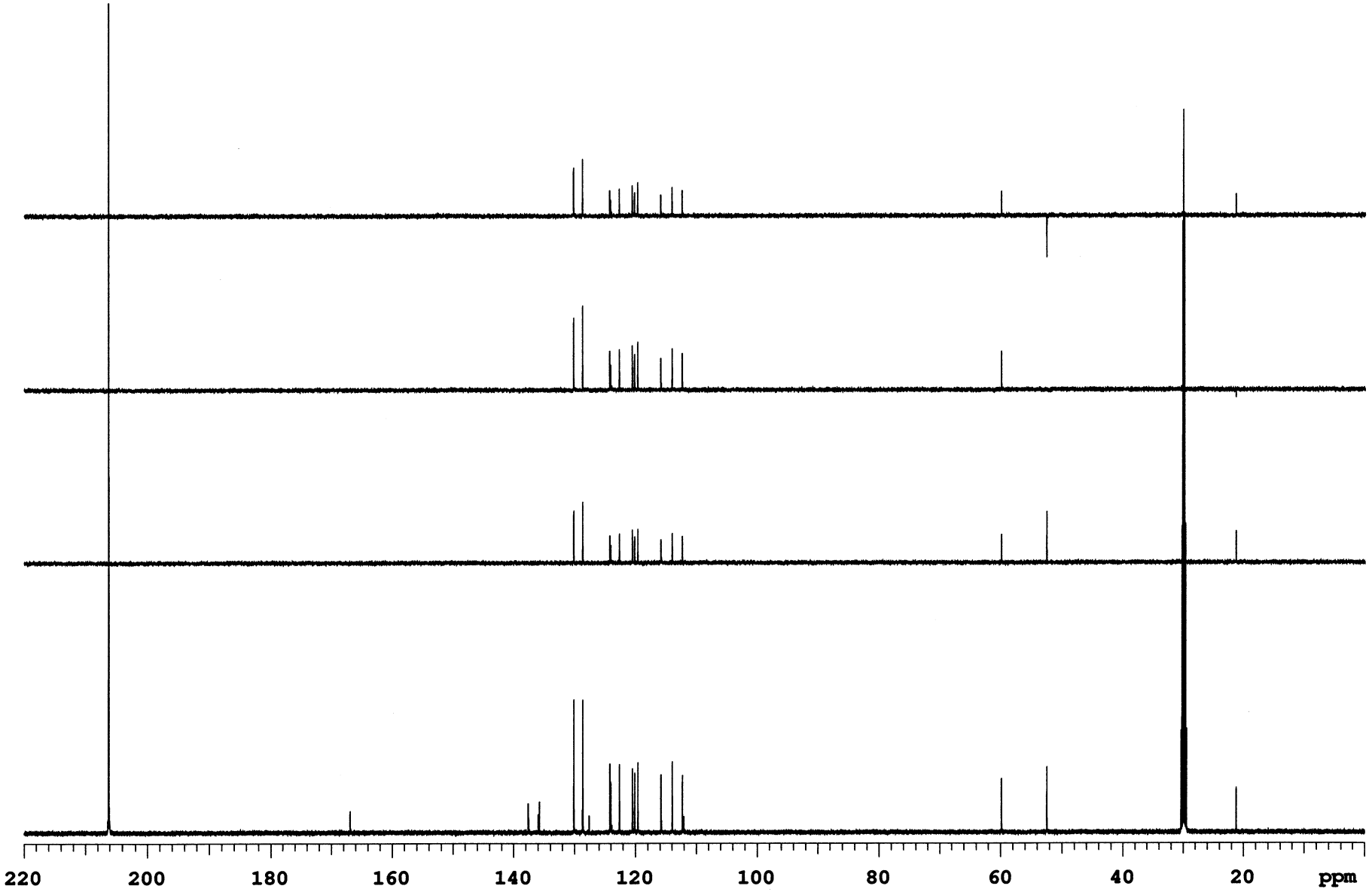


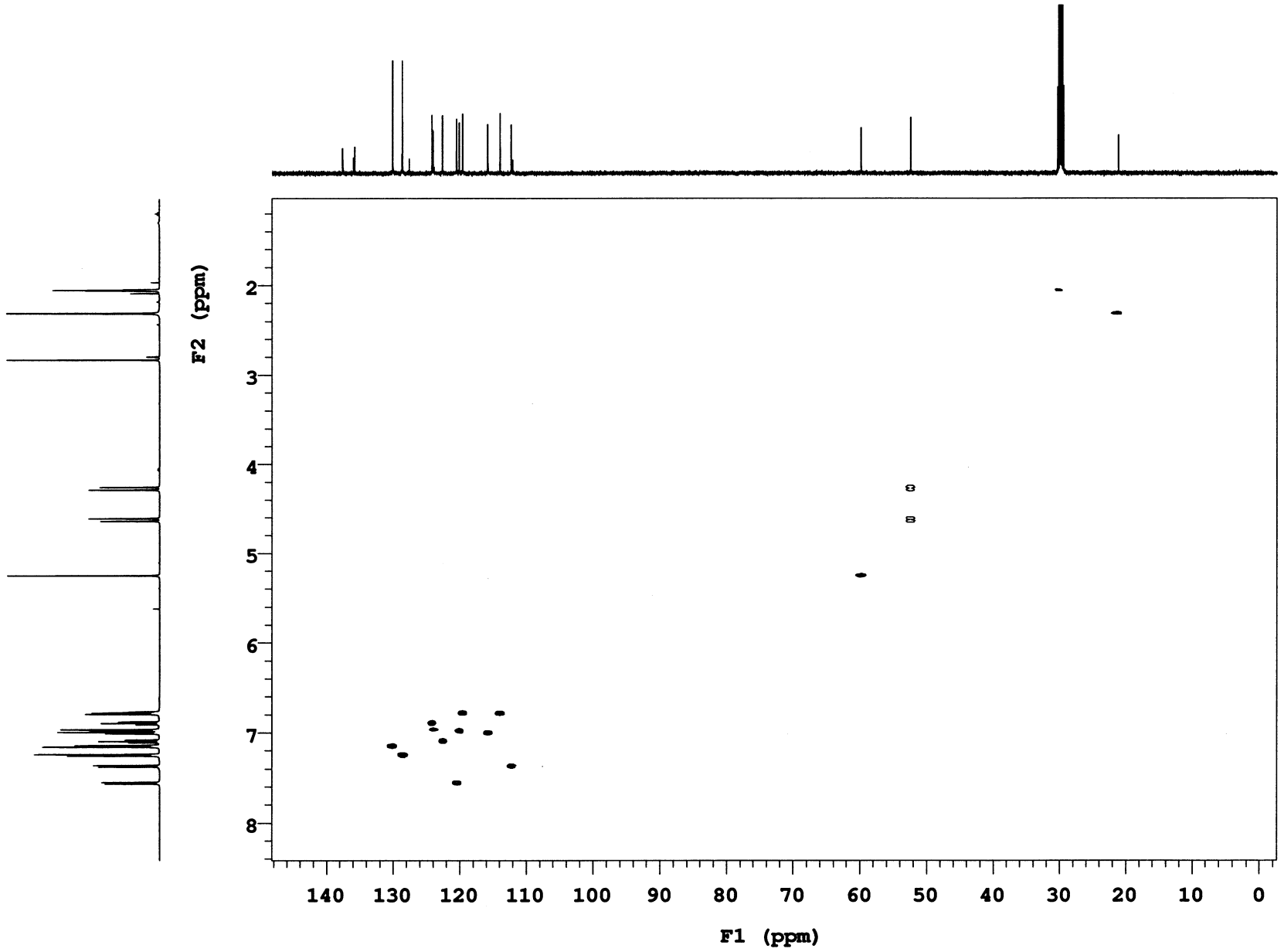
Fig S195. DEPT of compound 3ea

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-192/DEPT_01

Plot date 2017-01-04

APS-01-192

Sample Name	**APS-01-192**	Pulse sequence	**gHSQC**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-01-04**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-Inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-192/gHSQC_01

Fig S196. HSQC of compound 3ea

Plot date 2017-01-04

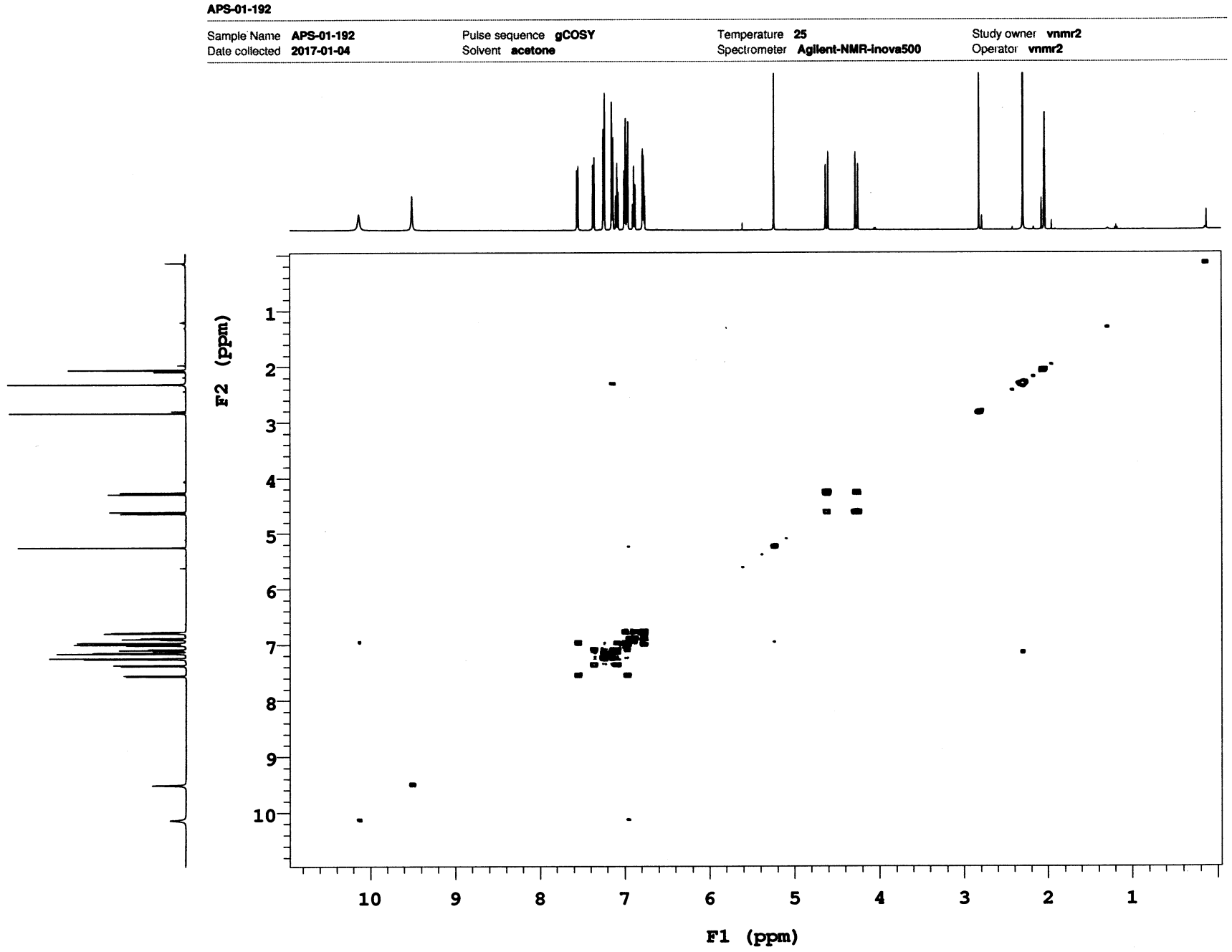
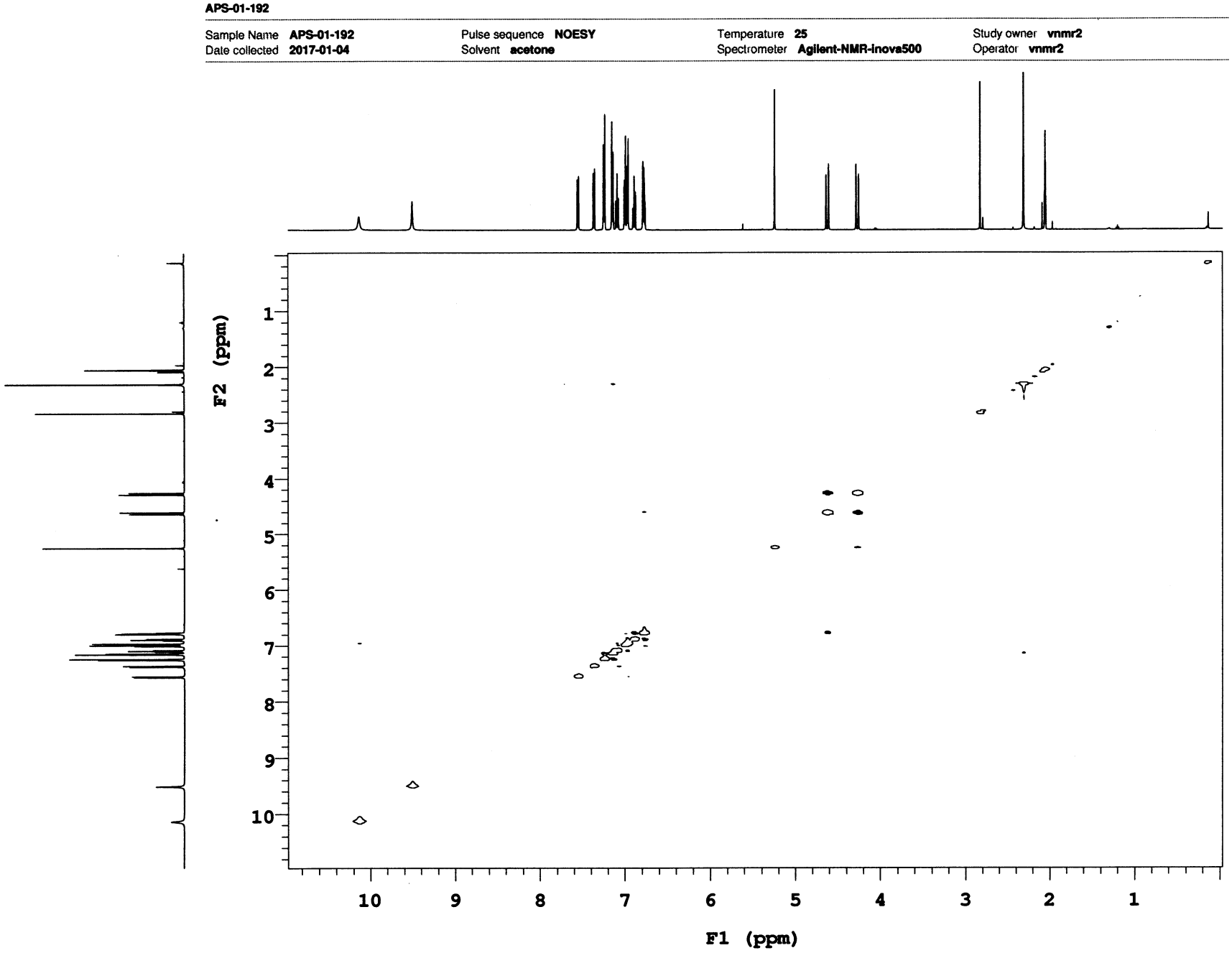


Fig S197. COSY of compound 3ea

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-192/gCOSY_01

Plot date 2017-01-04



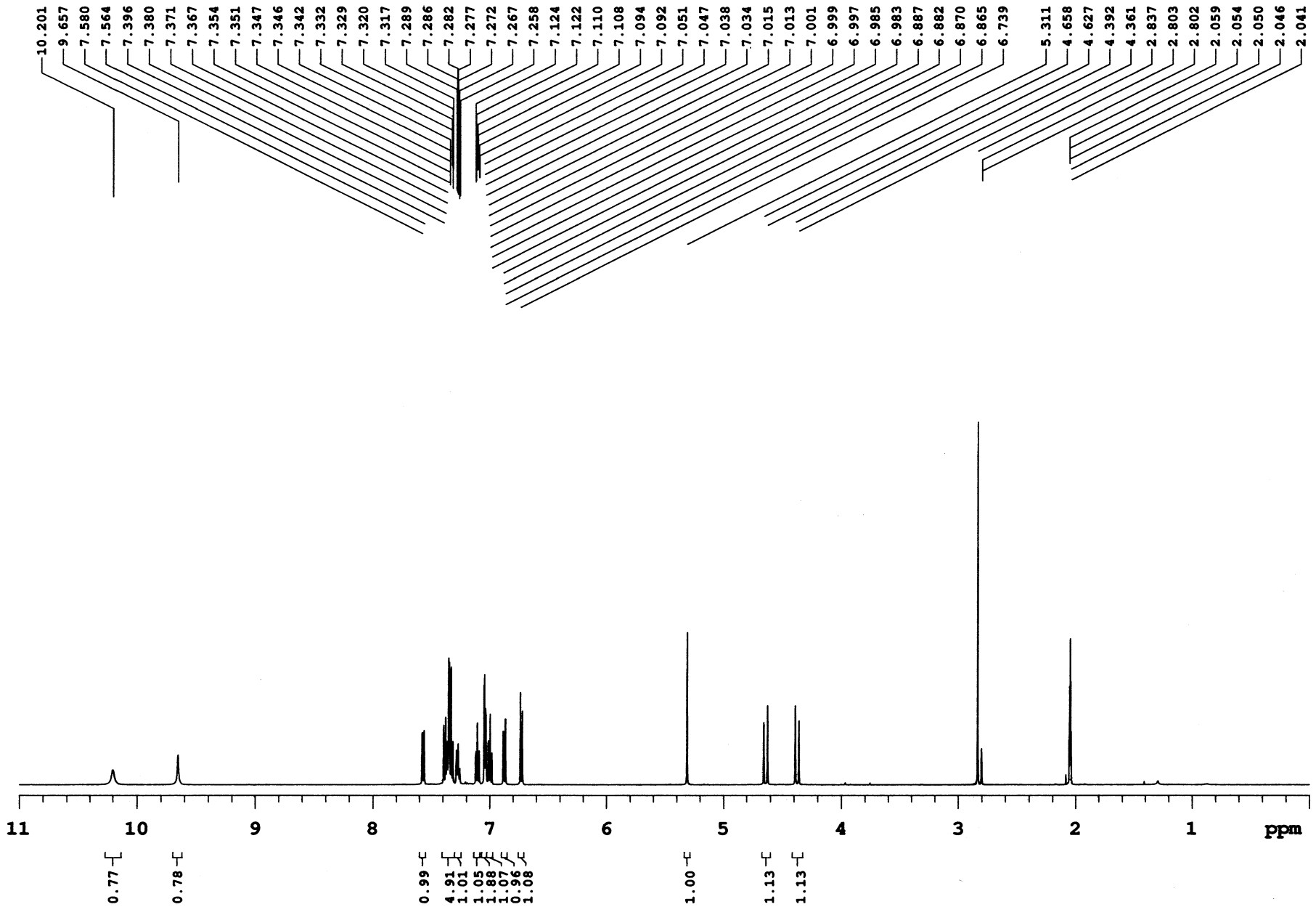
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-192/NOESY_01

Fig S198. NOESY of compound 3ea

Plot date 2017-01-04

APS-01-220-A

Sample Name	**APS-01-220-A**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-05-09**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-220-A/PROTON_03

Plot date 2017-05-15

Fig S199. 1H NMR (acetone-d6, 500 MHz) of compound 3ga

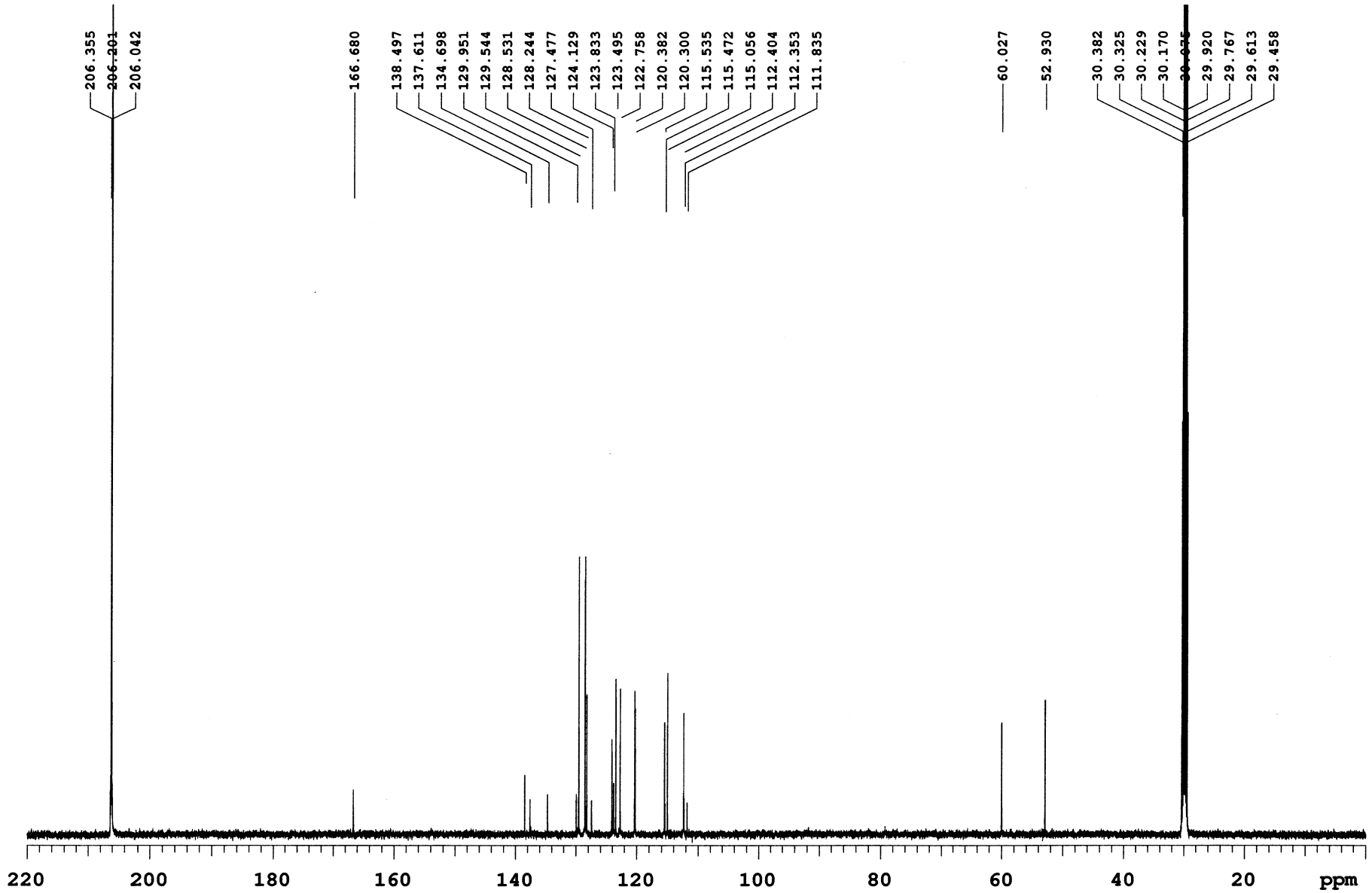


Fig S200. 13C NMR (acetone-d6, 125 MHz) of compound 3ga

APS-01-220

Sample Name **APS-01-220**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-19**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

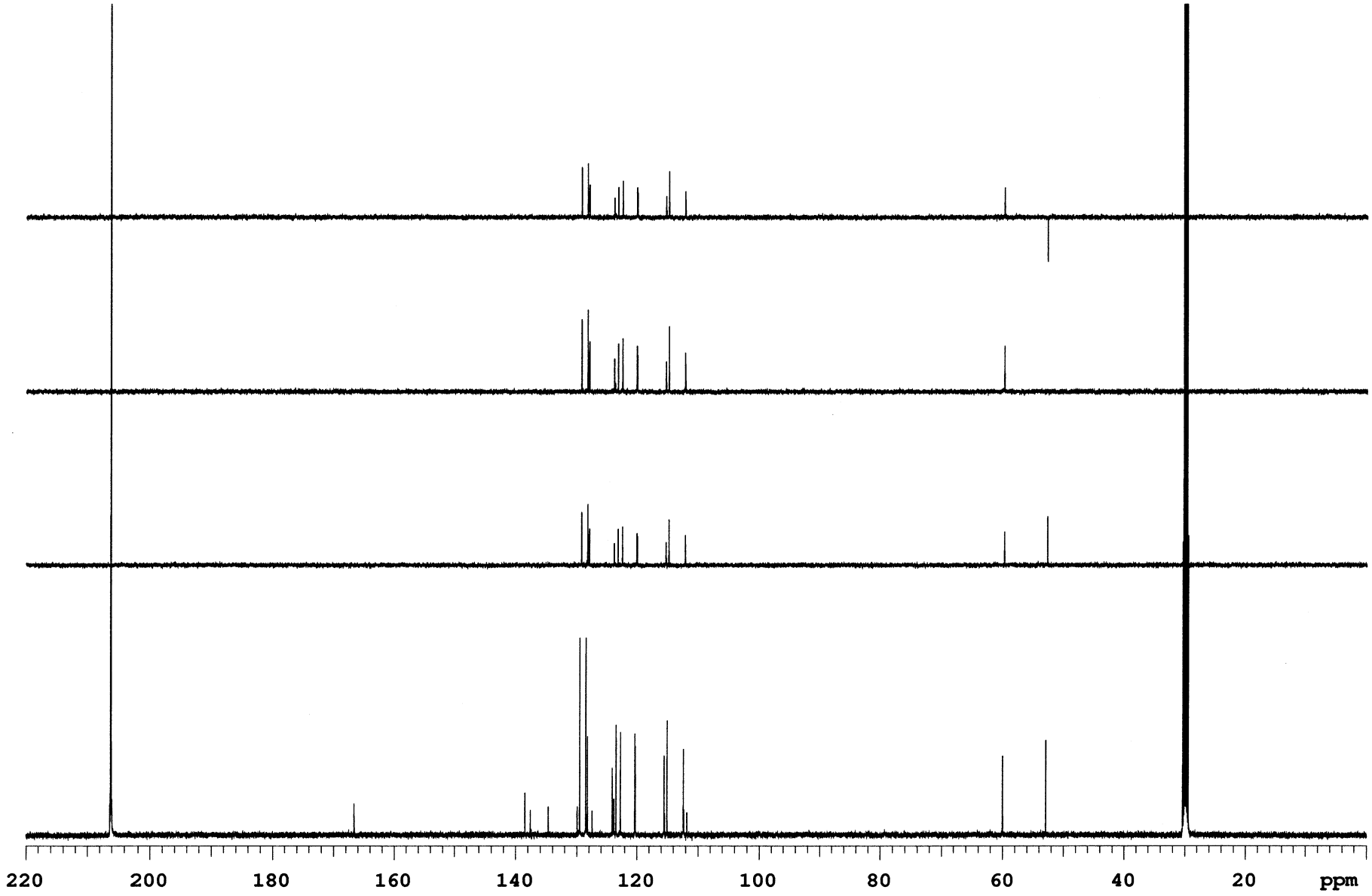
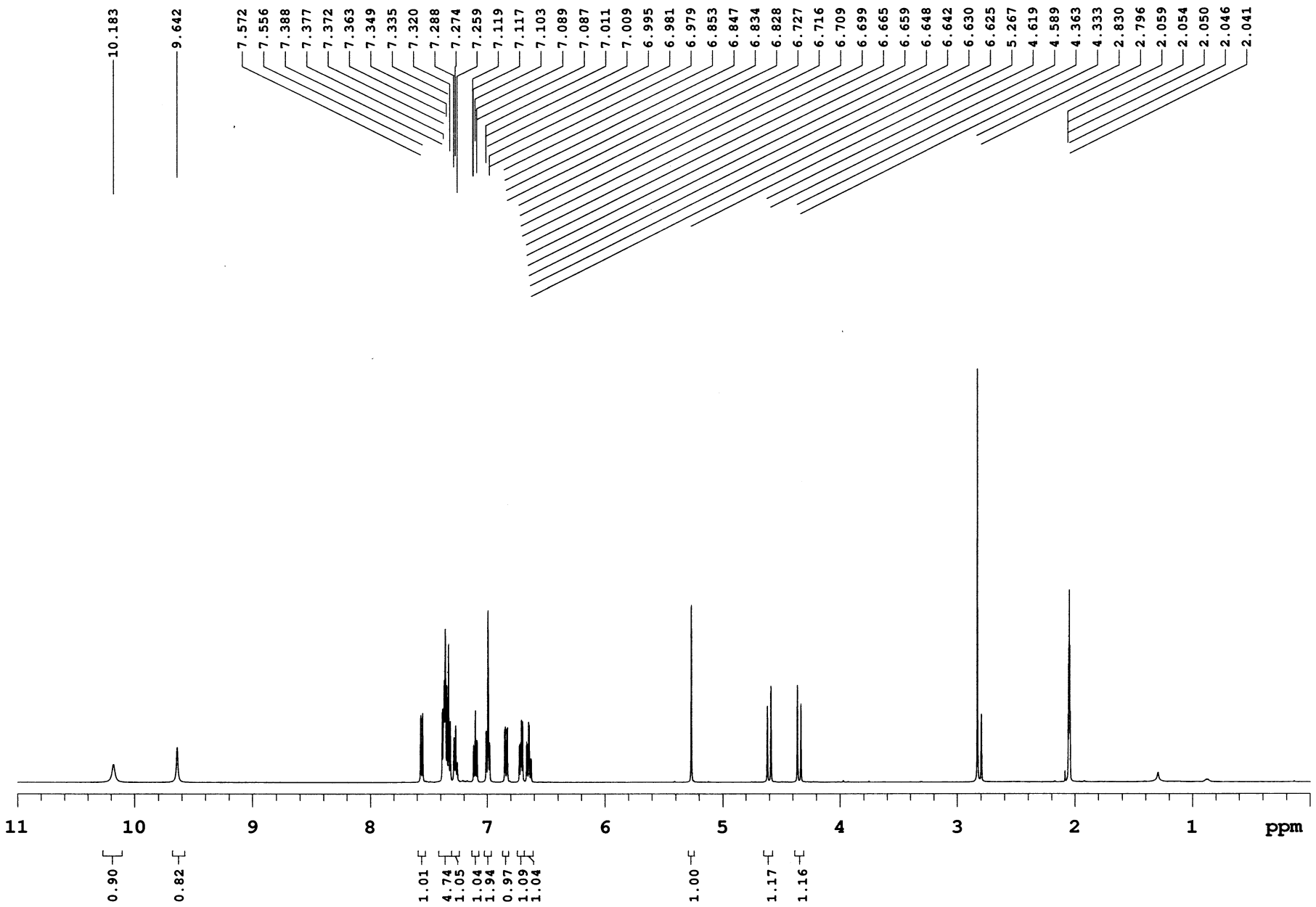


Fig S201. DEPT of compound 3ga

APS-01-225-A

Sample Name	**APS-01-225-A**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-05-06**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-225-A/PROTON_03

Fig S202. 1H NMR (acetone-d6, 500 MHz) of compound 3ia

Plot date 2017-05-15

APS-01-225-A

Sample Name **APS-01-225-A**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-06**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

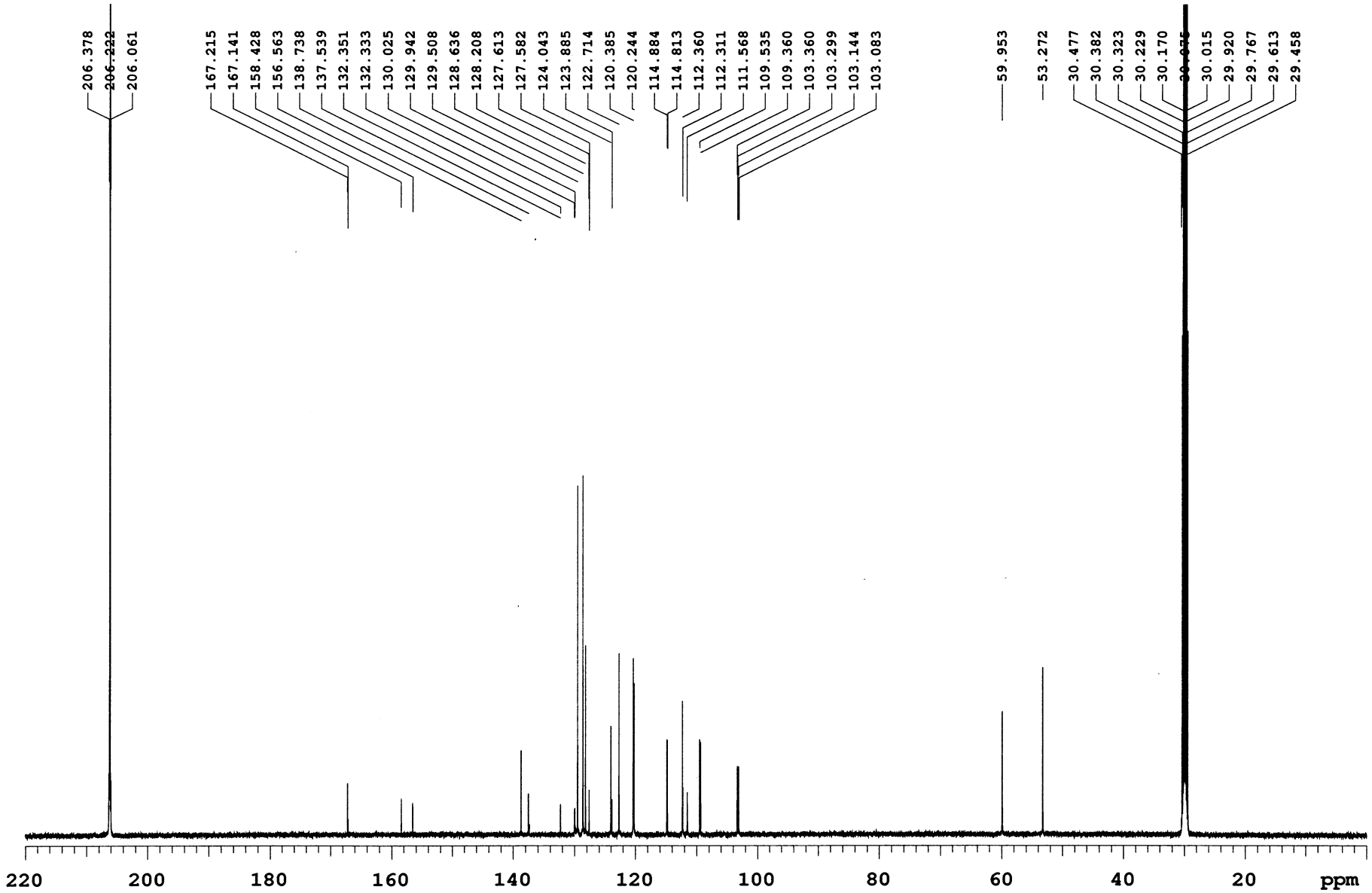


Fig S203. 13C NMR (acetone-d6, 125 MHz) of compound 3ia

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-225-A/CARBON_02

Plot date 2017-05-15

APS-01-225-A

Sample Name **APS-01-225-A**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-06**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

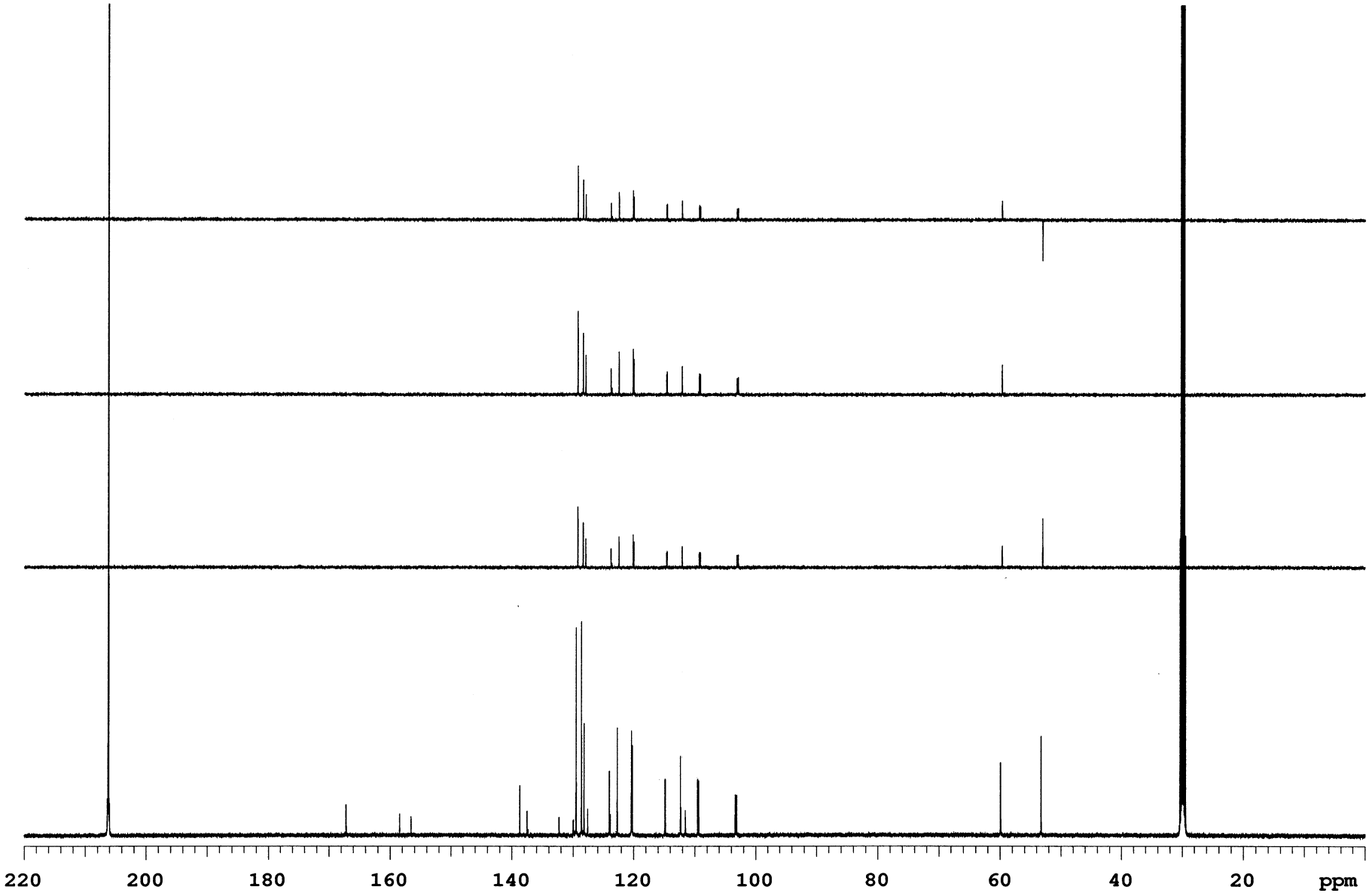


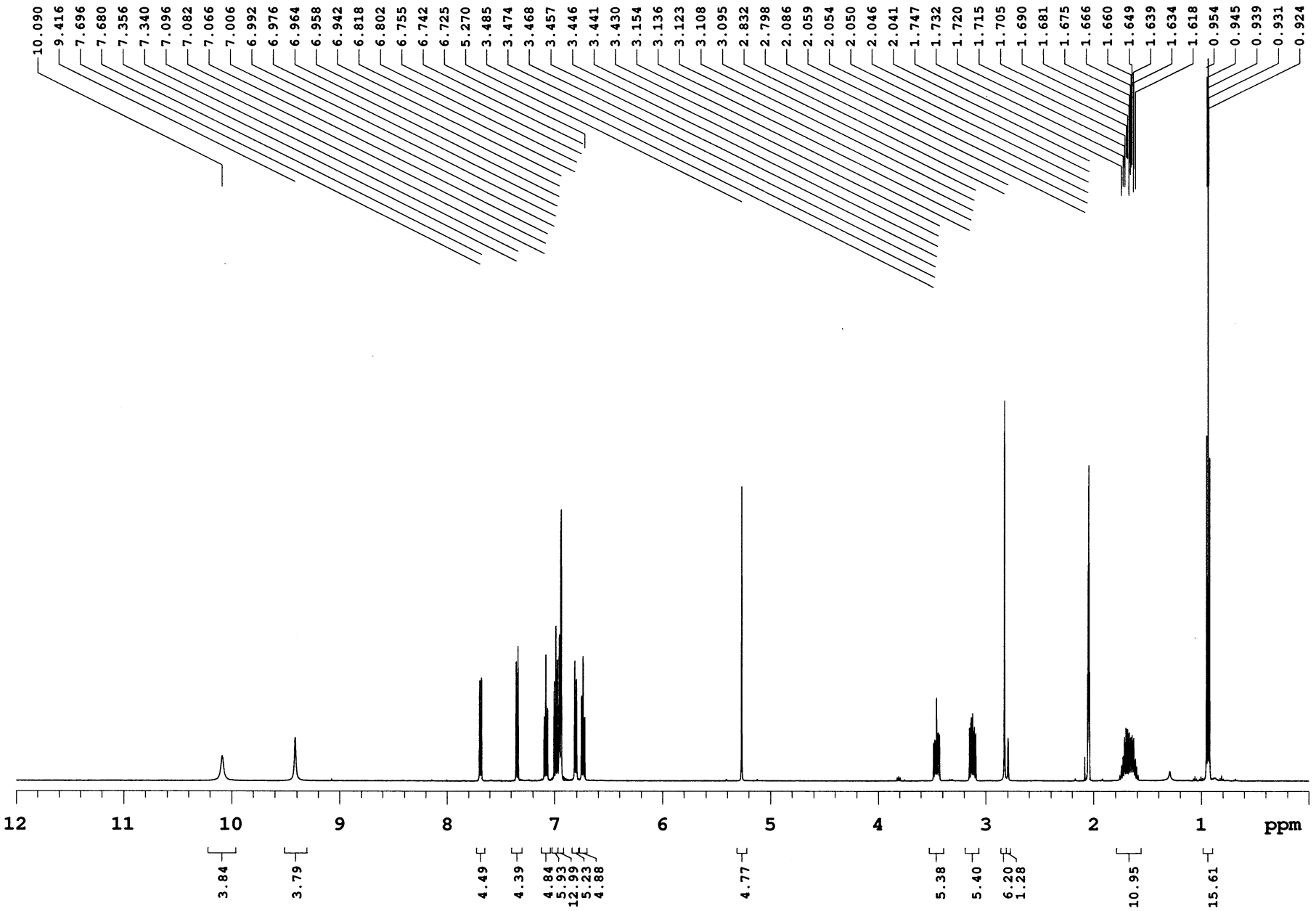
Fig S204. DEPT of compound 3ia

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-225-A/DEPT_01.fid

Plot date 2017-05-15

APS-01-180

Sample Name **APS-01-180**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-26**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-180/PROTON_03

Fig S205. 1H NMR (acetone-d6, 500 MHz) of compound 3ja

Plot date 2017-05-27

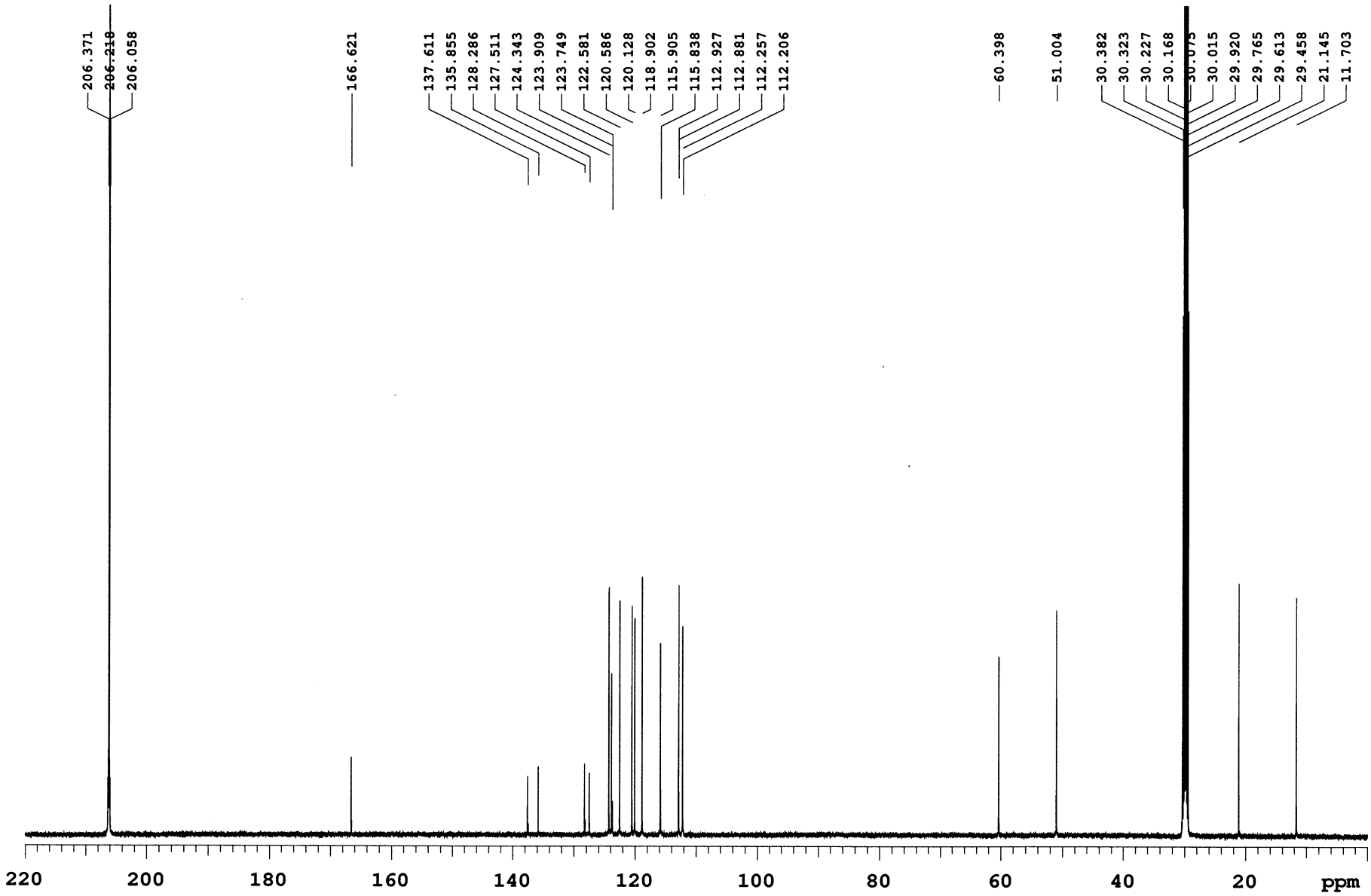


Fig S206. 13C NMR (acetone-d6, 125 MHz) of compound 3ja

APS-01-180

Sample Name **APS-01-180**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-27**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

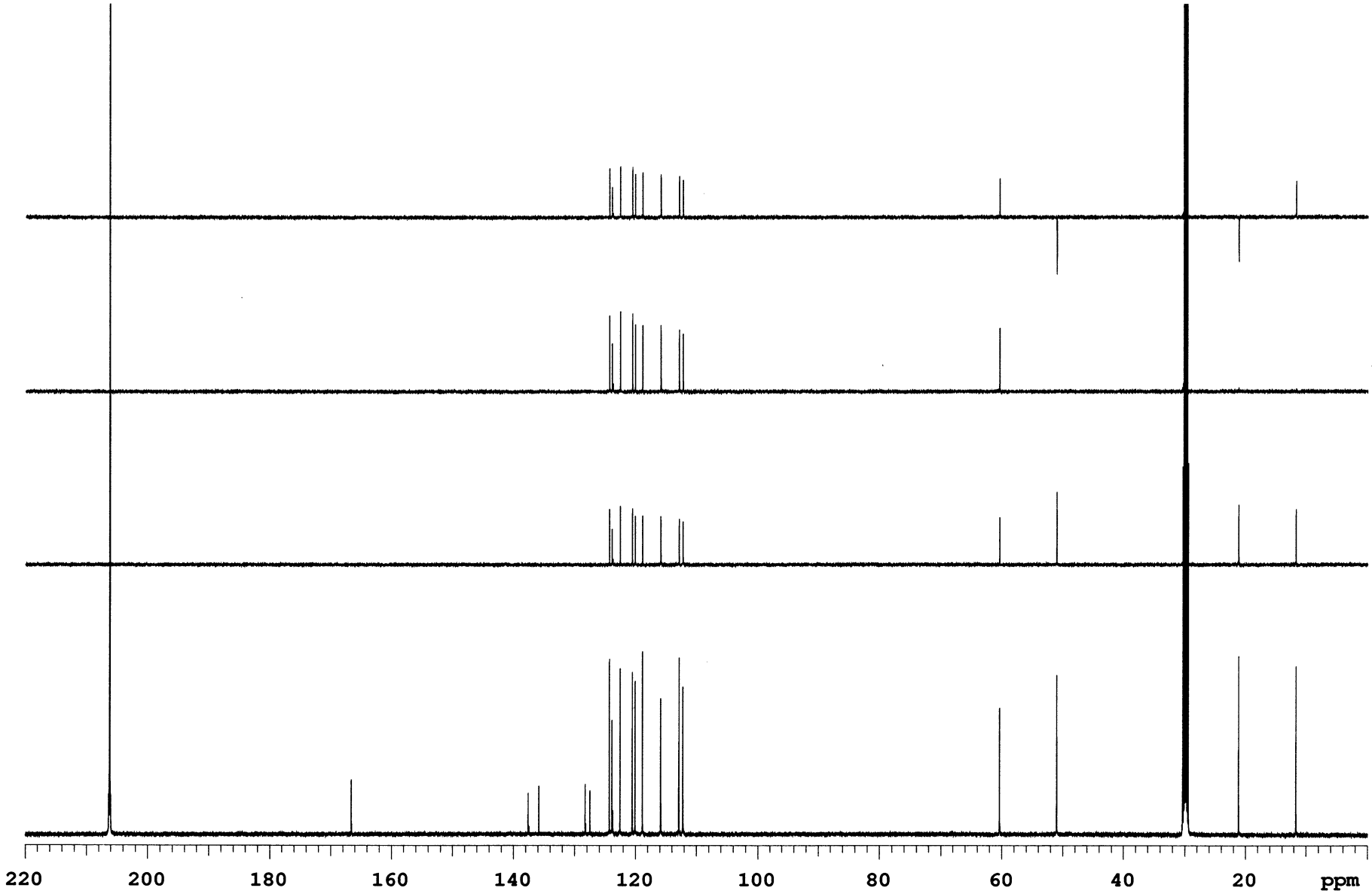
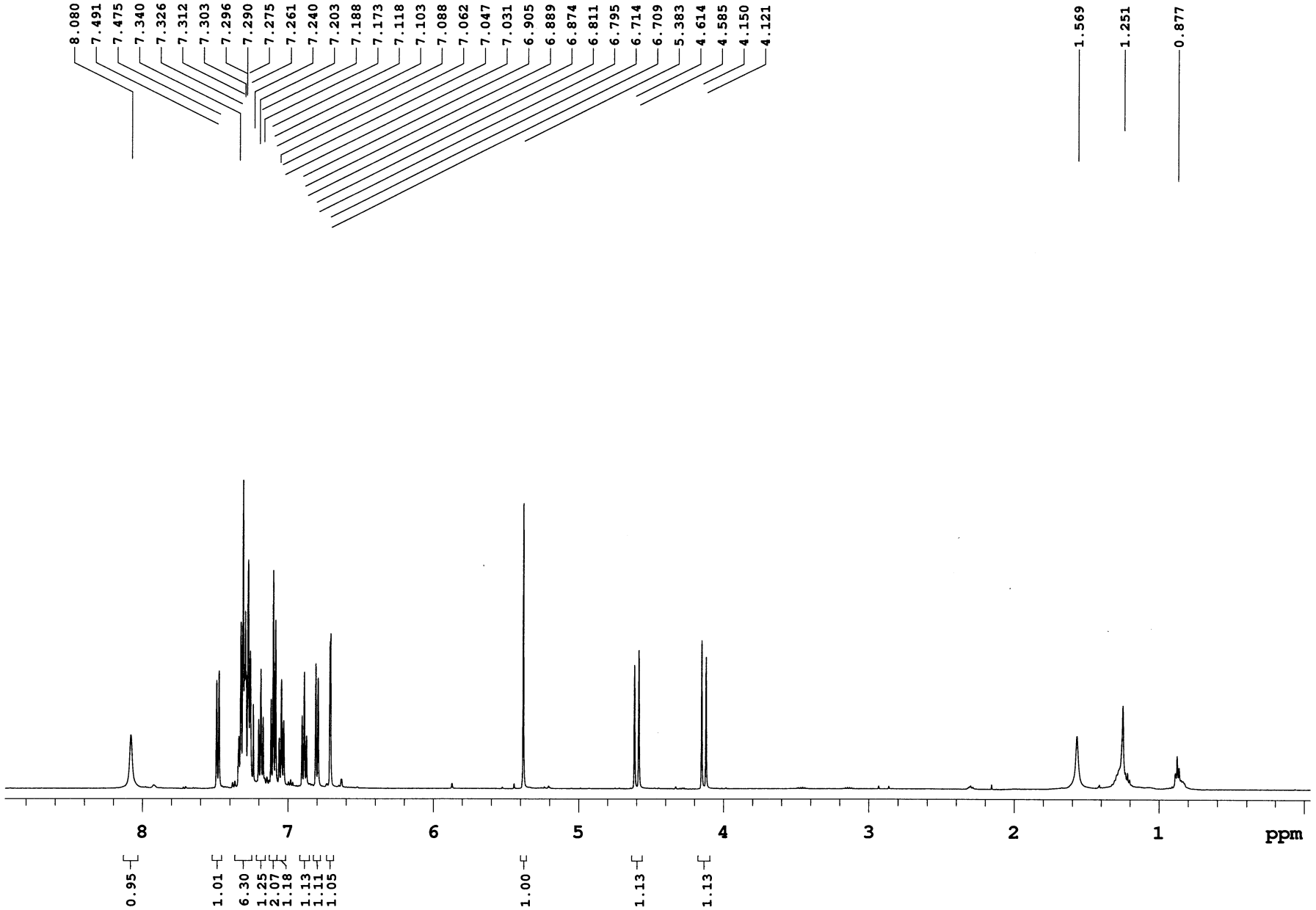


Fig S207. DEPT of compound 3ja

APS-01-195

Sample Name **APS-01-195**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-21**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-195/PROTON_04

Plot date 2017-03-21

Fig S208. 1H NMR (CDCl3, 500 MHz) of compound 3ka

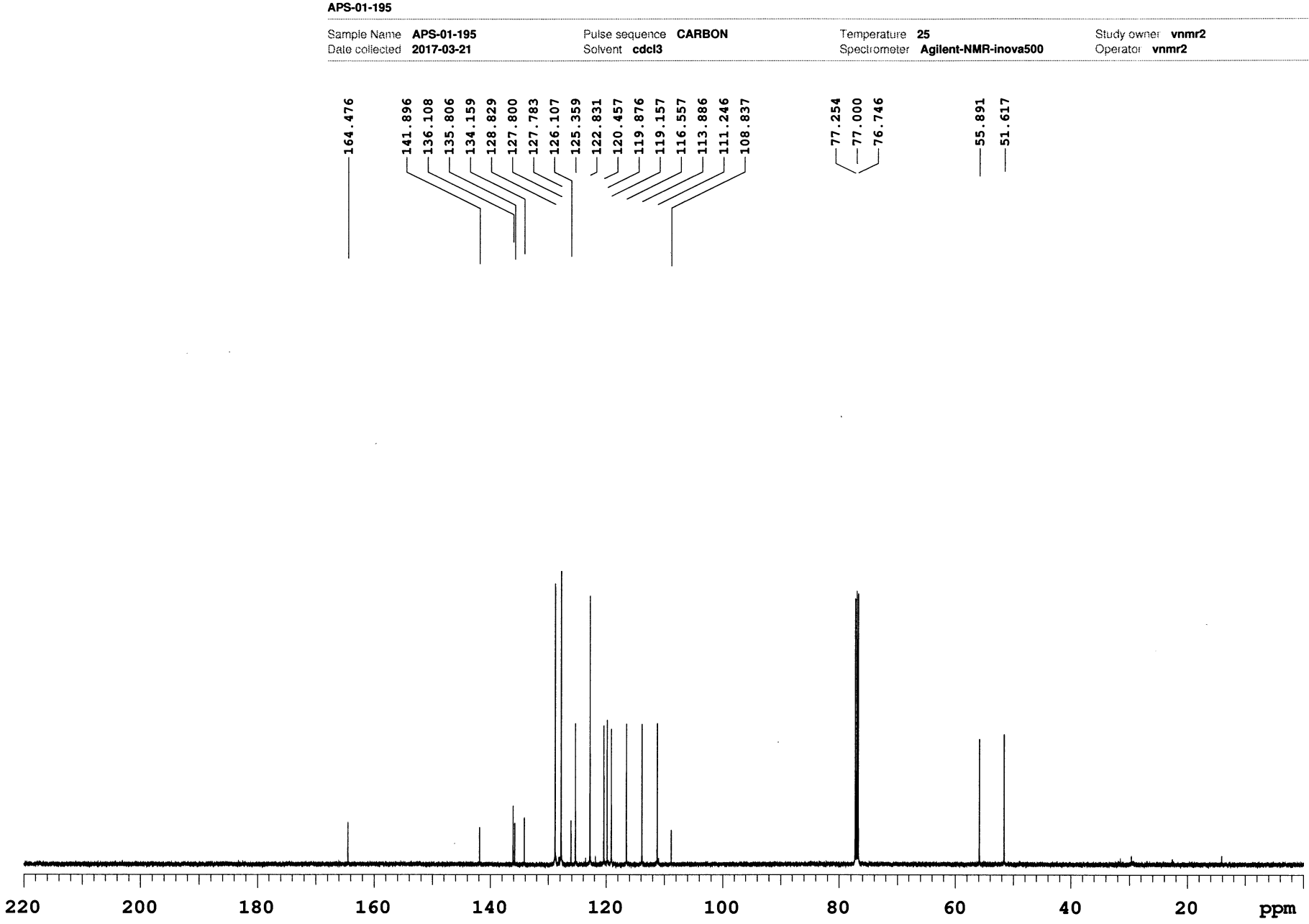


Fig S209. 13C NMR (CDCl3, 125 MHz) of compound 3ka

APS-01-195

Sample Name **APS-01-195**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-21**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

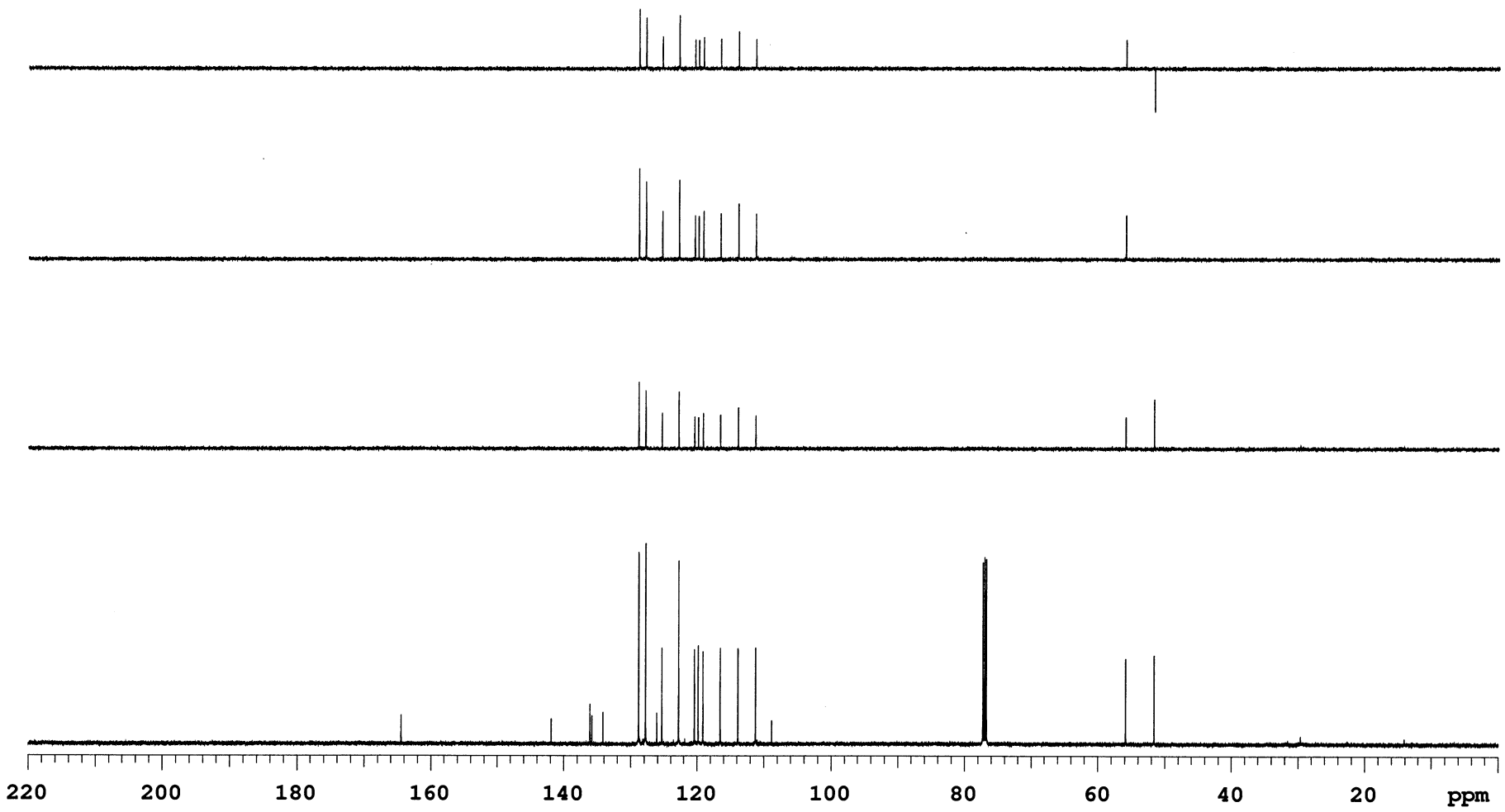


Fig S210. DEPT of compound 3ka

APS-01-195

Sample Name **APS-01-195**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-21**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

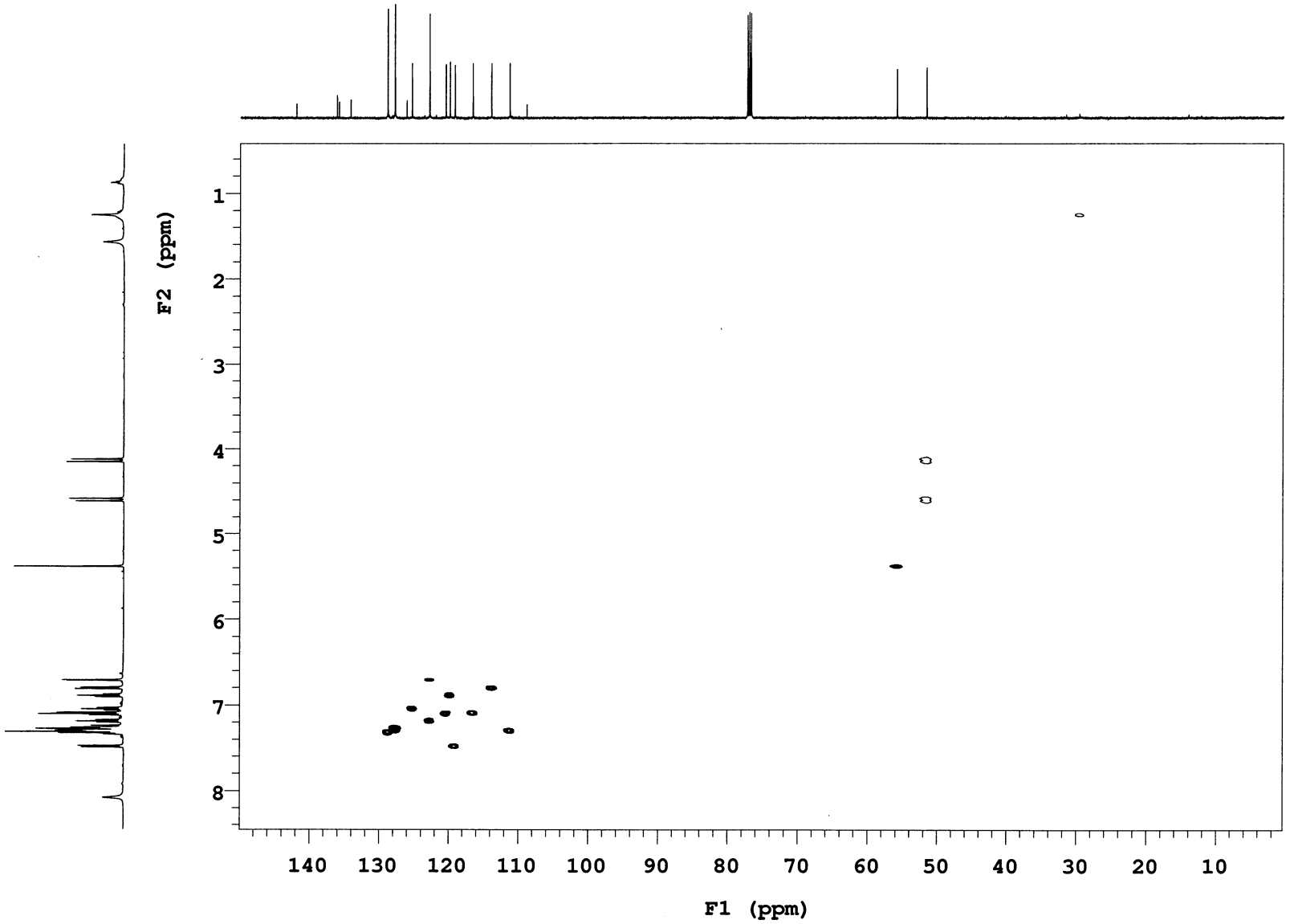


Fig S211. HSQC of compound 3ka

APS-01-195

Sample Name	**APS-01-195**	Pulse sequence	**gCOSY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-21**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

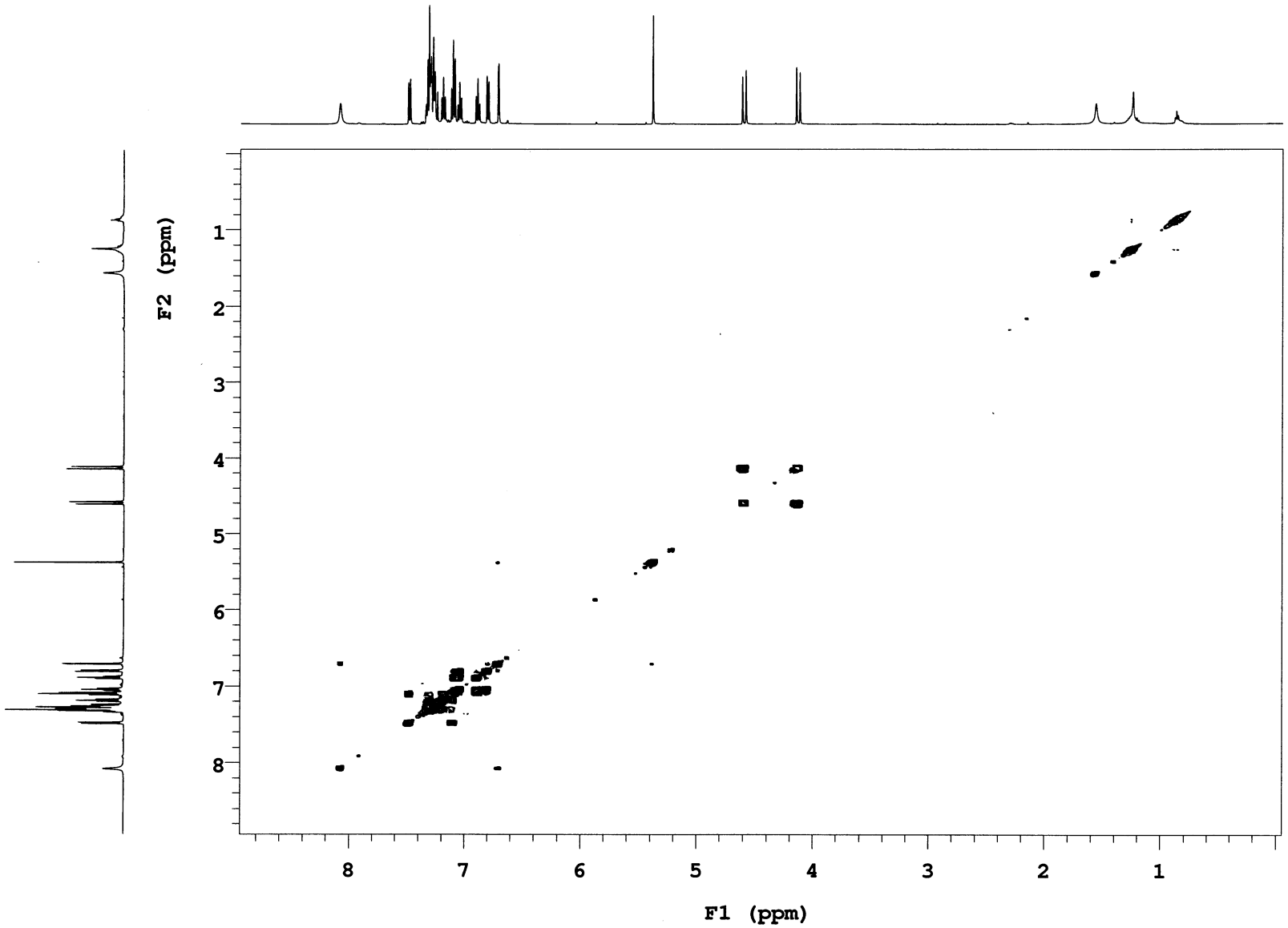


Fig S212. COSY of compound 3ka

APS-01-195

Sample Name **APS-01-195**	Pulse sequence **NOESY**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-21**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

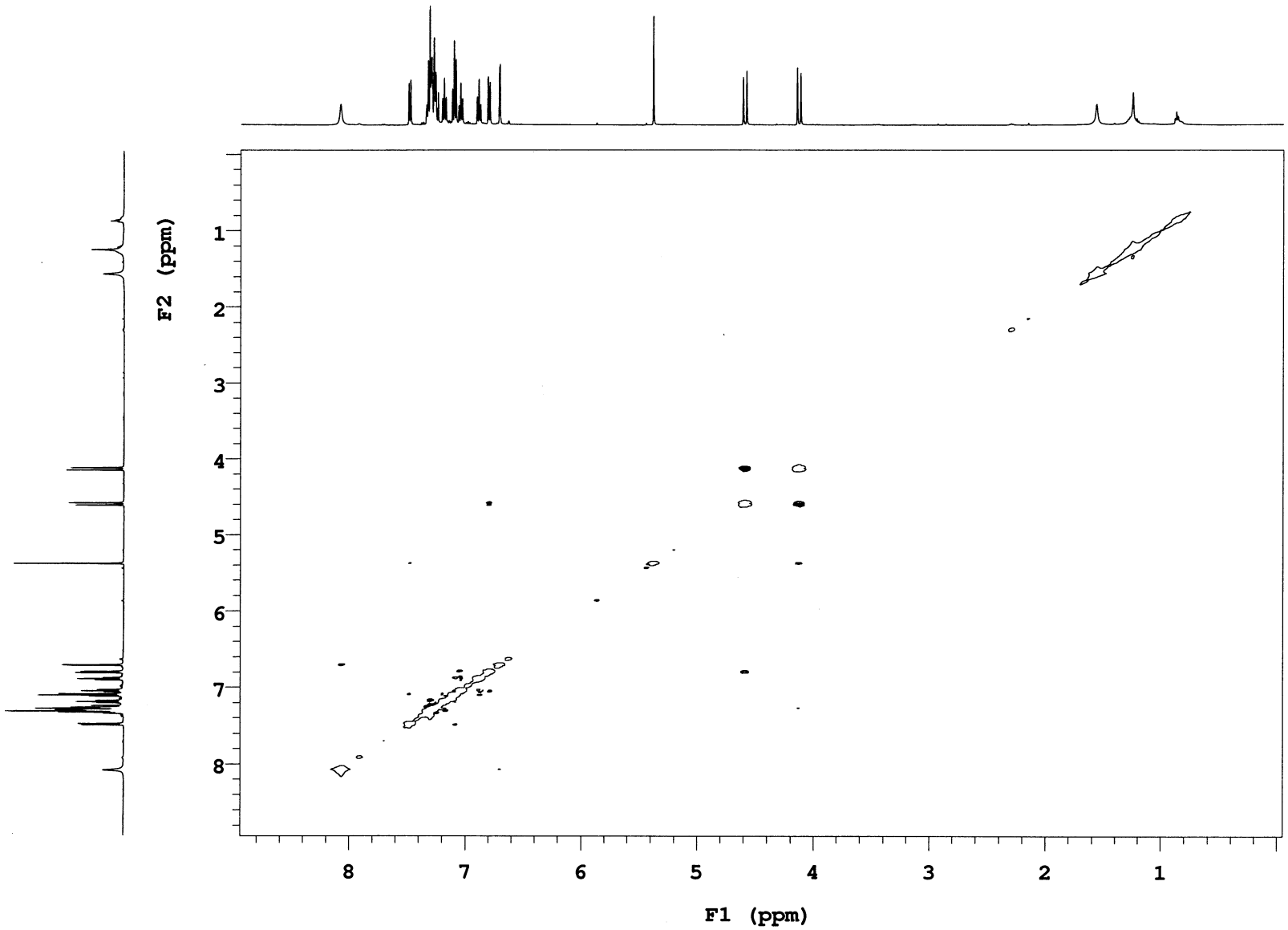
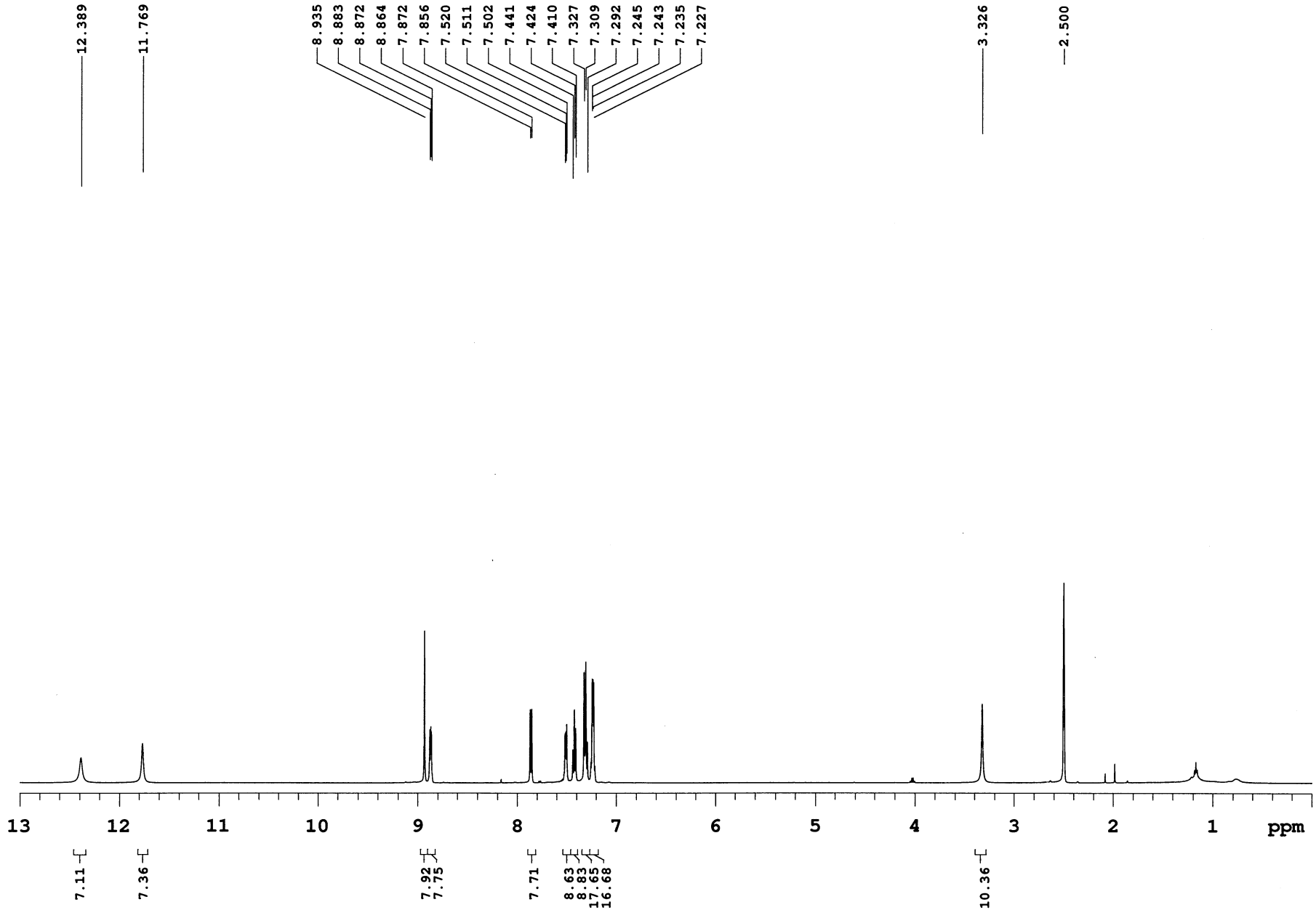


Fig S213. NOESY of compound 3ka

APS-01-249

Sample Name **APS-01-249**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-11-23**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-249/PROTON_08

Plot date 2017-11-28

Fig S214. 1H NMR (DMSO-d6, 500 MHz) of compound 4aa

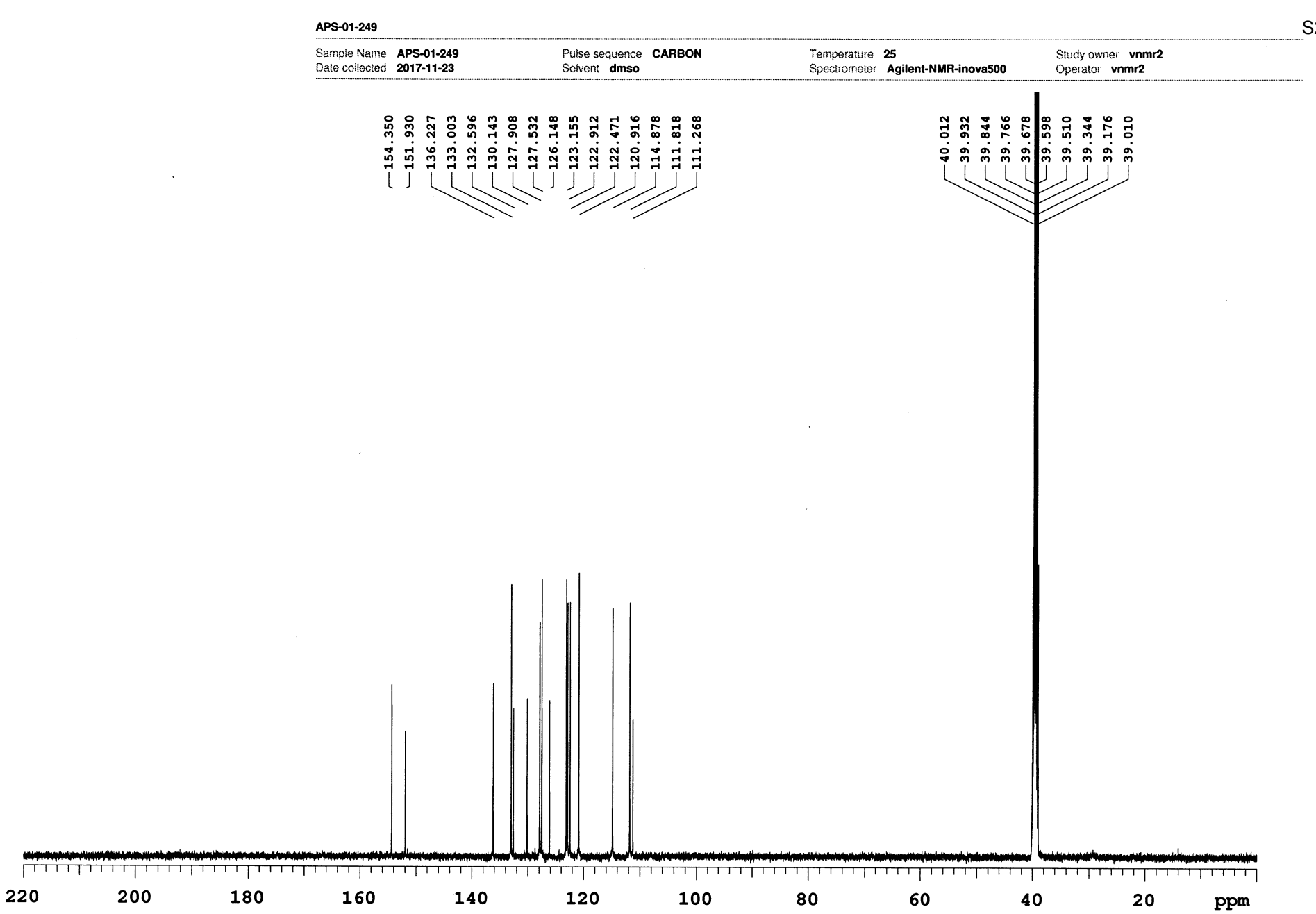


Fig S215. 13C NMR (DMSO-d6, 125 MHz) of compound 4aa

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-249/CARBON_03

Plot date 2017-11-28

APS-01-249

Sample Name **APS-01-249**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-11-24**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

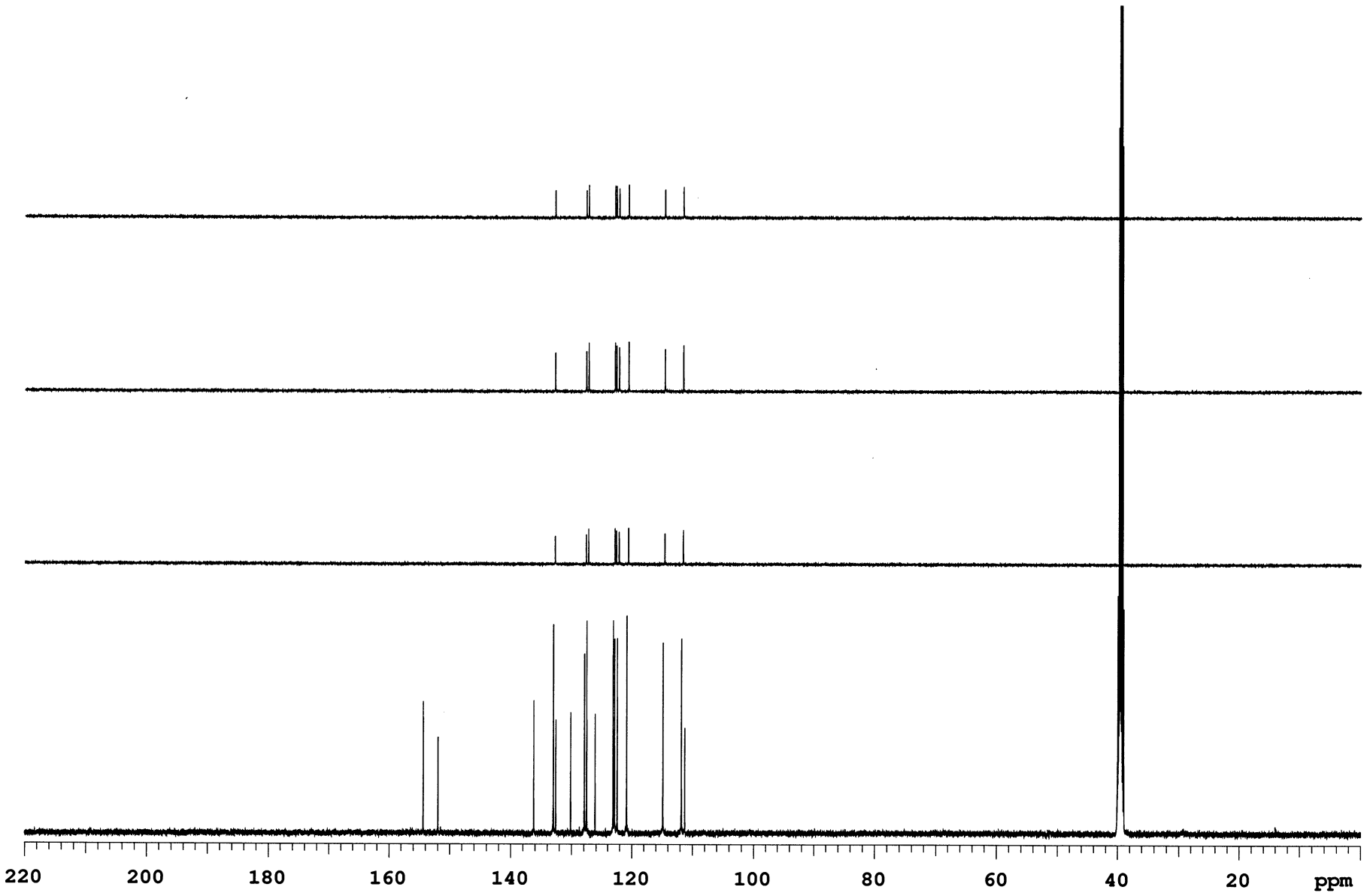
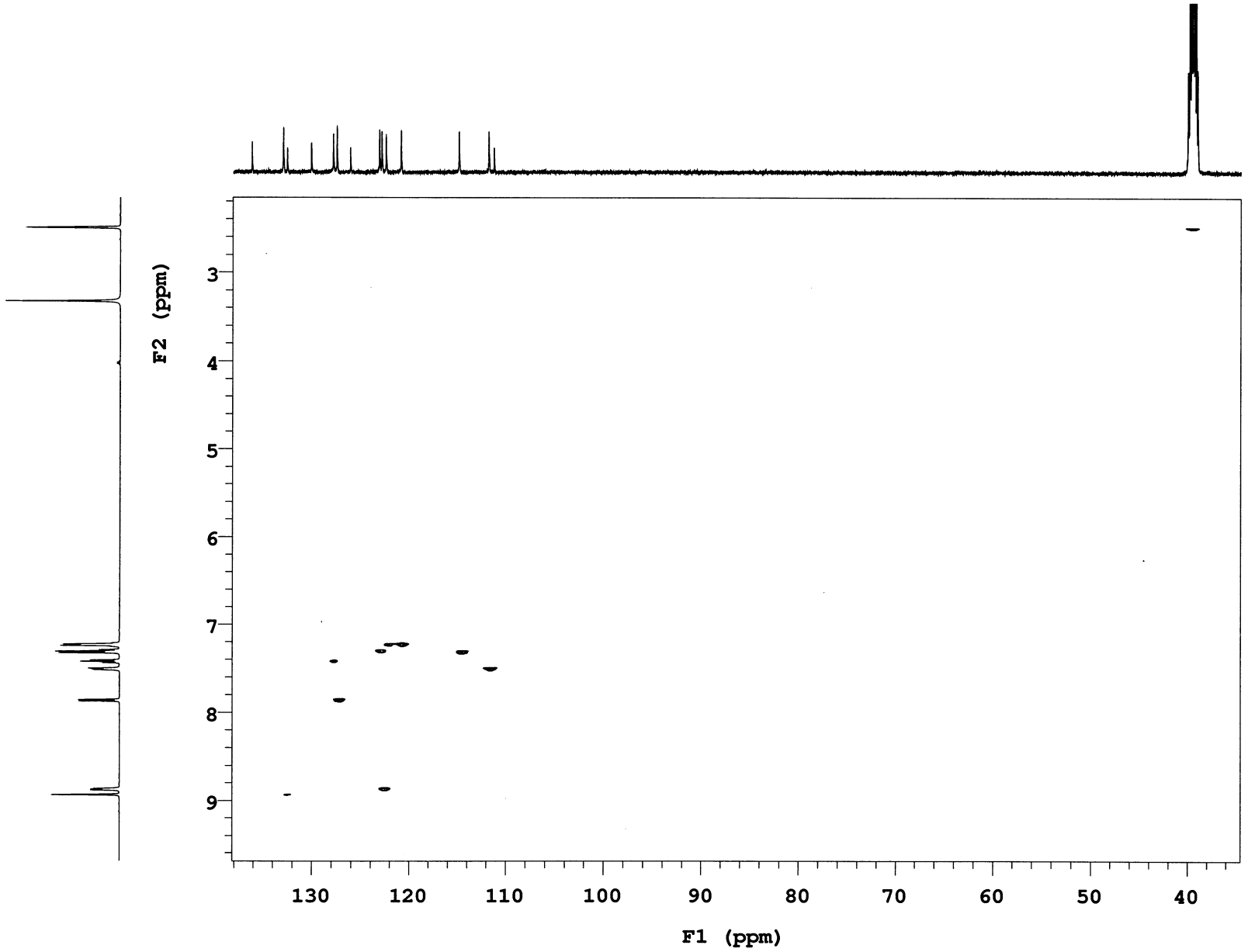


Fig S216. DEPT of compound 4aa

APS-161

Sample Name	**APS-161**	Pulse sequence	**gHSQC**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2018-01-05**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



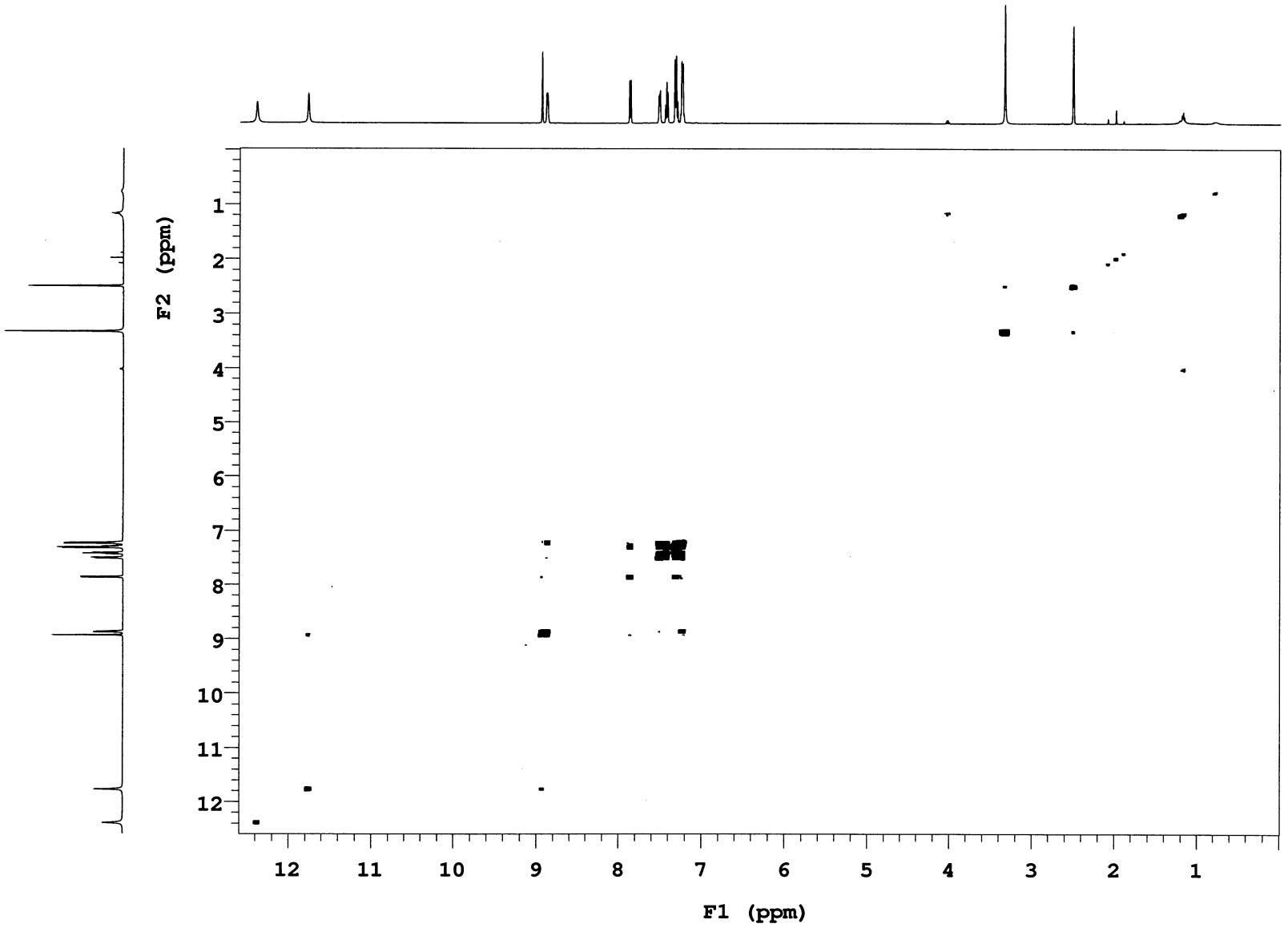
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-161/gHSQC_01

Fig S217. HSQC of compound 4aa

Plot date 2018-01-05

APS-161

Sample Name	**APS-161**	Pulse sequence	**gCOSY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2018-01-05**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



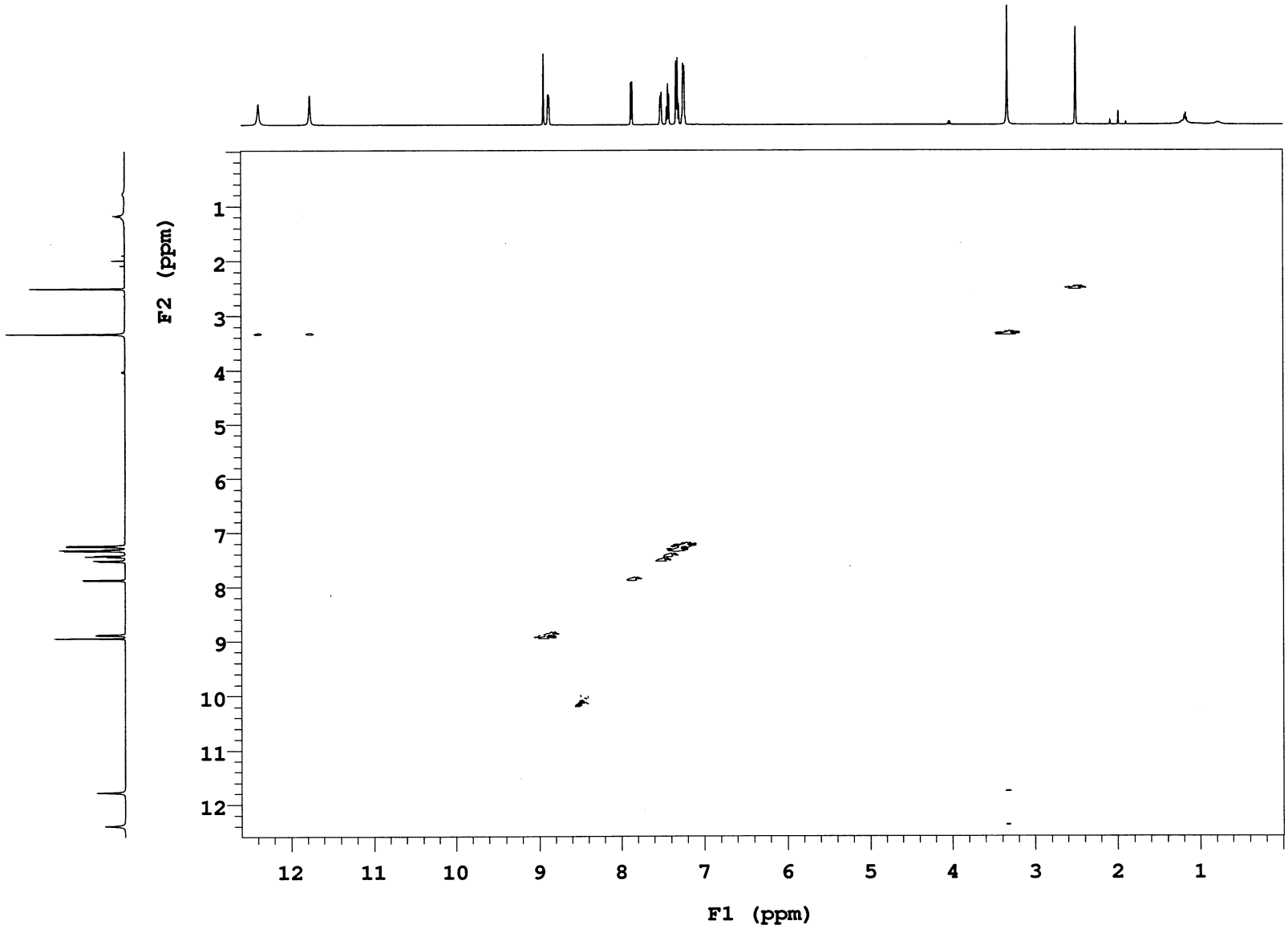
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-161/gCOSY_01

Fig S218. COSY of compound 4aa

Plot date 2018-01-05

APS-161

Sample Name	**APS-161**	Pulse sequence	**NOESY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2018-01-05**	Solvent	**dmso**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



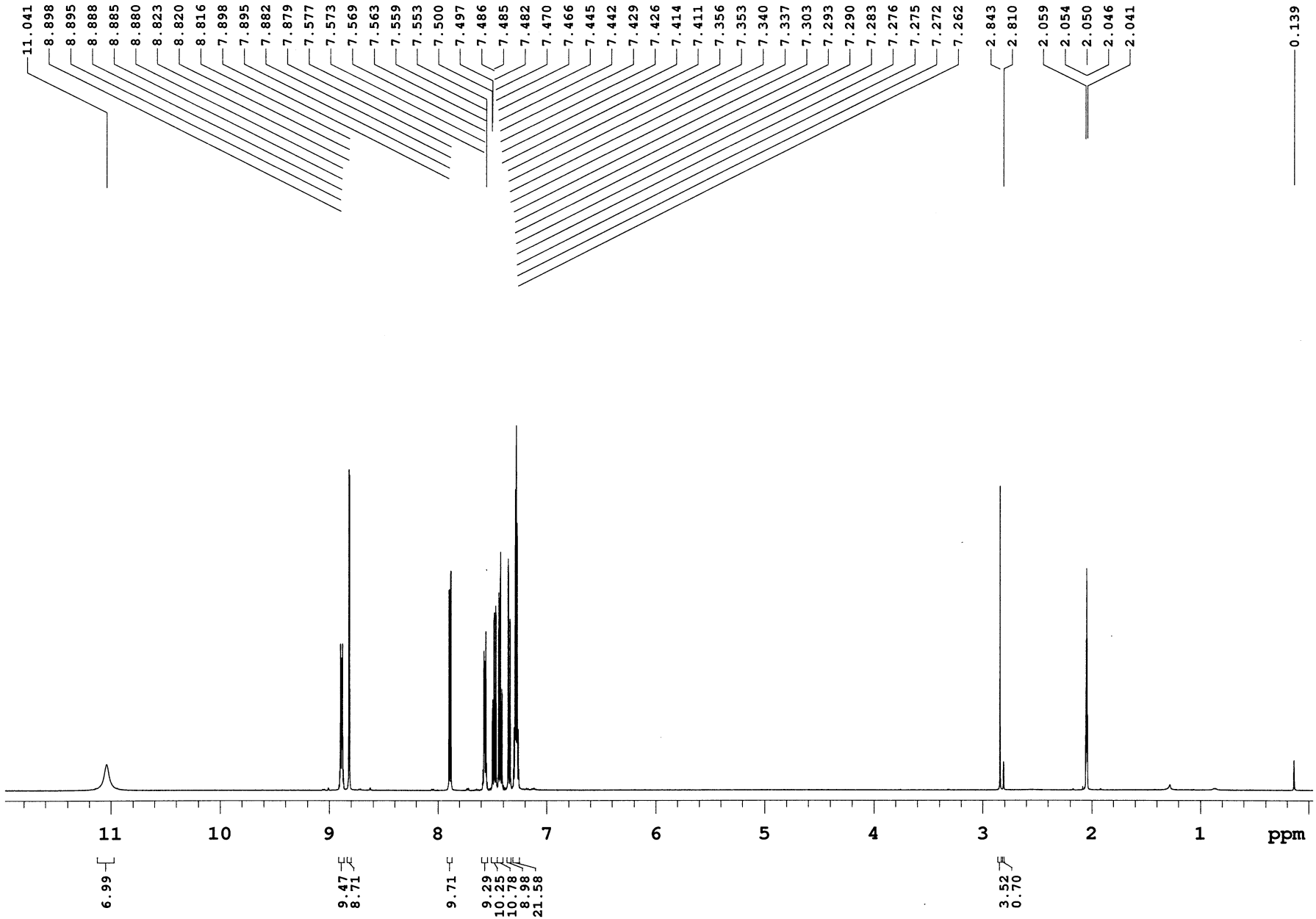
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-161/NOESY_01

Fig S219. NOESY of compound 4aa

Plot date 2018-01-05

APS-01-214

Sample Name **APS-01-214**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-27**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-214/PROTON_03

Fig S220. 1H NMR (acetone-d6, 500 MHz) of compound 4ka

Plot date 2017-03-28

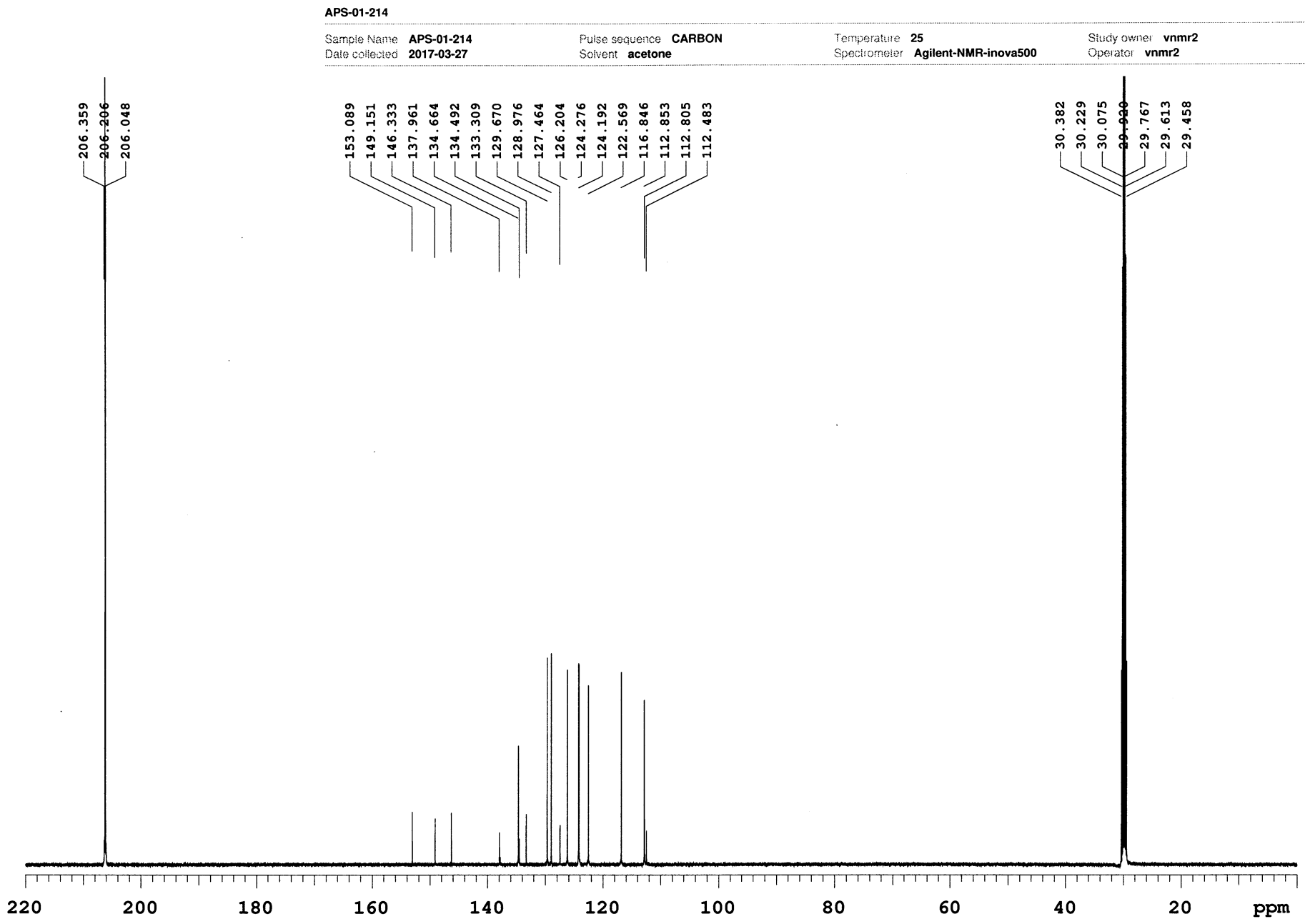


Fig S221. 13C NMR (acetone-d6, 125 MHz) of compound 4ka

APS-01-214

Sample Name **APS-01-214**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-28**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

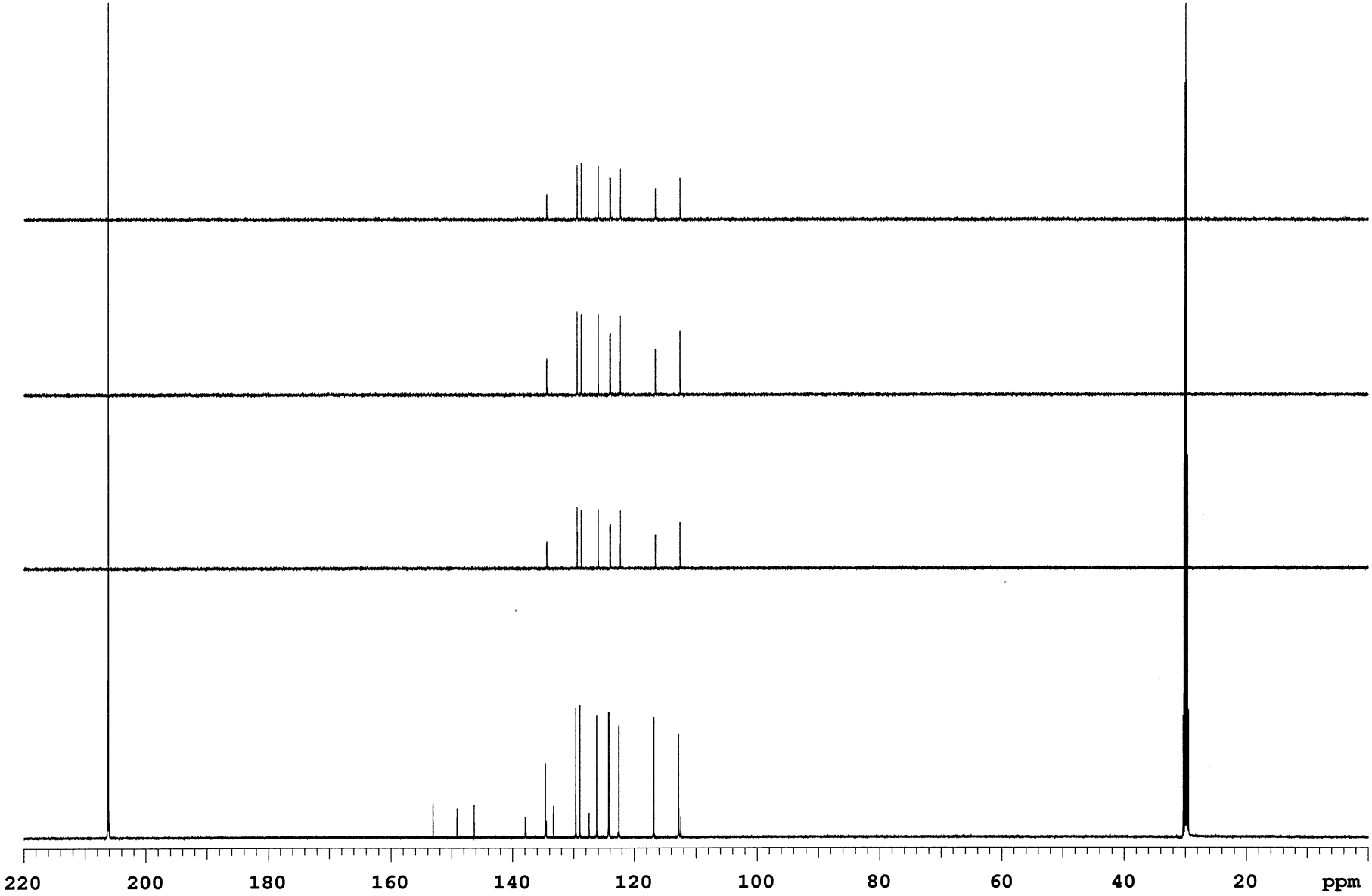


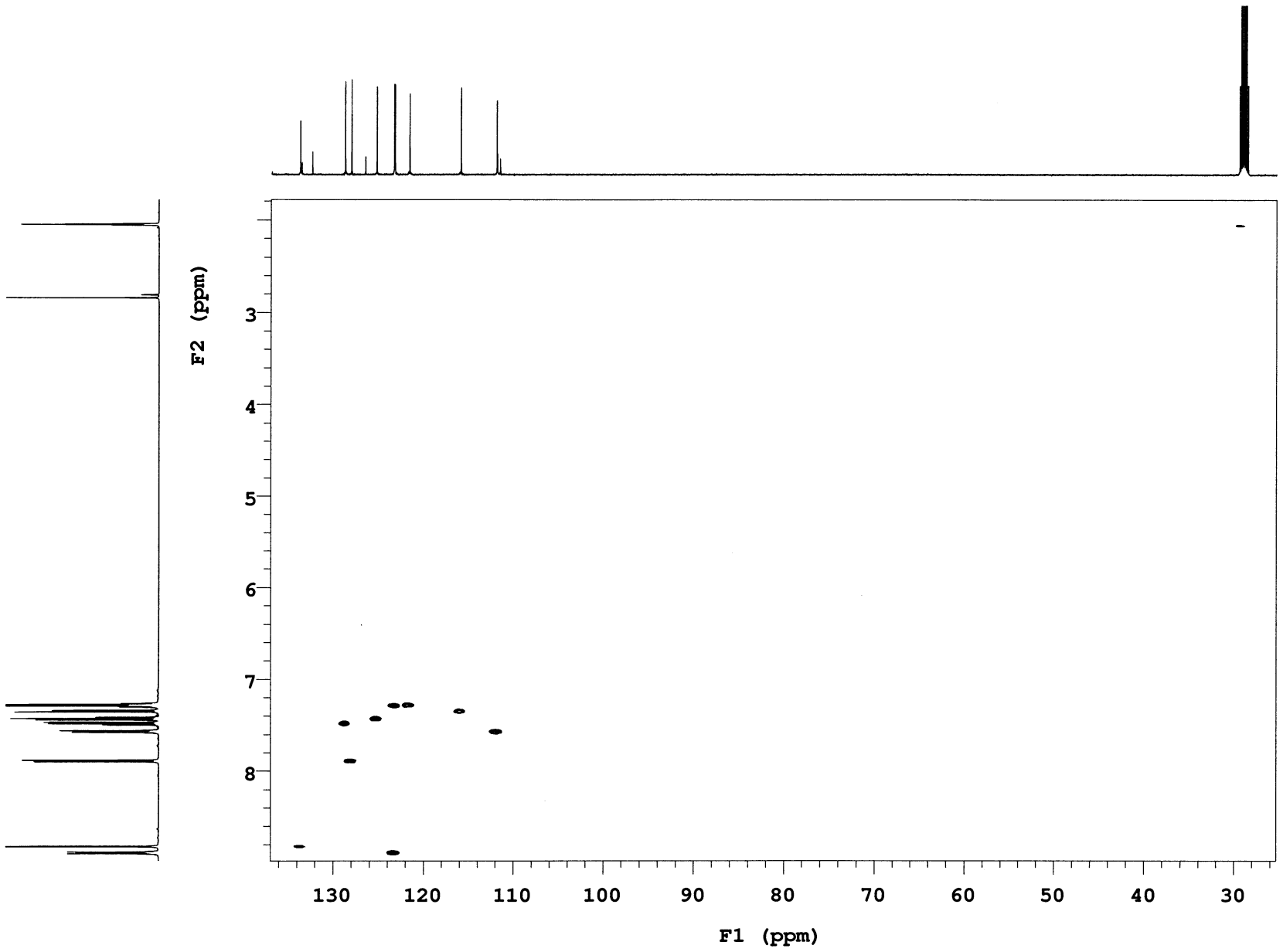
Fig S222. DEPT of compound 4ka

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-214/DEPT_01

Plot date 2017-03-28

APS-01-214

Sample Name **APS-01-214**	Pulse sequence **gHSQC**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-28**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-214/gHSQC_01

Fig S223. HSQC of compound 4ka

Plot date 2017-03-28

APS-01-214

Sample Name **APS-01-214**	Pulse sequence **gCOSY**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-03-28**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

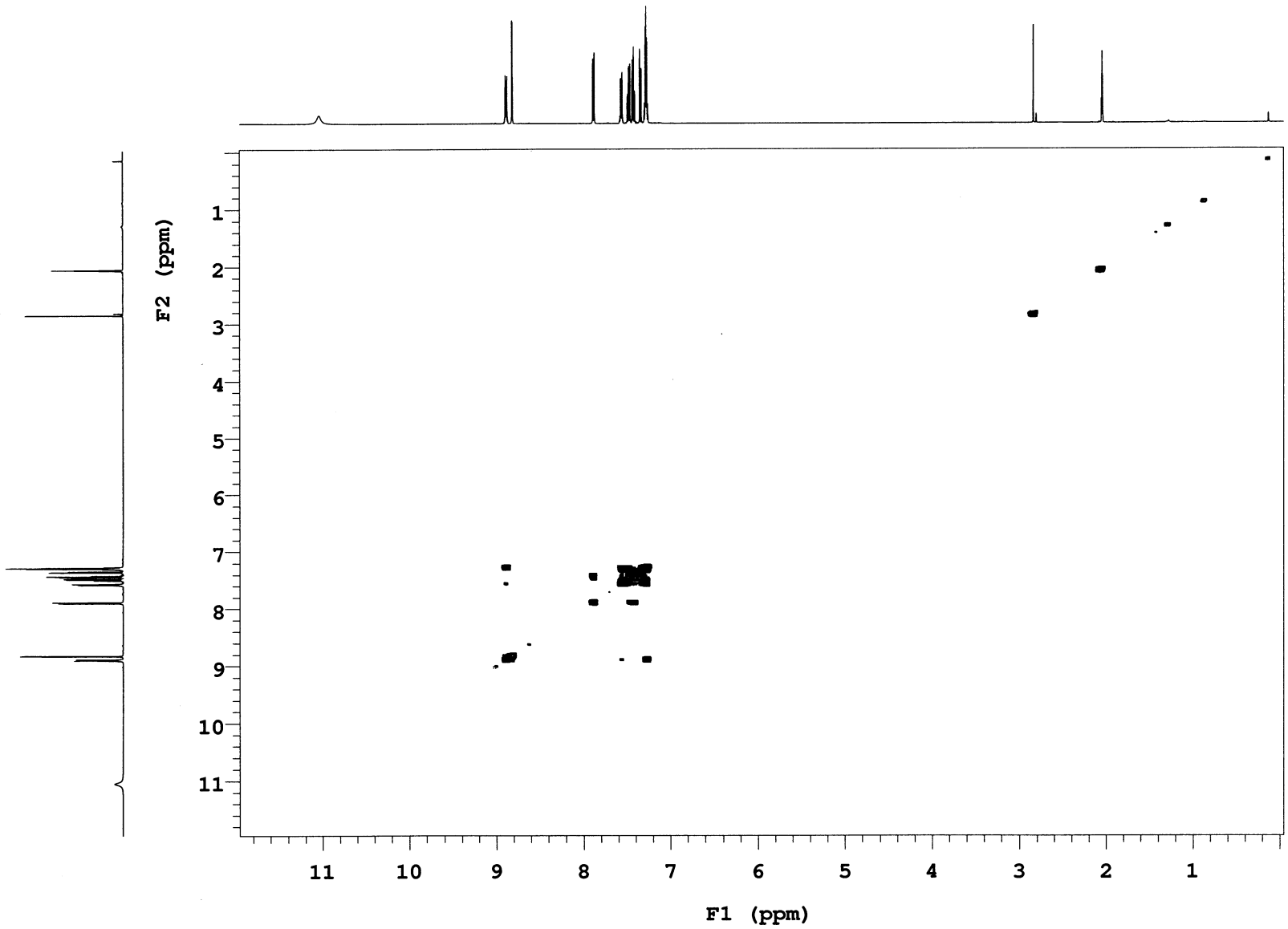


Fig S224. COSY of compound 4ka

APS-01-214

Sample Name	**APS-01-214**	Pulse sequence	**NOESY**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-03-28**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**

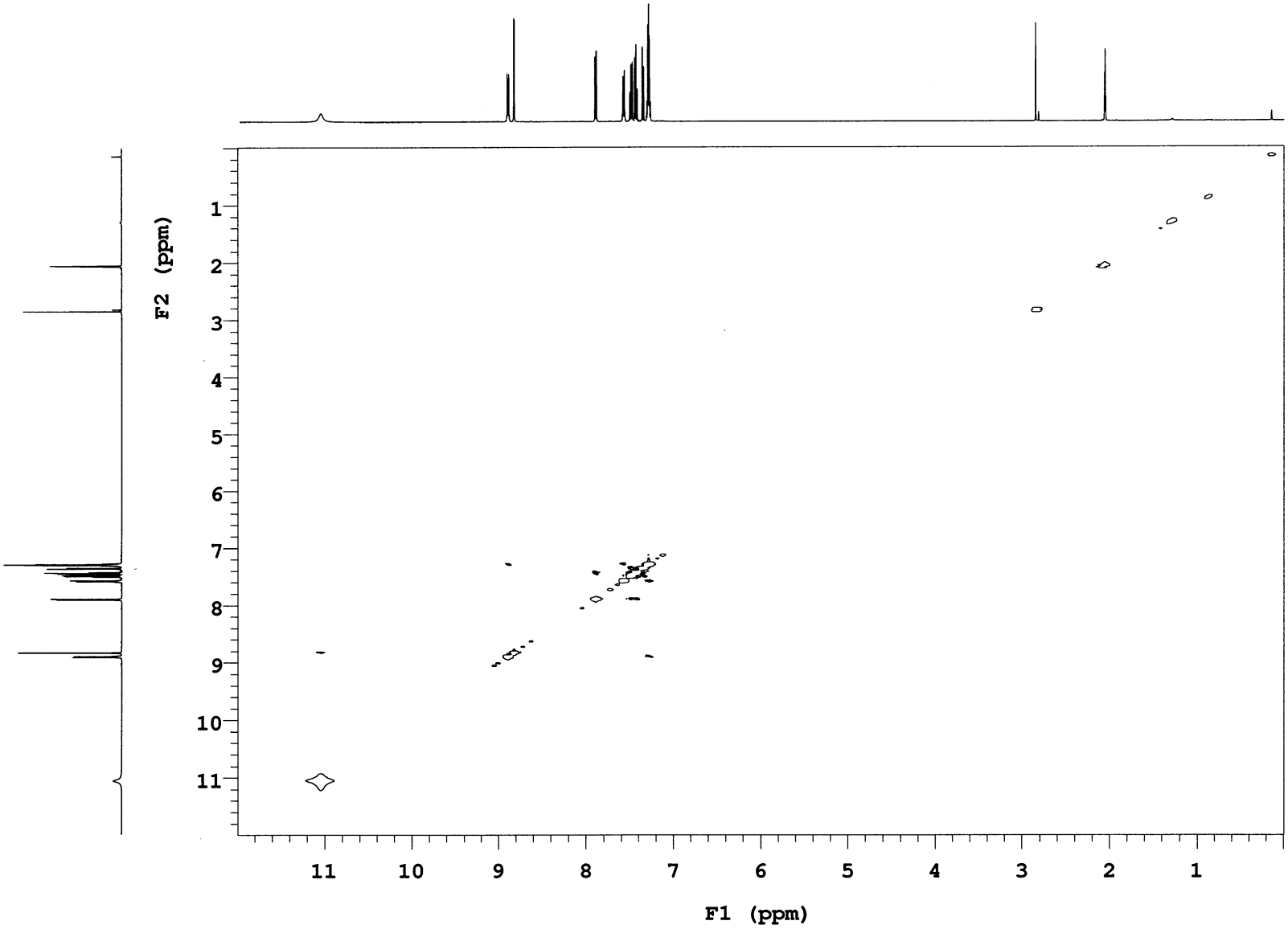
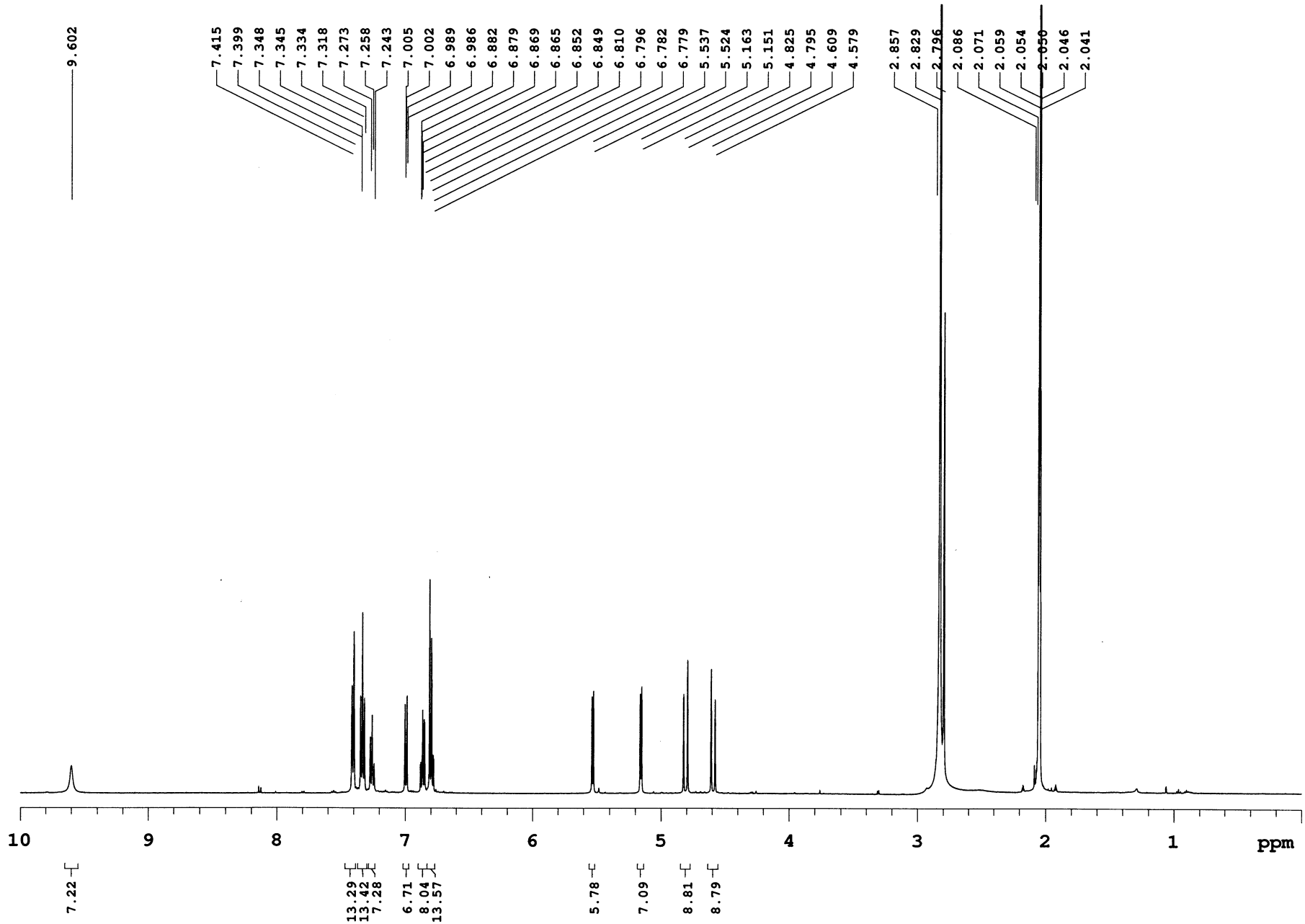


Fig S225. NOESY of compound 4ka

APS-01-215-Alcohol

Sample Name	**APS-01-215-Alcohol**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-06-15**	Solvent	**acetone**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-215-Alcohol/PROTON_04

Fig S226. 1H NMR (acetone-d6, 500 MHz) of compound 5

Plot date 2017-06-15

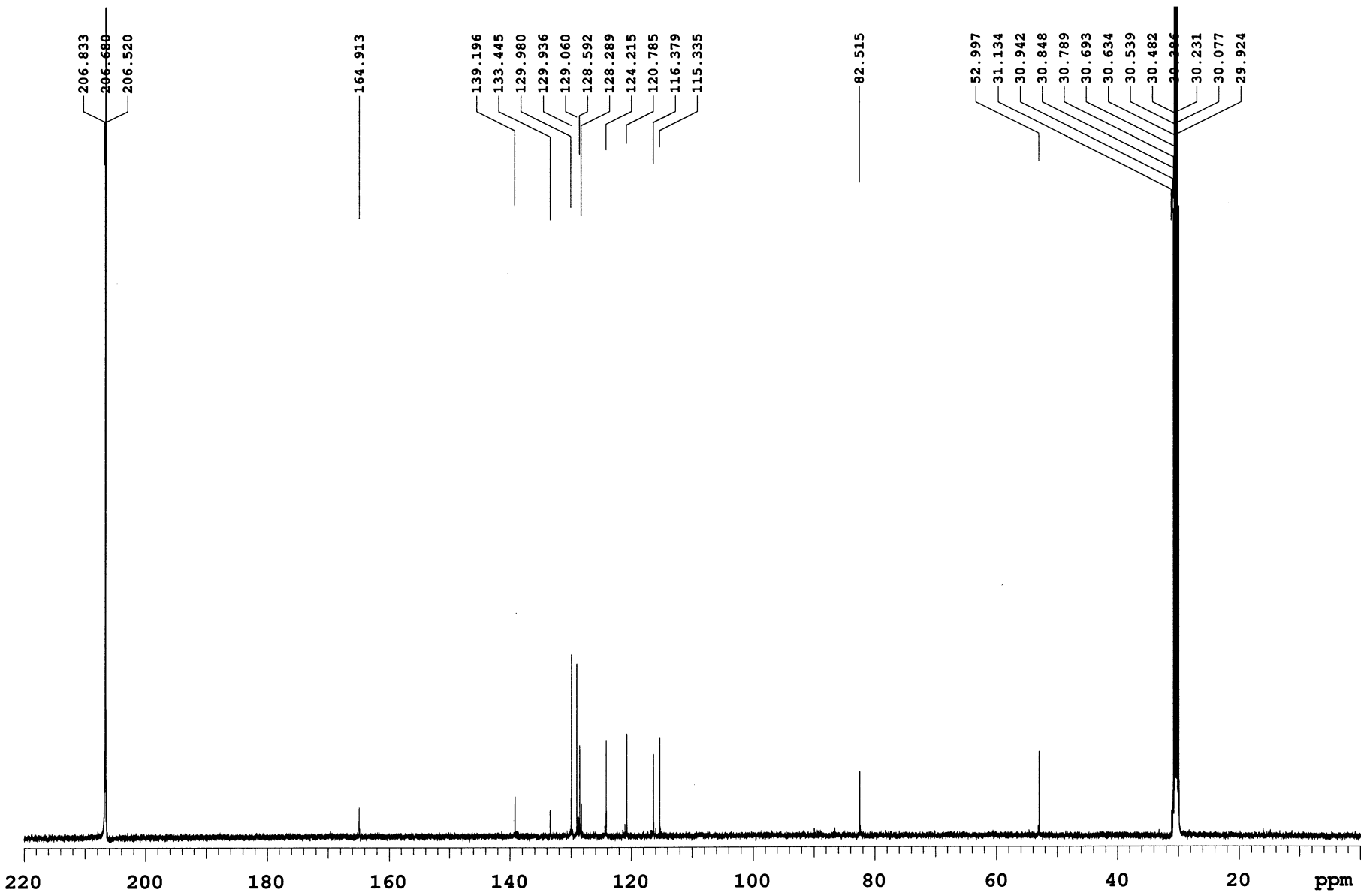


Fig S227. 13C NMR (acetone-d6, 125 MHz) of compound 5

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-156/CARBON_04

Plot date 2018-03-02

APS-01-215-Alcohol

Sample Name **APS-01-215-Alcohol**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-15**	Solvent **acetone**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

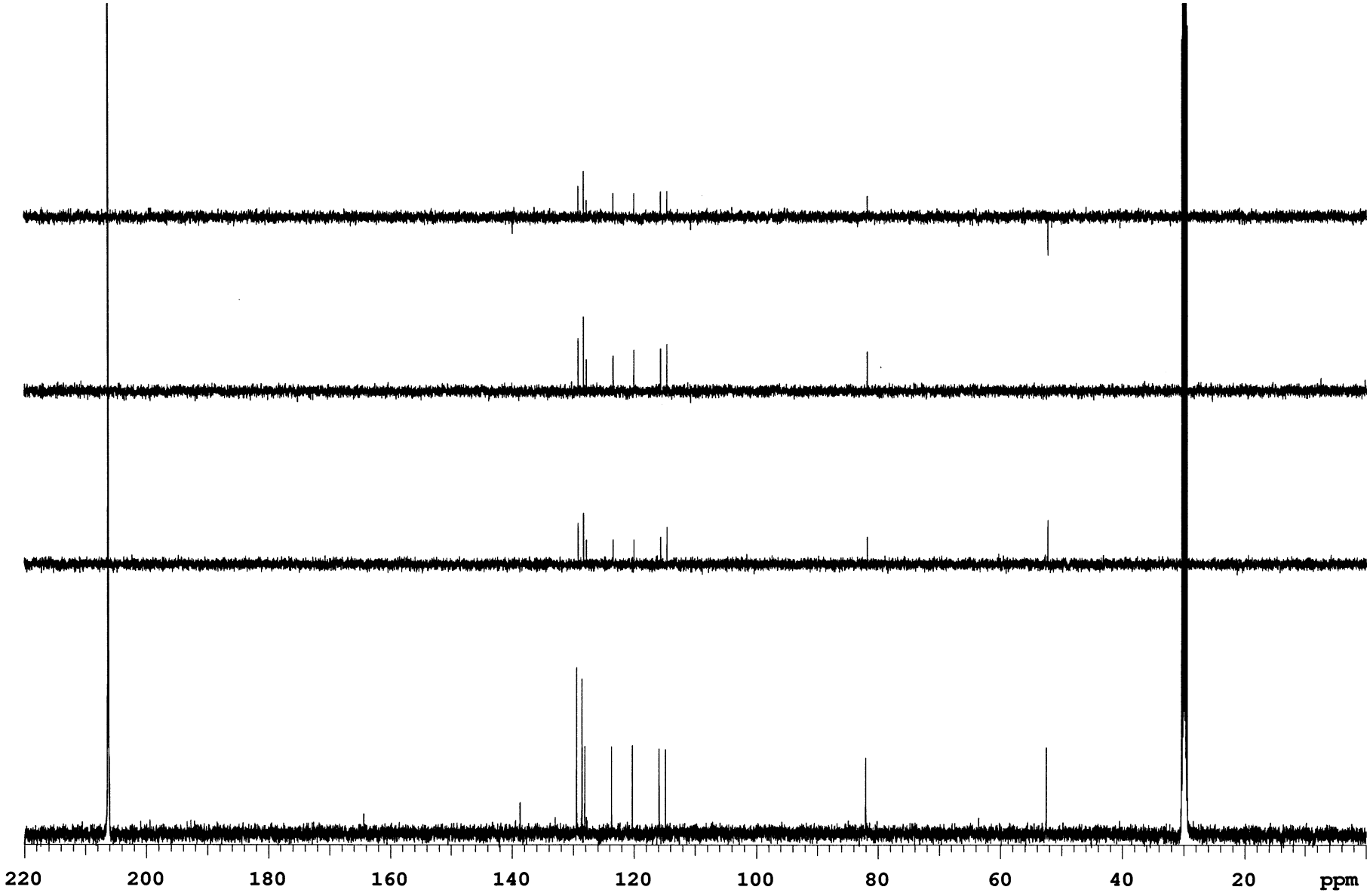
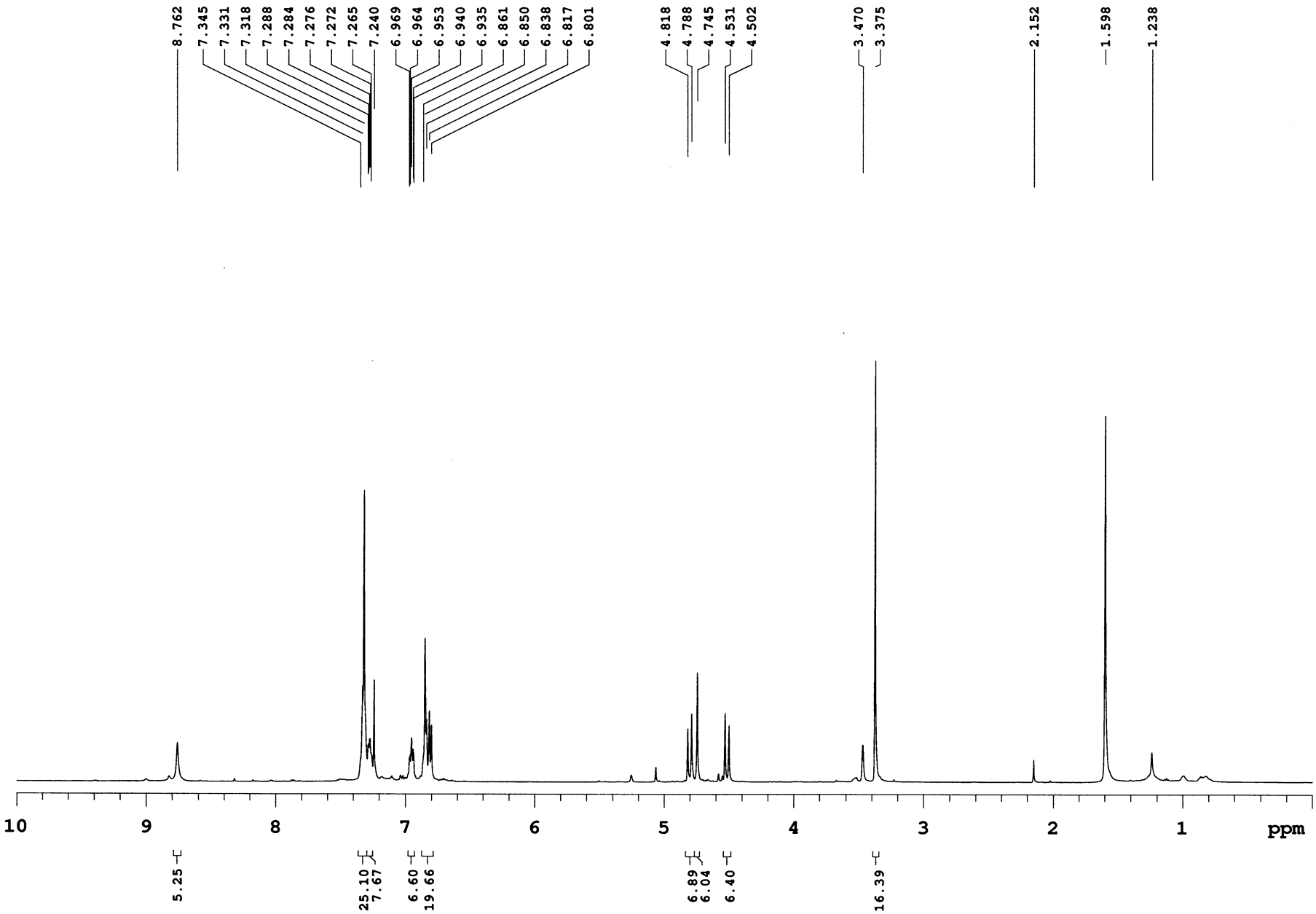


Fig S228. DEPT of compound 5

APS-01-215

Sample Name **APS-01-215**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-02**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-215/PROTON_07

Fig S229. 1H NMR (CDCl3, 500 MHz) of compound 6

Plot date 2017-06-05

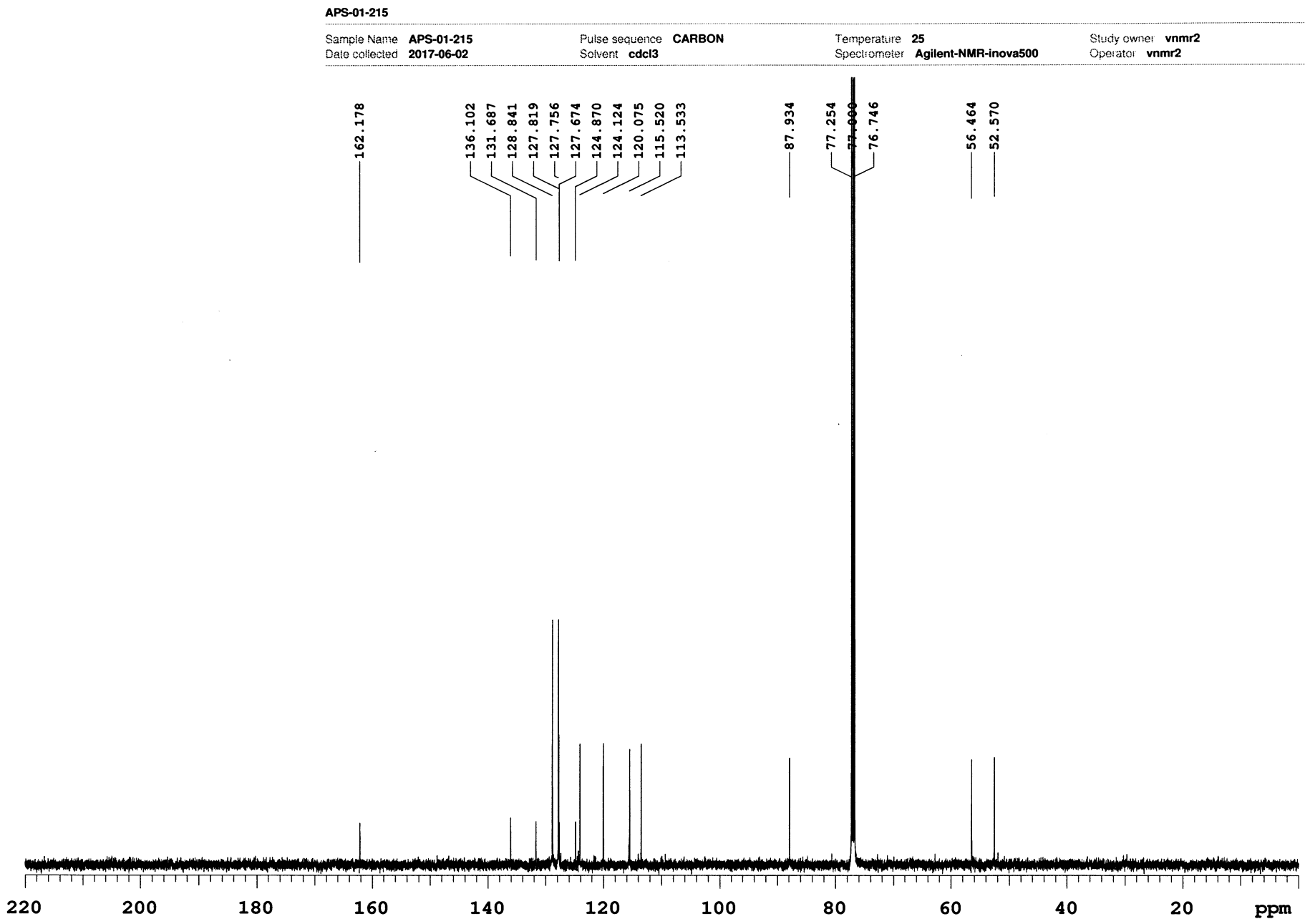


Fig S230. 13C NMR (CDCl3, 125 MHz) of compound 6

APS-01-215

Sample Name **APS-01-215**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-06-02**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

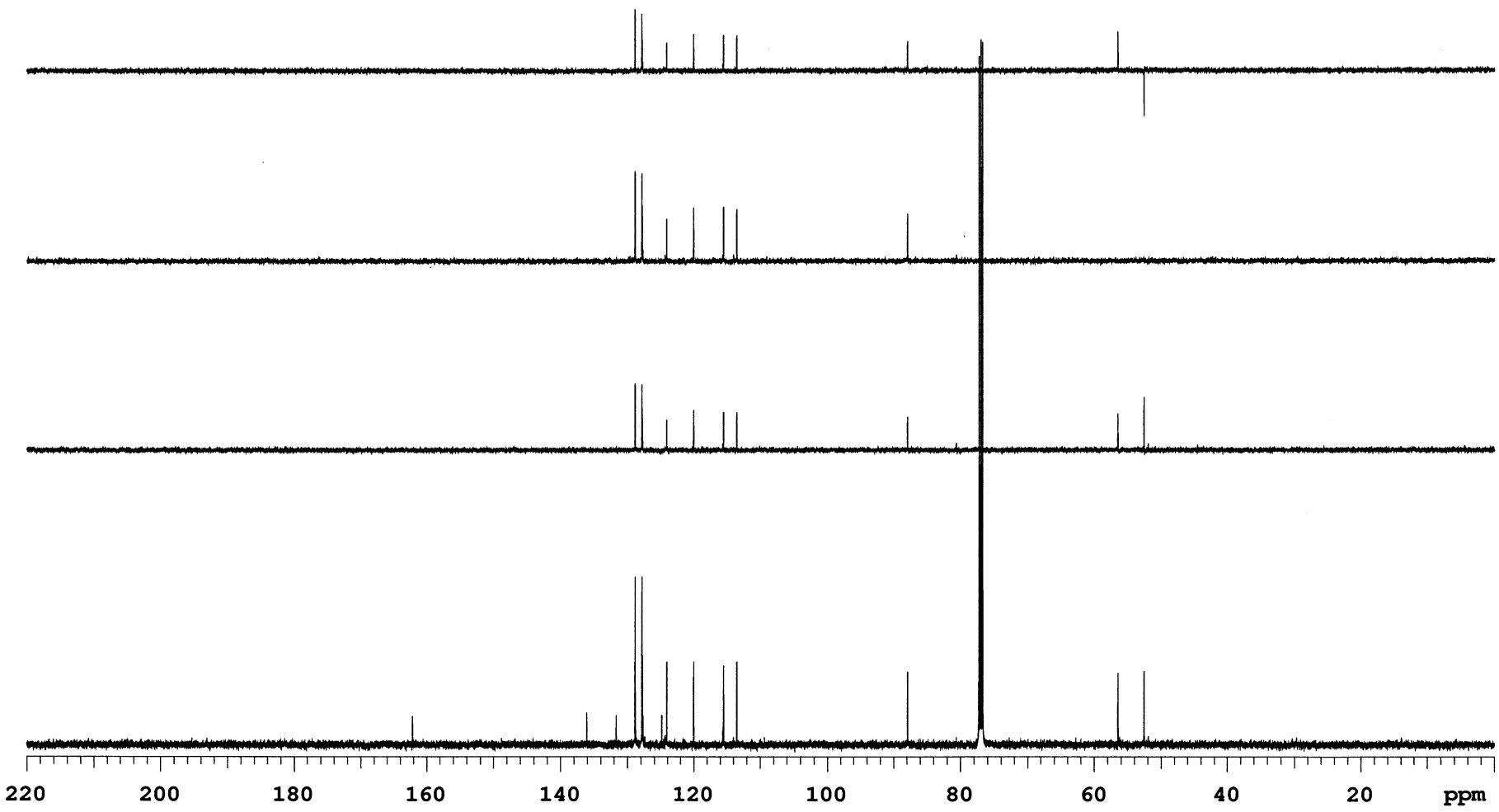
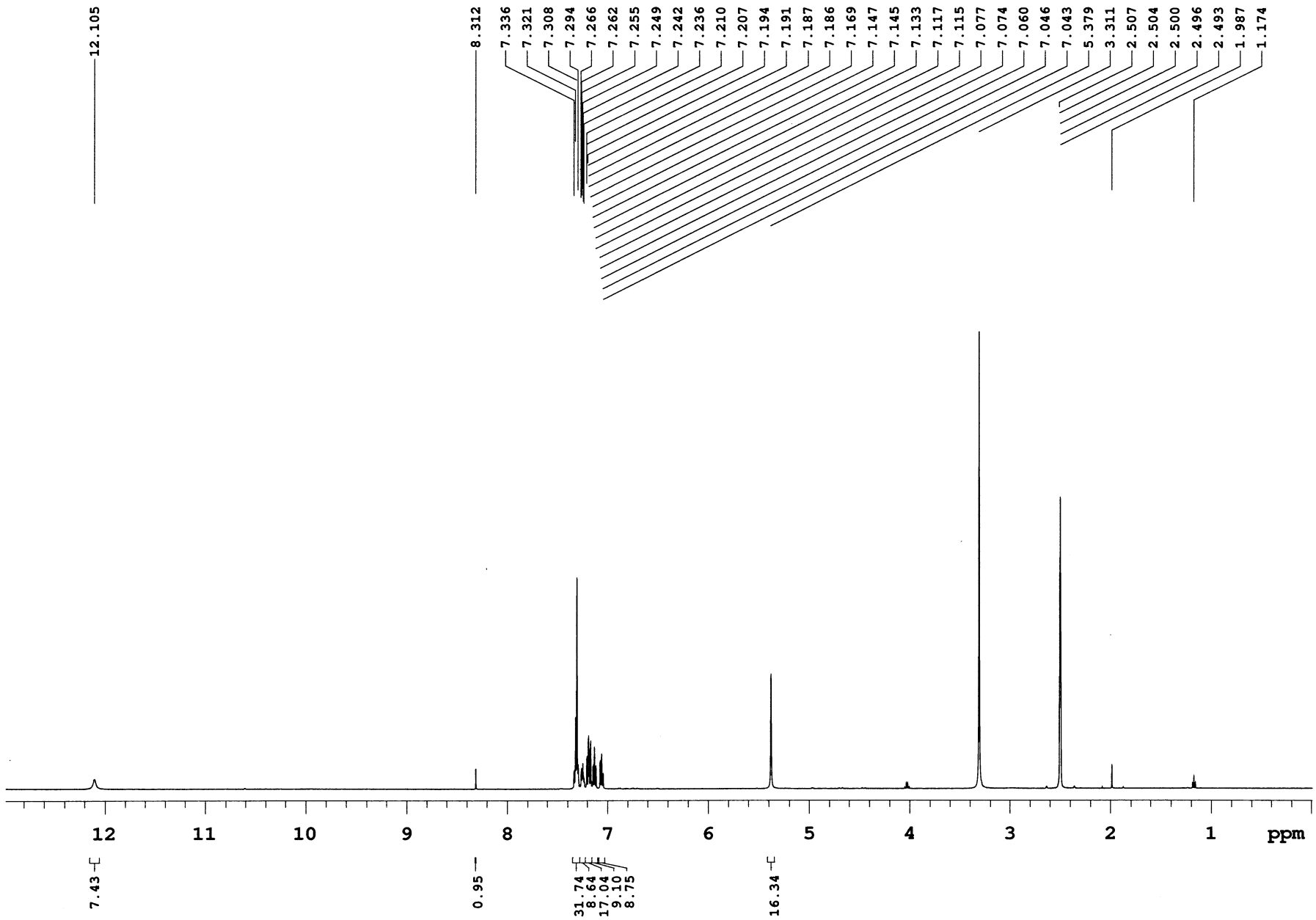


Fig S231. DEPT of compound 6

APS-01-234-polar

Sample Name **APS-01-234-polar**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-29**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-234-polar/PROTON_03

Plot date 2017-06-01

Fig S232. 1H NMR (DMSO-d6, 500 MHz) of compound 7

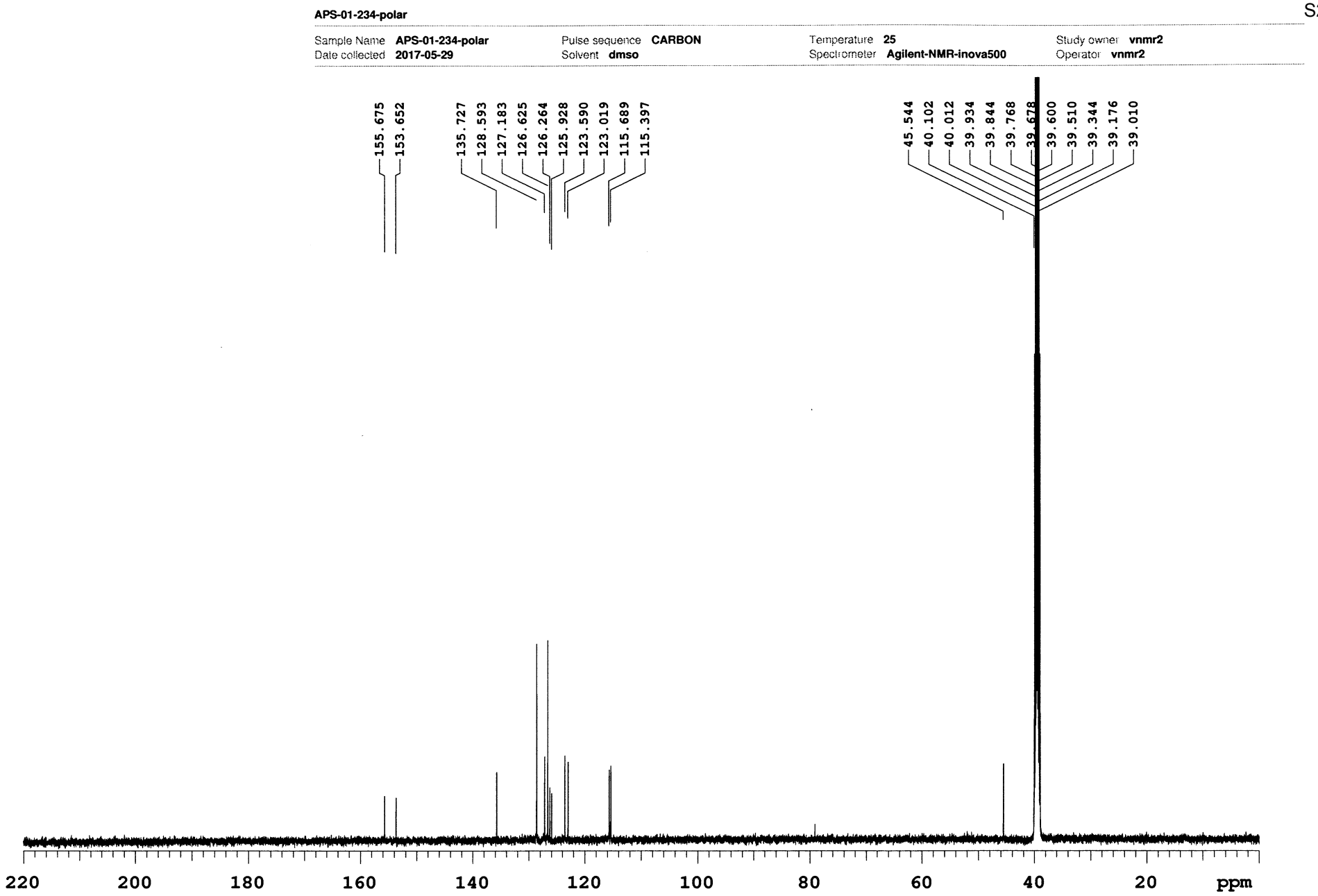


Fig S233. 13C NMR (DMSO-d6, 125 MHz) of compound 7

APS-01-234-polar

Sample Name **APS-01-234-polar**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-05-29**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

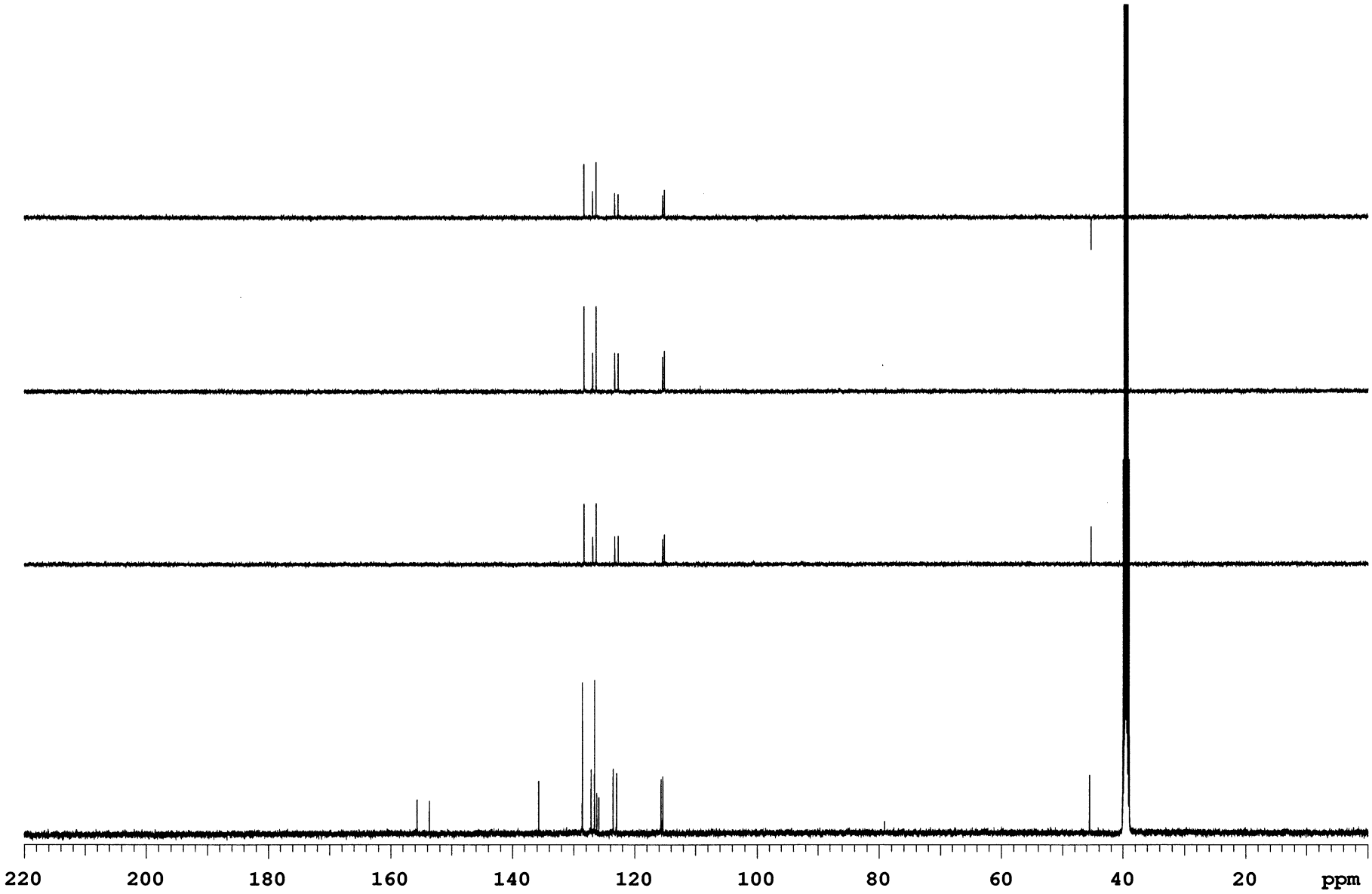
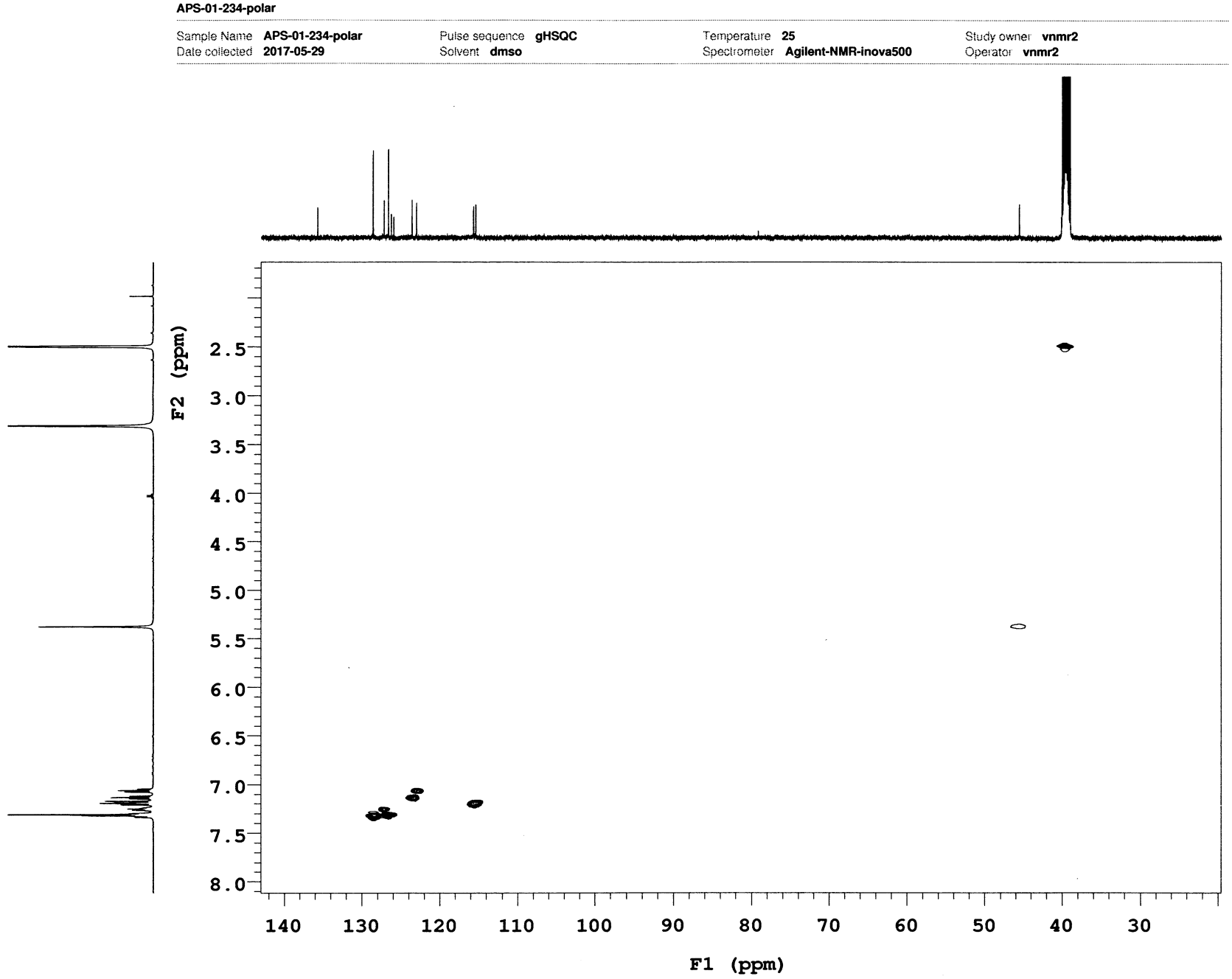


Fig S234. DEPT of compound 7

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-234-polar/DEPT_01

Plot date 2017-06-01



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-234-polar/gHSQC_01

Plot date 2017-06-01

Fig S235. HSQC of compound 7

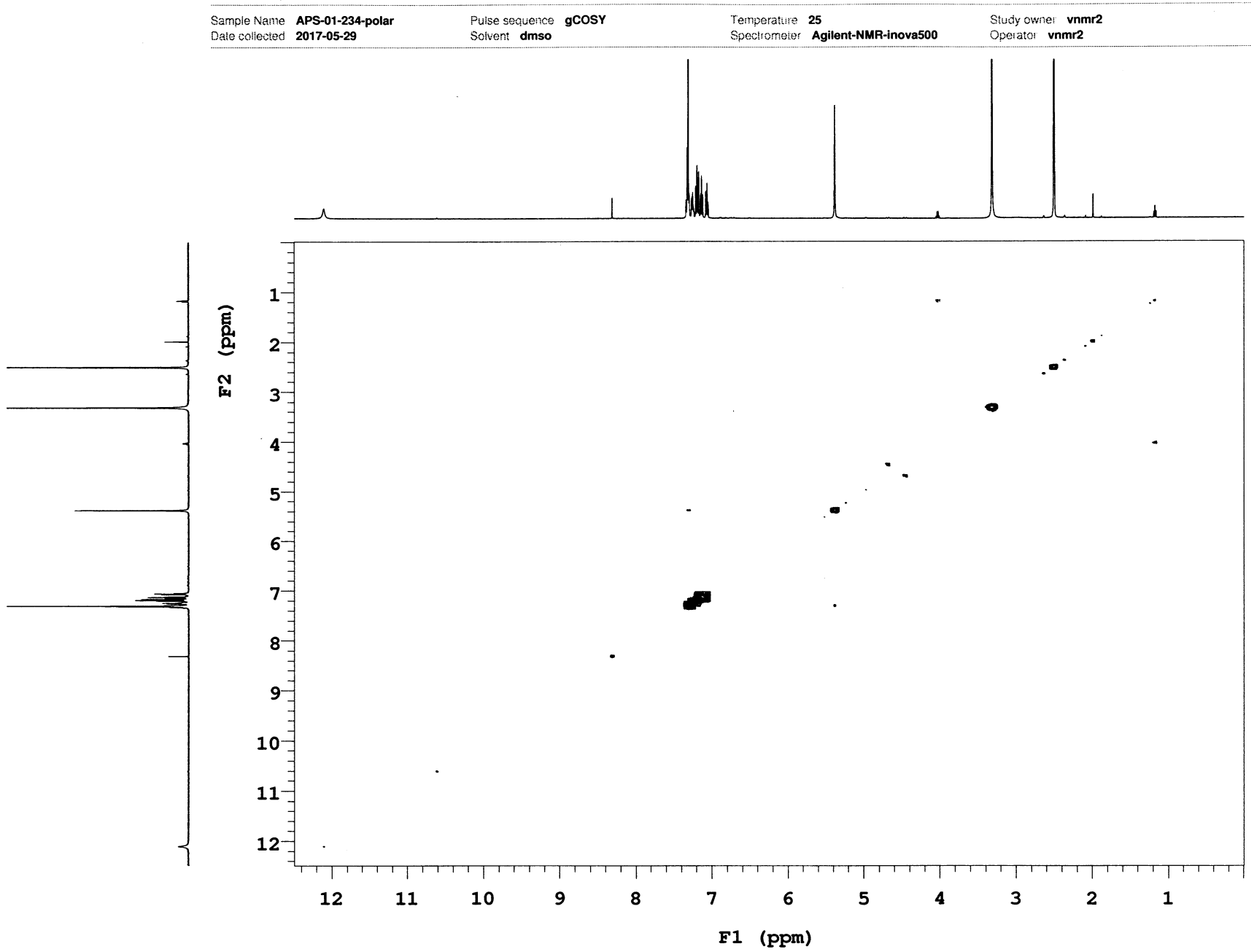
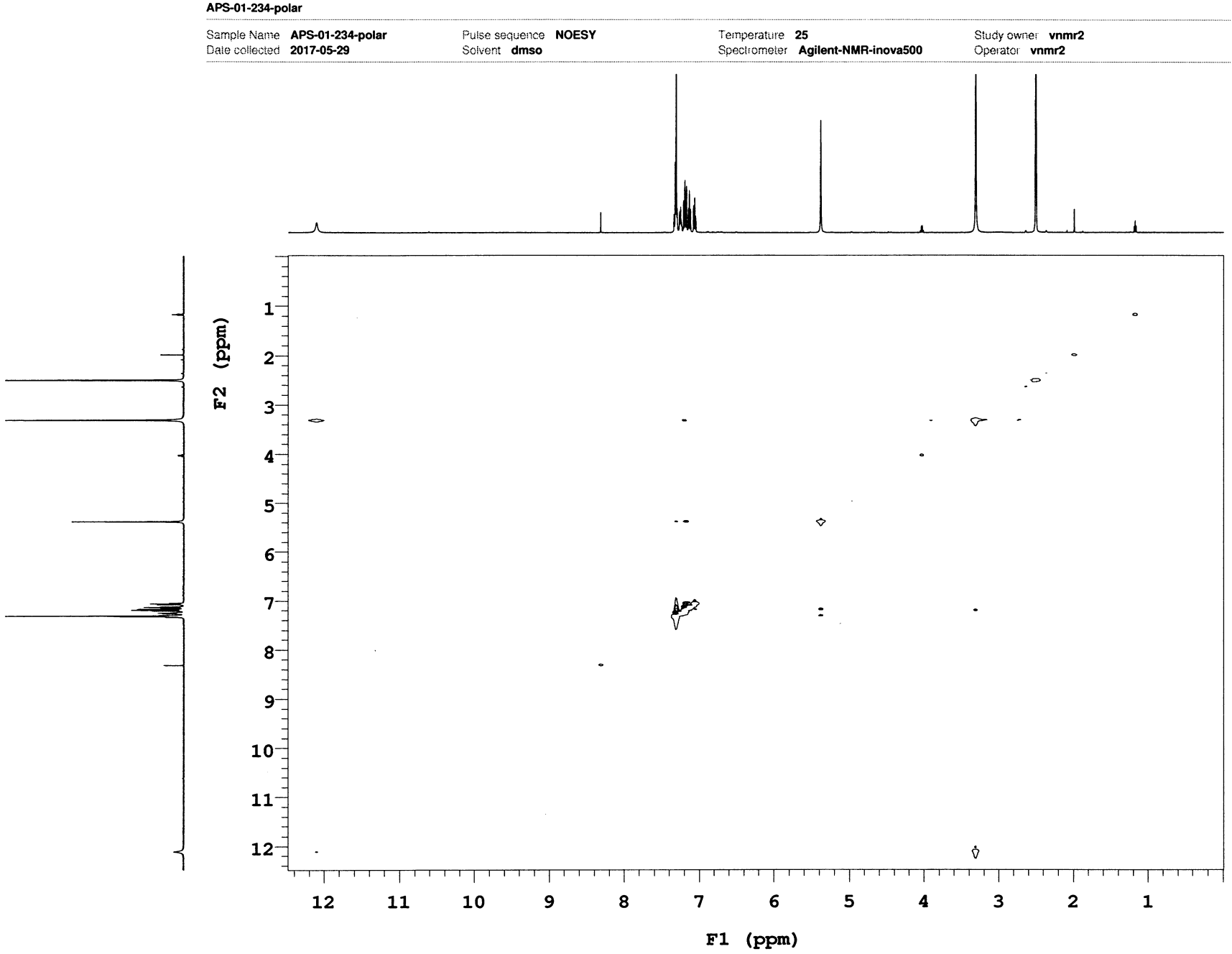


Fig S236. COSY of compound 7

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-234-polar/gCOSY_01

Plot date 2017-06-01



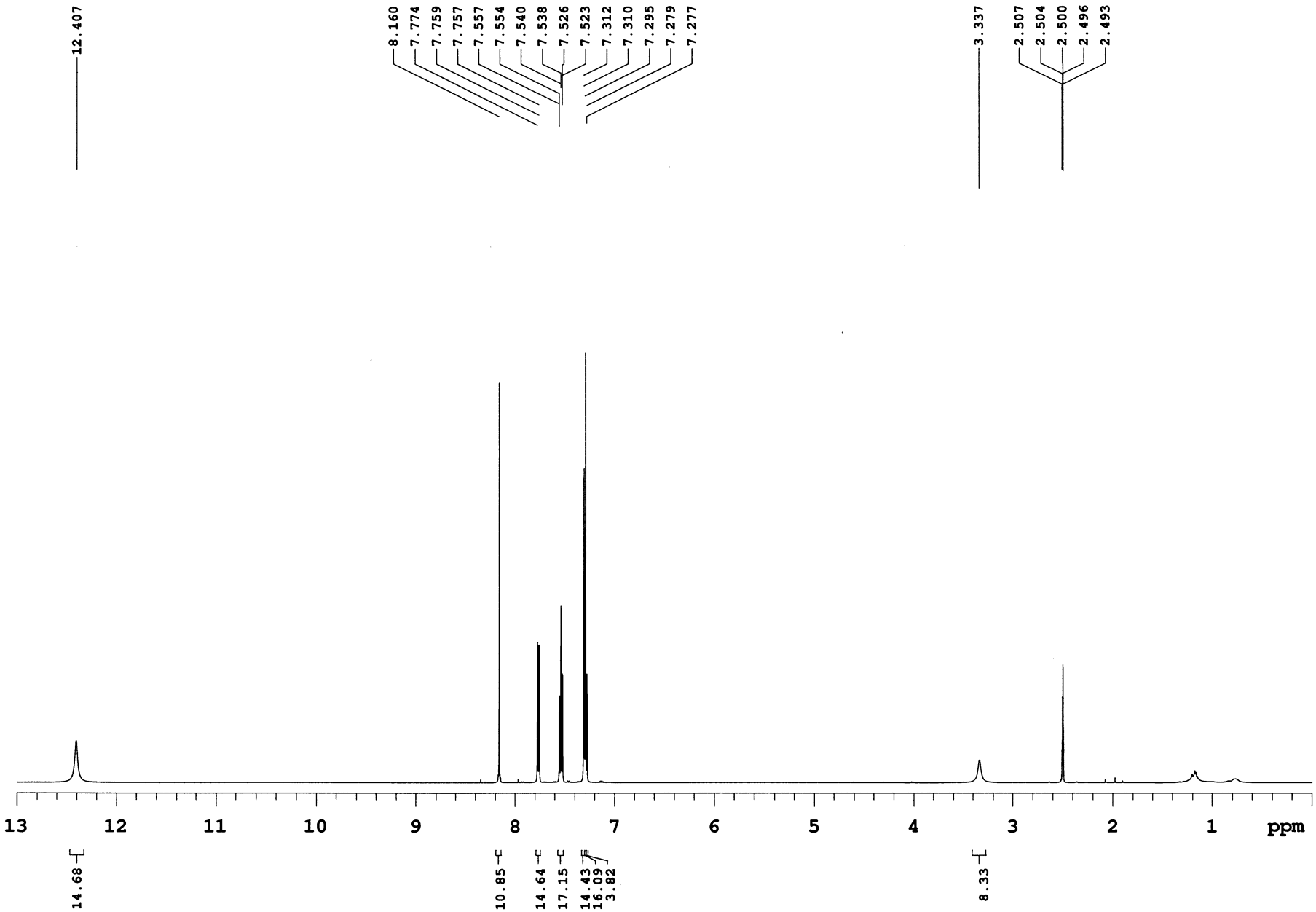
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-234-polar/NOESY_01

Fig S237. NOESY of compound 7

Plot date 2017-06-01

APS-162

Sample Name **APS-162**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2018-01-23**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-162/PROTON_04

Fig S238. 1H NMR (DMSO-d6, 500 MHz) of compound 8

Plot date 2018-01-23

APS-162

Sample Name **APS-162** | Pulse sequence **CARBON** | Temperature **25** | Study owner **vnmr2**
Date collected **2018-01-23** | Solvent **dmso** | Spectrometer **Agilent-NMR-inova500** | Operator **vnmr2**

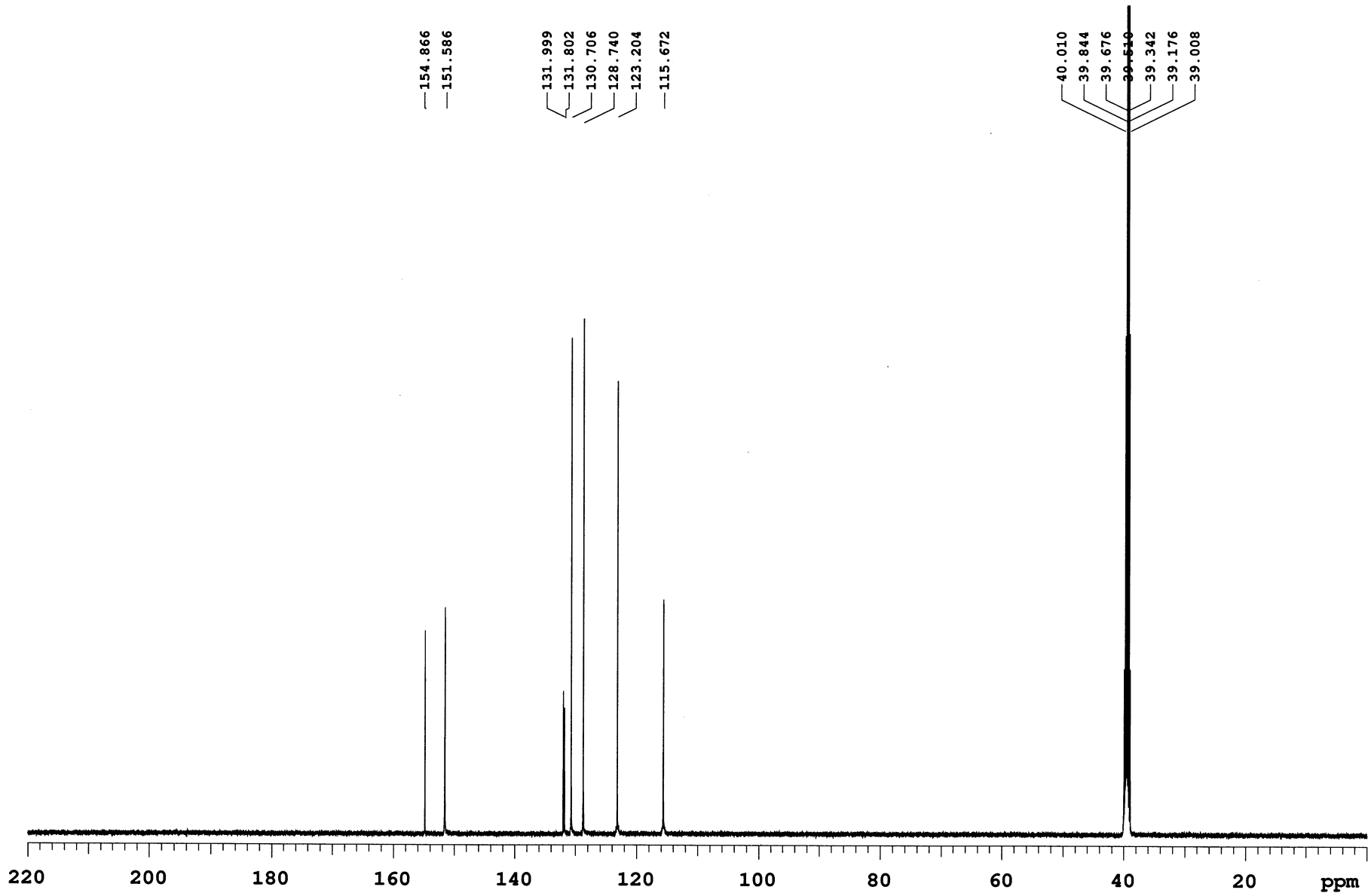


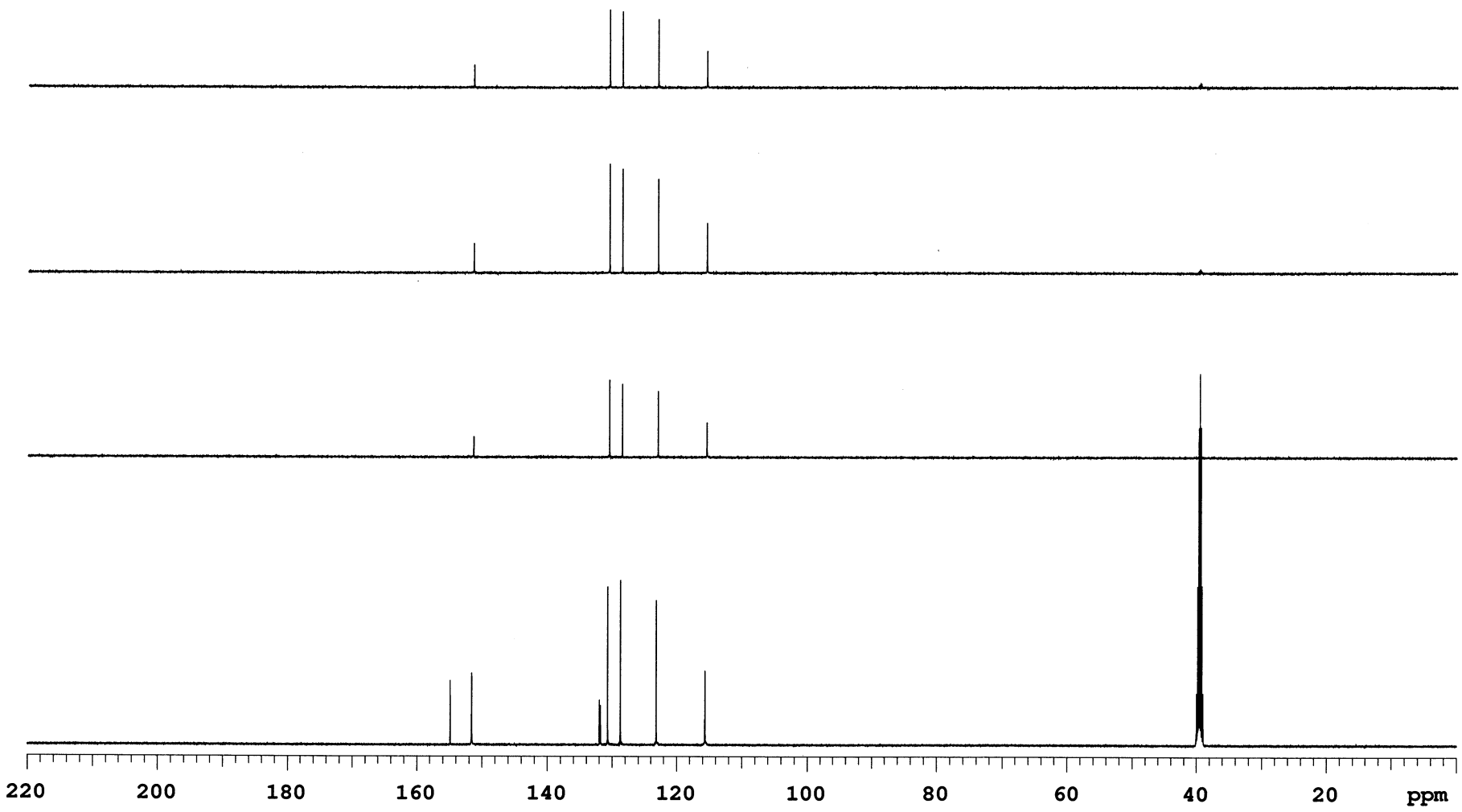
Fig S239. 13C NMR (DMSO-d6, 125 MHz) of compound 8

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-162/CARBON_02

Plot date 2018-01-23

APS-162

Sample Name **APS-162**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2018-01-23**	Solvent **dmso**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



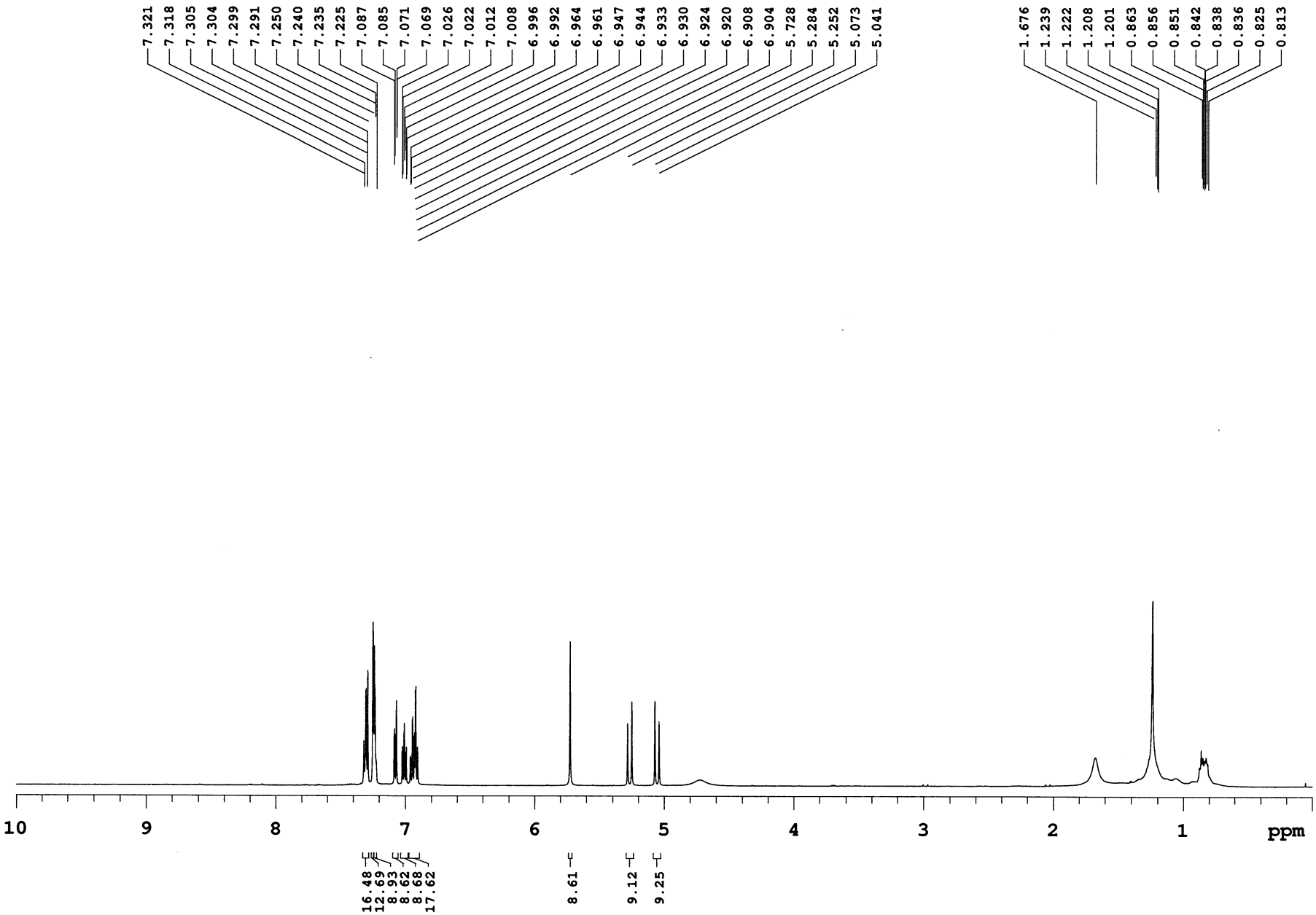
Data file /home/vnmr2/vnmrsys/data/511/APS/APS-162/DEPT_01

Fig S240. DEPT of compound 8

Plot date 2018-01-23

APS-01-195-f1

Sample Name	**APS-01-195-f1**	Pulse sequence	**PROTON**	Temperature	**25**	Study owner	**vnmr2**
Date collected	**2017-10-14**	Solvent	**cdcl3**	Spectrometer	**Agilent-NMR-inova500**	Operator	**vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-195-f1/PROTON_04

Fig S241. 1H NMR (CDCl3, 500 MHz) of compound 9

Plot date 2017-10-16

APS-01-195-f1

Sample Name **APS-01-195-f1**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-10-14**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

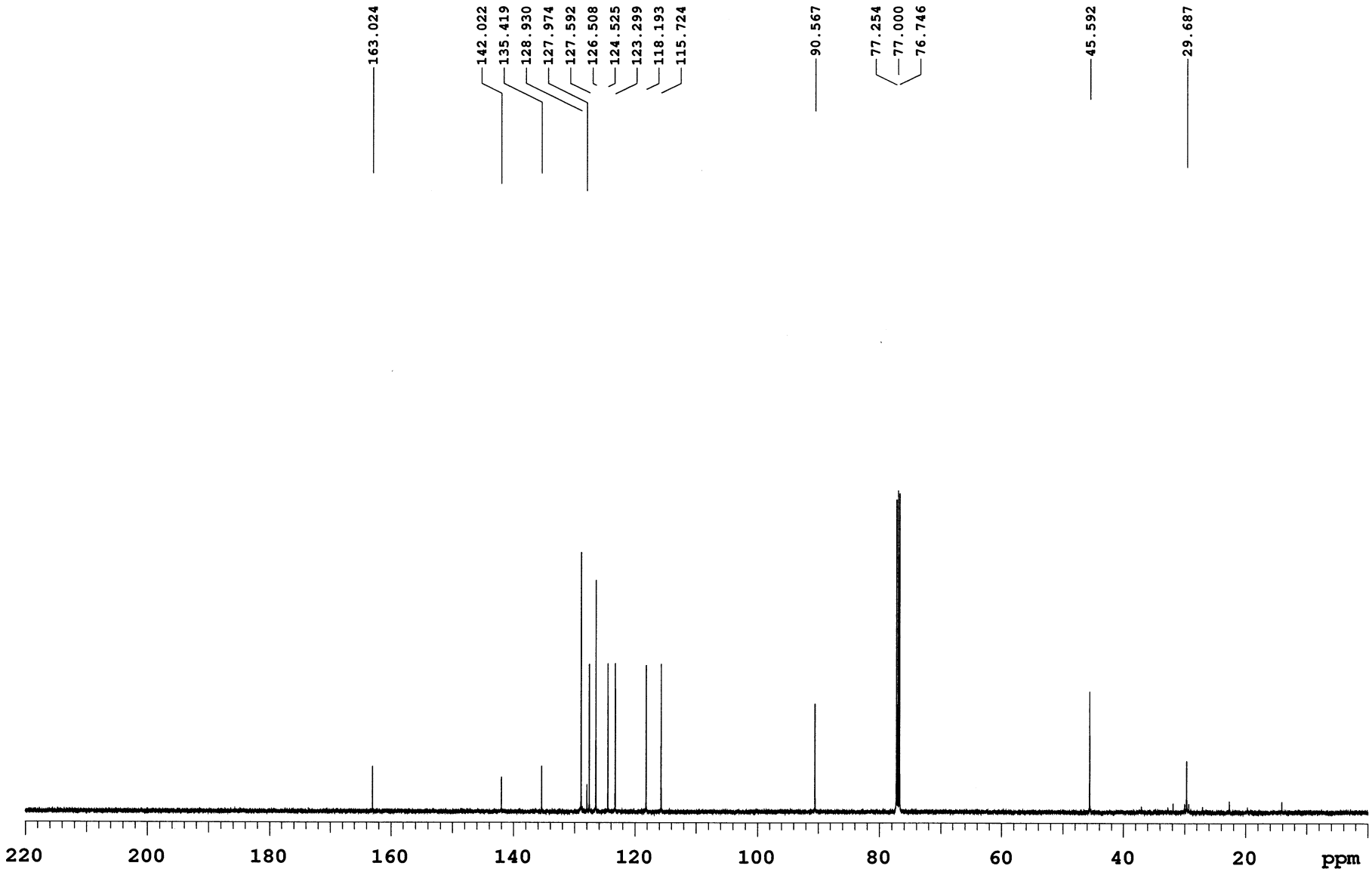


Fig S242. 13C NMR (CDCl3, 125 MHz) of compound 9

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-195-f1/CARBON_02

Plot date 2017-10-16

APS-01-195-f1

Sample Name **APS-01-195-f1**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-10-14**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

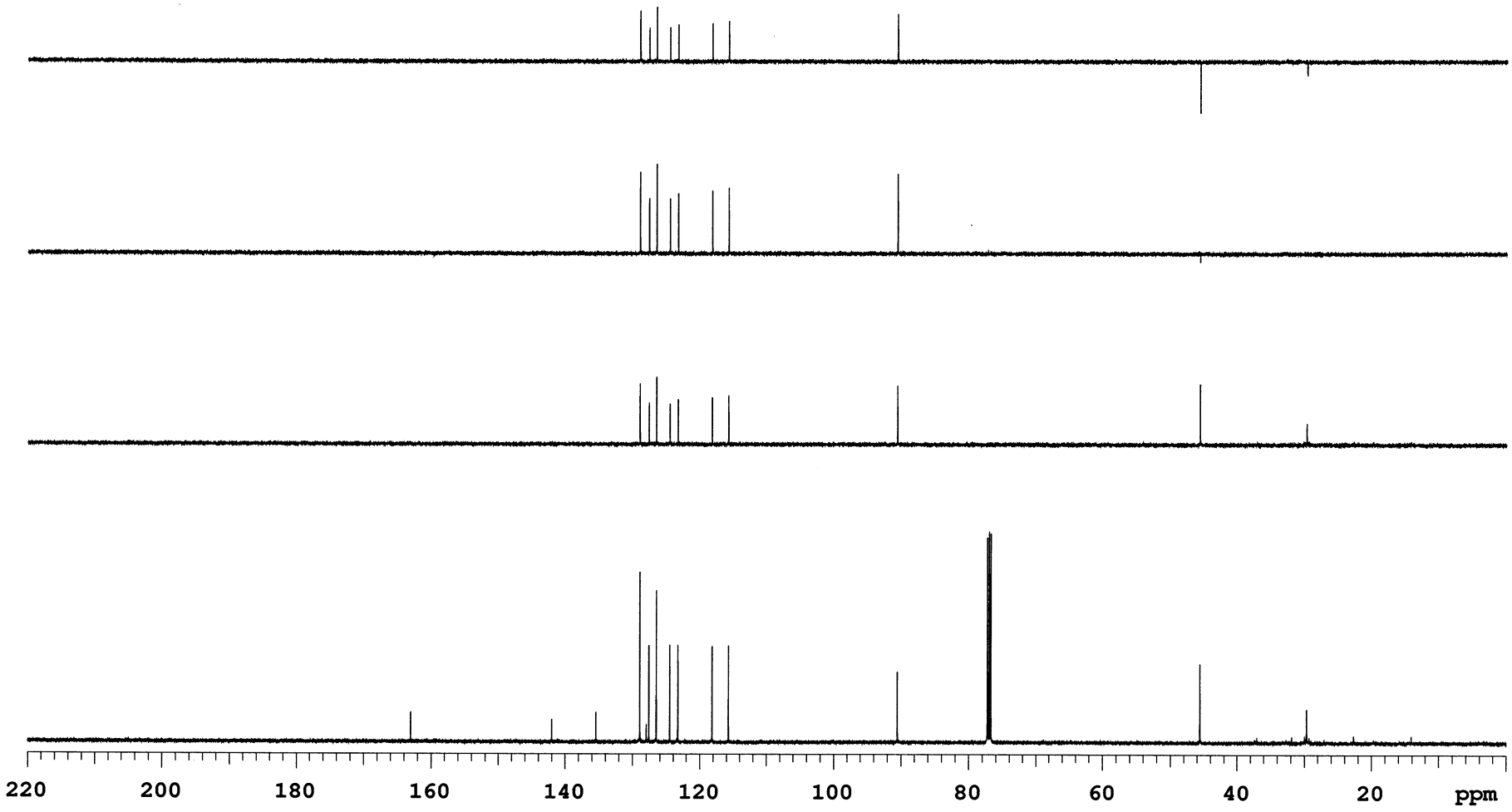
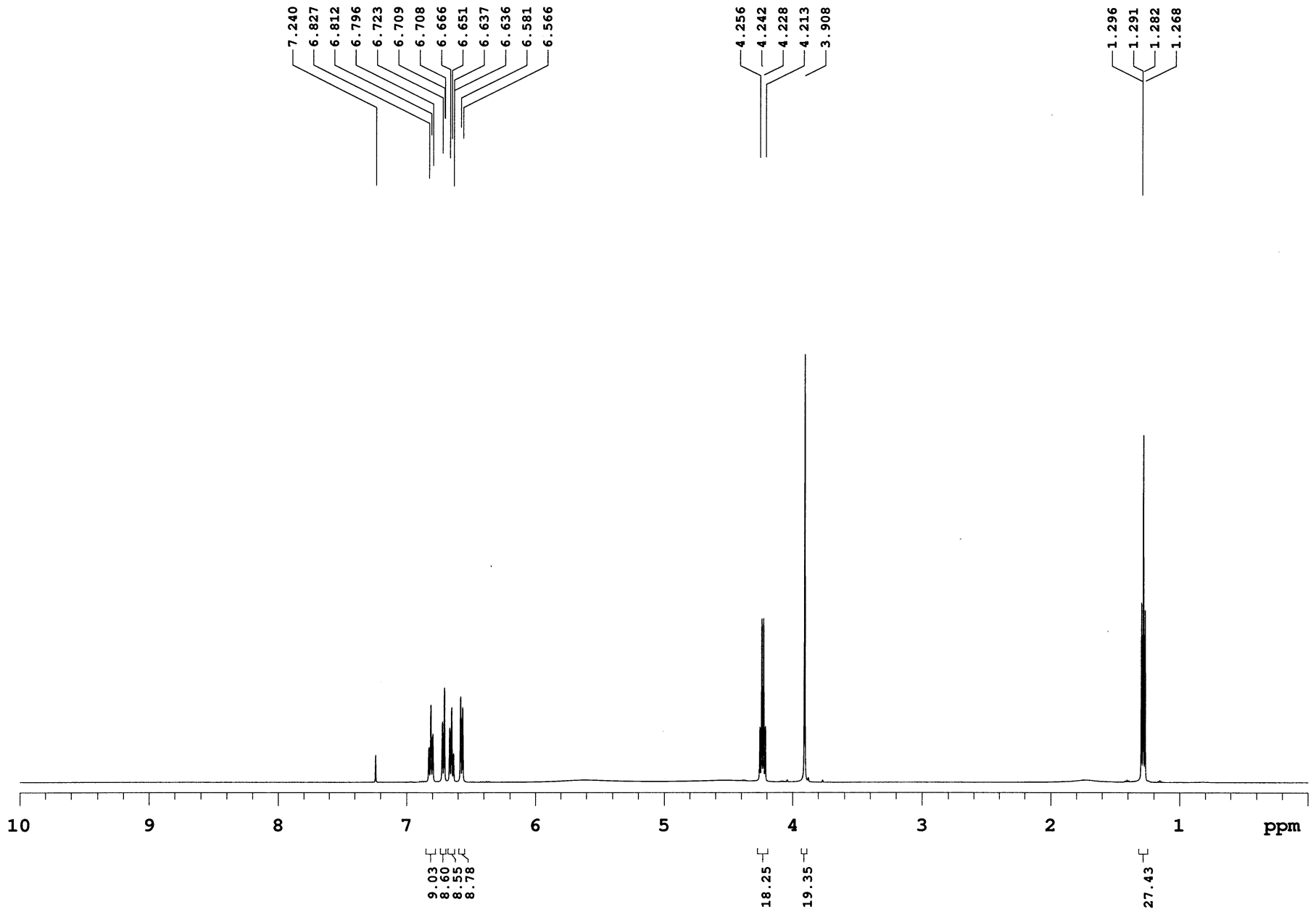


Fig S243. DEPT of compound 9

APS-01-209

Sample Name **APS-01-209**	Pulse sequence **PROTON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-06**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**



Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-209/PROTON_03

Plot date 2017-04-07

Fig S244. 1H NMR (CDCl3, 500 MHz) of compound APS-135

APS-01-209

Sample Name **APS-01-209**	Pulse sequence **CARBON**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-06**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

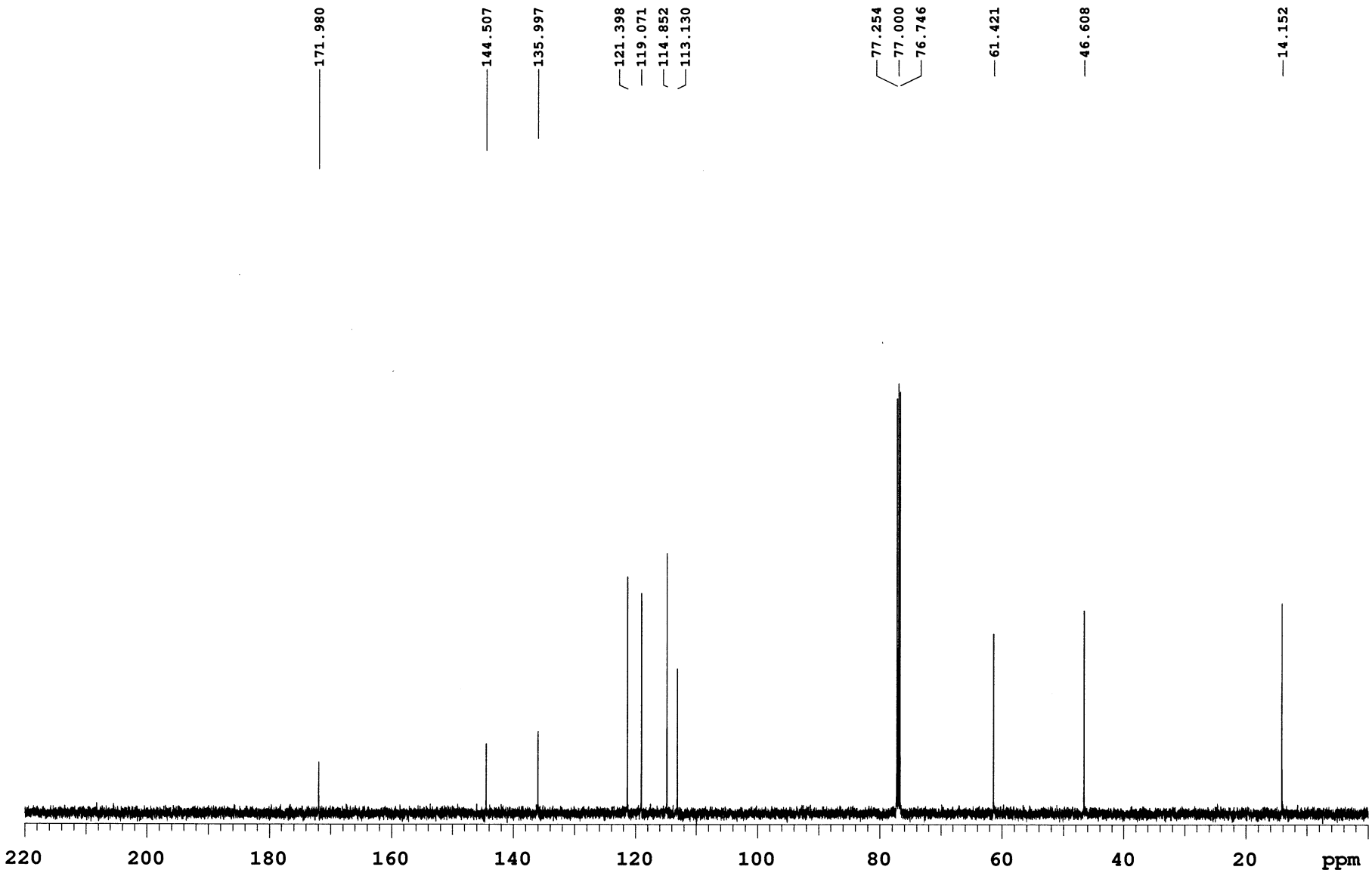


Fig S245. 13C NMR (CDCl3, 125 MHz) of compound APS-135

Data file /home/vnmr2/vnmrsys/data/511/APS/APS-01-209/CARBON_02

Plot date 2017-04-07

APS-01-209

Sample Name **APS-01-209**	Pulse sequence **DEPT**	Temperature **25**	Study owner **vnmr2**
Date collected **2017-04-06**	Solvent **cdcl3**	Spectrometer **Agilent-NMR-inova500**	Operator **vnmr2**

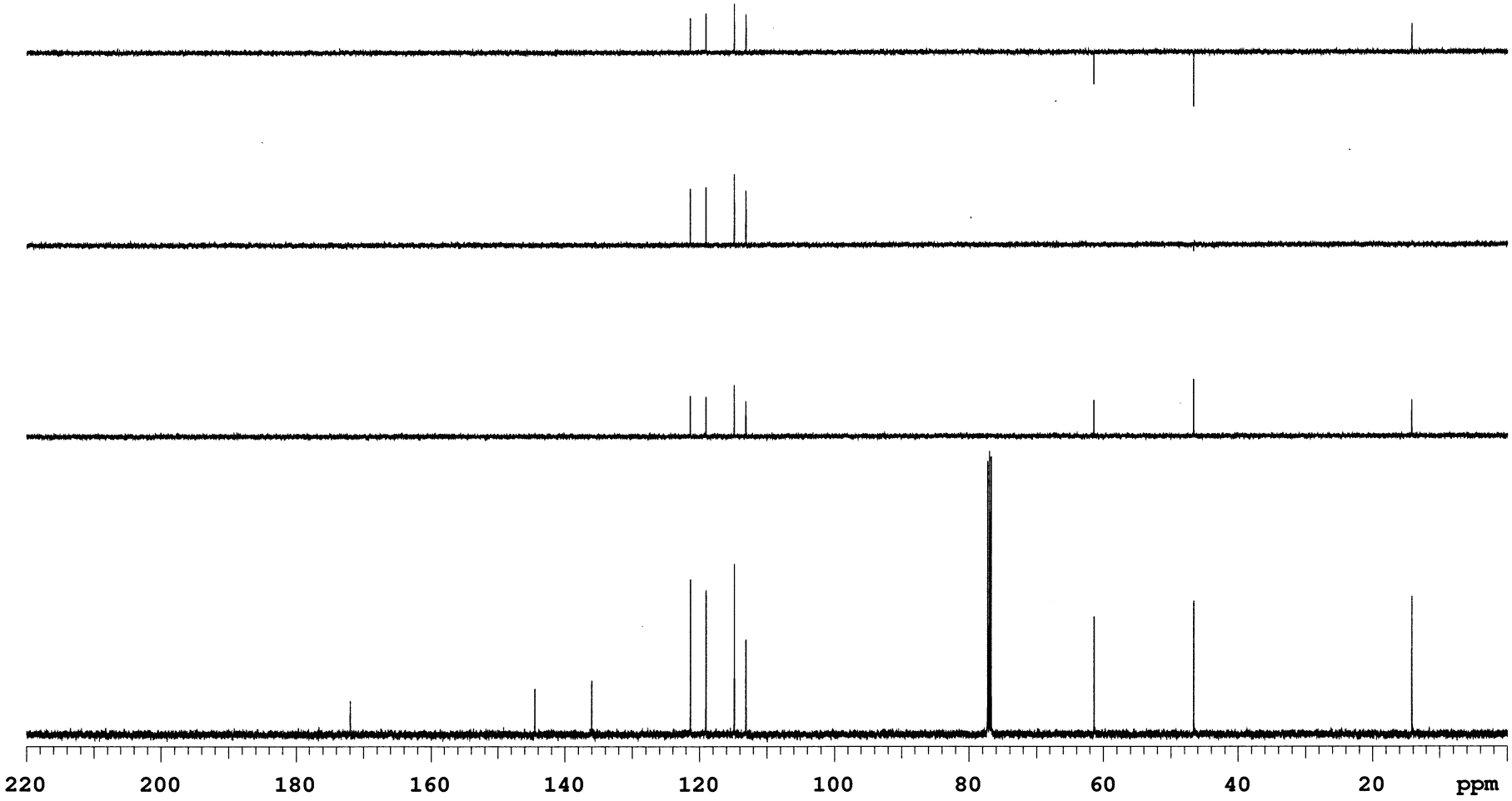


Fig S246. DEPT of compound APS-135