

Supporting Information

Asymmetric Synthesis of Spirocyclopentane Oxindoles Containing Four Consecutive Stereocenters and Quaternary α -Nitro Esters via Organocatalytic Enantioselective Michael–Michael Cascade Reactions

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SUPPORTING INFORMATION:

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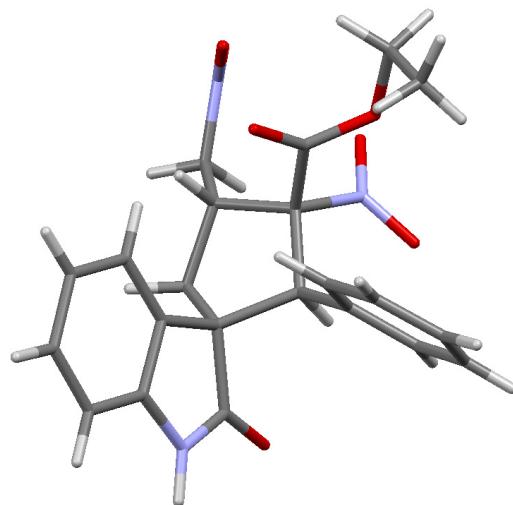
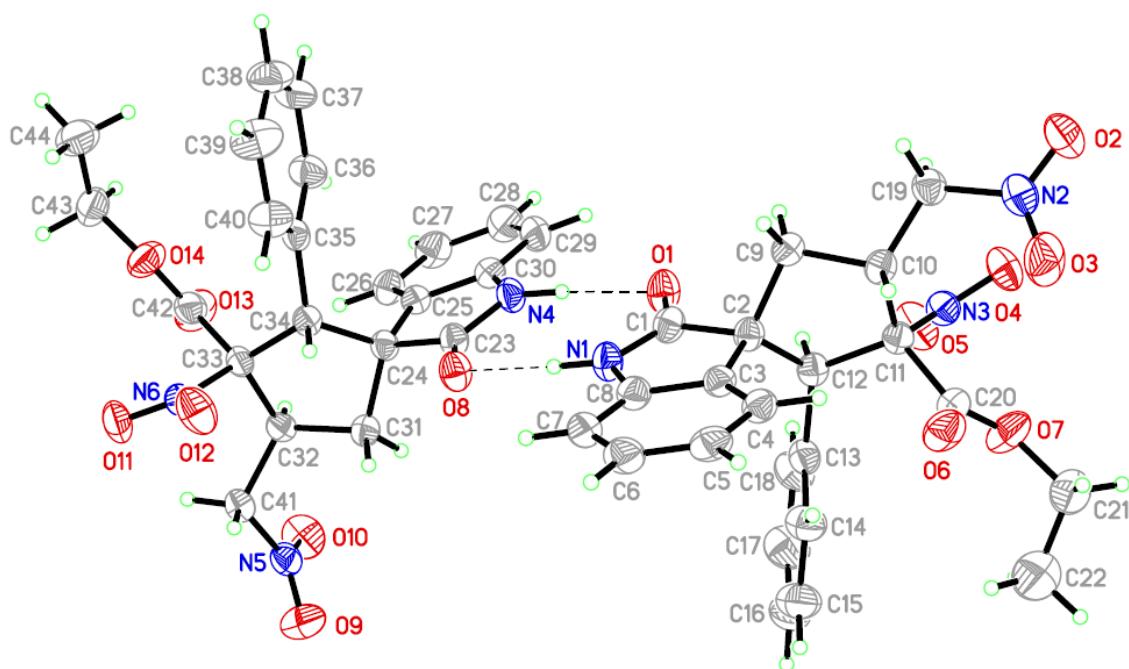


Figure S1. ORTEP and Stereo plots for X-ray crystal structures of (\pm)-3a (ic18895).

CCDC 1867291 contains the supplementary crystallographic data for (\pm)-3a (ic18895). 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 (\pm)-**3a** (**ic18895**).

Table 1. Crystal data and structure refinement for ic18895.

Identification code	ic18895		
Empirical formula	C ₂₂ H ₂₁ N ₃ O ₇		
Formula weight	439.42		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Monoclinic		
Space group	P2 ₁ /c		
Unit cell dimensions	a = 12.6555(3) Å	α= 90°.	
	b = 32.3648(7) Å	β= 104.6466(12)°.	
	c = 10.7780(2) Å	γ = 90°.	
Volume	4271.13(16) Å ³		
Z	8		
Density (calculated)	1.367 Mg/m ³		
Absorption coefficient	0.869 mm ⁻¹		
F(000)	1840		
Crystal size	0.410 x 0.027 x 0.025 mm ³		
Theta range for data collection	2.730 to 69.992°.		
Index ranges	-15<=h<=14, -32<=k<=39, -13<=l<=13		
Reflections collected	18688		
Independent reflections	8049 [R(int) = 0.0340]		
Completeness to theta = 67.679°	100.0 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7533 and 0.6358		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	8049 / 34 / 604		
Goodness-of-fit on F ²	1.075		
Final R indices [I>2sigma(I)]	R1 = 0.0783, wR2 = 0.2337		
R indices (all data)	R1 = 0.0981, wR2 = 0.2506		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.450 and -0.539 e.Å ⁻³		

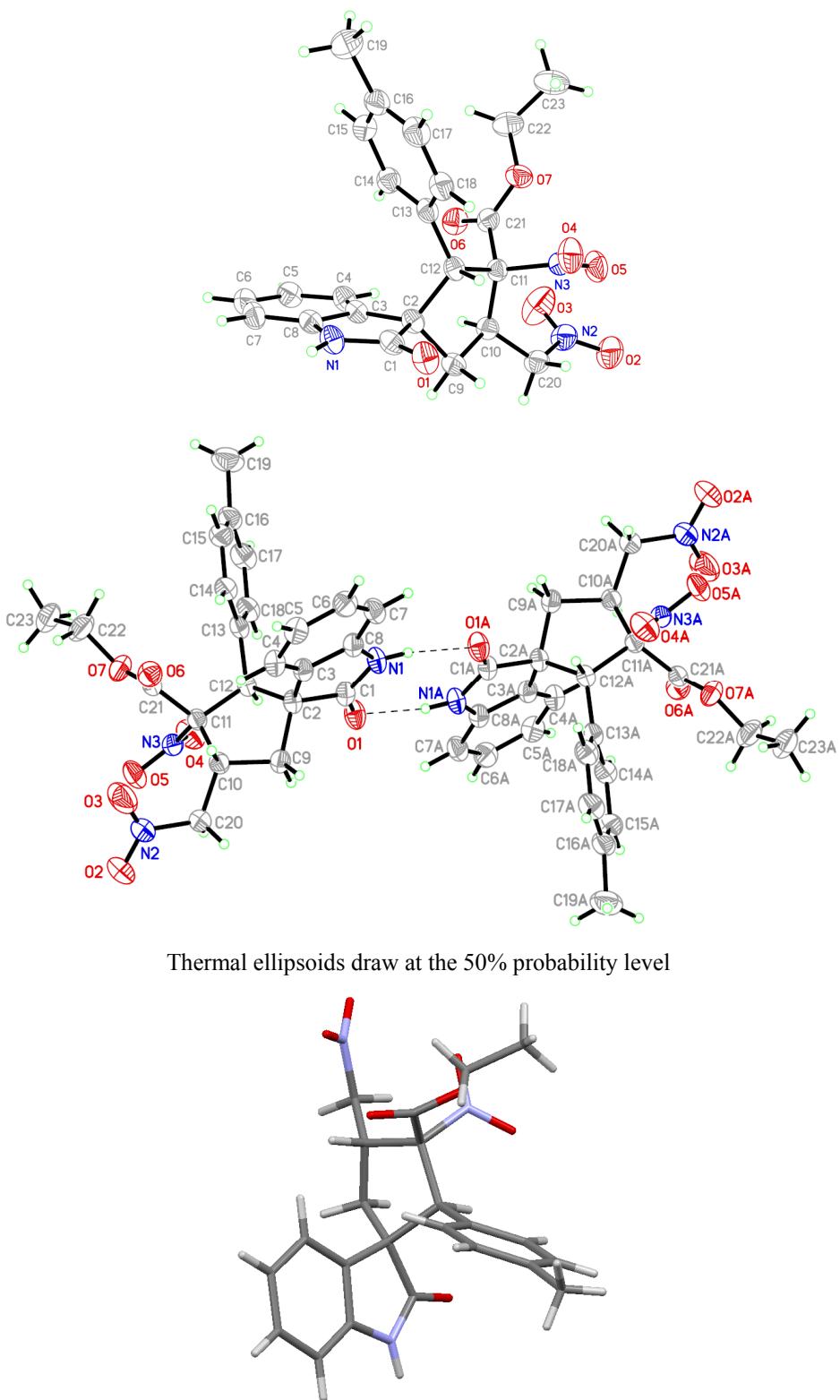
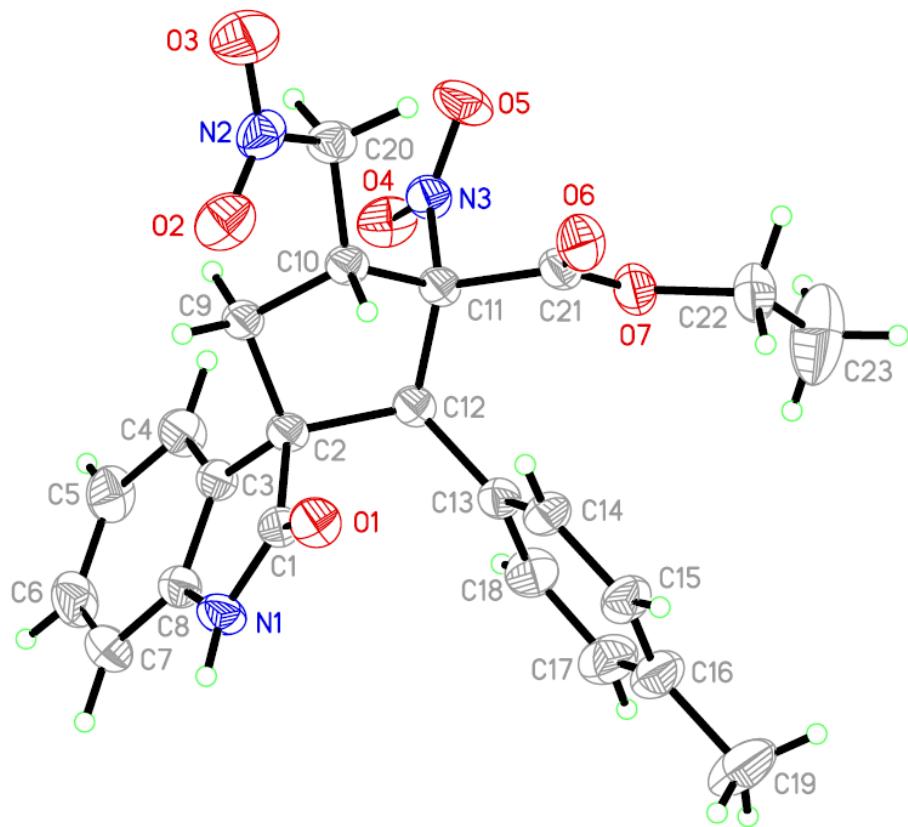


Figure S2. ORTEP and Stereo plots for X-ray crystal structures of (\pm) -3b (**ic18906**).

CCDC 1867292 contains the supplementary crystallographic data for (\pm) -3b (**ic18906**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S2. Crystal data and structure refinement for (\pm)-**3b** (**ic18906**).

Identification code	ic18906		
Empirical formula	C23 H23 N3 O7		
Formula weight	453.44		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Monoclinic		
Space group	P2 ₁ /c		
Unit cell dimensions	a = 7.2684(2) Å	α= 90°.	
	b = 24.3971(5) Å	β= 93.9065(7)°.	
	c = 12.3277(3) Å	γ = 90°.	
Volume	2180.97(9) Å ³		
Z	4		
Density (calculated)	1.381 Mg/m ³		
Absorption coefficient	0.867 mm ⁻¹		
F(000)	952		
Crystal size	0.249 x 0.103 x 0.093 mm ³		
Theta range for data collection	3.623 to 74.983°.		
Index ranges	-9<=h<=7, -30<=k<=30, -15<=l<=15		
Reflections collected	12341		
Independent reflections	4476 [R(int) = 0.0219]		
Completeness to theta = 67.679°	99.8 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7539 and 0.6203		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	4476 / 1 / 309		
Goodness-of-fit on F ²	1.029		
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.1123		
R indices (all data)	R1 = 0.0487, wR2 = 0.1159		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.291 and -0.231 e.Å ⁻³		



Thermal ellipsoids draw at the 50% probability level

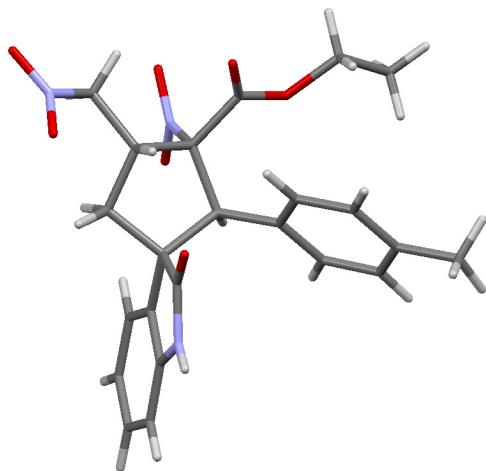


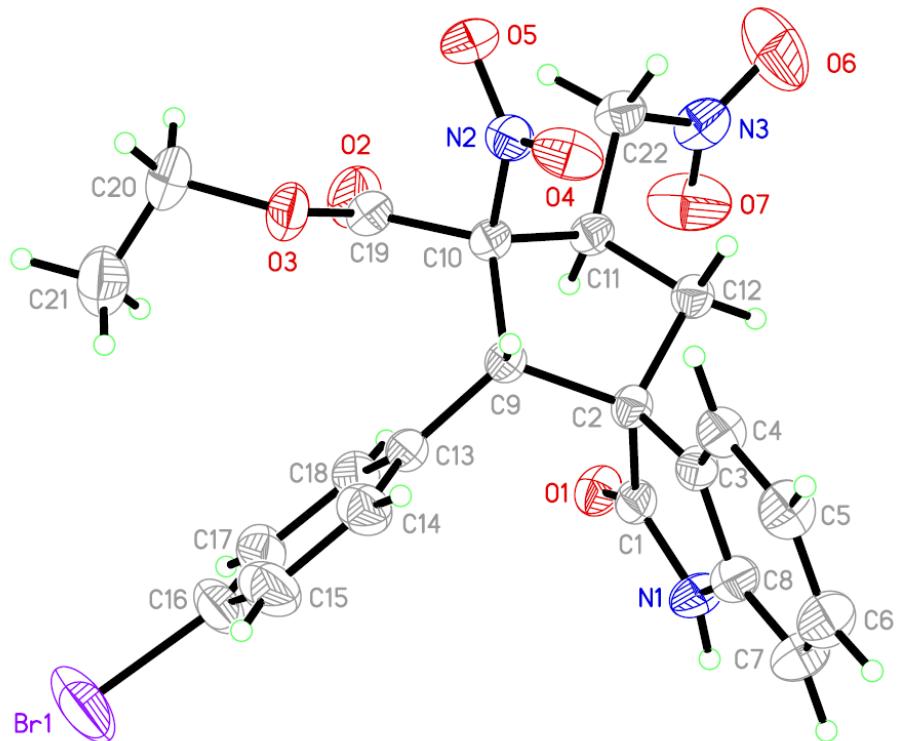
Figure S3. ORTEP and Stereo plots for X-ray crystal structures of (\pm)-4b (ic18910).

CCDC 1867293 contains the supplementary crystallographic data for (\pm)-4b (ic18910). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S3. Crystal data and structure refinement for (\pm)-**4b** (**ic18910**).

Table 1. Crystal data and structure refinement for ic18910.

Identification code	ic18910		
Empirical formula	C ₂₃ H ₂₃ N ₃ O ₇		
Formula weight	453.44		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Monoclinic		
Space group	P2 ₁ /c		
Unit cell dimensions	a = 11.7400(2) Å	α= 90°.	
	b = 11.8392(2) Å	β= 109.7658(7)°.	
	c = 16.8209(4) Å	γ = 90°.	
Volume	2200.23(7) Å ³		
Z	4		
Density (calculated)	1.369 Mg/m ³		
Absorption coefficient	0.860 mm ⁻¹		
F(000)	952		
Crystal size	0.252 x 0.130 x 0.024 mm ³		
Theta range for data collection	4.664 to 74.994°.		
Index ranges	-14<=h<=14, -14<=k<=14, -21<=l<=21		
Reflections collected	15262		
Independent reflections	4516 [R(int) = 0.0268]		
Completeness to theta = 67.679°	99.8 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7539 and 0.6446		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	4516 / 0 / 305		
Goodness-of-fit on F ²	1.067		
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0958		
R indices (all data)	R1 = 0.0472, wR2 = 0.1055		
Extinction coefficient	0.0025(2)		
Largest diff. peak and hole	0.299 and -0.197 e.Å ⁻³		



Thermal ellipsoids draw at the 50% probability level

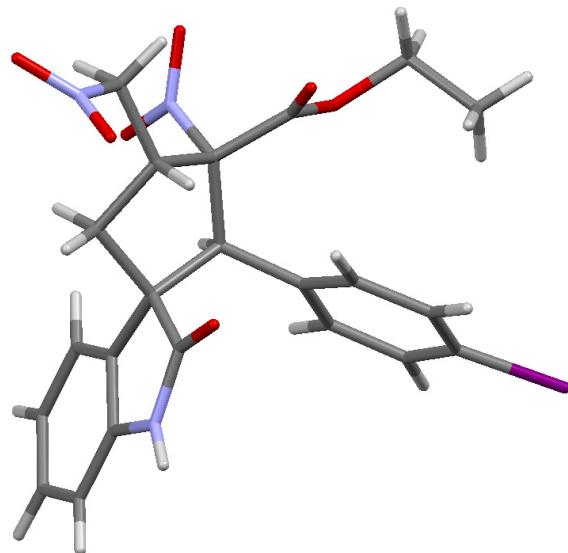


Figure S4. ORTEP and Stereo plots for X-ray crystal structures of (\pm) -4d (ic19210).

CCDC 1867294 contains the supplementary crystallographic data for (\pm) -4d (ic19210). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S4. Crystal data and structure refinement for (\pm)-**4d** (**ic19210**).

Identification code	ic19210		
Empirical formula	C48 H48 Br2 N6 O16		
Formula weight	1124.74		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Triclinic		
Space group	P-1		
Unit cell dimensions	$a = 11.3435(4)$ Å	$\alpha = 105.2163(11)^\circ$.	
	$b = 14.1708(5)$ Å	$\beta = 96.8216(12)^\circ$.	
	$c = 17.3486(6)$ Å	$\gamma = 109.1621(12)^\circ$.	
Volume	2476.78(15) Å ³		
Z	2		
Density (calculated)	1.508 Mg/m ³		
Absorption coefficient	2.733 mm ⁻¹		
F(000)	1152		
Crystal size	0.135 x 0.115 x 0.058 mm ³		
Theta range for data collection	2.709 to 74.996°.		
Index ranges	-14 <= h <= 14, -17 <= k <= 17, -21 <= l <= 21		
Reflections collected	19447		
Independent reflections	10155 [R(int) = 0.0151]		
Completeness to theta = 67.679°	99.9 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7539 and 0.6701		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	10155 / 17 / 656		
Goodness-of-fit on F ²	1.045		
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1196		
R indices (all data)	R1 = 0.0480, wR2 = 0.1244		
Extinction coefficient	n/a		
Largest diff. peak and hole	1.191 and -1.026 e.Å ⁻³		

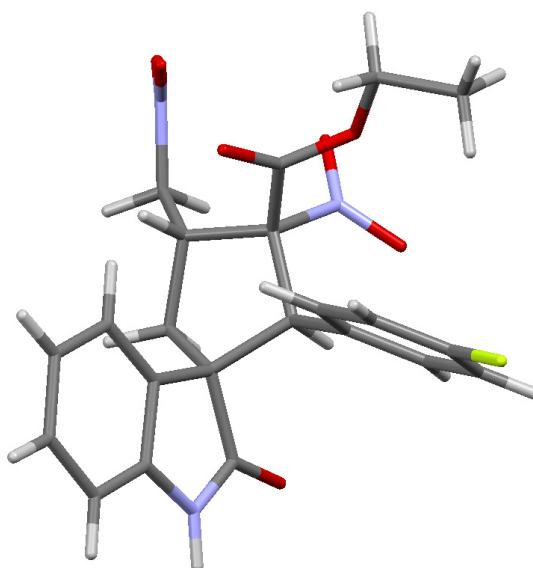
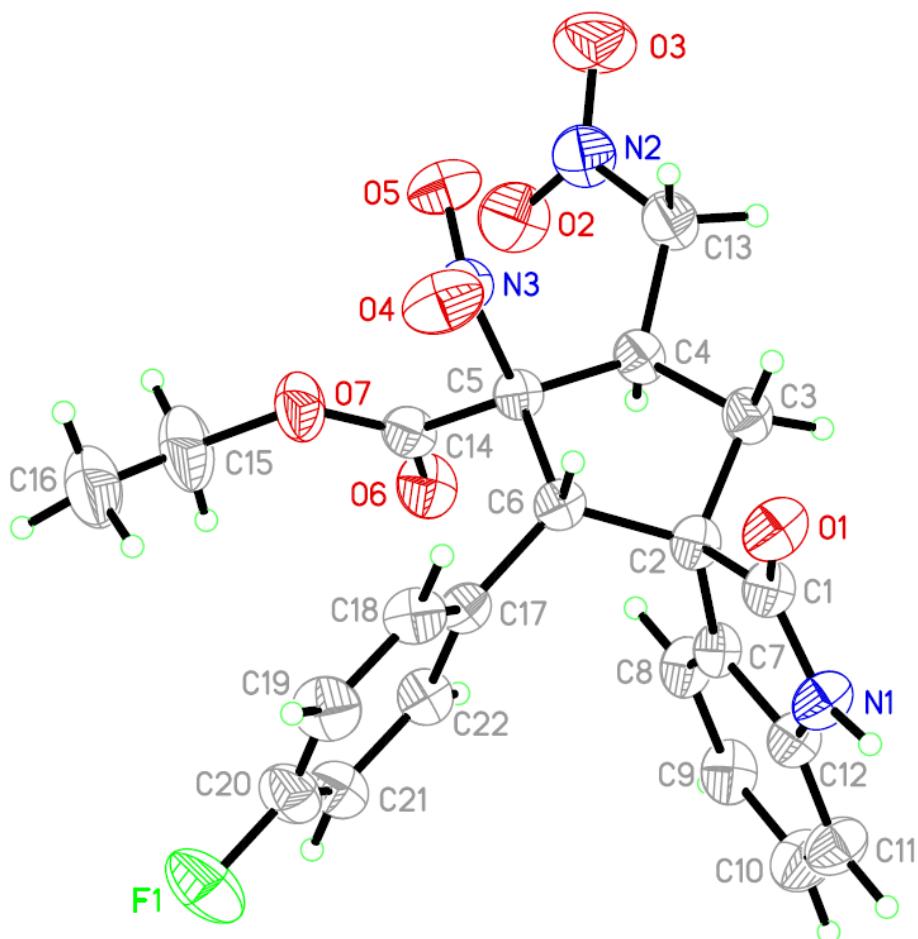
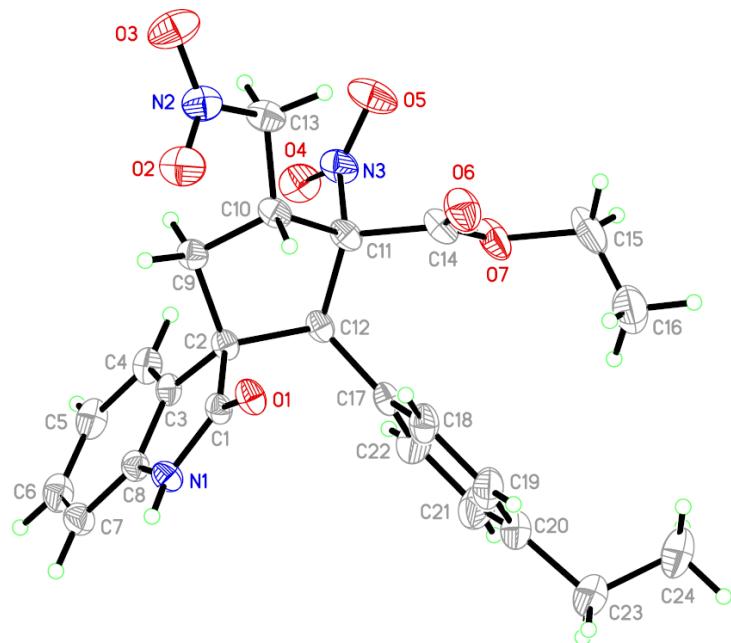


Figure S5. ORTEP and Stereo plots for X-ray crystal structures of (\pm) -3f (ic18973).

CCDC 1867295 contains the supplementary crystallographic data for (\pm) -3f (ic18973). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S5. Crystal data and structure refinement for (\pm)-3f (ic18973).

Identification code	ic18973		
Empirical formula	C23 H21 Cl3 F N3 O7		
Formula weight	576.78		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Triclinic		
Space group	P-1		
Unit cell dimensions	$a = 7.1303(2)$ Å	$\alpha = 82.5101(13)^\circ$.	
	$b = 11.6870(4)$ Å	$\beta = 82.4547(13)^\circ$.	
	$c = 15.7104(5)$ Å	$\gamma = 88.0256(13)^\circ$.	
Volume	1286.57(7) Å ³		
Z	2		
Density (calculated)	1.489 Mg/m ³		
Absorption coefficient	3.723 mm ⁻¹		
F(000)	592		
Crystal size	0.167 x 0.150 x 0.117 mm ³		
Theta range for data collection	2.860 to 74.964°.		
Index ranges	-8<=h<=8, -14<=k<=14, -19<=l<=19		
Reflections collected	7351		
Independent reflections	5246 [R(int) = 0.0197]		
Completeness to theta = 67.679°	99.7 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7539 and 0.6394		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	5246 / 0 / 335		
Goodness-of-fit on F ²	1.070		
Final R indices [I>2sigma(I)]	R1 = 0.0619, wR2 = 0.1726		
R indices (all data)	R1 = 0.0683, wR2 = 0.1808		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.956 and -0.852 e.Å ⁻³		



Thermal ellipsoids draw at the 30% probability level

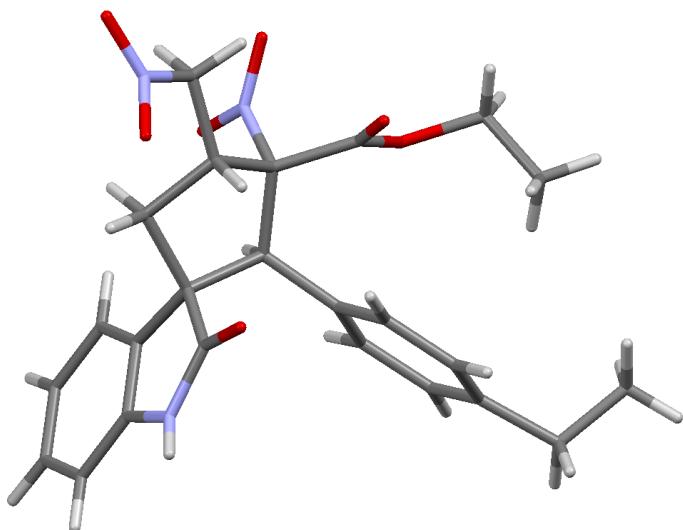
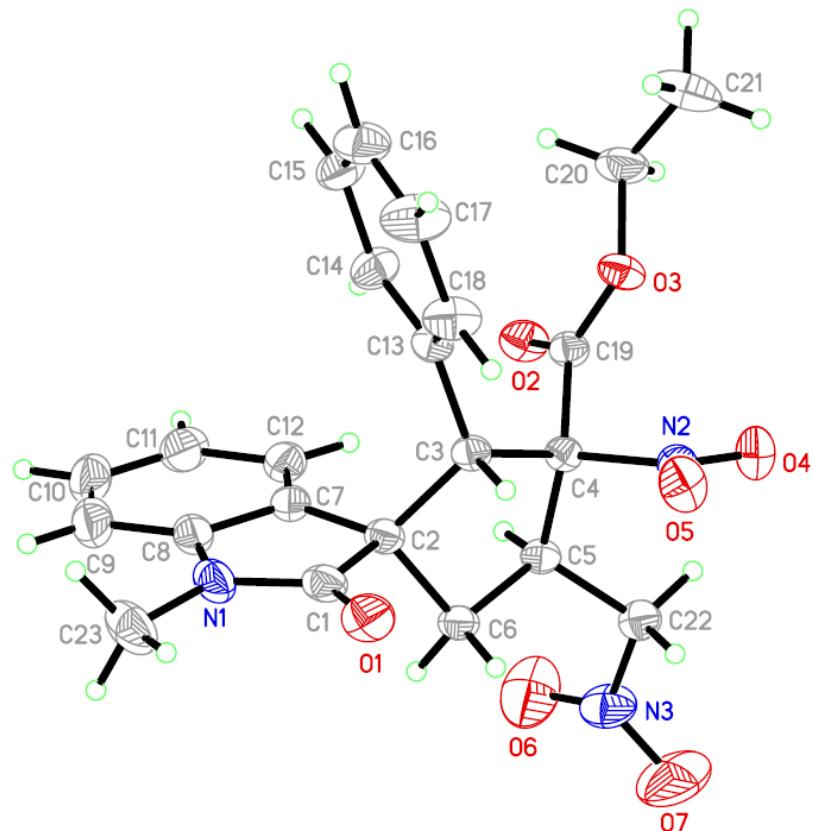


Figure S6. ORTEP and Stereo plots for X-ray crystal structures of (\pm) -4i (ic19221).

CCDC 1867296 contains the supplementary crystallographic data for (\pm) -4i (ic19221). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S6. Crystal data and structure refinement for (\pm)-**4i** (ic19221).

Identification code	ic19221		
Empirical formula	C ₂₄ H ₂₅ N ₃ O ₇		
Formula weight	467.47		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Monoclinic		
Space group	P2 ₁ /n		
Unit cell dimensions	a = 11.4775(4) Å	α= 90°.	
	b = 29.4193(10) Å	β= 108.3567(11)°.	
	c = 14.3936(5) Å	γ = 90°.	
Volume	4612.8(3) Å ³		
Z	8		
Density (calculated)	1.346 Mg/m ³		
Absorption coefficient	0.836 mm ⁻¹		
F(000)	1968		
Crystal size	0.188 x 0.164 x 0.156 mm ³		
Theta range for data collection	3.004 to 74.982°.		
Index ranges	-14<=h<=14, -36<=k<=36, -18<=l<=18		
Reflections collected	29853		
Independent reflections	9501 [R(int) = 0.0252]		
Completeness to theta = 67.679°	99.9 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7539 and 0.5429		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	9501 / 7 / 636		
Goodness-of-fit on F ²	1.028		
Final R indices [I>2sigma(I)]	R1 = 0.0530, wR2 = 0.1294		
R indices (all data)	R1 = 0.0605, wR2 = 0.1378		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.455 and -0.352 e.Å ⁻³		



Thermal ellipsoids draw at the 50% probability level

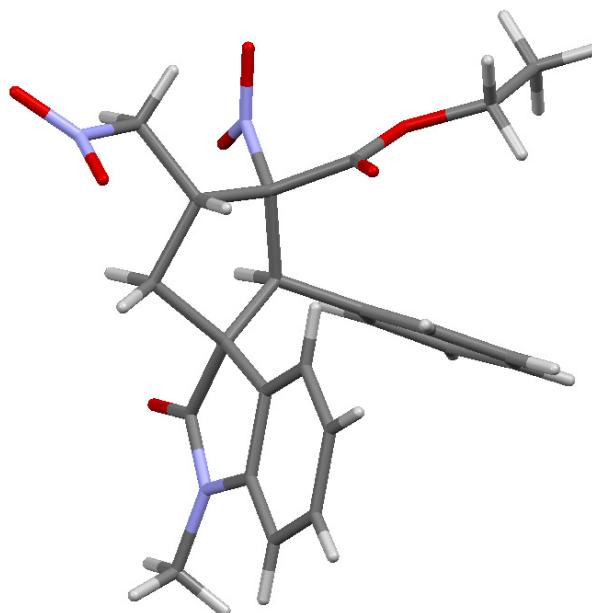


Figure S7. ORTEP and Stereo plots for X-ray crystal structures of (+)-3j (**ic18855**).

CCDC 1867297 contains the supplementary crystallographic data for (+)-3j (**ic18855**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S7. Crystal data and structure refinement for (+)-3j (ic18855).

Identification code	ic18855		
Empirical formula	C23.50 H23.50 Cl1.50 N3 O7		
Formula weight	513.13		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Orthorhombic		
Space group	P2 ₁ 2 ₁ 2		
Unit cell dimensions	a = 12.1872(3) Å	α= 90°.	
	b = 19.6134(4) Å	β= 90°.	
	c = 10.1516(2) Å	γ = 90°.	
Volume	2426.56(9) Å ³		
Z	4		
Density (calculated)	1.405 Mg/m ³		
Absorption coefficient	2.330 mm ⁻¹		
F(000)	1068		
Crystal size	0.195 x 0.190 x 0.147 mm ³		
Theta range for data collection	4.271 to 74.649°.		
Index ranges	-14<=h<=15, -24<=k<=24, -12<=l<=12		
Reflections collected	15293		
Independent reflections	4944 [R(int) = 0.0179]		
Completeness to theta = 67.679°	99.1 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7538 and 0.6161		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	4944 / 19 / 343		
Goodness-of-fit on F ²	1.048		
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1426		
R indices (all data)	R1 = 0.0503, wR2 = 0.1448		
Absolute structure parameter	0.026(6)		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.462 and -0.404 e.Å ⁻³		

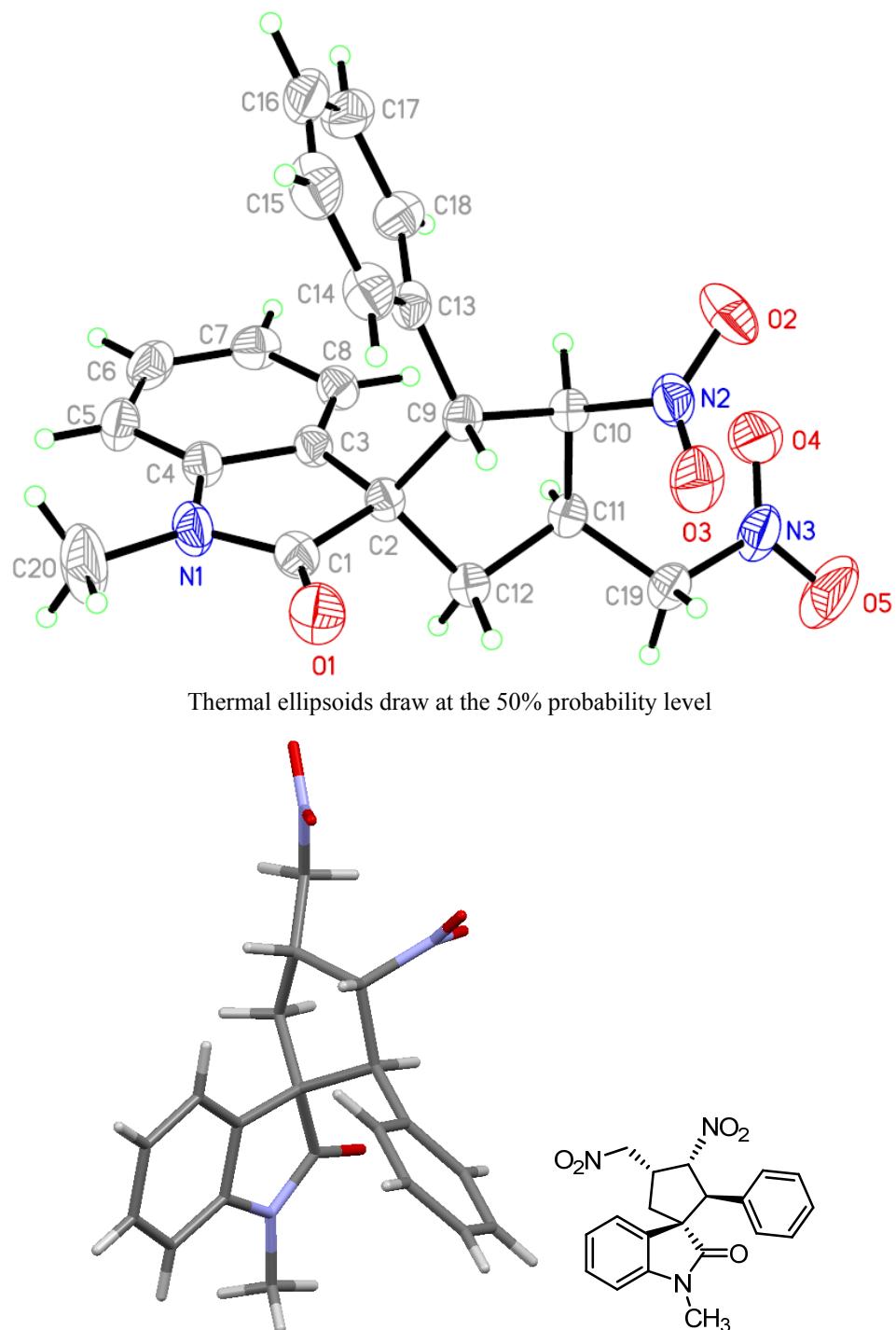
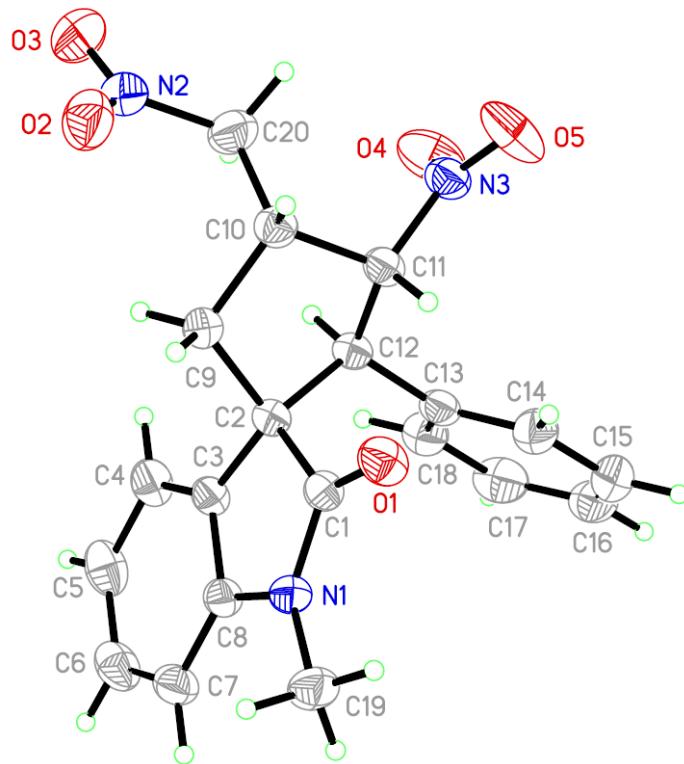


Figure S8. ORTEP and Stereo plots for X-ray crystal structures of (+)-7a (ic18616).

CCDC 1867298 contains the supplementary crystallographic data for (+)-7a (ic18616). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S8. Crystal data and structure refinement for (+)-**7a** (ic18616).

Identification code	ic18616		
Empirical formula	C ₂₀ H ₁₉ N ₃ O ₅		
Formula weight	381.38		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Orthorhombic		
Space group	P ₂ 1 ₂ 1 ₂ 1		
Unit cell dimensions	a = 9.5902(2) Å	α= 90°.	
	b = 9.6661(2) Å	β= 90°.	
	c = 20.3410(4) Å	γ = 90°.	
Volume	1885.61(7) Å ³		
Z	4		
Density (calculated)	1.343 Mg/m ³		
Absorption coefficient	0.817 mm ⁻¹		
F(000)	800		
Crystal size	0.269 x 0.192 x 0.054 mm ³		
Theta range for data collection	5.066 to 69.997°.		
Index ranges	-9<=h<=11, -11<=k<=11, -24<=l<=24		
Reflections collected	12192		
Independent reflections	3565 [R(int) = 0.0192]		
Completeness to theta = 67.679°	99.8 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7533 and 0.5362		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	3565 / 0 / 254		
Goodness-of-fit on F ²	1.039		
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0881		
R indices (all data)	R1 = 0.0344, wR2 = 0.0896		
Absolute structure parameter	0.00(4)		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.396 and -0.308 e.Å ⁻³		



Thermal ellipsoids draw at the 50% probability level

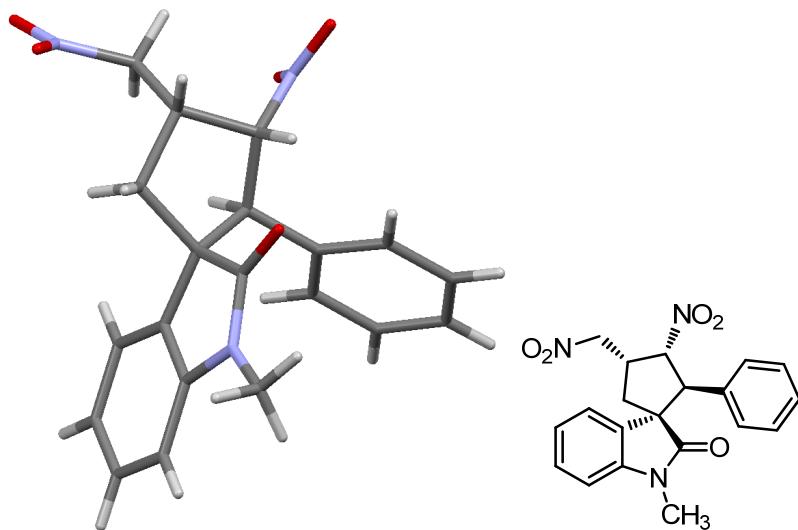


Figure S9. ORTEP and Stereo plots for X-ray crystal structures of (\pm) -8a (ic19258).

CCDC 1867312 contains the supplementary crystallographic data for (\pm) -8a (ic19258). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S9. Crystal data and structure refinement for (\pm)-**8a** (**ic19258**).

Identification code	ic19258	
Empirical formula	C ₂₀ H ₁₉ N ₃ O ₅	
Formula weight	381.38	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P ₂ 1/n	
Unit cell dimensions	a = 9.2665(3) Å	α = 90°.
	b = 10.5833(3) Å	β = 90.9476(8)°.
	c = 17.9618(5) Å	γ = 90°.
Volume	1761.28(9) Å ³	
Z	4	
Density (calculated)	1.438 Mg/m ³	
Absorption coefficient	0.874 mm ⁻¹	
F(000)	800	
Crystal size	0.181 x 0.163 x 0.150 mm ³	
Theta range for data collection	4.850 to 74.997°.	
Index ranges	-11<=h<=11, -13<=k<=13, -21<=l<=22	
Reflections collected	12081	
Independent reflections	3614 [R(int) = 0.0183]	
Completeness to theta = 67.679°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7539 and 0.6444	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3614 / 0 / 254	
Goodness-of-fit on F ²	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0478, wR2 = 0.1411	
R indices (all data)	R1 = 0.0497, wR2 = 0.1439	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.351 and -0.294 e.Å ⁻³	

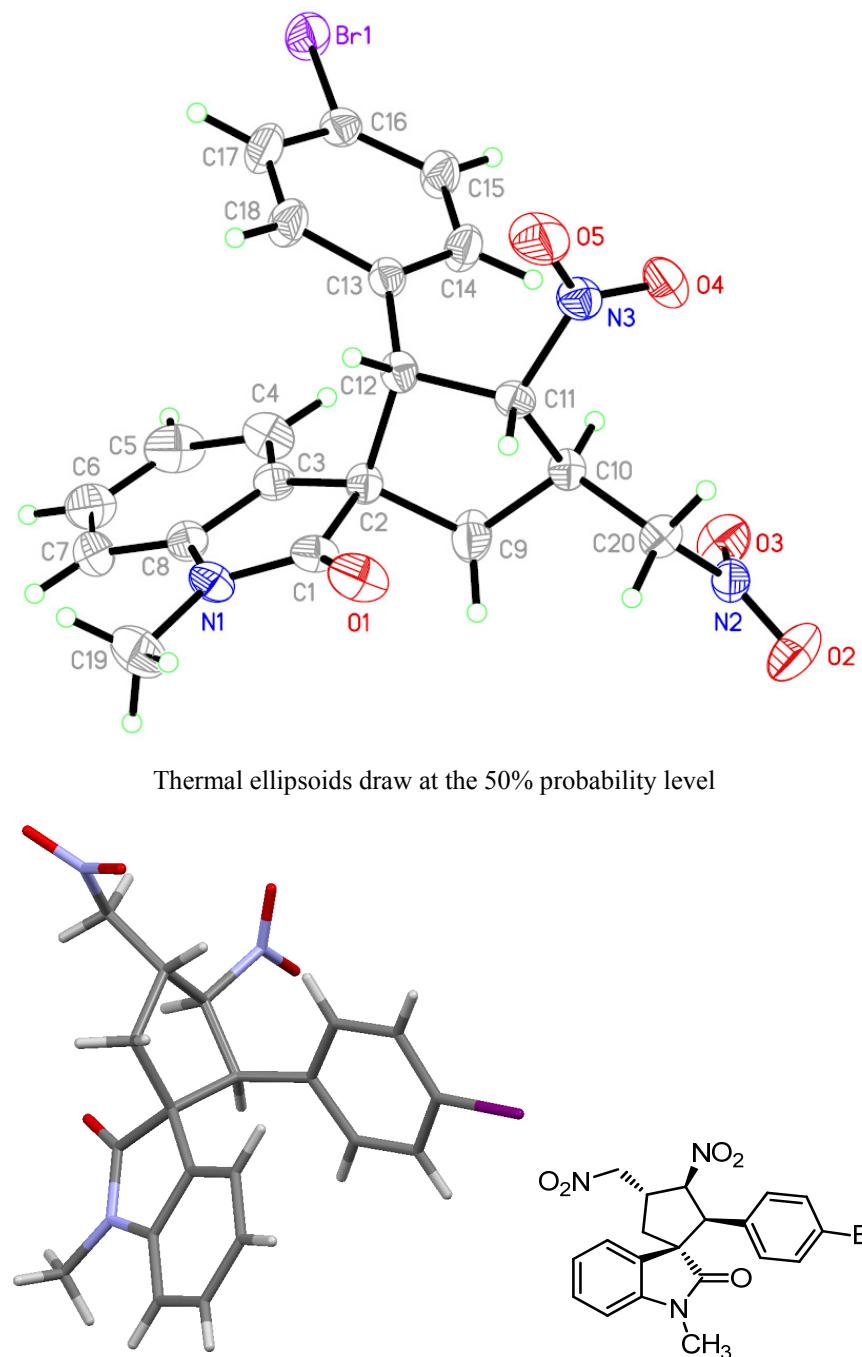
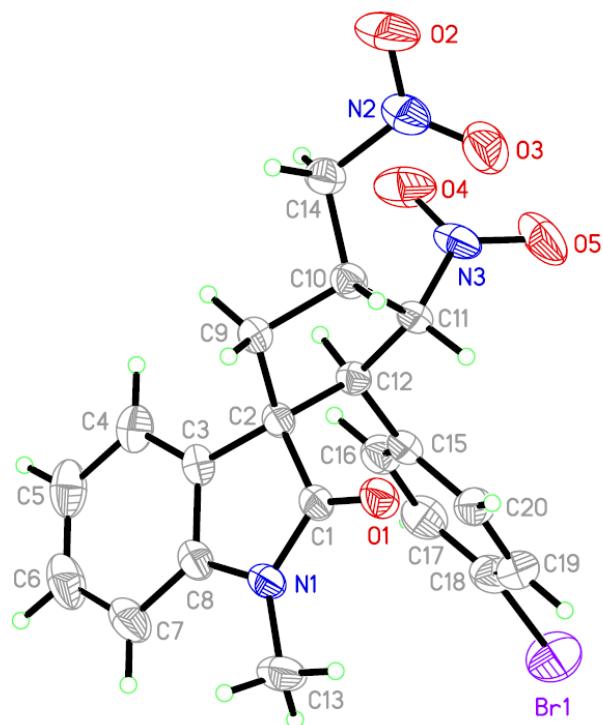


Figure S10. ORTEP and Stereo plots for X-ray crystal structures of (+)-9b (ic18876).

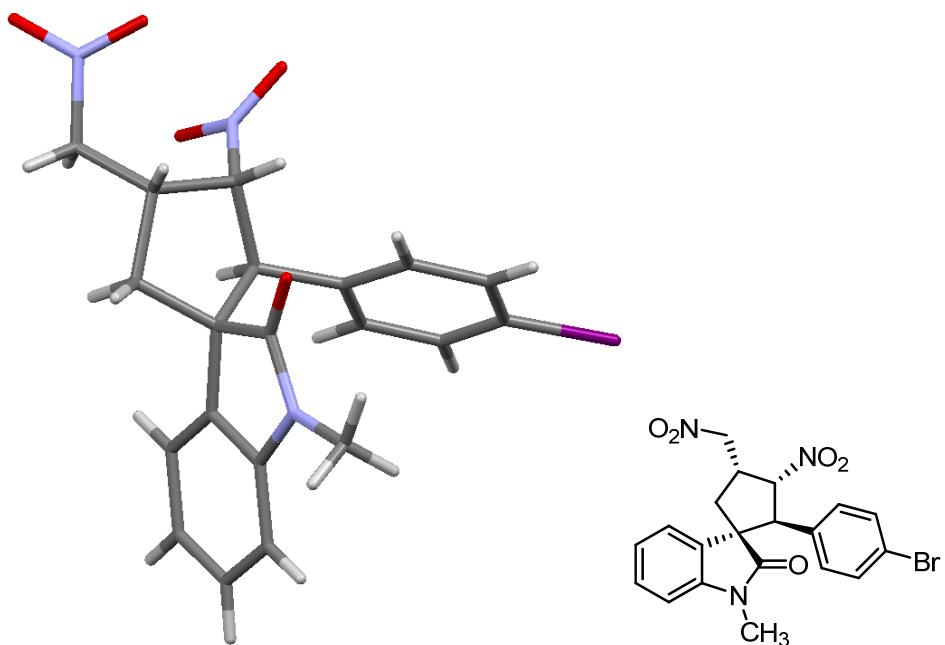
CCDC 1867299 contains the supplementary crystallographic data for (+)-9b (ic18876). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

Table S10. Crystal data and structure refinement for (+)-**9b** (ic18876).

Identification code	ic18876		
Empirical formula	C ₂₀ H ₁₈ BrN ₃ O ₅		
Formula weight	460.28		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Orthorhombic		
Space group	P ₂ 12 ₁ 2 ₁		
Unit cell dimensions	a = 5.88470(10) Å	α= 90°.	
	b = 10.0526(2) Å	β= 90°.	
	c = 31.9302(7) Å	γ = 90°.	
Volume	1888.88(6) Å ³		
Z	4		
Density (calculated)	1.619 Mg/m ³		
Absorption coefficient	3.314 mm ⁻¹		
F(000)	936		
Crystal size	0.271 x 0.095 x 0.081 mm ³		
Theta range for data collection	2.768 to 74.982°.		
Index ranges	-7<=h<=6, -12<=k<=12, -39<=l<=39		
Reflections collected	10463		
Independent reflections	3864 [R(int) = 0.0190]		
Completeness to theta = 67.679°	99.5 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7539 and 0.5660		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	3864 / 0 / 263		
Goodness-of-fit on F ²	1.091		
Final R indices [I>2sigma(I)]	R1 = 0.0230, wR2 = 0.0591		
R indices (all data)	R1 = 0.0232, wR2 = 0.0592		
Absolute structure parameter	0.030(5)		
Extinction coefficient	n/a		
Largest diff. peak and hole	0.414 and -0.293 e.Å ⁻³		



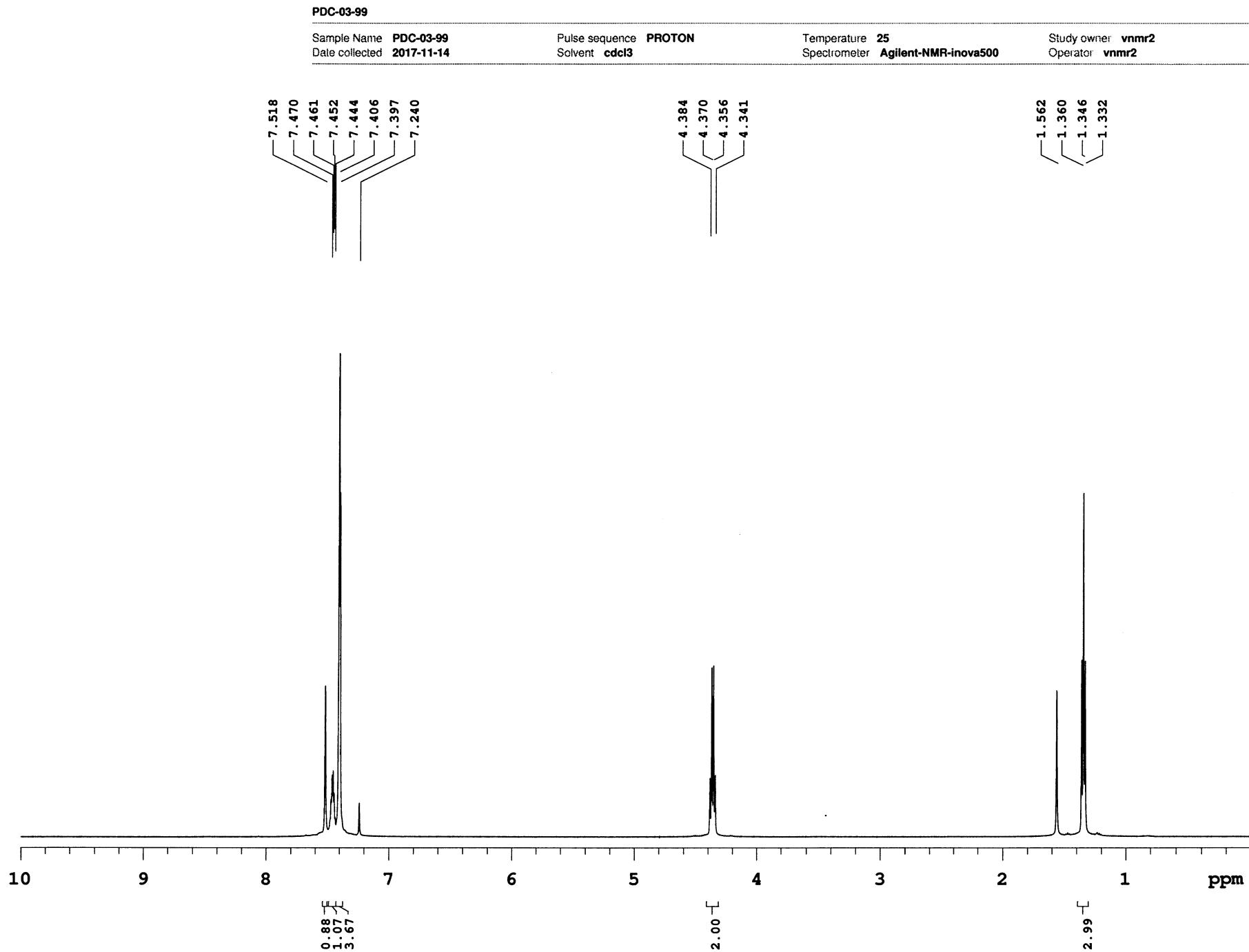
Thermal ellipsoids draw at the 50% probability level

**Figure S11.** ORTEP and Stereo plots for X-ray crystal structures of (\pm)-8b (ic19242).

CCDC 1867308 contains the supplementary crystallographic data for (\pm)-8b (ic19242). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk

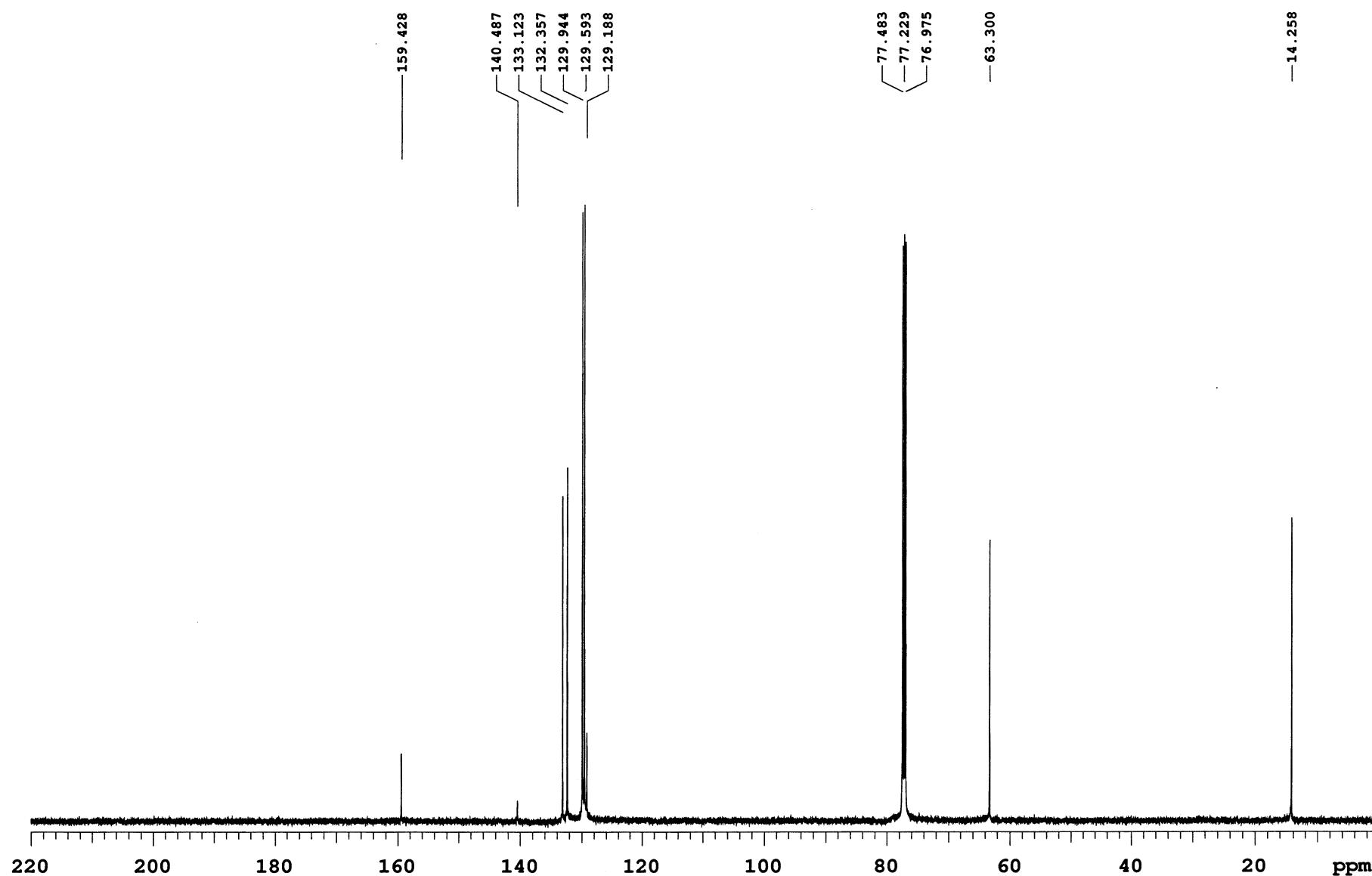
Table S11. Crystal data and structure refinement for (\pm)-**8b** (ic19242).

Identification code	ic19242		
Empirical formula	C ₂₀ H ₁₈ BrN ₃ O ₅		
Formula weight	460.28		
Temperature	200(2) K		
Wavelength	1.54178 Å		
Crystal system	Triclinic		
Space group	P-1		
Unit cell dimensions	a = 10.6940(2) Å	α = 104.6578(6)°.	
	b = 10.6945(3) Å	β = 95.9501(6)°.	
	c = 18.4813(4) Å	γ = 99.2596(7)°.	
Volume	1995.01(8) Å ³		
Z	4		
Density (calculated)	1.532 Mg/m ³		
Absorption coefficient	3.138 mm ⁻¹		
F(000)	936		
Crystal size	0.178 x 0.139 x 0.107 mm ³		
Theta range for data collection	2.500 to 74.969°.		
Index ranges	-13≤h≤13, -13≤k≤12, -23≤l≤23		
Reflections collected	15747		
Independent reflections	8181 [R(int) = 0.0132]		
Completeness to theta = 67.679°	99.8 %		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.7539 and 0.6381		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	8181 / 43 / 541		
Goodness-of-fit on F ²	1.039		
Final R indices [I>2sigma(I)]	R1 = 0.0435, wR2 = 0.1150		
R indices (all data)	R1 = 0.0462, wR2 = 0.1182		
Extinction coefficient	n/a		
Largest diff. peak and hole	1.047 and -0.751 e.Å ⁻³		

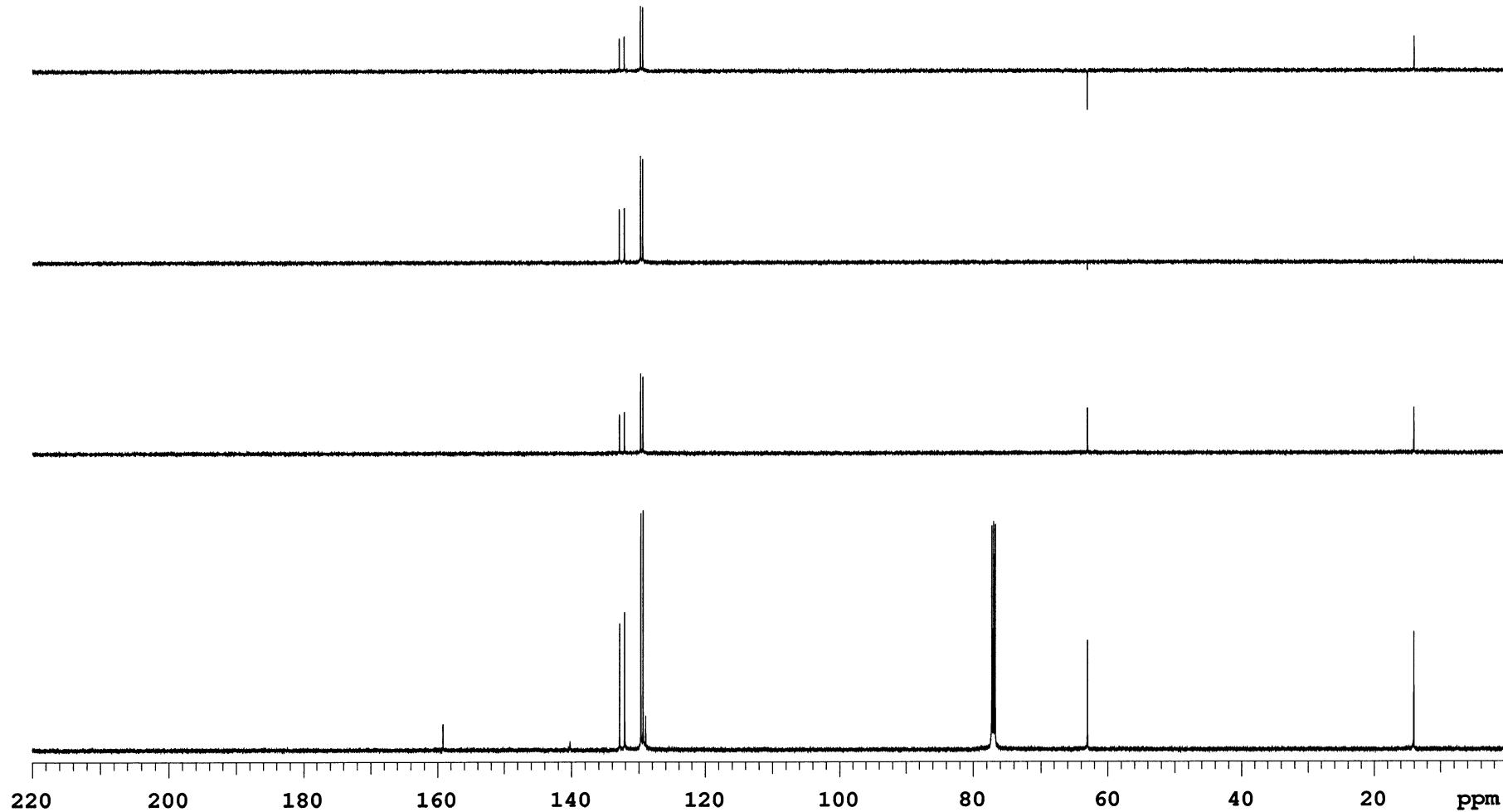
Figure S12. ^1H NMR (CDCl₃, 500 MHz) of **2a**

PDC-03-99

Sample Name	PDC-03-99	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2017-11-14	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

Figure S13. ¹³C NMR (CDCl₃, 125 MHz) of **2a**

PDC-03-99

Sample Name **PDC-03-99**
Date collected **2017-11-14**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S14. DEPT of **2a**

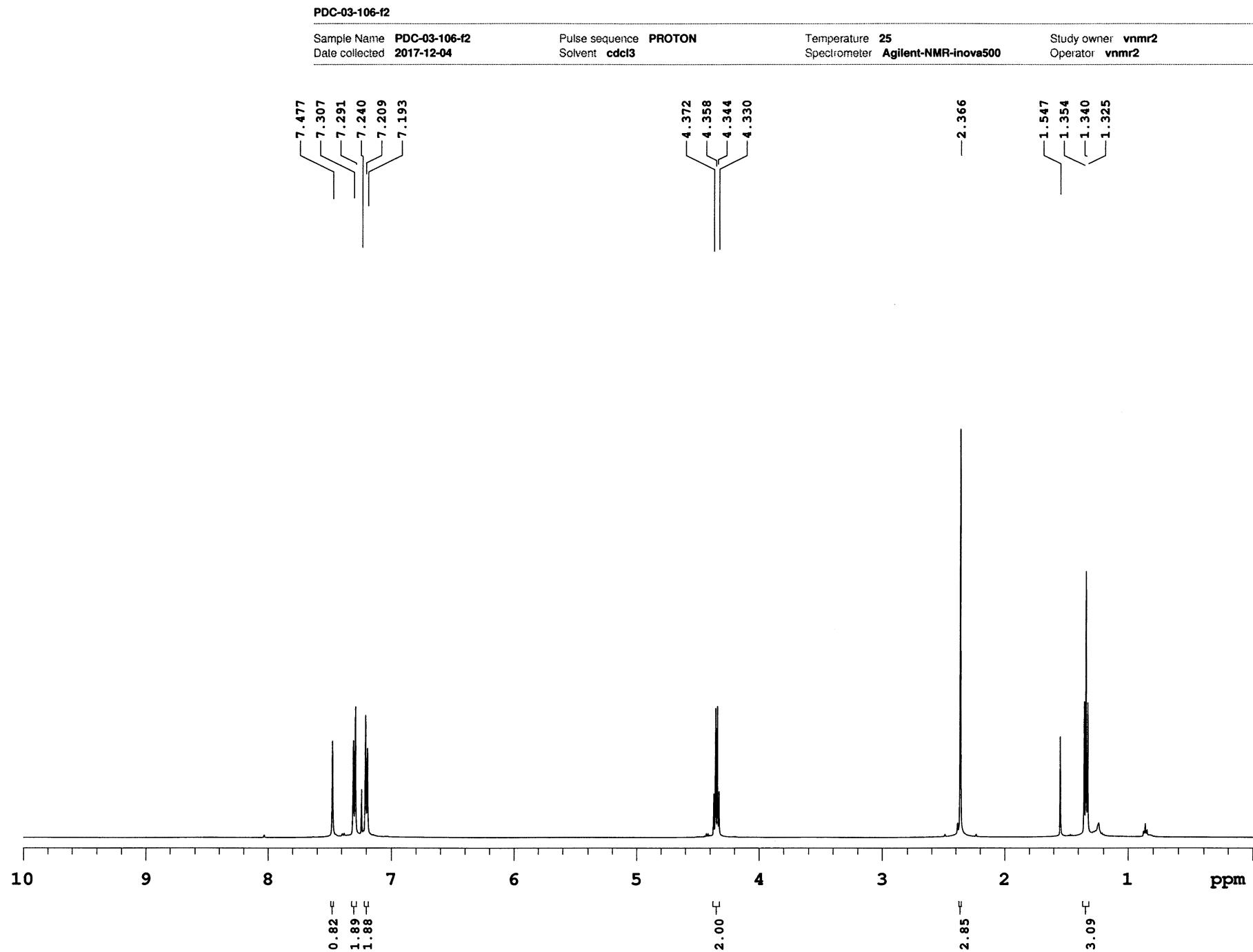
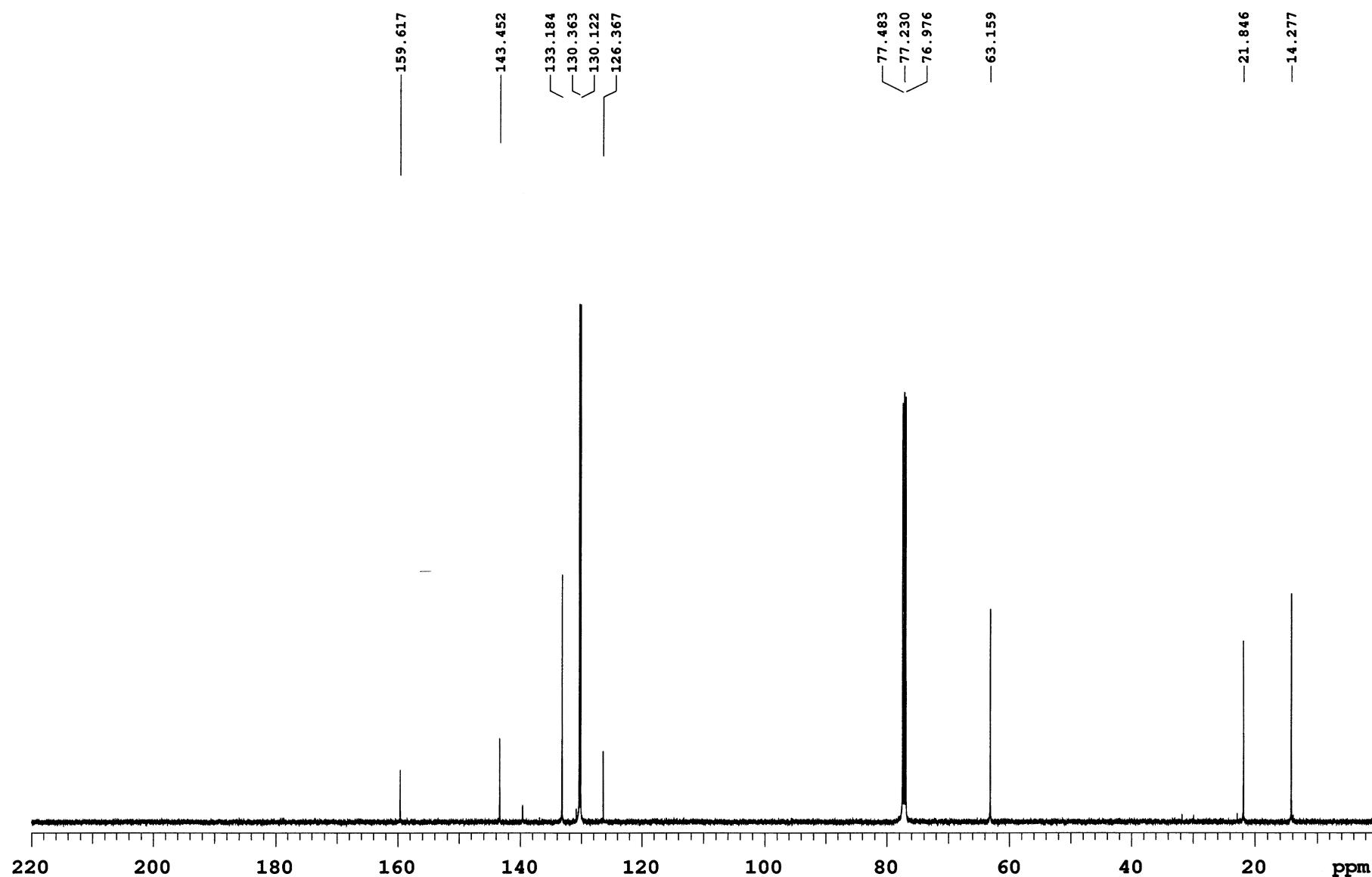


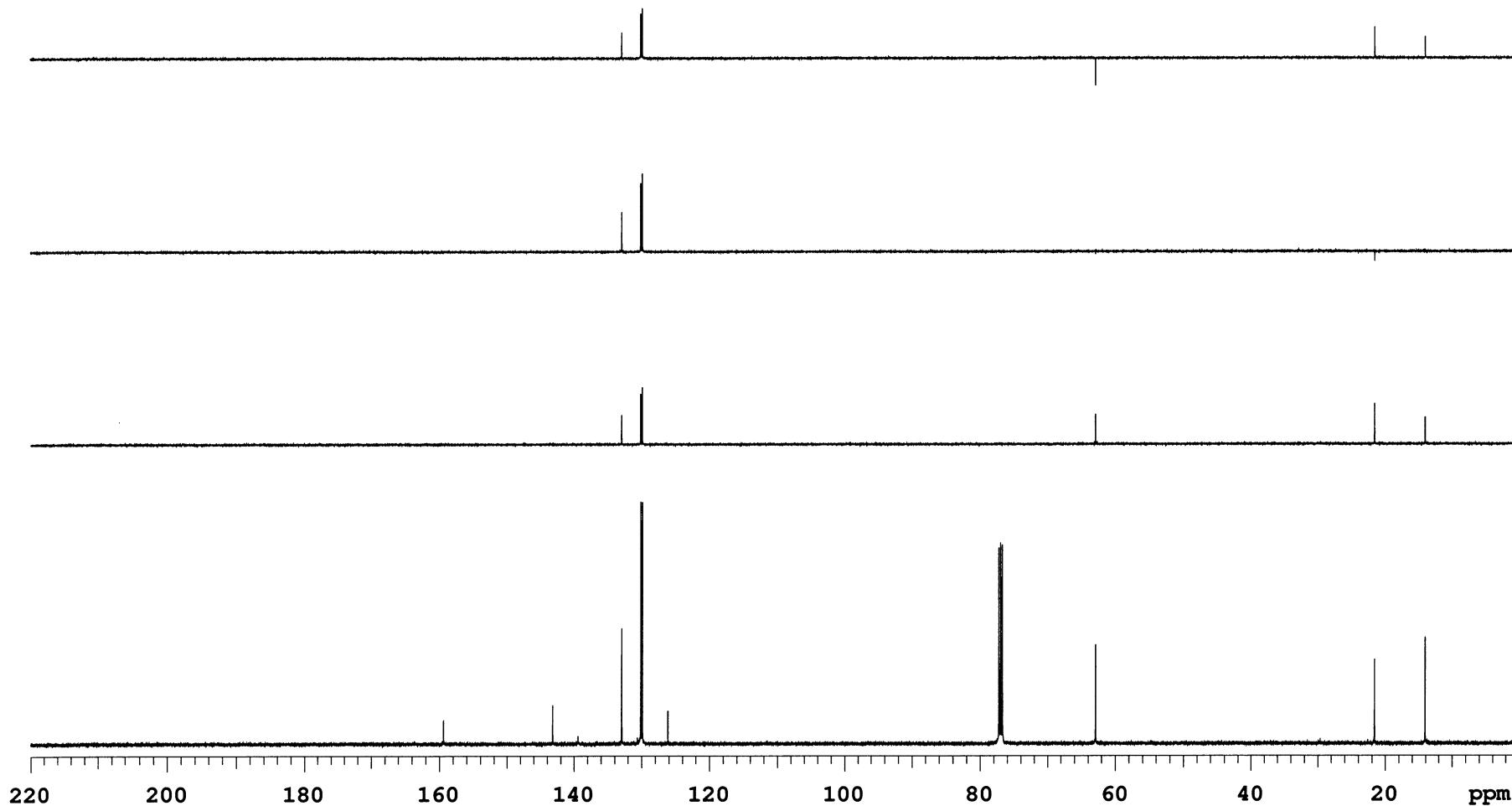
Figure S15. 1H NMR (CDCl3, 500 MHz) of 2b

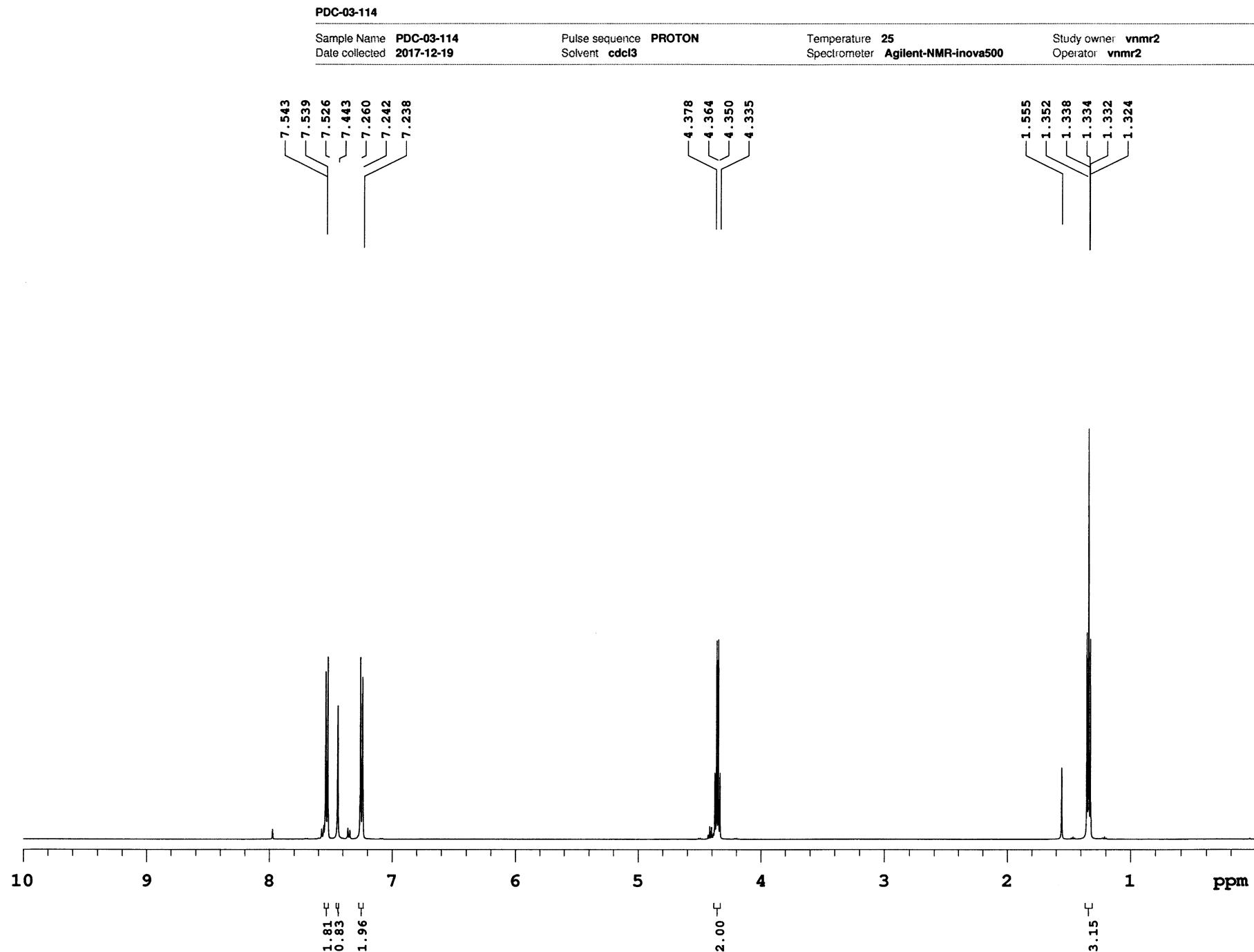
PDC-03-106-f2

Sample Name	PDC-03-106-f2	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2017-12-04	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

Figure S16. ¹³C NMR (CDCl₃, 125 MHz) of **2b**

PDC-03-106-f2

Sample Name **PDC-03-106-f2**
Date collected **2017-12-05**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S17. DEPT of **2b**

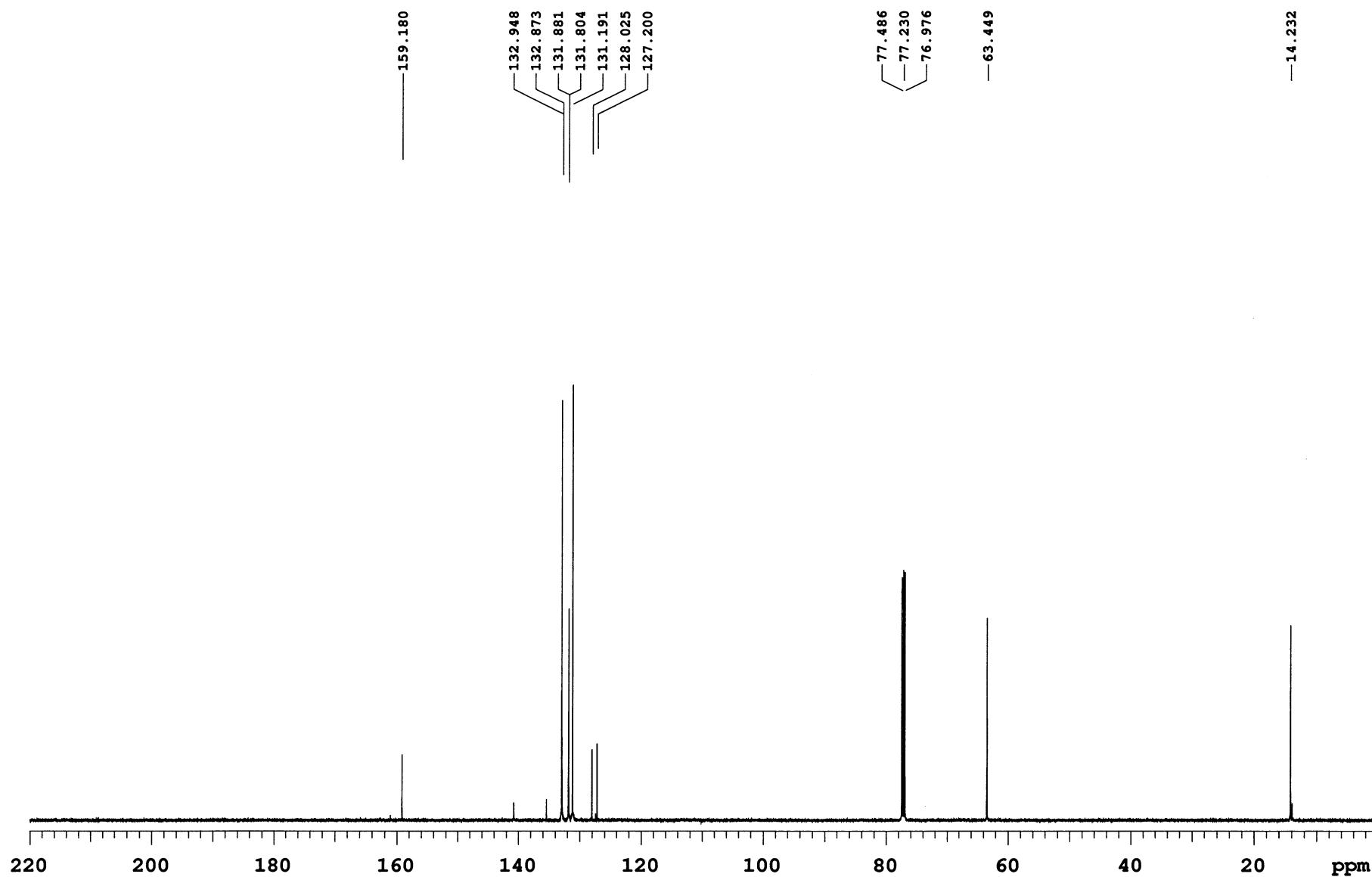
Figure S18. ¹H NMR (*CDCl*₃, 500 MHz) of **2c**

Data file /home/vnmr2/vnmrsys/data/511/PDC/PDC-03-114/PROTON_03

Plot date 2018-11-21

PDC-03-114

Sample Name	PDC-03-114	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2017-12-19	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

Figure S19. ¹³C NMR (CDCl₃, 125 MHz) of **2c**

PDC-03-114

Sample Name **PDC-03-114**
Date collected **2017-12-20**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

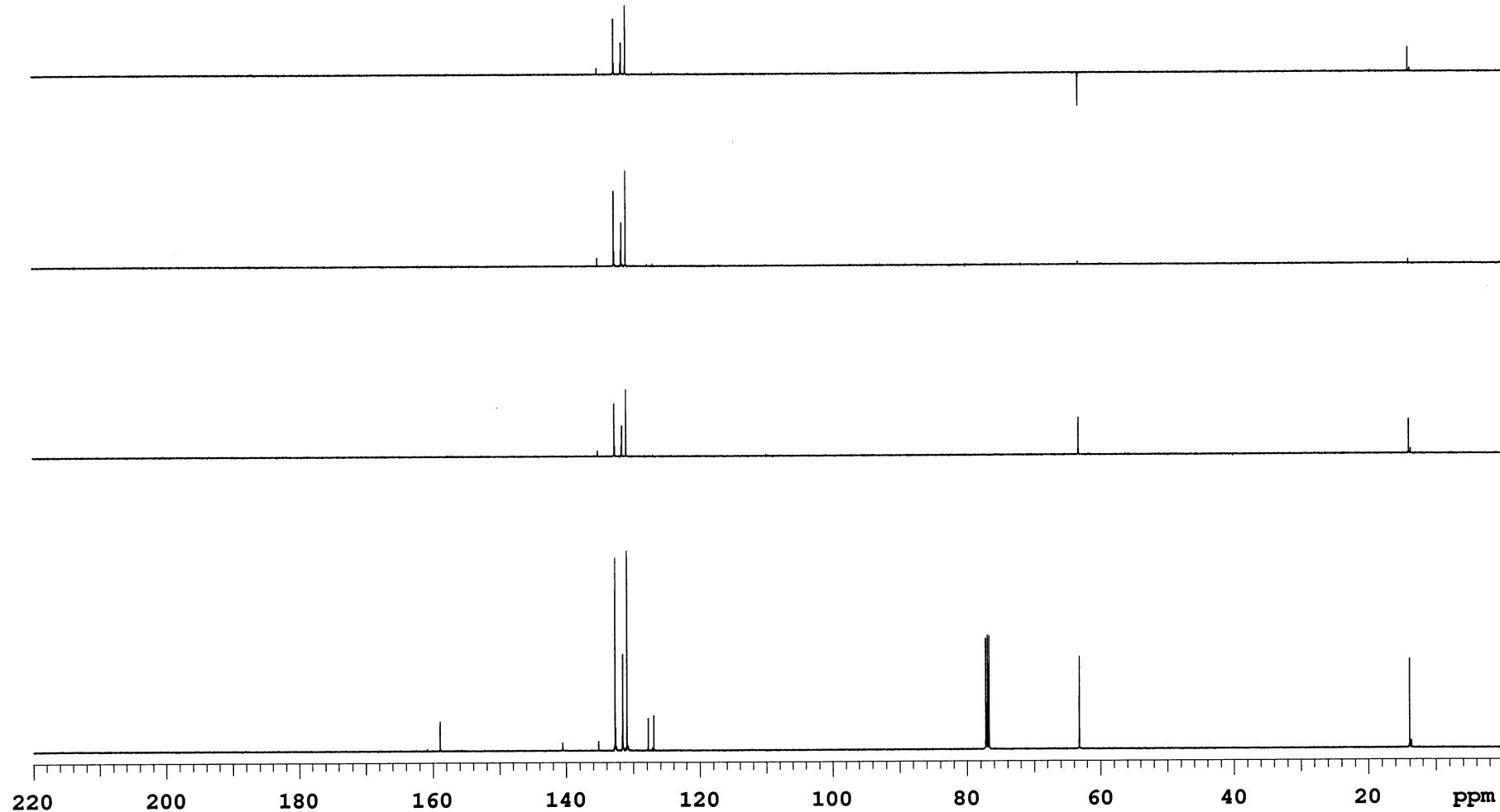
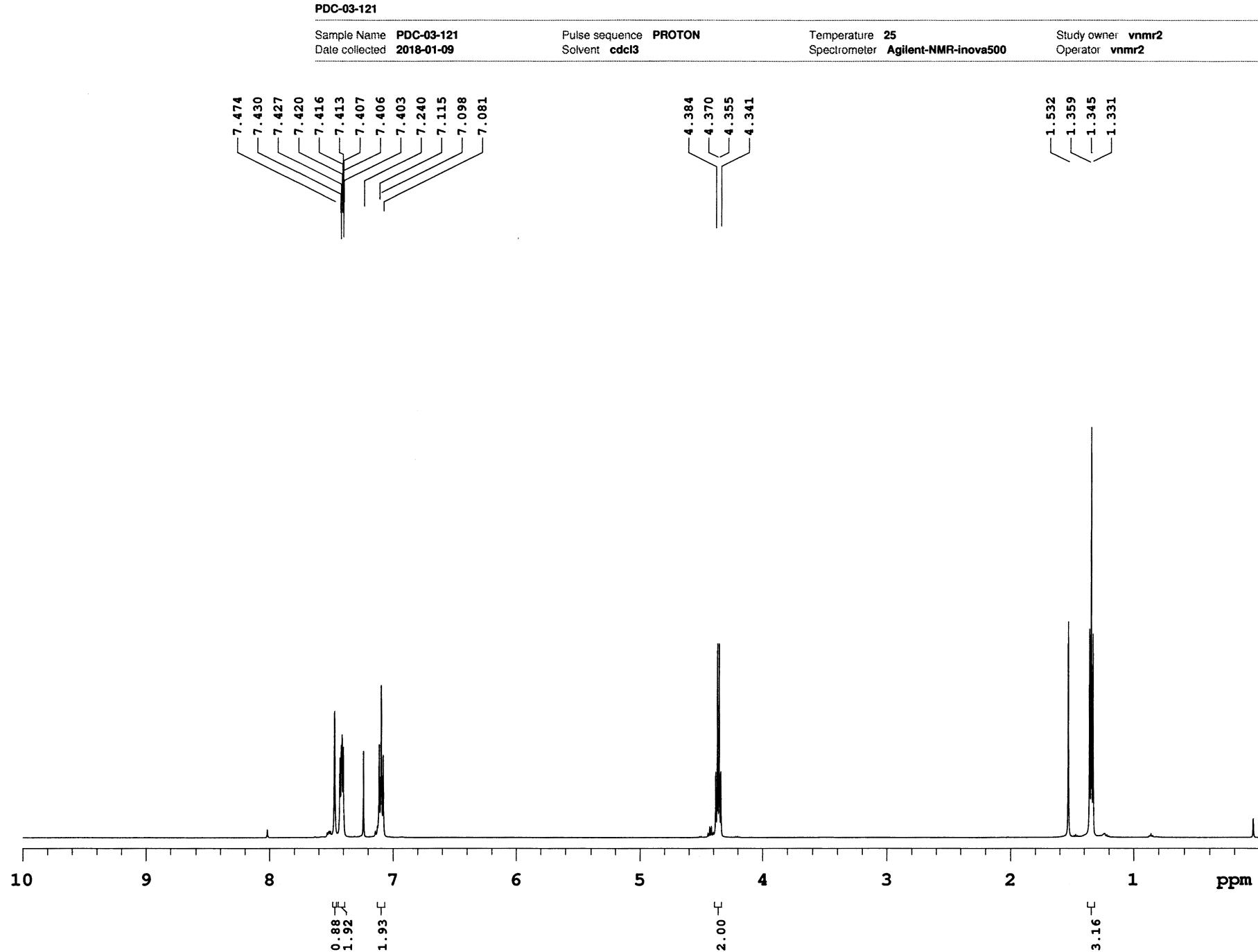


Figure S20. DEPT of **2c**

Figure S21. ^1H NMR (CDCl_3 , 500 MHz) of **2d**

PDC-03-12

Sample Name **PDC-03-12**
Date collected **2018-01-09**

Pulse sequence **CARBO**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova50**

Study owner **vnmr1**
Operator **vnmr2**

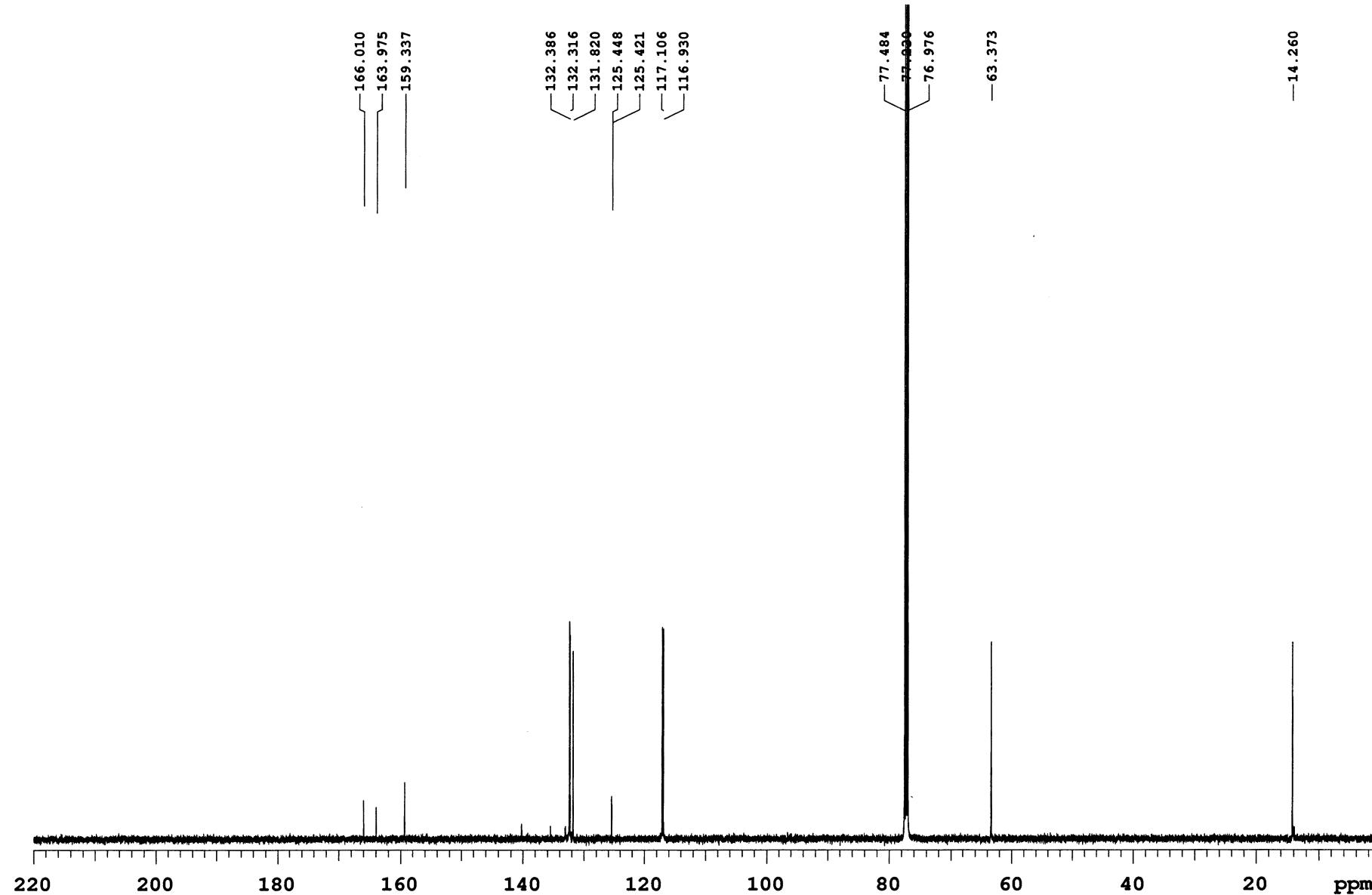


Figure S22. ^{13}C NMR (CDCl_3 , 125 MHz) of **2c**

PDC-03-121

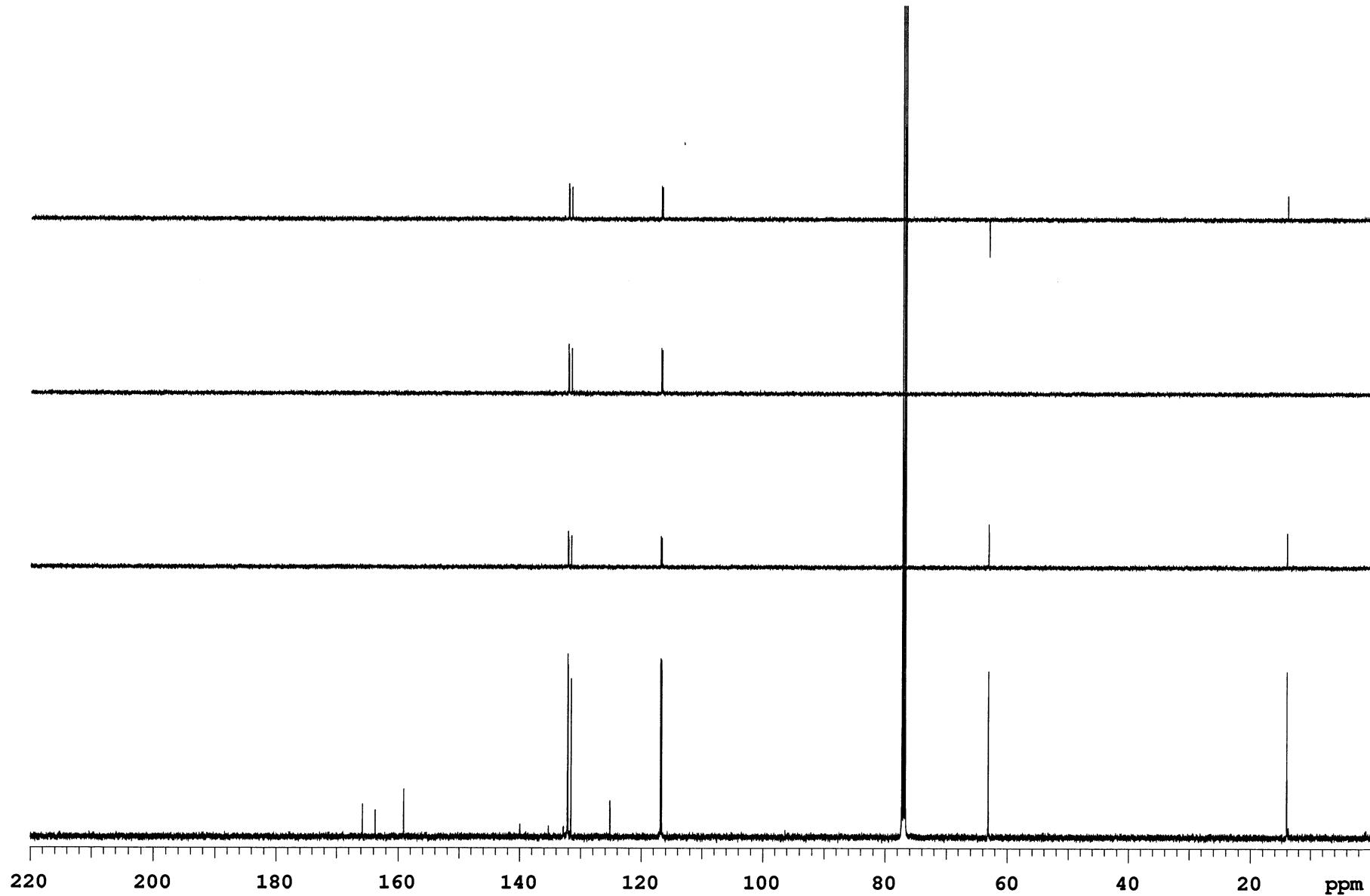
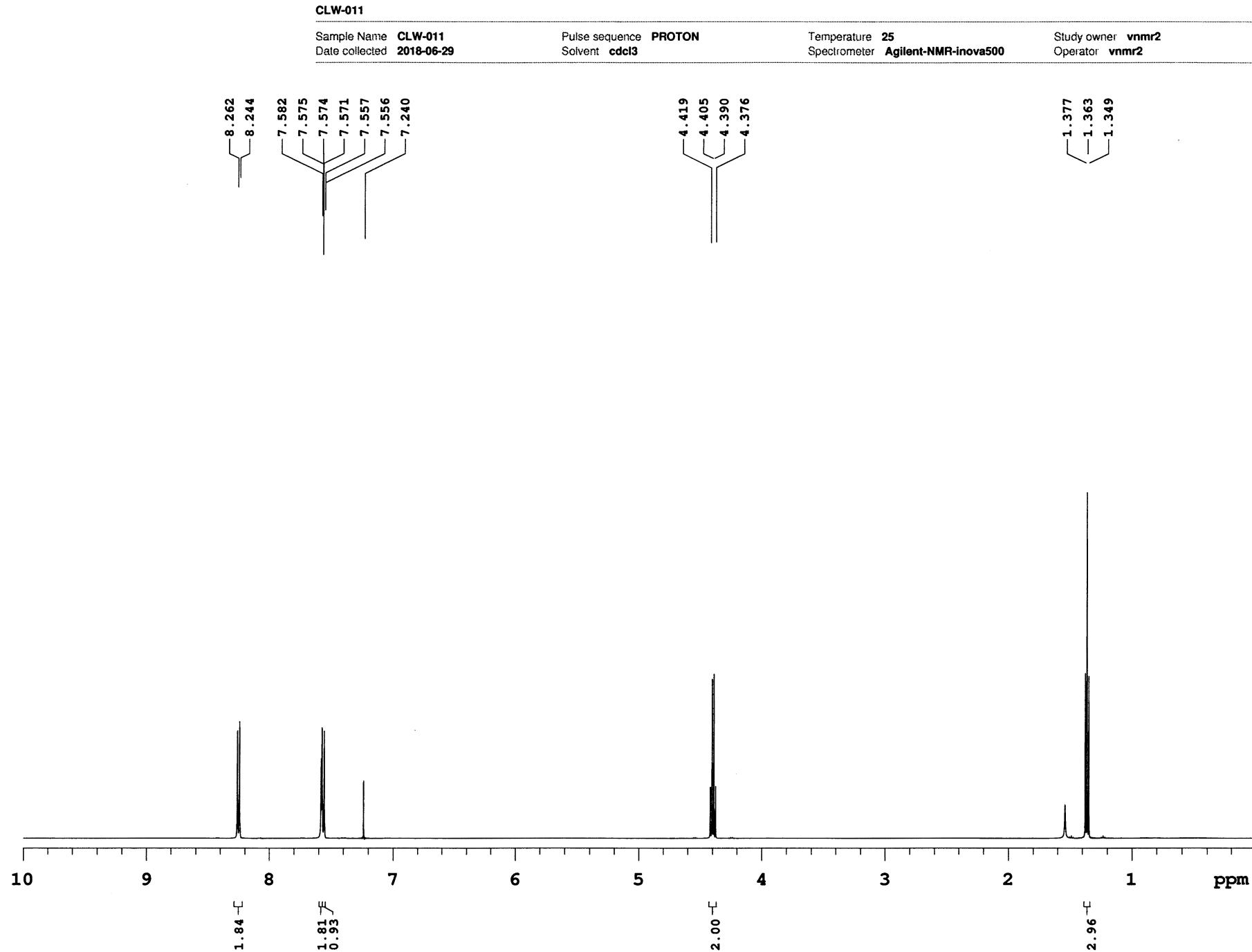
Sample Name PDC-03-121
Date collected 2018-01-10Pulse sequence DEPT
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner *vnmr2*
Operator *vnmr2*

Figure S23. DEPT of 2d

Figure S24. ^1H NMR (CDCl_3 , 500 MHz) of compound **2e**

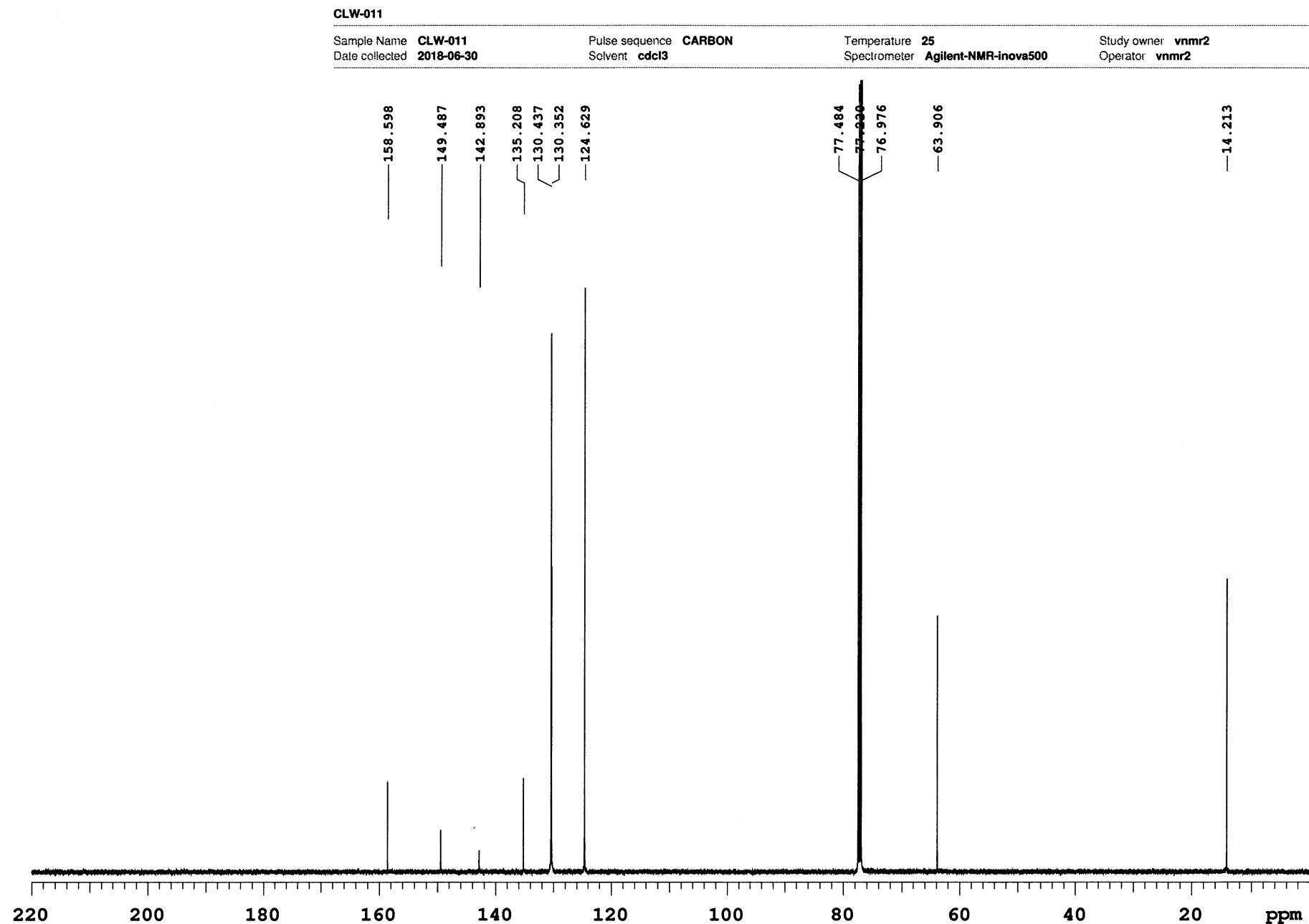
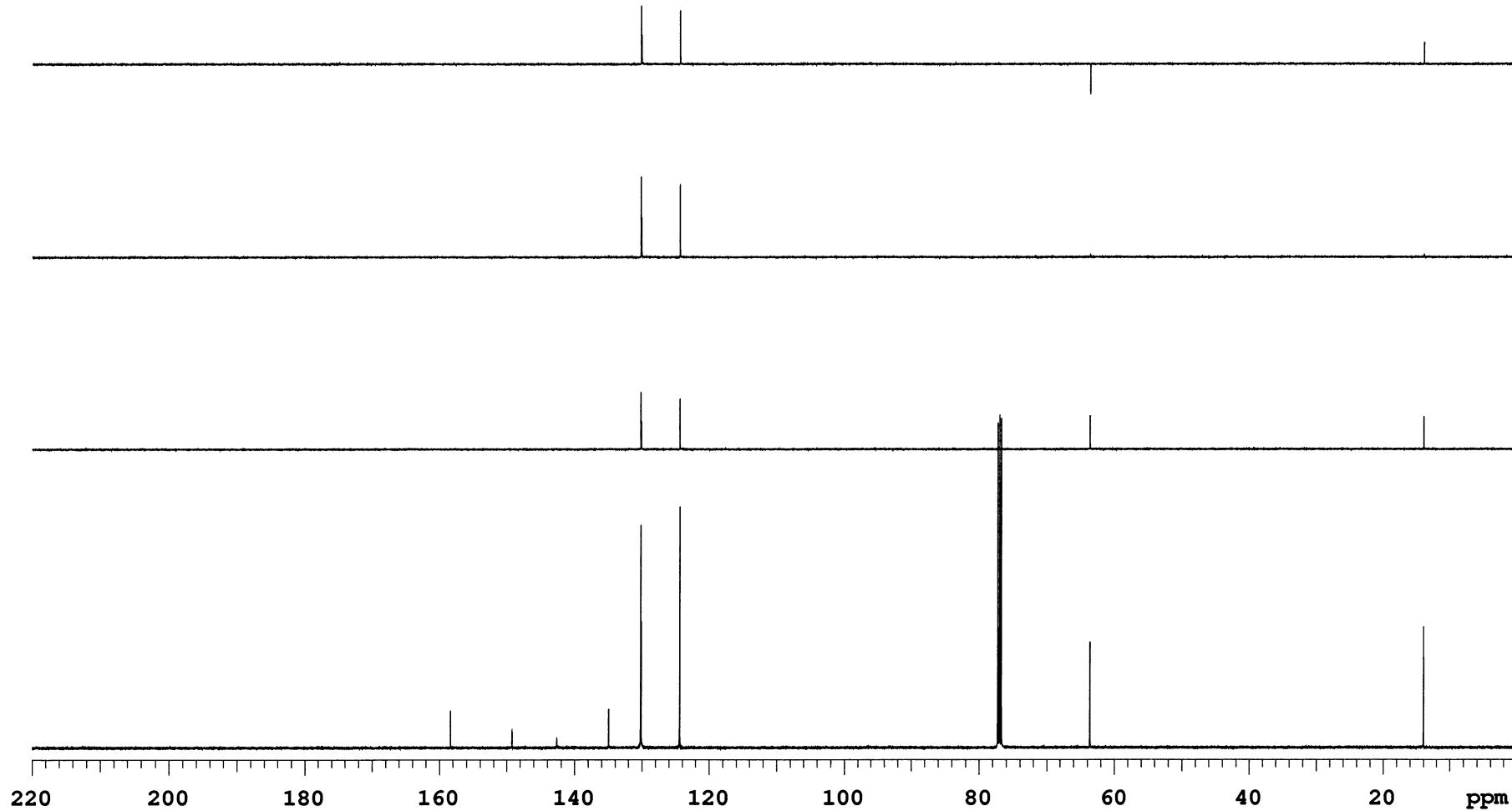
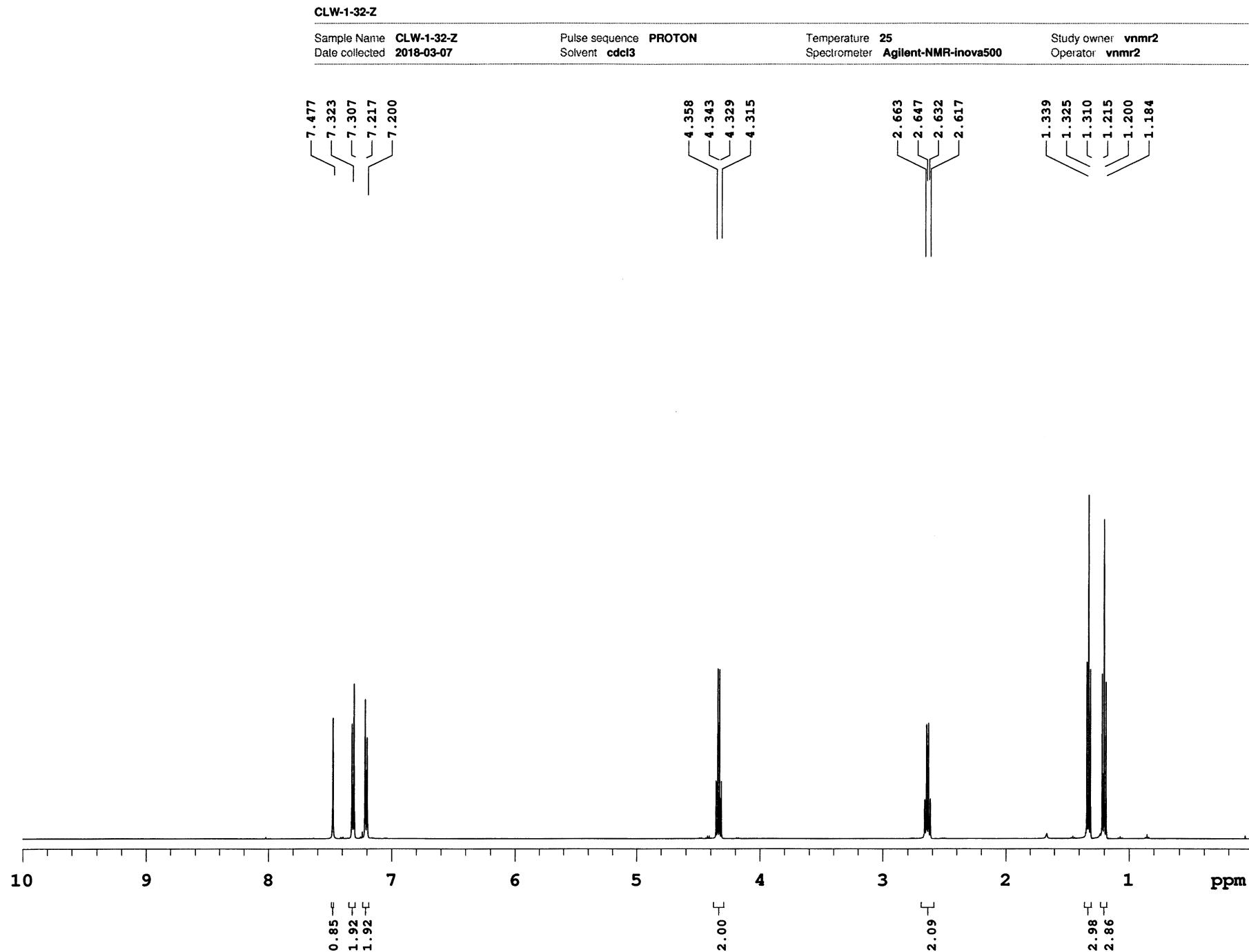


Figure S25. ^{13}C NMR (CDCl_3 , 125 MHz) of compound **2e**

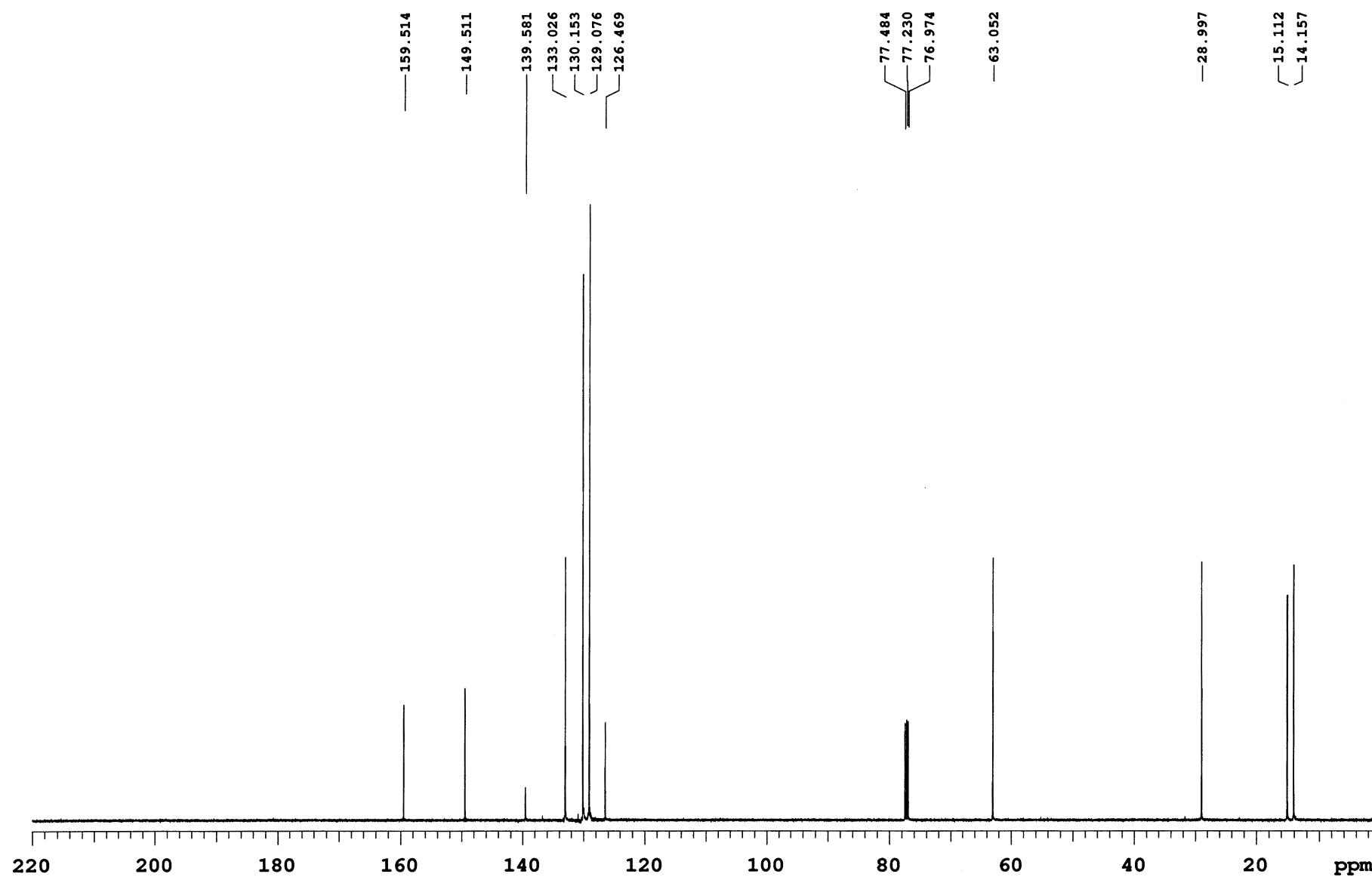
CLW-011

Sample Name **CLW-011**
Date collected **2018-06-30**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S26. DEPT of compound **2e**



CLW-1-32-Z

Sample Name	CLW-1-32-Z	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2018-03-07	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

Figure S28. ¹³C NMR (CDCl₃, 125 MHz) of compound **2f**

CLW-1-32-Z

Sample Name	CLW-1-32-Z	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr2
Date collected	2018-03-07	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

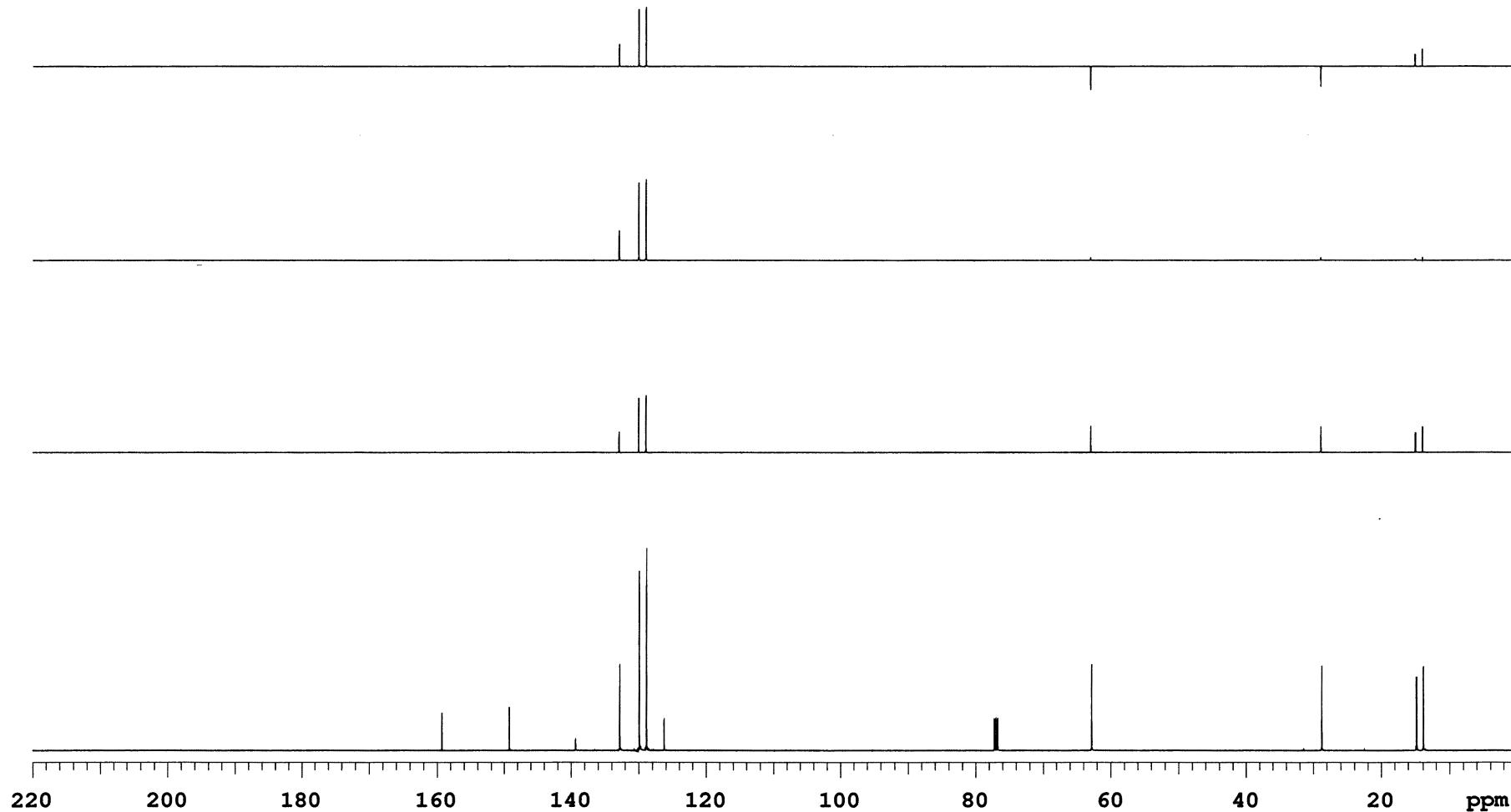


Figure S29. DEPT of compound 2f

PDC-03-107

Sample Name **PDC-03-10**
Date collected **2017-11-29**

Pulse sequence PROTON
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova50**

Study owner **vnmr**
Operator **vnmr2**

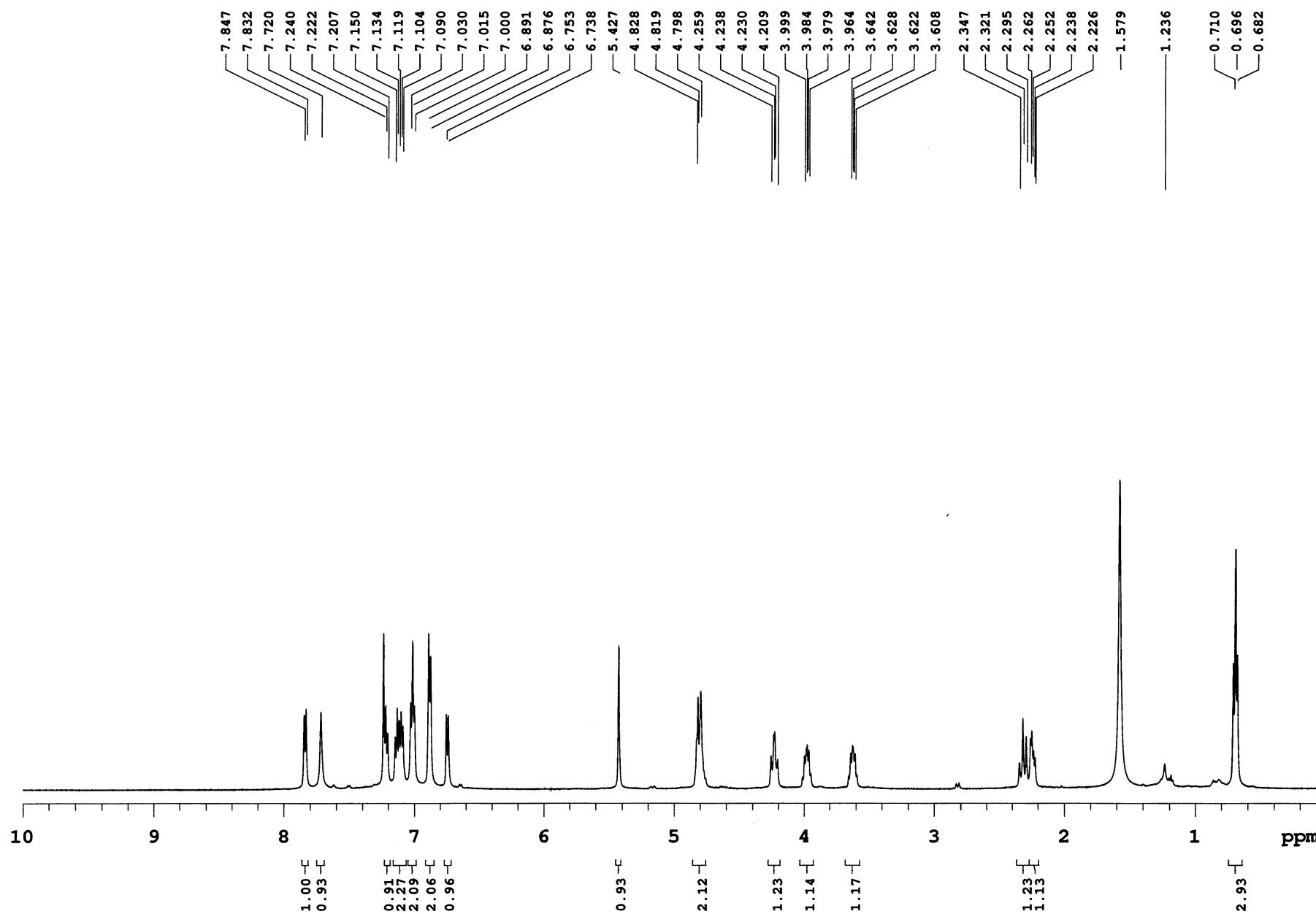
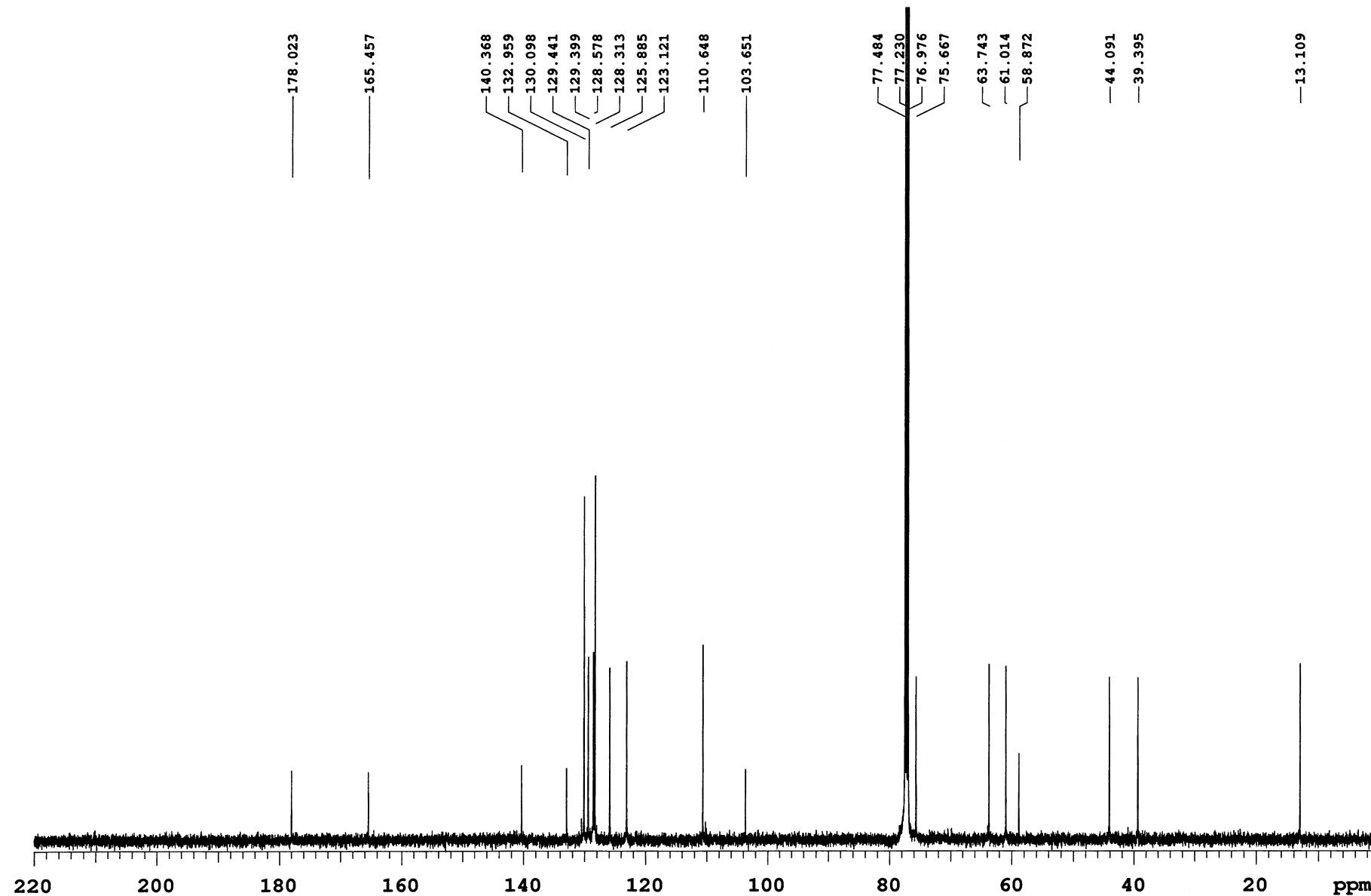


Figure S30. ^1H NMR (CDCl_3 , 500 MHz) of **3a**

PDC-03-107

Sample Name	PDC-03-107	Pulse sequence	CARBON	Temperature	25	Study owner	vnmr2
Date collected	2017-11-29	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

Figure S31. ¹³C NMR (CDCl₃, 125 MHz) of **3a**

PDC-03-107

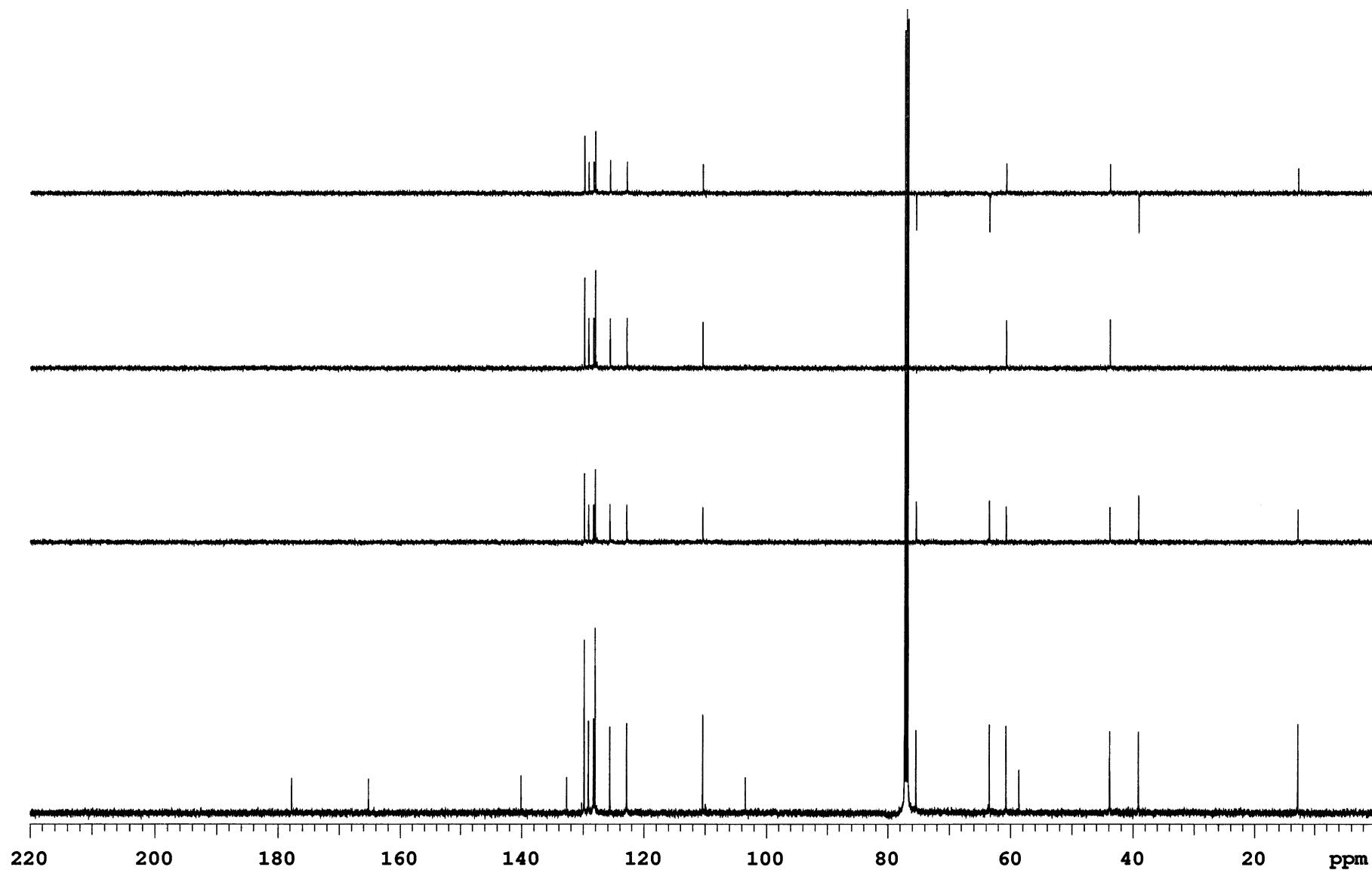
Sample Name PDC-03-107
Date collected 2017-11-30Pulse sequence DEPT
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S32. DEPT of 3a

PDC-03-107

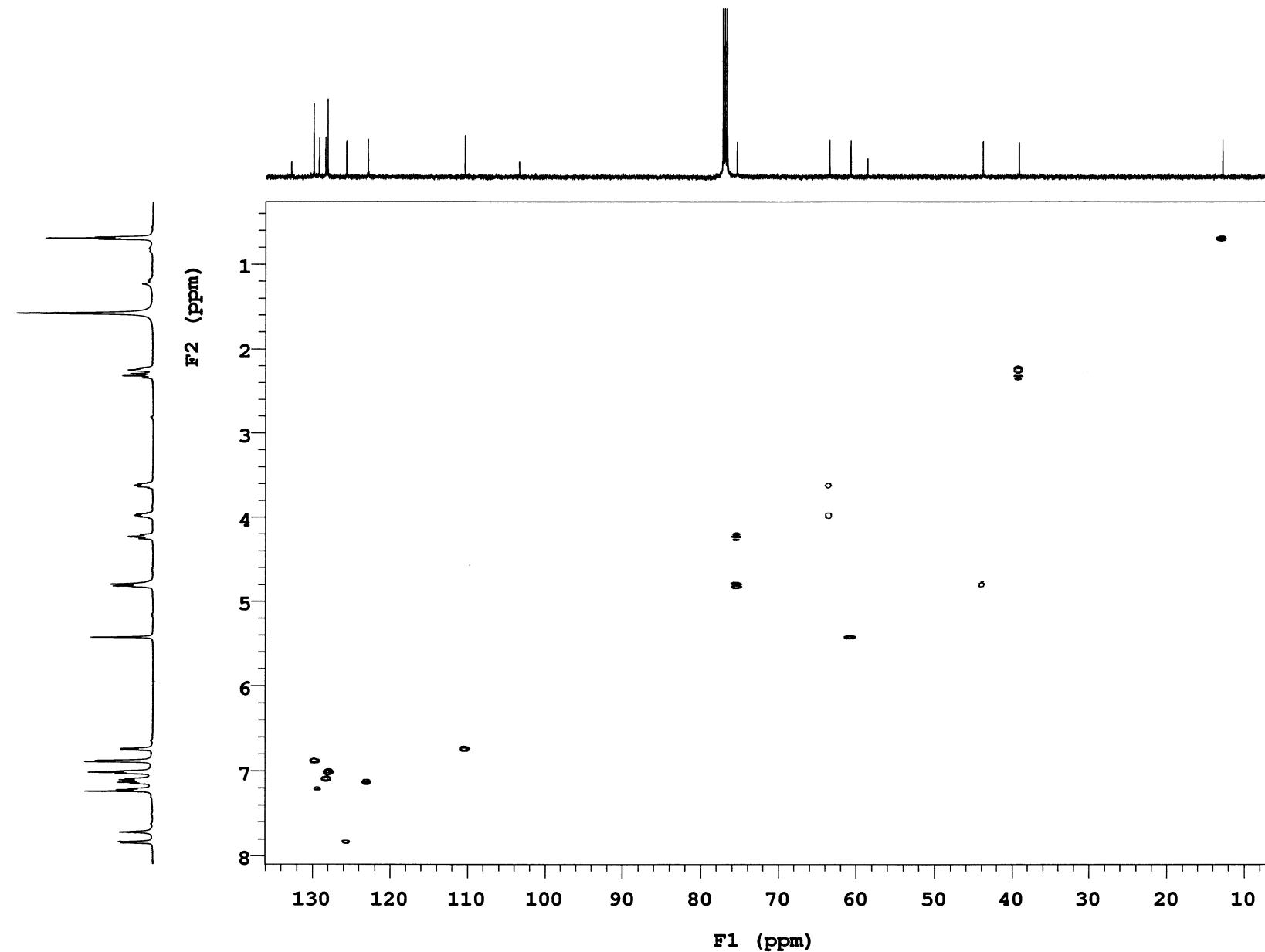
Sample Name PDC-03-107
Date collected 2017-11-30Pulse sequence gHMQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner **vnmr2**
Operator **vnmr2**

Figure S33. HMQC of 3a

PDC-03-107

Sample Name **PDC-03-107**
Date collected **2017-11-30**

Pulse sequence **gCOSY**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-Inova500**

Study owner **vnmr2**
Operator **vnmr2**

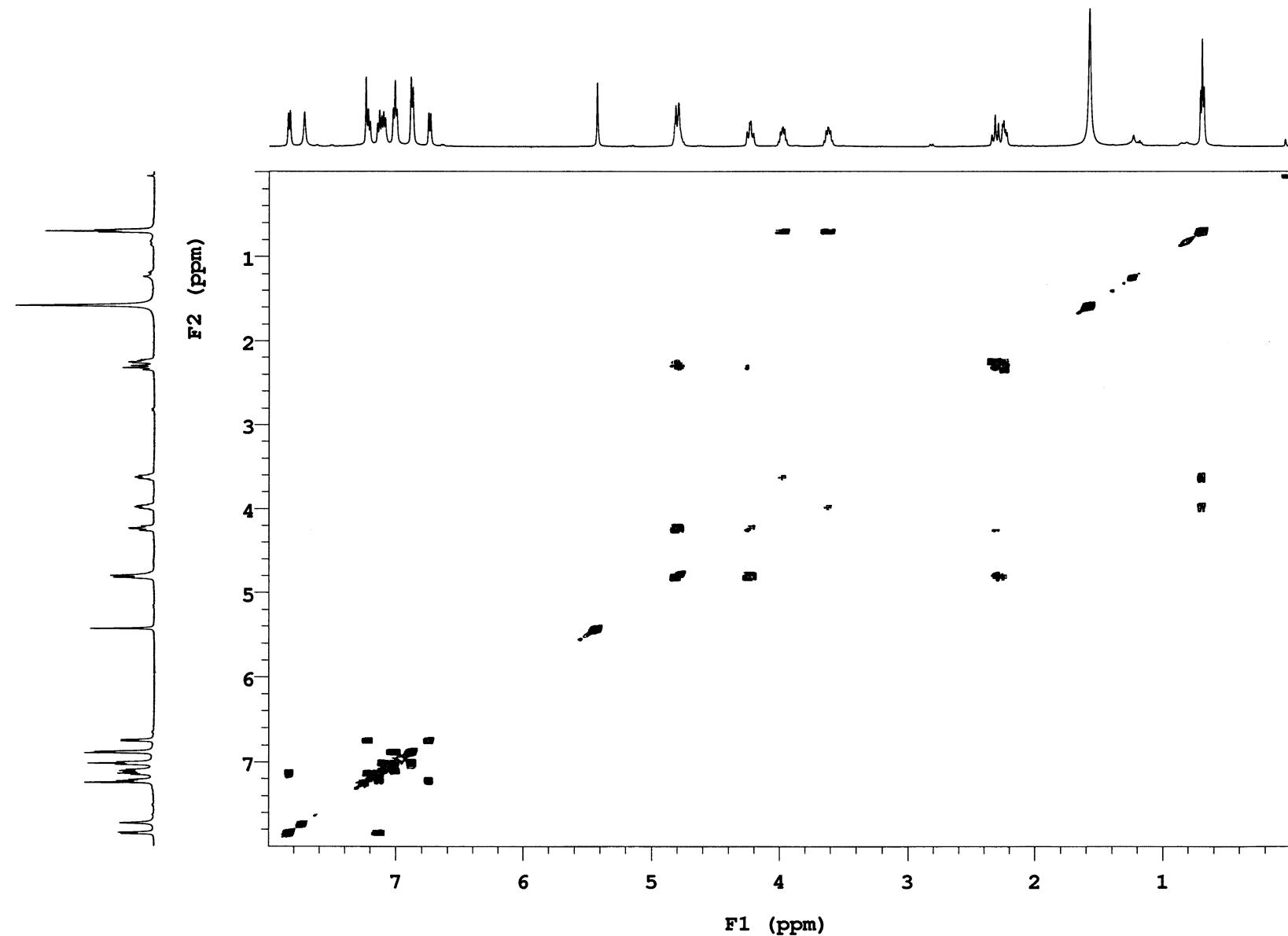


Figure S34. COSY of 3a

PDC-03-107

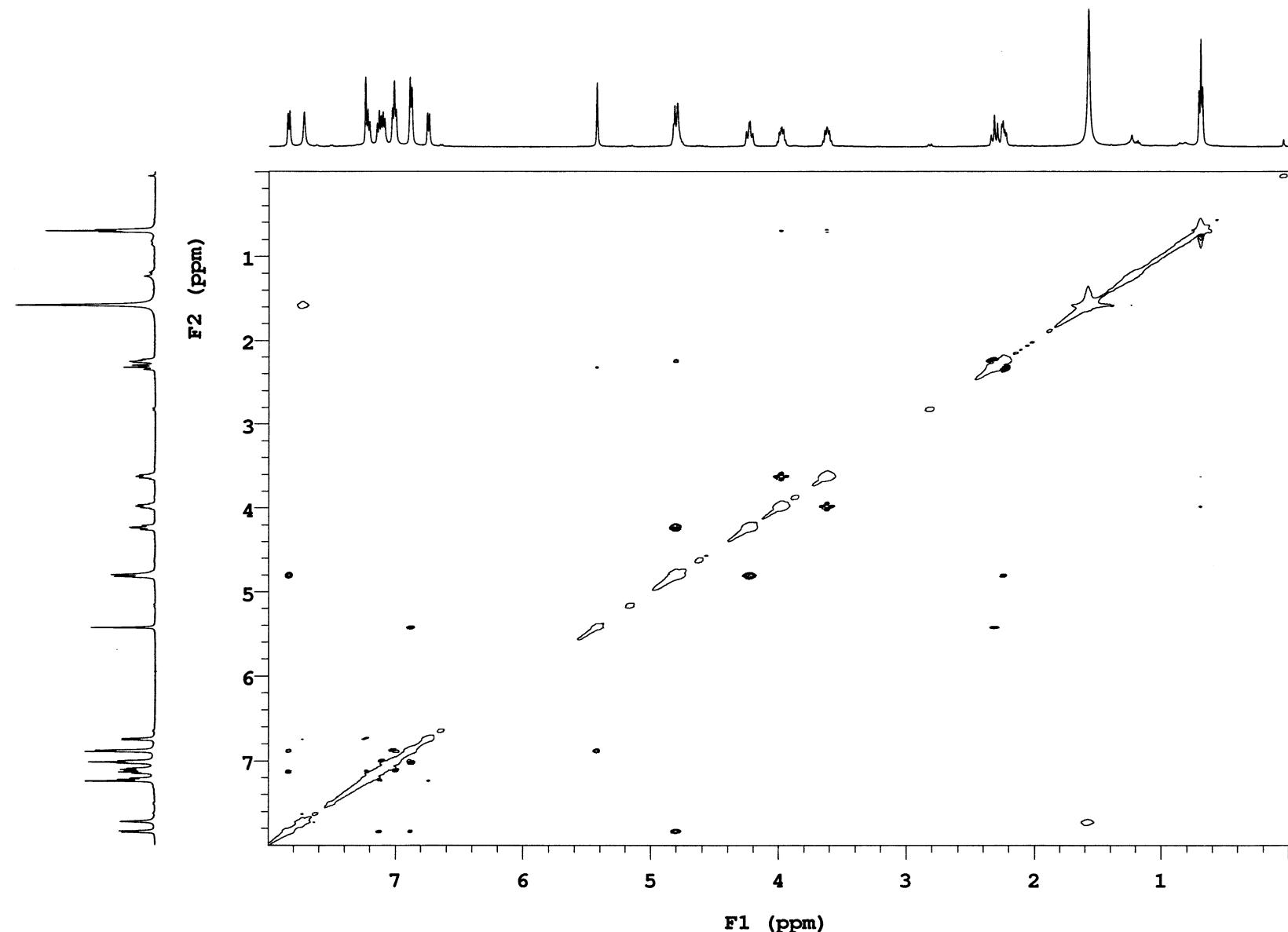
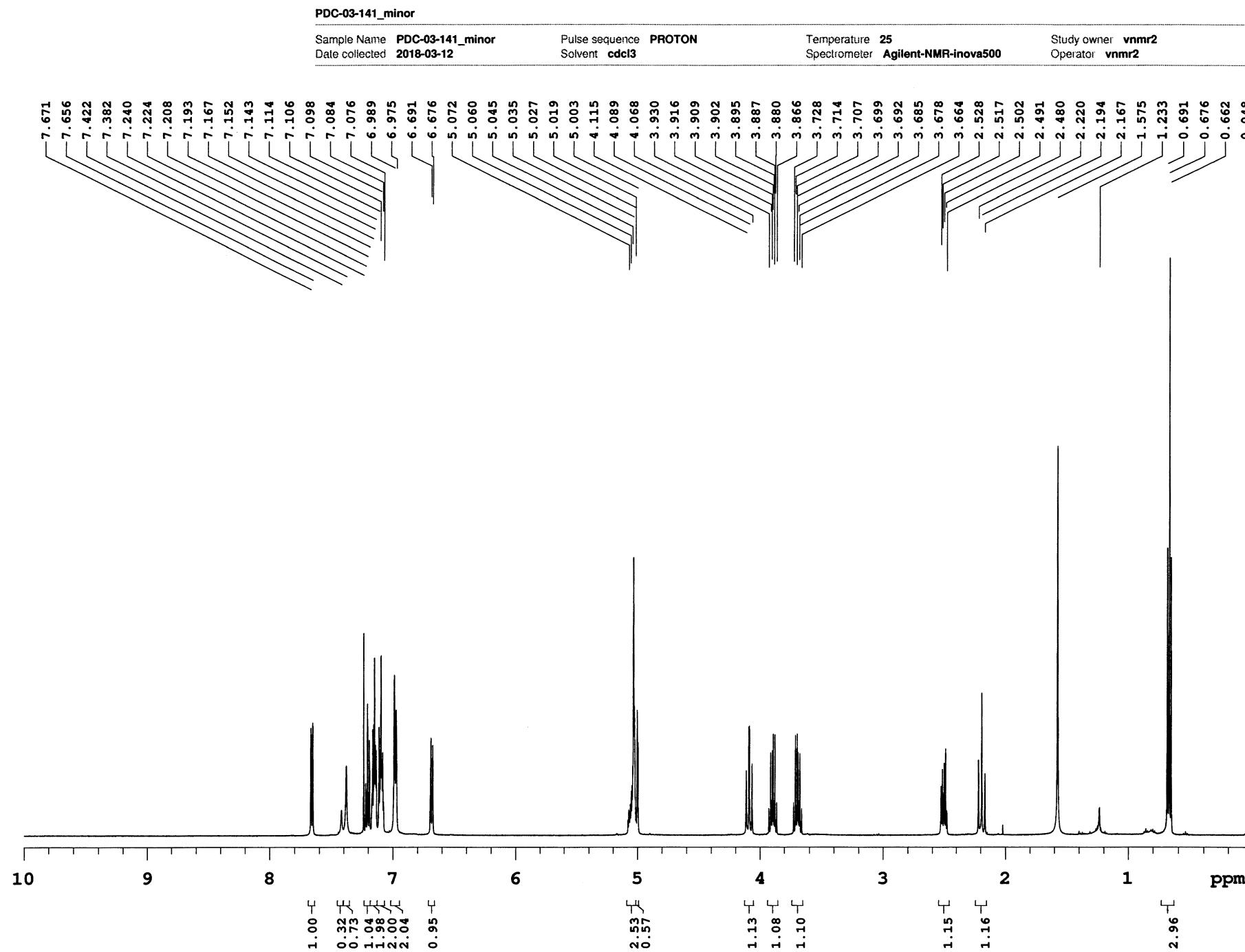
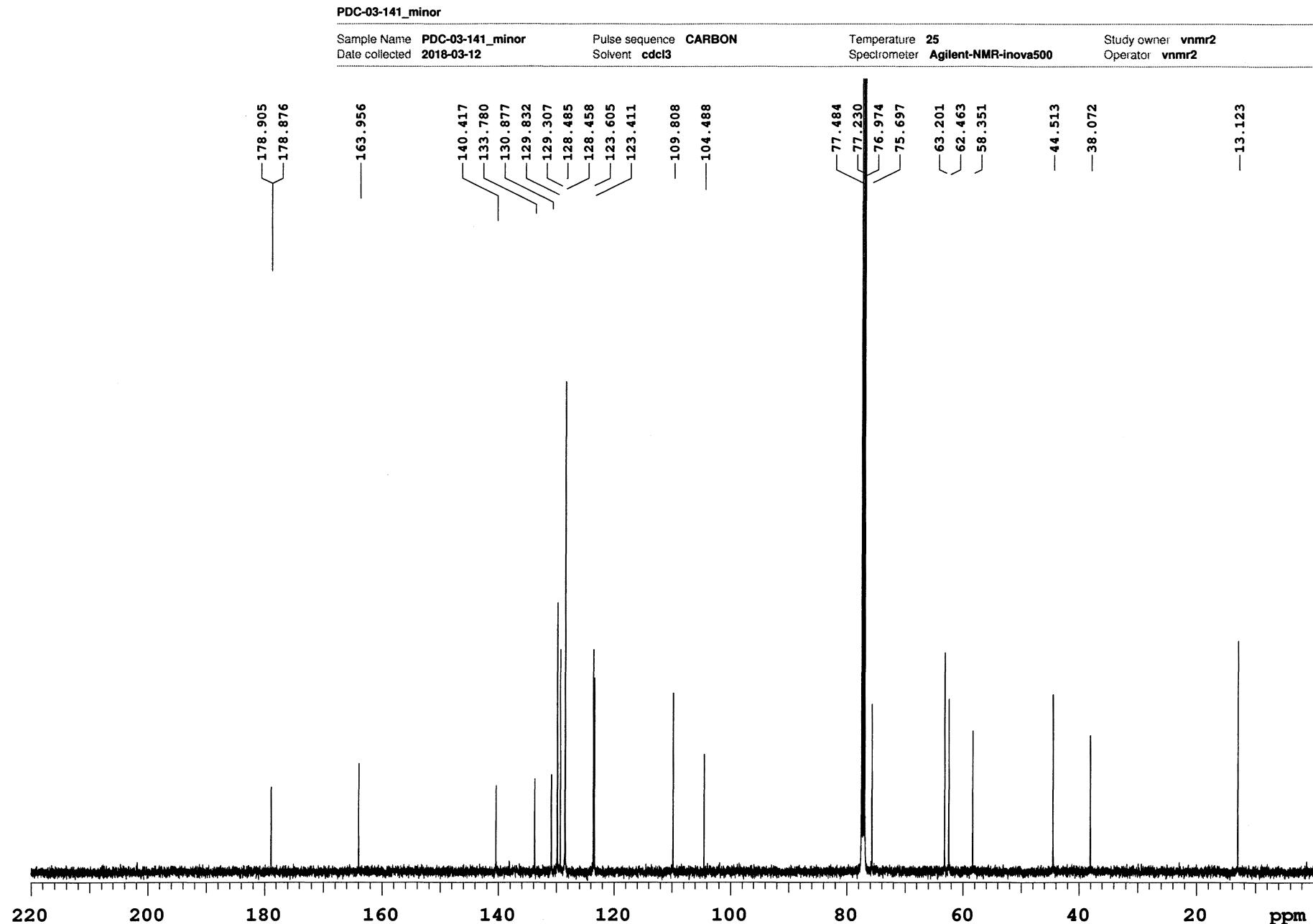
Sample Name PDC-03-107
Date collected 2017-11-30Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S35. NOESY of 3a



Figure S37. ^{13}C NMR (CDCl₃, 125 MHz) of **4a**

PDC-03-141_minor

Sample Name **PDC-03-141_minor**
Date collected **2018-03-13**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

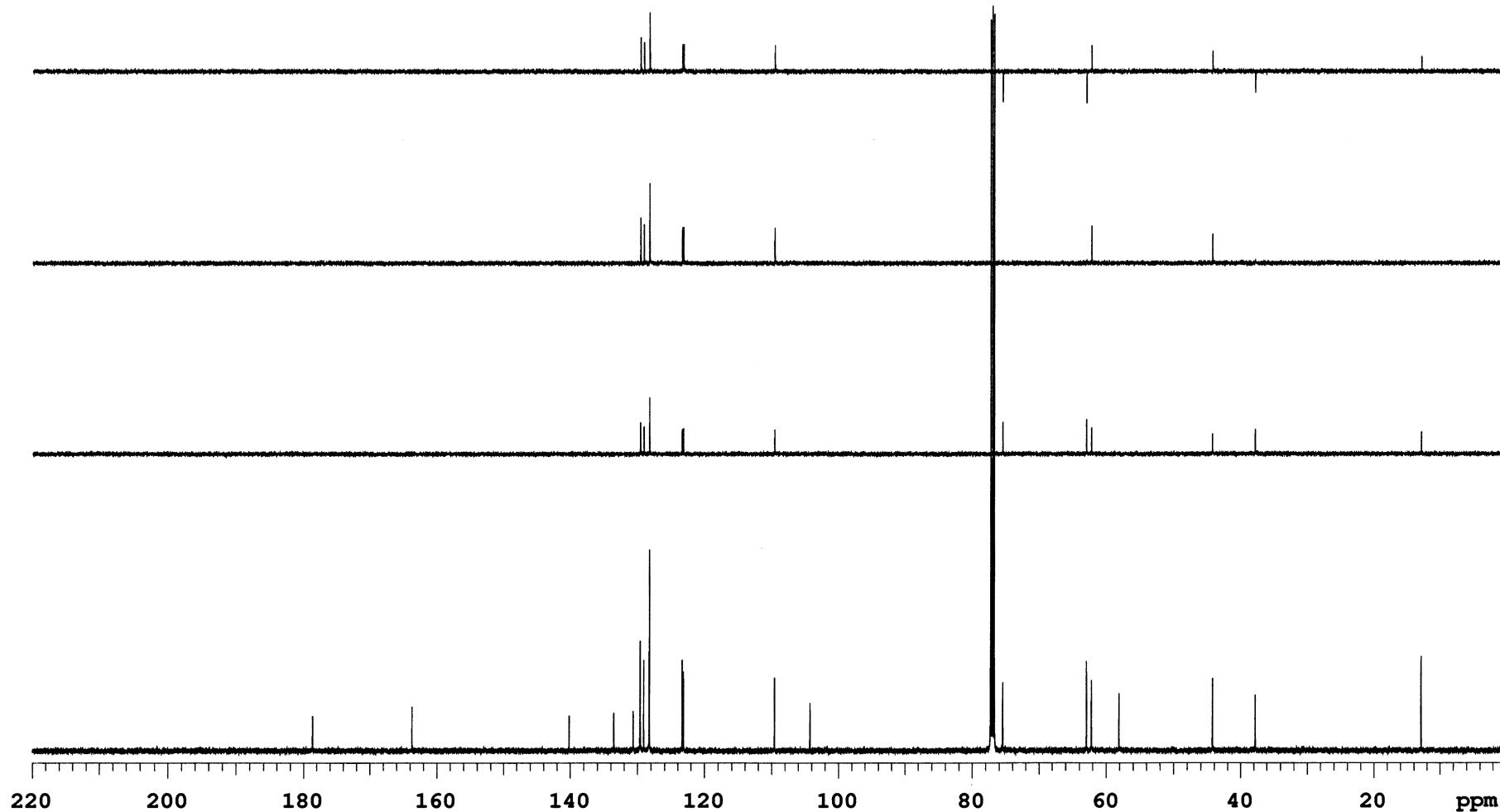
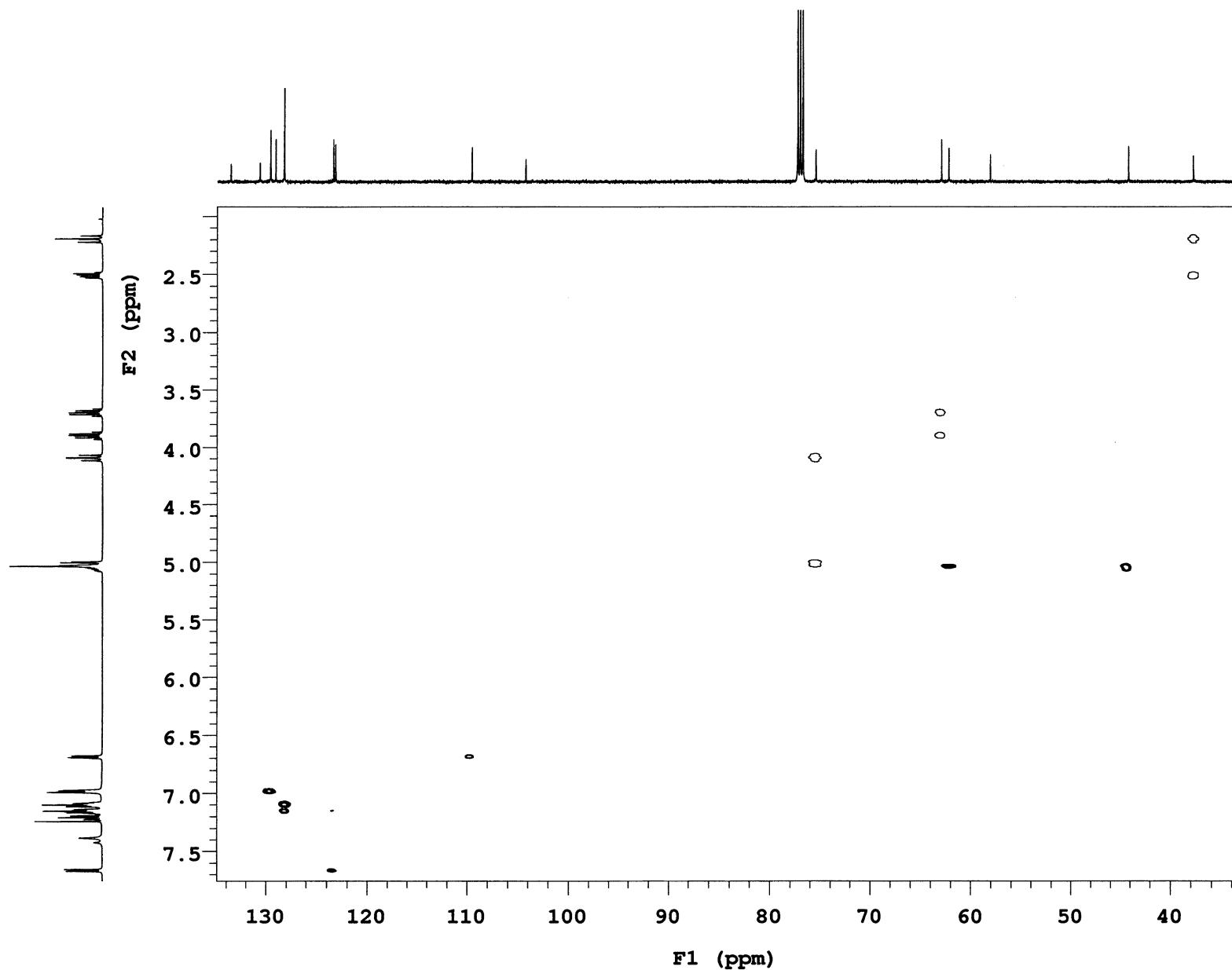


Figure S38. DEPT of **4a**

PDC-03-141_minor

Sample Name **PDC-03-141_minor**
Date collected **2018-03-13**Pulse sequence **gHSQC**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S39. HSQC of **4a**

PDC-03-141_minor

Sample Name PDC-03-141_minor
Date collected 2018-03-13

Pulse sequence gCOSY
Solvent *cdcl*3

Temperature 25
Specrometer Agilent-NMR-inova500

Study owner vnmr2
Operator vnmr2

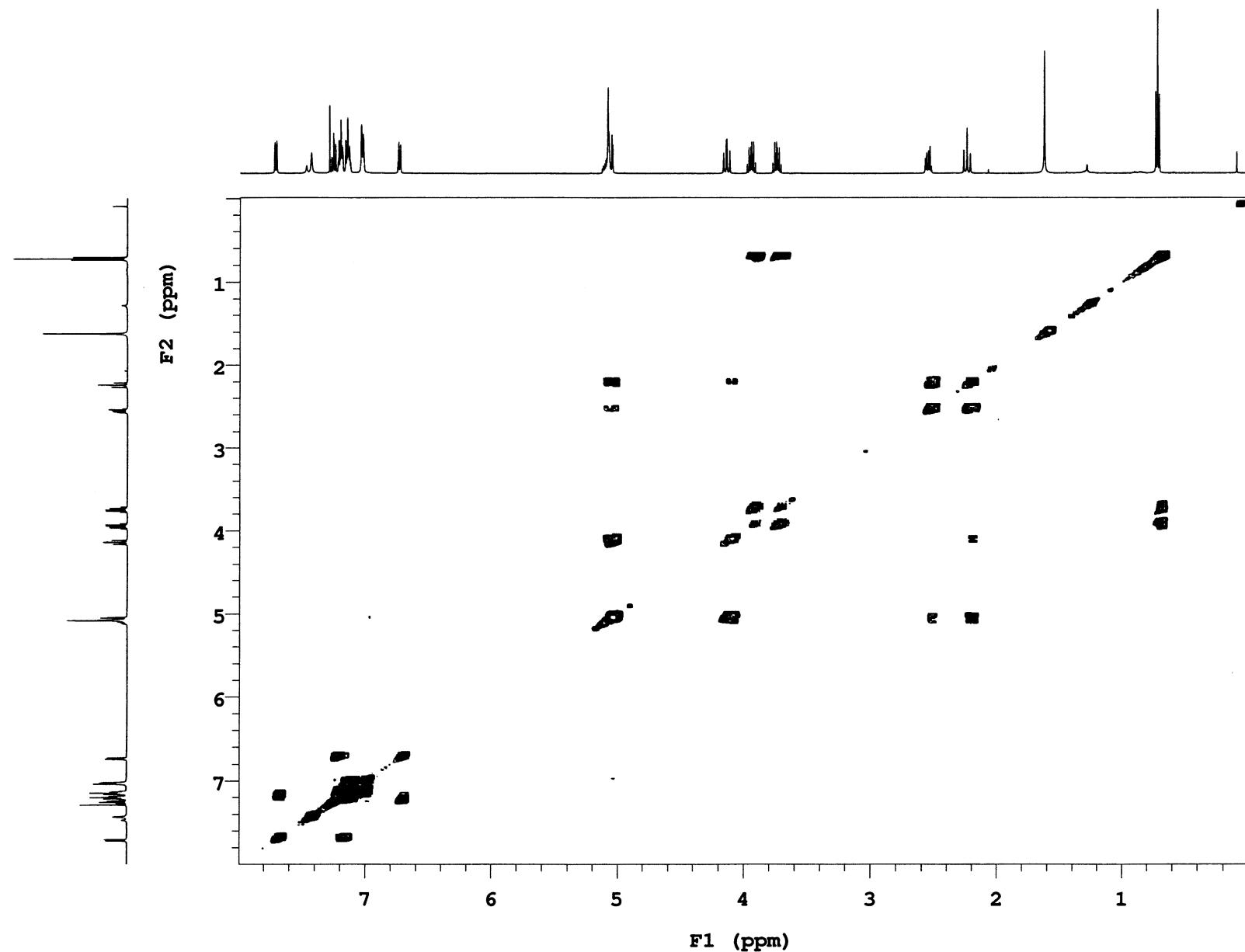


Figure S40. COSY of 4a

PDC-03-141_minor

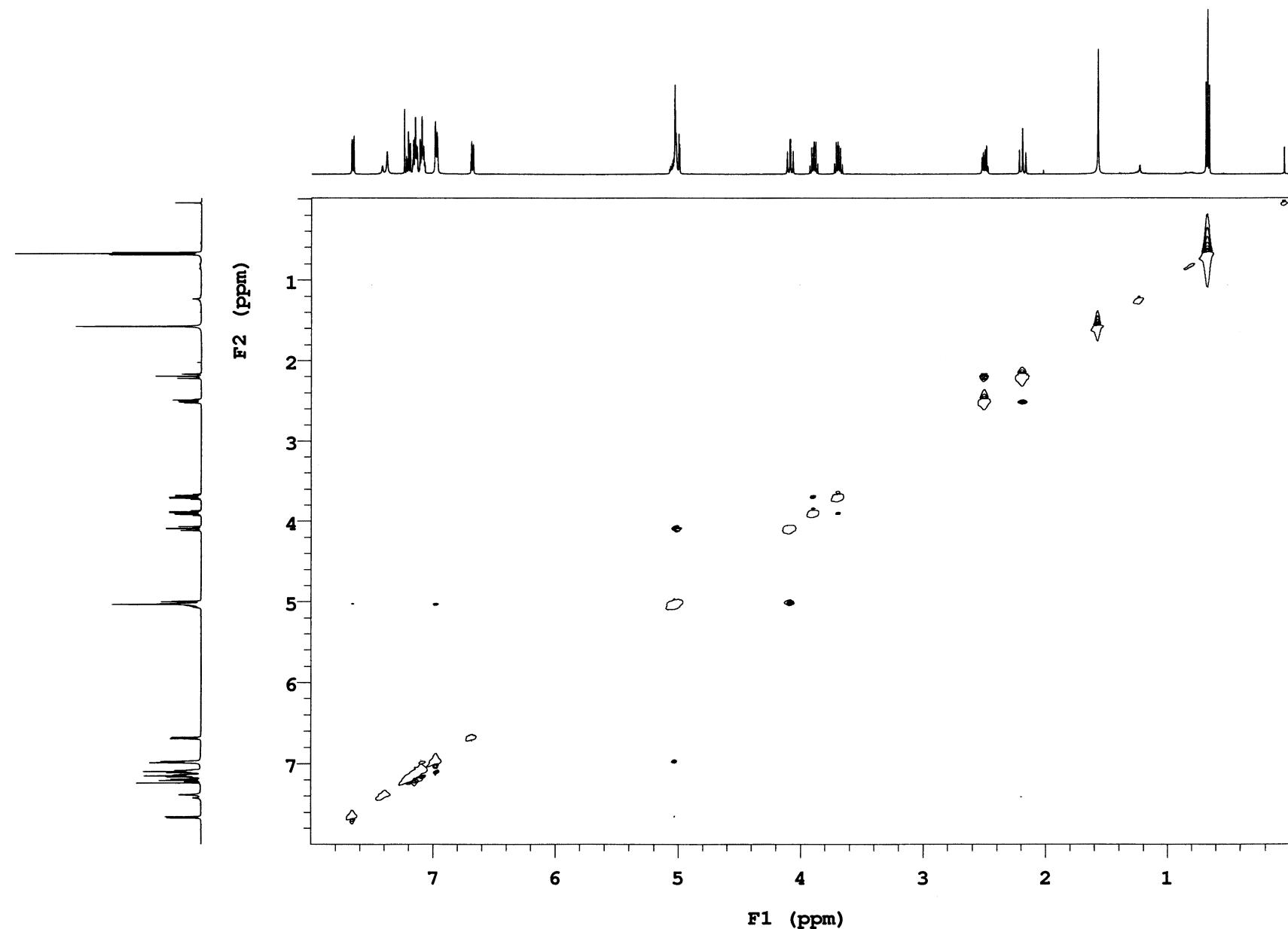
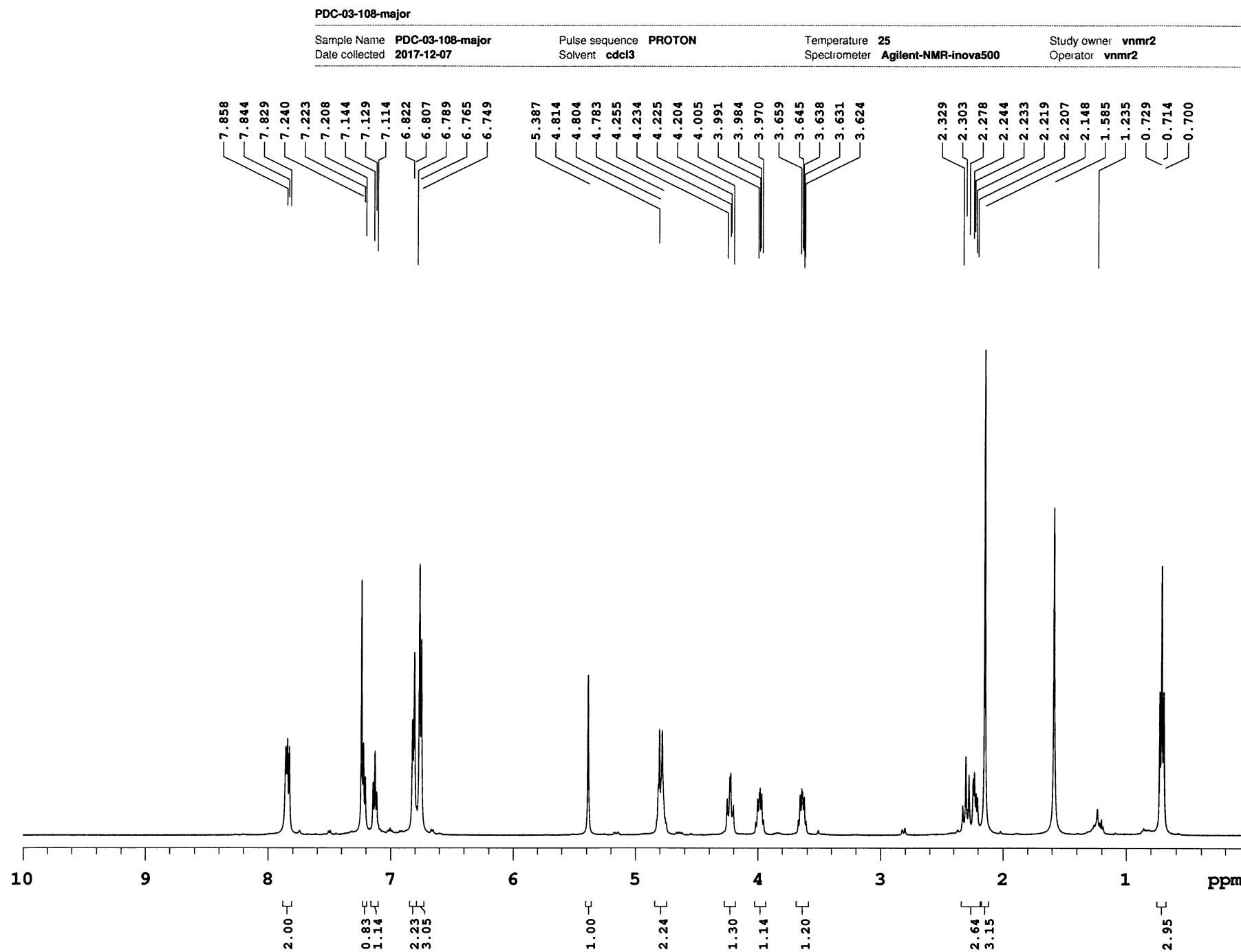
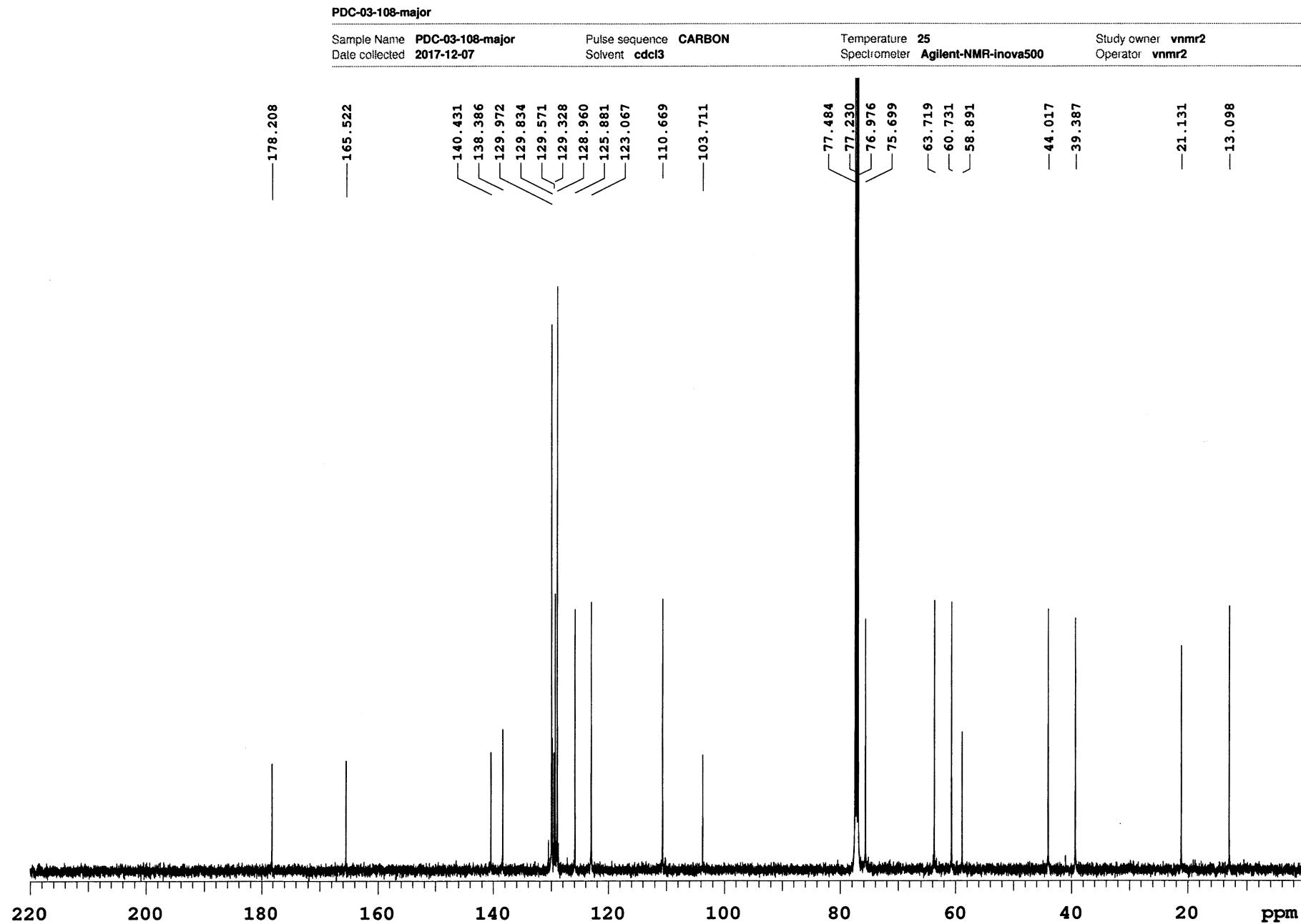
Sample Name PDC-03-141_minor
Date collected 2018-03-13Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Specrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S41. NOESY of 4a

Figure S42. ^1H NMR (CDCl_3 , 500 MHz) of **3b**

Figure S43. ¹³C NMR (CDCl₃, 125 MHz) of 3b

PDC-03-108-major

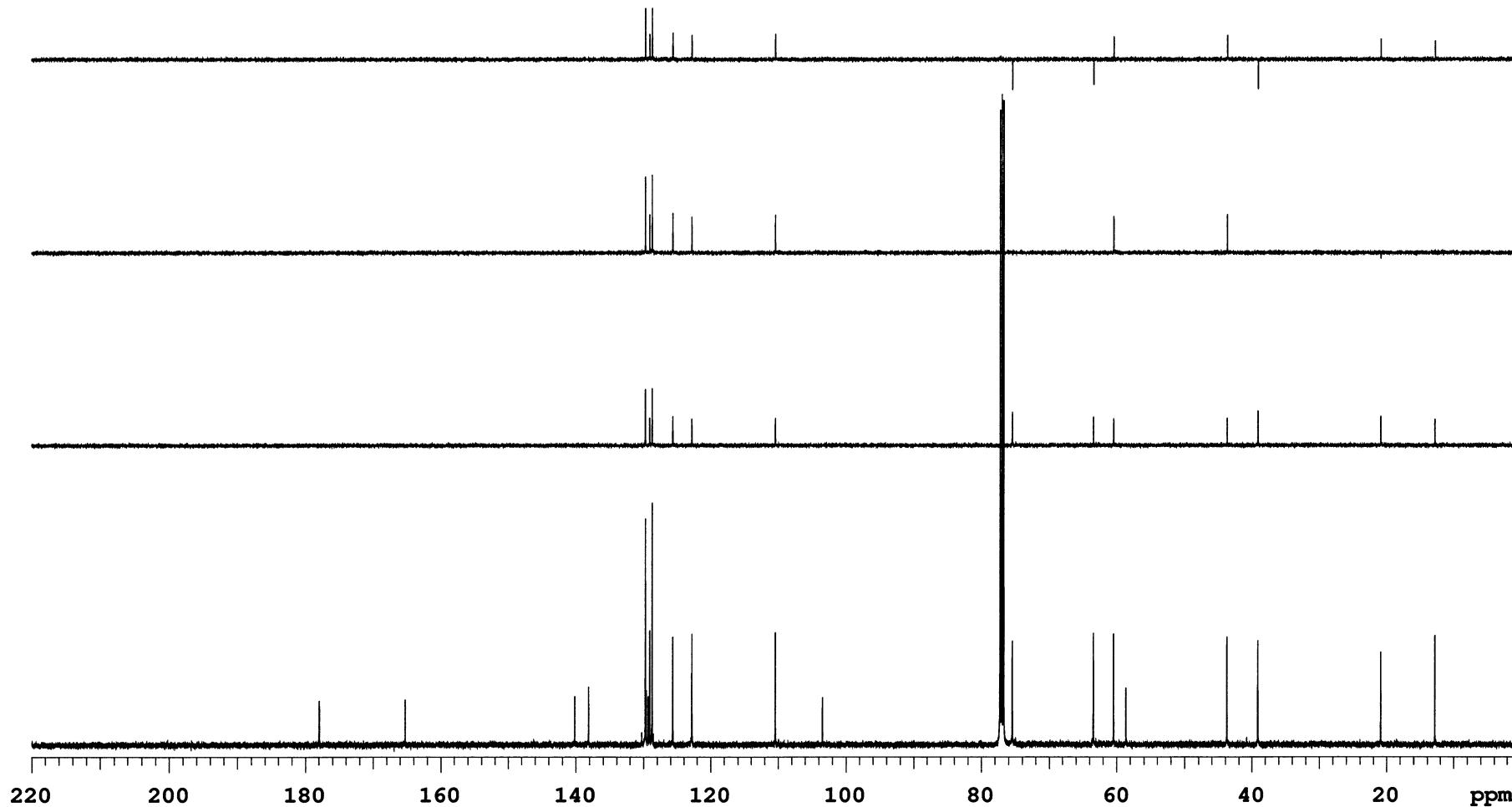
Sample Name PDC-03-108-major
Date collected 2017-12-08Pulse sequence DEPT
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S44. DEPT of 3b

PDC-03-108-major

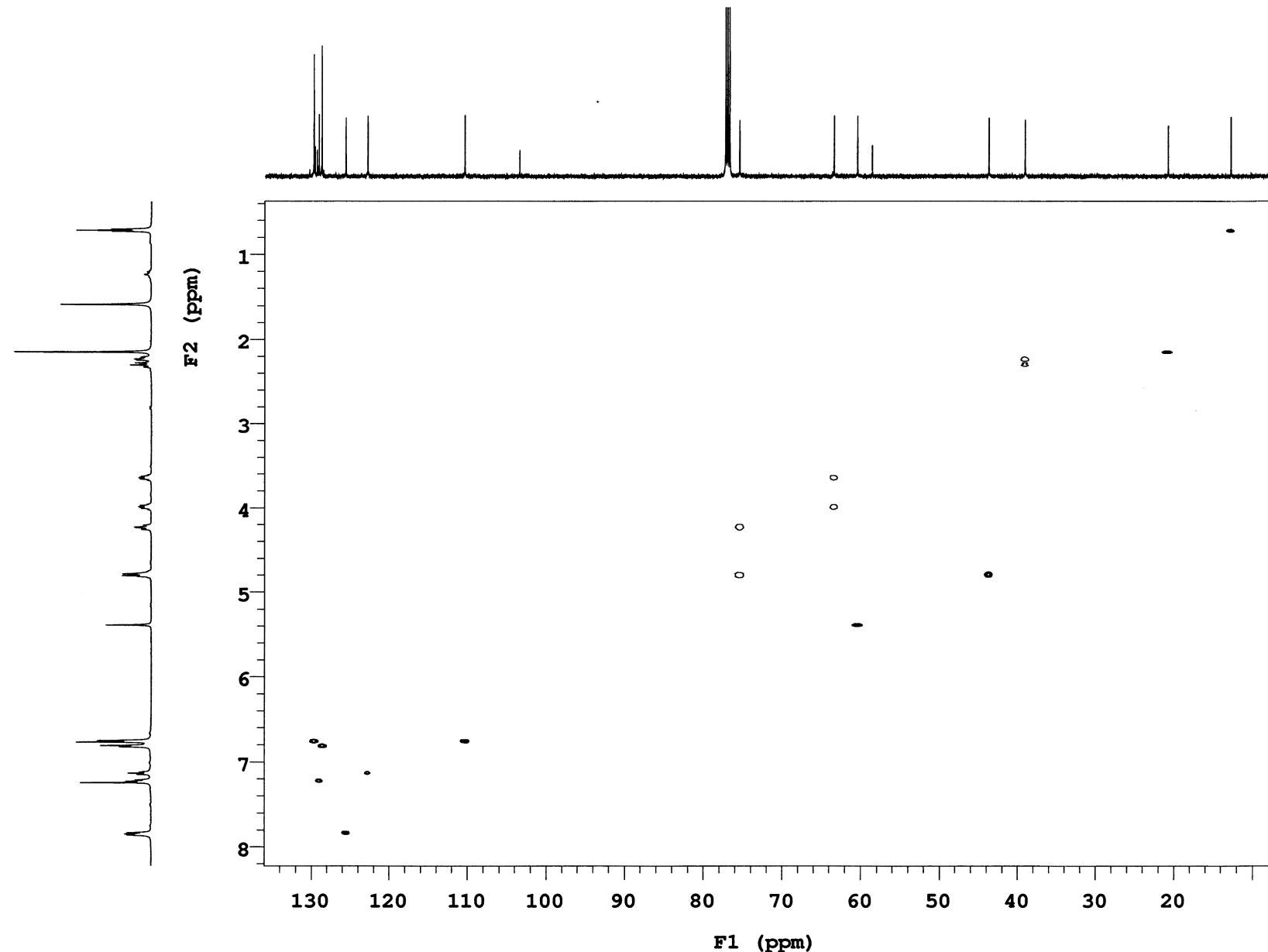
Sample Name PDC-03-108-major
Date collected 2017-12-08Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2

Figure S45. HSQC of 3b

PDC-03-108-major

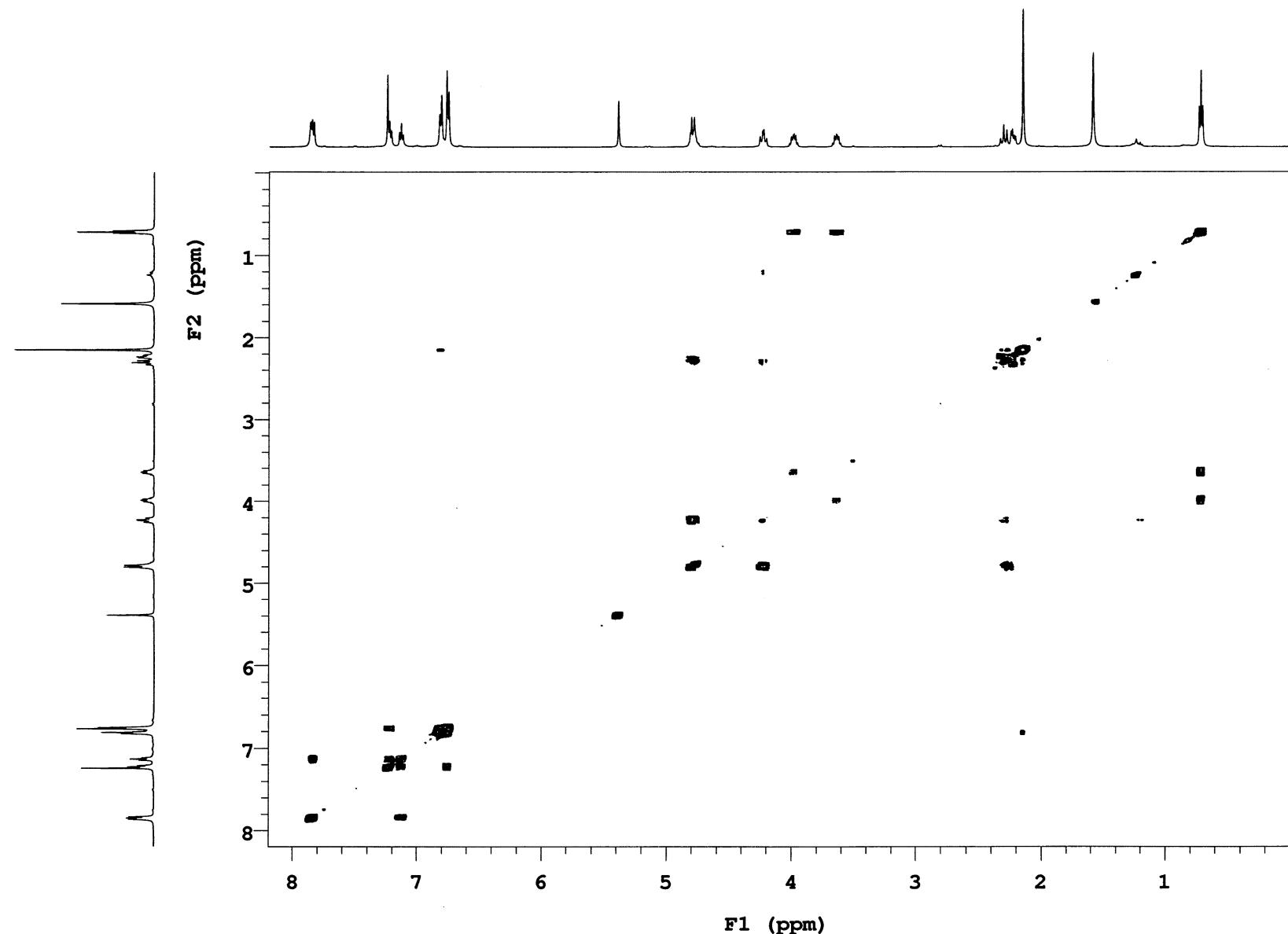
Sample Name **PDC-03-108-major**
Date collected **2017-12-08**Pulse sequence **gCOSY**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**

Figure S46. COSY of 3b

PDC-03-108-major

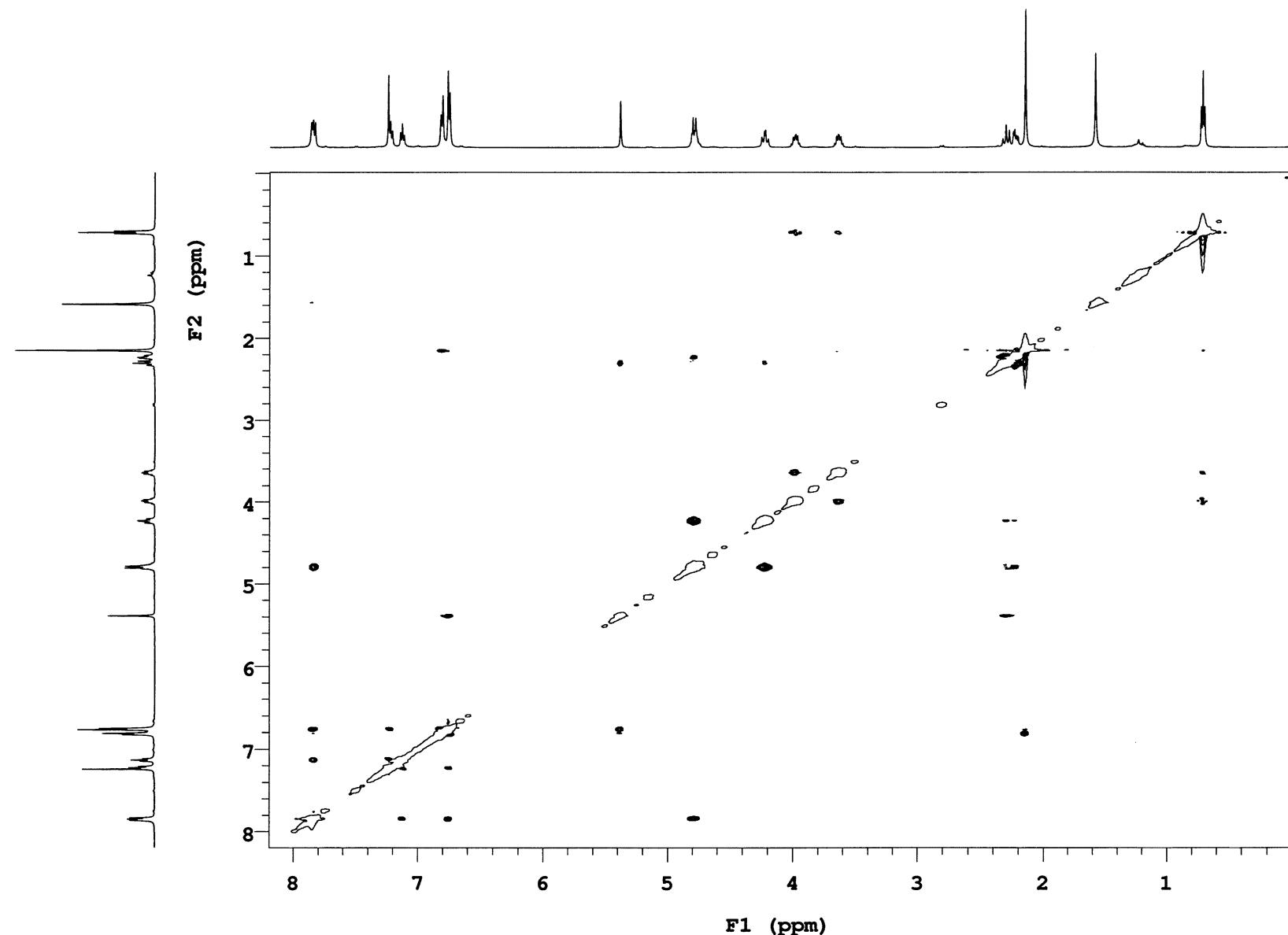
Sample Name PDC-03-108-major
Date collected 2017-12-08Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Specrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S47. NOESY of 3b

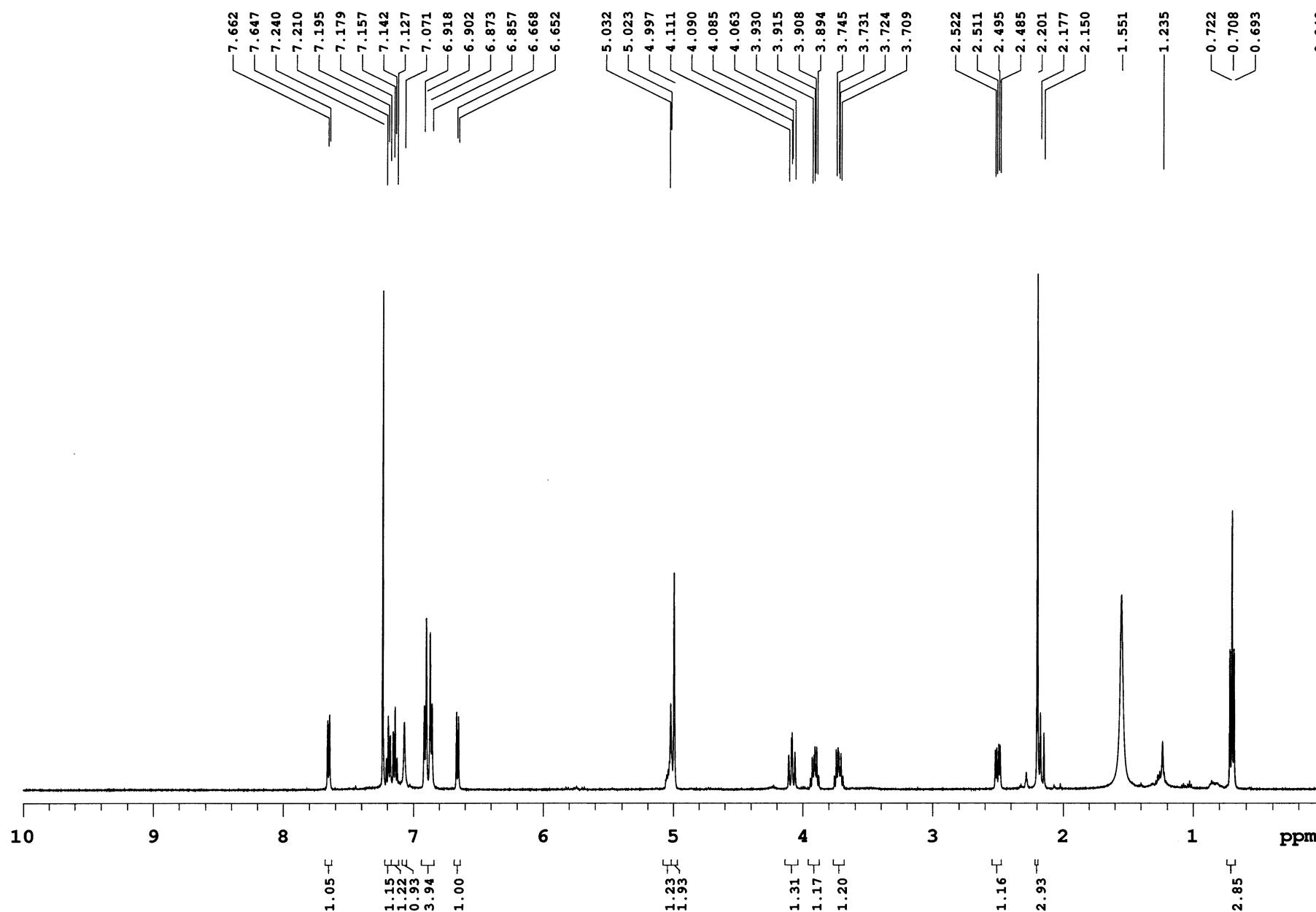
PDC-02-109

Sample Name **PDC-02-10**
Date collected **2018-03-24**

Pulse sequence PROTON
Solvent **cdcl3**

Temperature 25
Spectrometer Agilent-NMR-inova500

Study owner: **vnmr**
Operator: **vnmr2**



PDC-02-109

Sample Name **PDC-02-109**
Date collected **2018-03-24**

Pulse sequence **CARBON**
Solvent **cdcl3**

Temperature **25**
Specrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

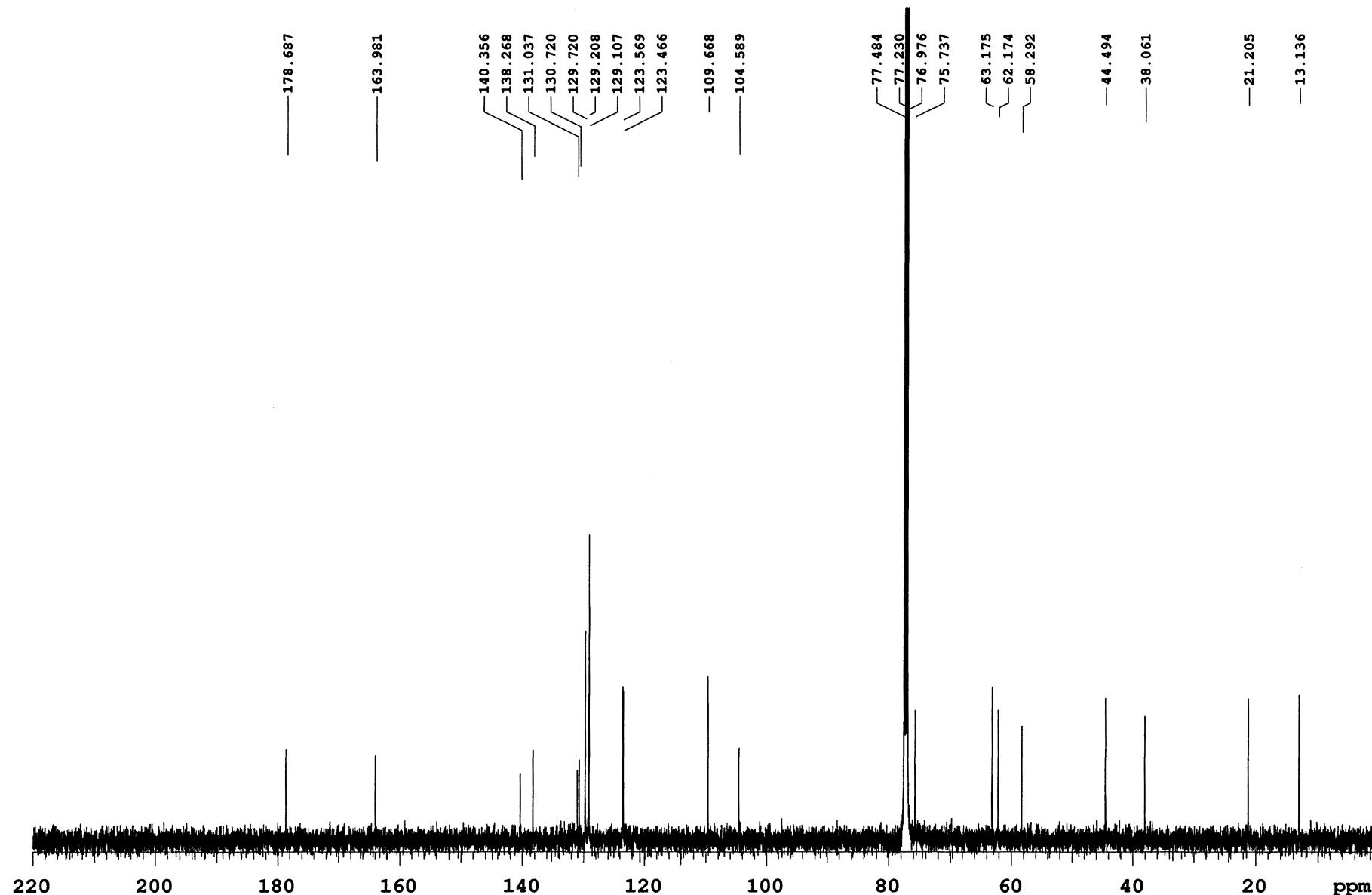


Figure S49. 13C NMR (CDCl₃, 125 MHz) of **4b**

Sample Name **PDC-02-109**
Date collected **2018-03-25**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Specrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

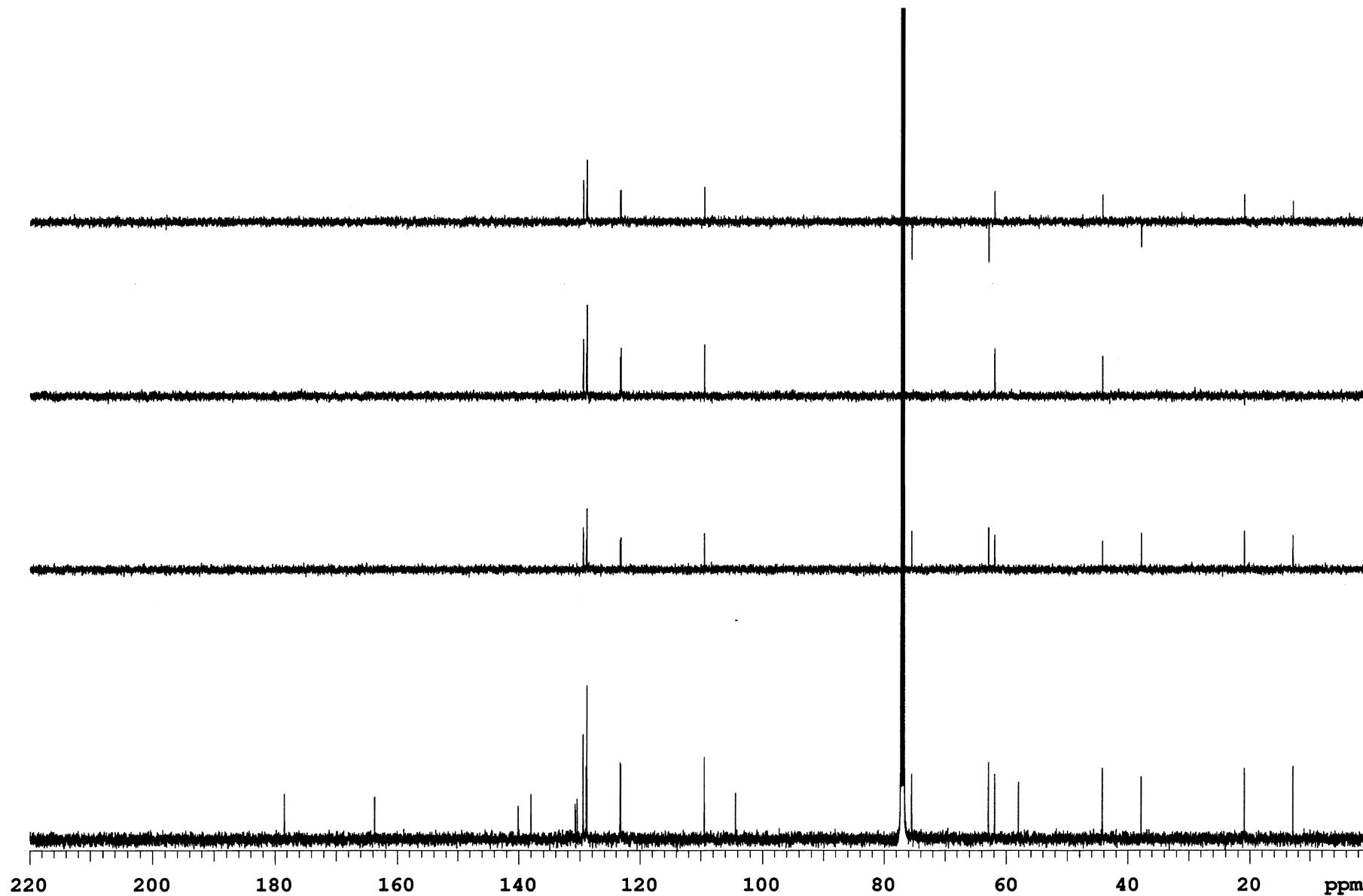
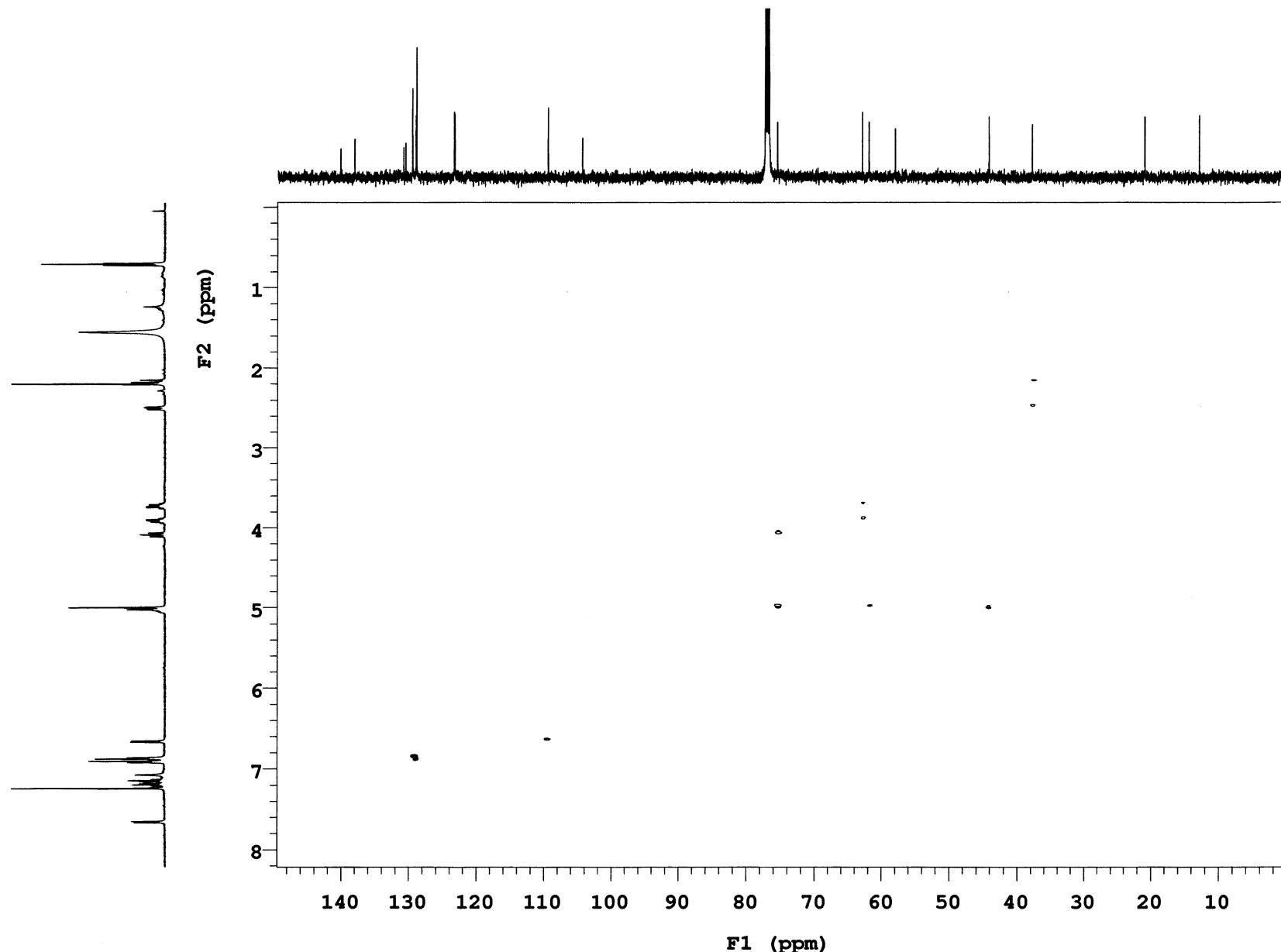


Figure S50. DEPT of **4b**

PDC-02-109

Sample Name PDC-02-109
Date collected 2018-03-25Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2Figure S51. HSQC of **4b**

PDC-03-109

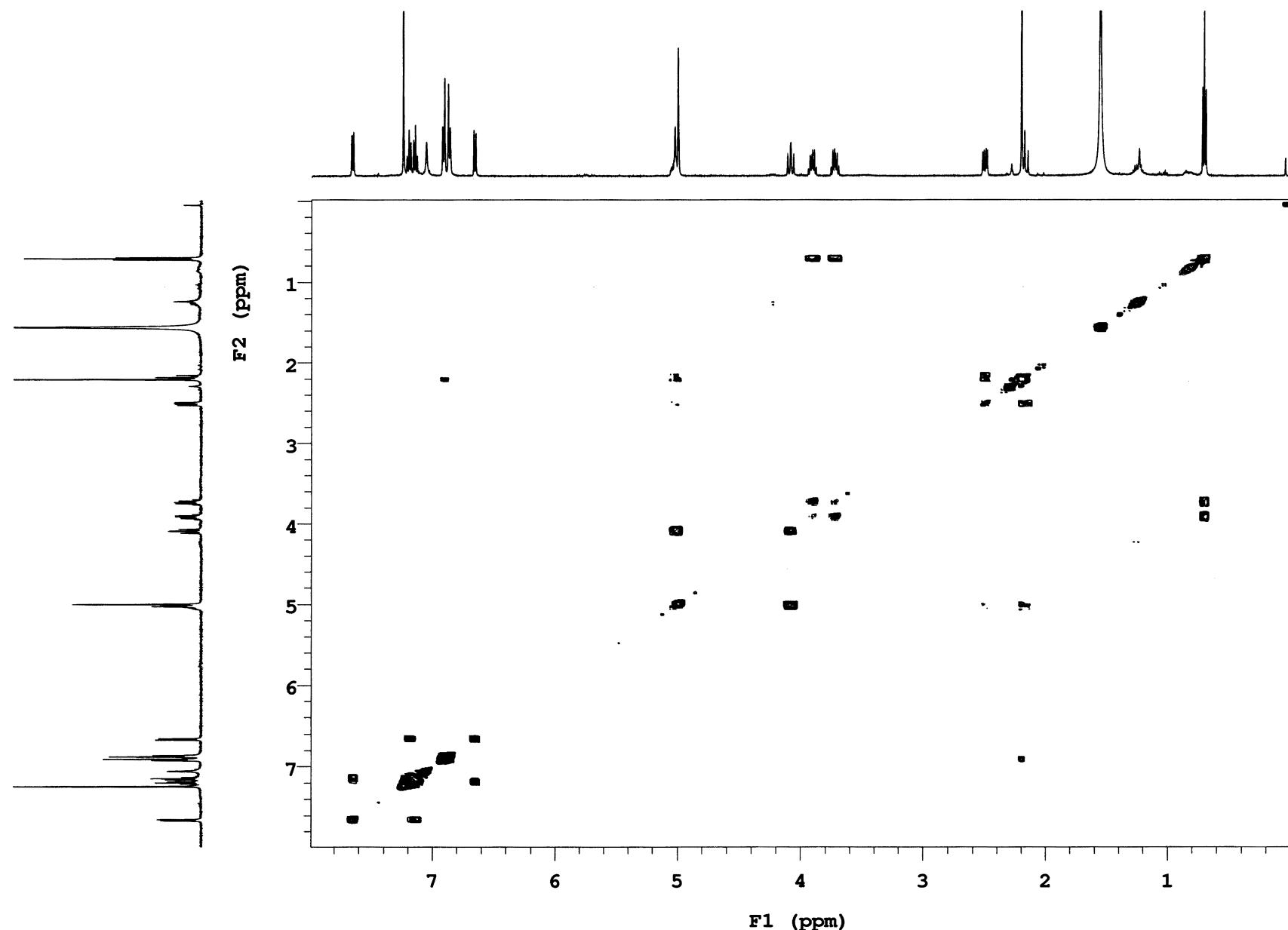
Sample Name PDC-03-109
Date collected 2018-03-20Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S52. COSY 4b

PDC-03-109

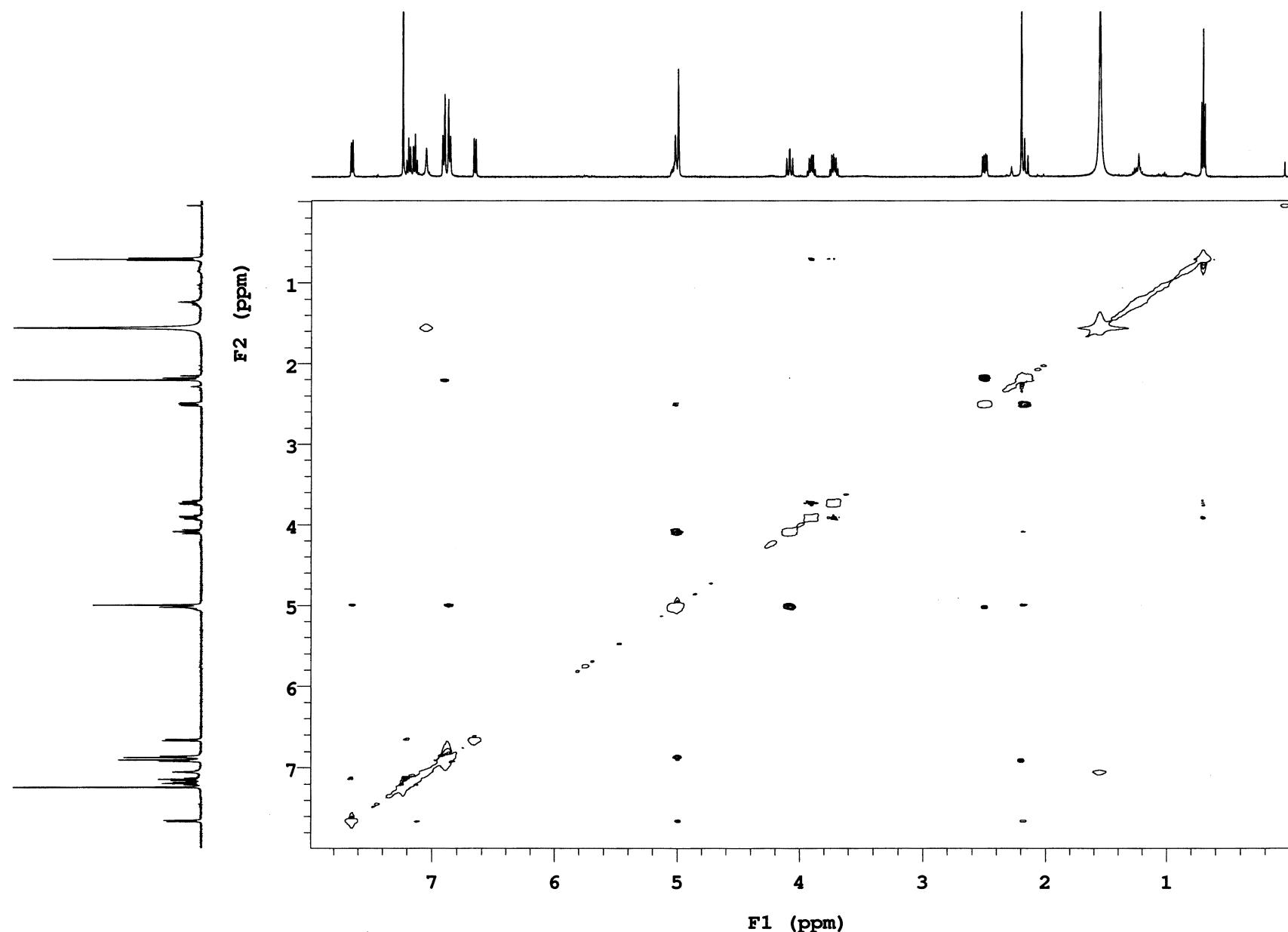
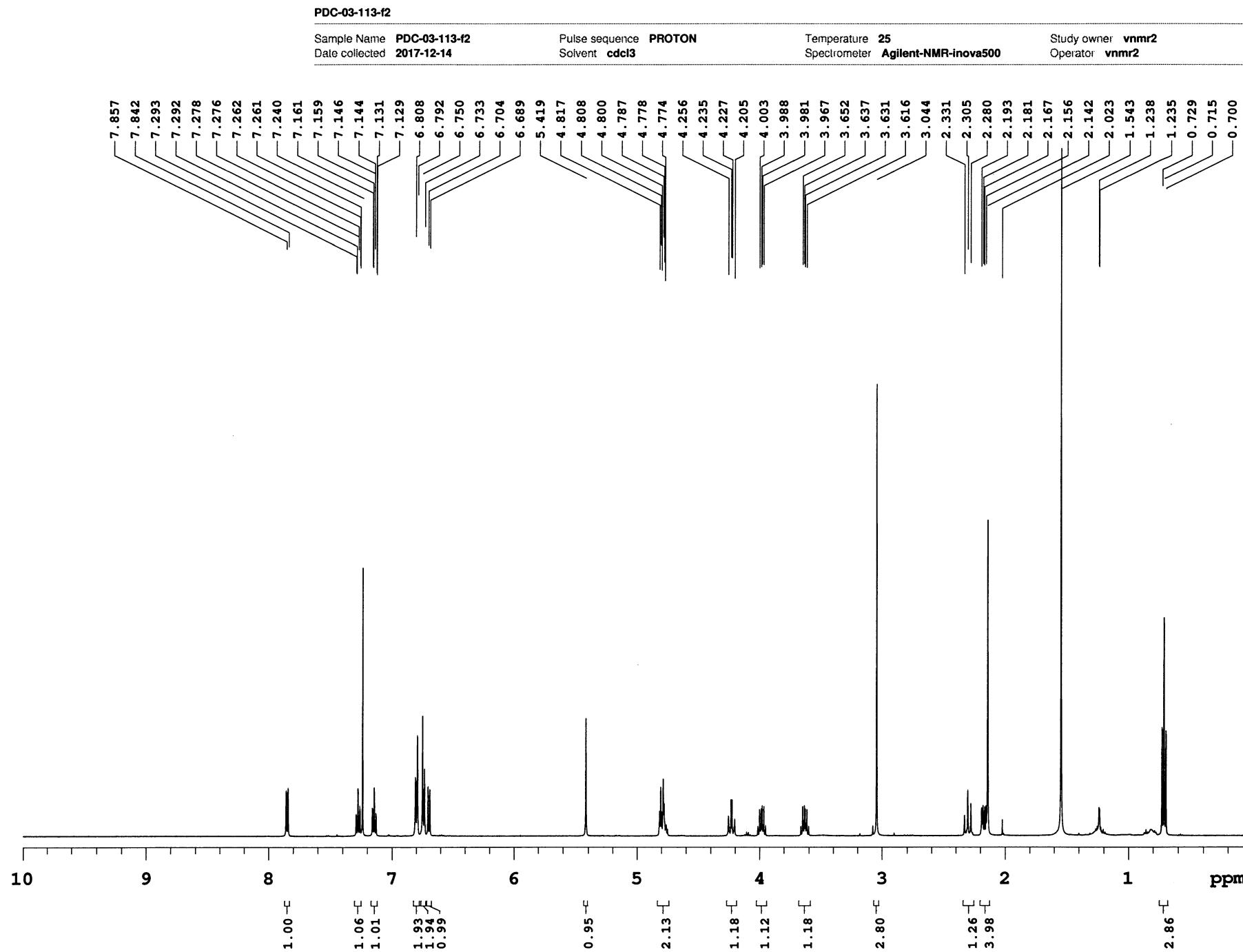
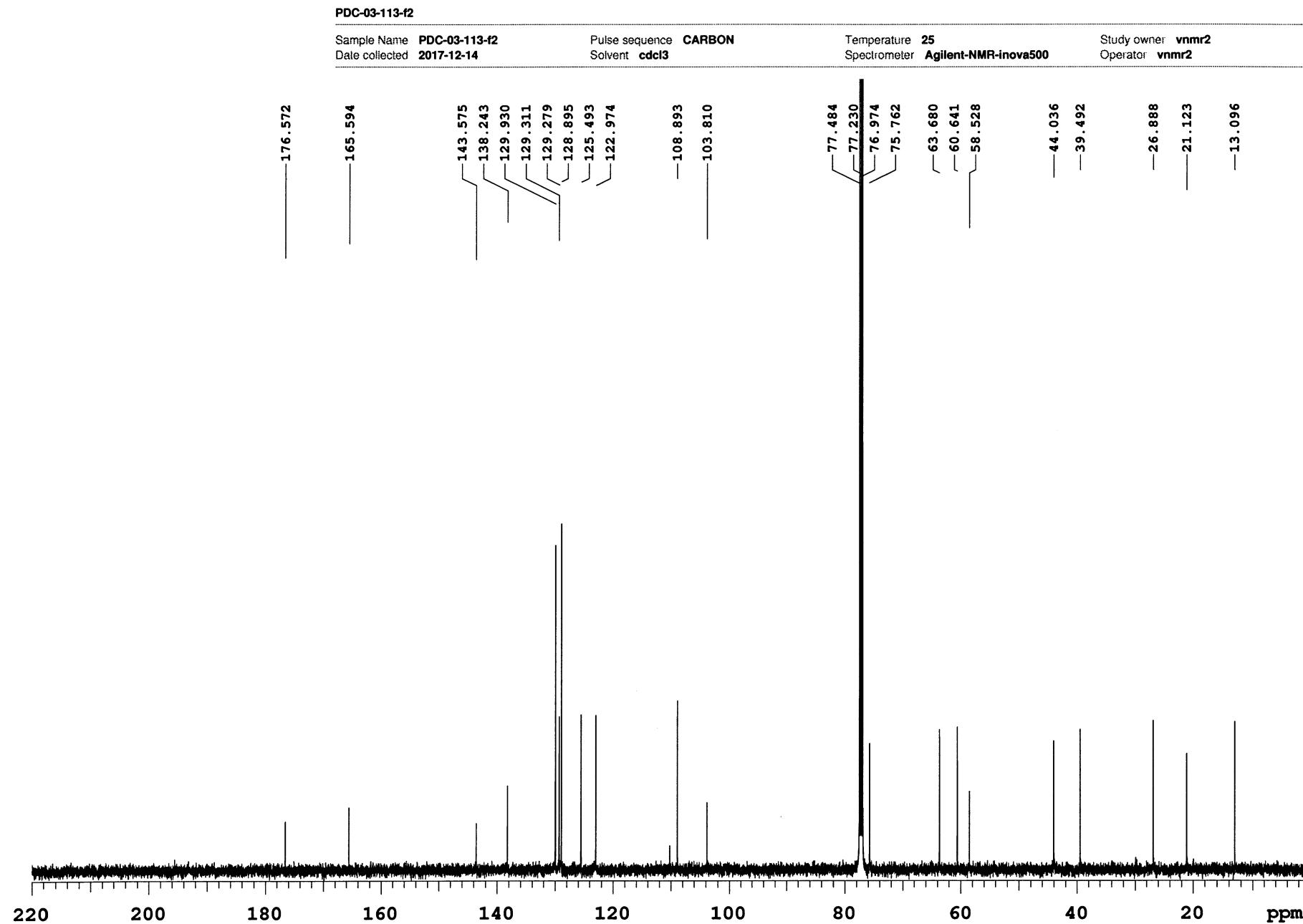
Sample Name PDC-03-109
Date collected 2018-03-20Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S53. NOESY of 4b



Figure S55. ^{13}C NMR (CDCl_3 , 125 MHz) of **3c**

PDC-03-113-f2

Sample Name **PDC-03-113-f2**
Date collected **2017-12-15**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-Inova500**

Study owner **vnmr2**
Operator **vnmr2**

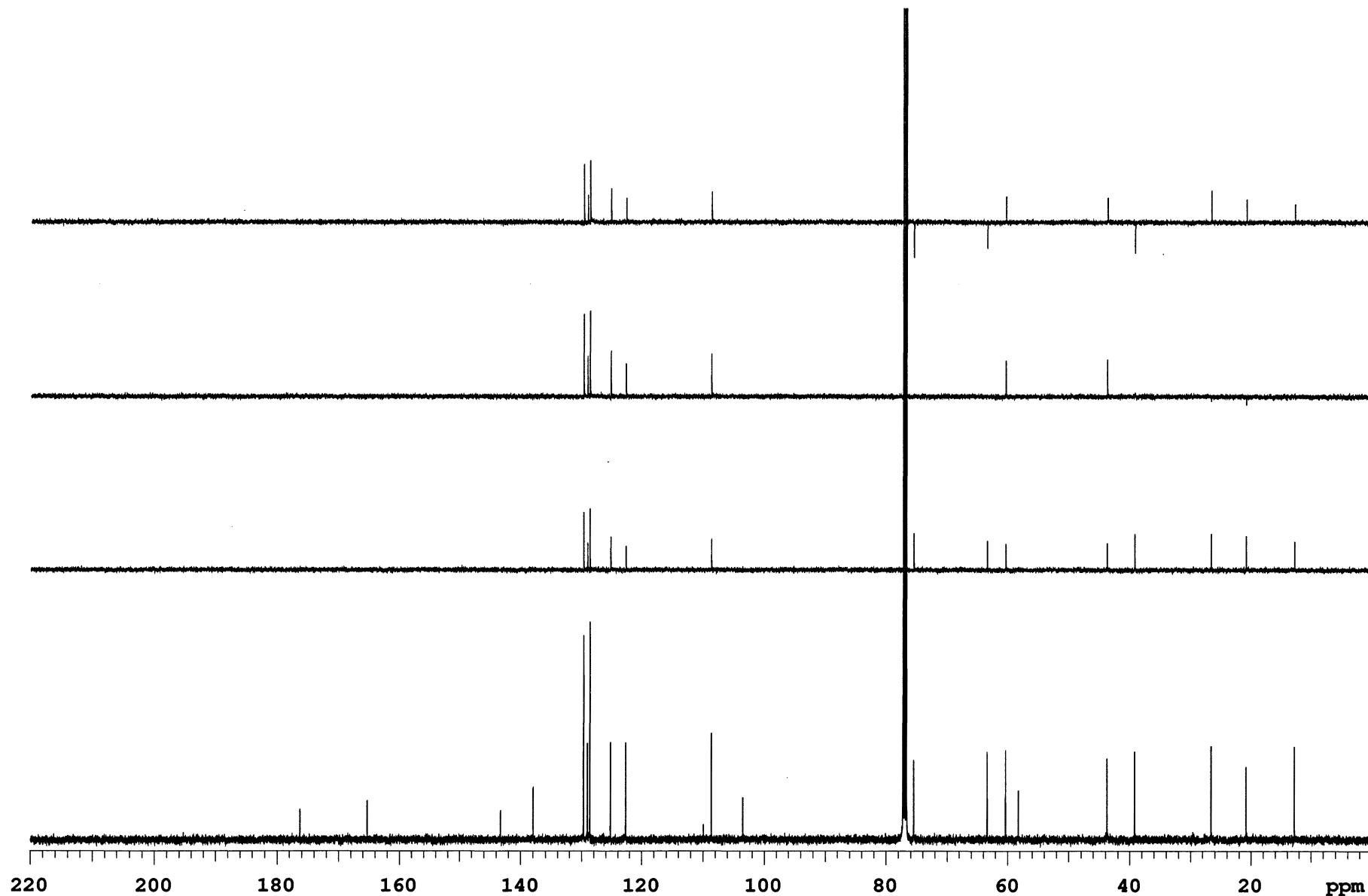
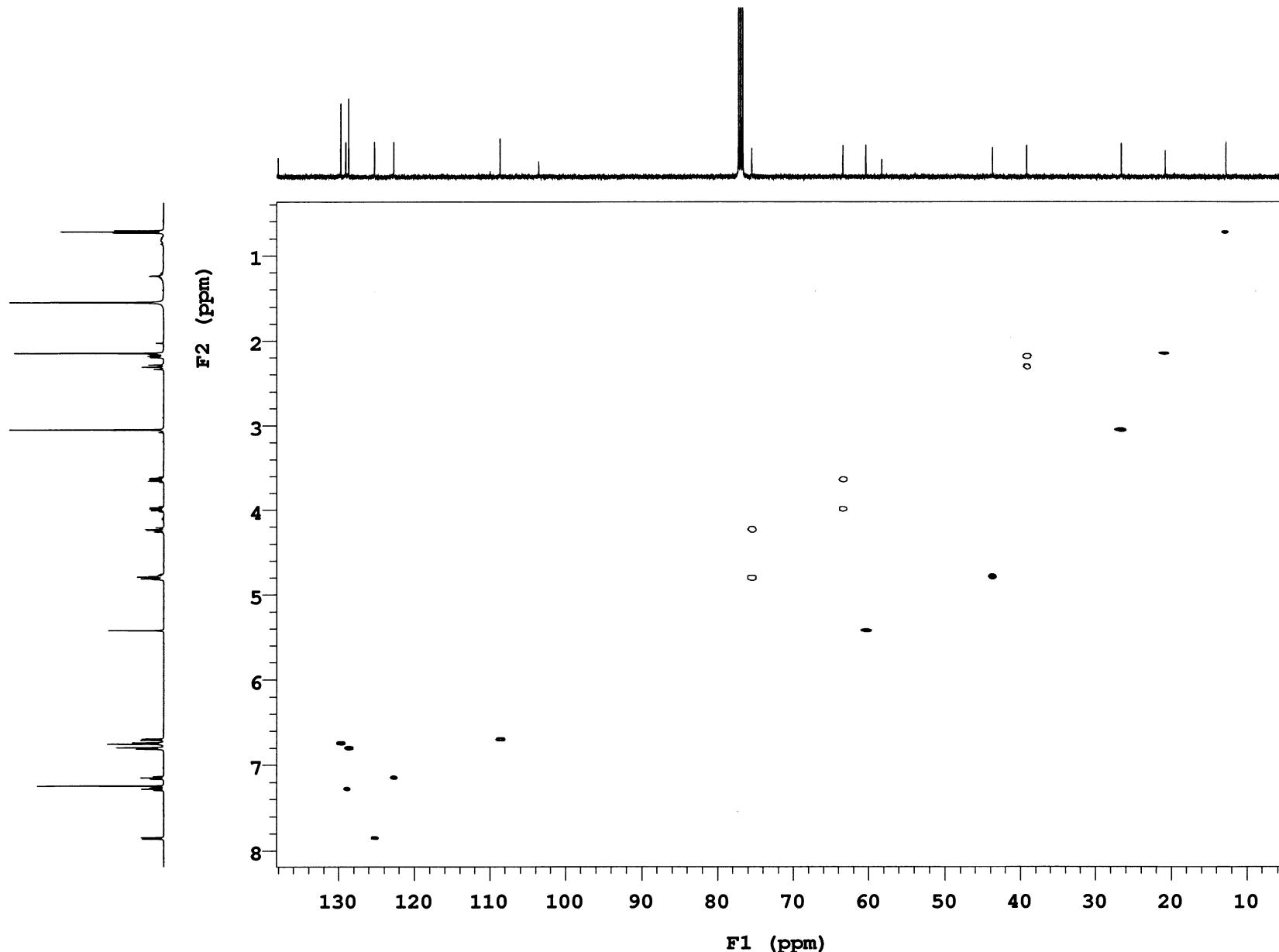


Figure S56. DEPT of 3c

PDC-03-113-f2

Sample Name **PDC-03-113-f2**
Date collected **2017-12-15**Pulse sequence **gHSQC**
Solvent **cdcl3**Temperature **25**
Specrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S57. HSQC of **3c**

Data file /home/vnmr2/vnmrsys/data/511/AD/PDC-03-113-f2/gHSQC_01

Plot date 2017-12-15

PDC-03-113-f2

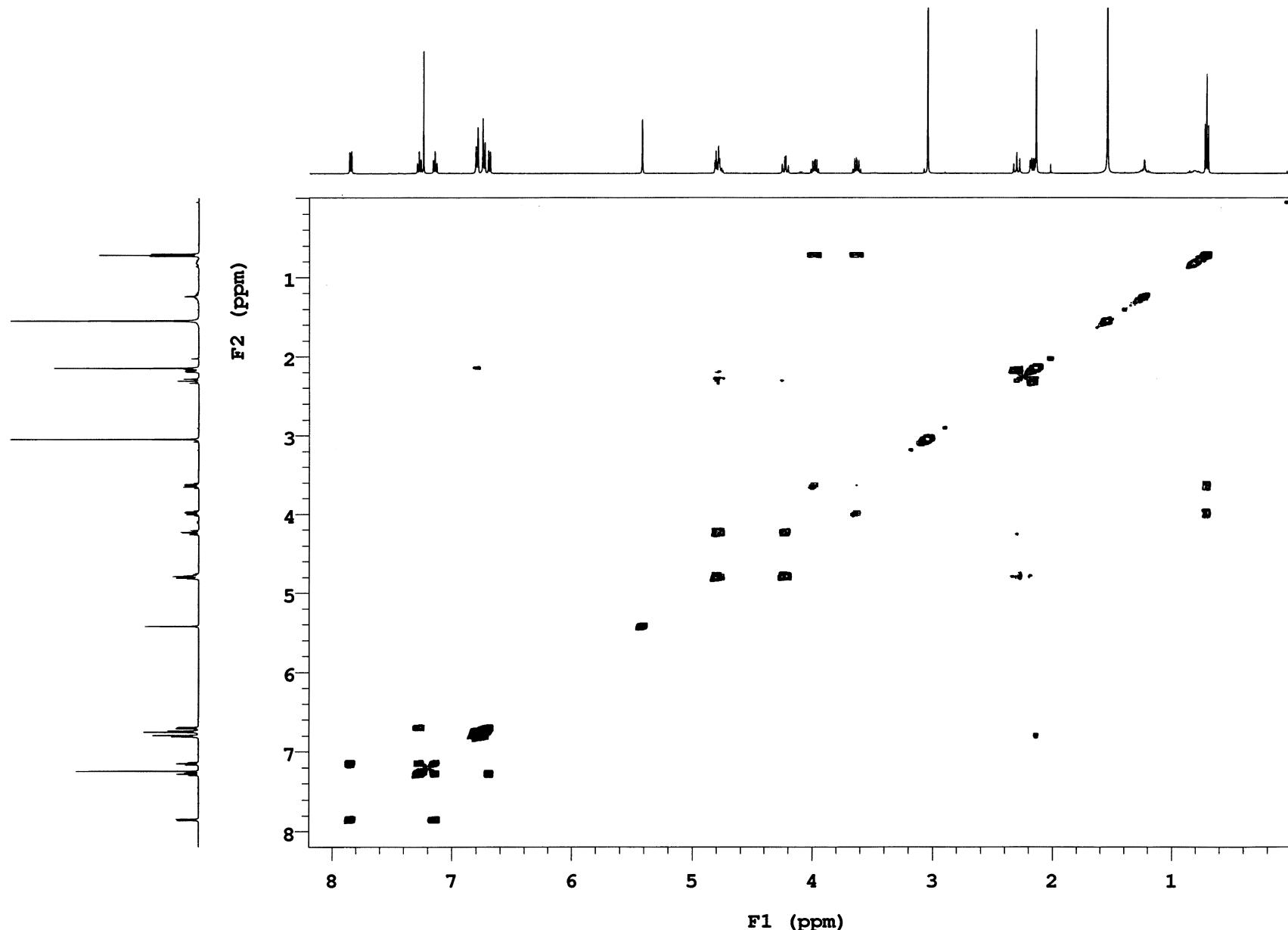
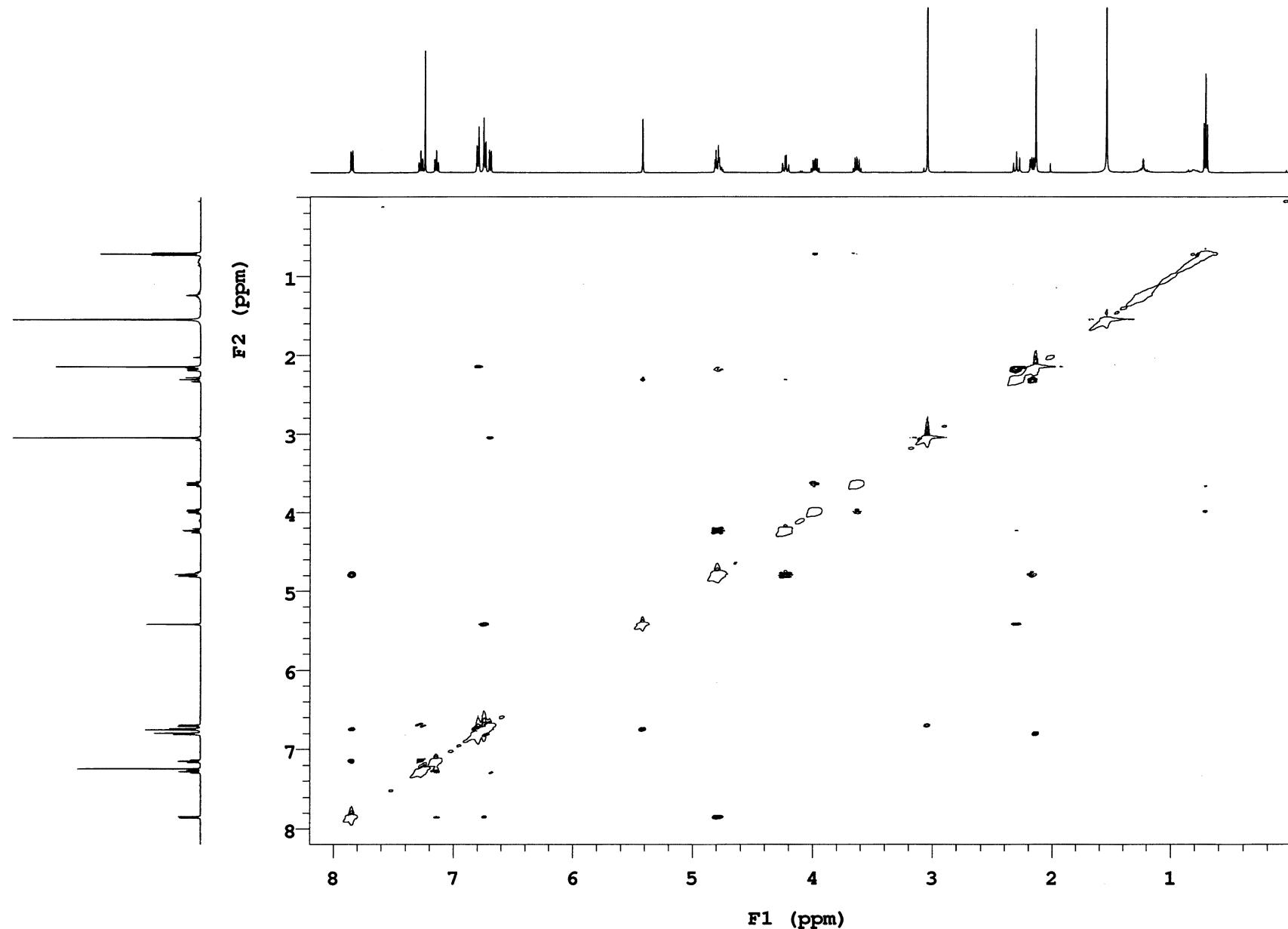
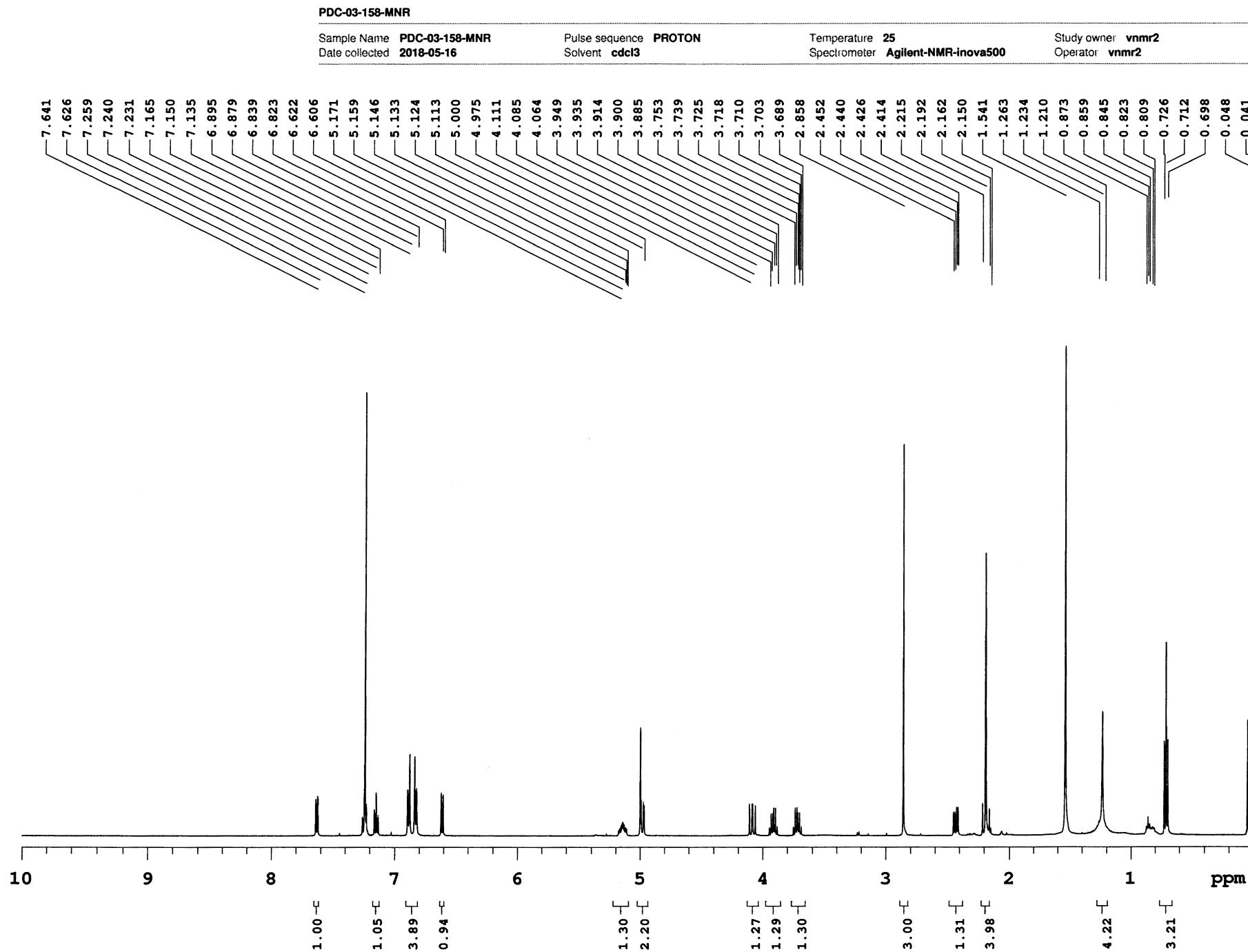
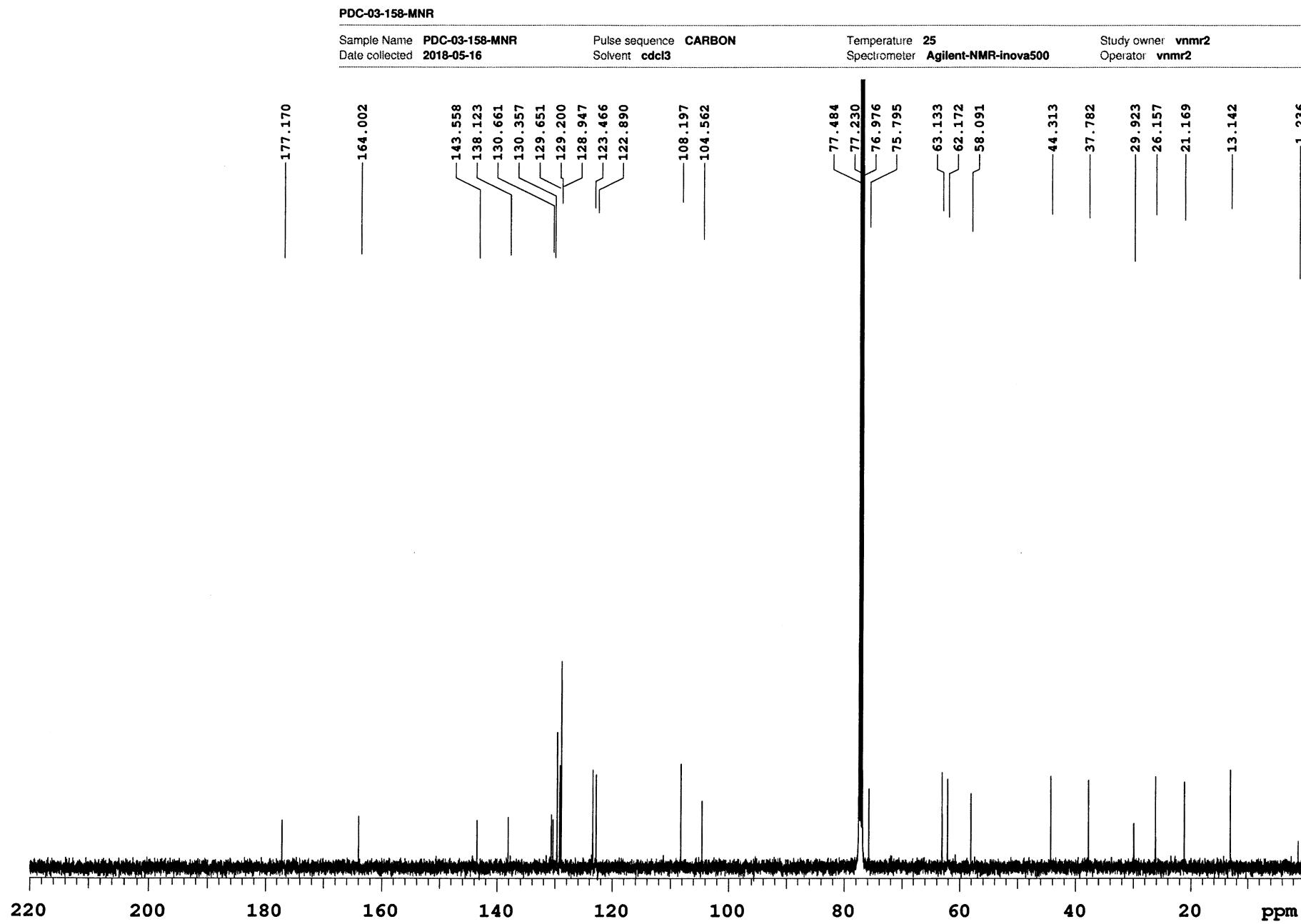
Sample Name PDC-03-113-f2
Date collected 2017-12-15Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S58. COSY of 3c

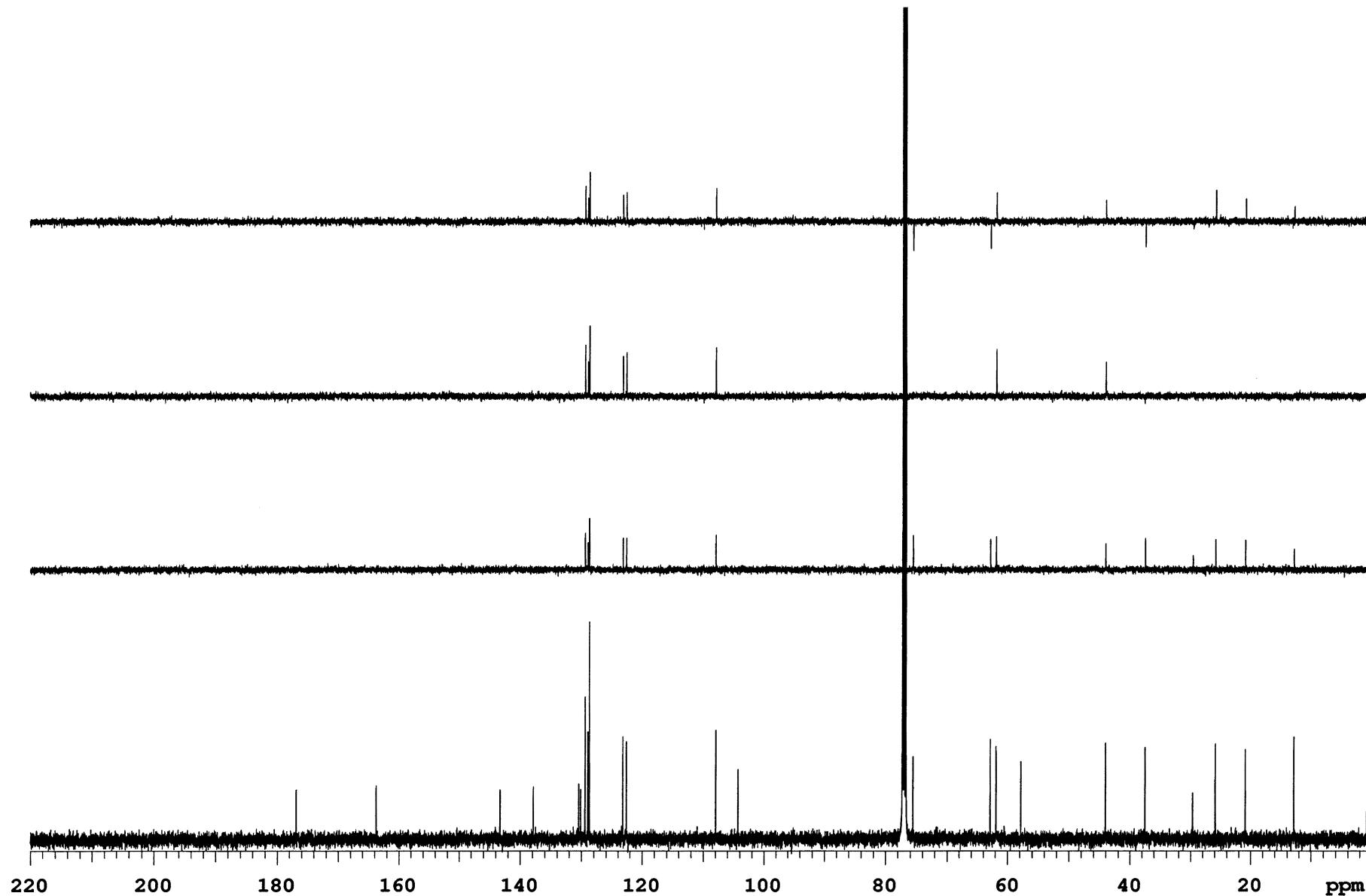
PDC-03-113-f2

Sample Name **PDC-03-113-f2**
Date collected **2017-12-15**Pulse sequence **NOESY**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S59. NOESY of **3c**

Figure S60. ^1H NMR (CDCl₃, 500 MHz) of **4c**

Figure S61. ¹³C NMR (CDCl₃, 125 MHz) of **4c**

PDC-03-158-MNR

Sample Name **PDC-03-158-MNR**
Date collected **2018-05-16**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S62. DEPT of **4c**

PDC-03-118-MNR

Sample Name **PDC-03-118-MNR**
Date collected **2018-05-03**

Pulse sequence **gHSQC**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

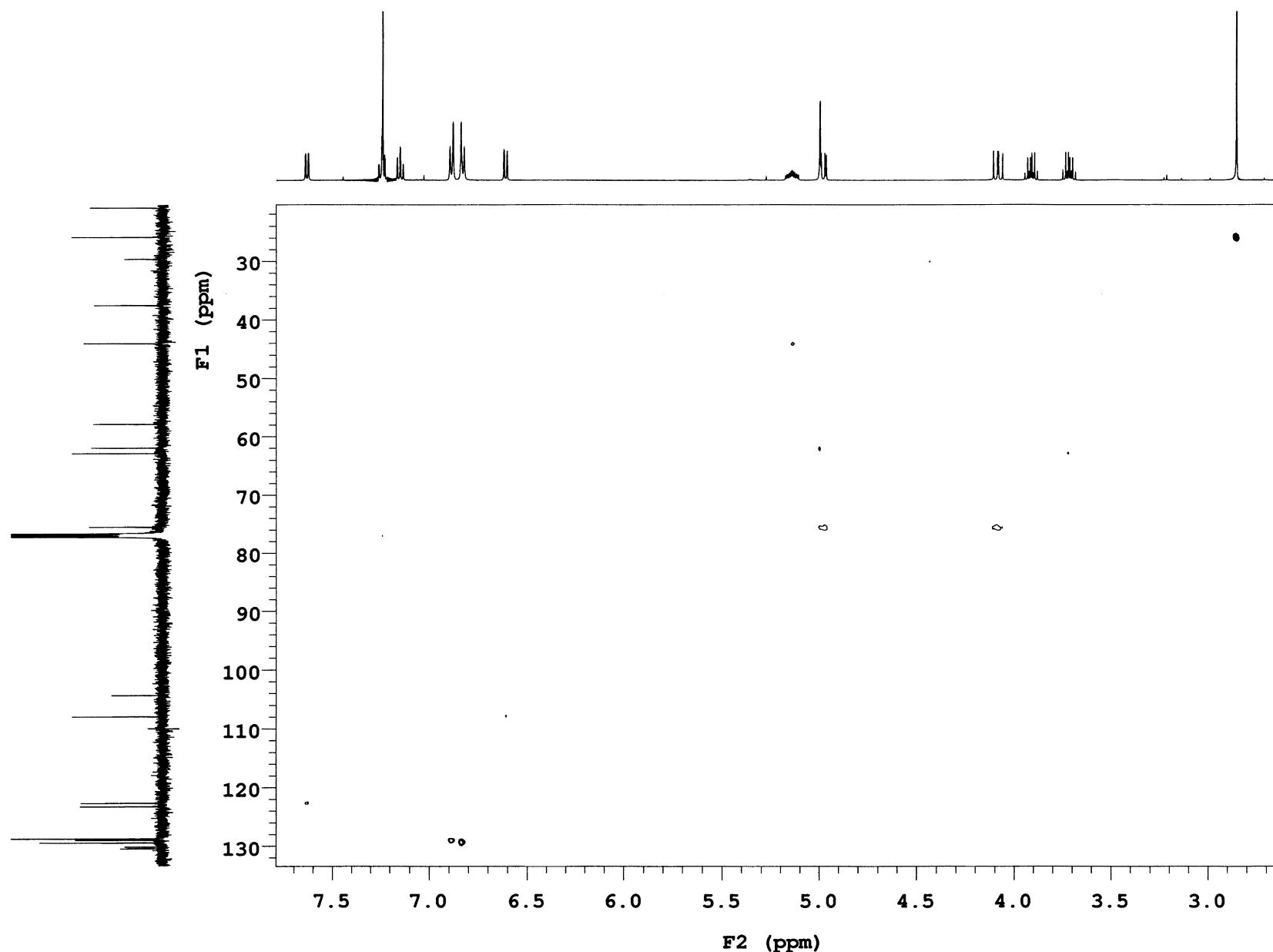
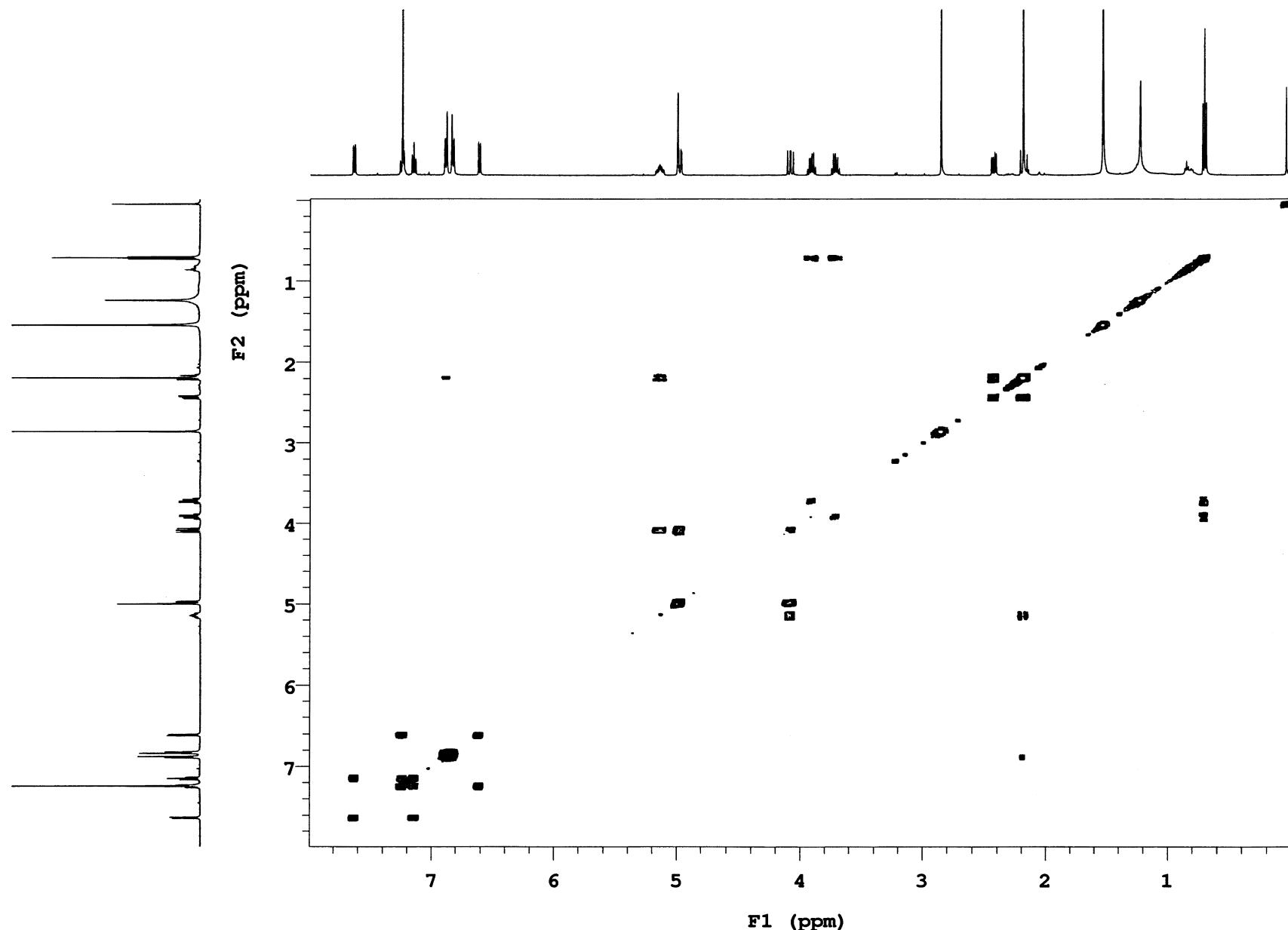


Figure S63. HSQC of **4c**

PDC-03-158-MNR

Sample Name **PDC-03-158-MNR**
Date collected **2018-05-16**Pulse sequence **gCOSY**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S64. COSY of **4c**

PDC-03-158-MNR

Sample Name PDC-03-158-MNR
Date collected 2018-05-16

Pulse sequence NOESY
Solvent *cdcl*3

Temperature 25
Spectrometer Agilent-NMR-inova500

Study owner vnmr2
Operator vnmr2

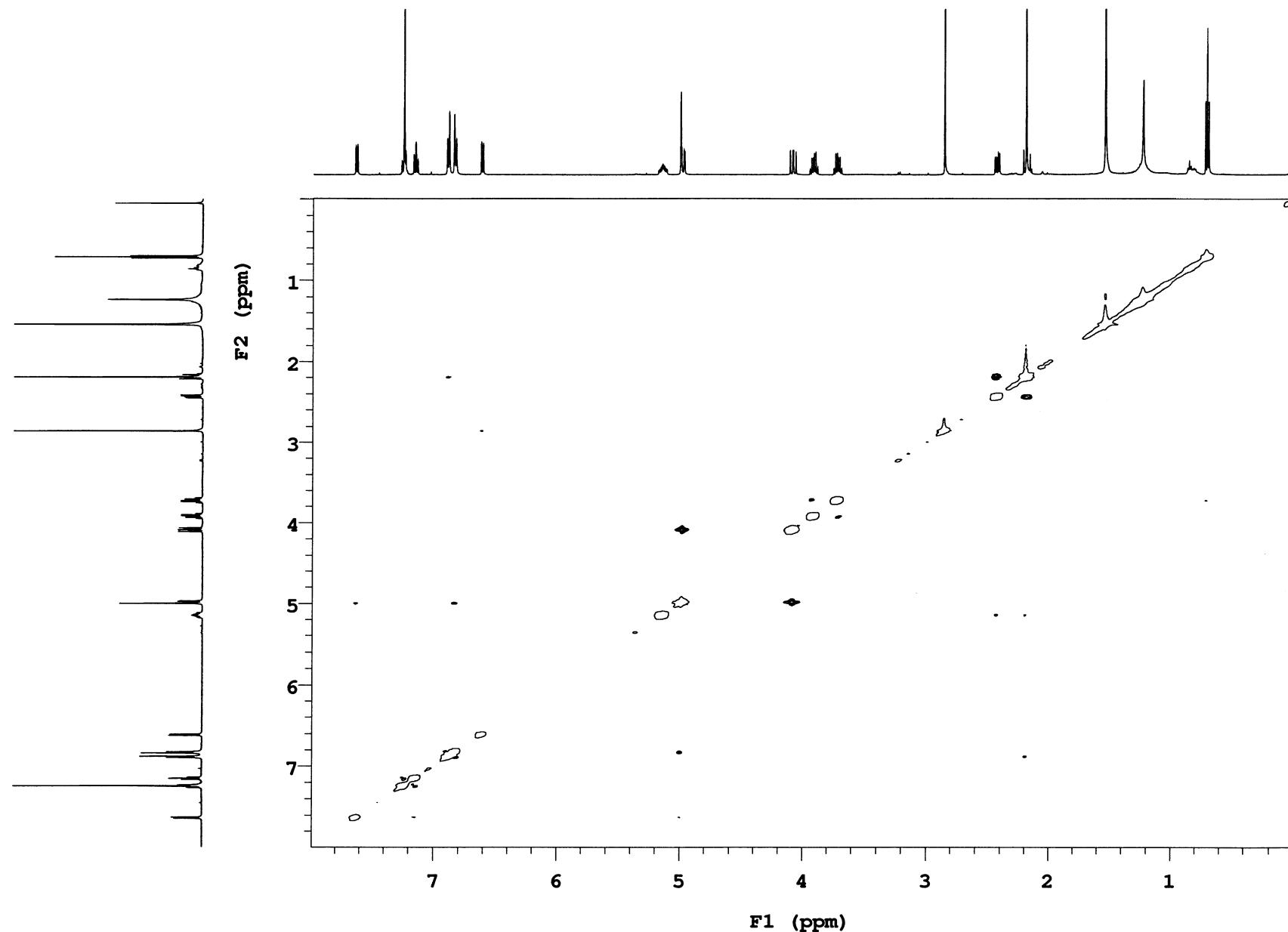


Figure S65. NOESY of 4c

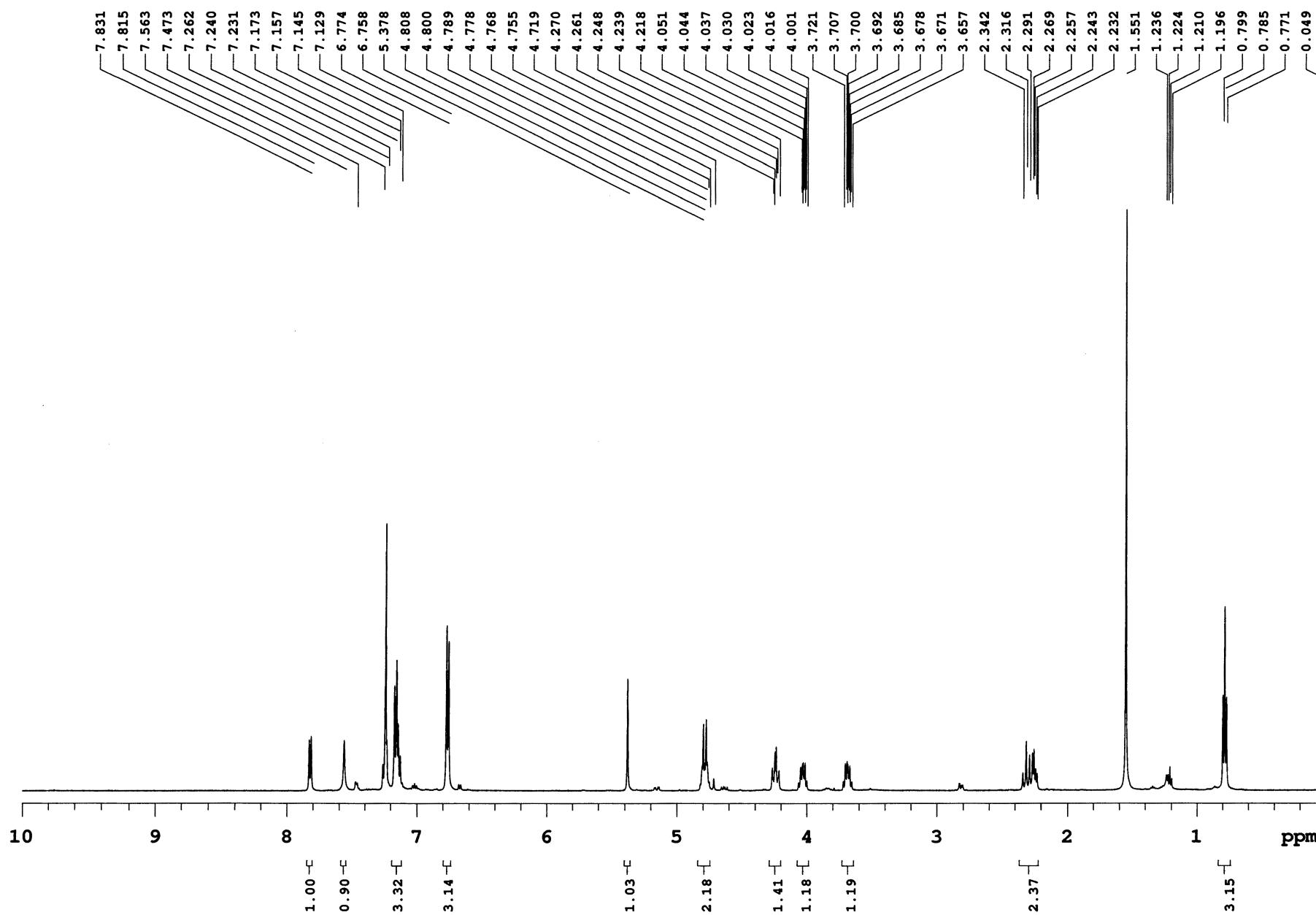
PDC-03-115

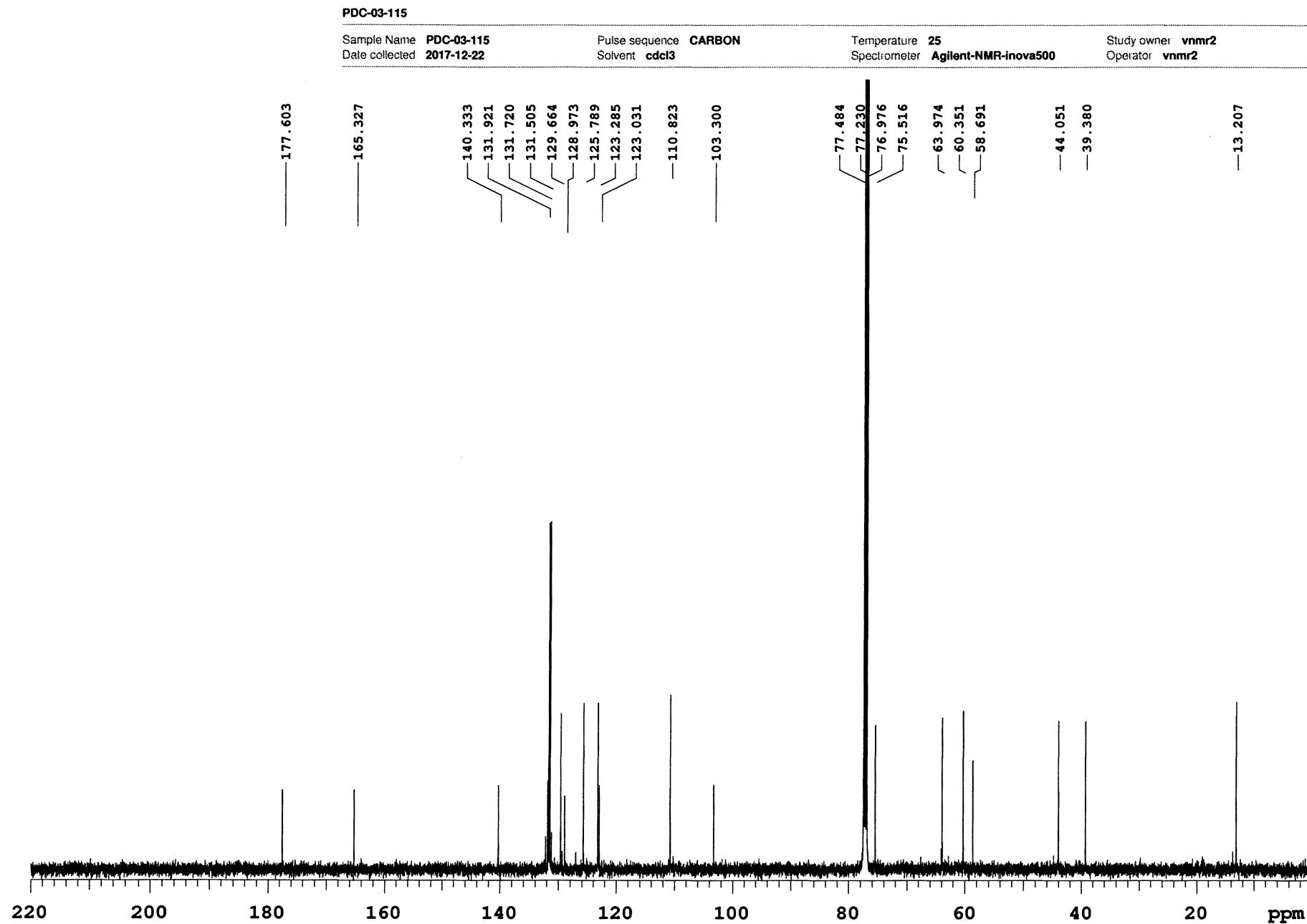
Sample Name **PDC-03-115**
 Date collected **2017-12-22**

Pulse sequence **PROTON**
 Solvent **cdcl3**

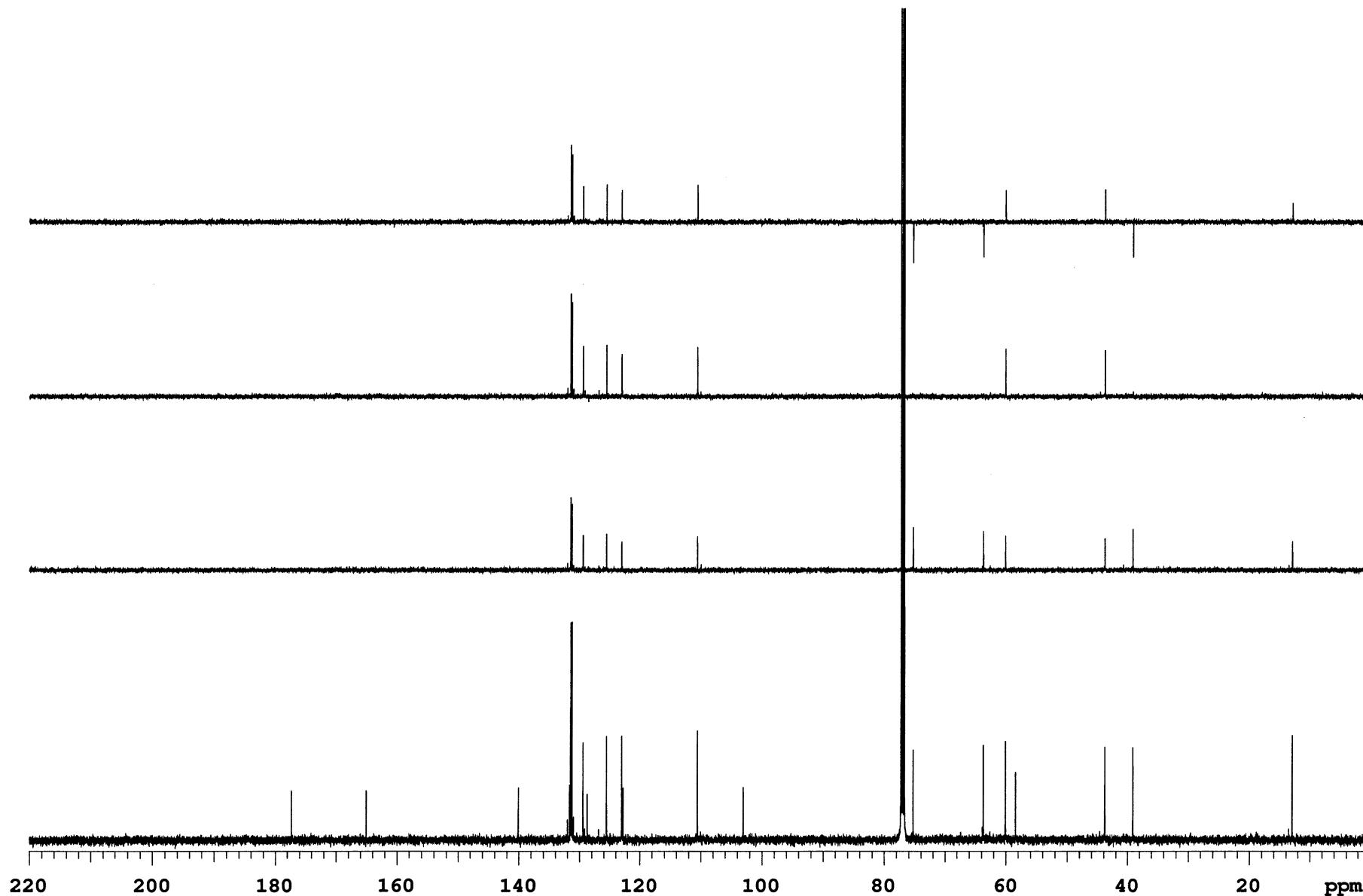
Temperature **25**
 Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
 Operator **vnmr2**



Figure S67. ^{13}C NMR (CDCl_3 , 125 MHz) of 3d

PDC-03-115

Sample Name **PDC-03-115**
Date collected **2017-12-22**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-Inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S68. DEPT of **3d**

PDC-03-115

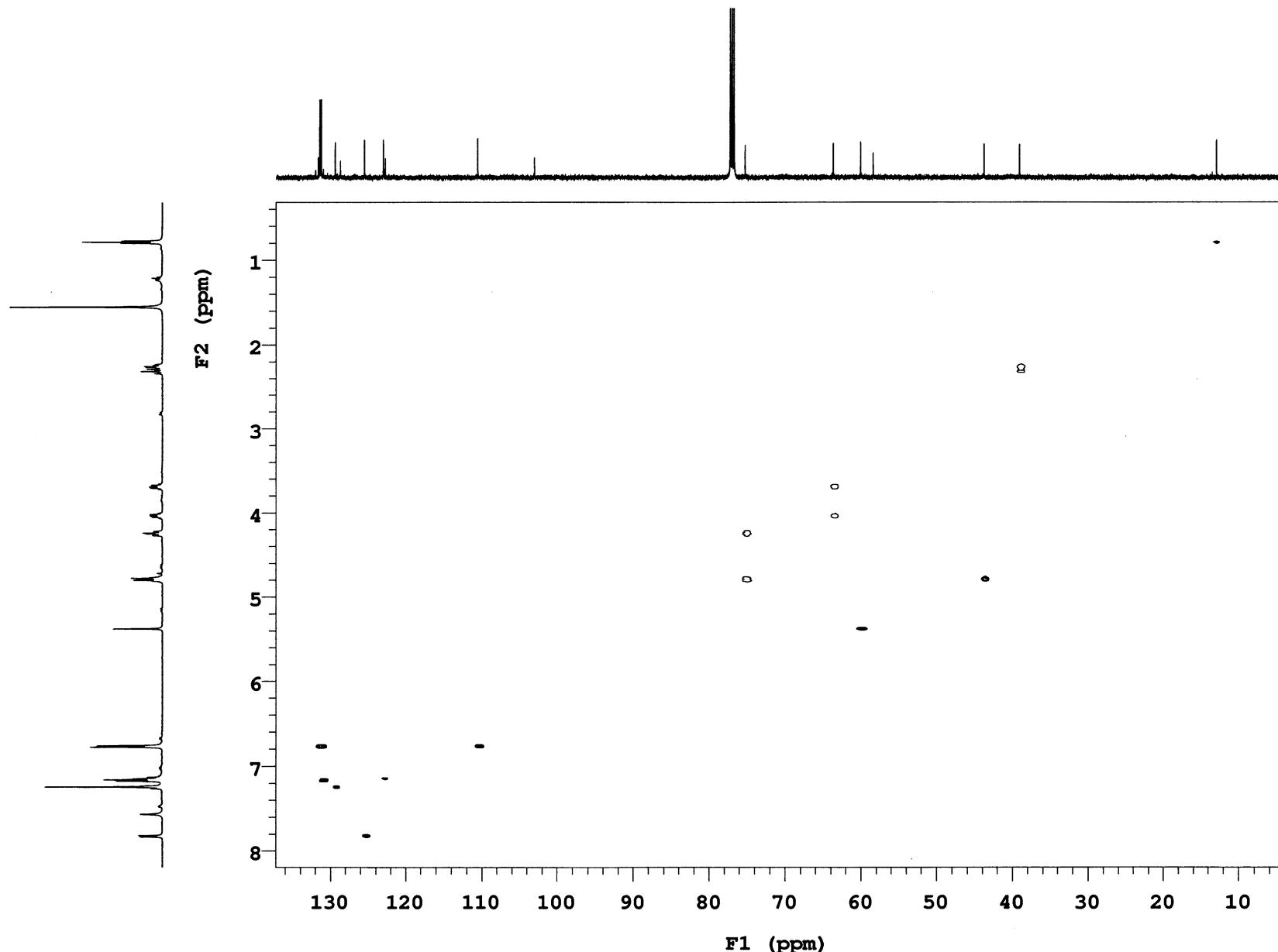
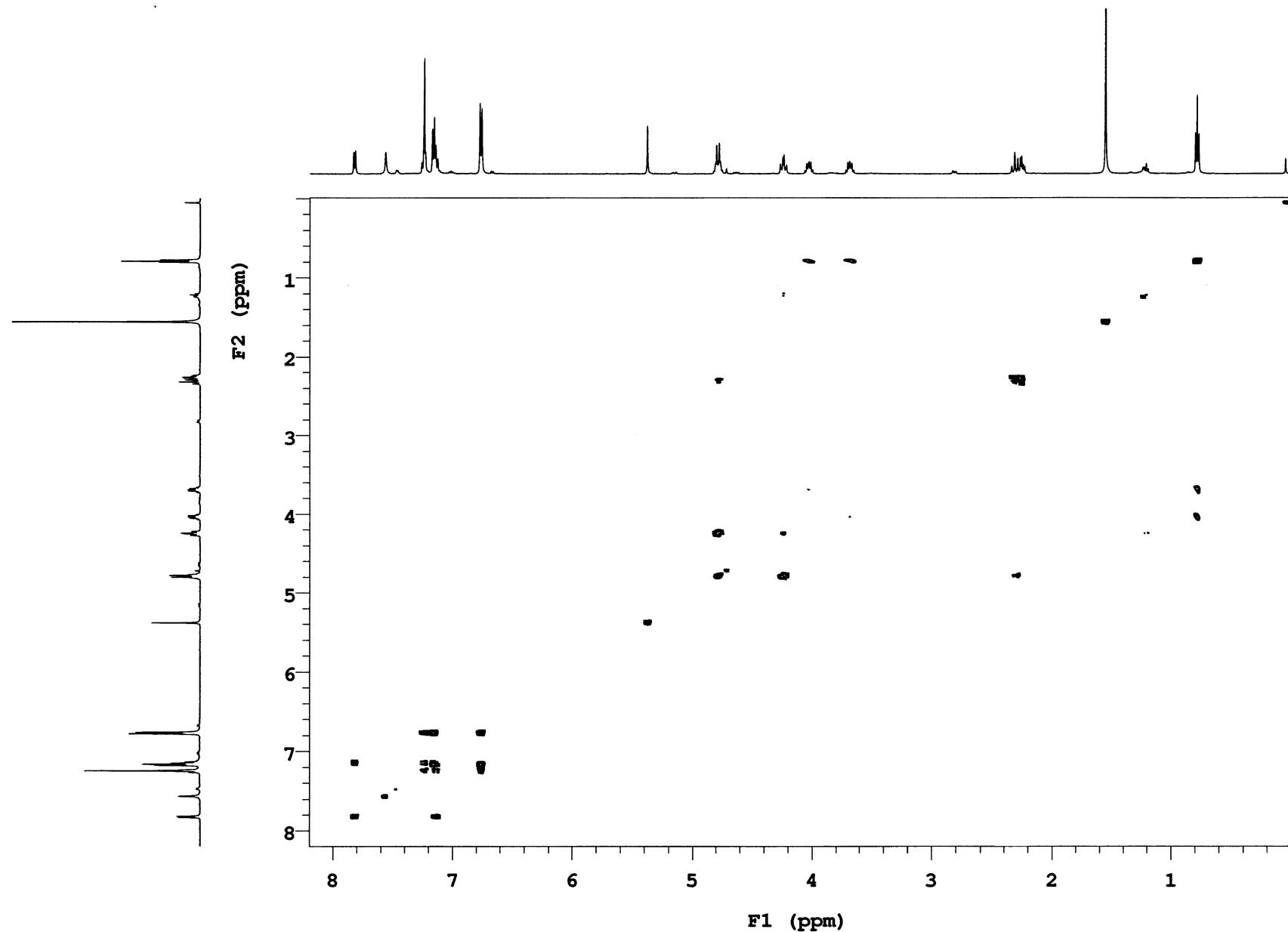
Sample Name PDC-03-115
Date collected 2017-12-22Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S69. HSQC of 3d

PDC-03-115

Sample Name PDC-03-115
Date collected 2017-12-22Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2Figure S70. COSY of **3d**

PDC-03-115

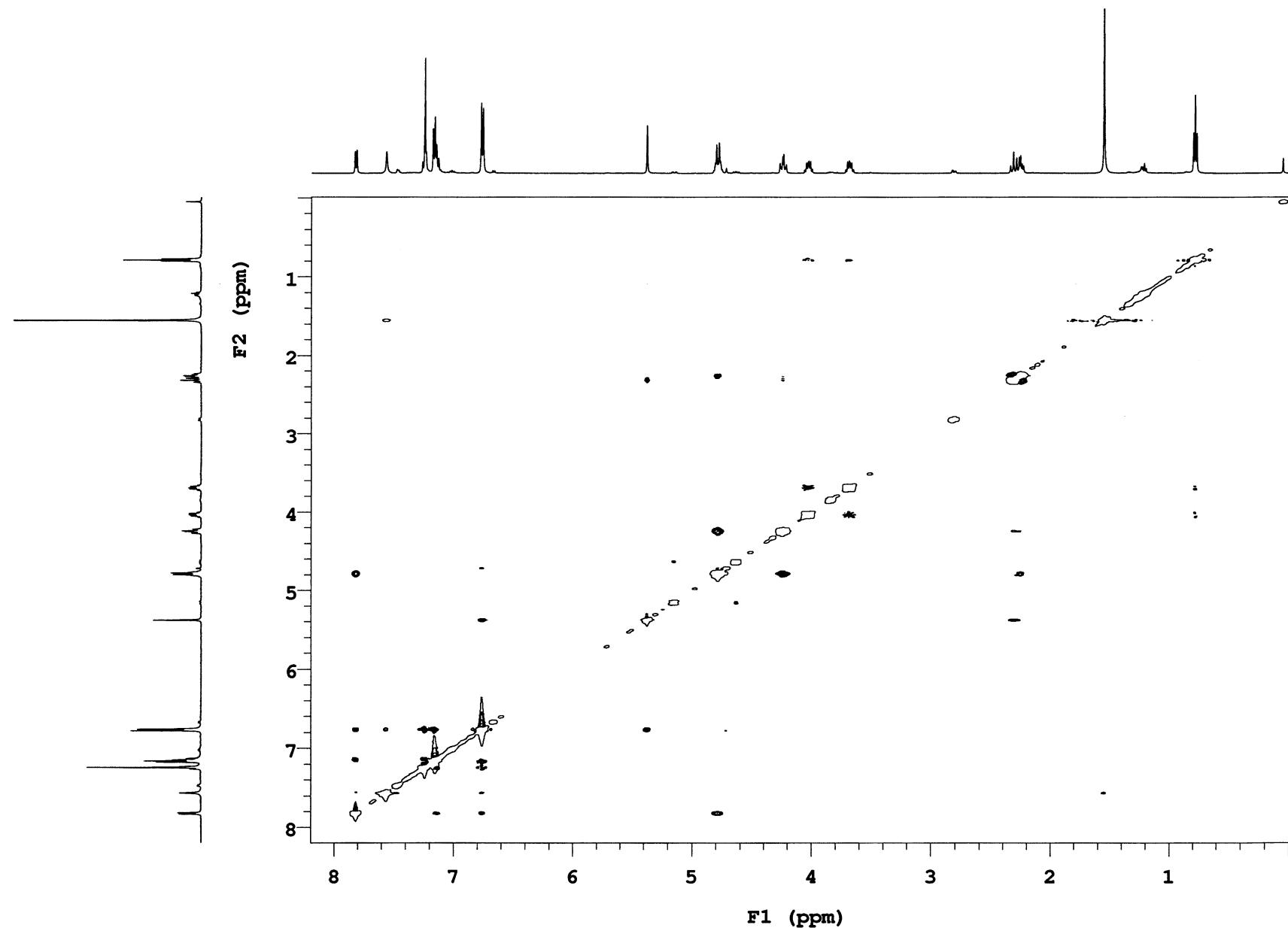
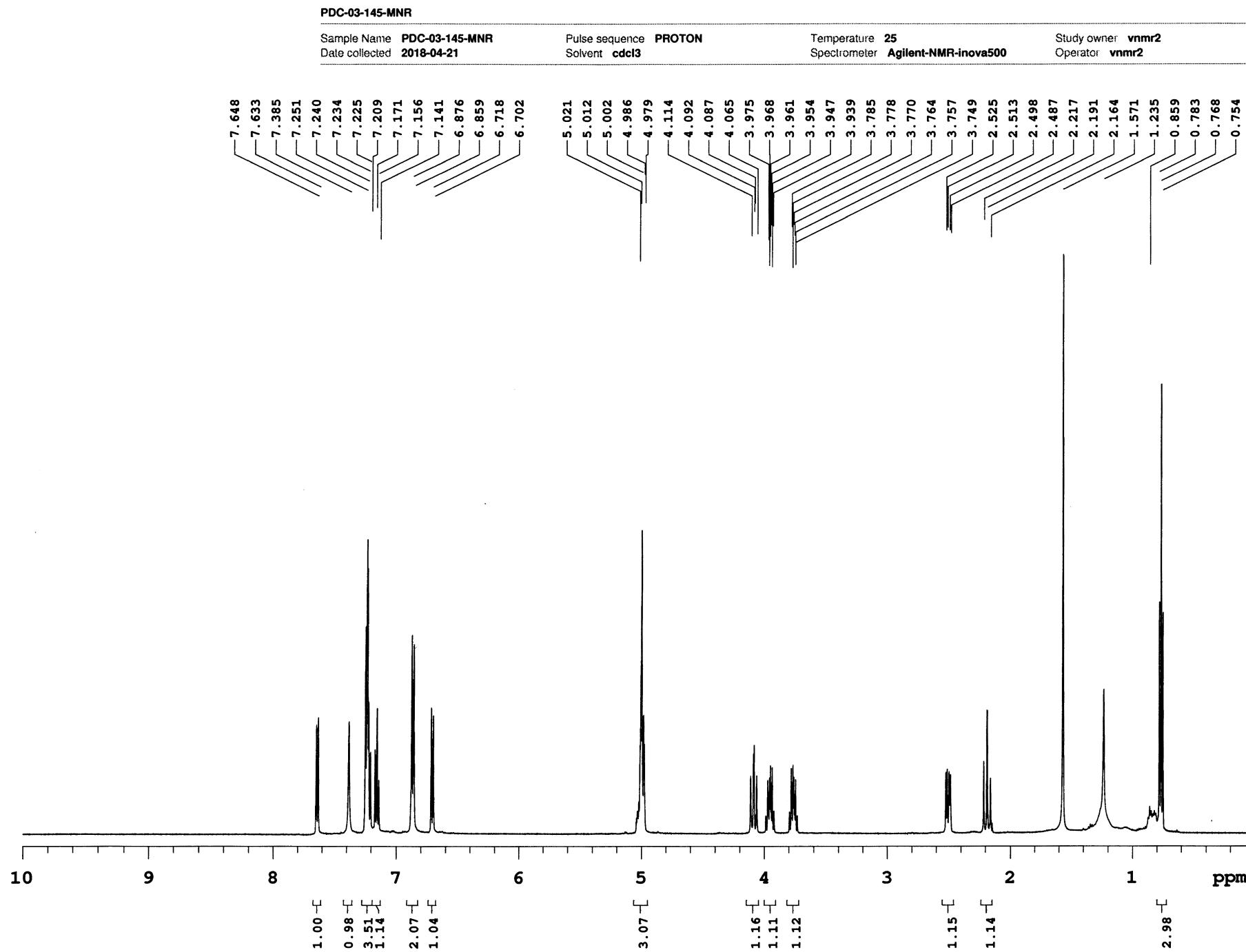
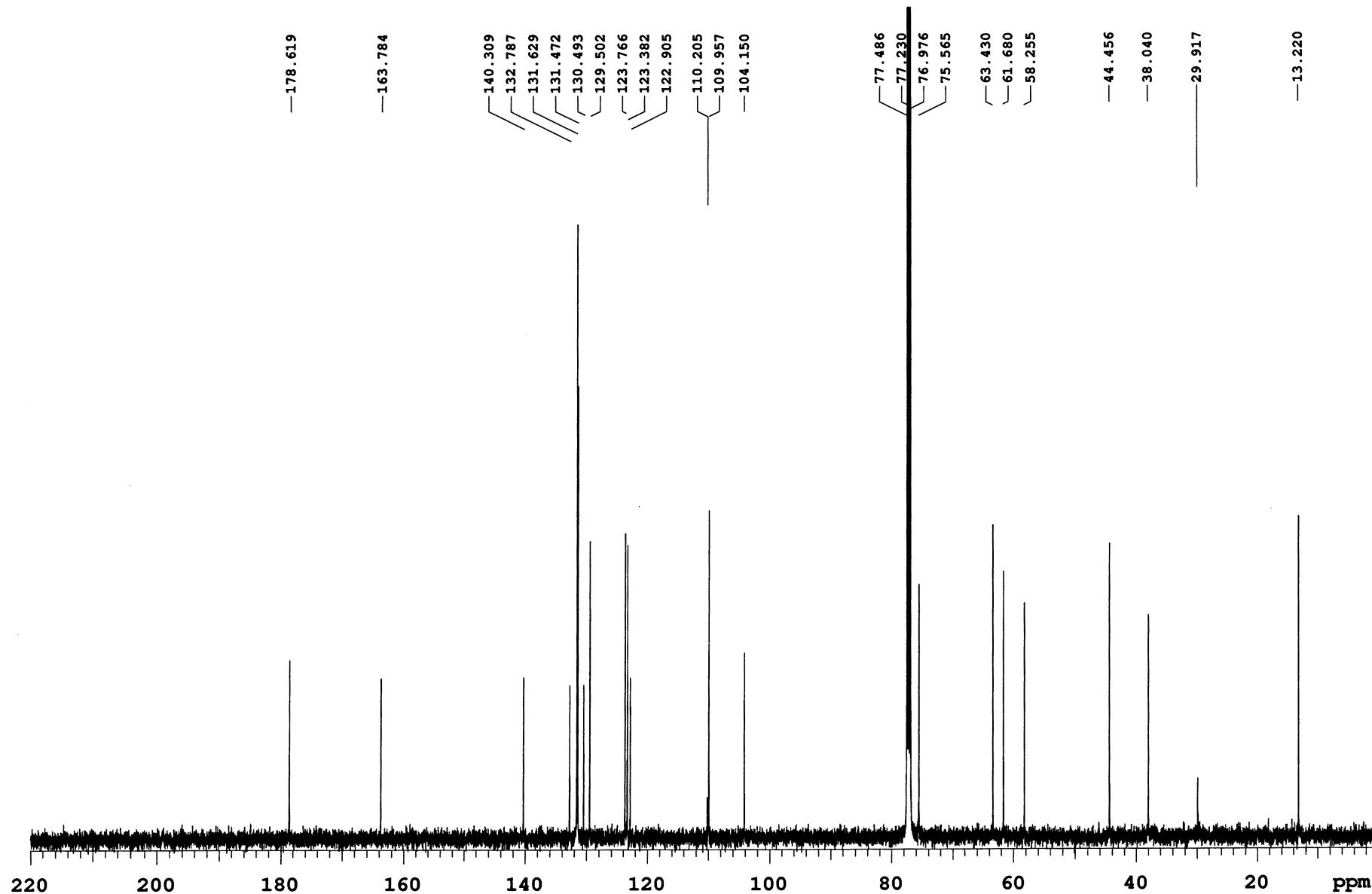
Sample Name PDC-03-115
Date collected 2017-12-22Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2

Figure S71. NOESY of 3d

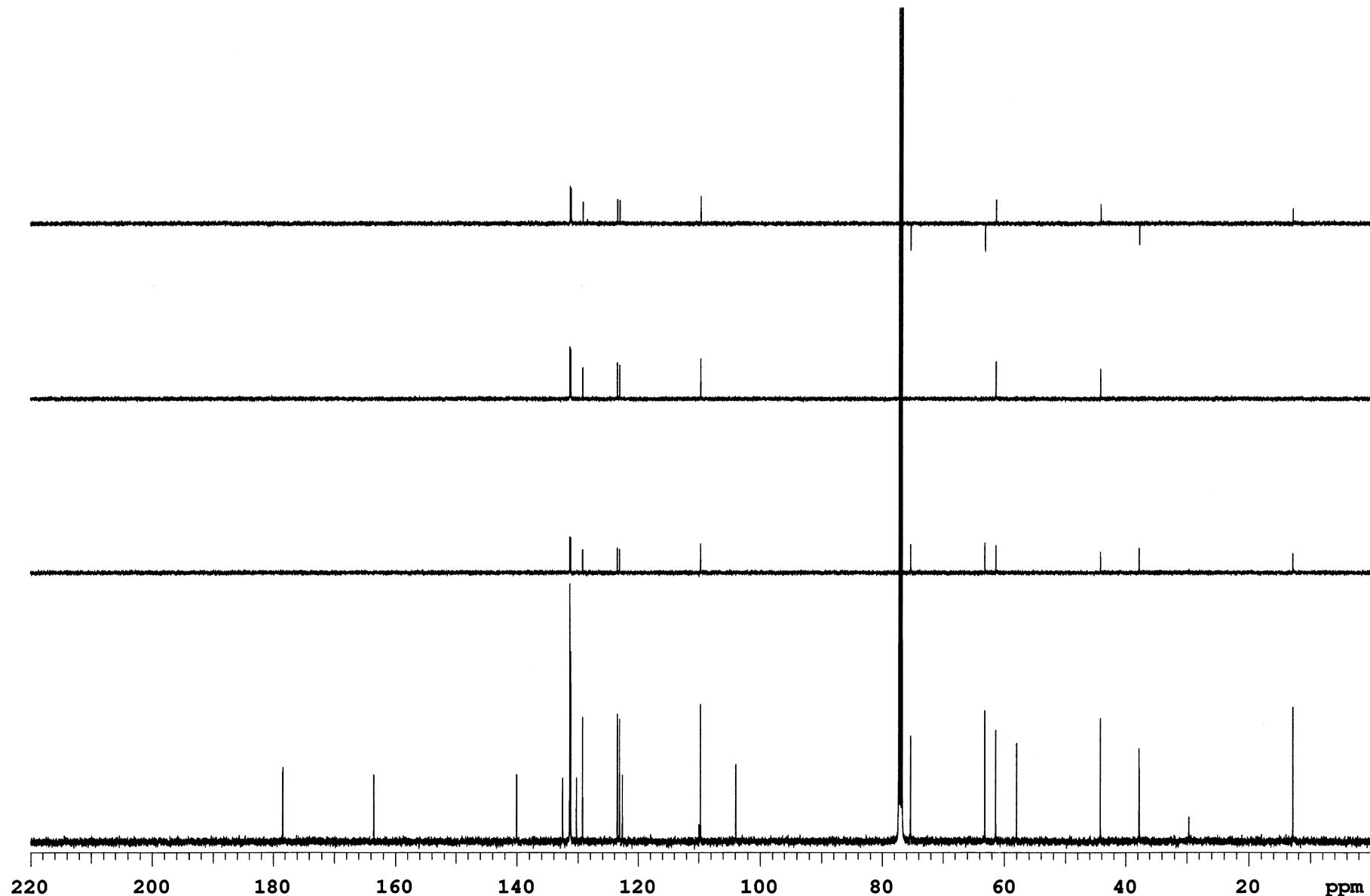


PDC-03-145-MNR

Sample Name PDC-03-145-MNR Date collected 2018-04-21 Pulse sequence CARBON Solvent cdcl_3 Temperature 25 Spectrometer Agilent-NMR-inova500 Study owner vnmr2 Operator vnmr2

Figure S73. ^{13}C NMR (CDCl_3 , 125 MHz) of **4d**

PDC-03-145-MNR

Sample Name **PDC-03-145-MNR**
Date collected **2018-04-21**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-Inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S74. DEPT of **4d**

PDC-03-145-MNR

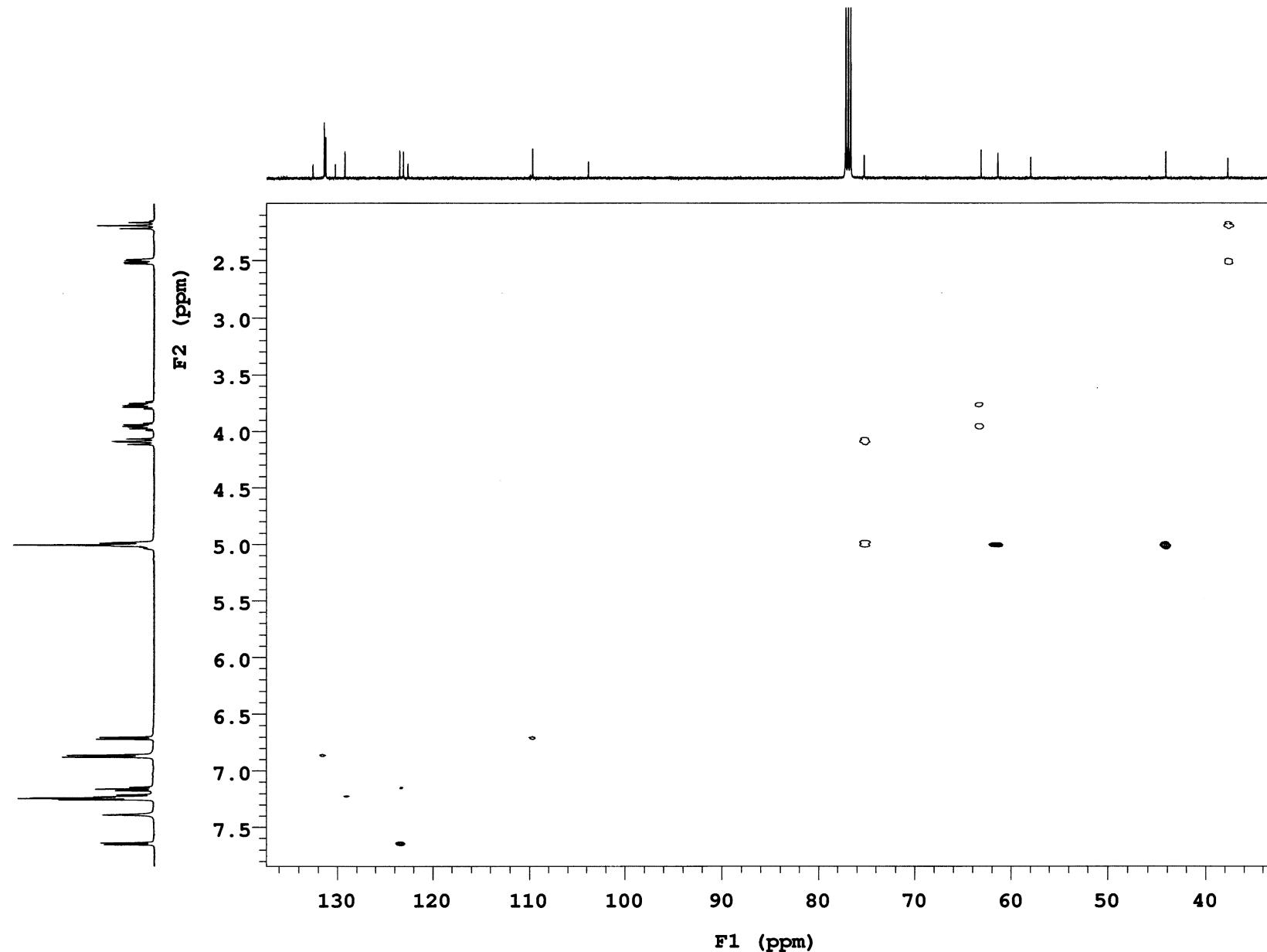
Sample Name PDC-03-145-MNR
Date collected 2018-04-22Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S75. HSQC of 4d

PDC-03-145-MNR

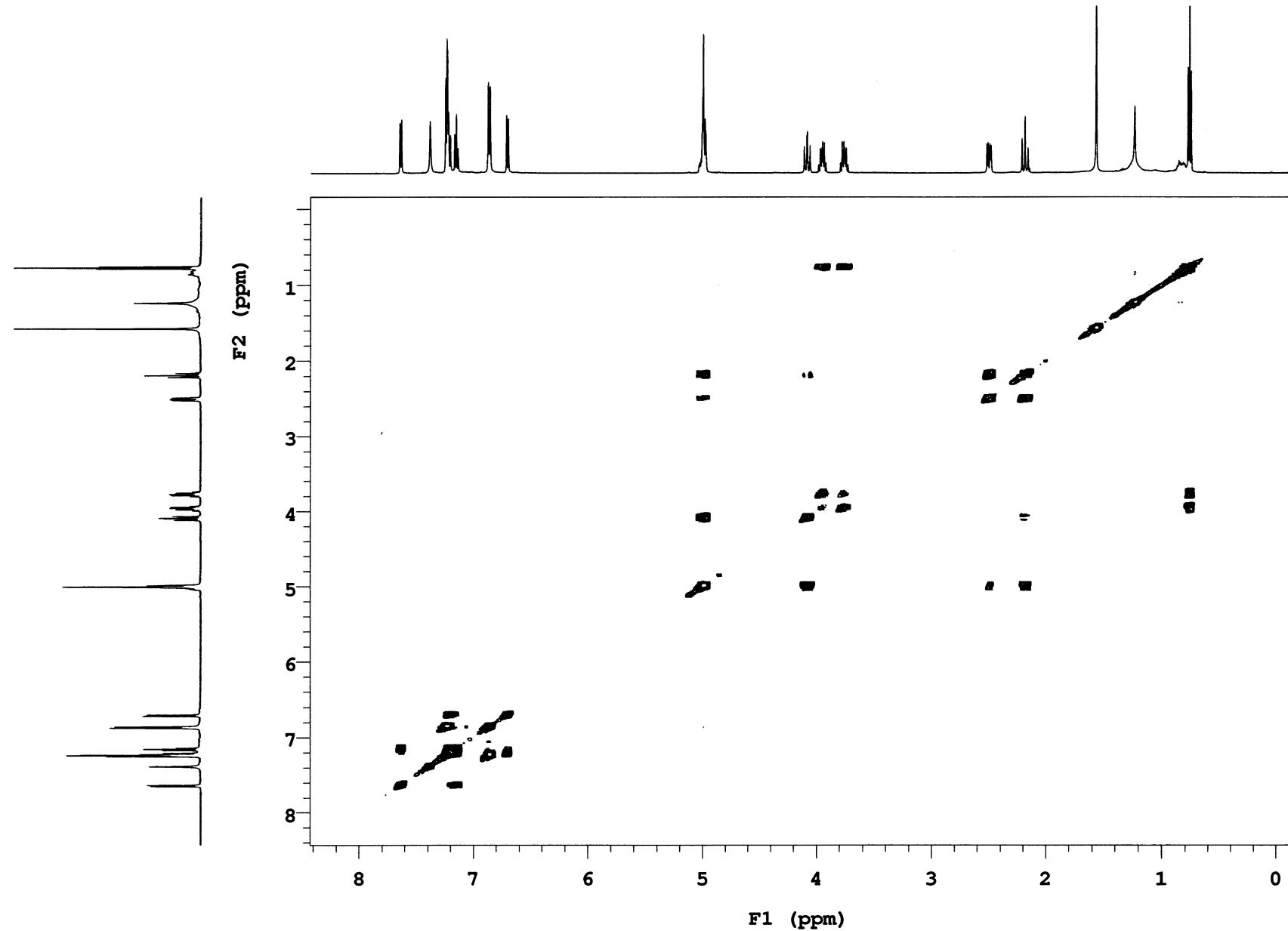
Sample Name PDC-03-145-MNR
Date collected 2018-04-22Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner **vnmr2**
Operator **vnmr2**

Figure S76. COSY of 4d

PDC-03-145-MNR

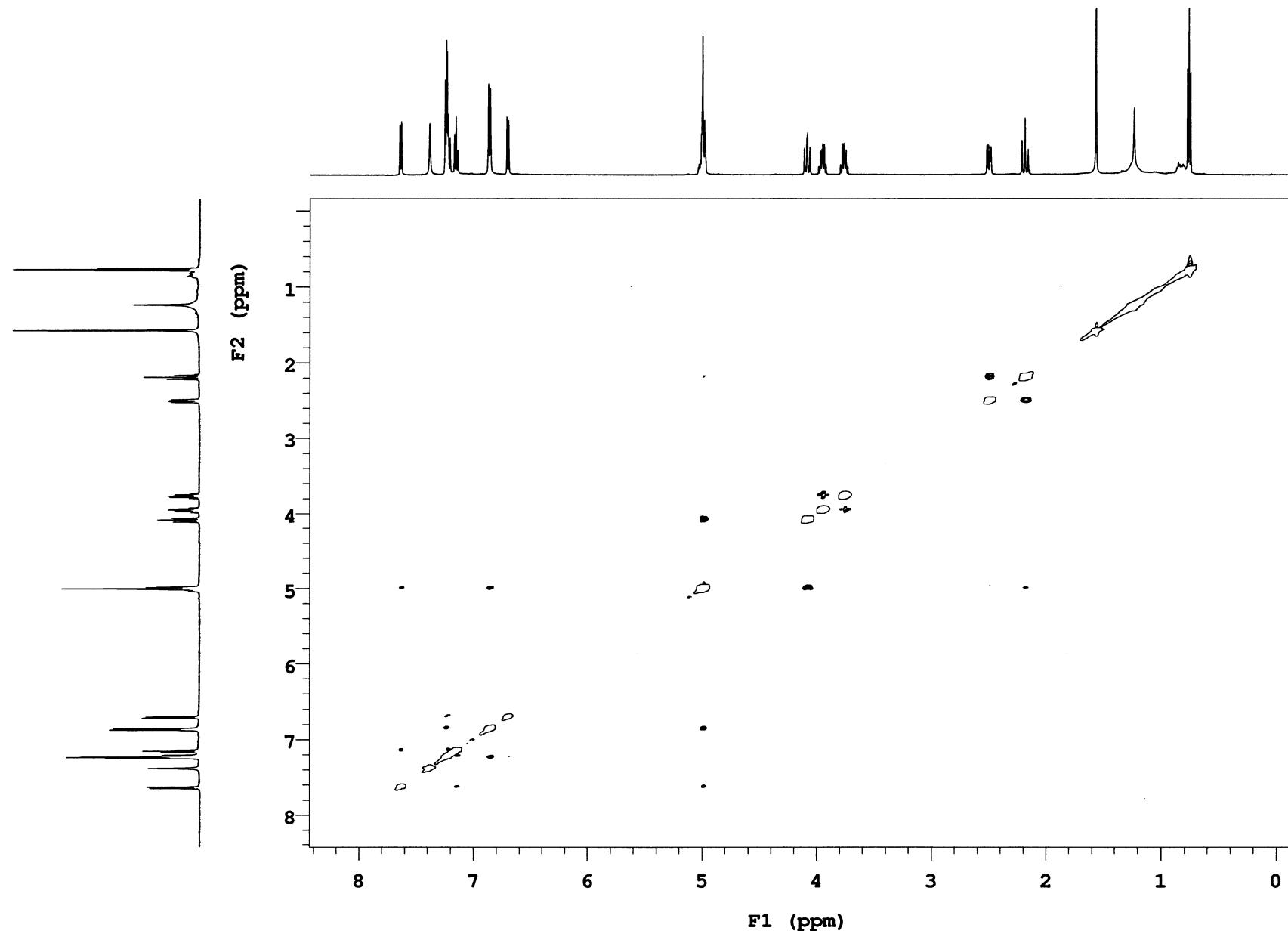
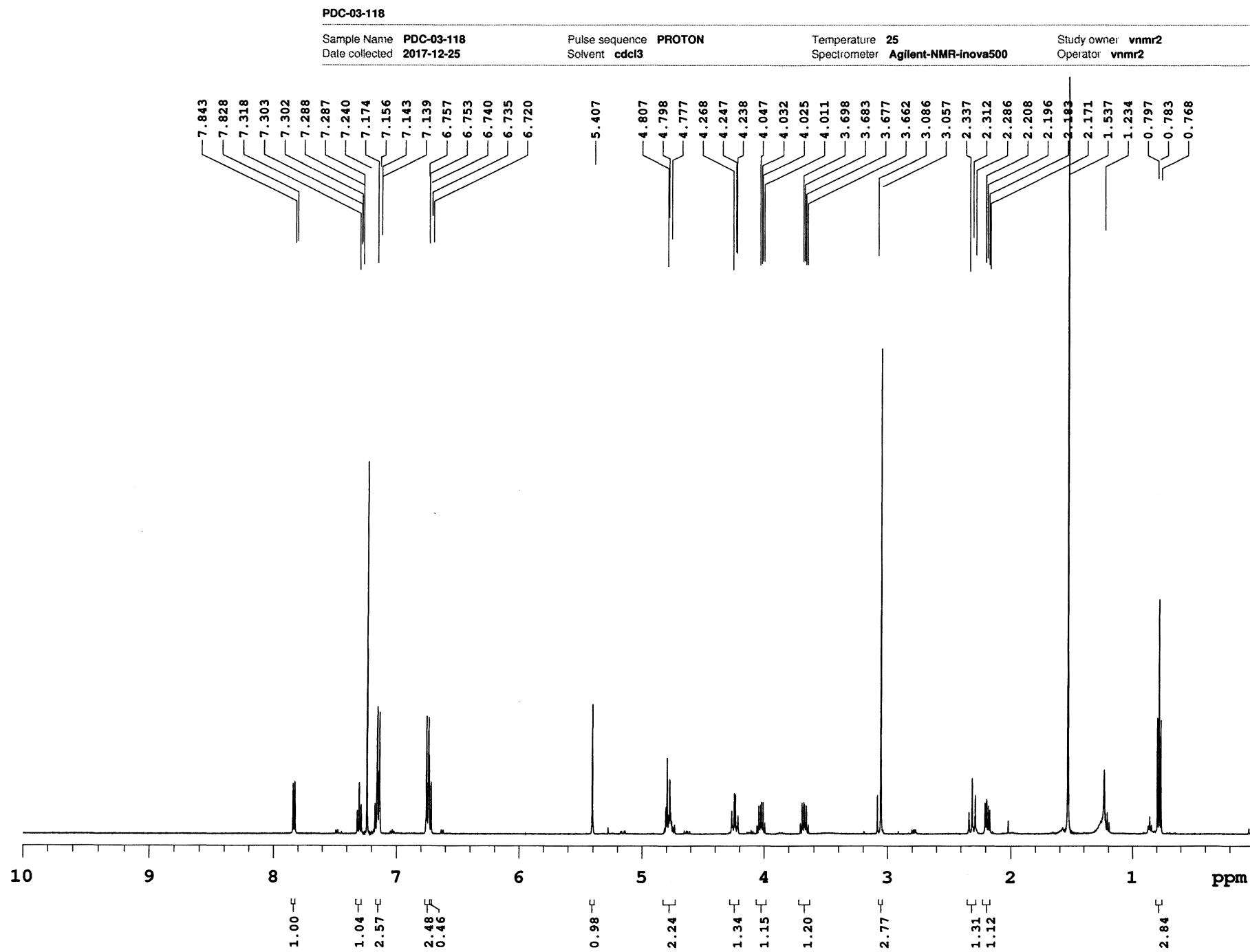
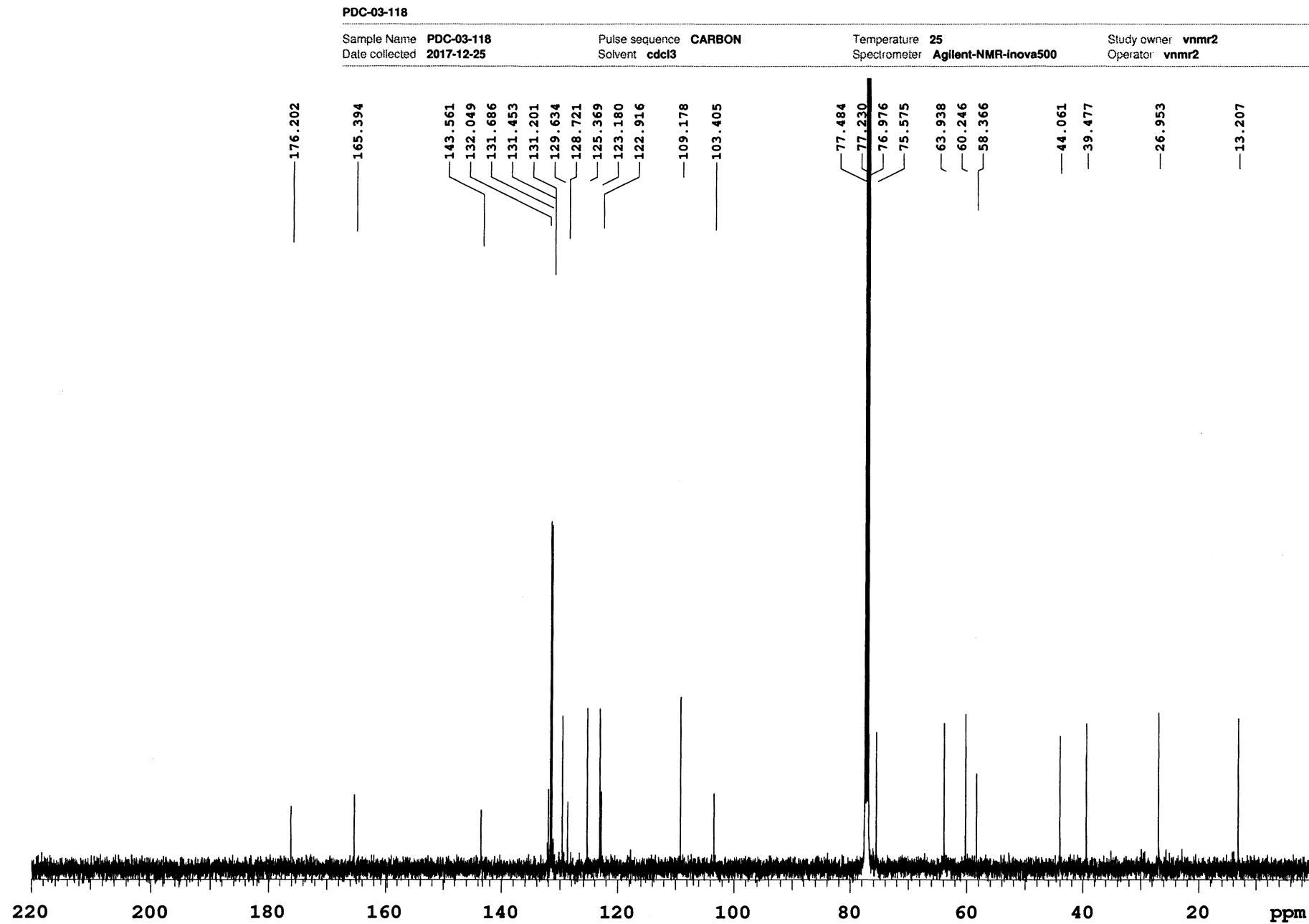
Sample Name PDC-03-145-MNR
Date collected 2018-04-22Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner *vnmr2*
Operator *vnmr2*

Figure S77. NOESY of 4d



Figure S79. ^{13}C NMR (CDCl_3 , 125 MHz) of **3e**

PDC-03-118

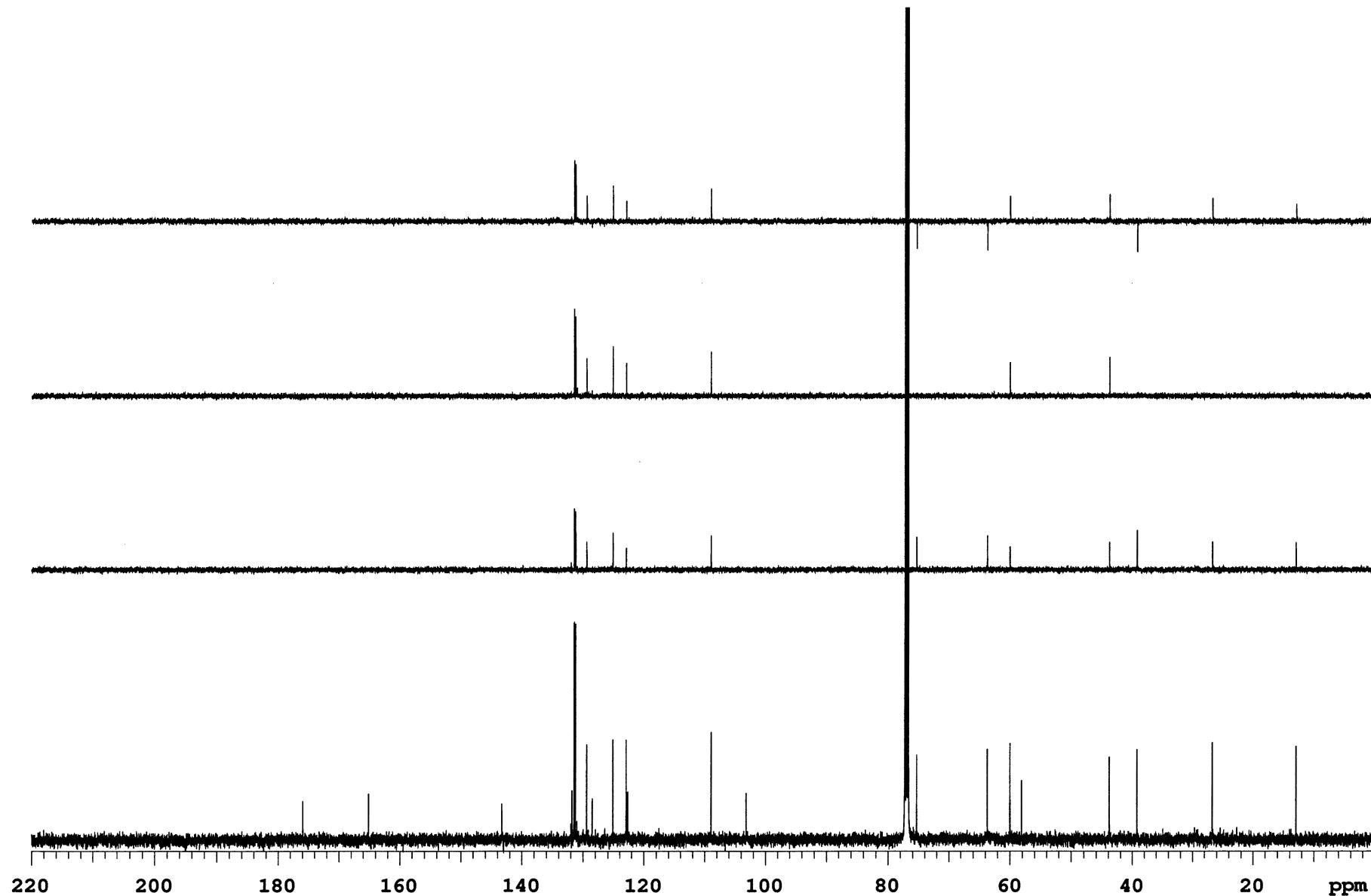
Sample Name **PDC-03-118**
Date collected **2017-12-26**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-Inova500**Study owner **vnmr2**
Operator **vnmr2**

Figure S80. DEPT of 3e

PDC-03-118

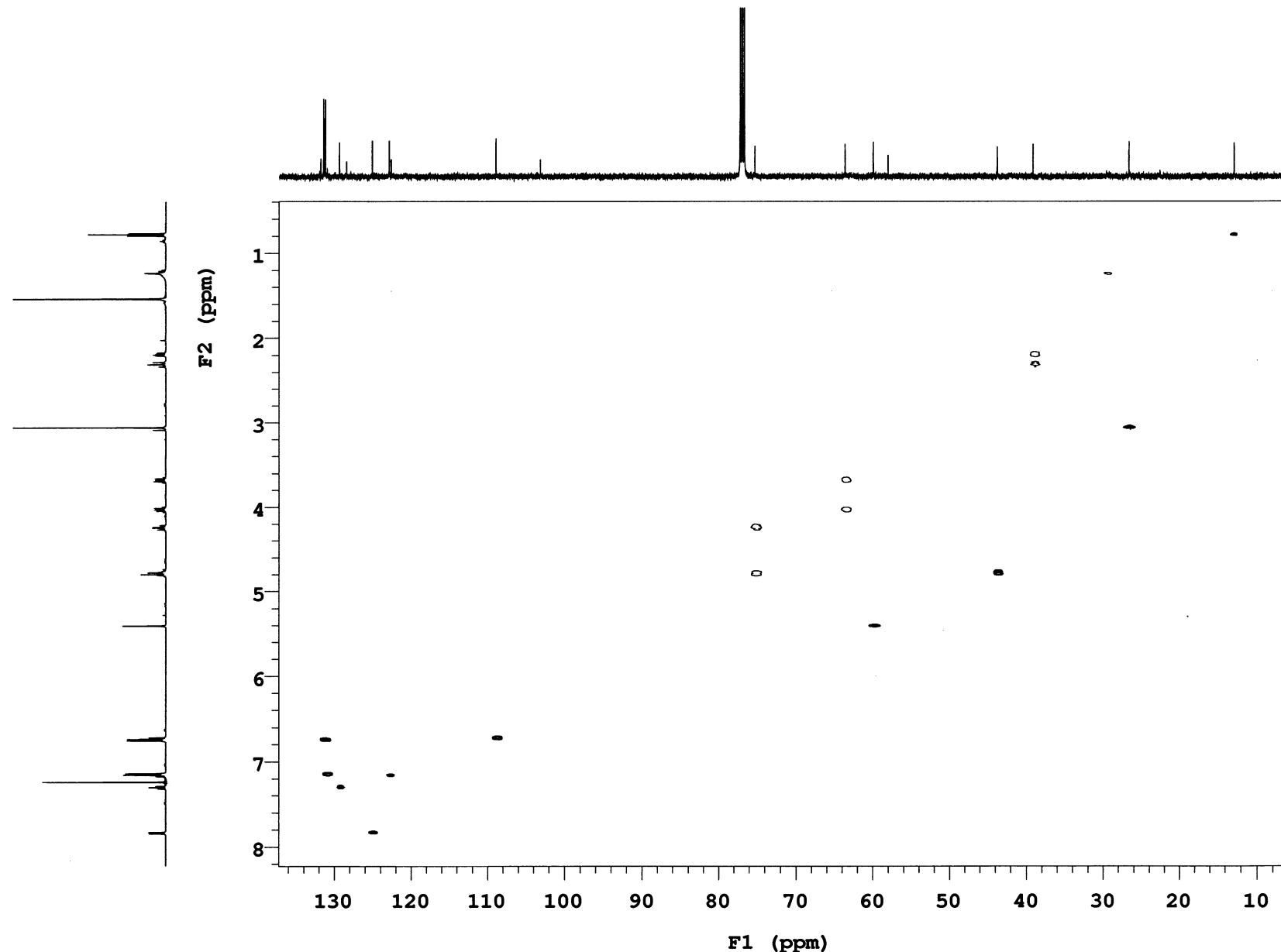
Sample Name PDC-03-118
Date collected 2017-12-26Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S81. HSQC of 3e

PDC-03-118

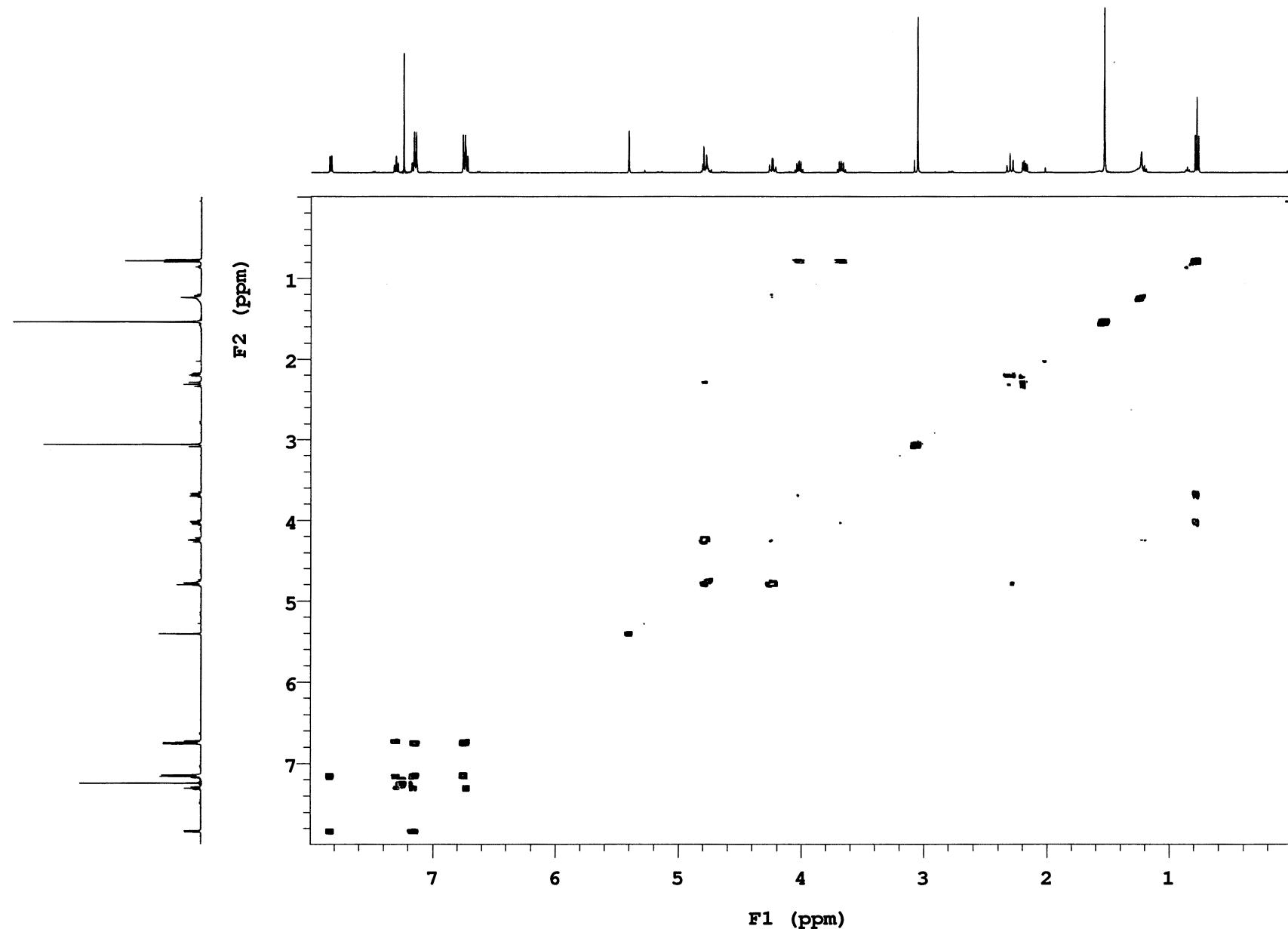
Sample Name PDC-03-118
Date collected 2017-12-26Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2

Figure S82. COSY of 3e

PDC-03-118

Sample Name **PDC-03-118**
Date collected **2017-12-26**

Pulse sequence NOESY
Solvent cdcl3

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr1**
Operator **vnmr2**

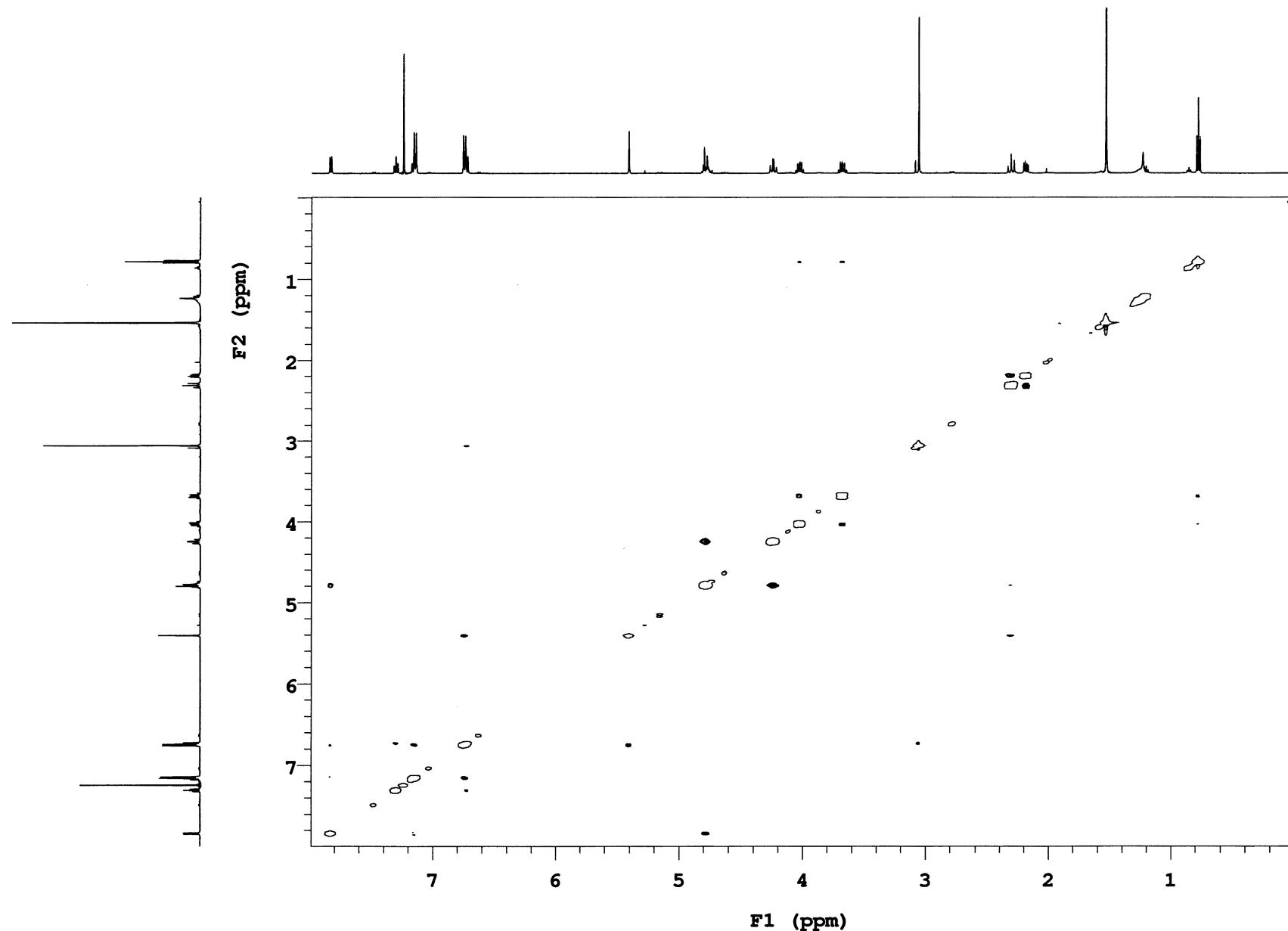
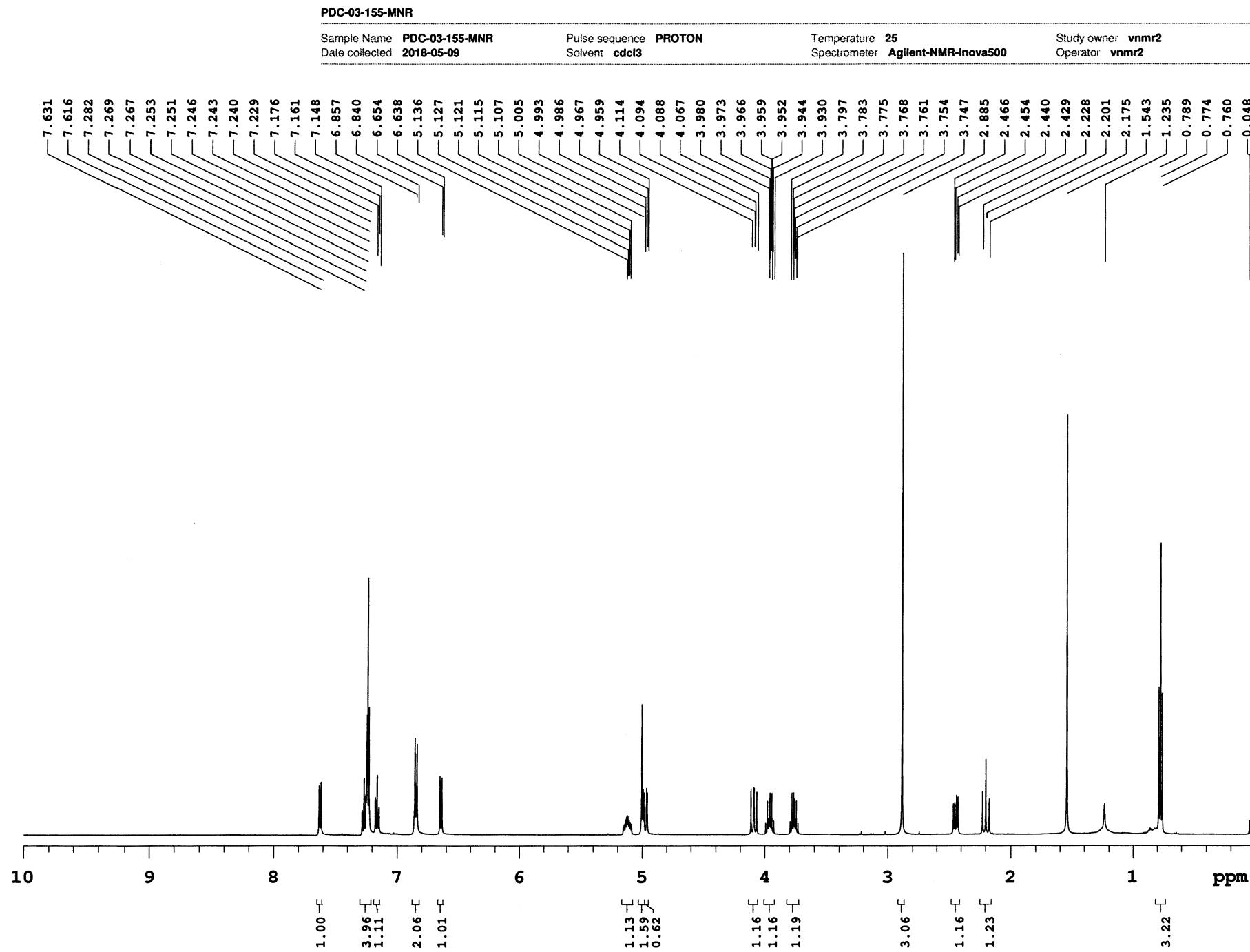
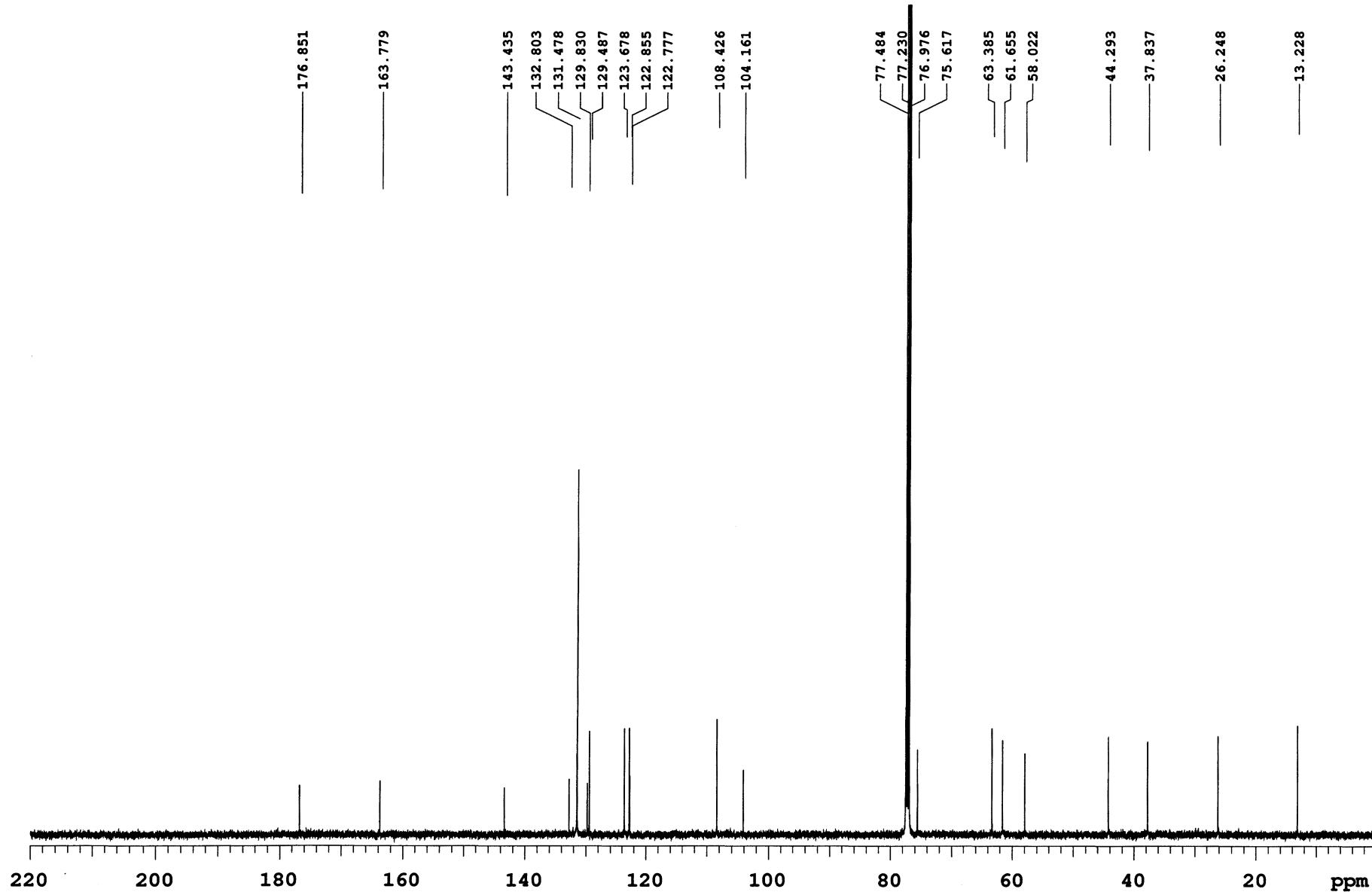


Figure S83. NOESY of **3e**



PDC-03-155-MNR

Sample Name PDC-03-155-MNR Date collected 2018-05-09 Pulse sequence CARBON Solvent *cdcl3* Temperature 25 Spectrometer Agilent-NMR-inova500 Study owner **vnmr2** Operator **vnmr2**

Figure S85. 13C NMR (*CDCl*3, 125 MHz) of **4e**

PDC-03-155-MNR

Sample Name **PDC-03-155-MNR**
Date collected **2018-05-10**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner: **vnmr2**
Operator: **vnmr2**

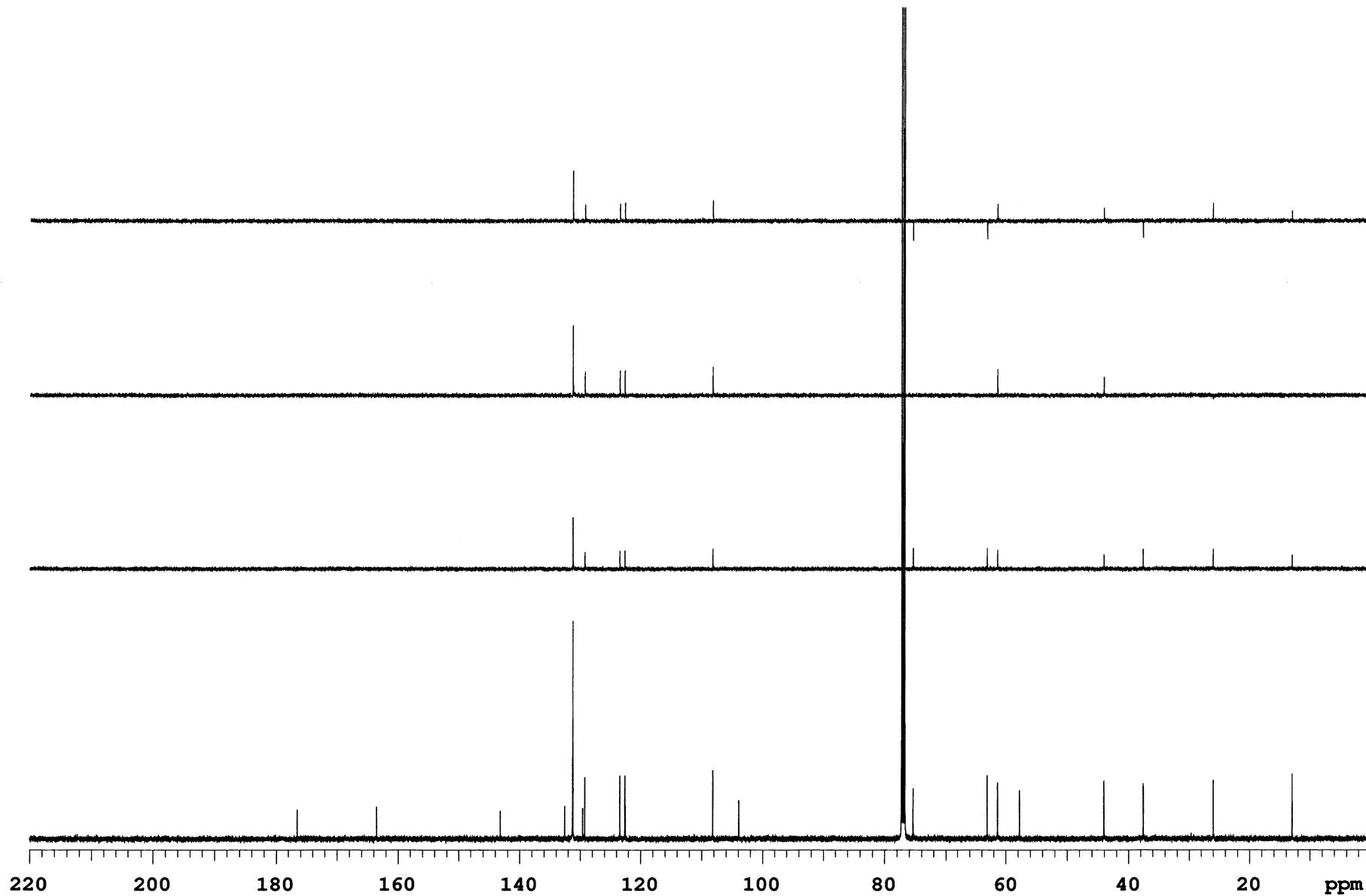
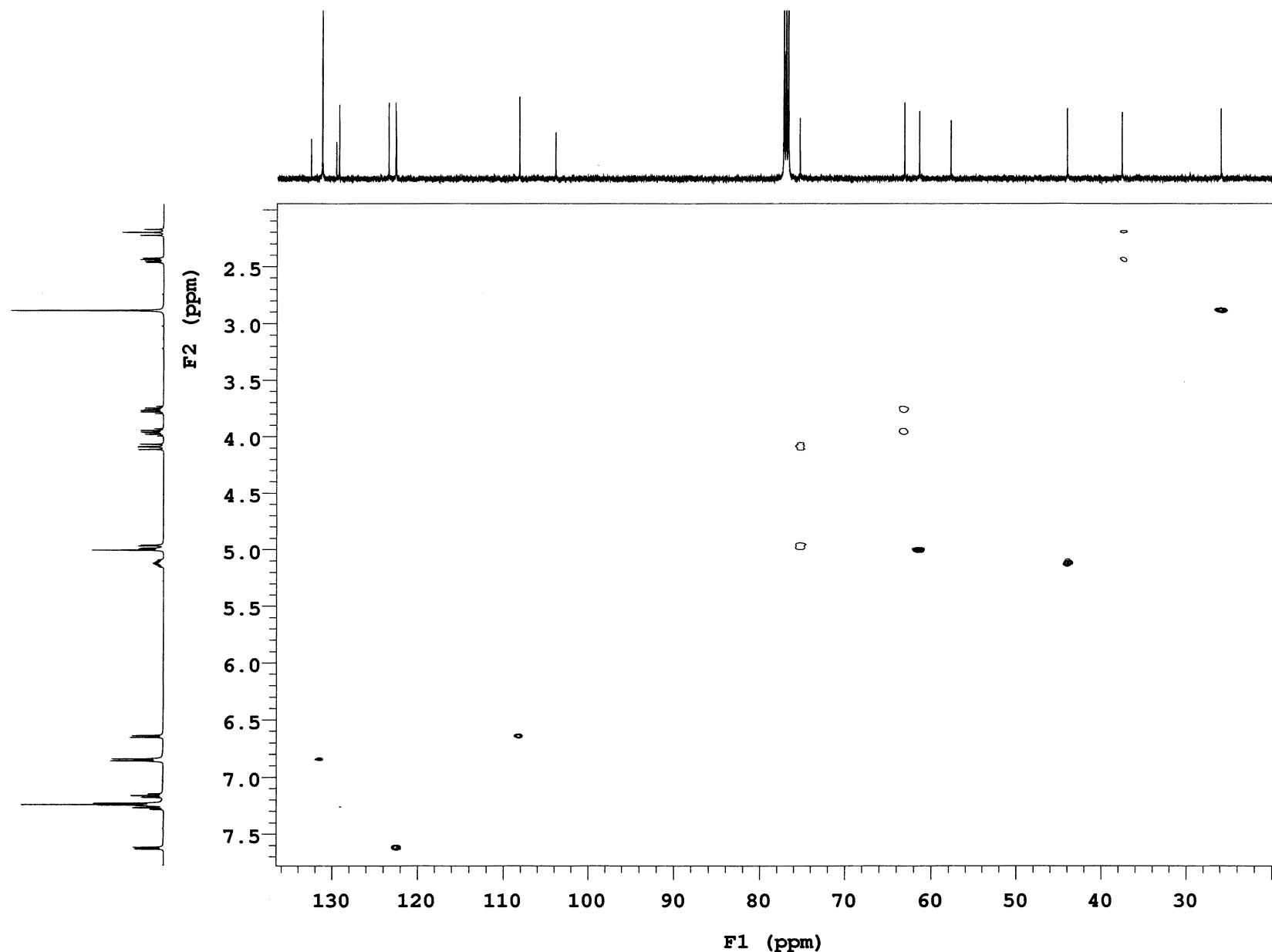
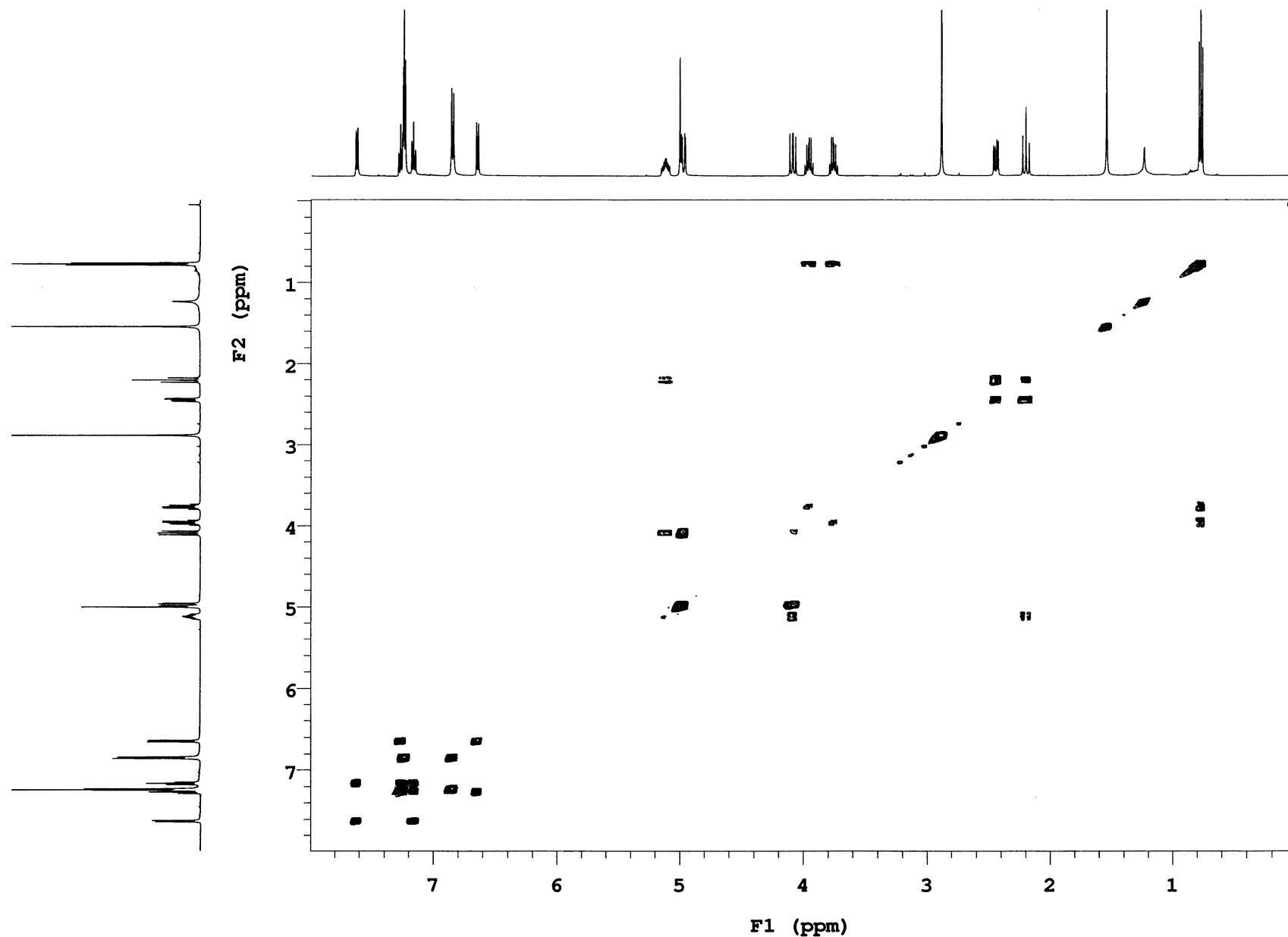


Figure S86. DEPT of **4e**

PDC-03-155-MNR

Sample Name PDC-03-155-MNR
Date collected 2018-05-10Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S87. HSQC of **4e**

PDC-03-155-MNR

Sample Name PDC-03-155-MNR
Date collected 2018-05-10Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S88. COSY of **4e**

PDC-03-155-MNR

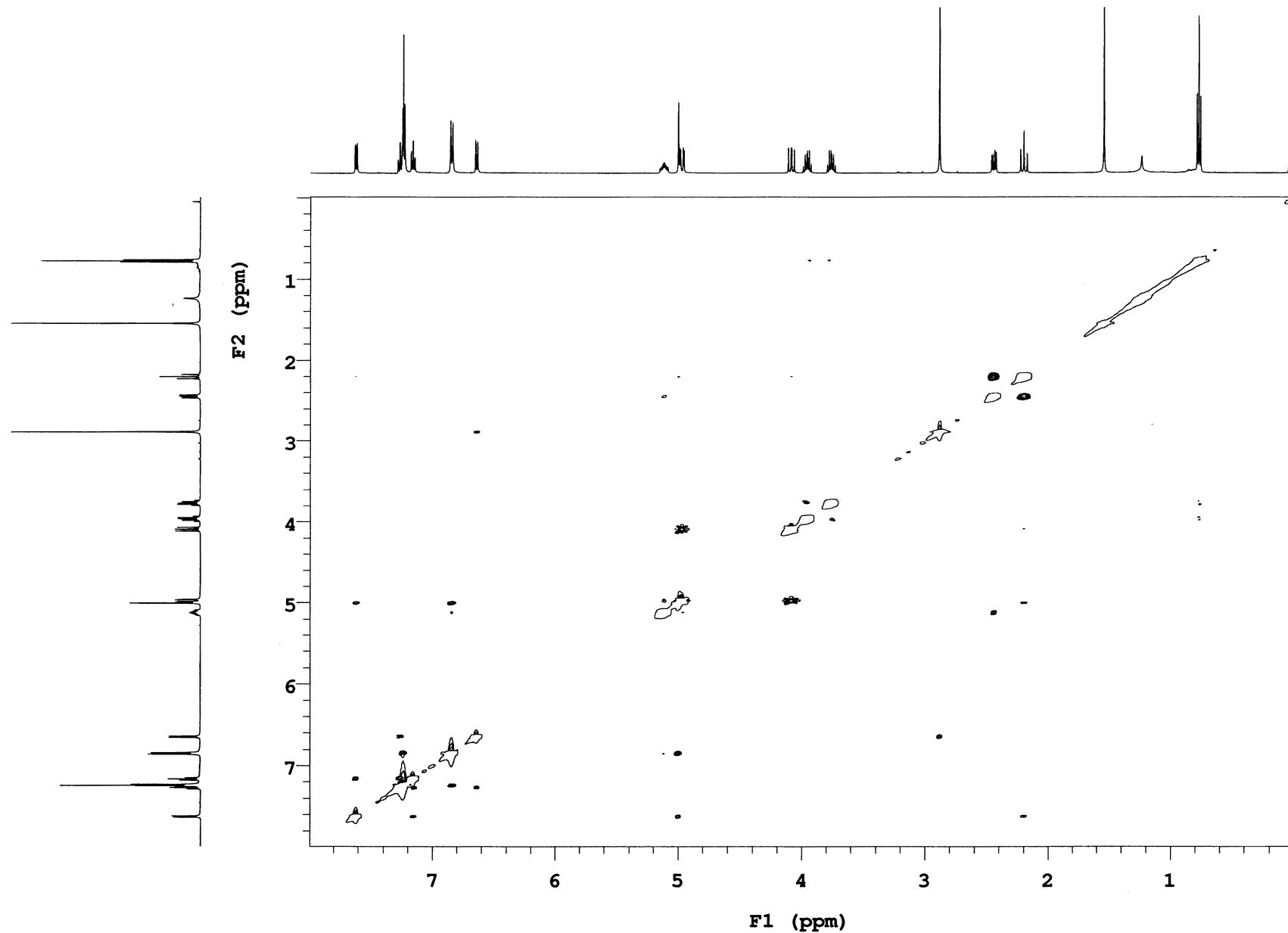
Sample Name PDC-03-155-MNR
Date collected 2018-05-10Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S89. NOESY of 4e

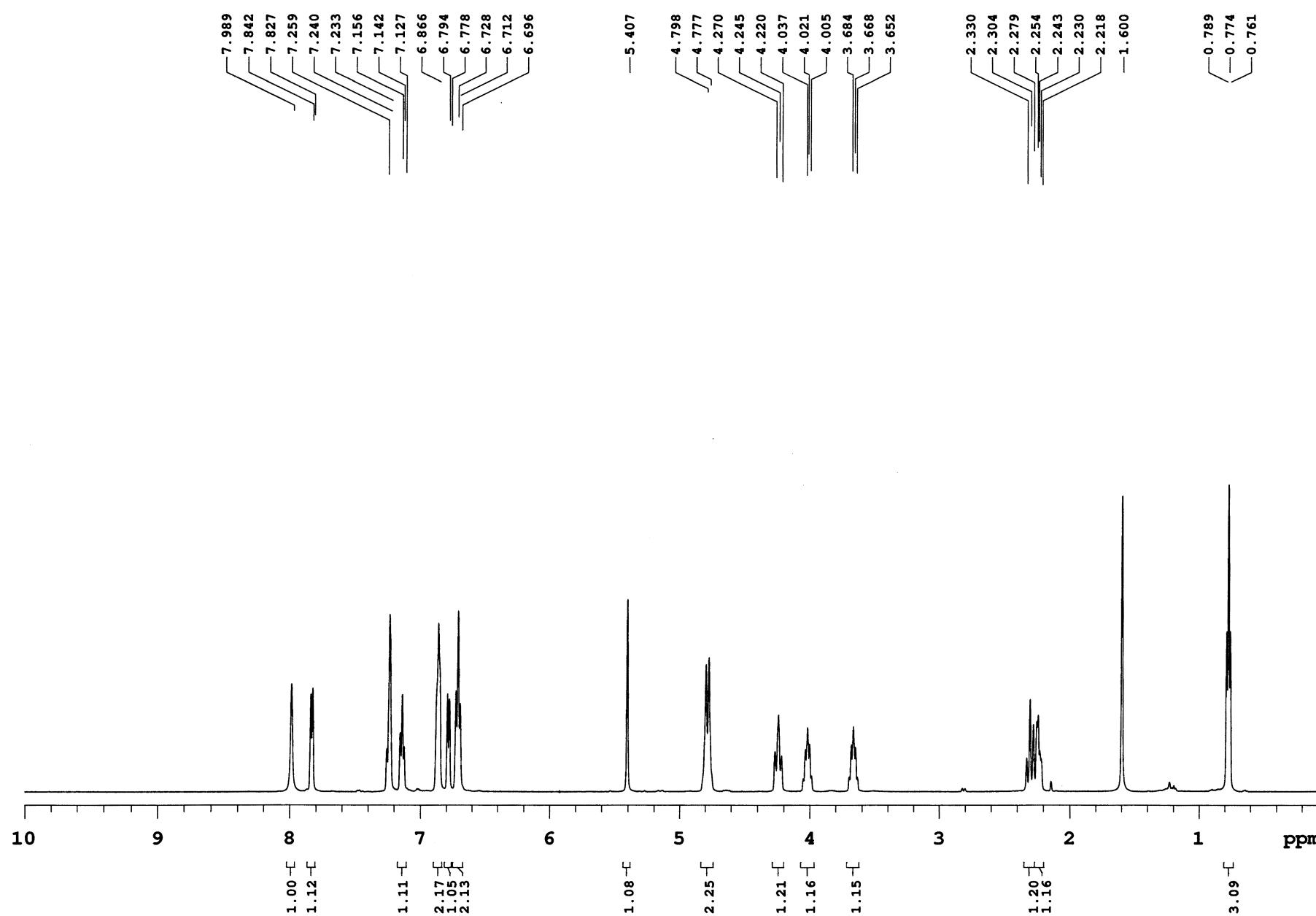
PDC-03-124

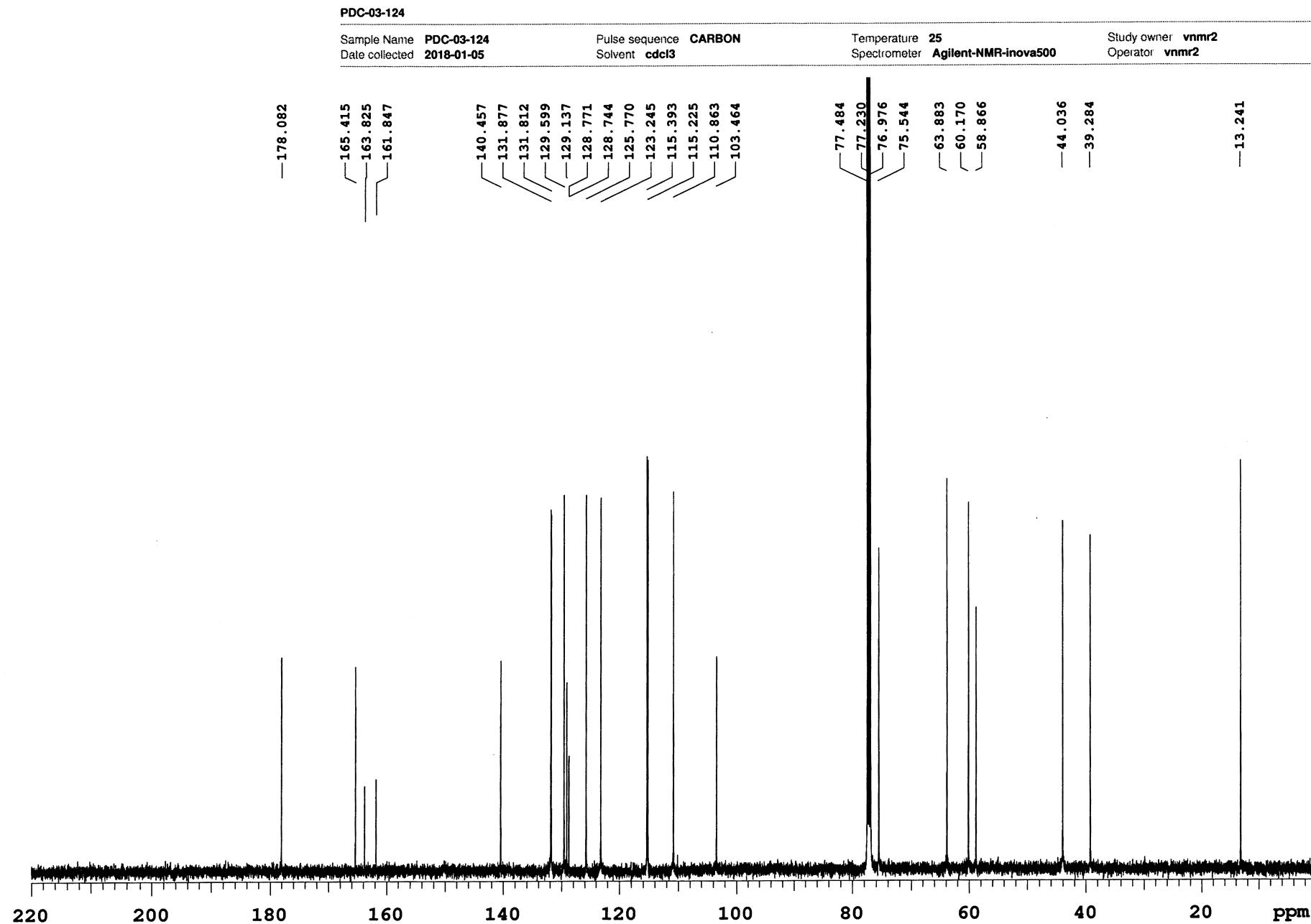
Sample Name **PDC-03-12**
Date collected **2018-01-05**

Pulse sequence PROTON
Solvent cdcl3

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr**
Operator **vnmr2**



Figure S91. ^{13}C NMR (CDCl₃, 125 MHz) of **3f**

PDC-03-124

Sample Name **PDC-03-124**
Date collected **2018-01-06**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

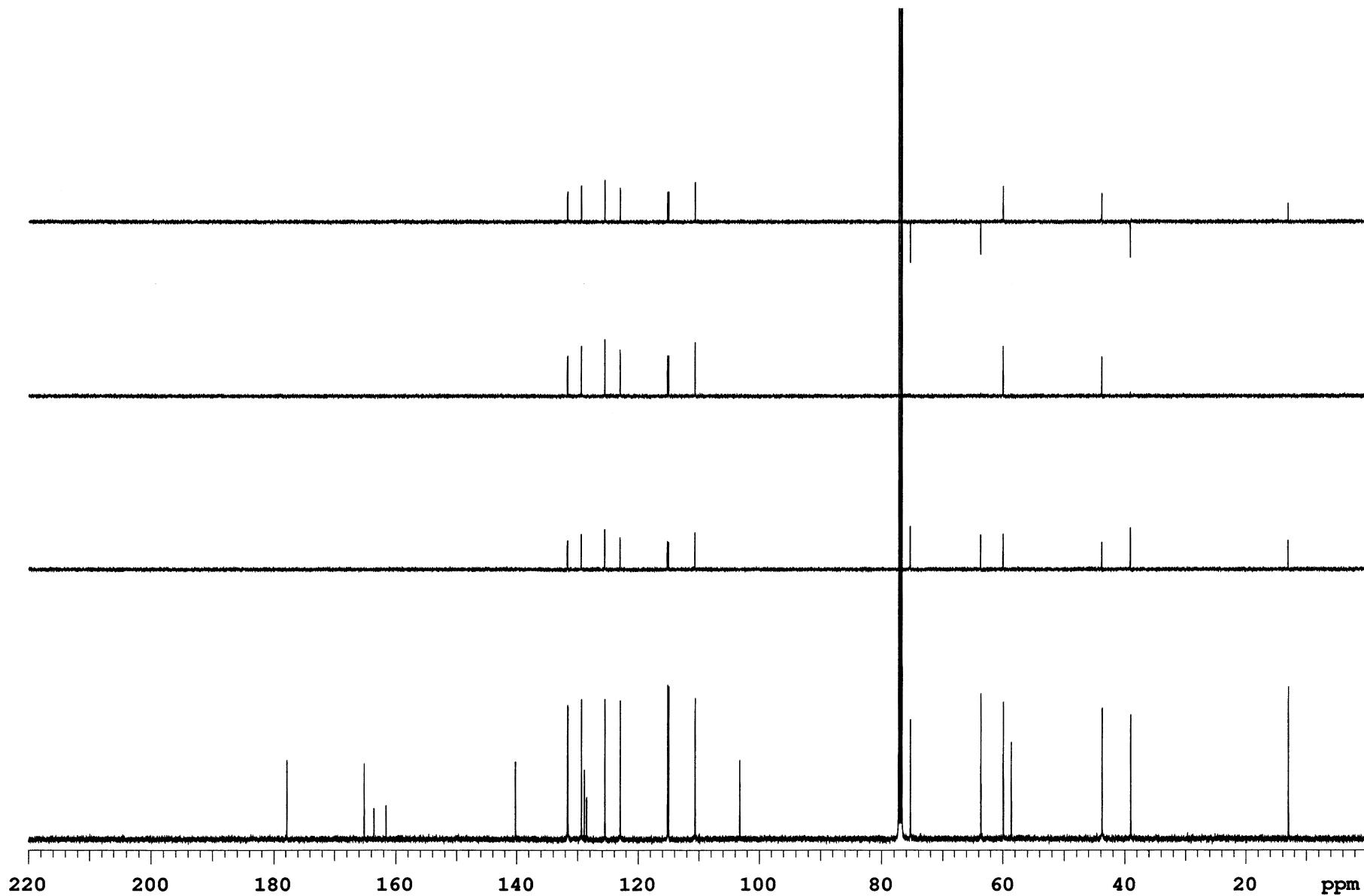


Figure S92. DEPT of **3f**

PDC-03-124

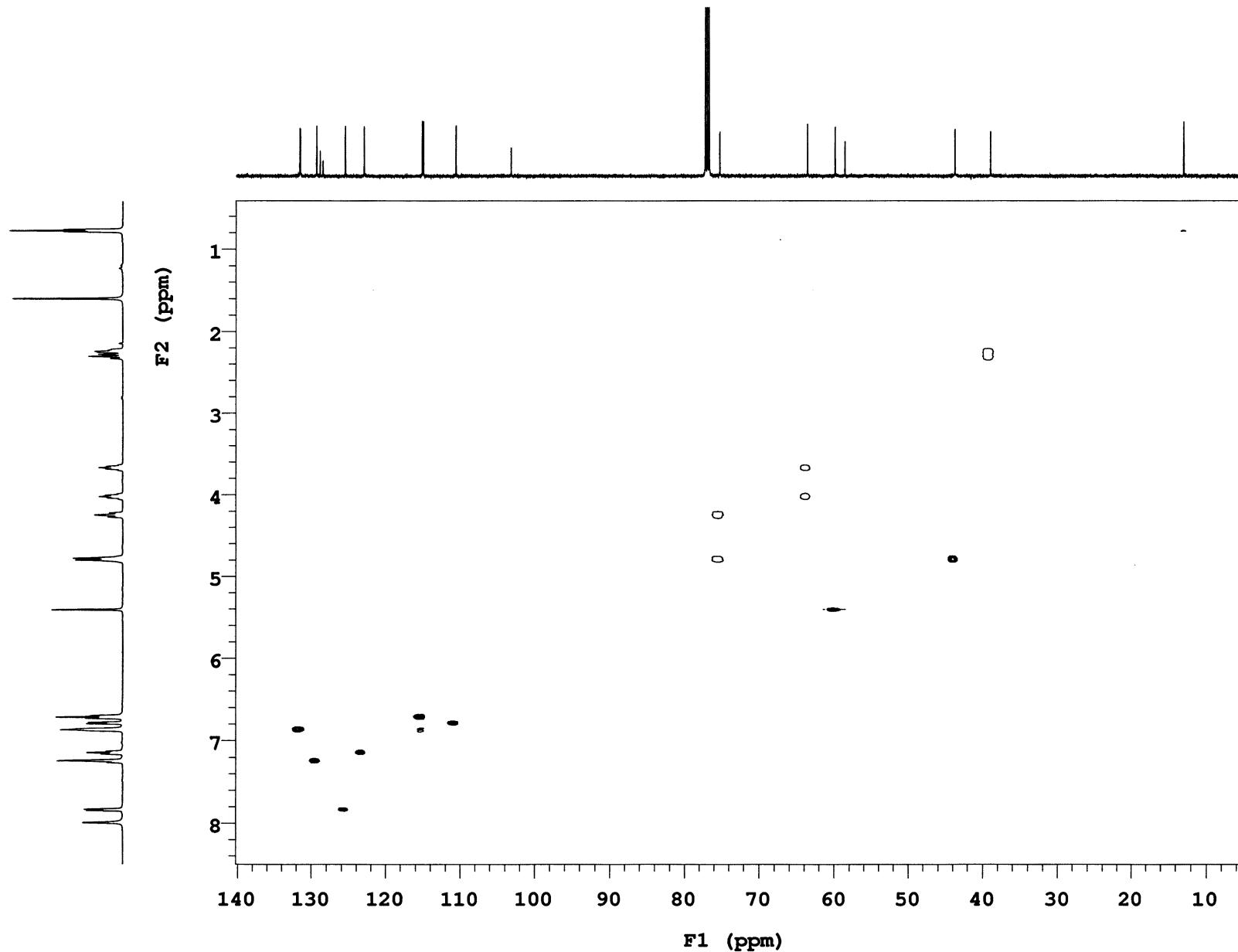
Sample Name PDC-03-124
Date collected 2018-01-06Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S93. HSQC of 3f

PDC-03-124

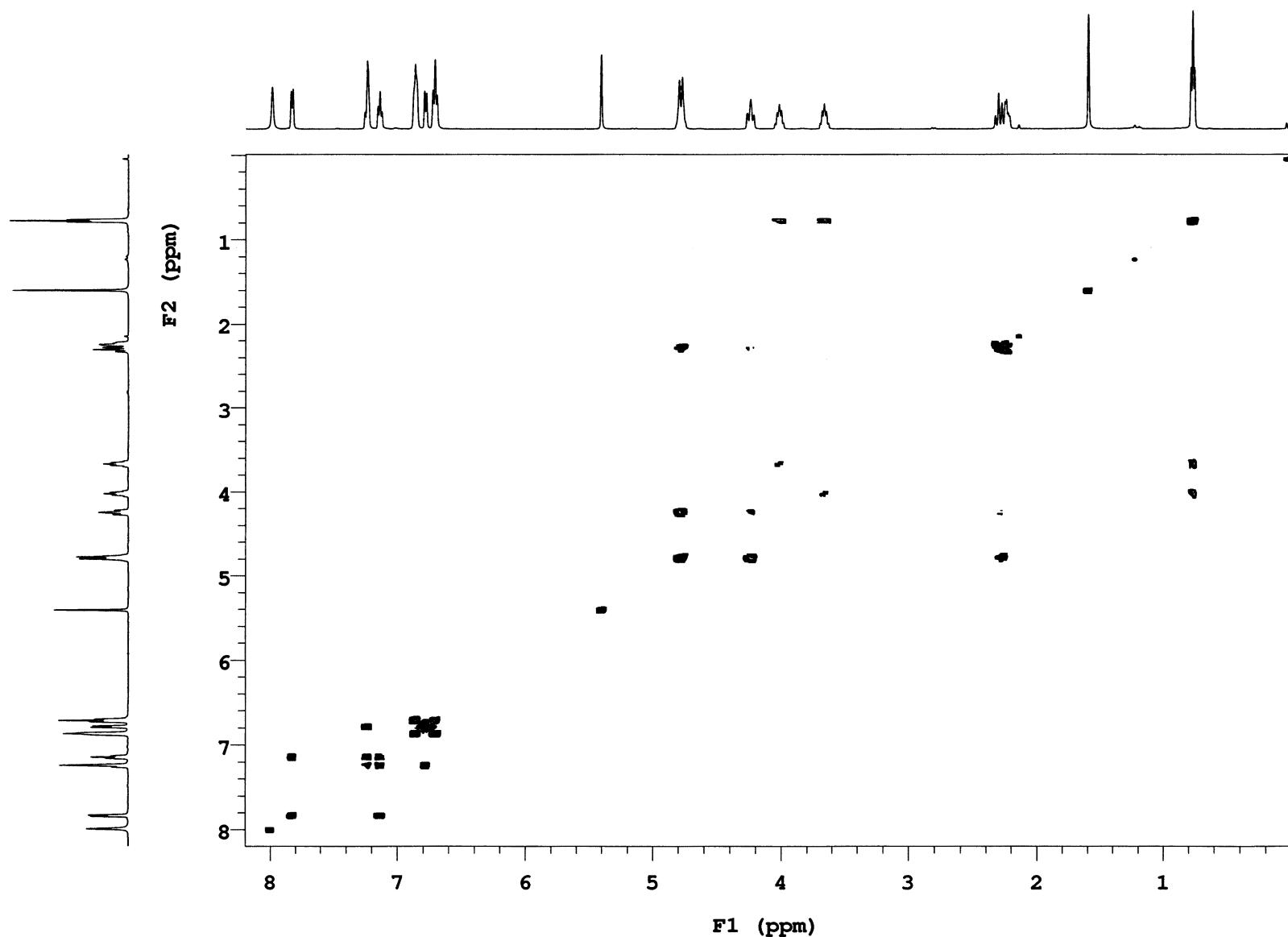
Sample Name PDC-03-124
Date collected 2018-01-06Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2

Figure S94. COSY of 3f

PDC-03-124

Sample Name PDC-03-124
Date collected 2018-01-06

Pulse sequence NOESY
Solvent *cdcl*3

Temperature 25
Spectrometer Agilent-NMR-inova500

Study owner vnmr2
Operator vnmr2

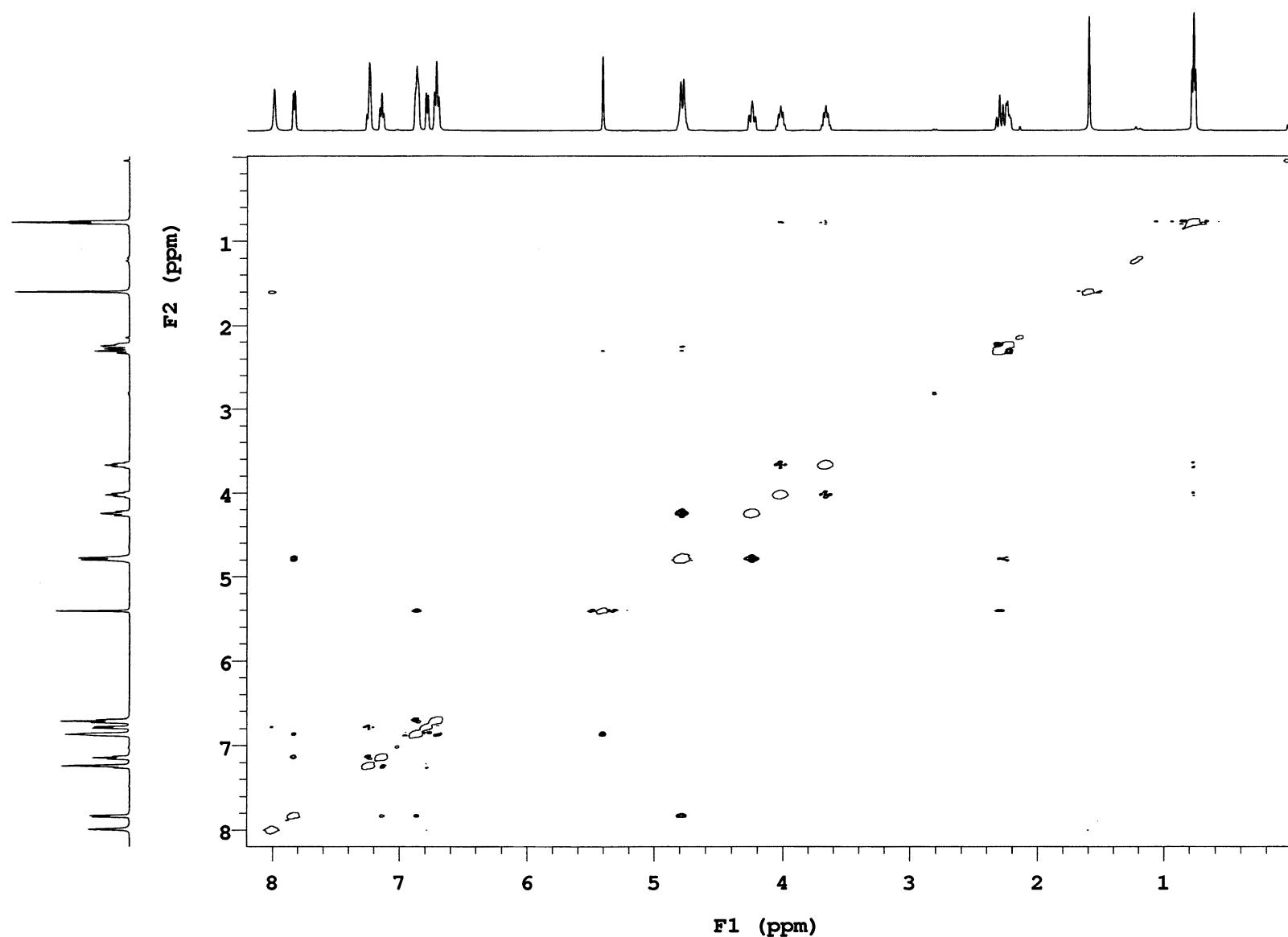
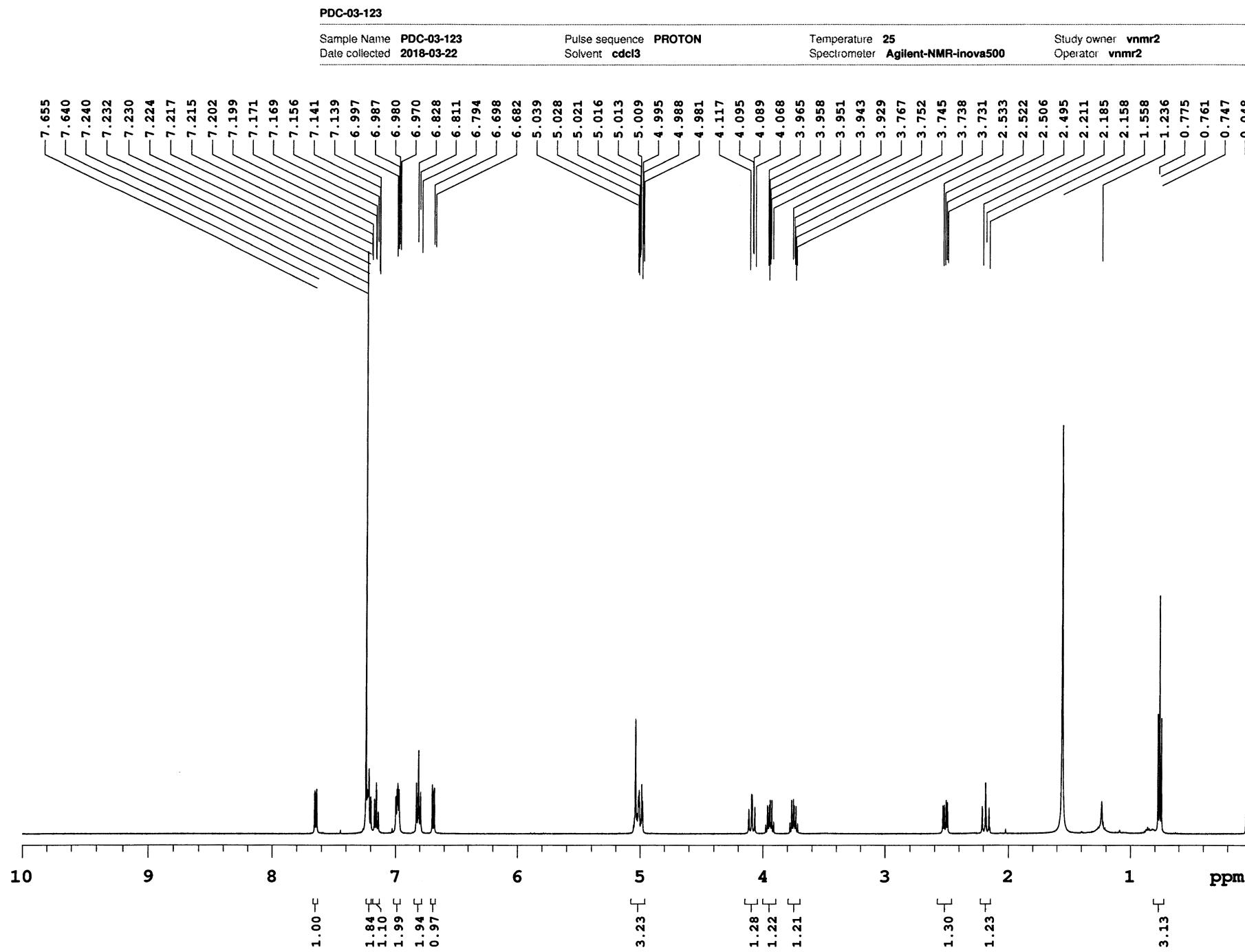
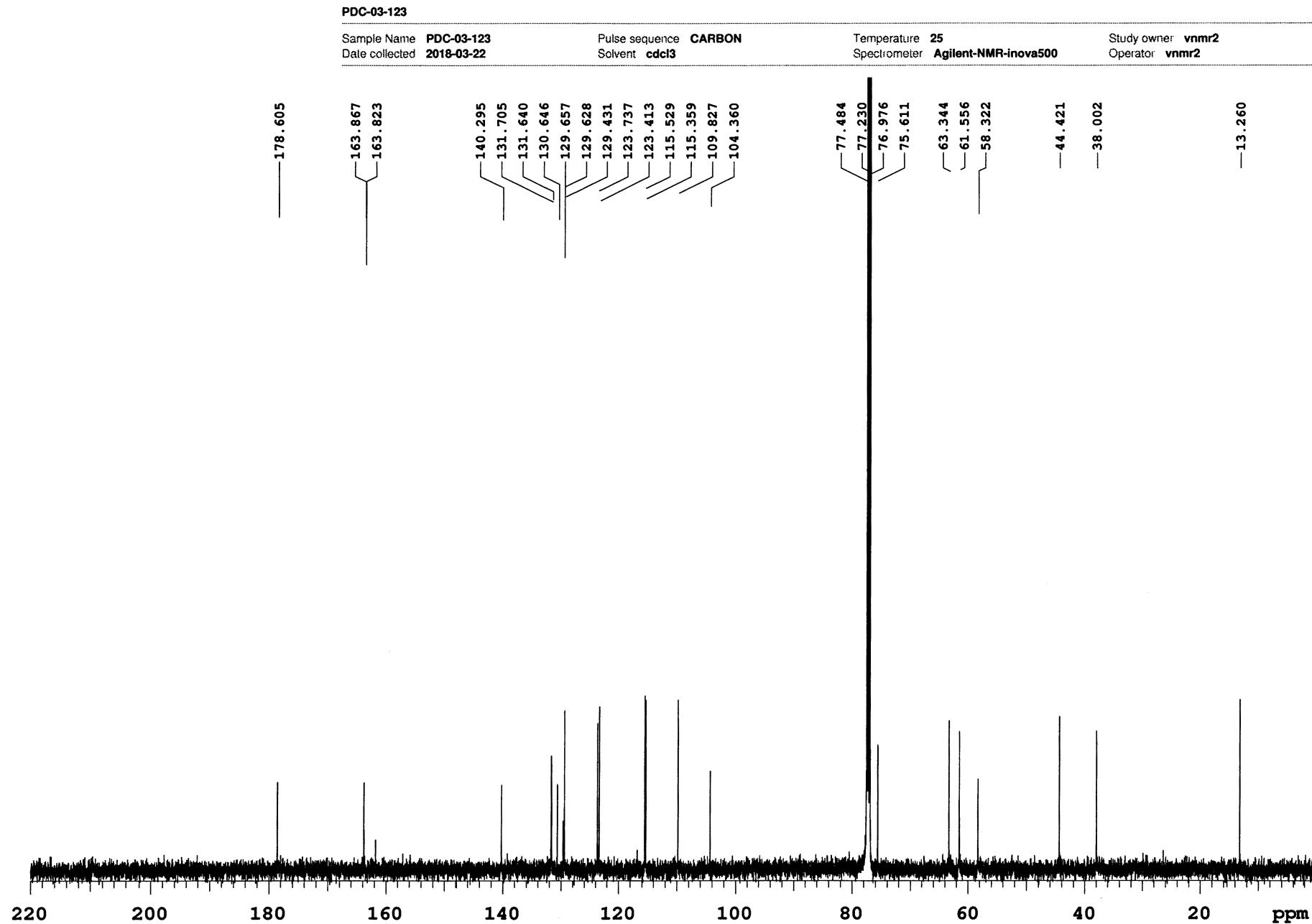
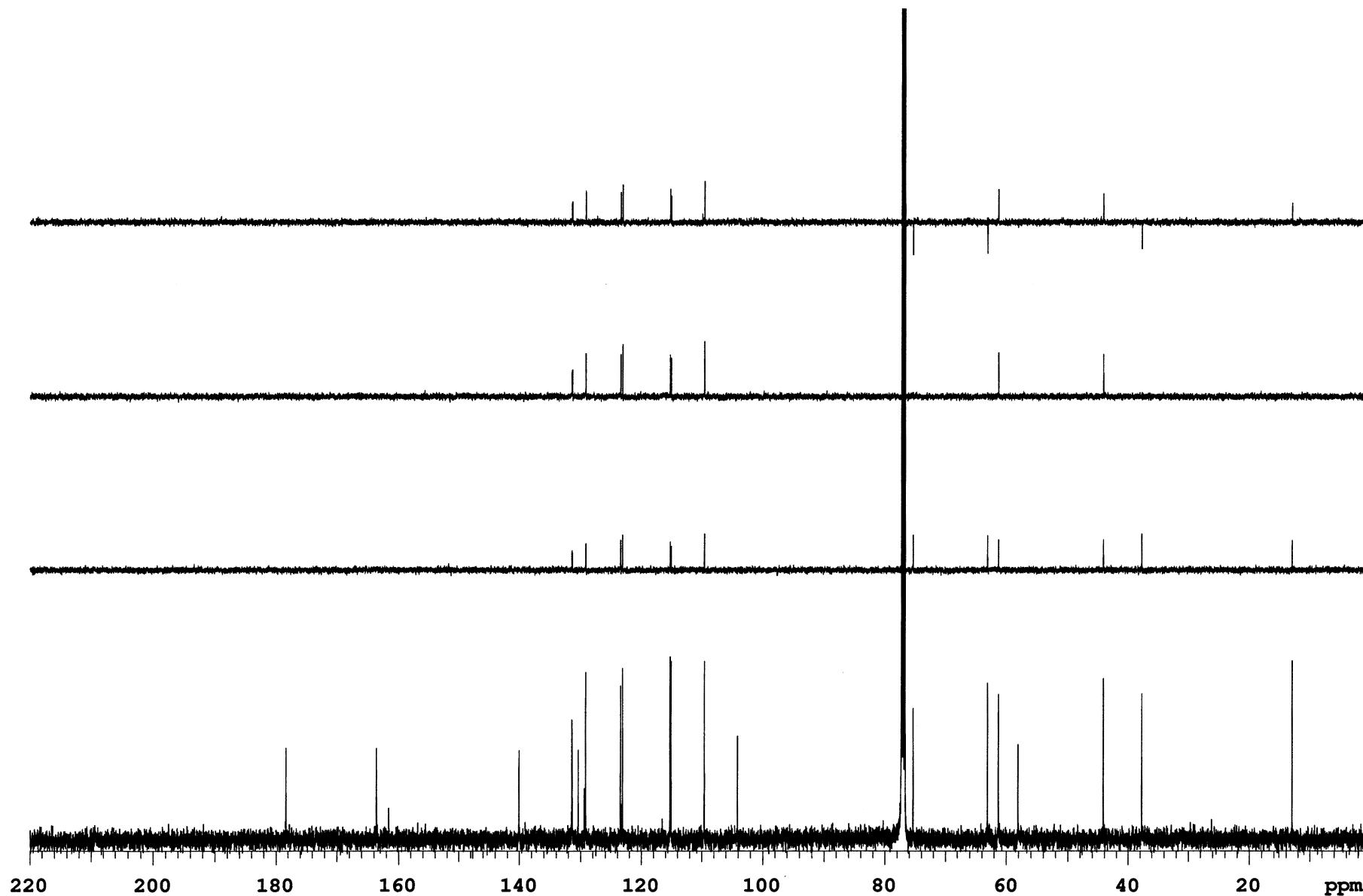


Figure S95. NOESY of 3f

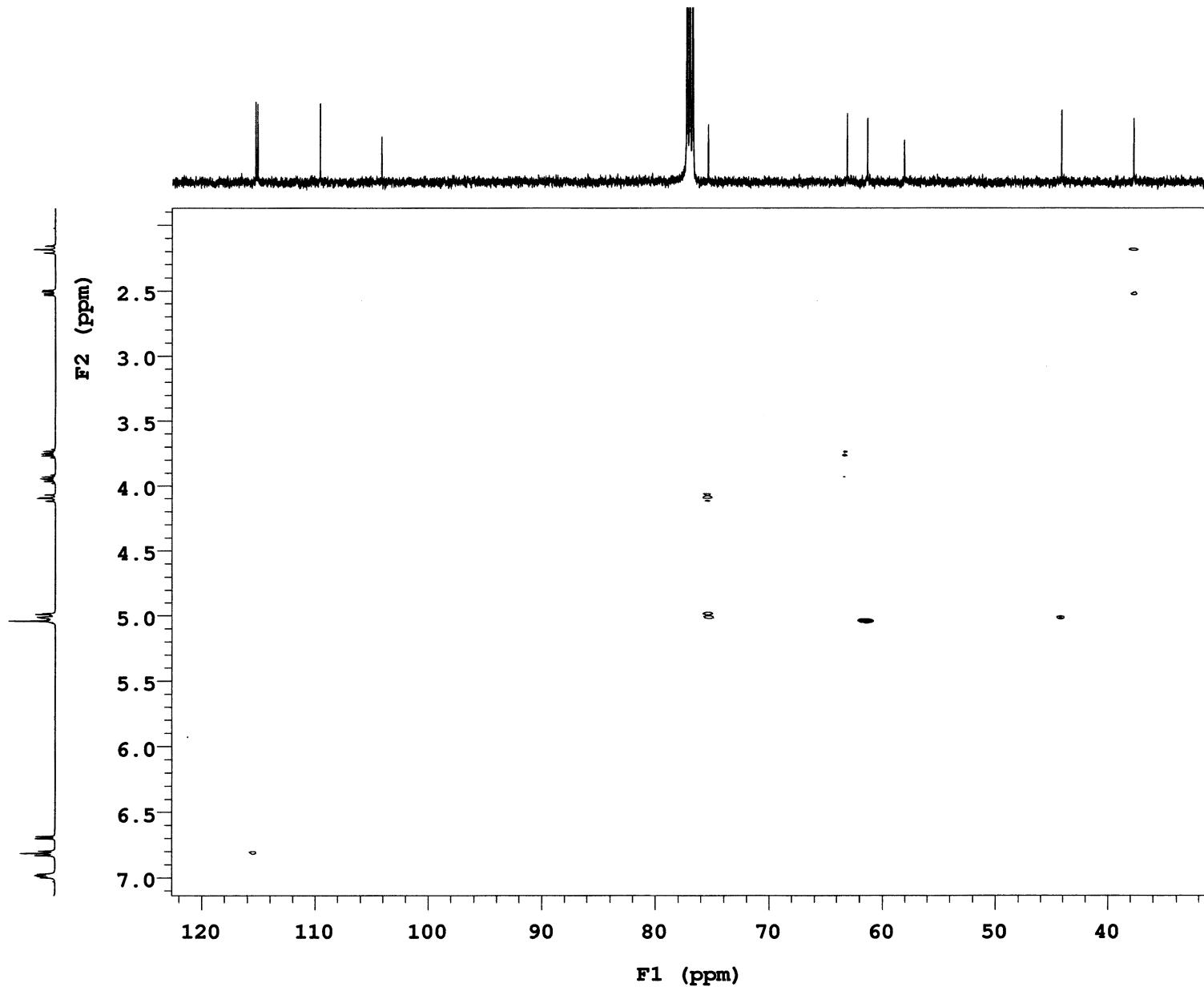


Figure S97. ^{13}C NMR (CDCl₃, 125 MHz) of **4f**

PDC-03-123

Sample Name PDC-03-123
Date collected 2018-03-22Pulse sequence DEPT
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner **vnmr2**
Operator **vnmr2**Figure S98. DEPT of **4f**

PDC-03-123

Sample Name PDC-03-123
Date collected 2018-03-22Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S99. HSQC of **4f**

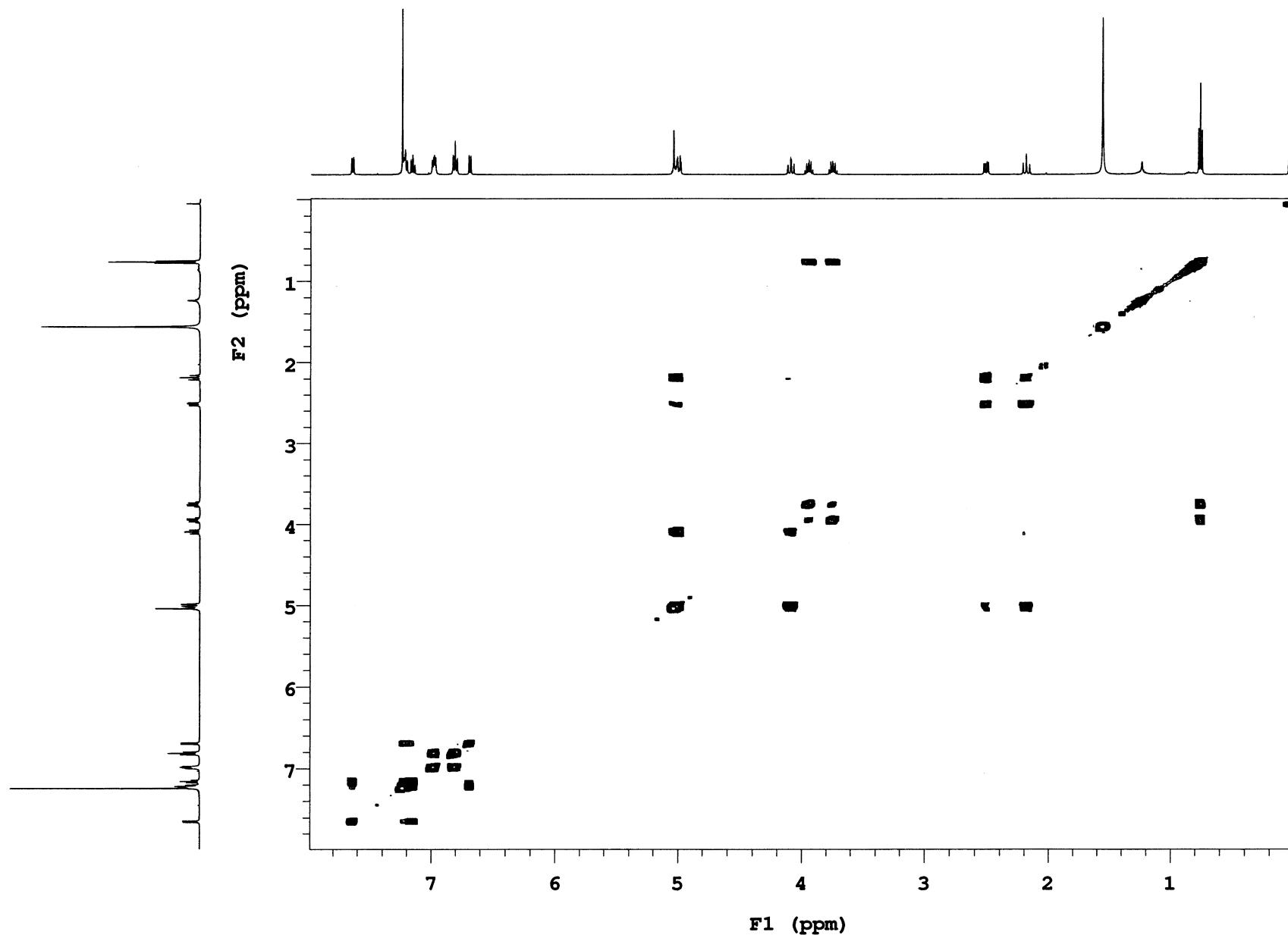
PDC-03-123

Sample Name PDC-03-123
Date collected 2018-03-22

Pulse sequence gCOSY
Solvent *cdcl*3

Temperature 25
Spectrometer Agilent-NMR-inova500

Study owner vnmr2
Operator vnmr2

Figure S100. COSY of **4f**

PDC-03-123

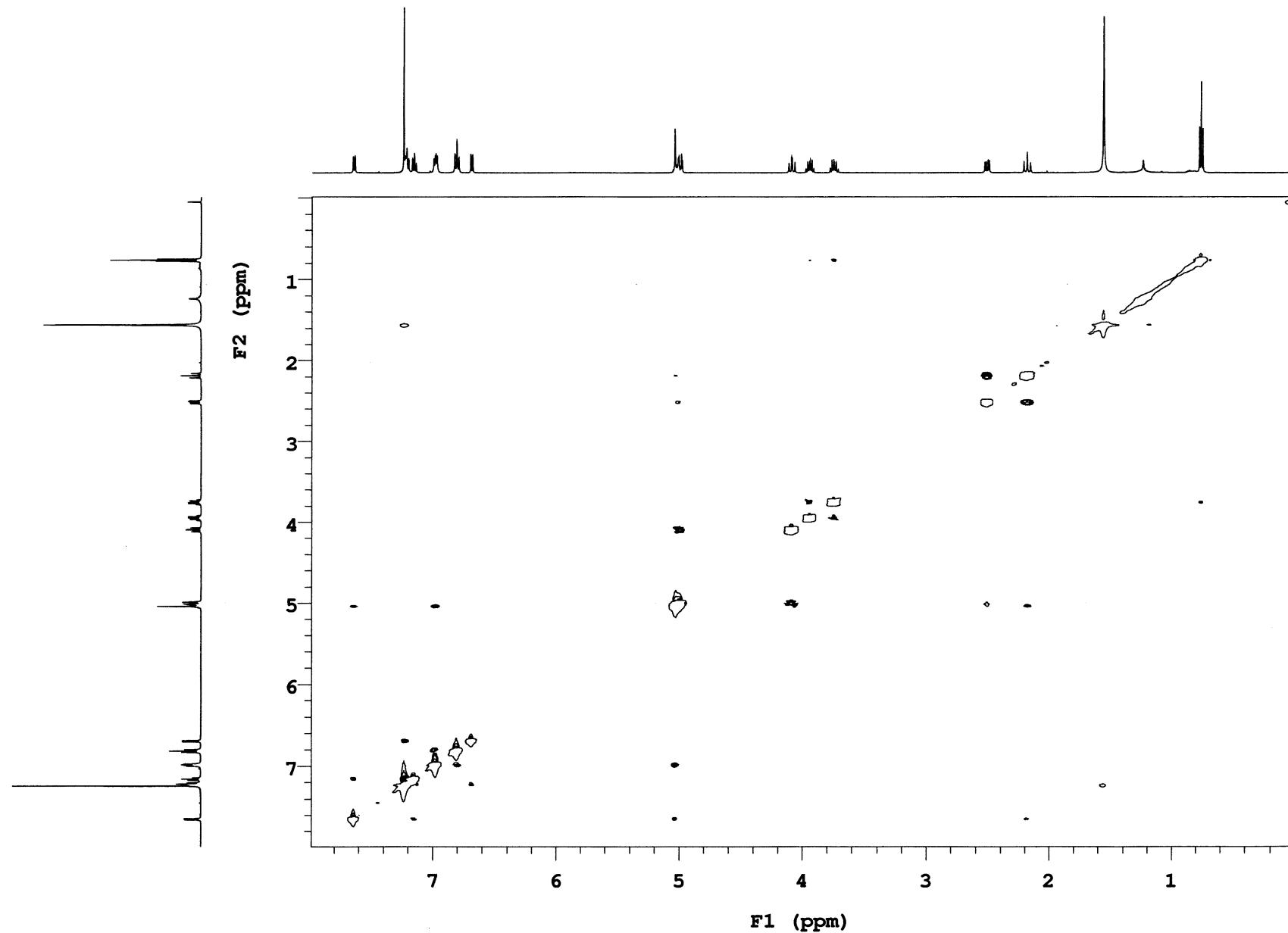
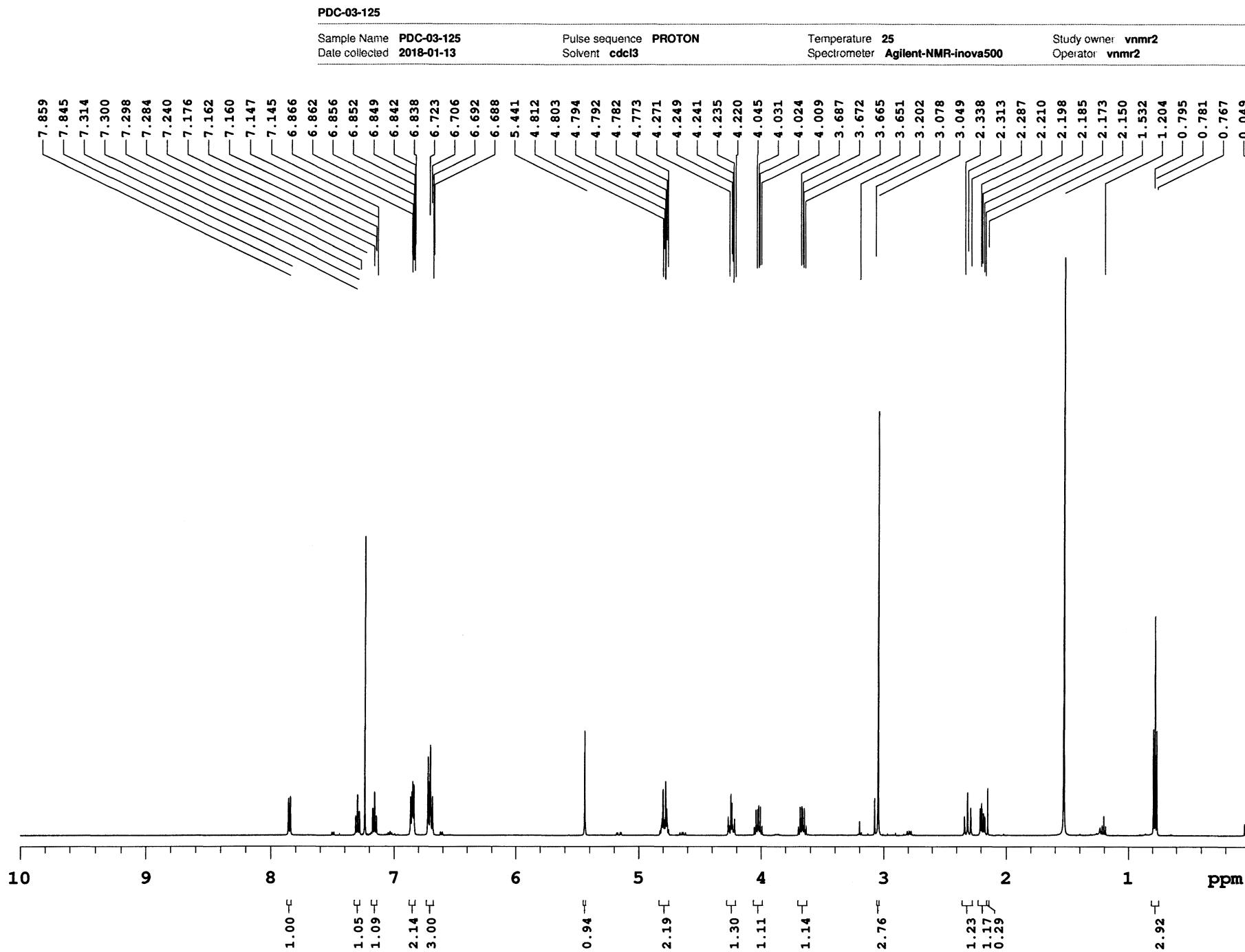
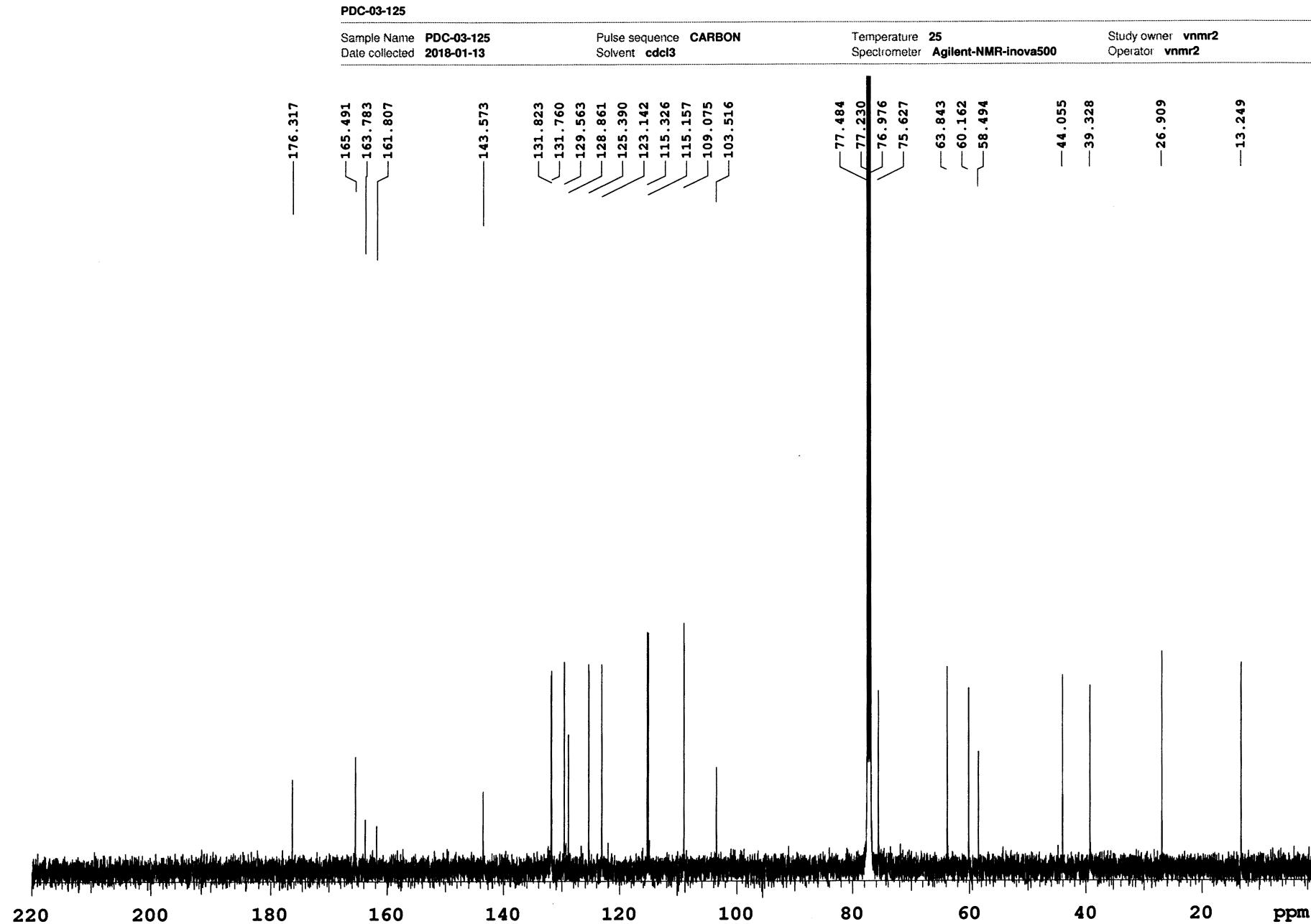
Sample Name PDC-03-123
Date collected 2018-03-22Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner *vnmr2*
Operator *vnmr2*

Figure S101. NOESY of 4f



Figure S103. ^{13}C NMR (CDCl_3 , 125 MHz) of **3g**

PDC-03-125

Sample Name **PDC-03-125**
Date collected **2018-01-13**

Pulse sequence DEPT
Solvent cdcl_3

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner: **vnmr**
Operator: **vnmr2**

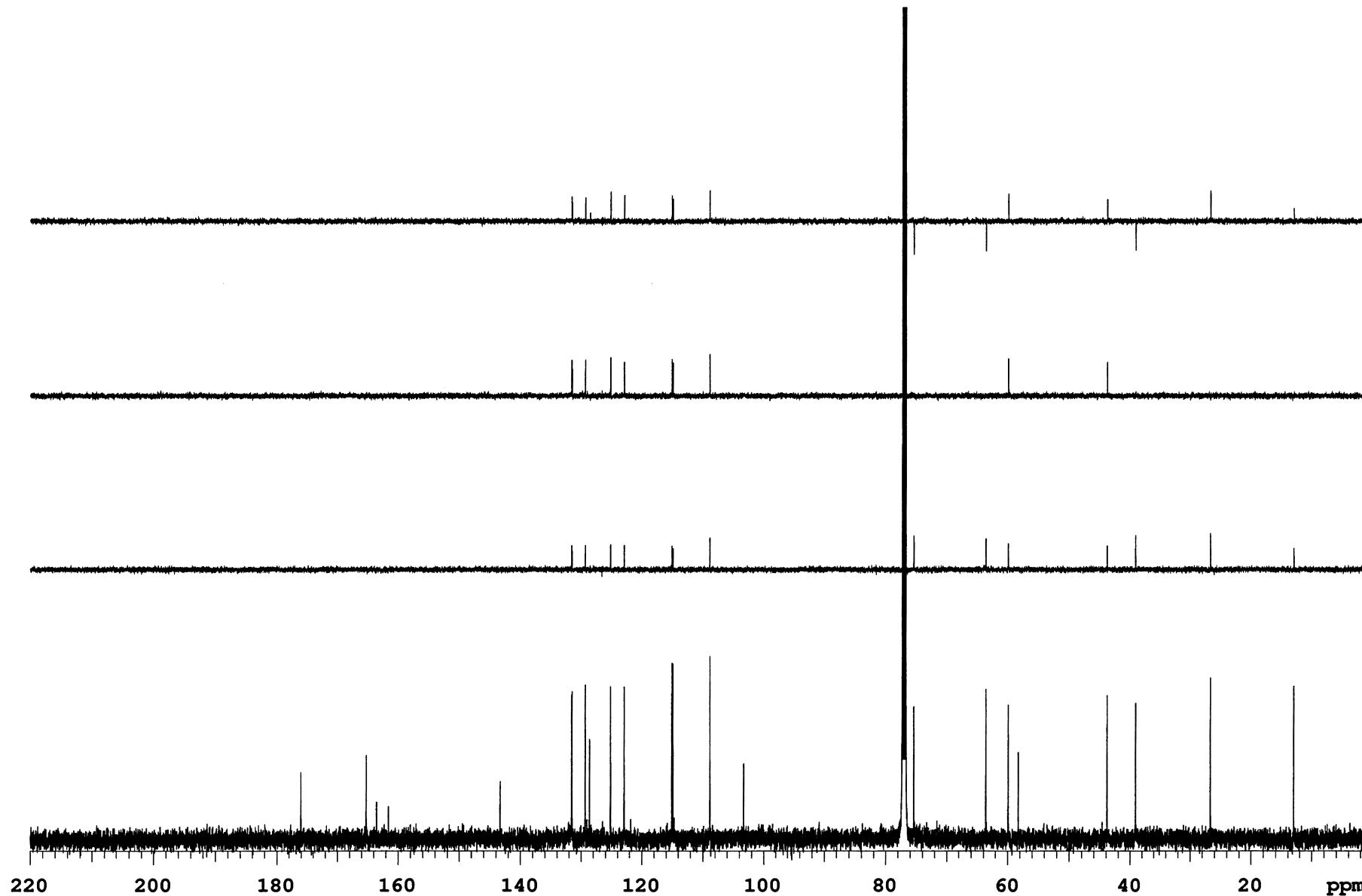
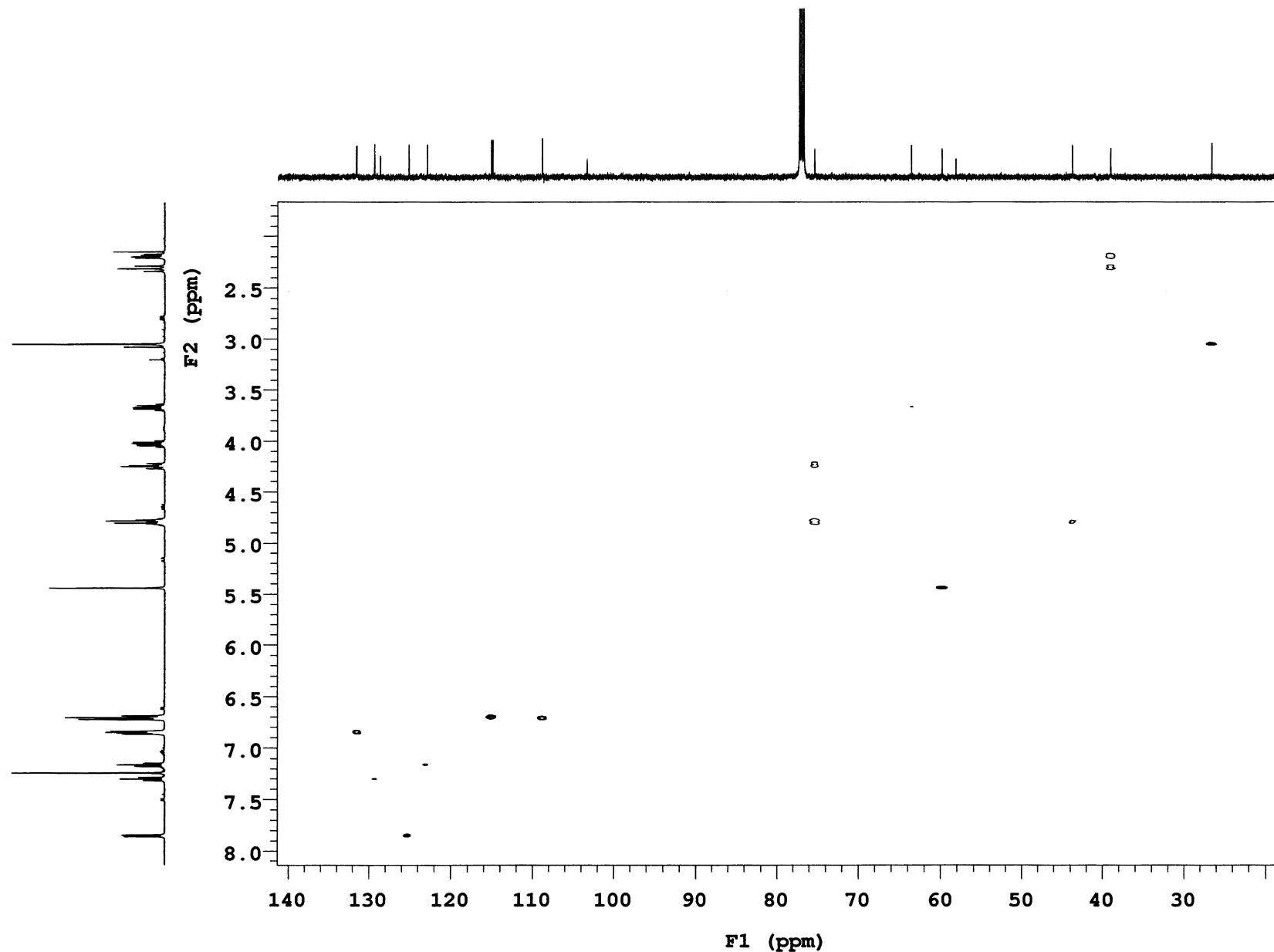


Figure S104. DEPT of 3g

PDC-03-125

Sample Name PDC-03-125
Date collected 2018-01-13Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner **vnmr2**
Operator **vnmr2**Figure S105. HSQC of **3g**

PDC-03-125

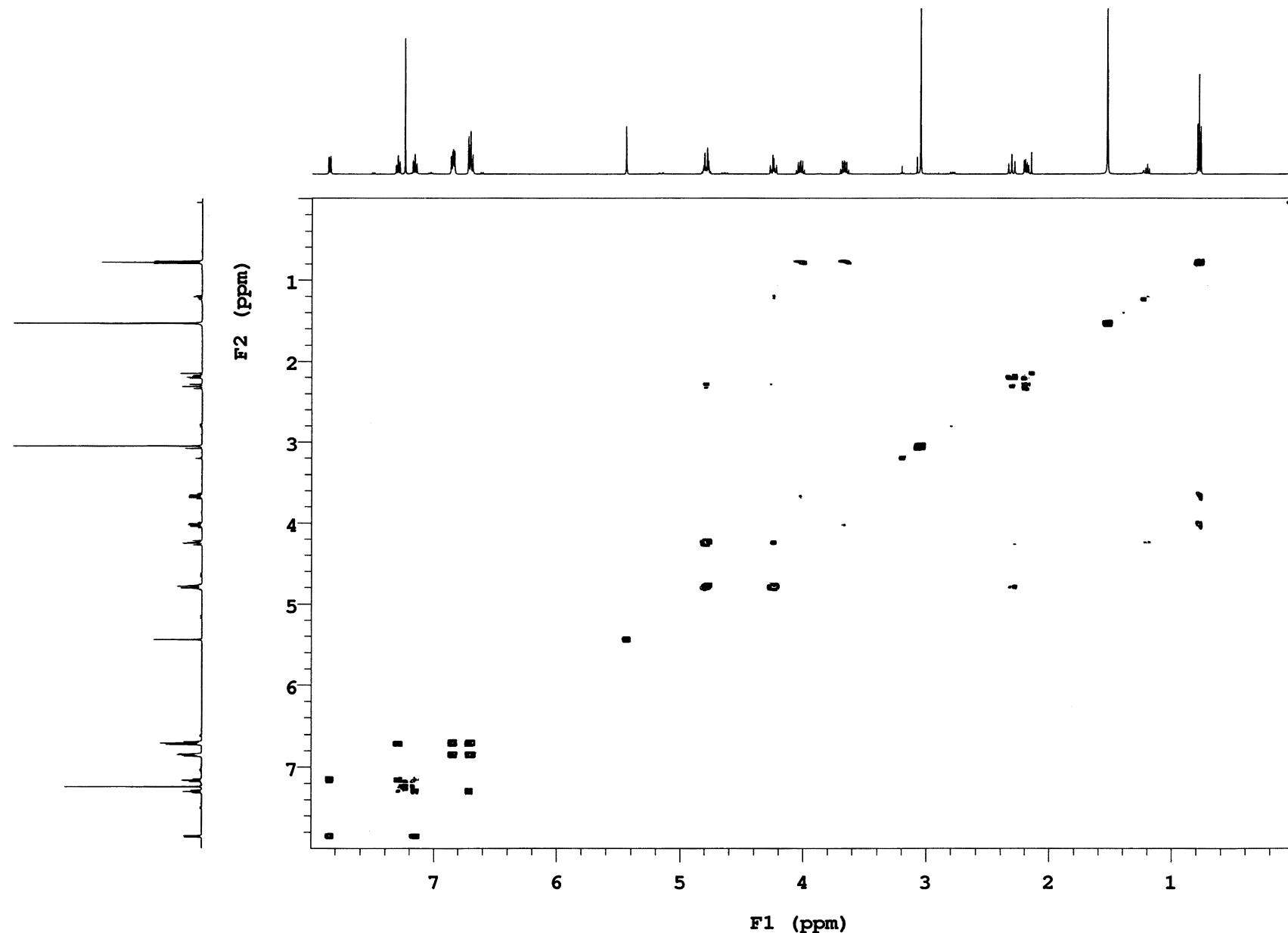
Sample Name PDC-03-125
Date collected 2018-01-13Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2

Figure S106. COSY of 3g

PDC-03-125

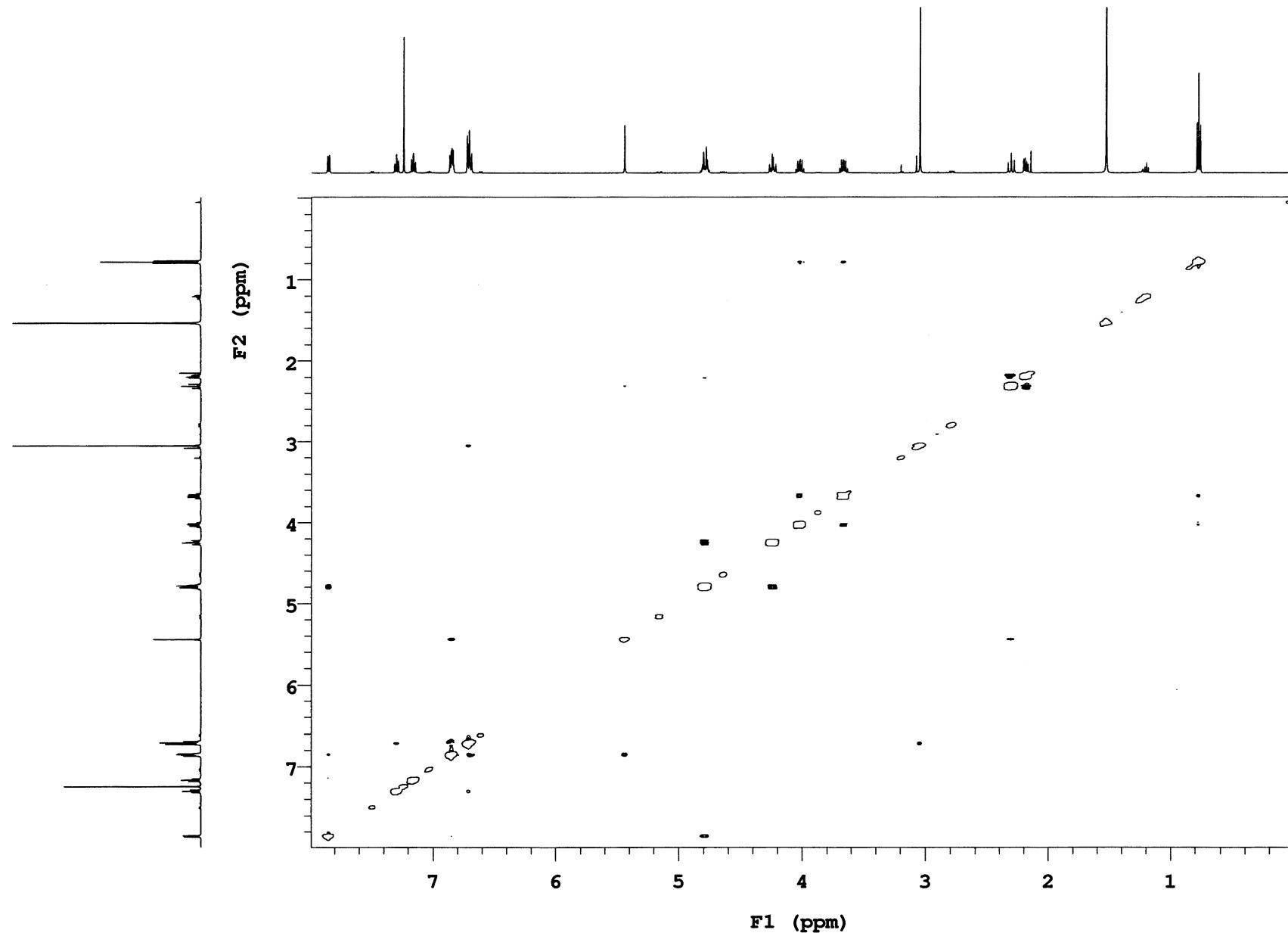
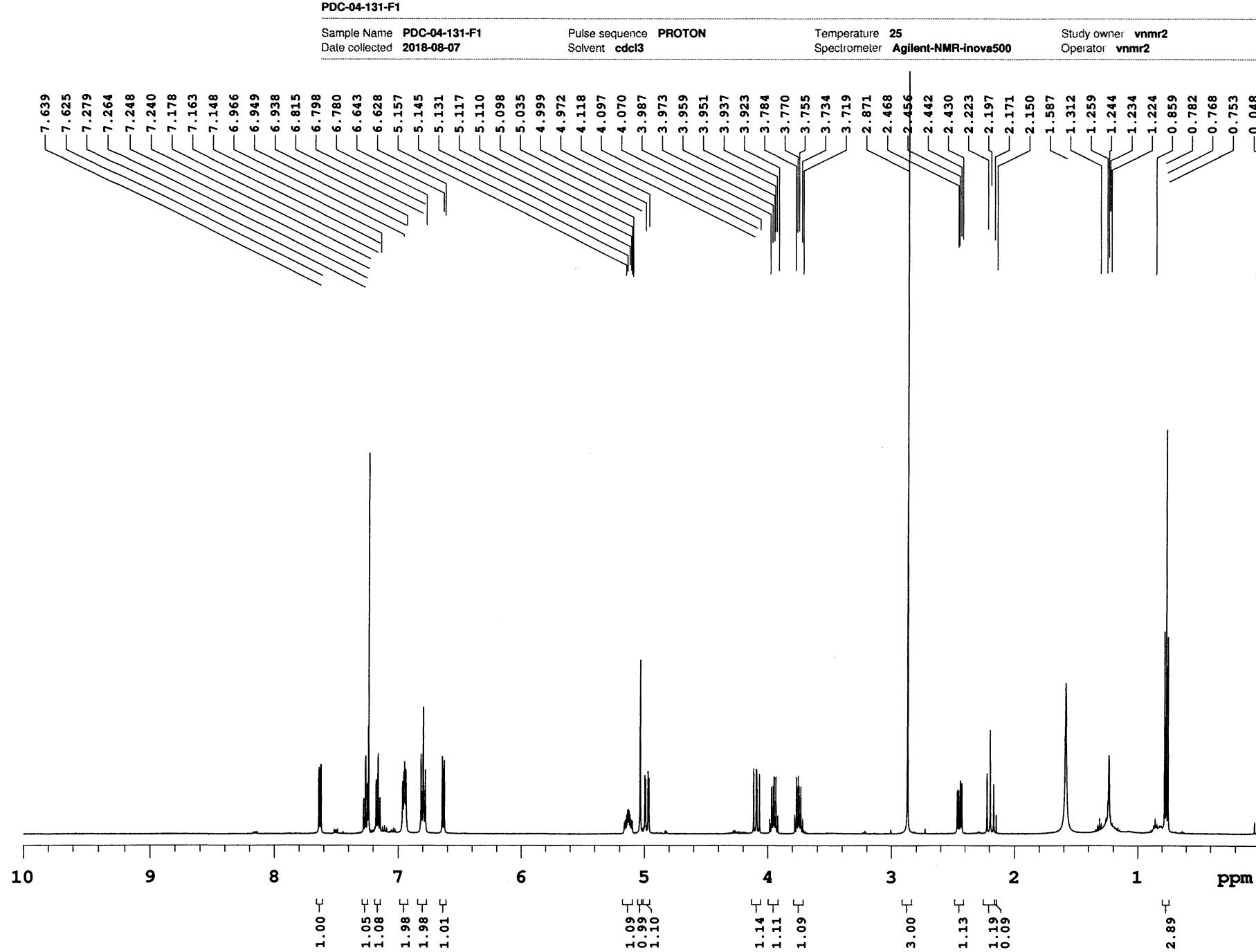
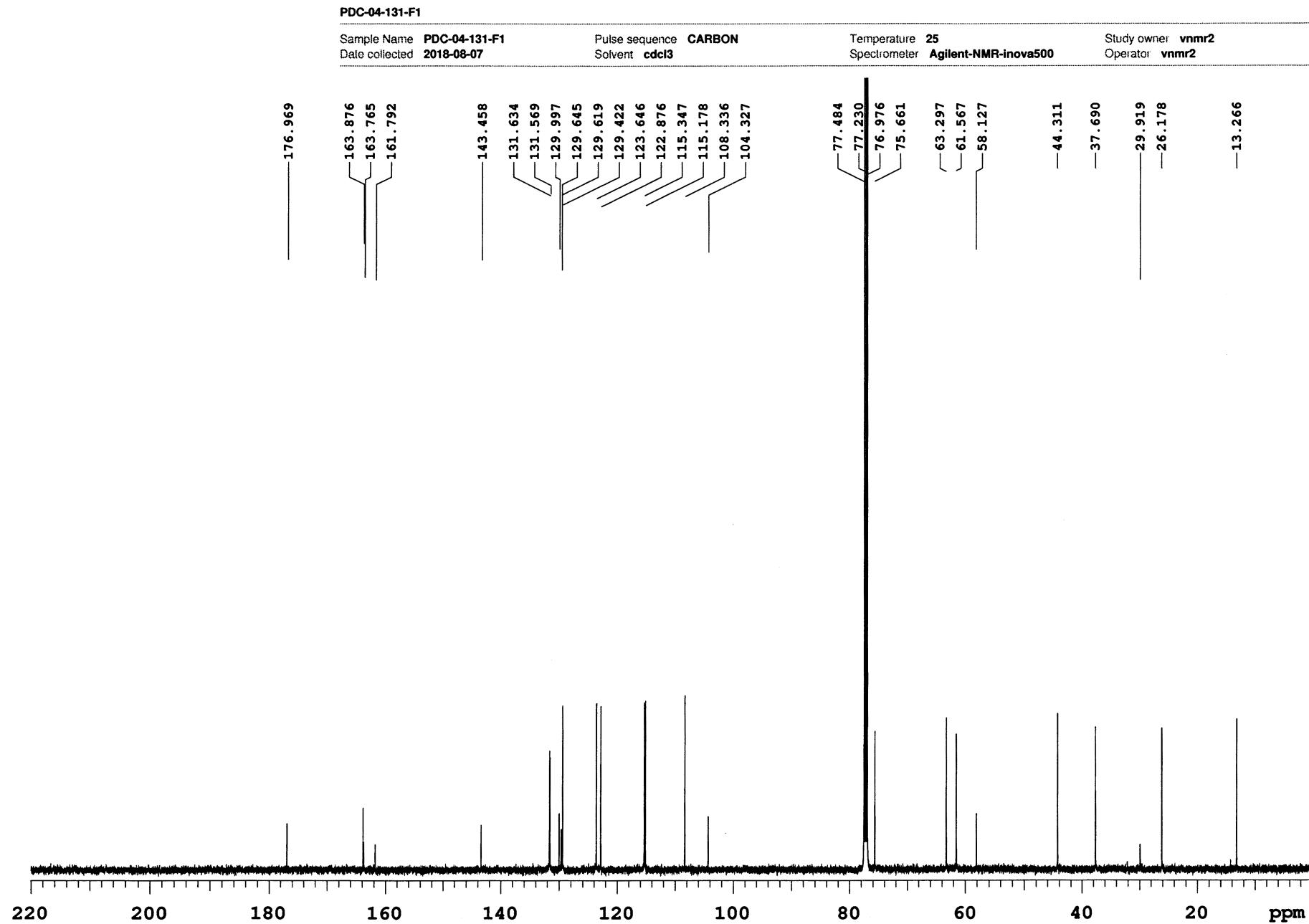
Sample Name PDC-03-125
Date collected 2018-01-13Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2

Figure S107. NOESY of 3g



Figure S109. ^{13}C NMR (CDCl₃, 125 MHz) of **4g**

PDC-04-131-F1

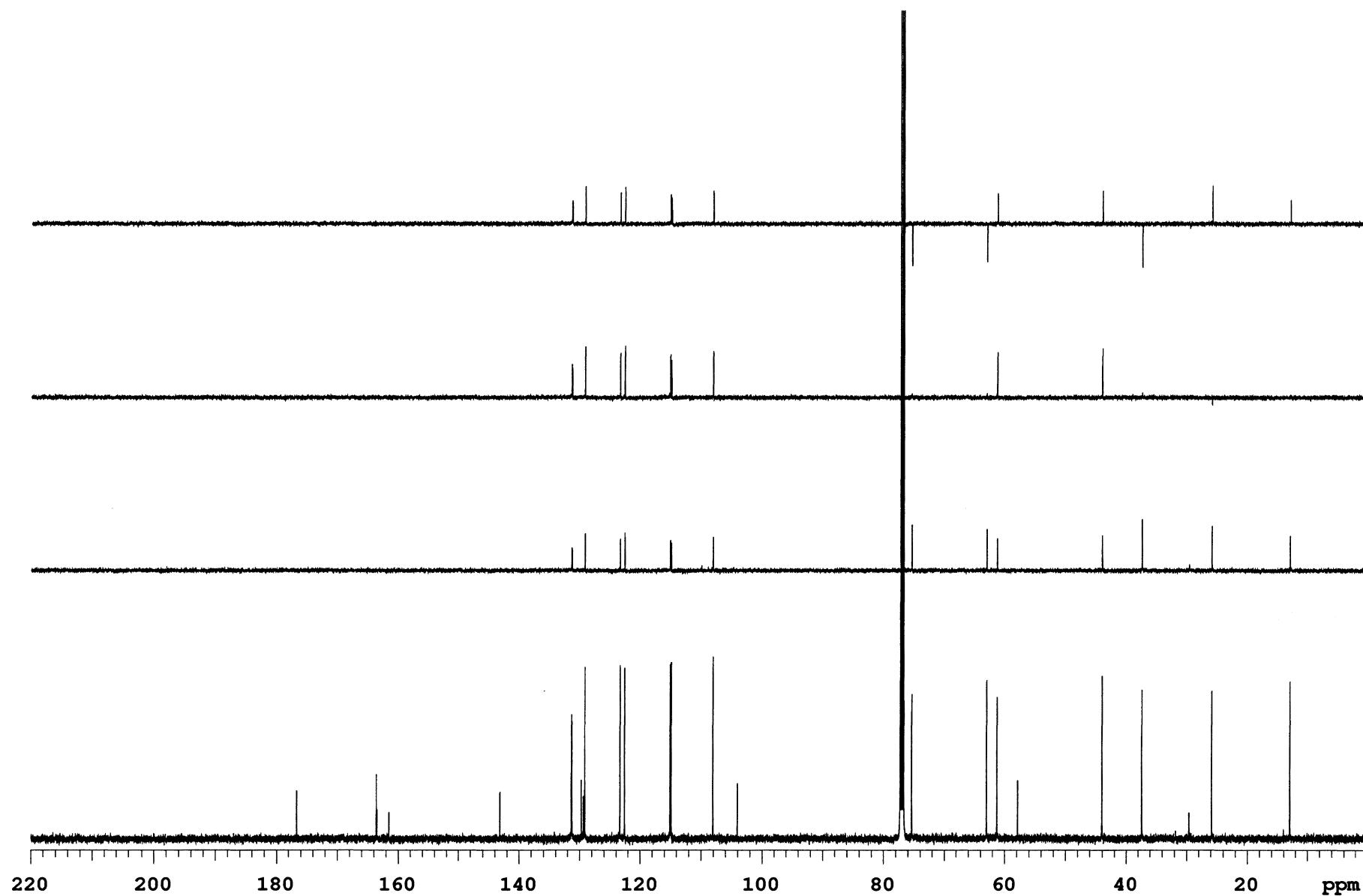
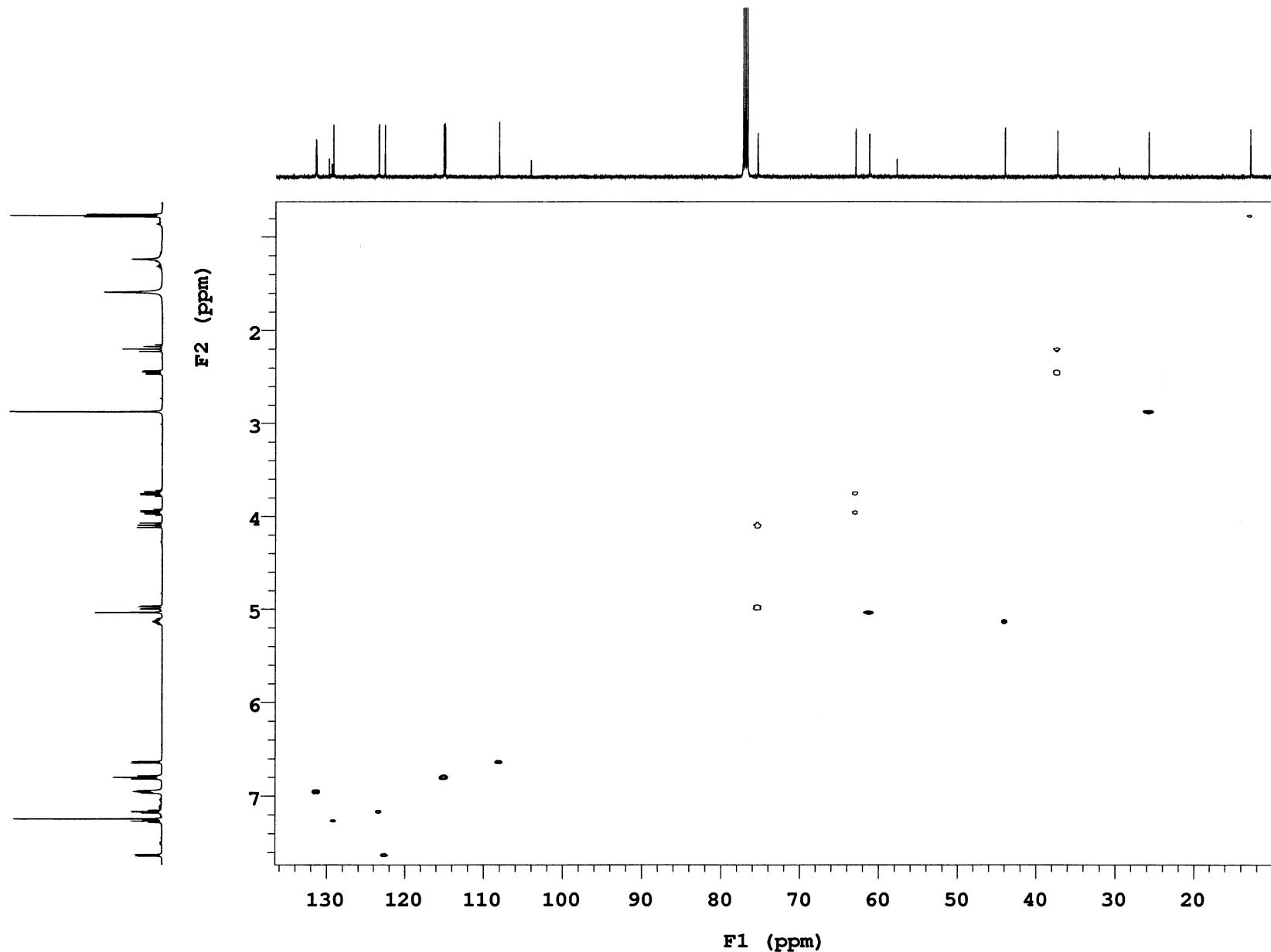
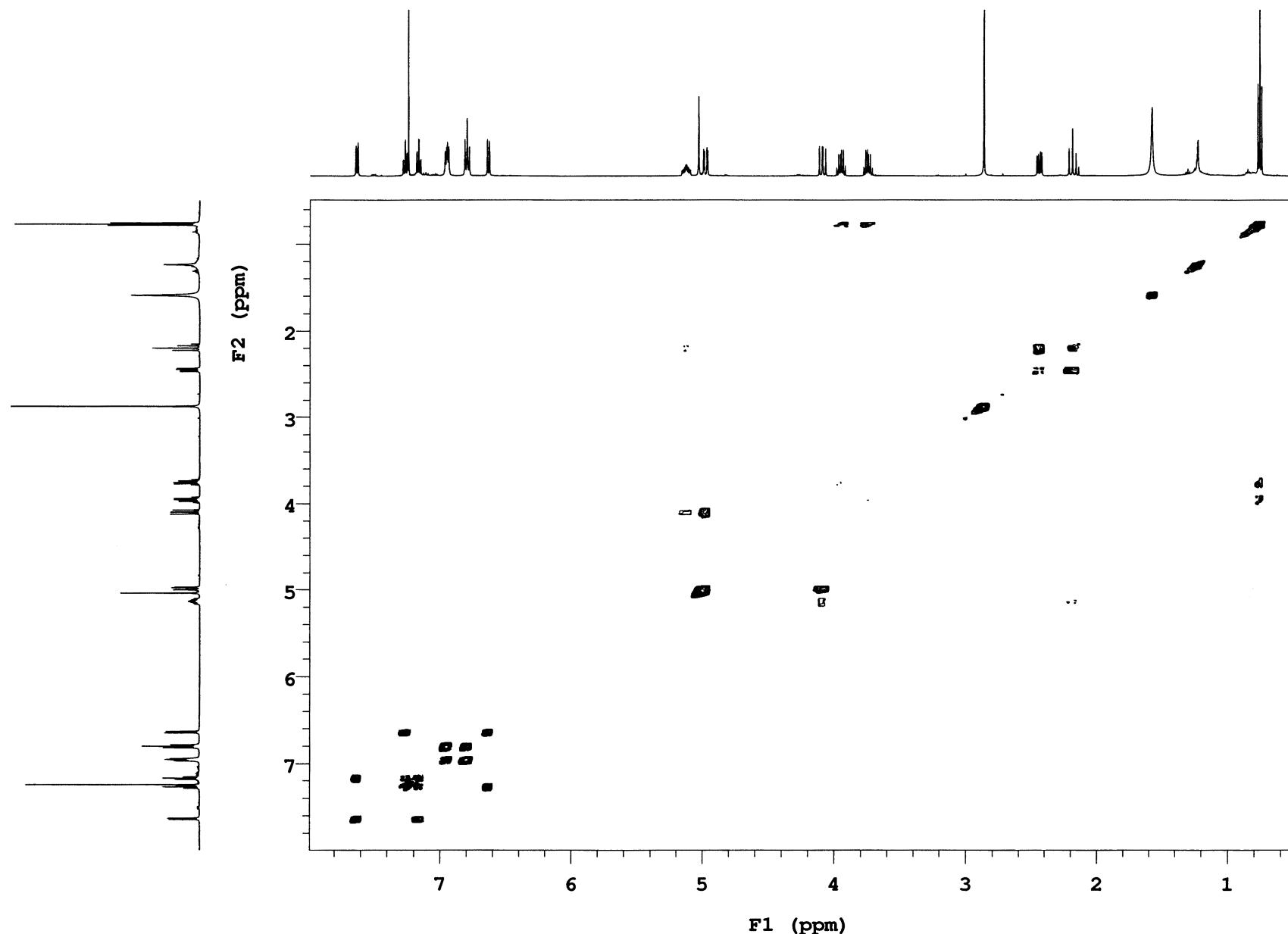
Sample Name **PDC-04-131-F1**
Date collected **2018-08-07**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Specrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**

Figure S110. DEPT of 4g

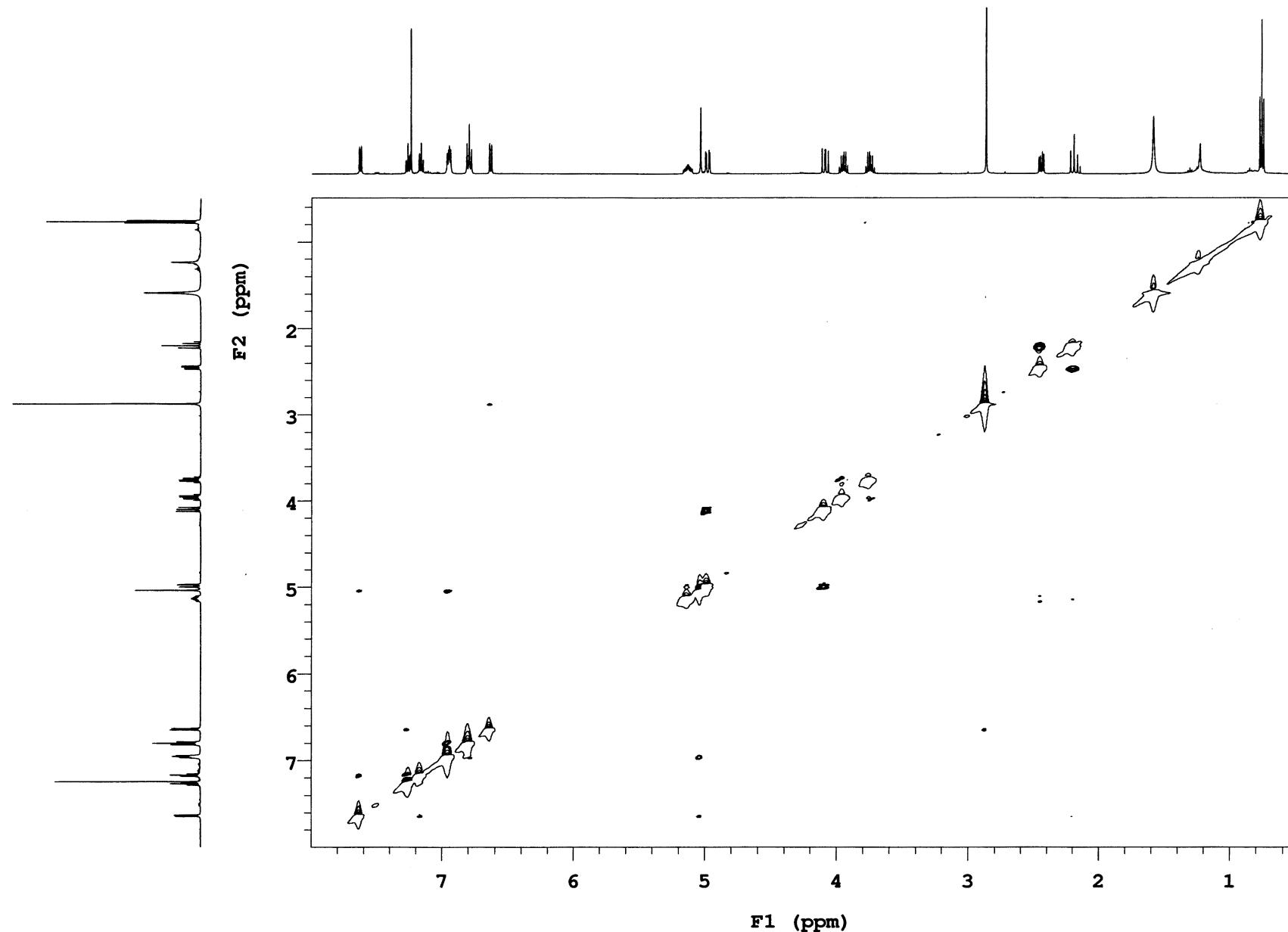
PDC-04-131-F1

Sample Name PDC-04-131-F1
Date collected 2018-08-07Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner **vnmr2**
Operator **vnmr2**Figure S111. HSQC of **4g**

PDC-04-131-F1

Sample Name PDC-04-131-F1
Date collected 2018-08-07Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Specrometer Agilent-NMR-inova500Study owner **vnmr2**
Operator **vnmr2**Figure S112. COSY of **4g**

PDC-04-131-F1

Sample Name **PDC-04-131-F1**
Date collected **2018-08-07**Pulse sequence **NOESY**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S113. NOESY of **4g**

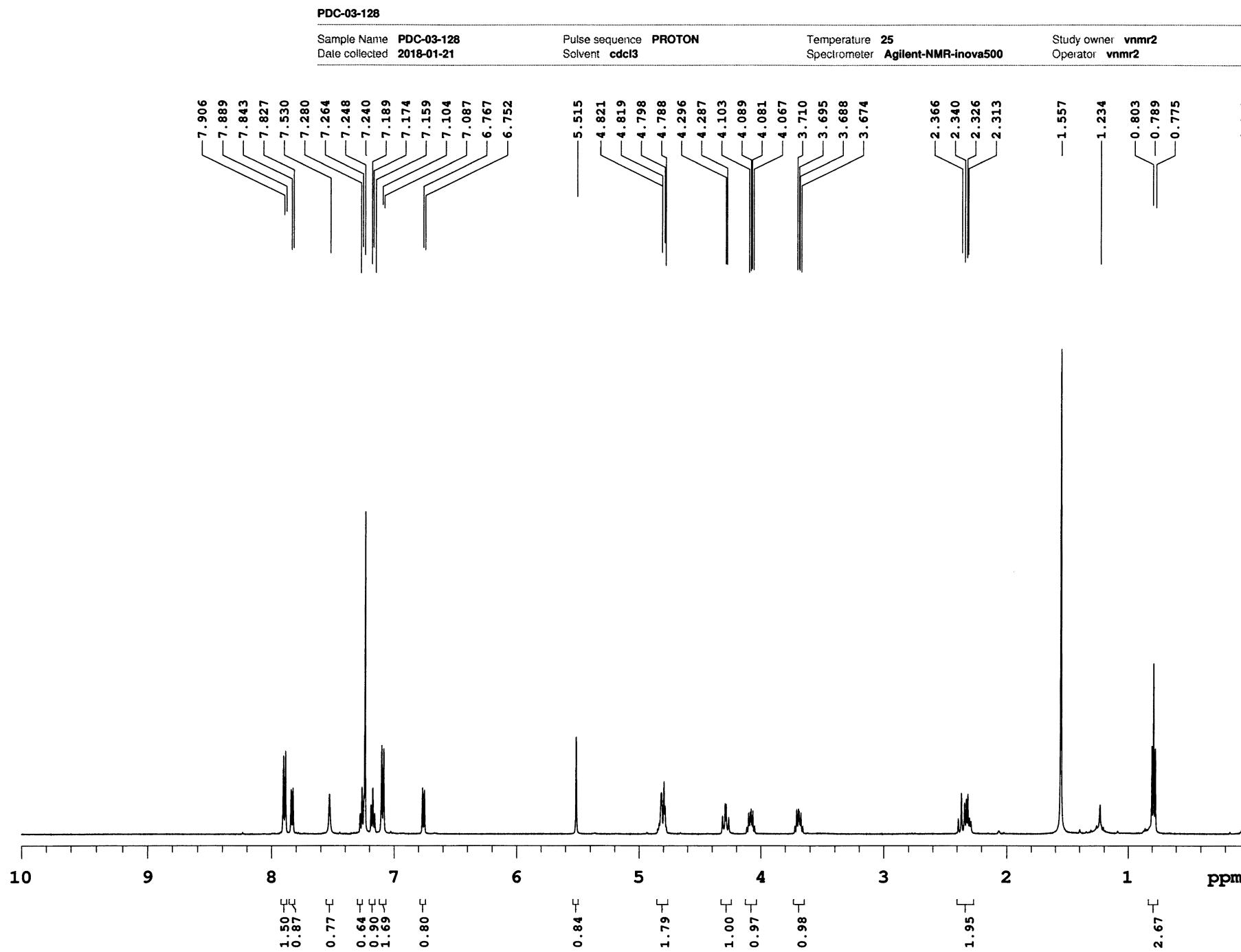
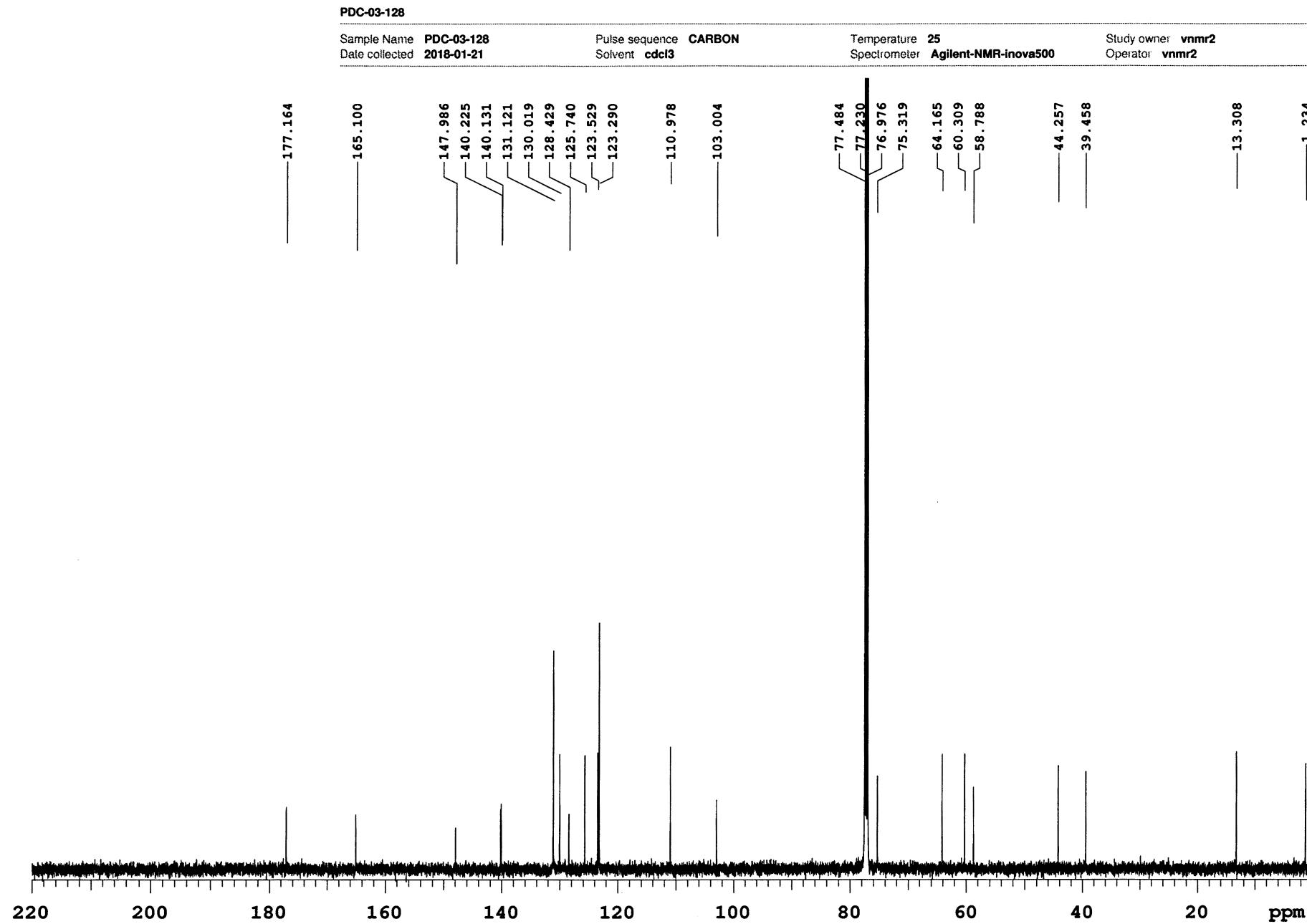


Figure S114. ¹H NMR (CDCl₃, 500 MHz) of **3h**

Data file :/home/vnmr2/vnmrsys/data/511/PDC/PDC-03-128/PROTON_05

Plot date 2018-11-21

Figure S115. ^{13}C NMR (CDCl_3 , 125 MHz) of **3h**

PDC-03-128

Sample Name **PDC-03-128**
Date collected **2018-01-21**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

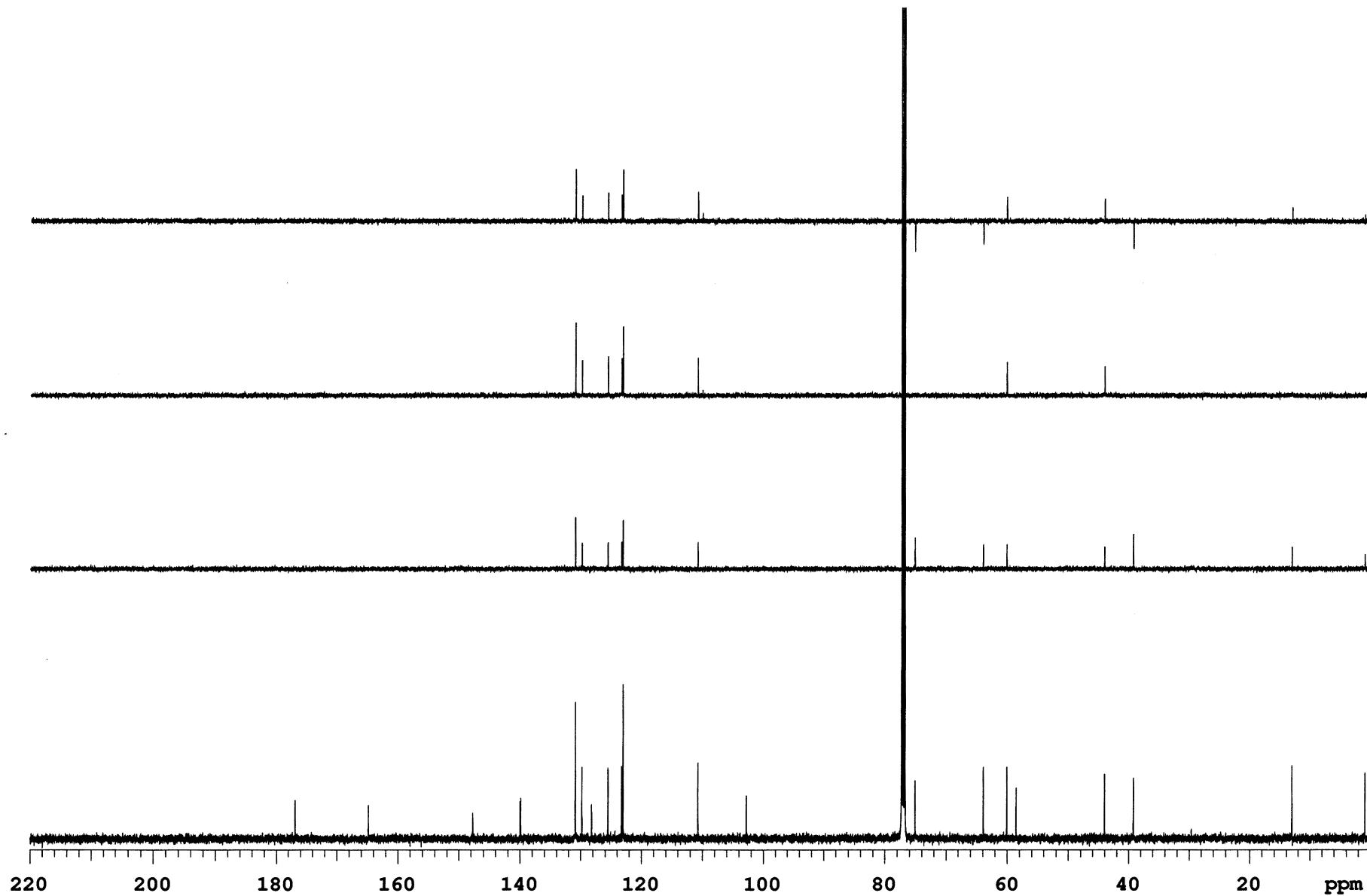


Figure S116. DEPT of **3h**

PDC-03-128

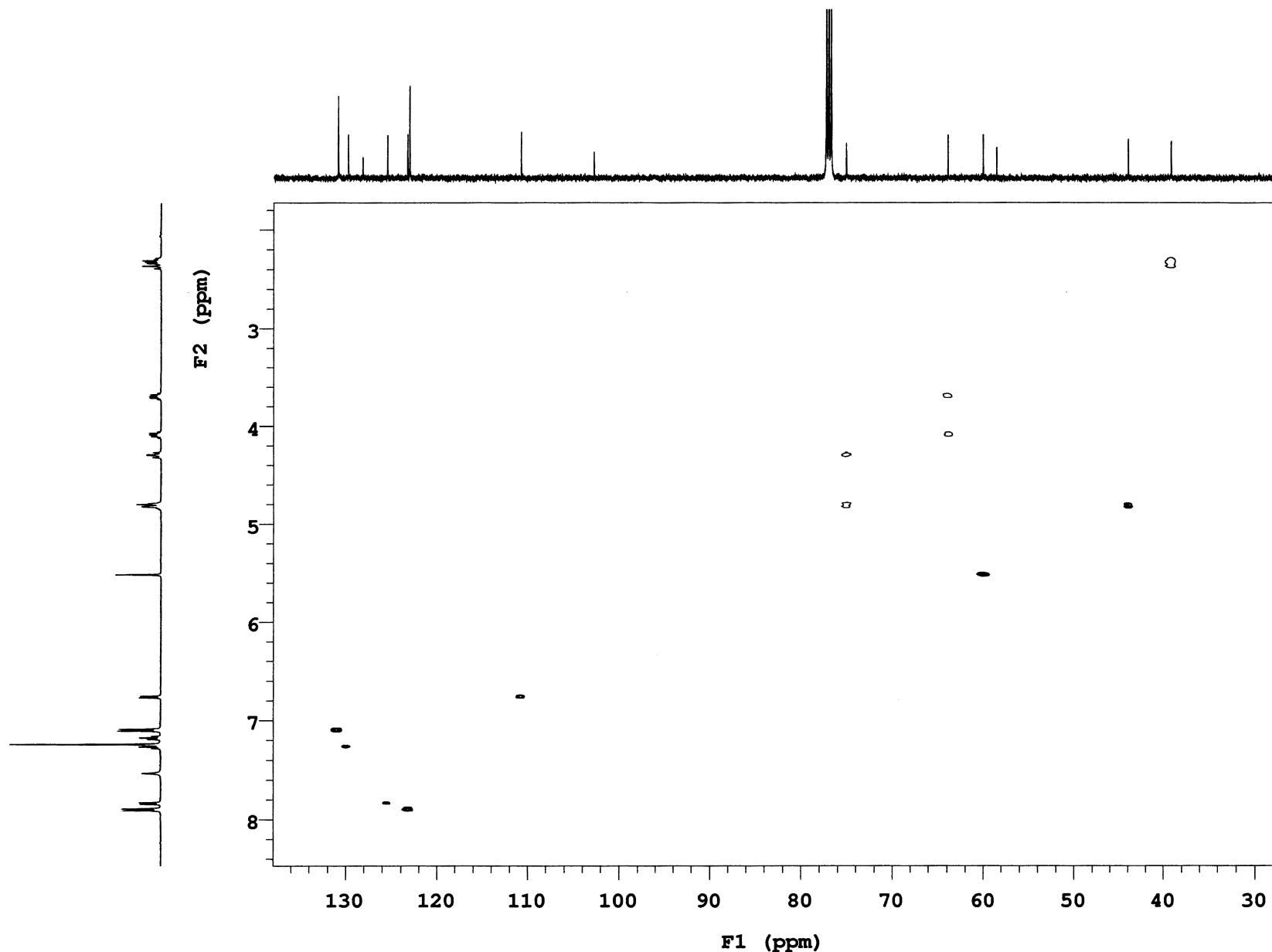
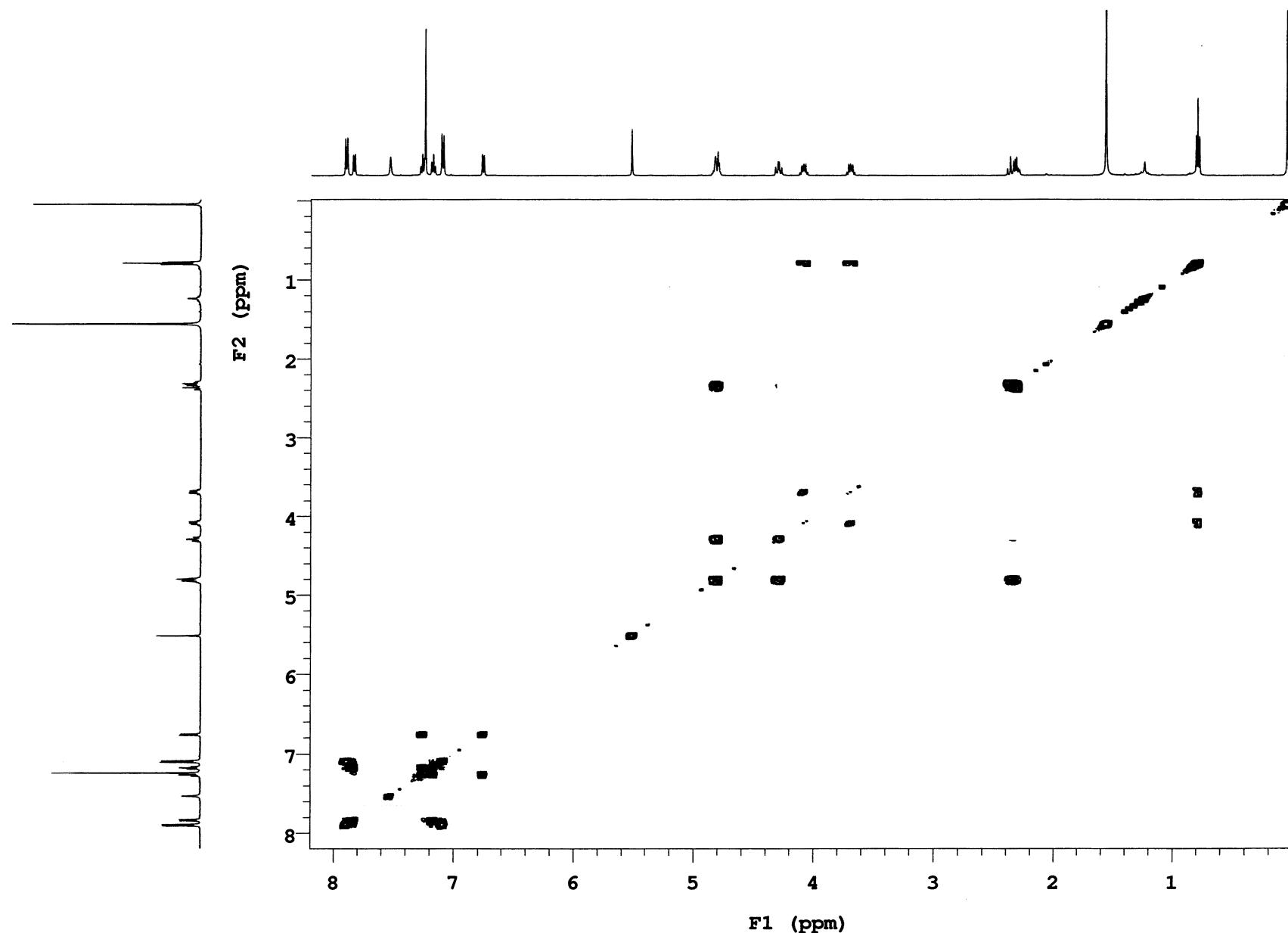
Sample Name PDC-03-128
Date collected 2018-01-22Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S117. HSQC of 3h

PDC-03-128

Sample Name PDC-03-128
Date collected 2018-01-22Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S118. COSY of **3h**

PDC-03-128

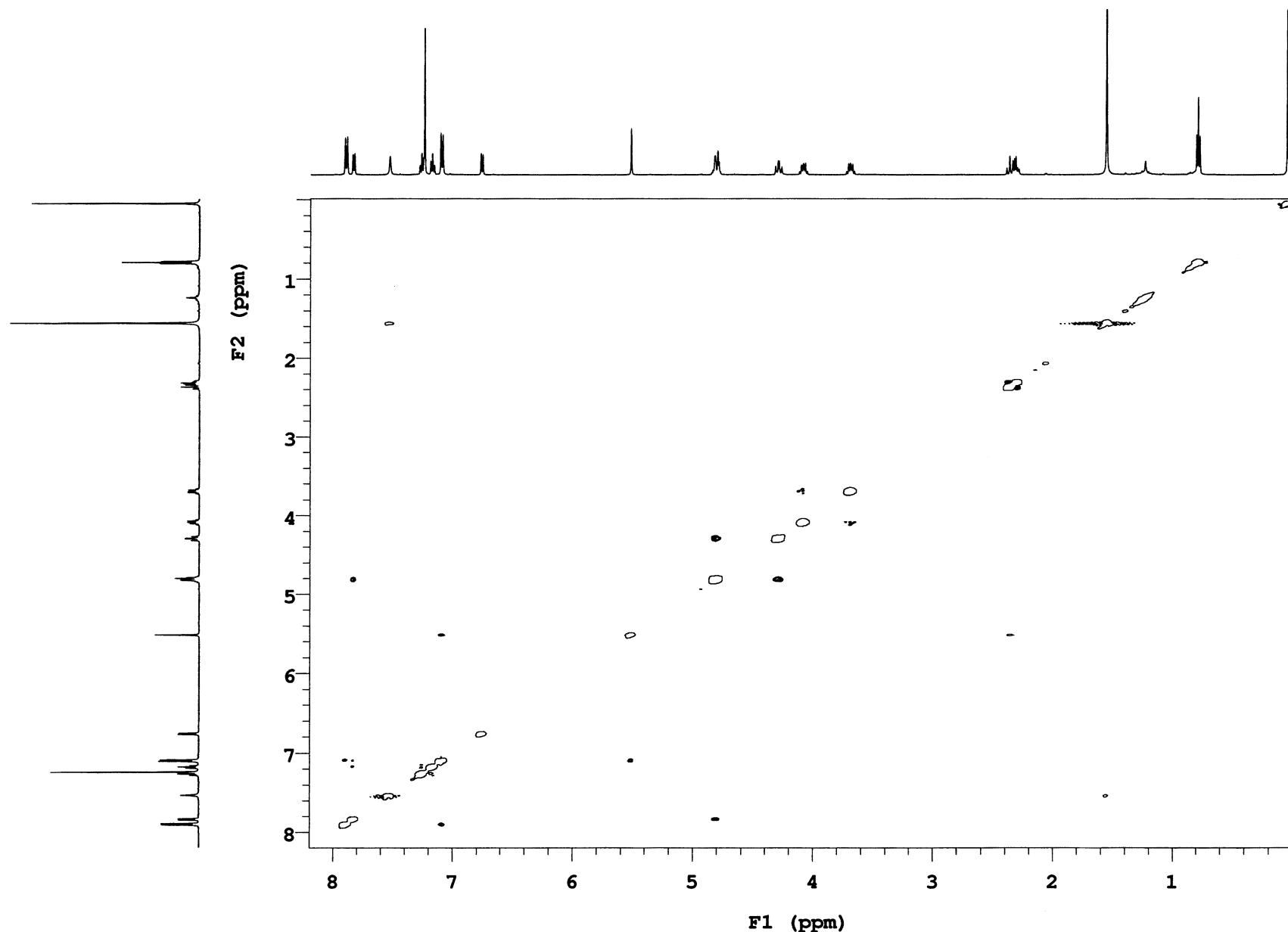
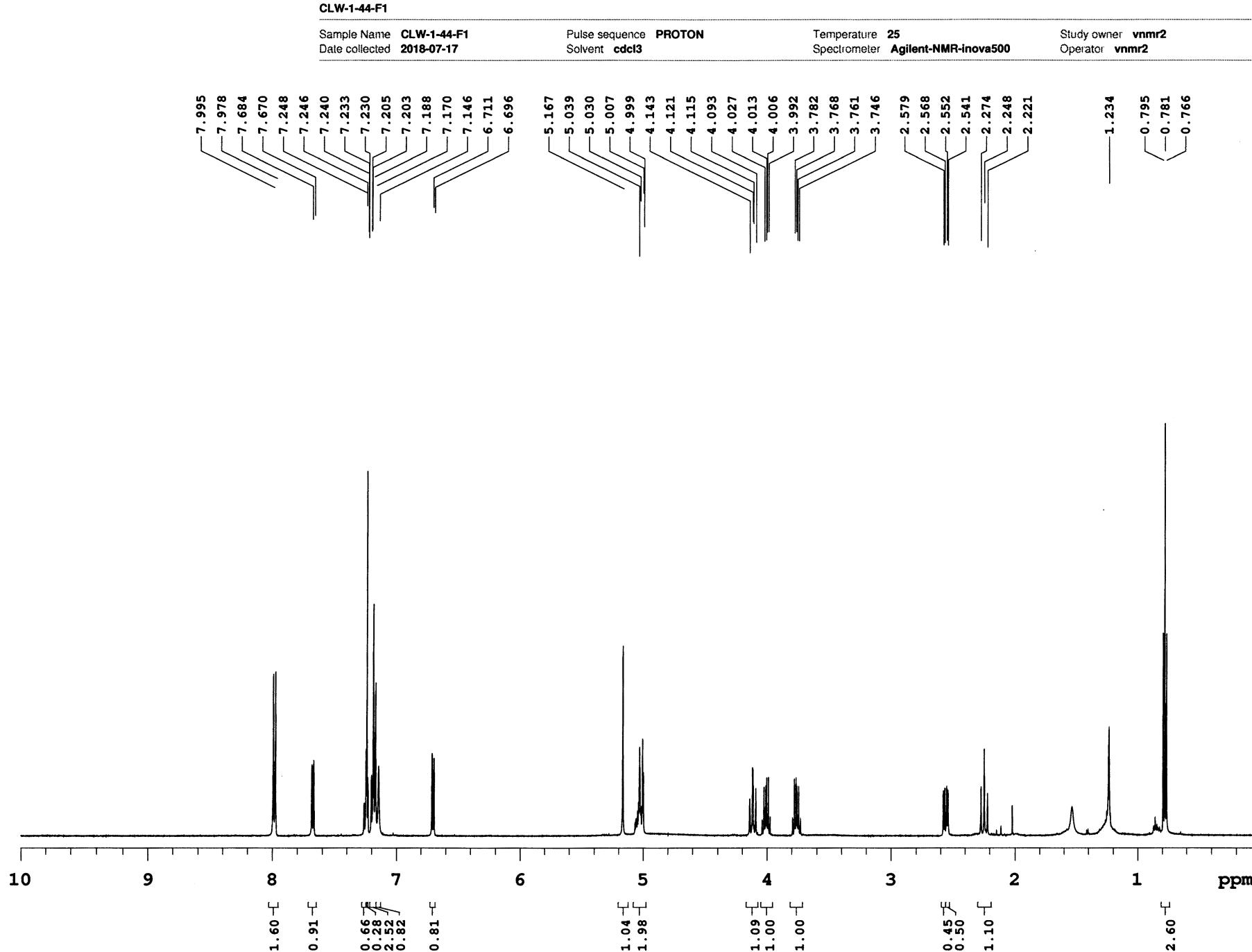
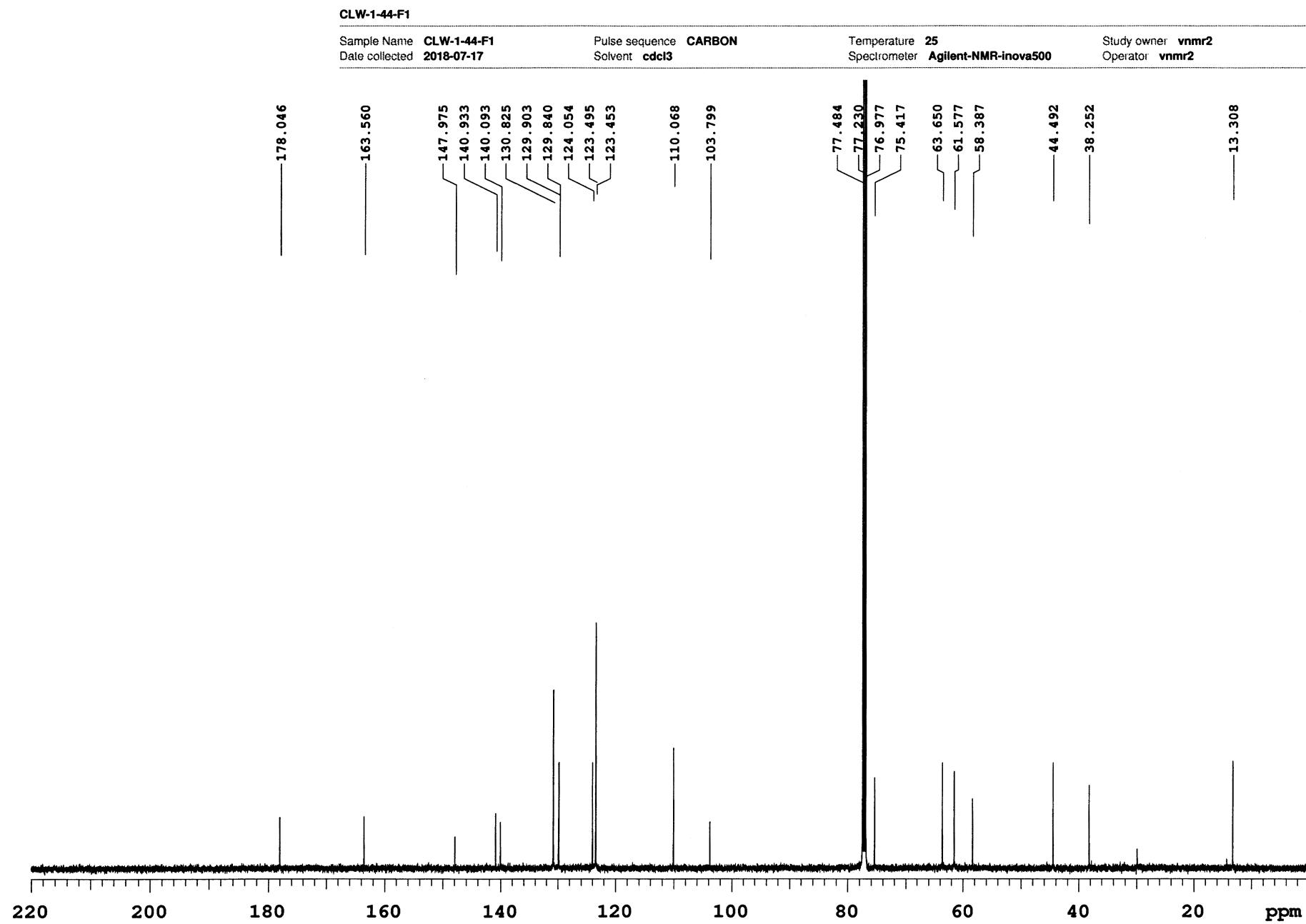
Sample Name PDC-03-128
Date collected 2018-01-22Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S119. NOESY of 3h

Figure S120. ^1H NMR (CDCl₃, 500 MHz) of **4h**

Figure S121. ¹³C NMR (CDCl₃, 125 MHz) of **4h**

CLW-1-44-F1

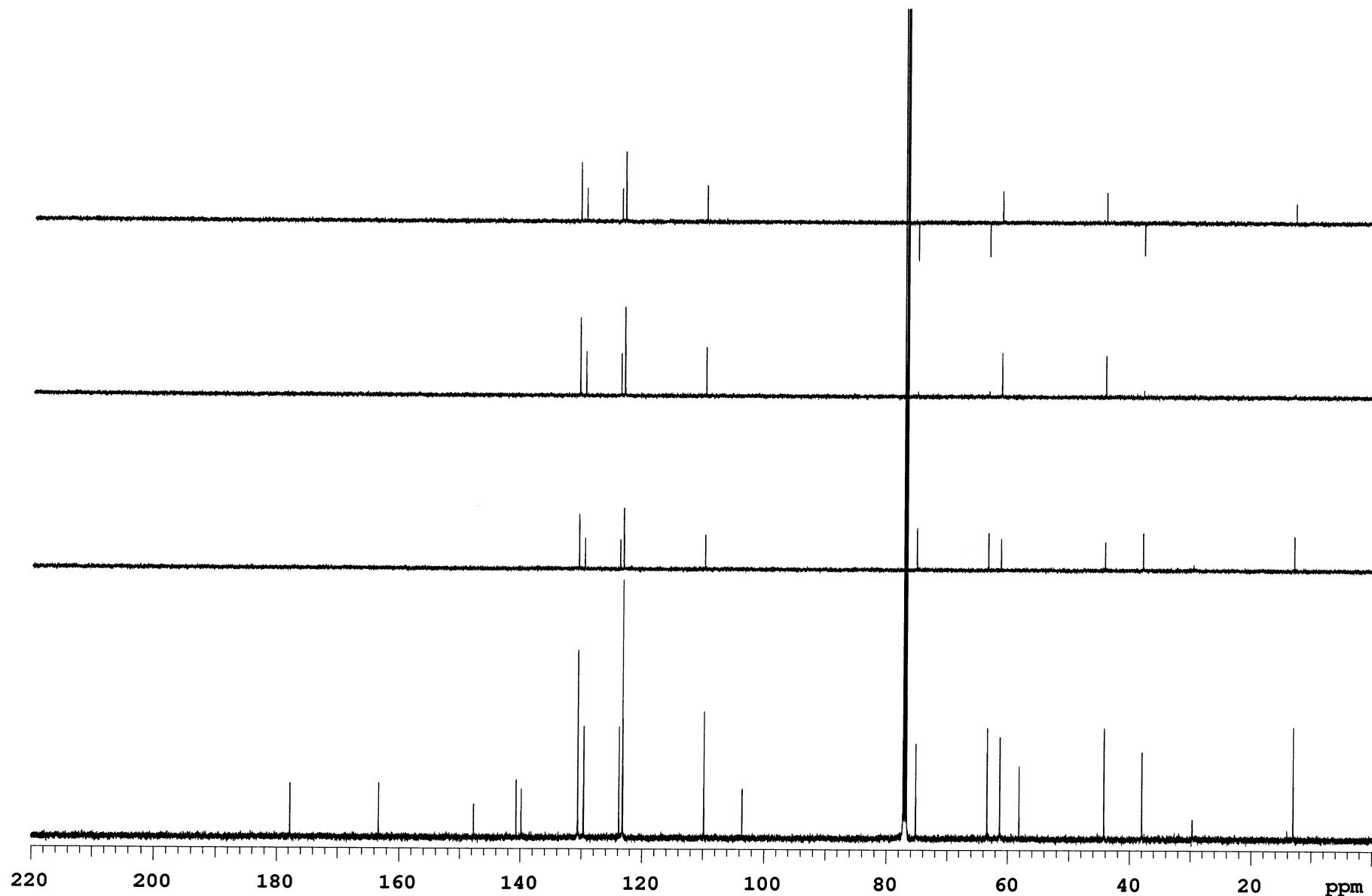
Sample Name **CLW-1-44-F1**
Date collected **2018-07-18**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**

Figure S122. DEPT of 4h

CLW-1-44-F1

Sample Name CLW-1-44-F1 Date collected 2018-07-18 Pulse sequence gHSQC Solvent *cdcl*3 Temperature 25 Spectrometer Agilent-NMR-inova500 Study owner vnmr2 Operator vnmr2

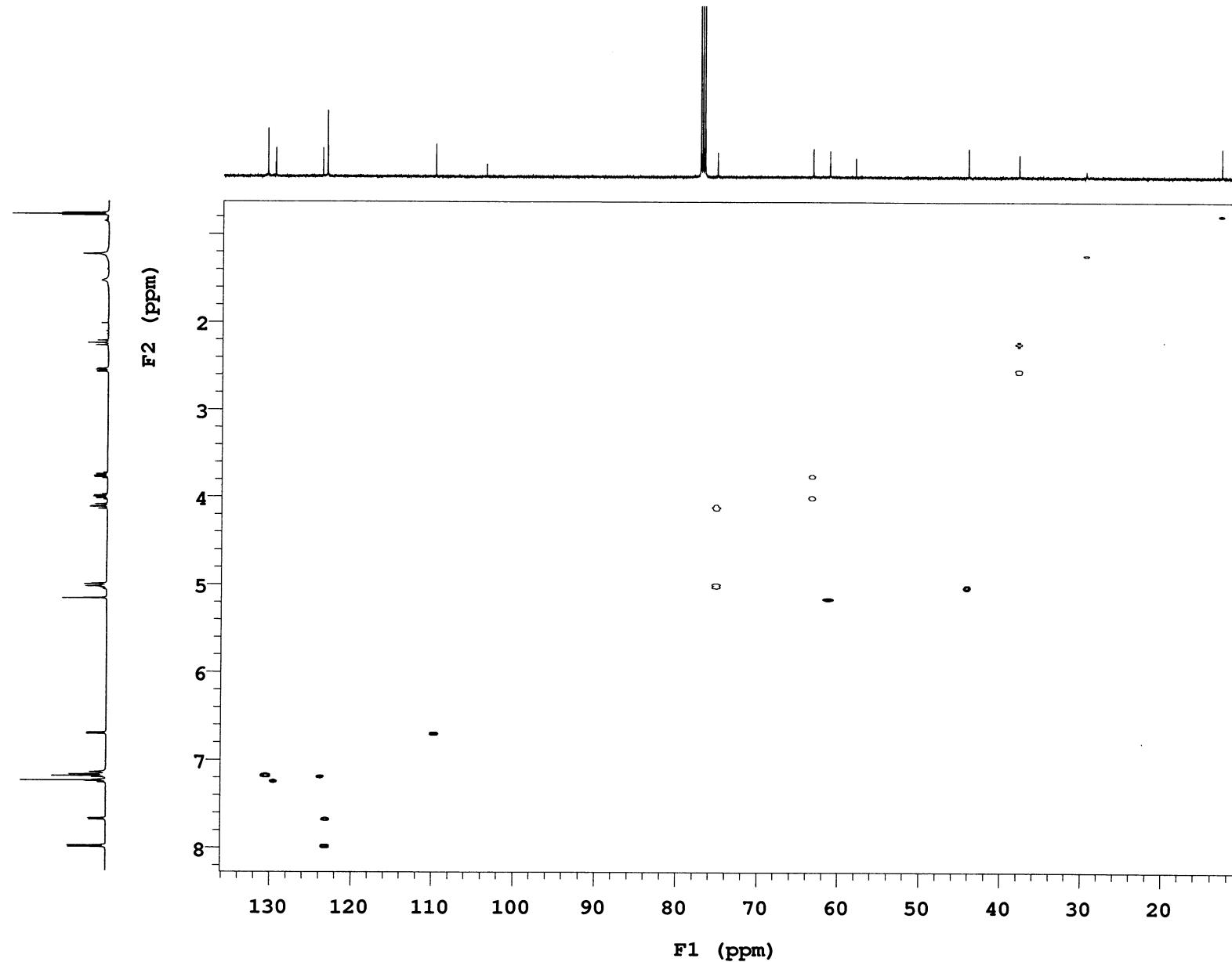
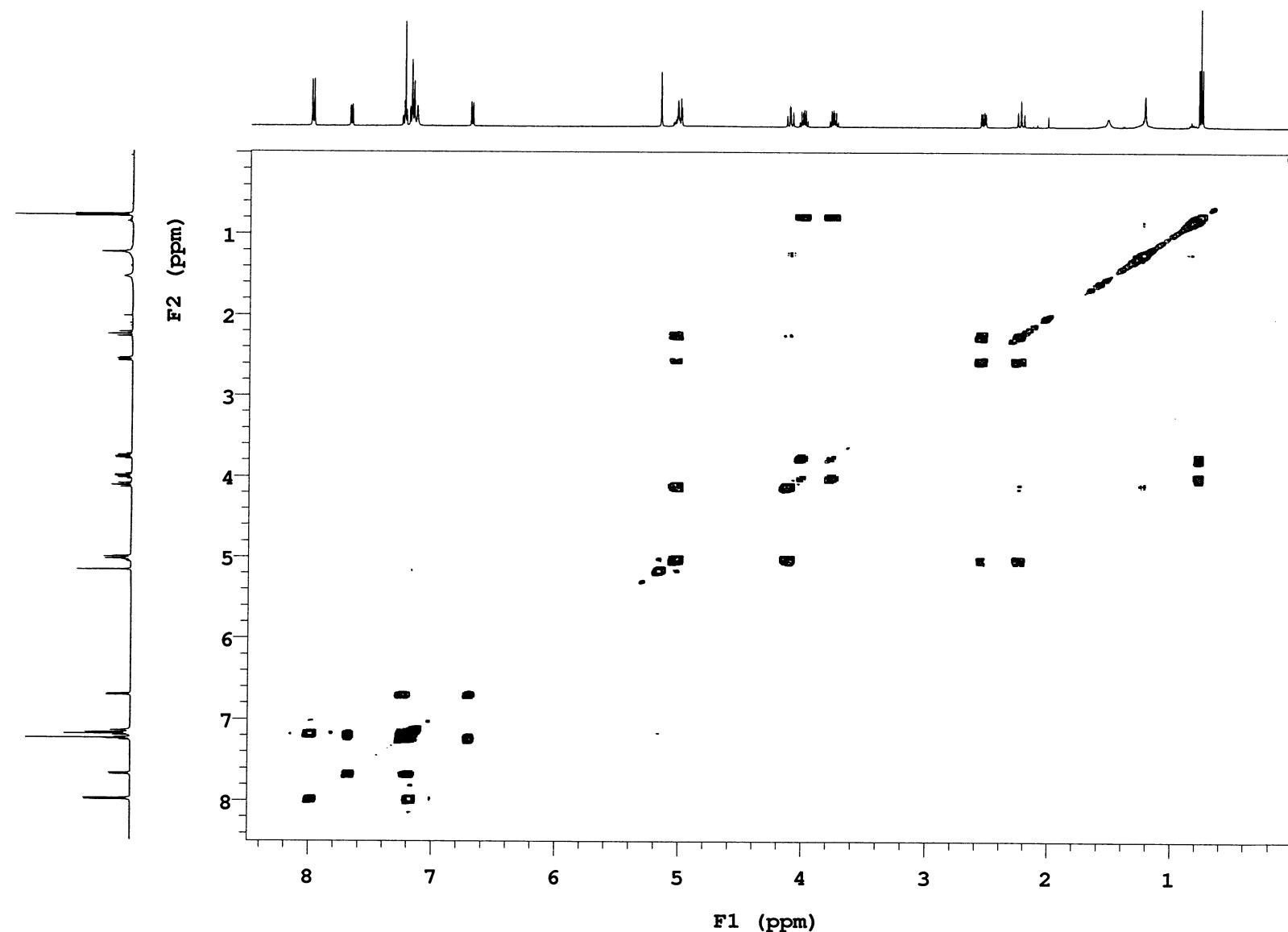


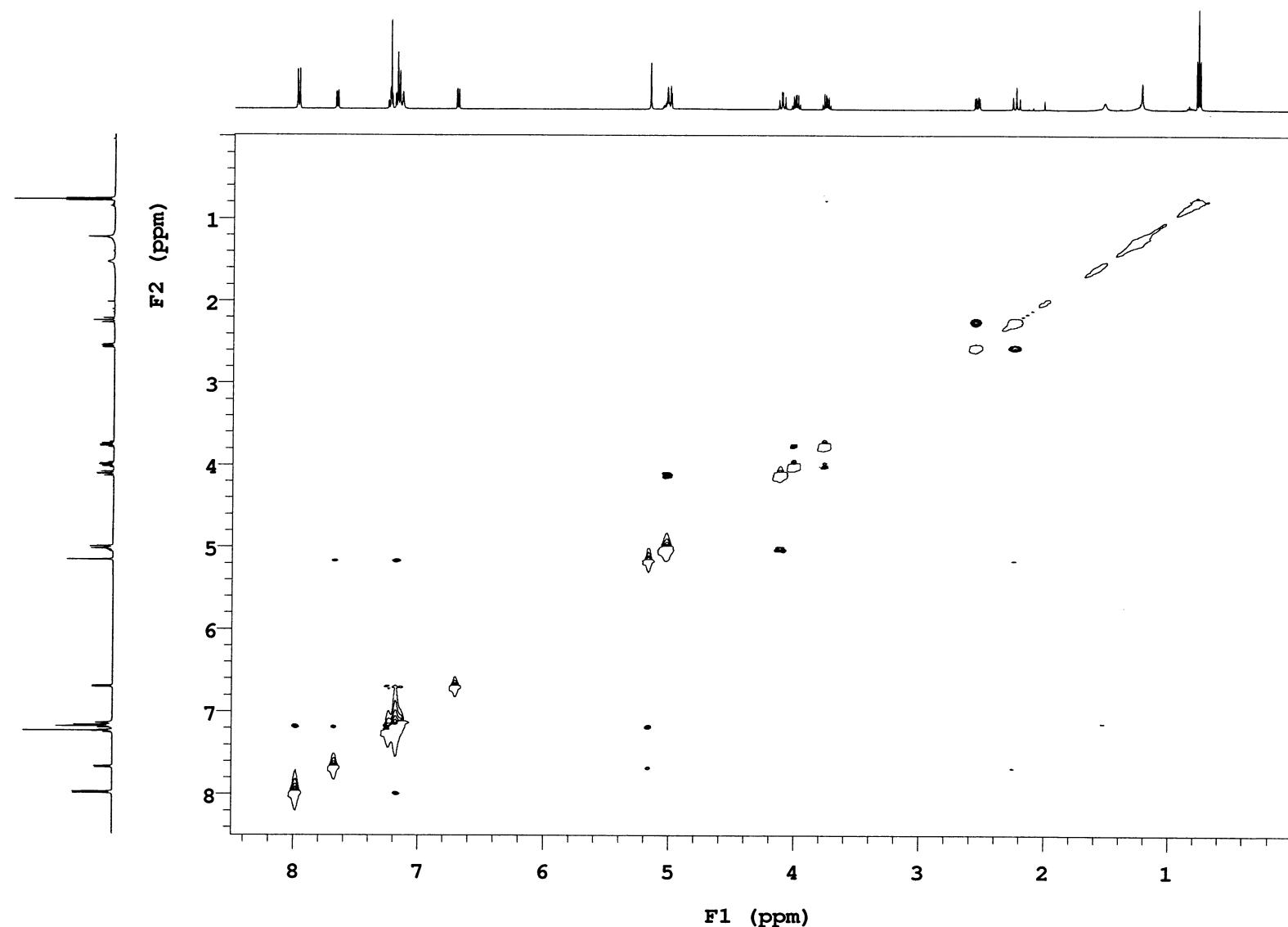
Figure S123. HSQC of 4h

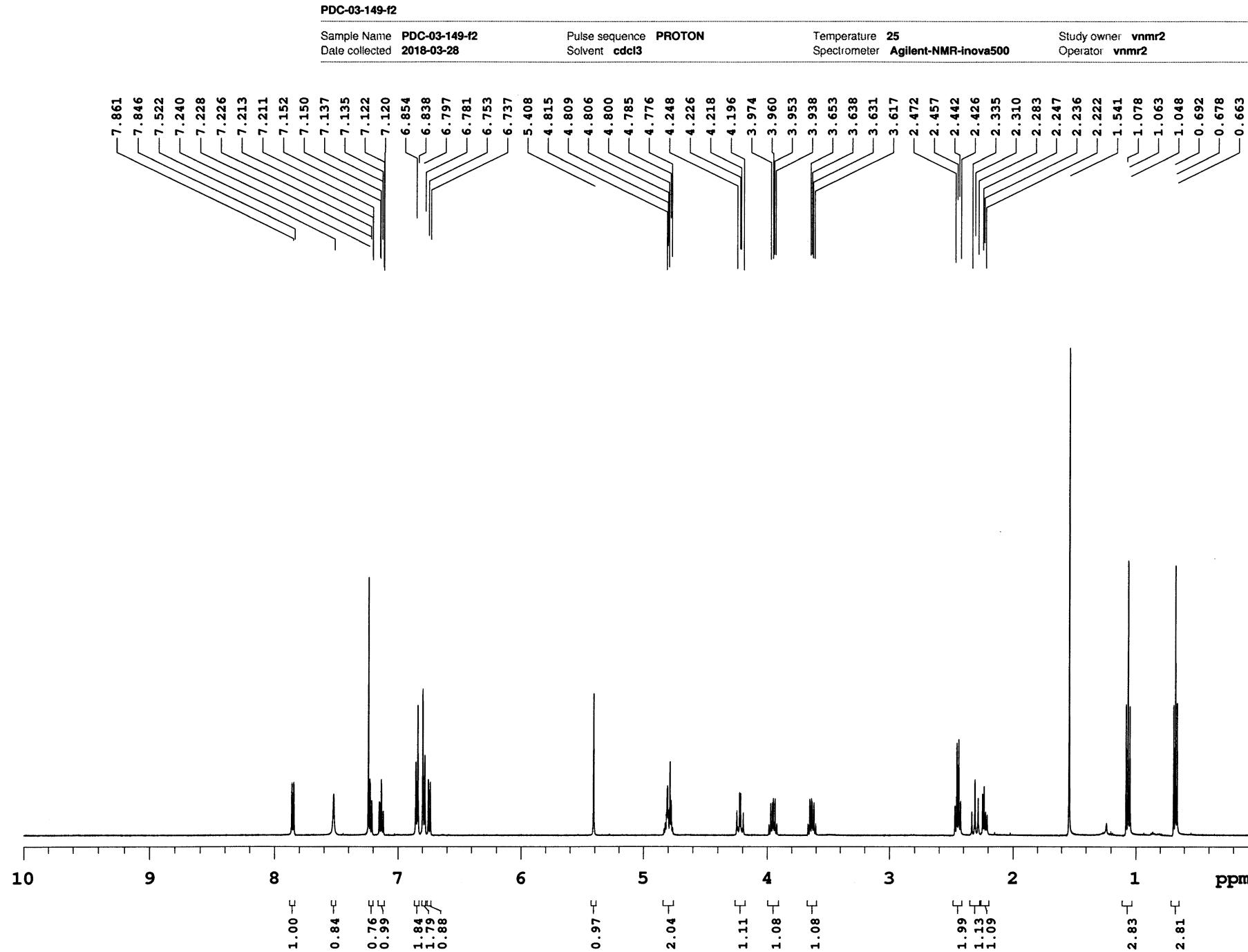
CLW-1-44-F1

Sample Name CLW-1-44-F1 Pulse sequence gCOSY
Date collected 2018-07-18 Solvent CDCl_3 Temperature 25
Temperature 25 Spectrometer Agilent-NMR-inova500
Study owner vnmr2
Operator vnmr2

Figure S124. COSY of **4h**

CLW-1-44-F1

Sample Name CLW-1-44-F1
Date collected 2018-07-18Pulse sequence NOESY
Solvent CDCl_3 Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S125. NOESY of **4h**



PDC-03-149-f2

Sample Name PDC-03-149-f2
Date collected 2018-03-28

Pulse sequence CARBON
Solvent *cdcl*3

Temperature 25
25 Spectrometer Agilent-NMR-inova500

Study owner vnmr2
Operator vnmr2

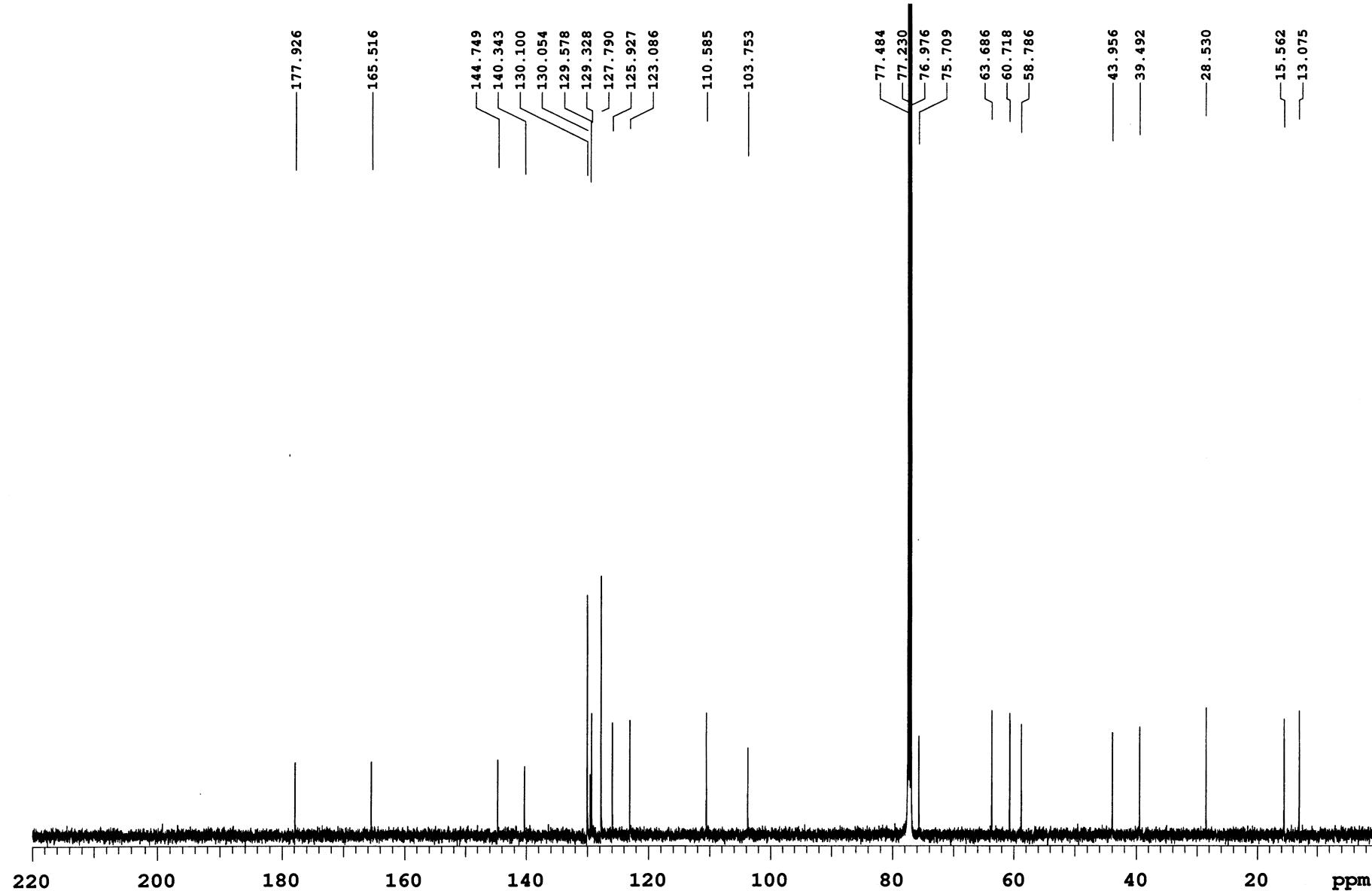
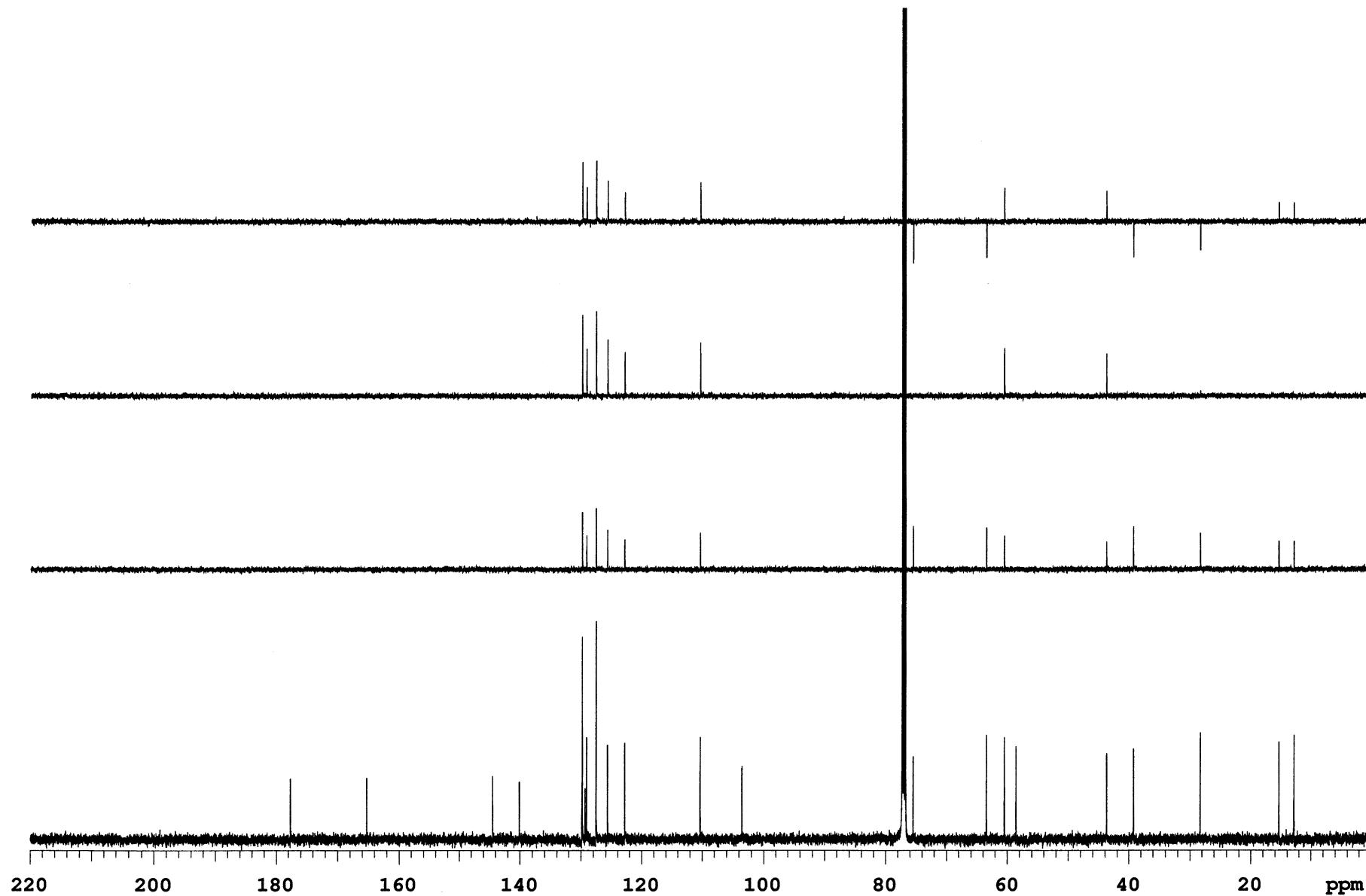


Figure S127. 13C NMR (*CDCl*3, 125 MHz) of **3i**

PDC-03-149-f2

Sample Name **PDC-03-149-f2**
Date collected **2018-03-28**Pulse sequence **DEPT**
Solvent **cdcl3**Temperature **25**
Specrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S128. DEPT of **3i**

PDC-03-149-f2

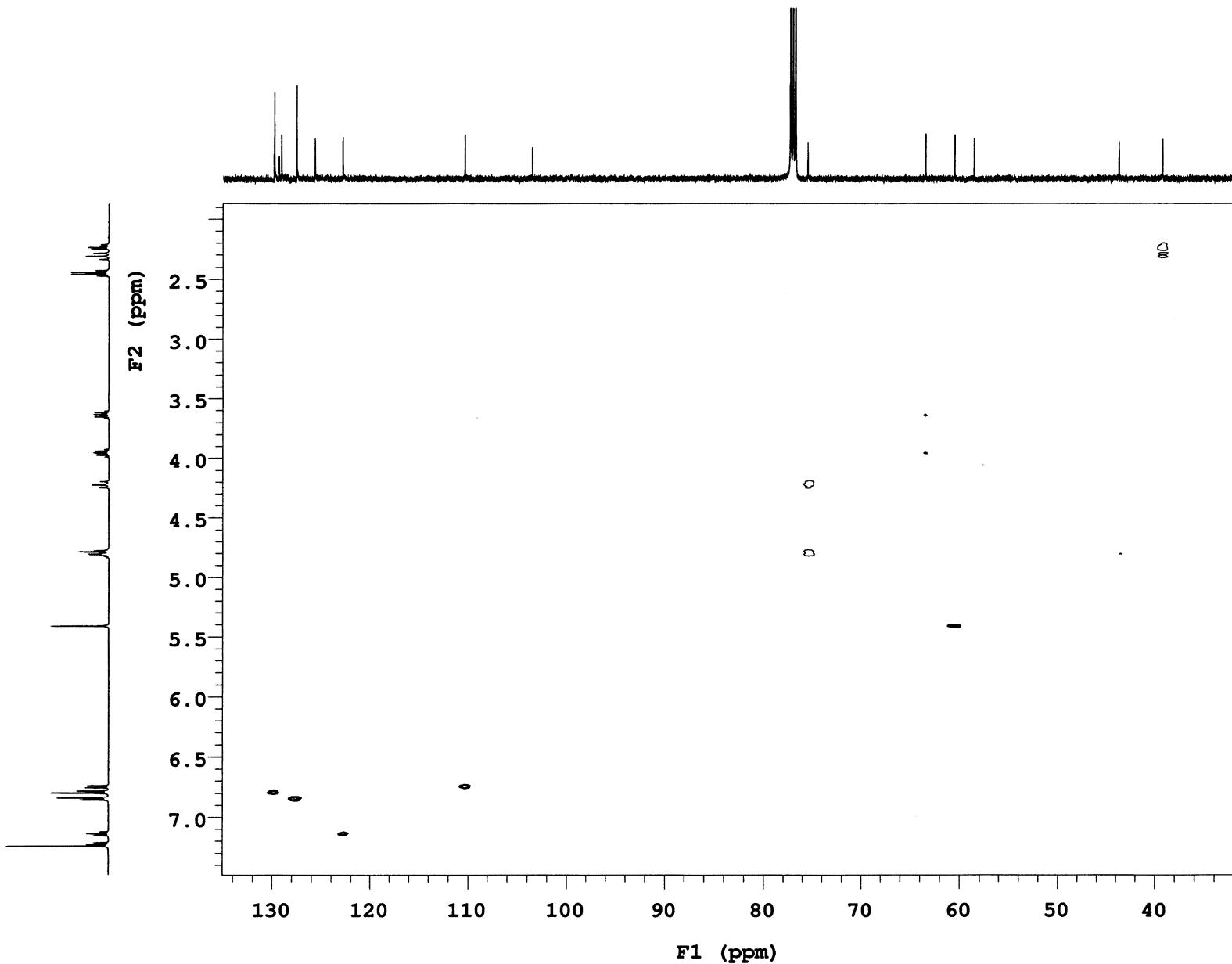
Sample Name **PDC-03-149-f2**
Date collected **2018-03-28**Pulse sequence **gHSQC**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**

Figure S129. HSQC of 3i

PDC-03-149-f2

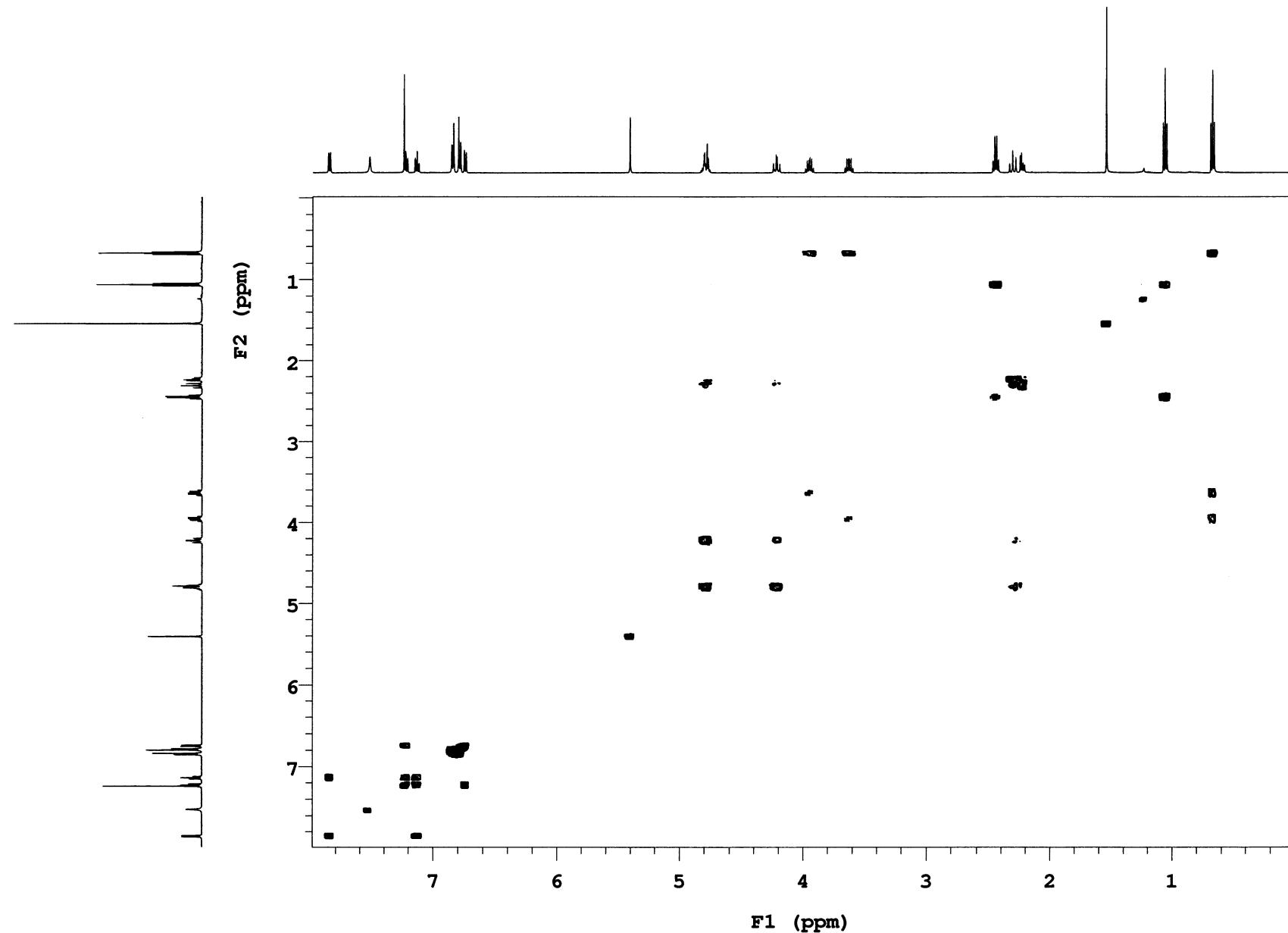
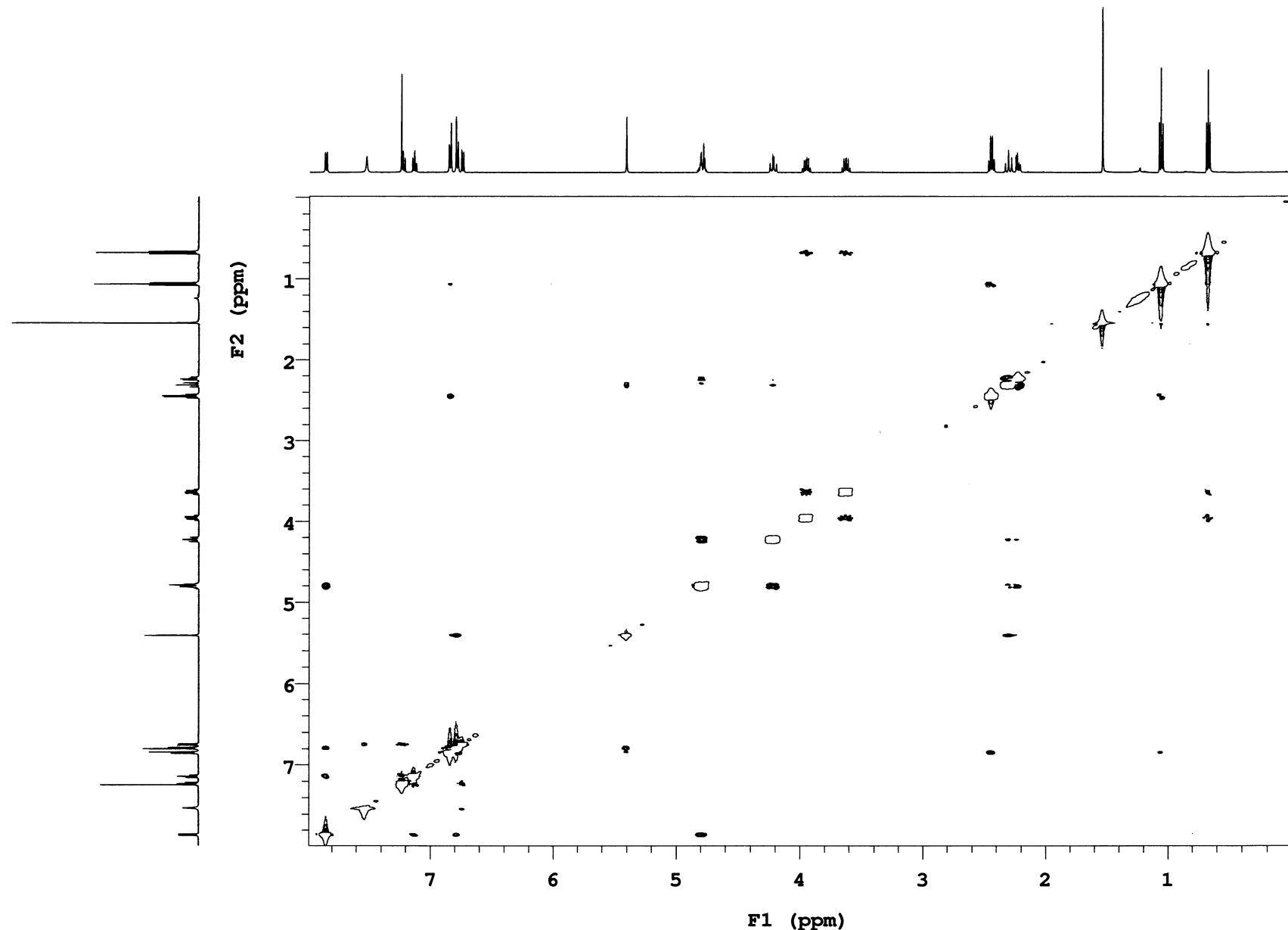
Sample Name PDC-03-149-f2
Date collected 2018-03-28Pulse sequence gCOSY
Solvent cdcl_3 Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S130. COSY of 3i

PDC-03-149-f2

Sample Name PDC-03-149-f2
Date collected 2018-03-28Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

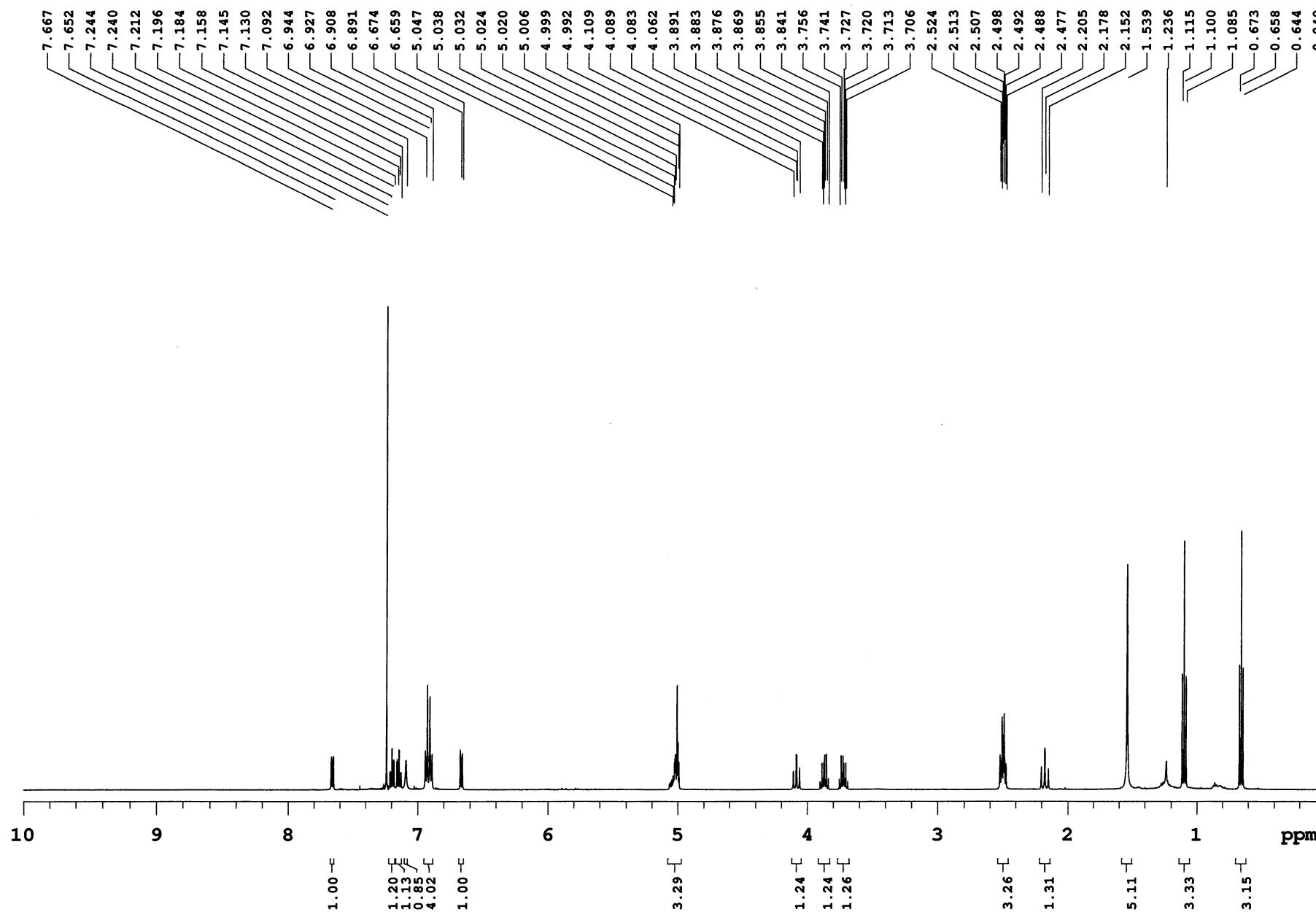
PDC-03-150-f1

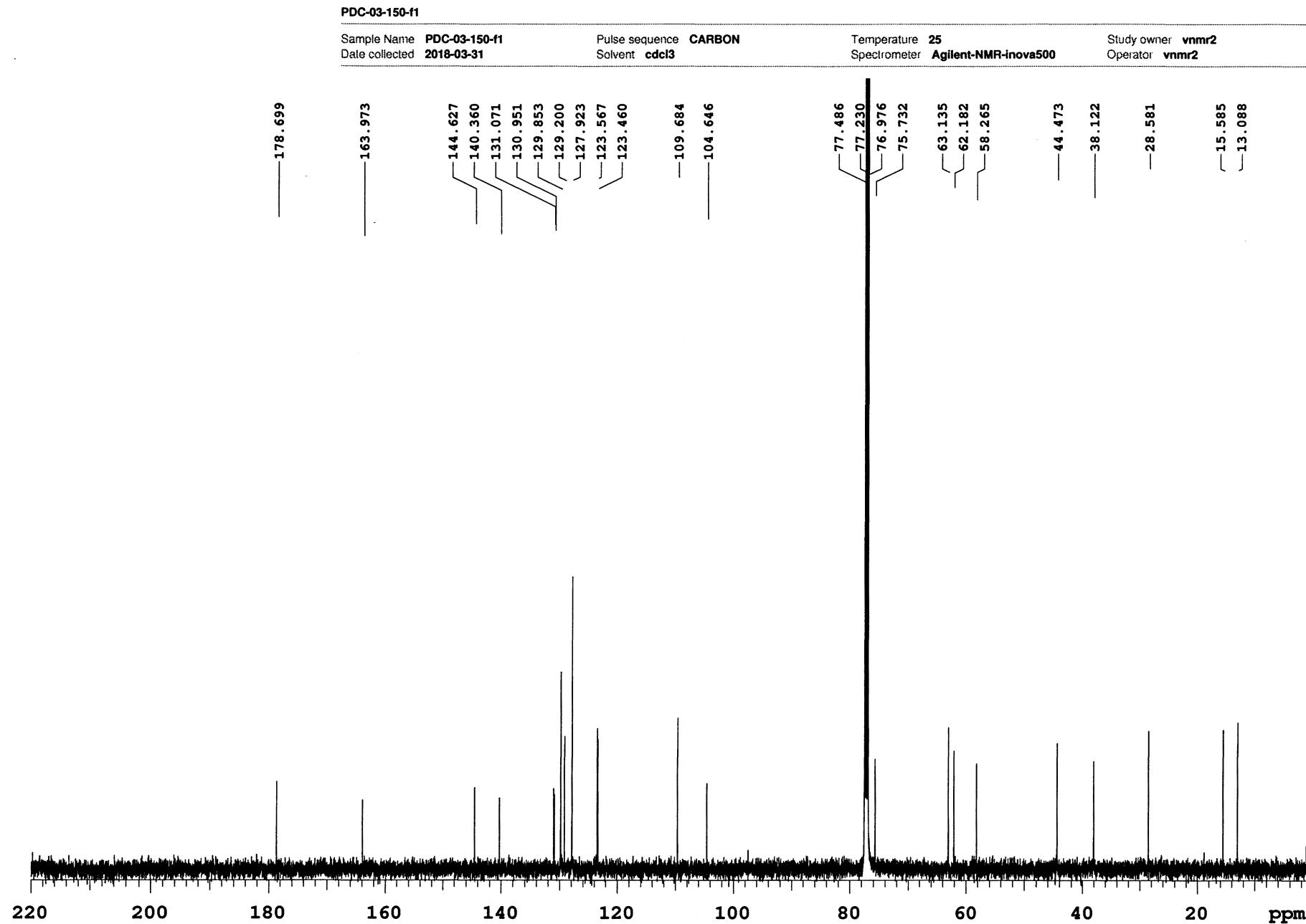
Sample Name PDC-03-150-f1
 Date collected 2018-03-31

Pulse sequence PROTON
 Solvent *cdcl*3

Temperature 25
 Spectrometer Agilent-NMR-inova500

Study owner vnmr2
 Operator vnmr2



Figure S133. ^{13}C NMR (CDCl₃, 125 MHz) of **4i**

Sample Name **PDC-03-150-f1**
Date collected **2018-03-31**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

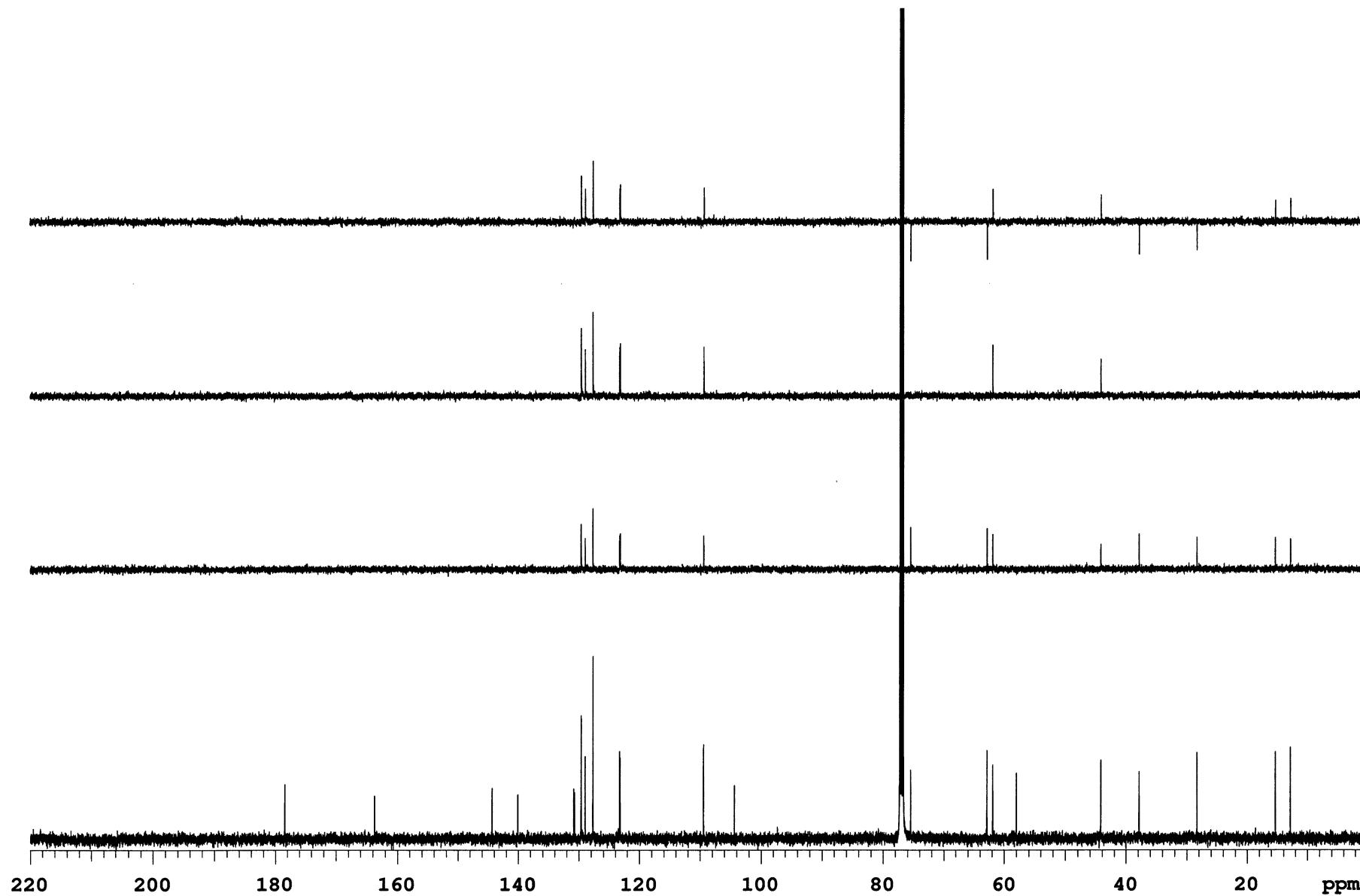


Figure S134. DEPT of **4i**

PDC-03-150-f1

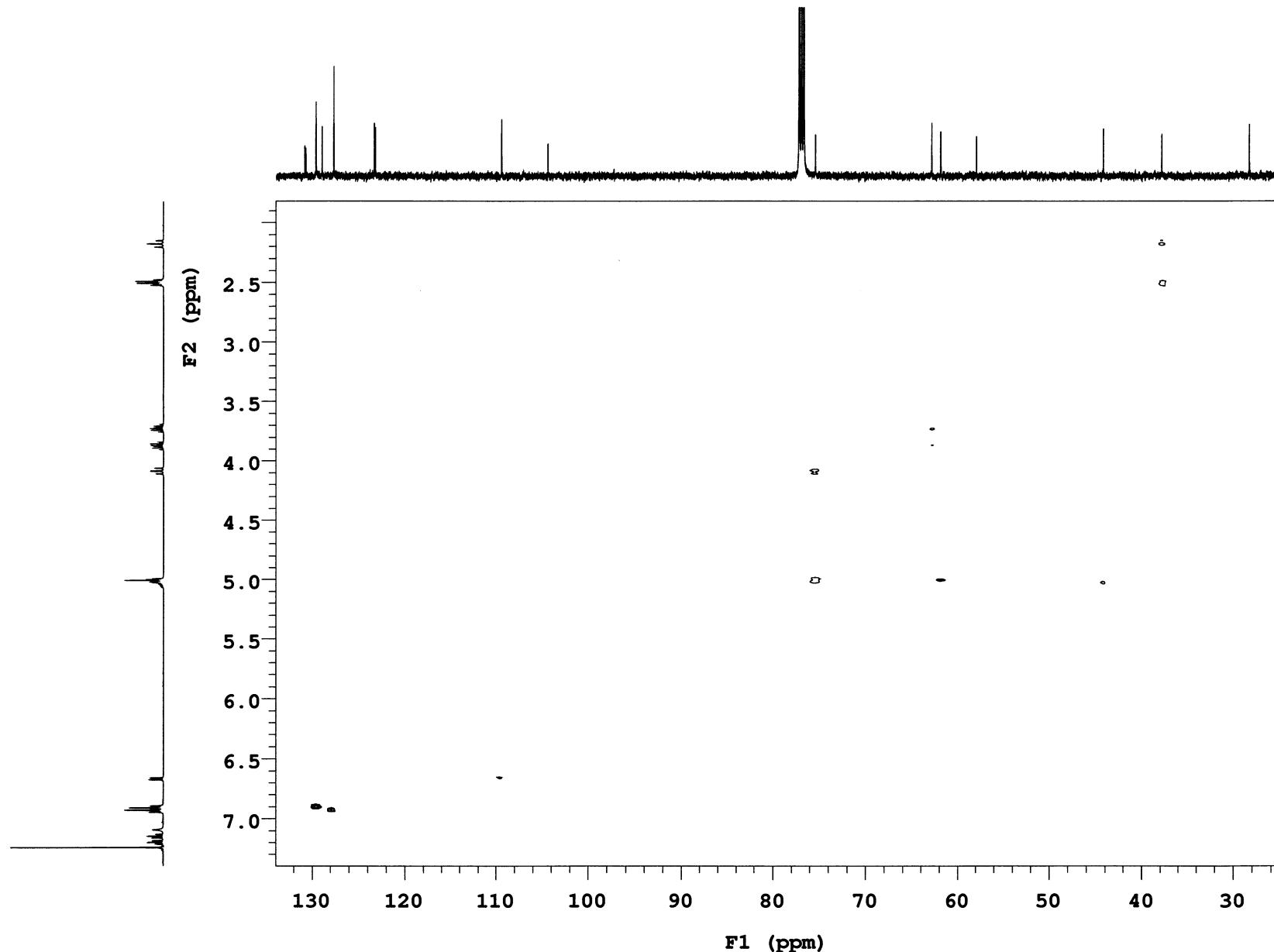
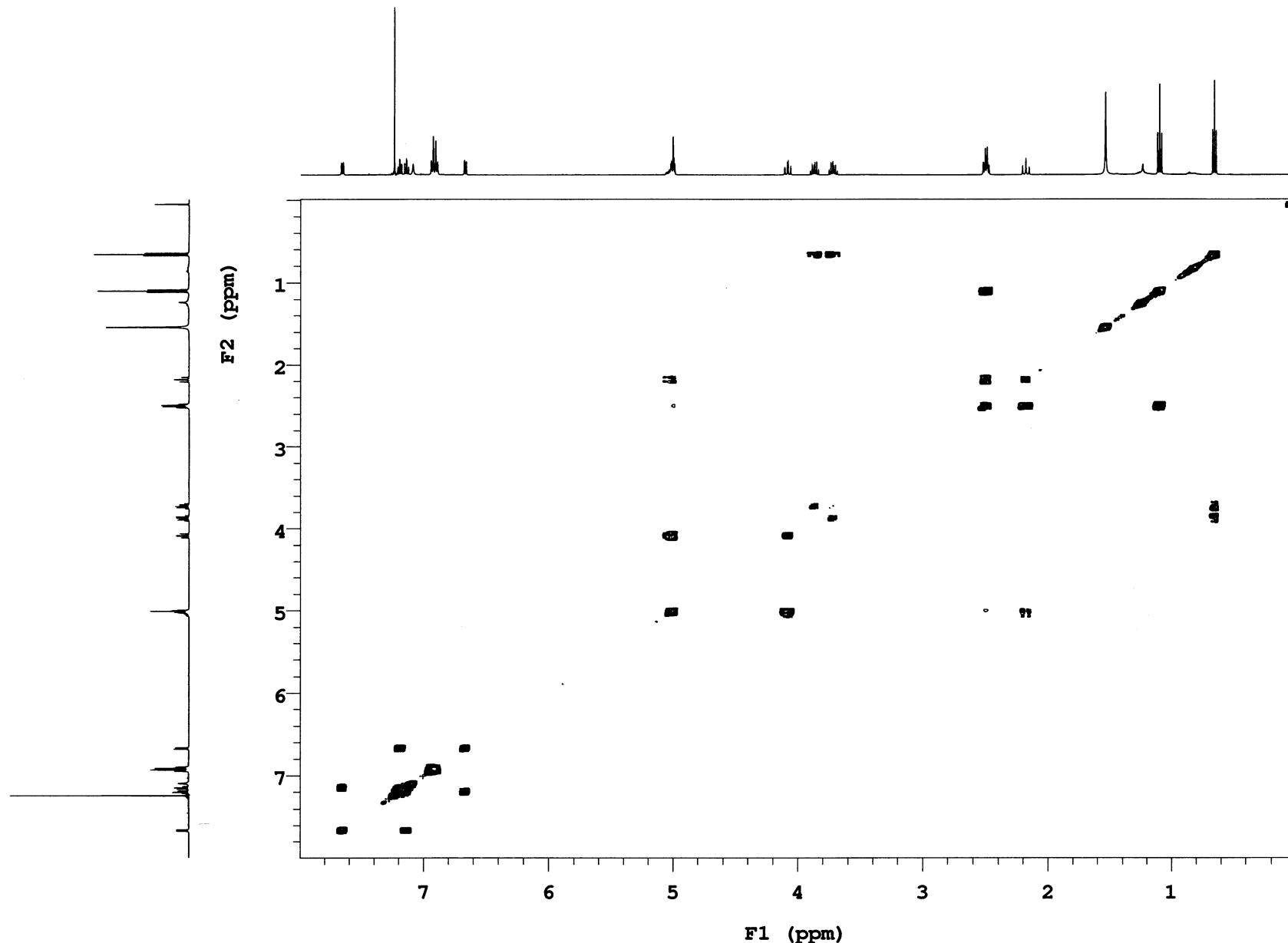
Sample Name PDC-03-150-f1
Date collected 2018-03-31Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S135. HSQC of 4i

PDC-03-150-f1

Sample Name PDC-03-150-f1
Date collected 2018-03-31Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S136. COSY of **4i**

PDC-03-150-f1

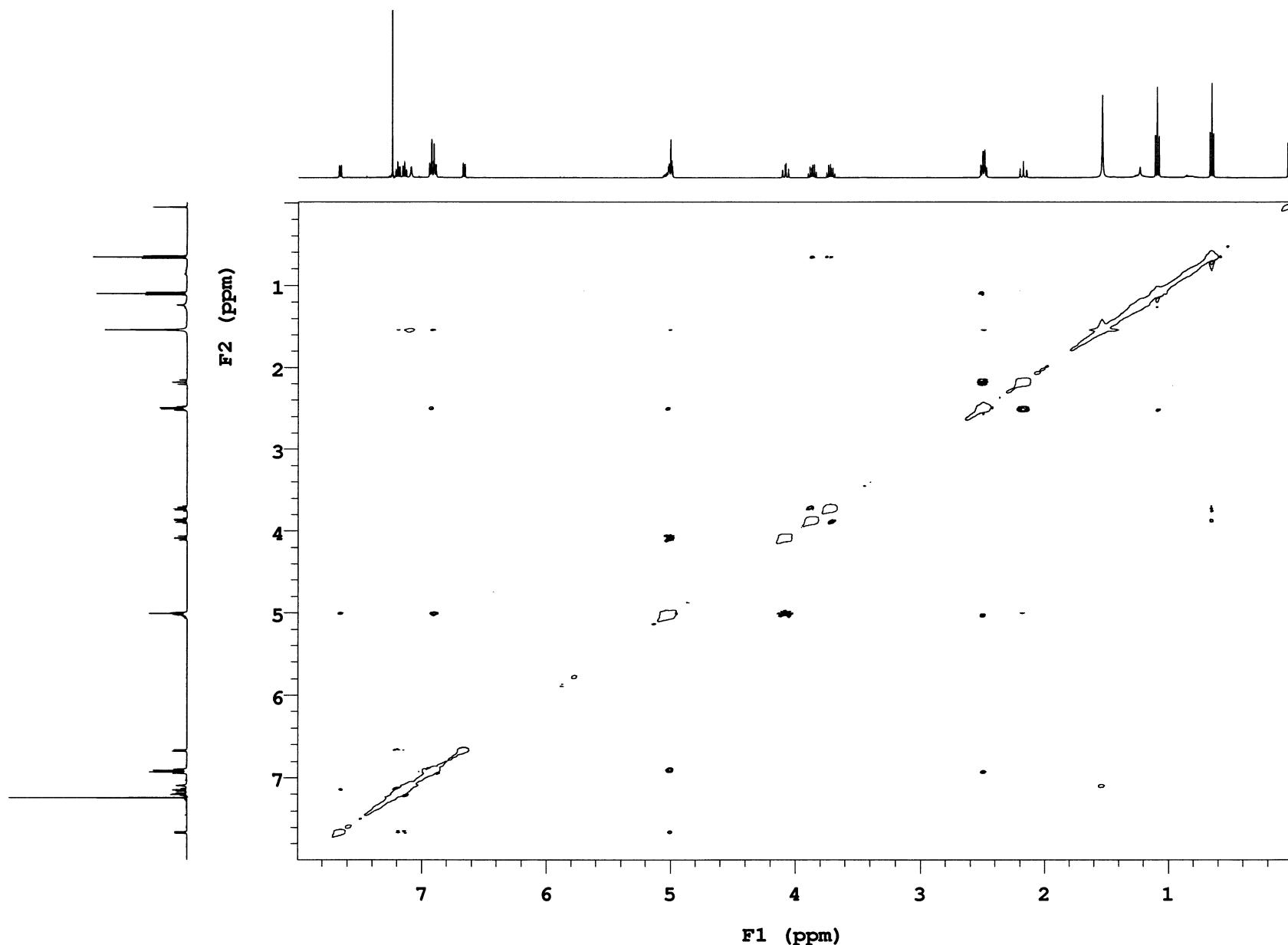
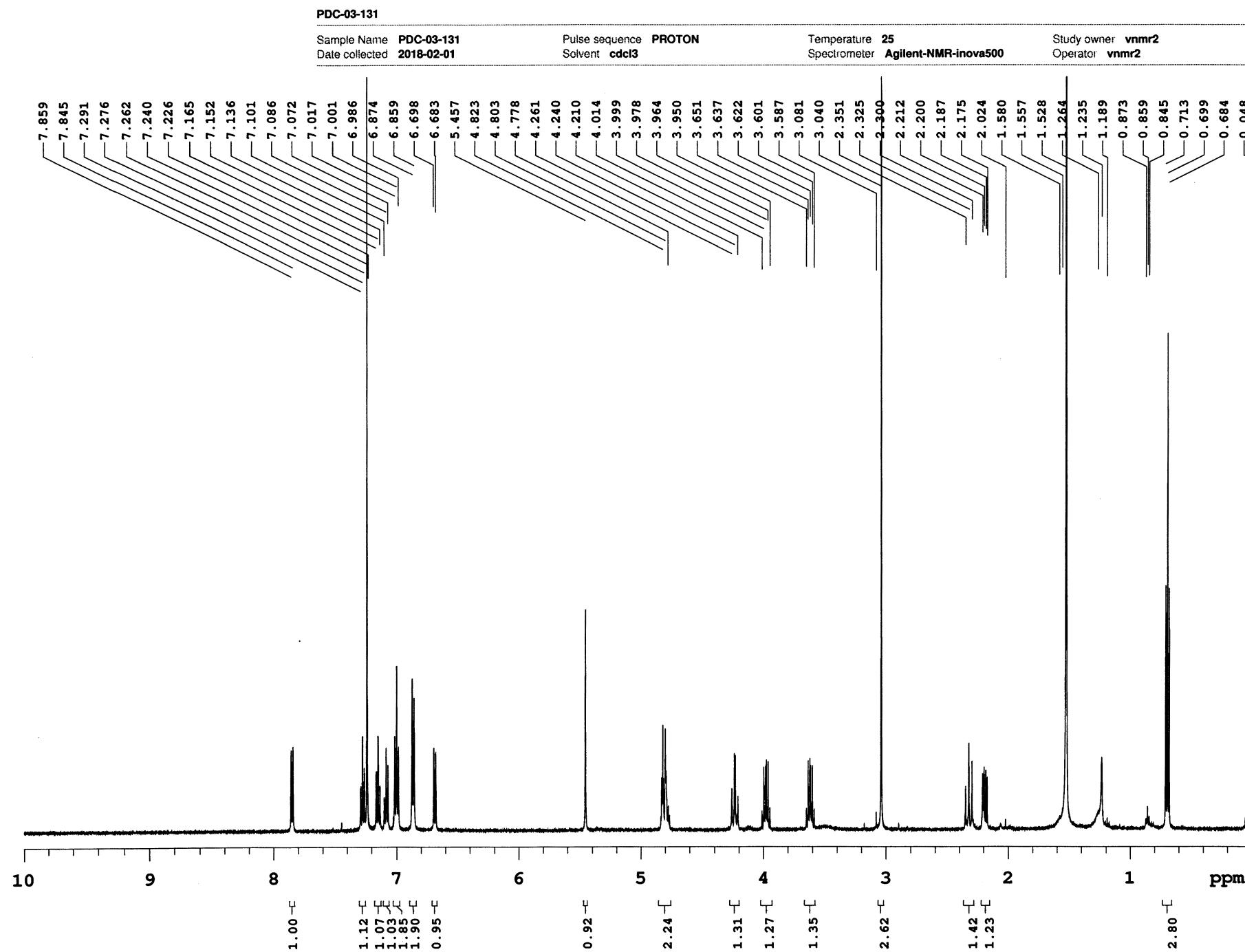
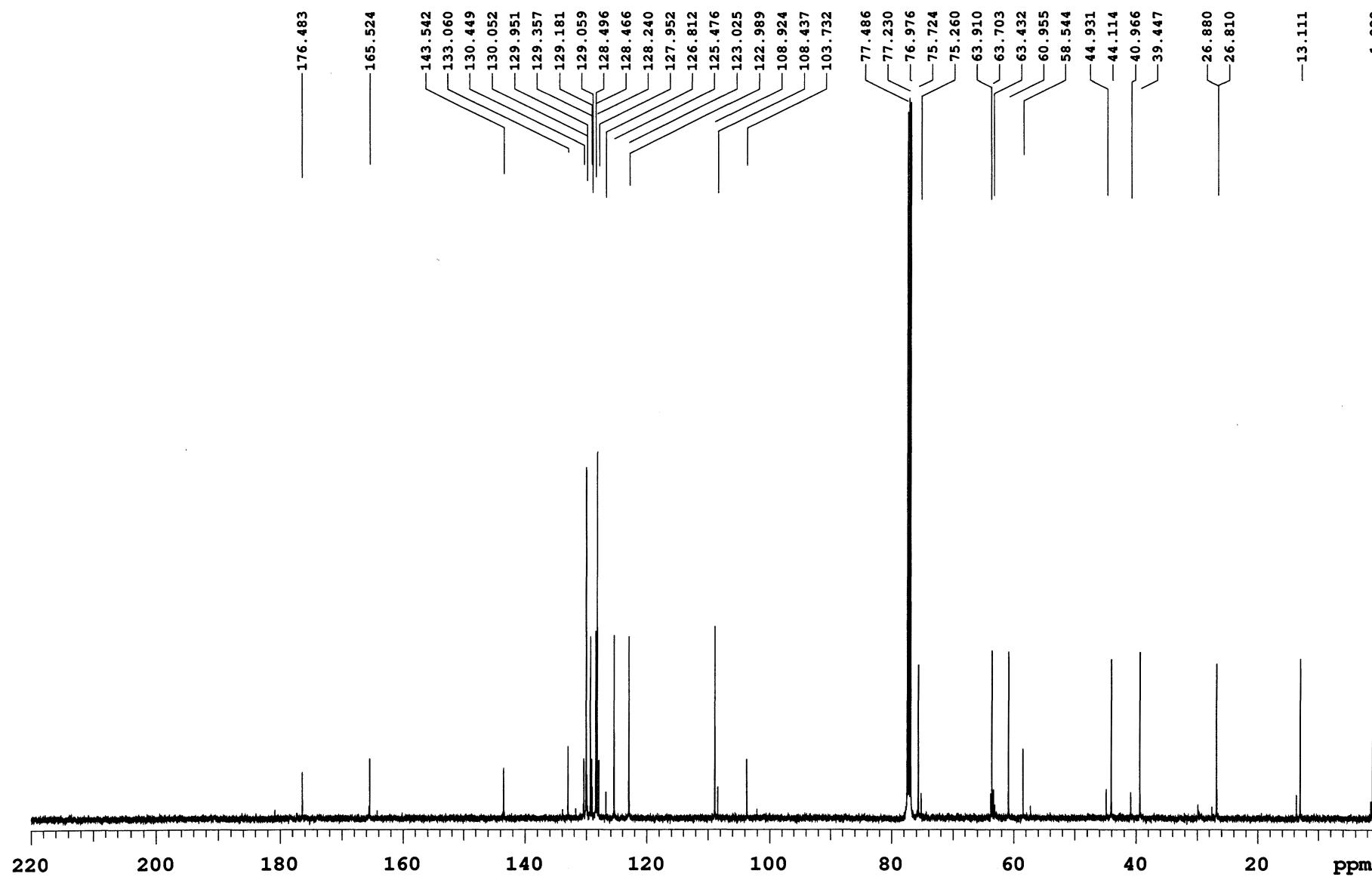
Sample Name PDC-03-150-f1
Date collected 2018-03-31Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S137. NOESY of 4i



PDC-03-101-f2

Sample Name PDC-03-101-f2
Date collected 2017-11-03Pulse sequence CARBON
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S139. 13C NMR (CDCl₃, 125 MHz) of 3j

PDC-03-101-f2

Sample Name	PDC-03-101-f2	Pulse sequence	DEPT	Temperature	25	Study owner	vnmr2
Date collected	2017-11-04	Solvent	cdcl3	Spectrometer	Agilent-NMR-inova500	Operator	vnmr2

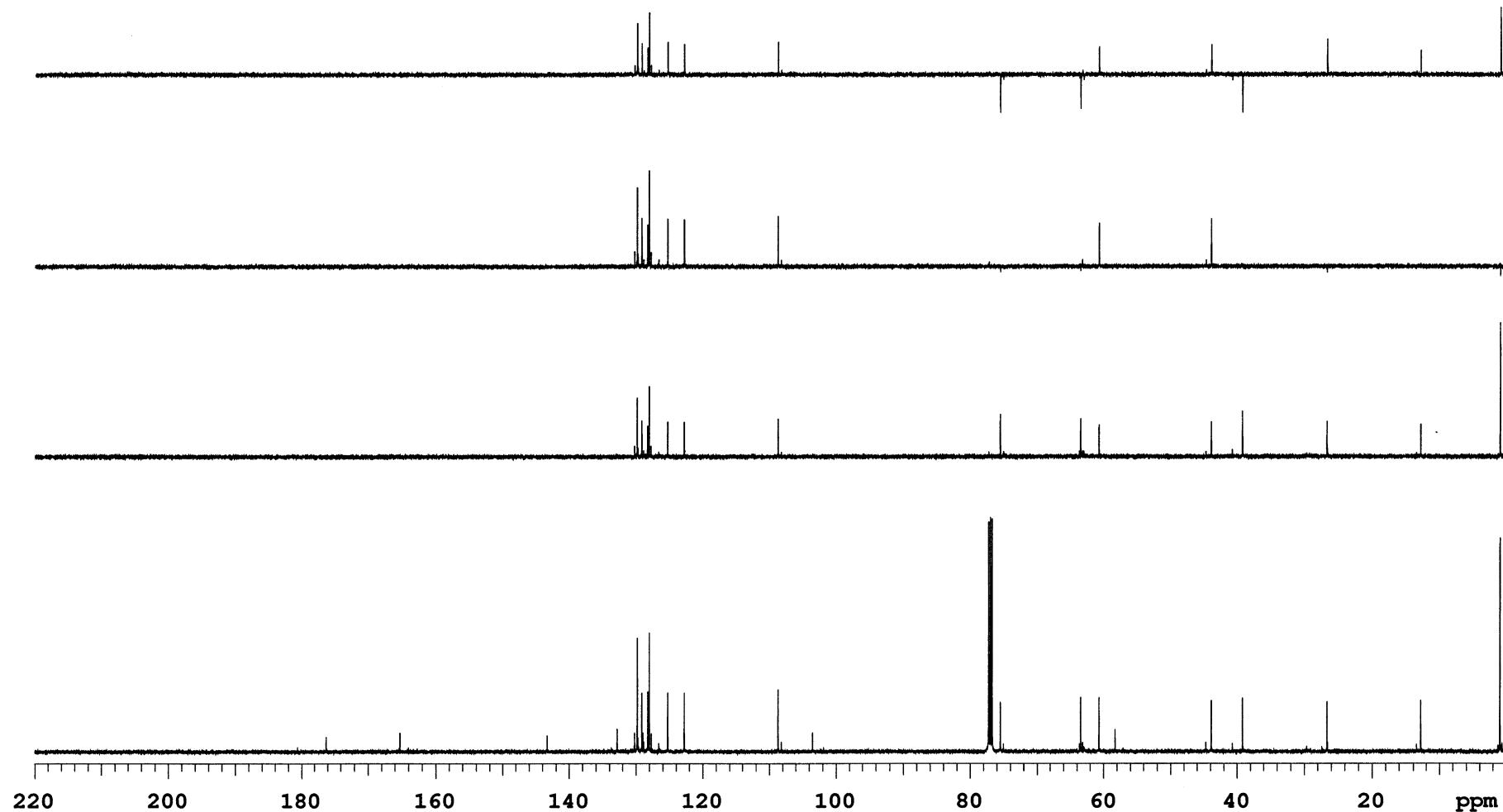
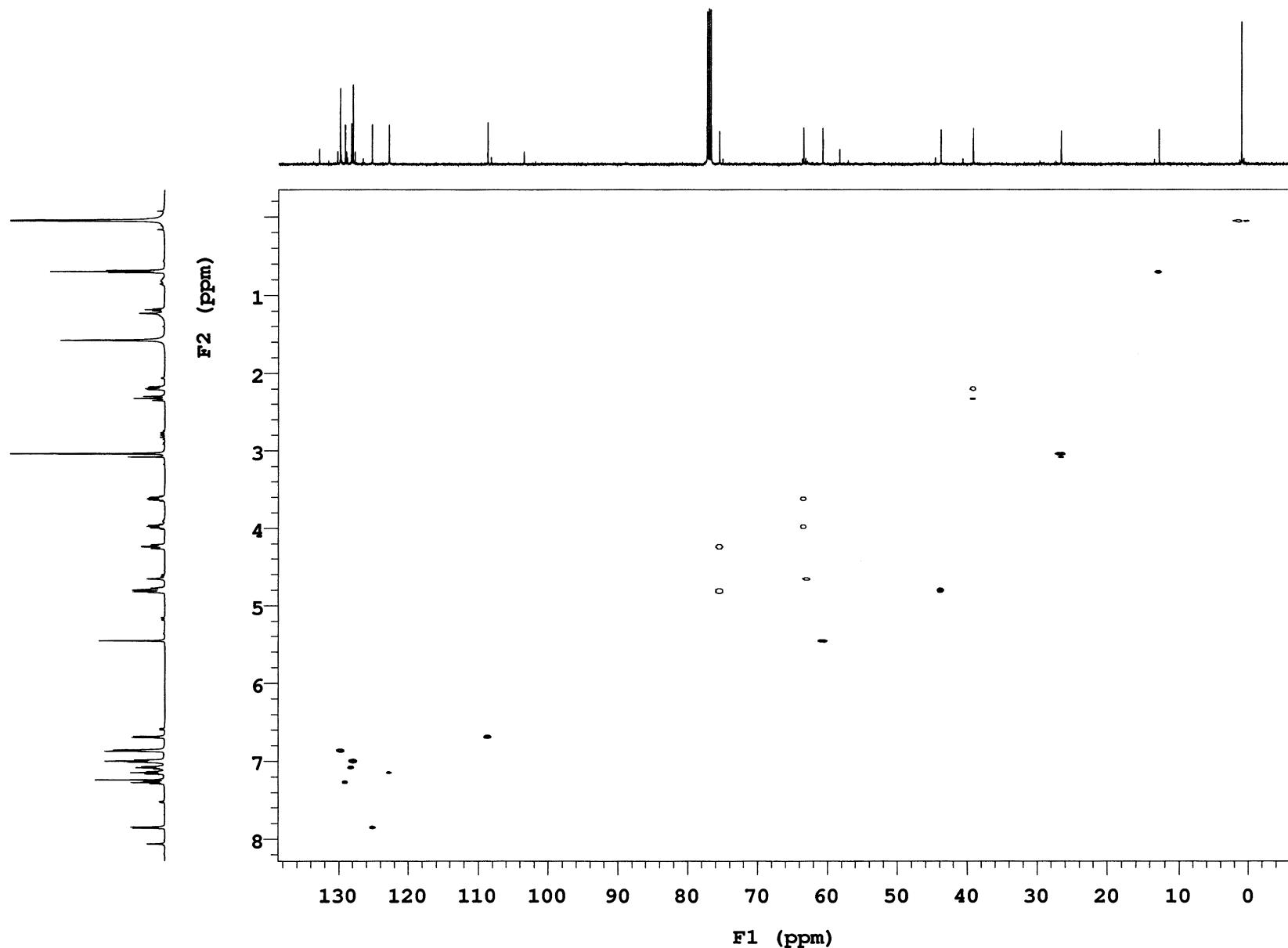


Figure S140. DEPT of 3j

PDC-03-101-f2

Sample Name PDC-03-101-f2
Date collected 2017-11-04Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S141. HSQC of **3j**

PDC-03-101-f2

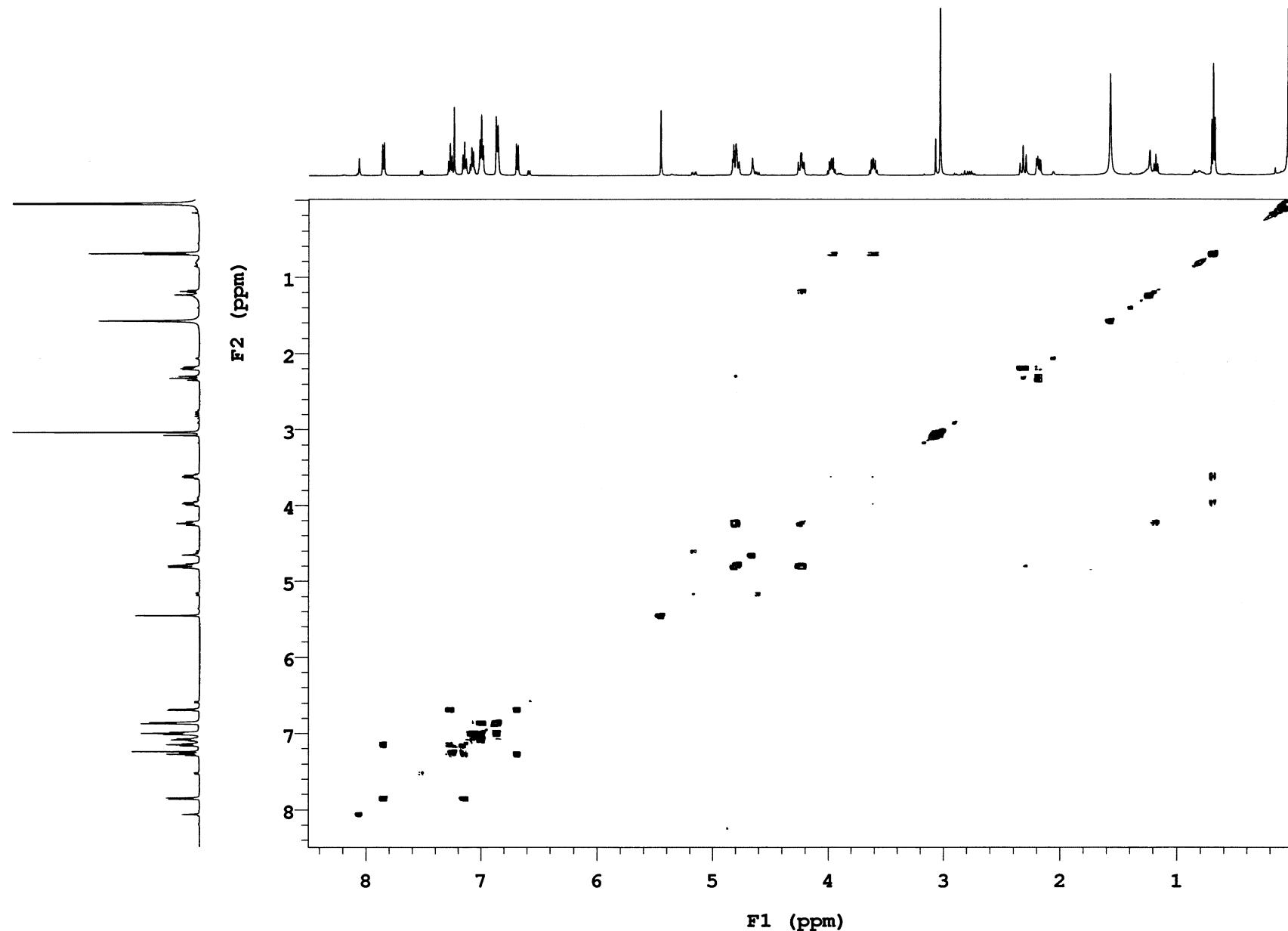
Sample Name PDC-03-101-f2
Date collected 2017-11-04Pulse sequence gCOSY
Solvent cdcl_3 Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S142. COSY of 3j

PDC-03-101-f2

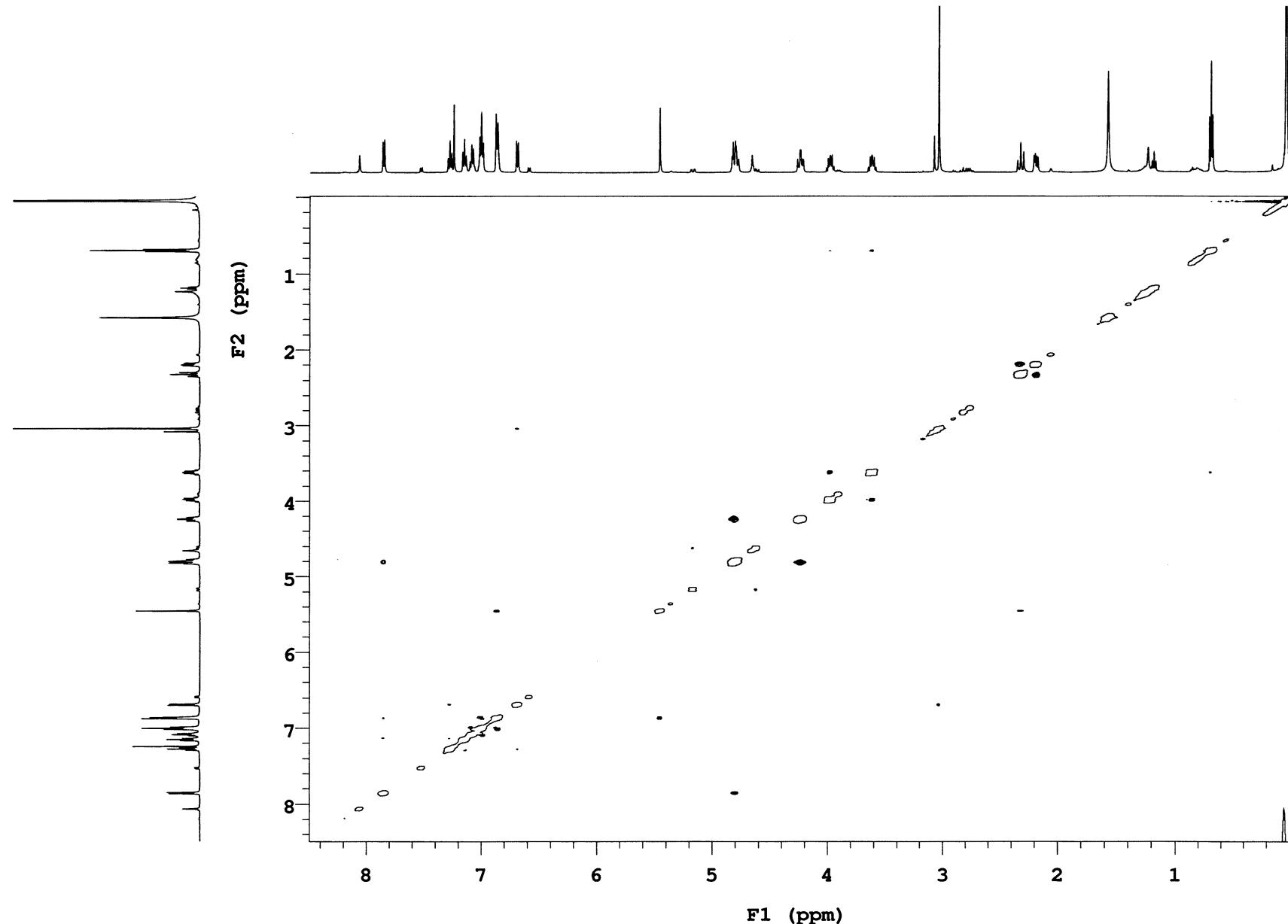
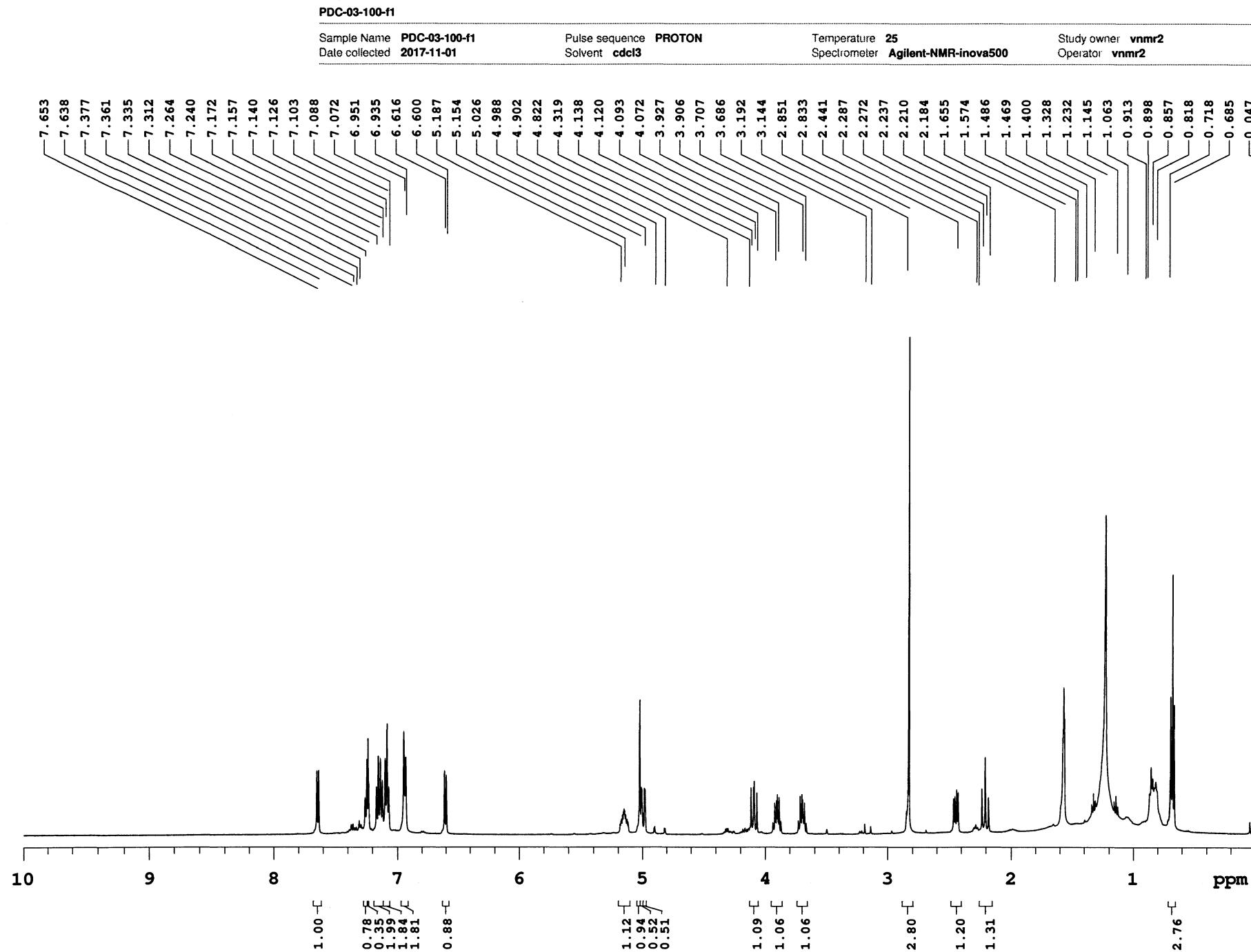
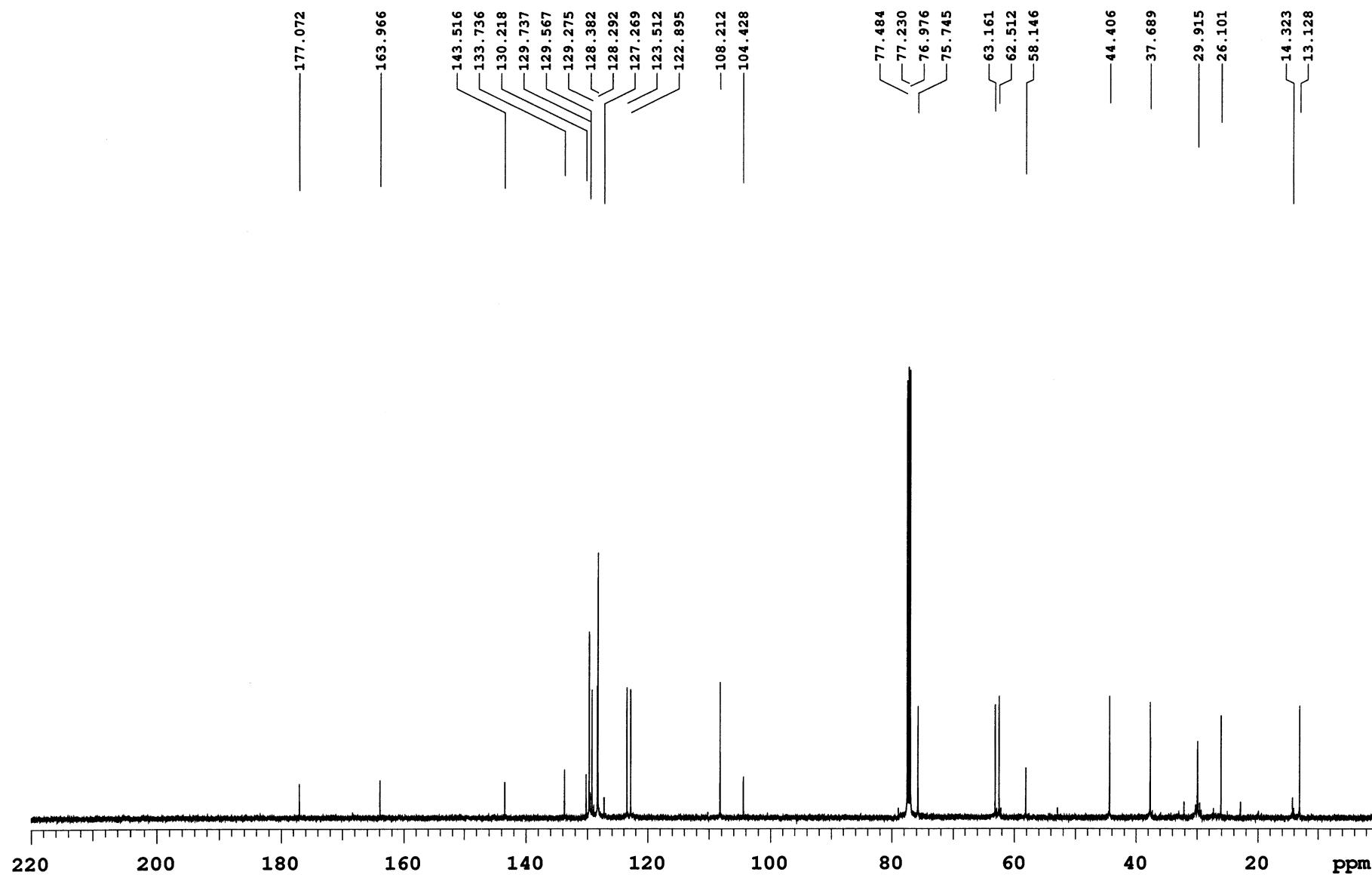
Sample Name PDC-03-101-f2
Date collected 2017-11-04Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S143. NOESY of 3j



PDC-03-100-f1

Sample Name PDC-03-100-f1
Date collected 2017-11-01Pulse sequence CARBON
Solvent *cdcl*3Temperature 25
Specrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S145. 13C NMR (*CDCl*3, 125 MHz) of **4j**

Sample Name **PDC-03-100-f1**
Date collected **2017-11-02**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

S158

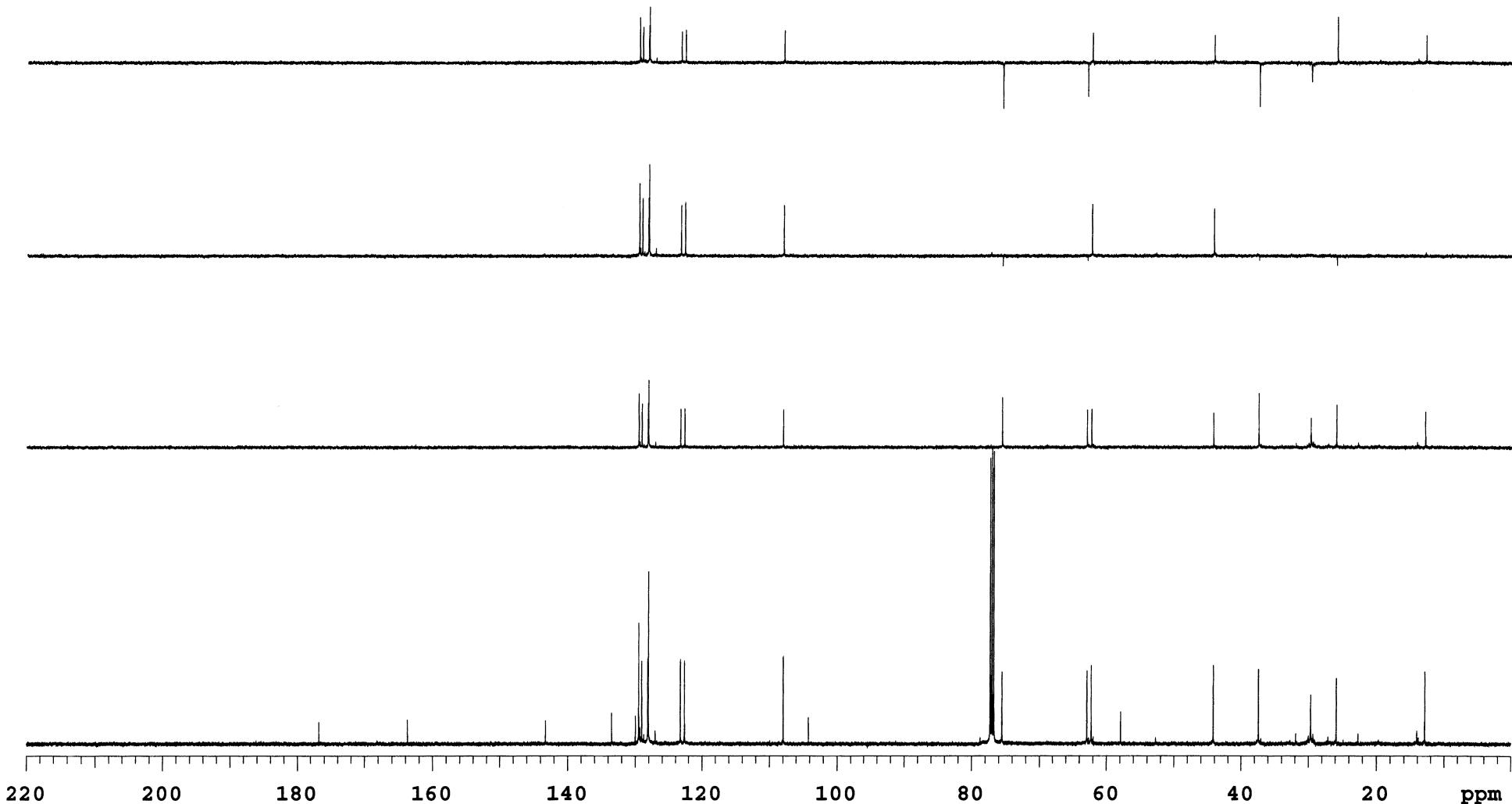


Figure S146. DEPT of **4j**

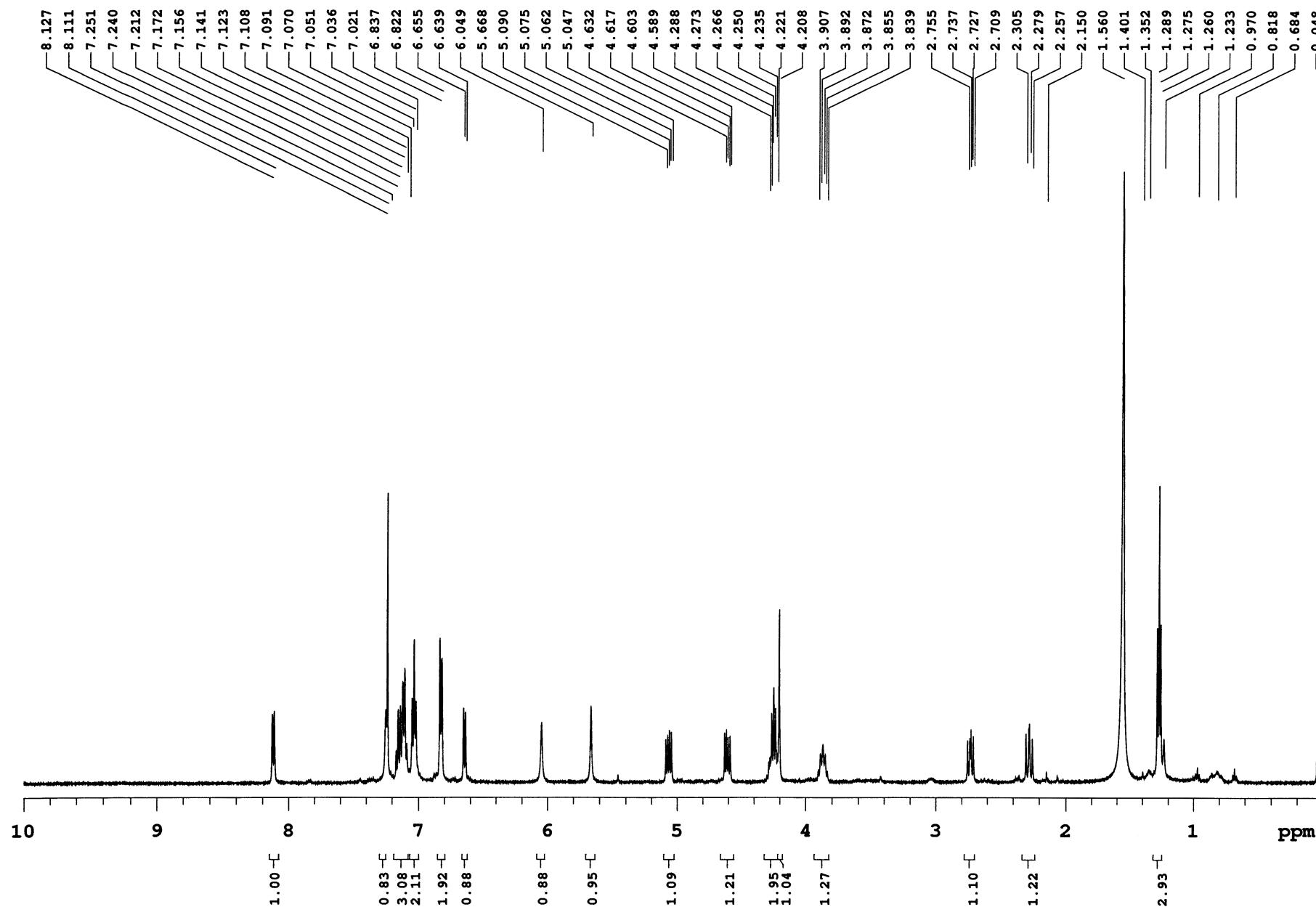
PDC-03-157

Sample Name **PDC-03-15**
Date collected **2018-05-08**

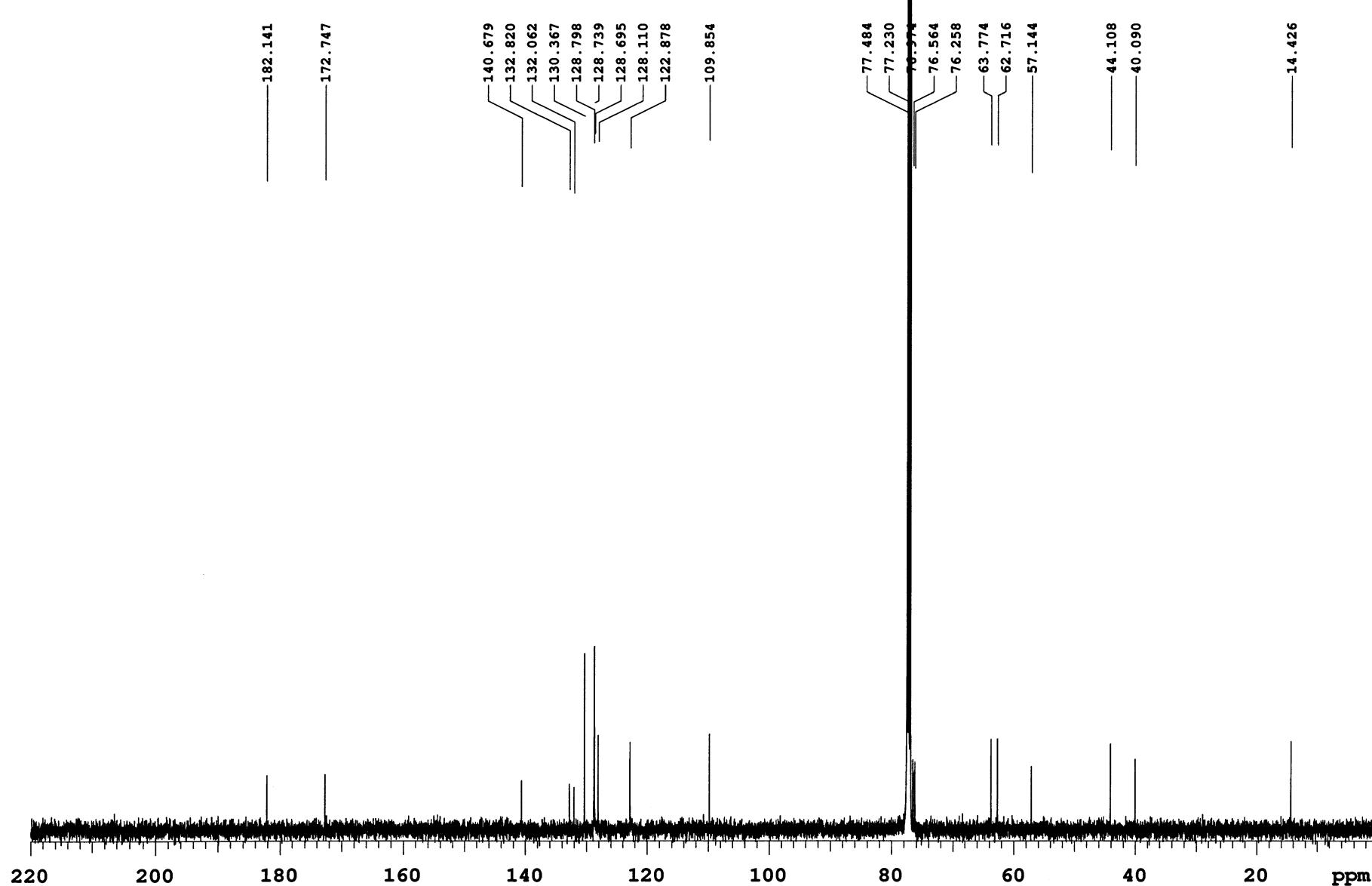
Pulse sequence PROTON
Solvent cdcl3

Temperature **25**
Spectrometer **Agilent-NMR-inova50**

Study owner **vnmr2**
Operator **vnmr2**



PDC-03-157

Sample Name PDC-03-157
Date collected 2018-05-08Pulse sequence CARBON
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S148. ¹³C NMR (*CDCl*3, 125 MHz) of 5a

Sample Name **PDC-03-157**
Date collected **2018-05-08**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-Inova500**

Study owner **vnmr2**
Operator **vnmr2**

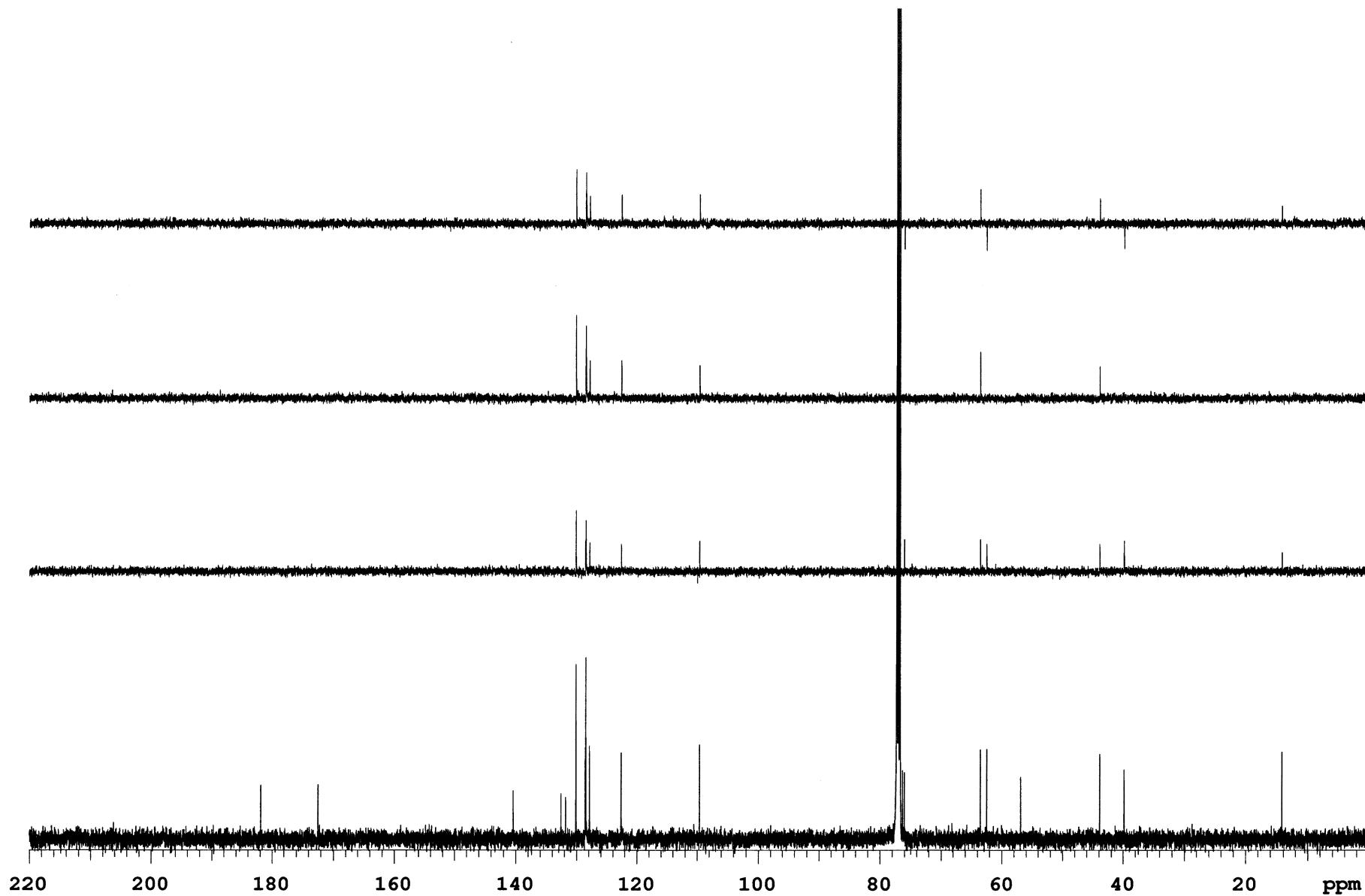
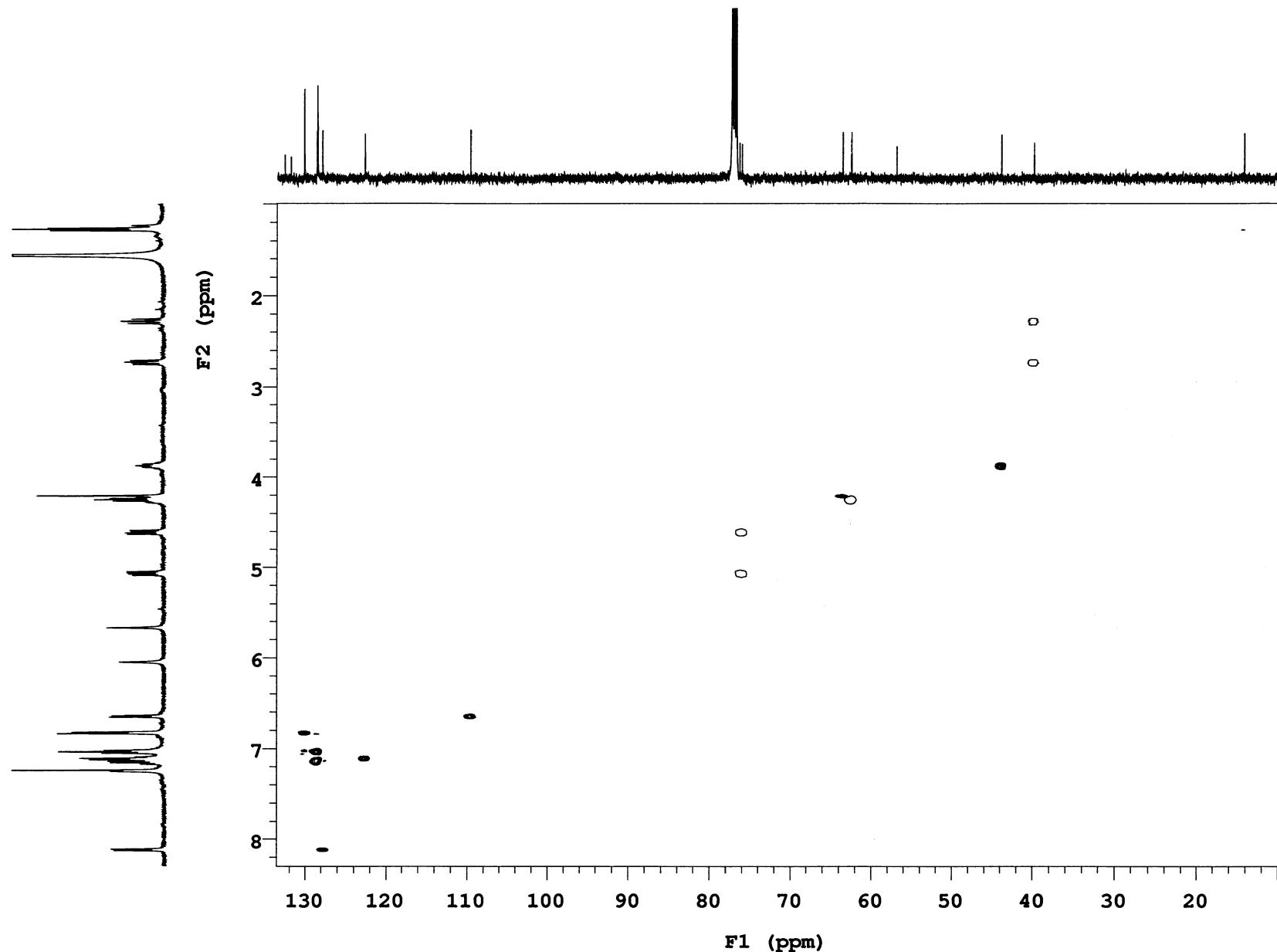
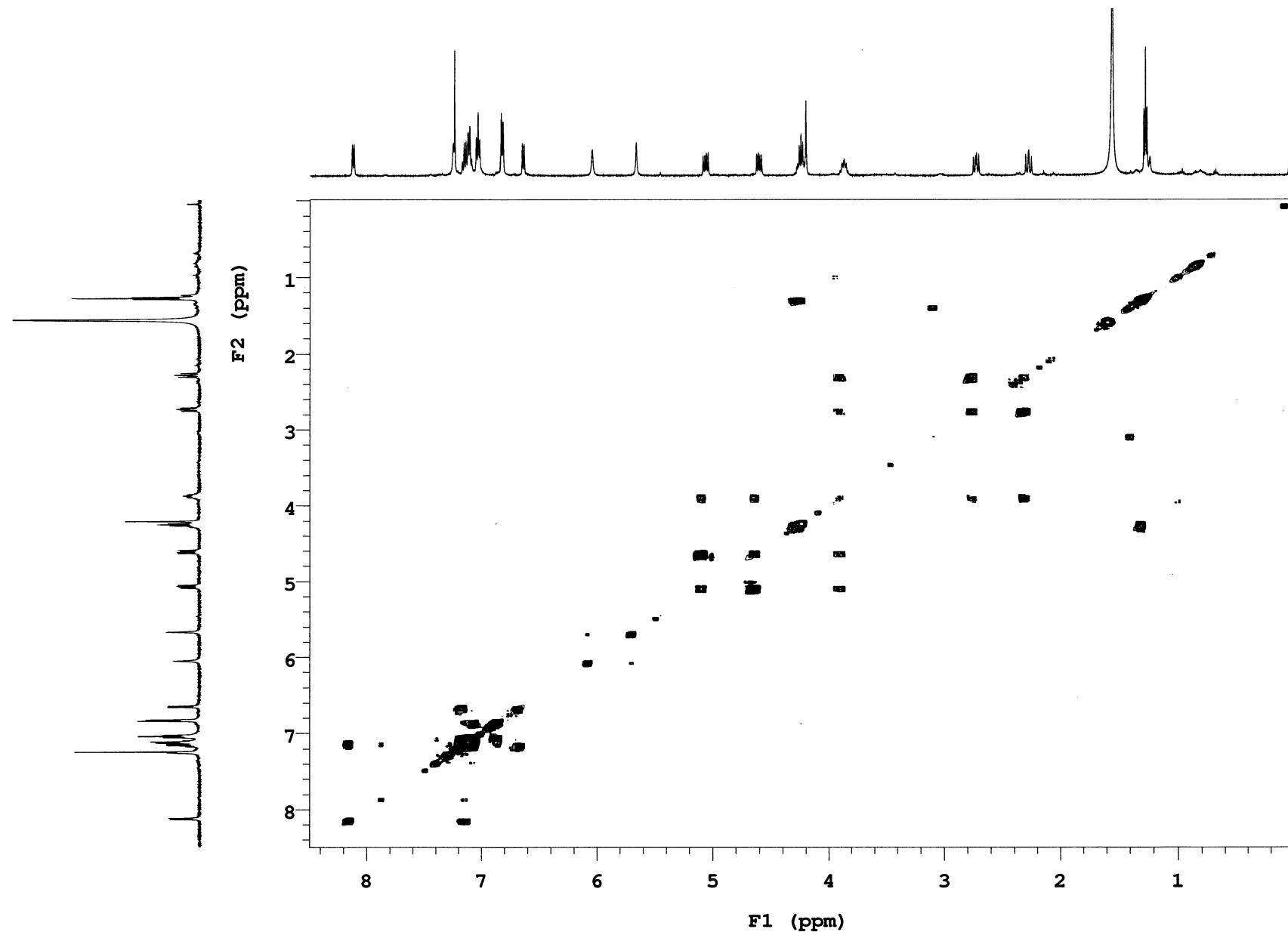


Figure S149. DEPT of **5a**

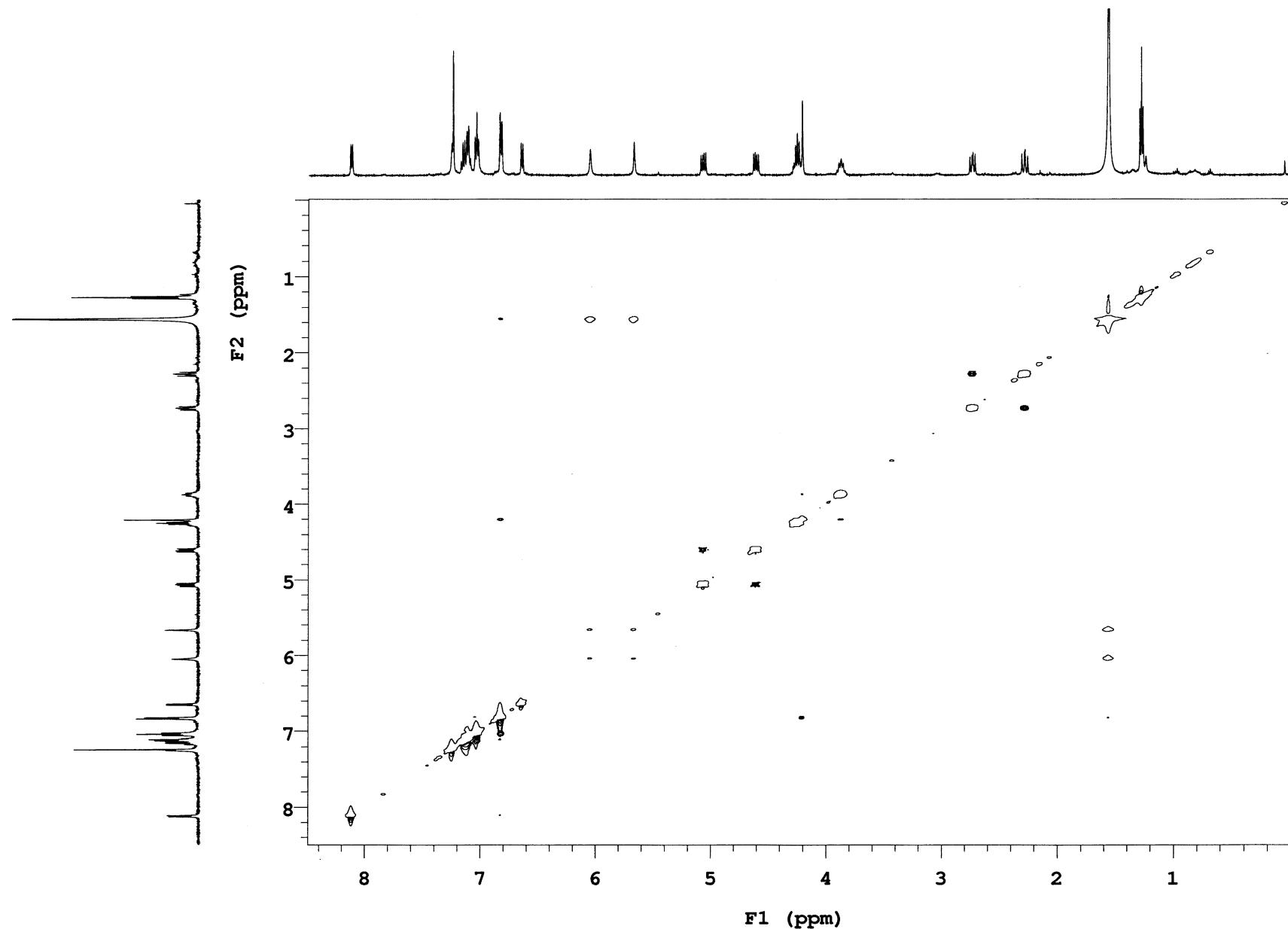
PDC-03-157

Sample Name PDC-03-157
Date collected 2018-05-26Pulse sequence gHSQC
Solvent *cdcl*3Temperature 26
Spectrometer Agilent-NMR-Inova500Study owner vnmr2
Operator vnmr2Figure S150. HSQC of **5a**

PDC-03-157

Sample Name PDC-03-157
Date collected 2018-05-08Pulse sequence gCOSY
Solvent cdcl_3 Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S151. COSY of **5a**

PDC-03-157

Sample Name **PDC-03-157**
Date collected **2018-05-08**Pulse sequence **NOESY**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S152. NOESY of **5a**

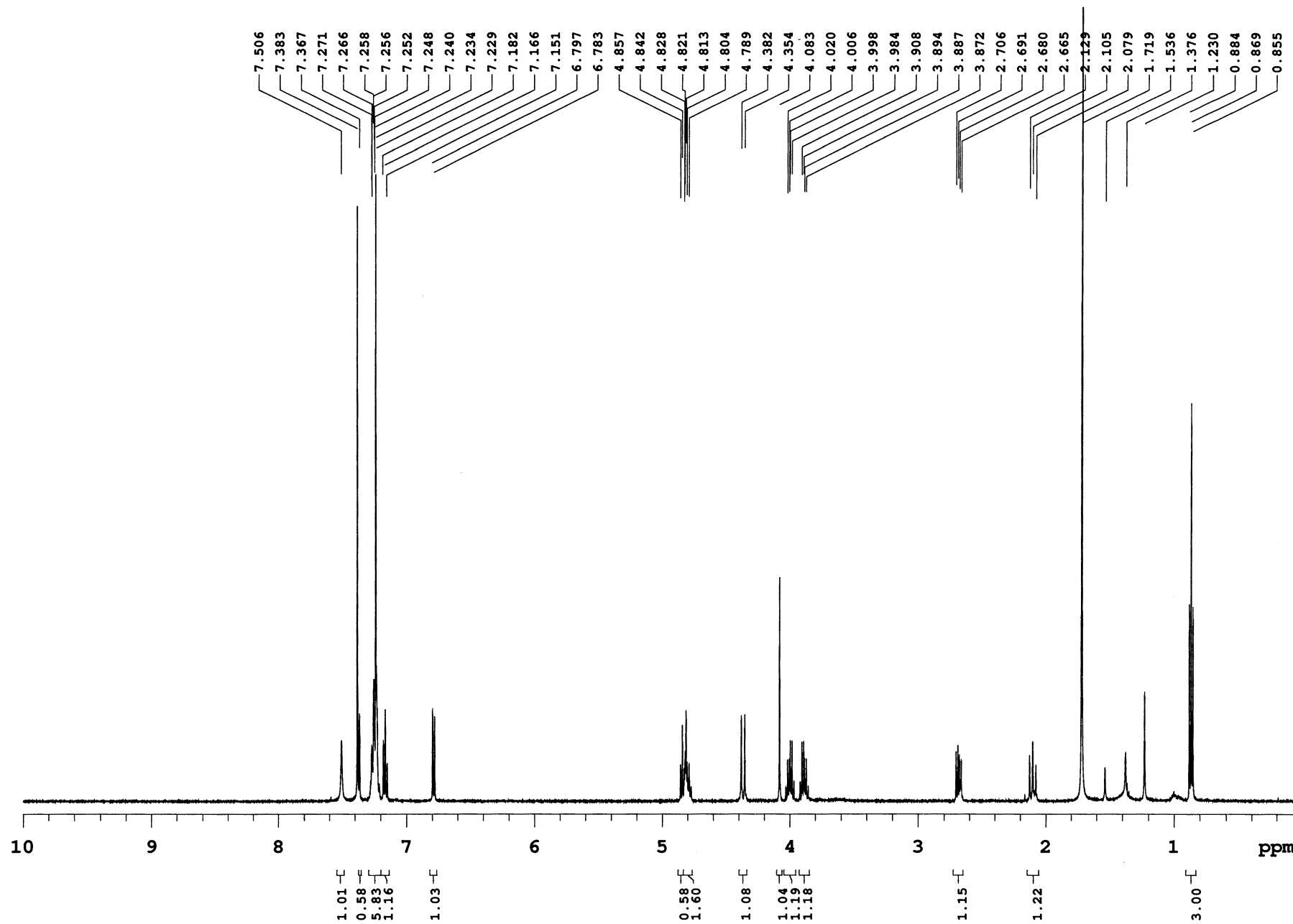
PDC-03-157-MNR

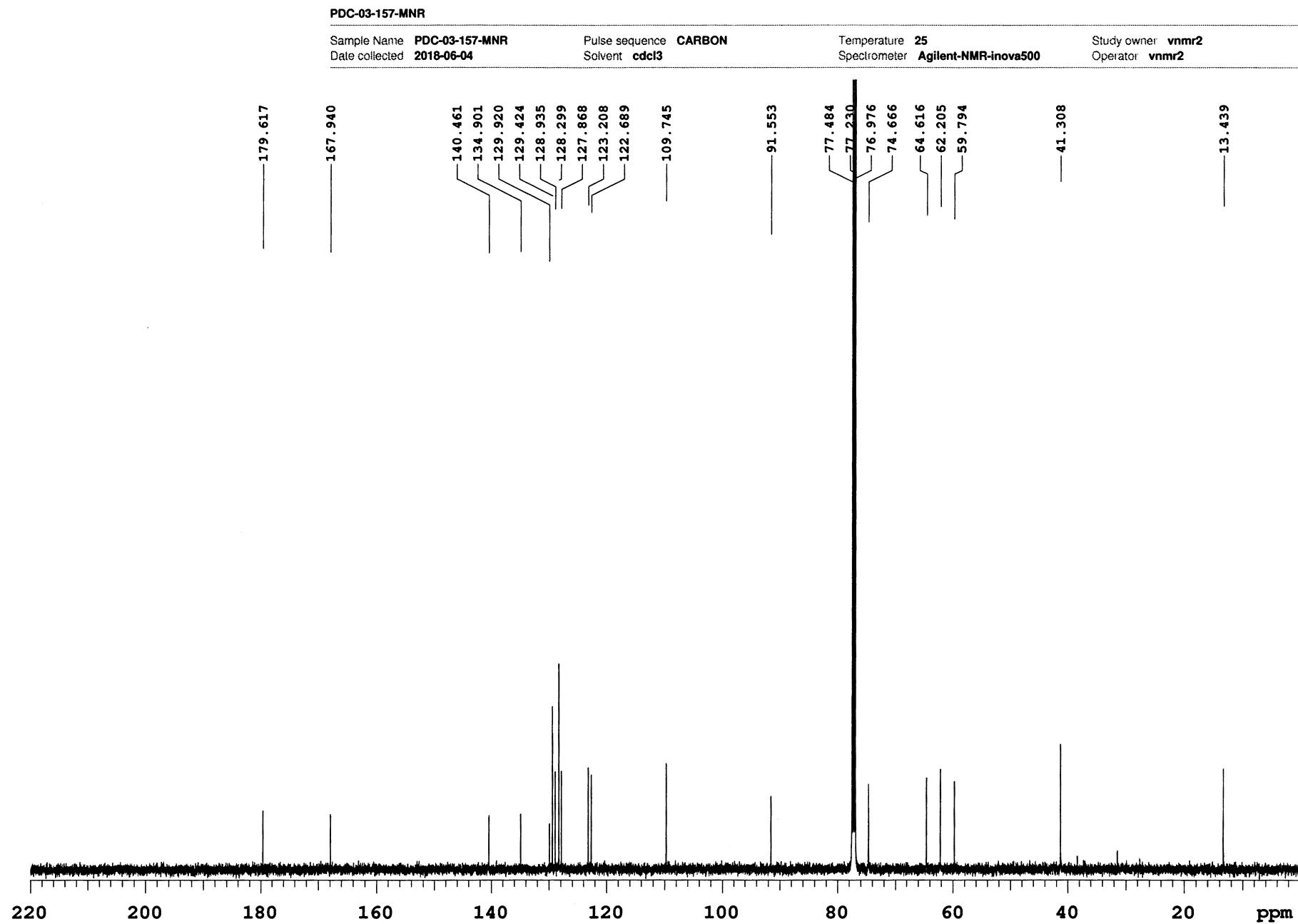
Sample Name **PDC-03-157-MNR**
 Date collected **2018-06-04**

Pulse sequence **PROTON**
 Solvent **cdcl3**

Temperature **25**
 Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
 Operator **vnmr2**



Figure S154. ^{13}C NMR (CDCl_3 , 125 MHz) of **6a**

PDC-03-157-MNR

Sample Name **PDC-03-157-MNR**
Date collected **2018-06-05**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Specrometer **Agilent-NMR-inova500**

Study owner: **vnmr2**
Operator: **vnmr2**

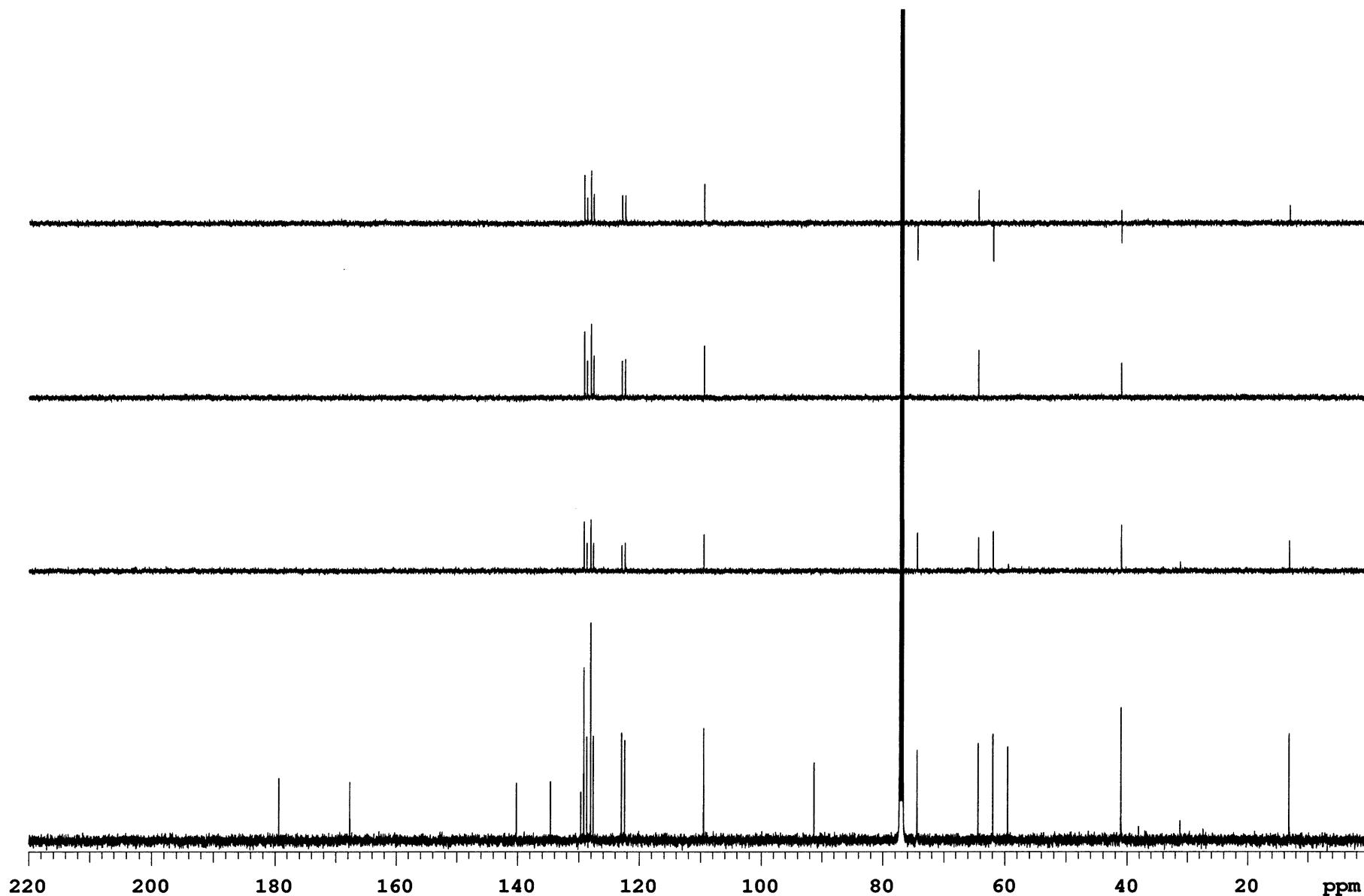


Figure S155. DEPT of **6a**

PDC-03-157-MNR

Sample Name **PDC-03-157-MNR**
Date collected **2018-06-05**

Pulse sequence **gHSQC**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

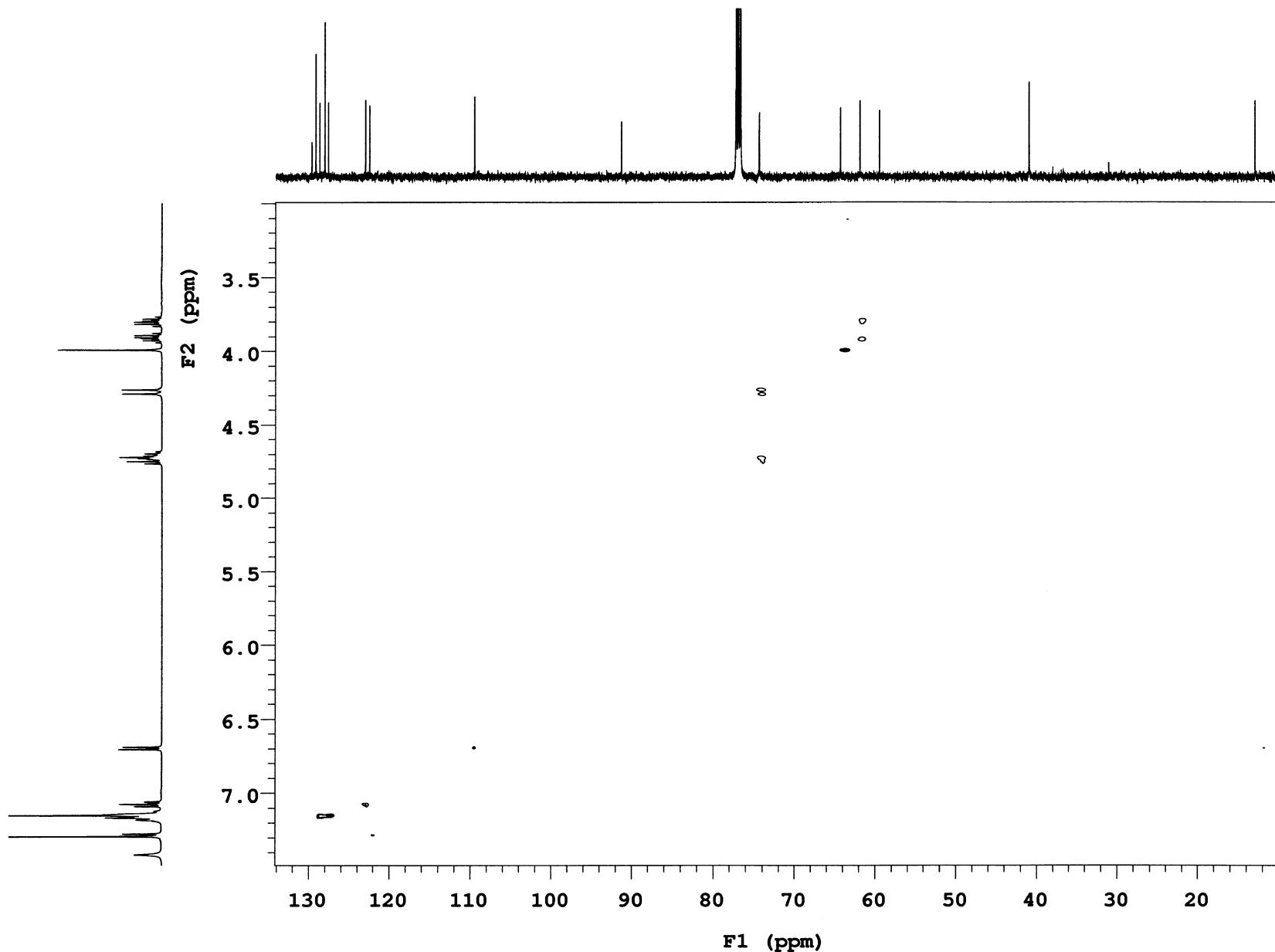
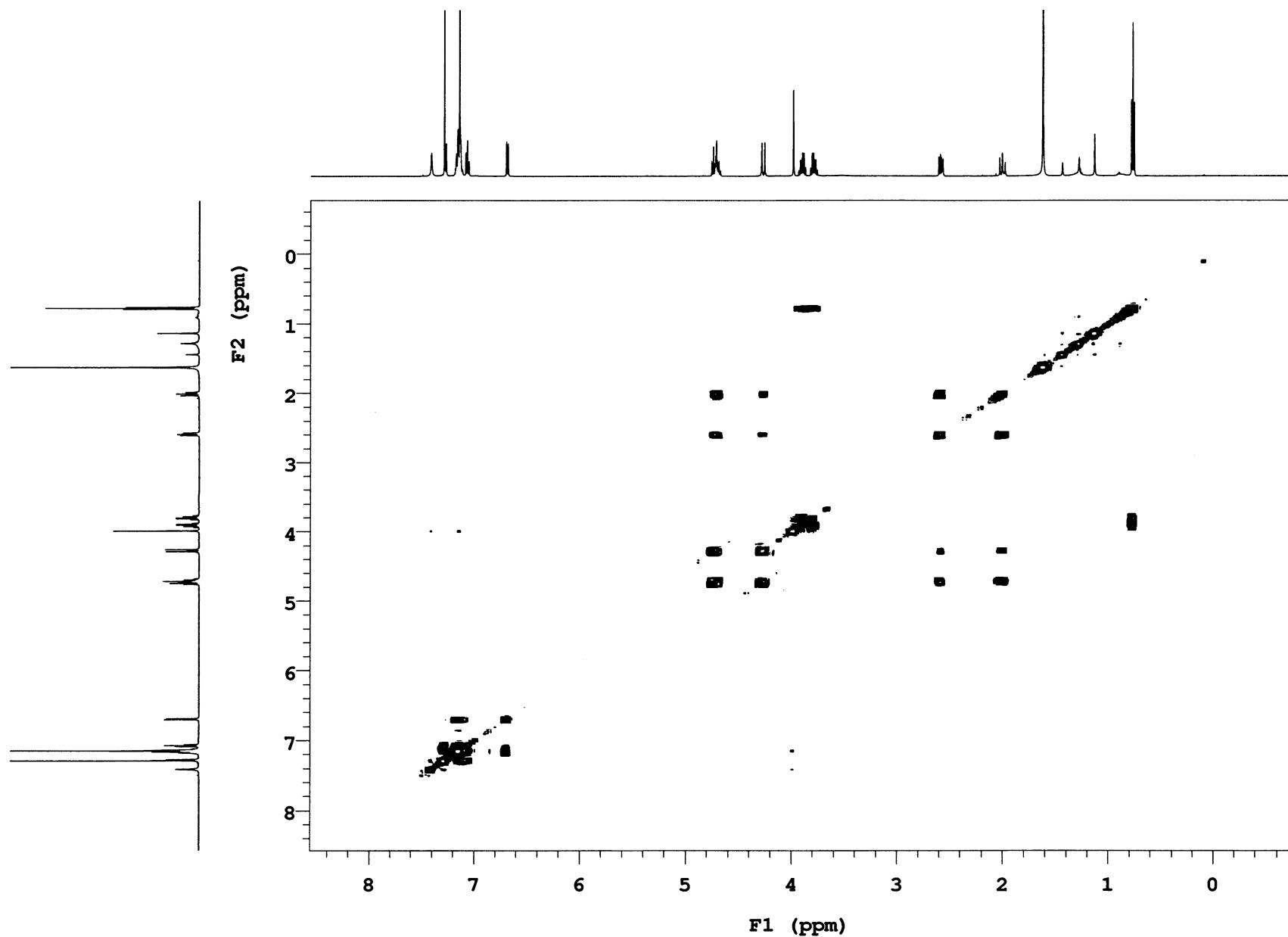
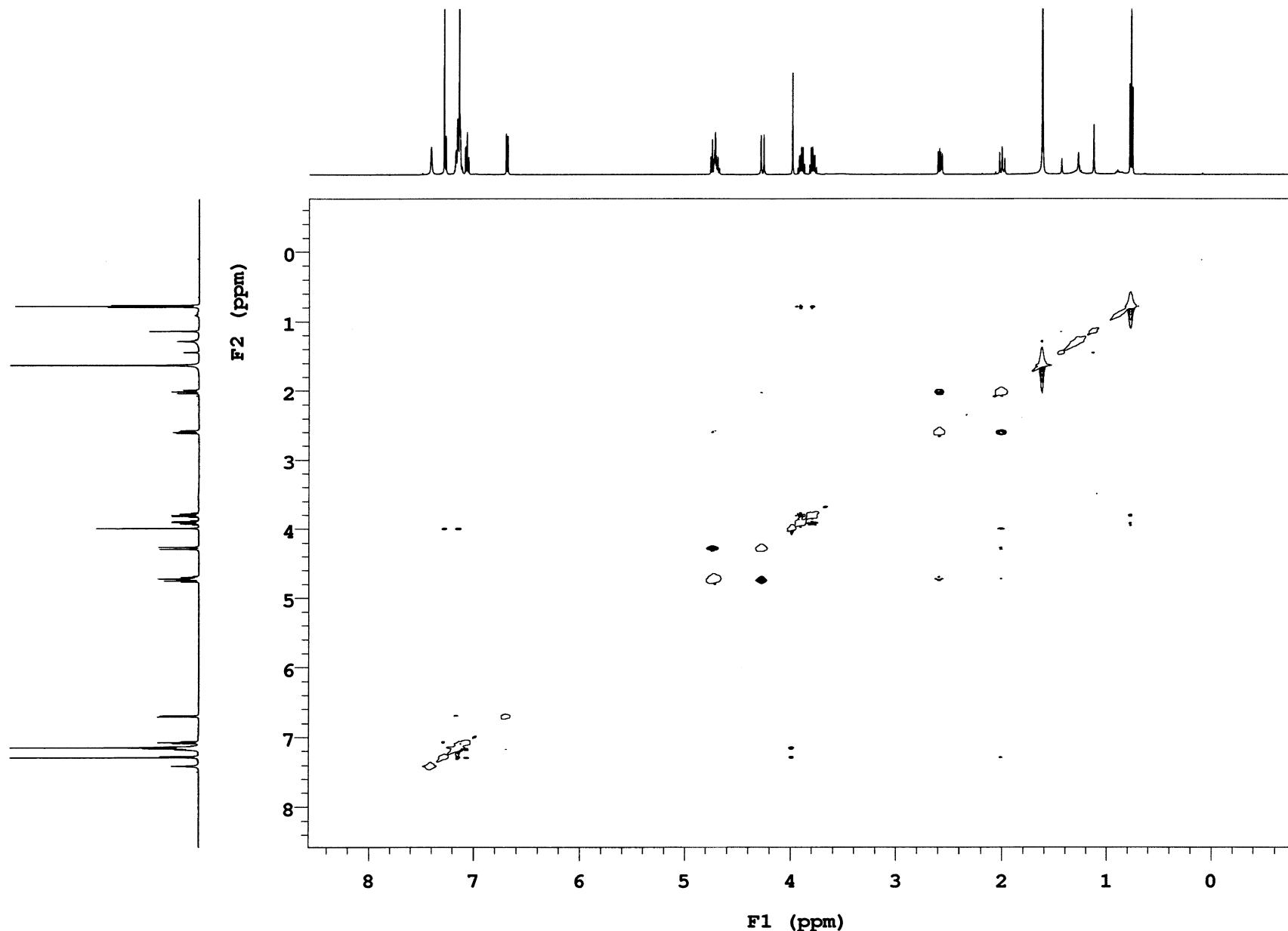


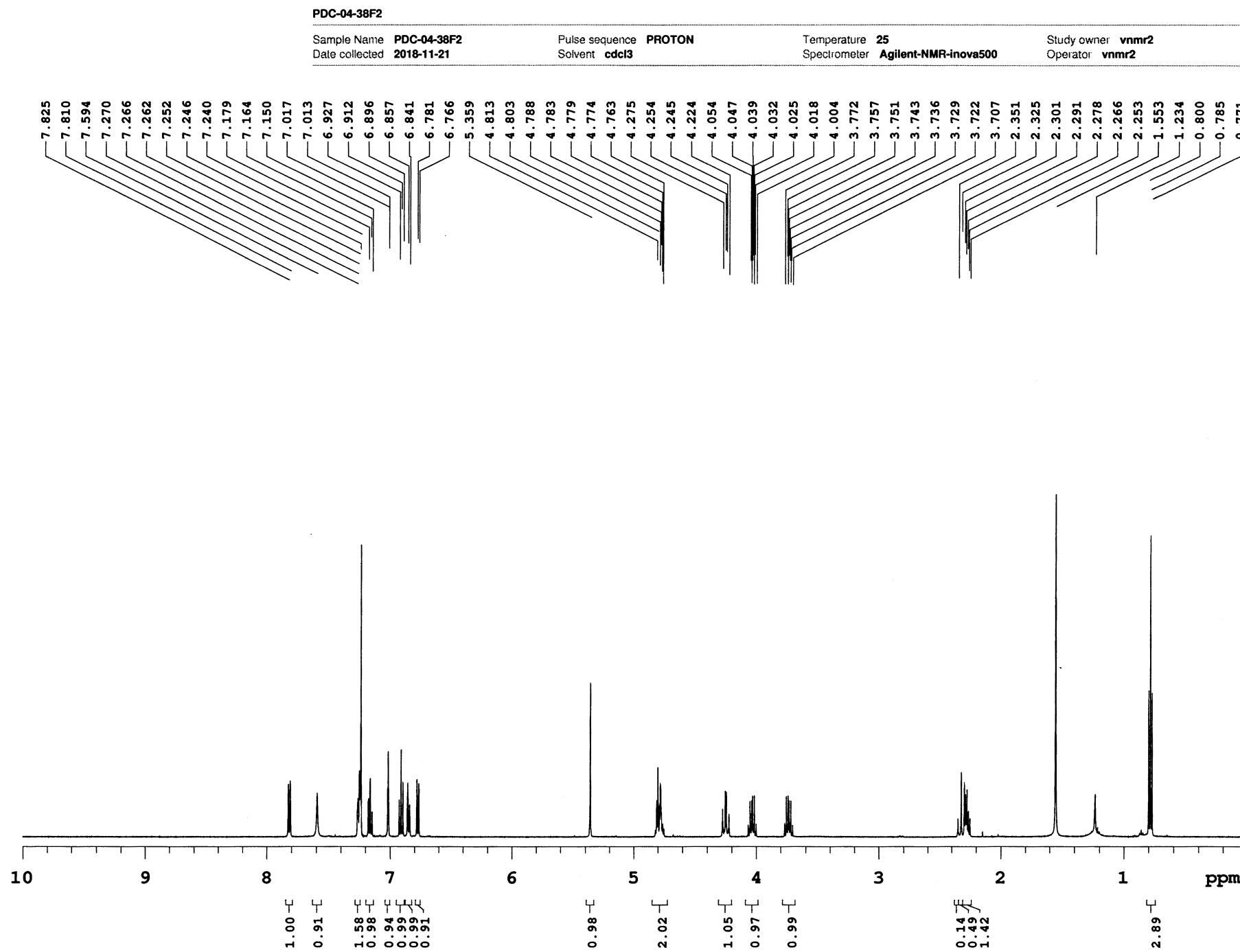
Figure S156. HSQC of **6a**

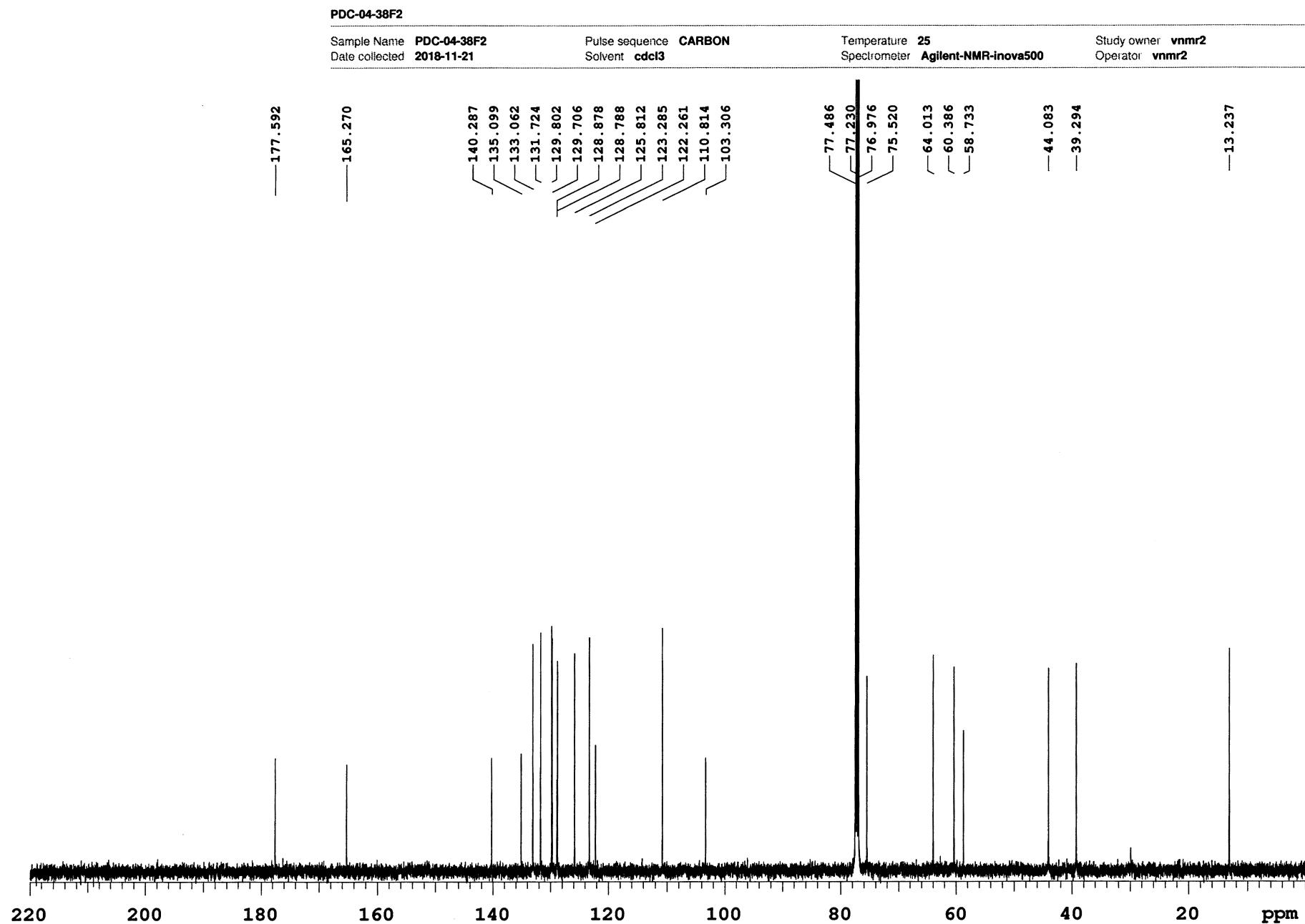
PDC-03-157-MNR

Sample Name PDC-03-157-MNR
Date collected 2018-06-05Pulse sequence gCOSY
Solvent cdcl_3 Temperature 25
Specrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S157. COSY of **6a**

PDC-03-157-MNR

Sample Name **PDC-03-157-MNR**
Date collected **2018-06-05**Pulse sequence **NOESY**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S158. NOESY of **6a**



Figure S160. ^{13}C NMR (CDCl₃, 125 MHz) of **3k**

PDC-04-38F2

Sample Name **PDC-04-38F2**
Date collected **2018-11-22**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

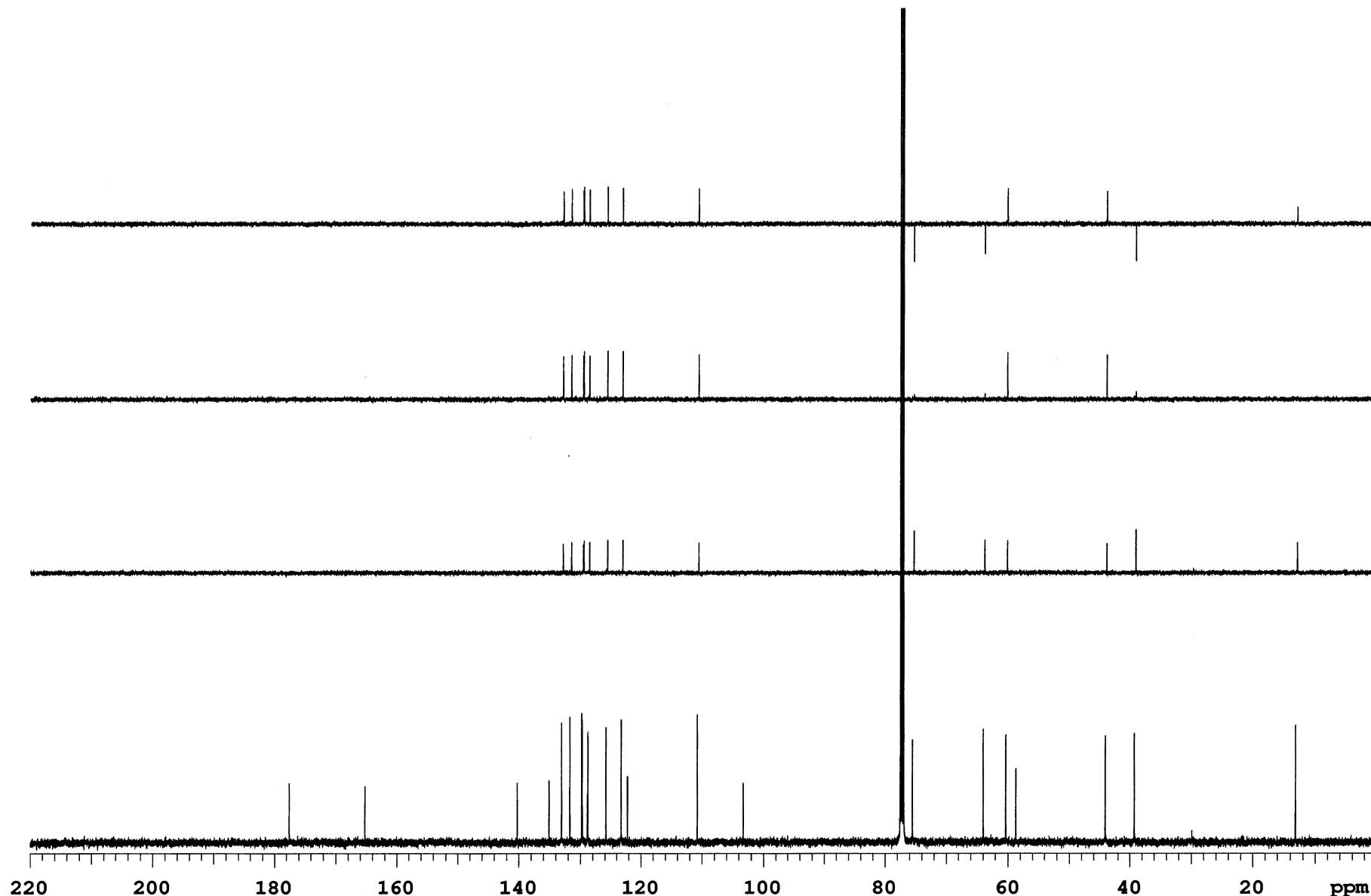


Figure S161. DEPT of **3k**

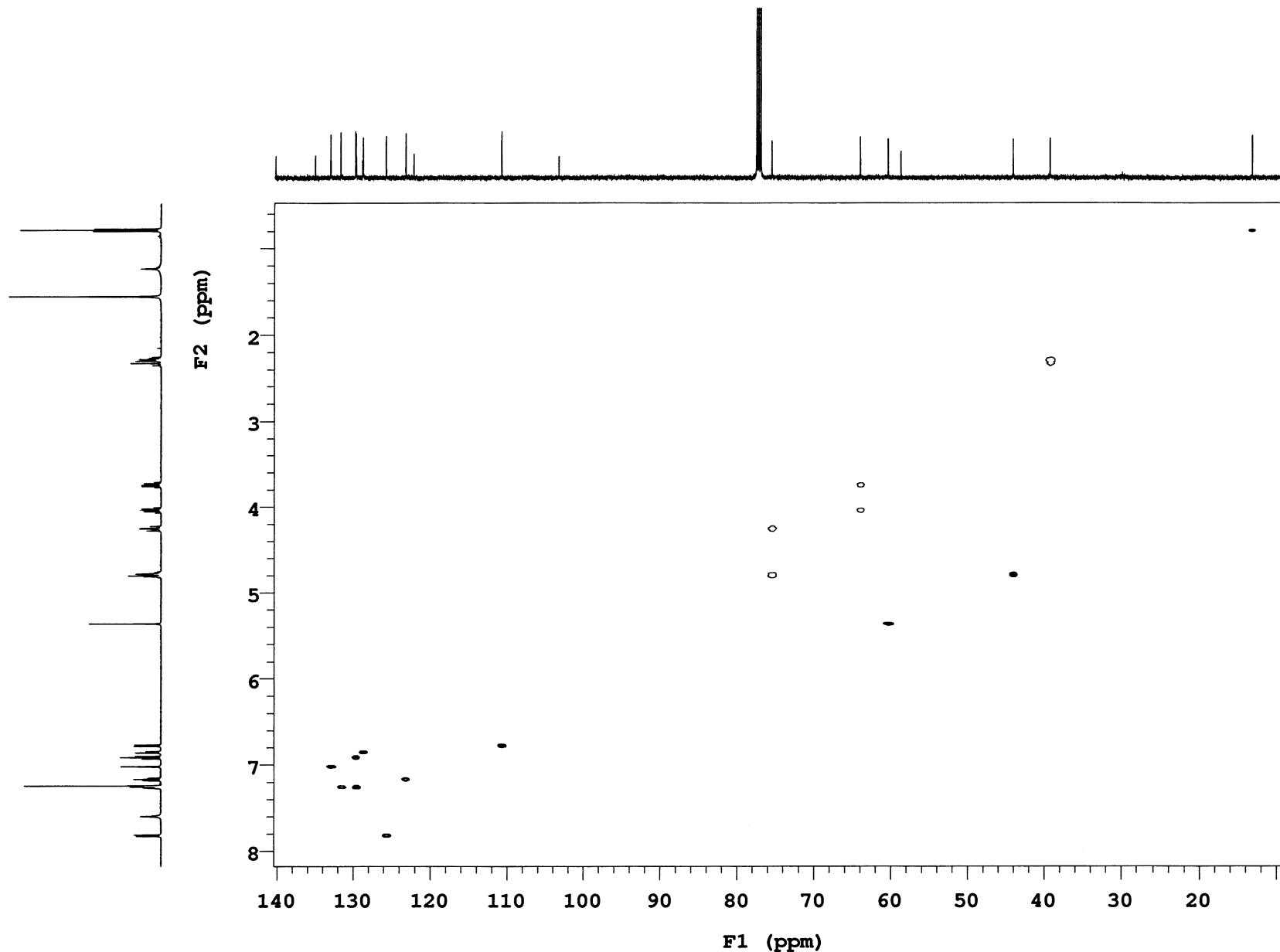
PDC-04-38F2

Sample Name **PDC-04-38F2**
Date collected **2018-11-22**

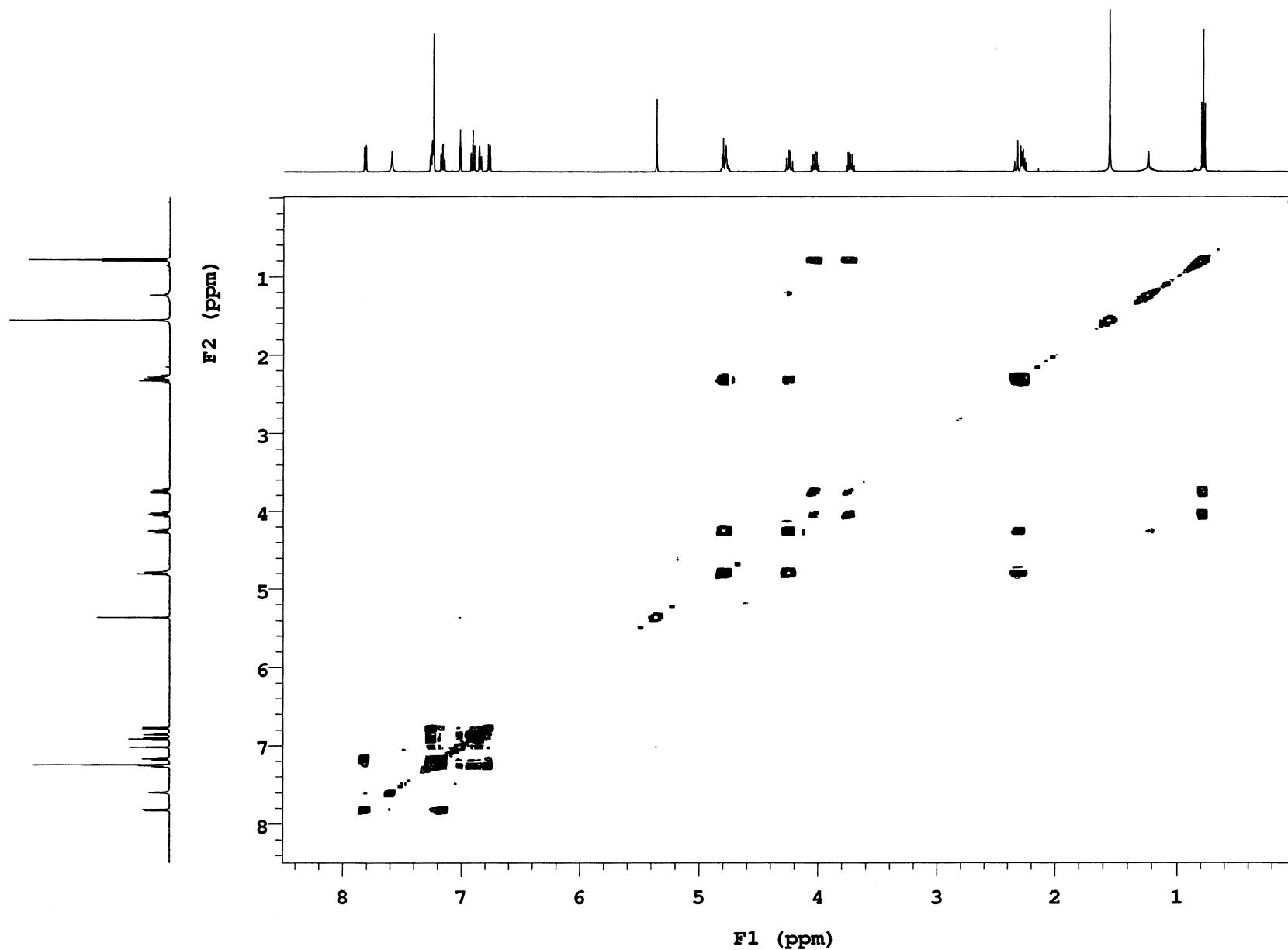
Pulse sequence **gHSQC**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

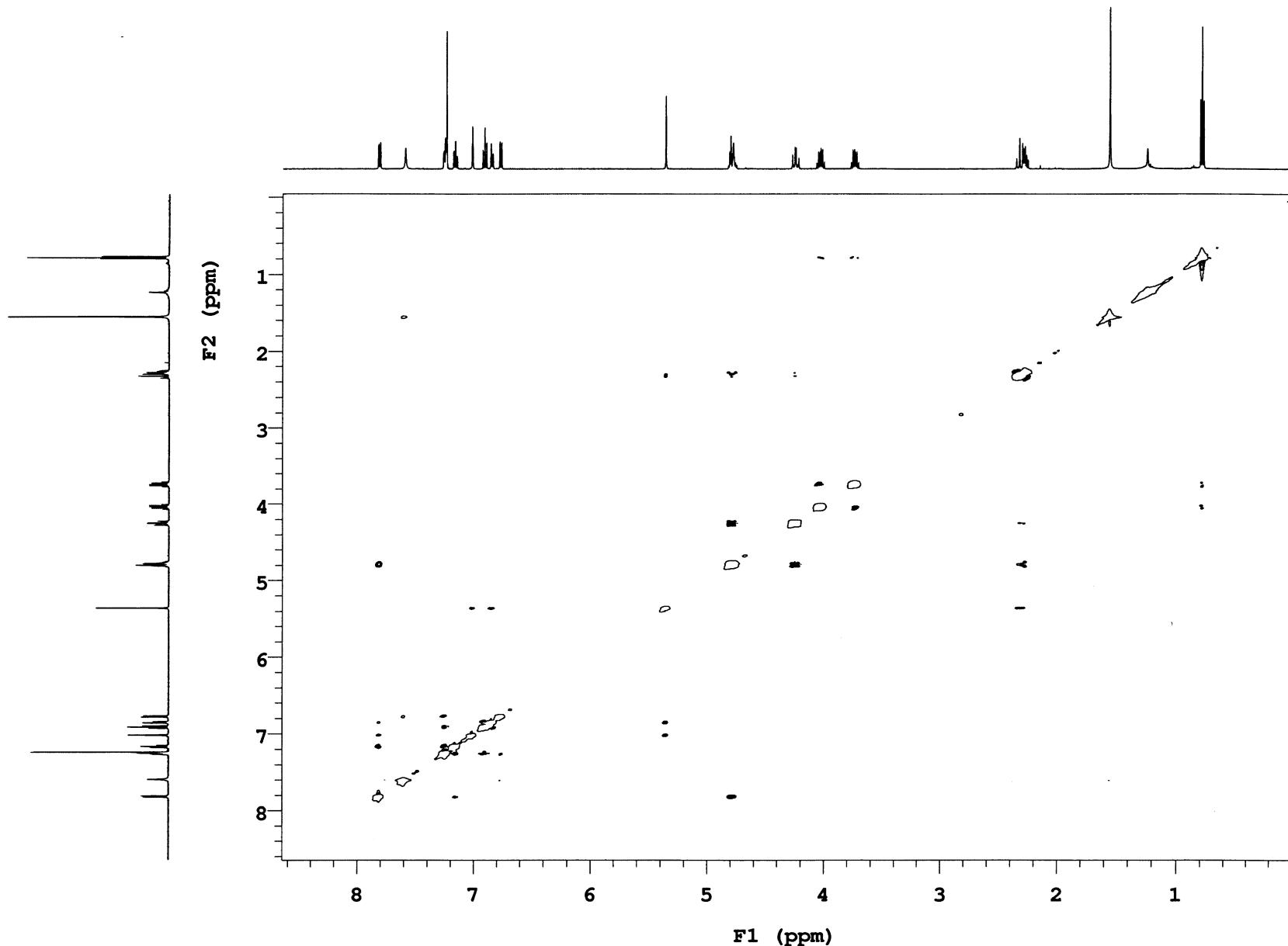
Study owner **vnmr2**
Operator **vnmr2**

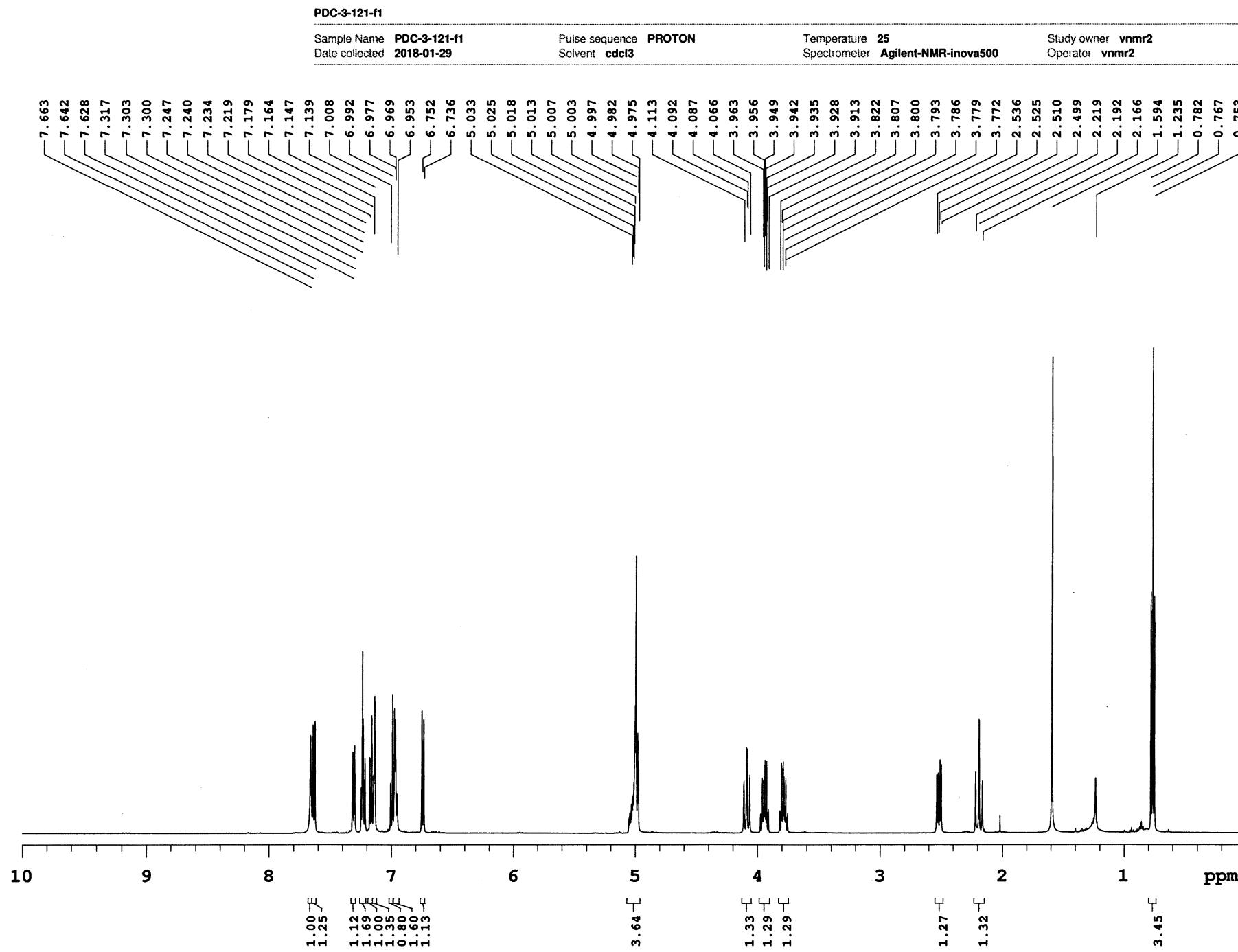
Figure S162. HSQC of **3k**

PDC-04-38F2

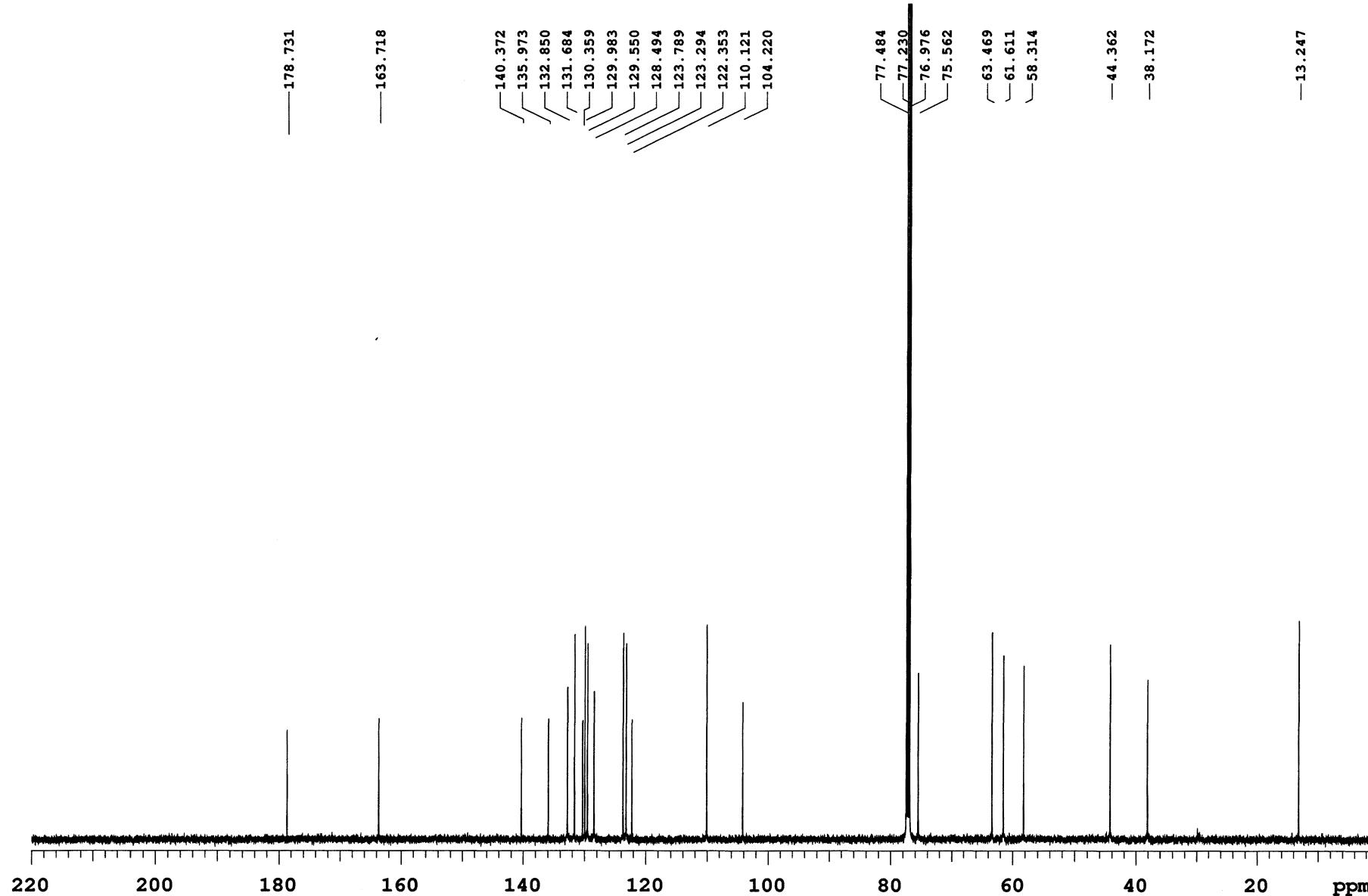
Sample Name PDC-04-38F2
Date collected 2018-11-22Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S163. COSY of **3k**

PDC-04-38F2

Sample Name **PDC-04-38F2**
Date collected **2018-11-22**Pulse sequence **NOESY**
Solvent **cdcl3**Temperature **25**
Specrometer **Agilent-NMR-Inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S164. NOESY of **3k**



Sample Name **PDC-3-121-f1**
 Date collected **2018-01-29**
 Pulse sequence **CARBON**
 Solvent **cdcl3**
 Temperature **25**
Spectrometer 25 Agilent-NMR-inova500
 Study owner **vnmr2**
 Operator **vnmr2**

Figure S166. 13C NMR (CDCl₃, 125 MHz) of **4k**

PDC-3-121-f1

Sample Name **PDC-3-121-f1**
Date collected **2018-01-30**

Pulse sequence **DEPT**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

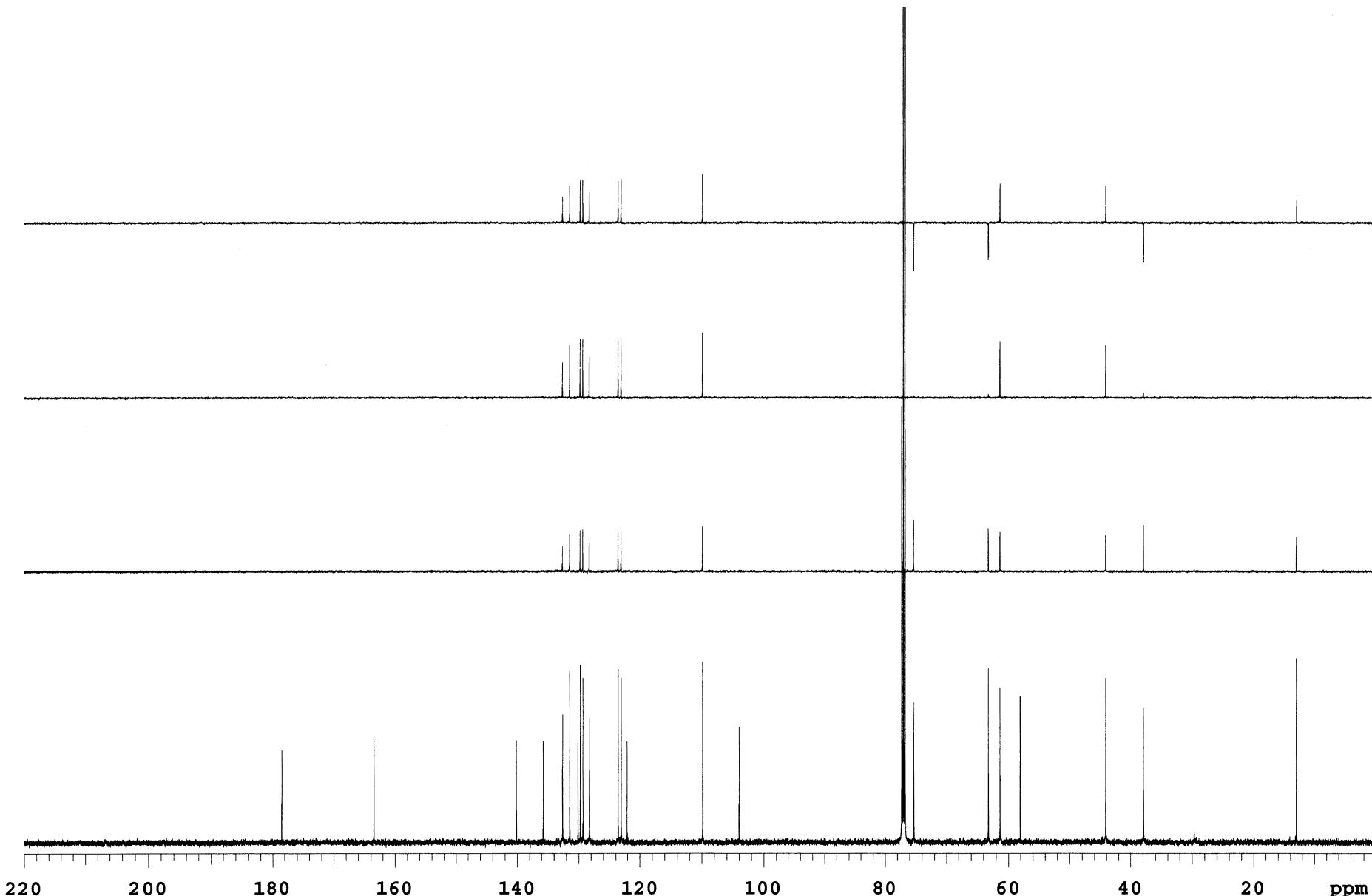


Figure S167. DEPT of 4k

PDC-3-121-f1

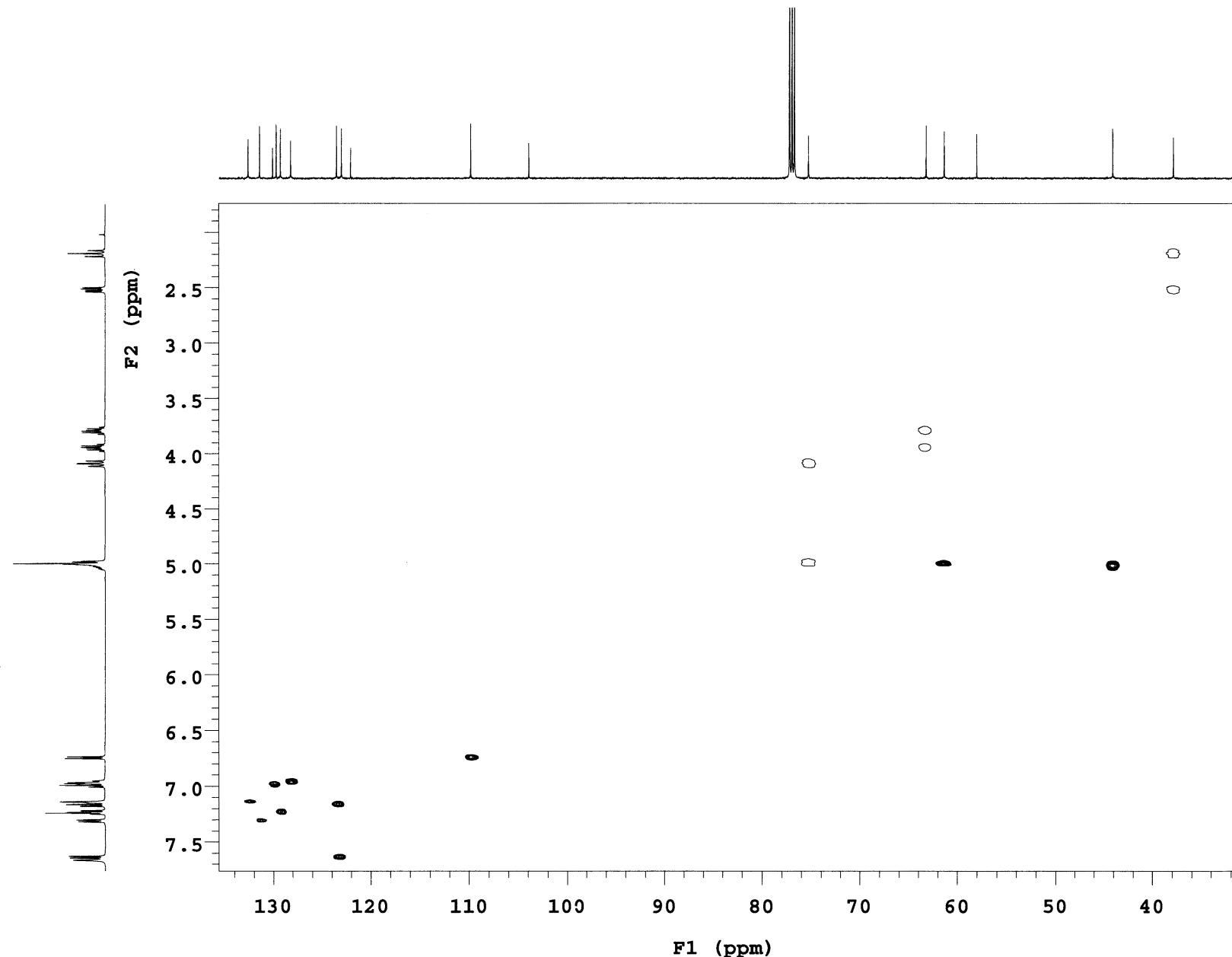
Sample Name PDC-3-121-f1
Date collected 2018-01-30Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S168. HSQC of 4k

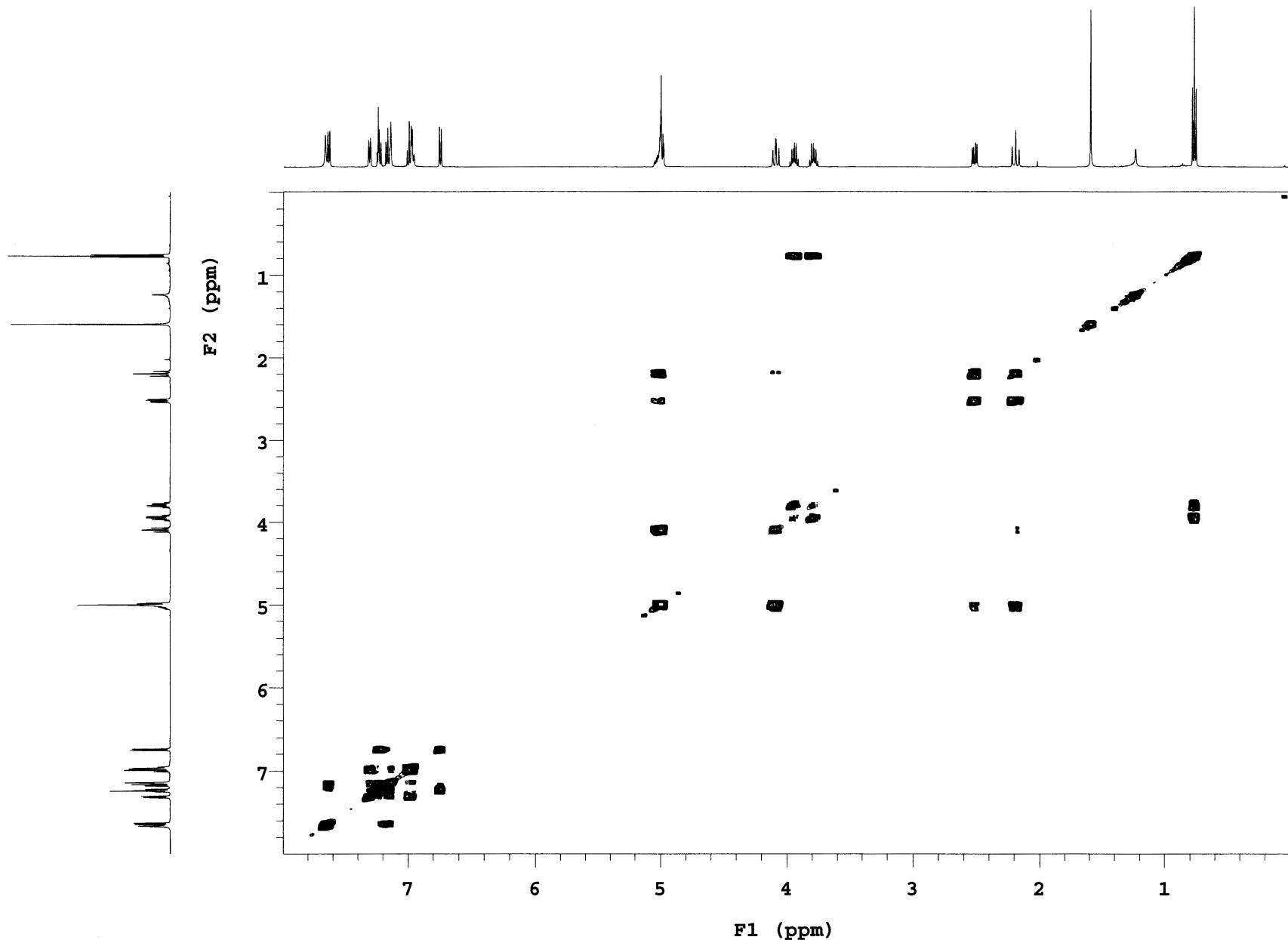
PDC-3-121-f1

Sample Name **PDC-3-121-f1**
Date collected **2018-01-30**

Pulse sequence **gCOSY**
Solvent **cdcl3**

Temperature **25**
Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
Operator **vnmr2**

Figure S169. COSY of **4k**

PDC-3-121-f1

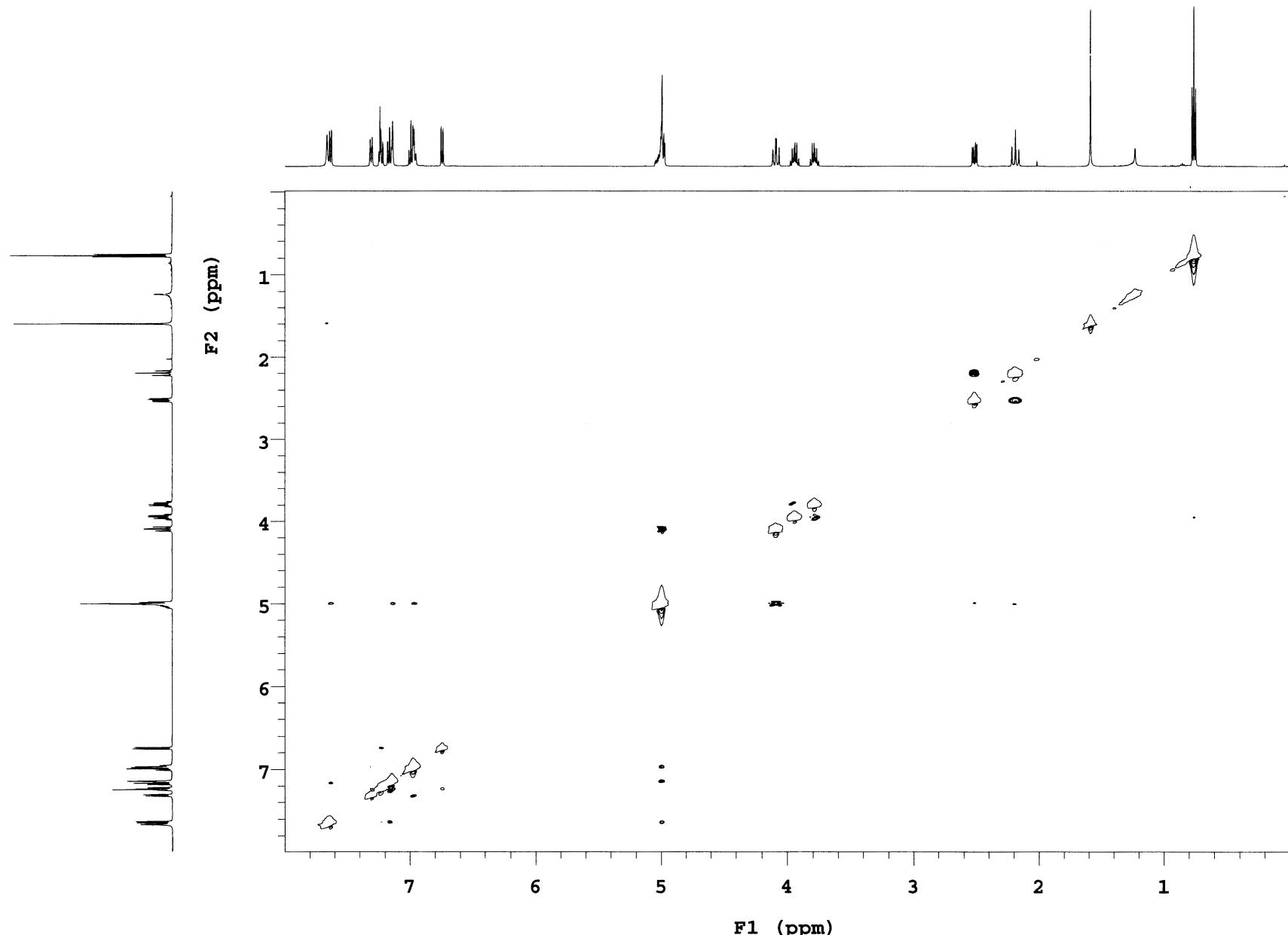
Sample Name PDC-3-121-f1
Date collected 2018-01-30Pulse sequence NOESY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner *vnmr2*
Operator *vnmr2*

Figure S170. NOESY of 4k

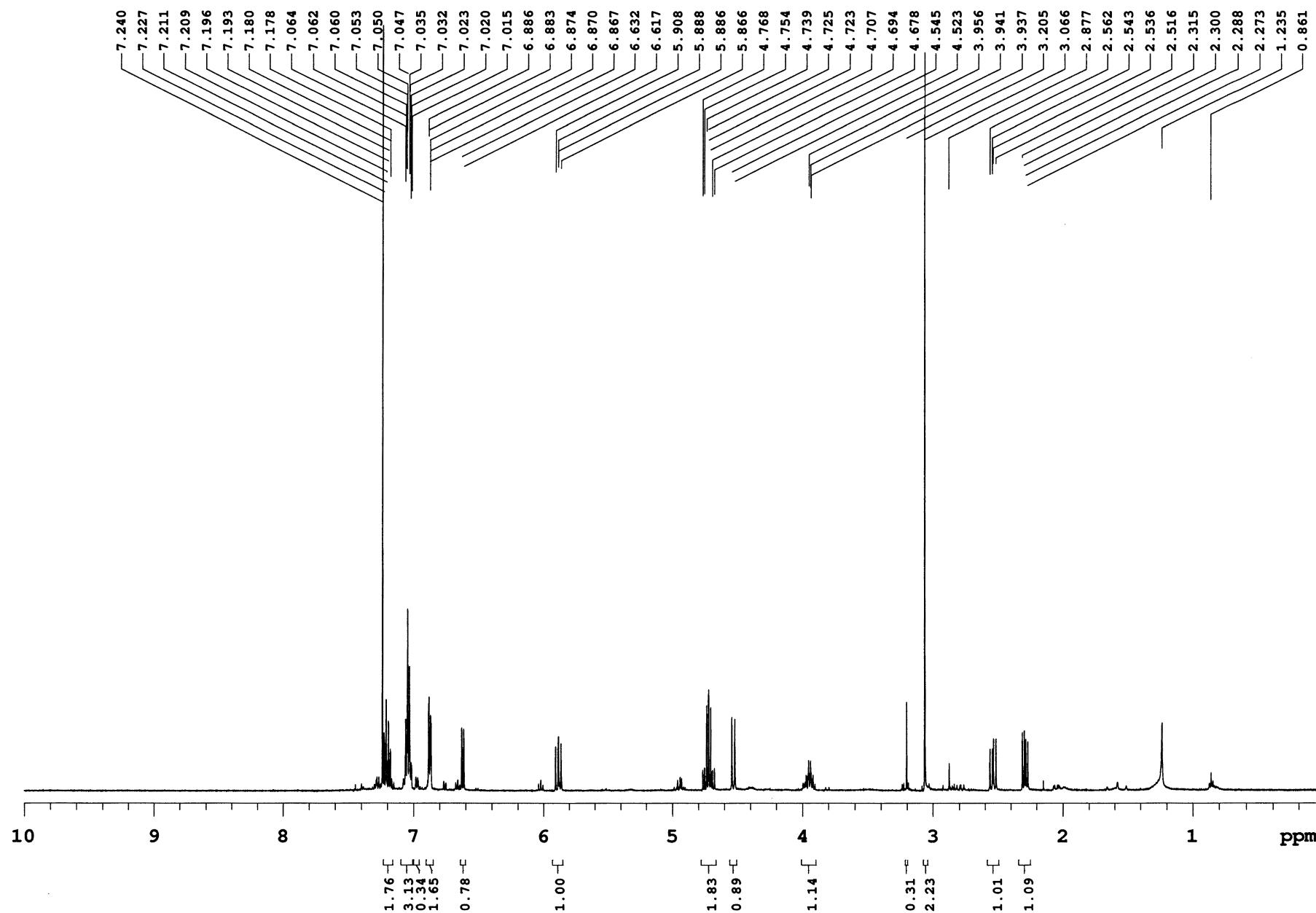
CLW-1-52-F2

Sample Name **CLW-1-52-F2**
 Date collected **2018-07-27**

Pulse sequence **PROTON**
 Solvent **cdcl3**

Temperature **25**
 Spectrometer **Agilent-NMR-inova500**

Study owner **vnmr2**
 Operator **vnmr2**



CLW-1-52-F2

Sample Name CLW-1-52-F2
Date collected 2018-07-26

Pulse sequence CARBON
Solvent *cdcl*3

Temperature 25
Spectrometer 25
Agilent-NMR-inova500

Study owner vnmr2
Operator vnmr2

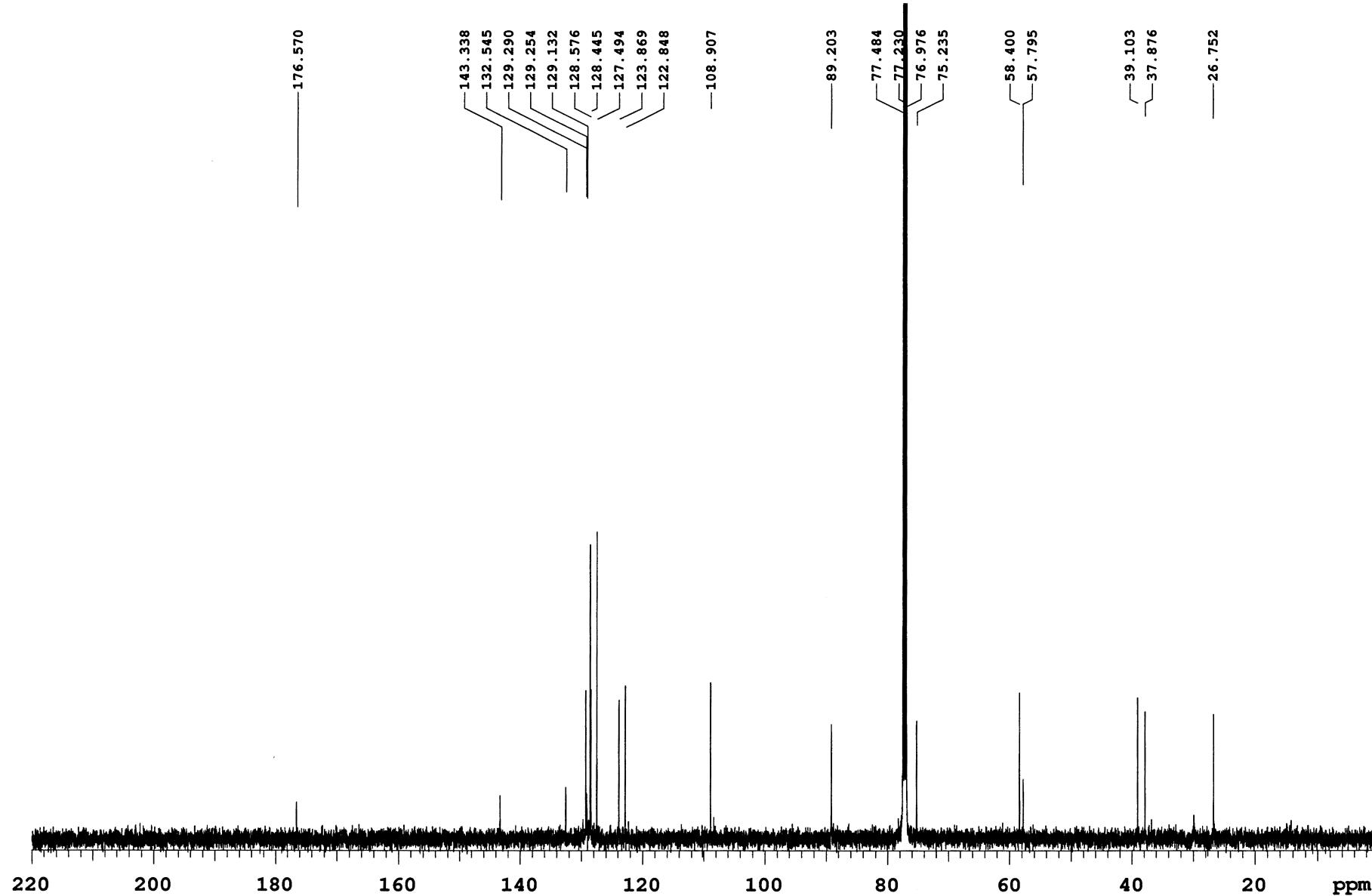


Figure S172. 13C NMR (*CDCl*3, 125 MHz) of 7a

CLW-1-52-F2

Sample Name CLW-1-52-F2
Date collected 2018-07-27

Pulse sequence DEPT
Solvent *cdcl*3

Temperature 25
Spectrometer Agilent-NMR-inova500

Study owner vnmr2
Operator vnmr2

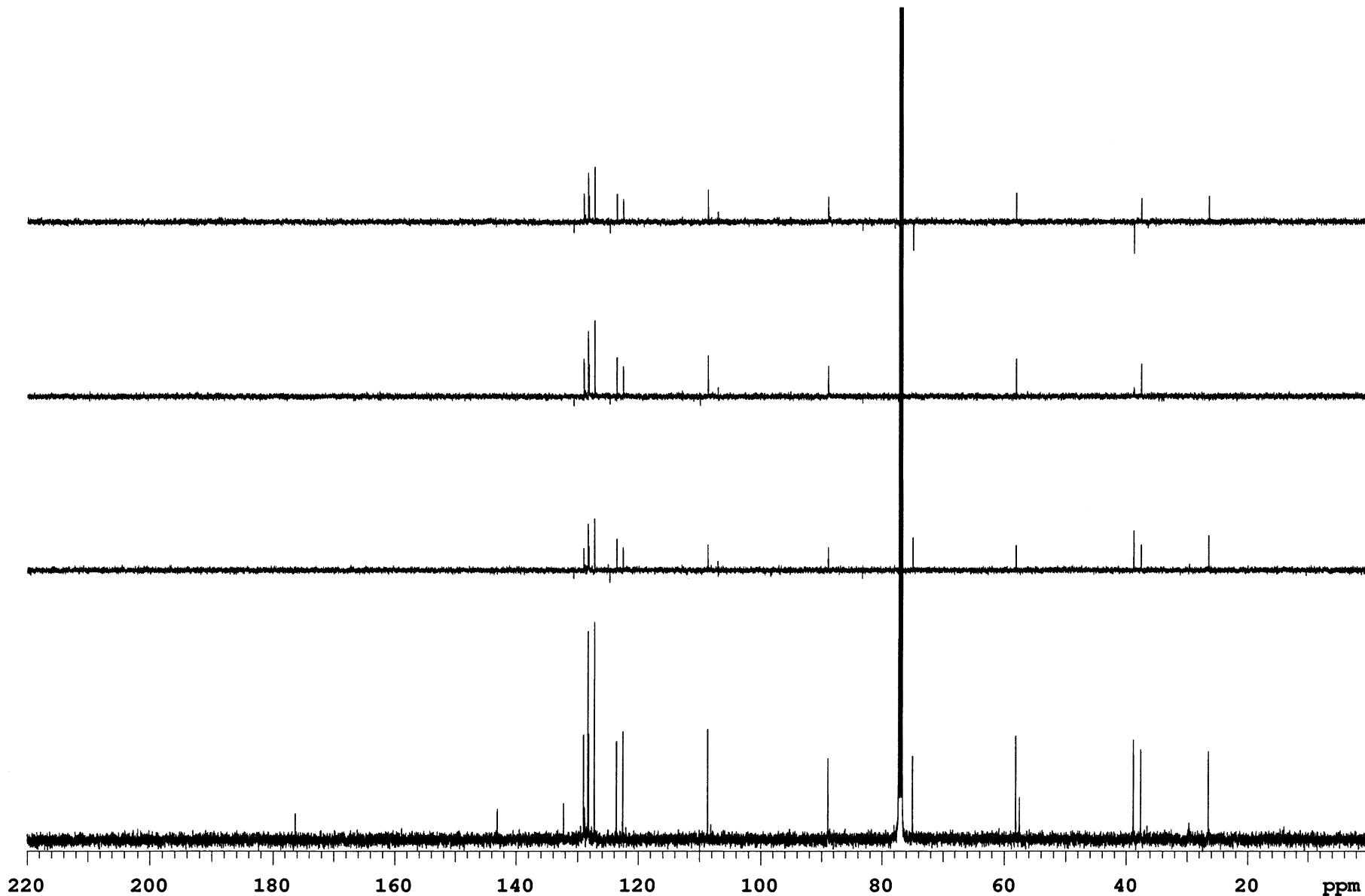


Figure S173. DEPT of 7a

CLW-1-52-F2

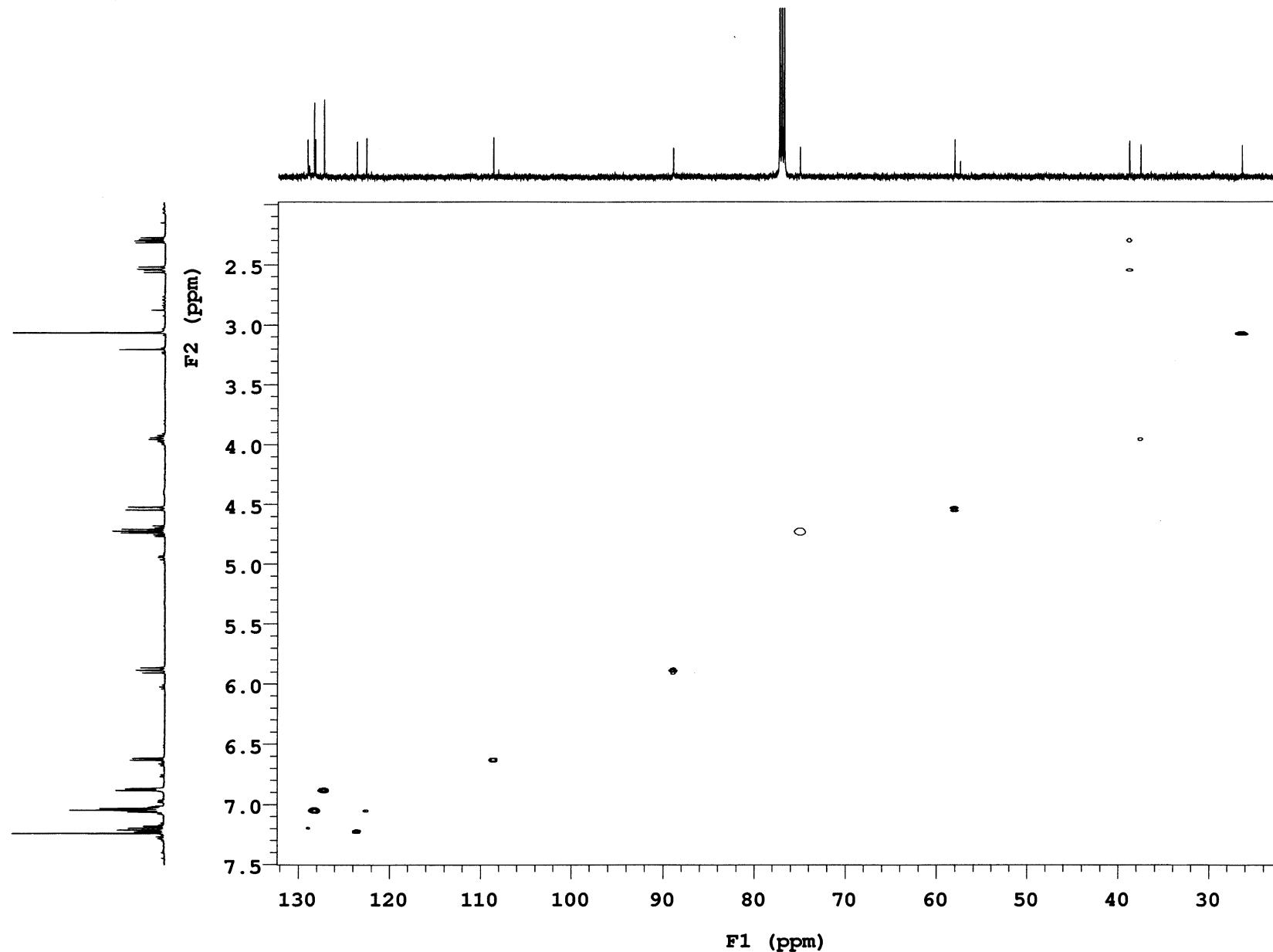
Sample Name CLW-1-52-F2
Date collected 2018-07-27Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S174. HSQC of 7a

CLW-1-52-F2

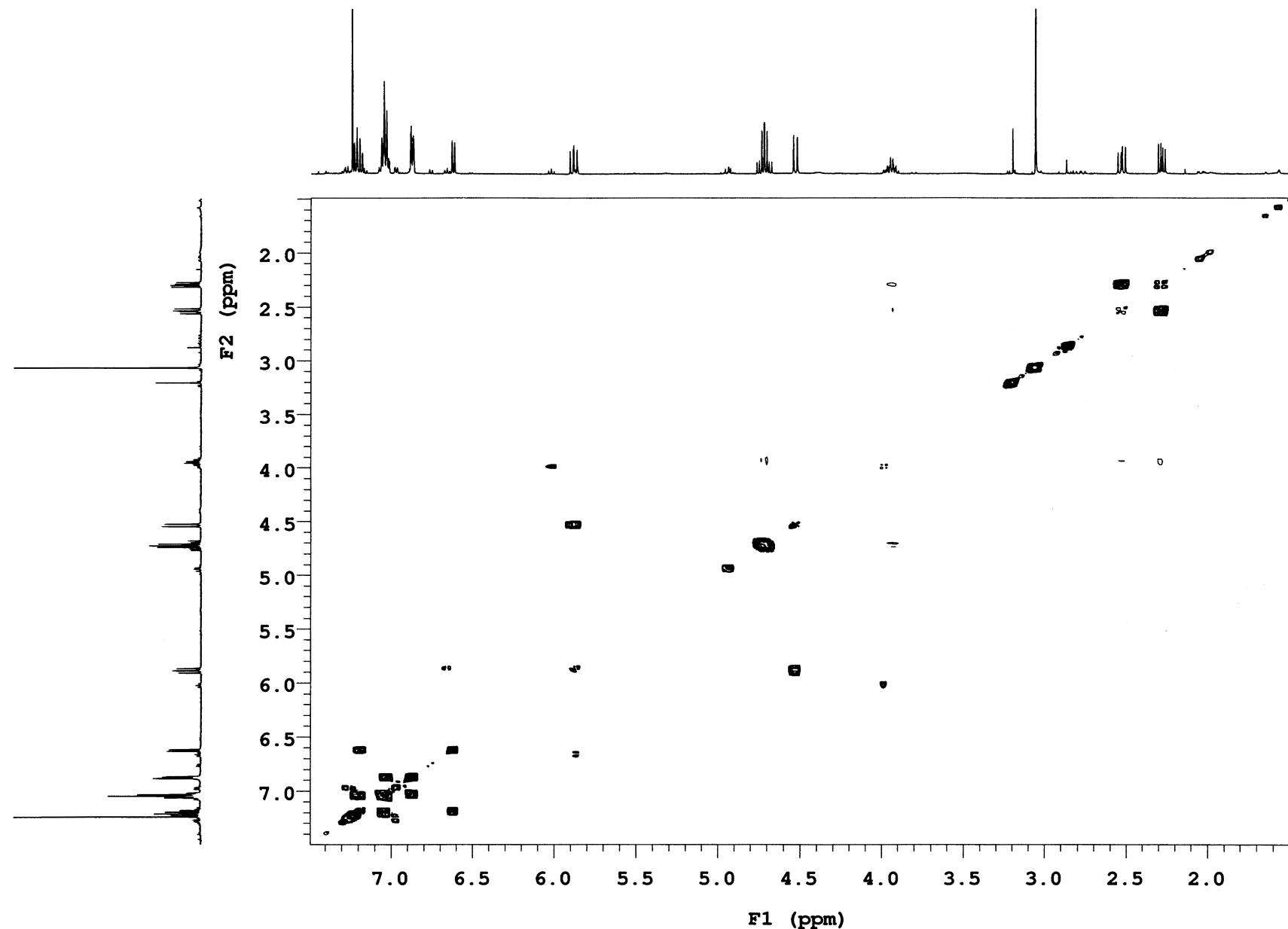
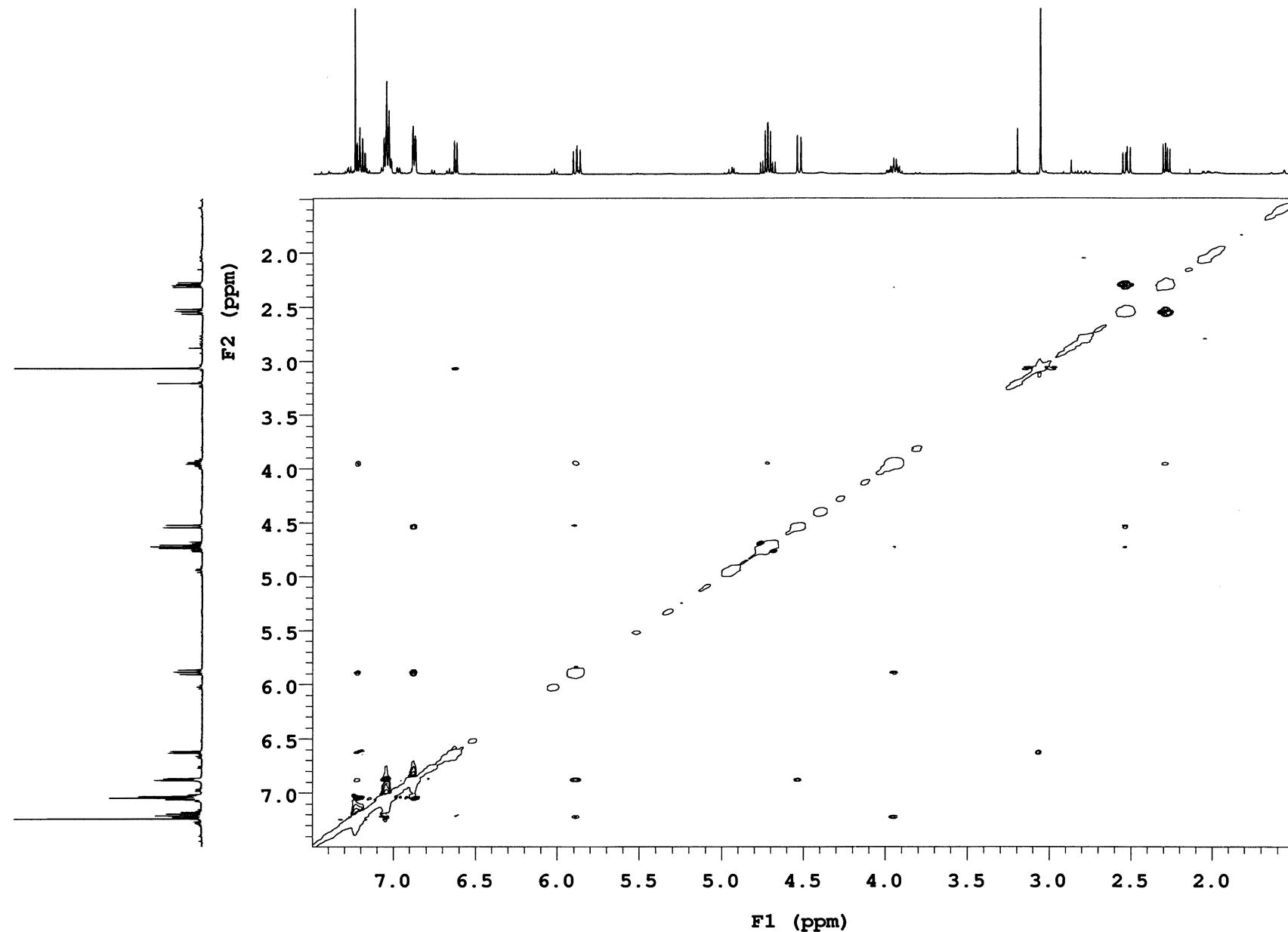
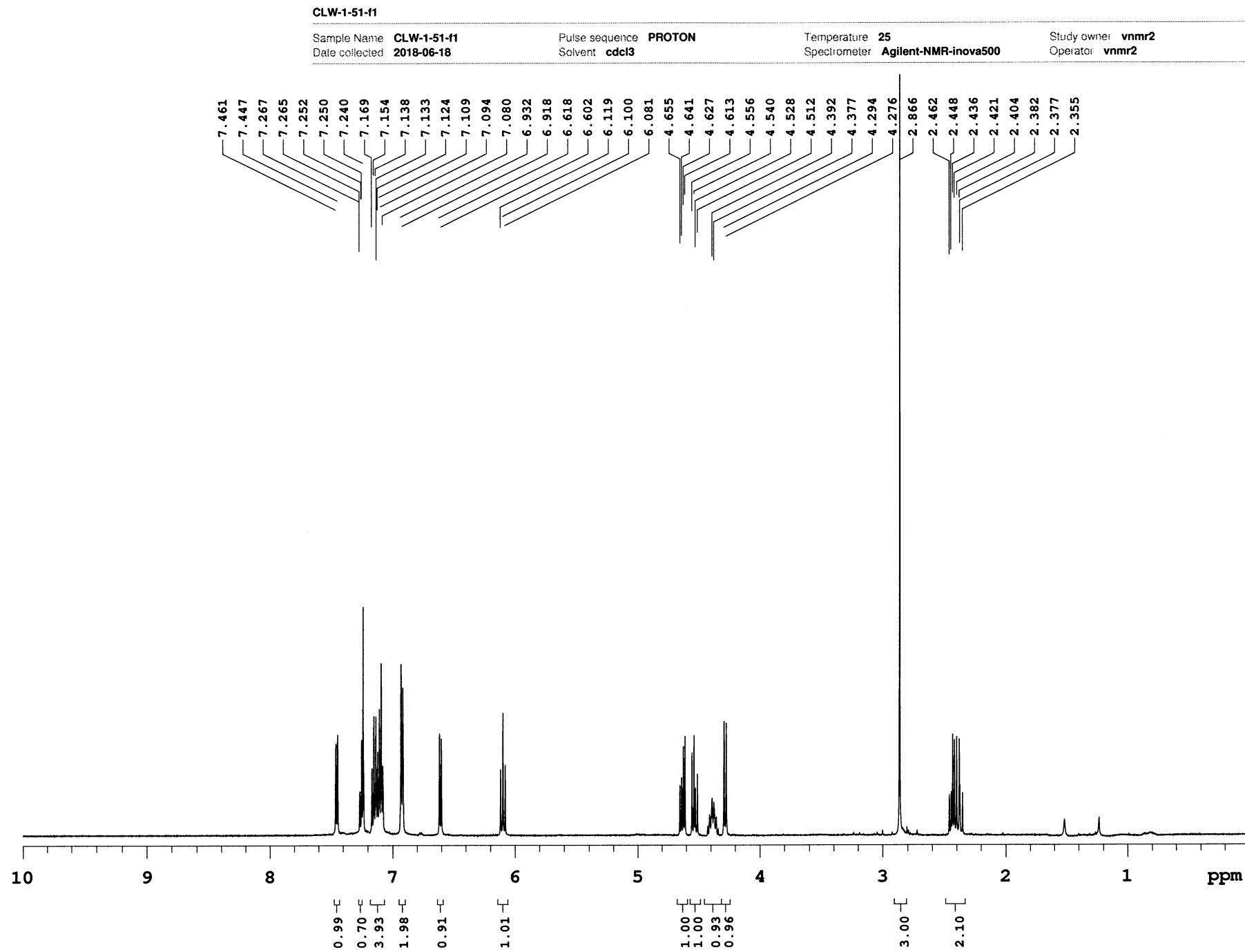
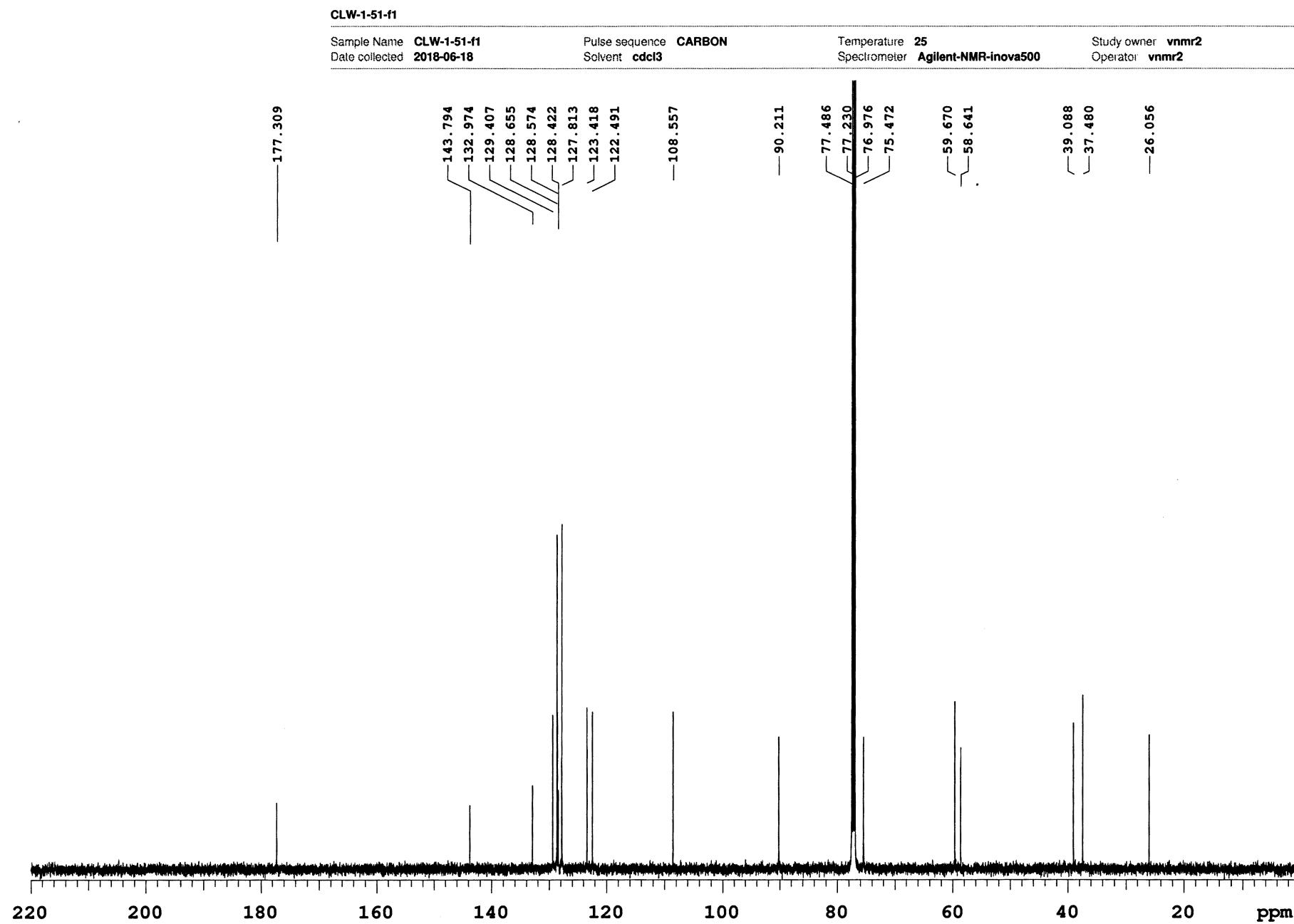
Sample Name CLW-1-52-F2
Date collected 2018-07-27Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

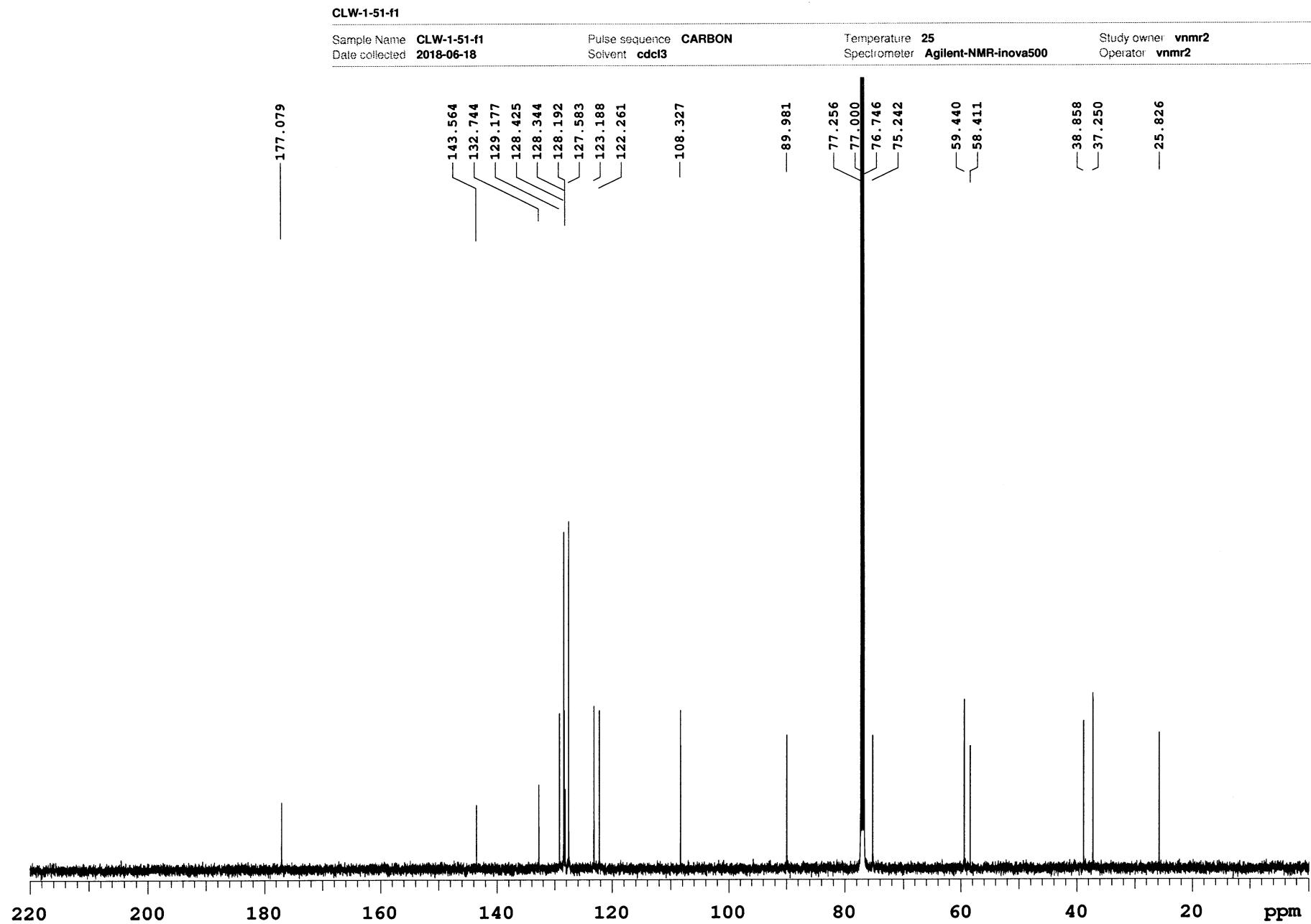
Figure S175. COSY of 7a

CLW-1-52-F2

Sample Name CLW-1-52-F2
Date collected 2018-07-27Pulse sequence NOESY
Solvent cdcl_3 Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S176. NOESY of **7a**



Figure S178. ^{13}C NMR (CDCl₃, 125 MHz) of **8a**

Figure S179. ^{13}C NMR (CDCl_3 , 125 MHz) of **8a**

CLW-1-51-f1

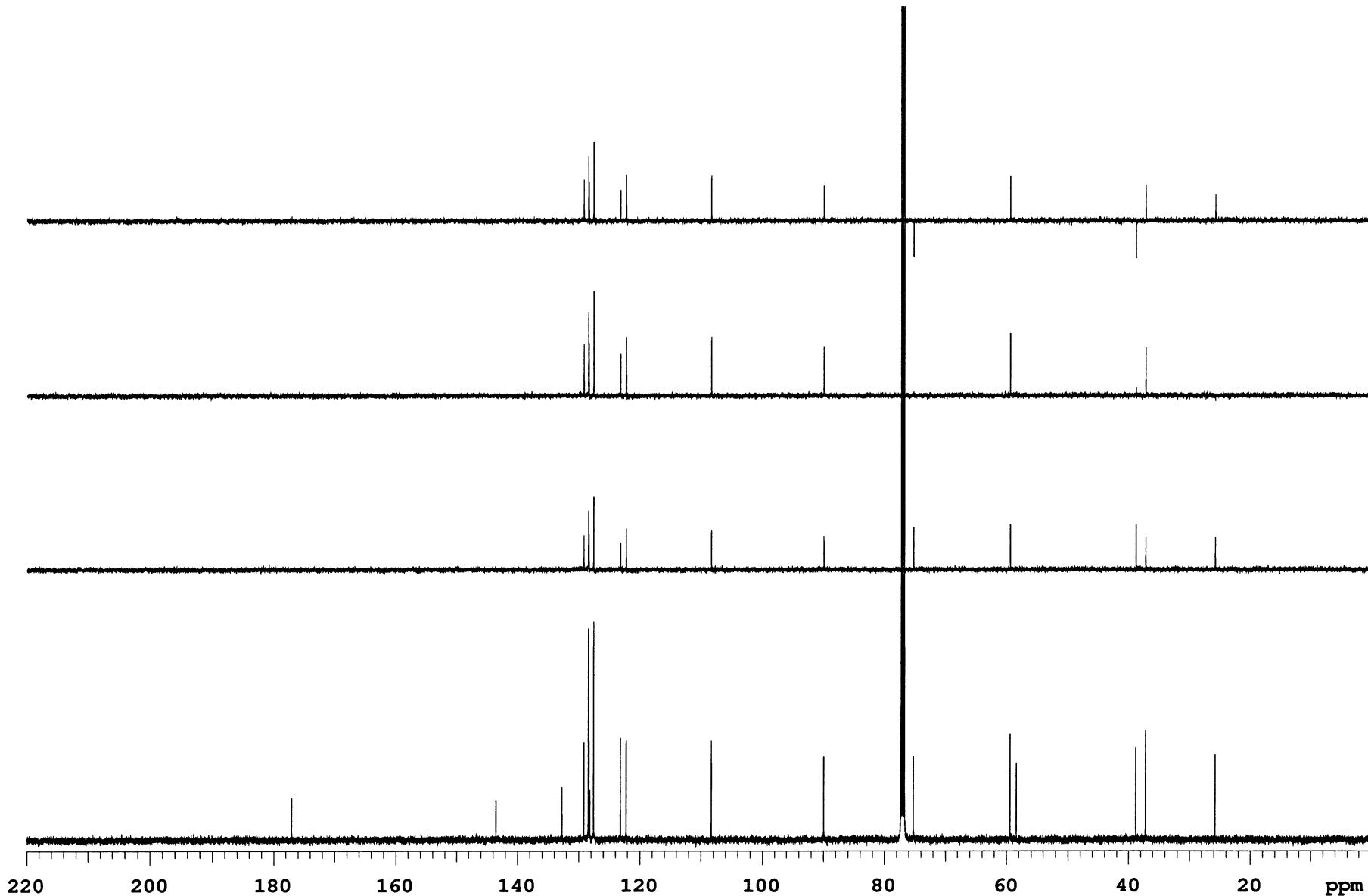
Sample Name CLW-1-51-f1
Date collected 2018-06-19Pulse sequence DEPT
Solvent CDCl_3 Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S180. DEPT of 8a

CLW-1-51-f1

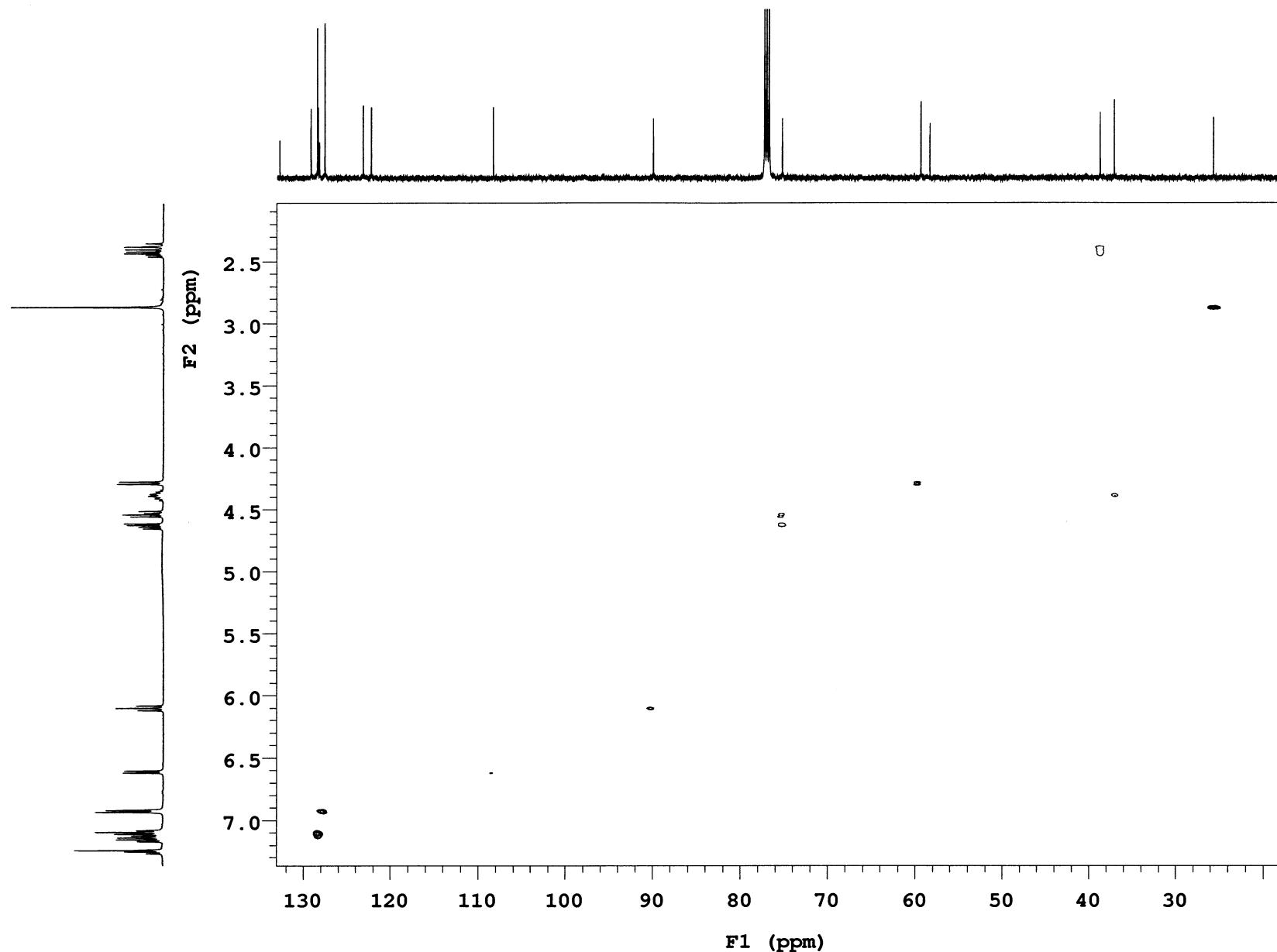
Sample Name CLW-1-51-f1
Date collected 2018-06-19Pulse sequence gHSQC
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S181. HSQC of 8a

CLW-1-51-f1

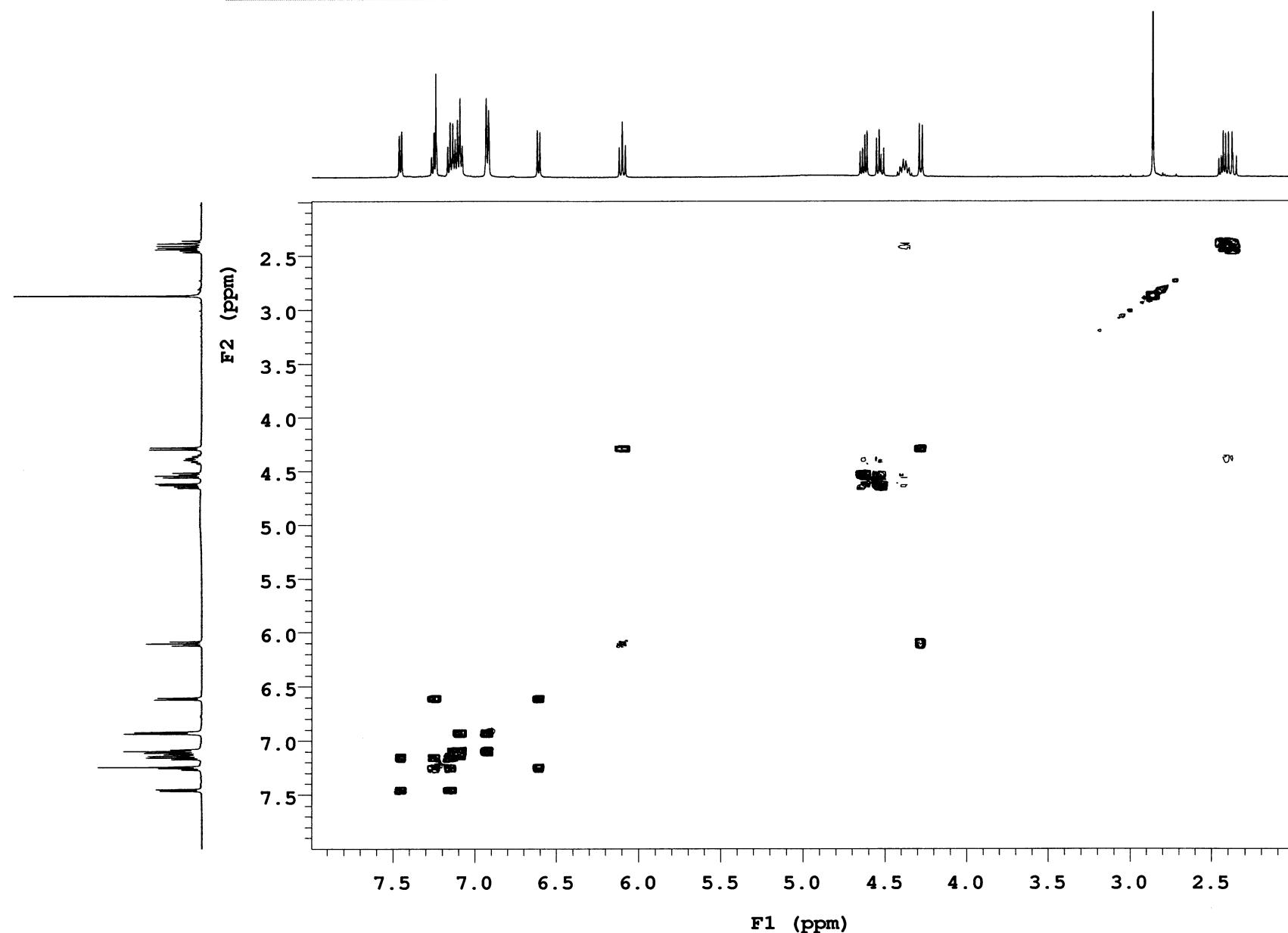
Sample Name CLW-1-51-f1
Date collected 2018-06-19Pulse sequence gCOSY
Solvent CDCl_3 Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S182. COSY of 8a

CLW-1-51-f1

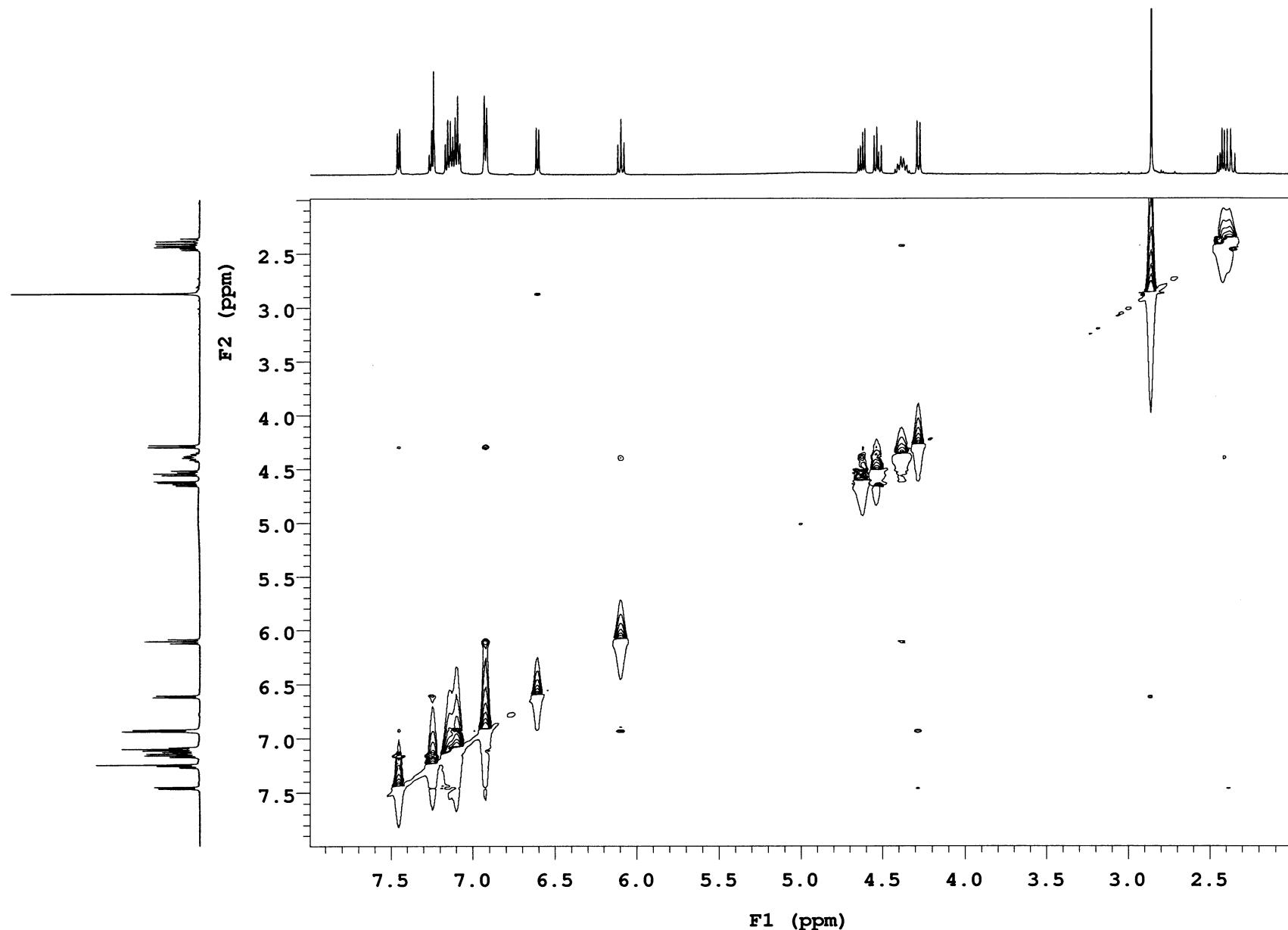
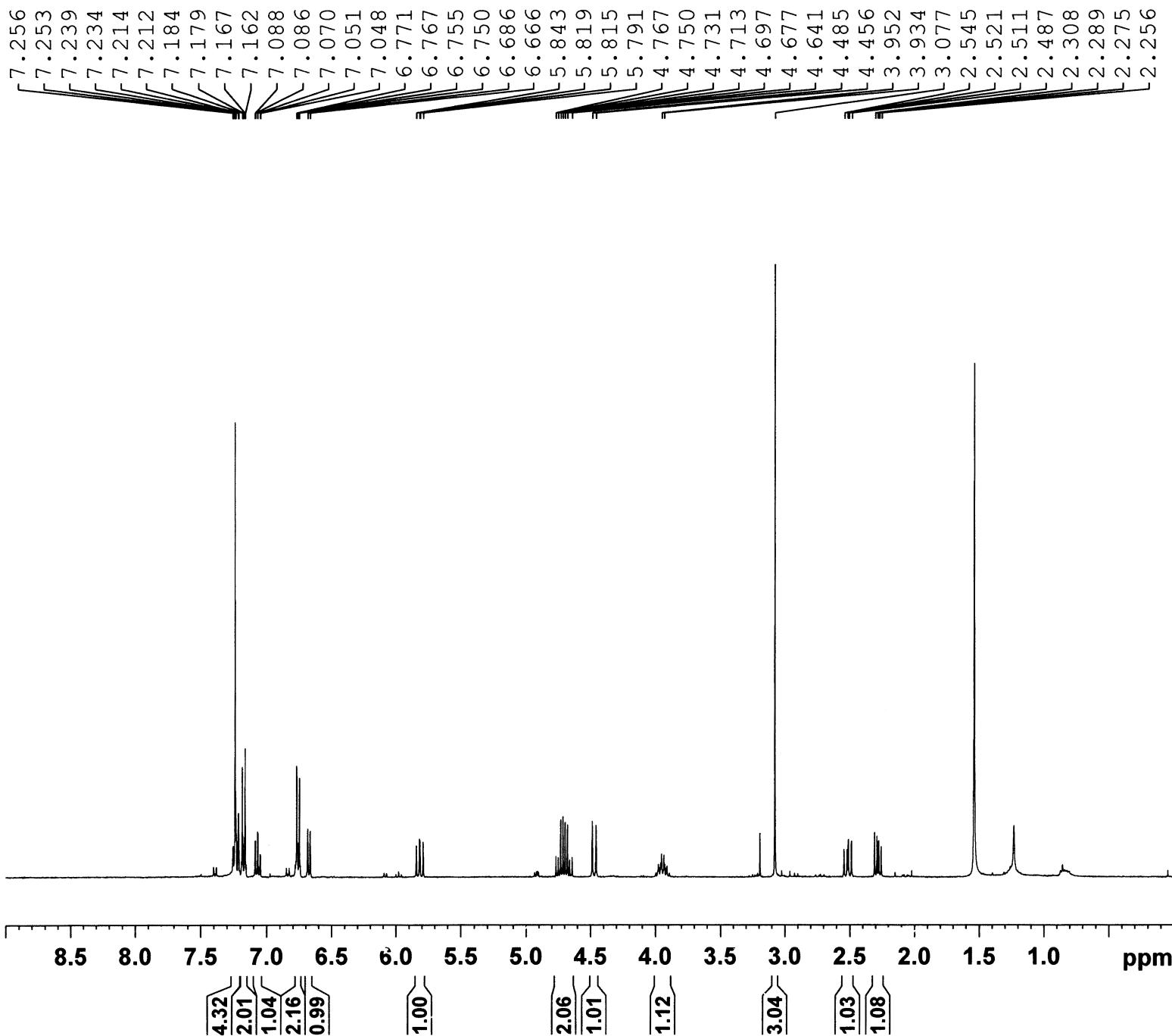
Sample Name CLW-1-51-f1
Date collected 2018-06-19Pulse sequence NOESY
Solvent *cdcl*3Temperature 120
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2

Figure S183. NOESY of 8a

Figure S184. ^1H NMR (CDCl_3 , 400 MHz) of **9b**

S196



Current Data Parameters
 NAME PDC-04-028F2
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180811
 Time 15.53 h
 INSTRUM spect
 PROBHD Z108618_0922 (zg30
 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 298.1 K
 D1 2.00000000 sec
 TDO 1
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 14.50 usec
 PLW1 12.50000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300181 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

Figure S185. ^{13}C NMR (CDCl_3 , 100 MHz) of **9b**

S197

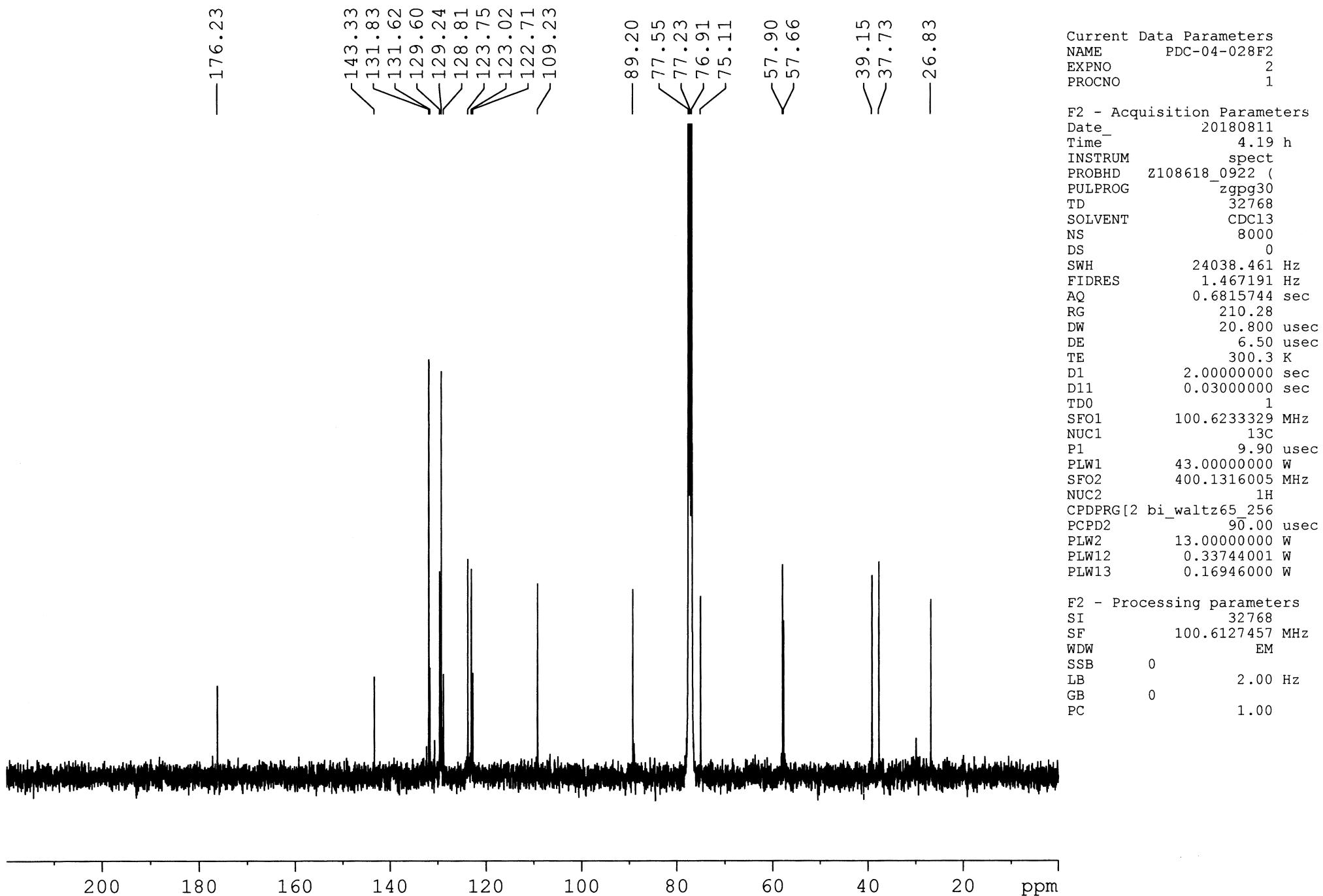
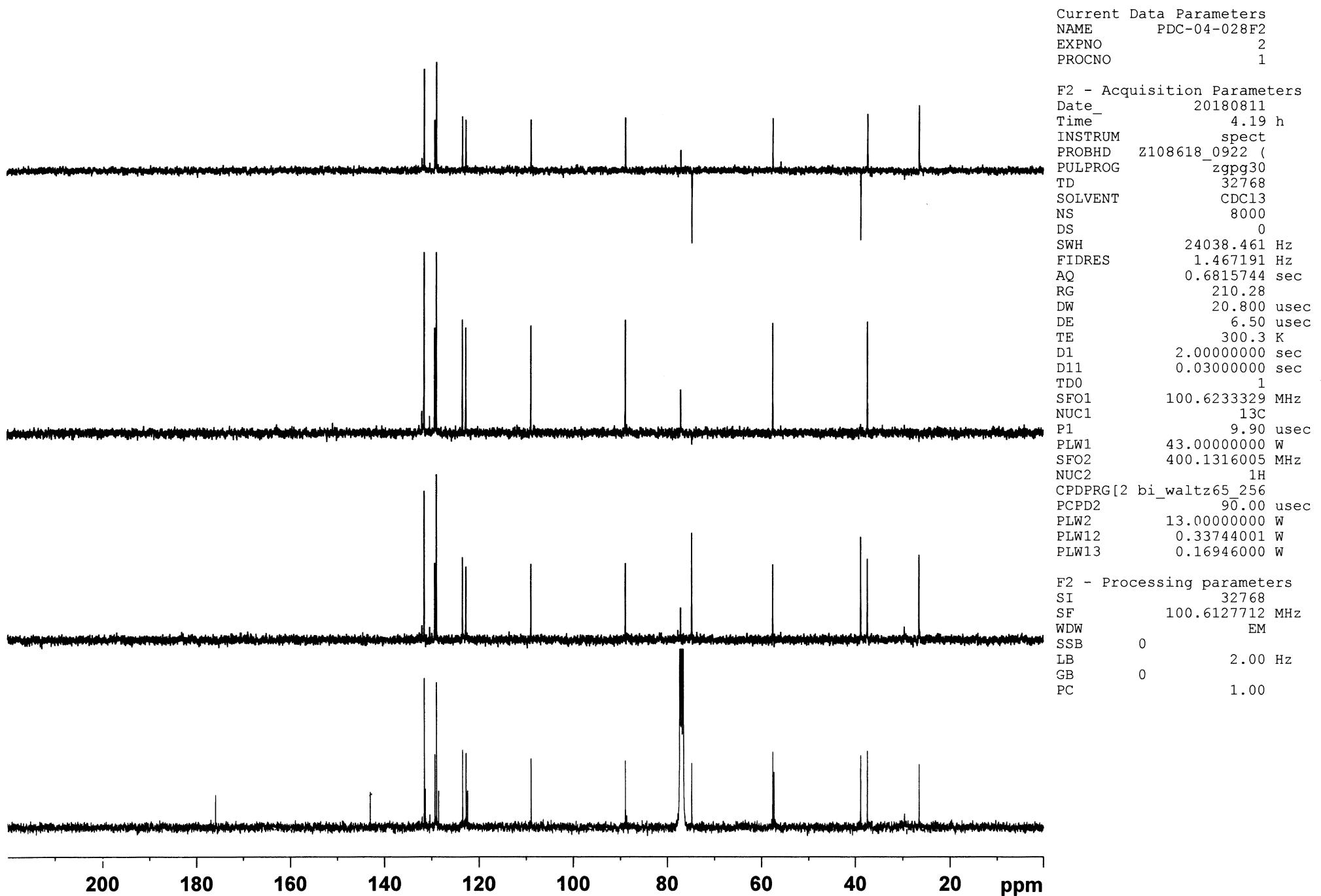
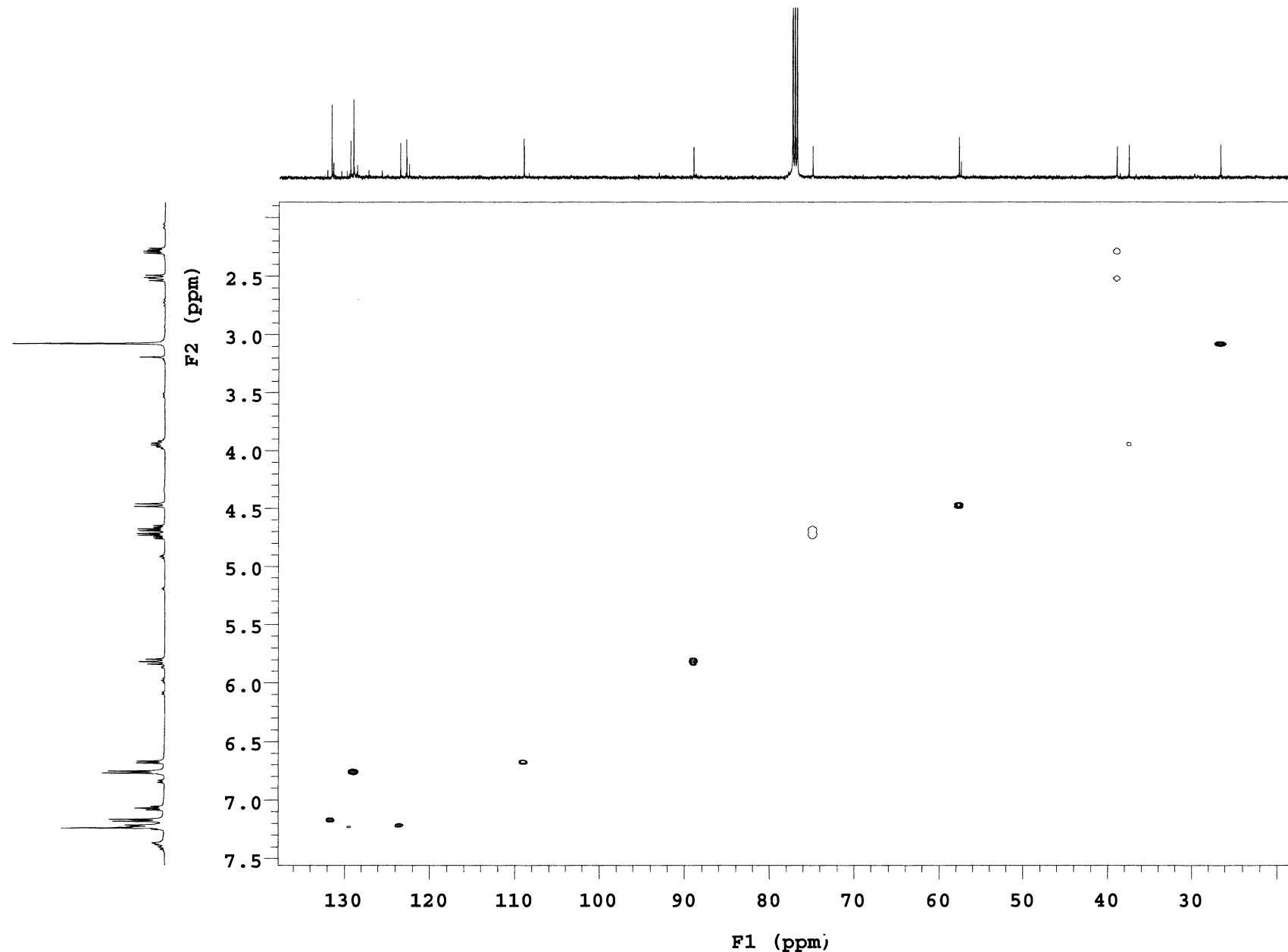


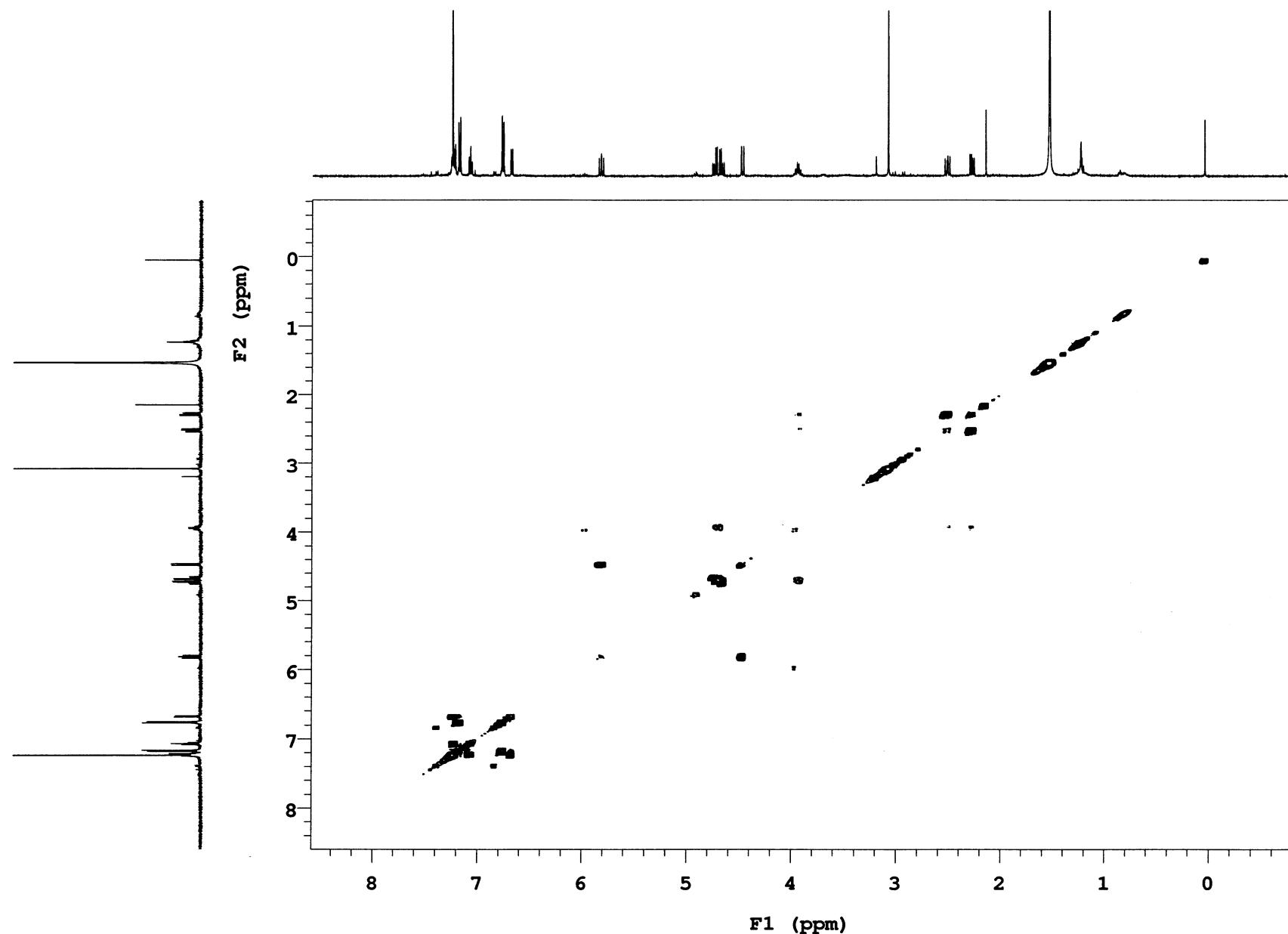
Figure S186. DEPT of 9b



PDC-03-102-f2

Sample Name **PDC-03-102-f2**
Date collected **2017-11-10**Pulse sequence **HSQC**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S187. HSQC of **9b**

PDC-04-022F3

Sample Name PDC-04-022F3
Date collected 2018-07-21Pulse sequence gCOSY
Solvent *cdcl*3Temperature 25
Spectrometer Agilent-NMR-inova500Study owner vnmr2
Operator vnmr2Figure S188. COSY of **9b**

PDC-04-022F3

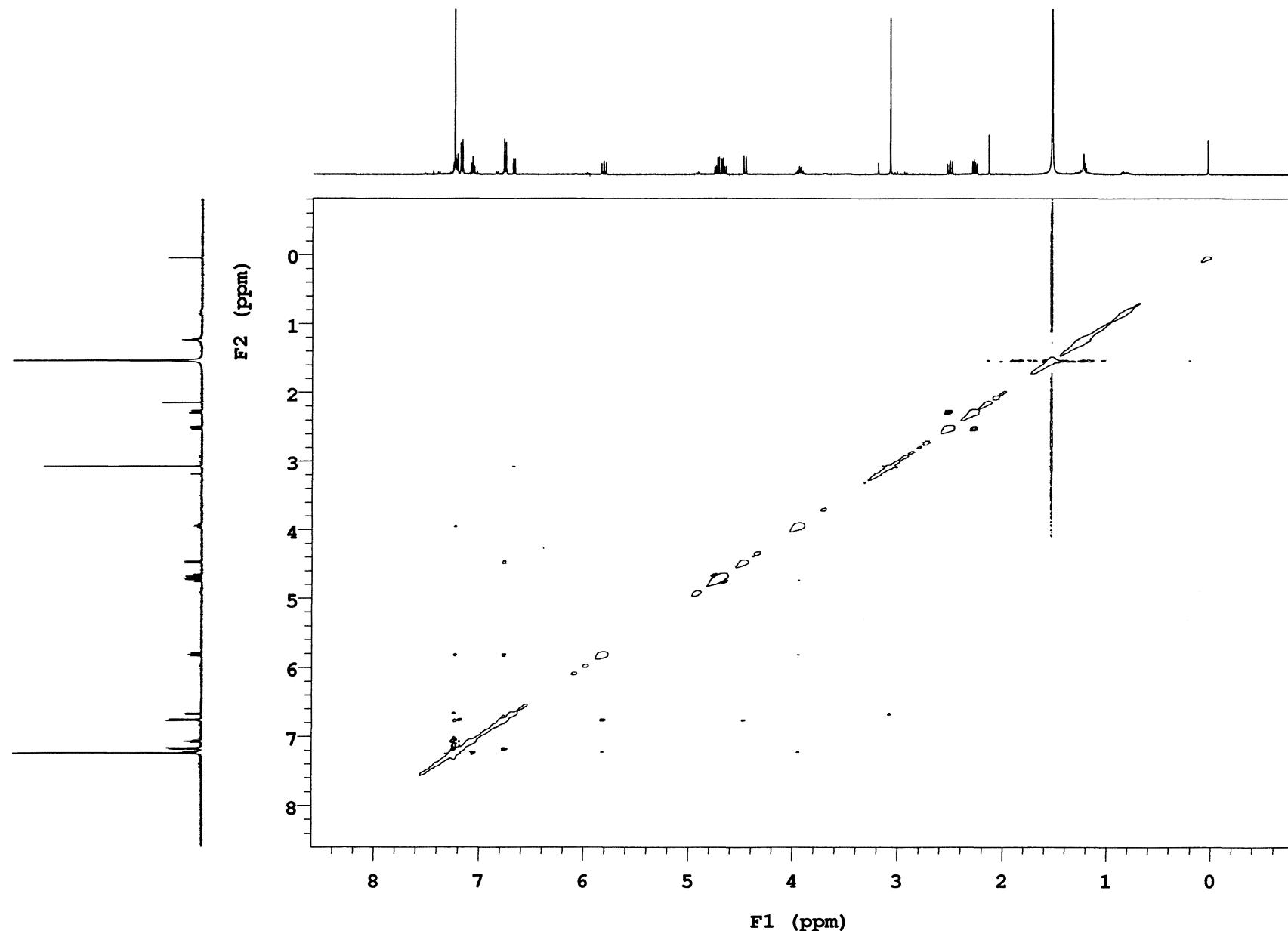
Sample Name **PDC-04-022F3**
Date collected **2018-07-21**Pulse sequence **NOESY**
Solvent **cdcl3**Temperature **25**
Spectrometer **Agilent-NMR-inova500**Study owner **vnmr2**
Operator **vnmr2**Figure S189. NOESY of **9b**

Figure S190. ^1H NMR (CDCl_3 , 400 MHz) of **8b**

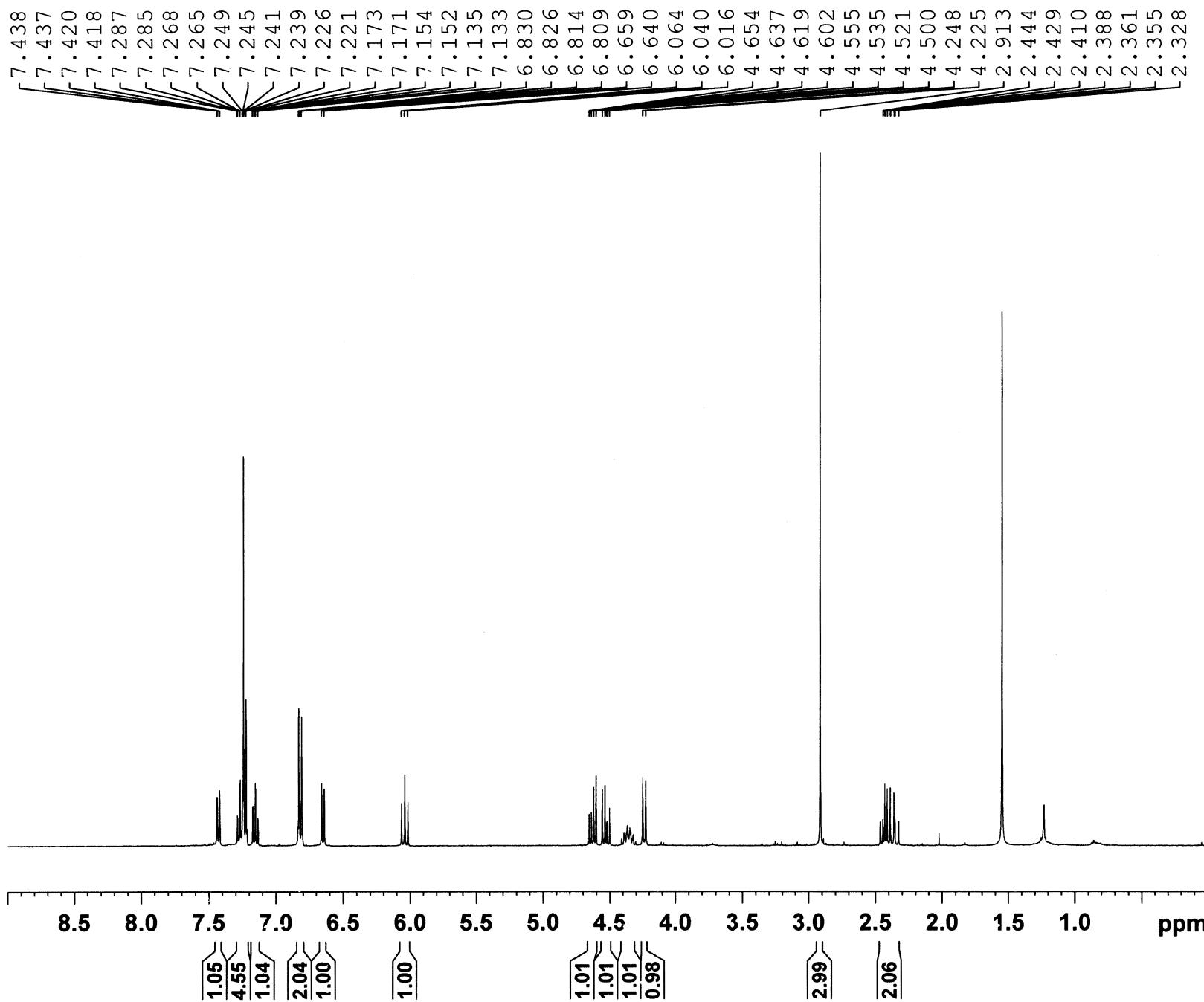


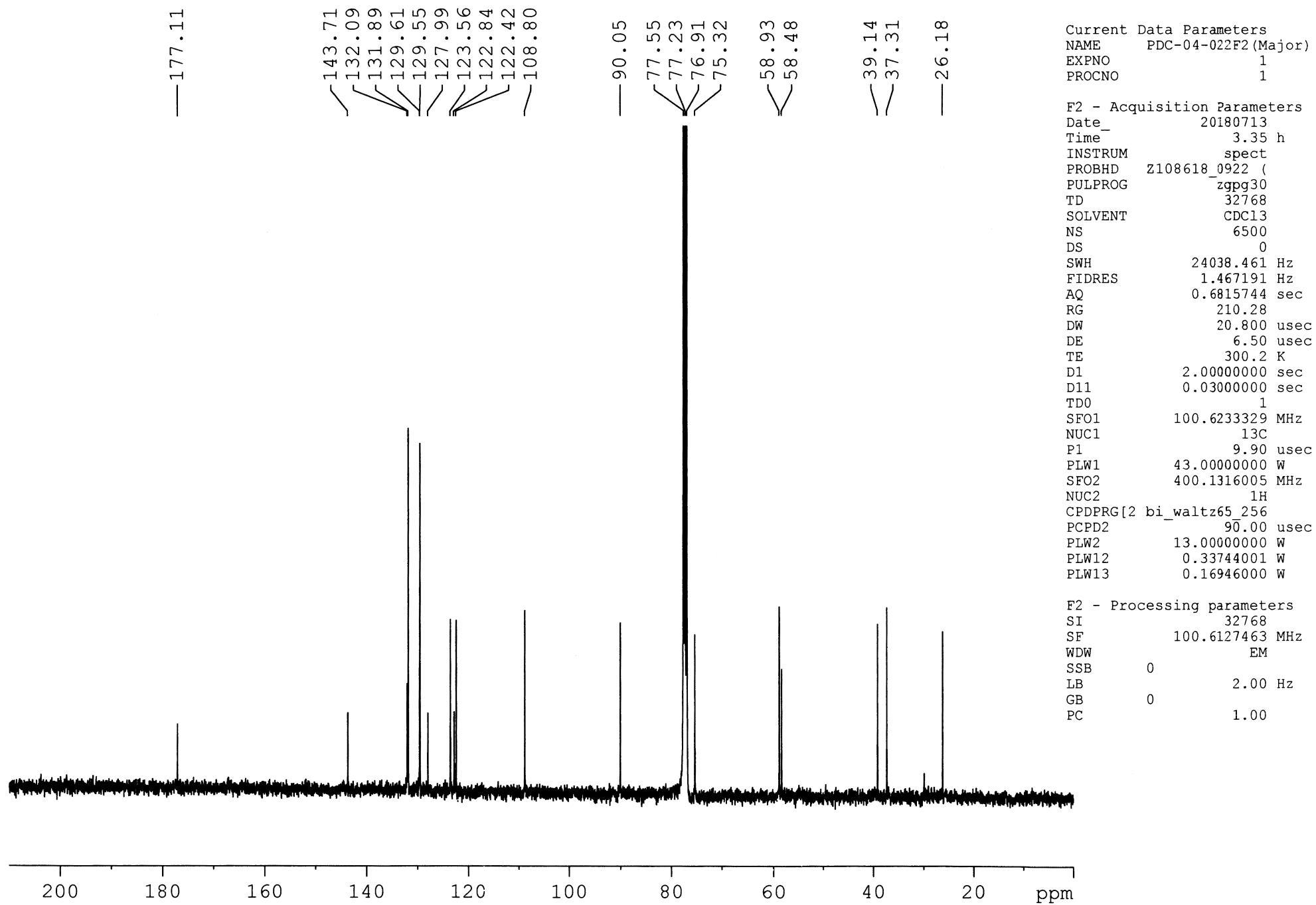
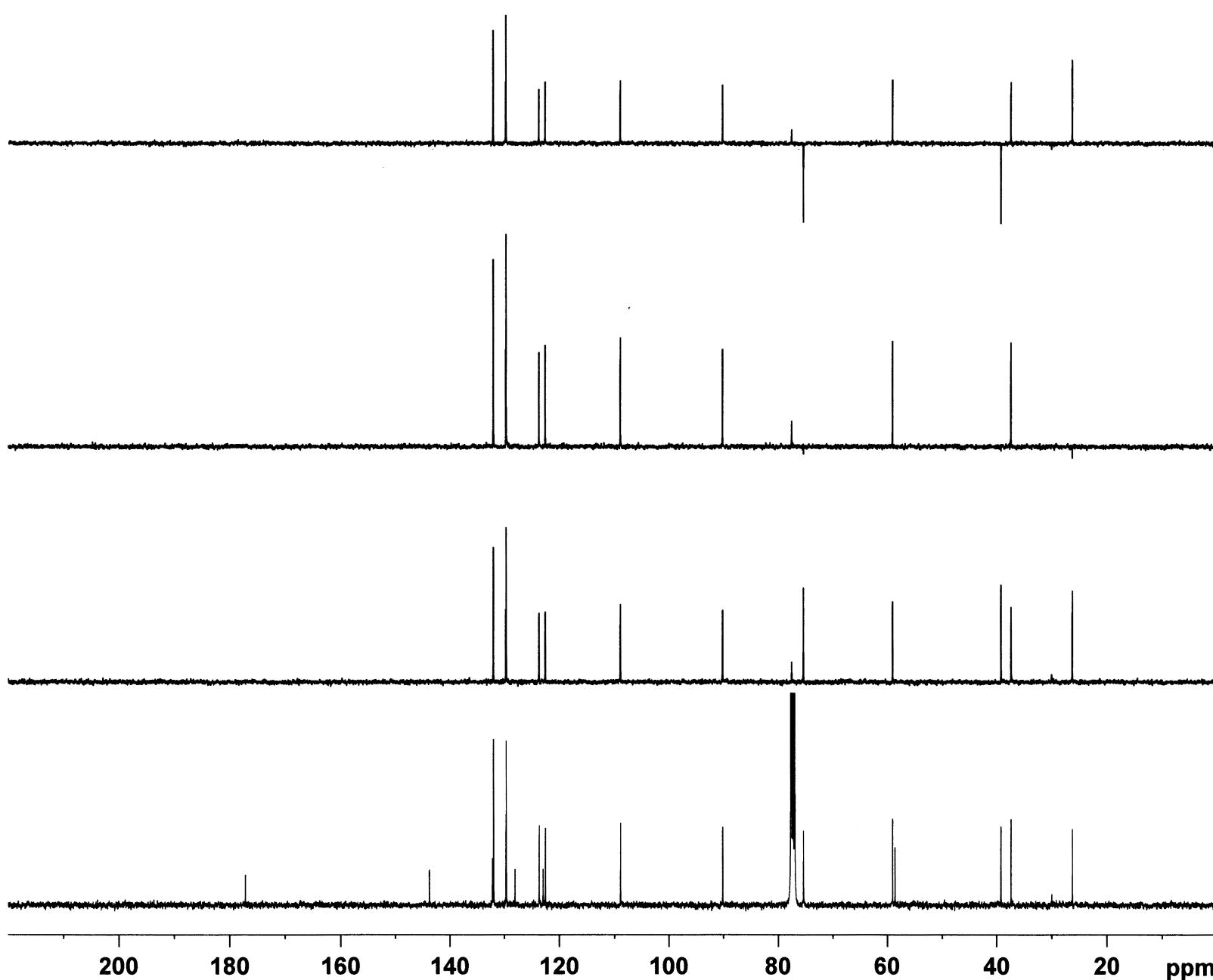
Figure S191. ^{13}C NMR (CDCl_3 , 100 MHz) of **8b**

Figure S192. DEPT of 8b



Current Data Parameters
 NAME PDC-04-022F2(Major)
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180713
 Time 3.35 h
 INSTRUM spect
 PROBHD Z108618_0922_()
 PULPROG zgpg30
 TD 32768
 SOLVENT CDC13
 NS 6500
 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 300.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 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 100.6127334 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

Figure S193. HSQC of **8b**

S205

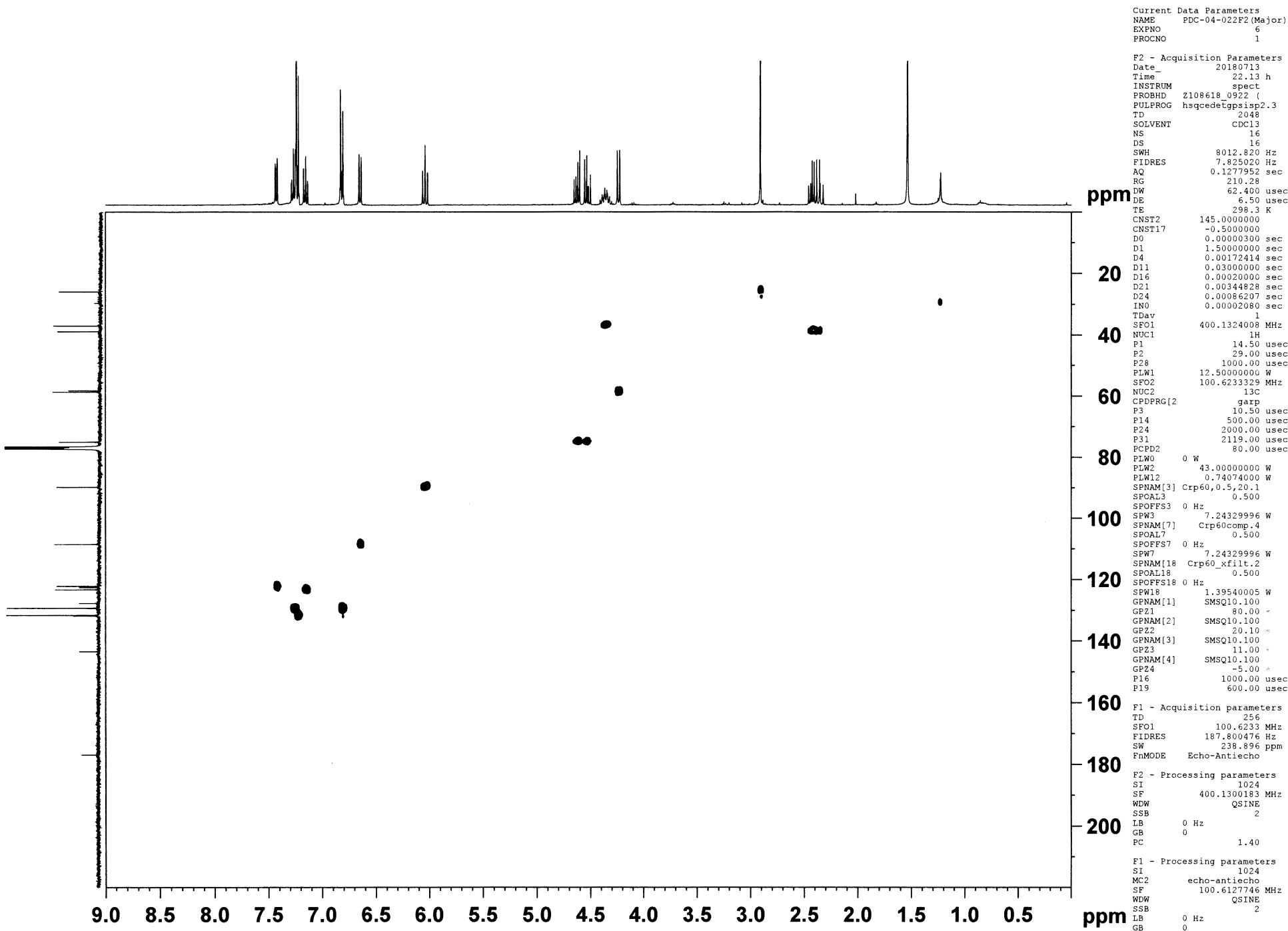
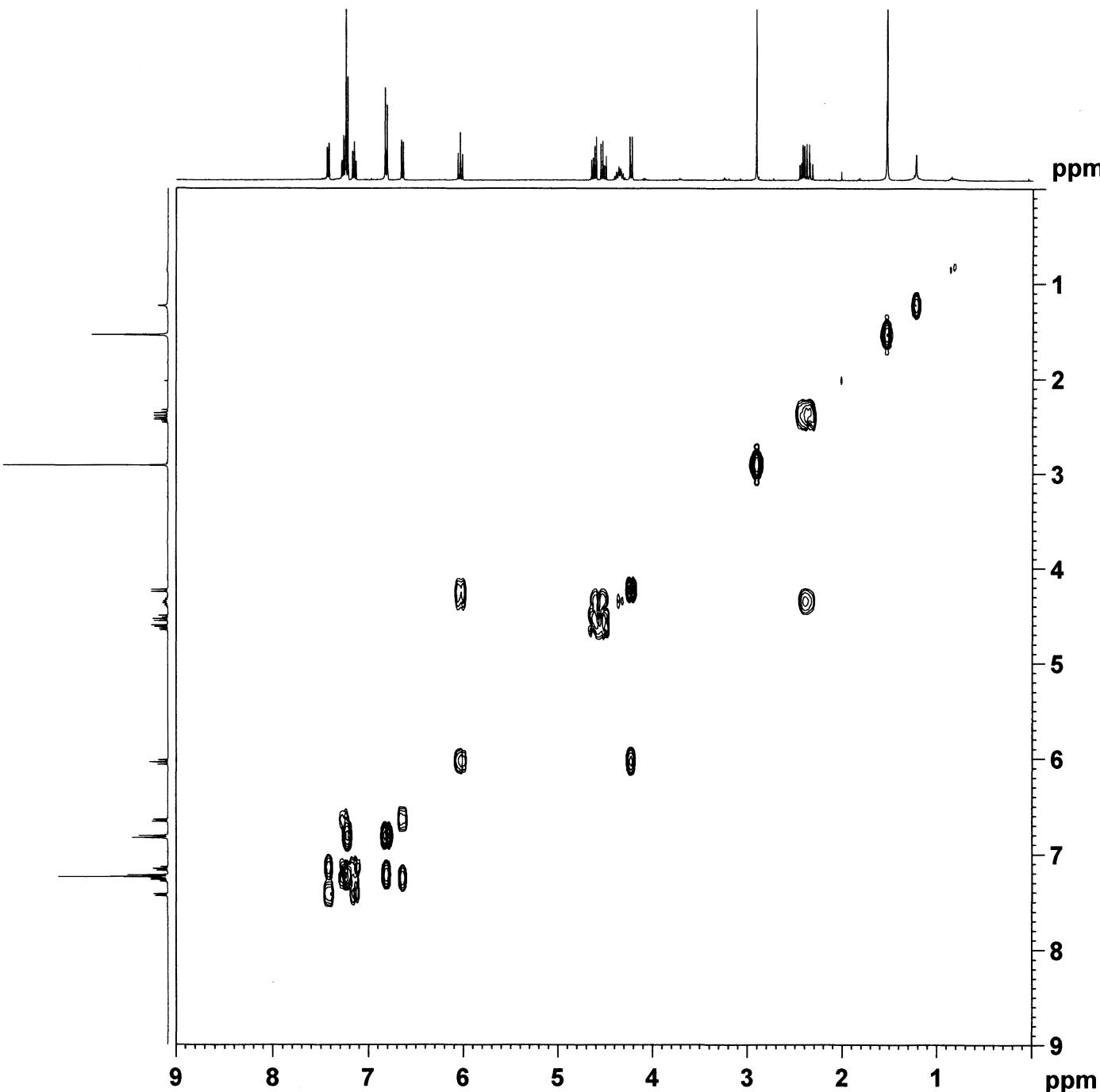


Figure S194. COSY of **8b**

S206



Current Data Parameters
 NAME PDC-04-022F2(Major)
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180714
 Time_ 0.07 h
 INSTRUM spect
 PROBHD Z108618_0922 (
 PULPROG cosygpppaf
 TD 2048
 SOLVENT CDC13
 NS 16
 DS 16
 SWH 8012.820 Hz
 FIDRES 7.825020 Hz
 AQ 0.1277952 sec
 RG 210.28
 DW 62.400 usec
 DE 6.50 usec
 TE 299.1 K
 D0 0.00000300 sec
 D1 2.0000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00012480 sec
 TDav 1
 SFO1 400.1324008 MHz
 NUC1 1H
 P0 14.50 usec
 P1 14.50 usec
 P17 2500.00 usec
 PLW1 12.5000000 W
 PLW10 2.92009997 W
 GPNAM[1] SMSQ10.100
 GPZ1 10.00 %
 P16 1000.00 usec

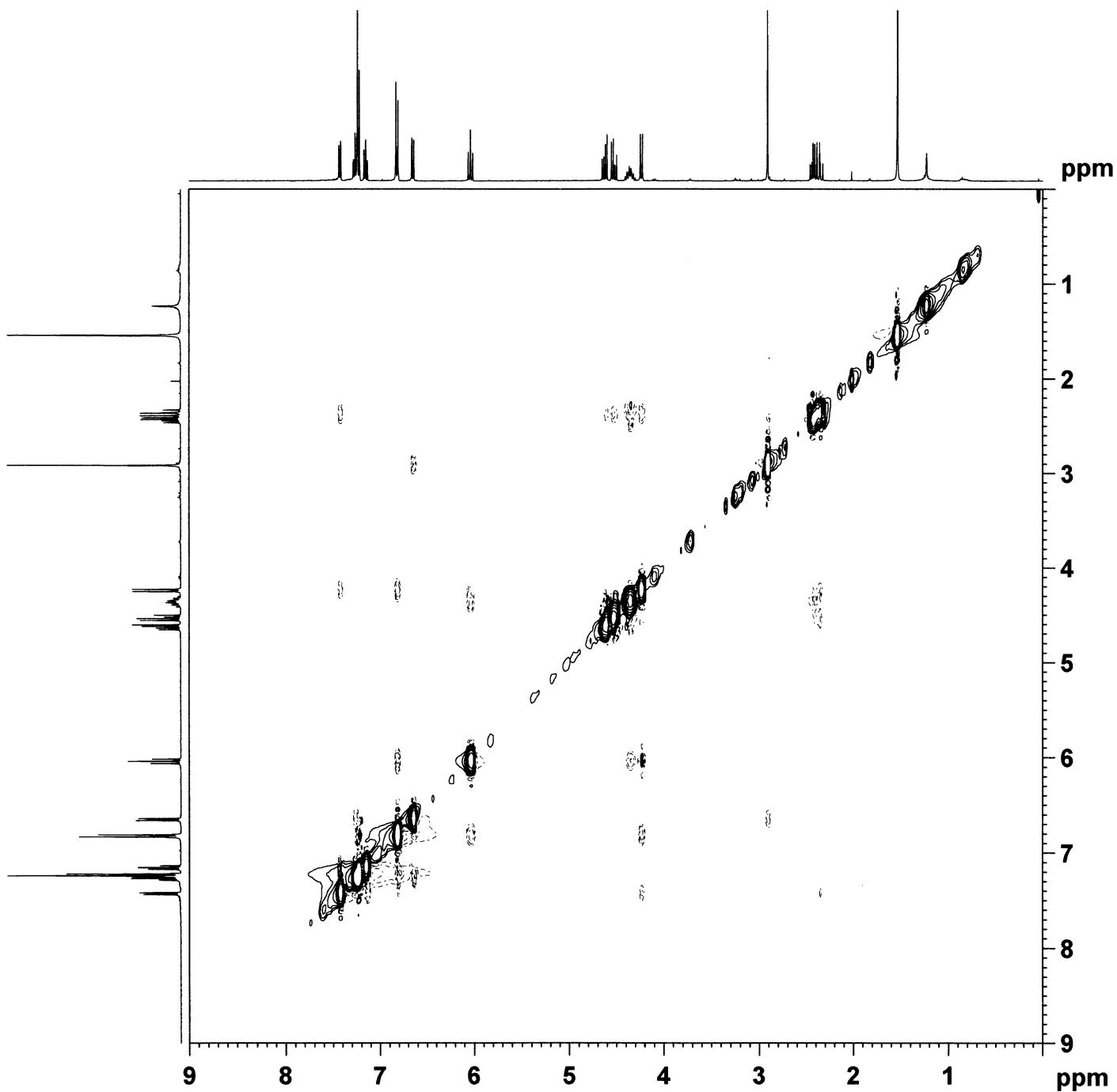
F1 - Acquisition parameters
 TD 256
 SFO1 400.1324 MHz
 FIDRES 62.600159 Hz
 SW 20.025 ppm
 FnMODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300183 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300183 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0

Figure S195. NOESY of 8b

S207



Current Data Parameters
 NAME PDC-04-022F2 (Major)
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180714
 Time 2.37 h
 INSTRUM spect
 PROBHD Z108618_0922 (
 PULPROG noesypphp
 TD 2048
 SOLVENT CDCl3
 NS 16
 DS 16
 SWH 8012.820 Hz
 FIDRES 7.825020 Hz
 AQ 0.1277952 sec
 RG 210.28
 DW 62.400 usec
 DE 6.50 usec
 TE 298.4 K
 D0 0.00004394 sec
 D1 2.0000000 sec
 D8 0.40000001 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 INO 0.00012480 sec
 TDav 1
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 14.50 usec
 P2 29.00 usec
 P17 2500.00 usec
 PLW1 12.50000000 W
 PLW10 2.92009997 W
 GPNAM[1] SMSQ10.100
 GPZ1 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 256
 SFO1 400.1324 MHz
 FIDRES 62.600159 Hz
 SW 20.025 ppm
 FnMODE States-TPPI

F2 - Processing parameters
 SI 1024
 SF 400.1300183 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 States-TPPI
 SF 400.1300183 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/04/2018 03:28 PM Reported Date and Time: 02/04/2018 03:52 PM

Processed Date and Time: 02/04/2018 03:52 PM

Data Path: D:\Prakash\DATA\0806\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0806

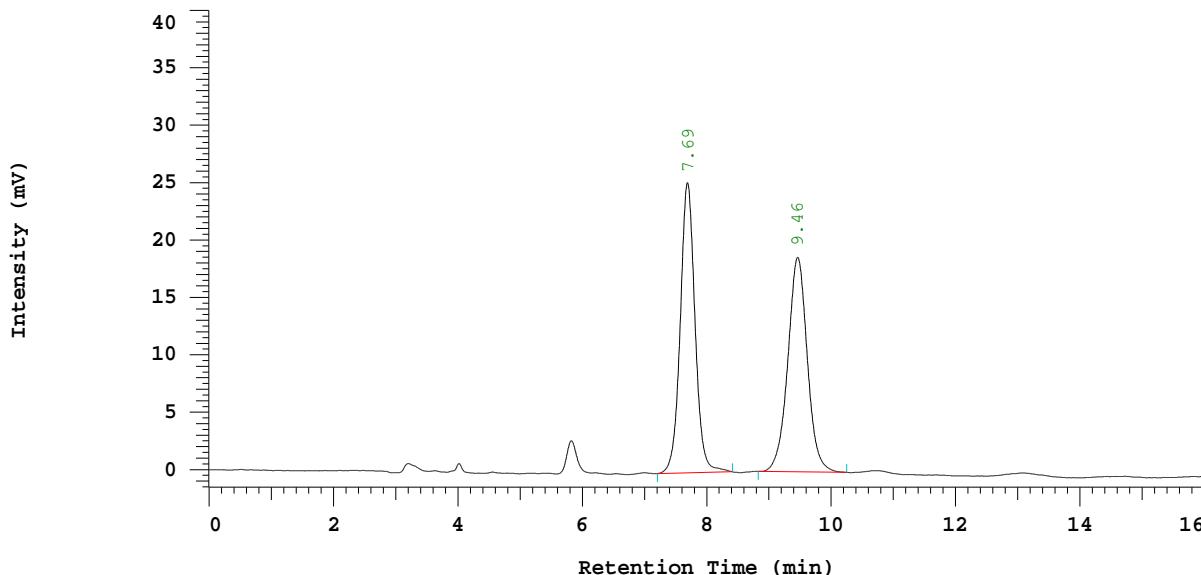
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-137 (Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.69	417263	25263	50.594
2	9.46	407470	18687	49.406
		824733	43950	100.000

Peak rejection level: 200000

Figure S196. HPLC analysis of the racemic **3a**, for comparison (Table 1, entry 3)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/04/2018 05:07 PM Reported Date and Time: 02/04/2018 05:29 PM

Processed Date and Time: 02/04/2018 05:28 PM

Data Path: D:\Prakash\DATA\0805\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0805

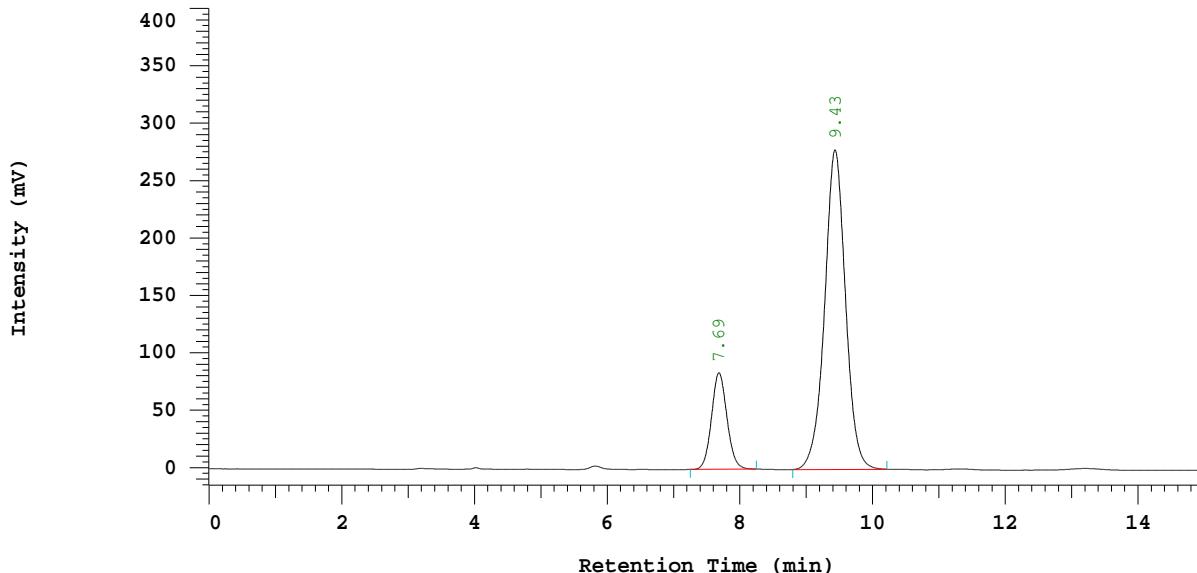
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-137F2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.69	1357778	84049	18.245
2	9.43	6084087	278183	81.755
		7441865	362232	100.000

Peak rejection level: 200000

Figure S197. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst II (Table 1, entry 3).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/04/2018 05:57 PM Reported Date and Time: 02/04/2018 05:23 PM

Processed Date and Time: 02/04/2018 05:22 PM

Data Path: D:\Prakash\DATA\0807\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0807

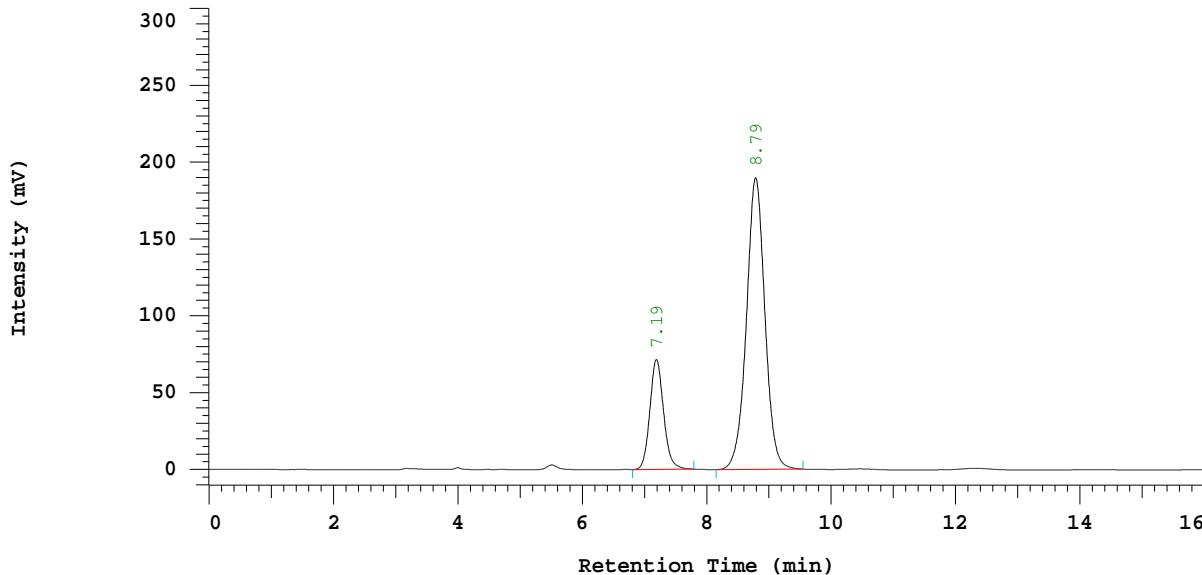
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-137F2(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.19	1096246	71597	21.877
2	8.79	3914799	189814	78.123
		5011045	261411	100.000

Peak rejection level: 200000

Figure S198. HPLC analysis of the mixture of chiral **3a** and racemic **3a**, for comparison (Table 1, entry 3)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/30/2018 07:26 PM Reported Date and Time: 07/30/2018 07:50 PM

Processed Date and Time: 07/30/2018 07:49 PM

Data Path: D:\Prakash\DATA\0972\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0972

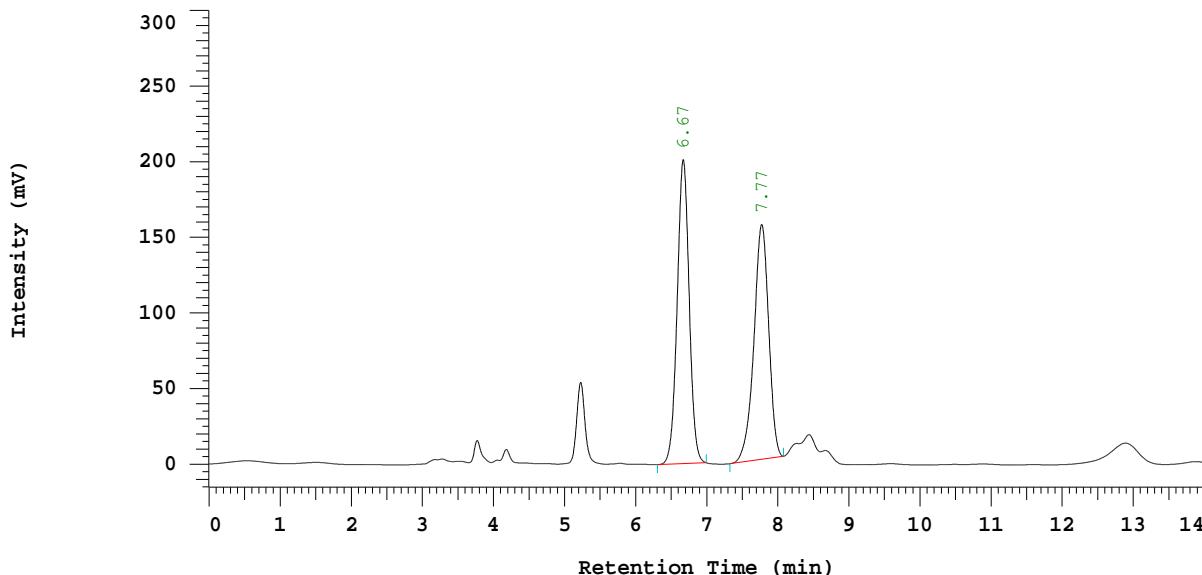
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-029F2(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.67	2349922	200920	51.222
2	7.77	2237793	155208	48.778
		4587715	356128	100.000

Peak rejection level: 1000

Figure S199. HPLC analysis of the racemic **3a**, for comparison (Table 1, entry 4)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/28/2018 07:10 PM Reported Date and Time: 07/28/2018 07:35 PM

Processed Date and Time: 07/28/2018 07:34 PM

Data Path: D:\Prakash\DATA\0961\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0961

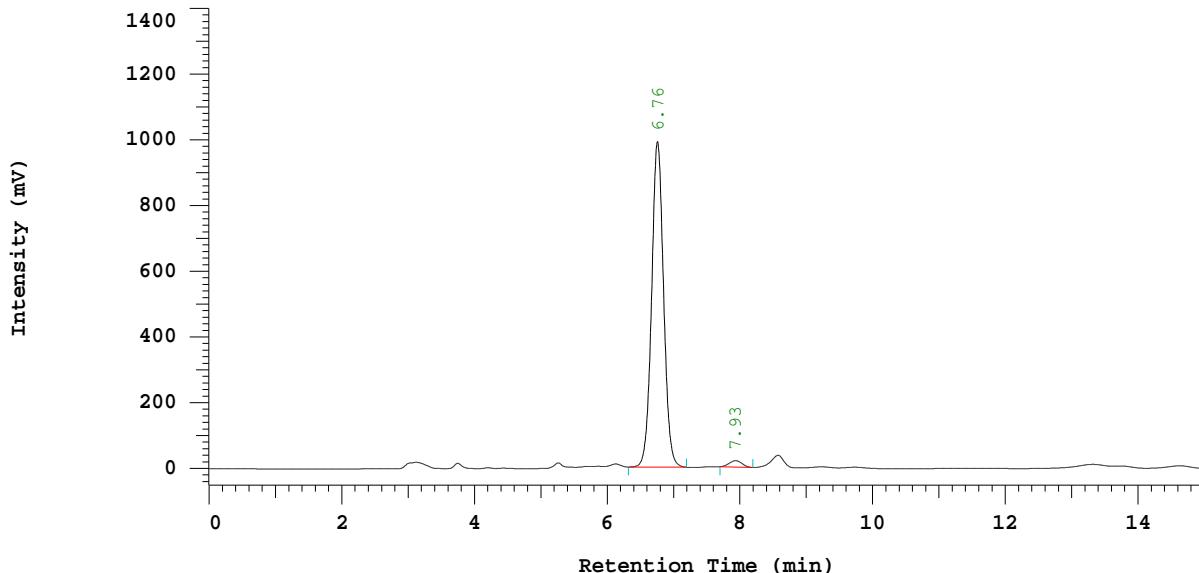
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-029F2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 235 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 235 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.76	12400809	990303	97.954
2	7.93	258999	19350	2.046
		12659808	1009653	100.000

Peak rejection level: 1000

Figure S200. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst III (Table 1, entry 4).

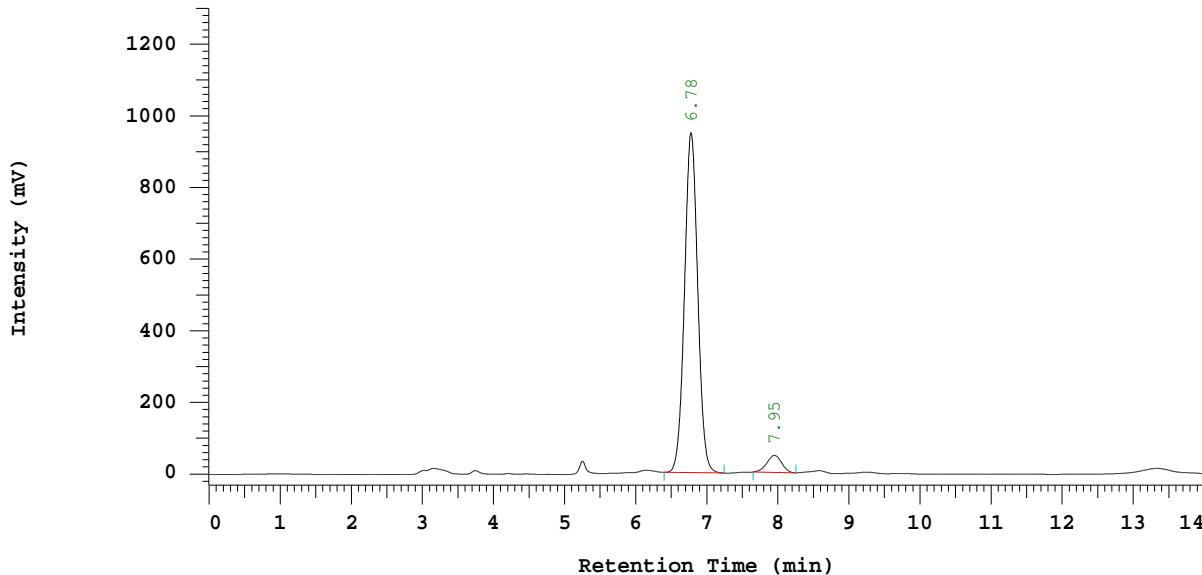
D-2000 Elite HPLC System Manager ReportAnalyzed Date and Time: 07/28/2018 Reported Date and Time: 07/29/2018
 09:44 PM 04:43 PMProcessed Date and Time: 07/29/2018
 04:42 PM

Data Path: D:\Prakash\DATA\0963\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0963
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-04-029F2(Co) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 ul
Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.78	12276204	948794	94.706
2	7.95	686211	47517	5.294
		12962415	996311	100.000

Peak rejection level: 1000

Figure S201. HPLC analysis of the mixture of chiral **3a** and racemic **3a**, for comparison (Table 1, entry 4)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/28/2018 05:36 PM Reported Date and Time: 07/28/2018 06:53 PM

Processed Date and Time: 07/28/2018 06:53 PM

Data Path: D:\Prakash\DATA\0958\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0958

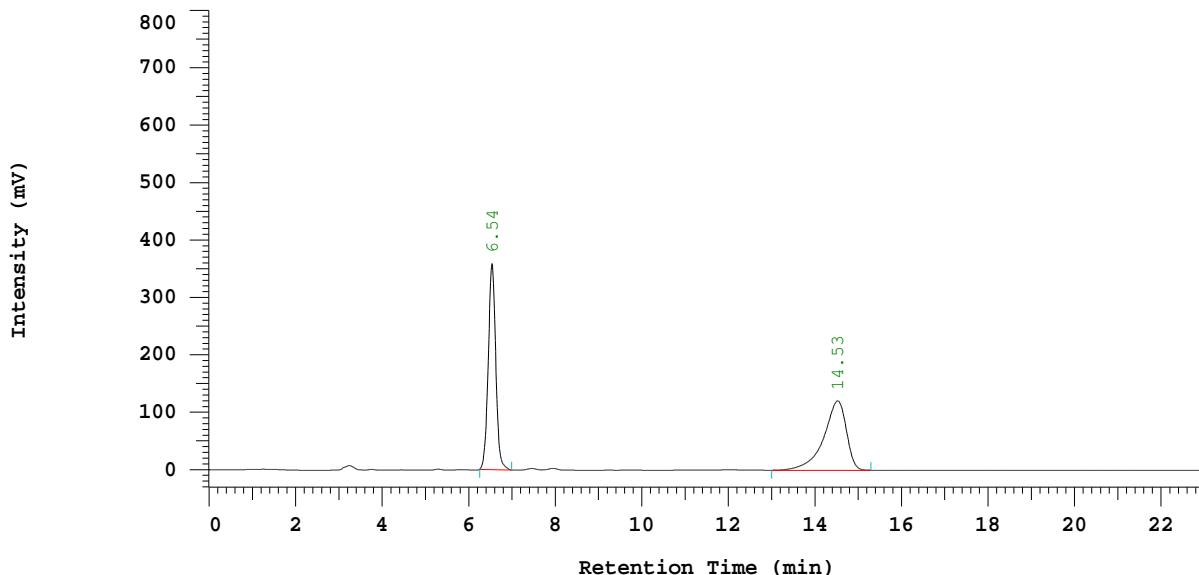
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-105F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.54	4301246	358702	49.406
2	14.53	4404702	120777	50.594
		8705948	479479	100.000

Peak rejection level: 1000

Figure S202. HPLC analysis of the racemic **4a**, for comparison (Table 1, entry 4)

D-2000: Prakash Series: 0959
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/28/2018 06:20 PM Reported Date and Time: 07/28/2018 06:52 PM

Processed Date and Time: 07/28/2018 06:50 PM

Data Path: D:\Prakash\DATA\0959\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0959

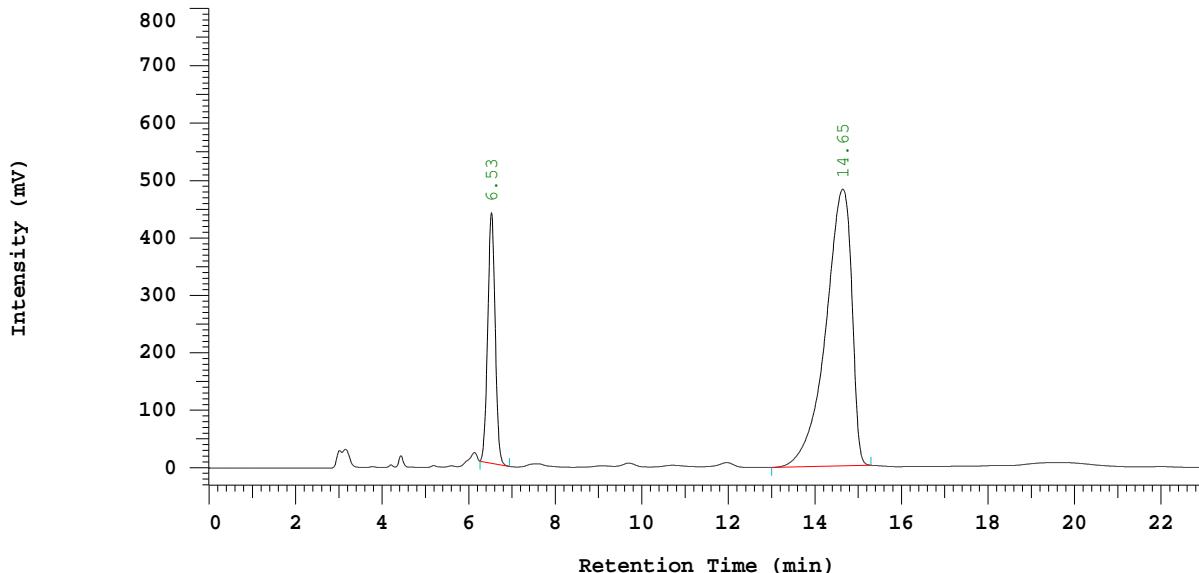
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-129F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.53	5189554	436049	20.555
2	14.65	20058004	481877	79.445
		25247558	917926	100.000

Peak rejection level: 1000

Figure S203. HPLC analysis of chiral **4a**, obtained from the reaction with catalyst **III** (Table 1, entry 4).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/28/2018 06:45 PM Reported Date and Time: 07/30/2018 11:22 AM

Processed Date and Time: 07/30/2018 11:21 AM

Data Path: D:\Prakash\DATA\0960\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0960

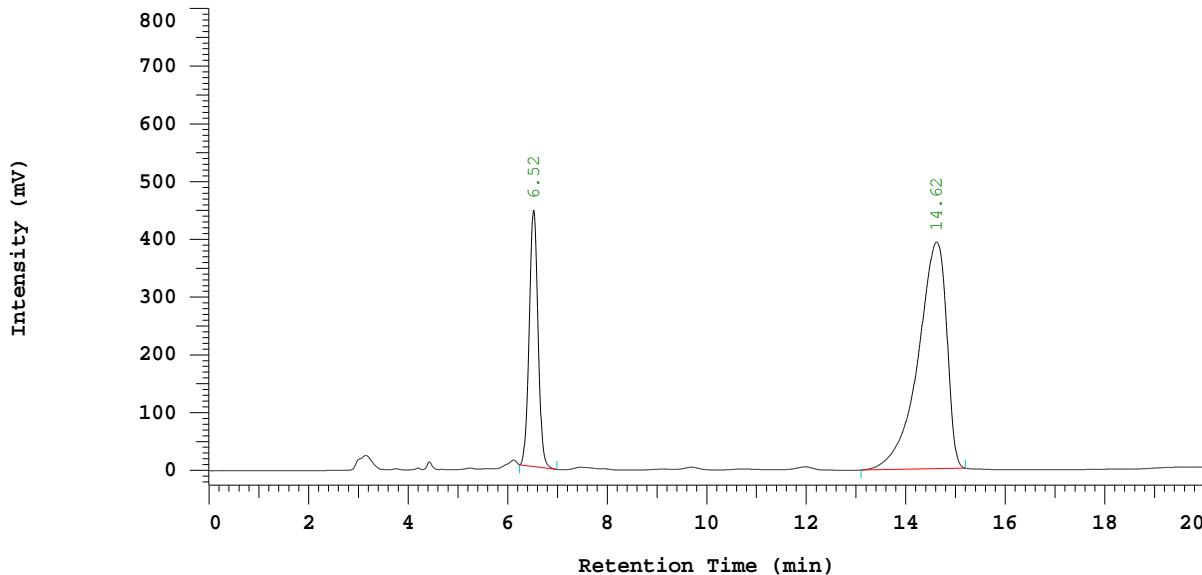
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-029F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.52	5454109	443921	25.843
2	14.62	15651078	392382	74.157
		21105187	836303	100.000

Peak rejection level: 1000

Figure S204. HPLC analysis of the mixture of chiral **4a** and racemic **4a**, for comparison (Table 1, entry 4)

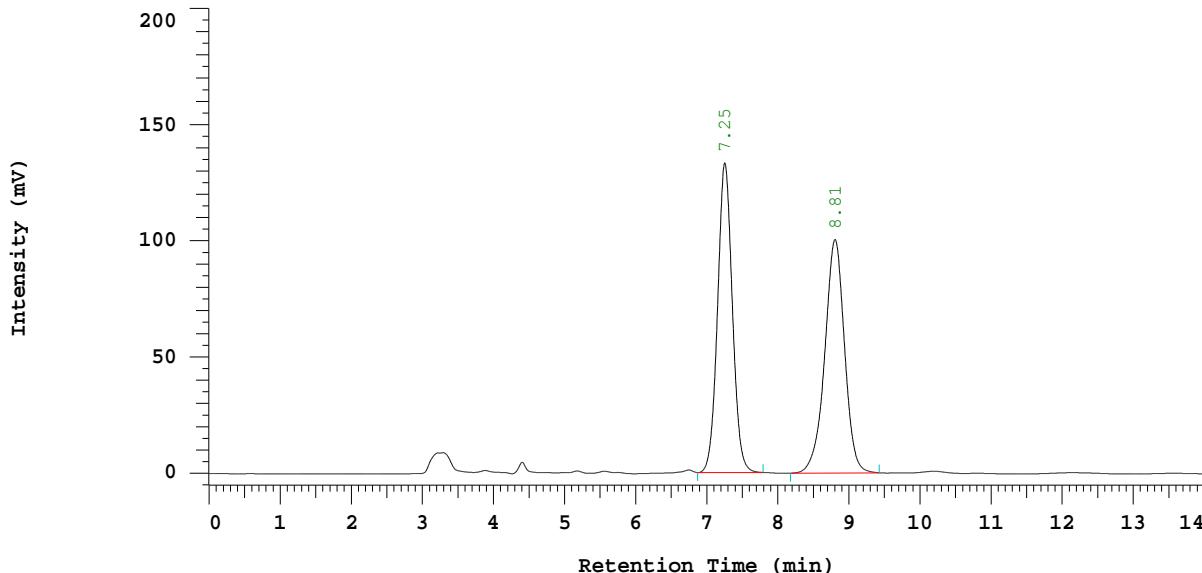
D-2000 Elite HPLC System Manager ReportAnalyzed Date and Time: 01/15/2018 Reported Date and Time: 06/18/2018
07:10 PM 01:05 PMProcessed Date and Time: 06/18/2018
01:04 PM

Data Path: D:\Prakash\DATA\0750\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0750
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-03-096F2Racemic) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 ul
Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.25	1926313	133169	49.813
2	8.81	1940768	100397	50.187
		3867081	233566	100.000

Peak rejection level: 200000

Figure S205. HPLC analysis of the racemic **3a**, for comparison (Table 1, entry 5)

D-2000 Elite HPLC System Manager Report

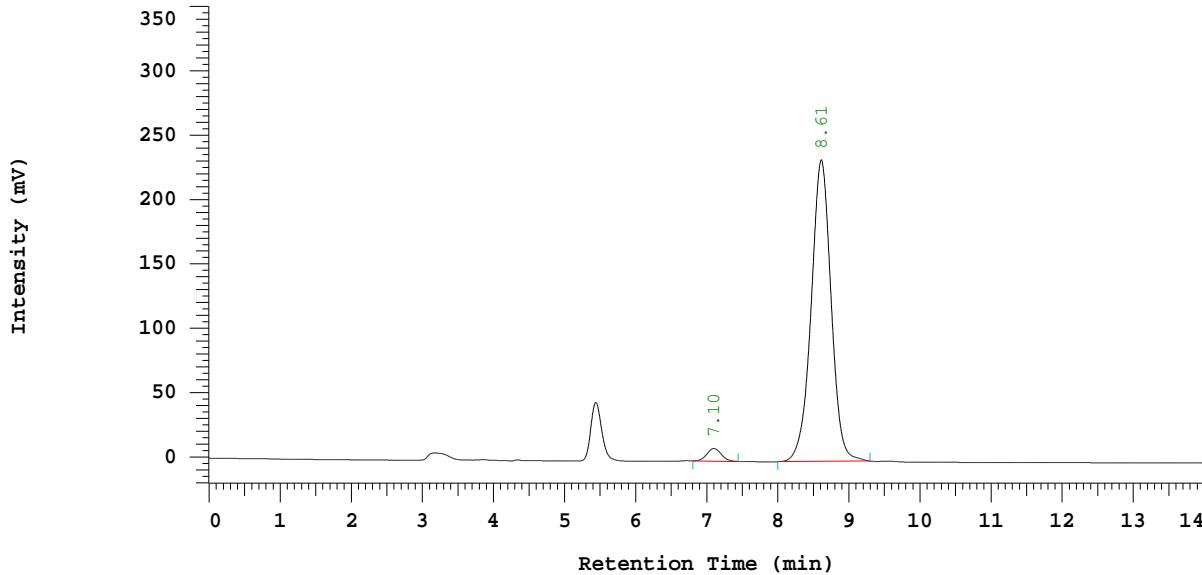
Analyzed Date and Time: 01/16/2018 11:04 AM Reported Date and Time: 06/18/2018 12:00 PM

Processed Date and Time: 06/18/2018
11:59 AM

Data Path: D:\Prakash\DATA\0753\
Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0753
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-03-096F2(Chiral) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 uL
Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1,000

No.	RT	Area	Height	Area %
1	7.10	137391	9815	2.922
2	8.61	4564397	234086	97.078
		4701788	243901	100.000

Peak rejection level: 10000

Figure S206. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst **IV** (Table 1, entry 5).

D-2000: Prakash Series: 0814
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/05/2018 06:02 PM Reported Date and Time: 02/05/2018 07:39 PM

Processed Date and Time: 02/05/2018 07:38 PM

Data Path: D:\Prakash\DATA\0814\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0814

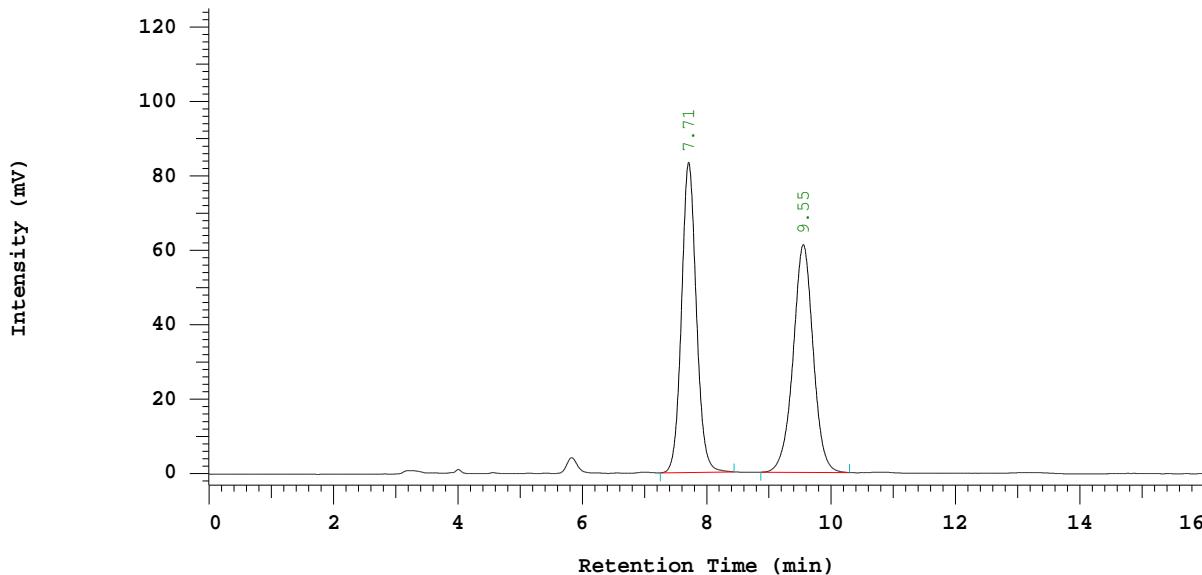
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-138F2(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.71	1378991	83264	50.148
2	9.55	1370846	61138	49.852
		2749837	144402	100.000

Peak rejection level: 200000

Figure S207. HPLC analysis of the mixture of chiral 3a and racemic 3a, for comparison (Table 1, entry 6)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/05/2018 05:42 PM Reported Date and Time: 02/05/2018 07:43 PM

Processed Date and Time: 02/05/2018 07:42 PM

Data Path: D:\Prakash\DATA\0813\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0813

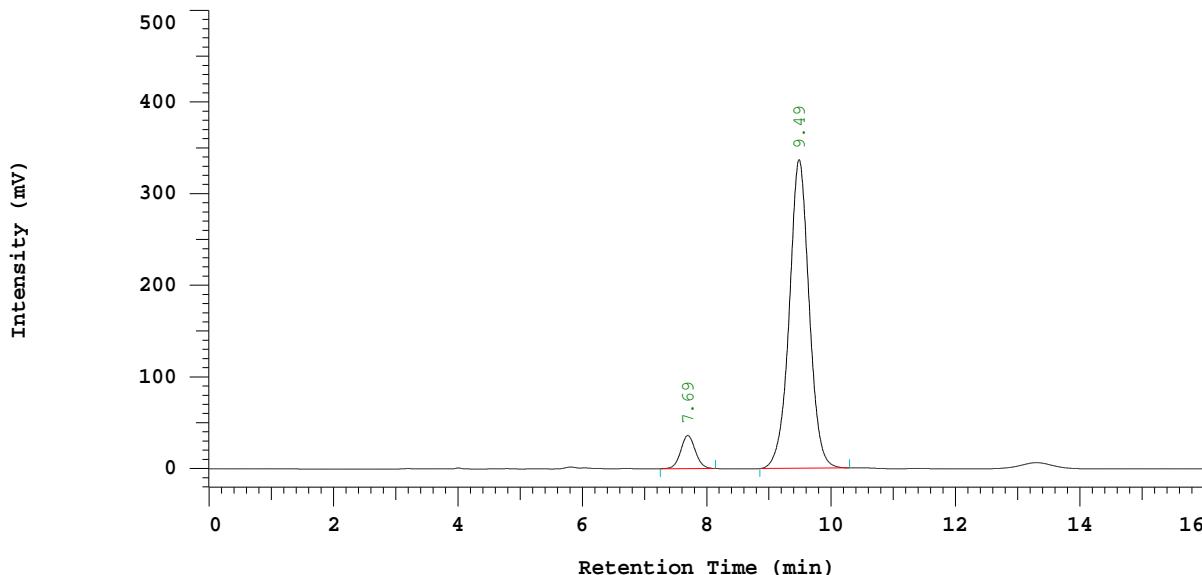
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-138F2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.69	590601	36253	7.328
2	9.49	7468989	336612	92.672
		8059590	372865	100.000

Peak rejection level: 200000

Figure S208. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst **V** (Table 1, entry 6).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/05/2018 05:23 PM Reported Date and Time: 06/17/2018 08:38 PM

Processed Date and Time: 06/17/2018 08:37 PM

Data Path: D:\Prakash\DATA\0809\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0809

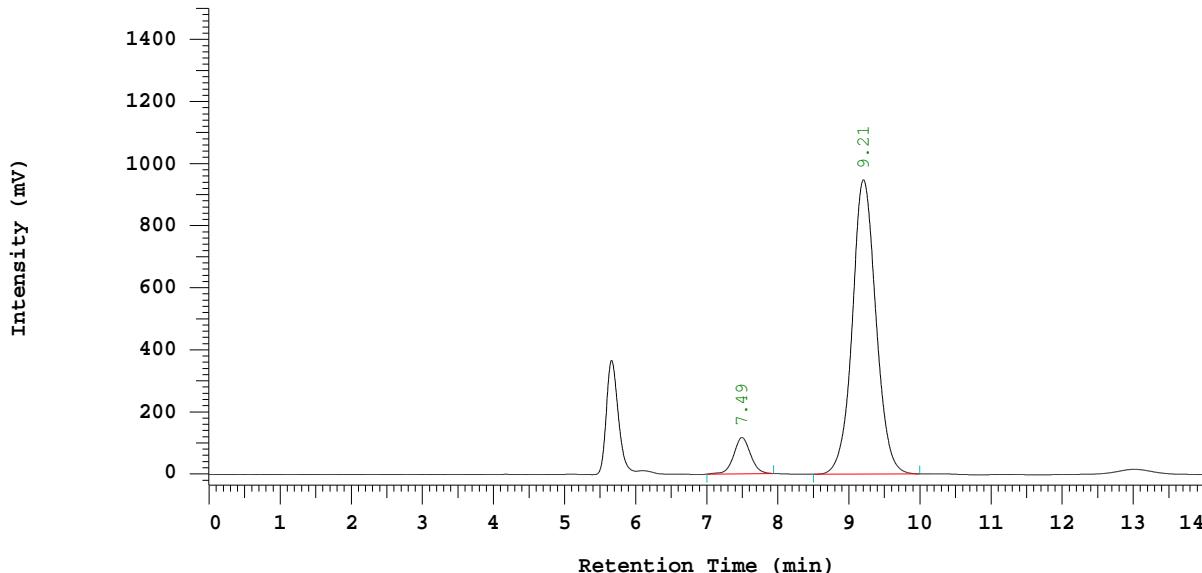
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-138F2(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.49	1935849	117024	8.124
2	9.21	21891873	948076	91.876
		23827722	1065100	100.000

Peak rejection level: 200000

Figure S209. HPLC analysis of the mixture of chiral **3a** and racemic **3a**, for comparison (Table 1, entry 6)

D-2000: Prakash Series: 0979
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/01/2018 03:18 PM Reported Date and Time: 08/01/2018 03:54 PM

Processed Date and Time: 08/01/2018 03:54 PM

Data Path: D:\Prakash\DATA\0979\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0979

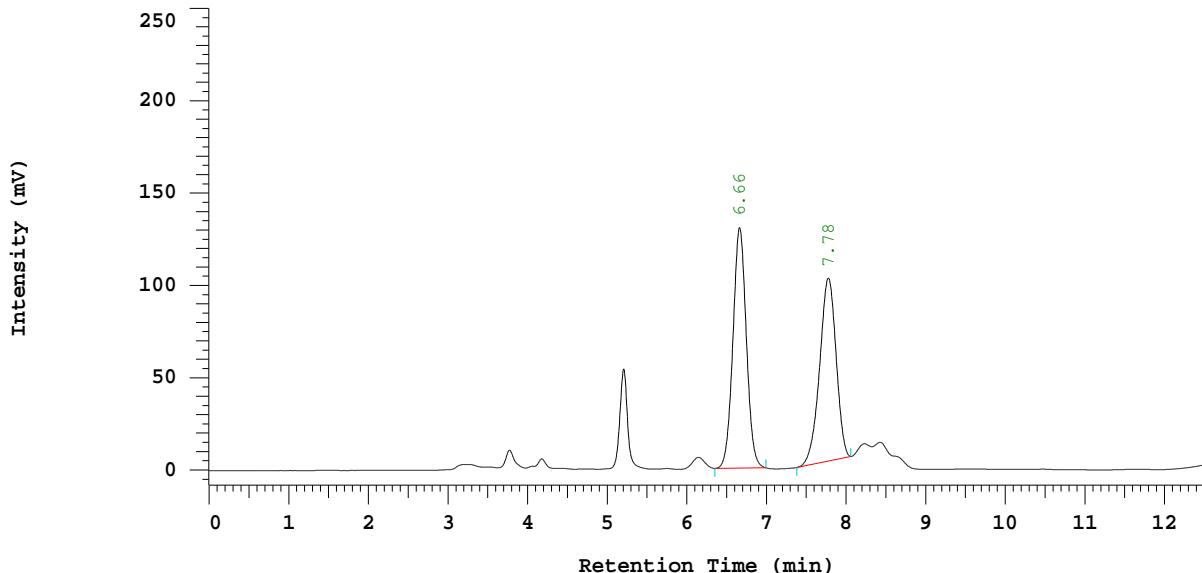
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-030F2(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.66	1528635	130233	51.822
2	7.78	1421126	99157	48.178
		2949761	229390	100.000

Peak rejection level: 1000

Figure S210. HPLC analysis of the racemic **3a**, for comparison (Table 1, entry 7)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/01/2018 01:52 PM Reported Date and Time: 08/01/2018 03:23 PM

Processed Date and Time: 08/01/2018 03:22 PM

Data Path: D:\Prakash\DATA\0978\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0978

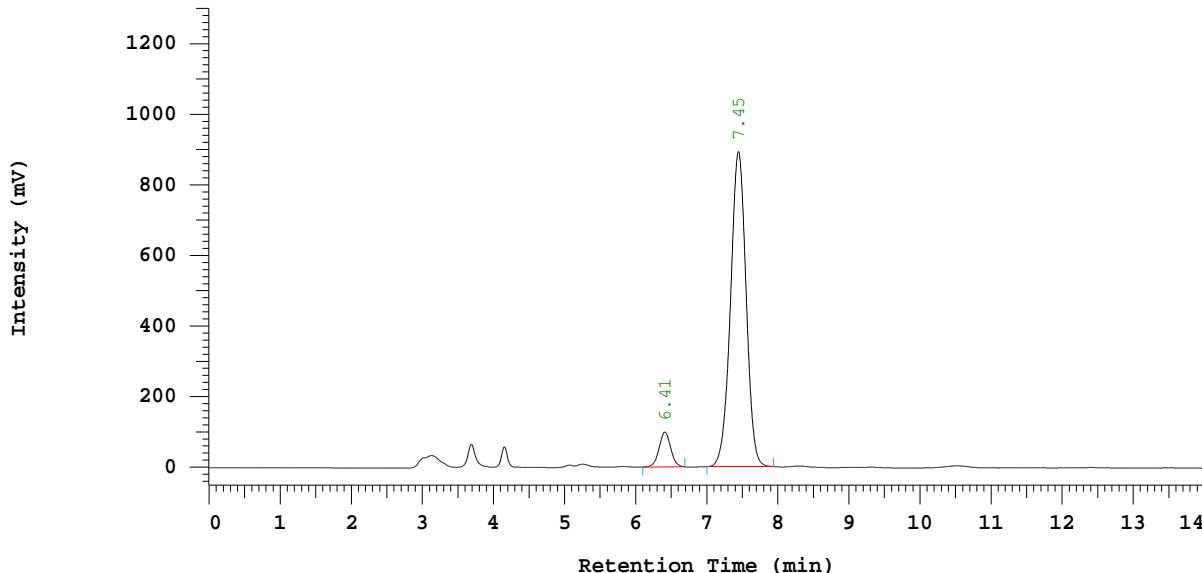
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-030FF2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.41	1124197	99108	7.641
2	7.45	13588798	892465	92.359
		14712995	991573	100.000

Peak rejection level: 1000

Figure S211. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst **VI** (Table 1, entry 7).

D-2000: Prakash Series: 0980
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/01/2018 03:38 PM Reported Date and Time: 08/01/2018 04:01 PM

Processed Date and Time: 08/01/2018 04:00 PM

Data Path: D:\Prakash\DATA\0980\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0980

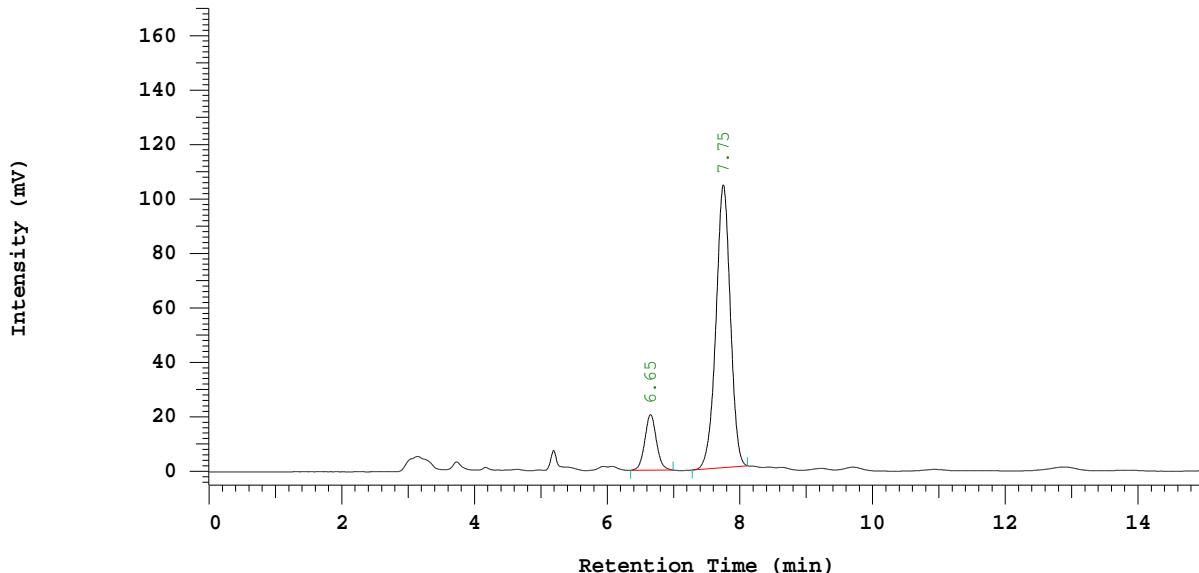
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-170F2(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.65	248392	20429	13.703
2	7.75	1564277	103791	86.297
		1812669	124220	100.000

Peak rejection level: 1000

Figure S212. HPLC analysis of the mixture of chiral **3a** and racemic **3a**, for comparison (Table 1, entry 7)

D-2000: Prakash Series: 0976
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/01/2018 02:16 PM Reported Date and Time: 08/01/2018 06:17 PM

Processed Date and Time: 08/01/2018 06:17 PM

Data Path: D:\Prakash\DATA\0976\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0976

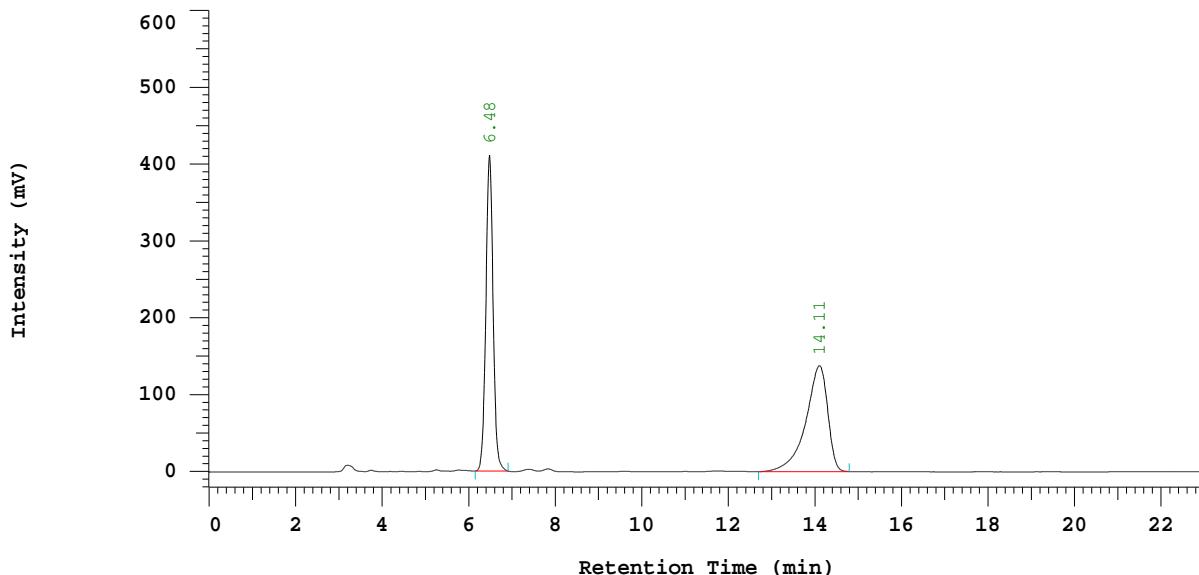
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-030F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.48	4748470	411005	49.559
2	14.11	4832894	137663	50.441
		9581364	548668	100.000

Peak rejection level: 1000

Figure S213. HPLC analysis of the racemic **4a**, for comparison (Table 1, entry 7)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/01/2018 11:51 AM Reported Date and Time: 08/01/2018 12:25 PM

Processed Date and Time: 08/01/2018 12:24 PM

Data Path: D:\Prakash\DATA\0975\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0975

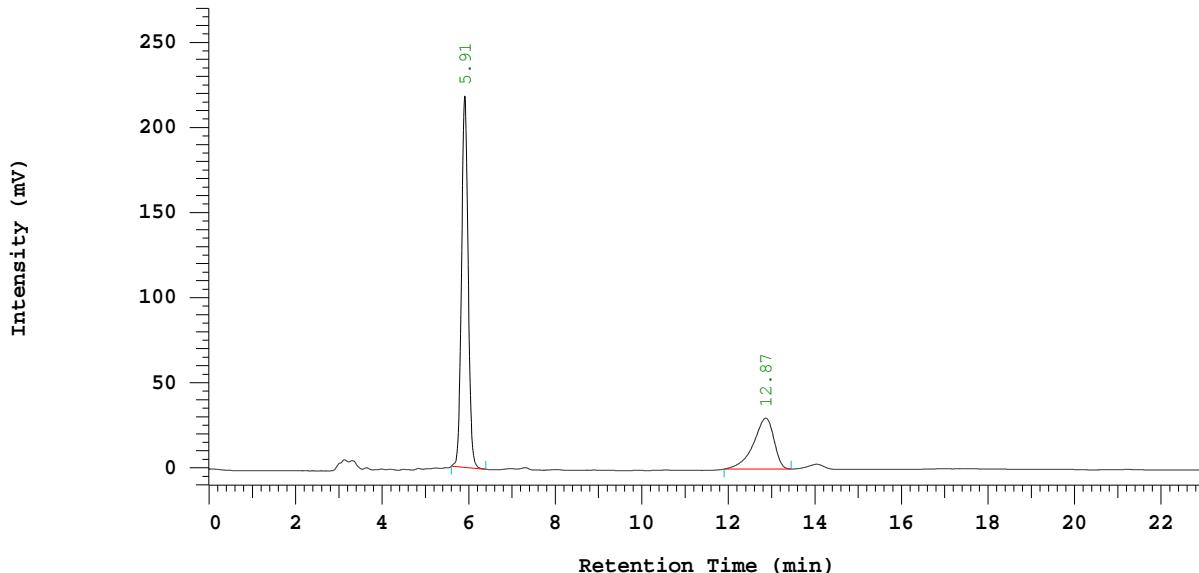
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-030F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 271 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Column Type: IC

Method Description:

Chrom Type: Fixed WL Chromatogram, 271 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.91	2308546	218088	70.045
2	12.87	987242	29938	29.955
		3295788	248026	100.000

Peak rejection level: 1000

Figure S214. HPLC analysis of chiral **4a**, obtained from the reaction with catalyst **VI** (Table 1, entry 7).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/01/2018 02:42 PM Reported Date and Time: 08/01/2018 06:19 PM

Processed Date and Time: 08/01/2018 06:18 PM

Data Path: D:\Prakash\DATA\0977\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0977

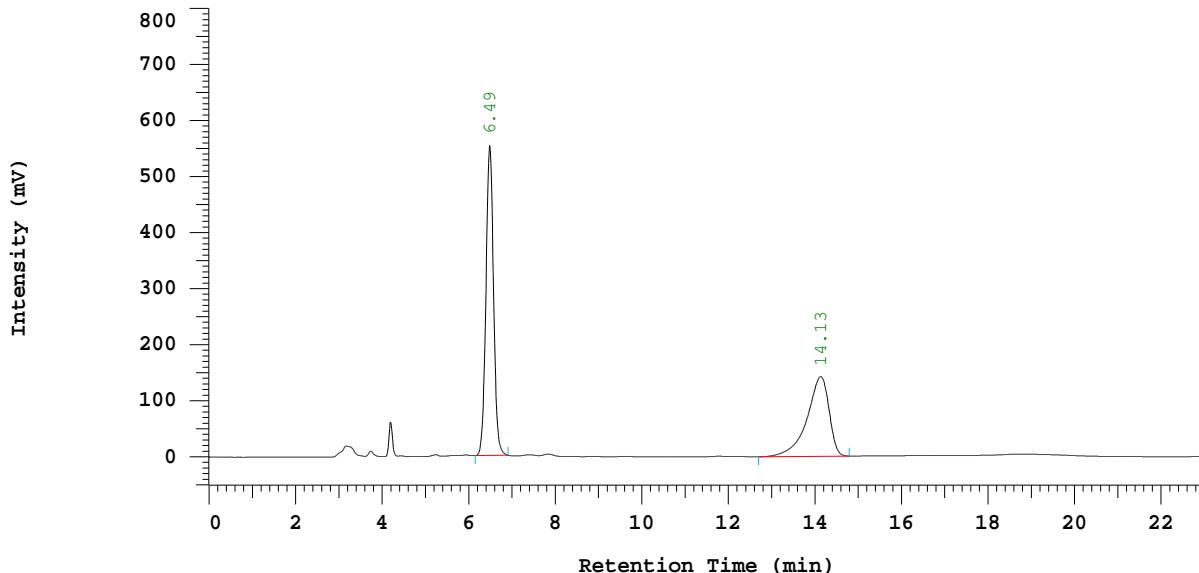
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-030F1(CO) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.49	6701076	553218	57.200
2	14.13	5014012	142141	42.800
		11715088	695359	100.000

Peak rejection level: 1000

Figure S215. HPLC analysis of the mixture of chiral **4a** and racemic **4a**, for comparison (Table 1, entry 7)

D-2000: Prakash Series: 0756
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/16/2018 12:06 PM Reported Date and Time: 01/16/2018 01:47 PM

Processed Date and Time: 01/16/2018 01:47 PM

Data Path: D:\Prakash\DATA\0756\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0756

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-105 (Racemic)

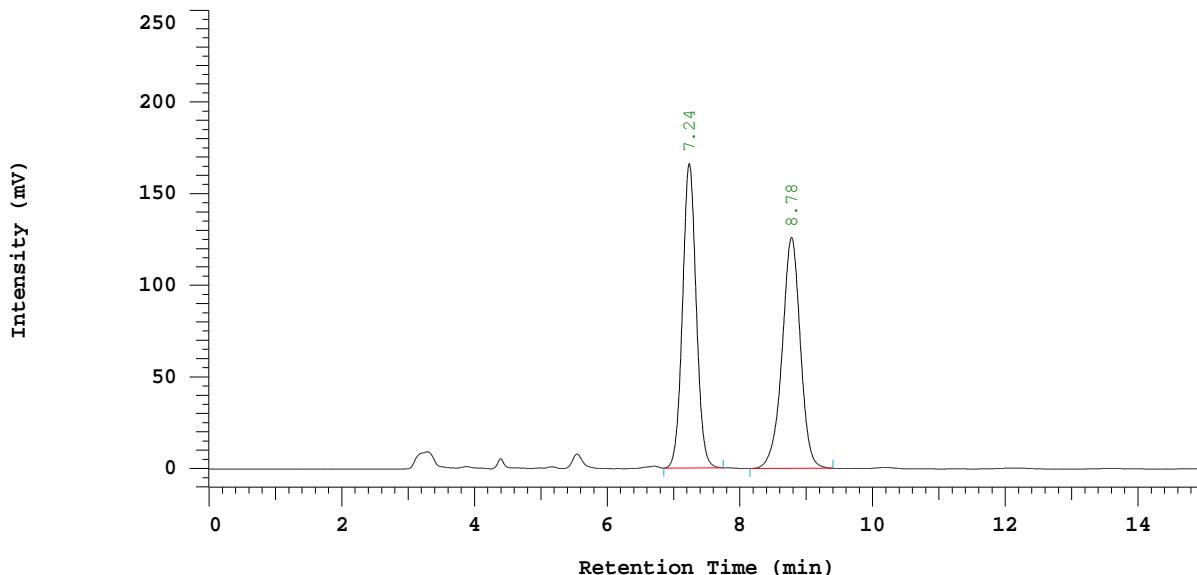
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.24	2382158	166083	49.723
2	8.78	2408664	125957	50.277
		4790822	292040	100.000

Peak rejection level: 200000

Figure S216. HPLC analysis of the racemic **3a**, for comparison (Table 1, entry 11)

D-2000: Prakash Series: 0755
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/16/2018 11:47 AM Reported Date and Time: 01/16/2018 01:54 PM

Processed Date and Time: 01/16/2018 01:53 PM

Data Path: D:\Prakash\DATA\0755\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0755

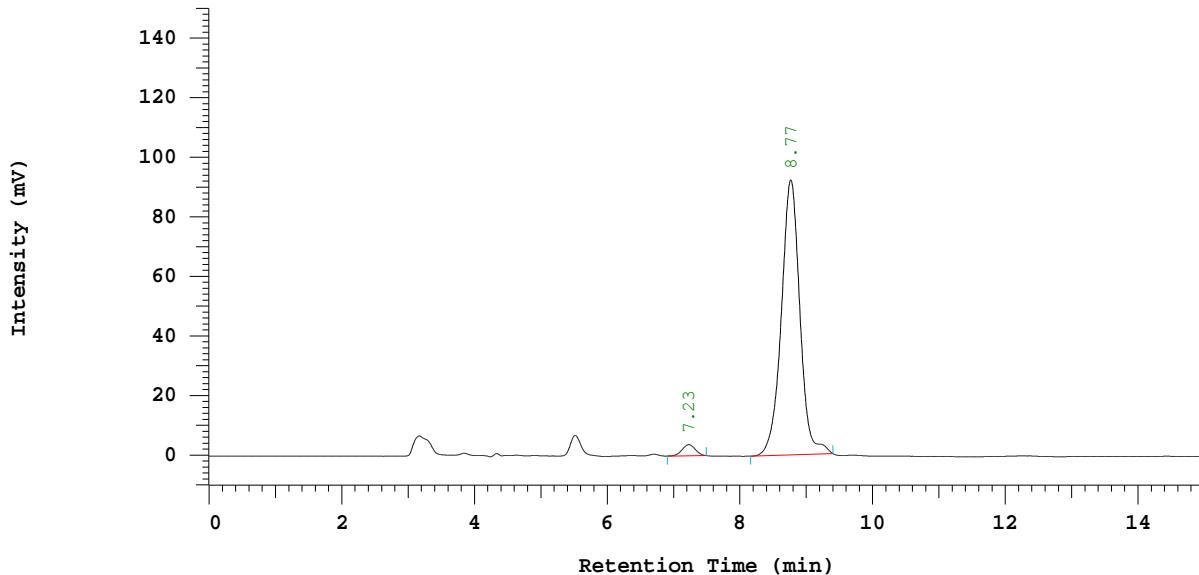
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.23	51465	3734	2.790
2	8.77	1793097	92305	97.210
		1844562	96039	100.000

Peak rejection level: 100

Figure S217. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst **IV** (Table 1, entry 11).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/16/2018 01:16 PM Reported Date and Time: 01/16/2018 01:43 PM

Processed Date and Time: 01/16/2018 01:41 PM

Data Path: D:\Prakash\DATA\0757\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0757

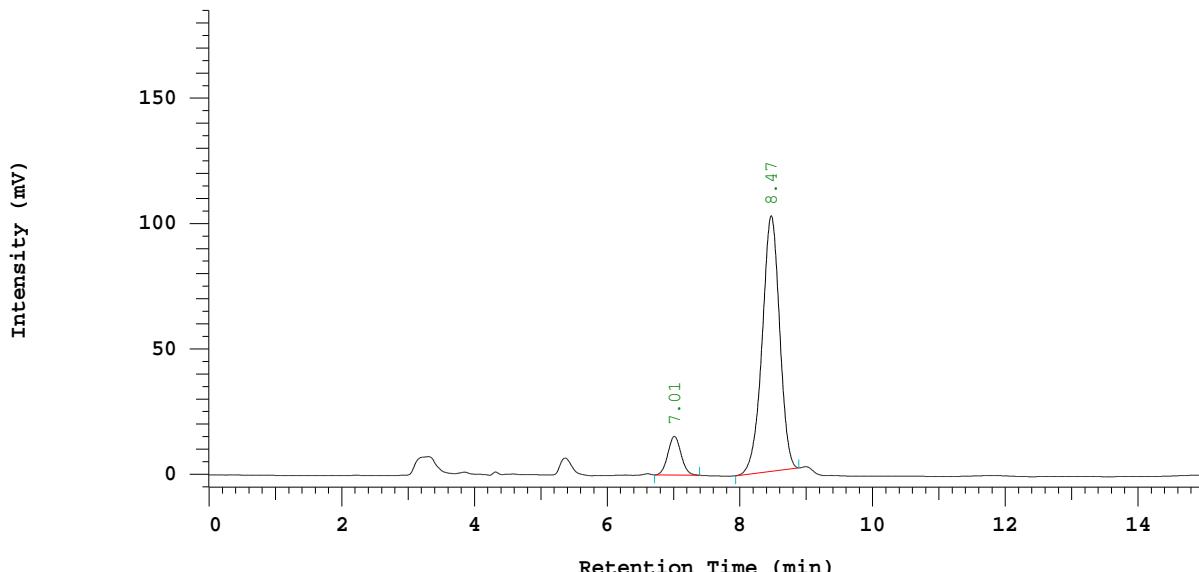
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.01	212810	15460	10.254
2	8.47	1862675	101910	89.746
		2075485	117370	100.000

Peak rejection level: 200000

Figure S218. HPLC analysis of the mixture of chiral **3a** and racemic **3a**, for comparison (Table 1, entry 11)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/12/2018 02:51 PM Reported Date and Time: 06/18/2018 12:25 PM

Processed Date and Time: 06/18/2018 12:19 PM

Data Path: D:\Prakash\DATA\0829\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0829

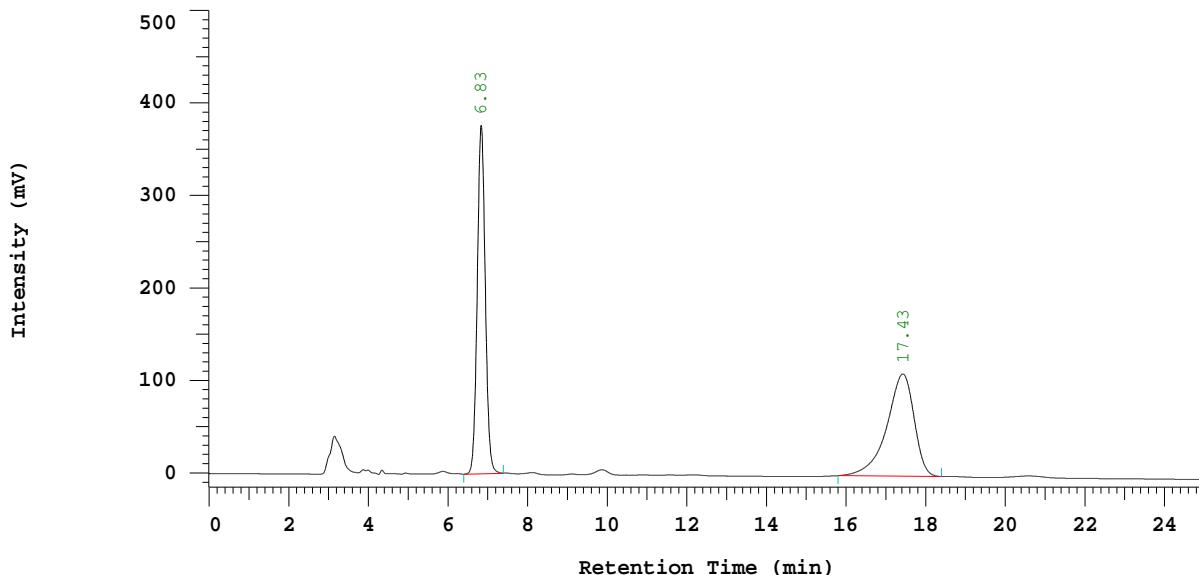
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.83	5223057	376339	49.861
2	17.43	5252176	110438	50.139
		10475233	486777	100.000

Peak rejection level: 200000

Figure S219. HPLC analysis of the racemic **4a**, for comparison (Table 1, entry 11)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/12/2018 03:30 PM Reported Date and Time: 06/18/2018 12:17 PM

Processed Date and Time: 06/18/2018 12:16 PM

Data Path: D:\Prakash\DATA\0830\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0830

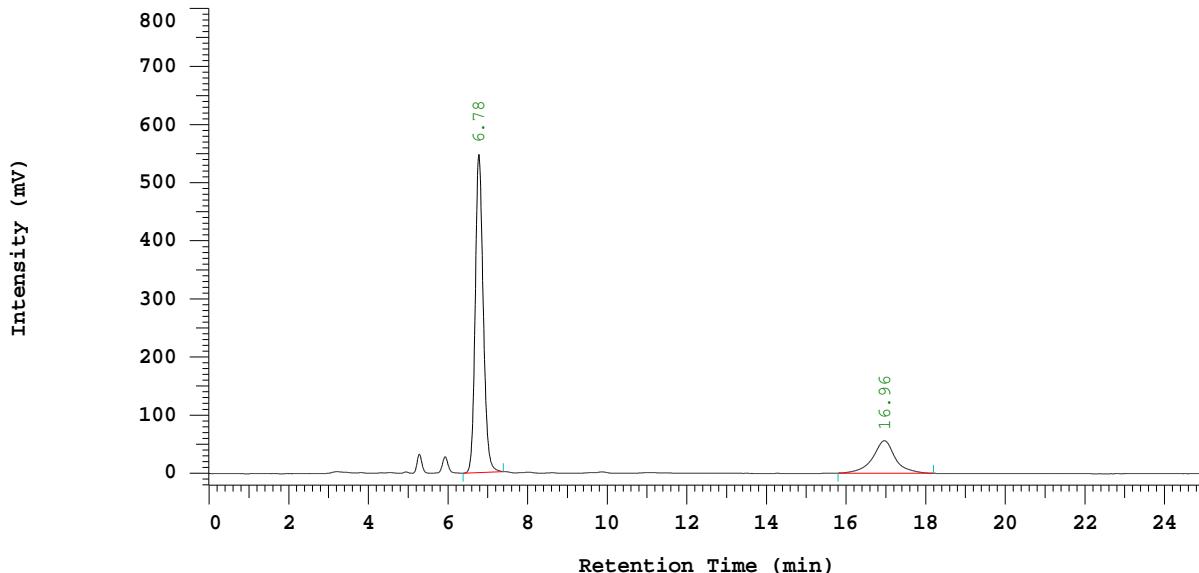
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Column Type: IC

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.78	7577790	547187	77.432
2	16.96	2208627	55986	22.568
		9786417	603173	100.000

Peak rejection level: 200000

Figure S220. HPLC analysis of chiral **4a**, obtained from the reaction with catalyst **IV** (Table 1, entry 11).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/12/2018 05:49 PM Reported Date and Time: 06/18/2018 12:27 PM

Processed Date and Time: 06/18/2018 12:27 PM

Data Path: D:\Prakash\DATA\0835\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0835

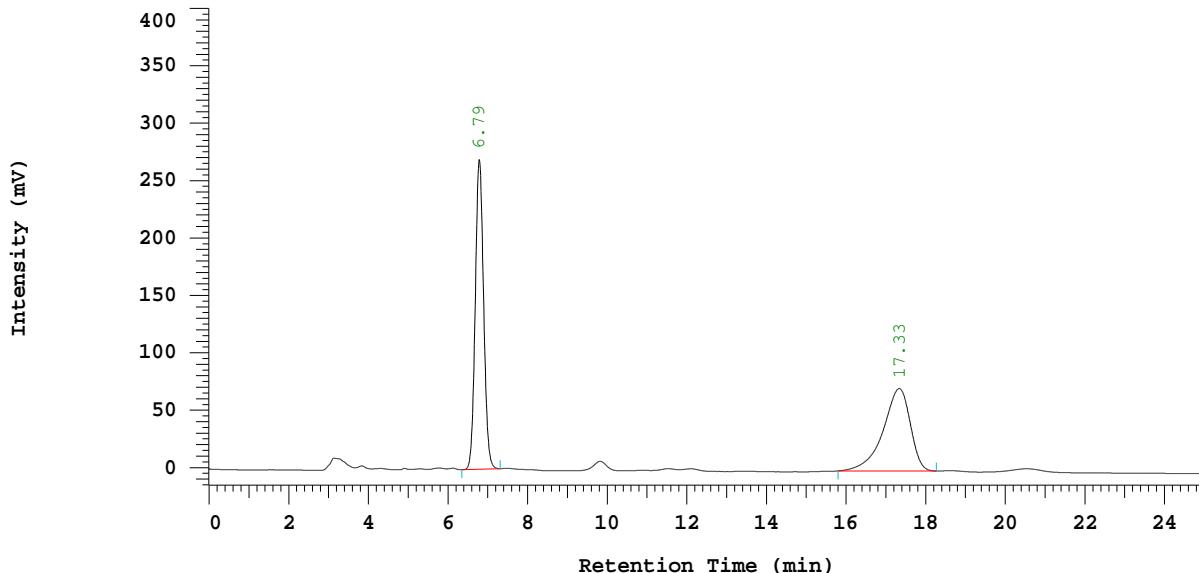
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.79	3904749	269710	53.491
2	17.33	3395115	71712	46.509
		7299864	341422	100.000

Peak rejection level: 200000

Figure S221. HPLC analysis of the mixture of chiral **4a** and racemic **4a**, for comparison (Table 1, entry 11)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/23/2018 10:32 PM Reported Date and Time: 07/23/2018 10:18 PM

Processed Date and Time: 07/23/2018 10:17 PM

Data Path: D:\Prakash\DATA\0937\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0937

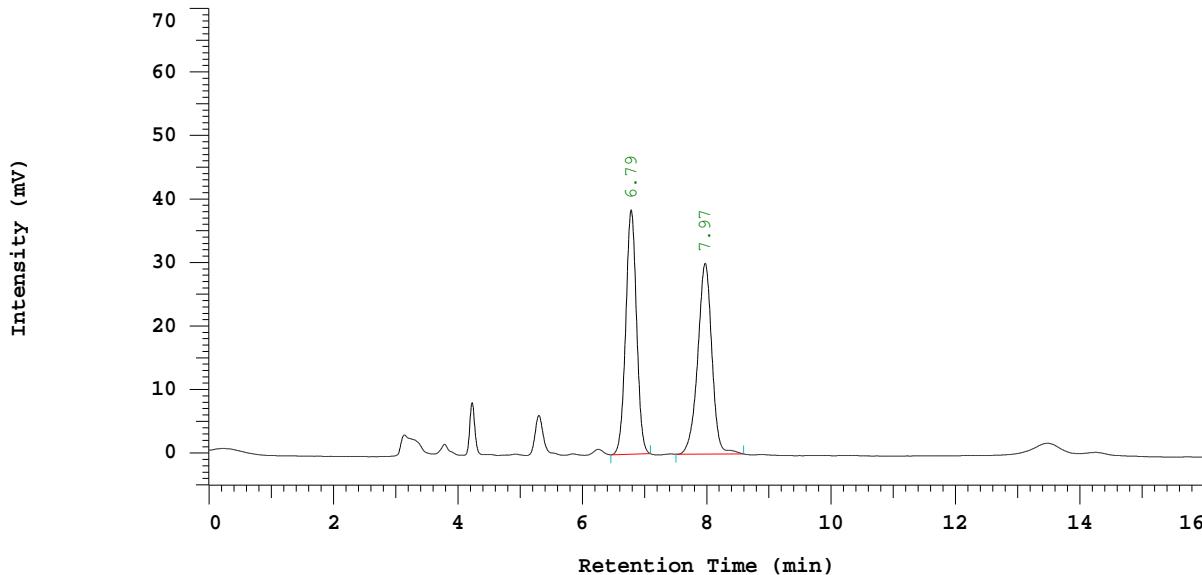
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-125F2(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.79	463526	38460	49.415
2	7.97	474502	30053	50.585
		938028	68513	100.000

Peak rejection level: 1000

Figure S222. HPLC analysis of the racemic **3a**, for comparison (Table 1, entry 12)

D-2000: Prakash Series: 0935
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/23/2018 07:50 PM Reported Date and Time: 07/23/2018 08:47 PM

Processed Date and Time: 07/23/2018 08:46 PM

Data Path: D:\Prakash\DATA\0935\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0935

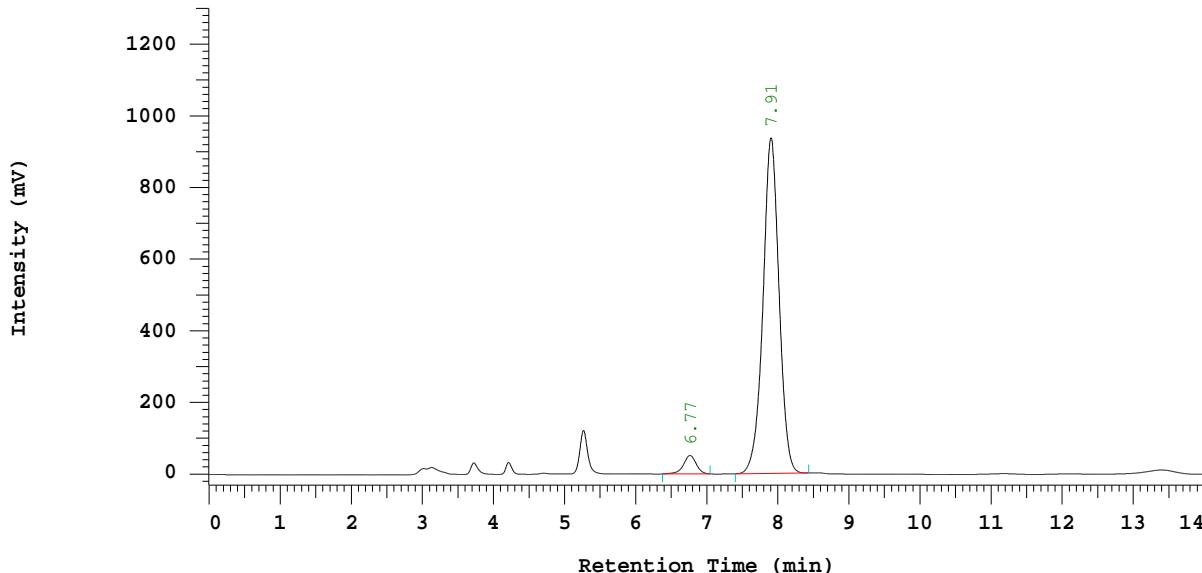
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-125F2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.77	647047	51743	4.209
2	7.91	14727374	936150	95.791
		15374421	987893	100.000

Peak rejection level: 1000

Figure S223. HPLC analysis of chiral 3a, obtained from the reaction with catalyst VII (Table 1, entry 12).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/23/2018 10:50 PM Reported Date and Time: 07/23/2018 10:16 PM

Processed Date and Time: 07/23/2018 10:15 PM

Data Path: D:\Prakash\DATA\0938\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0938

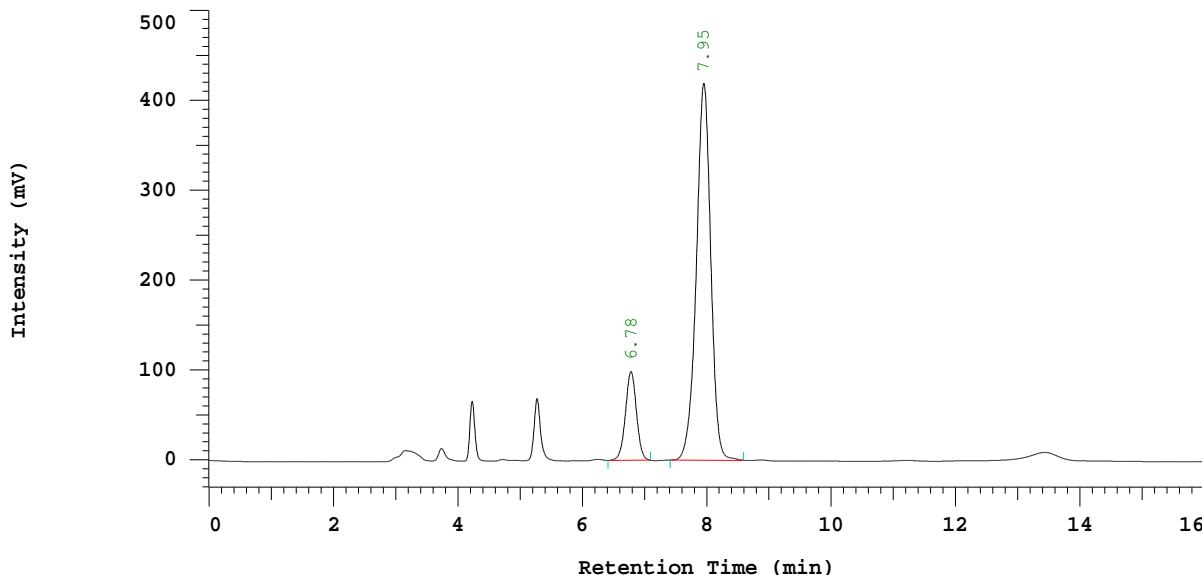
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-125F2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.78	1215502	98689	15.264
2	7.95	6747800	419179	84.736
		7963302	517868	100.000

Peak rejection level: 1000

Figure S224. HPLC analysis of the mixture of chiral **3a** and racemic **3a**, for comparison (Table 1, entry 12)

D-2000: Prakash Series: 0932
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/23/2018 05:13 PM Reported Date and Time: 07/23/2018 05:46 PM

Processed Date and Time: 07/23/2018 05:45 PM

Data Path: D:\Prakash\DATA\0932\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0932

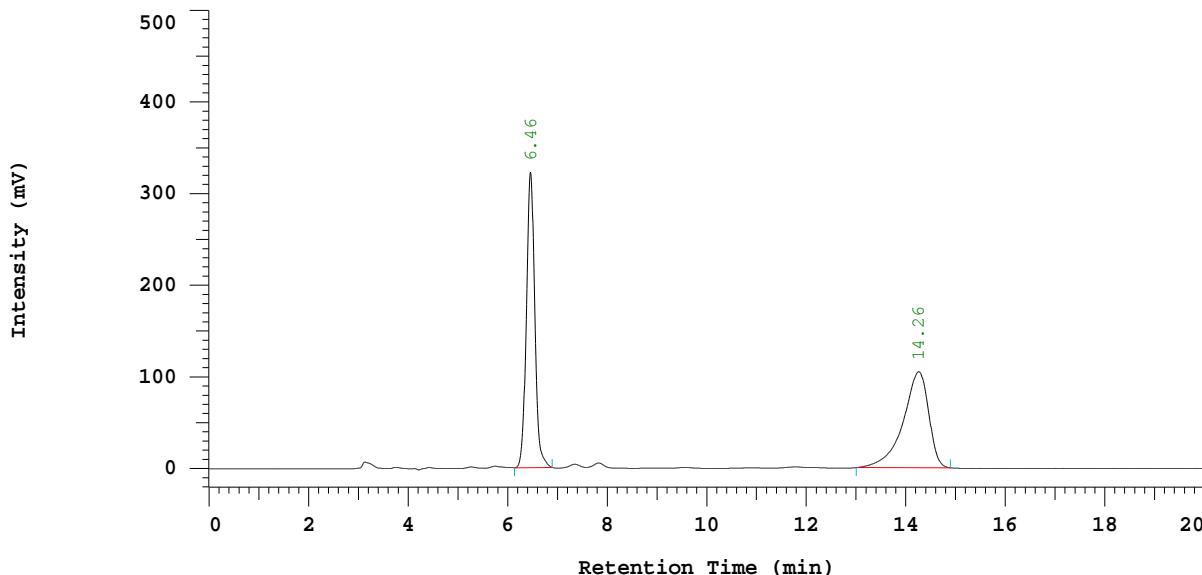
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-125F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.46	3785859	322226	50.318
2	14.26	3738029	104801	49.682
		7523888	427027	100.000

Peak rejection level: 1000

Figure S225. HPLC analysis of the racemic **4a**, for comparison (Table 1, entry 12)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/23/2018 04:32 PM Reported Date and Time: 07/23/2018 05:19 PM

Processed Date and Time: 07/23/2018 05:18 PM

Data Path: D:\Prakash\DATA\0931\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0931

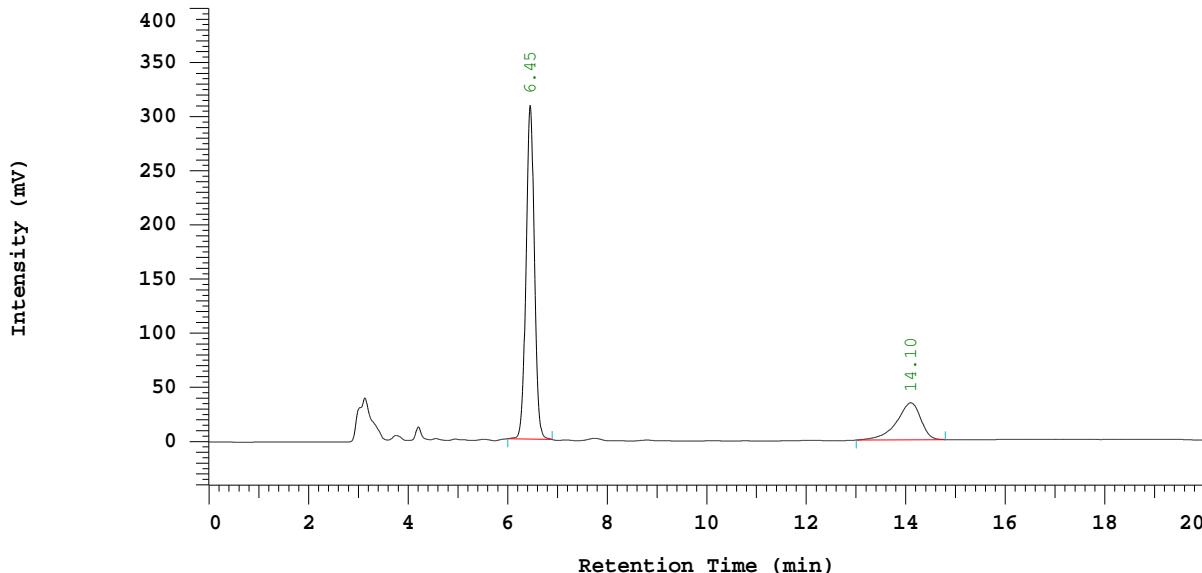
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-125F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.45	3598636	307961	75.622
2	14.10	1160068	34202	24.378
		4758704	342163	100.000

Peak rejection level: 1000

Figure S226. HPLC analysis of chiral **4a**, obtained from the reaction with catalyst **VII** (Table 1, entry 12)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/23/2018 07:34 PM Reported Date and Time: 07/23/2018 06:58 PM

Processed Date and Time: 07/23/2018 06:58 PM

Data Path: D:\Prakash\DATA\0933\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0933

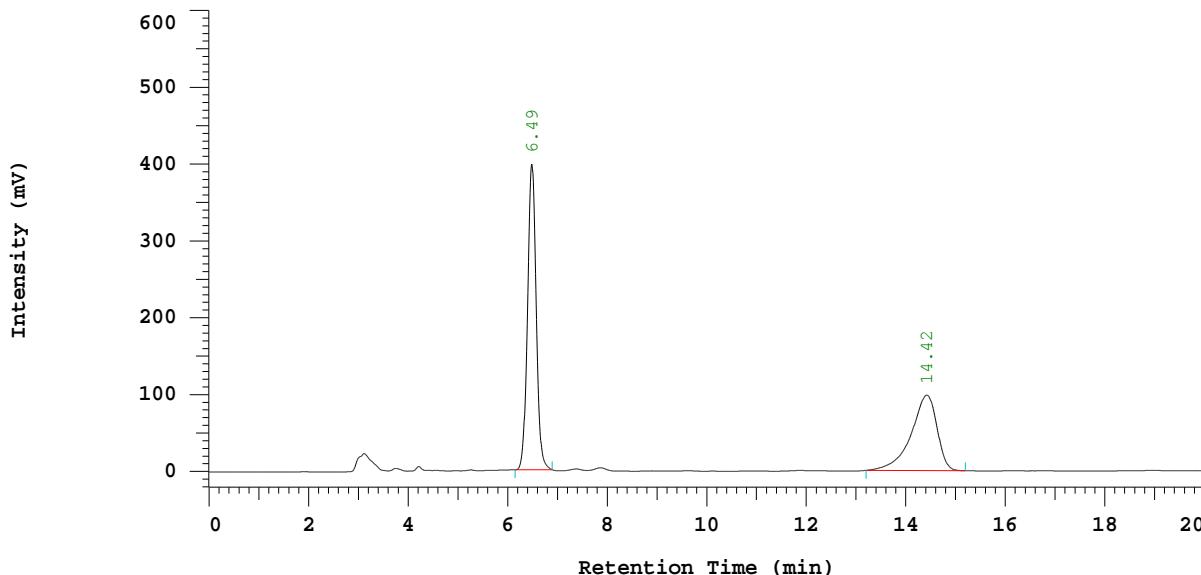
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-125F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Column Type: IC

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.49	4786445	397635	57.375
2	14.42	3555924	98203	42.625
		8342369	495838	100.000

Peak rejection level: 1000

Figure S227. HPLC analysis of the mixture of chiral **4a** and racemic **4a**, for comparison (Table 1, entry 12)

D-2000: Prakash Series: 0944
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/25/2018 Reported Date and Time: 11/28/2018
 08:02 PM 08:37 PM

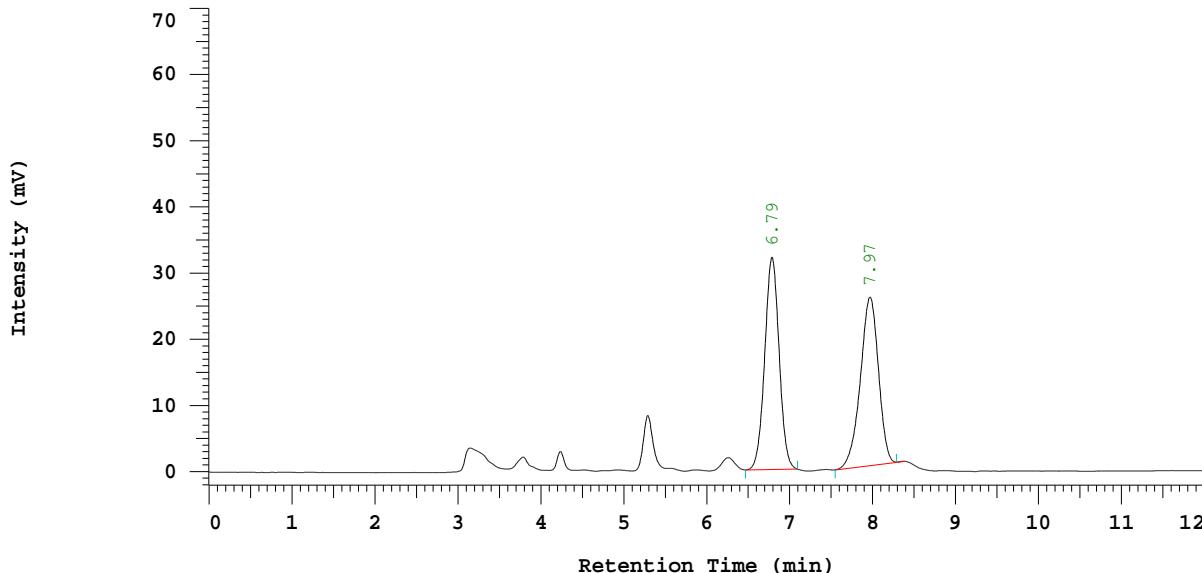
Processed Date and Time: 11/28/2018
 08:37 PM

Data Path: D:\Prakash\DATA\0944\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0944
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-04-026F2(Racemic) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 ul
Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.79	386515	32081	50.036
2	7.97	385951	25460	49.964
		772466	57541	100.000

Peak rejection level: 200000

Figure S228. HPLC analysis of the racemic **3a**, for comparison (Table 1, entry 13)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/25/2018 05:43 PM Reported Date and Time: 11/28/2018 07:05 PM

Processed Date and Time: 11/28/2018 07:03 PM

Data Path: D:\Prakash\DATA\0943\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0943

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-04-026F2(chiral)

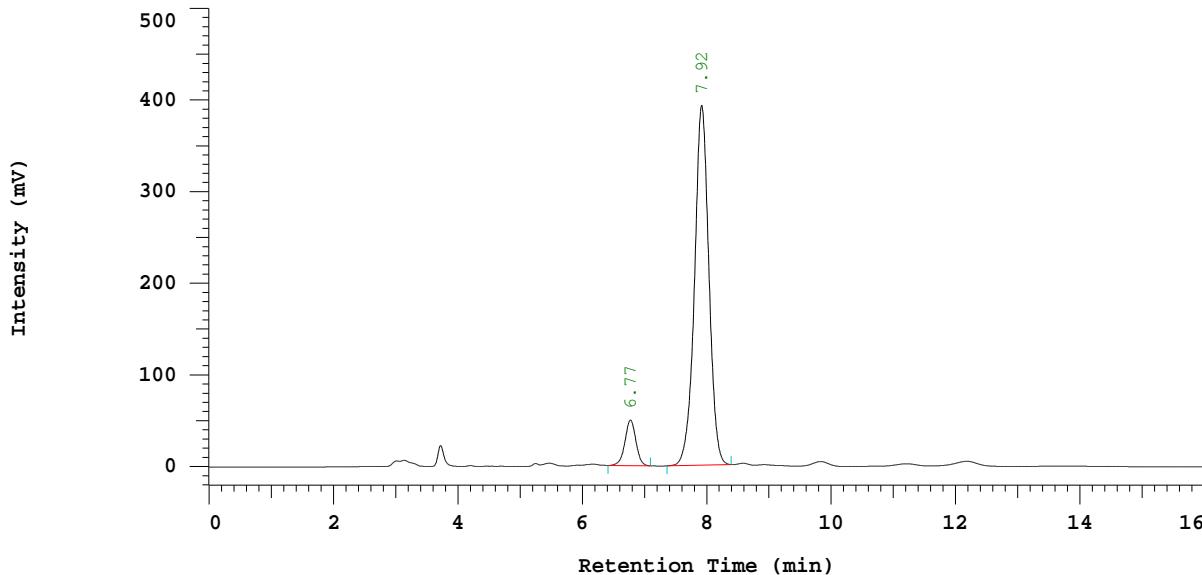
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 270 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 270 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.77	610055	49765	8.826
2	7.92	6302246	392709	91.174
		6912301	442474	100.000

Peak rejection level: 200000

Figure S229. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst **IV** (Table 1, entry 13)

D-2000: Prakash Series: 0945
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/25/2018 Reported Date and Time: 11/28/2018
 08:24 PM 08:34 PM

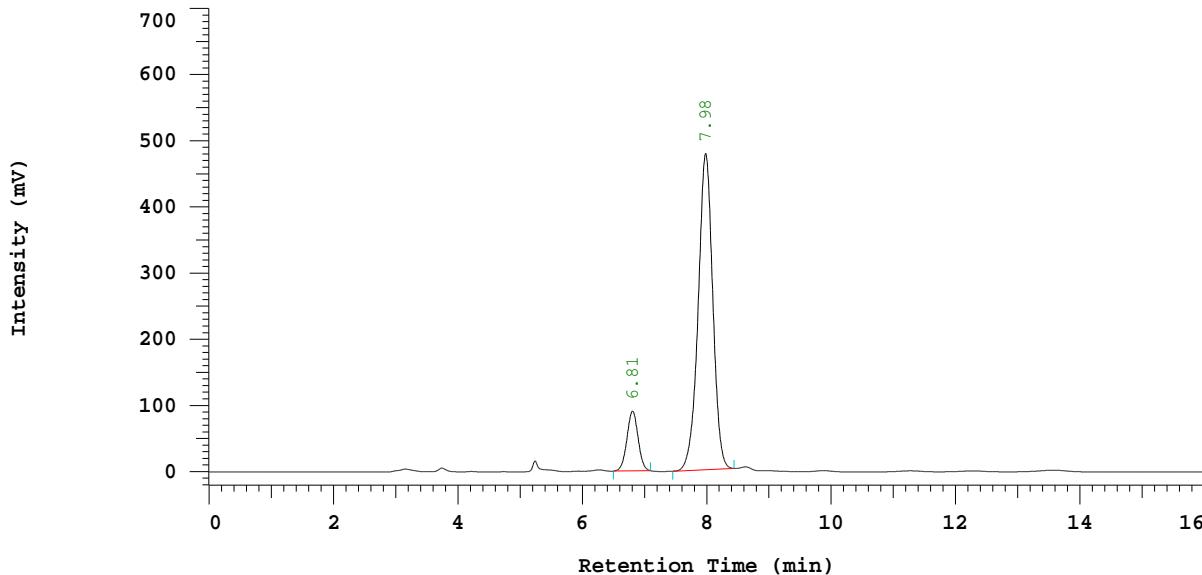
Processed Date and Time: 11/28/2018
 08:33 PM

Data Path: D:\Prakash\DATA\0945\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0945
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-04-026F2(Co) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 ul
Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.81	1124962	90435	12.631
2	7.98	7781369	477760	87.369
		8906331	568195	100.000

Peak rejection level: 200000

Figure S230. HPLC analysis of the mixture of chiral 3a and racemic 3a, for comparison (Table 1, entry 13)

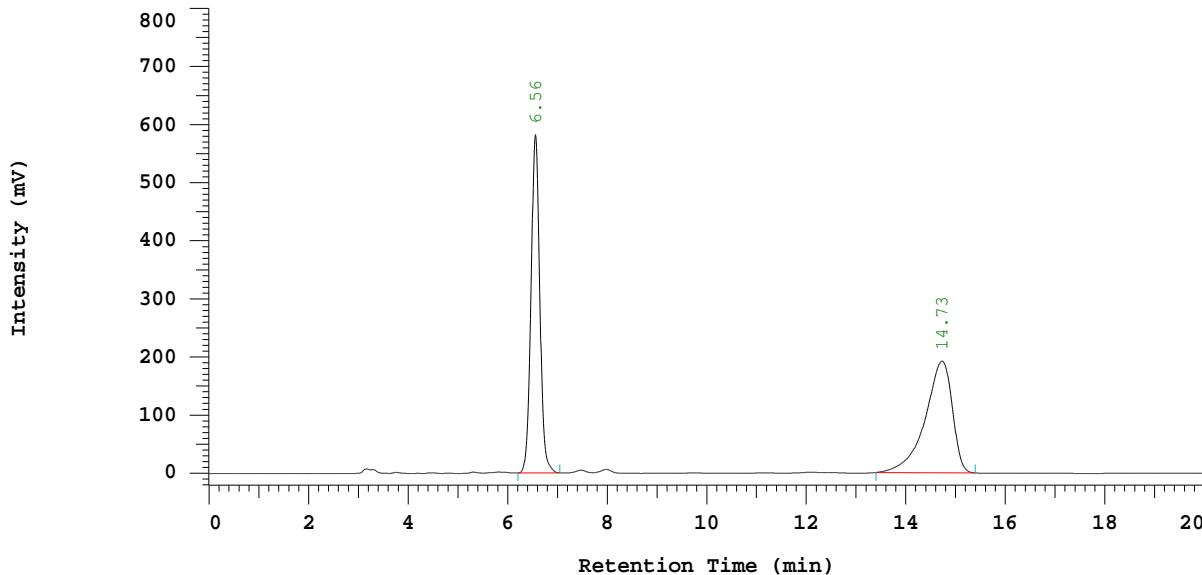
D-2000 Elite HPLC System Manager ReportAnalyzed Date and Time: 07/25/2018 Reported Date and Time: 11/28/2018
06:33 PM 08:29 PMProcessed Date and Time: 11/28/2018
08:27 PM

Data Path: D:\Prakash\DATA\0940\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0940
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-04-026F1(Racemic) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 ul
Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.56	7131622	581460	49.492
2	14.73	7278093	192186	50.508
		14409715	773646	100.000

Peak rejection level: 200000

Figure S231. HPLC analysis of the racemic **4a**, for comparison (Table 1, entry 13)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/25/2018
06:03 PM

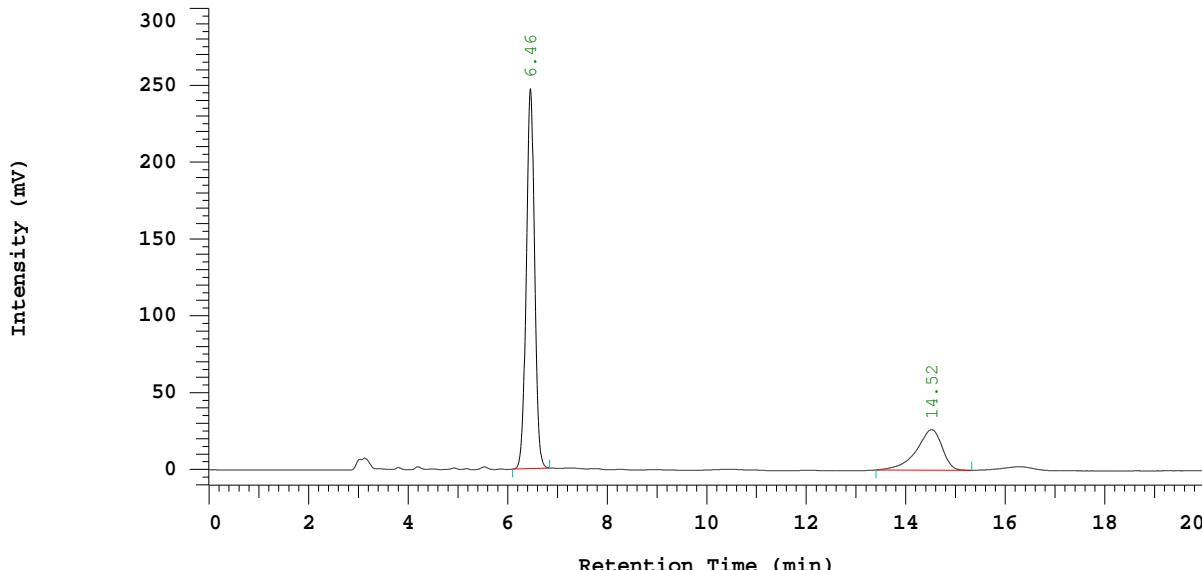
Reported Date and Time: 11/28/2018
08:23 PM

Processed Date and Time: 11/28/2018
08:22 PM

Data Path: D:\Prakash\DATA\0939\
Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0939
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-04-026F1(chiral) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 uL
Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.46	2872246	247030	75.208
2	14.52	946835	26309	24.792
		3819081	273339	100.000

Peak rejection level: 200000

Figure S232. HPLC analysis of chiral **4a**, obtained from the reaction with catalyst **IV** (Table 1, entry 13)

D-2000: Prakash Series: 0941
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/25/2018 07:00 PM Reported Date and Time: 11/28/2018 08:18 PM

Processed Date and Time: 11/28/2018 08:17 PM

Data Path: D:\Prakash\DATA\0941\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0941

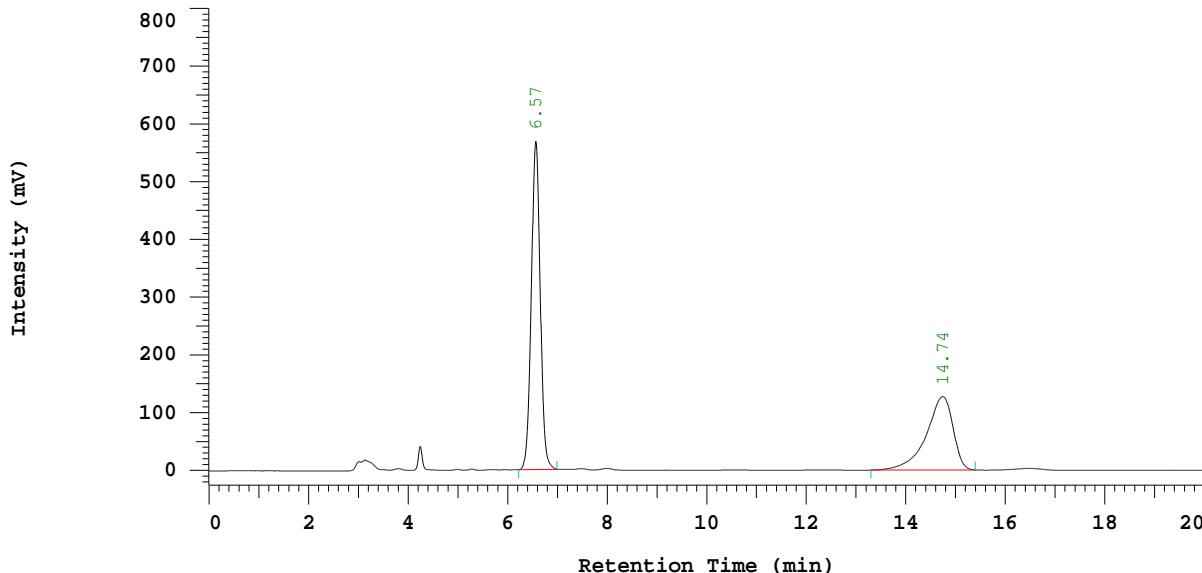
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-026F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.57	7096924	568247	59.871
2	14.74	4756846	127177	40.129
		11853770	695424	100.000

Peak rejection level: 200000

Figure S233. HPLC analysis of the mixture of chiral 4a and racemic 4a, for comparison (Table 1, entry 13)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/16/2018 12:06 PM Reported Date and Time: 01/16/2018 01:47 PM

Processed Date and Time: 01/16/2018 01:47 PM

Data Path: D:\Prakash\DATA\0756\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0756

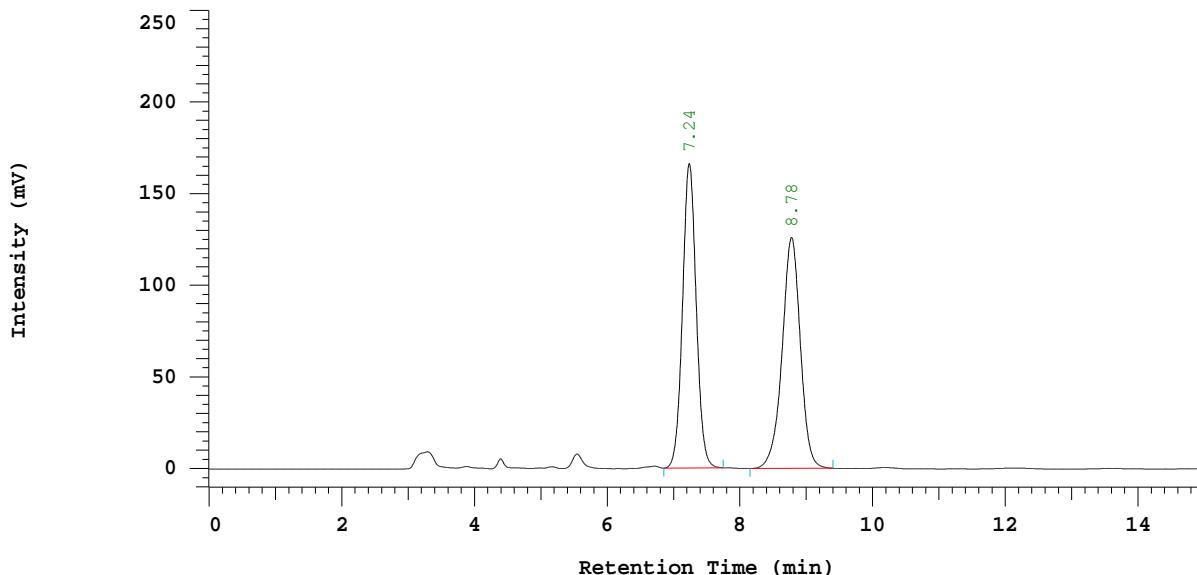
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105 (Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.24	2382158	166083	49.723
2	8.78	2408664	125957	50.277
		4790822	292040	100.000

Peak rejection level: 200000

Figure S234. HPLC analysis of the racemic **3a**, for comparison (Table 2, entry 1)

D-2000: Prakash Series: 0755
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/16/2018 11:47 AM Reported Date and Time: 01/16/2018 01:54 PM

Processed Date and Time: 01/16/2018 01:53 PM

Data Path: D:\Prakash\DATA\0755\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0755

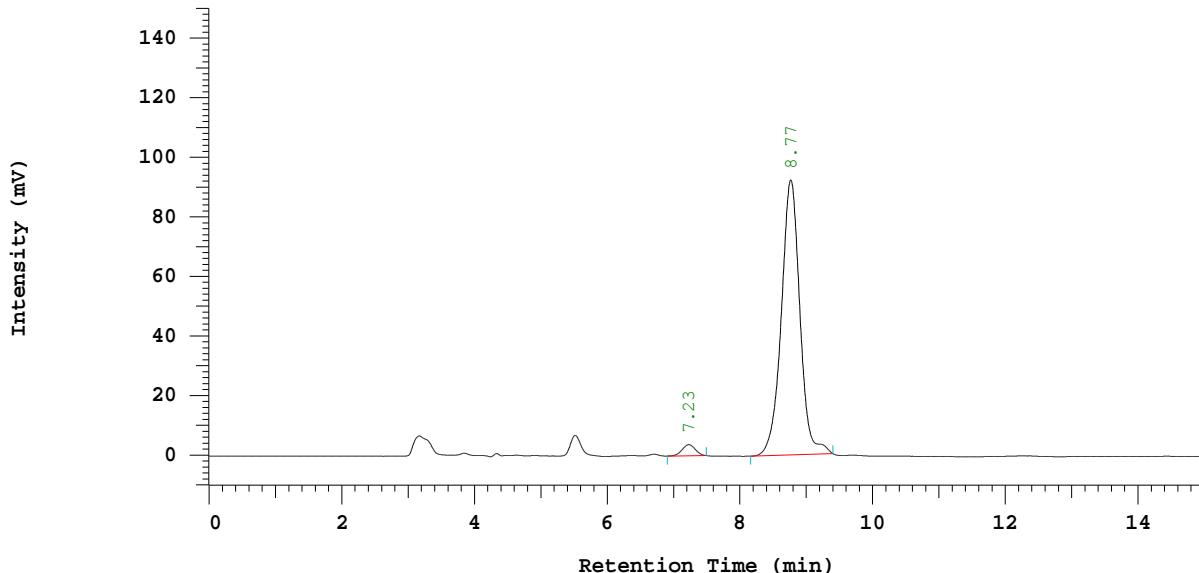
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.23	51465	3734	2.790
2	8.77	1793097	92305	97.210
		1844562	96039	100.000

Peak rejection level: 100

Figure S235. HPLC analysis of chiral **3a**, obtained from the reaction with catalyst **IV** (Table 2, entry 1)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/16/2018 01:16 PM Reported Date and Time: 01/16/2018 01:43 PM

Processed Date and Time: 01/16/2018 01:41 PM

Data Path: D:\Prakash\DATA\0757\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0757

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-105(Co)

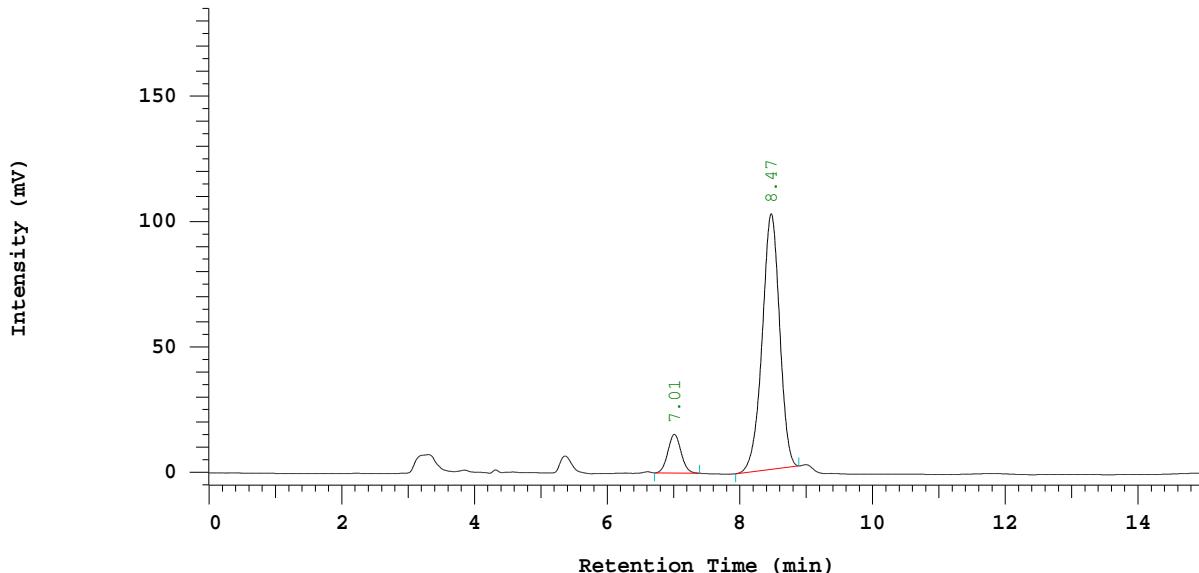
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.01	212810	15460	10.254
2	8.47	1862675	101910	89.746
		2075485	117370	100.000

Peak rejection level: 200000

Figure S236. HPLC analysis of the mixture of chiral **3a** and racemic **3a**, for comparison (Table 2, entry 1)

D-2000: Prakash Series: 0829
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/12/2018 02:51 PM Reported Date and Time: 06/18/2018 12:25 PM

Processed Date and Time: 06/18/2018 12:19 PM

Data Path: D:\Prakash\DATA\0829\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0829

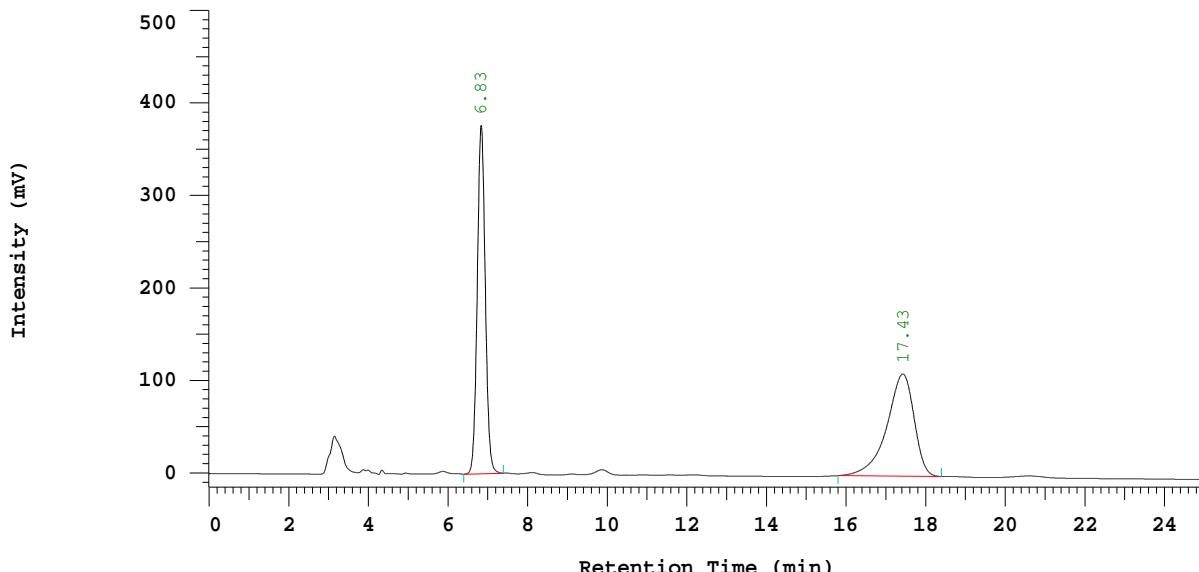
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.83	5223057	376339	49.861
2	17.43	5252176	110438	50.139
		10475233	486777	100.000

Peak rejection level: 200000

Figure S237. HPLC analysis of the racemic **4a**, for comparison (Table 2, entry 1)

D-2000: Prakash Series: 0830
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/12/2018 03:30 PM Reported Date and Time: 06/18/2018 12:17 PM

Processed Date and Time: 06/18/2018 12:16 PM

Data Path: D:\Prakash\DATA\0830\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0830

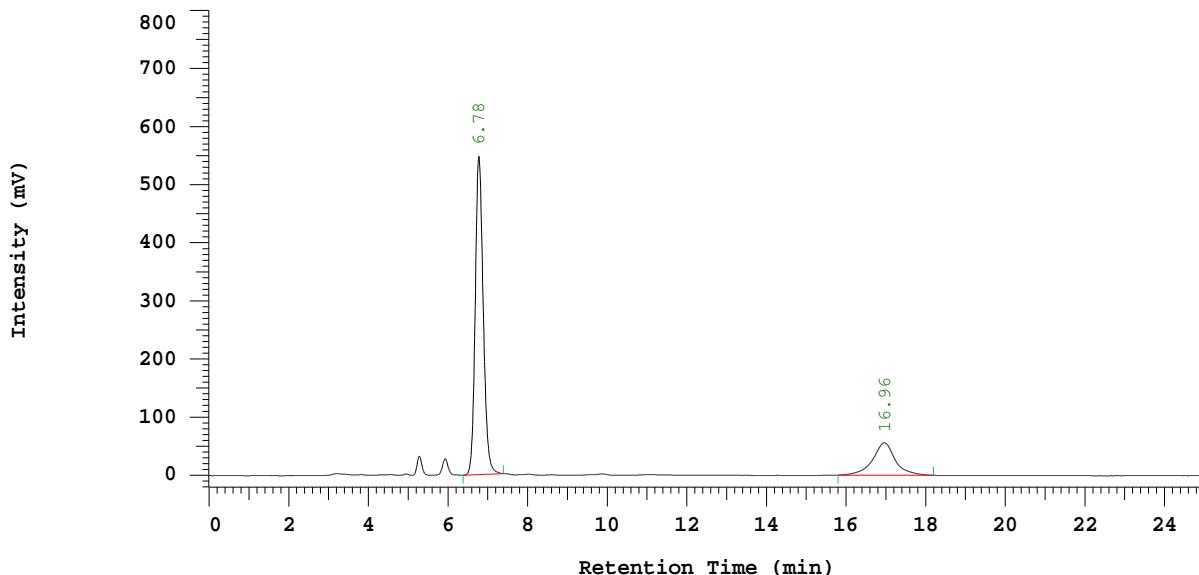
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-105F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.78	7577790	547187	77.432
2	16.96	2208627	55986	22.568
		9786417	603173	100.000

Peak rejection level: 200000

Figure S238. HPLC analysis of chiral **4a**, obtained from the reaction with catalyst **IV** (Table 2, entry 1)

D-2000: Prakash Series: 0835
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 02/12/2018 05:49 PM Reported Date and Time: 06/18/2018 12:27 PM

Processed Date and Time: 06/18/2018 12:27 PM

Data Path: D:\Prakash\DATA\0835\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0835

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-105F1(Co)

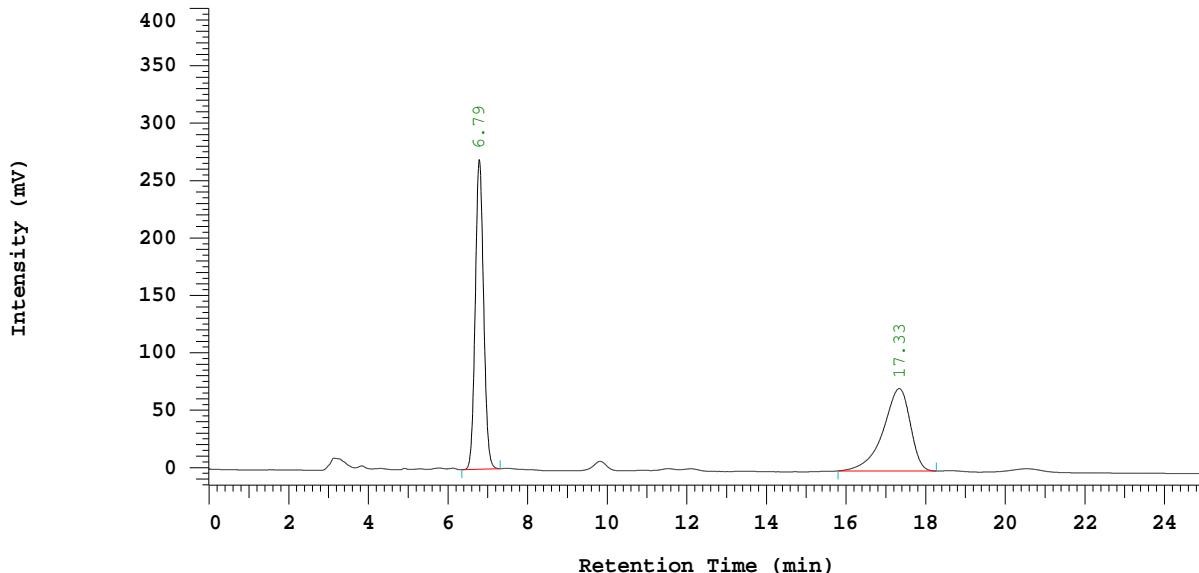
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.79	3904749	269710	53.491
2	17.33	3395115	71712	46.509
		7299864	341422	100.000

Peak rejection level: 200000

Figure S239. HPLC analysis of the mixture of chiral **4a** and racemic **4a**, for comparison (Table 2, entry 1)

D-2000: Prakash Series: 0734
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/13/2018 03:40 PM Reported Date and Time: 01/13/2018 08:38 PM

Processed Date and Time: 01/13/2018 08:37 PM

Data Path: D:\Prakash\DATA\0734\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0734

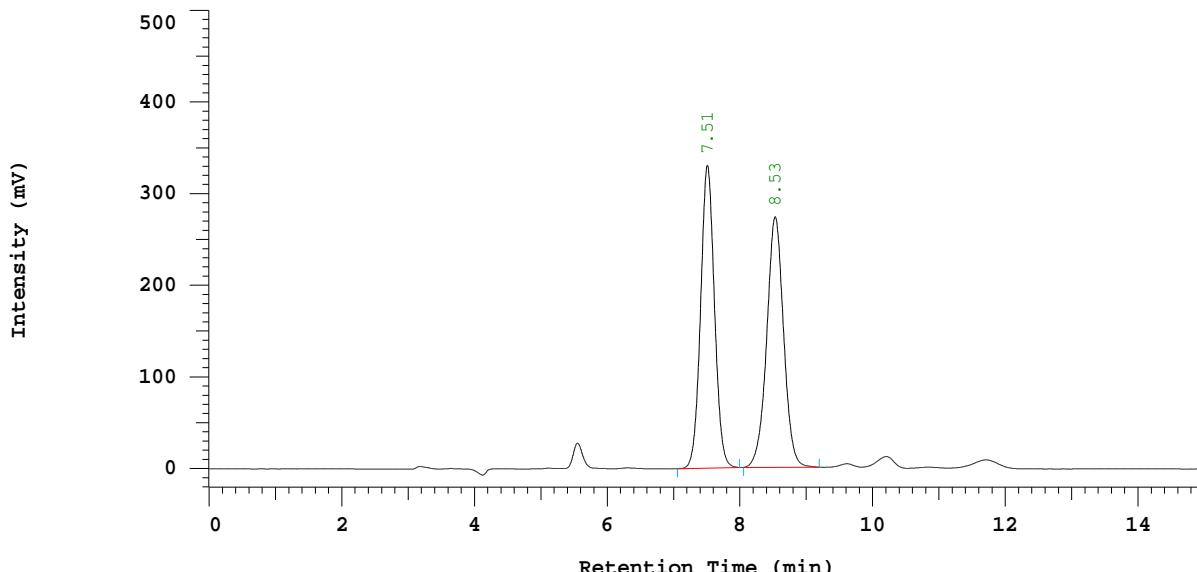
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-109(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.51	4788437	330228	49.747
2	8.53	4837108	273345	50.253
		9625545	603573	100.000

Peak rejection level: 2000

Figure S240. HPLC analysis of the racemic **3b**, for comparison (Table 2, entry 2)

D-2000: Prakash Series: 0740
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/13/2018 07:43 PM Reported Date and Time: 01/13/2018 08:32 PM

Processed Date and Time: 01/13/2018 08:31 PM

Data Path: D:\Prakash\DATA\0740\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0740

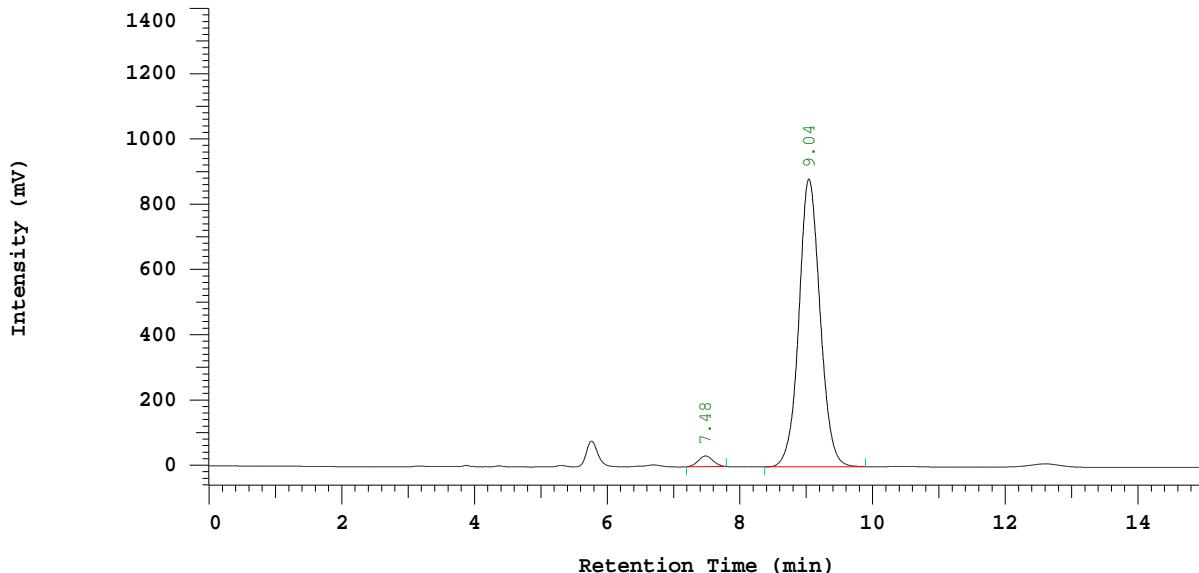
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-109(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.48	501591	32645	2.500
2	9.04	19564555	881513	97.500
		20066146	914158	100.000

Peak rejection level: 200000

Figure S241. HPLC analysis of chiral **3b**, obtained from the reaction with catalyst **IV** (Table 2, entry 2)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/13/2018 08:01 PM Reported Date and Time: 01/13/2018 08:26 PM

Processed Date and Time: 01/13/2018 08:25 PM

Data Path: D:\Prakash\DATA\0741\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0741

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-109(Co)

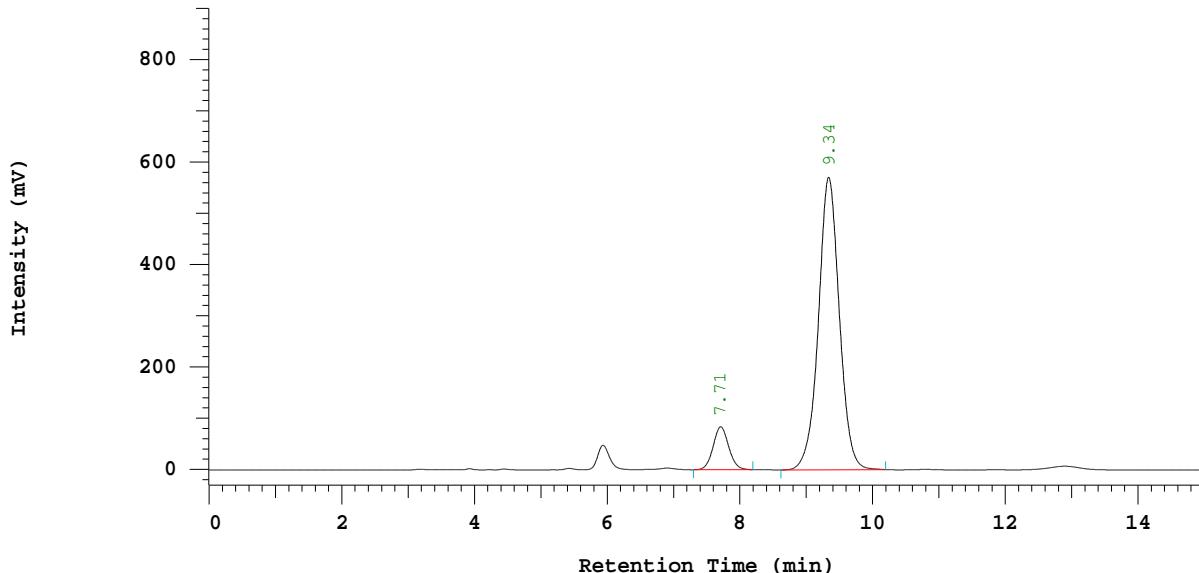
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.71	1374190	83907	9.908
2	9.34	12495925	570431	90.092
		13870115	654338	100.000

Peak rejection level: 200000

Figure S242. HPLC analysis of the mixture of chiral **3b** and racemic **3b**, for comparison (Table 2, entry 2)

D-2000: Prakash Series: 0861
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/11/2018 03:42 PM Reported Date and Time: 04/11/2018 04:04 PM

Processed Date and Time: 04/11/2018 04:03 PM

Data Path: D:\Prakash\DATA\0861\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0861

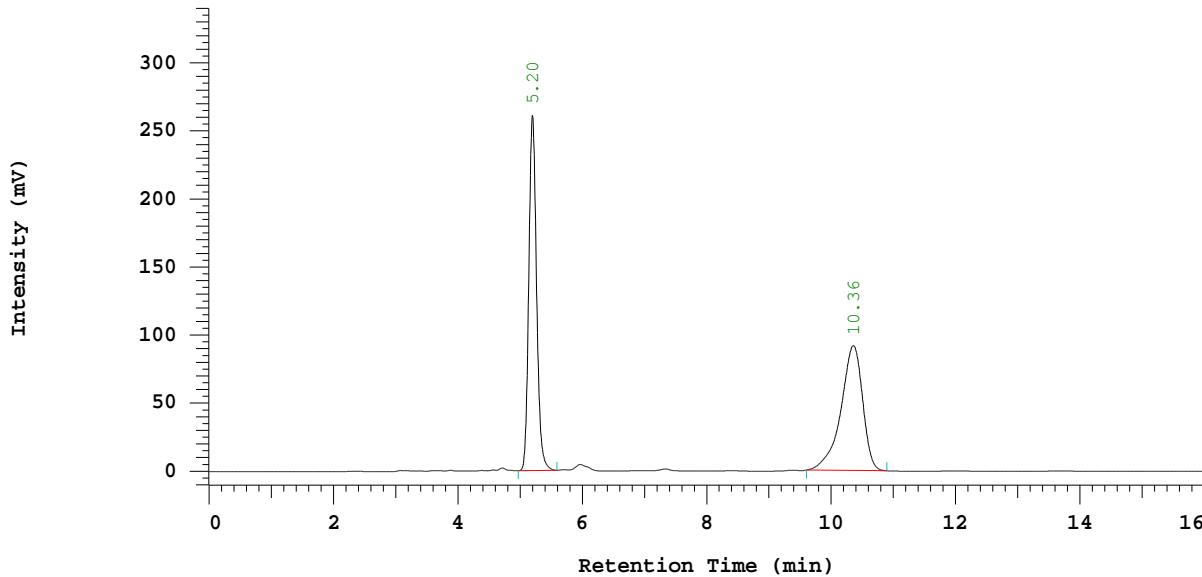
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-109F1Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.20	2253970	260811	50.218
2	10.36	2234408	91761	49.782
		4488378	352572	100.000

Peak rejection level: 200000

Figure S243. HPLC analysis of the racemic **4b**, for comparison (Table 2, entry 2)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/11/2018 03:24 PM Reported Date and Time: 04/11/2018 03:49 PM

Processed Date and Time: 04/11/2018 03:49 PM

Data Path: D:\Prakash\DATA\0860\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0860

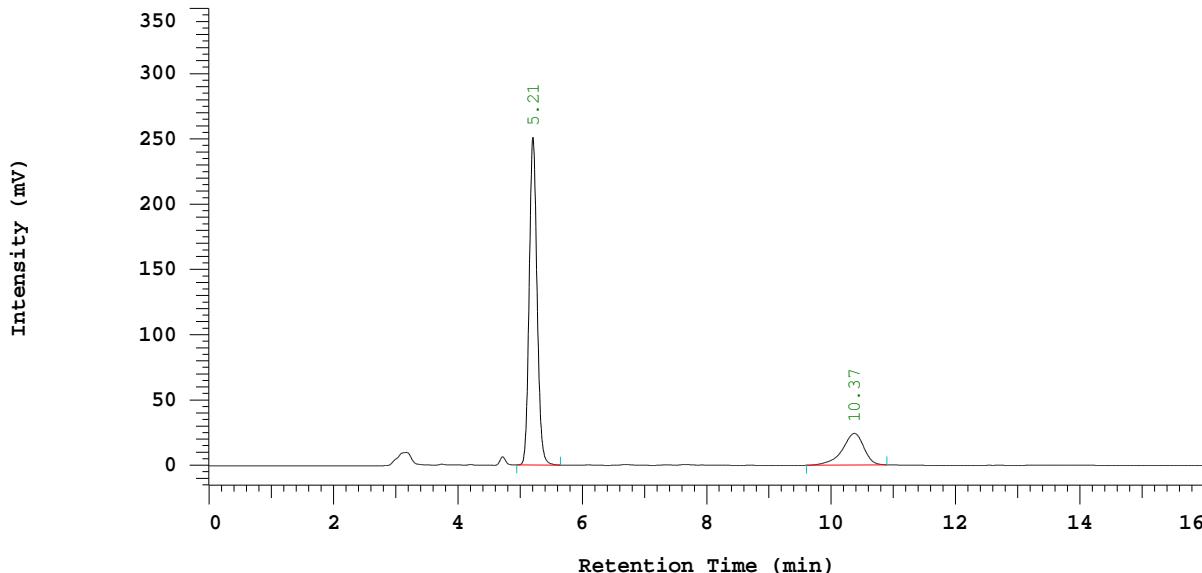
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-109F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.21	2194733	250917	79.014
2	10.37	582906	24242	20.986
		2777639	275159	100.000

Peak rejection level: 200000

Figure S244. HPLC analysis of chiral **4b**, obtained from the reaction with catalyst **IV** (Table 2, entry 2)

D-2000: Prakash Series: 0862
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/11/2018 06:01 PM Reported Date and Time: 04/11/2018 05:27 PM

Processed Date and Time: 04/11/2018 05:26 PM

Data Path: D:\Prakash\DATA\0862\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0862

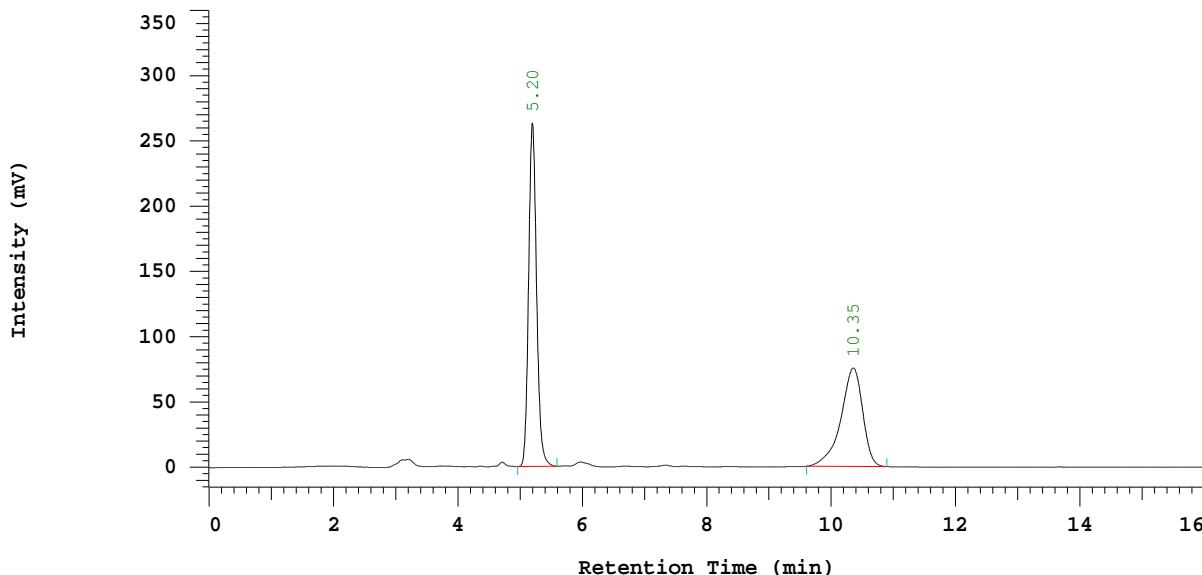
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-109F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.20	2335484	263157	55.924
2	10.35	1840676	75401	44.076
		4176160	338558	100.000

Peak rejection level: 200000

Figure S245. HPLC analysis of the mixture of chiral **4b** and racemic **4b**, for comparison (Table 2, entry 2)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/12/2018 04:17 PM Reported Date and Time: 01/12/2018 05:03 PM

Processed Date and Time: 01/12/2018 05:03 PM

Data Path: D:\Prakash\DATA\0724\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0724

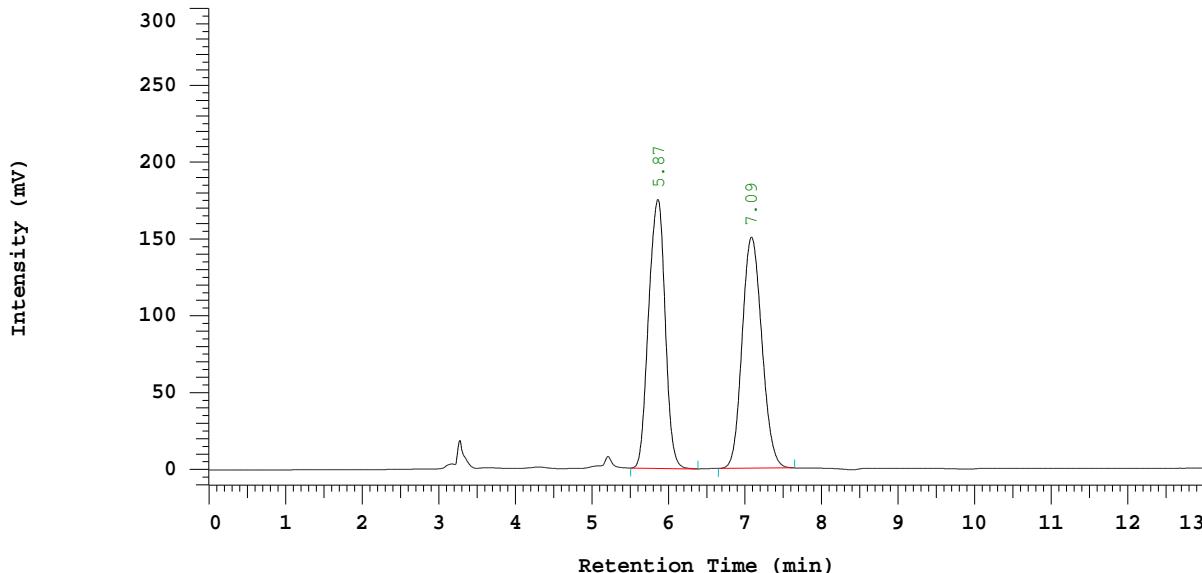
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-111(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.87	2616736	174934	49.276
2	7.09	2693578	150284	50.724
		5310314	325218	100.000

Peak rejection level: 2000

Figure S246. HPLC analysis of the racemic **3c**, for comparison (Table 2, entry 3)

D-2000: Prakash Series: 0725
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/12/2018 04:35 PM Reported Date and Time: 01/12/2018 05:00 PM

Processed Date and Time: 01/12/2018 05:00 PM

Data Path: D:\Prakash\DATA\0725\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0725

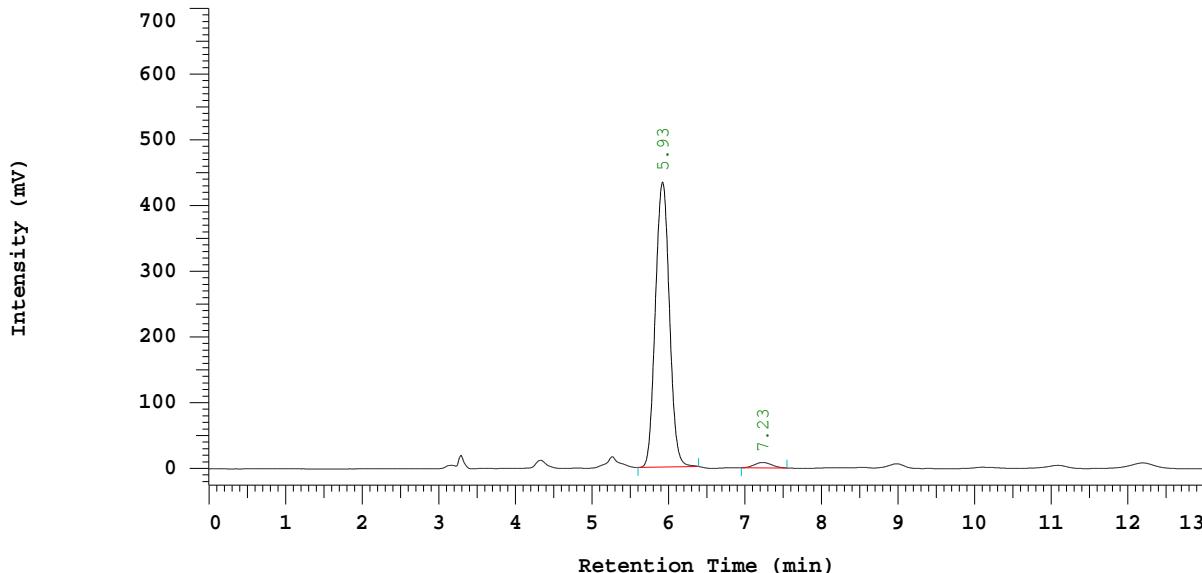
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-111(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.93	5517117	433566	97.675
2	7.23	131307	8262	2.325
		5648424	441828	100.000

Peak rejection level: 2000

Figure S247. HPLC analysis of chiral **3c**, obtained from the reaction with catalyst **IV** (Table 2, entry 3)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/12/2018 04:52 PM Reported Date and Time: 01/12/2018 05:28 PM

Processed Date and Time: 01/12/2018 05:27 PM

Data Path: D:\Prakash\DATA\0726\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0726

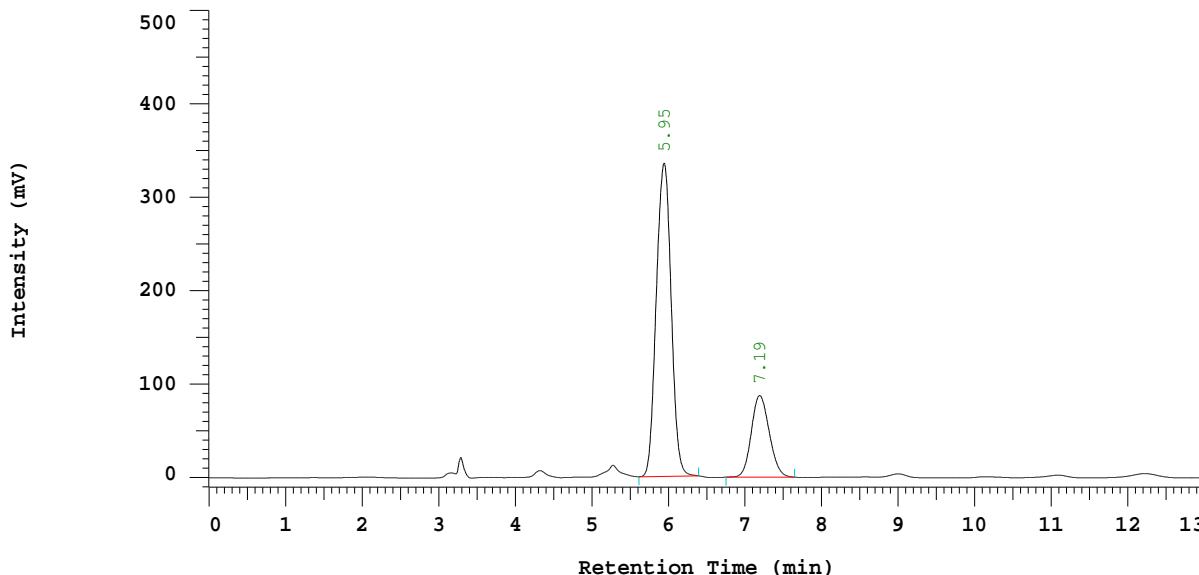
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-111(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.95	4524812	335010	76.036
2	7.19	1426064	87401	23.964
		5950876	422411	100.000

Peak rejection level: 2000

Figure S248. HPLC analysis of the mixture of chiral **3c** and racemic **3c**, for comparison (Table 2, entry 3)

D-2000: Prakash Series: 0882
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 06/23/2018 04:02 PM Reported Date and Time: 06/23/2018 04:11 PM

Processed Date and Time: 06/23/2018 04:10 PM

Data Path: D:\Prakash\DATA\0882\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0882

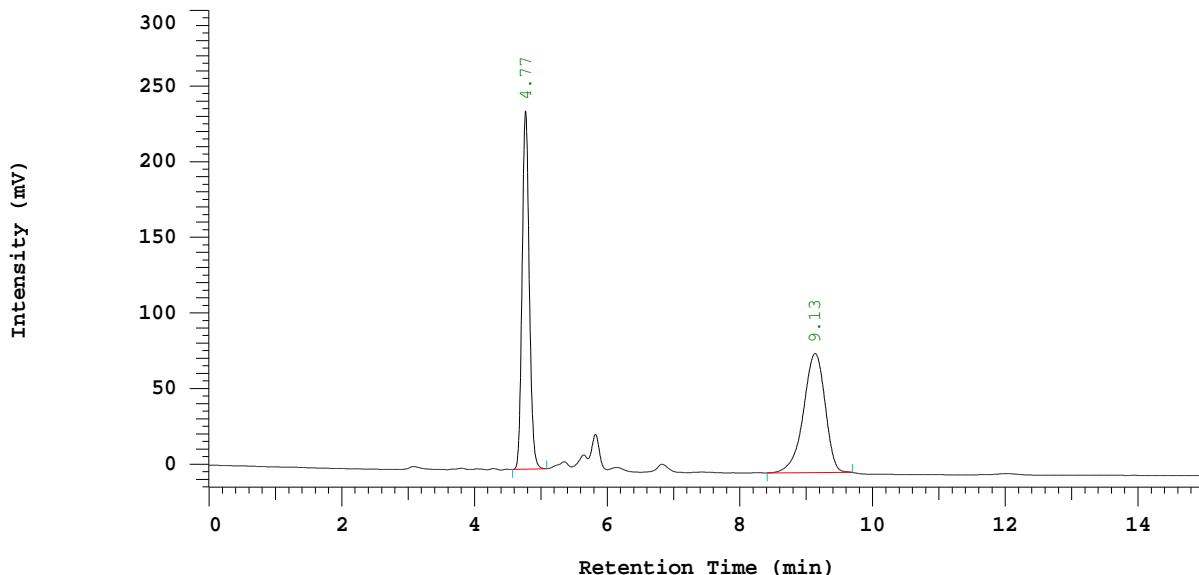
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-111F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	4.77	1770463	236665	49.785
2	9.13	1785784	78713	50.215
		3556247	315378	100.000

Peak rejection level: 200000

Figure S249. HPLC analysis of the racemic **4c**, for comparison (Table 2, entry 3)

D-2000: Prakash Series: 0883
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 06/23/2018 04:19 PM Reported Date and Time: 06/23/2018 04:06 PM

Processed Date and Time: 06/23/2018 04:05 PM

Data Path: D:\Prakash\DATA\0883\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0883

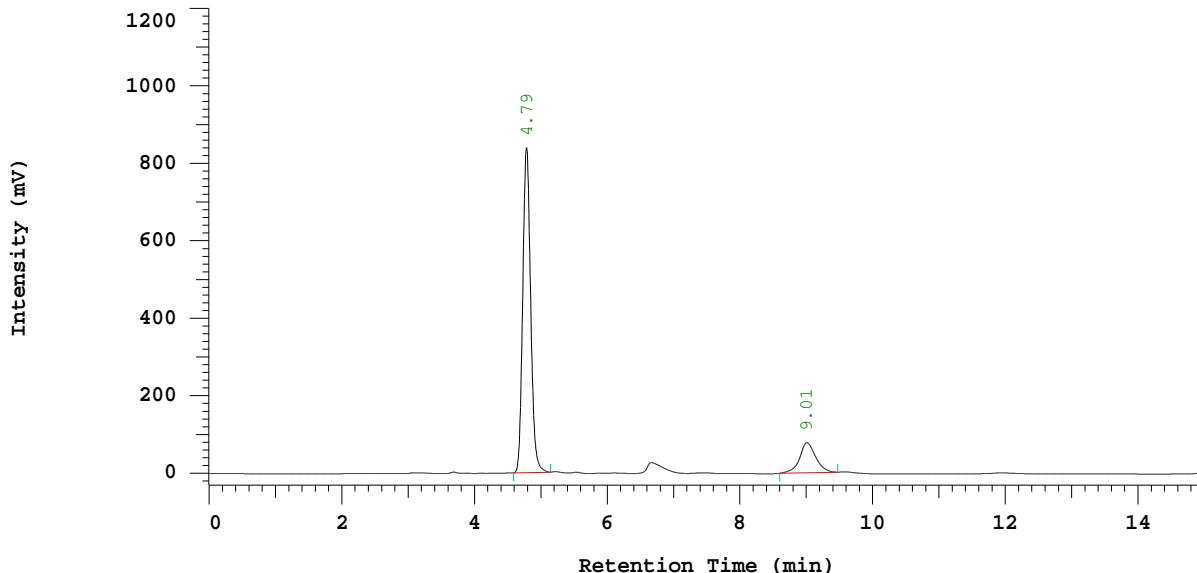
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-111F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	4.79	6944049	838802	84.195
2	9.01	1303541	77763	15.805
		8247590	916565	100.000

Peak rejection level: 200000

Figure S250. HPLC analysis of chiral **4c**, obtained from the reaction with catalyst **IV** (Table 2, entry 3)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 06/23/2018 04:37 PM Reported Date and Time: 06/23/2018 04:02 PM

Processed Date and Time: 06/23/2018 04:01 PM

Data Path: D:\Prakash\DATA\0884\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0884

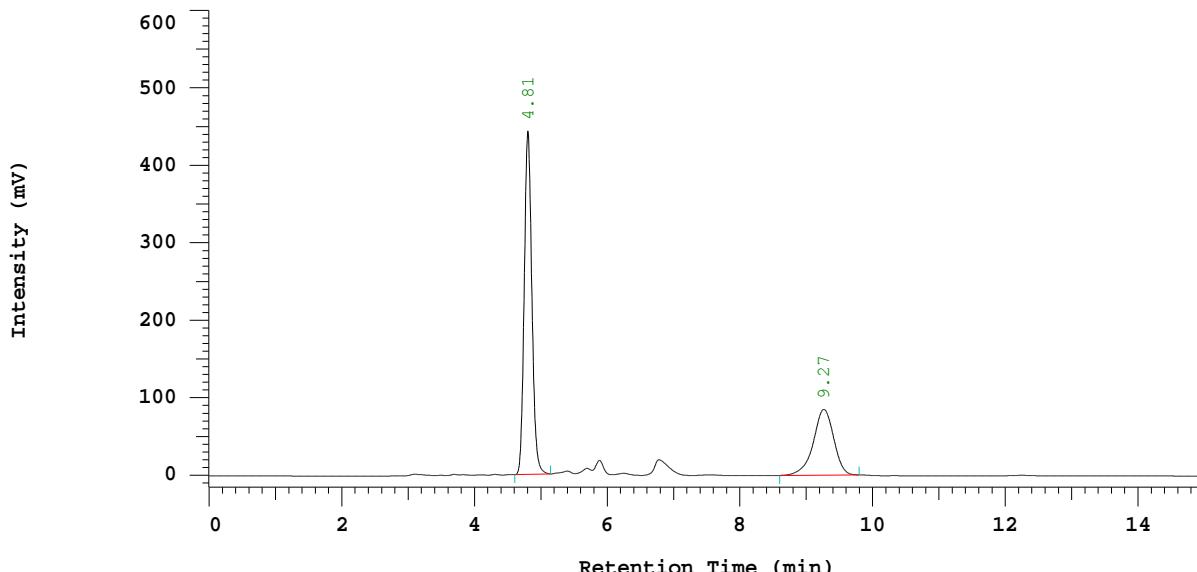
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-111F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	4.81	3539514	443251	66.121
2	9.27	1813542	84777	33.879
		5353056	528028	100.000

Peak rejection level: 200000

Figure S251. HPLC analysis of the mixture of chiral **4c** and racemic **4c**, for comparison (Table 2, entry 3)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/07/2018 04:30 PM Reported Date and Time: 01/07/2018 05:18 PM

Processed Date and Time: 01/07/2018 05:17 PM

Data Path: D:\Prakash\DATA\0712\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0712

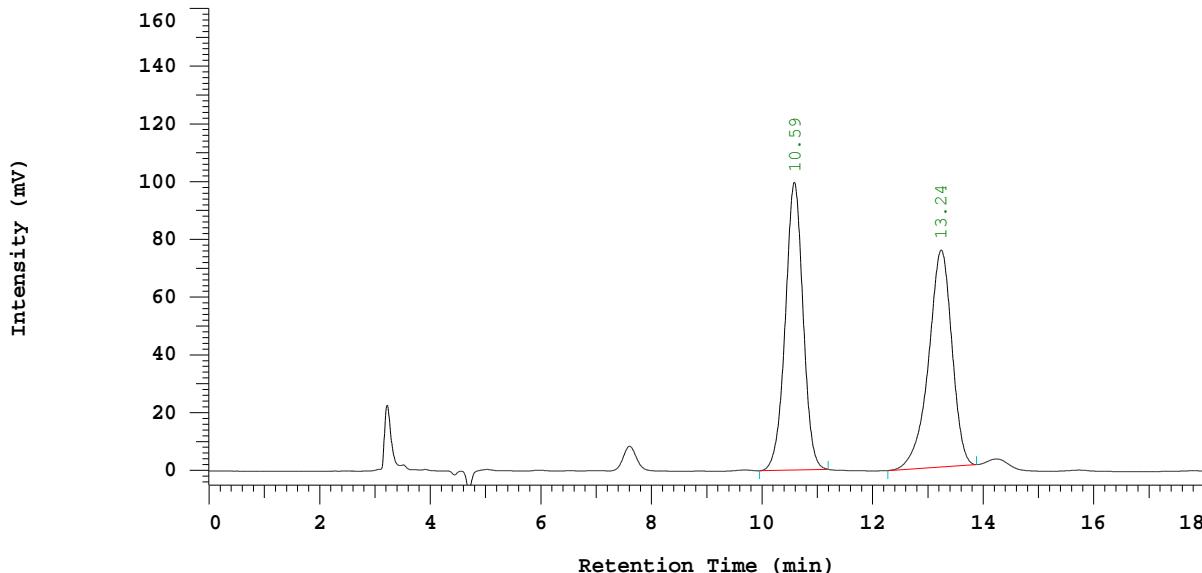
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-115Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	10.59	2226122	99589	50.234
2	13.24	2205339	75108	49.766
		4431461	174697	100.000

Peak rejection level: 200000

Figure S252. HPLC analysis of the racemic **3d**, for comparison (Table 2, entry 4)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/07/2018 04:54 PM Reported Date and Time: 01/07/2018 05:22 PM

Processed Date and Time: 01/07/2018 05:22 PM

Data Path: D:\Prakash\DATA\0713\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0713

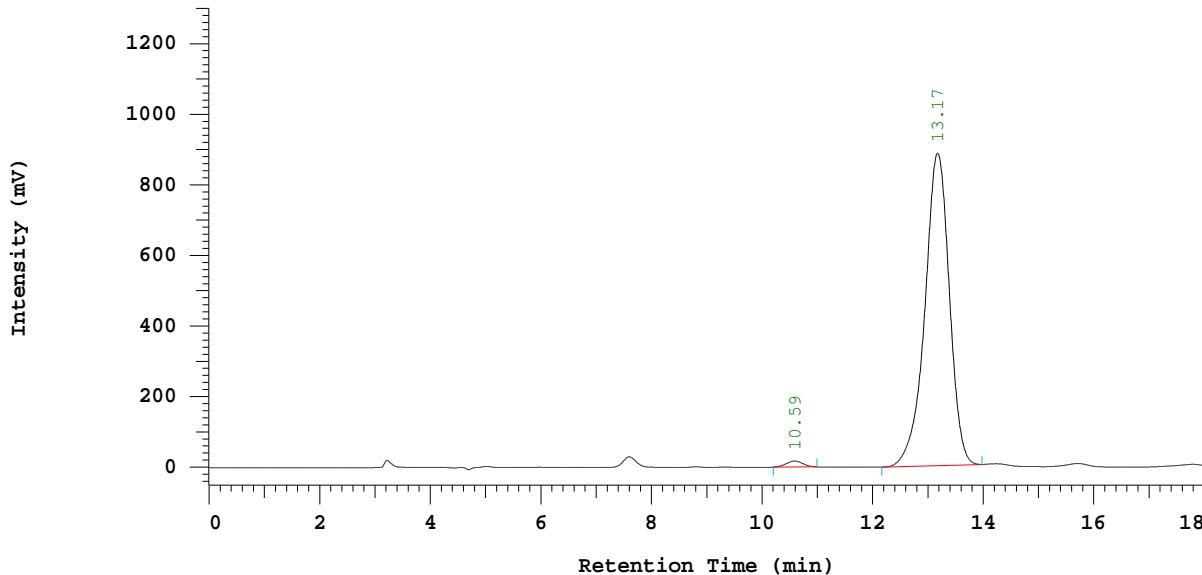
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-115(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	10.59	353477	16921	1.282
2	13.17	27226851	885139	98.718
		27580328	902060	100.000

Peak rejection level: 200000

Figure S253. HPLC analysis of chiral **3d**, obtained from the reaction with catalyst **IV** (Table 2, entry 4)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/07/2018 04:55 PM Reported Date and Time: 01/07/2018 05:26 PM

Processed Date and Time: 01/07/2018 05:26 PM

Data Path: D:\Prakash\DATA\0711\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0711

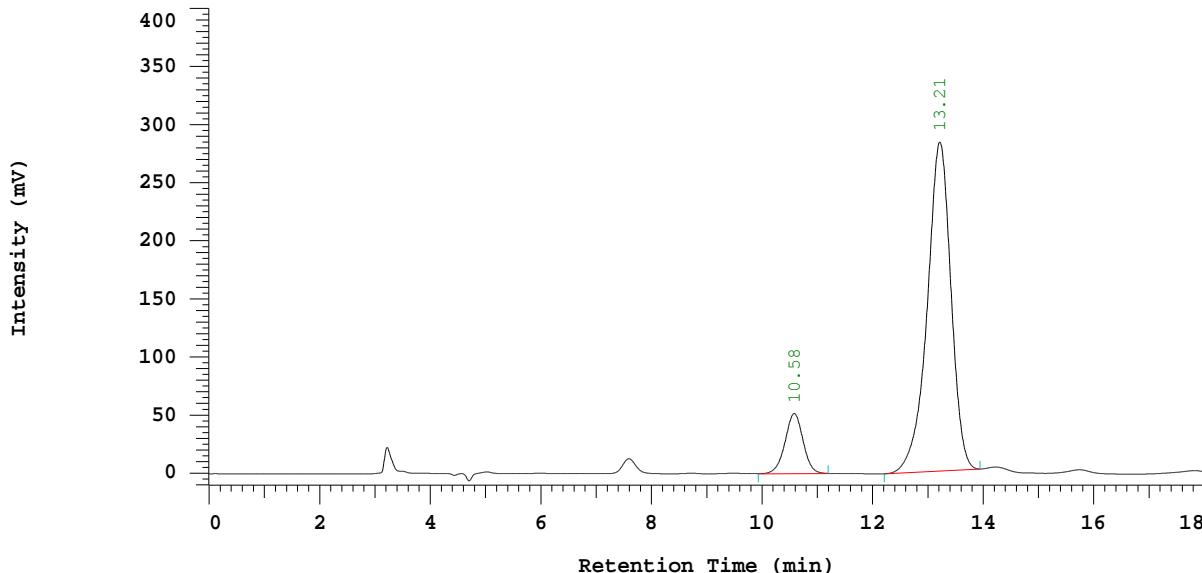
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-115(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	10.58	1170108	51685	12.162
2	13.21	8450840	283014	87.838
		9620948	334699	100.000

Peak rejection level: 200000

Figure S254. HPLC analysis of the mixture of chiral **3d** and racemic **3d**, for comparison (Table 2, entry 4)

D-2000: Prakash Series: 0866
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/20/2018 07:23 PM Reported Date and Time: 04/20/2018 08:04 PM

Processed Date and Time: 04/20/2018 08:03 PM

Data Path: D:\Prakash\DATA\0866\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0866

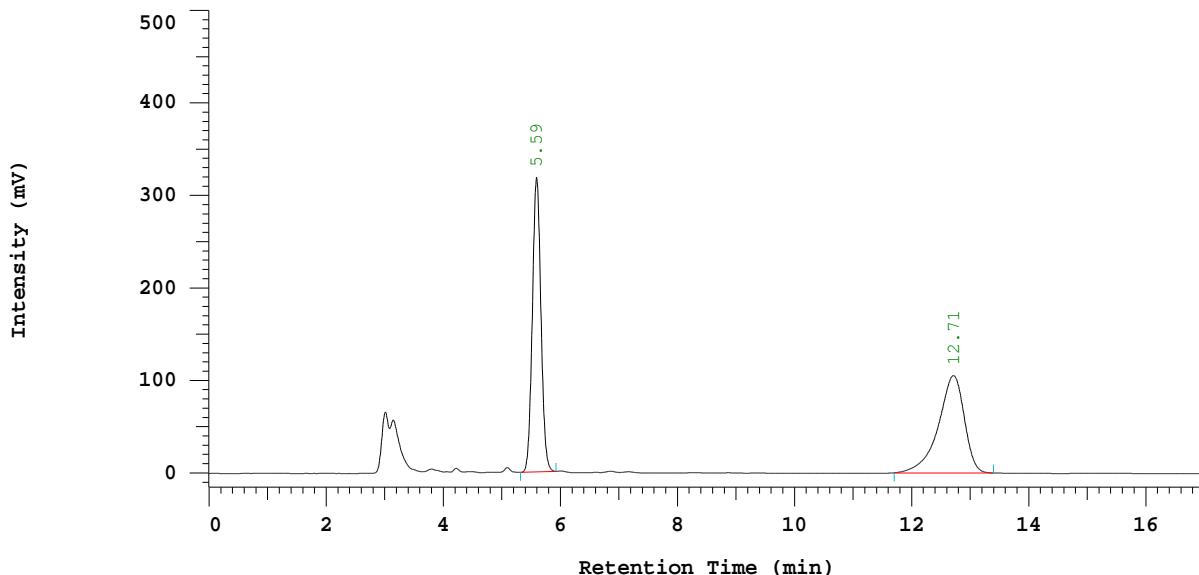
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-115F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.59	3241268	318301	49.986
2	12.71	3243109	105135	50.014
		6484377	423436	100.000

Peak rejection level: 200000

Figure S255. HPLC analysis of the racemic **4d**, for comparison (Table 2, entry 4)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/21/2018 03:38 PM Reported Date and Time: 04/21/2018 04:01 PM

Processed Date and Time: 04/21/2018 04:00 PM

Data Path: D:\Prakash\DATA\0870\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0870

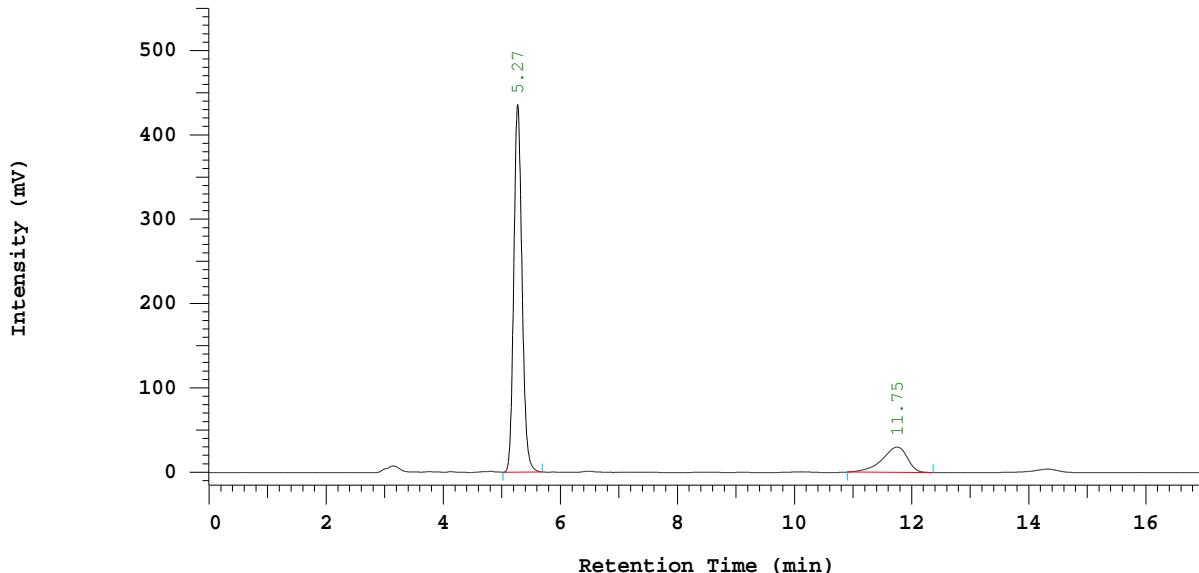
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-115F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Column Type: IC

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.27	4270438	435615	82.652
2	11.75	896342	29959	17.348
		5166780	465574	100.000

Peak rejection level: 200000

Figure S256. HPLC analysis of chiral **4d**, obtained from the reaction with catalyst **IV** (Table 2, entry 4)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/22/2018 11:34 AM Reported Date and Time: 04/22/2018 12:18 PM

Processed Date and Time: 04/22/2018 12:18 PM

Data Path: D:\Prakash\DATA\0873\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0873

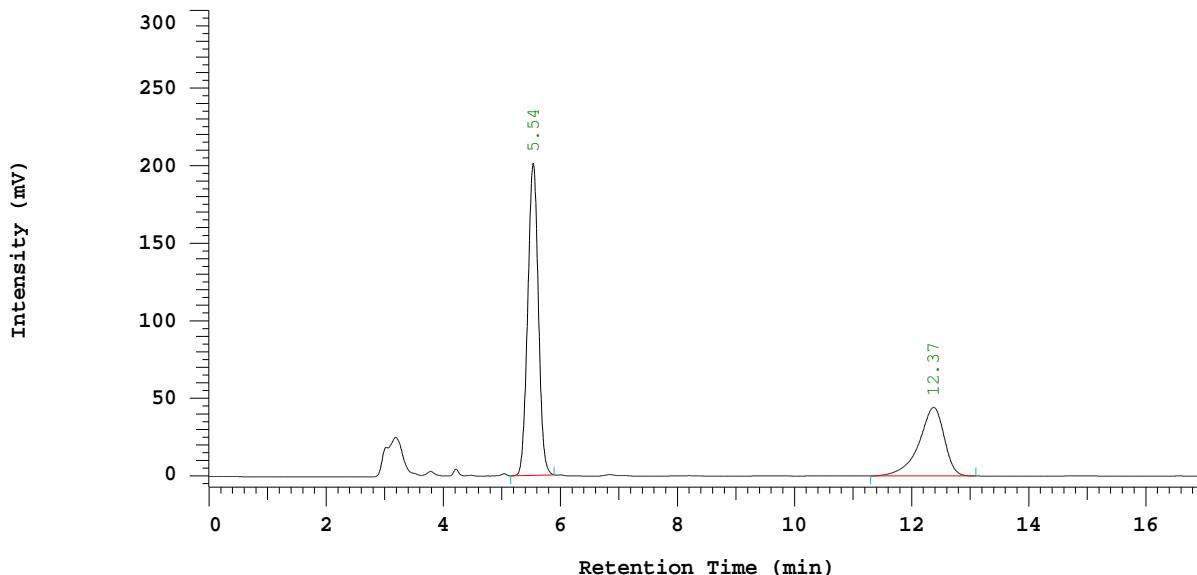
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-115F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.54	2532674	201149	65.580
2	12.37	1329262	44233	34.420
		3861936	245382	100.000

Peak rejection level: 200000

Figure S257. HPLC analysis of the mixture of chiral **4d** and racemic **4d**, for comparison (Table 2, entry 4)

D-2000: Prakash Series: 0717
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/11/2018 03:50 PM Reported Date and Time: 01/11/2018 04:49 PM

Processed Date and Time: 01/11/2018 04:48 PM

Data Path: D:\Prakash\DATA\0717\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0717

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-118Racemic)

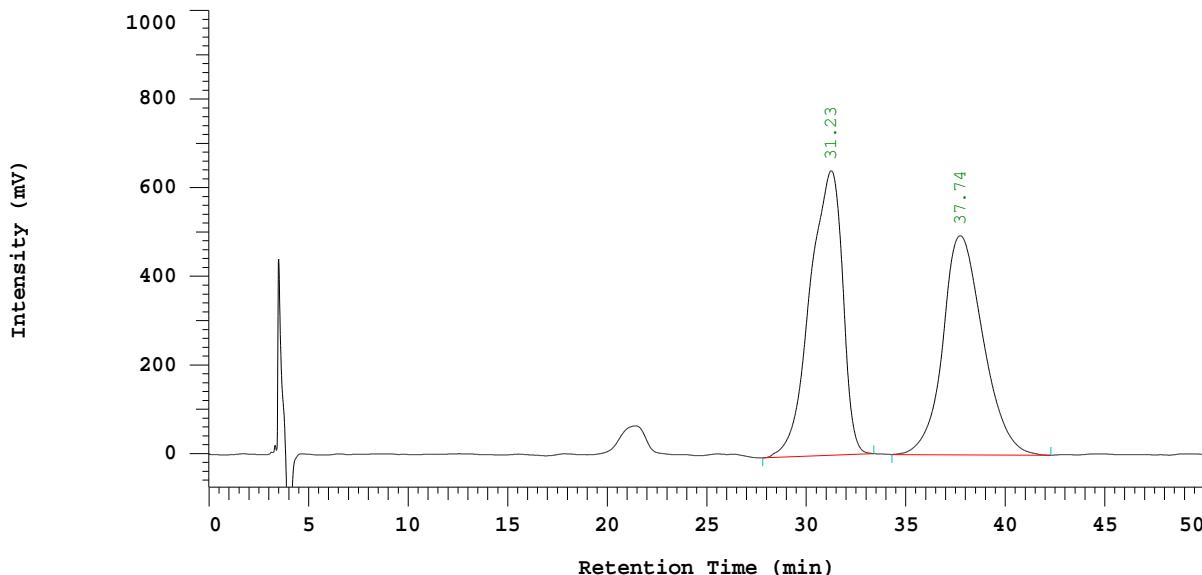
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 5%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-THF/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	31.23	72709324	641770	51.206
2	37.74	69284275	493701	48.794
		1.419E+08	1135471	100.000

Peak rejection level: 1000

Figure S258. HPLC analysis of the racemic **3e**, for comparison (Table 2, entry 5)

D-2000 Elite HPLC System Manager ReportAnalyzed Date and Time: 12/26/2017 03:06 PM
Reported Date and Time: 12/26/2017 04:15 PM

Processed Date and Time: 12/26/2017 04:14 PM

Data Path: D:\Prakash\DATA\0705\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0705

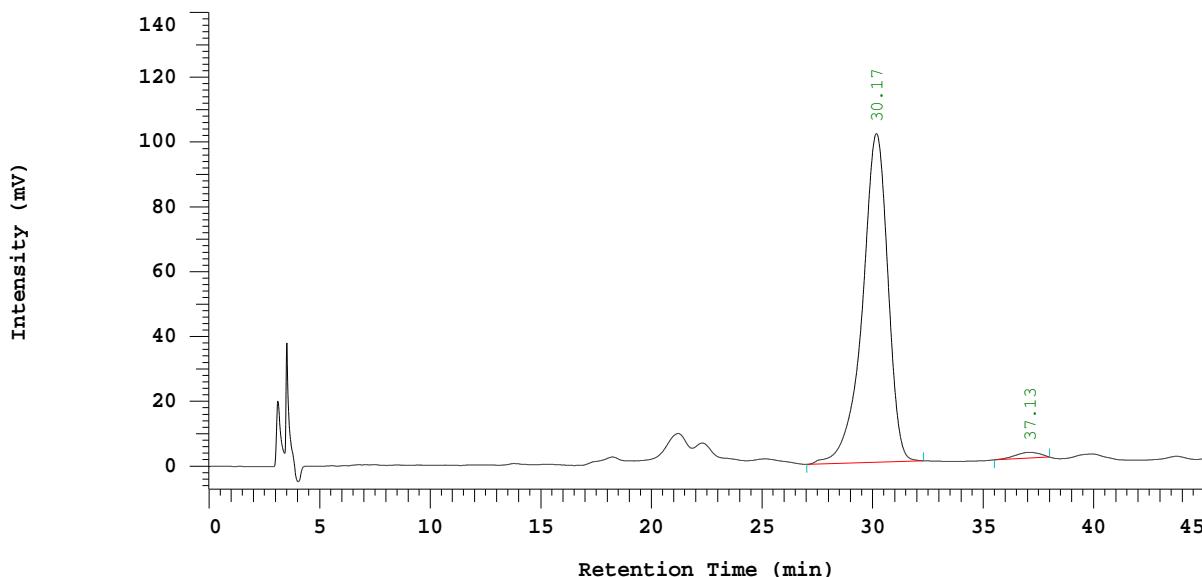
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-117Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 5%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	30.17	8076075	101329	98.321
2	37.13	137923	1771	1.679
		8213998	103100	100.000

Peak rejection level: 2000

Figure S259. HPLC analysis of chiral **3e**, obtained from the reaction with catalyst **IV** (Table 2, entry 5)

D-2000: Prakash Series: 0718
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/11/2018 04:41 PM Reported Date and Time: 01/12/2018 10:32 AM

Processed Date and Time: 01/12/2018 10:32 AM

Data Path: D:\Prakash\DATA\0718\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0718

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-118 (Co)

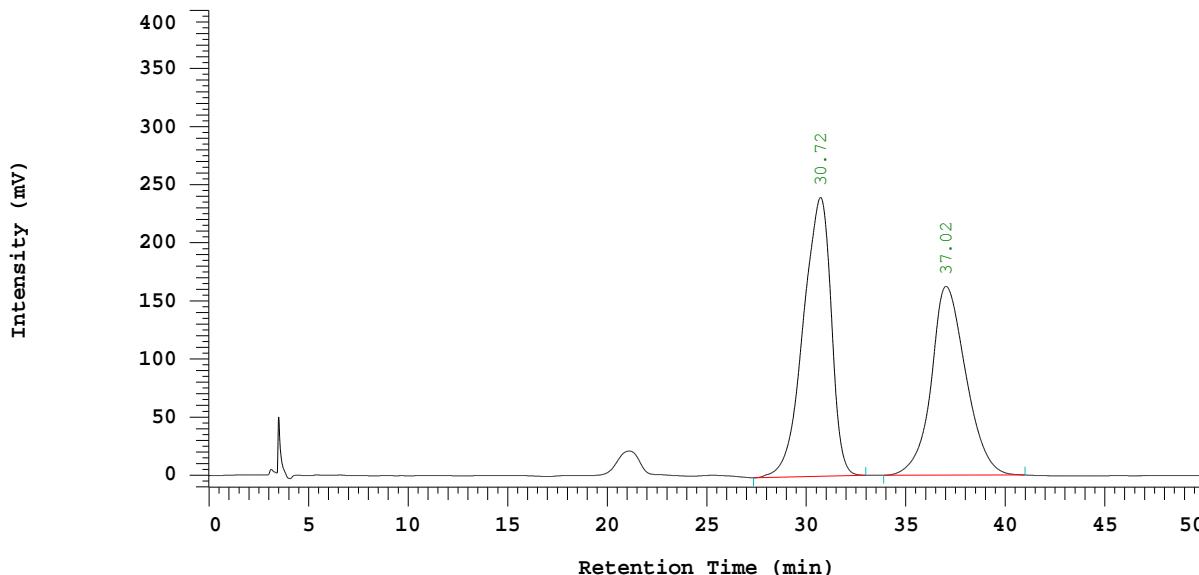
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 5%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	30.72	23306788	239811	54.353
2	37.02	19573529	162325	45.647
		42880317	402136	100.000

Peak rejection level: 2000

Figure S260. HPLC analysis of the mixture of chiral **3e** and racemic **3e**, for comparison (Table 2, entry 5)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/27/2018 01:57 PM Reported Date and Time: 04/27/2018 02:43 PM

Processed Date and Time: 04/27/2018 02:42 PM

Data Path: D:\Prakash\DATA\0874\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0874

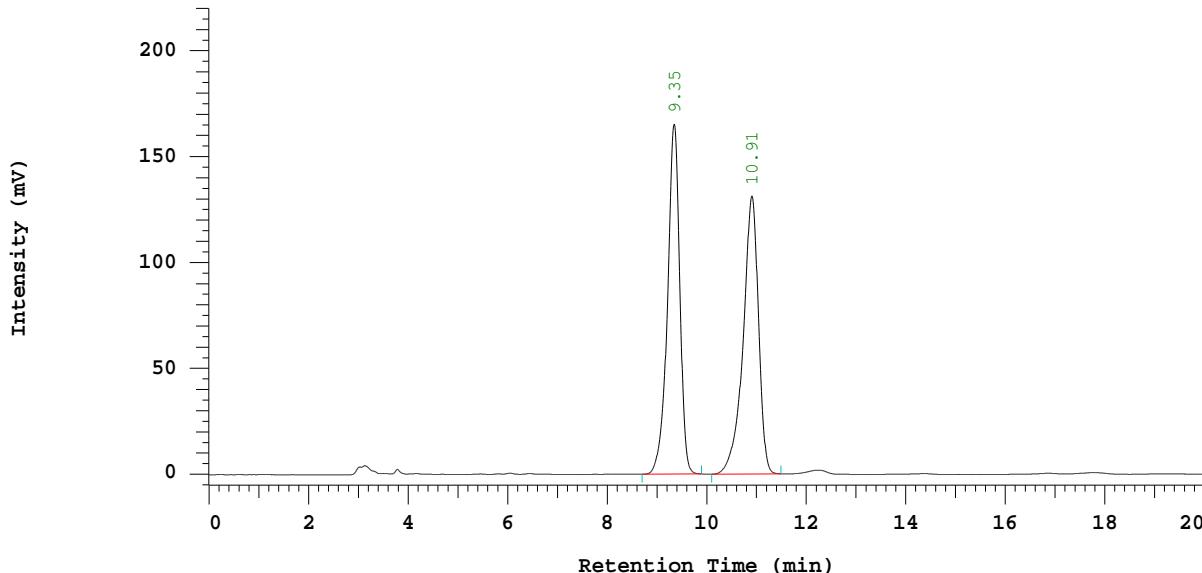
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-118F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.35	2823753	165179	50.039
2	10.91	2819404	131274	49.961
		5643157	296453	100.000

Peak rejection level: 200000

Figure S261. HPLC analysis of the racemic **4e**, for comparison (Table 2, entry 5)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/27/2018 02:26 PM Reported Date and Time: 04/27/2018 02:58 PM

Processed Date and Time: 04/27/2018 02:58 PM

Data Path: D:\Prakash\DATA\0875\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0875

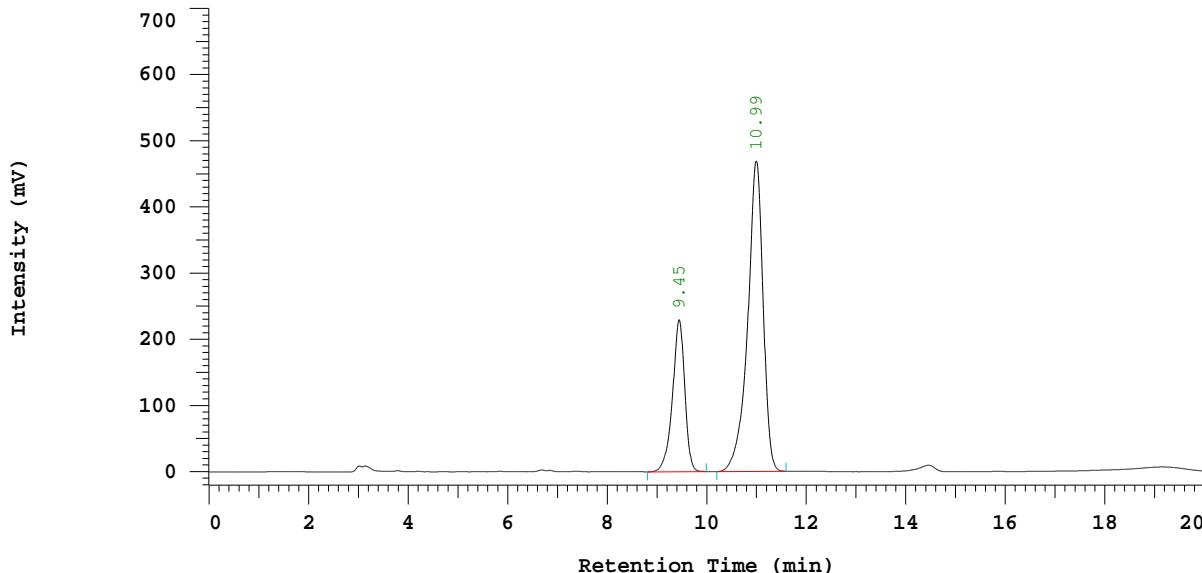
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-118F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.45	3931302	229499	28.018
2	10.99	10099860	468826	71.982
		14031162	698325	100.000

Peak rejection level: 200000

Figure S262. HPLC analysis of chiral **4e**, obtained from the reaction with catalyst **IV** (Table 2, entry 5)

D-2000: Prakash Series: 0876
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 04/27/2018 03:00 PM Reported Date and Time: 04/27/2018 03:24 PM

Processed Date and Time: 04/27/2018 03:24 PM

Data Path: D:\Prakash\DATA\0876\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0876

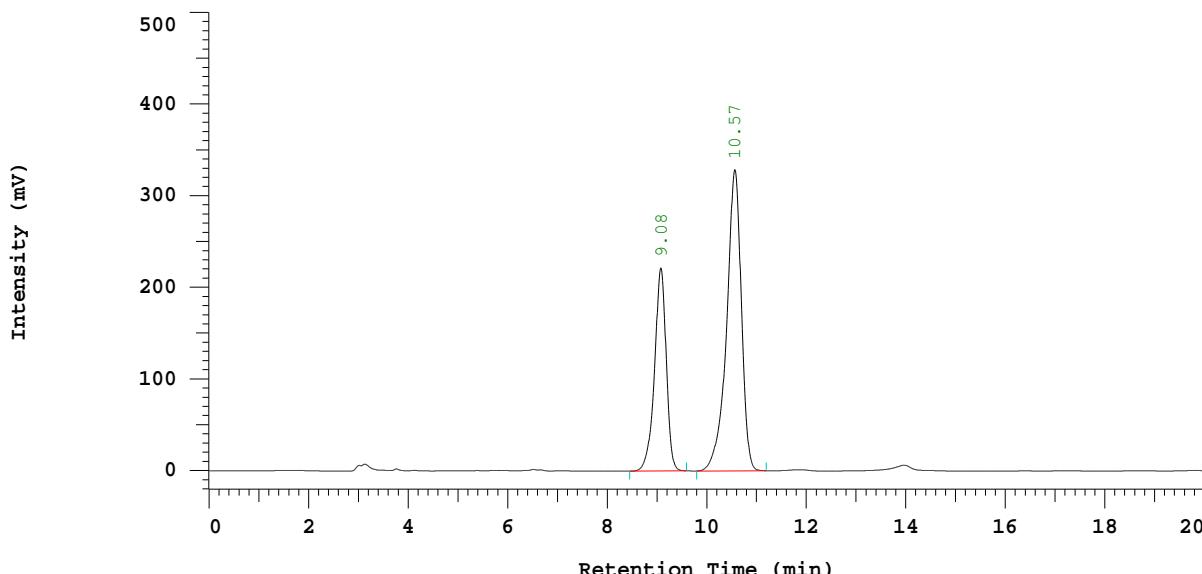
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-118F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.08	3623163	221563	34.846
2	10.57	6774534	328675	65.154
		10397697	550238	100.000

Peak rejection level: 200000

Figure S263. HPLC analysis of the mixture of chiral **4e** and racemic **4e**, for comparison (Table 2, entry 5)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/06/2018 05:40 PM Reported Date and Time: 01/06/2018 06:57 PM

Processed Date and Time: 01/06/2018 06:56 PM

Data Path: D:\Prakash\DATA\0708\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0708

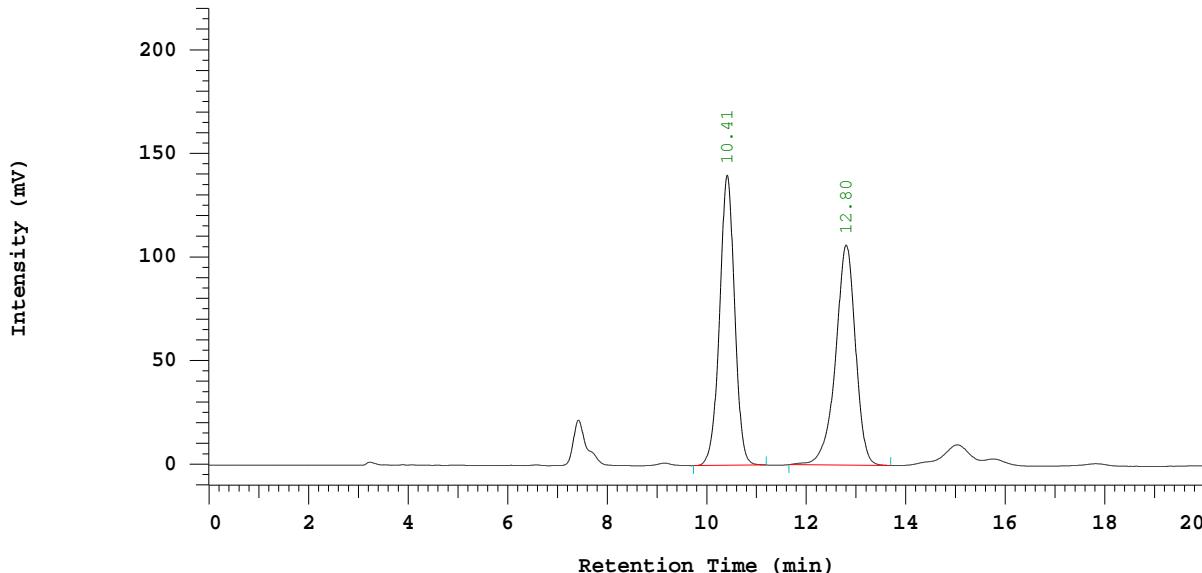
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-123Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	10.41	2947514	140039	49.930
2	12.80	2955831	106194	50.070
		5903345	246233	100.000

Peak rejection level: 200000

Figure S264. HPLC analysis of the racemic **3f**, for comparison (Table 2, entry 6)

D-2000: Prakash Series: 0709
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/06/2018 06:10 PM Reported Date and Time: 01/06/2018 06:54 PM

Processed Date and Time: 01/06/2018 06:53 PM

Data Path: D:\Prakash\DATA\0709\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0709

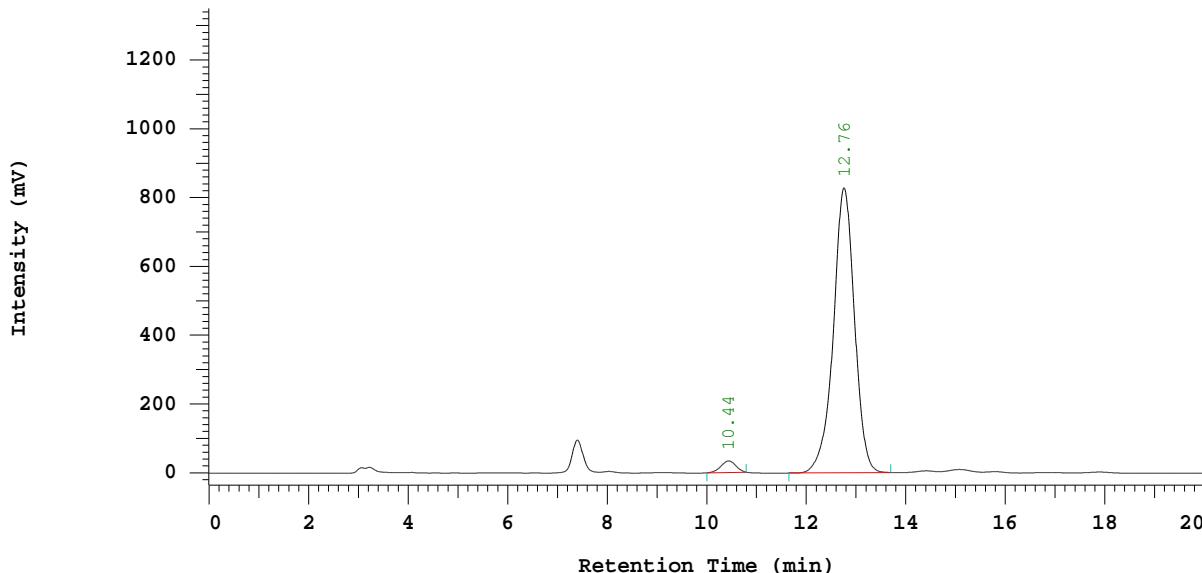
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-124(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	10.44	696400	33626	2.770
2	12.76	24446368	827885	97.230
		25142768	861511	100.000

Peak rejection level: 200000

Figure S265. HPLC analysis of chiral **3f**, obtained from the reaction with catalyst **IV** (Table 2, entry 6)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/07/2018 01:52 PM Reported Date and Time: 01/07/2018 02:20 PM

Processed Date and Time: 01/07/2018 02:19 PM

Data Path: D:\Prakash\DATA\0710\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0710

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-123(Co)

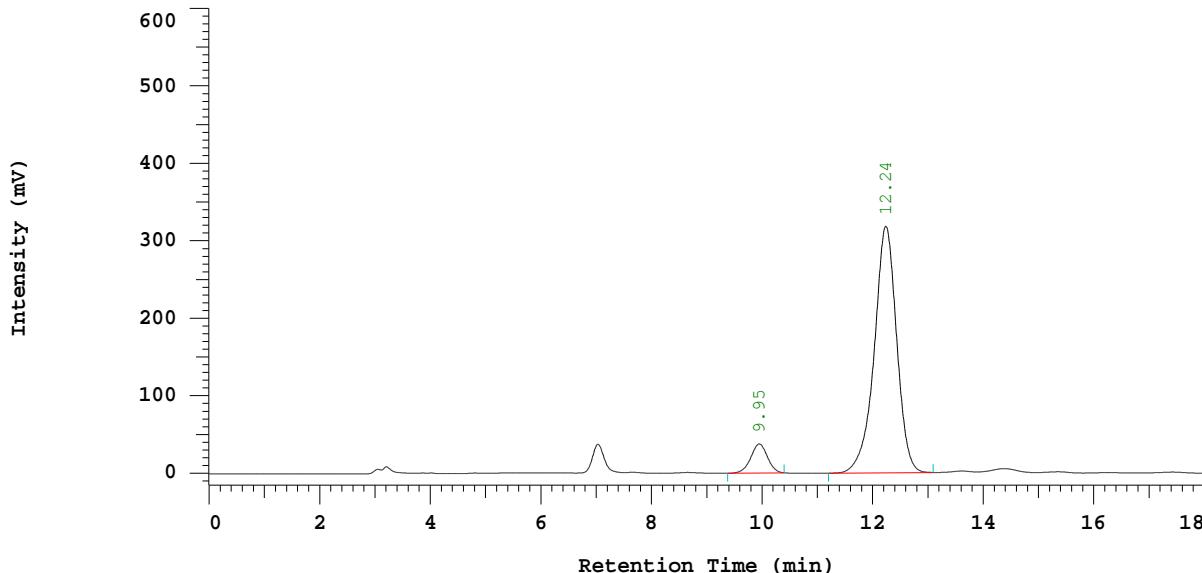
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 10%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.95	788283	37476	8.093
2	12.24	8952400	318222	91.907
		9740683	355698	100.000

Peak rejection level: 200000

Figure S266. HPLC analysis of the mixture of chiral **3f** and racemic **3f**, for comparison (Table 2, entry 6)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/26/2018 11:57 AM Reported Date and Time: 01/26/2018 01:51 PM

Processed Date and Time: 01/26/2018 01:50 PM

Data Path: D:\Prakash\DATA\0794\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0794

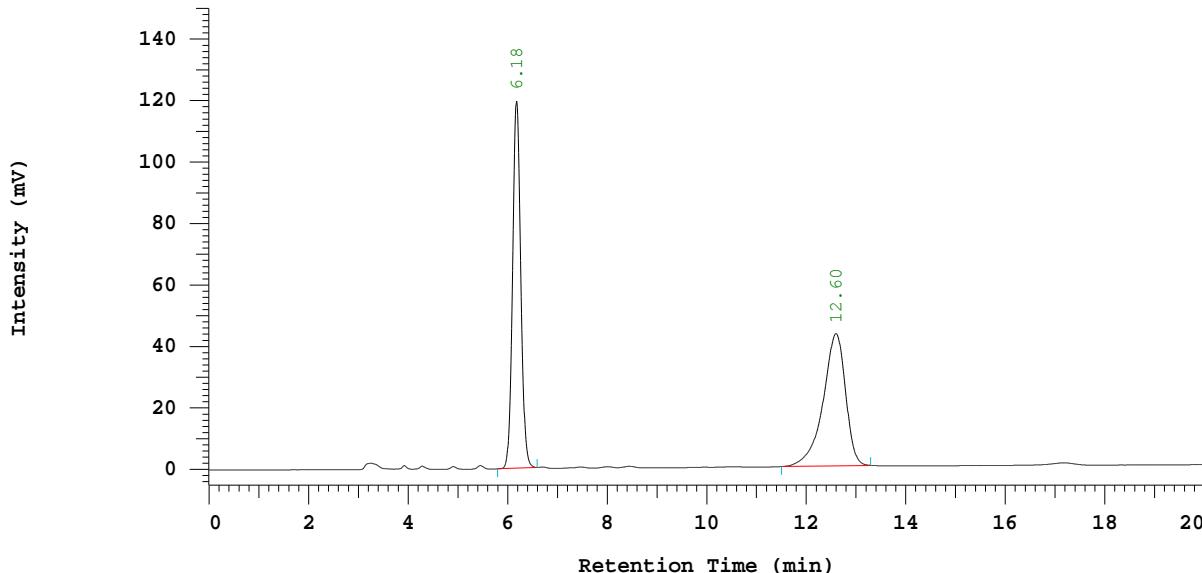
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-120 (Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.18	1355999	119304	50.119
2	12.60	1349544	43031	49.881
		2705543	162335	100.000

Peak rejection level: 200000

Figure S267. HPLC analysis of the racemic **4f**, for comparison (Table 2, entry 6)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/26/2018 01:47 PM Reported Date and Time: 01/26/2018 02:13 PM

Processed Date and Time: 01/26/2018 02:12 PM

Data Path: D:\Prakash\DATA\0795\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0795

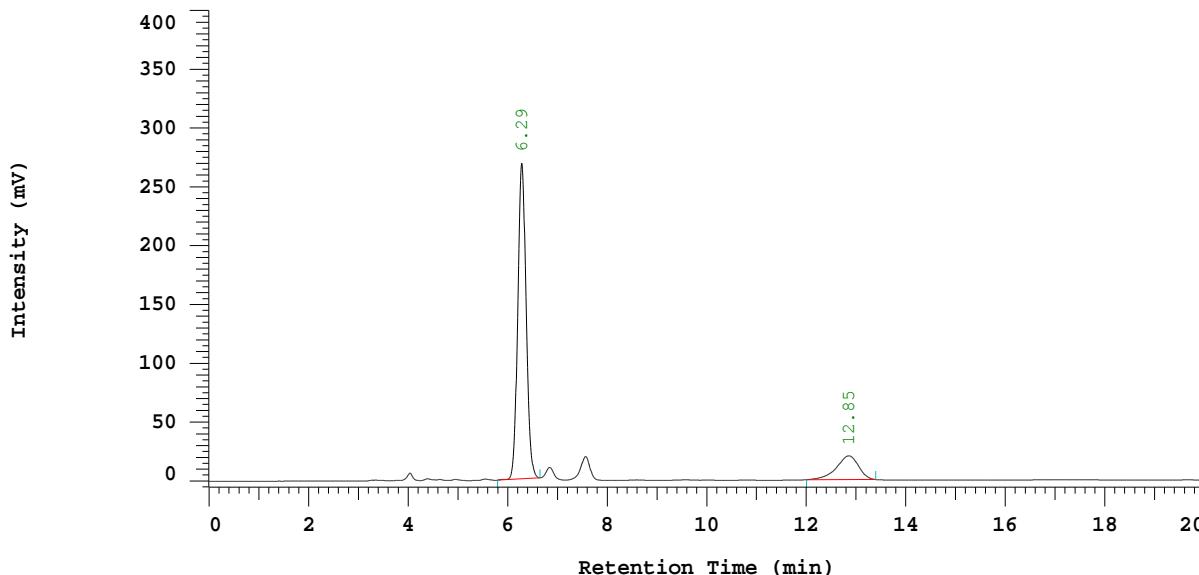
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-120(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.29	3131664	268158	83.348
2	12.85	625663	20191	16.652
		3757327	288349	100.000

Peak rejection level: 200000

Figure S268. HPLC analysis of chiral **4f**, obtained from the reaction with catalyst **IV** (Table 2, entry 6)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/26/2018 02:10 PM Reported Date and Time: 01/26/2018 02:40 PM

Processed Date and Time: 01/26/2018 02:39 PM

Data Path: D:\Prakash\DATA\0796\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0796

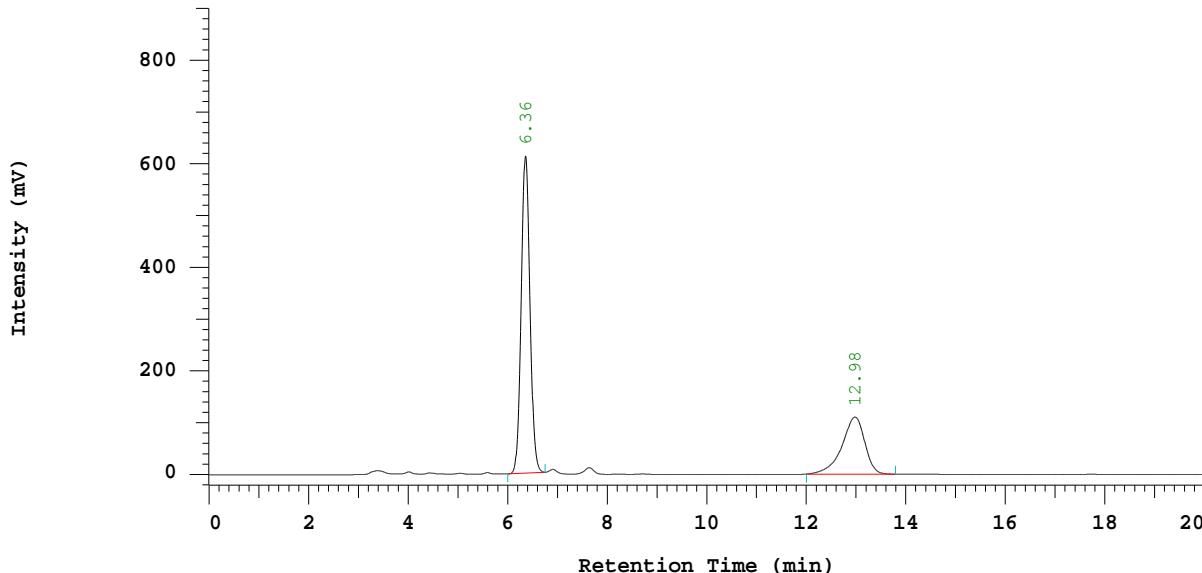
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-120(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Column Type: IC

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.36	7499082	612339	67.990
2	12.98	3530527	110210	32.010
		11029609	722549	100.000

Peak rejection level: 200000

Figure S269. HPLC analysis of the mixture of chiral **4f** and racemic **4f**, for comparison (Table 2, entry 6)

D-2000: Prakash Series: 0766
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/18/2018 01:32 PM Reported Date and Time: 01/18/2018 01:17 PM

Processed Date and Time: 01/18/2018 01:15 PM

Data Path: D:\Prakash\DATA\0766\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0766

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-125Racemic)

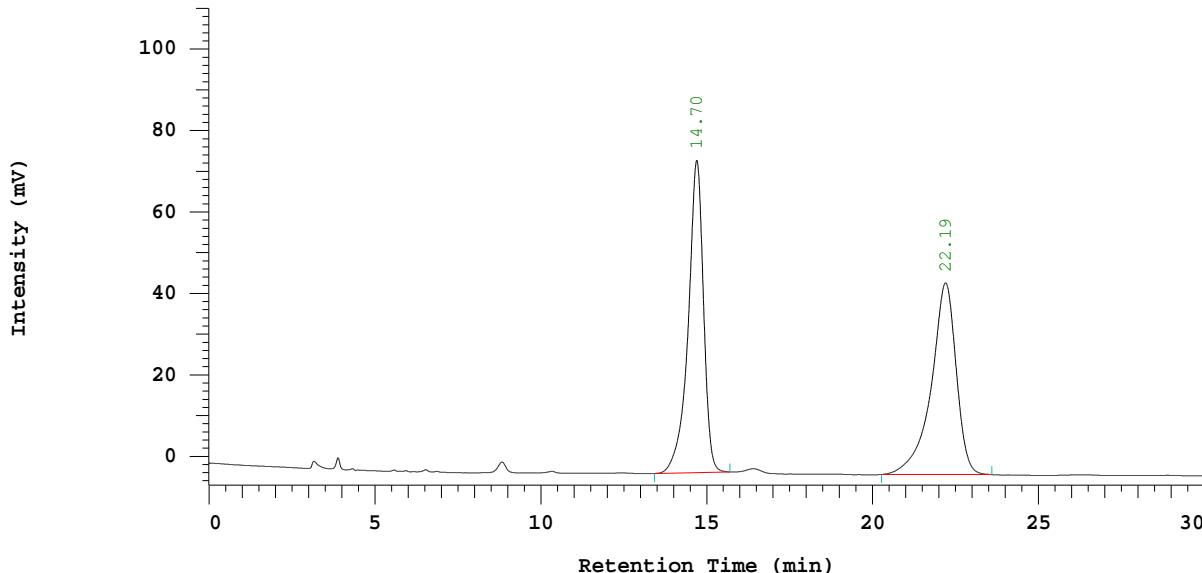
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 17%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	14.70	2451622	76681	49.930
2	22.19	2458542	47047	50.070
		4910164	123728	100.000

Peak rejection level: 200000

Figure S270. HPLC analysis of the racemic **3g**, for comparison (Table 2, entry 7)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/18/2018 04:25 PM Reported Date and Time: 01/18/2018 05:07 PM

Processed Date and Time: 01/18/2018 05:06 PM

Data Path: D:\Prakash\DATA\0772\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0772

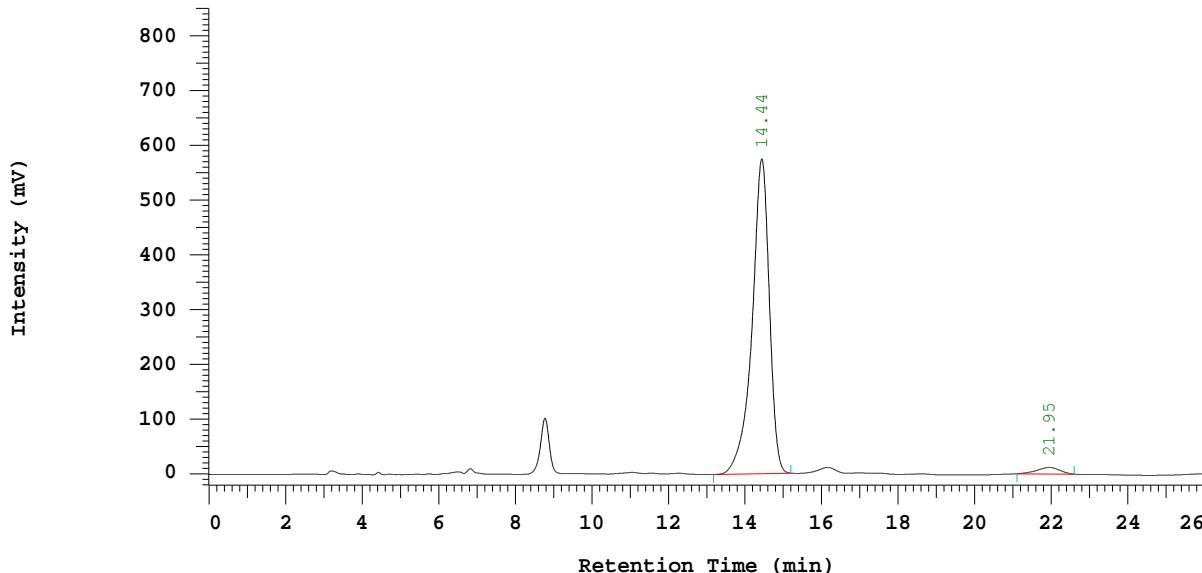
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-125(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 17%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	14.44	17925968	574213	97.325
2	21.95	492768	11892	2.675
		18418736	586105	100.000

Peak rejection level: 200000

Figure S271. HPLC analysis of chiral **3g**, obtained from the reaction with catalyst **IV** (Table 2, entry 7)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/18/2018 08:41 PM Reported Date and Time: 01/18/2018 09:23 PM

Processed Date and Time: 01/18/2018 09:23 PM

Data Path: D:\Prakash\DATA\0777\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0777

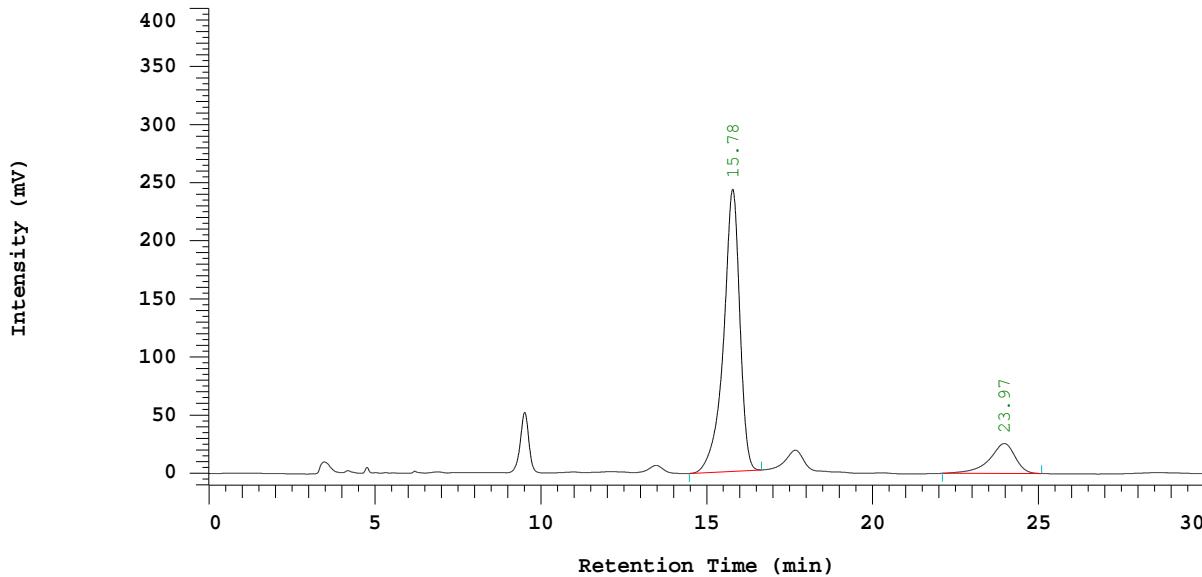
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-125(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 17%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Column Type: IC

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	15.78	8221081	242712	85.487
2	23.97	1395700	25815	14.513
		9616781	268527	100.000

Peak rejection level: 200000

Figure S272. HPLC analysis of the mixture of chiral **3g** and racemic **3g**, for comparison (Table 2, entry 7)

D-2000: Prakash Series: 0987
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/06/2018 Reported Date and Time: 08/06/2018
 08:12 PM 08:39 PM

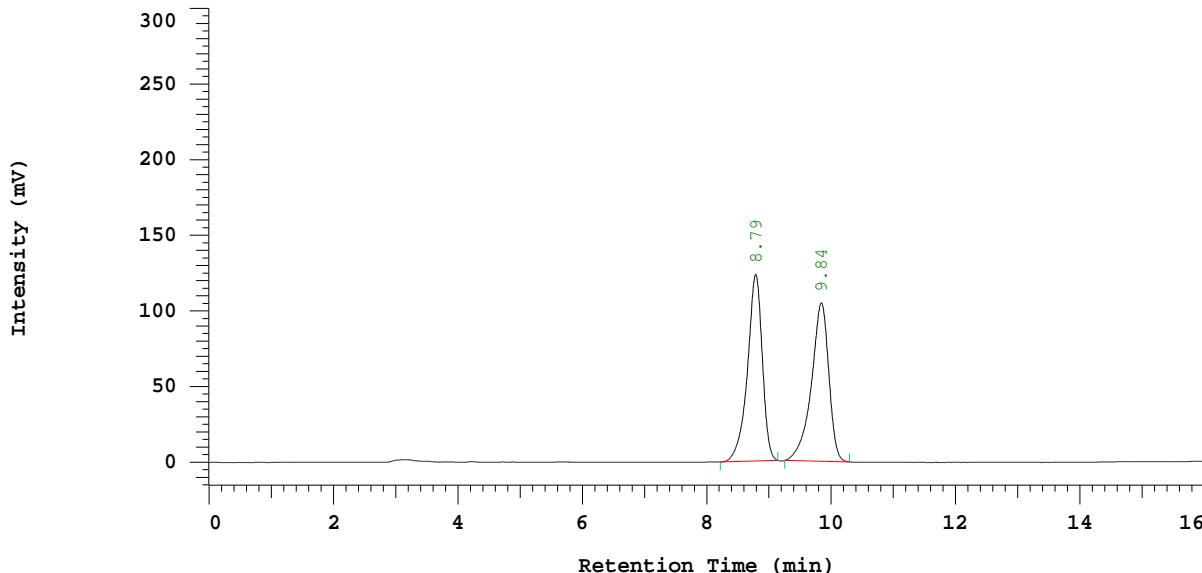
Processed Date and Time: 08/06/2018
 08:38 PM

Data Path: D:\Prakash\DATA\0987\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0987
Application(data): Prakash Chaudari Vial Number: 1
Sample Name: PDC-04-131F1(Racemic) Vial Type: UNK
Injection from this vial: 1 of 1 Volume: 20.0 ul
Sample Description: 15%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	8.79	2041937	123397	50.021
2	9.84	2040182	104790	49.979
		4082119	228187	100.000

Peak rejection level: 1000

Figure S273. HPLC analysis of the racemic **4g**, for comparison (Table 2, entry 7)

D-2000: Prakash Series: 0995
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/07/2018 04:41 PM Reported Date and Time: 08/07/2018 05:06 PM

Processed Date and Time: 08/07/2018 05:06 PM

Data Path: D:\Prakash\DATA\0995\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0995

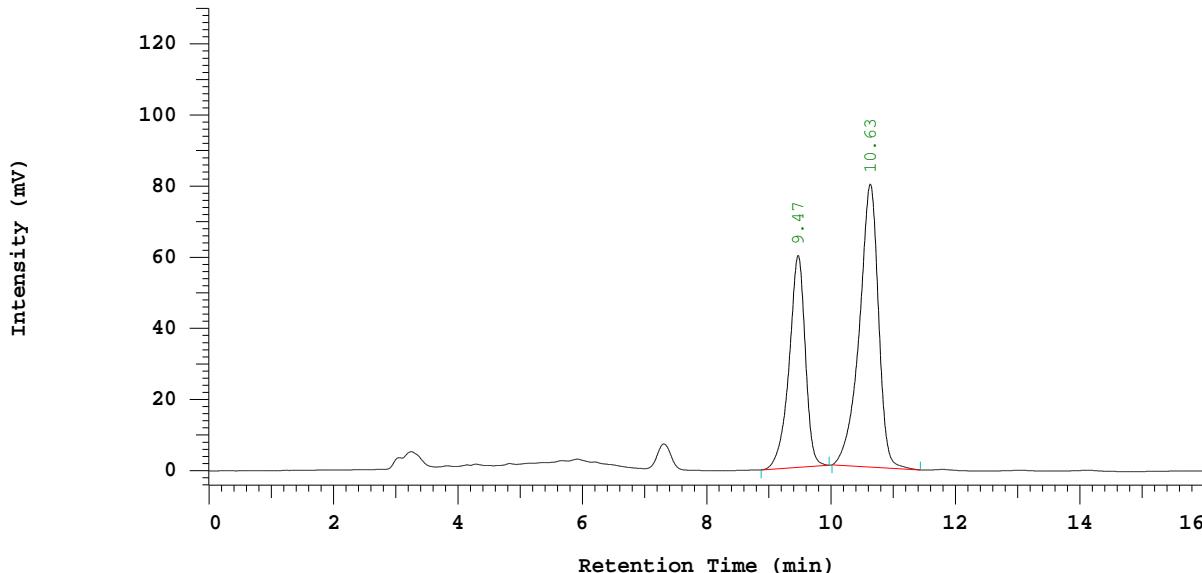
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-131F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 271 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 271 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.47	1075554	59604	38.730
2	10.63	1701479	79527	61.270
		2777033	139131	100.000

Peak rejection level: 1000

Figure S274. HPLC analysis of chiral **4g**, obtained from the reaction with catalyst **IV** (Table 2, entry 7).

D-2000: Prakash Series: 0991
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/07/2018 11:19 AM Reported Date and Time: 08/07/2018 11:53 AM

Processed Date and Time: 08/07/2018 11:52 AM

Data Path: D:\Prakash\DATA\0991\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0991

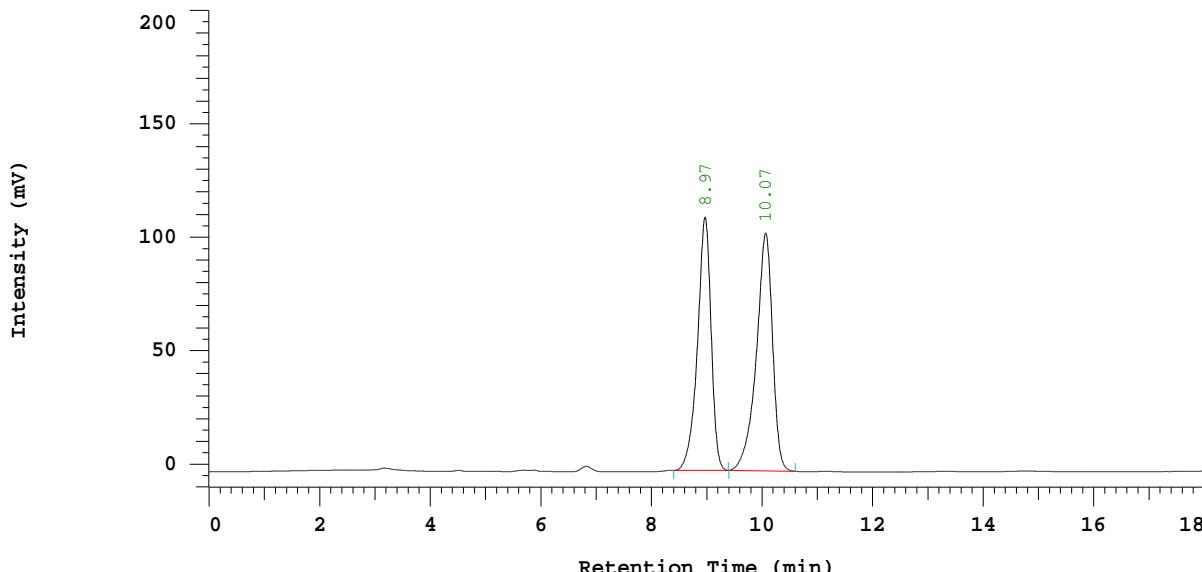
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-31F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 271 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 271 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	8.97	1910742	111564	47.166
2	10.07	2140346	104830	52.834
		4051088	216394	100.000

Peak rejection level: 1000

Figure S275. HPLC analysis of the mixture of chiral **4g** and racemic **4g**, for comparison (Table 2, entry 7)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/22/2018 02:43 PM Reported Date and Time: 01/23/2018 03:46 PM

Processed Date and Time: 01/23/2018 03:45 PM

Data Path: D:\Prakash\DATA\0778\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0778

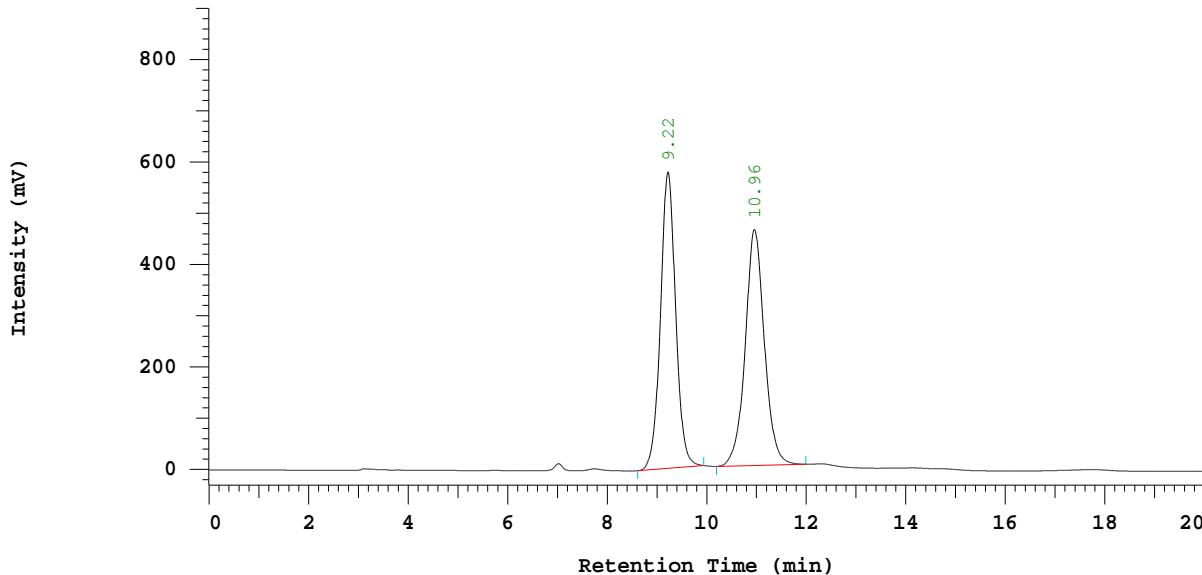
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-128 (Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.22	12273120	578413	49.882
2	10.96	12331228	460789	50.118
		24604348	1039202	100.000

Peak rejection level: 200000

Figure S276. HPLC analysis of the racemic **3h**, for comparison (Table 2, entry 8)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/23/2018 08:05 PM Reported Date and Time: 01/23/2018 07:31 PM

Processed Date and Time: 01/23/2018 07:31 PM

Data Path: D:\Prakash\DATA\0792\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0792

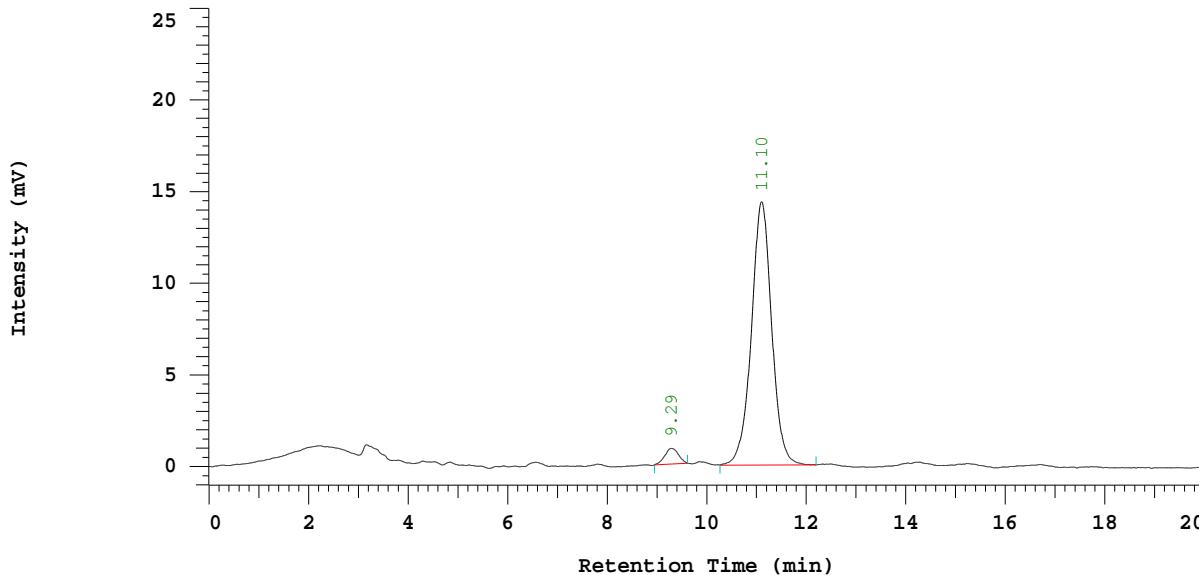
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-128Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.29	16182	852	3.830
2	11.10	406348	14364	96.170
		422530	15216	100.000

Peak rejection level: 100

Figure S277. HPLC analysis of chiral **3h**, obtained from the reaction with catalyst **IV** (Table 2, entry 8)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 01/23/2018 07:40 PM Reported Date and Time: 01/23/2018 08:04 PM

Processed Date and Time: 01/23/2018 08:03 PM

Data Path: D:\Prakash\DATA\0793\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0793

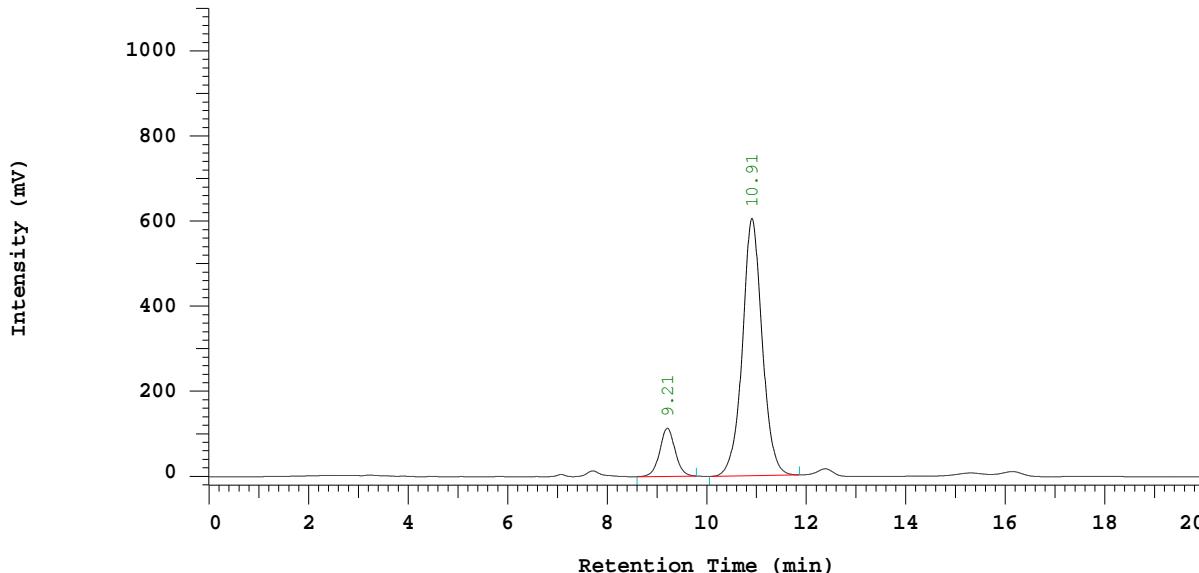
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-128(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.21	2436353	113236	12.702
2	10.91	16744424	604886	87.298
		19180777	718122	100.000

Peak rejection level: 200000

Figure S278. HPLC analysis of the mixture of chiral **3h** and racemic **3h**, for comparison (Table 2, entry 8)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/12/2018
10:14 PM

Reported Date and Time: 07/12/2018
11:14 PM

Processed Date and Time: 07/12/2018
11:13 PM

Data Path: D:\CLW\DATA\0006\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0006

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-44-f1-racemic

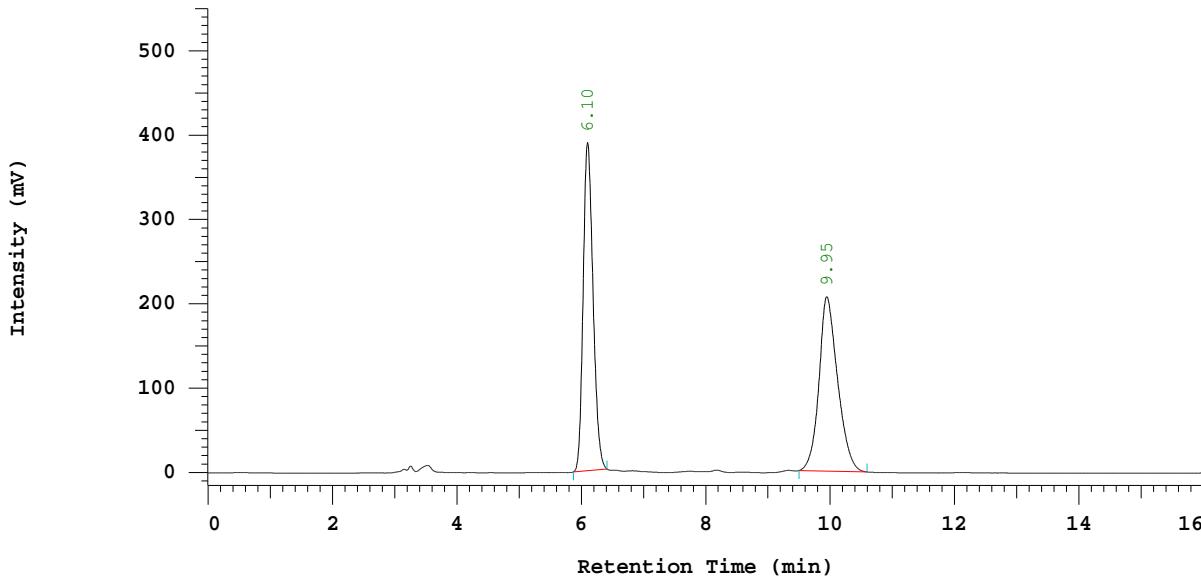
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%THF+80%HEX-IC

Chrom Type: Fixed WL Chromatogram, 301 nm



Processing Method: test-THF/Hx-IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 301 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.10	4282585	389004	49.891
2	9.95	4301273	206820	50.109
		8583858	595824	100.000

Peak rejection level: 1000

Figure S279. HPLC analysis of the racemic **4h**, for comparison (Table 2, entry 8)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/12/2018
09:55 PM

Reported Date and Time: 07/12/2018
11:19 PM

Processed Date and Time: 07/12/2018
11:18 PM

Data Path: D:\CLW\DATA\0005\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0005

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-44-f1-chiral

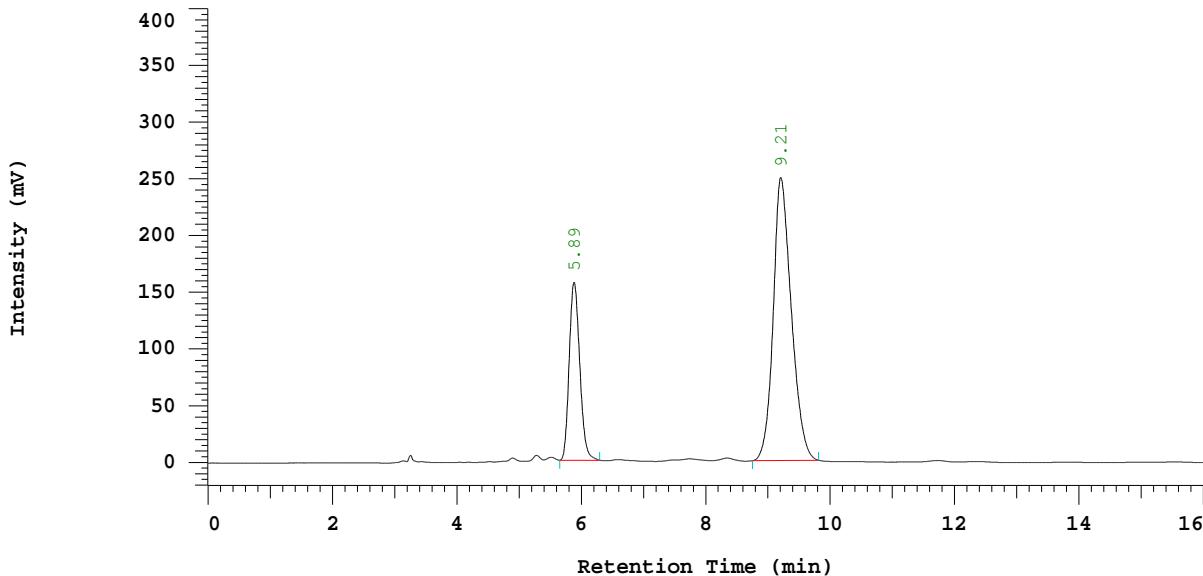
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%THF+80%HEX-IC

Chrom Type: Fixed WL Chromatogram, 301 nm



Processing Method: test-THF/Hx-IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 301 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.89	1849042	156770	26.828
2	9.21	5043132	249344	73.172
		6892174	406114	100.000

Peak rejection level: 1000

Figure S280. HPLC analysis of chiral **4h**, obtained from the reaction with catalyst **IV** (Table 2, entry 8)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/12/2018
10:33 PM

Reported Date and Time: 07/12/2018
11:07 PM

Processed Date and Time: 07/12/2018
11:06 PM

Data Path: D:\CLW\DATA\0007\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0007

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-44-f1-(Co)

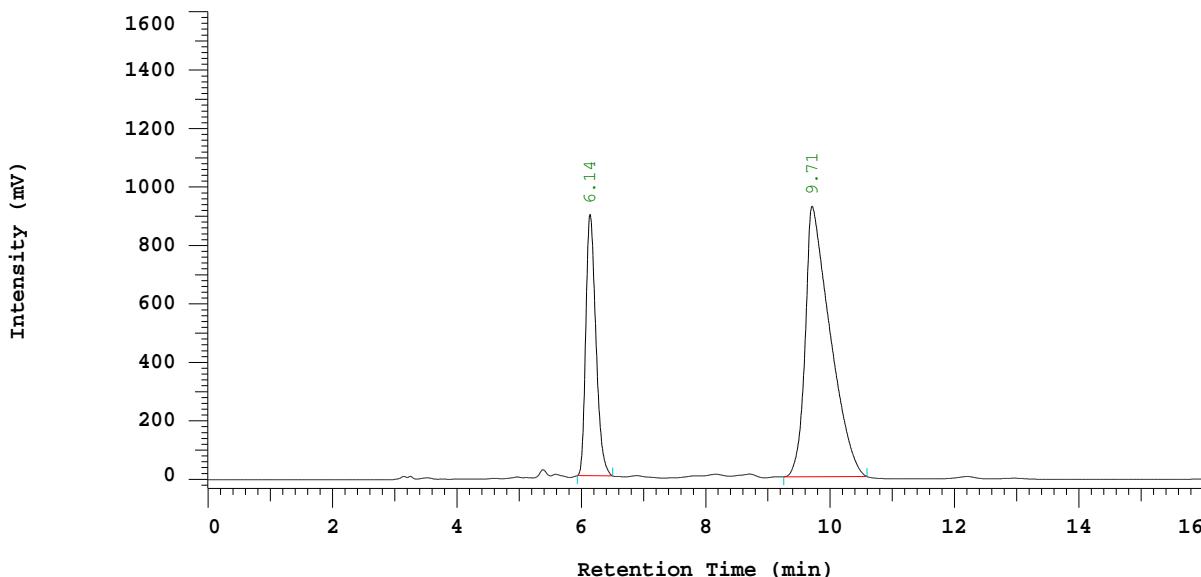
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 20%THF+80%HEX-IC

Chrom Type: Fixed WL Chromatogram, 302 nm



Processing Method: test-THF/Hx-IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 302 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.14	10087898	894628	28.163
2	9.71	25732057	925234	71.837
		35819955	1819862	100.000

Peak rejection level: 1000

Figure S281. HPLC analysis of the mixture of chiral **4h** and racemic **4h**, for comparison (Table 2, entry 8)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 03/27/2018 01:54 PM Reported Date and Time: 03/27/2018 03:08 PM

Processed Date and Time: 03/27/2018 03:07 PM

Data Path: D:\Prakash\DATA\0836\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0836

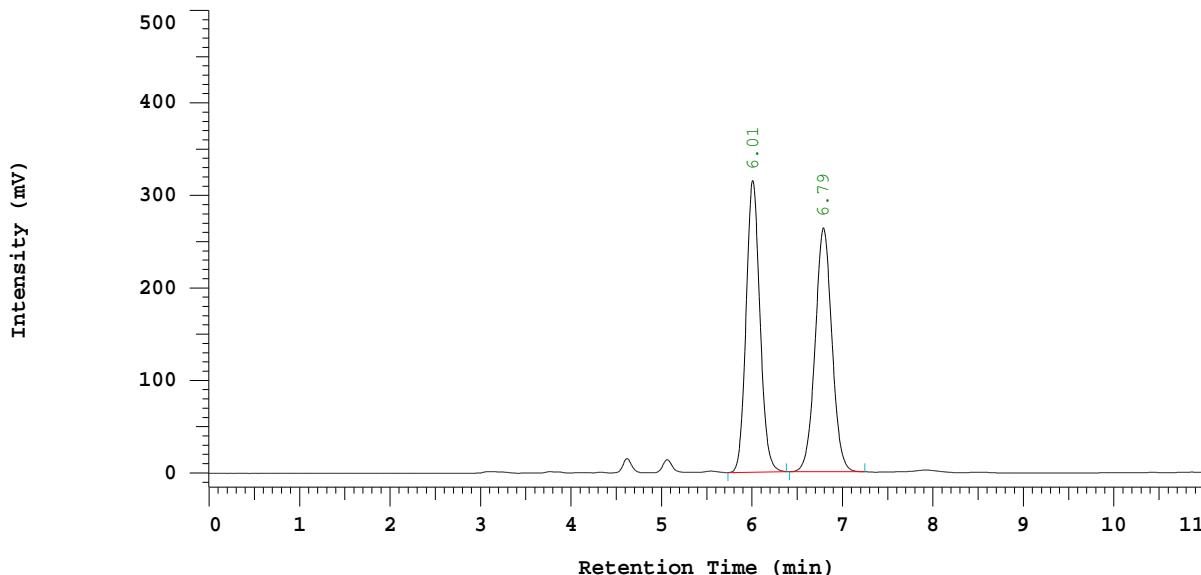
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-149 F2(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 25%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.01	3347789	315306	49.632
2	6.79	3397386	263430	50.368
		6745175	578736	100.000

Peak rejection level: 200000

Figure S282. HPLC analysis of the racemic **3i**, for comparison (Table 2, entry 9)

D-2000: Prakash Series: 0837
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 03/27/2018 02:18 PM Reported Date and Time: 03/27/2018 03:03 PM

Processed Date and Time: 03/27/2018 03:02 PM

Data Path: D:\Prakash\DATA\0837\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0837

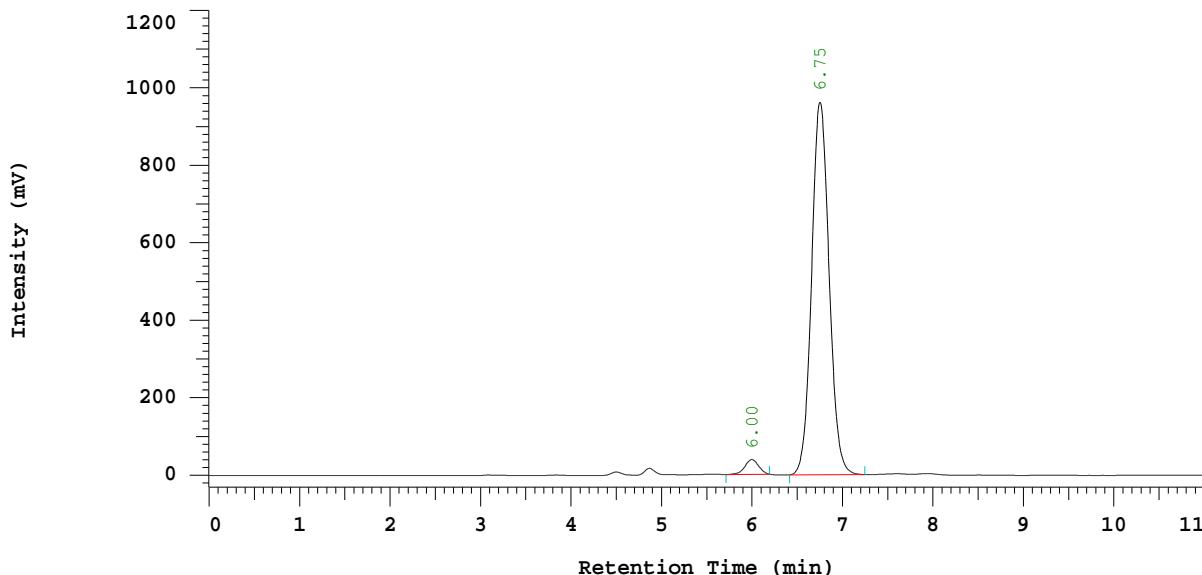
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-149 F2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 25%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.00	404394	38109	3.035
2	6.75	12919402	961560	96.965
		13323796	999669	100.000

Peak rejection level: 200000

Figure S283. HPLC analysis of chiral **3i**, obtained from the reaction with catalyst **IV** (Table 2, entry 9)

D-2000: Prakash Series: 0838
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 03/27/2018 02:37 PM Reported Date and Time: 03/27/2018 03:00 PM

Processed Date and Time: 03/27/2018 02:59 PM

Data Path: D:\Prakash\DATA\0838\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0838

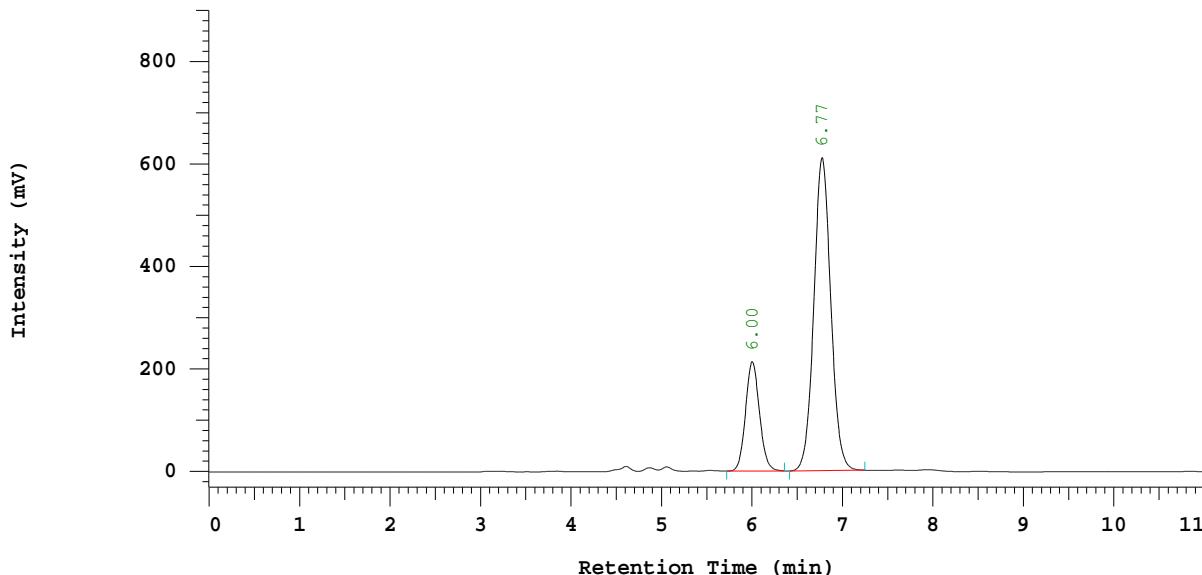
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-149 F2(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 25%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.00	2289460	213537	22.355
2	6.77	7952123	610930	77.645
		10241583	824467	100.000

Peak rejection level: 200000

Figure S284. HPLC analysis of the mixture of chiral **3i** and racemic **3i**, for comparison (Table 2, entry 9)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 03/28/2018 04:16 PM Reported Date and Time: 03/28/2018 05:27 PM

Processed Date and Time: 03/28/2018 05:27 PM

Data Path: D:\Prakash\DATA\0847\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1 Series: 0847

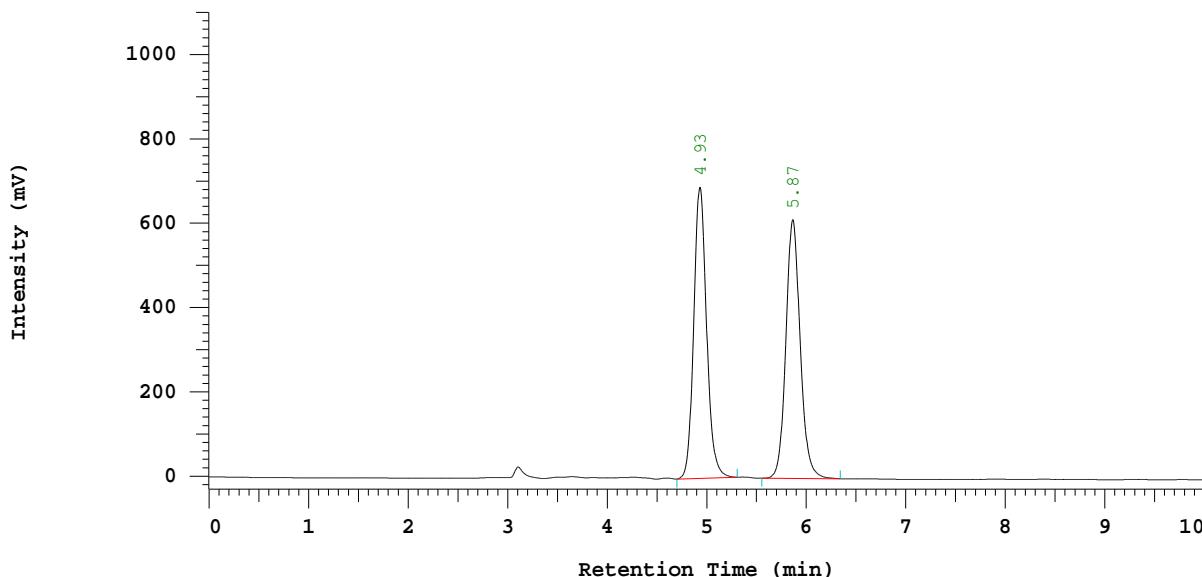
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-149 F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%THF+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IA

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	4.93	6200328	690214	50.187
2	5.87	6154244	613358	49.813
		12354572	1303572	100.000

Peak rejection level: 200000

Figure S285. HPLC analysis of the racemic **4i**, for comparison (Table 2, entry 9)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 03/28/2018 09:21 PM Reported Date and Time: 03/28/2018 09:36 PM

Processed Date and Time: 03/28/2018 09:36 PM

Data Path: D:\Prakash\DATA\0853\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1 Series: 0853

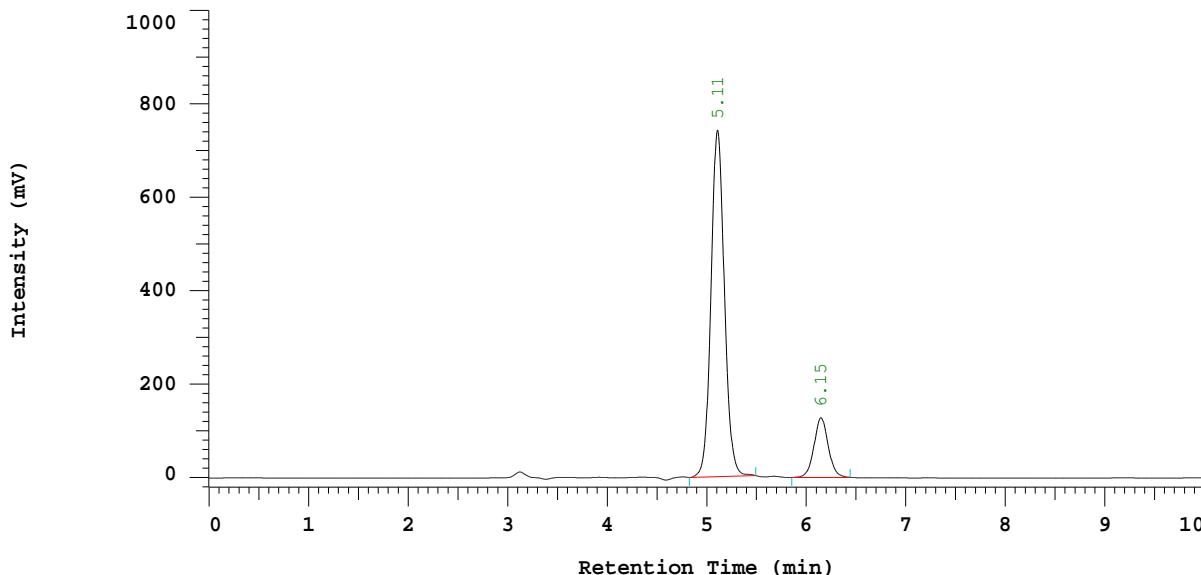
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-149 (Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%THF+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IA

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.11	6958220	741940	84.540
2	6.15	1272461	127807	15.460
		8230681	869747	100.000

Peak rejection level: 200000

Figure S286. HPLC analysis of chiral **4i**, obtained from the reaction with catalyst IV (Table 2, entry 9)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 03/29/2018 11:45 AM Reported Date and Time: 03/29/2018 12:05 PM

Processed Date and Time: 03/29/2018 12:04 PM

Data Path: D:\Prakash\DATA\0854\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1 Series: 0854

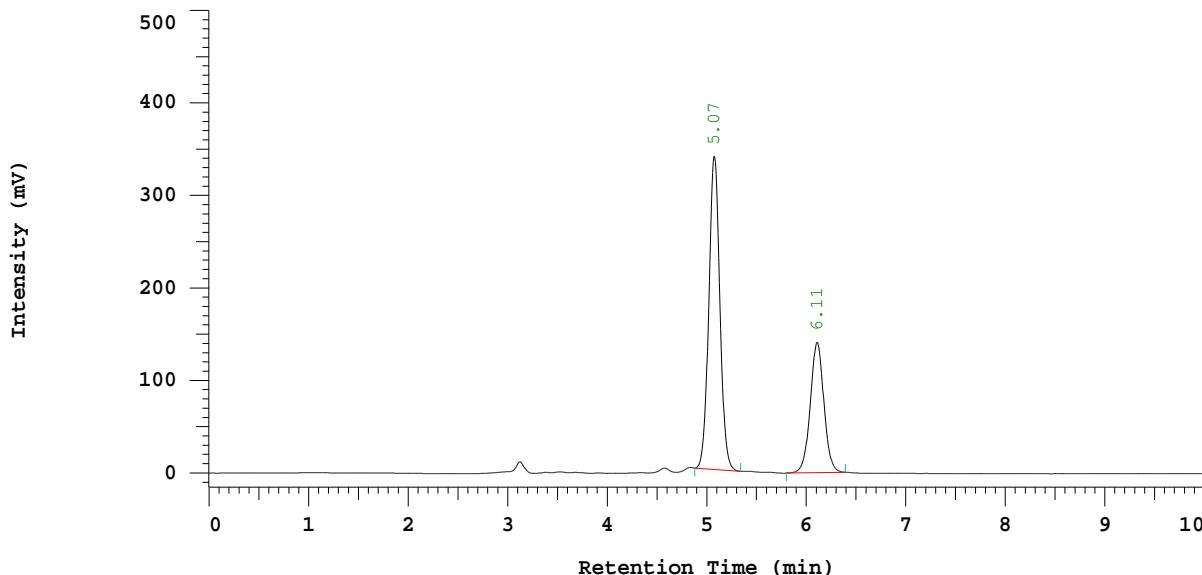
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-149 (Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%THF+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IA

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	5.07	2608817	338393	66.044
2	6.11	1341326	140954	33.956
		3950143	479347	100.000

Peak rejection level: 200000

Figure S287. HPLC analysis of the mixture of chiral **4i** and racemic **4i**, for comparison (Table 2, entry 9)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/06/2018 10:29 PM Reported Date and Time: 07/06/2018 10:16 PM

Processed Date and Time: 07/06/2018 10:15 PM

Data Path: D:\Prakash\DATA\0903\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0903

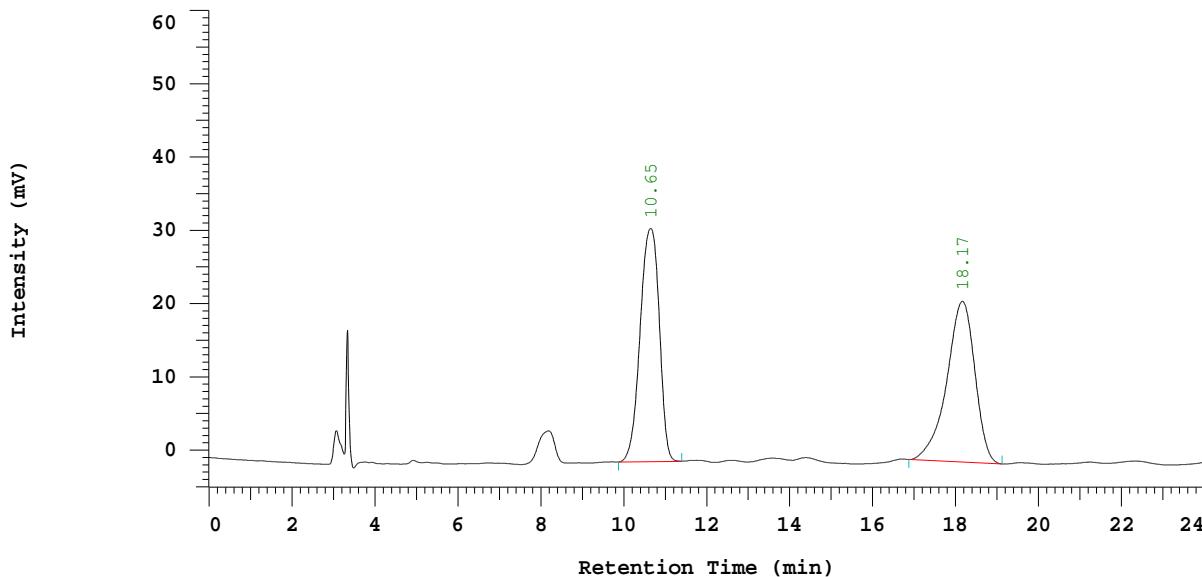
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-101F2(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	10.65	1017368	31792	49.634
2	18.17	1032393	21918	50.366
		2049761	53710	100.000

Peak rejection level: 2000

Figure S288. HPLC analysis of the racemic **3j**, for comparison (Table 2, entry 10)

D-2000: Prakash Series: 0895
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/05/2018 11:25 PM Reported Date and Time: 07/06/2018 10:33 PM

Processed Date and Time: 07/06/2018 10:31 PM

Data Path: D:\Prakash\DATA\0895\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0895

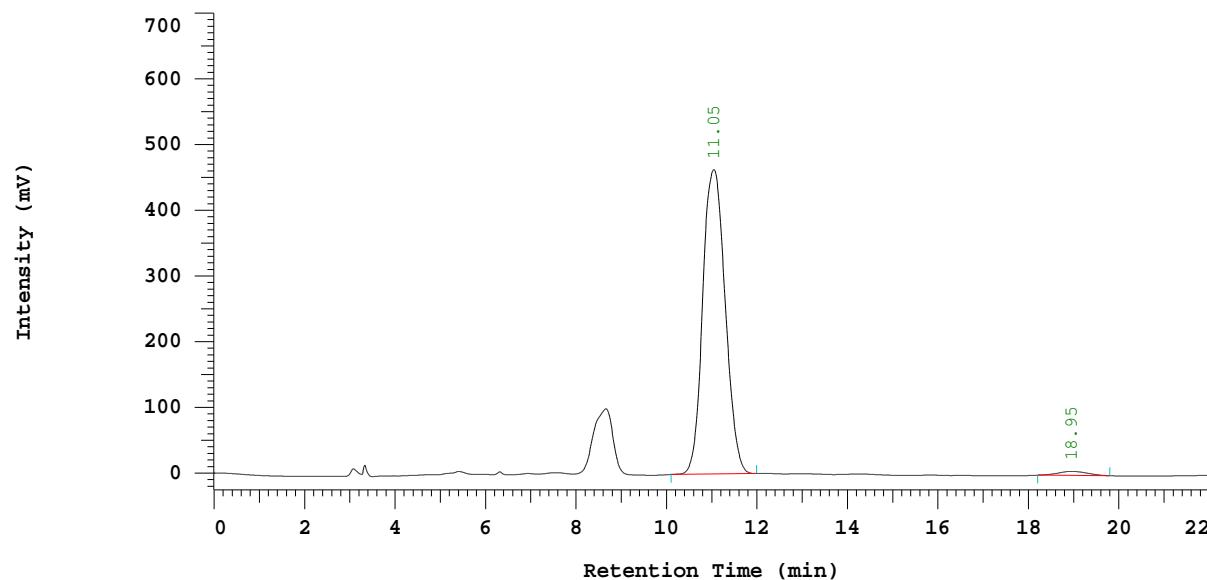
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-101F2(Major) (Chiral) Vial Type: UNK
Volume: 20.0 ul

Injection from this vial: 1 of 1

Sample Description: 10%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 295 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 295 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	11.05	15959388	462934	98.283
2	18.95	278827	6160	1.717
		16238215	469094	100.000

Peak rejection level: 1000

Figure S289. HPLC analysis of chiral **3j**, obtained from the reaction with catalyst **IV** (Table 2, entry 10)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/06/2018 09:43 PM Reported Date and Time: 07/06/2018 10:37 PM

Processed Date and Time: 07/06/2018 10:36 PM

Data Path: D:\Prakash\DATA\0902\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0902

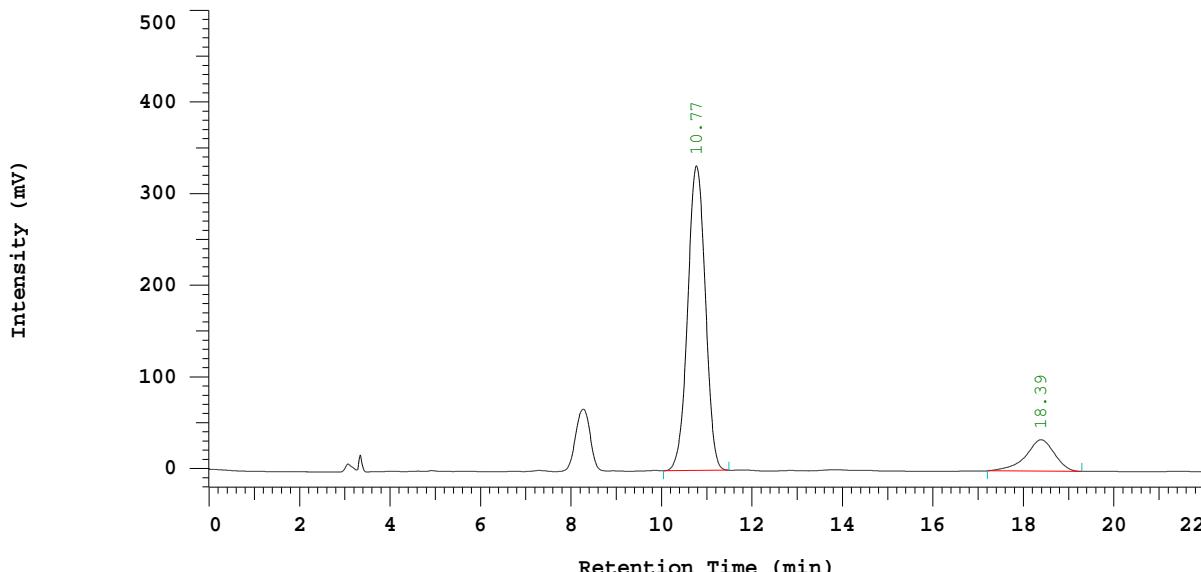
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-101F2(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	10.77	8990652	332337	85.553
2	18.39	1518162	34298	14.447
		10508814	366635	100.000

Peak rejection level: 2000

Figure S290. HPLC analysis of the mixture of chiral **3j** and racemic **3j**, for comparison (Table 2, entry 10)

D-2000 Elite HPLC System Manager ReportAnalyzed Date and Time: 07/05/2018
04:17 PMReported Date and Time: 07/05/2018
05:53 PMProcessed Date and Time: 07/05/2018
05:52 PM

Data Path: D:\Prakash\DATA\0891\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0891

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-03-101F1(Racemic)

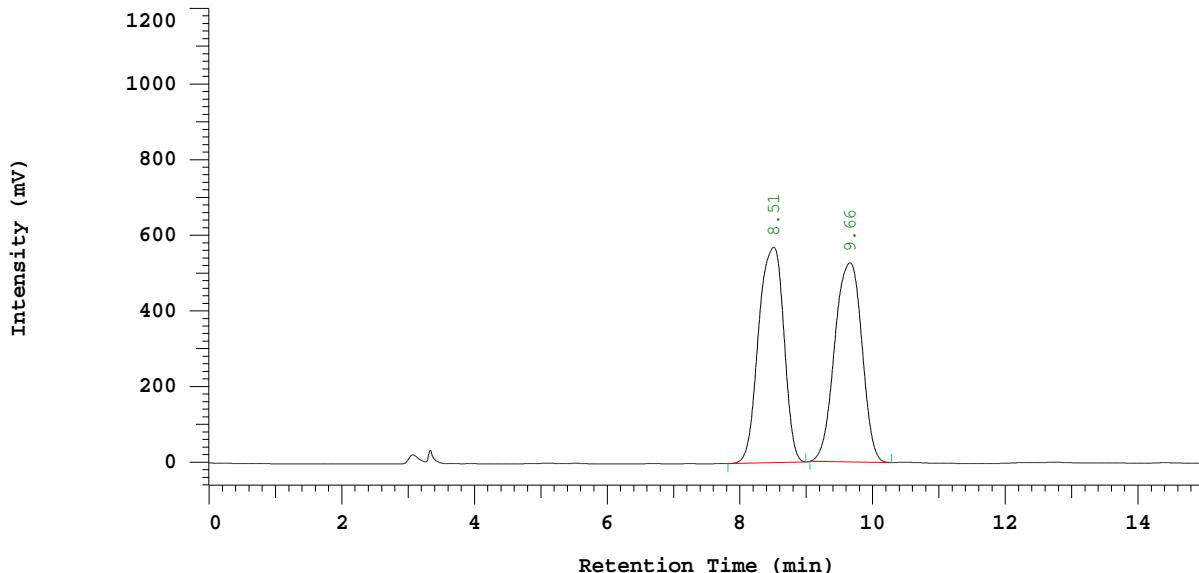
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 10%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Method Developer: Prakash

Column Type: IC

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	8.51	15063128	569364	50.102
2	9.66	15001995	526203	49.898
		30065123	1095567	100.000

Peak rejection level: 2000

Figure S291. HPLC analysis of the racemic **4j**, for comparison (Table 2, entry 10)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/05/2018 04:45 PM Reported Date and Time: 07/05/2018 06:00 PM

Processed Date and Time: 07/05/2018 05:59 PM

Data Path: D:\Prakash\DATA\0892\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0892

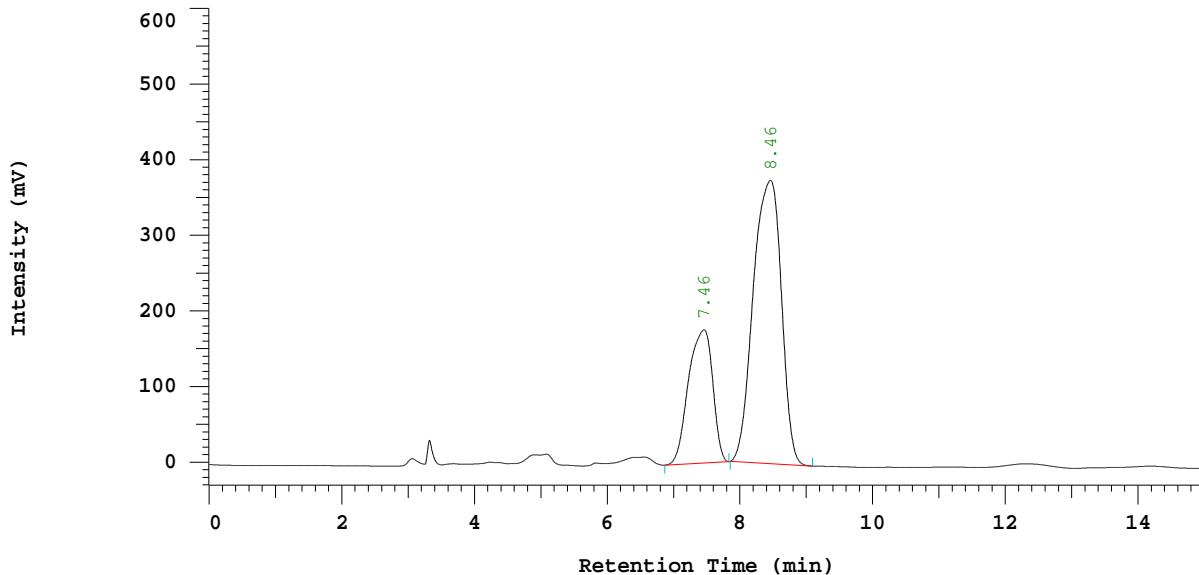
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-101F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.46	4474289	176025	28.878
2	8.46	11019678	374494	71.122
		15493967	550519	100.000

Peak rejection level: 2000

Figure S292. HPLC analysis of chiral **4j**, obtained from the reaction with catalyst **IV** (Table 2, entry 10)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/05/2018 05:43 PM Reported Date and Time: 07/05/2018 06:12 PM

Processed Date and Time: 07/05/2018 06:11 PM

Data Path: D:\Prakash\DATA\0893\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1 Series: 0893

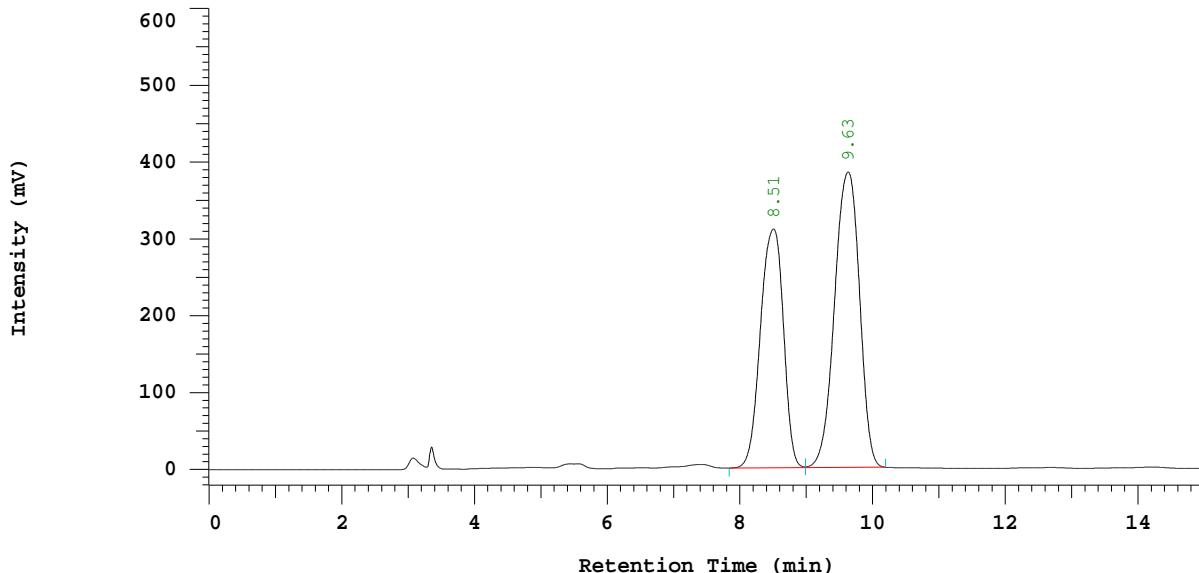
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-03-101F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 10%THF+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	8.51	7476348	310613	42.707
2	9.63	10029675	384328	57.293
		17506023	694941	100.000

Peak rejection level: 2000

Figure S293. HPLC analysis of the mixture of chiral **4j** and racemic **4j**, for comparison (Table 2, entry 10)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 11/22/2018 05:54 PM Reported Date and Time: 11/22/2018 10:19 PM

Processed Date and Time: 11/22/2018 10:18 PM

Data Path: D:\Prakash\DATA\0998\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 0998

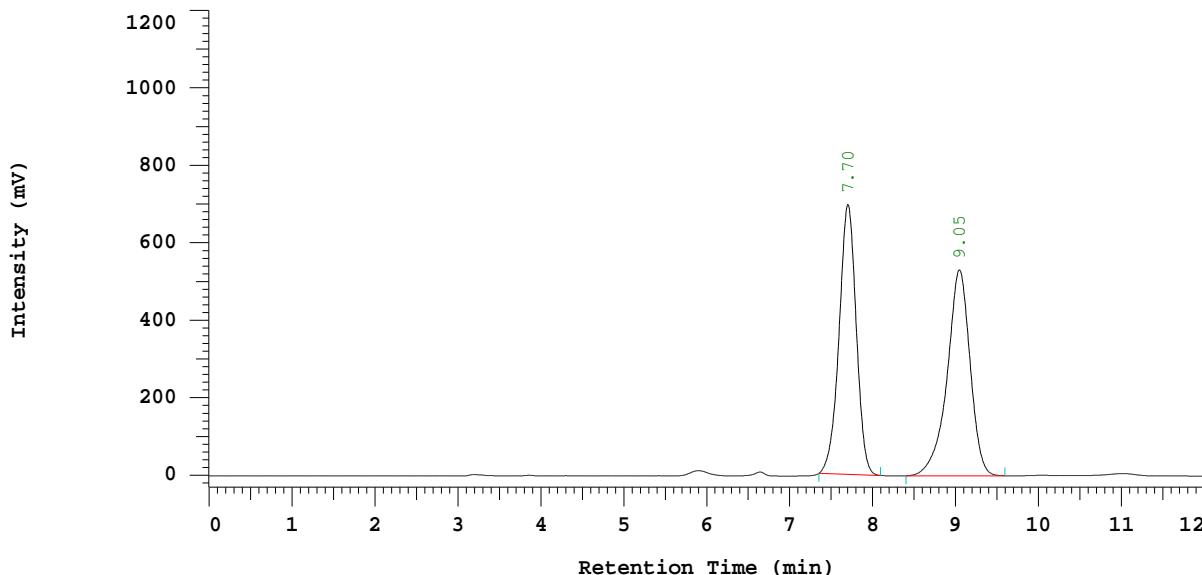
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-039 F2 (Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.70	10004240	695965	49.465
2	9.05	10220672	531322	50.535
		20224912	1227287	100.000

Peak rejection level: 1000

Figure S294. HPLC analysis of the racemic **3k**, for comparison (Scheme 3, b)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 11/22/2018 06:43 PM Reported Date and Time: 11/22/2018 10:17 PM

Processed Date and Time: 11/22/2018 10:16 PM

Data Path: D:\Prakash\DATA\1000\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 1000

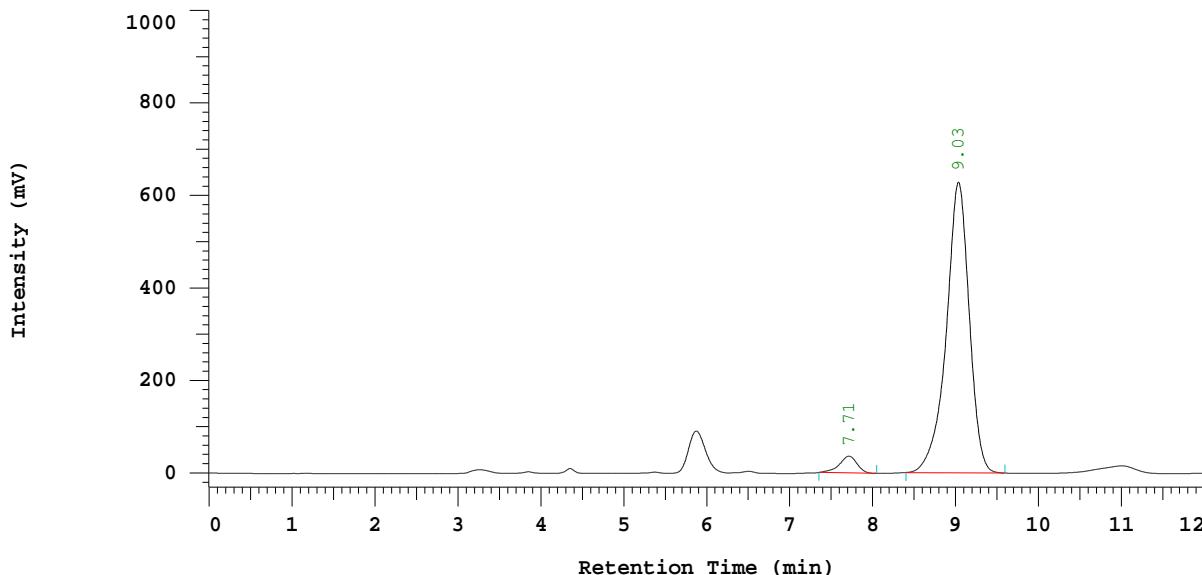
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-039 F2 (Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 240 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 240 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.71	538909	36377	4.273
2	9.03	12074068	627771	95.727
		12612977	664148	100.000

Peak rejection level: 1000

Figure S295. HPLC analysis of chiral **3k** obtained (Scheme 3, b)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 11/23/2018 04:51 PM Reported Date and Time: 11/23/2018 05:13 PM

Processed Date and Time: 11/23/2018 05:12 PM

Data Path: D:\Prakash\DATA\1008\

Processing Method: test-IPA/Hx-IC

System (acquisition): Sys 1 Series: 1008

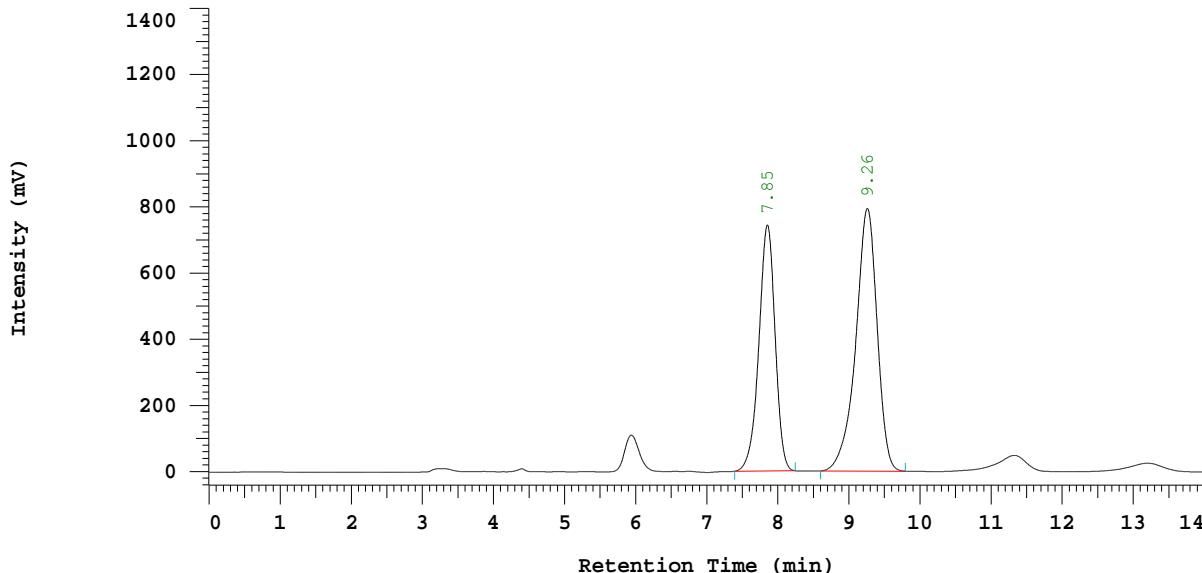
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-039 F2 (CO) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 15%IPA+HX 1.00mL/MIN COL-IC

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IC

Column Type: IC

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.85	11794310	743744	41.577
2	9.26	16572939	793494	58.423
		28367249	1537238	100.000

Peak rejection level: 1000

Figure S296. HPLC analysis of the mixture of chiral 3k and racemic 3k, for comparison (Scheme 3, b)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/15/2018
12:37 AM

Reported Date and Time: 08/15/2018
01:10 AM

Processed Date and Time: 08/15/2018
01:09 AM

Data Path: D:\CLW\DATA\0028\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0028

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-48-F1-racemic

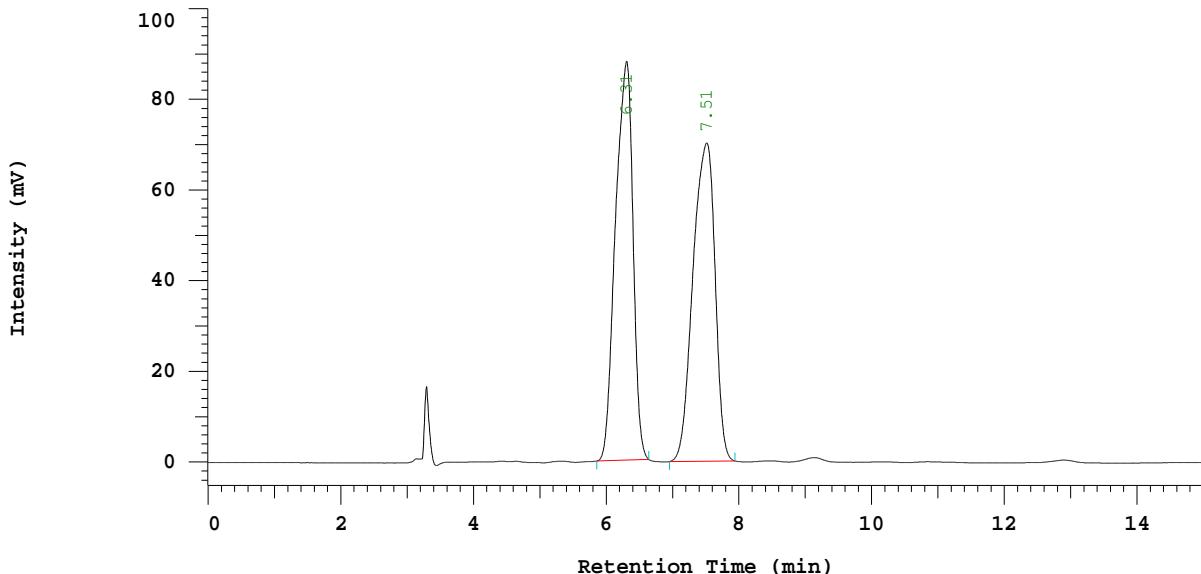
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IC

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.31	1607151	87901	49.828
2	7.51	1618270	70175	50.172
		3225421	158076	100.000

Peak rejection level: 1000

Figure S297. HPLC analysis of the racemic **4k**, for comparison (Scheme 3, b)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/15/2018
01:50 AM

Reported Date and Time: 10/30/2018
04:59 PM

Processed Date and Time: 10/30/2018
04:59 PM

Data Path: D:\CLW\DATA\0031\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0031

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-46-F1-chiral

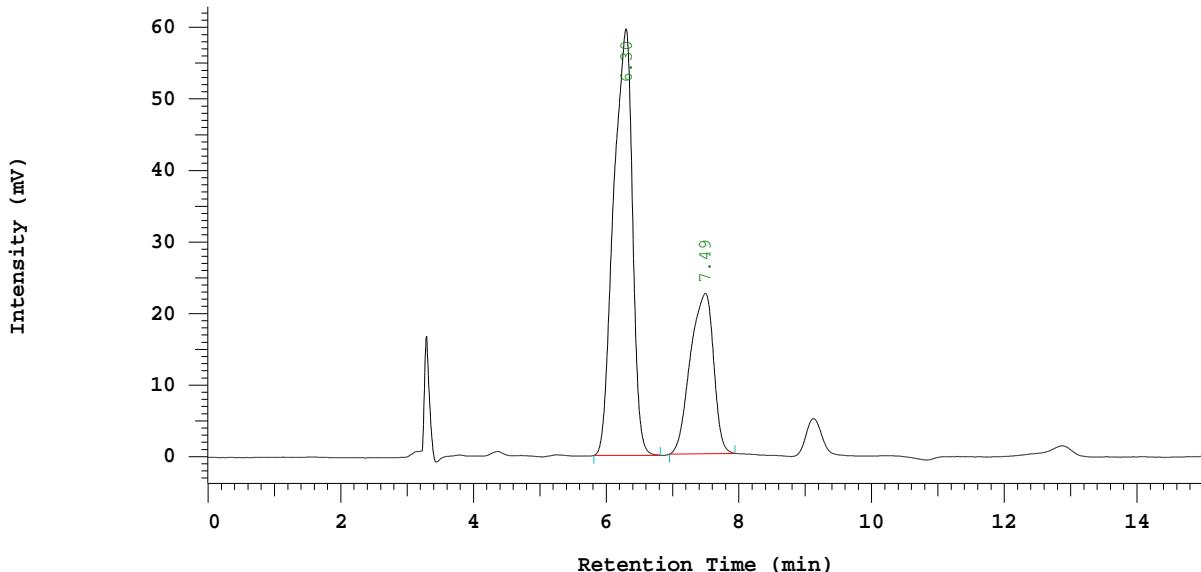
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IC

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-THF/Hx-IC

Column Type: IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.30	1175067	59605	68.404
2	7.49	542779	22402	31.596
		1717846	82007	100.000

Peak rejection level: 1000

Figure S298. HPLC analysis of chiral **4k** obtained (Scheme 3, b)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/02/2018
02:25 PM

Reported Date and Time: 10/30/2018
04:58 PM

Processed Date and Time: 10/30/2018
04:57 PM

Data Path: D:\CLW\DATA\0010\

Processing Method: test-THF/Hx-IC

System (acquisition): Sys 1

Series: 0010

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-46+48-F1-Co

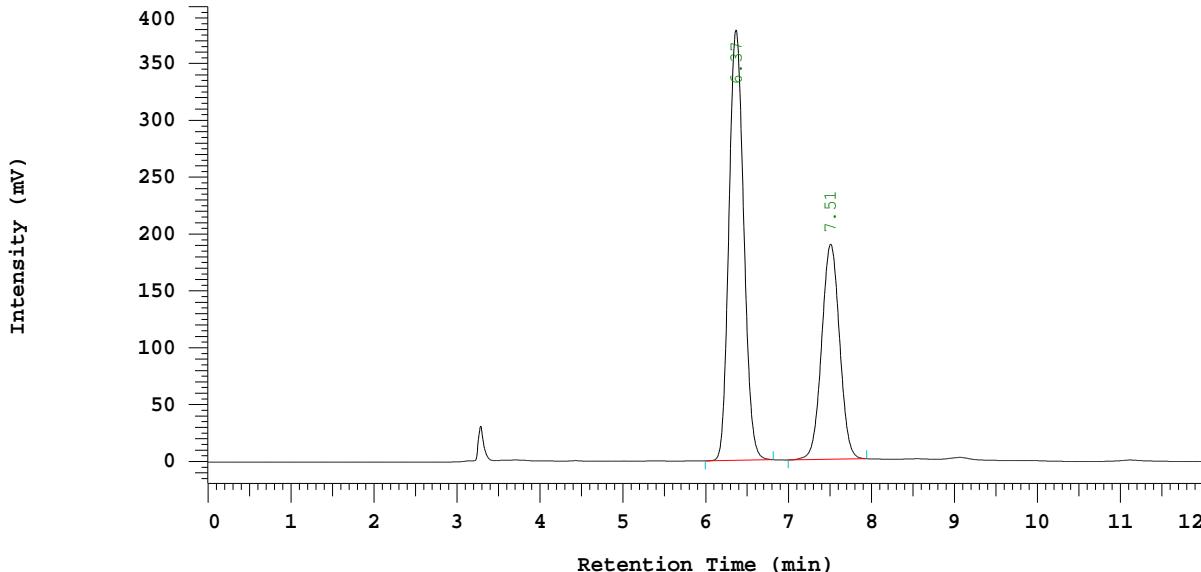
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-IC

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-THF/Hx-IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	6.37	4692249	378342	62.285
2	7.51	2841226	189077	37.715
		7533475	567419	100.000

Peak rejection level: 1000

Figure S299. HPLC analysis of the mixture of chiral 4k and racemic 4k, for comparison (Scheme 3, b)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/17/2018 Reported Date and Time: 08/17/2018
 01:04 AM 02:16 AM

Processed Date and Time: 08/17/2018
 02:15 AM

Data Path: D:\CLW\DATA\0039\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1

Series: 0039

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-51-F2-racemic

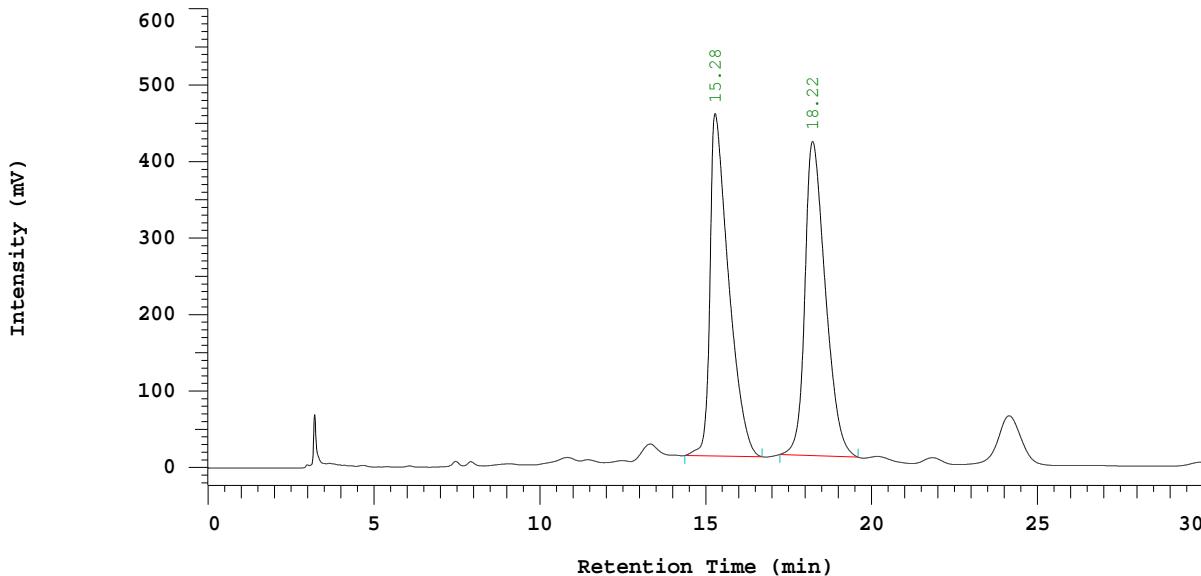
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IA

Chrom Type: Fixed WL Chromatogram, 265 nm



Processing Method: test-THF/Hx-IA

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 265 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	15.28	17407435	447606	49.783
2	18.22	17559259	410572	50.217
		34966694	858178	100.000

Peak rejection level: 1000

Figure S300. HPLC analysis of the racemic **7a for comparison (Scheme 3, c)**

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/16/2018 Reported Date and Time: 08/17/2018
 11:59 PM 06:01 PM

Processed Date and Time: 08/17/2018
 06:01 PM

Data Path: D:\CLW\DATA\0040\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1

Series: 0040

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-52-F2-chiral

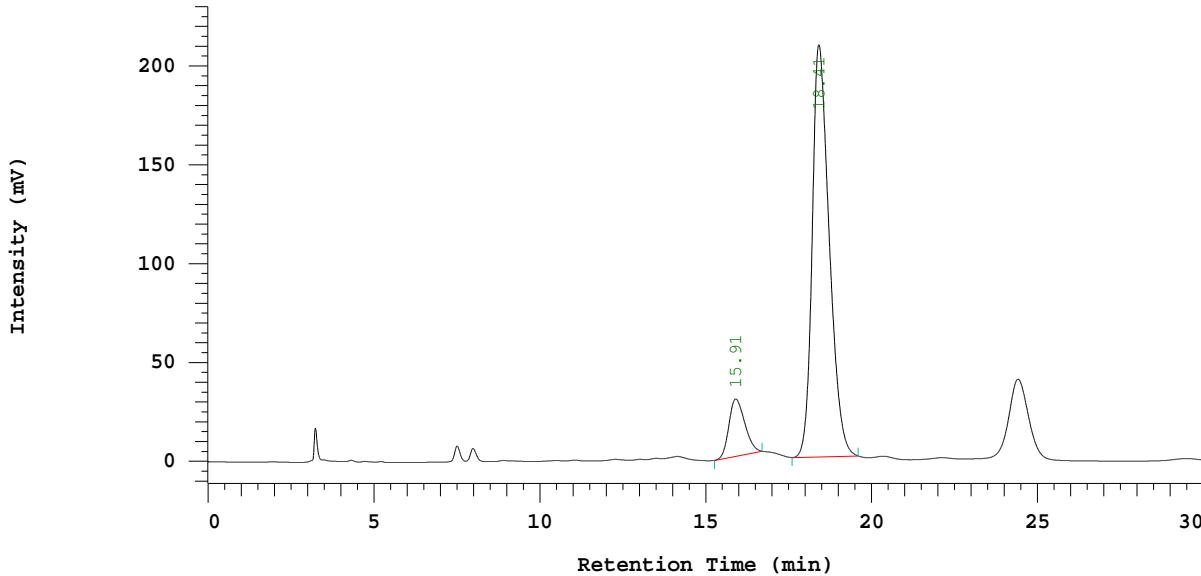
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IA

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-THF/Hx-IA

Column Type: IC Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	15.91	958367	29010	11.479
2	18.41	7390636	208373	88.521
		8349003	237383	100.000

Peak rejection level: 1000

Figure S301. HPLC analysis of chiral **7a**, obtained from the reaction with catalyst **IV** (Scheme 3, c).

D-2000 Elite HPLC System Manager ReportAnalyzed Date and Time: 08/21/2018
02:26 PMReported Date and Time: 08/21/2018
04:13 PMProcessed Date and Time: 08/21/2018
04:12 PM

Data Path: D:\CLW\DATA\0043\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1

Series: 0043

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-51+52-F2-Co

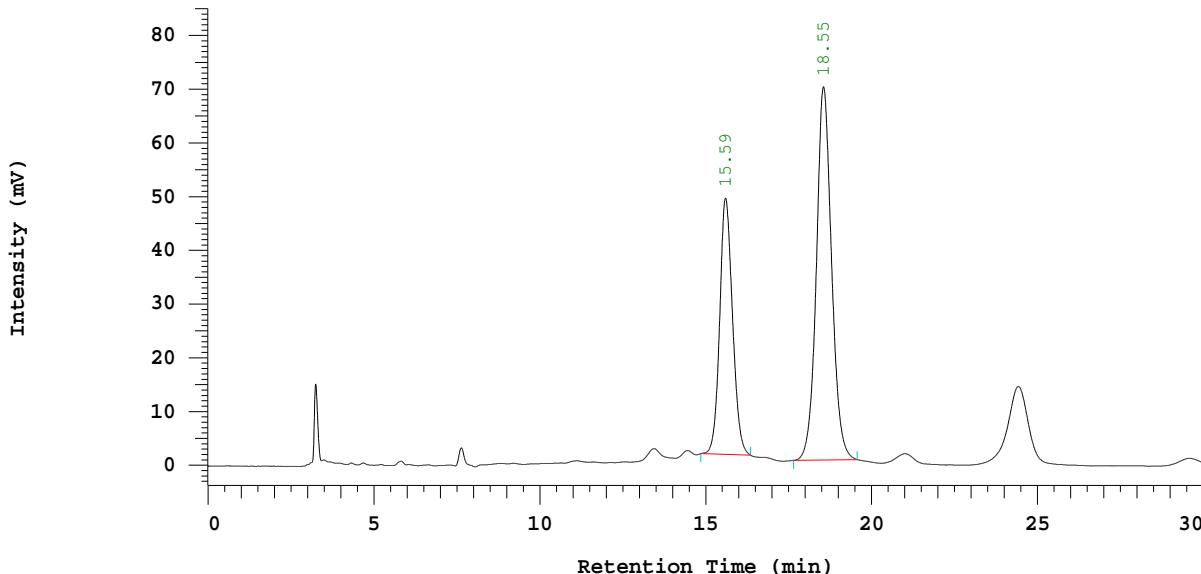
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IA

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-THF/Hx-IA

Column Type: IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	15.59	1271141	47697	36.582
2	18.55	2203645	69484	63.418
		3474786	117181	100.000

Peak rejection level: 1000

Figure S302. HPLC analysis of the mixture of chiral **7a** and racemic **7a**, for comparison (Scheme 3, c)

D-2000: CLW

Series: 0034

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/16/2018
07:35 PM

Reported Date and Time: 08/17/2018
12:59 AM

Processed Date and Time: 08/17/2018
12:58 AM

Data Path: D:\CLW\DATA\0034\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1

Series: 0034

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-51-F1-racemic

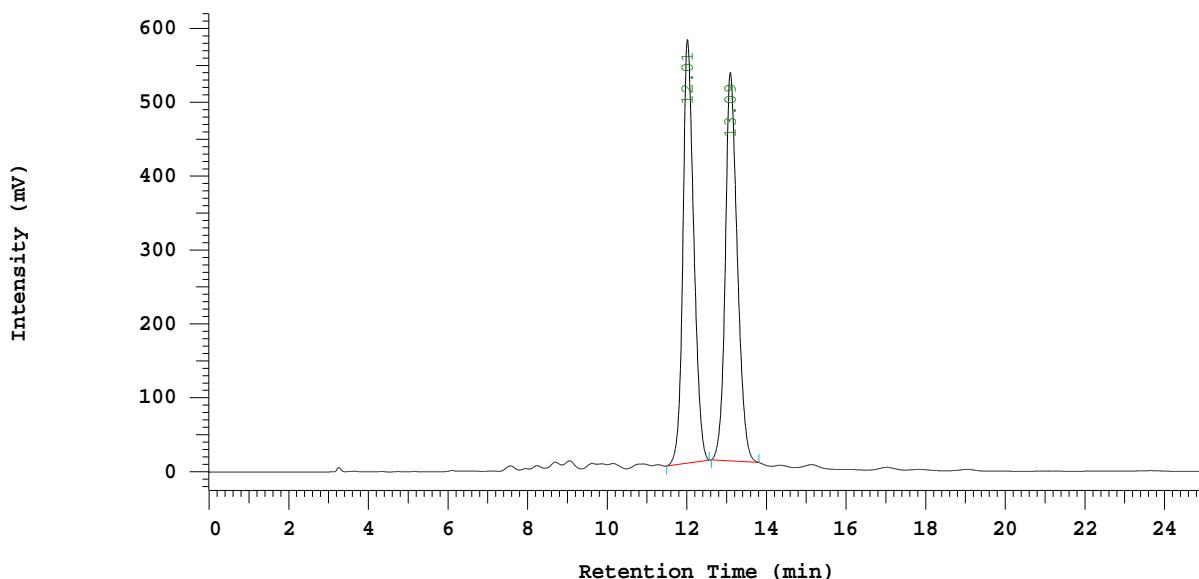
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IA

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-THF/Hx-IA

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	12.01	10851476	573057	49.717
2	13.09	10974988	525738	50.283
		21826464	1098795	100.000

Peak rejection level: 1000

Figure S303. HPLC analysis of the racemic **8a**, for comparison (Scheme 3, c)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/16/2018
10:34 PM

Reported Date and Time: 08/16/2018
11:26 PM

Processed Date and Time: 08/16/2018
11:26 PM

Data Path: D:\CLW\DATA\0037\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1

Series: 0037

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-52-F1-chiral

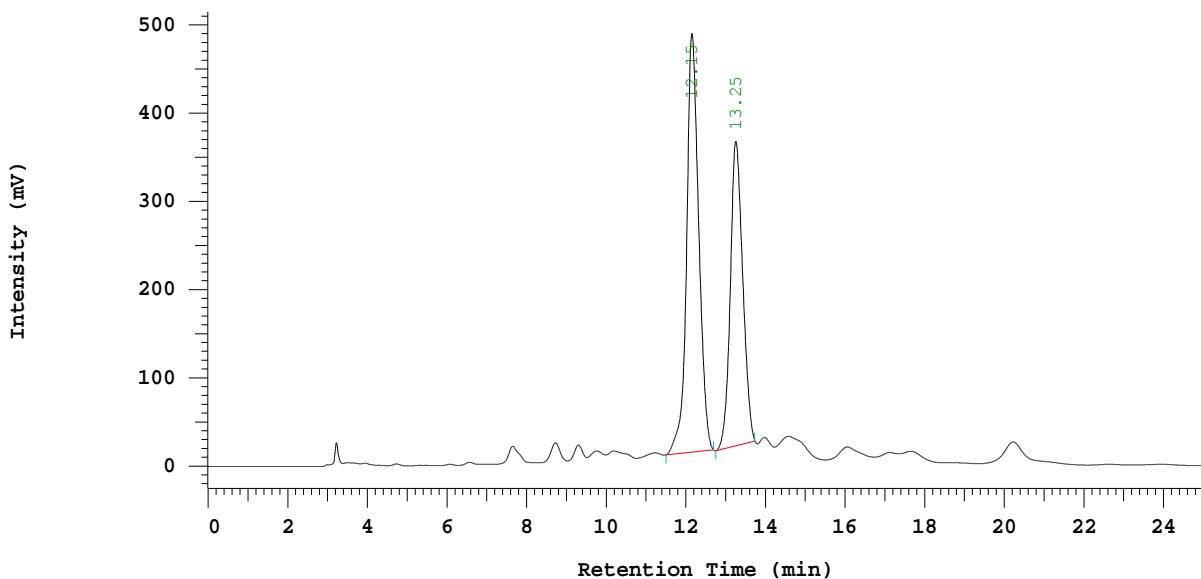
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IA

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-THF/Hx-IA

Column Type: IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	12.15	9998093	474512	57.350
2	13.25	7435222	345097	42.650
		17433315	819609	100.000

Peak rejection level: 1000

Figure S304. HPLC analysis of chiral **8a**, obtained from the reaction with catalyst **IV** (Scheme 3, c).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 08/16/2018
11:58 PM

Reported Date and Time: 08/17/2018
12:52 AM

Processed Date and Time: 08/17/2018
12:51 AM

Data Path: D:\CLW\DATA\0038\

Processing Method: test-THF/Hx-IA

System (acquisition): Sys 1

Series: 0038

Application(data): CLW

Vial Number: 1

Sample Name: CLW-1-51+52-F1-Co

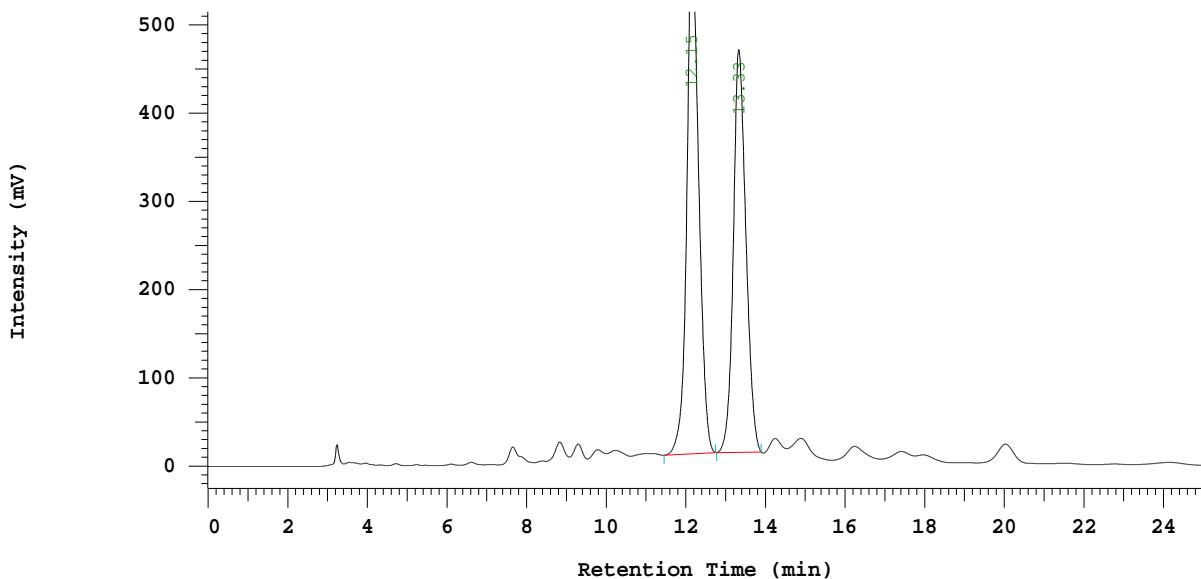
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 15%THF+85%Hex-1.0ml/min-col-IA

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-THF/Hx-IA

Column Type: IC

Method Developer: CLW

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	12.15	12052851	584003	54.653
2	13.33	10000500	456240	45.347
		22053351	1040243	100.000

Peak rejection level: 1000

Figure S305. HPLC analysis of the mixture of chiral **8a** and racemic **8a**, for comparison (Scheme 3, c)

D-2000: Prakash Series: 0925
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/20/2018 12:40 PM Reported Date and Time: 07/20/2018 01:17 PM

Processed Date and Time: 07/20/2018 01:16 PM

Data Path: D:\Prakash\DATA\0925\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0925

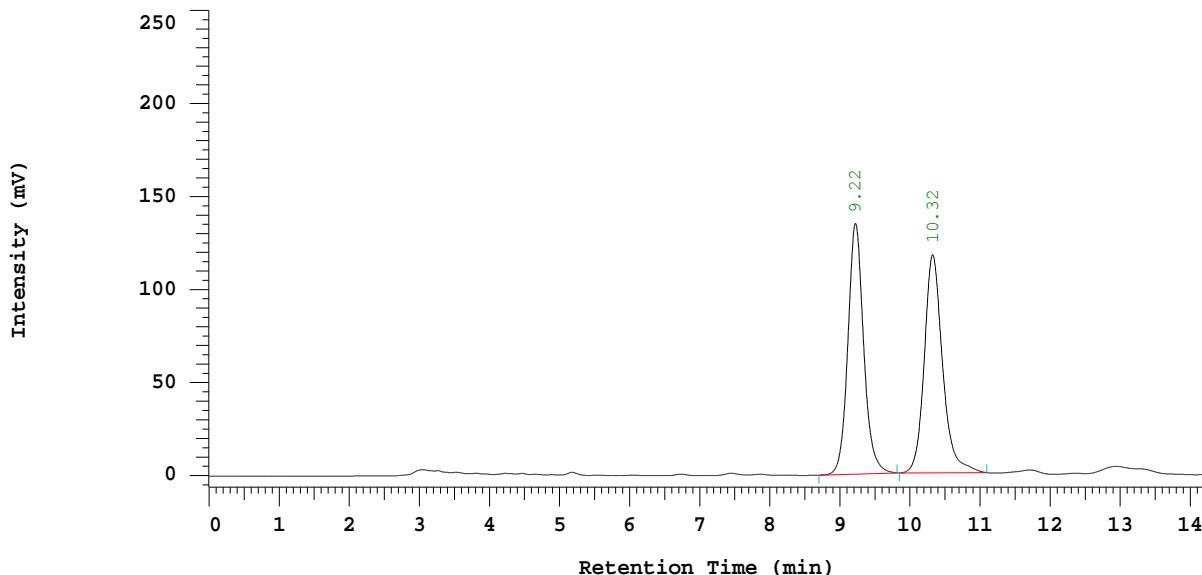
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-022F3(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.22	2107004	134650	49.748
2	10.32	2128360	117259	50.252
		4235364	251909	100.000

Peak rejection level: 200000

Figure S306. HPLC analysis of the racemic **9b**, for comparison (Scheme 3, d)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/20/2018 01:06 PM Reported Date and Time: 07/20/2018 01:34 PM

Processed Date and Time: 07/20/2018 01:33 PM

Data Path: D:\Prakash\DATA\0926\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0926

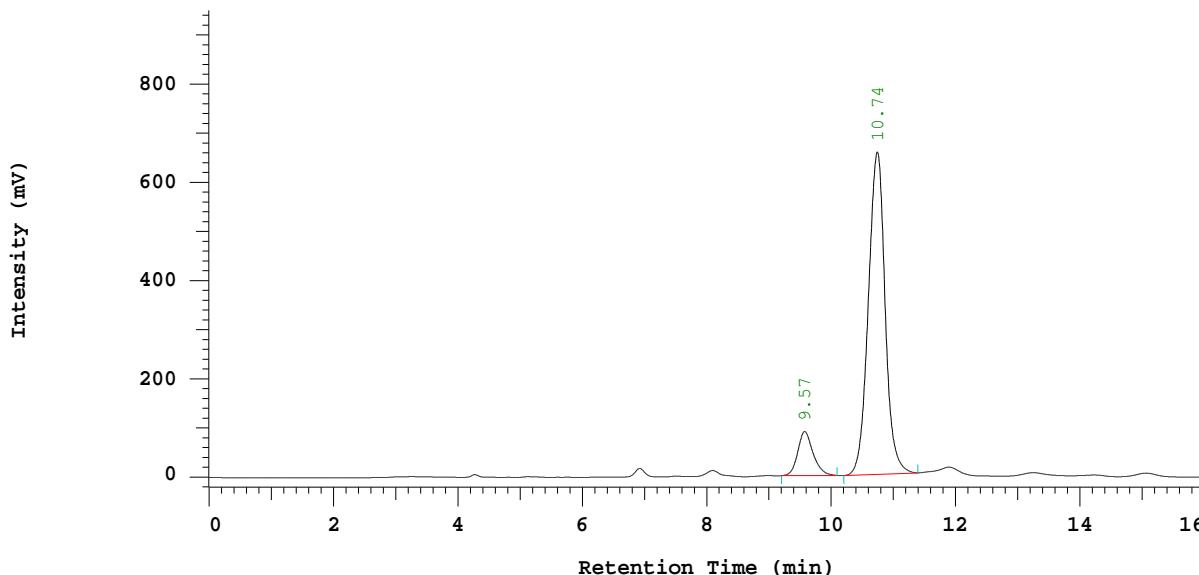
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-022F3(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.57	1537740	89761	11.117
2	10.74	12294292	656189	88.883
		13832032	745950	100.000

Peak rejection level: 200000

Figure S307. HPLC analysis of chiral **9b**, obtained from the reaction with catalyst **IV** (Scheme 3, d).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/20/2018 01:27 PM Reported Date and Time: 07/20/2018 01:57 PM

Processed Date and Time: 07/20/2018 01:56 PM

Data Path: D:\Prakash\DATA\0927\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0927

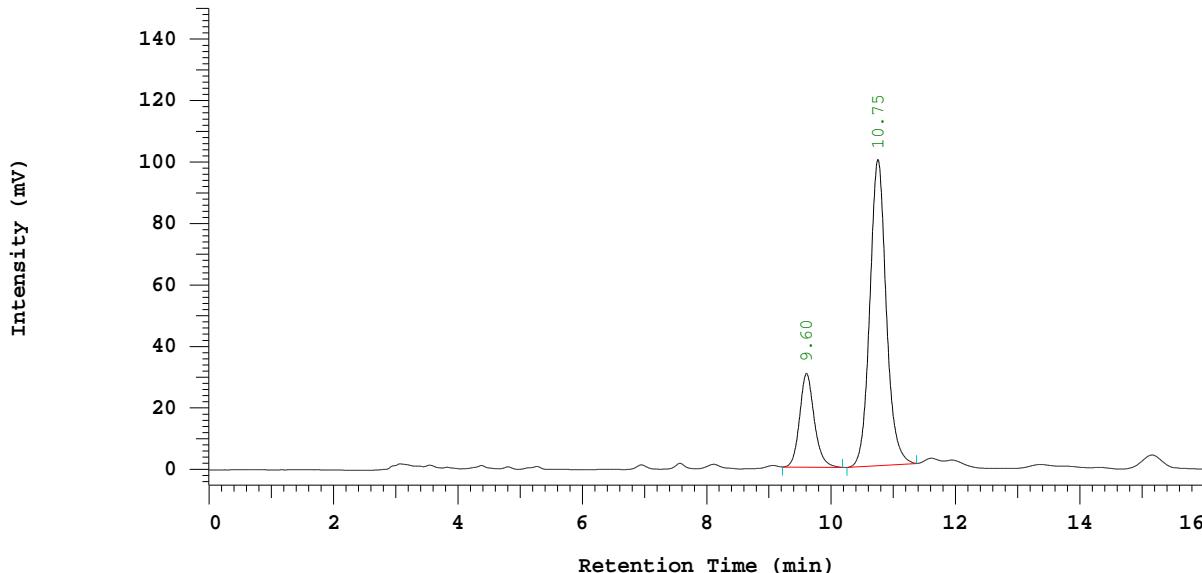
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-022F3(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 280 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Column Type: IA
Method Description:

Chrom Type: Fixed WL Chromatogram, 280 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.60	499270	30488	21.465
2	10.75	1826655	99588	78.535
		2325925	130076	100.000

Peak rejection level: 200000

Figure S308. HPLC analysis of the mixture of chiral **9b** and racemic **9b**, for comparison (Scheme 3, d)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/17/2018 02:24 PM Reported Date and Time: 07/18/2018 05:58 PM

Processed Date and Time: 07/18/2018 05:57 PM

Data Path: D:\Prakash\DATA\0919\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0919

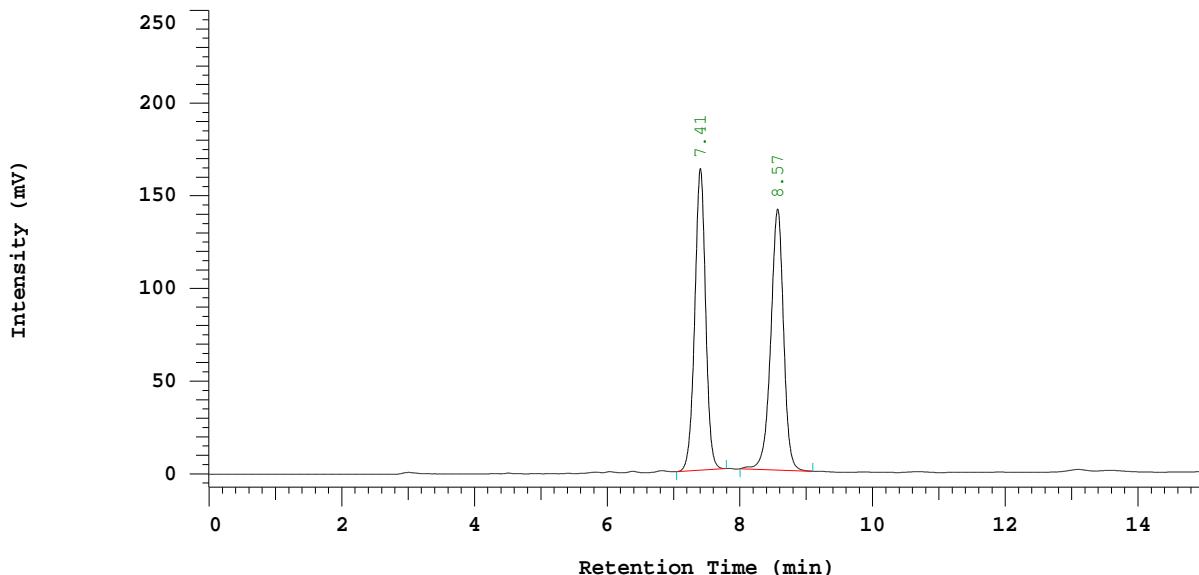
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-022F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 270 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Column Type: IA
Method Description:

Chrom Type: Fixed WL Chromatogram, 270 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.41	1849752	162816	49.445
2	8.57	1891270	140780	50.555
		3741022	303596	100.000

Peak rejection level: 200000

Figure S309. HPLC analysis of the racemic **8b**, for comparison (Scheme 3, d)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/18/2018 05:22 PM Reported Date and Time: 07/18/2018 06:04 PM

Processed Date and Time: 07/18/2018 06:03 PM

Data Path: D:\Prakash\DATA\0922\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0922

Application(data): Prakash Chaudari

Vial Number: 1

Sample Name: PDC-04-022F1(Chiral)

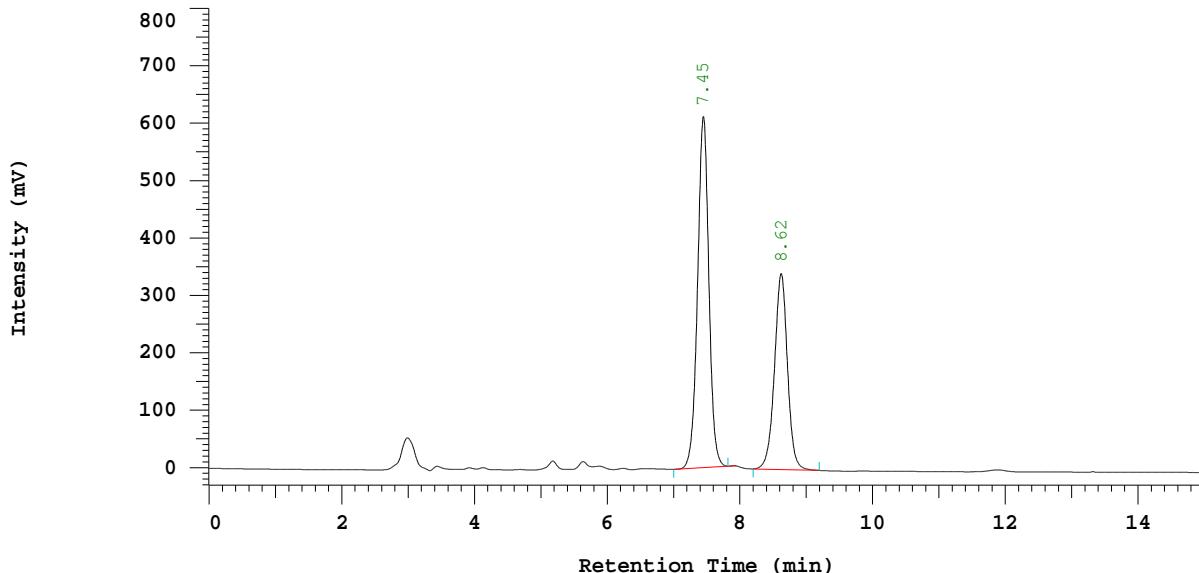
Vial Type: UNK

Injection from this vial: 1 of 1

Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 215 nm



Processing Method: test-IPA/Hx-IA

Column Type: IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 215 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.45	7223716	611280	60.816
2	8.62	4654258	341395	39.184
		11877974	952675	100.000

Peak rejection level: 200000

Figure S310. HPLC analysis of chiral **8b**, obtained from the reaction with catalyst **IV** (Scheme 3, d).

D-2000: Prakash Series: 0923
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/18/2018 05:42 PM Reported Date and Time: 07/18/2018 06:06 PM

Processed Date and Time: 07/18/2018 06:06 PM

Data Path: D:\Prakash\DATA\0923\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0923

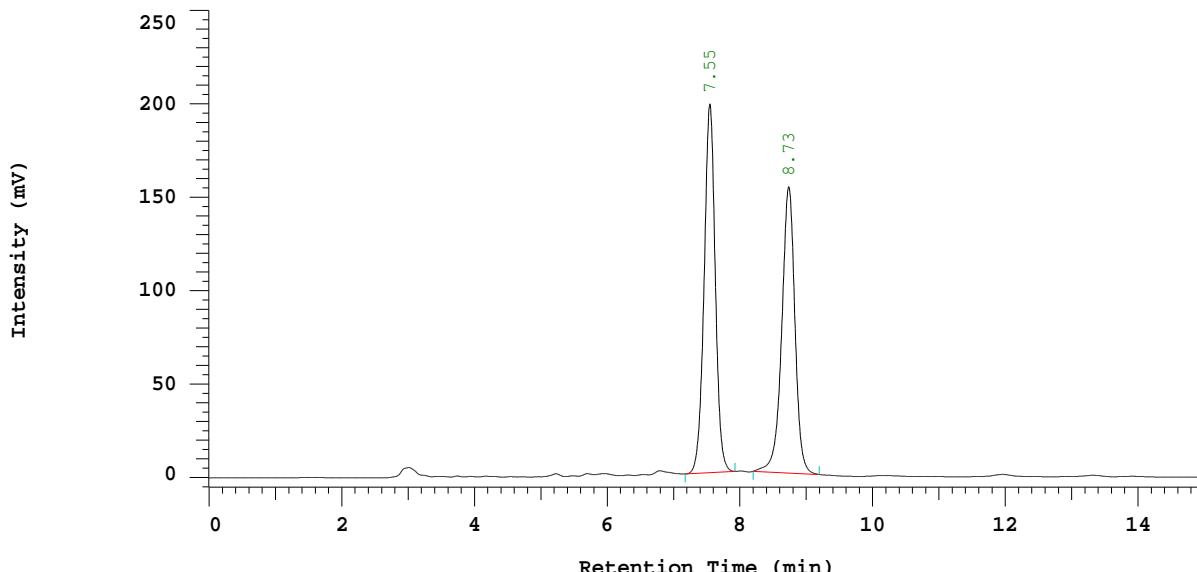
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-022F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.55	2302835	197310	52.083
2	8.73	2118632	153224	47.917
		4421467	350534	100.000

Peak rejection level: 200000

Figure S311. HPLC analysis of the mixture of chiral **8b** and racemic **8b**, for comparison (Scheme 3, d)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/26/2018 08:48 PM Reported Date and Time: 07/27/2018 11:51 AM

Processed Date and Time: 07/27/2018 11:51 AM

Data Path: D:\Prakash\DATA\0952\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0952

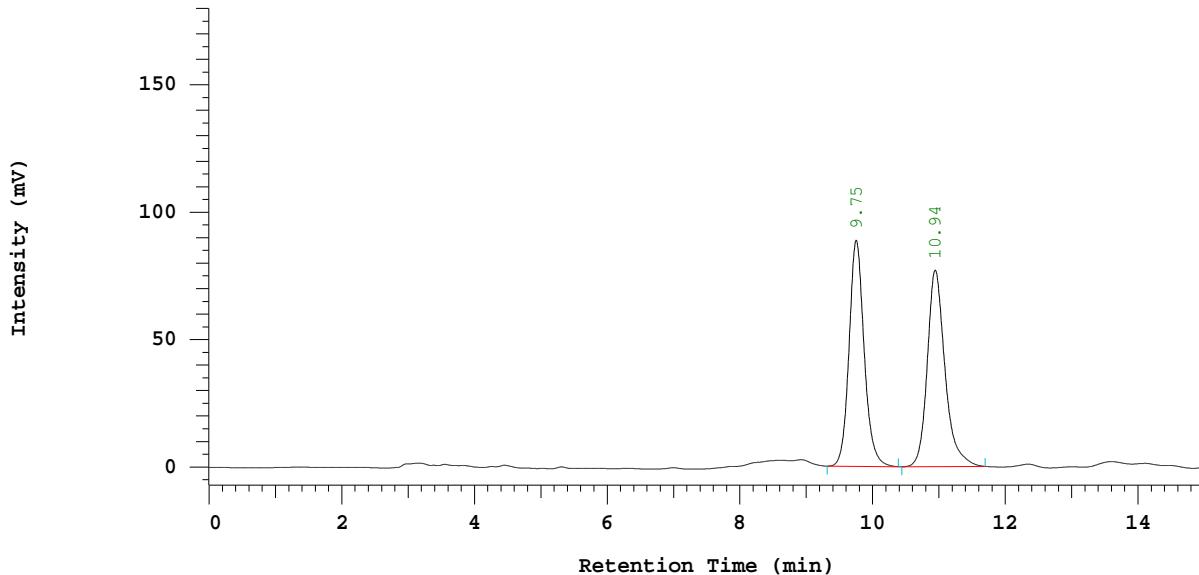
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-028F2(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 260 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Column Type: IA
Method Description:

Chrom Type: Fixed WL Chromatogram, 260 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.75	1404119	88747	49.479
2	10.94	1433680	77156	50.521
		2837799	165903	100.000

Peak rejection level: 200000

Figure S312. HPLC analysis of the racemic **9b**, for comparison (Scheme 3, e)

D-2000: Prakash Series: 0955
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/27/2018 01:44 PM Reported Date and Time: 07/27/2018 02:13 PM

Processed Date and Time: 07/27/2018 02:12 PM

Data Path: D:\Prakash\DATA\0955\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0955

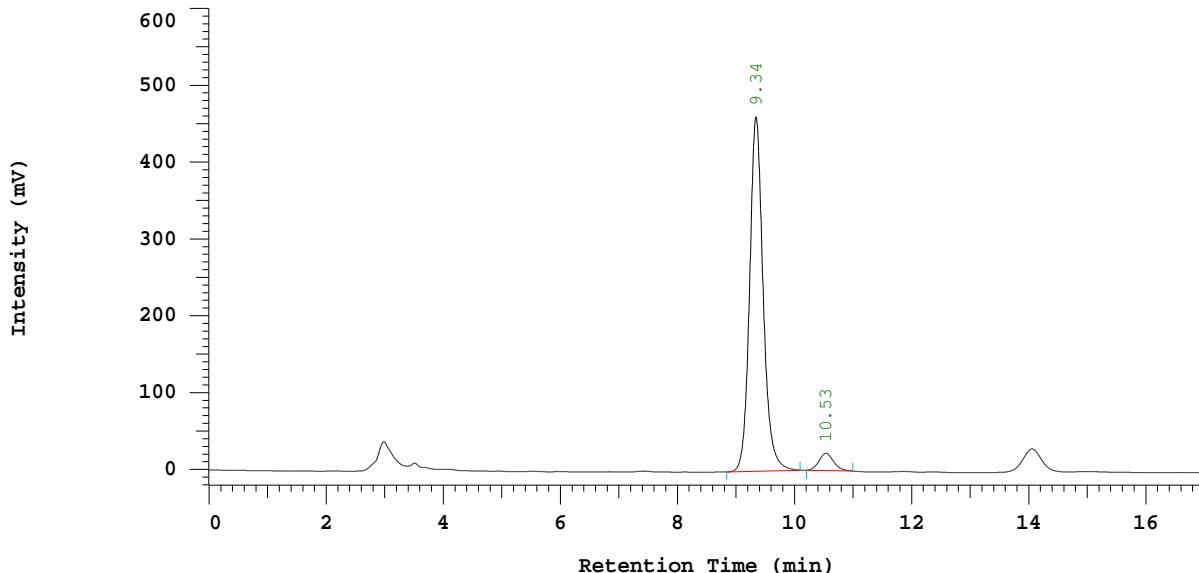
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-028F2(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 215 nm



Processing Method: test-IPA/Hx-IA

Column Type: IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 215 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.34	7419539	461068	94.979
2	10.53	392189	22486	5.021
		7811728	483554	100.000

Peak rejection level: 200000

Figure S313. HPLC analysis of chiral **9b**, obtained from the reaction with catalyst **III** (Scheme 3, e).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/27/2018 02:07 PM Reported Date and Time: 07/27/2018 02:32 PM

Processed Date and Time: 07/27/2018 02:32 PM

Data Path: D:\Prakash\DATA\0956\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0956

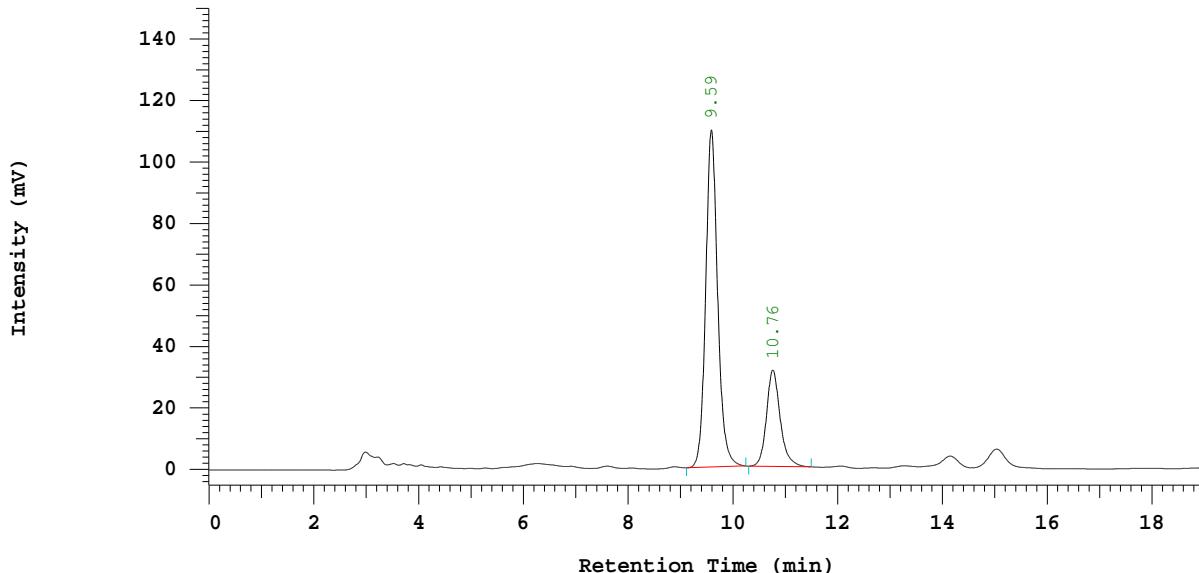
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-028F3(C0) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 20%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 254 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Column Type: IA
Method Description:

Chrom Type: Fixed WL Chromatogram, 254 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	9.59	1738881	109649	75.257
2	10.76	571716	31349	24.743
		2310597	140998	100.000

Peak rejection level: 200000

Figure S314. HPLC analysis of the mixture of chiral **9b** and racemic **9b**, for comparison (Scheme 3, e)

D-2000: Prakash Series: 0948
Chaudari

Report Name: modified System: Sys 1

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/26/2018 06:49 PM Reported Date and Time: 07/26/2018 09:01 PM

Processed Date and Time: 07/26/2018 09:00 PM

Data Path: D:\Prakash\DATA\0948\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0948

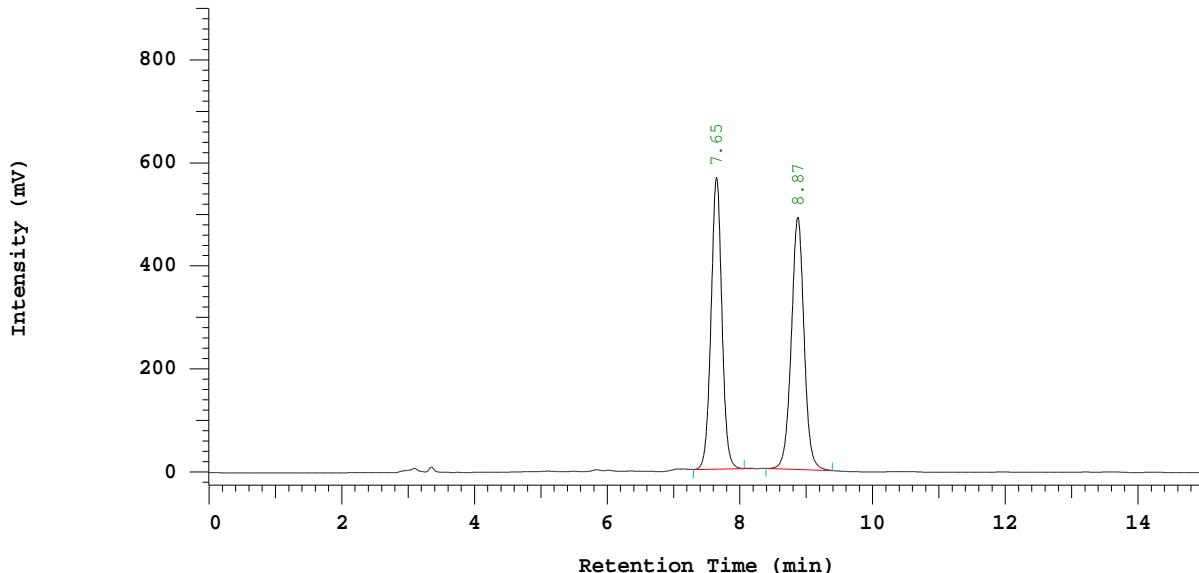
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-028F1(Racemic) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 215 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 215 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.65	6428707	566473	49.534
2	8.87	6549688	489549	50.466
		12978395	1056022	100.000

Peak rejection level: 200000

Figure S315. HPLC analysis of the racemic **8b**, for comparison (Scheme 3, e)

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/26/2018 06:30 PM Reported Date and Time: 07/26/2018 09:05 PM

Processed Date and Time: 07/26/2018 09:04 PM

Data Path: D:\Prakash\DATA\0947\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0947

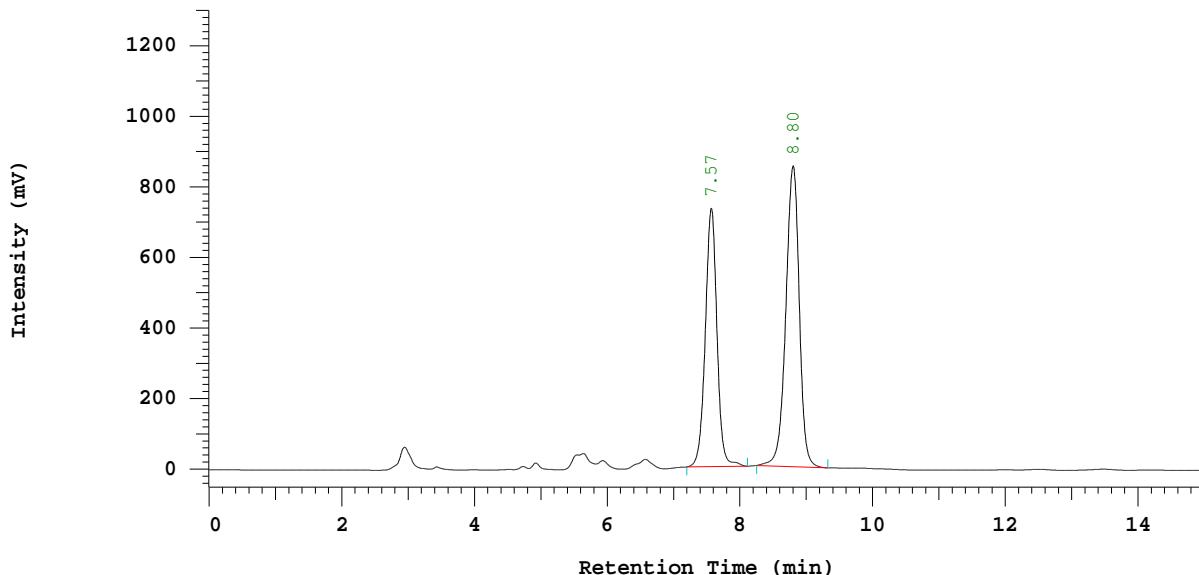
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-028F1(Chiral) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 225 nm



Processing Method: test-IPA/Hx-IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 225 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.57	8938622	731760	42.664
2	8.80	12012588	852648	57.336
		20951210	1584408	100.000

Peak rejection level: 200000

Figure S316. HPLC analysis of chiral **8b**, obtained from the reaction with catalyst **III** (Scheme 3, e).

D-2000 Elite HPLC System Manager Report

Analyzed Date and Time: 07/26/2018 07:07 PM Reported Date and Time: 07/26/2018 08:59 PM

Processed Date and Time: 07/26/2018 08:58 PM

Data Path: D:\Prakash\DATA\0949\

Processing Method: test-IPA/Hx-IA

System (acquisition): Sys 1 Series: 0949

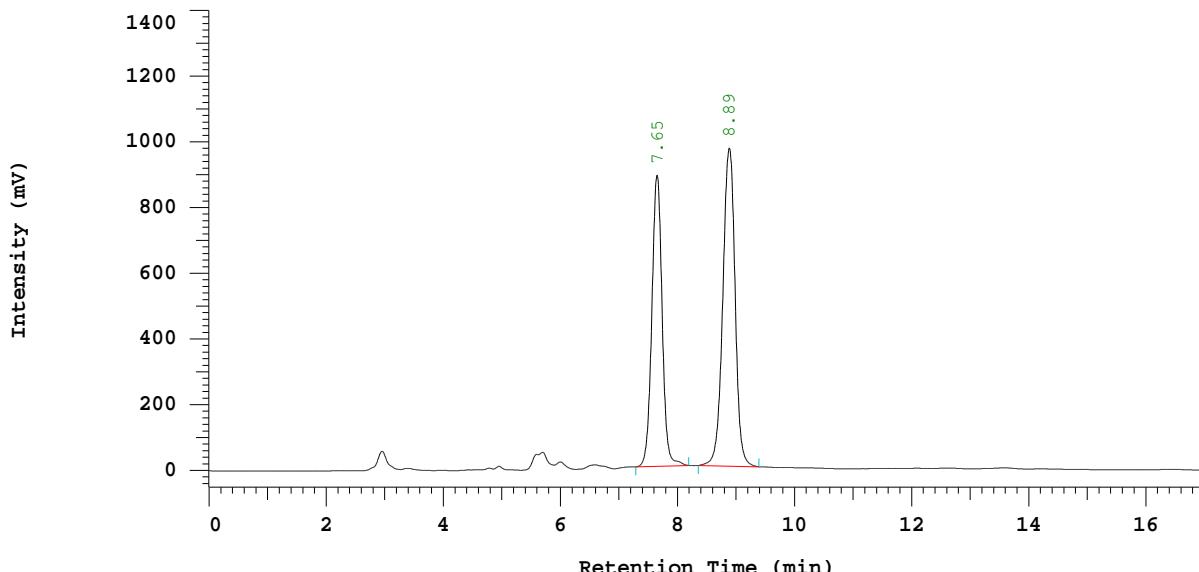
Application(data): Prakash Chaudari Vial Number: 1

Sample Name: PDC-04-028F1(Co) Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 20.0 ul

Sample Description: 30%IPA+HX 1.00mL/MIN COL-IA

Chrom Type: Fixed WL Chromatogram, 215 nm



Processing Method: test-IPA/Hx-IA

Column Type: IA

Method Developer: Prakash

Method Description:

Chrom Type: Fixed WL Chromatogram, 215 nm

Peak Quantitation: AREA

Calculation Method: EXT-STD

Scale Factor 1: 1.000

No.	RT	Area	Height	Area %
1	7.65	10835806	886034	43.357
2	8.89	14156222	967478	56.643
		24992028	1853512	100.000

Peak rejection level: 200000

Figure S317. HPLC analysis of the mixture of chiral **8b** and racemic **8b**, for comparison (Scheme 3, e)