Electronic Supporting Information

Understand, elucidate and rationalize the coordination mode of pyrimidylmethylamines: an intertwined study combining NMR and DFT methods

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Experimental details, NMR data and tables

Experimental details:

Unless otherwise noted, all starting materials were obtained from commercial suppliers and used without purification. Petroleum ether was distilled under Argon. NMR spectra were recorded on a 400 MHz, 300 MHz and 200 MHz Bruker spectrometers. ^{15}N-^{1}H HMBC spectra were recorded by acquiring 3072 x 256 points with 96 scans per transient. Chemical shifts were reported in ppm relative to the residual solvent peak (DMSO). For ^{15}N the CH_3NO_2 has been used as a reference at 0 ppm. High Resolution Mass Spectroscopy data were recorded on an Autospec Ultima (Waters/Micromass) device with a resolution of 5000 RP at 5%. Ligand **1** and complexes **7**, **9** were prepared according to literature. [1-3]

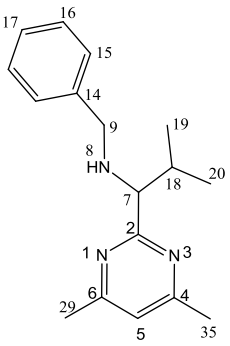
*General procedure for the preparation of pyrma ligands **2-6***

Boc-protected pyrma were prepared as follows: A sealed tube was charged with CBn-protected β-enaminones (1 mmol, 1 equiv.), carboxamide (1.5 mmol, 1.5 equiv.), activated MS 4Å (350 mg) and anhydrous toluene (10 mL). *t*-BuOK (2 mmol, 2 equiv.) was added in one portion and the tube was sealed and stirred at 110°C for 1.5 h. After cooling back to room temperature, the crude mixture was filtered over a short pad of silica gel (2 cm), washed with AcOEt and the filtrate was evaporated. The crude product was used as such for the next deprotection and reductive amination steps.

Boc deprotection step: The Boc-protected pyrma (1 mmol), was dissolved in CH_2Cl_2 (5 mL) and TFA (5 mL) was added at 0°C. The reaction mixture was then stirred at room temperature for 1 h. It was then quenched by addition of saturated aqueous $NaHCO_3$ at 0°C, extracted with CH_2Cl_2 (3 X 10 mL), the combined organic layers were washed with brine (10 mL), dried ($MgSO_4$) and evaporated.

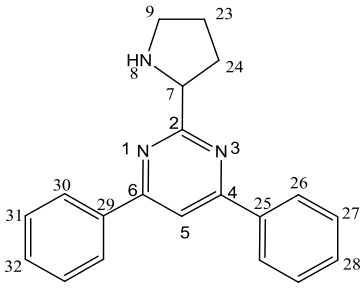
Reductive amination: The amine (1 equiv.) and benzaldehyde (1.5 equiv.) were dissolved in THF (7 mL) and $MgSO_4$ (1.5 g) was added. The reaction mixture was then stirred at room temperature for 12h. It was then filtered and the solvent was evaporated. The resulting crude imine was dissolved in MeOH (5 mL) and $NaBH_4$ (3 equiv.) was added and the mixture was stirred for further 12 h at room temperature. Saturated aqueous $NaHCO_3$ (10 mL) was added. The product was extracted with CH_2Cl_2 (3 X 10 mL), the combined organic layers were washed with brine (10 mL), dried ($MgSO_4$) and evaporated. It was then purified by flash column chromatography (see each case for detail).

Ligand **2:**



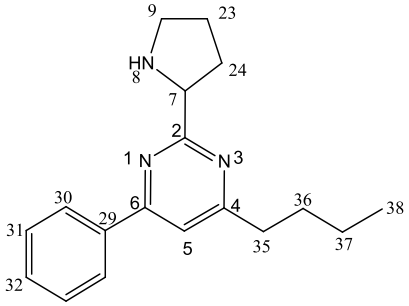
Ligand **2** was obtained following the aforementioned general procedure on 0.5 mmol scale. After purification on silica gel (PE/AcOEt : 90/10), **2** was obtained in 13 % yield (3 steps). ^{1}H NMR (300 MHz, DMSO): δ 7.28 (m, H-15 and H-16), 7.20 (m, H-17), 7.09 (s, H-5), 3.58 (d, J = 9Hz, H-9a), 3.39 (d, J = 9Hz, H-9b), 3.32 (m, H-7), 2.41 (s, H-21 and H-22), 1.92 (m, H-18), 0.90 (d, J = 6Hz, H-19), 0.75 (d, J = 6Hz, H-20). ^{13}C NMR (75 MHz, DMSO): δ 172.9 (C-2), 165.9 (C-6, C-4), 140.9 (C-14), 128.0 (C-16), 127.8 (C-15), 117.7 (C-6), 68.6 (C-7), 51.3 (C-9), 33.1 (C-18), 23.5 (C-21 and C-22), 20.0 (C-20), 18.6 (C-19). HRMS-ESI: m/z $[M + H]^+$ calcd for $C_{17}H_{24}N_3$: 270.1970; found: 270.1963.

Ligand **3**



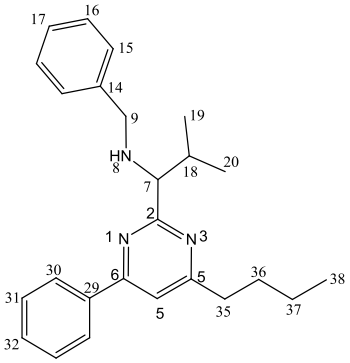
Ligand **3** was obtained following the aforementioned general procedure on 0.3 mmol scale. After purification on silica gel (AcOEt : 100%), **3** was obtained in 19 % yield (3 steps). ^{1}H NMR (300 MHz, DMSO): δ 8.45 (s, H-5), 8.38 (m, H-26 and H-30), 7.58 (m, H-27, H-28, H-31 and H-32), 4.34 (m, H-7), 3.23 (m, H-9a), 2.9 (m, H-9b), 2.25 (m, H-24a), 1.94 (m, H-24b). ^{13}C NMR (75 MHz, DMSO): δ 172.0 (C-2), 163.9 (C-6, C-4), 136.5 (C-25, C-29), 131.0 (C-28, C-32), 128.9 (C-27, C-31), 127.3 (C-26, C-30), 110.5 (C-5), 63.9 (C-7), 46.9 (C-9), 32.7 (C-24), 25.8 (C-23). HRMS-ESI: m/z $[M + H]^+$ calcd for $C_{20}H_{20}N_3$: 302.1657; found: 302.1659.

Ligand **4**



Ligand **4** was obtained following the aforementioned general procedure on 0.2 mmol scale. After purification on silica gel (AcOEt : 100%), **4** was obtained in 37 % yield (3 steps). ^{1}H NMR (300 MHz, DMSO): δ 8.26 (m, H-30), 7.89 (s, H-5), 7.56 (m, H-31 and H-32), 4.48 (m, H-7), 3.28 (m, H-9a), 3.05 (m, H-9b), 2.79 (m, H-35), 2.31 (m, H-24a), 1.95 (m, H-24b), 1.73 (m, H-36), 1.36 (m, H-37), 0.93 (H-38). ^{13}C NMR (75 MHz, DMSO): δ 171.8 (C-4), 168.7 (C-2), 162.7 (C-6), 136.1 (C-29), 131.1 (C-32), 128.9 (C-31), 127.2 (C-30), 113.9 (C-5), 63.2 (C-7), 46.3 (C-9), 36.8 (C-35), 31.8 (C-24), 30.3 (C-36), 24.7 (C-23), 21.8 (C-37), 13.7 (C-38). HRMS-ESI: m/z $[M + H]^+$ calcd for $C_{18}H_{24}N_3$: 282.1970; found: 282.1967.

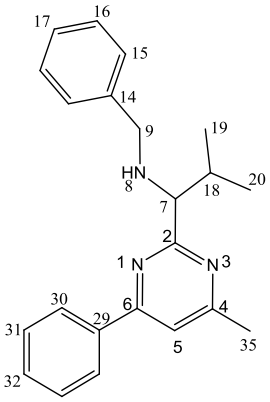
Ligand **5**



Ligand **5** was obtained following the aforementioned general procedure on 1 mmol scale. After purification on silica gel (PE/AcOEt : 90/10), **5** was obtained in 25 % yield (3 steps). ^{1}H NMR (300 MHz, DMSO): δ 8.23 (m, H-

30), 7.79 (s, H-5), 7.5 (m, H-31 and H-32), 7.27 (m, H-15, H-16), 7.18 (m, H-17), 3.66 (m, H-9a), 3.49 (m, H-7), 3.48 (m, H-9b), 2.77 (m, H-35), 2.04 (m, H-18), 1.71 (m, H-36), 1.32 (m, H-37), 0.94 (d, H-19), 0.89 (H-38), 0.79 (d, H-20). ^{13}C NMR (75 MHz, DMSO): δ 171.6 (C-2), 171.5 (C-4), 162.8 (C-6), 141.0 (C-14), 137.1 (C-29), 131.3 (C-32), 129.3 (C-31), 128.5 (C-16), 128.4 (C-15), 127.5 (C-30), 127.0 (C-17), 113.9 (C-5), 69.2 (C-7), 52.0 (C-9), 37.2 (C-35), 33.6 (C-18), 31.0 (C-36), 22.2 (C-37), 20.2 (C-20), 19.2 (C-19), 14.2 (C-38). HRMS-ESI: m/z [M + H]$^+$ calcd for $C_{25}H_{32}N_3$: 373.2881; found: 374.2587.

Ligand **6**

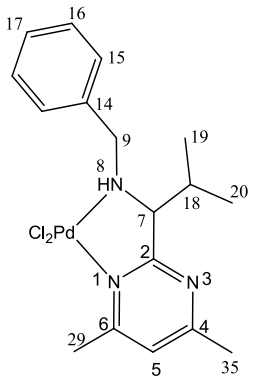


Ligand **6** was obtained following the general procedure on 1 mmol scale. After purification on silica gel (PE/AcOEt : 90/10), **6** was obtained in 21 % yield (3 steps). ^{1}H NMR (300 MHz, DMSO): δ 8.21 (m, H-30), 7.82 (s, H-5), 7.54 (m, H-31, H-32), 7.25 (m, H-15, H-16), 7.19 (m, H-17), 3.66 (d, H-9a), 3.49 (m, H-7, H-9b), 2.52 (s, H-35), 2.05 (m, H-18), 0.91 (d, H-19), 0.79 (d, H-20). ^{13}C NMR (75 MHz, DMSO): δ 171.4 (C-2), 167.5 (C-4), 162.1 (C-6), 140.9 (C-14), 136.5 (C-29), 130.8 (C-32), 128.9 (C-31), 128.0 (C-16), 127.8 (C-15), 127.0 (C-30), 126.5 (C-17), 113.9 (C-5), 68.7 (C-7), 51.4 (C-9), 33.1 (C-18), 24.0 (C-35), 19.4 (C-20), 18.6 (C-19). HRMS-ESI: m/z [M + H]$^+$ calcd for $C_{22}H_{26}N_3$: 332.2127; found: 332.2129.

*General procedure for the preparation of complexes **8-17***

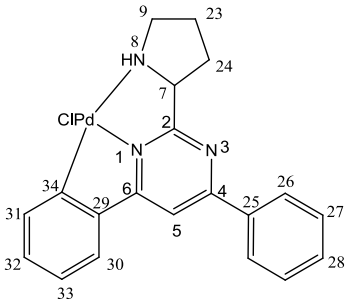
To a stirred solution of ligand **1-6** (0.25 mmol) in 5 mL of freshly distilled MeOH was added Na_2PdCl_4 (74 mg, 0.25 mmol). The mixture was stirred at room temperature for 16 h, filtered over silica gel pad and the solvent was then removed by evaporation under vacuum.

Complex **8** (86%)



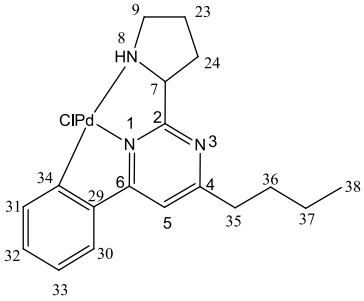
^{1}H NMR (300 MHz, DMSO): δ 7.03 (s, H-5), 7.69 (m, H-15), 7.28 (m, H-16), 7.18 (m, H-17), 5.82 (brs, H-8), 3.97 (m, H-7), 3.97 (m, H-9a), 3.59 (m, H-9b), 2.99 (m, H-18), 2.45 (s, H-29), 2.36 (s, H-35), 1.45 (d, H-19), 1.33 (d, H-20). ^{13}C NMR (75 MHz, DMSO): δ 171.8 (C-2), 169.1 (C-6), 168.1 (C-4), 120.9 (C-5), 76.5 (C-7), 57.9 (C-9), 135.1 (C-14), 131.2 (C-15), 128.8 (C-17), 128.6 (C-16), 33.6 (C-18), 25.8 (C-29), 23.6 (C_35), 19.8 (C-19), 20.5 (C-20). HRMS-ESI: m/z [M –Cl+MeCN]$^{+}$ calcd for $C_{19}H_{26}ClN_4Pd$: 453.0879; found: 453.0911.

Complex **10** (38%)



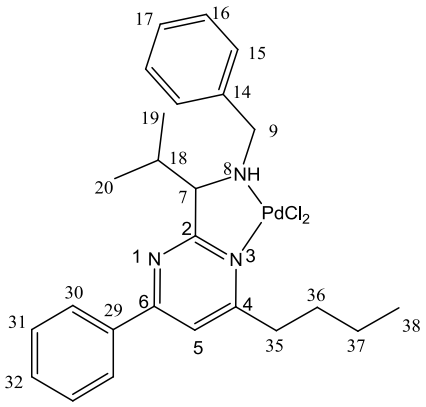
^{1}H NMR (300 MHz, DMSO): δ 8.38 (s, H-5), 8.30 (m, H-26), 7.92 (m, H-30), 7.62 (m, H-27, H-28), 7.53 (H-33), 7.11 (m, H-31, H-32), 5.50 (brs, H-8), 4.87 (m, H-7), 3.23 (m, H-9a), 3.08 (m, H-9b), 2.46 (m, H-24a), 2.08 (m, H-24b). ^{13}C NMR (75 MHz, DMSO): δ 168.6 (C-2), 165.0 (C-4), 173.4 (C-6), 157.2 (C-34), 146.9 (C-29), 136.0 (C-25, C-33), 132.5 (C-28), 131.4 (C-32), 129.6 (C-27), 128.2 (C-26), 126.5 (C-30), 124.9 (C-31), 109.1 (C-5), 67.9 (C-7), 49.7 (C-9), 32.4 (C-24), 26.4 (C-23). HRMS-ESI: m/z [M –Cl+MeCN]$^{+}$ calcd for $C_{22}H_{21}N_4Pd$: 447.0810; found: 447.0830.

Complex **13** (31%)



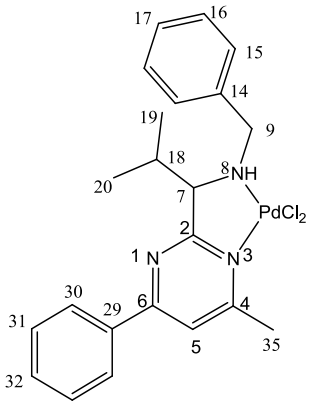
^{1}H NMR (300 MHz, DMSO): δ 7.81(s, H-5), 7.74 (m, H-30), 7.54 (m, H-33), 7.12 (m, H-31, H-32), 5.55 (brs, H-8), 4.77 (m, H-7), 3.19 (m, H-9a), 3.03 (m, H-9b), 2.78 (m, H-35), 2.38 (m, H-24a), 1.95 (m, H-24b), 1.73 (m, H-36), 1.36 (m, H-37), 0.92 (H-38). ^{13}C NMR (75 MHz, DMSO): δ 173.3 (C-4), 172.7 (C-2), 167.6 (C-6), 156.8 (C-8), 146.2 (C-29), 135.6 (C-33), 130.7 (C-32), 125.5 (C-30), 124.3 (C-31), 111.8 (C-5), 67.2 (C-7), 49.1 (C-9), 37.3 (C-35), 31.9 (C-24), 30.2 (C-36), 25.9 (C-23), 21.8 (C-37), 13.7 (C-38). HRMS-ESI: m/z [M –Cl–HCl +MeCN]$^{+}$ calcd for $C_{20}H_{25}N_4Pd$: 427.1122; found: 427.1132.

Complex **15** (69%)



^{1}H NMR (300 MHz, DMSO): δ 8.18 (m, H-30), 7.83 (s, H-5), 7.66 (m, H-15), 7.60 (m, H-31 and H-32), 7.21 (m, H-17, H-16), 5.76 (brs, H-8), 4.06 (m, H-7), 3.97 (m, H-9a), 3.69 (m, H-9b), 3.08 (m, H-18, H-35), 1.62 (m, H-36), 1.49 (d, H-19), 1.38 (m, H-37), 1.34 (d, H-20), 0.97 (H-38). ^{13}C NMR (75 MHz, DMSO): δ 172.0 (C-2), 174.7 (C-4), 162.8 (C-6), 135.0 (C-14), 134.6 (C-29), 129.5 (C-32), 129.7 (C-31), 128.7 (C-16), 131.2 (C-15), 128.2 (C-30), 128.5 (C-17), 116.0 (C-5), 76.7 (C-7), 57.7 (C-9), 37.6 (C-35), 33.3 (C-18), 31.8 (C-36), 22.4 (C-37), 20.6 (C-20), 19.8 (C-19), 14.3 (C-38). HRMS-ESI: m/z $[M + Na]^{+}$ calcd for $C_{25}H_{31}Cl_2N_3PdNa$: 574.0822; found: 574.0853.

Complex **17** (71%)



^{1}H NMR (300 MHz, DMSO): δ 8.14 (m, H-30), 7.78 (s, H-5), 7.72 (m, H-15), 7.58 (m, H-31, H-32), 7.20 (m, H-16, H-17), 5.95 (brs, H-8), 4.10 (m, H-7), 4.03 (m, H-9b), 3.65 (d, H-9a), 3.05 (m, H-18), 2.51 (s, H-35), 1.55 (d, H-19), 1.37 (d, H-20). ^{13}C NMR (75 MHz, DMSO): δ 171.6 (C-2), 170.2 (C-4), 162.0 (C-2), 134.7 (C-14), 134.1 (C-29), 132.3 (C-31), 130.8 (C-15), 129.2 (C-32), 128.3 (C-16), 128.1 (C-17), 127.5 (C-30), 116.3 (C-5), 76.1 (C-7), 57.4 (C-9), 32.7 (C-18), 25.7 (C-35), 20.1 (C-20), 19.2 (C-19). HRMS-ESI: m/z $[M –Cl+MeCN]^{+}$ calcd for $C_{24}H_{28}ClN_3Pd$: 513.1044; found: 513.1074.

Table 1. Characteristic ^{15}N chemical shifts for ligands **1-6** and complexes **7-17.** An error of ± 2ppm has been measured for ΔδN.

Nitrogen 15		N1	N3	N8
1	δ1 (ppm)	-87,5	-87,5	-331,2
7	δ2 (ppm)	-163,2	-85,3	-345
	Δ=δ2−δ1	-75,7	2,2	-13,8
2	δ1 (ppm)	-96,1	-96,1	-332,6
8	δ2 (ppm)	-164,8	-92,6	-349,9
	Δ=δ2−δ1	-68,7	3,5	-17,3
3	δ1 (ppm)	-103,8	-103,8	-330,8
10	δ2 (ppm)	-158,6	-104,7	-343,2
	Δ=δ2−δ1	-54,8	-0,9	-12,4
4	δ1 (ppm)	-107,9	-95,7	-327,7
13	δ2 (ppm)	-159,3	-95,4	-342,8
	Δ=δ2−δ1	-51,4	0,3	-15,1
5	δ1 (ppm)	-103,4	-91,6	-334,4
15	δ2 (ppm)	-101,8	-163,8	-349,9
	Δ=δ2−δ1	1,6	-72,2	-15,5
6	δ1 (ppm)	-104,3	-90,8	-334,9
17	δ2 (ppm)	-102,9	-163,1	-349,9
	Δ=δ2−δ1	1,4	-72,3	-15

Table 2: Geometrical data of all pyrma ligands (A) and their $PdCl_2$ complexes (B) obtained by DFT calculations considering the solvent effect by the means of the SCRF calculation scheme, having DMSO as implicit solvent (see computational methods and 3D atomic coordinates schemed on Figure 6 SI) Bond distances as well as pyrimidine – benzylic aromatic ring distances ($d_{inter\text{-}rings}$) are expressed in Angstroms (Å) whilst torsional angles are depicted in degrees (deg). Pyrimidine – benzylic interplanar ring angles (IA) are also expressed in degrees. For Pd(*C*,*N*,*N*) complexes **10**, **13** and **17'** it is also expressed the bond distance between carbon and palladium (Cortho-Pd) in Angströms.

A

	N1-N8 (Å)	**N3-N8 (Å)**	**N1CCN8(deg.)**	**N3CCN8 (deg.)**	**$d_{inter\text{-}rings}$ (Å)**	**IA (deg.)**
1	2.97	3.53	54.48	-127.92	4.5875	-8.41
2	3.01	3.42	65.71	-115.6	4.605	-12.21
3	2.96	3.49	57.92	-122.74	x	x
4	2.96	3.49	57.82	-122.65	x	x
5	2.93	3.42	61.65	-117.98	5.6675	48.66
6	2.9	3.57	50.12	-131.27	4.5275	15.79

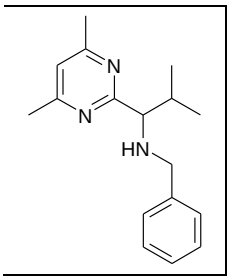
B

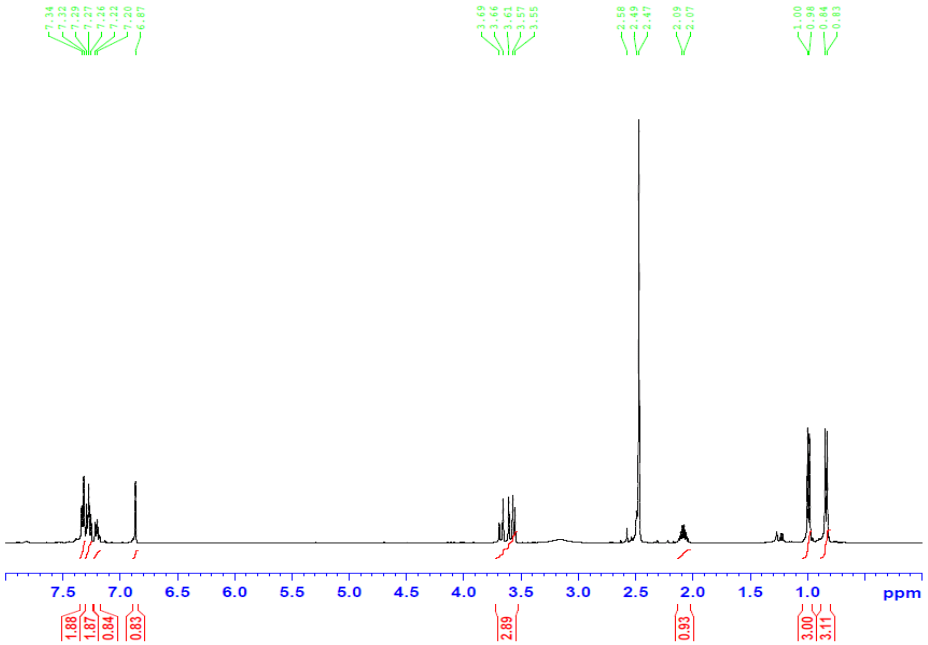
	N1-N8 (Å)	**N3-N8 (Å)**	**N1CCN8(deg.)**	**N3CCN8 (deg.)**	**$d_{inter\text{-}rings}$ (Å)**	**IA (deg.)**
7	2.71	3.67	23.63	-157.63	4.6825	29.92
8	2.69	3.6	29.06	-149.9	4.39	22.13
10	2.72	3.73	8.13	-172.91	x	x
10'	2.67	3.67	-10.81	169.26	x	x
13	2.72	3.74	8.18	-172.77	x	x
12	3.64	2.66	160.26	-19.48	x	x
15	3.6	2.69	-150.29	28.82	4.36	22.26
14	2.71	3.61	27.87	-151.89	4.565	23.31
17	3.59	2.69	-149.17	29.72	4.3875	19.34
17'	2.71	3.66	32.18	-151.01	4.665	33.65

B (continue)

	N1-Pd (Å)	N3-Pd (Å)	N8-Pd (Å)	Cortho-Pd (Å)	Cl1Pd (Å)	Cl2Pd (Å)
7	2.07	x	2.09	x	2.42	2.41
8	2.12	x	2.08	x	2.44	2.42
10	1.99	x	2.26	2.01	2.43	x
10'	2.11	x	2.06	x	2.42	2.41
13	1.99	x	2.26	2.01	2.43	x
12	x	2.13	2.06	x	2.44	2.42
15	x	2.12	2.08	x	2.44	2.42
14	2.11		2.09	x	2.43	2.42
17	x	2.12	2.08	x	2.44	2.42
17'	1.99	x	2.29	2.01	2.43	x

Ligand 2



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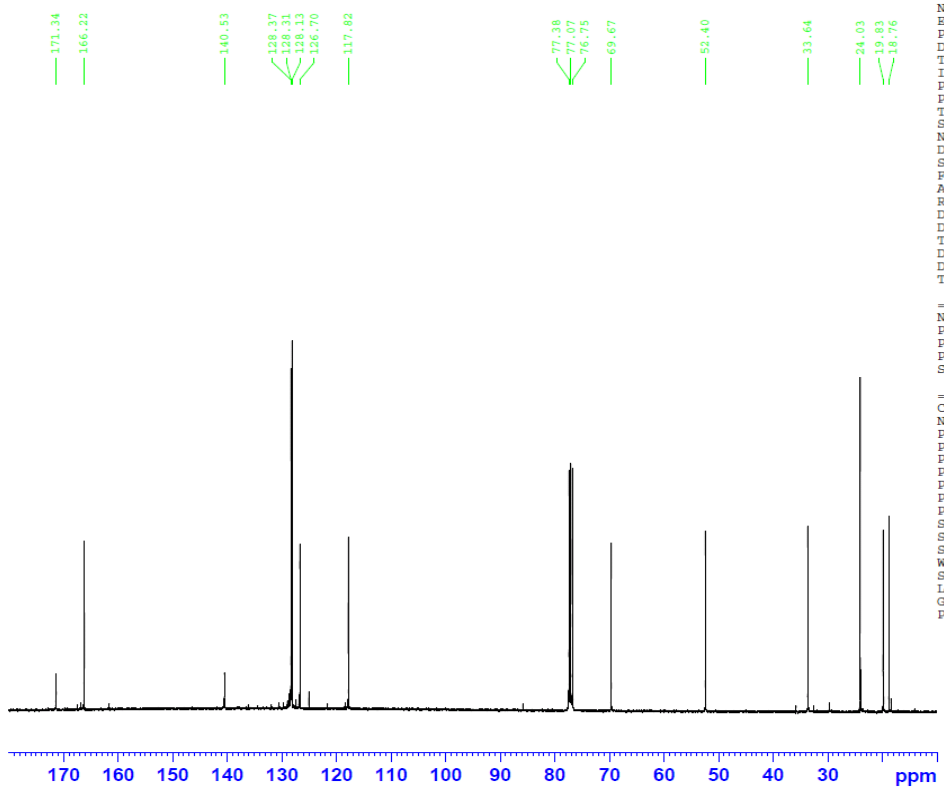
DS                    2
SWH           5580.357 Hz
FIDRES        0.340598 Hz
AQ            1.4681460 sec
RG                  7.1
DW                89.600 usec
DE                 6.50 usec
TE                300.0 K
D1            1.00000000 sec
TD0                   1

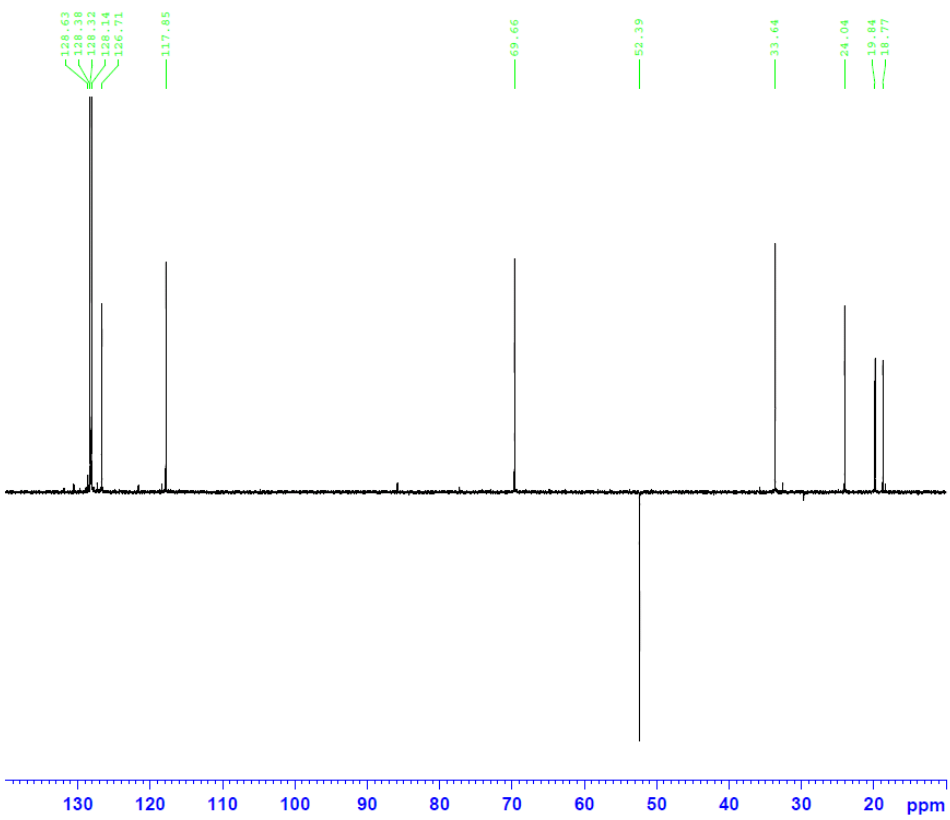
======== CHANNEL f1 ========
NUC1                 1H
P1                 7.80 usec
PL1               -3.00 dB
PL1W       30.07123375 W
SFO1       400.1326008 MHz
SI                32768
SF         400.1300016 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```




```
NAME          dp141abex01L3
EXPNO               405
PROCNO                1
Date_          20130410
Time               4.51
INSTRUM           spect
PROBHD   5 mm BBI 1H/2H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 8192
DS                    4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3632196 sec
RG              11585.2
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -6.00 dB
PL1W      150.00000000 W
SFO1       100.6228298 MHz

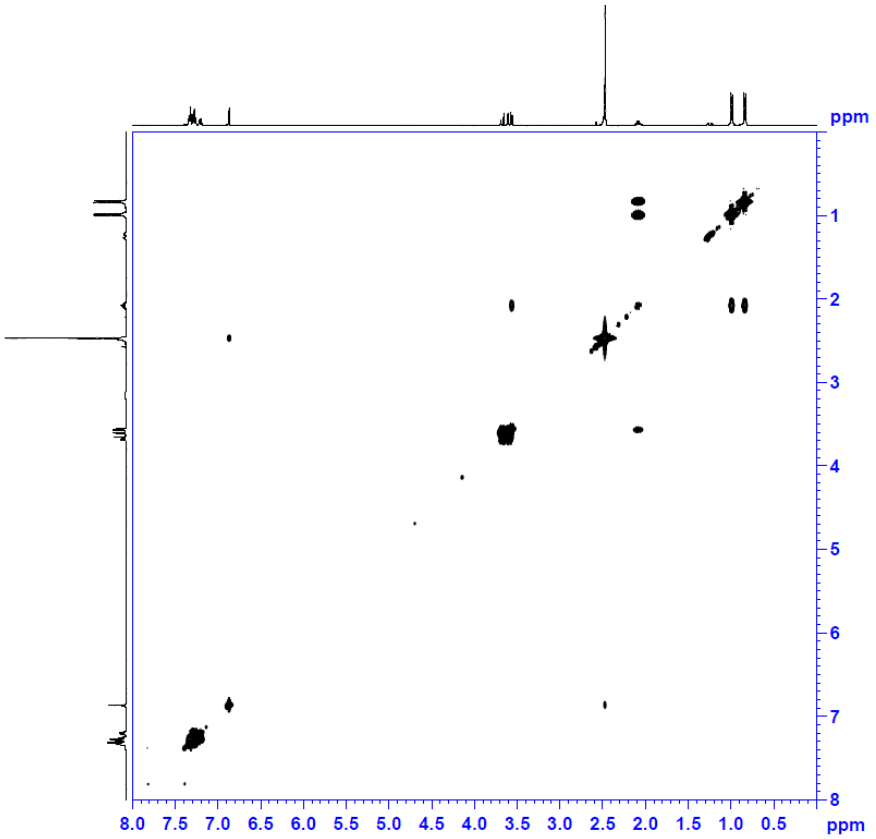
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              18.00 dB
PL13              18.00 dB
PL2W       30.07123375 W
PL12W       0.23886430 W
PL13W       0.23886430 W
SFO2       400.1316005 MHz
SI                65536
SF         100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
NAME          dp141abex01L3
EXPNO               403
PROCNO                1
Date_          20130409
Time              19.12
INSTRUM           spect
PROBHD   5 mm BBI 1H/2H
PULPROG         dept135
TD                32768
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           16025.641 Hz
FIDRES         0.489064 Hz
AQ             1.0224428 sec
RG                16384
DW               31.200 usec
DE                6.50 usec
TE               300.0 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
P2                 20.00 usec
PL1                -6.00 dB
PL1W        150.00000000 W
SFO1         100.6198119 MHz

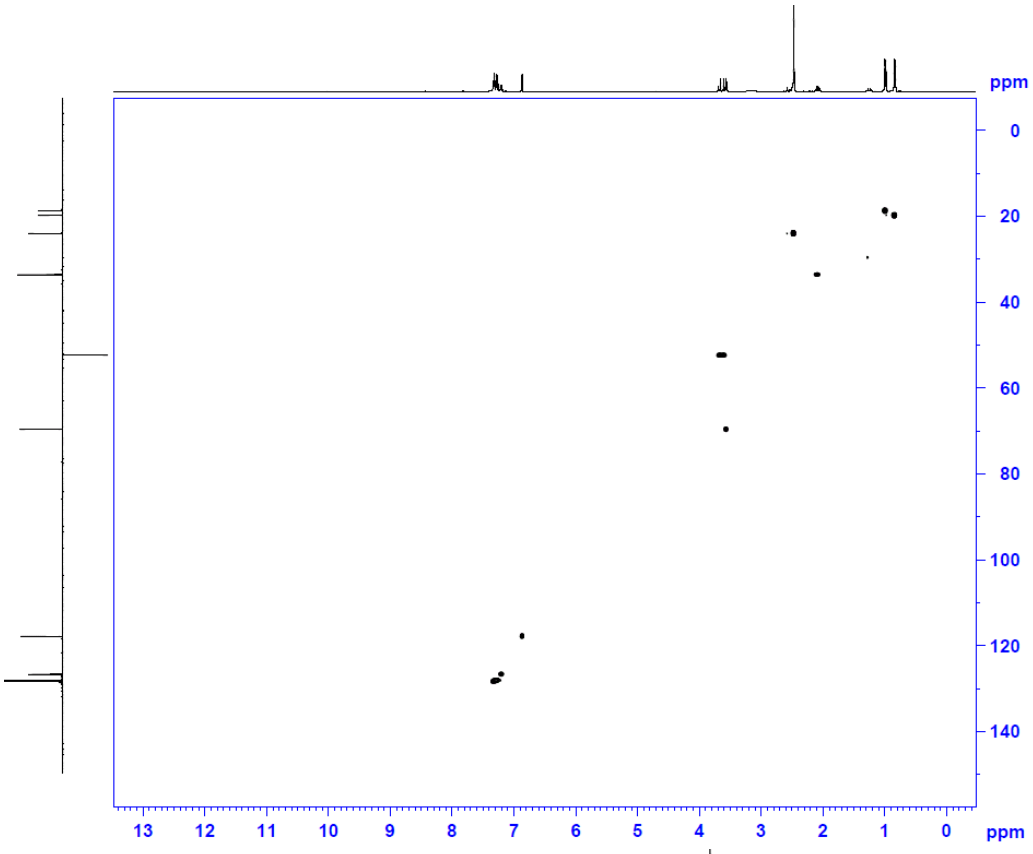
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
P3                 7.00 usec
P4                14.00 usec
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              18.00 dB
PL2W         30.07123375 W
PL12W         0.23886430 W
SFO2        400.1316005 MHz
SI                65536
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
NAME          dp141abex01L3
EXPNO               402
PROCNO                1
Date_          20130409
Time              16.29
INSTRUM           spect
PROBHD   5 mm BBI 1H/2H
PULPROG         cosygpqf
TD                 2048
SOLVENT           CDCl3
NS                    8
DS                    8
SWH            5580.357 Hz
FIDRES         2.724784 Hz
AQ             0.1836404 sec
RG                 71.8
DW                89.600 usec
DE                 6.50 usec
TE                300.0 K
D0             0.00000300 sec
D1             1.50000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00017920 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                 7.00 usec
P1                 7.00 usec
PL1               -3.00 dB
PL1W         30.07123375 W
SFO1         400.1326008 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1              10.00 %
P16             1000.00 usec
ND0                   1
TD                  256
SFO1          400.1326 MHz
FIDRES        21.798281 Hz
SW               13.946 ppm
FnMODE              QF
SI                  2048
SF          400.1300000 MHz
WDW                SINE
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40
SI                 1024
MC2                 QF
SF          400.1300000 MHz
WDW                SINE
SSB                   0
LB                 0.00 Hz
GB                    0
```

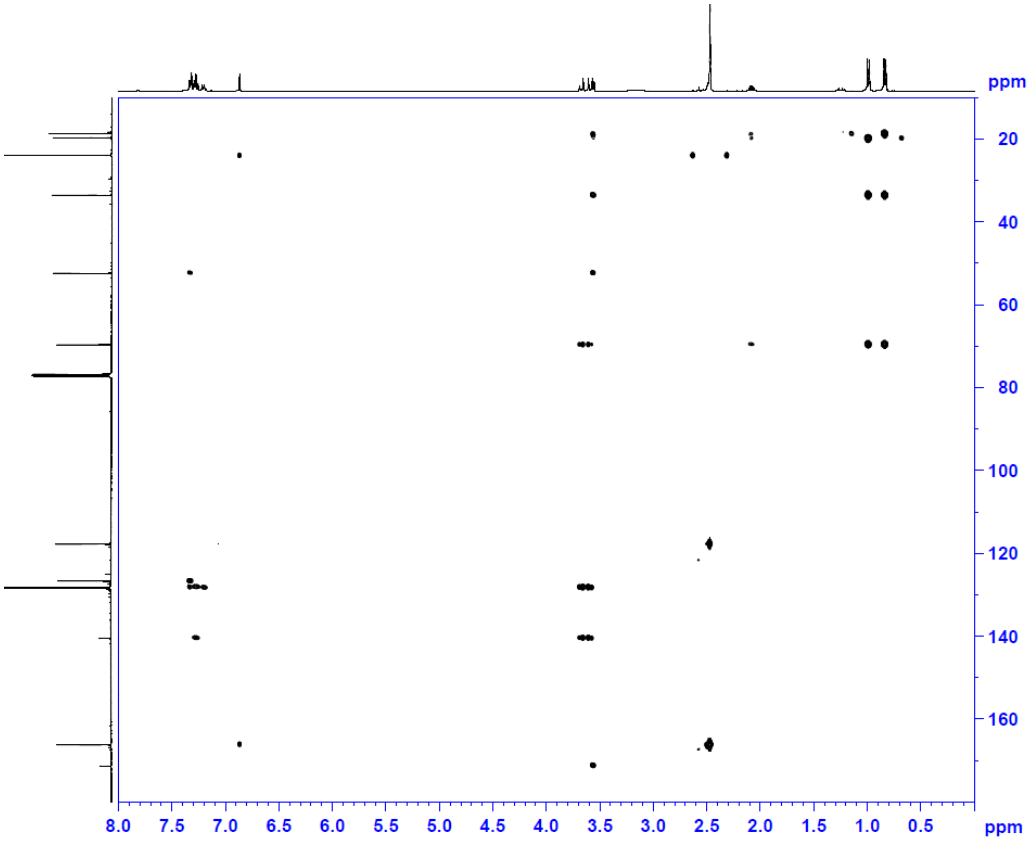



```
NAME          dp141abex01L3
EXPNO                  404
PROCNO                   1
Date_             20130409
Time                 19.13
INSTRUM              spect
PROBHD    5 mm BBI 1H/2H
PULPROG          hsqcetgp
TD                    1024
SOLVENT              CDCl3
NS                      16
DS                      16
SWH              5580.357 Hz
FIDRES           5.449567 Hz
AQ               0.0918900 sec
RG                  9195.2
DW                 89.600 usec
DE                  6.50 usec
TE                 300.0 K
CNST2           145.0000000
D0               0.00000300 sec
D1               1.50000000 sec
D4               0.00172414 sec
D11              0.03000000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00003010 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                    7.00 usec
P2                   14.00 usec
P28                1000.00 usec
PL1                  -3.00 dB
PL1W           30.07123375 W
SFO1          400.1326008 MHz

======== CHANNEL f2 ========
CPDPRG2              garp
NUC2                   13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                80.00 usec
PL2                  -6.00 dB
PL12                 12.00 dB
PL2W          150.00000000 W
PL12W           2.37733984 W
SFO2          100.6203150 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPZ1                 80.00 %
GPZ2                 20.10 %
P16                1000.00 usec
ND0                     2
TD                    256
SFO1          100.6203 MHz
FIDRES         64.852936 Hz
SW               165.000 ppm
FnMODE      Echo-Antiecho
SI                   2048
SF            400.1300000 MHz
WDW                  QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2         echo-antiecho
SF            100.6127690 MHz
WDW                  QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

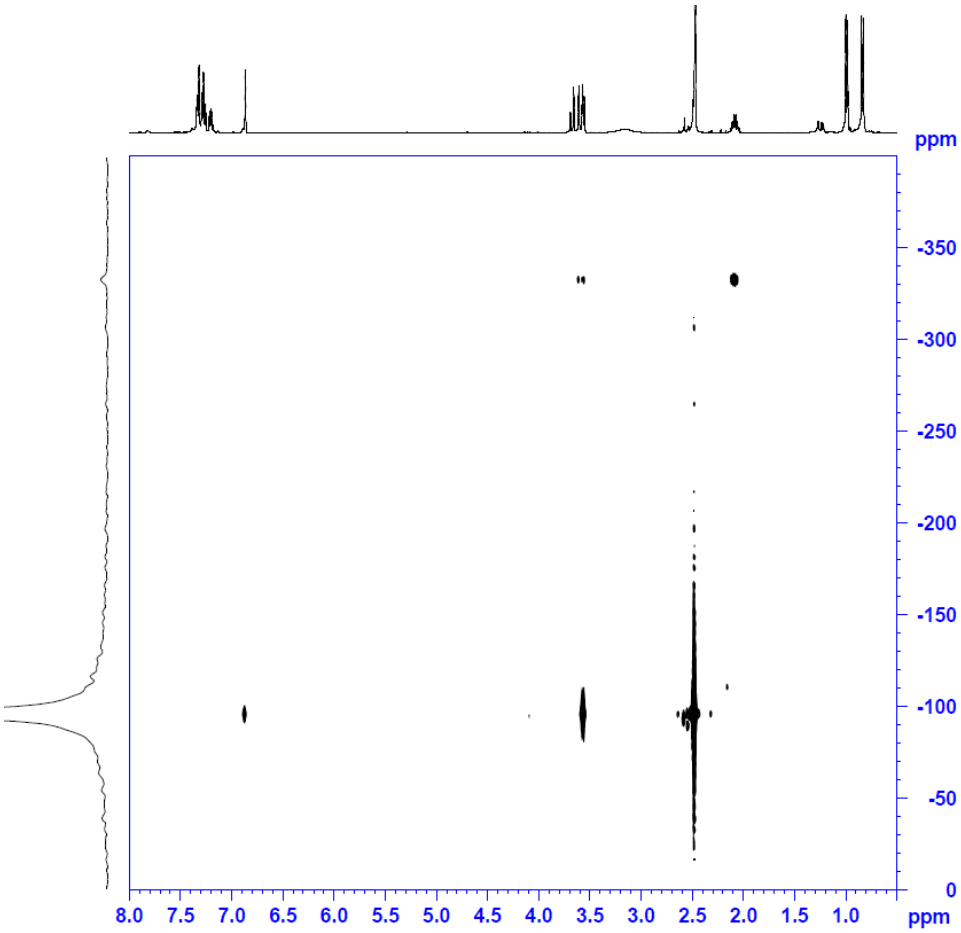



```
NAME          dp141abex01L3
EXPNO                  406
PROCNO                   1
Date_             20130410
Time                  4.52
INSTRUM              spect
PROBHD    5 mm BBI 1H/2H
PULPROG     hmbcgplpndqf
TD                    2048
SOLVENT              CDCl3
NS                      32
DS                      16
SWH              4006.410 Hz
FIDRES           1.956255 Hz
AQ               0.2557652 sec
RG                  11585.2
DW                 124.800 usec
DE                  6.50 usec
TE                 300.0 K
CNST2           145.0000000
CNST13           10.0000000
D0               0.00000300 sec
D1               1.50000000 sec
D2               0.00344828 sec
D6               0.05000000 sec
D16              0.00020000 sec
IN0              0.00002070 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                    7.00 usec
P2                   14.00 usec
PL1                  -3.00 dB
PL1W           30.07123375 W
SFO1          400.1318006 MHz

======== CHANNEL f2 ========
NUC2                   13C
P3                   10.00 usec
PL2                  -6.00 dB
PL2W          150.00000000 W
SFO2          100.6243395 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPNAM3             SINE.100
GPZ1                 50.00 %
GPZ2                 30.00 %
GPZ3                 40.10 %
P16                1000.00 usec
ND0                     2
TD                    256
SFO1          100.6243 MHz
FIDRES         94.335320 Hz
SW               240.000 ppm
FnMODE                QF
SI                   2048
SF            400.1300000 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2                   QF
SF            100.6127690 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

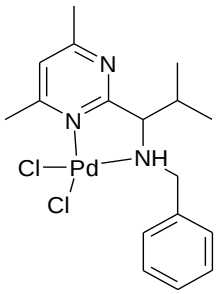


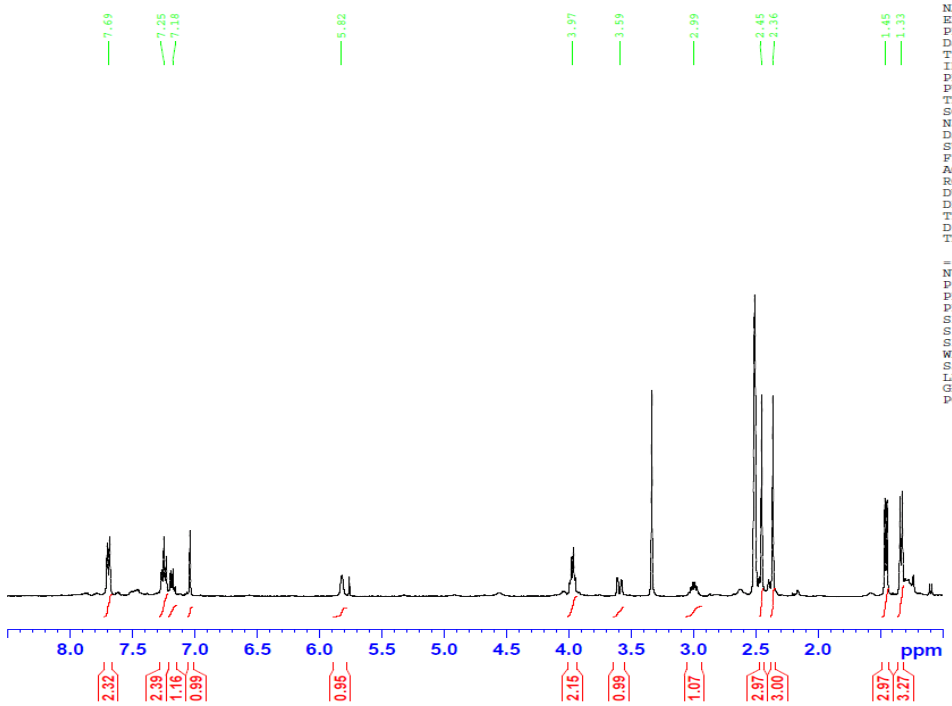

```
NAME          dp141abex01L3
EXPNO                  411
PROCNO                   1
Date_             20130406
Time                 8.48
INSTRUM             spect
PROBHD   5 mm BBI 1H/2H
PULPROG       hmbcgpndqf
TD                   3072
SOLVENT             CDCl3
NS                    256
DS                     16
SWH             4006.410 Hz
FIDRES          1.304170 Hz
AQ              0.3835604 sec
RG                  16384
DW                124.800 usec
DE                  6.50 usec
TE                 300.0 K
CNST13          6.0000000
D0              0.00000300 sec
D1              1.50000000 sec
D6              0.08333334 sec
D16             0.00020000 sec
IN0             0.00002055 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.00 usec
P2                  14.00 usec
PL1                 -3.00 dB
PL1W          30.07123375 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
NUC2                  15N
P3                  17.00 usec
PL2                 -6.00 dB
PL2W         150.00000000 W
SFO2          40.5529300 MHz

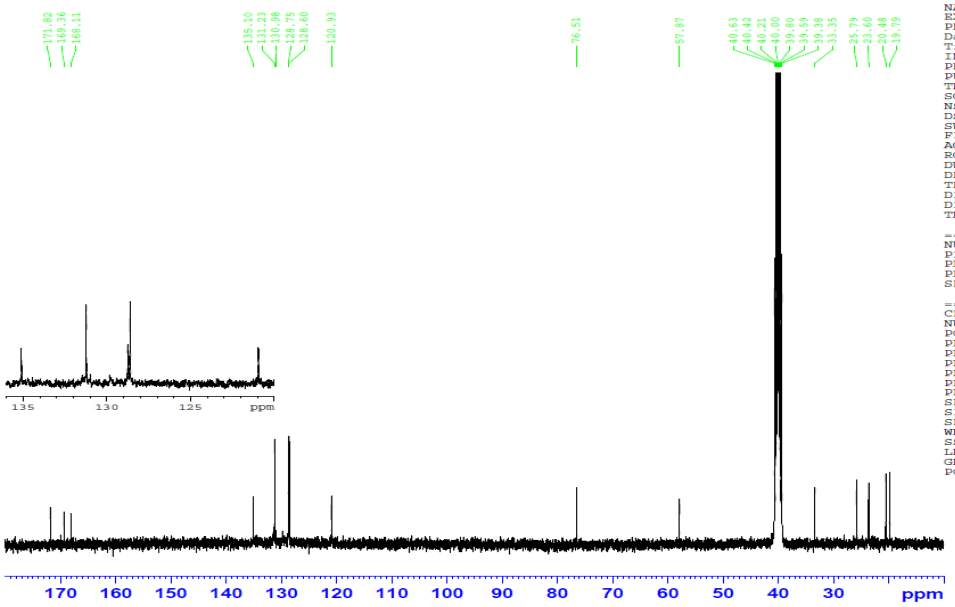
====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1                70.00 %
GPZ2                30.00 %
GPZ3                50.10 %
P16               1000.00 usec
ND0                    2
TD                   128
SFO1            40.55293 MHz
FIDRES        190.091858 Hz
SW               600.000 ppm
FnMODE                QF
SI                  4096
SF           400.1300000 MHz
WDW                QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
PC                  1.40
SI                   512
MC2                   QF
SF           40.5601462 MHz
WDW                QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
```

Complex 8	




```
NAME                dp46dp76
EXPNO                    401
PROCNO                     1
Date_               20131121
Time                   11.02
INSTRUM                spect
PROBHD     5 mm BBI 1H/2H
PULPROG                zg30
TD                    16384
SOLVENT                DMSO
NS                        16
DS                         2
SWH                5580.357 Hz
FIDRES             0.340598 Hz
AQ                 1.4681460 sec
RG                       6.3
DW                    89.600 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                        1

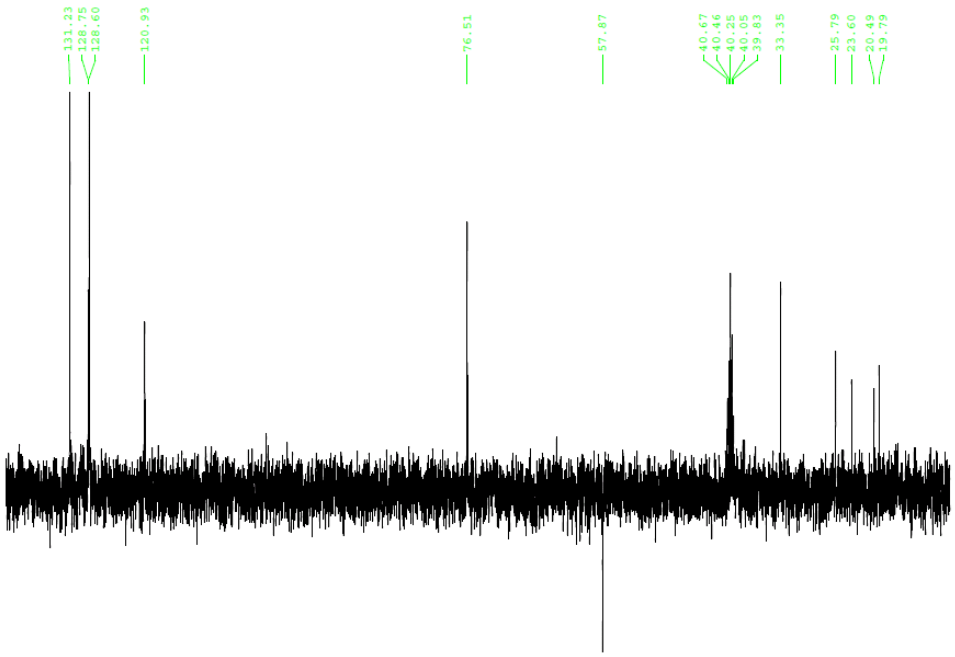
======== CHANNEL f1 ========
NUC1                      1H
P1                     7.80 usec
PL1                   -3.00 dB
PL1W          30.07123375 W
SFO1          400.1326008 MHz
SI                     32768
SF            400.1300000 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```




```
NAME                dp46dp76
EXPNO                    406
PROCNO                     1
Date_               20131121
Time                   16.31
INSTRUM                spect
PROBHD     5 mm BBI 1H/2H
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      2560
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3632196 sec
RG                    4597.6
DW                    20.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                    10.00 usec
PL1                   -6.00 dB
PL1W         150.00000000 W
SFO1          100.6228298 MHz

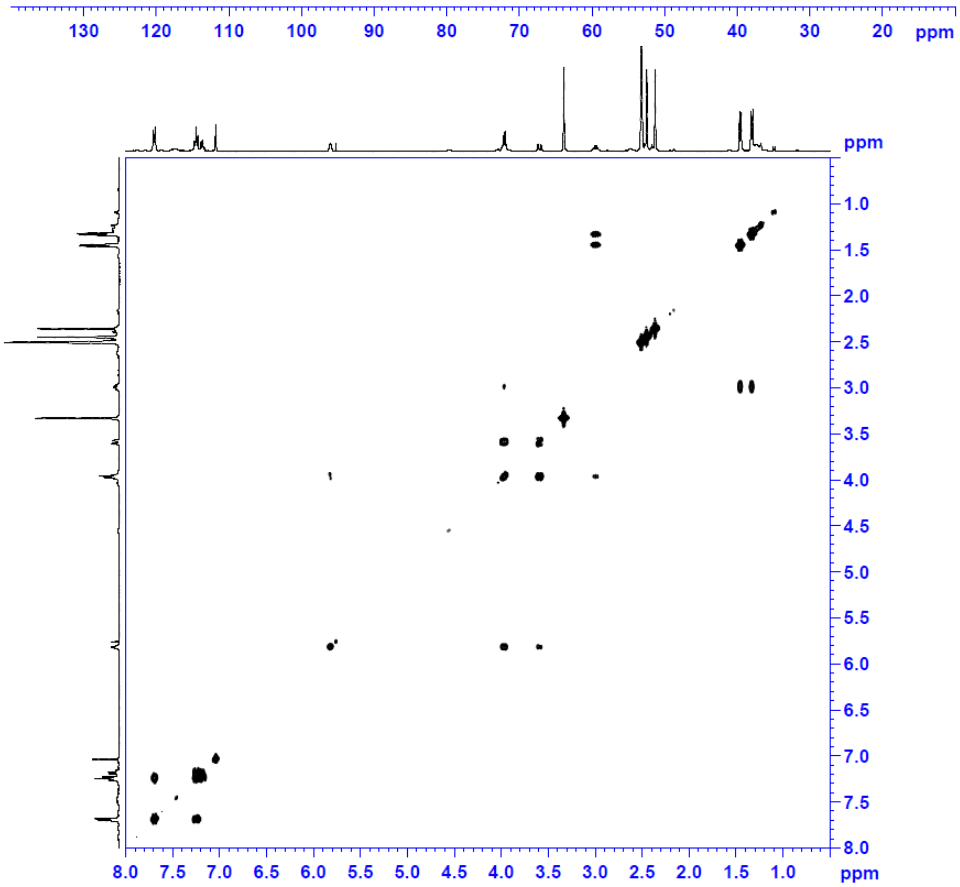
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                   -3.00 dB
PL12                  18.00 dB
PL13                  18.00 dB
PL2W          30.07123375 W
PL12W          0.23886430 W
PL13W          0.23886430 W
SFO2          400.1316005 MHz
SI                     65536
SF            100.6127690 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      1.40
```




```
NAME            dp46dp76
EXPNO                403
PROCNO                 1
Date_           20131121
Time               11.31
INSTRUM            spect
PROBHD   5 mm BBI 1H/2H
PULPROG          dept135
TD                 32768
SOLVENT             DMSO
NS                   256
DS                     4
SWH            16025.641 Hz
FIDRES         0.489064 Hz
AQ             1.0224428 sec
RG                 16384
DW                31.200 usec
DE                 6.50 usec
TE                300.0 K
CNST2         145.0000000
D1              2.00000000 sec
D2              0.00344828 sec
D12             0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
P2                 20.00 usec
PL1                -6.00 dB
PL1W        150.00000000 W
SFO1         100.6198119 MHz

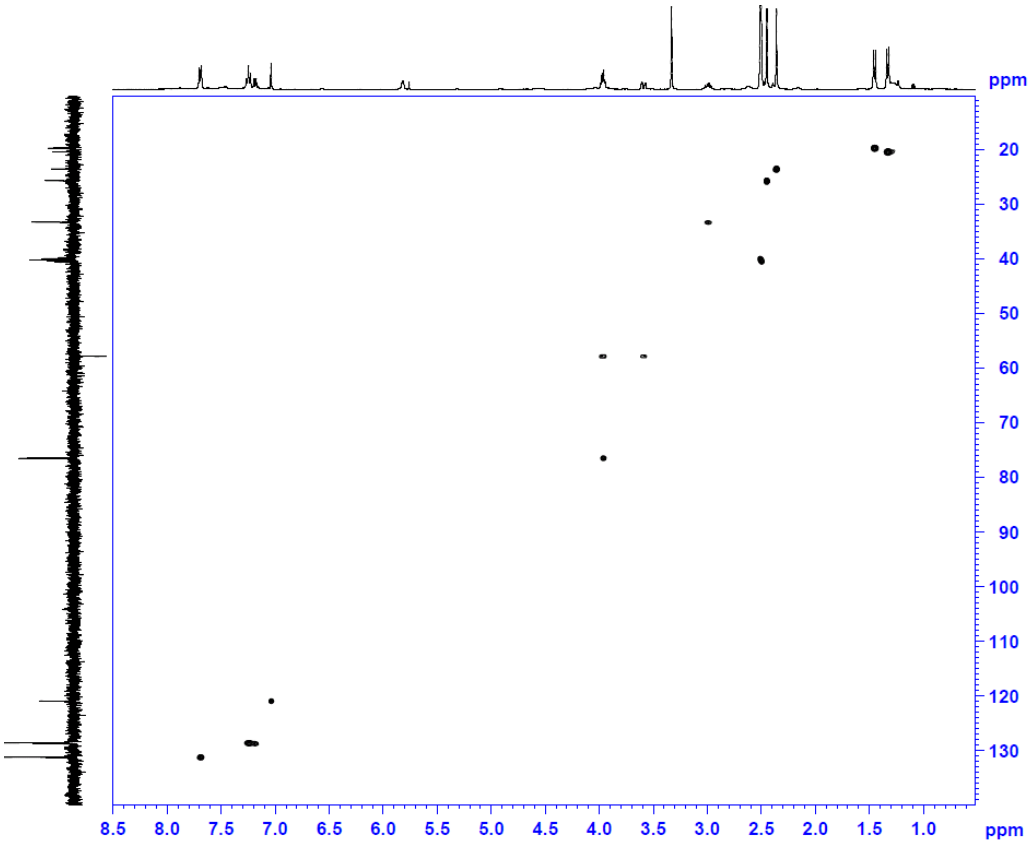
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
P3                 7.00 usec
P4                14.00 usec
PCPD2             80.00 usec
PL2                -3.00 dB
PL12               18.00 dB
PL2W        30.07123375 W
PL12W        0.23886430 W
SFO2        400.1316005 MHz
SI                 65536
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
NAME            dp46dp76
EXPNO                402
PROCNO                 1
Date_           20131121
Time               11.09
INSTRUM            spect
PROBHD   5 mm BBI 1H/2H
PULPROG          cosygpqf
TD                  2048
SOLVENT             DMSO
NS                     2
DS                     8
SWH             5580.357 Hz
FIDRES         2.724784 Hz
AQ             0.1836404 sec
RG                   256
DW                89.600 usec
DE                 6.50 usec
TE                300.0 K
D0             0.00000300 sec
D1             1.50000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00017920 sec

======== CHANNEL f1 ========
NUC1                 1H
P0                 7.00 usec
P1                 7.00 usec
PL1                -3.00 dB
PL1W        30.07123375 W
SFO1        400.1326008 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPZ1               10.00 %
P16              1000.00 usec
ND0                    1
TD                   256
SFO1            400.1326 MHz
FIDRES         21.798281 Hz
SW                13.946 ppm
FnMODE                QF
SI                  2048
SF          400.1300000 MHz
WDW                 SINE
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.40
SI                  1024
MC2                   QF
SF          400.1300000 MHz
WDW                 SINE
SSB                    0
LB                 0.00 Hz
GB                     0
```

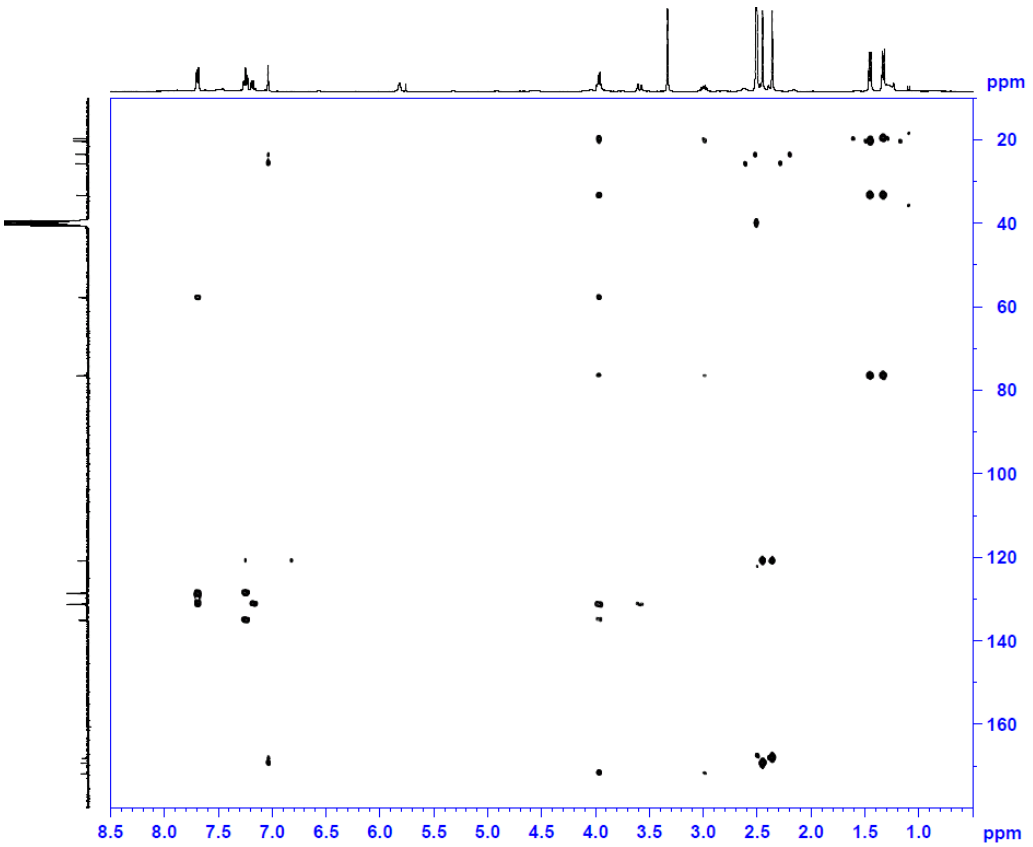



```
NAME              dp46dp76
EXPNO                  404
PROCNO                   1
Date_             20131121
Time                 11.38
INSTRUM              spect
PROBHD   5 mm BBI 1H/2H
PULPROG          hsqcetgp
TD                    1024
SOLVENT               DMSO
NS                       8
DS                      16
SWH               4807.692 Hz
FIDRES            4.695012 Hz
AQ                0.1066500 sec
RG                  18390.4
DW                  104.000 usec
DE                     6.50 usec
TE                   300.0 K
CNST2           145.0000000
D0                0.00000300 sec
D1                1.50000000 sec
D4                0.00172414 sec
D11               0.03000000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00003000 sec
EGOPTNS

======== CHANNEL f1 =========
NUC1                     1H
P1                     7.00 usec
P2                    14.00 usec
P28                 1000.00 usec
PL1                   -3.00 dB
PL1W           30.07123375 W
SFO1           400.1320007 MHz

======== CHANNEL f2 =========
CPDPRG2               garp
NUC2                    13C
P3                    10.00 usec
P4                    20.00 usec
PCPD2                 80.00 usec
PL2                   -6.00 dB
PL12                  12.00 dB
PL2W          150.00000000 W
PL12W          2.37733984 W
SFO2           100.6202727 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec
ND0                      2
TD                     256
SFO1           100.6203 MHz
FIDRES           65.104164 Hz
SW                 165.639 ppm
FnMODE     Echo-Antiecho
SI                    2048
SF             400.1300000 MHz
WDW                  QSINE
SSB                      2
LB                    0.00 Hz
GB                       0
PC                    1.40
SI                    1024
MC2          echo-antiecho
SF             100.6127625 MHz
WDW                  QSINE
SSB                      2
LB                    0.00 Hz
GB                       0
```

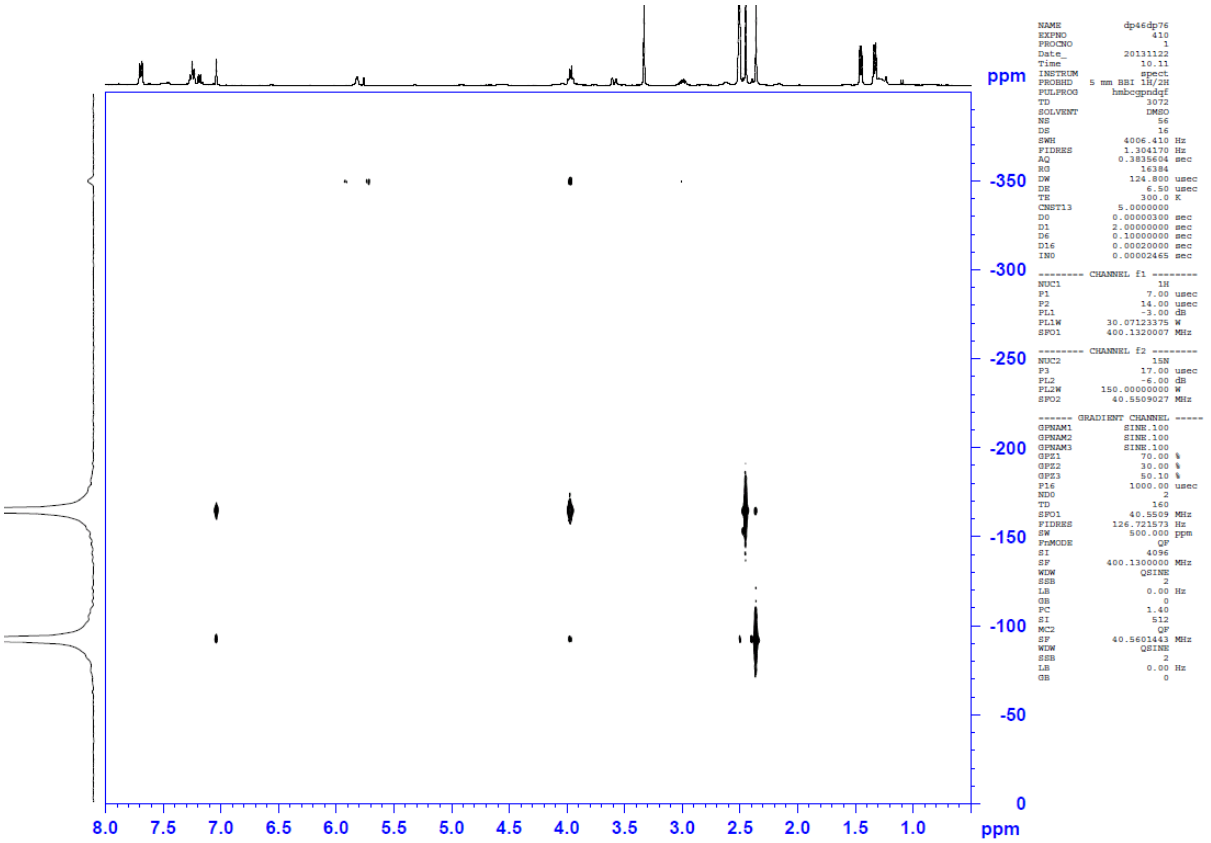



```
NAME              dp46dp76
EXPNO                  405
PROCNO                   1
Date_             20131121
Time                 12.34
INSTRUM              spect
PROBHD   5 mm BBI 1H/2H
PULPROG     hmbcgplpndqf
TD                    2048
SOLVENT               DMSO
NS                      12
DS                      16
SWH               4807.692 Hz
FIDRES            2.347506 Hz
AQ                0.2131460 sec
RG                   16384
DW                  104.000 usec
DE                     6.50 usec
TE                   300.0 K
CNST2           145.0000000
CNST13           10.0000000
D0                0.00000300 sec
D1                1.50000000 sec
D2                0.00344828 sec
D6                0.05000000 sec
D16               0.00020000 sec
IN0               0.00002070 sec

======== CHANNEL f1 =========
NUC1                     1H
P1                     7.00 usec
P2                    14.00 usec
PL1                   -3.00 dB
PL1W           30.07123375 W
SFO1           400.1320007 MHz

======== CHANNEL f2 =========
NUC2                    13C
P3                    10.00 usec
PL2                   -6.00 dB
PL2W          150.00000000 W
SFO2           100.6243395 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPNAM3             SINE.100
GPZ1                  50.00 %
GPZ2                  30.00 %
GPZ3                  40.10 %
P16                 1000.00 usec
ND0                      2
TD                     256
SFO1           100.6243 MHz
FIDRES           94.335320 Hz
SW                 240.000 ppm
FnMODE                  QF
SI                    2048
SF             400.1300000 MHz
WDW                  SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
SI                    1024
MC2                     QF
SF             100.6127690 MHz
WDW                  SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```



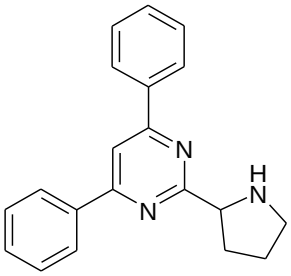

```
NAME              dp46dp76
EXPNO                  410
PROCNO                   1
Date_             20131122
Time                 10.11
INSTRUM              spect
PROBHD    5 mm BBI 1H/2H
PULPROG       hmbcgpndqf
TD                    3072
SOLVENT               DMSO
NS                      56
DS                      16
SWH               4006.410 Hz
FIDRES            1.304170 Hz
AQ                0.3835604 sec
RG                    16384
DW                  124.800 usec
DE                    6.50 usec
TE                  300.0 K
CNST13            5.0000000
D0                0.00000300 sec
D1                2.00000000 sec
D6                0.10000000 sec
D16               0.00020000 sec
IN0               0.00002465 sec

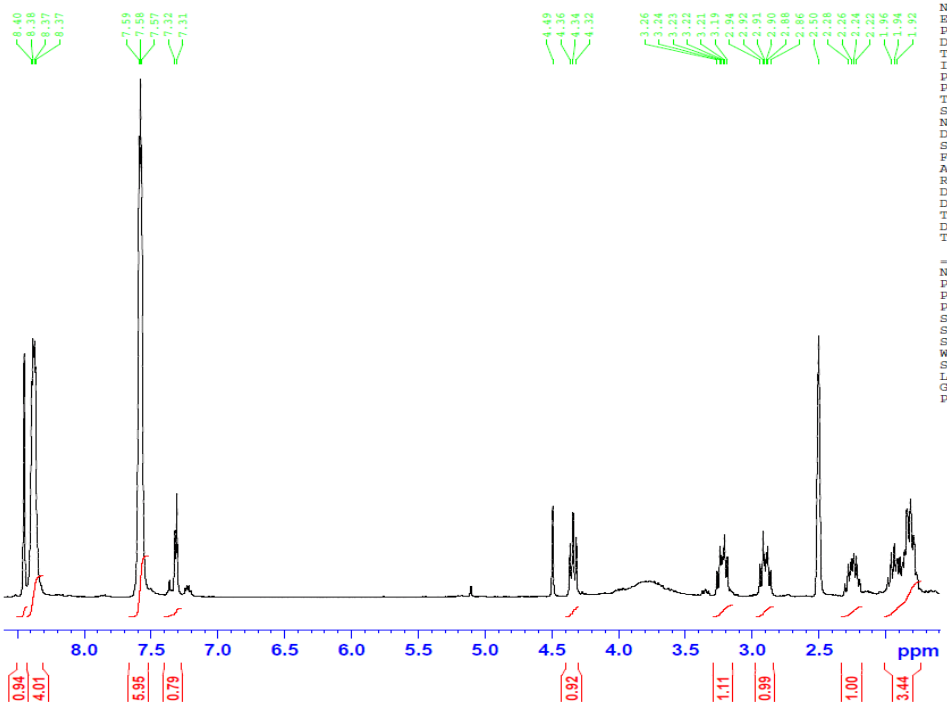
======== CHANNEL f1 ========
NUC1                    1H
P1                    7.00 usec
P2                   14.00 usec
PL1                  -3.00 dB
PL1W          30.07123375 W
SFO1          400.1320007 MHz

======== CHANNEL f2 ========
NUC2                   15N
P3                   17.00 usec
PL2                  -6.00 dB
PL2W         150.00000000 W
SFO2           40.5509027 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPNAM3             SINE.100
GPZ1                 70.00 %
GPZ2                 30.00 %
GPZ3                 50.10 %
P16                1000.00 usec
ND0                     2
TD                    160
SFO1           40.5509 MHz
FIDRES        126.721573 Hz
SW                500.000 ppm
FnMODE                QF
SI                    4096
SF            400.1300000 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                    512
MC2                   QF
SF             40.5601443 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

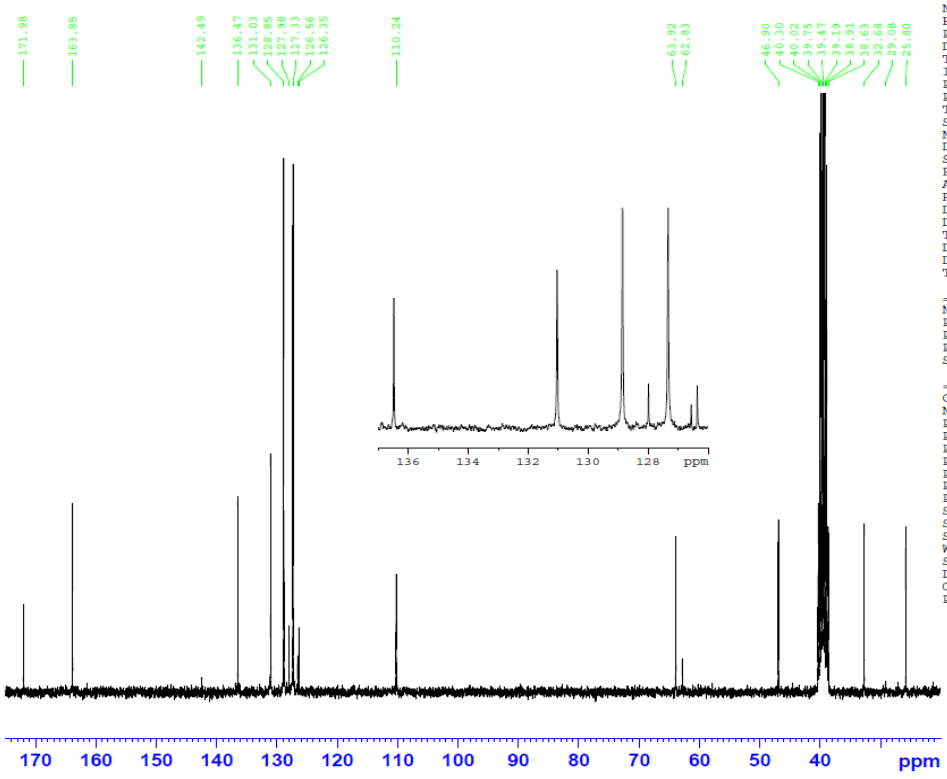
Ligand 3






```
NAME            dp21dp141
EXPNO                  10
PROCNO                  1
Date_            20130522
Time                 1.46
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH             4194.631 Hz
FIDRES          0.256020 Hz
AQ              1.9530228 sec
RG                   181
DW               119.200 usec
DE                 6.50 usec
TE                294.3 K
D1              1.00000000 sec
TD0                    1

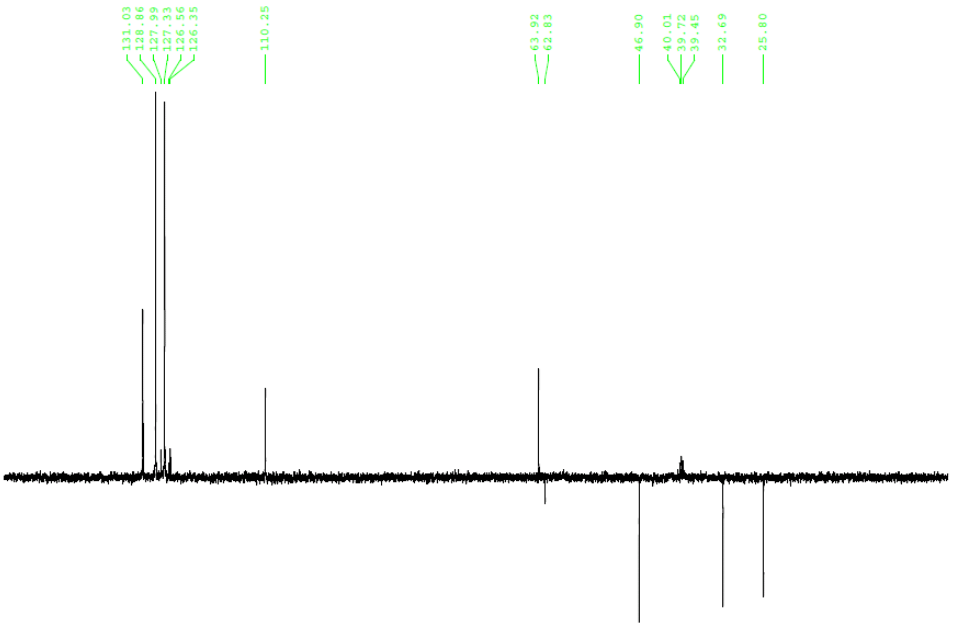
======== CHANNEL f1 ========
NUC1                  1H
P1                 6.70 usec
PL1                0.00 dB
PL1W        15.07131863 W
SFO1        300.1319508 MHz
SI                 32768
SF          300.1300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```




```
NAME            dp21dp141
EXPNO                  14
PROCNO                  1
Date_            20130522
Time                 6.47
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  4000
DS                     4
SWH            17985.611 Hz
FIDRES          0.548877 Hz
AQ              0.9110004 sec
RG                3649.1
DW               27.800 usec
DE                10.00 usec
TE                294.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.20 usec
PL1               -6.00 dB
PL1W       150.00000000 W
SFO1        75.4760505 MHz

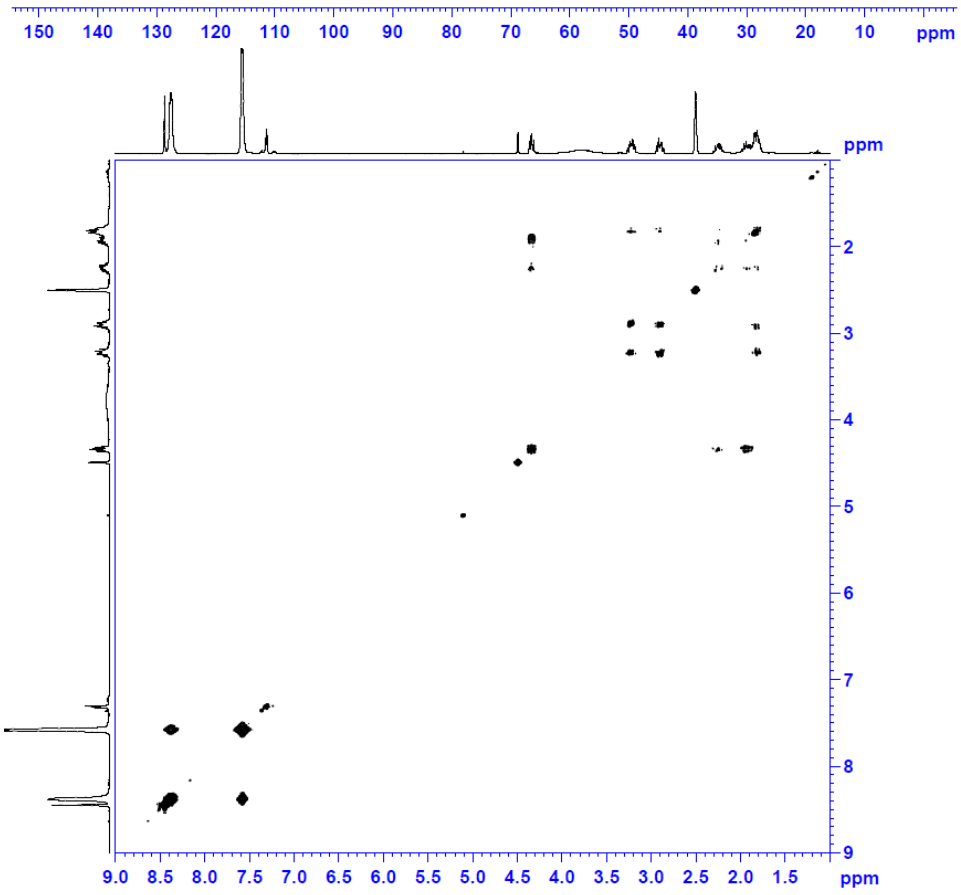
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              21.54 dB
PL13              21.54 dB
PL2W        15.07131863 W
PL12W        0.10571854 W
PL13W        0.10571854 W
SFO2        300.1312005 MHz
SI                 32768
SF          75.4677867 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```




```
NAME            dp21dp141
EXPNO                  12
PROCNO                  1
Date_            20130522
Time                2.59
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG          dept135
TD                 32768
SOLVENT             DMSO
NS                  1000
DS                     2
SWH           12077.295 Hz
FIDRES         0.368570 Hz
AQ             1.3566452 sec
RG                 16384
DW                41.400 usec
DE                10.00 usec
TE                294.4 K
CNST2         145.0000000
D1              2.00000000 sec
D2              0.00344828 sec
D12             0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.20 usec
P2                  16.40 usec
PL1                 -6.00 dB
PL1W        150.00000000 W
SFO1          75.4734091 MHz

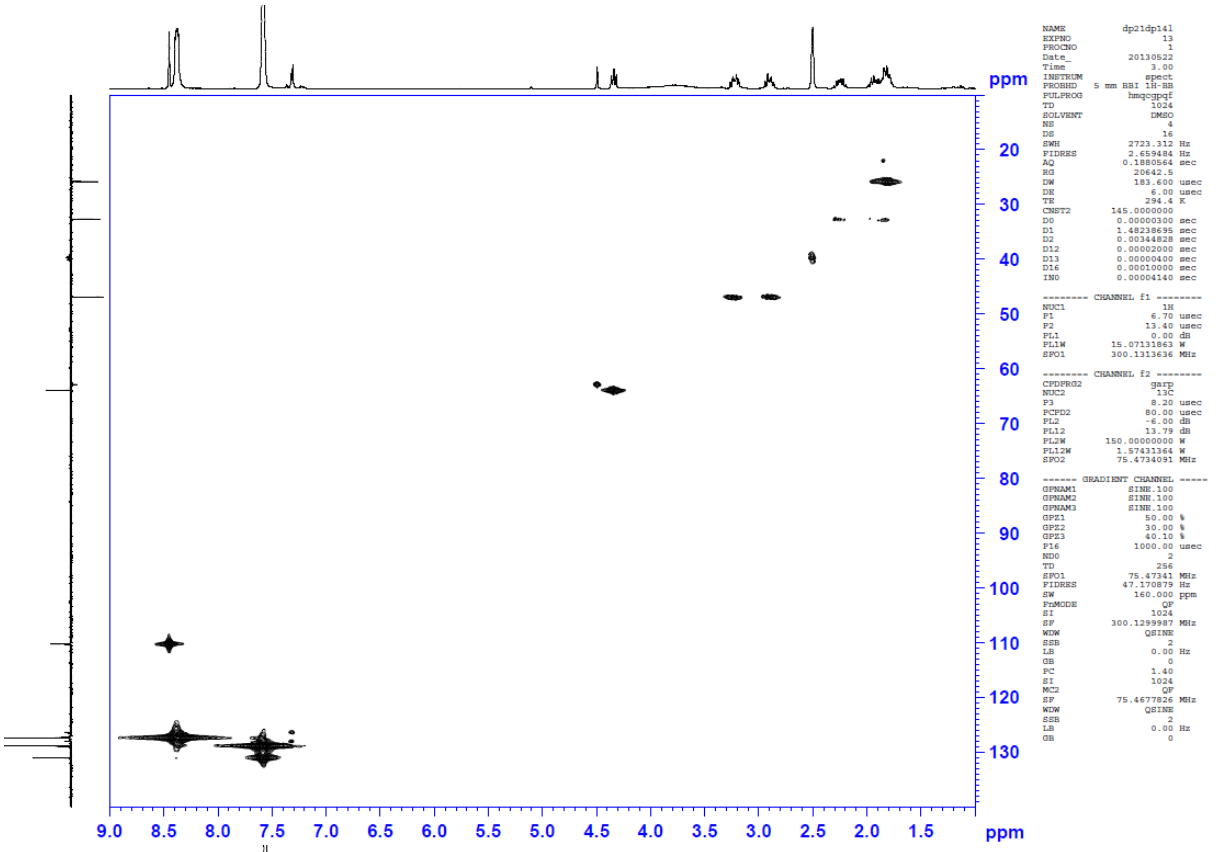
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
P3                   6.70 usec
P4                  13.40 usec
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                21.54 dB
PL2W         15.07131863 W
PL12W         0.10571854 W
SFO2         300.1312005 MHz
SI                  32768
SF            75.4677867 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
NAME            dp21dp141
EXPNO                  11
PROCNO                  1
Date_            20130522
Time                1.47
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG          cosygpqf
TD                  1024
SOLVENT             DMSO
NS                     2
DS                     8
SWH            2723.312 Hz
FIDRES         2.659484 Hz
AQ             0.1880564 sec
RG                   128
DW                183.600 usec
DE                 10.00 usec
TE                 294.3 K
D0              0.00000300 sec
D1              1.48238695 sec
D13             0.00000400 sec
D16             0.00010000 sec
IN0             0.00036720 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                   6.70 usec
P1                   6.70 usec
PL1                  0.00 dB
PL1W         15.07131863 W
SFO1         300.1313636 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPZ1                10.00 %
P16               1000.00 usec
ND0                    1
TD                   256
SFO1           300.1314 MHz
FIDRES         10.637936 Hz
SW                 9.074 ppm
FnMODE                QF
SI                  2048
SF           300.1300000 MHz
WDW                 SINE
SSB                    1
LB                  0.00 Hz
GB                     0
PC                  1.40
SI                  1024
MC2                   QF
SF           300.1300000 MHz
WDW                 SINE
SSB                    1
LB                  0.00 Hz
GB                     0
```

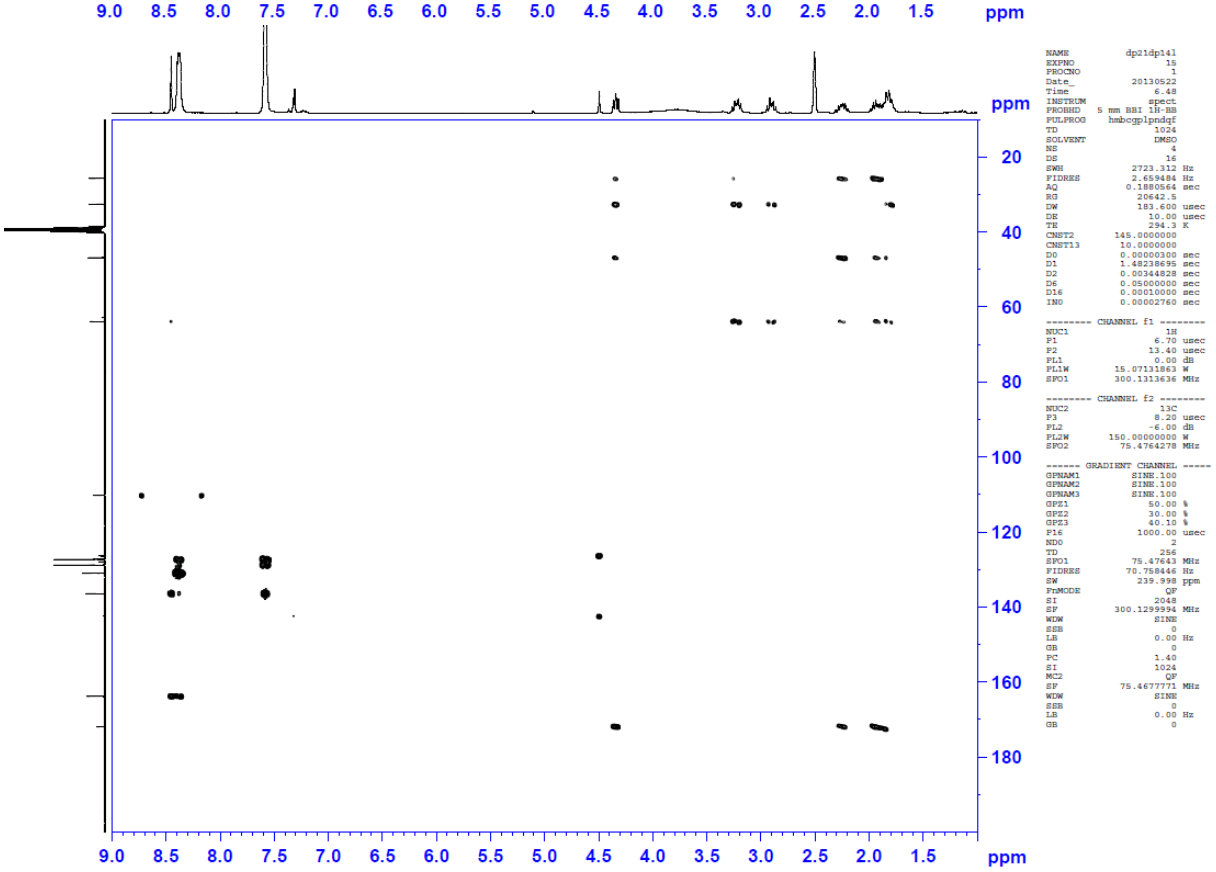



```
NAME                dp21dp141
EXPNO                      13
PROCNO                      1
Date_                20130522
Time                     3.00
INSTRUM                 spect
PROBHD   5 mm BBI 1H-BB
PULPROG             hmqcgpqf
TD                       1024
SOLVENT                  DMSO
NS                          4
DS                         16
SWH                2723.312 Hz
FIDRES             2.659484 Hz
AQ                 0.1880564 sec
RG                   20642.5
DW                   183.600 usec
DE                     6.00 usec
TE                    294.4 K
CNST2              145.0000000
D0                 0.00000300 sec
D1                 1.48238695 sec
D2                 0.00344828 sec
D12                0.00002000 sec
D13                0.00000400 sec
D16                0.00010000 sec
IN0                0.00004140 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       6.70 usec
P2                      13.40 usec
PL1                      0.00 dB
PL1W               15.07131863 W
SFO1              300.1313636 MHz

======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                      13C
P3                       8.20 usec
PCPD2                   80.00 usec
PL2                     -6.00 dB
PL12                    13.79 dB
PL2W              150.00000000 W
PL12W               1.57431364 W
SFO2               75.4734091 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPNAM3                SINE.100
GPZ1                     50.00 %
GPZ2                     30.00 %
GPZ3                     40.10 %
P16                    1000.00 usec
ND0                           2
TD                          256
SFO1               75.47341 MHz
FIDRES             47.170879 Hz
SW                   160.000 ppm
FnMODE                     QF
SI                       1024
SF                300.1299987 MHz
WDW                     QSINE
SSB                           2
LB                       0.00 Hz
GB                            0
PC                       1.40
SI                       1024
MC2                        QF
SF                75.4677826 MHz
WDW                     QSINE
SSB                           2
LB                       0.00 Hz
GB                            0
```

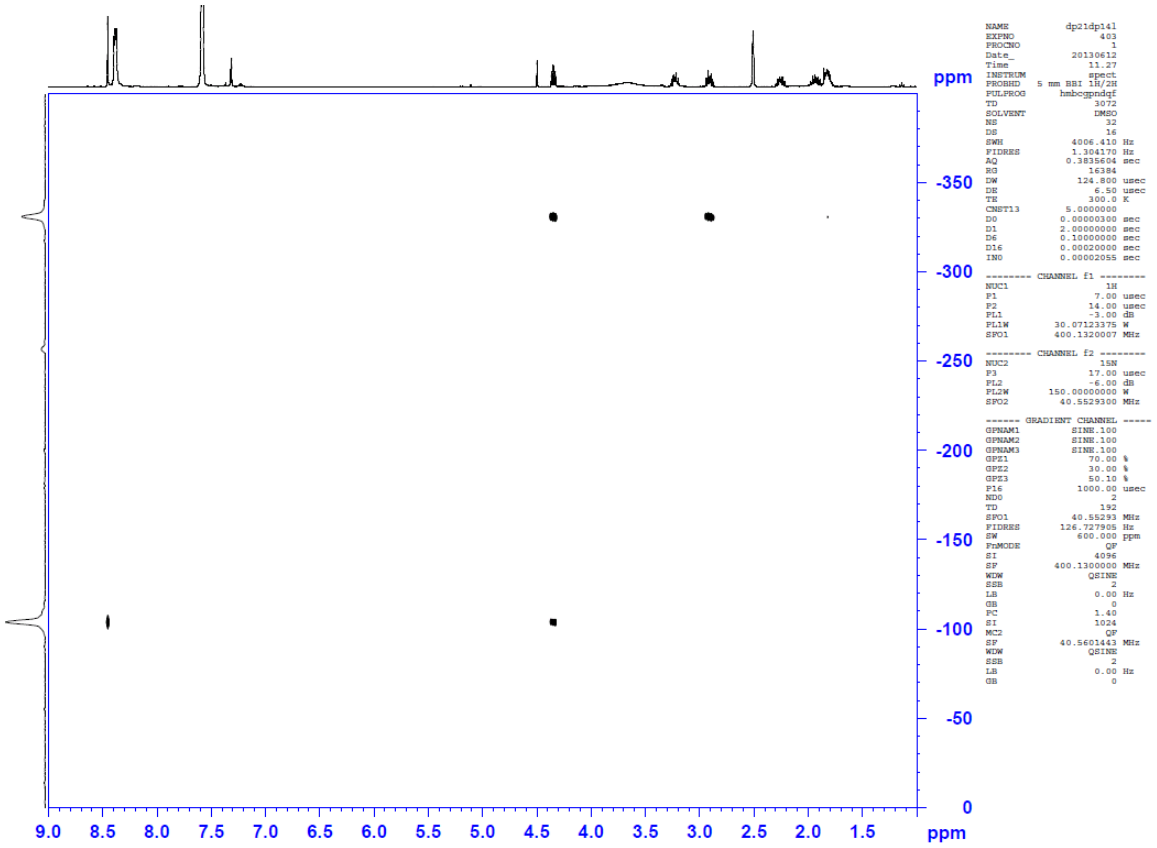



```
NAME                dp21dp141
EXPNO                      15
PROCNO                      1
Date_                20130522
Time                     6.48
INSTRUM                 spect
PROBHD   5 mm BBI 1H-BB
PULPROG          hmbcgplpndqf
TD                       1024
SOLVENT                  DMSO
NS                          4
DS                         16
SWH                2723.312 Hz
FIDRES             2.659484 Hz
AQ                 0.1880564 sec
RG                   20642.5
DW                   183.600 usec
DE                     10.00 usec
TE                    294.3 K
CNST2              145.0000000
CNST13              10.0000000
D0                 0.00000300 sec
D1                 1.48238695 sec
D2                 0.00344828 sec
D6                 0.05000000 sec
D16                0.00010000 sec
IN0                0.00002760 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       6.70 usec
P2                      13.40 usec
PL1                      0.00 dB
PL1W               15.07131863 W
SFO1              300.1313636 MHz

======== CHANNEL f2 ========
NUC2                      13C
P3                       8.20 usec
PL2                     -6.00 dB
PL2W              150.00000000 W
SFO2               75.4764278 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPNAM3                SINE.100
GPZ1                     50.00 %
GPZ2                     30.00 %
GPZ3                     40.10 %
P16                    1000.00 usec
ND0                           2
TD                          256
SFO1               75.47643 MHz
FIDRES             70.758446 Hz
SW                   239.998 ppm
FnMODE                     QF
SI                       2048
SF                300.1299994 MHz
WDW                      SINE
SSB                           0
LB                       0.00 Hz
GB                            0
PC                       1.40
SI                       1024
MC2                        QF
SF                75.4677771 MHz
WDW                      SINE
SSB                           0
LB                       0.00 Hz
GB                            0
```



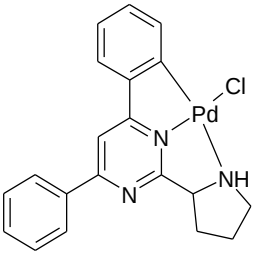

```
NAME            dp21dp141
EXPNO                 403
PROCNO                  1
Date_            20130612
Time                11.27
INSTRUM             spect
PROBHD   5 mm BBI 1H/2H
PULPROG       hmbcgpndqf
TD                    3072
SOLVENT               DMSO
NS                      32
DS                      16
SWH              4006.410 Hz
FIDRES           1.304170 Hz
AQ               0.3835604 sec
RG                    16384
DW                124.800 usec
DE                  6.50 usec
TE                300.0 K
CNST13          5.0000000
D0              0.00000300 sec
D1              2.00000000 sec
D6              0.10000000 sec
D16             0.00020000 sec
IN0             0.00002055 sec

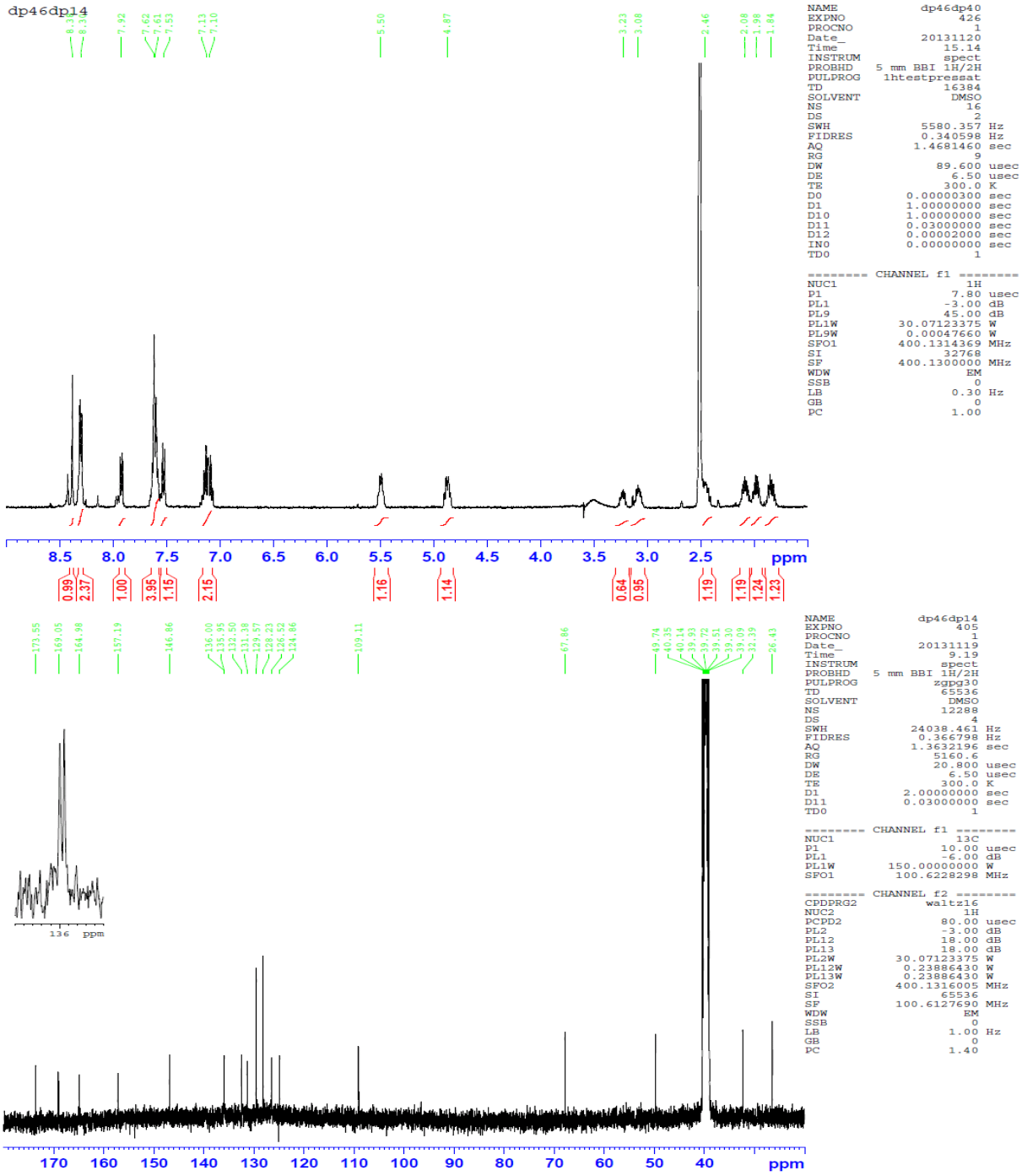
======== CHANNEL f1 ========
NUC1                  1H
P1                  7.00 usec
P2                 14.00 usec
PL1                -3.00 dB
PL1W         30.07123375 W
SFO1         400.1320007 MHz

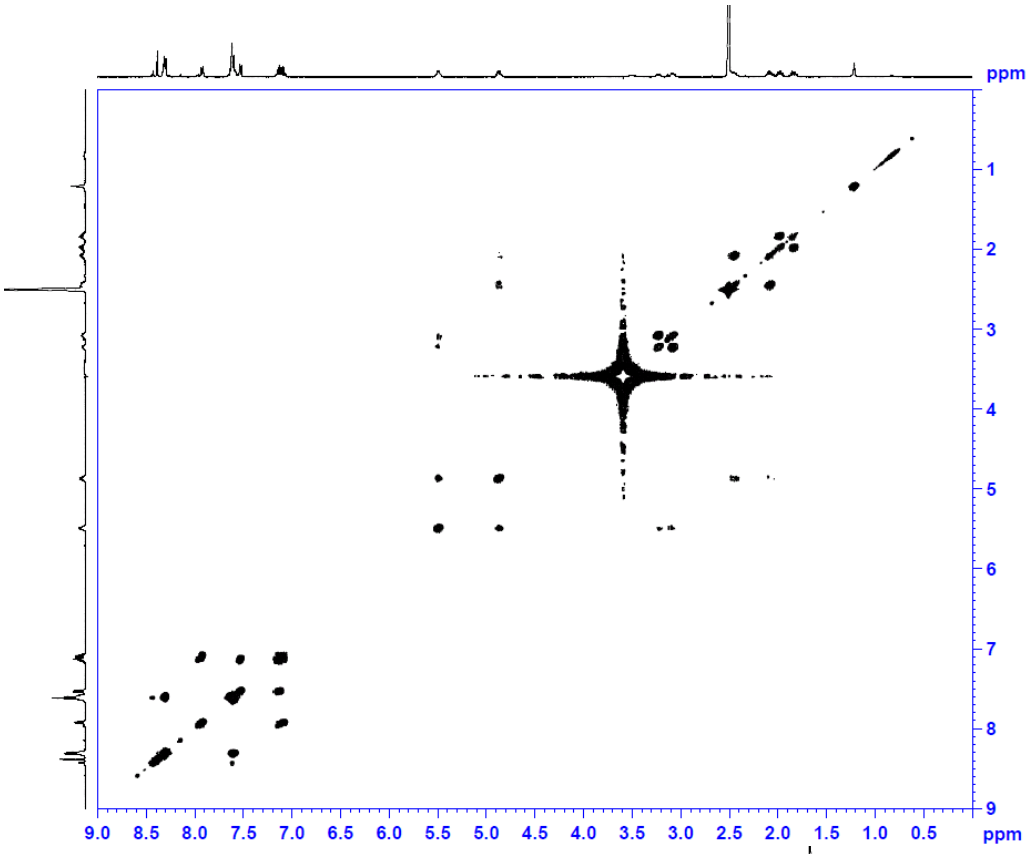
======== CHANNEL f2 ========
NUC2                 15N
P3                 17.00 usec
PL2                -6.00 dB
PL2W        150.00000000 W
SFO2         40.5529300 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1                70.00 %
GPZ2                30.00 %
GPZ3                50.10 %
P16               1000.00 usec
ND0                     2
TD                    192
SFO1             40.55293 MHz
FIDRES          126.727905 Hz
SW                600.000 ppm
FnMODE                 QF
SI                   4096
SF               400.1300000 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2                    QF
SF               40.5601443 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

Complex 10


Cl
Pd
N
N
NH

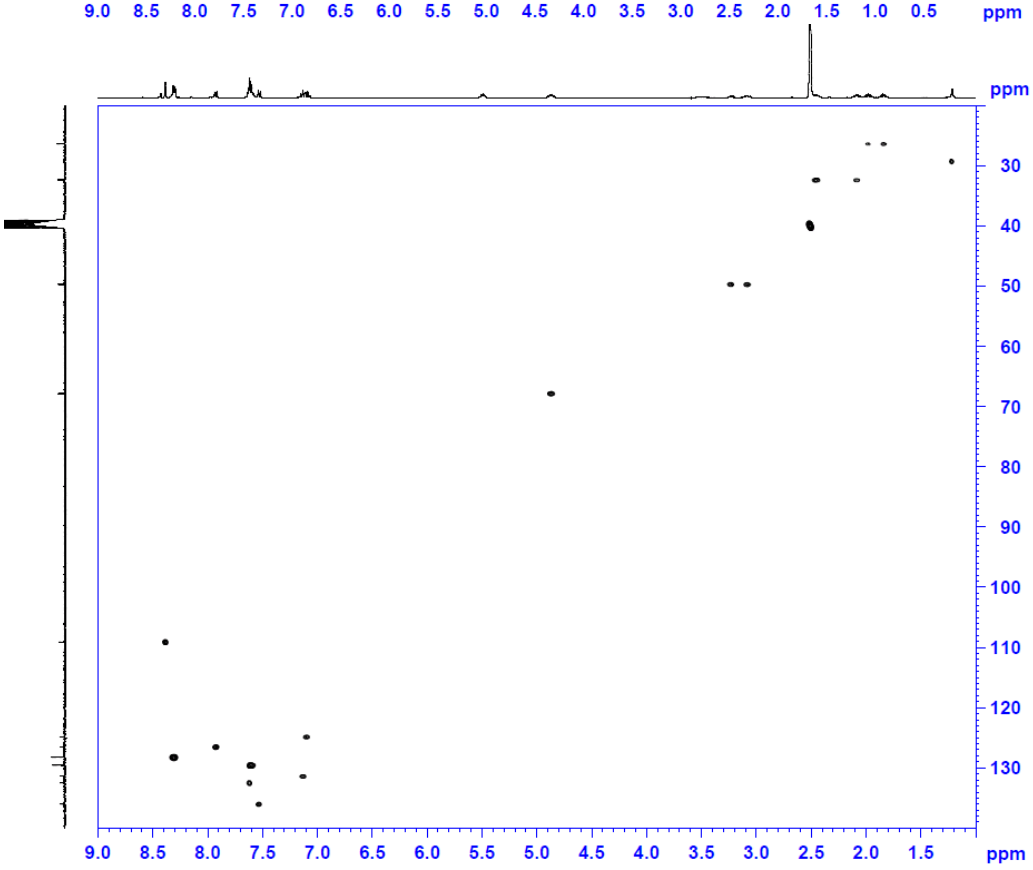

dp46dp14
8.39
8.34
7.92
7.62
7.61
7.53
7.13
7.10
5.50
4.87
3.23
3.08
2.46
2.08
1.98
1.84
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
0.99
2.37
1.00
3.85
1.15
2.15
1.16
1.14
0.64
0.95
1.19
1.19
1.24
1.23
NAME dp46dp40
EXPNO 426
PROCNO 1
Date_ 20131120
Time 15.14
INSTRUM spect
PROBHD 5 mm BBI 1H/2H
PULPROG 1htestpressat
TD 16384
SOLVENT DMSO
NS 16
DS 2
SWH 5580.357 Hz
FIDRES 0.340598 Hz
AQ 1.4681460 sec
RG 9
DW 89.600 usec
DE 6.50 usec
TE 300.0 K
D0 0.00000300 sec
D1 1.00000000 sec
D10 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
IN0 0.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.80 usec
PL1 -3.00 dB
PL9 45.00 dB
PL1W 30.07123375 W
PL9W 0.00047660 W
SFO1 400.1314369 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
173.55
169.05
164.98
157.19
146.86
136.00
135.95
132.50
131.38
129.57
128.23
126.52
124.86
109.11
67.86
49.74
40.35
40.14
39.93
39.72
39.51
39.30
39.09
32.39
26.43
136 ppm
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm
NAME dp46dp14
EXPNO 405
PROCNO 1
Date_ 20131119
Time 9.19
INSTRUM spect
PROBHD 5 mm BBI 1H/2H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 12288
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 5160.6
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -6.00 dB
PL1W 150.00000000 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 18.00 dB
PL2W 30.07123375 W
PL12W 0.23886430 W
PL13W 0.23886430 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
NAME                dp46dp14
EXPNO                    402
PROCNO                     1
Date_              20131118
Time                   16.43
INSTRUM                spect
PROBHD   5 mm BBI 1H/2H
PULPROG            copyjpqf
TD                       2048
SOLVENT                  DMSO
NS                          8
DS                          8
SWH                5580.357 Hz
FIDRES             2.724784 Hz
AQ                 0.1836404 sec
RG                      35.9
DW                   89.600 usec
DE                    6.50 usec
TE                   300.0 K
D0                 0.00000300 sec
D1                 1.50000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00017920 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                     7.00 usec
P1                     7.00 usec
PL1                   -3.00 dB
PL1W          30.07123375 W
SFO1          400.1326008 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPZ1                  10.00 %
P16                 1000.00 usec
ND0                        1
TD                       256
SFO1              400.1326 MHz
FIDRES            21.798281 Hz
SW                   13.946 ppm
FnMODE                    QF
SI                       2048
SF              400.1300000 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                       1024
MC2                       QF
SF              400.1300000 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
```

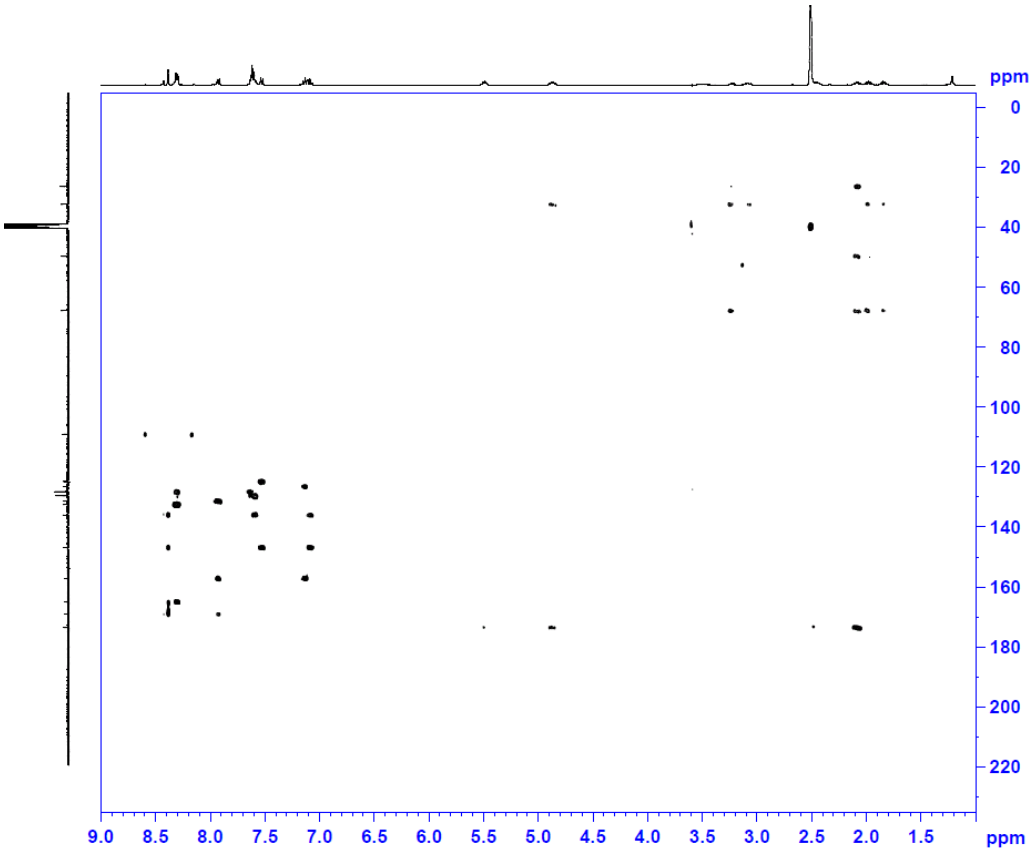



```
NAME                dp46dp14
EXPNO                    403
PROCNO                     1
Date_              20131118
Time                   17.43
INSTRUM                spect
PROBHD   5 mm BBI 1H/2H
PULPROG            hsqcetgp
TD                       1024
SOLVENT                  DMSO
NS                         16
DS                         16
SWH                5341.880 Hz
FIDRES             5.216680 Hz
AQ                 0.0959900 sec
RG                   18390.4
DW                   93.600 usec
DE                    6.50 usec
TE                   300.0 K
CNST2             145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                     7.00 usec
P2                    14.00 usec
P28                 1000.00 usec
PL1                   -3.00 dB
PL1W          30.07123375 W
SFO1          400.1324057 MHz

======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                     13C
P3                    10.00 usec
P4                    20.00 usec
PCPD2                 80.00 usec
PL2                   -6.00 dB
PL12                  12.00 dB
PL2W          150.00000000 W
PL12W          2.37733984 W
SFO2          100.6202727 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec
ND0                        2
TD                       256
SFO1              100.6203 MHz
FIDRES            65.104164 Hz
SW                  165.639 ppm
FnMODE     Echo-Antiecho
SI                       2048
SF              400.1299986 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                       1024
MC2          echo-antiecho
SF              100.6127613 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```

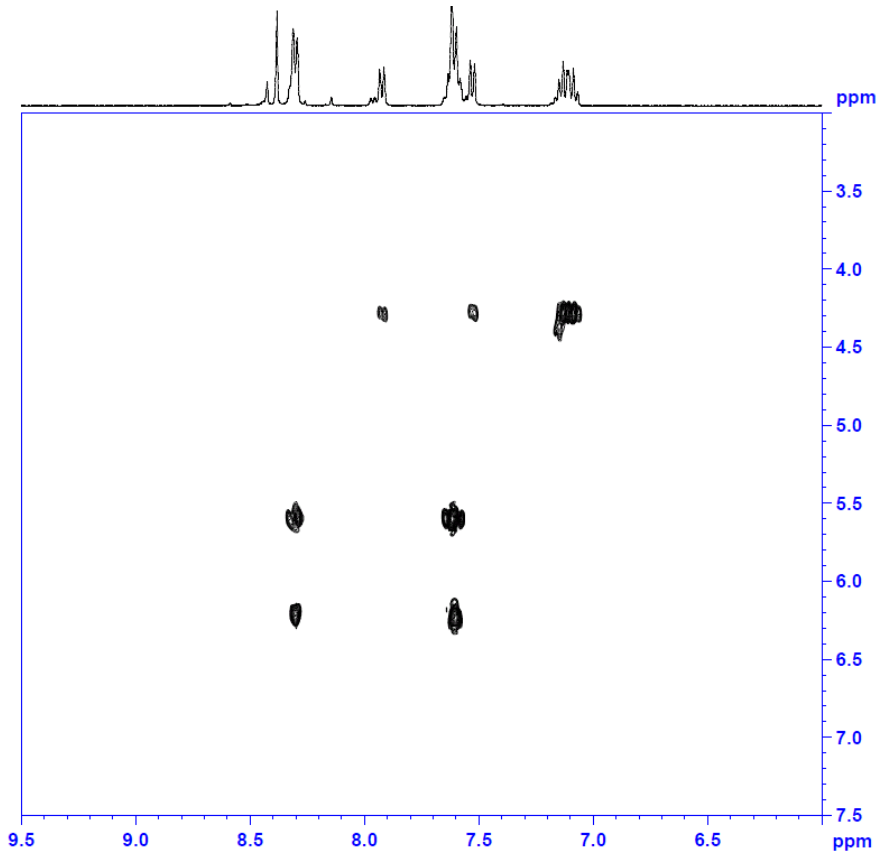



```
NAME                dp46dp14
EXPNO                    404
PROCNO                     1
Date_               20131118
Time                   19.33
INSTRUM                spect
PROBHD    5 mm BBI 1H/2H
PULPROG     hmbcgplpndqf
TD                      2048
SOLVENT                 DMSO
NS                        16
DS                        16
SWH                 4006.410 Hz
FIDRES              1.956255 Hz
AQ                  0.2557652 sec
RG                      16384
DW                    124.800 usec
DE                      6.50 usec
TE                     300.0 K
CNST2               145.0000000
CNST13               10.0000000
D0                   0.00000300 sec
D1                   1.50000000 sec
D2                   0.00344828 sec
D6                   0.05000000 sec
D16                  0.00020000 sec
IN0                  0.00002070 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       7.00 usec
P2                      14.00 usec
PL1                     -3.00 dB
PL1W               30.07123375 W
SFO1               400.1318006 MHz

======== CHANNEL f2 ========
NUC2                      13C
P3                      10.00 usec
PL2                     -6.00 dB
PL2W              150.00000000 W
SFO2              100.6243395 MHz

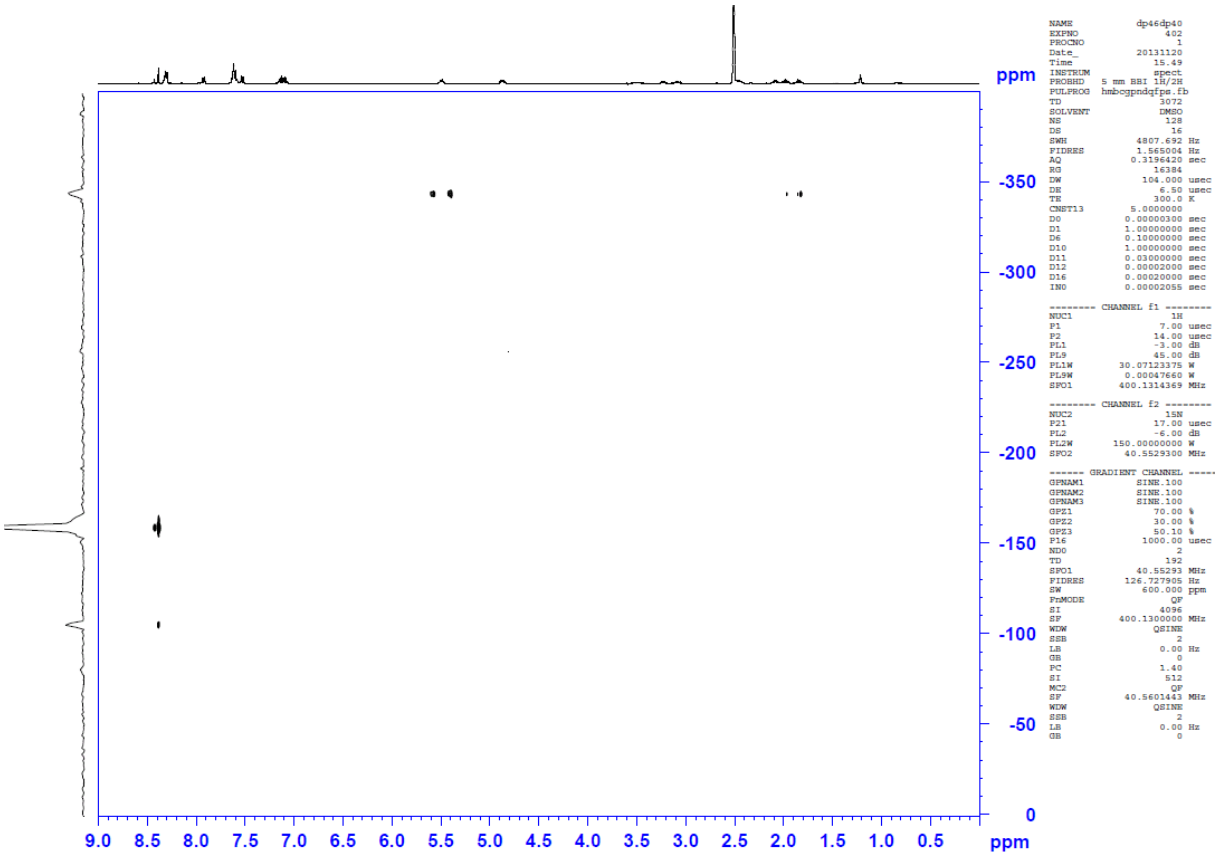
====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPNAM3               SINE.100
GPZ1                    50.00 %
GPZ2                    30.00 %
GPZ3                    40.10 %
P16                   1000.00 usec
ND0                         2
TD                        256
SFO1              100.6243 MHz
FIDRES             94.335320 Hz
SW                   240.000 ppm
FnMODE                    QF
SI                      2048
SF                400.1300000 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                      1024
MC2                       QF
SF                100.6127548 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
```




```
NAME                dp46dp14
EXPNO                    408
PROCNO                     1
Date_               20131121
Time                   17.04
INSTRUM                spect
PROBHD    5 mm BBI 1H/2H
PULPROG   cosymqgpqf.txt
TD                      2048
SOLVENT                 DMSO
NS                         8
DS                        16
SWH                 4807.692 Hz
FIDRES              2.347506 Hz
AQ                  0.2131460 sec
RG                     11585.2
DW                    104.000 usec
DE                      6.50 usec
TE                     300.0 K
D0                   0.00000300 sec
D1                   1.50000000 sec
D13                  0.00000400 sec
D16                  0.00020000 sec
D20                  0.03750000 sec
IN0                  0.00018720 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       7.00 usec
P2                       7.00 usec
P3                      14.00 usec
PL1                     -3.00 dB
PL1W               30.07123375 W
SFO1               400.1316005 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPZ1                    10.00 %
GPZ2                    40.00 %
P16                   1000.00 usec
ND0                         1
TD                        127
SFO1               400.1316 MHz
FIDRES             37.855824 Hz
SW                     12.015 ppm
FnMODE                    QF
SI                      2048
SF                400.1300000 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                       512
MC2                       QF
SF                400.1300000 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
```



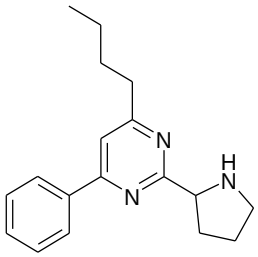

```
NAME                dp46dp40
EXPNO                    402
PROCNO                     1
Date_              20131120
Time                   15.49
INSTRUM                spect
PROBHD    5 mm BBI 1H/2H
PULPROG   hmbcgpndqfpe.fb
TD                       3072
SOLVENT                  DMSO
NS                        128
DS                         16
SWH                4807.692 Hz
FIDRES             1.565004 Hz
AQ                 0.3196420 sec
RG                       16384
DW                   104.000 usec
DE                     6.50 usec
TE                    300.0 K
CNST13             5.0000000
D0                 0.00000300 sec
D1                 1.00000000 sec
D6                 0.10000000 sec
D10                1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D16                0.00020000 sec
IN0                0.00002055 sec

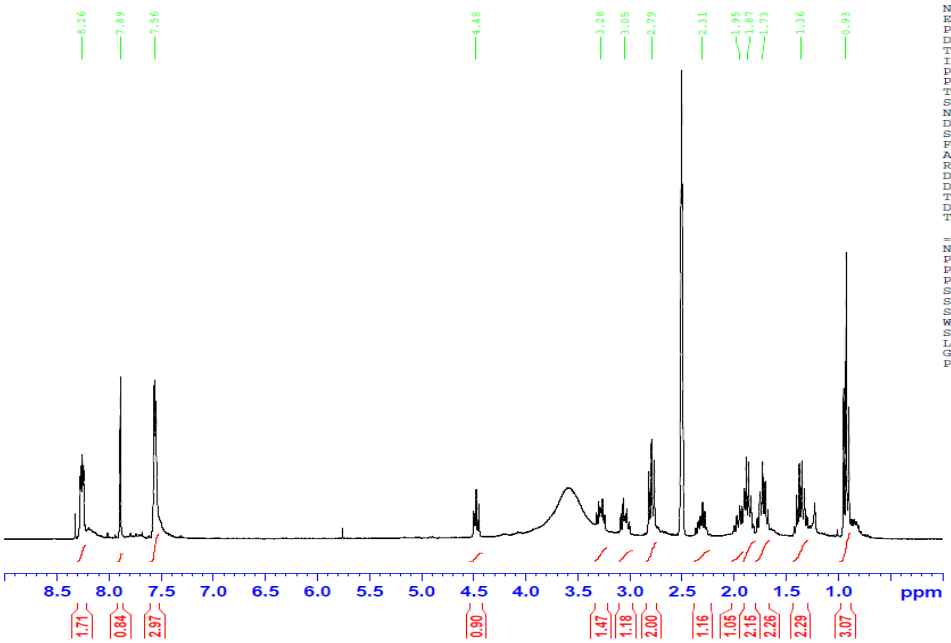
======== CHANNEL f1 ========
NUC1                       1H
P1                       7.00 usec
P2                      14.00 usec
PL1                     -3.00 dB
PL9                     45.00 dB
PL1W            30.07123375 W
PL9W             0.00047660 W
SFO1            400.1314369 MHz

======== CHANNEL f2 ========
NUC2                      15N
P21                     17.00 usec
PL2                     -6.00 dB
PL2W           150.00000000 W
SFO2            40.5529300 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPNAM3               SINE.100
GPZ1                    70.00 %
GPZ2                    30.00 %
GPZ3                    50.10 %
P16                   1000.00 usec
ND0                        2
TD                       192
SFO1                40.55293 MHz
FIDRES             126.727905 Hz
SW                  600.000 ppm
FnMODE                    QF
SI                       4096
SF                 400.1300000 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                        512
MC2                       QF
SF                 40.5601443 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```

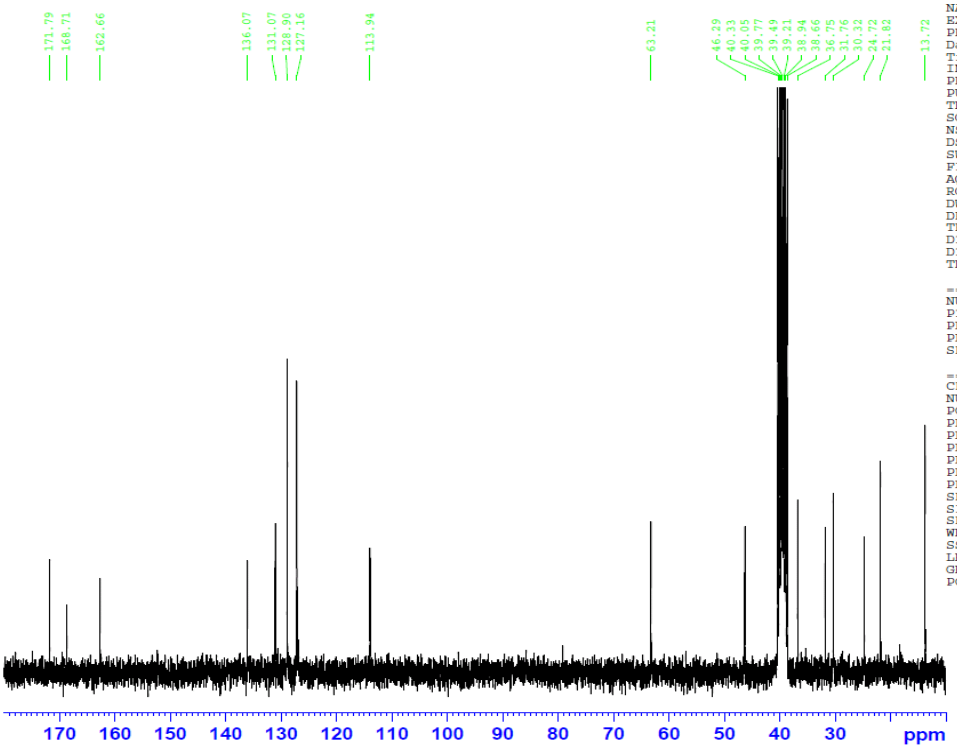
Ligand 4






```
NAME                dp161
EXPNO                  10
PROCNO                  1
Date_            20130711
Time                21.55
INSTRUM             spect
PROBHD    5 mm BBI 1H-BB
PULPROG              zg30
TD                  16384
SOLVENT              DMSO
NS                      32
DS                       2
SWH              4194.631 Hz
FIDRES           0.256020 Hz
AQ               1.9530228 sec
RG                   322.5
DW                 119.200 usec
DE                    6.50 usec
TE                   300.0 K
D1             1.00000000 sec
TD0                     1

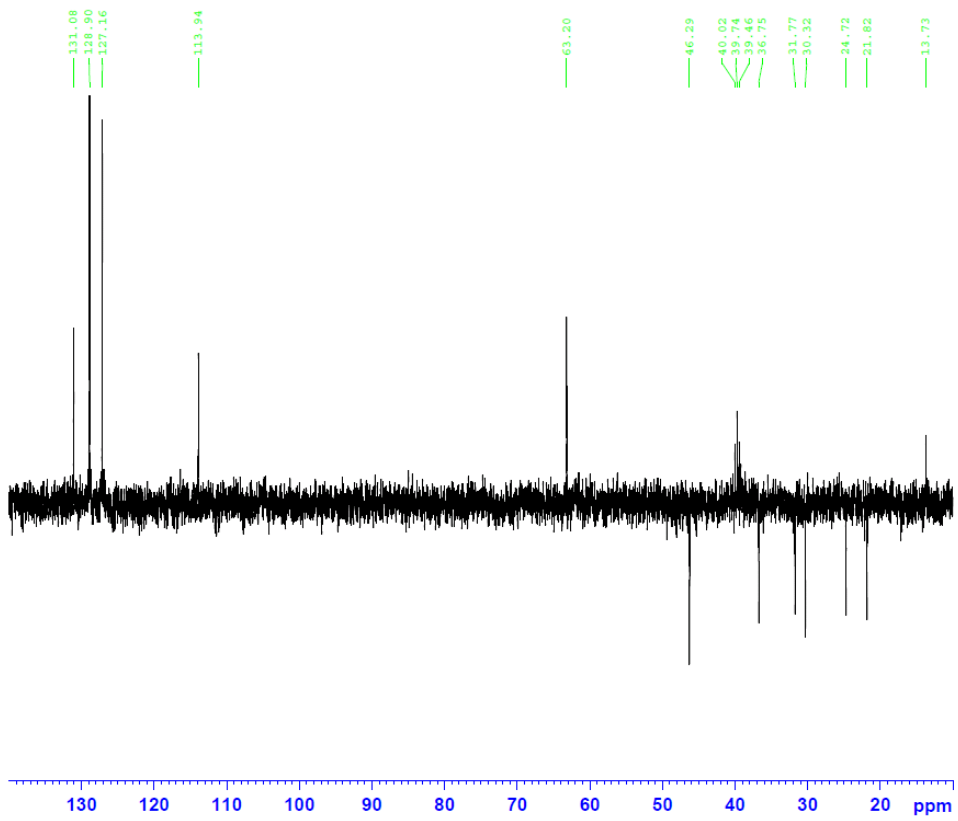
======== CHANNEL f1 ========
NUC1                   1H
P1                   6.70 usec
PL1                  0.00 dB
PL1W          15.07131863 W
SFO1         300.1319508 MHz
SI                   32768
SP           300.1300000 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```




```
NAME                dp161
EXPNO                  14
PROCNO                  1
Date_            20130712
Time                 3.36
INSTRUM             spect
PROBHD    5 mm BBI 1H-BB
PULPROG           zgpg30
TD                  32768
SOLVENT              DMSO
NS                    4096
DS                       4
SWH             17985.611 Hz
FIDRES           0.548877 Hz
AQ               0.9110004 sec
RG                    3251
DW                 27.800 usec
DE                   10.00 usec
TE                   300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.20 usec
PL1                 -6.00 dB
PL1W         150.00000000 W
SFO1          75.4760505 MHz

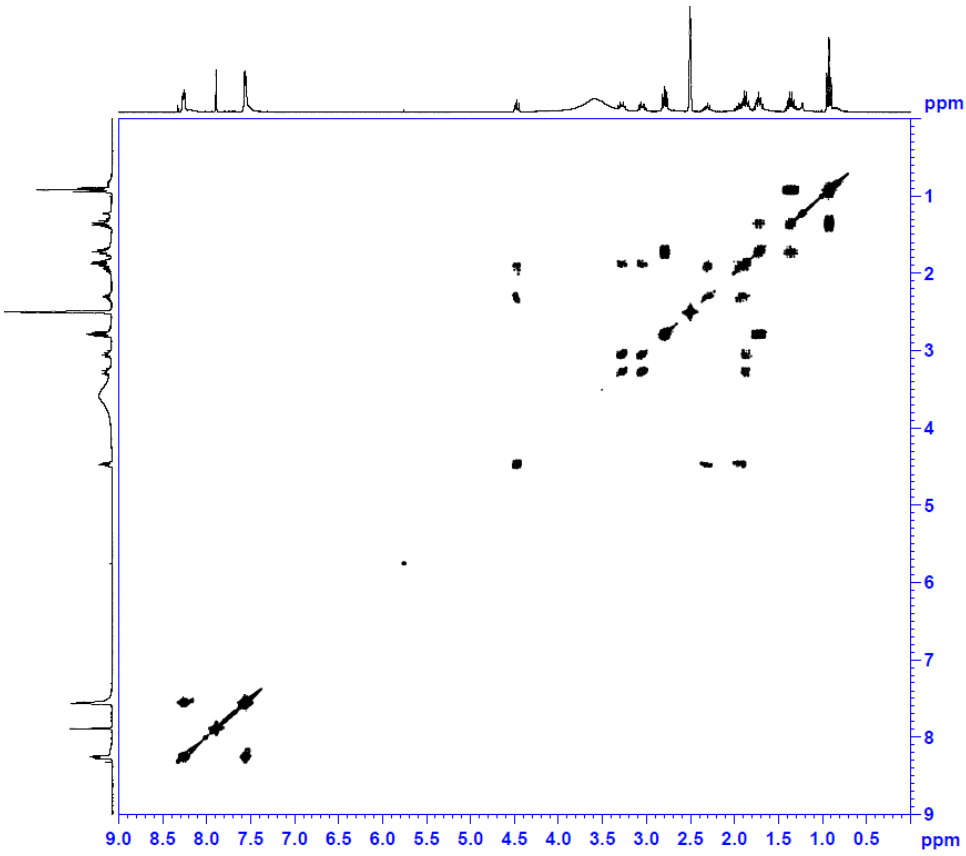
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  0.00 dB
PL12                21.54 dB
PL13                21.54 dB
PL2W          15.07131863 W
PL12W          0.10571854 W
PL13W          0.10571854 W
SFO2         300.1312005 MHz
SI                   65536
SF            75.4677867 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
NAME                dp161
EXPNO                  12
PROCNO                  1
Date_            20130711
Time                23.15
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG           dept135
TD                  32768
SOLVENT              DMSO
NS                   1024
DS                      4
SWH            12077.295 Hz
FIDRES          0.368570 Hz
AQ              1.3566452 sec
RG                  16384
DW                41.400 usec
DE                10.00 usec
TE                300.0 K
CNST2         145.0000000
D1              1.50000000 sec
D2              0.00344828 sec
D12             0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.20 usec
P2                  16.40 usec
PL1                 -6.00 dB
PL1W        150.00000000 W
SFO1          75.4734091 MHz

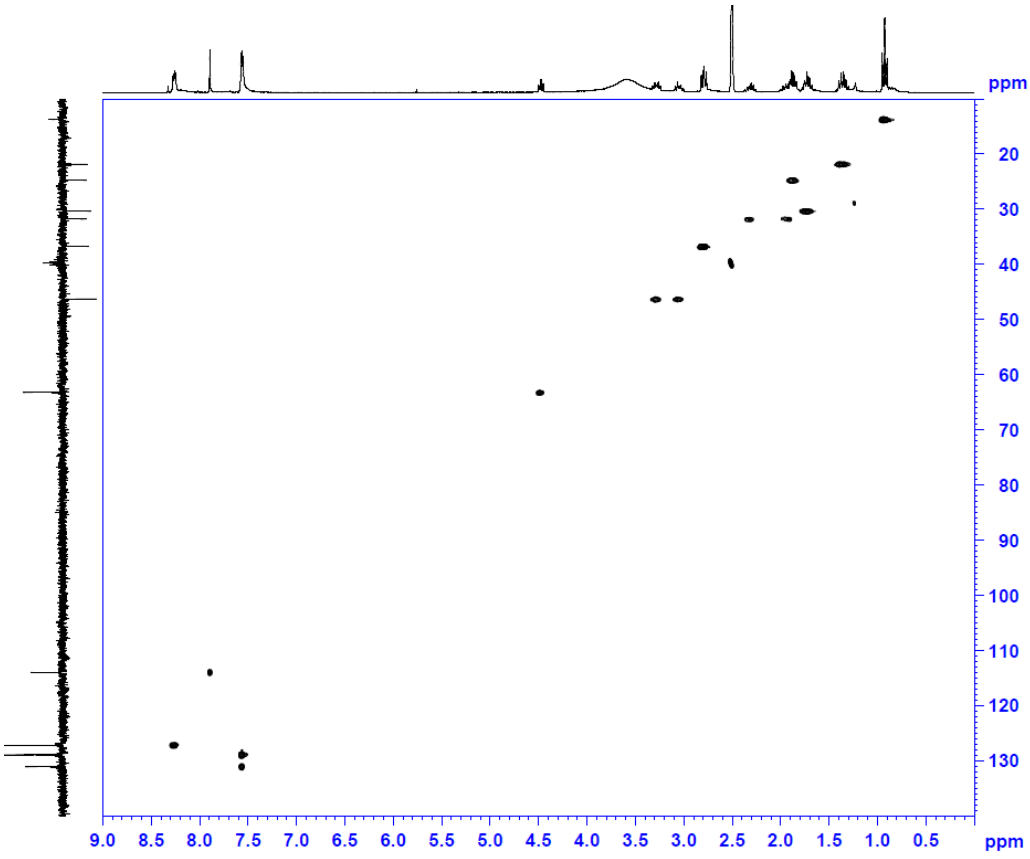
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
P3                   6.70 usec
P4                  13.40 usec
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                21.54 dB
PL2W         15.07131863 W
PL12W         0.10571854 W
SFO2         300.1312005 MHz
SI                  65536
SF            75.4677867 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
NAME                dp161
EXPNO                  11
PROCNO                  1
Date_            20130711
Time                21.56
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG         cosygpqf
TD                  1024
SOLVENT              DMSO
NS                      4
DS                     16
SWH             2759.382 Hz
FIDRES          2.694709 Hz
AQ              0.1855988 sec
RG                  161.3
DW                181.200 usec
DE                10.00 usec
TE                300.0 K
D0              0.00000300 sec
D1              1.45719695 sec
D13             0.00000400 sec
D16             0.00010000 sec
IN0             0.00036240 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                   6.70 usec
P1                   6.70 usec
PL1                  0.00 dB
PL1W         15.07131863 W
SFO1         300.1312978 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1                10.00 %
P16               1000.00 usec
ND0                     1
TD                    256
SFO1            300.1313 MHz
FIDRES          10.778835 Hz
SW                  9.194 ppm
FnMODE                 QF
SI                   2048
SF           300.1300000 MHz
WDW                  SINE
SSB                     1
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2                    QF
SF           300.1300000 MHz
WDW                  SINE
SSB                     1
LB                   0.00 Hz
GB                      0
```

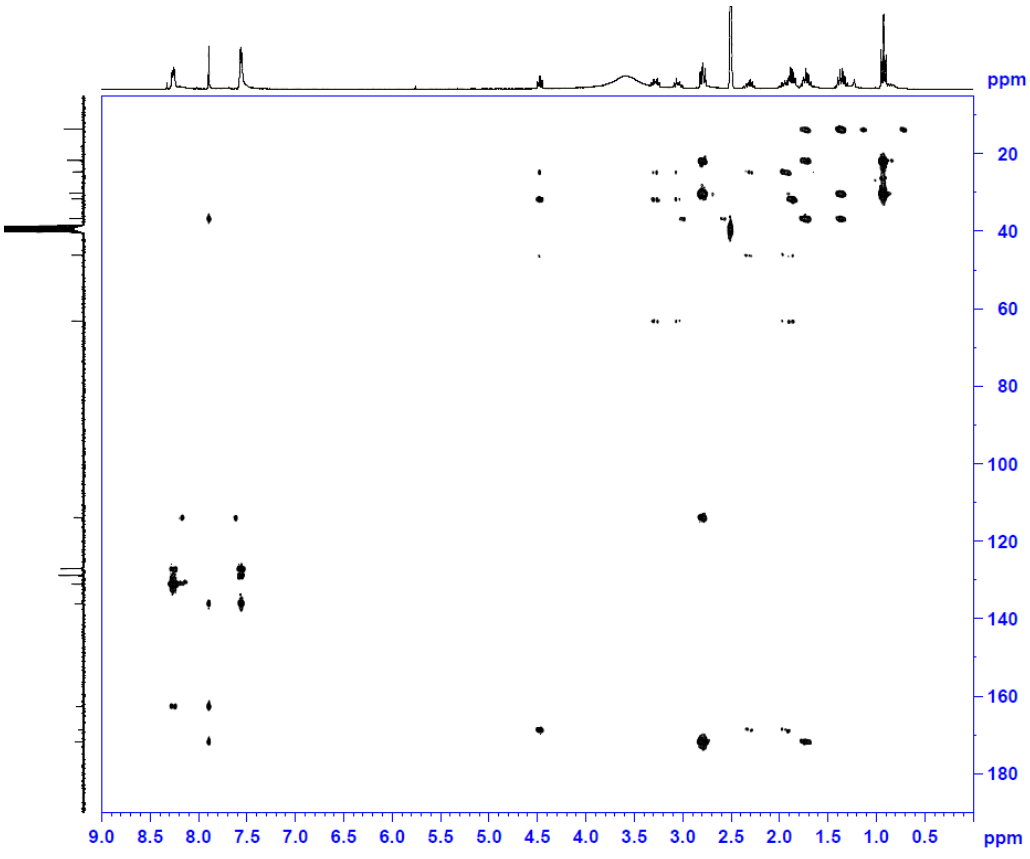



```
NAME                dp161
EXPNO                  13
PROCNO                  1
Date_            20130711
Time                23.16
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG         hsqcgpph
TD                   1024
SOLVENT              DMSO
NS                      8
DS                     16
SWH              2759.382 Hz
FIDRES           2.694709 Hz
AQ               0.1855988 sec
RG                   26008
DW                181.200 usec
DE                 10.00 usec
TE                 300.0 K
CNST2          145.0000000
D0               0.00000300 sec
D1               1.45719695 sec
D4               0.00172414 sec
D11              0.03000000 sec
D13              0.00000400 sec
D16              0.00010000 sec
IN0              0.00004140 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   6.70 usec
P2                  13.40 usec
PL1                  0.00 dB
PL1W          15.07131863 W
SFO1         300.1312978 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                  13C
P3                   8.20 usec
P4                  16.40 usec
PCPD2               80.00 usec
PL2                 -6.00 dB
PL12                13.79 dB
PL2W         150.00000000 W
PL12W          1.57431364 W
SFO2          75.4734091 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1                80.00 %
GPZ2                30.00 %
GPZ3                20.10 %
P16               1000.00 usec
ND0                     2
TD                    256
SFO1           75.47341 MHz
FIDRES         47.170879 Hz
SW                160.009 ppm
FnMODE               TPPI
SI                   2048
SF           300.1299972 MHz
WDW                QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2                  TPPI
SF            75.4677788 MHz
WDW                QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

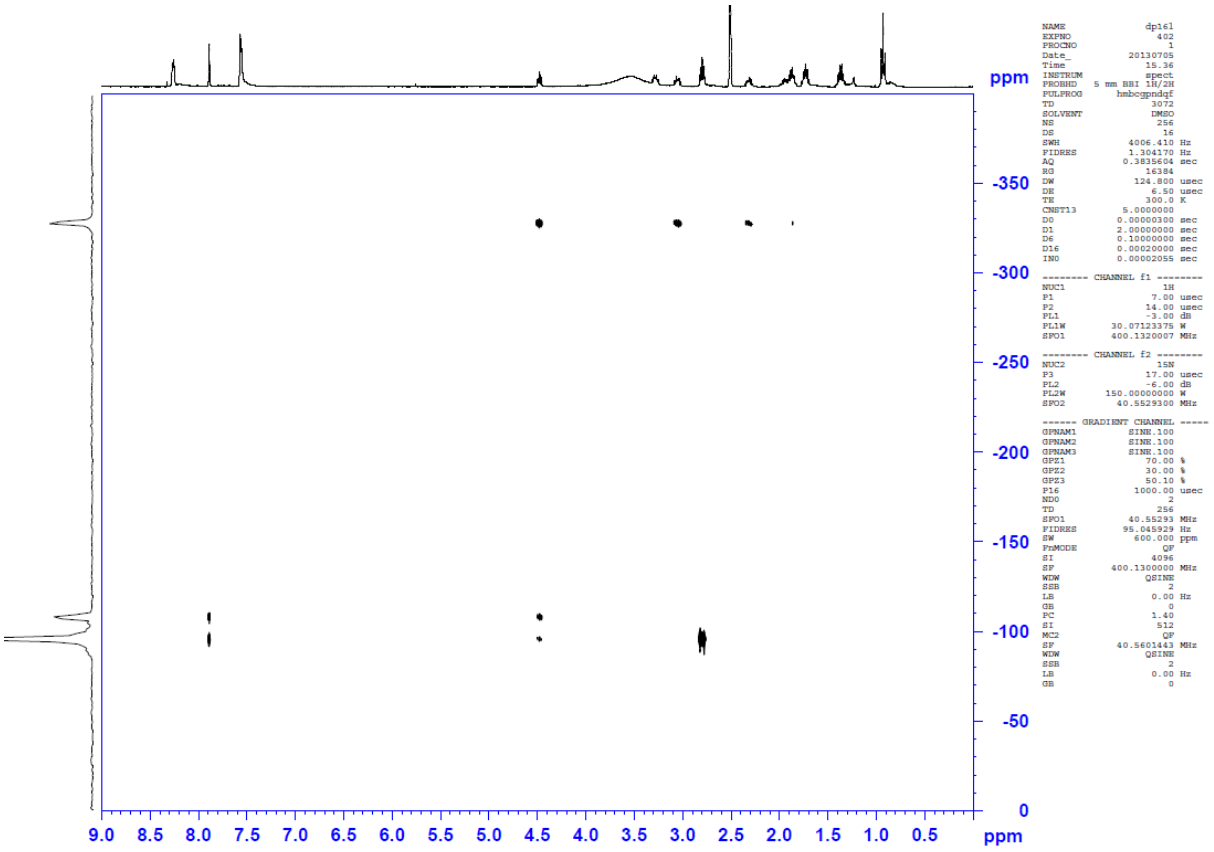



```
NAME                dp161
EXPNO                  15
PROCNO                  1
Date_            20130712
Time                 3.38
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG     hmbcgplpndqf
TD                   2048
SOLVENT              DMSO
NS                     16
DS                     16
SWH              2759.382 Hz
FIDRES           1.347354 Hz
AQ               0.3711476 sec
RG                 20642.5
DW                181.200 usec
DE                 10.00 usec
TE                 300.0 K
CNST2          145.0000000
CNST13          10.0000000
D0               0.00000300 sec
D1               1.41439295 sec
D2               0.00344828 sec
D6               0.05000000 sec
D16              0.00010000 sec
IN0              0.00002760 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   6.70 usec
P2                  13.40 usec
PL1                  0.00 dB
PL1W          15.07131863 W
SFO1         300.1312978 MHz

======== CHANNEL f2 ========
NUC2                  13C
P3                   8.20 usec
PL2                 -6.00 dB
PL2W         150.00000000 W
SFO2          75.4764278 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1                50.00 %
GPZ2                30.00 %
GPZ3                40.10 %
P16               1000.00 usec
ND0                     2
TD                    256
SFO1           75.47643 MHz
FIDRES         70.758446 Hz
SW                239.998 ppm
FnMODE                QF
SI                   2048
SF           300.1299989 MHz
WDW                QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2                   QF
SF            75.4677756 MHz
WDW                QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```



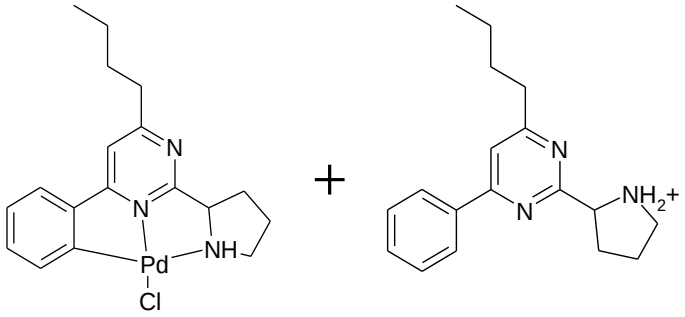

```
NAME                dp161
EXPNO                 402
PROCNO                  1
Date_            20130705
Time                15.36
INSTRUM             spect
PROBHD   5 mm BBI 1H/2H
PULPROG       hmbcgpndqf
TD                  3072
SOLVENT             DMSO
NS                   256
DS                    16
SWH              4006.410 Hz
FIDRES           1.304170 Hz
AQ               0.3835604 sec
RG                  16384
DW                124.800 usec
DE                  6.50 usec
TE                 300.0 K
CNST13          5.0000000
D0              0.00000300 sec
D1              2.00000000 sec
D6              0.10000000 sec
D16             0.00020000 sec
IN0             0.00002055 sec

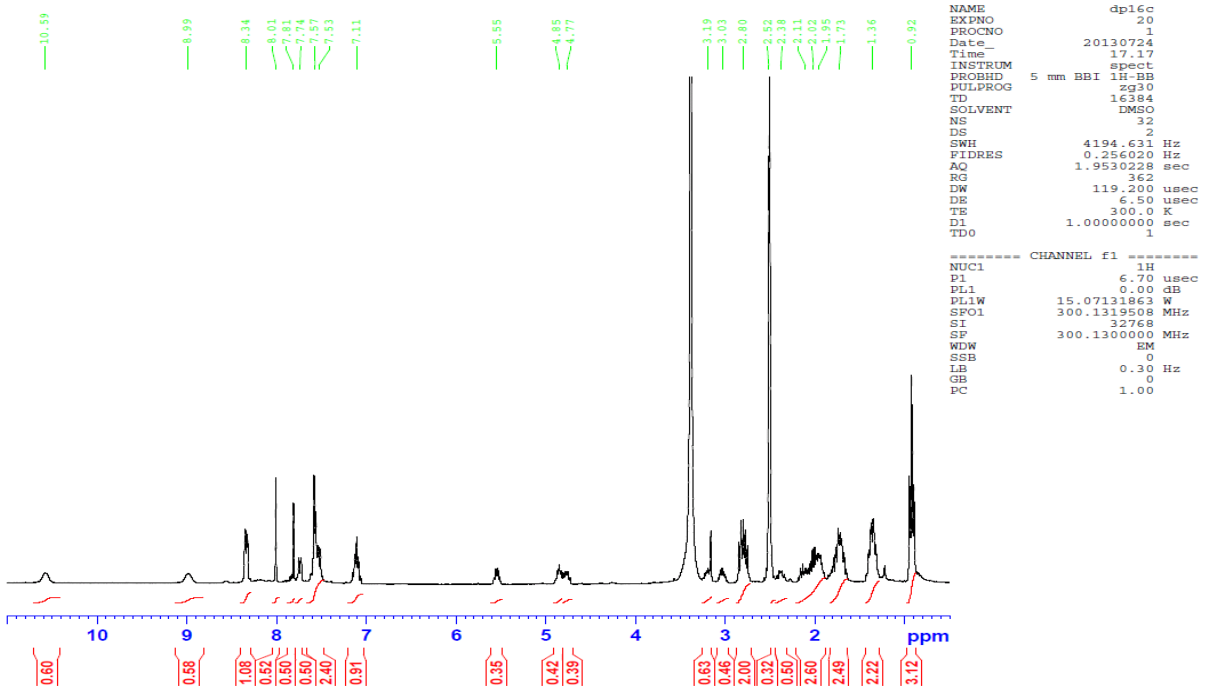
======== CHANNEL f1 ========
NUC1                  1H
P1                  7.00 usec
P2                 14.00 usec
PL1                -3.00 dB
PL1W         30.07123375 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
NUC2                 15N
P3                 17.00 usec
PL2                -6.00 dB
PL2W        150.00000000 W
SFO2         40.5529300 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1                70.00 %
GPZ2                30.00 %
GPZ3                50.10 %
P16               1000.00 usec
ND0                    2
TD                   256
SFO1         40.55293 MHz
FIDRES       95.045929 Hz
SW             600.000 ppm
FnMODE              QF
SI                  4096
SF           400.1300000 MHz
WDW               QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
PC                  1.40
SI                   512
MC2                 QF
SF           40.5601443 MHz
WDW               QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
```

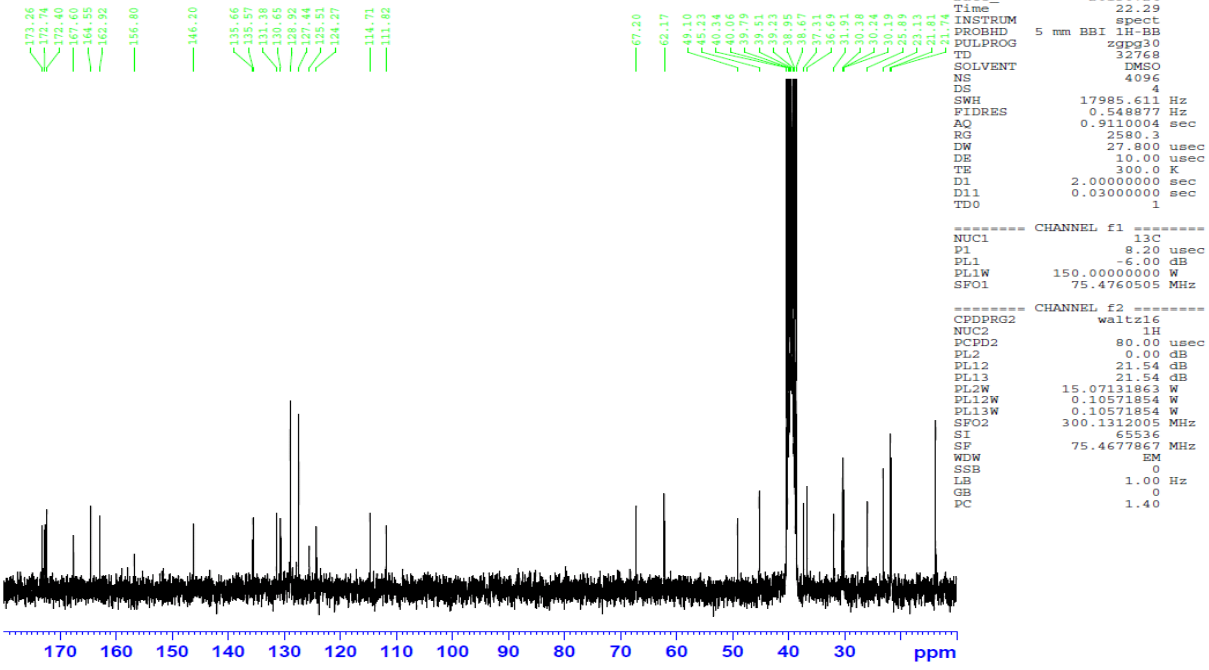
Complex 13






```
NAME                 dp16c
EXPNO                   20
PROCNO                   1
Date_             20130724
Time                 17.17
INSTRUM              spect
PROBHD     5 mm BBI 1H-BB
PULPROG              zg30
TD                  16384
SOLVENT              DMSO
NS                      32
DS                       2
SWH              4194.631 Hz
FIDRES           0.256020 Hz
AQ               1.9530228 sec
RG                     362
DW               119.200 usec
DE                  6.50 usec
TE                 300.0 K
D1               1.00000000 sec
TD0                      1

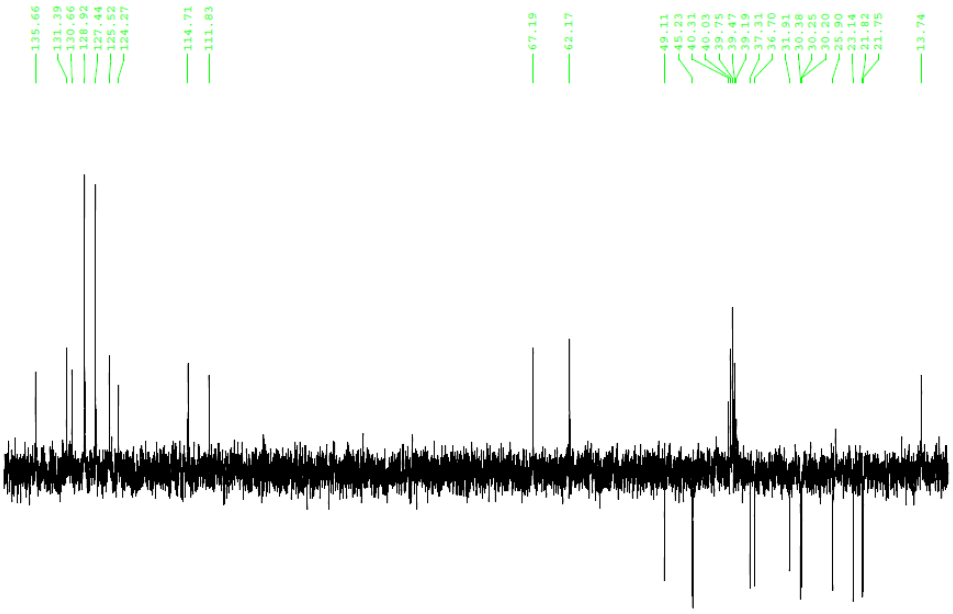
======== CHANNEL f1 ========
NUC1                    1H
P1                   6.70 usec
PL1                  0.00 dB
PL1W          15.07131863 W
SFO1          300.1319508 MHz
SI                   32768
SF            300.1300000 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```




```
NAME                 dp16c
EXPNO                   24
PROCNO                   1
Date_             20130724
Time                 22.29
INSTRUM              spect
PROBHD     5 mm BBI 1H-BB
PULPROG             zgpg30
TD                  32768
SOLVENT              DMSO
NS                    4096
DS                       4
SWH             17985.611 Hz
FIDRES           0.548877 Hz
AQ               0.9110004 sec
RG                  2580.3
DW                27.800 usec
DE                10.00 usec
TE                 300.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   8.20 usec
PL1                 -6.00 dB
PL1W          150.00000000 W
SFO1           75.4760505 MHz

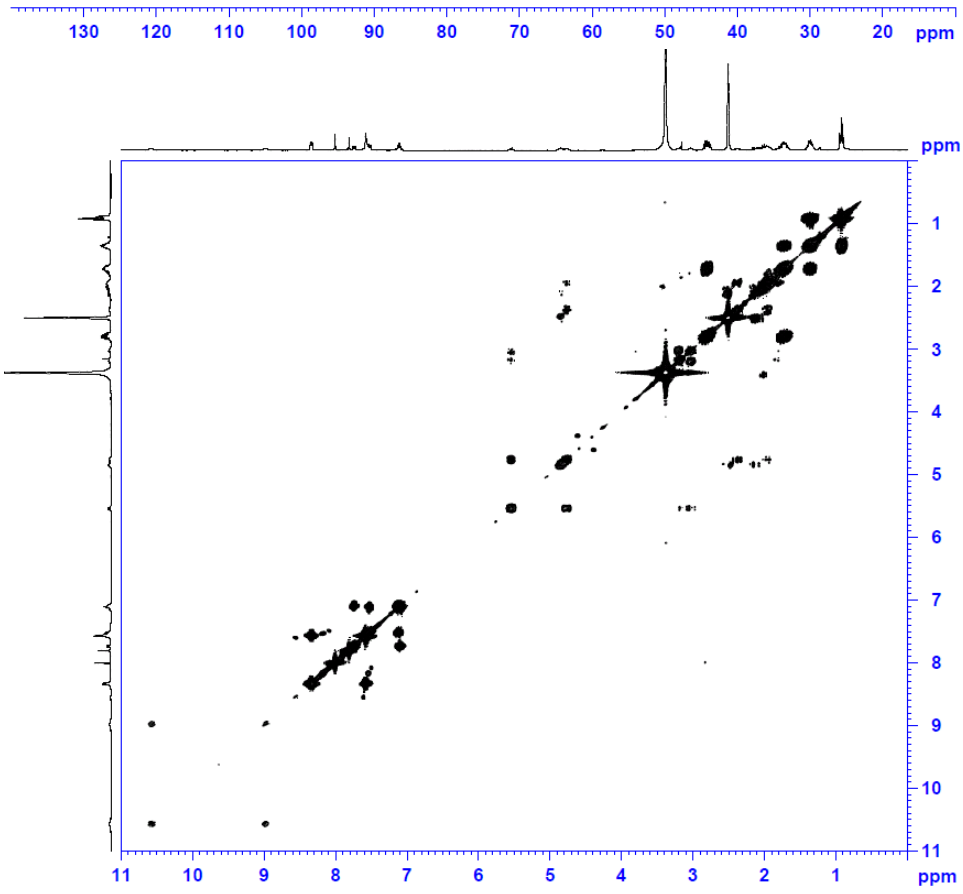
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                21.54 dB
PL13                21.54 dB
PL2W          15.07131863 W
PL12W          0.10571854 W
PL13W          0.10571854 W
SFO2          300.1312005 MHz
SI                   65536
SF             75.4677867 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```




```
NAME                dp16c
EXPNO                  22
PROCNO                  1
Date_            20130724
Time                18.07
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG           dept135
TD                  32768
SOLVENT              DMSO
NS                   1024
DS                      4
SWH           12077.295 Hz
FIDRES         0.368570 Hz
AQ             1.3566452 sec
RG                  16384
DW                41.400 usec
DE                10.00 usec
TE                300.0 K
CNST2        145.0000000
D1             1.50000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.20 usec
P2                16.40 usec
PL1               -6.00 dB
PL1W       150.00000000 W
SFO1         75.4734091 MHz

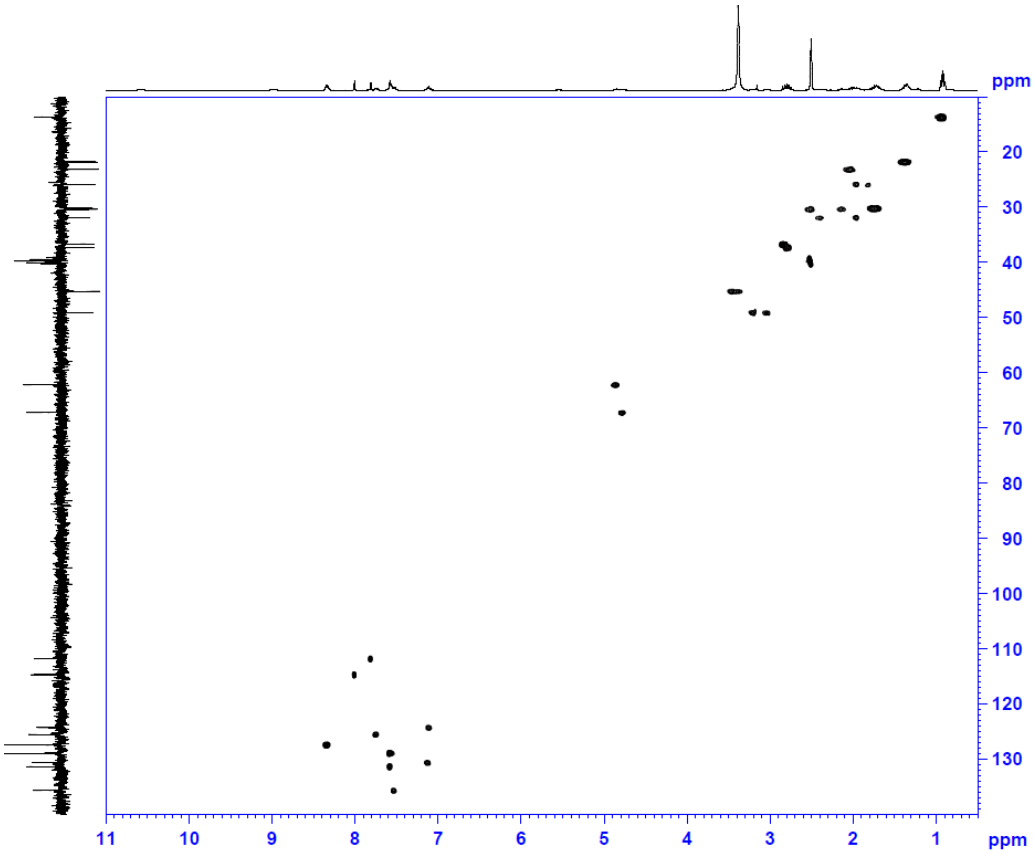
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
P3                 6.70 usec
P4                13.40 usec
PCPD2             80.00 usec
PL2                0.00 dB
PL12              21.54 dB
PL2W       15.07131863 W
PL12W       0.10571854 W
SFO2       300.1312005 MHz
SI                65536
SF           75.4677867 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
NAME                dp16c
EXPNO                  11
PROCNO                  1
Date_            20130724
Time                0.50
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG         cosygpqf
TD                  1024
SOLVENT              DMSO
NS                      4
DS                     16
SWH           3289.474 Hz
FIDRES        3.212377 Hz
AQ            0.1556980 sec
RG                    128
DW                152.000 usec
DE                10.00 usec
TE                300.0 K
D0            0.00000300 sec
D1            1.48689306 sec
D13           0.00000400 sec
D16           0.00010000 sec
IN0           0.00030400 sec

======== CHANNEL f1 ========
NUC1                1H
P0                 6.70 usec
P1                 6.70 usec
PL1                0.00 dB
PL1W       15.07131863 W
SFO1       300.1317276 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1               10.00 %
P16              1000.00 usec
ND0                     1
TD                    256
SFO1          300.1317 MHz
FIDRES        12.849506 Hz
SW               10.960 ppm
FnMODE                QF
SI                  2048
SF         300.1300000 MHz
WDW                 SINE
SSB                    1
LB                 0.00 Hz
GB                     0
PC                 1.40
SI                  1024
MC2                   QF
SF         300.1300000 MHz
WDW                 SINE
SSB                    1
LB                 0.00 Hz
GB                     0
```

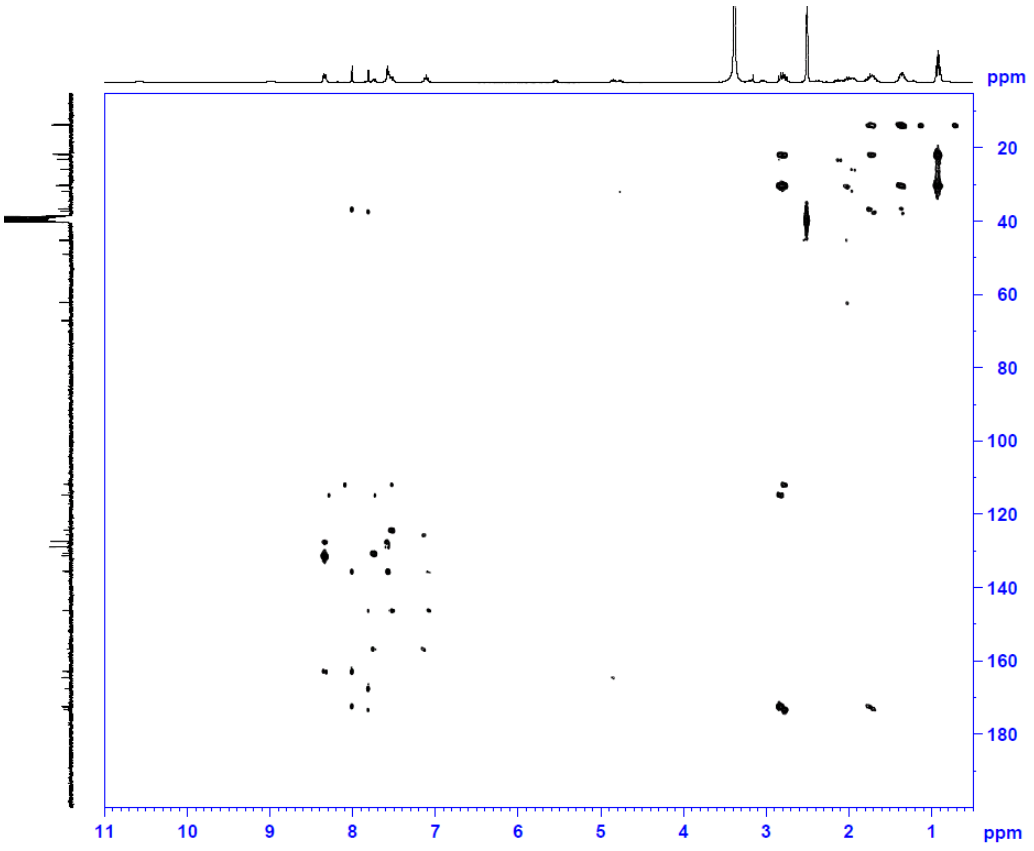



```
NAME                dp16c
EXPNO                  23
PROCNO                  1
Date_            20130724
Time_                18.09
INSTRUM              spect
PROBHD   5 mm BBI 1H-BB
PULPROG          hsqcgpph
TD                   1024
SOLVENT              DMSO
NS                      8
DS                     16
SWH              3324.468 Hz
FIDRES           3.246551 Hz
AQ               0.1540596 sec
RG                  18390.4
DW                150.400 usec
DE                 10.00 usec
TE                 300.0 K
CNST2           145.0000000
D0              0.00000300 sec
D1              1.48894095 sec
D4              0.00172414 sec
D11             0.03000000 sec
D13             0.00000400 sec
D16             0.00010000 sec
IN0             0.00004140 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   6.70 usec
P2                  13.40 usec
PL1                  0.00 dB
PL1W           15.07131863 W
SFO1          300.1317179 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                  13C
P3                   8.20 usec
P4                  16.40 usec
PCPD2               80.00 usec
PL2                 -6.00 dB
PL12                13.79 dB
PL2W          150.00000000 W
PL12W          1.57431364 W
SFO2           75.4734091 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPNAM3             SINE.100
GPZ1                 80.00 %
GPZ2                 30.00 %
GPZ3                 20.10 %
P16                1000.00 usec
ND0                     2
TD                    256
SFO1           75.47341 MHz
FIDRES         47.170879 Hz
SW                160.000 ppm
FnMODE               TPPI
SI                    2048
SF            300.1299974 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                    1024
MC2                  TPPI
SF             75.4677794 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

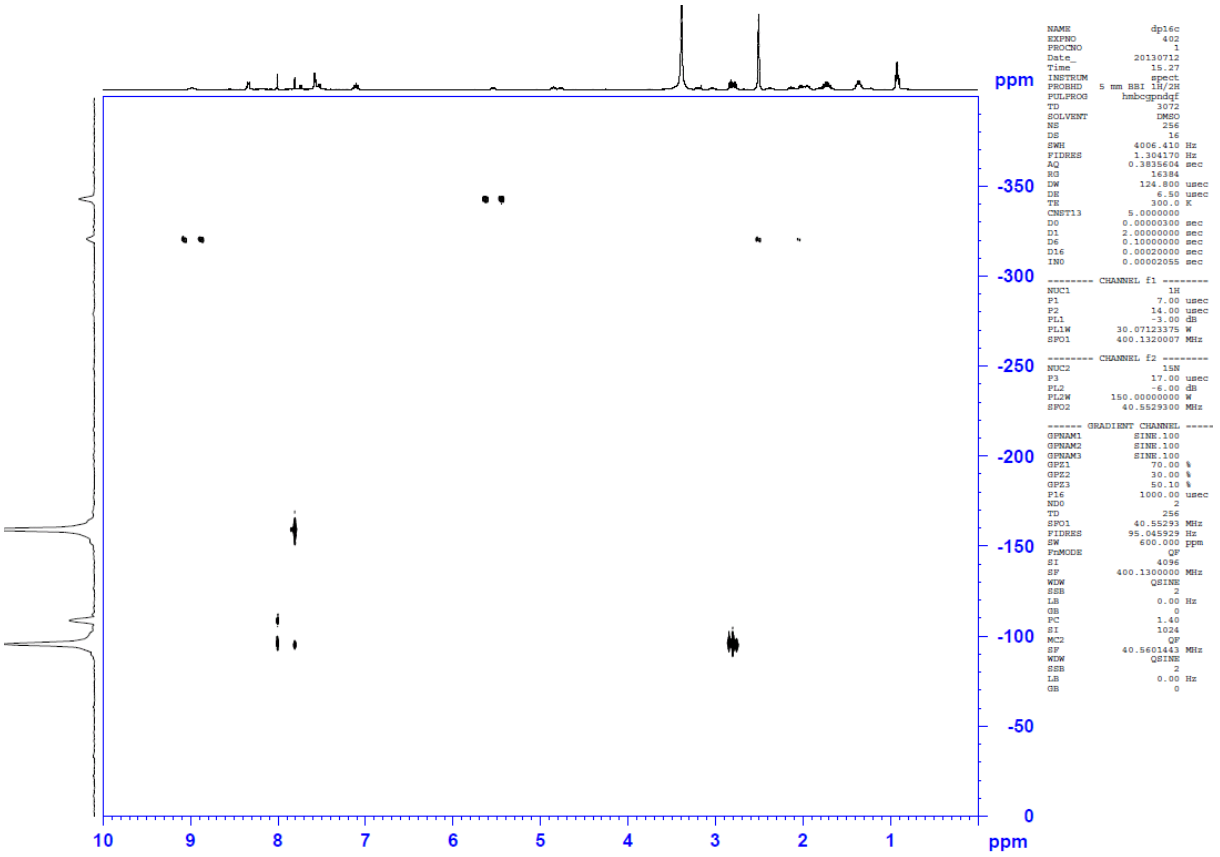



```
NAME                dp16c
EXPNO                  25
PROCNO                  1
Date_            20130724
Time                 22.30
INSTRUM              spect
PROBHD   5 mm BBI 1H-BB
PULPROG     hmbcgplpndqf
TD                   2048
SOLVENT              DMSO
NS                     16
DS                     16
SWH              3324.468 Hz
FIDRES           1.623275 Hz
AQ               0.3080692 sec
RG                 20642.5
DW                150.400 usec
DE                 10.00 usec
TE                 300.0 K
CNST2           145.0000000
CNST13           10.0000000
D0              0.00000300 sec
D1              1.47788095 sec
D2              0.00344828 sec
D6              0.05000000 sec
D16             0.00010000 sec
IN0             0.00002760 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   6.70 usec
P2                  13.40 usec
PL1                  0.00 dB
PL1W           15.07131863 W
SFO1          300.1317179 MHz

======== CHANNEL f2 ========
NUC2                  13C
P3                   8.20 usec
PL2                 -6.00 dB
PL2W          150.00000000 W
SFO2           75.4764278 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPNAM3             SINR.100
GPZ1                 50.00 %
GPZ2                 30.00 %
GPZ3                 40.10 %
P16                1000.00 usec
ND0                     2
TD                    256
SFO1           75.47643 MHz
FIDRES         70.758446 Hz
SW                239.998 ppm
FnMODE                QF
SI                    2048
SF            300.1300000 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                    1024
MC2                    QF
SF             75.4677733 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```



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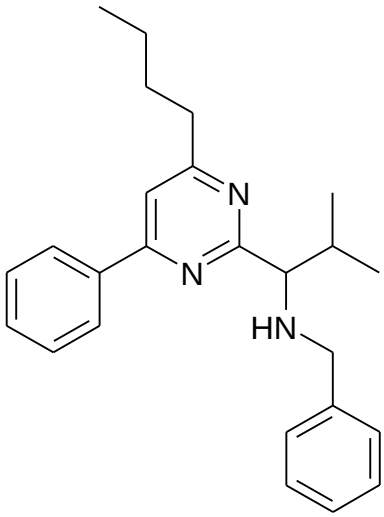
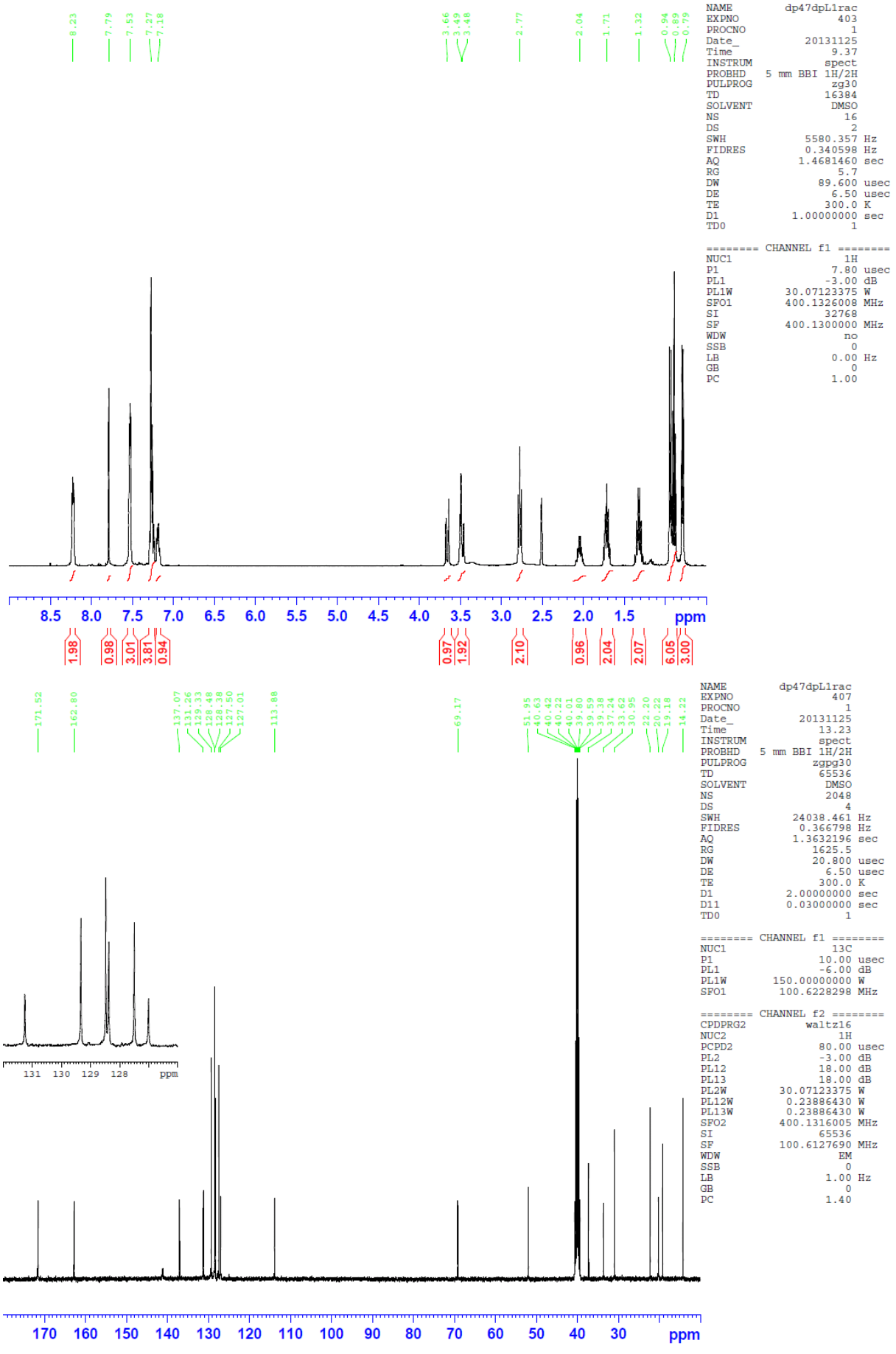
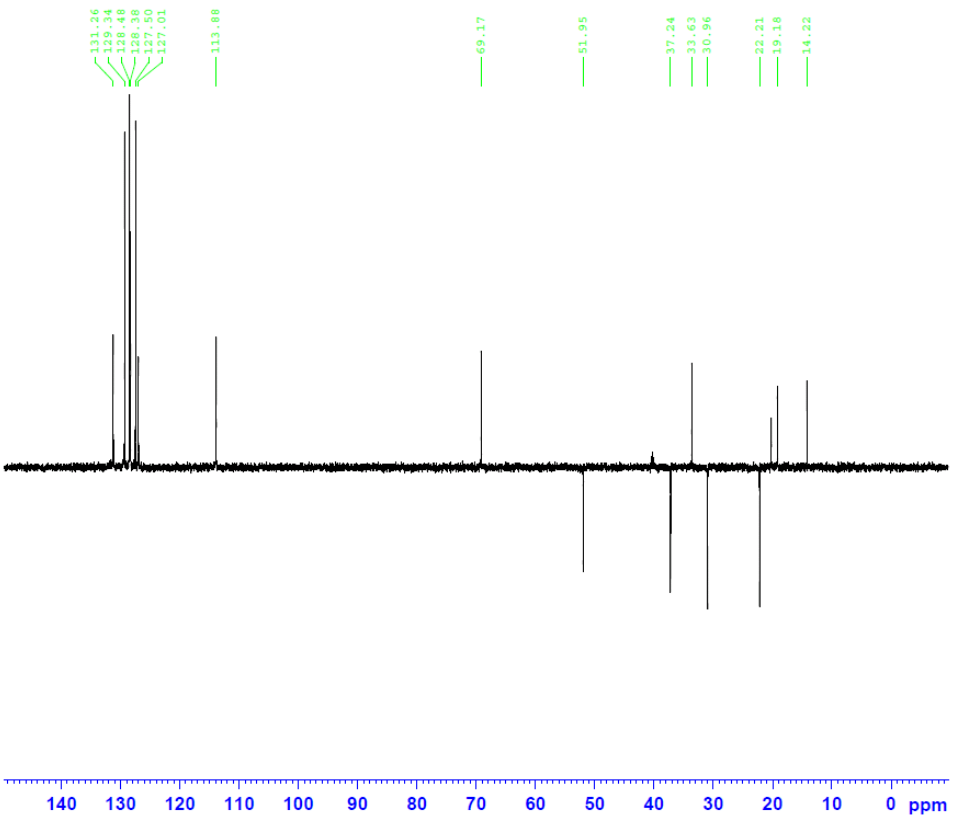


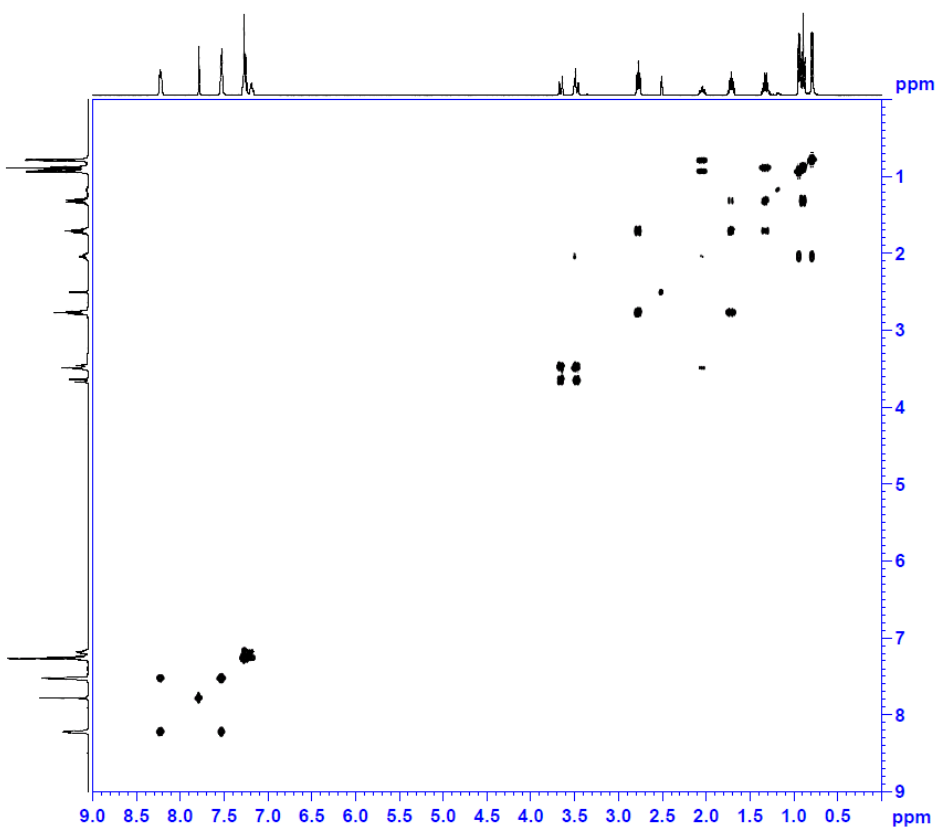

8.23
7.79
7.53
7.27
7.18
3.66
3.49
3.48
2.77
2.04
1.71
1.32
0.94
0.89
0.79
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.98
0.98
3.01
3.81
0.94
0.97
1.92
2.10
0.96
2.04
2.07
6.05
3.00
NAME dp47dpL1rac
EXPNO 403
PROCNO 1
Date_ 20131125
Time 9.37
INSTRUM spect
PROBHD 5 mm BBI 1H/2H
PULPROG zg30
TD 16384
SOLVENT DMSO
NS 16
DS 2
SWH 5580.357 Hz
FIDRES 0.340598 Hz
AQ 1.4681460 sec
RG 5.7
DW 89.600 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.80 usec
PL1 -3.00 dB
PL1W 30.07123375 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
171.52
162.80
137.07
131.26
129.33
128.48
128.38
127.50
127.01
113.88
69.17
51.95
40.63
40.42
40.22
40.01
39.80
39.59
39.38
37.24
33.62
30.95
22.20
20.22
19.18
14.22
131 130 129 128 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm
NAME dp47dpL1rac
EXPNO 407
PROCNO 1
Date_ 20131125
Time 13.23
INSTRUM spect
PROBHD 5 mm BBI 1H/2H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 1625.5
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -6.00 dB
PL1W 150.00000000 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 18.00 dB
PL2W 30.07123375 W
PL12W 0.23886430 W
PL13W 0.23886430 W
SFO2 400.1316005 MHz
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
NAME          dp47dpL1rac
EXPNO                 405
PROCNO                  1
Date_            20131125
Time                10.30
INSTRUM             spect
PROBHD   5 mm BBI 1H/2H
PULPROG           dept135
TD                  32768
SOLVENT               DMSO
NS                    256
DS                      4
SWH             16025.641 Hz
FIDRES          0.489064 Hz
AQ              1.0224428 sec
RG                  16384
DW                31.200 usec
DE                 6.50 usec
TE                300.0 K
CNST2         145.0000000
D1              2.00000000 sec
D2              0.00344828 sec
D12             0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PL1                -6.00 dB
PL1W        150.00000000 W
SFO1         100.6198119 MHz

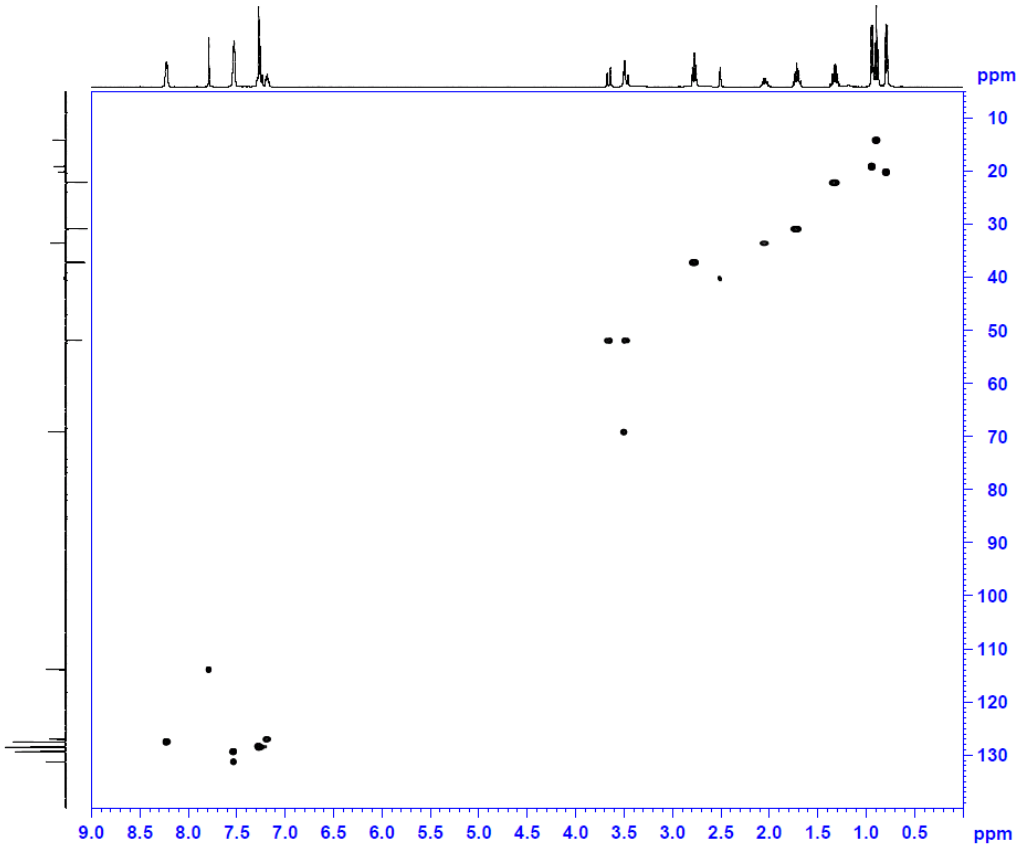
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
P3                 7.00 usec
P4                14.00 usec
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              18.00 dB
PL2W         30.07123375 W
PL12W         0.23886430 W
SFO2         400.1316005 MHz
SI                 65536
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```




```
NAME          dp47dpL1rac
EXPNO                 404
PROCNO                  1
Date_            20131125
Time                 9.47
INSTRUM             spect
PROBHD   5 mm BBI 1H/2H
PULPROG          cosygpqf
TD                  2048
SOLVENT               DMSO
NS                      4
DS                      8
SWH              4807.692 Hz
FIDRES          2.347506 Hz
AQ              0.2131460 sec
RG                     57
DW                104.000 usec
DE                 6.50 usec
TE                300.0 K
D0              0.00000300 sec
D1              1.50000000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00020800 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                 7.00 usec
P1                 7.00 usec
PL1                -3.00 dB
PL1W         30.07123375 W
SFO1         400.1320007 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPZ1               10.00 %
P16              1000.00 usec
ND0                    1
TD                   256
SFO1             400.132 MHz
FIDRES         18.780018 Hz
SW                12.015 ppm
FnMODE                QF
SI                  2048
SF           400.1300000 MHz
WDW                 SINE
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.40
SI                  1024
MC2                   QF
SF           400.1300000 MHz
WDW                 SINE
SSB                    0
LB                 0.00 Hz
GB                     0
```

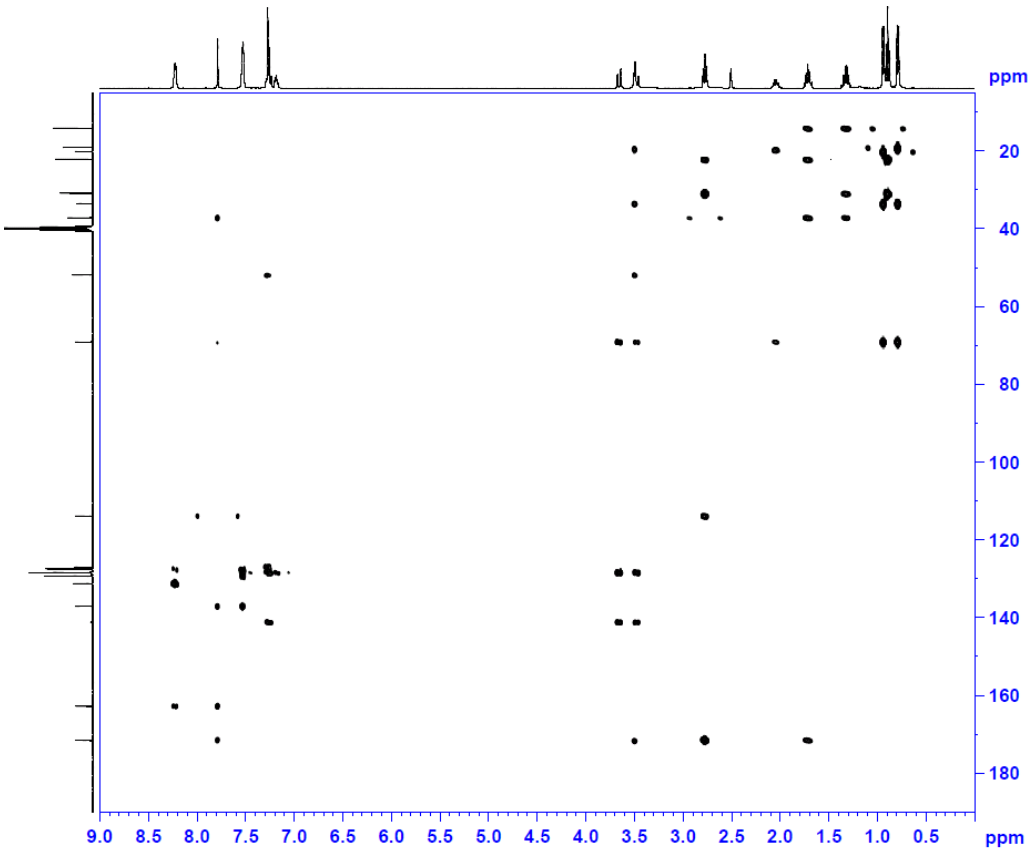



```
NAME            dp47dpL1rac
EXPNO                   406
PROCNO                    1
Date_              20131125
Time                  10.31
INSTRUM               spect
PROBHD   5 mm BBI 1H/2H
PULPROG          hsqcetgp
TD                    1024
SOLVENT               DMSO
NS                       8
DS                      16
SWH                4807.692 Hz
FIDRES             4.695012 Hz
AQ                 0.1066600 sec
RG                    7298.2
DW                  104.000 usec
DE                    6.50 usec
TE                   300.0 K
CNST2              145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                      7.00 usec
P2                     14.00 usec
P28                  1000.00 usec
PL1                    -3.00 dB
PL1W             30.07123375 W
SFO1             400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                     13C
P3                     10.00 usec
P4                     20.00 usec
PCPD2                  80.00 usec
PL2                    -6.00 dB
PL12                   12.00 dB
PL2W            150.00000000 W
PL12W            2.37733984 W
SFO2             100.6202727 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPZ1                    80.00 %
GPZ2                    20.10 %
P16                   1000.00 usec
ND0                          2
TD                         256
SFO1             100.6203 MHz
FIDRES           65.104164 Hz
SW                  165.639 ppm
FnMODE       Echo-Antiecho
SI                        2048
SF               400.1299983 MHz
WDW                     QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                        1024
MC2           echo-antiecho
SF               100.6127610 MHz
WDW                     QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
```

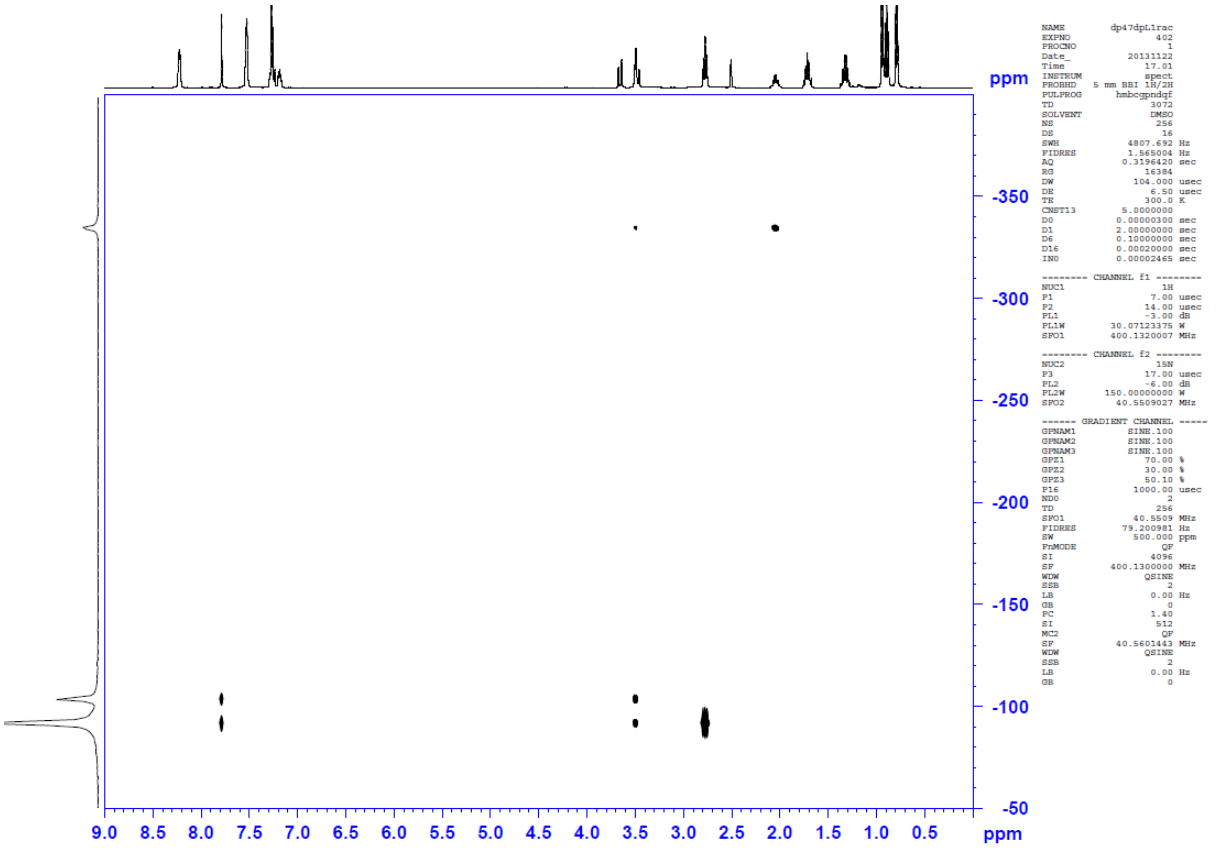



```
NAME            dp47dpL1rac
EXPNO                   408
PROCNO                    1
Date_              20131125
Time                  13.24
INSTRUM               spect
PROBHD   5 mm BBI 1H/2H
PULPROG       hmbcgplpndqf
TD                    2048
SOLVENT               DMSO
NS                      16
DS                      16
SWH                4807.692 Hz
FIDRES             2.347506 Hz
AQ                 0.2131460 sec
RG                   14596.5
DW                  104.000 usec
DE                    6.50 usec
TE                   300.0 K
CNST2              145.0000000
CNST13              10.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D2                 0.00344828 sec
D6                 0.05000000 sec
D16                0.00020000 sec
IN0                0.00002070 sec

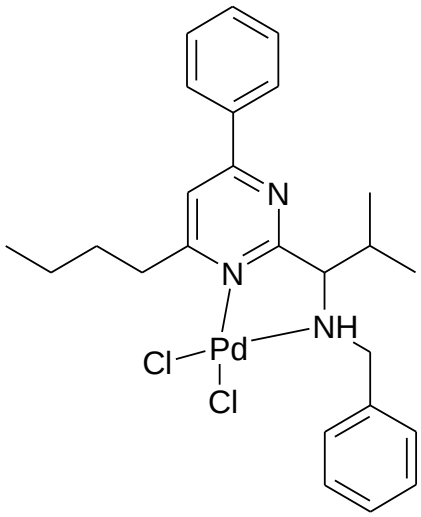
======== CHANNEL f1 ========
NUC1                      1H
P1                      7.00 usec
P2                     14.00 usec
PL1                    -3.00 dB
PL1W             30.07123375 W
SFO1             400.1320007 MHz

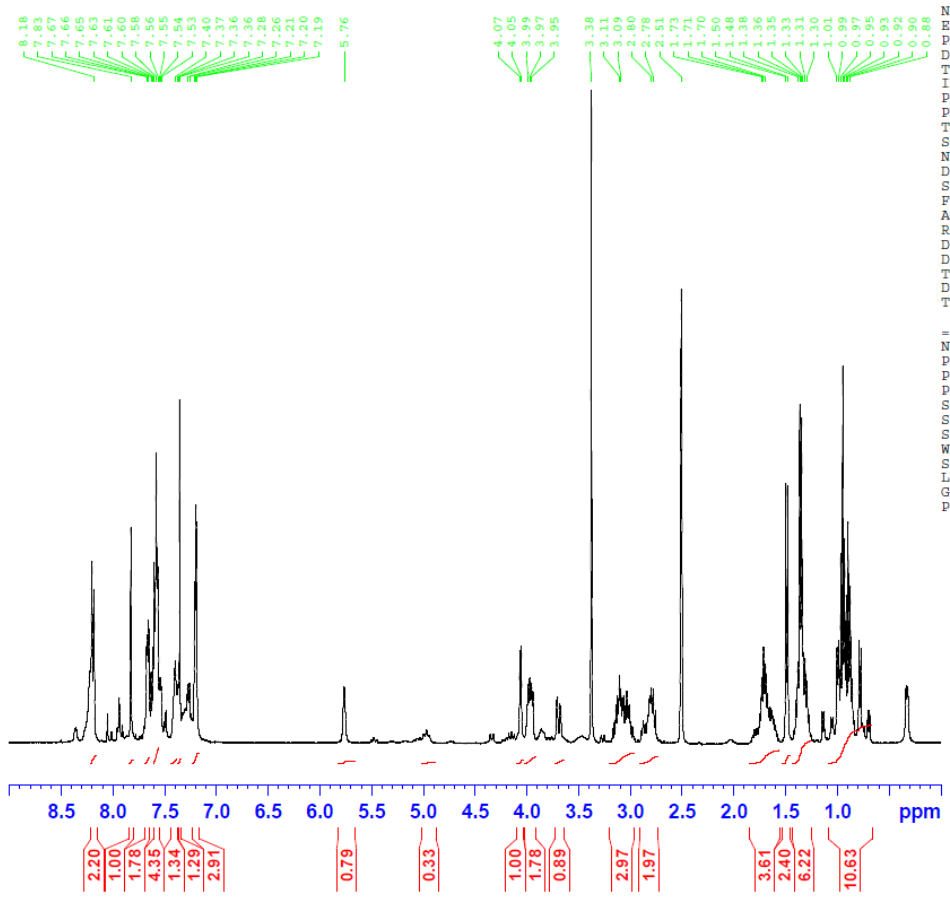
======== CHANNEL f2 ========
NUC2                     13C
P3                     10.00 usec
PL2                    -6.00 dB
PL2W            150.00000000 W
SFO2             100.6243395 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPNAM3               SINE.100
GPZ1                    50.00 %
GPZ2                    30.00 %
GPZ3                    40.10 %
P16                   1000.00 usec
ND0                          2
TD                         226
SFO1             100.6243 MHz
FIDRES           106.857704 Hz
SW                  240.000 ppm
FnMODE                   QF
SI                        2048
SF               400.1299991 MHz
WDW                     SINE
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                        1024
MC2                      QF
SF               100.6127514 MHz
WDW                     SINE
SSB                          0
LB                        0.00 Hz
GB                           0
```


ppm
-350
-300
-250
-200
-150
-100
-50
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm
NAME dp47dpL1rac
EXPNO 402
PROCNO 1
Date 20131122
Time 17.01
INSTRUM spect
PROBHD 5 mm BBI 1H/2H
PULPROG hmbcgpndqf
TD 3072
SOLVENT DMSO
NS 256
DS 16
SWH 4807.692 Hz
FIDRES 1.565004 Hz
AQ 0.3196420 sec
RG 16384
DW 104.000 usec
DE 6.50 usec
TE 300.0 K
CNST13 5.0000000
D0 0.00000300 sec
D1 2.00000000 sec
D6 0.10000000 sec
D16 0.00020000 sec
IN0 0.00002465 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.00 usec
P2 14.00 usec
PL1 -3.00 dB
PLW 30.07123375 W
SFO1 400.1320007 MHz
======== CHANNEL f2 ========
NUC2 15N
P3 17.00 usec
PL2 -6.00 dB
PLW 150.00000000 W
SFO2 40.5509027 MHz
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 70.00 %
GPZ2 30.00 %
GPZ3 50.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 40.5509 MHz
FIDRES 79.200981 Hz
SW 500.000 ppm
FnMODE QF
SI 4096
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 QF
SF 40.5601443 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

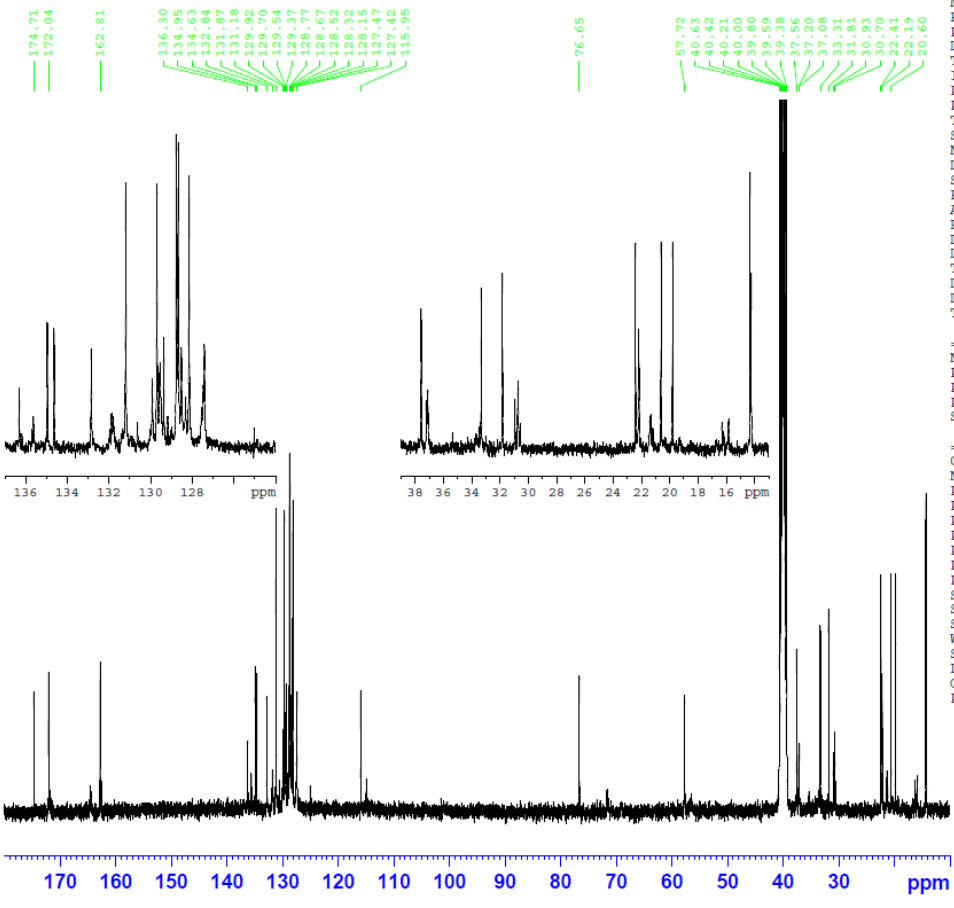
Complex **15**


N
N
NH
Cl
Pd
Cl




```
NAME            dp46dp42
EXPNO                420
PROCNO                 1
Date_           20131128
Time               20.00
INSTRUM            spect
PROBHD    5 mm BBI 1H/2H
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH           5580.357 Hz
FIDRES       0.340598 Hz
AQ           1.4681460 sec
RG                   7.1
DW              89.600 usec
DE               6.50 usec
TE              300.0 K
D1           1.00000000 sec
TD0                    1

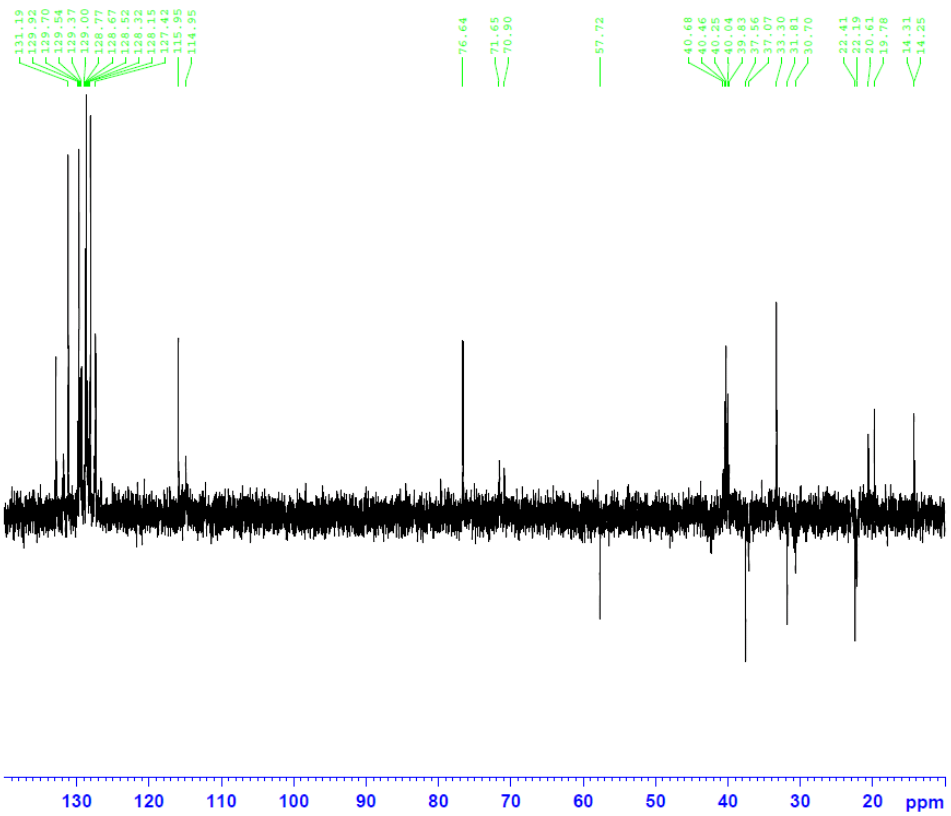
======== CHANNEL f1 ========
NUC1                  1H
P1                 7.80 usec
PL1               -3.00 dB
PL1W        30.07123375 W
SFO1       400.1326008 MHz
SI                 32768
SF         400.1300000 MHz
WDW                   no
SSB                    0
LB              0.00 Hz
GB                     0
PC                  1.00
```




```
NAME            dp46dp42
EXPNO                415
PROCNO                 1
Date_           20131128
Time               10.03
INSTRUM            spect
PROBHD    5 mm BBI 1H/2H
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  8192
DS                     4
SWH          24038.461 Hz
FIDRES       0.366798 Hz
AQ           1.3632196 sec
RG              7298.2
DW              20.800 usec
DE               6.50 usec
TE              300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -6.00 dB
PL1W       150.00000000 W
SFO1        100.6228298 MHz

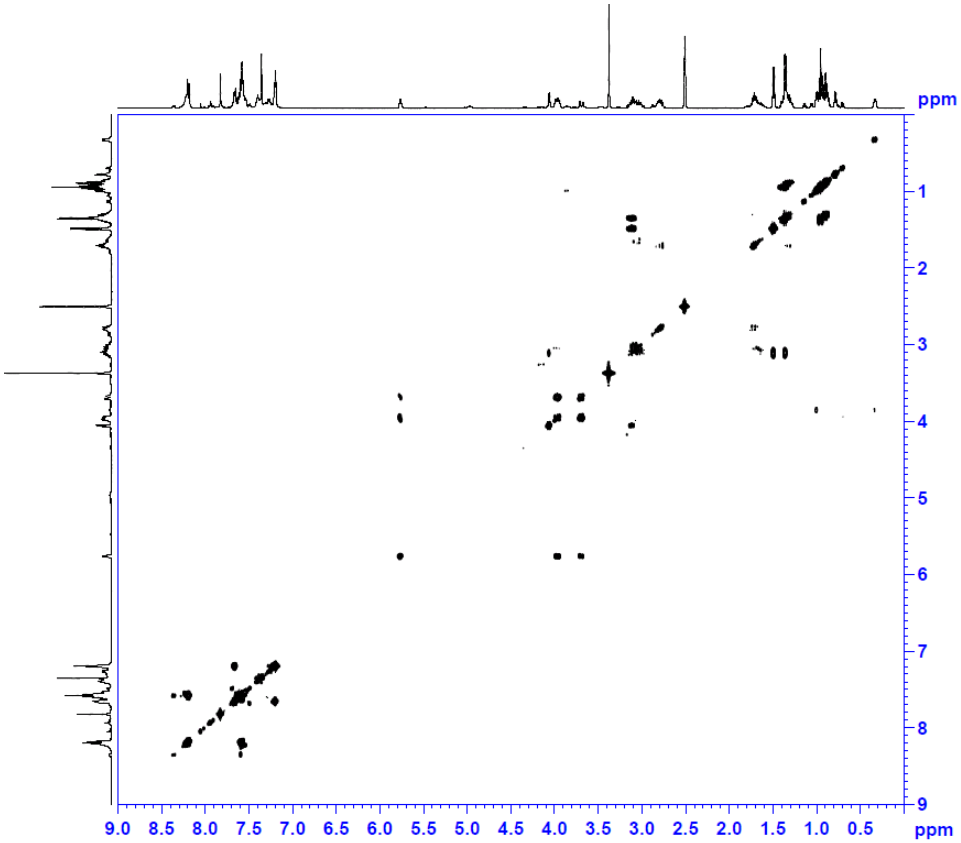
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              18.00 dB
PL13              18.00 dB
PL2W        30.07123375 W
PL12W        0.23886430 W
PL13W        0.23886430 W
SFO2       400.1316005 MHz
SI                 65536
SF         100.6127690 MHz
WDW                   EM
SSB                    0
LB              1.00 Hz
GB                     0
PC                  1.40
```




```
NAME            dp46dp42
EXPNO                411
PROCNO                 1
Date_           20131127
Time               16.11
INSTRUM            spect
PROBHD   5 mm BBI 1H/2H
PULPROG          dept135
TD                 32768
SOLVENT             DMSO
NS                   256
DS                     4
SWH          16025.641 Hz
FIDRES        0.489064 Hz
AQ           1.0224428 sec
RG                 16384
DW              31.200 usec
DE               6.50 usec
TE              300.0 K
CNST2       145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
P2               20.00 usec
PL1               -6.00 dB
PL1W       150.00000000 W
SFO1        100.6198119 MHz

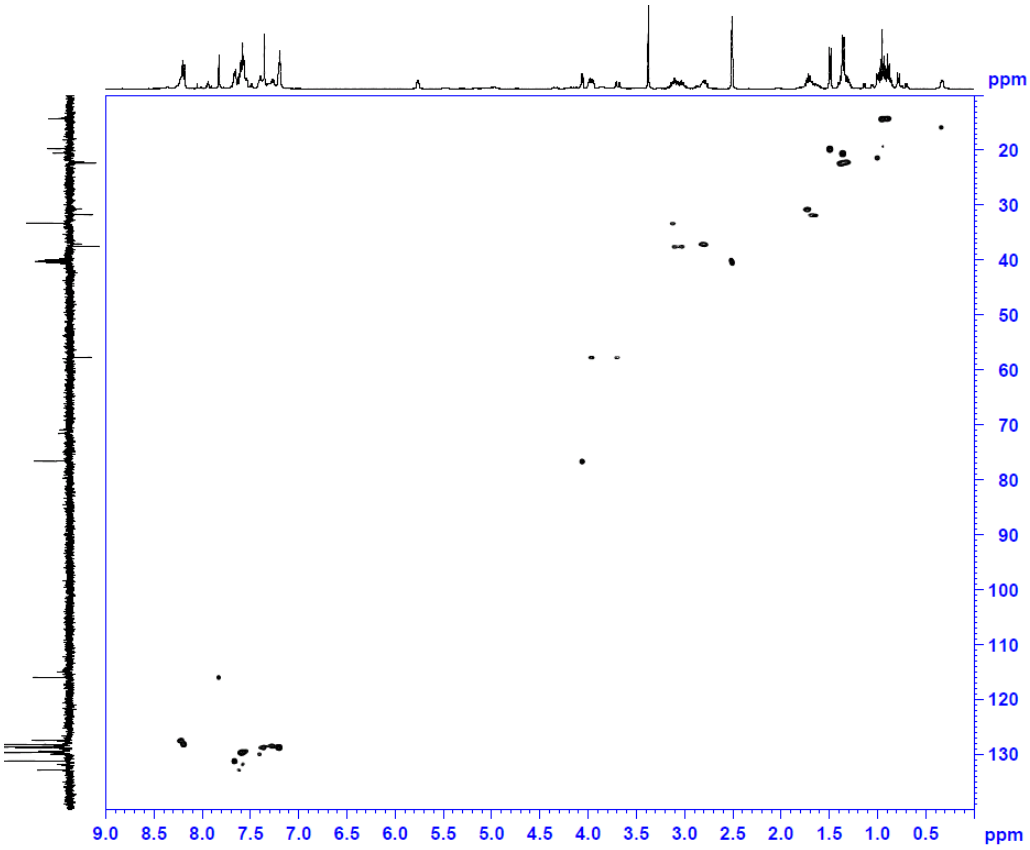
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
P3                7.00 usec
P4               14.00 usec
PCPD2            80.00 usec
PL2               -3.00 dB
PL12              18.00 dB
PL2W        30.07123375 W
PL12W        0.23886430 W
SFO2        400.1316005 MHz
SI                 65536
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```




```
NAME            dp46dp42
EXPNO                410
PROCNO                 1
Date_           20131127
Time               14.58
INSTRUM            spect
PROBHD   5 mm BBI 1H/2H
PULPROG         cosygpqf
TD                  2048
SOLVENT             DMSO
NS                     8
DS                     8
SWH           4807.692 Hz
FIDRES        2.347506 Hz
AQ            0.2131460 sec
RG                  90.5
DW              104.000 usec
DE               6.50 usec
TE              300.0 K
D0            0.00000300 sec
D1            1.50000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00020825 sec

======== CHANNEL f1 ========
NUC1                1H
P0               7.00 usec
P1               7.00 usec
PL1              -3.00 dB
PL1W        30.07123375 W
SFO1        400.1320007 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1             10.00 %
P16            1000.00 usec
ND0                    1
TD                   256
SFO1          400.132 MHz
FIDRES       18.756187 Hz
SW              12.000 ppm
FnMODE                QF
SI                  2048
SF          400.1300000 MHz
WDW                SINE
SSB                    0
LB                0.00 Hz
GB                     0
PC                1.40
SI                  1024
MC2                   QF
SF          400.1300000 MHz
WDW                SINE
SSB                    0
LB                0.00 Hz
GB                     0
```

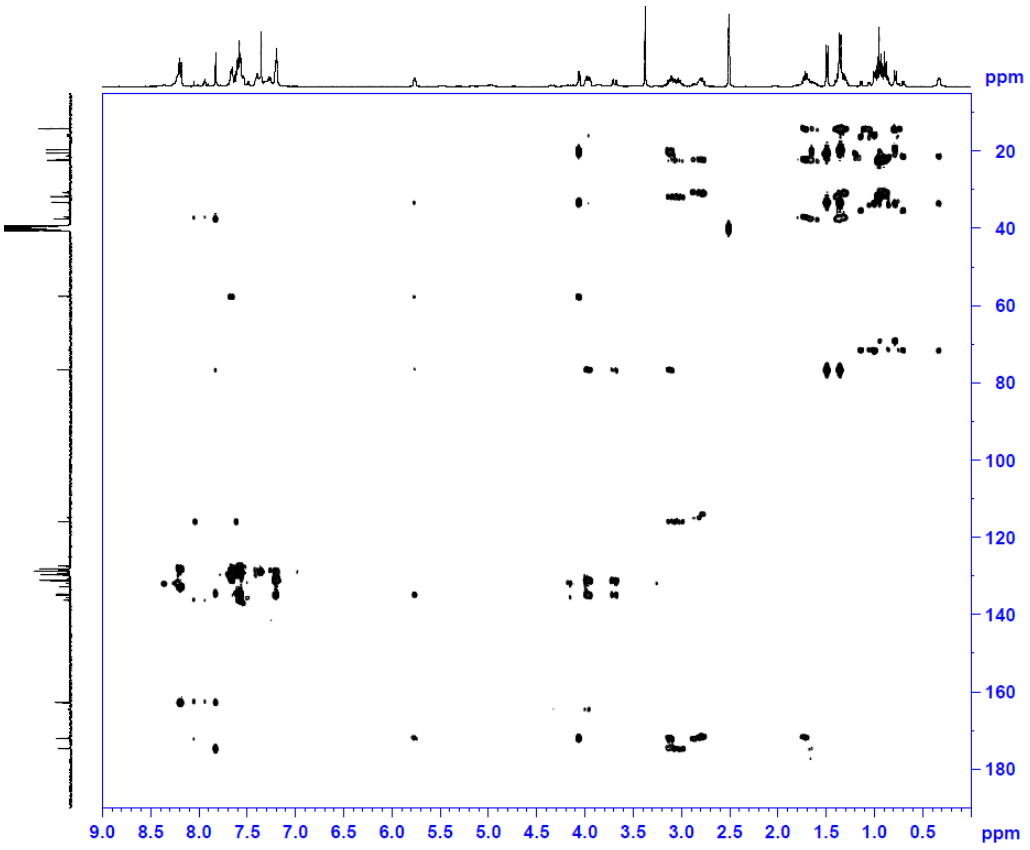



```
NAME              dp46dp42
EXPNO                  412
PROCNO                   1
Date_             20131127
Time                 16.12
INSTRUM              spect
PROBHD   5 mm BBI 1H/2H
PULPROG          hsqcetgp
TD                    1024
SOLVENT               DMSO
NS                      24
DS                      16
SWH               4807.692 Hz
FIDRES            4.695012 Hz
AQ                0.1066500 sec
RG                   11585.2
DW                 104.000 usec
DE                    6.50 usec
TE                  300.0 K
CNST2             145.0000000
D0                0.00000300 sec
D1                1.50000000 sec
D4                0.00172414 sec
D11               0.03000000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00003000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                     1H
P1                     7.00 usec
P2                    14.00 usec
P28                 1000.00 usec
PL1                   -3.00 dB
PL1W          30.07123375 W
SFO1          400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG2               garp
NUC2                    13C
P3                    10.00 usec
P4                    20.00 usec
PCPD2                 80.00 usec
PL2                   -6.00 dB
PL12                  12.00 dB
PL2W          150.00000000 W
PL12W          2.37733984 W
SFO2          100.6202727 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec
ND0                      2
TD                     256
SFO1              100.6203 MHz
FIDRES            65.104164 Hz
SW                  165.639 ppm
FnMODE        Echo-Antiecho
SI                    2048
SF                400.1299979 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
PC                     1.40
SI                     1024
MC2           echo-antiecho
SF                100.6127612 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
```

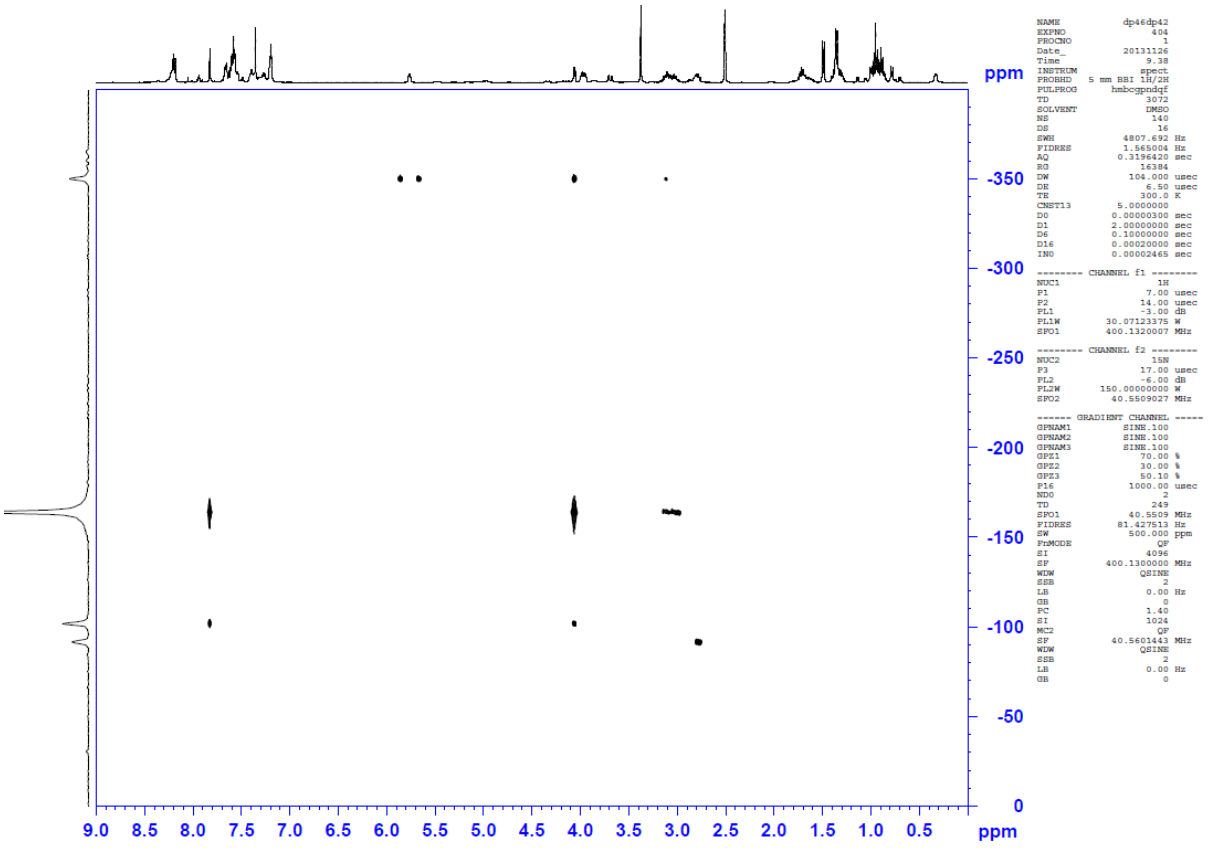



```
NAME              dp46dp42
EXPNO                  413
PROCNO                   1
Date_             20131127
Time                 18.59
INSTRUM              spect
PROBHD   5 mm BBI 1H/2H
PULPROG     hmbcgplpndqf
TD                    2048
SOLVENT               DMSO
NS                      32
DS                      16
SWH               4807.692 Hz
FIDRES            2.347506 Hz
AQ                0.2133460 sec
RG                   16384
DW                 104.000 usec
DE                    6.50 usec
TE                  300.0 K
CNST2             145.0000000
CNST13             10.0000000
D0                0.00000300 sec
D1                1.50000000 sec
D2                0.00344828 sec
D6                0.05000000 sec
D16               0.00020000 sec
IN0               0.00002070 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                     7.00 usec
P2                    14.00 usec
PL1                   -3.00 dB
PL1W          30.07123375 W
SFO1          400.1320007 MHz

======== CHANNEL f2 ========
NUC2                    13C
P3                    10.00 usec
PL2                   -6.00 dB
PL2W          150.00000000 W
SFO2          100.6243395 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPNAM3             SINE.100
GPZ1                  50.00 %
GPZ2                  30.00 %
GPZ3                  40.10 %
P16                 1000.00 usec
ND0                      2
TD                     256
SFO1              100.6243 MHz
FIDRES            94.335320 Hz
SW                  240.000 ppm
FnMODE                   QF
SI                    2048
SF                400.1299989 MHz
WDW                   SINE
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.40
SI                     1024
MC2                      QF
SF                100.6127565 MHz
WDW                   SINE
SSB                       0
LB                     0.00 Hz
GB                        0
```

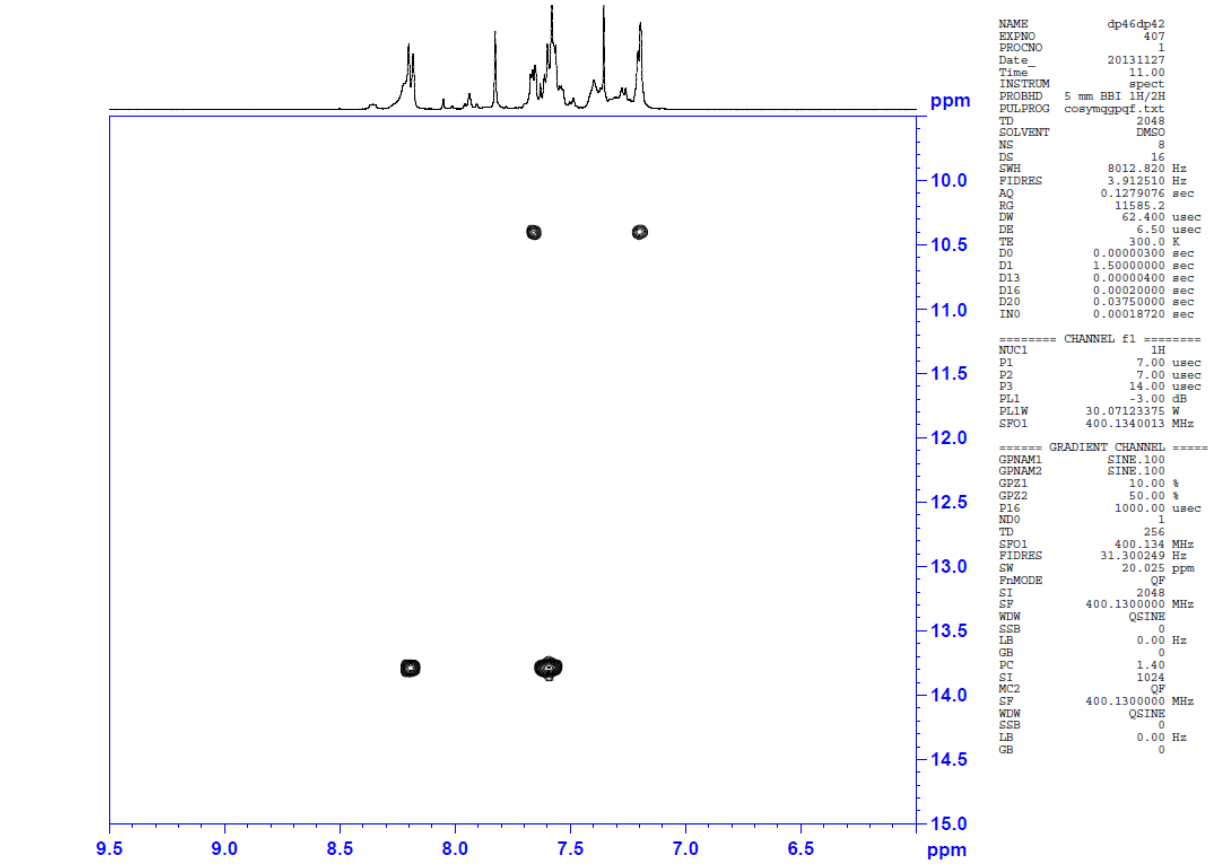



```
NAME                dp46dp42
EXPNO                    404
PROCNO                     1
Date_               20131126
Time                    9.38
INSTRUM                spect
PROBHD    5 mm BBI 1H/2H
PULPROG          hmbcgpndqf
TD                      3072
SOLVENT                 DMSO
NS                       140
DS                        16
SWH                4807.692 Hz
FIDRES             1.565004 Hz
AQ                 0.3196420 sec
RG                     16384
DW                   104.000 usec
DE                      6.50 usec
TE                     300.0 K
CNST13             5.0000000
D0                 0.00000300 sec
D1                 2.00000000 sec
D6                 0.10000000 sec
D16                0.00020000 sec
IN0                0.00002465 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       7.00 usec
P2                      14.00 usec
PL1                     -3.00 dB
PL1W               30.07123375 W
SFO1              400.1320007 MHz

======== CHANNEL f2 ========
NUC2                      15N
P3                      17.00 usec
PL2                     -6.00 dB
PL2W              150.00000000 W
SFO2               40.5509027 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPNAM3                SINE.100
GPZ1                     70.00 %
GPZ2                     30.00 %
GPZ3                     50.10 %
P16                    1000.00 usec
ND0                          2
TD                         249
SFO1                  40.5509 MHz
FIDRES               81.427513 Hz
SW                      500.000 ppm
FnMODE                       QF
SI                         4096
SF                400.1300000 MHz
WDW                      QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                        1024
MC2                          QF
SF                 40.5601443 MHz
WDW                      QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
```

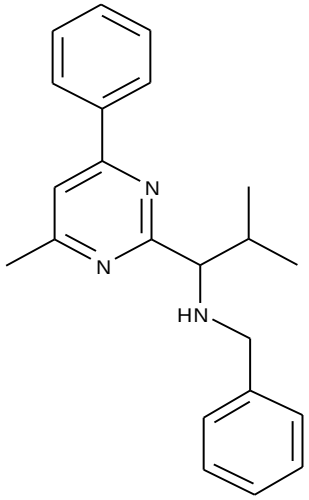


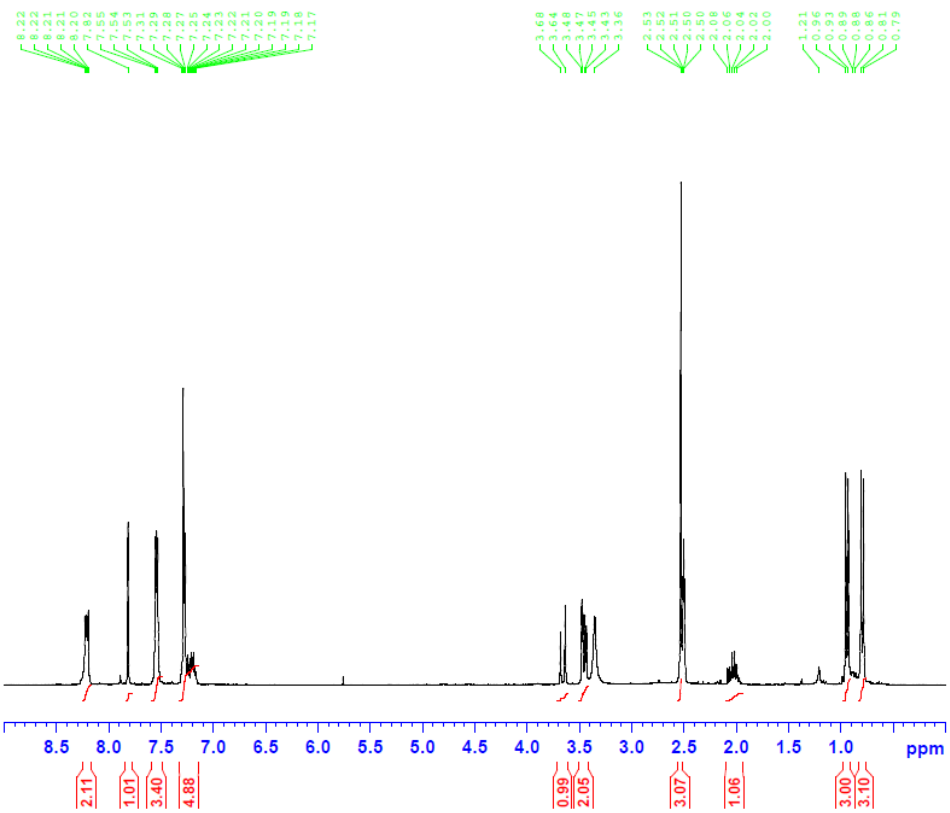

```
NAME                dp46dp42
EXPNO                    407
PROCNO                     1
Date_               20131127
Time                   11.00
INSTRUM                spect
PROBHD    5 mm BBI 1H/2H
PULPROG   cosymqgpqf.txt
TD                      2048
SOLVENT                 DMSO
NS                         8
DS                        16
SWH                8012.820 Hz
FIDRES             3.912510 Hz
AQ                 0.1279076 sec
RG                   11585.2
DW                    62.400 usec
DE                      6.50 usec
TE                     300.0 K
D0                 0.00000300 sec
D1                 1.50000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
D20                0.03750000 sec
IN0                0.00018720 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       7.00 usec
P2                       7.00 usec
P3                      14.00 usec
PL1                     -3.00 dB
PL1W               30.07123375 W
SFO1              400.1340013 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPZ1                     10.00 %
GPZ2                     50.00 %
P16                    1000.00 usec
ND0                          1
TD                         256
SFO1                400.134 MHz
FIDRES             31.300249 Hz
SW                      20.025 ppm
FnMODE                       QF
SI                         2048
SF                400.1300000 MHz
WDW                      QSINE
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                        1024
MC2                          QF
SF                400.1300000 MHz
WDW                      QSINE
SSB                          0
LB                        0.00 Hz
GB                           0
```

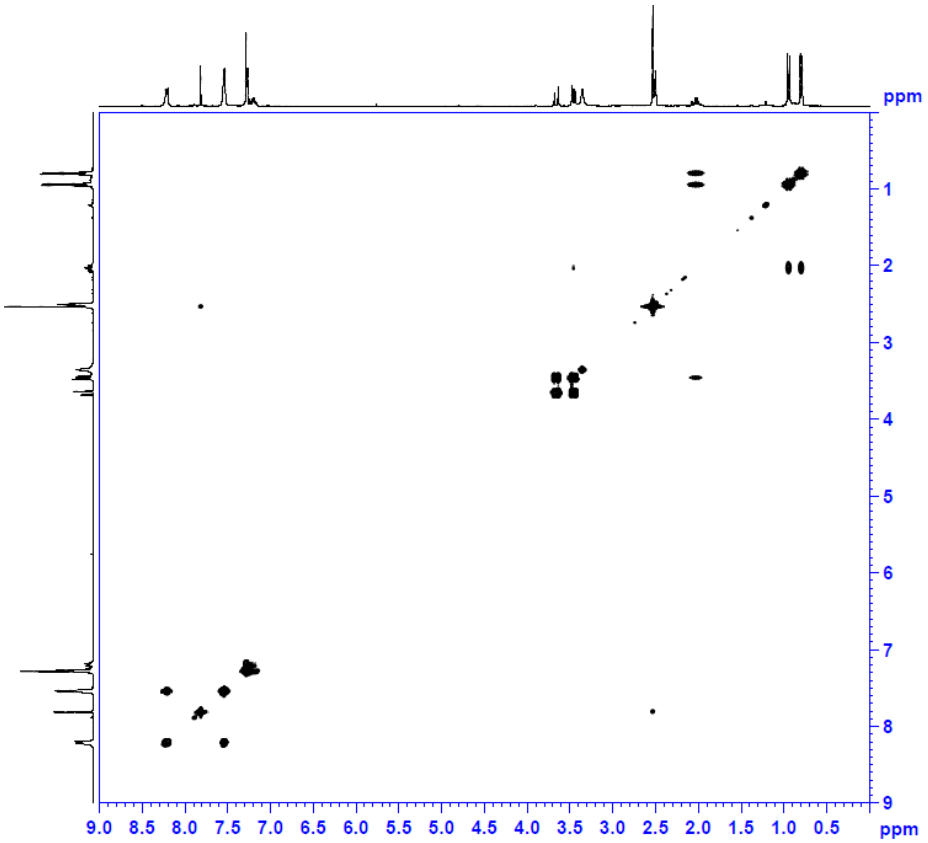
Ligand **6**






```
NAME          ligand-damien
EXPNO                    10
PROCNO                    1
Date_              20140209
Time                   6.52
INSTRUM               spect
PROBHD    5 mm Multinucl
PULPROG                zg30
TD                    16384
SOLVENT                DMSO
NS                       16
DS                        2
SWH                4194.631 Hz
FIDRES             0.256020 Hz
AQ                 1.9530228 sec
RG                      181
DW                  119.200 usec
DE                    6.50 usec
TE                   295.8 K
D1                 1.00000000 sec
TD0                       1

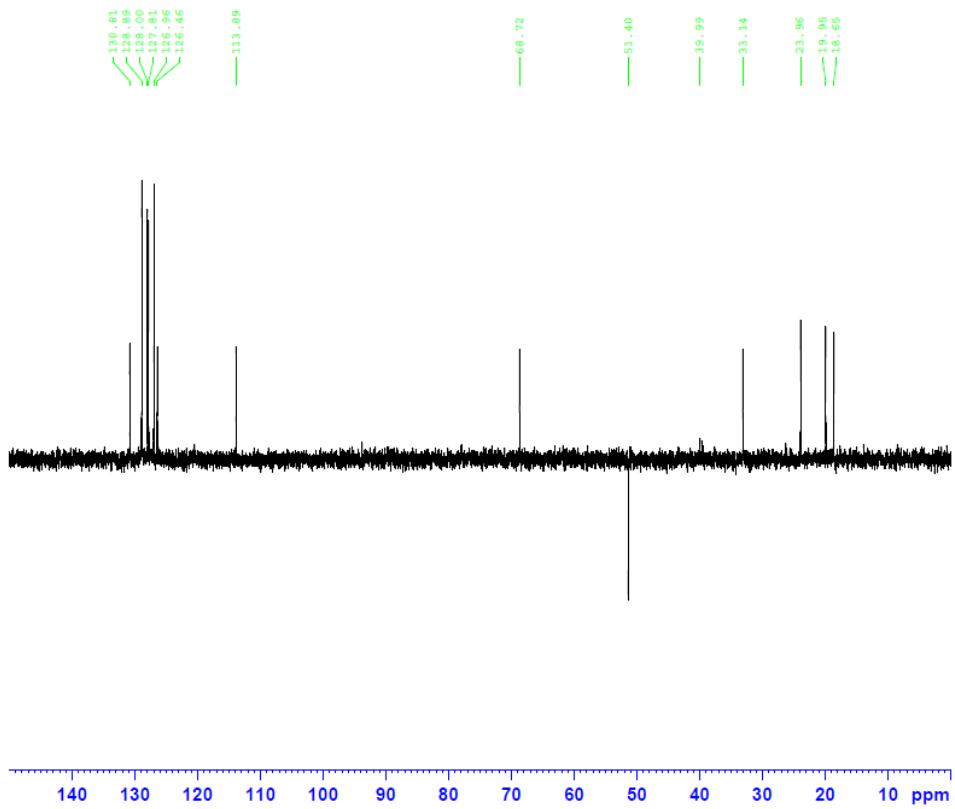
======== CHANNEL f1 ========
NUC1                     1H
P1                    6.70 usec
PL1                   0.00 dB
PL1W             15.07131863 W
SFO1             300.1319508 MHz
SI                    32768
SF               300.1300000 MHz
WDW                      no
SSB                       0
LB                    0.00 Hz
GB                        0
PC                    1.00
```




```
NAME          ligand-damien
EXPNO                    11
PROCNO                    1
Date_              20140209
Time                   6.53
INSTRUM               spect
PROBHD   5 mm Multinucl
PULPROG           cosygpqf
TD                     1024
SOLVENT                DMSO
NS                        4
DS                       16
SWH                2913.753 Hz
FIDRES             2.845462 Hz
AQ                 0.1757684 sec
RG                      90.5
DW                   171.600 usec
DE                    10.00 usec
TE                    295.8 K
D0                 0.00000300 sec
D1                 1.46641302 sec
D13                0.00000400 sec
D16                0.00010000 sec
IN0                0.00034320 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                     6.70 usec
P1                     6.70 usec
PL1                    0.00 dB
PL1W              15.07131863 W
SFO1              300.1312991 MHz

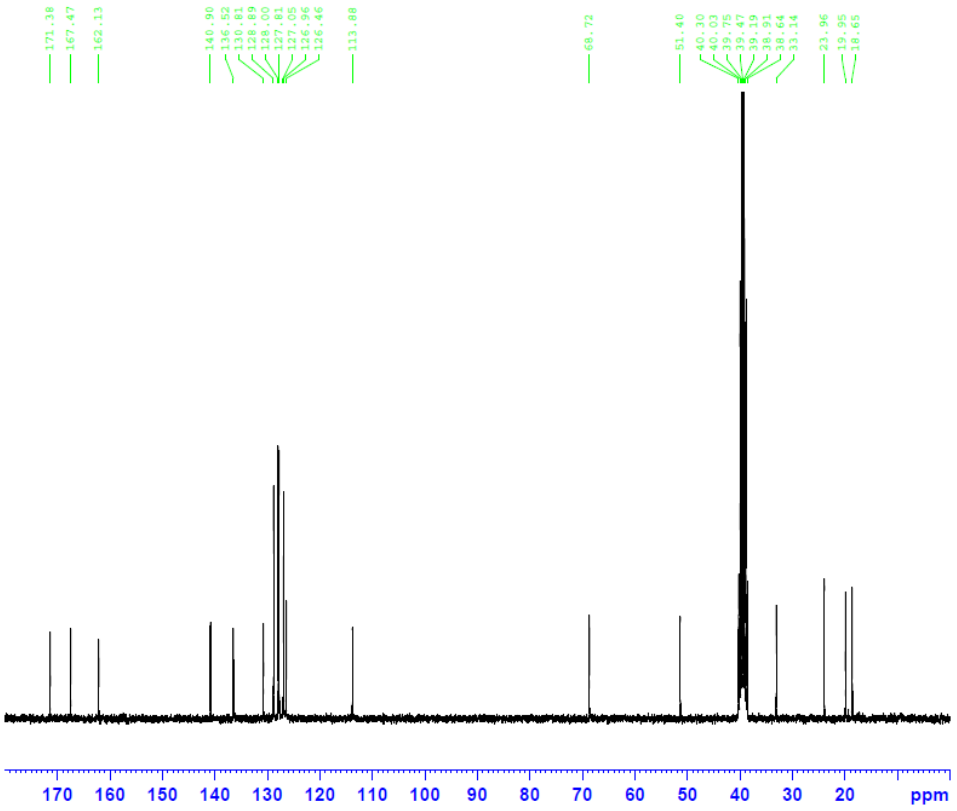
====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPZ1                    10.00 %
P16                   1000.00 usec
ND0                        1
TD                       256
SFO1              300.1313 MHz
FIDRES             11.381847 Hz
SW                     9.708 ppm
FnMODE                    QF
SI                      2048
SF                300.1300000 MHz
WDW                     SINE
SSB                        1
LB                     0.00 Hz
GB                         0
PC                      1.40
SI                      1024
MC2                       QF
SF                300.1300000 MHz
WDW                     SINE
SSB                        1
LB                     0.00 Hz
GB                         0
```




```
NAME          ligand-damien
EXPNO                    12
PROCNO                    1
Date_              20140209
Time                   7.35
INSTRUM               spect
PROBHD   5 mm Multinucl
PULPROG           dept135
TD                    32768
SOLVENT                DMSO
NS                      256
DS                        4
SWH               12077.295 Hz
FIDRES             0.368570 Hz
AQ                 1.3566452 sec
RG                    16384
DW                   41.400 usec
DE                    10.00 usec
TE                    295.8 K
CNST2            145.0000000
D1                 1.50000000 sec
D2                 0.00344828 sec
D12                0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     8.20 usec
P2                    16.40 usec
PL1                   -6.00 dB
PL1W          150.00000000 W
SFO1               75.4734091 MHz

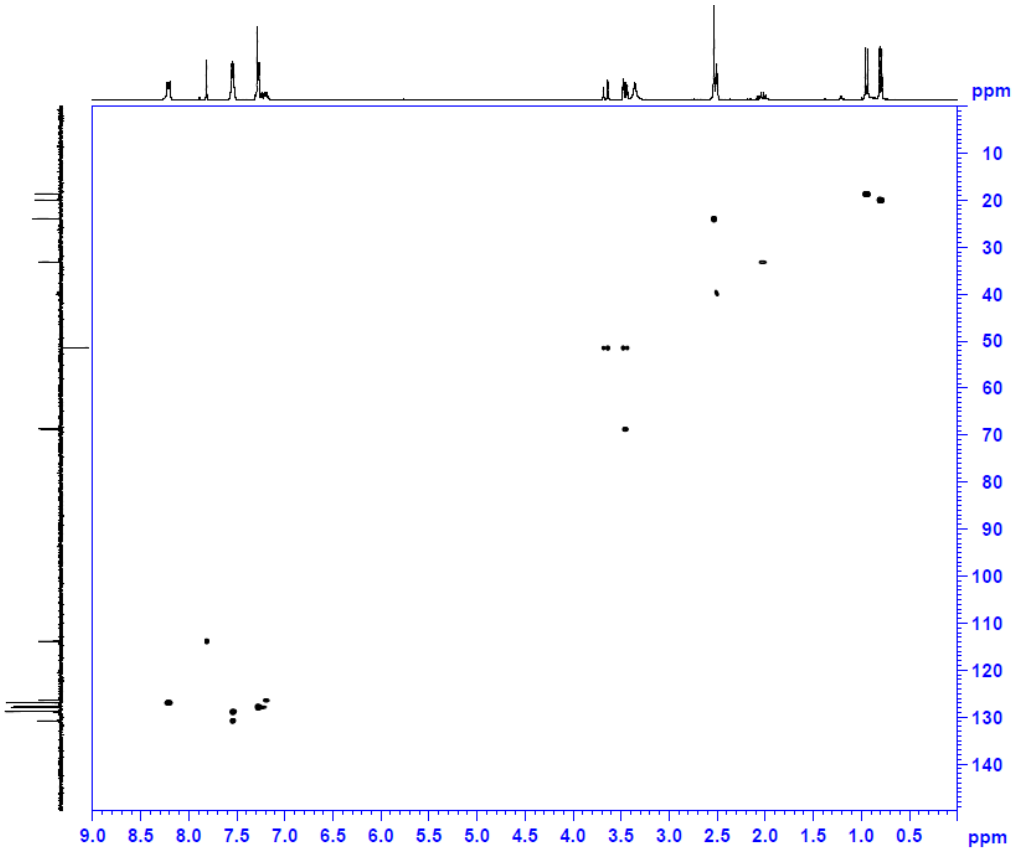
======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
P3                     6.70 usec
P4                    13.40 usec
PCPD2                 80.00 usec
PL2                    0.00 dB
PL12                  21.54 dB
PL2W              15.07131863 W
PL12W              0.10571854 W
SFO2              300.1312005 MHz
SI                     65536
SF                75.4677867 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                      1.40
```




```
NAME            ligand-damien
EXPNO                      14
PROCNO                      1
Date_                20140209
Time                    11.56
INSTRUM                 spect
PROBHD   5 mm Multinucl
PULPROG                 zgpg30
TD                       32768
SOLVENT                  DMSO
NS                       4096
DS                          4
SWH                17985.611 Hz
FIDRES              0.548877 Hz
AQ                  0.9110004 sec
RG                     4597.6
DW                     27.800 usec
DE                     10.00 usec
TE                     295.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       8.20 usec
PL1                     -6.00 dB
PL1W            150.00000000 W
SFO1              75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    21.54 dB
PL13                    21.54 dB
PL2W             15.07131863 W
PL12W             0.10571854 W
PL13W             0.10571854 W
SFO2            300.1312005 MHz
SI                       65536
SF                75.4677867 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

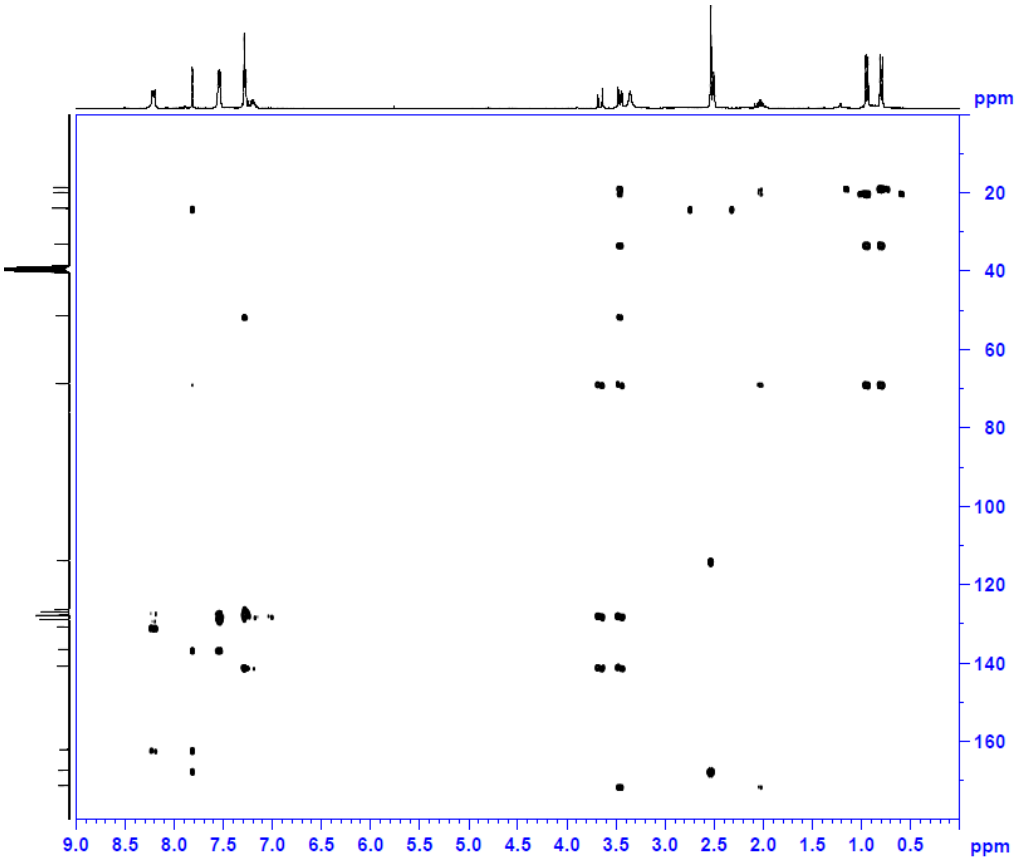



```
NAME            ligand-damien
EXPNO                      13
PROCNO                      1
Date_                20140209
Time                     7.36
INSTRUM                 spect
PROBHD   5 mm Multinucl
PULPROG              hsqcgpph
TD                       1024
SOLVENT                  DMSO
NS                          8
DS                         16
SWH                2913.753 Hz
FIDRES             2.845462 Hz
AQ                 0.1757684 sec
RG                     18390.4
DW                     171.600 usec
DE                     10.00 usec
TE                     295.8 K
CNST2              145.0000000
D0                 0.00000300 sec
D1                 1.46641302 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D13                0.00000400 sec
D16                0.00010000 sec
IN0                0.00004140 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       6.70 usec
P2                      13.40 usec
PL1                      0.00 dB
PL1W             15.07131863 W
SFO1            300.1312991 MHz

======== CHANNEL f2 ========
CPDPRG2                 garp
NUC2                      13C
P3                       8.20 usec
P4                      16.40 usec
PCPD2                   80.00 usec
PL2                     -6.00 dB
PL12                    13.79 dB
PL2W            150.00000000 W
PL12W             1.57431364 W
SFO2              75.4734091 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPNAM3              SINE.100
GPZ1                    80.00 %
GPZ2                    30.00 %
GPZ3                    20.10 %
P16                   1000.00 usec
ND0                         2
TD                        256
SFO1              75.47341 MHz
FIDRES           47.170879 Hz
SW                    160.000 ppm
FnMODE                  TPPI
SI                      2048
SF                300.1300000 MHz
WDW                     QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
PC                       1.40
SI                       1024
MC2                     TPPI
SF                75.4677800 MHz
WDW                     QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
```

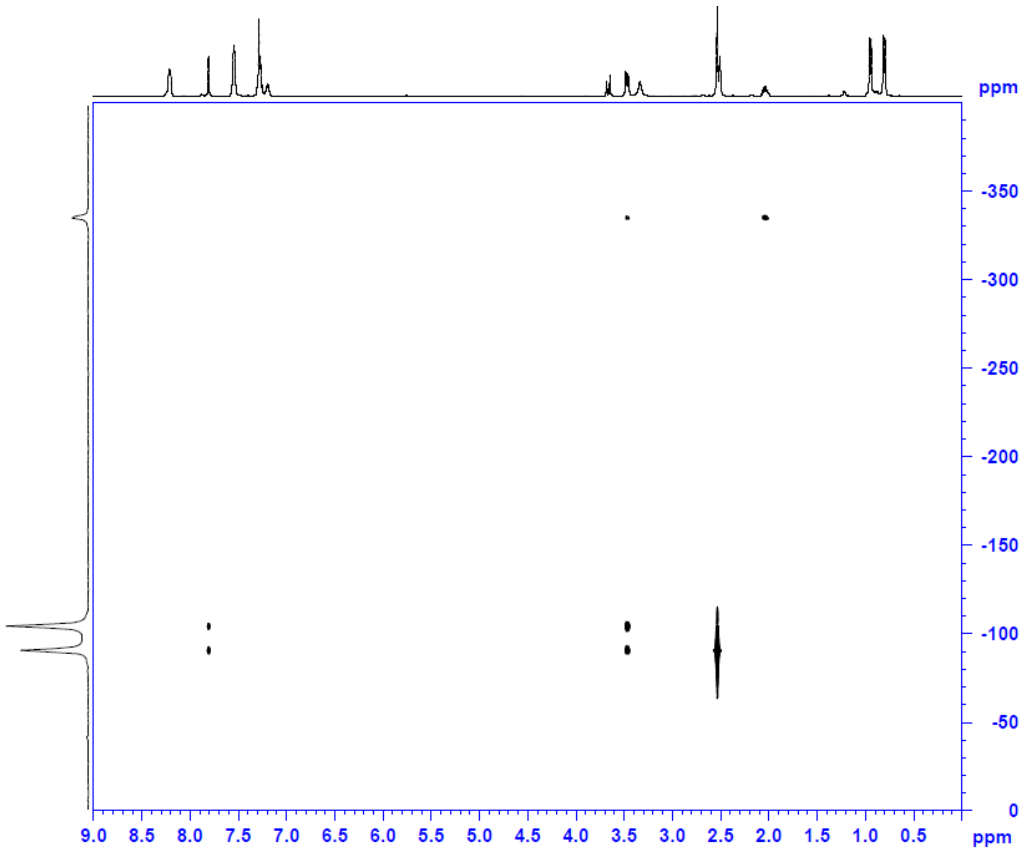



```
NAME          11gand-damien
EXPNO                    15
PROCNO                    1
Date_              20140209
Time                  11.57
INSTRUM               spect
PROBHD   5 mm Multinucl
PULPROG    hmbcgplpndqf
TD                     2048
SOLVENT                DMSO
NS                        8
DS                       16
SWH               2913.753 Hz
FIDRES            1.422731 Hz
AQ                0.3514868 sec
RG                  20642.5
DW                  171.600 usec
DE                    10.00 usec
TE                   295.9 K
CNST2             145.0000000
CNST13             10.0000000
D0                0.00000300 sec
D1                1.43282497 sec
D2                0.00344828 sec
D6                0.05000000 sec
D16               0.00010000 sec
IN0               0.00002760 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                      6.70 usec
P2                     13.40 usec
PL1                     0.00 dB
PL1W           15.07131863 W
SFO1          300.1312991 MHz

======== CHANNEL f2 ========
NUC2                     13C
P3                      8.20 usec
PL2                    -6.00 dB
PL2W          150.00000000 W
SFO2           75.4764278 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPNAM3               SINE.100
GPZ1                    50.00 %
GPZ2                    30.00 %
GPZ3                    40.10 %
P16                   1000.00 usec
ND0                         2
TD                        256
SFO1               75.47643 MHz
FIDRES            70.758446 Hz
SW                   239.998 ppm
FnMODE                   QF
SI                       2048
SF            300.1300000 MHz
WDW                    QSINE
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                       1024
MC2                      QF
SF             75.4677490 MHz
WDW                    QSINE
SSB                        0
LB                      0.00 Hz
GB                         0
```

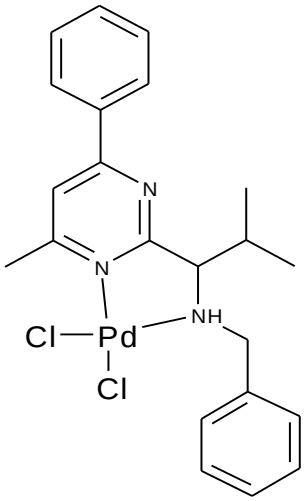



```
NAME          11gand-Damien
EXPNO                   403
PROCNO                    1
Date_              20140124
Time                  20.54
INSTRUM               spect
PROBHD   5 mm BBI 1H/2H
PULPROG    hmbcgpndqf
TD                     3072
SOLVENT                DMSO
NS                       256
DS                        16
SWH               4807.692 Hz
FIDRES            1.565004 Hz
AQ                0.3196420 sec
RG                    16384
DW                  104.000 usec
DE                     6.50 usec
TE                    300.0 K
CNST13              5.0000000
D0                0.00000300 sec
D1                2.00000000 sec
D6                0.10000000 sec
D16               0.00020000 sec
IN0               0.00002465 sec

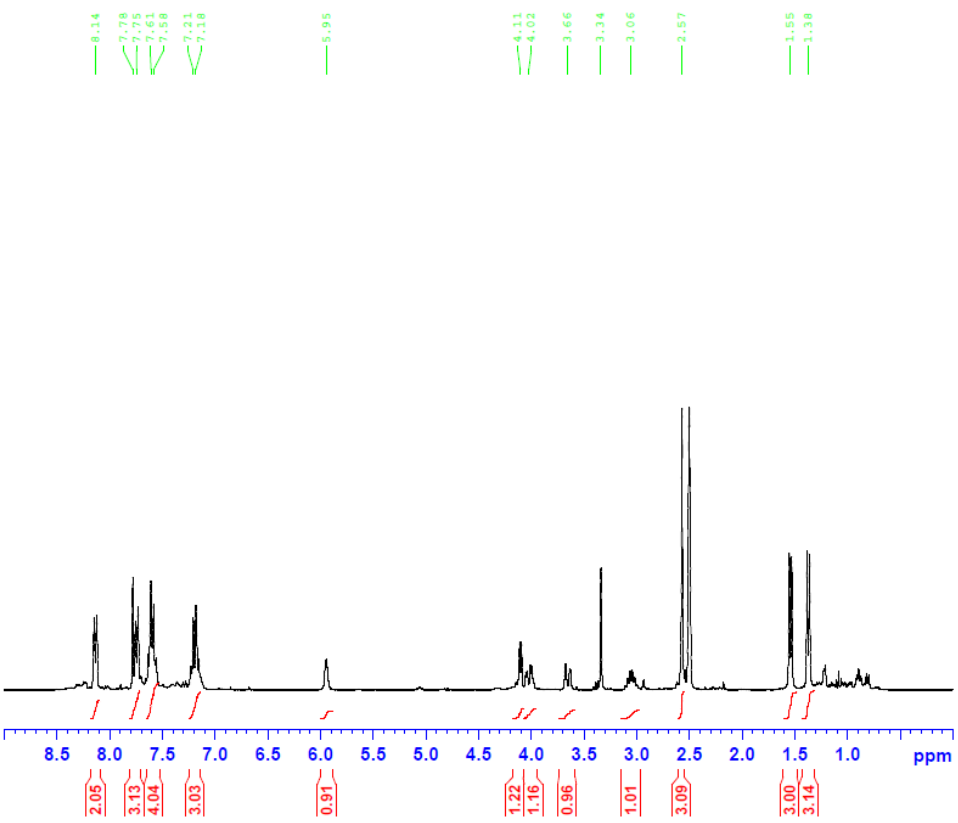
======== CHANNEL f1 ========
NUC1                      1H
P1                      7.00 usec
P2                     14.00 usec
PL1                    -3.00 dB
PL1W           30.07123375 W
SFO1          400.1320007 MHz

======== CHANNEL f2 ========
NUC2                     15N
P3                     17.00 usec
PL2                    -6.00 dB
PL2W          150.00000000 W
SFO2           40.5509027 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPNAM3               SINE.100
GPZ1                    70.00 %
GPZ2                    30.00 %
GPZ3                    50.10 %
P16                   1000.00 usec
ND0                         2
TD                        256
SFO1               40.5509 MHz
FIDRES            79.200981 Hz
SW                   500.000 ppm
FnMODE                   QF
SI                       4096
SF            400.1300000 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                        512
MC2                      QF
SF             40.5601443 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```



Complex **17**

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DW                    119.200 usec
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TE                     295.8 K
D1                  1.00000000 sec
TD0                        1

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PL1                     0.00 dB
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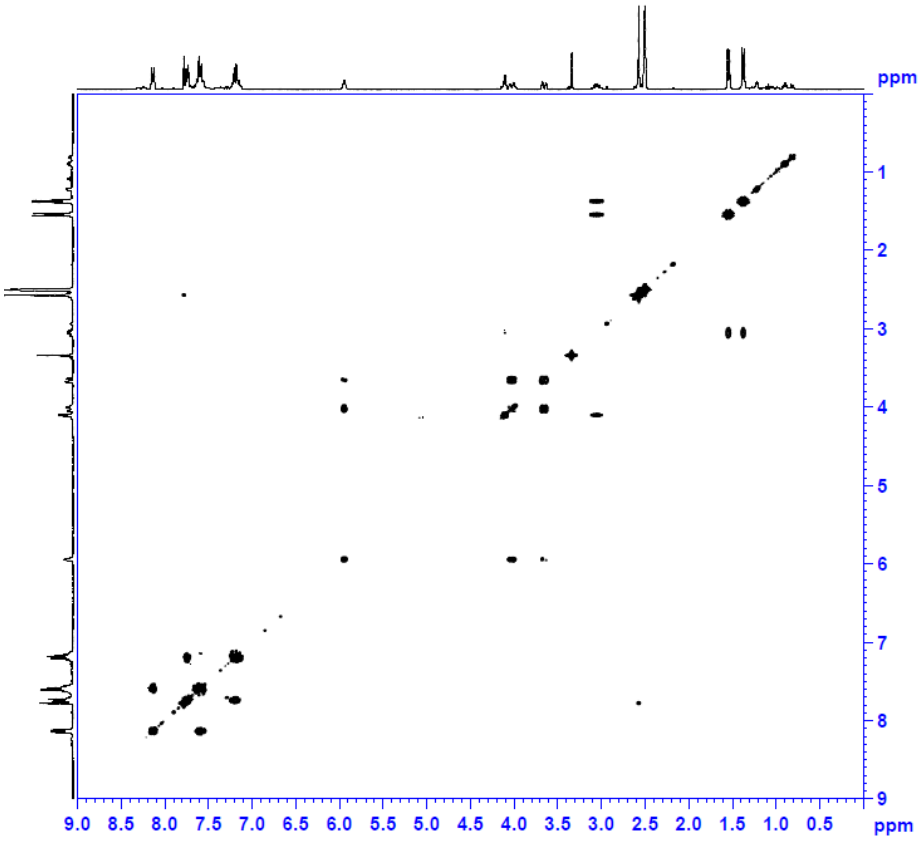


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D1           1.44798100 sec
D13          0.00000400 sec
D16          0.00010000 sec
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======== CHANNEL f1 ========
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SW                8.787 ppm
FnMODE               QF
SI                 2048
SF          300.1300000 MHz
WDW                SINE
SSB                   0
LB                 0.00 Hz
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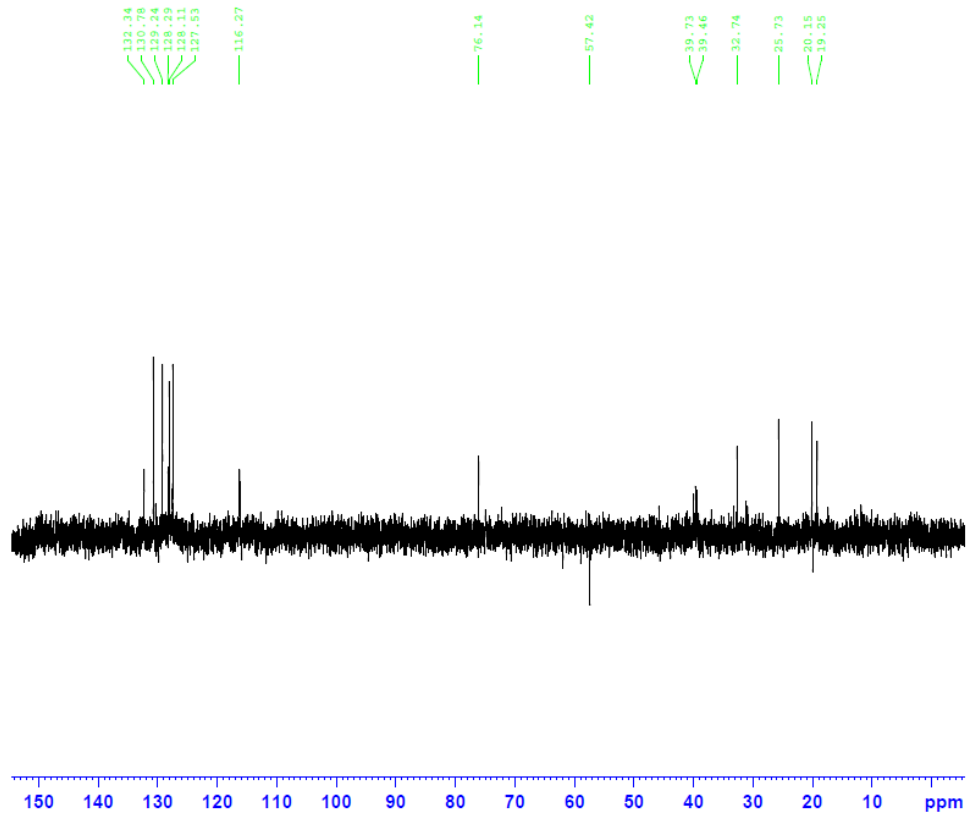


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SOLVENT             DMSO
NS                   256
DS                     4
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FIDRES         0.368570 Hz
AQ             1.3566452 sec
RG                 16384
DW                41.400 usec
DE                10.00 usec
TE                295.9 K
CNST2       145.0000000
D1           1.50000000 sec
D2           0.00344828 sec
D12          0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                8.20 usec
P2               16.40 usec
PL1              -6.00 dB
PL1W       150.00000000 W
SFO1        75.4734091 MHz

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NUC2                 1H
P3                6.70 usec
P4               13.40 usec
PCPD2            80.00 usec
PL2               0.00 dB
PL12             21.54 dB
PL2W        15.07131863 W
PL12W        0.10571854 W
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SF          75.4677867 MHz
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SSB                   0
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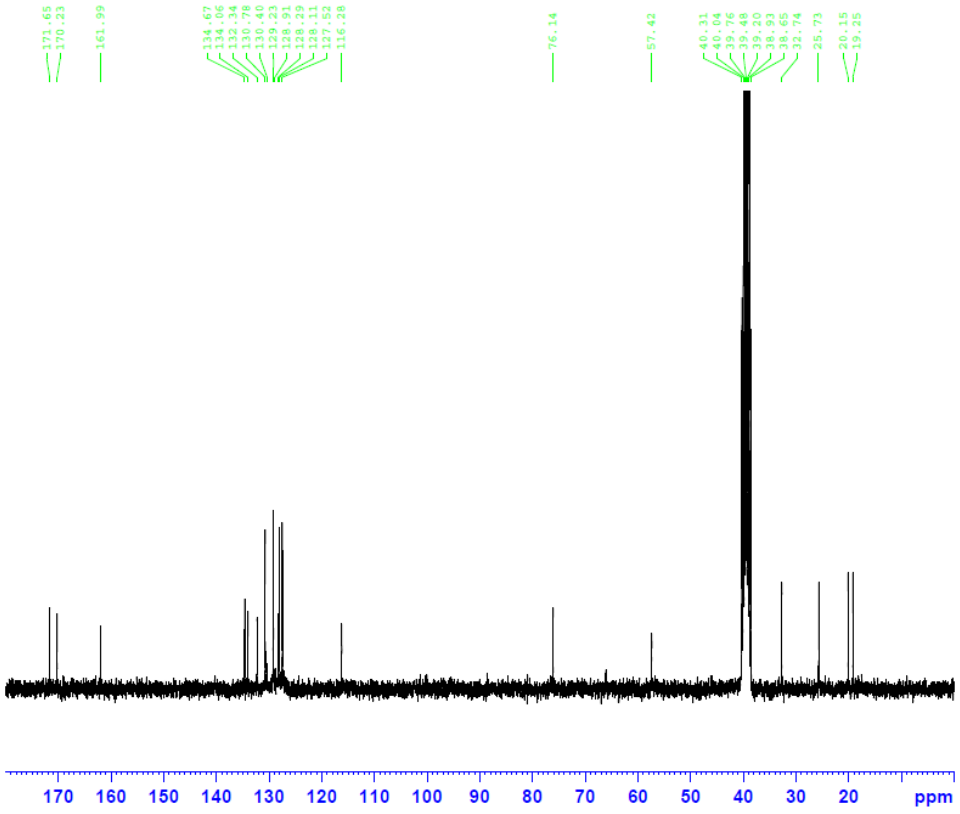


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TD               32768
SOLVENT           DMSO
NS                4096
DS                   4
SWH          17985.611 Hz
FIDRES         0.548877 Hz
AQ             0.9110004 sec
RG                5160.6
DW                27.800 usec
DE                10.00 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.20 usec
PL1               -6.00 dB
PL1W       150.00000000 W
SFO1         75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               21.54 dB
PL13               21.54 dB
PL2W        15.07131863 W
PL12W        0.10571854 W
PL13W        0.10571854 W
SFO2       300.1312005 MHz
SI                65536
SF           75.4677867 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
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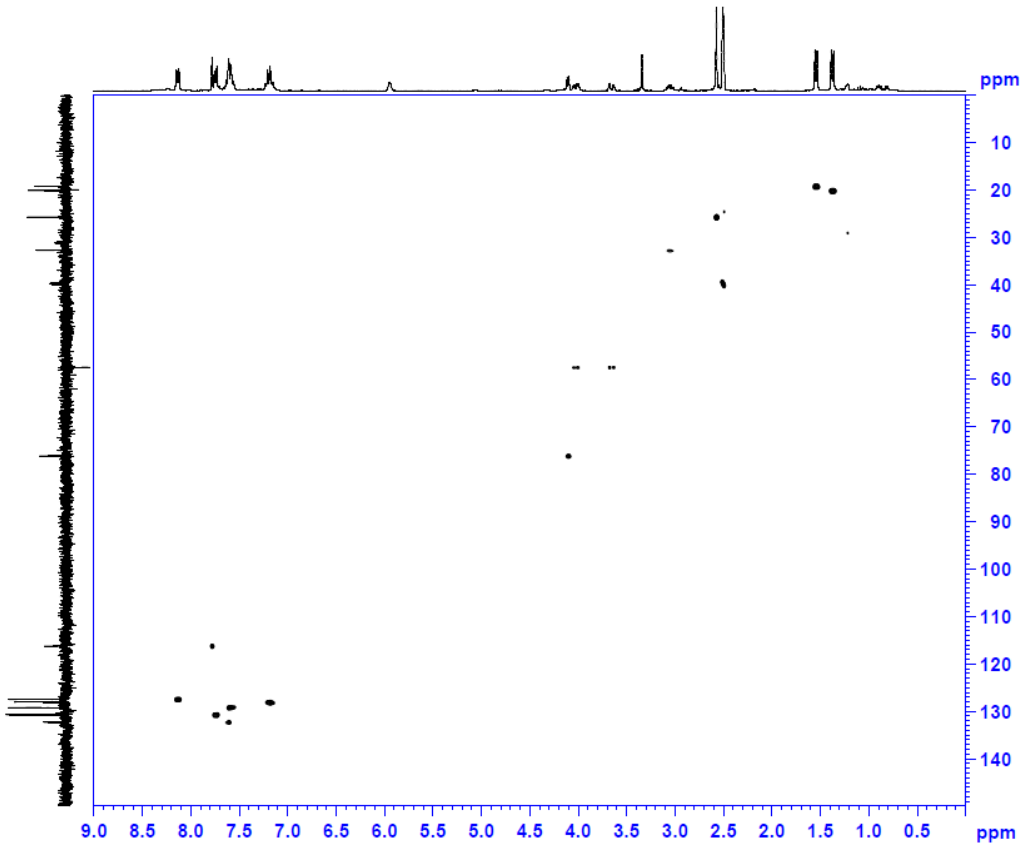


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SOLVENT           DMSO
NS                   8
DS                  16
SWH          2637.131 Hz
FIDRES         2.575323 Hz
AQ             0.1942004 sec
RG                18390.4
DW                189.600 usec
DE                10.00 usec
TE                295.9 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.44798100 sec
D4             0.00172414 sec
D11            0.03000000 sec
D13            0.00000400 sec
D16            0.00010000 sec
IN0            0.00004140 sec

======== CHANNEL f1 ========
NUC1                1H
P1                 6.70 usec
P2                13.40 usec
PL1                0.00 dB
PL1W        15.07131863 W
SFO1       300.1313665 MHz

======== CHANNEL f2 ========
CPDPRG2             garp
NUC2                13C
P3                 8.20 usec
P4                16.40 usec
PCPD2              80.00 usec
PL2               -6.00 dB
PL12               13.79 dB
PL2W        150.00000000 W
PL12W        1.57431364 W
SFO2         75.4734091 MHz

====== GRADIENT CHANNEL =====
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GPNAM2          SINE.100
GPNAM3          SINE.100
GPZ1               80.00 %
GPZ2               30.00 %
GPZ3               20.10 %
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ND0                   2
TD                  256
SFO1         75.47341 MHz
FIDRES       47.170879 Hz
SW             160.000 ppm
FnMODE             TPPI
SI                 2048
SF         300.1300000 MHz
WDW              QSINE
SSB                   2
LB                 0.00 Hz
GB                    0
PC                 1.40
SI                 1024
MC2                TPPI
SF           75.4677761 MHz
WDW              QSINE
SSB                   2
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GB                    0
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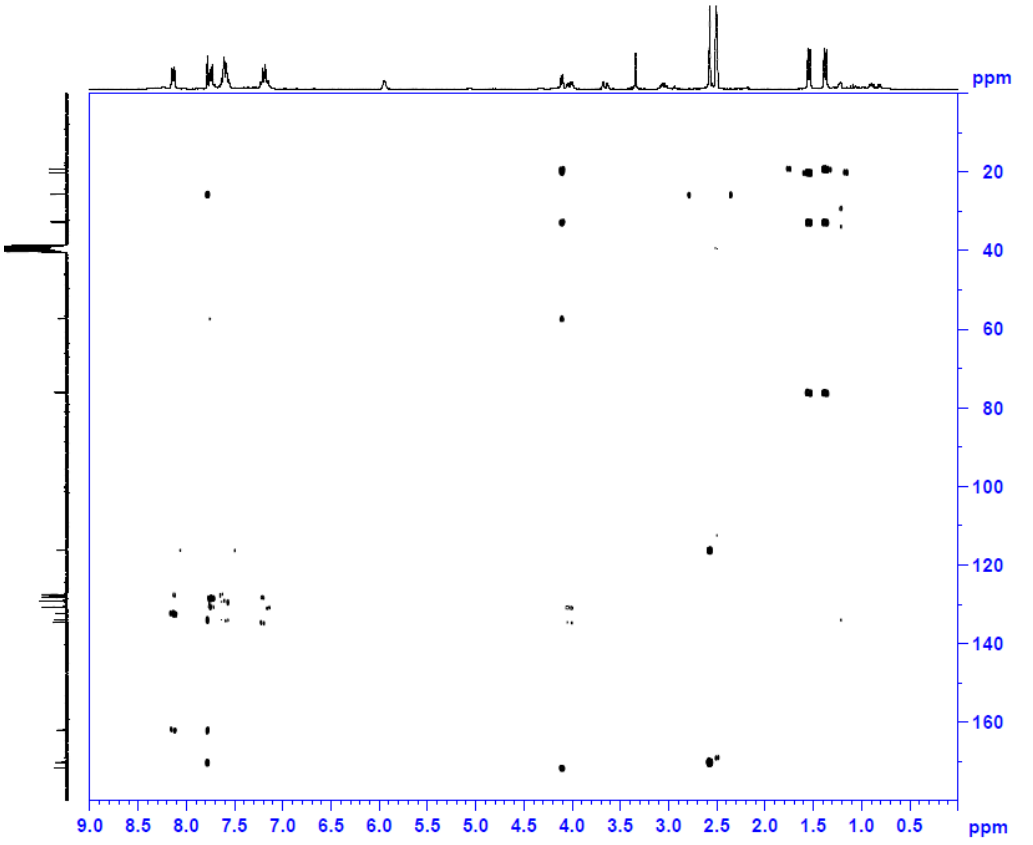


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Time                   18.11
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TD                      2048
SOLVENT                 DMSO
NS                         8
DS                        16
SWH                2637.131 Hz
FIDRES             1.287662 Hz
AQ                 0.3883508 sec
RG                   20642.5
DW                   189.600 usec
DE                     10.00 usec
TE                     296.0 K
CNST2              145.0000000
CNST13              10.0000000
D0                 0.00000300 sec
D1                 1.39596105 sec
D2                 0.00344828 sec
D6                 0.05000000 sec
D16                0.00010000 sec
IN0                0.00002760 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                      6.70 usec
P2                     13.40 usec
PL1                     0.00 dB
PL1W            15.07131863 W
SFO1           300.1313665 MHz

======== CHANNEL f2 ========
NUC2                     13C
P3                      8.20 usec
PL2                    -6.00 dB
PL2W           150.00000000 W
SFO2            75.4764278 MHz

====== GRADIENT CHANNEL =====
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GPNAM2               SINE.100
GPNAM3               SINE.100
GPZ1                    50.00 %
GPZ2                    30.00 %
GPZ3                    40.10 %
P16                   1000.00 usec
NDO                         2
TD                        256
SFO1            75.47643 MHz
FIDRES          70.758446 Hz
SW                 239.998 ppm
FnMODE                    QF
SI                      2048
SF             300.1300000 MHz
WDW                   QSINE
SSB                       0
LB                     0.00 Hz
GB                        0
PC                      1.40
SI                      1024
MC2                       QF
SF              75.4677732 MHz
WDW                   QSINE
SSB                       0
LB                     0.00 Hz
GB                        0
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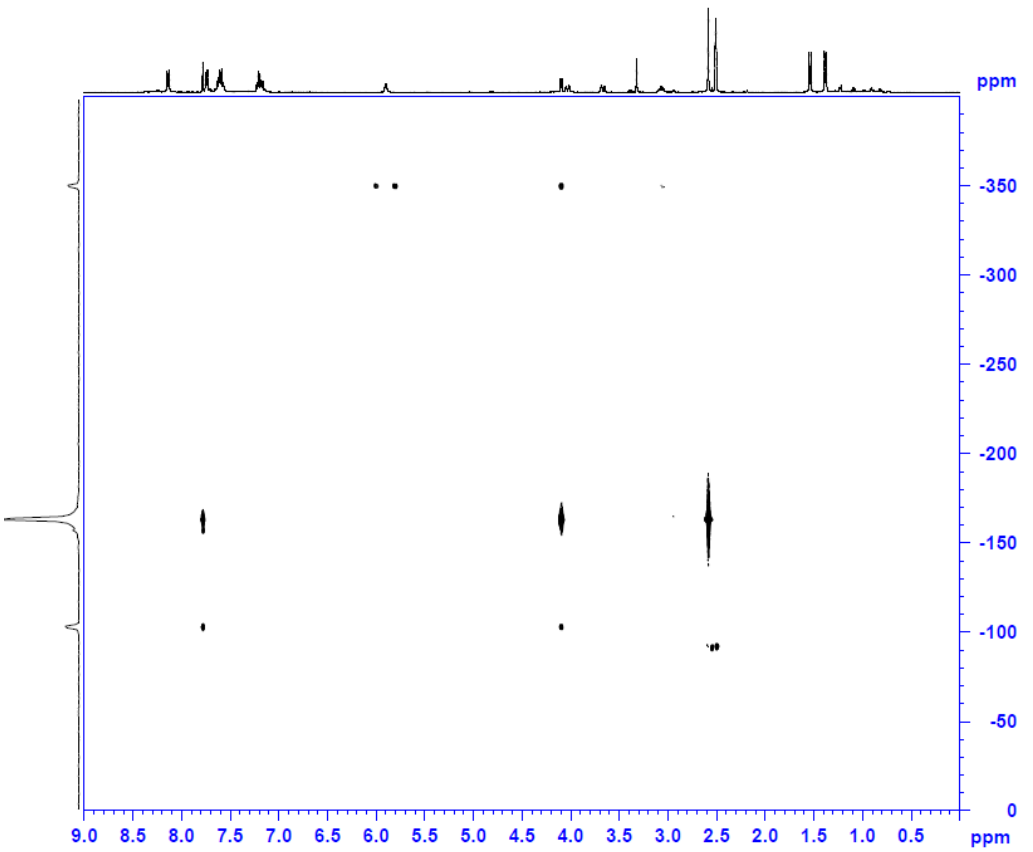


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TD                      3072
SOLVENT                 DMSO
NS                       128
DS                        16
SWH                4807.692 Hz
FIDRES             1.565004 Hz
AQ                 0.3196420 sec
RG                     16384
DW                   104.000 usec
DE                      6.50 usec
TE                     300.0 K
CNST13              5.0000000
D0                 0.00000300 sec
D1                 2.00000000 sec
D6                 0.10000000 sec
D16                0.00020000 sec
IN0                0.00002465 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                      7.00 usec
P2                     14.00 usec
PL1                    -3.00 dB
PL1W            30.07123375 W
SFO1           400.1320007 MHz

======== CHANNEL f2 ========
NUC2                     15N
P3                     17.00 usec
PL2                    -6.00 dB
PL2W           150.00000000 W
SFO2            40.5509027 MHz

====== GRADIENT CHANNEL =====
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GPNAM2               SINE.100
GPNAM3               SINE.100
GPZ1                    70.00 %
GPZ2                    30.00 %
GPZ3                    50.10 %
P16                   1000.00 usec
NDO                         2
TD                        256
SFO1            40.5509 MHz
FIDRES          79.200981 Hz
SW                 500.000 ppm
FnMODE                    QF
SI                      4096
SF             400.1300000 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
PC                      1.40
SI                       512
MC2                       QF
SF              40.5601443 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
```
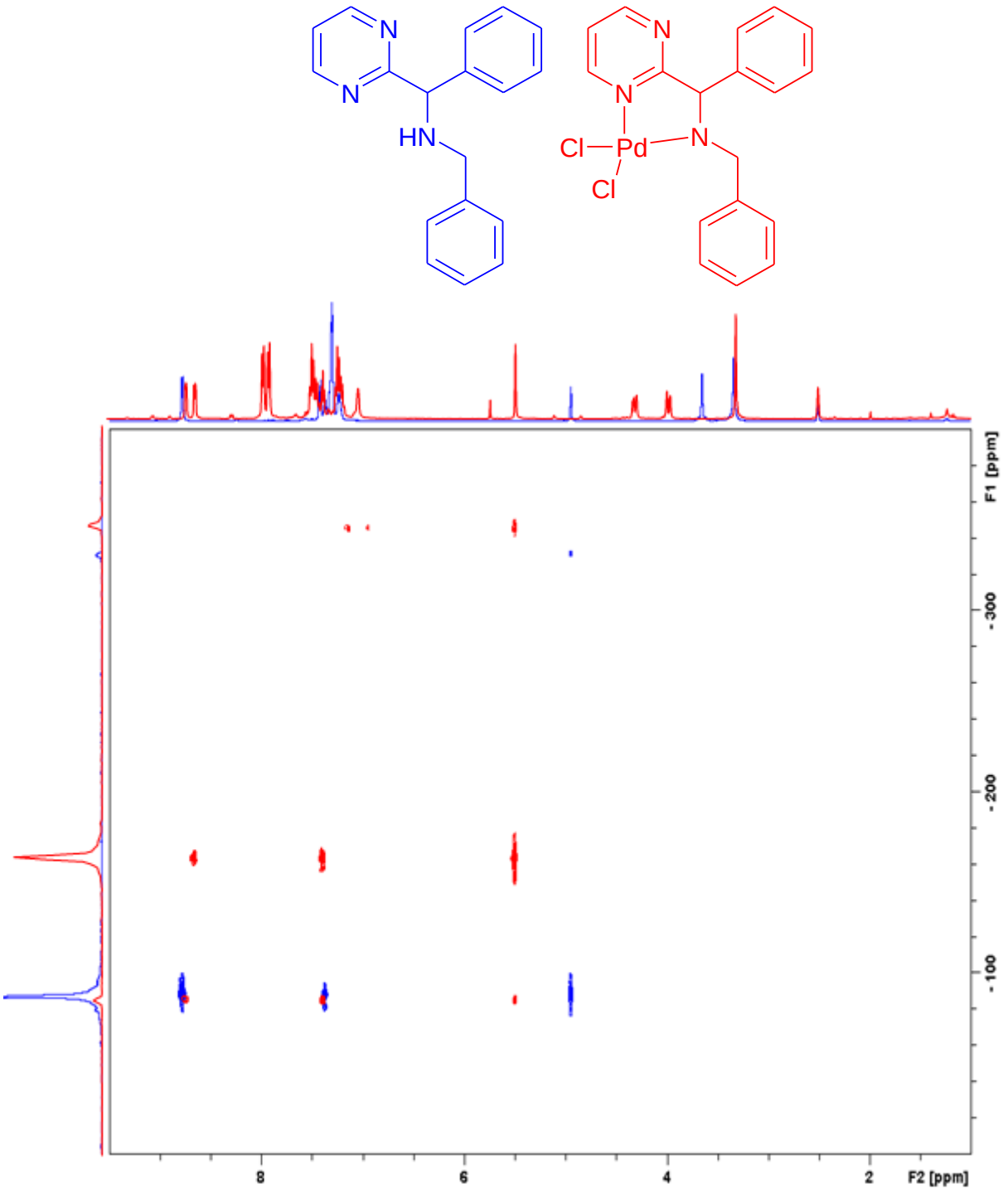
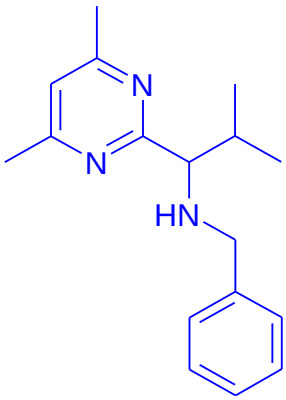
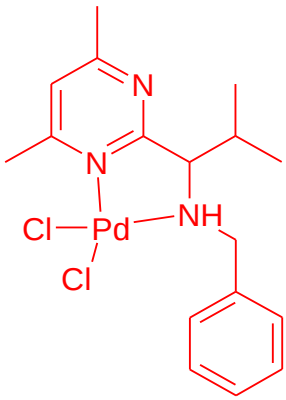

Figure 1 SI ^{1}H-^{15}N HMBC spectra overlay
A) ligand 1 and the symmetric Pd-pyrma 7



B) ligand 2 and the symmetric Pd-pyrma 8





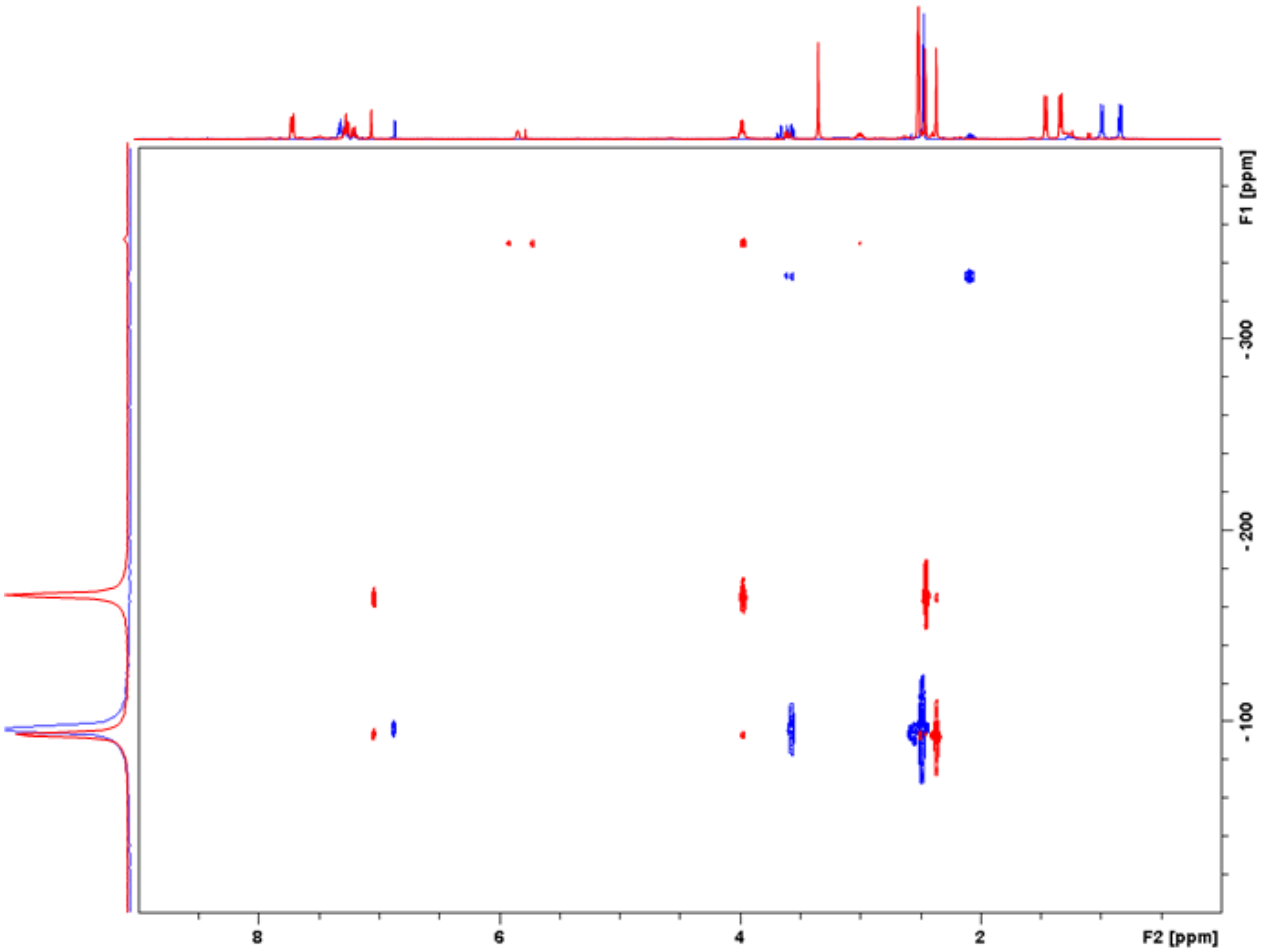


Figure 2 SI: Overlapped ^{1}H-^{15}N HMBC for the ligand 4 and the complex **13.** Asterix (*) represents a peak coming from an impurity.

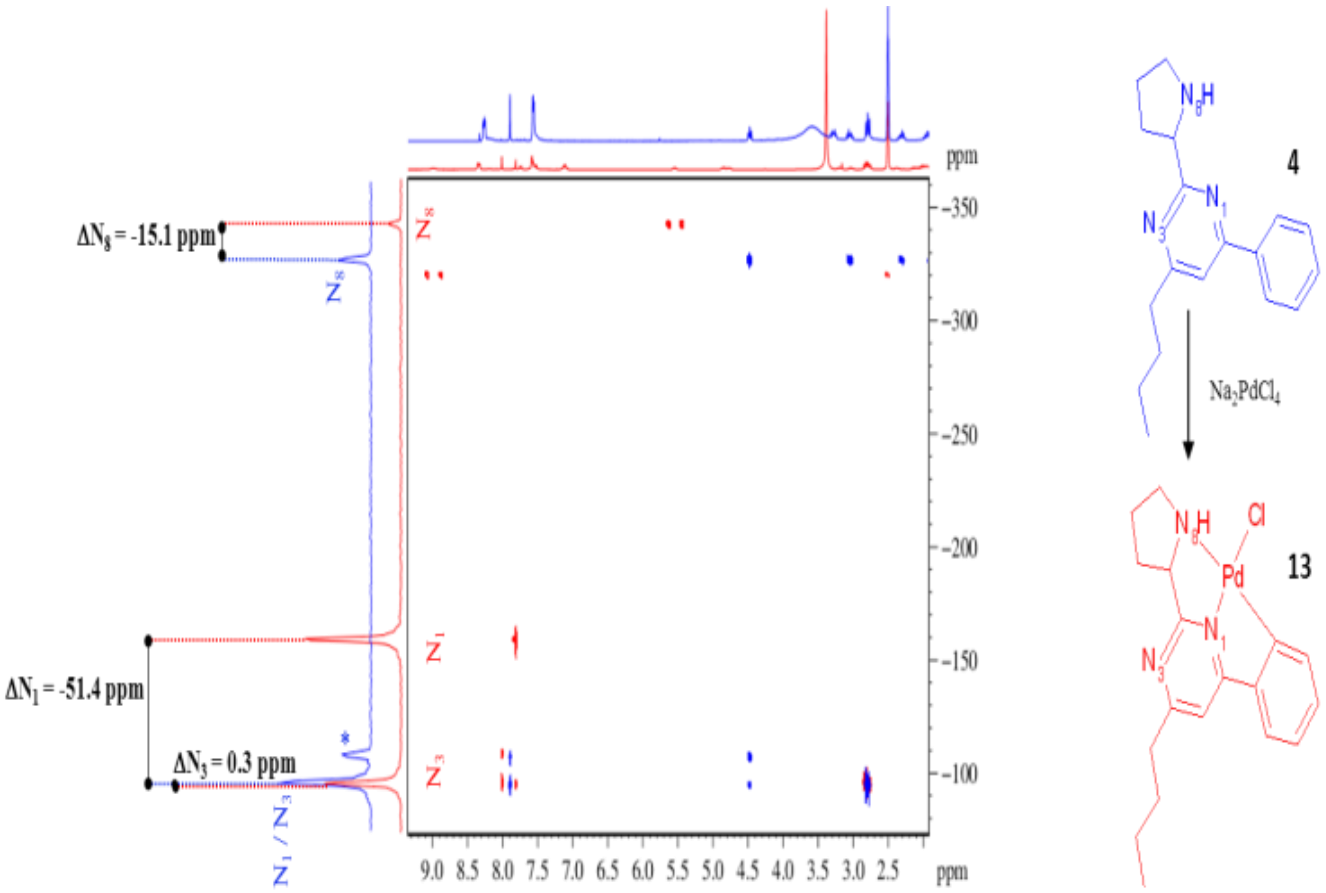
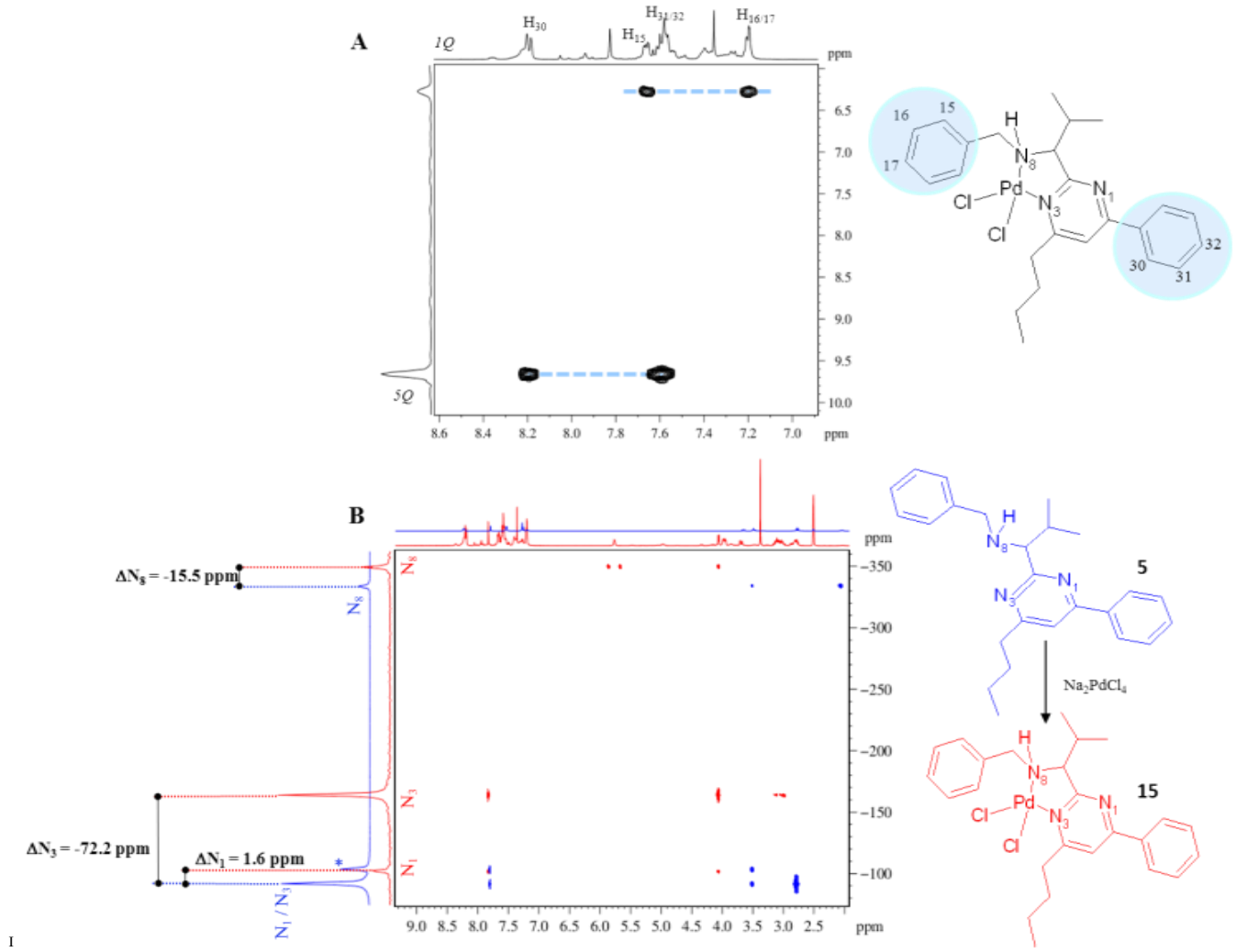
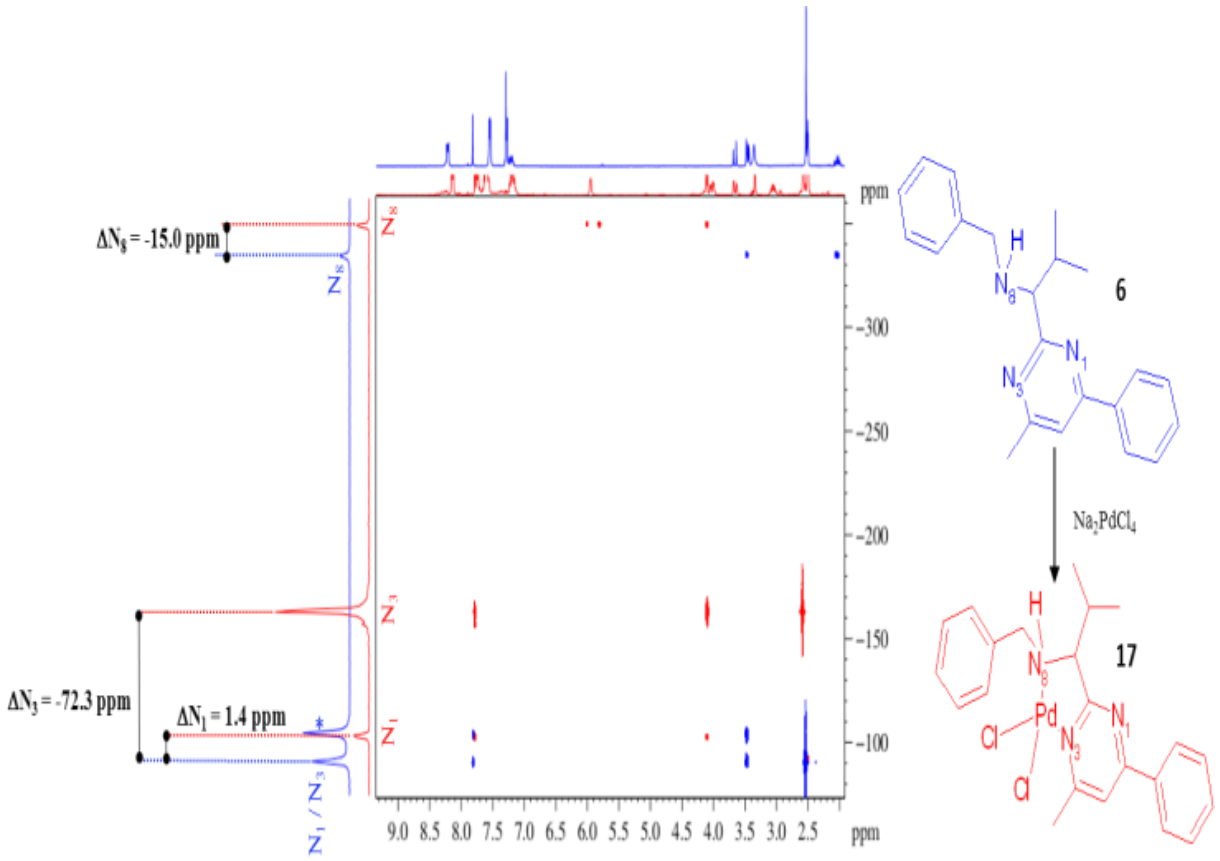


Figure 3 SI



*A) 5Q-1Q Maximum Quantum experiment recorded on both ligand **5** and complex **15**. Phenyl groups have the same spectral fingerprint confirming coordination to the Pd(II) (in light blue) B) Overlapped ^{1}H-^{15}N HMBC for the ligand **5** (in blue) and the complex **15** (in red). Asterix (*) represents a peak coming from an impurity.*

Figure 4 SI:

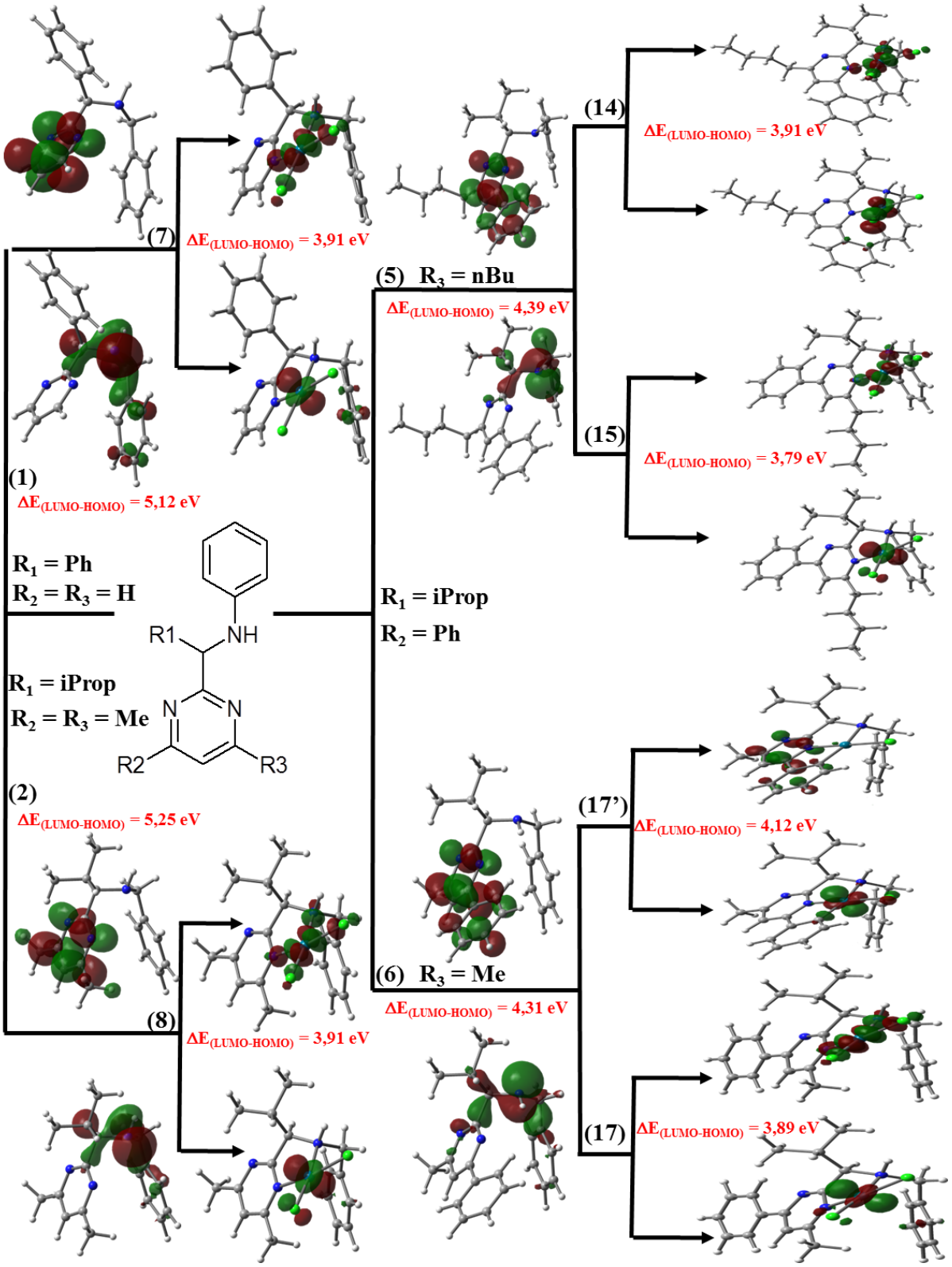


*Overlapped ^{1}H-^{15}N HMBC for the ligand **6** (in blue) and the complex **17** (in red). Asterix (*) represents a peak coming from an impurity*

Computational methods

All computations of geometry optimizations, electronic structure determinations and NMR chemical shift values were carried out using the Gaussian 09 program [5]. All geometries were optimized by minimizing energies with respect to all the geometrical parameters, without imposing any molecular constraints. Restricted Hartree – Fock method was used as geometry pre-optimization scheme. Density Functional Theory (DFT) Self Consistent Field (SCF) procedure for energy minimizations and description of orbitals were performed with the hybrid method B3LYP, whereas electronic correlation and exchange were respectively described by the use of the Becke [6] and Lee-Yang Parr [7] functionals. Relativistic effective core potentials (ECP) were used to describe electrons of heavy atoms (Pd and Cl) with the valence double ζ quality basis sets LANL2DZ [8]. The standard 6-311G(d,p) basis sets were used for the rest of the atoms on PYRMA ligands and their Pd complexes (i.e. H, C and N). Geometrical results are similar when chlorine atoms are described even with LANL2DZ and 6-311G(d,p) basis sets but the former case was used for the rest of calculations. Stable structures were confirmed with the calculation of harmonic vibrational frequencies of all structures. None of the predicted vibrational spectra has any imaginary frequency (data not shown), implying that the optimized geometry of each of the molecules under study lay at a local point on the potential energy surface. The electronic properties such as Molecular Electrostatic Potential (MEP), frontier molecular HOMO – LUMO orbital energies and Mulliken atomic charges have been obtained with the same level of theory as previously described. Gauge – Invariant Atomic Orbital (GIAO) [10] scheme was used to compute ^{1}H, ^{13}C and ^{15}N chemical shift values, theoretically referenced with respect to TMS / 6-311G(d,p) (^{1}H and ^{13}C, *vide infra*) and NH_3 with later subtraction of all values with respect the calculated theoretical chemical shift of CH_3NO_2 (^{15}N). As for geometry optimizations and electronic properties, B3LYP functional with 6-311G(d,p) for H,C and N and LANL2DZ / ECP basis sets for heavier atoms were used as levels of theory for NMR parameters. Higher accuracy of the full set of computed carbon resonances for all PYRMA complexes were obtained with the basis set 6-311G(d,p), in comparison with the IGLO-III basis functions, popularly used to calculate NMR tensors (Figure 13 SI). Basis Set Superposition Error (BSSE) Counterpoise correction [9] in the gas phase prior to NMR GIAO computations was carried out for all palladium pyrma complexes. In the limits of both types of basis functions LANL2DZ /ECP (Pd, Cl atoms) and 6-311G(d,p) (H, C, N atoms), electronic environments are poorly described without the BSSE correction, which would eventually produce important ^{13}C chemical shifts overestimations especially for the C-Pd quaternary carbons in Pd *(C, N, N)* complexes **10** and **13**, when correction is ignored. Systematic overestimation of the *overall* solvent dependent isotropic ^{13}C calculated resonances in the range of 0 to -8 ppm were obtained for all energetically favored PYRMA complexes (7, 8, 10, 13, 15 and 17) when B3LYP / 6-311G(d,p) with the TMS (tetramethylsilane) reference standard was used. In deep contrast, loss of systematic estimation with ranges of $\Delta\delta^{13}C$ between -30 and +10 ppm were observed for all energetically disfavored PYRMA complexes (10', 12, 14 and 17') with the same reference standard. As a result, we suggest that both $\Delta\delta^{13}C$ within the 0 to -8 ppm ranges as well as systematic overestimations of the full set of carbon resonances per complex could be used as fingerprints to qualitatively assign the preferred coordination modes for each type of PYRMA complex. $\Delta\delta^{13}C$ values of energetically favored complexes can be significantly lowered to ± 3 ppm (compensated by the loss of systematic overestimations) when calculated shifts are referenced with different standards [12], such as B3LYP / 6-311G(d,p) optimized benzene as reference standard (Figure 14 SI). Self-Consistent Reaction Field (SCRF) Tomasi's Polarized Continuum Model (PCM) for solvation [11] was used in all calculations (except BSSE) to describe implicitly the solvent (DMSO), which was the selected solvent to obtain experimental NMR data. Further details are highlighted on SI figure captions.

Figure 5 SI:
Frontier Molecular Orbitals HOMO / LUMO of PYRMA ligands at their $PdCl_2$ complexes.



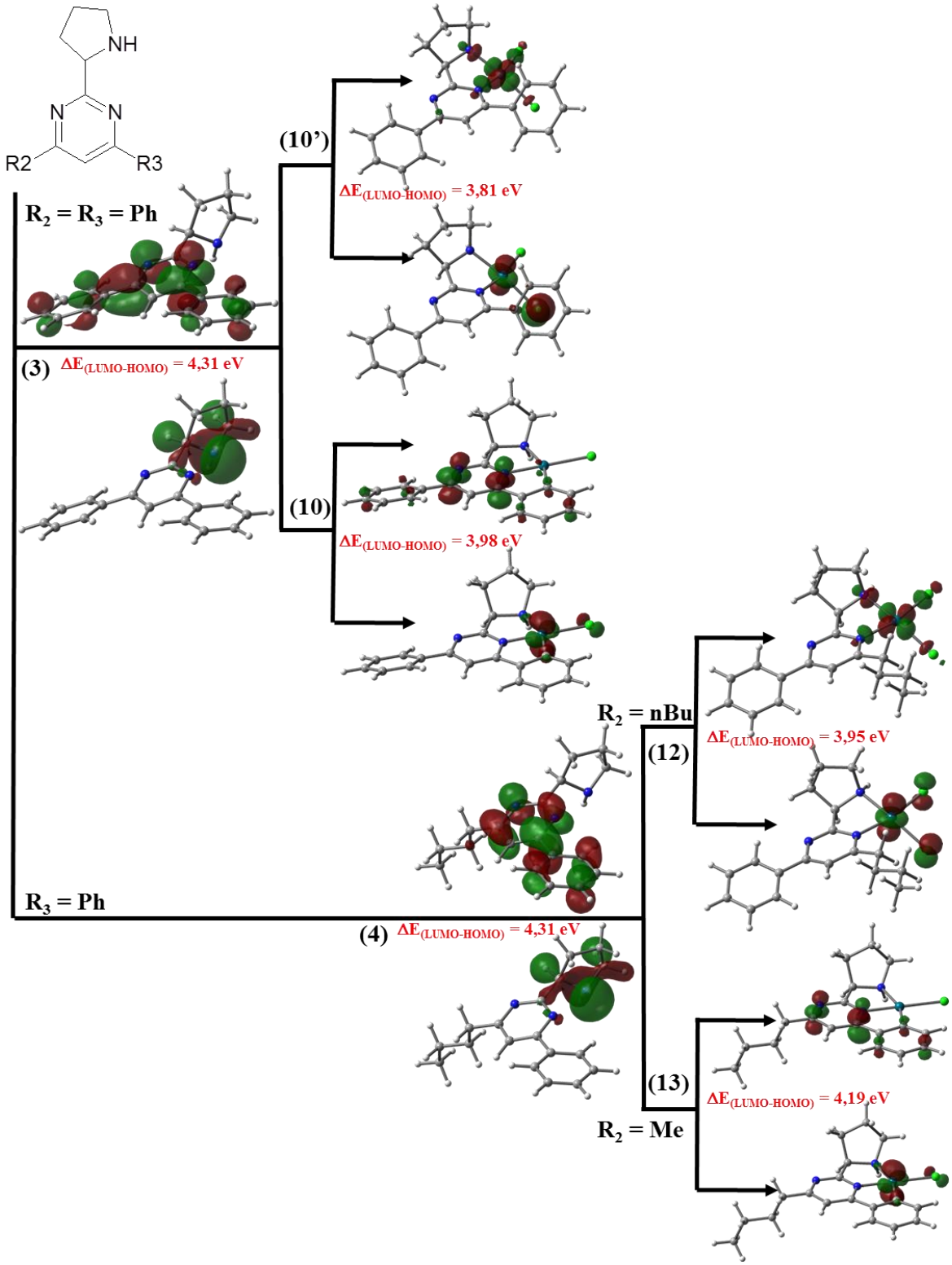
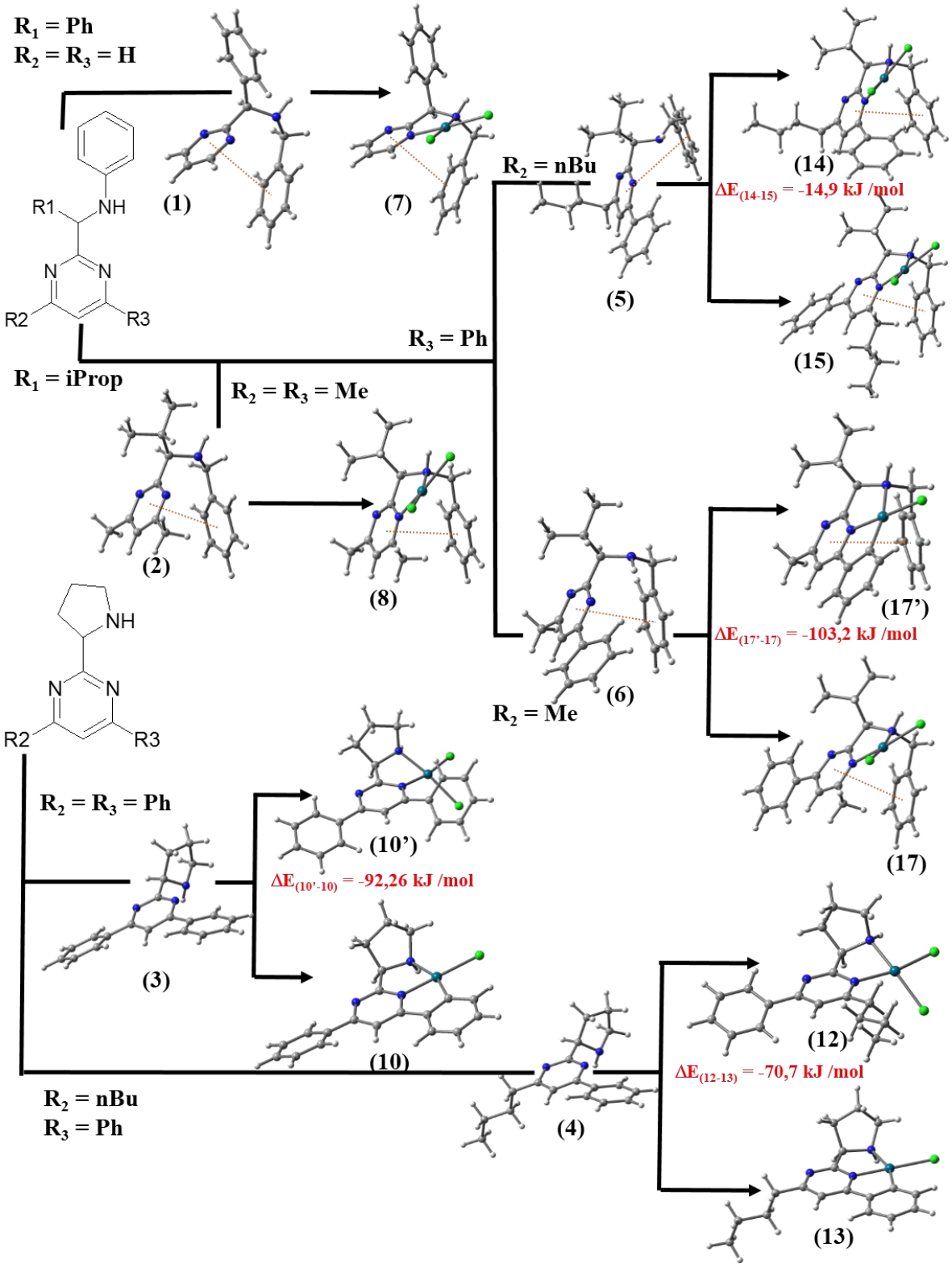

NH
N
N
R2
R3
R2 = R3 = Ph
(3) ΔE(LUMO-HOMO) = 4,31 eV
(10')
ΔE(LUMO-HOMO) = 3,81 eV
(10)
ΔE(LUMO-HOMO) = 3,98 eV
R2 = nBu
(12)
ΔE(LUMO-HOMO) = 3,95 eV
R3 = Ph
(4) ΔE(LUMO-HOMO) = 4,31 eV
(13)
ΔE(LUMO-HOMO) = 4,19 eV
R2 = Me

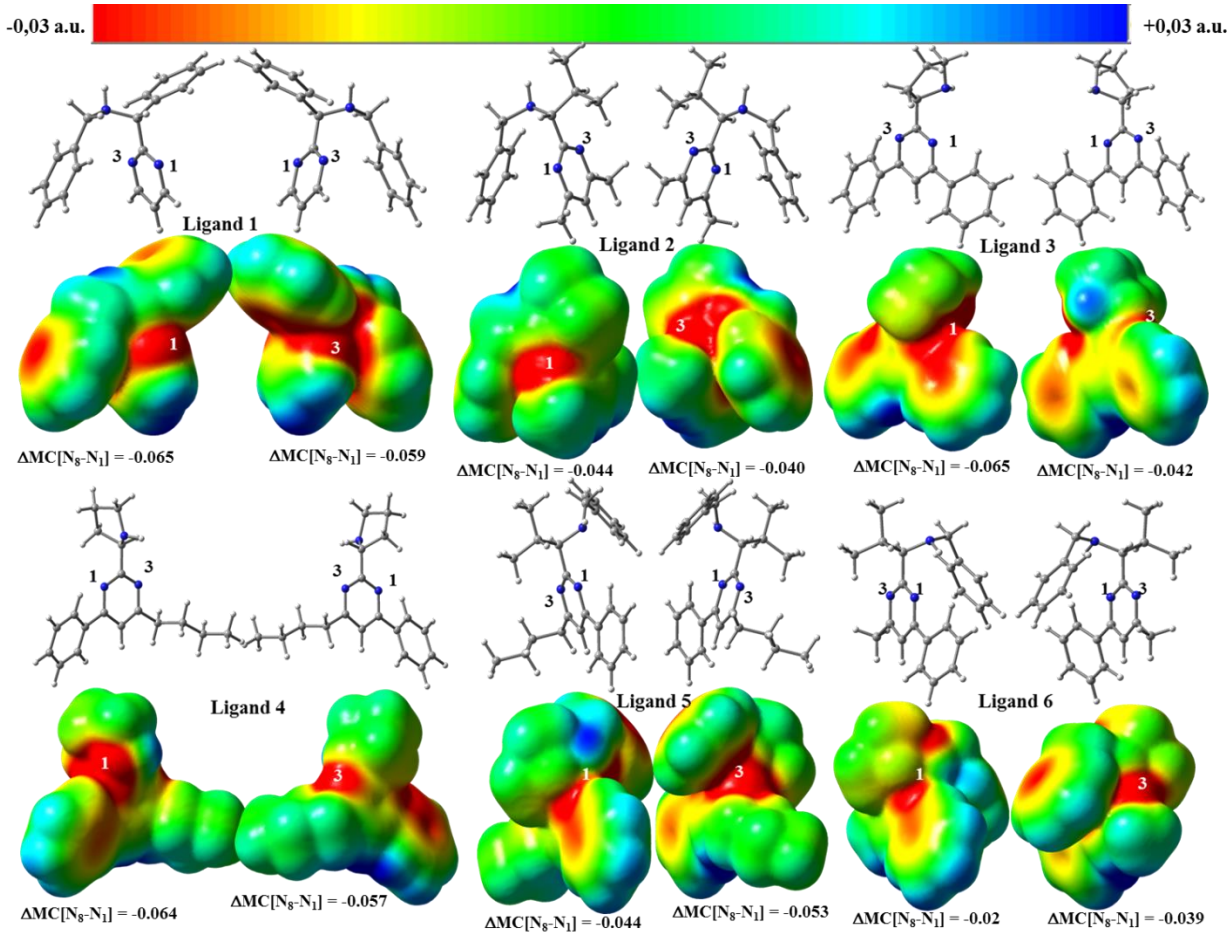
Figure 6 SI:



*Electronic optimized structures of all pyrma ligands (**1** to **6**) and their PdCl2 complexes (**7**, **8**, **10**, **10'**, **12**, **13**, **14**, **15**, **17** and **17'**; referring the labelling to Schemes 2 and 3) obtained by DFT calculations (see computational methods, ESI), ,considering the solvent effect by the means of the SCRF calculation scheme, having DMSO as implicit solvent. Electronic energy differences between the lowest local minimum (consistent with experimental data,) and other observed local minimum for each complexation possibility are highlighted in red. Dotted orange lines represent the shortest distance between pyrmidine*

*– benzylic aromatic rings ($d_{inter\text{-}rings}$, see Table 2 SI), the last one coming from the NHBn moiety in the pyrma methylamine-capped ligands and their Pd(II) complexes. Despite the dispersion-correction protocol [13] was not used to confirm the presence of π stacking weak dipole-dipole interaction, pyrma complexes bearing a valine-capped substitution present geometries deeply comparable to X-Ray diffraction data of their pma analogues with known π stack interaction [14] Thus, we inquire that $d_{inter\text{-}rings}$ observed in PYRMA at the B3LYP level of theory is a consequence of the accuracy of calculation to predict geometries at the level of metallic center. The last suggest that $d_{inter\text{-}rings}$ distances are comparable to the expected π stack interactions in NHBn PYRMA complexation, being a non-essential weak interaction to explain the sterical arrangement around the metallic core and thus not responsible of the electronic structural stability. For balanced energy equations between energetically favored Pd(C,N,N) species (**10** and **13**) with respect their less favorable Pd(N,N) counterparts as well as for complexes **17** and **17'** (with inverse energetic tendency respect **10** or **13**), it is considered the released HCl moiety in Pd(C,N,N) complex formation for ΔE computations. The orientation of HCl release respect the Pd(II) complex plane is also depicted in the Figure.*

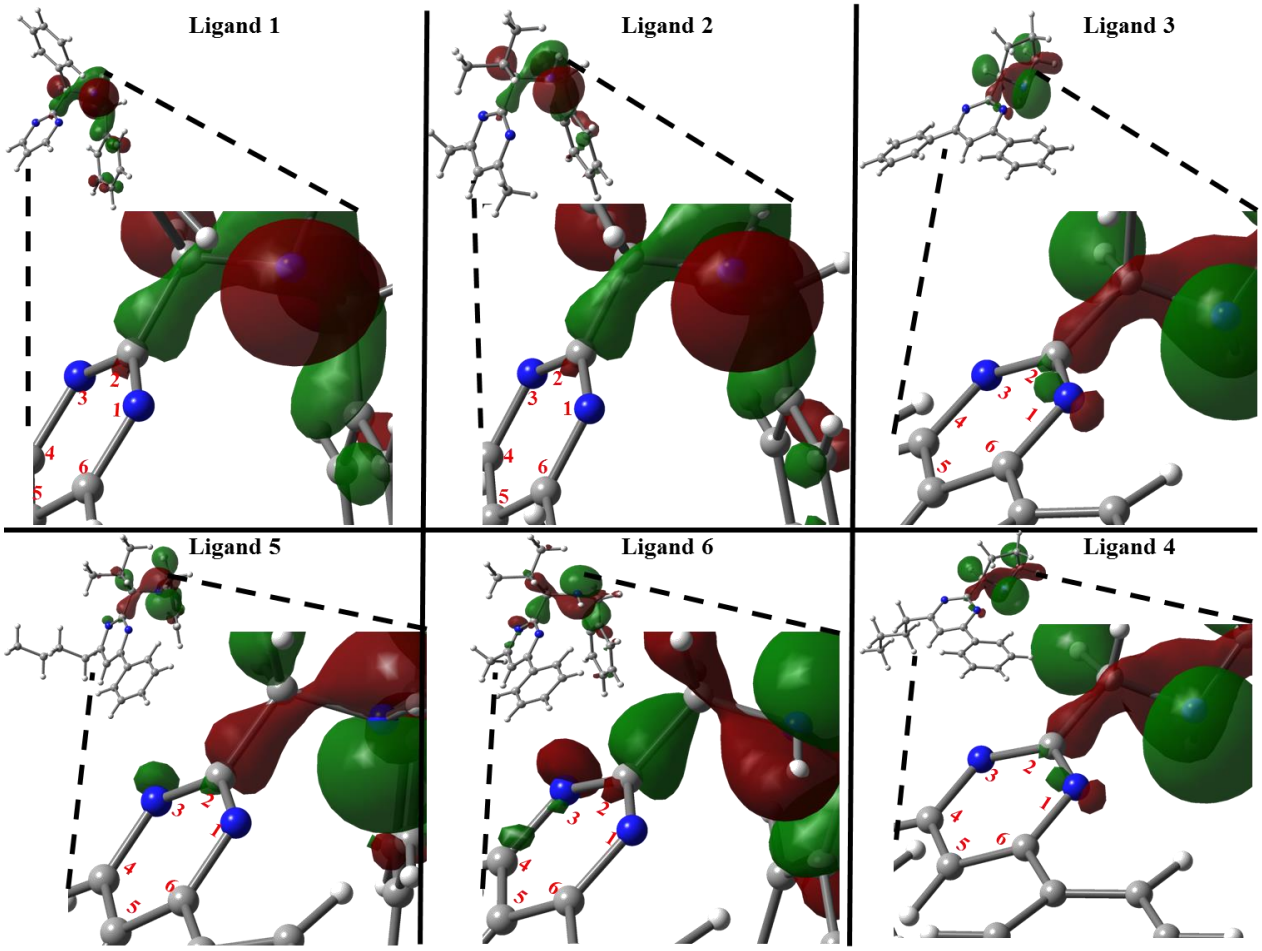
Figure 7 SI:



*Molecular electrostatic potential (MEP) mapped on the SCF total electronic density surface calculated by DFT / B3LYP method for pyrma ligands **1-6**. For visualisation of the most electronegative sites within each molecule, it is presented a pair of MEP surfaces for each ligand by just turning each projection 180° around the plane and thus showing the faces of N1 or N3 as depicted in the Figure. Developed ball-sticks formulae of ligands are projected on top of each MEP surface, showing the numbering of each N atom as well as the 3D arrangement of atoms that are depicted on the MEP surface. Similar electronegativities are observed for N1 and N3 in*

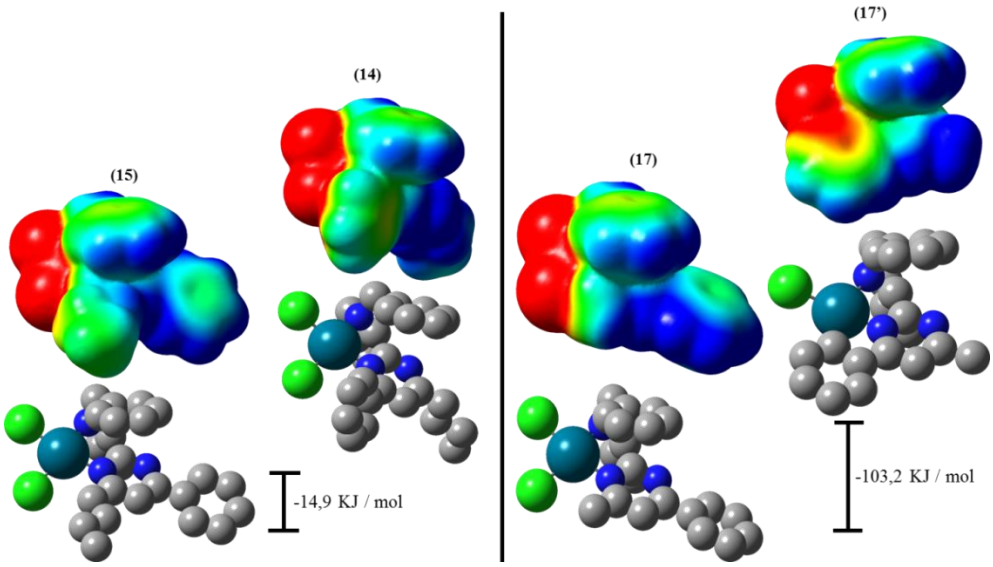
*ligands **1** and **2**. In contrast, pyrrolidine-capped pyrma ligands (**3** and **4**) show a striking higher negative electronic density over N1 whilst N3 atoms are considerably more electronegative in non-symmetrical methylamine-capped pyrma ligands (**5** and **6**). Numeric representation of electron availability of each pair of N1 / N3 atoms per PYRMA ligand is given by computing the difference of Mulliken's charges (MC) between N8 and each of the aromatic N PYRMA nitrogens ($\Delta MC[N_8\text{-}N_i]$, whereas i = 1 or 3). Highest negative values of ΔMC show the most electronegative aromatic nitrogen which chelates the palladium, consistent to the graphical analysis by MEP.*

Figure 8 SI:



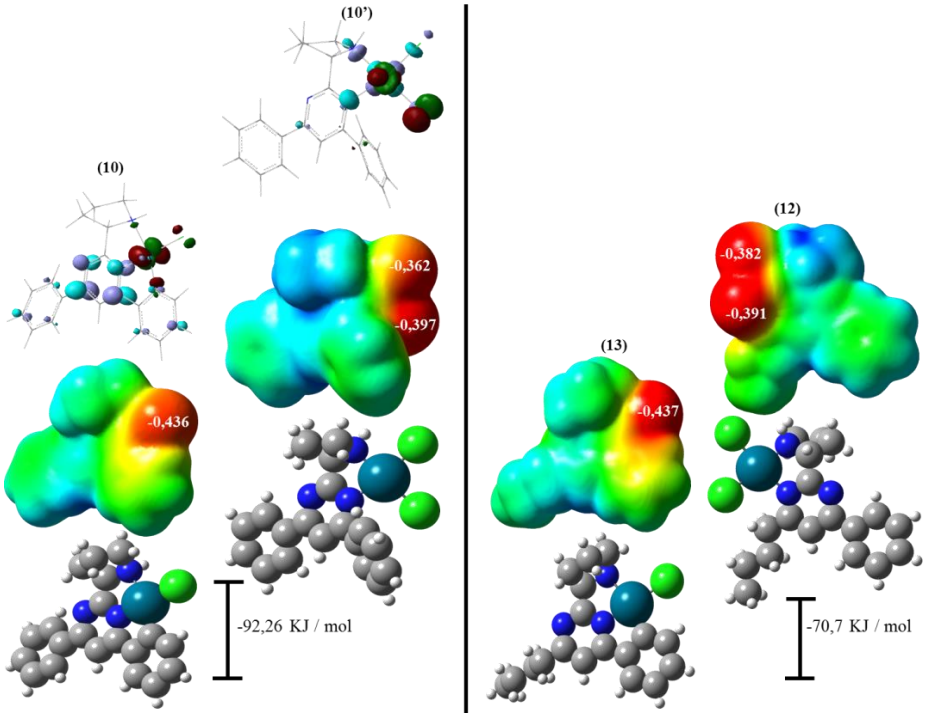
*Ground state isodensity surfaces for the frontier molecular HOMO orbitals calculated with DFT/B3LYP level of theory for pyrma ligands **1**-**6**. For observing the Pi lobes of nitrogens N1 and N3 for each ligand, an expansion is depicted along the dotted lines.*

Figure 9 SI:



*Valine-capped complexes **15, 14, 17** and **17'**. MEP maps (top) and Van der Waals radii formulae (bottom) depicting the relative SCRF electronic-energy differences (ΔE) of each pair of complexes, as stated above in Figure 6 SI.*

Figure 10 SI:



*Proline-capped complexes **10**, **10'**, **13** and **12**: HOMO(red/ green)/ LUMO (blue / purple) orbitals (top), MEP maps with chlorine electronic charges obtained by Mulliken population analysis (middle) and Van der Waals radii formulae (bottom), depicting the relative SCRF electronic-energy differences (ΔE) of each pair of complexes. As stated above for Figure 6 SI, ΔE was obtained by balanced equations between [*Pd(C,N,N)* + HCl] and [*Pd(N,N)]* energy values. For visualization purposes, the HCl expelled prior to Pd(C,N,N) complexation is not depicted on the Figure.*

Figure 11 SI:

Agreement between DFT calculated and NMR measured ^{1}H and ^{13}C chemical shifts for PYRMA / Pd-PYRMA couples under study

Figure 11.1 SI

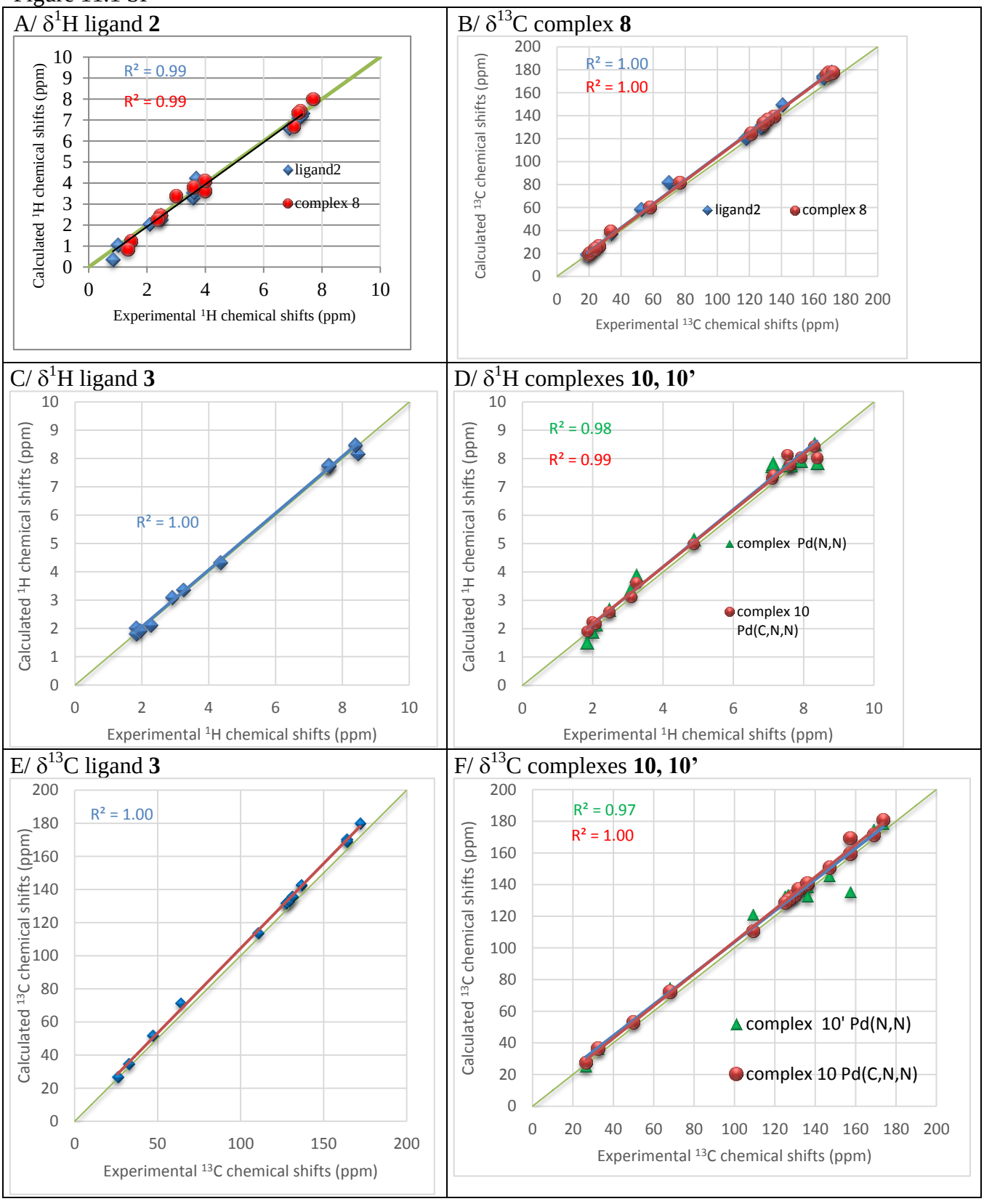


Figure 11.2 SI

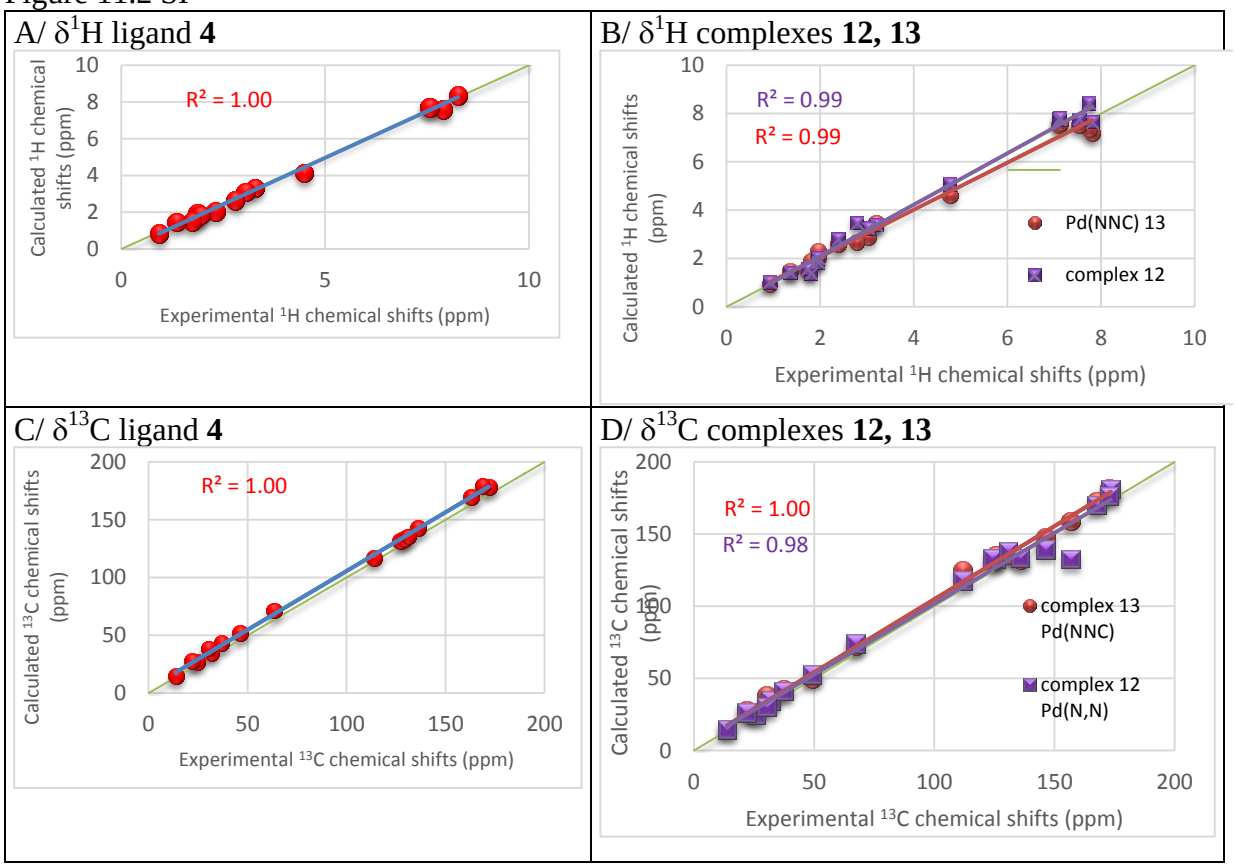


Figure 11.3 SI

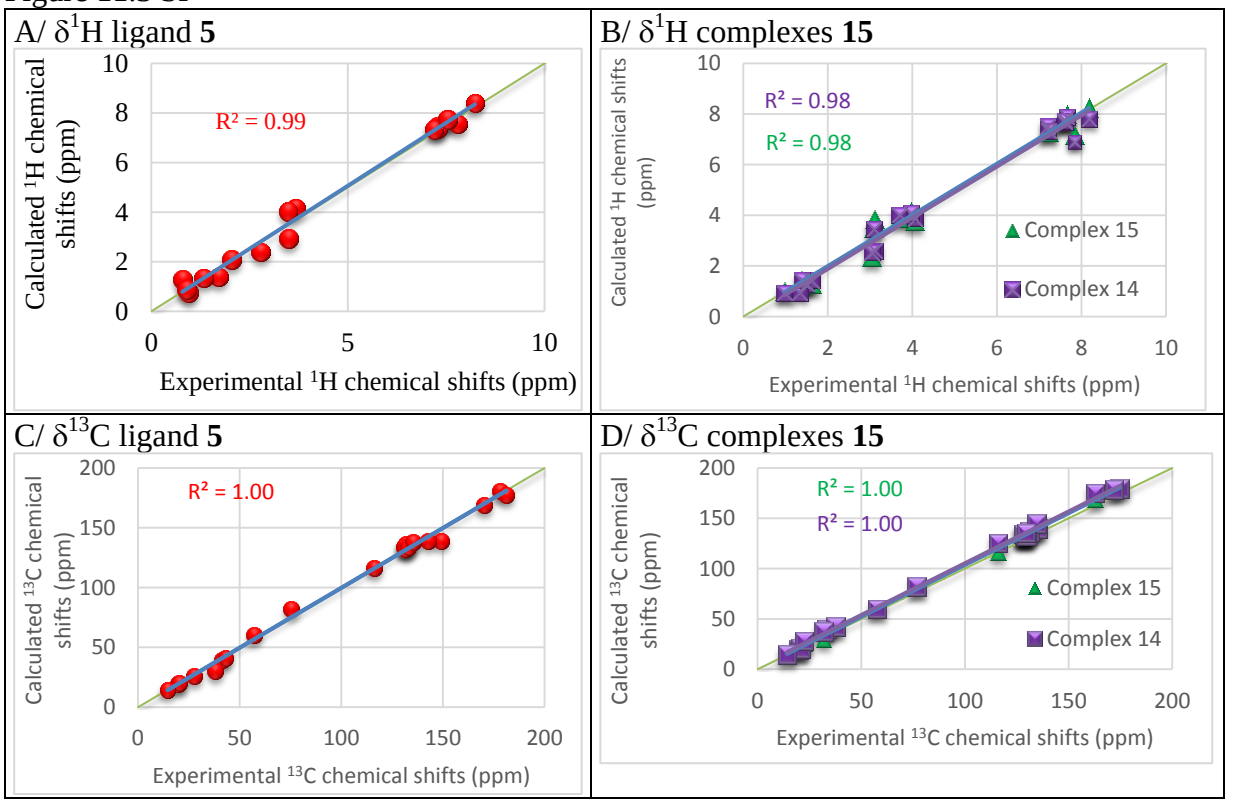
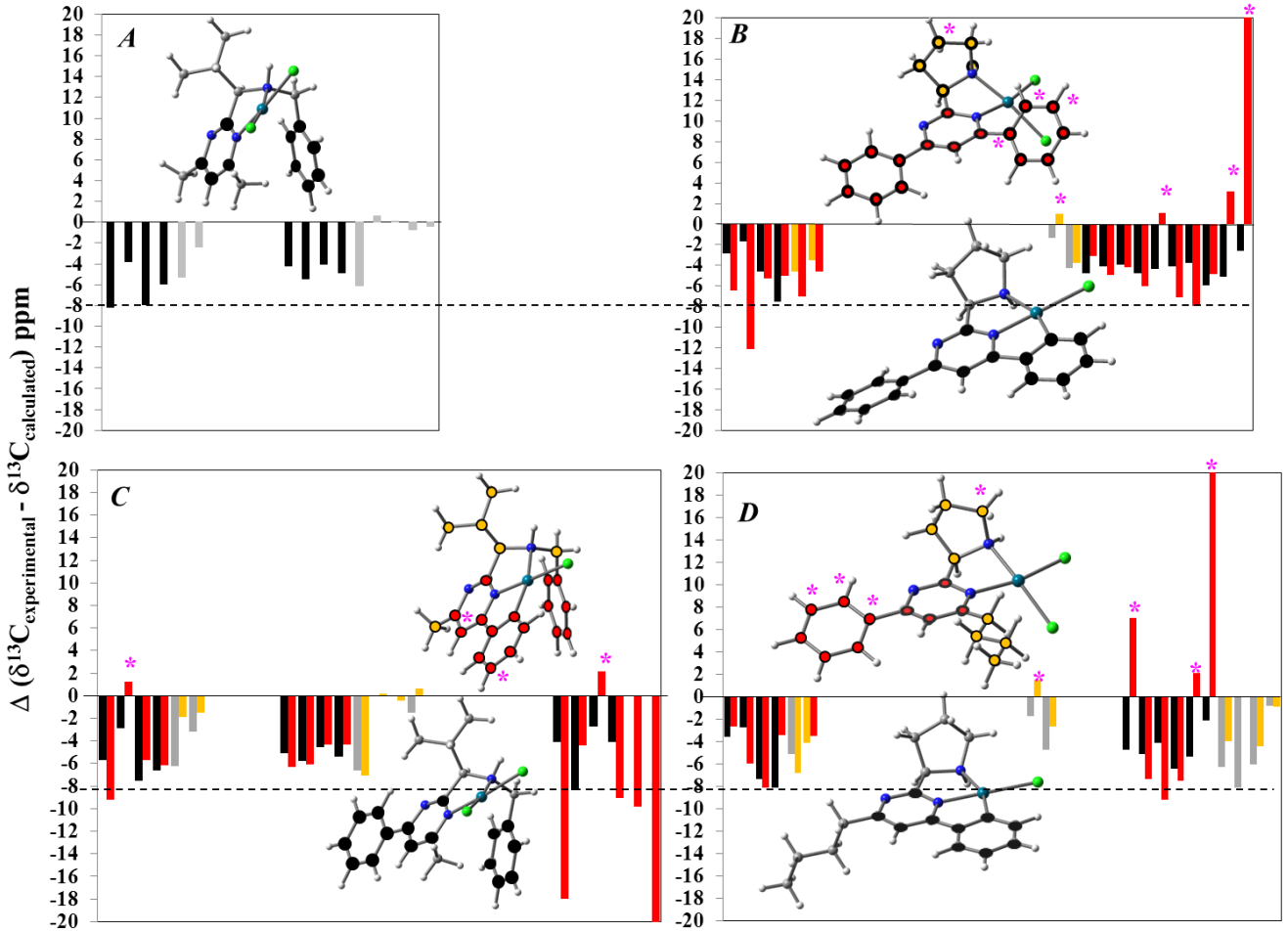


***Figure 12 SI**: $\Delta\delta^{13}C$ fingerprints between Pd(N,N) and Pd(C,N,N) obtained by the difference of experimental ^{13}C chemical shifts of symmetric (A, B) and non-symmetric (C, D) pyrma complexes, with respect to the DFT – GIAO predicted shifts.*
*Electronically favourable (**8**, **10**, **13**, **17**) and unfavourable (**10'**, **12**, **17'**) pyrma complexes present the following colour code for histograms*

- *Black- gray to describe respectively aromatic and aliphatic carbons of **8**, **10**, **13**, **17**.*
- *Red - yellow to describe respectively aromatic and aliphatic carbons of **10'**, **12**, **17'**.*

DFT GIAO shifts were obtained by using TMS (tetramethylsilane) as a reference standard Dotted black line limits the interval of statistical confidence, which scales up to $\Delta\delta$ values of - 8 ppm. Magenta asterisk highlight the relevant aliphatic and aromatic carbons of unfavourable electronic states that are non-systematically underestimated. It is worth noting to remark that isopropyl methyls ^{13}C shift's estimations (A and C) are close to $\Delta\delta$= 0 but slightly underestimated and are not considered in our analysis. The B3LYP – GIAO approach, using a 6-311G basis set, has been used to compute $\Delta\delta^{13}C$values in the present figure. The use of different basis sets or reference standard are discussed below.



*Systematic overestimation of the overall solvent dependent isotropic ^{13}C calculated resonances in the range of 0 to -8 ppm were obtained for all energetically favored PYRMA complexes (**7** (data not shown), **8**, **10**, **13**, **15** (data not shown) and **17**) when B3LYP / 6-311G(d,p) using TMS as reference standard. In deep contrast, loss of systematic estimation with ranges of $\Delta\delta^{13}C$ between -30 and +10 ppm were observed for all energetically disfavored PYRMA complexes (**10'**, **12**, **14** (data not shown) and **17'**) with the same reference standard and mostly for aromatic carbons close to the coordination sphere. (red histograms with magenta stars) Thus, not only inaccurate overestimations of ^{13}C shifts above - 8 ppm, but mostly non-systematic underestimations of key $\delta^{13}C$ shifts could serve as fingerprints to discriminate incorrect entries of local minima palladium complexes of higher electronic energy.*

Analysis of non-symmetric PYRMA complexes $\Delta\delta^{13}C$ histograms (also applied to the symmetric cases)

*First, systematic overestimations of predicted ^{13}C shifts (between 0 to -8 ppm) of complex **13** show that the Pd(C,N,N) coordination mode is the electronic structure that best fits the experimental evidence, in agreement with the energetics coming from the full optimization of electronic geometries of non-symmetric proline headed pyrma complex (Figure 6 SI). Important non – systematic underestimations even above + 20 ppm are observed for its Pd(N3,N8) analog **12** of higher electronic energy.*

*The pair of complexes **17** and **17'** were also subjected to the analysis of $\Delta\delta^{13}C$ dispersions. As seen by the energetics in Figure 6 SI, the most stable electronic structure was assigned to the complex **17** (i.e. Pd(N3,N8) coordination mode), whereas a second local minimum of 103 KJ/mol of higher energy with respect complex **17**, was founded to be the Pd(C,N,N) mode. Again, systematic overestimations of experimental and predicted $\Delta\delta^{13}C$ shifts between 0 to –8 ppm were only observed for the stable coordination mode Pd(N3,N8) valine-capped pyrma complex. In contrast, complex **17'** can be rejected as observable by the fact of presenting nonsystematic underestimations as well as overestimations of several ^{13}C predicted shifts below the limit of - 8 ppm. Some of these highly overestimated $\Delta\delta^{13}C$ values of complex **17'** correspond to spin systems that are not experimentally observed like the hypothetic quaternary C-ortho linked to Pd at $\delta^{13}C_{(calculated)}$= 160 ppm which is dispersed by -32 ppm with respect the experimental CH-ortho at $\delta^{13}C_{(experimental)}$= 128 ppm (extreme right histogram bar at Figure 12 SI C). The last proves the fact that this simple qualitative analysis is independent of the capped pyrma complex to distinguish complexation modes of pyrma by only N-Pd coordination or by a third C-Pd bound.*

Figure 13 SI:

*Effect of the basis set used in the NMR B3LYP/GIAO calculations of ^{13}C chemical shifts of PYRMA complexes **10** and **10'** by comparing $\Delta(\delta^{13}C_{experimental} - \delta^{13}C_{calculated})$; displayed as histograms and overall $\Delta\delta^{13}C$ ranges per calculated complex. Color codes for sp3 and sp2 carbons are the same as in Figure 12 SI.*

Proton, carbon and nitrogen -s, -p and -d atomic orbitals were respectively described with

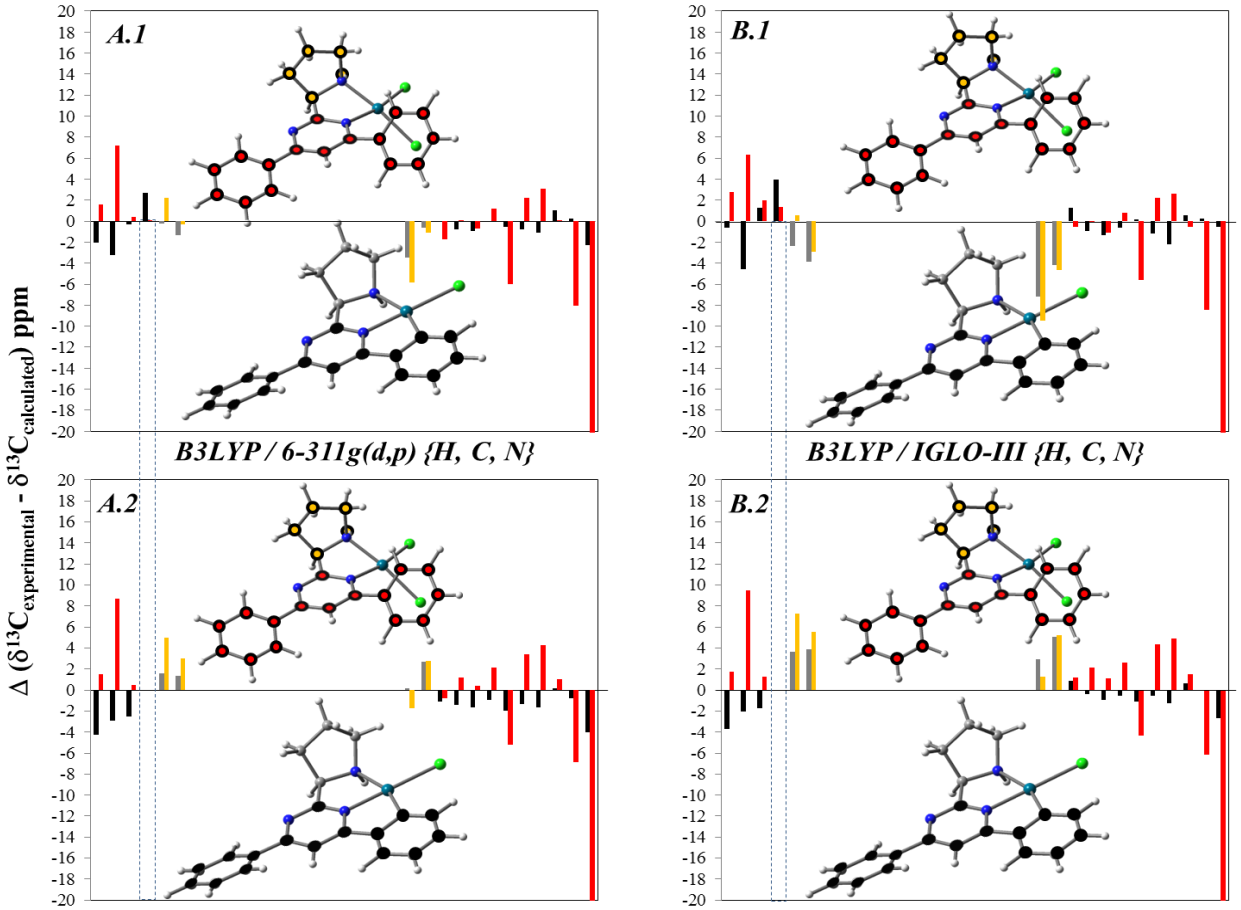
A) 6-311g(d,p)

B) IGLO-III

For fair comparisons between both basis sets and due to the scarcity of default reference standards implemented within the Gaussian software [5], $\delta^{13}C_{calculated}$ shifts were referenced as follows:

1. *Using Benzene isotopic magnetic shielding values as reference standard, obtained by SCRF (cpcm, solvent = DMSO) / B3LYP / GIAO calculations, computed at the same level of theory ($\sigma_{Benzene/6\text{-}311g(d,p)}$ = 133.24 ppm, $\sigma_{Benzene/IGLO\text{-}III}$ = 141.34 ppm) and referencing all carbon signals with respect the experimental value of benzene's $\delta^{13}C_{experimental}$ shift = 128.37 ppm [12].*
2. *Referencing C6 of both complexes at each level of theory, with respect the $\delta^{13}C_{experimental}$ shift of 173.4 ppm for **10** (page 5 ESI). $\Delta\delta^{13}C6$ =0 of the internal reference standard is depicted with blue dotted squares. The scaling factor produced by each $\Delta\delta^{13}C$ is applied for the rest of the ^{13}C calculated shifts, for both levels of theory.*

Computation of overall ^{13}C resonances of both expected and unexpected complexes, as a function of the basis set and comparison with experimental data run as follows:



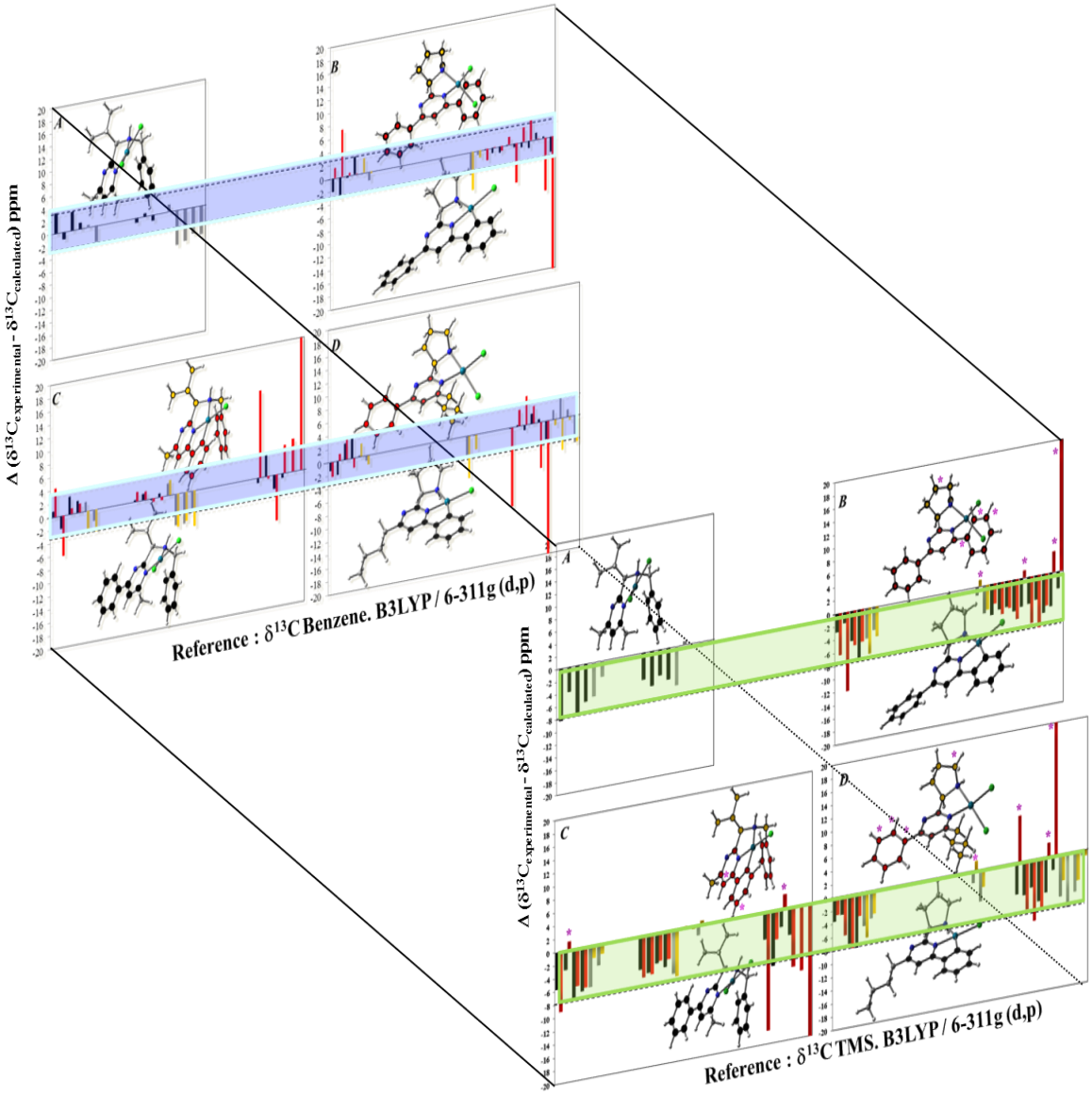
6-311g(d,p)	$-3.5 \leq \Delta\delta^{13}C$ (complex 10) ≤ 2.7	Reference standard: $\sigma^{13}C$ benzene (1)
	$-26.4 \leq \Delta\delta^{13}C$ (complex 10') ≤ 7.2	
IGLO-III	$-7.2 \leq \Delta\delta^{13}C$ (complex 10) ≤ 4.0	
	$-26.3 \leq \Delta\delta^{13}C$ (complex 10') ≤ 6.3	
6-311g(d,p)	$-4.3 \leq \Delta\delta^{13}C$ (complex 10) ≤ 2.7	Reference standard: $\delta^{13}C6_{experimental}$ complex 10 (2)
	$-25.3 \leq \Delta\delta^{13}C$ (complex 10') ≤ 8.7	
IGLO-III	$-3.7 \leq \Delta\delta^{13}C$ (complex 10) ≤ 5.1	
	$-24.3 \leq \Delta\delta^{13}C$ (complex 10') ≤ 9.5	

Intervals of $\Delta\delta^{13}C$ ranges show that independently of the selected reference standard, 6-311G(d,p) basis functions describes with higher accuracy the electronic environment under the influence of the magnetic shielding tensors and thus the overall calculated sp3 and sp2 carbon chemical shifts of PYRMA complex ***10****. Similar trends were observed for the rest of the complexes described in the main text (data not shown).*

In terms of the selected reference standard, TMS gives differences between experimental and calculated ^{13}C from 0 to -8 ppm for all type of carbons (Figure 12 SI). The benzene (commonly used as reference for sp2 ^{13}C) allows the reduction of $\Delta\delta^{13}C$ range between - 3 and +3 ppm, but leads a loss of the systematic calculated $\delta^{13}C$ overestimation. Finally the utilization of an internal ^{13}C reference chosen as $\delta C6$ gives comparable $\Delta\delta^{13}C$ to the ones coming from the benzene.

In conclusion, the IGLO-III data set is not better than the 6-311G. The reference has to be judiciously chosen for reducing the prediction discrepancies, like with benzene. However, using the benzene leads to the removing of the systematic over-estimation obtained by using the TMS (see Figure 14 SI) and preventing to get an additional qualitative fingerprint of the most stable complexes.

Figure 14 SI:



*$\Delta\delta^{13}C$ stacked plots of PYRMA complexes **8** (A), **10-10'** (B), 17-17' (C) and **12-13** (D) referenced with TMS (lower case) and Benzene (upper case) at the level of theory B3LYP / 6-311G(d,p). Systematic overestimations from 0 to -8 ppm of predicted ^{13}C resonances of the favored complexes are obtained when the former reference standard was used (green region). Accuracy of overall ^{13}C resonances' prediction (± 3 ppm, blue region) but loss of systematic estimation is given when benzene is used as reference standard. The over estimations are not existing for all ^{13}C and are especially localized on some ^{13}C of the diazine or phenyl rings heart of the coordination sphere.*

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