

Supporting information

Ergostane-Type Sterols from King Trumpet Mushroom (*Pleurotus eryngii*) and Their Inhibitory Effects on Aromatase

Takashi Kikuchi¹, Naoki Motoyashiki¹, Takeshi Yamada¹, Kanae Shibatani², Kiyofumi Ninomiya², Toshio Morikawa^{2,*}, Reiko Tanaka^{1,*}

¹ Osaka University of Pharmaceutical Sciences, 4-20-1 Nasahara, Takatsuki, Osaka 569-1094, Japan

² Pharmaceutical Research and Technology Institute, Kindai University, 3-4-1 Kowakae, Higashi-osaka, Osaka 577-8502, Japan

* Correspondence: tanakar@gly.oups.ac.jp (R.T.); morikawa@kindai.ac.jp (T.M.);

Tel.: +81-72-690-1084 (R.T.); +81-6-4307-4306 (T.M.); Fax: +81-72-690-1084 (R.T.); +81-6-6729-3577 (T.M.)

Supporting Information

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Table S1. NMR Data for Compound 1 in CDCl₃ (δ in ppm; J in Hz)

	δ_{H}	^1H - ^1H COSY	NOE	δ_{C}	HMBC (H to C)
1 α	2.01 (1H, m)	1 β , 2	3	31.0	t 2, 3, 19
1 β	1.86 (1H, m)	1 α , 2			
2	1.68 (2H, m)	1 α , 1 β , 3	19	30.9	t
3	3.96 (1H, tt, $J = 11.5, 5.4$)	2, 4 α , 4 β	1 α	68.4	d
4 α	1.50 (1H, m)	3	6	39.0	t 3, 5
4 β	2.21 (1H, m)	3	19		3
5				63.3	s
6	3.24 (1H, d, $J = 2.4$)	7	4 α , 7	59.5	d 7, 8
7	4.85 (1H, br s)		6, 15	63.8	d 5, 6, 8, 14
8				122.2	s
9				138.8	s
10				38.3	s
11	2.19 (2H, m)	12 α , 12 β		22.2	t 9
12 α	1.47 (1H, m)	11		35.4	t
12 β	1.99 (1H, m)	11	21		
13				44.6	s
14				147.7	s
15	5.55 (1H, br s)	16 α , 16 β	7	118.7	d 13, 16, 17
16 α	2.27 (1H, m)	15, 17	17		13, 14, 15, 17
16 β	2.08 (1H, m)	15, 17	18	36.8	t 14, 15, 17
17	1.55 (1H, m)	16, 20		56.4	d 12, 13, 16
18	0.82 (3H, s)		16 β , 20	15.6	q 12, 13, 14, 17
19	1.30 (3H, s)		2 β , 4 β	23.6	q 1, 5, 9, 10
20	2.24 (1H, m)	17, 21, 22	18	38.8	d 22, 23
21	1.04 (3H, d, $J = 6.5$)	20	12 β	21.0	q 17, 20, 22
22	5.20 (1H, dd, $J = 15.2, 7.6$)	20, 23		135.1	d 21, 23, 24
23	5.28 (1H, dd, $J = 15.2, 7.9$)	22		132.4	d 22, 24, 28
24	1.88 (1H, m)	23, 28		42.8	d 22, 23, 25, 26
25	1.48 (1H, m)	26, 27		33.1	d 23, 24, 26, 28
26	0.85 (3H, d, $J = 6.8$)	25		19.9	q 24, 25, 27
27	0.83 (3H, d, $J = 6.8$)	25		19.6	q 24, 25, 26
28	0.93 (3H, d, $J = 6.8$)	24		17.6	q 23, 24, 25

Table S2. NMR Data for Compound 2 in CDCl₃ (δ in ppm; J in Hz)

	δ_{H}	^1H - ^1H COSY	NOE	δ_{C}	HMBC (H to C)
1 α	1.46 (1H, m)	1 β , 2 α , 2 β	3	32.2	t 2, 3, 5, 9, 10
1 β	1.67 (1H, m)	1 α , 2 α , 2 β			2, 3, 5, 10
2 α	1.96 (1H, m)	1 α , 1 β , 2 β , 3		31.1	t 9
2 β	1.56 (1H, m)	1 α , 1 β , 2 α , 3	19		1
3	3.92 (1H, tt, J = 11.4, 3.0)	2 α , 2 β , 4 α , 4 β	1 α	68.7	d
4 α	1.42 (1H, m)	3, 4 β	6	39.6	t 2, 3, 5, 6, 10
4 β	2.13 (1H, dd, J = 13.2, 11.4)	3, 4 α	19		2, 3
5				67.8	s
6	3.15 (1H, d, J = 3.5)	7	4 α , 19	61.3	d 4, 5, 7, 8
7	4.43 (1H, dd, J = 9.6, 3.5)	6	19	65.1	d 8
8				125.1	s
9	2.35 (1H, m)	11 α , 11 β		38.7	d 8, 10, 11, 14, 19
10				35.8	s
11 α	1.49 (1H, m)	9, 11 β		19.0	t 8, 13
11 β	1.40 (1H, m)	9, 11 α	18		9, 10, 13
12 α	1.16 (1H, m)	11 α , 11 β , 12 β	17	36.7	t 18
12 β	1.95 (1H, m)	11 α , 11 β , 12 α			13, 14, 18
13				43.1	s
14				152.7	s
15 α	2.65 (1H, m)	15 β , 16 α , 16 β		25.0	t 8, 13, 14, 16
15 β	2.30 (1H, m)	15 α , 16 β	18		8, 10, 14, 16, 17
16 α	1.89 (1H, m)	15 α , 16 β		26.6	t 13, 14, 15, 17
16 β	1.41 (1H, m)	15 α , 15 β , 16 α	18		13, 15, 17, 20
17	1.21 (1H, m)	16 α , 16 β , 20	12 α	56.6	d 12, 13, 20, 22
18	0.85 (3H, s)		11 β , 15 β , 16 β	17.9	q 12, 13, 14, 17
19	0.87 (3H, s)		2 β , 4 β , 6, 7	16.5	q 1, 5, 9, 10
20	1.46 (1H, m)	17, 21, 22A, 22B		34.9	d 13, 17
21	0.93 (3H, d, J = 6.8)	20		19.1	q 17, 20, 22
22A	1.03 (1H, m)	20, 22B, 23A, 23B		33.4	t 20, 21, 23
22B	1.44 (1H, m)	20, 22A, 23A, 23B			20, 24
23A	0.95 (1H, m)	22A, 22B, 23B, 24		30.4	t
23B	1.37 (1H, m)	22A, 22B, 23A, 24			22, 24, 25, 28
24	1.21 (1H, m)	26		39.1	d 22, 23, 24, 26, 28
25	1.58 (1H, m)	23A, 23B, 28		31.5	d 23, 25, 26, 28
26	0.85 (3H, d, J = 7.1)	24		20.5	q 24, 27
27	0.78 (3H, d, J = 7.0)	25		17.6	q 24, 26
28	0.77 (3H, d, J = 6.9)	25		15.4	q 23, 24, 25

Figure S1. ^1H NMR spectrum of compound **1**.

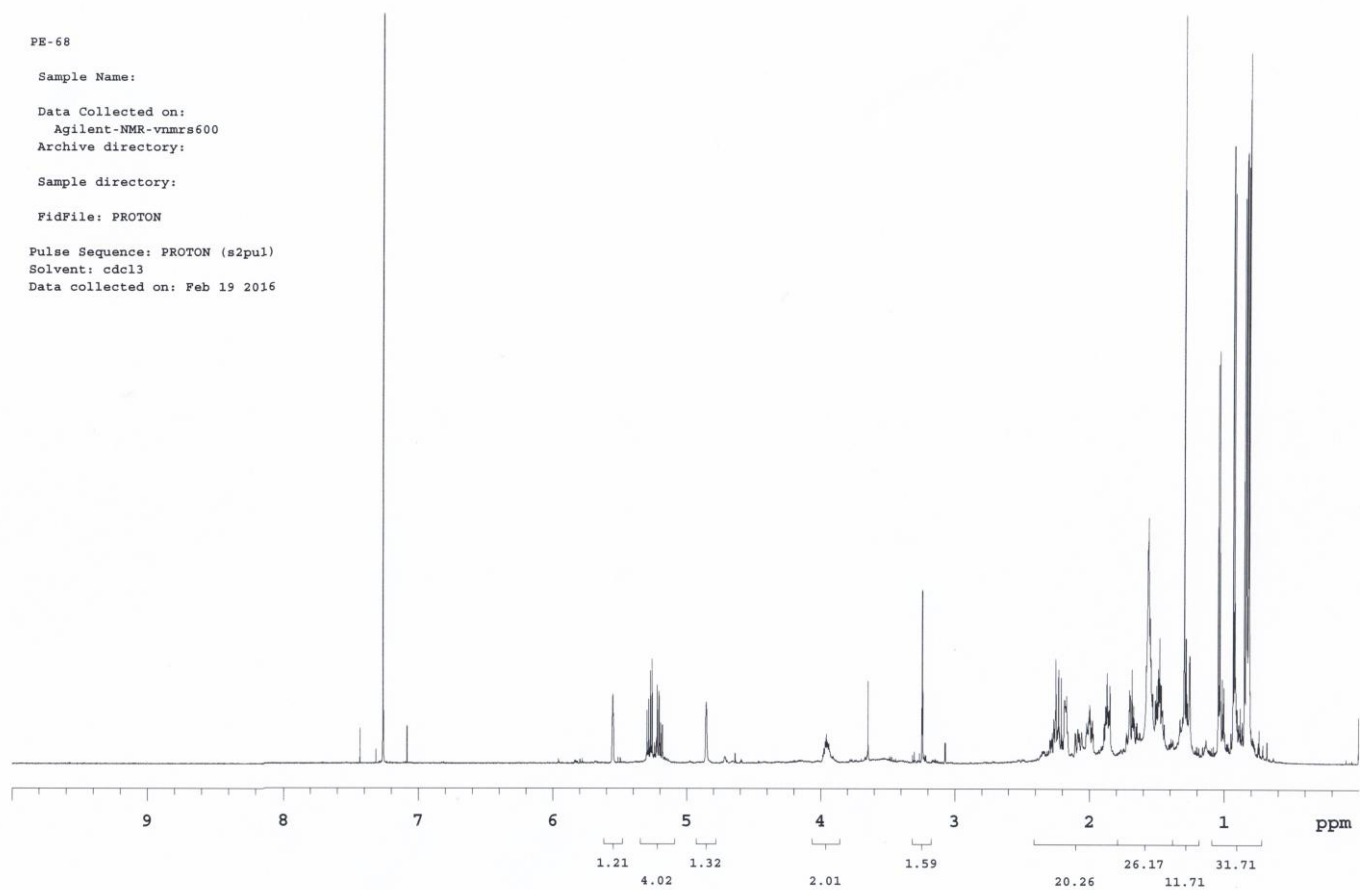


Figure S2. ^{13}C NMR spectrum of compound 1.

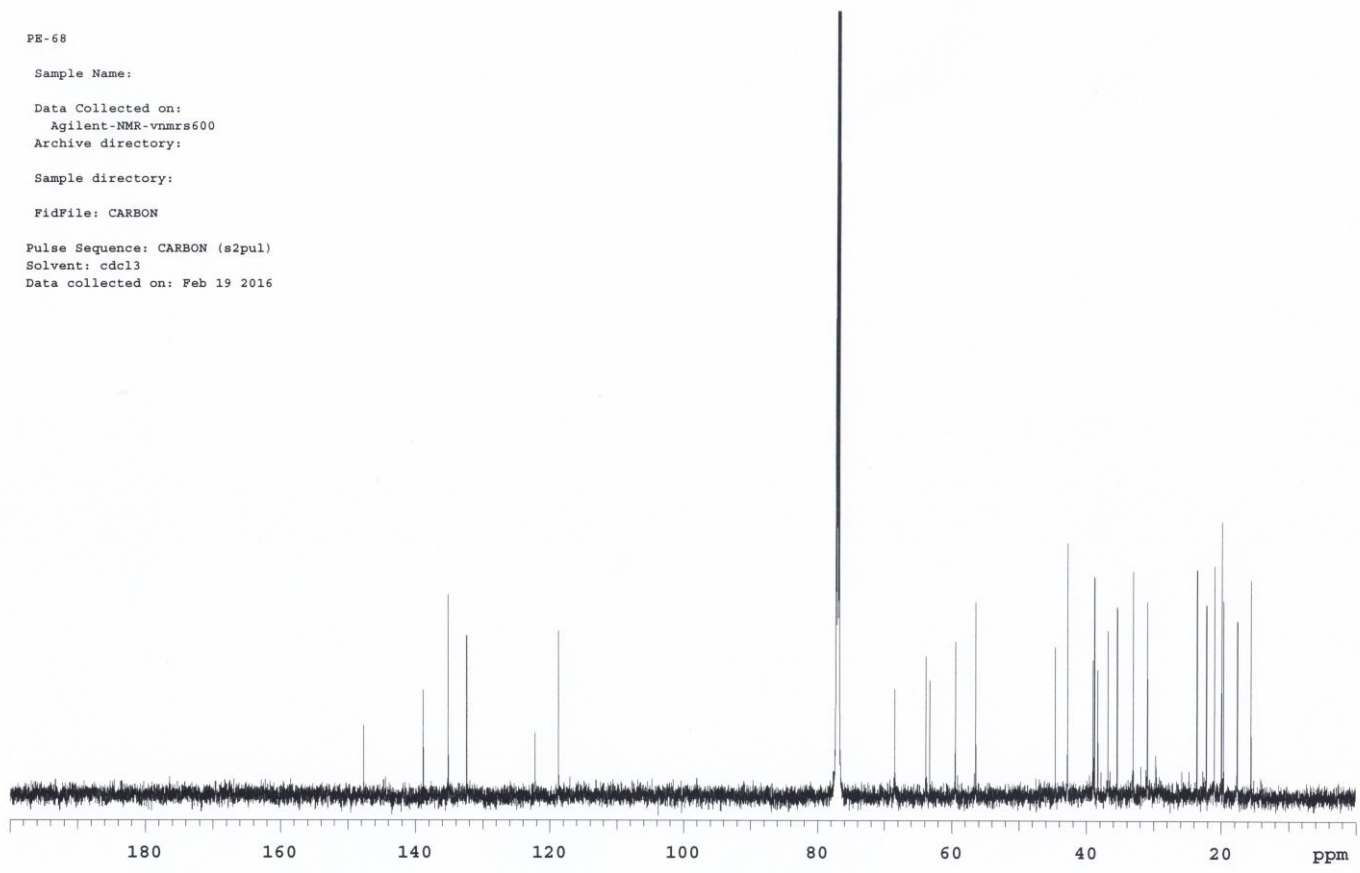


Figure S3. DEPT spectrum of compound **1**.

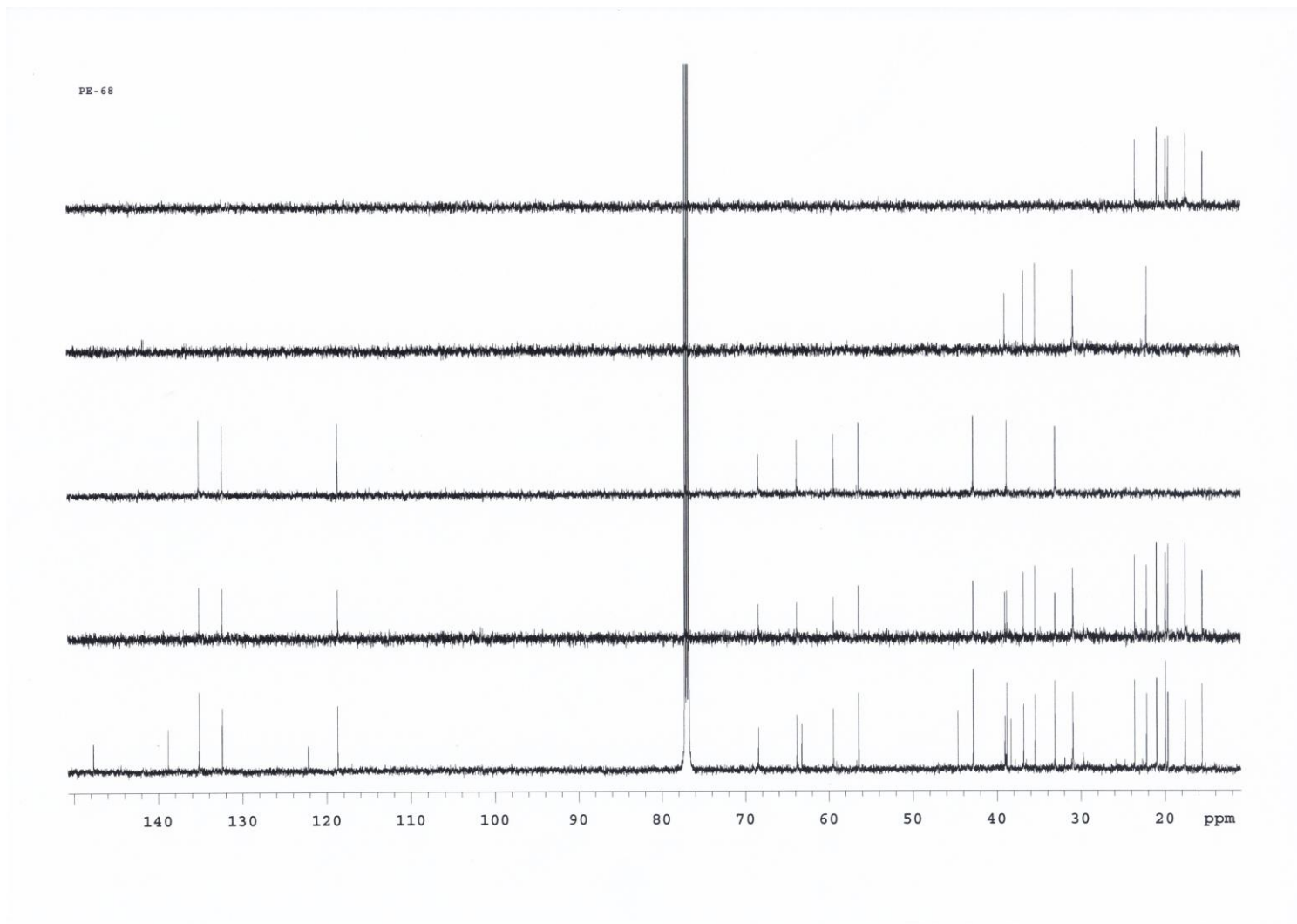


Figure S4. HSQC spectrum of compound 1.

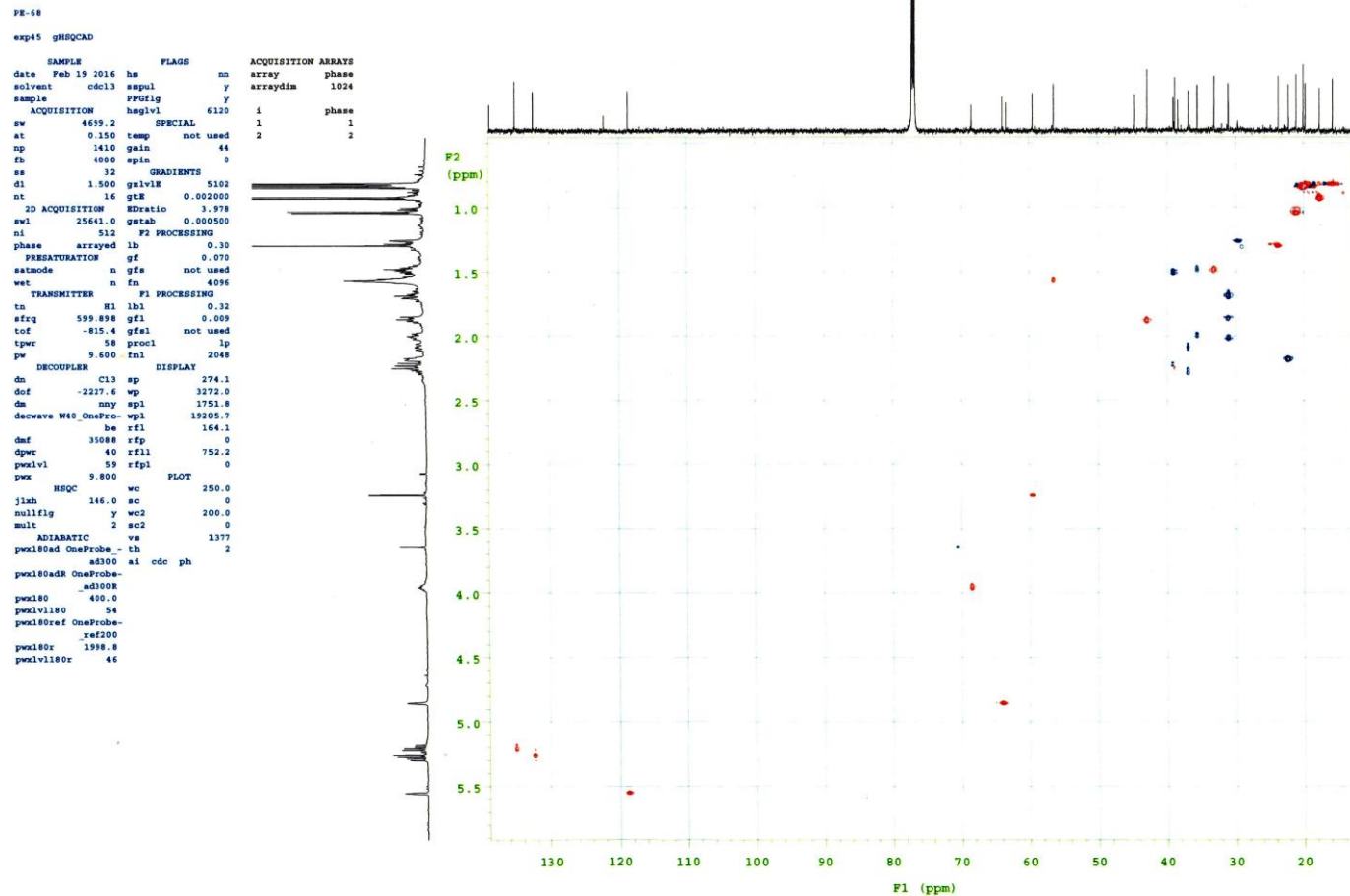


Figure S5. HMBC spectrum of compound 1.

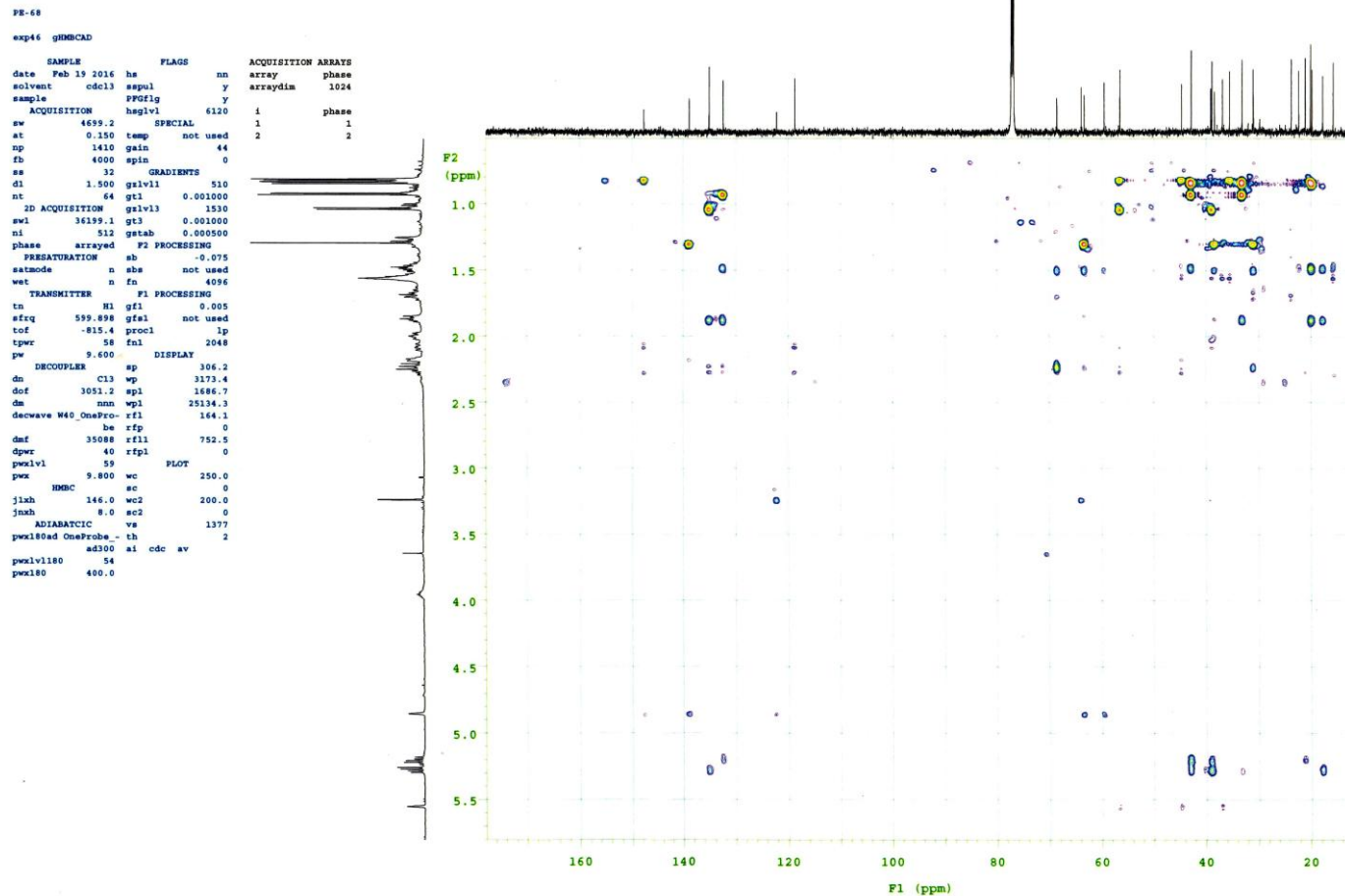


Figure S6. ^1H - ^1H COSY spectrum of compound **1**.

```
PE-68
exp43 gCOSY
SAMPLE          FLAGS
date Feb 19 2016 hs      nn
solvent cdcl3  espul    y
sample          hsglwl   6120
ACQUISITION     SPECIAL
sw 4734.8 temp not used
at 0.150 gain 48
np 1420 spin 0
fb 4000 F2 PROCESSING 0
ss 32 sb -0.075
d1 1.000 sbs not used
nt 16 fn 2048
2D ACQUISITION  F1 PROCESSING
sw1 4734.8 sb1 -0.027
ni 256 sbel not used
d2 0 procl lp
PREHEATURATION fnl 2048
satmode n sp DISPLAY 317.3
set TRANSMITTER wp 3366.2
tn N1 sp1 317.3
sfrq 599.898 wp1 3352.3
tof -755.4 rf1 121.9
tpr 58 rfp 0
pw 5.600 rf11 121.9
GRADIENTS rfpl 0
gr1v1E 5102 PLOT
g1E 0.001000 wc 200.0
EDratio 1.000 sc 0
gstab 0.000500 wc2 200.0
DECOUPLER sc2 0
dn C13 va 5702
dm mnn th
ai cdc av 2
```

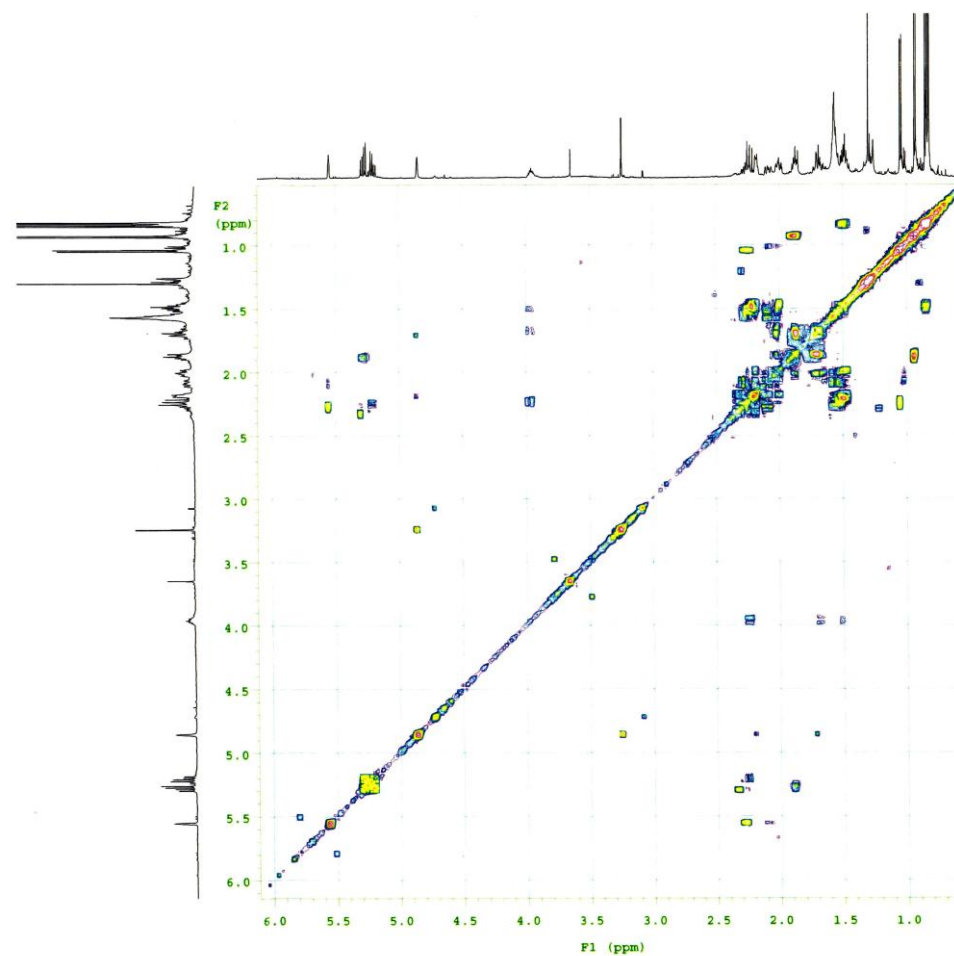


Figure S7. NOESY spectrum of compound 1.

```

PE-68
exp44 NOESY
SAMPLE          FLAGS
date Feb 19 2016 ha      nn
solvent cdc13  sspul    y
sample  PPO1g    PPO1g    y
ACQUISITION    hsg1v1  6120
sw 4699.2      SPECIAL
at 0.150 temp    not used
np 1410 gain     48
fb 4000 spin     0
ss 32          F2 PROCESSING 0
dl 1.300 gf     0.060
nt 24          gfs     not used
2D ACQUISITION fn      2048
sw1 4699.2     F1 PROCESSING
ni 256         gfl     0.030
TRANSMITTER    gfs1    not used
tn N1         procl   lp
sfrq 559.898  fnl     2048
tof -815.4    DISPLAY
tpwr 58       sp      313.1
pw 5.600     wp      3363.8
NOESY         sp1     313.1
mixN 0.800   wp1     3350.0
PRESATURATION  rfl     164.1
satmode n     rfp     0
wet n       rfl1    164.1
DECOUPLER     rfp1    0
dm C13       nnn     PLOT 200.0
nnn          wc      0
sc           ac2     200.0
wc2         ac2     0
va          va      200
th          th      2
a1 cdc ph
  
```

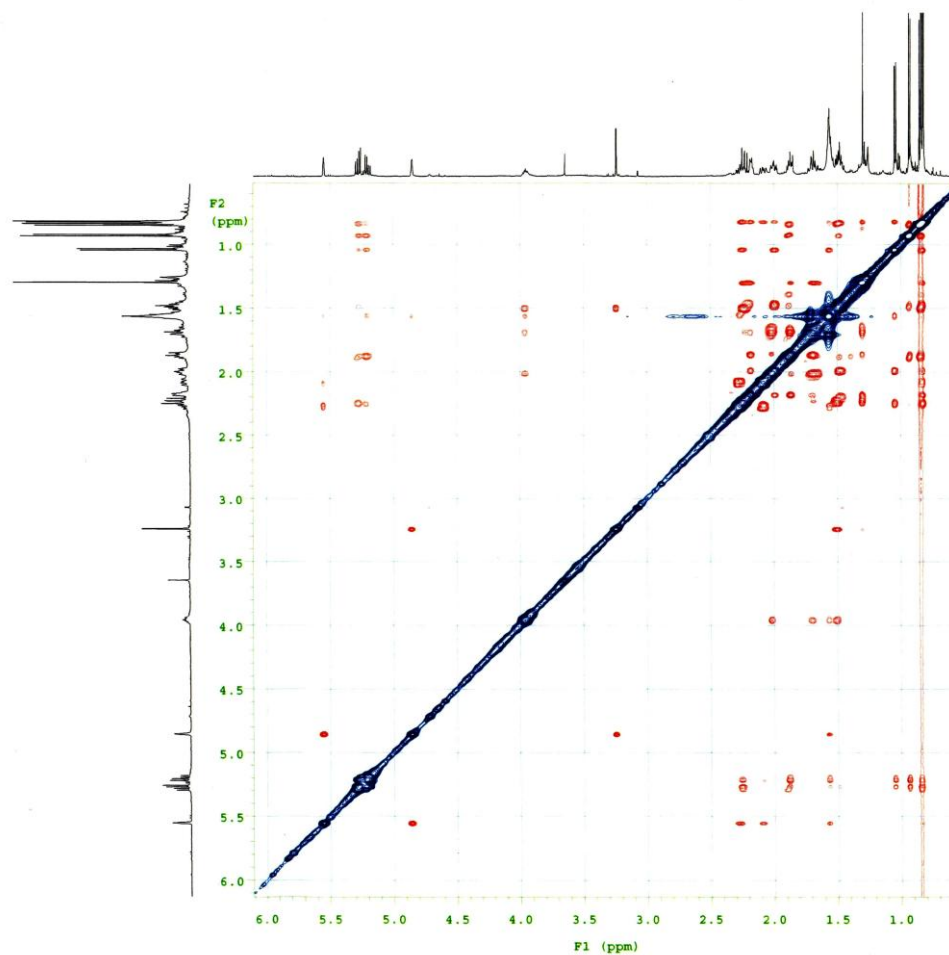


Figure S8. ^1H NMR spectrum of compound 2.

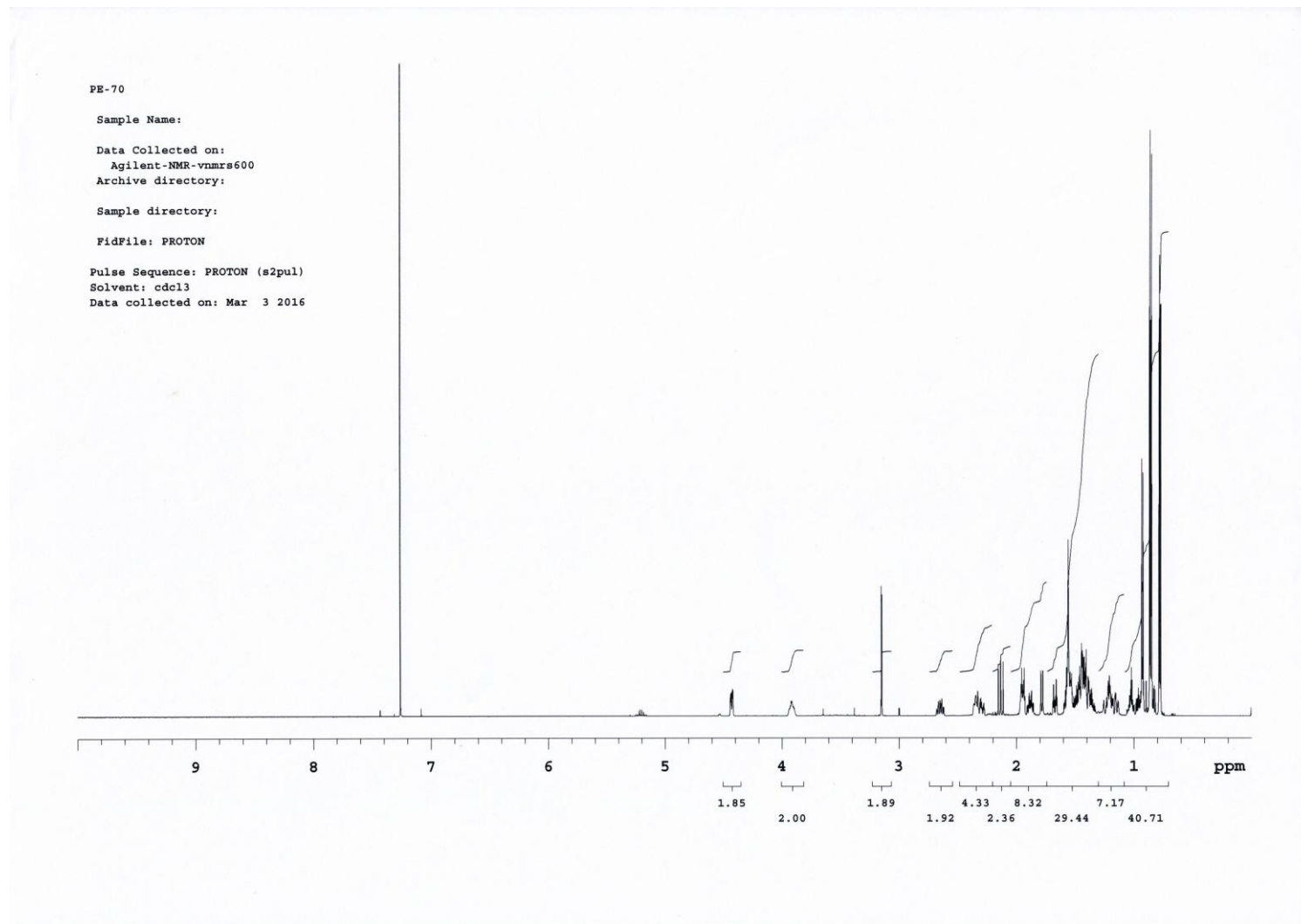


Figure S9. ^{13}C NMR spectrum of compound 2.

PE-70

Sample Name:

Data Collected on:
Agilent-NMR-vnmrs600
Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 3 2016

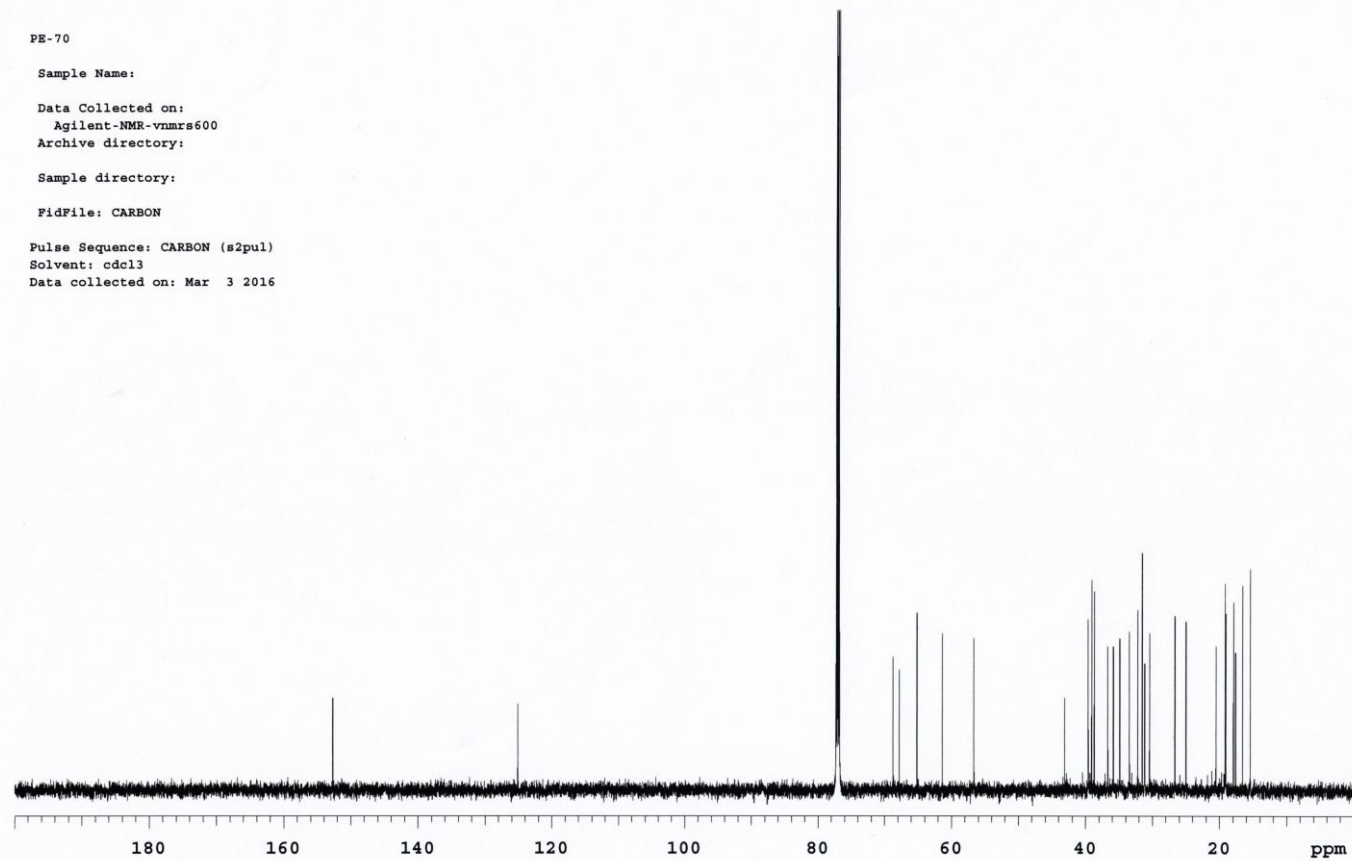


Figure S10. DEPT spectrum of compound 2.

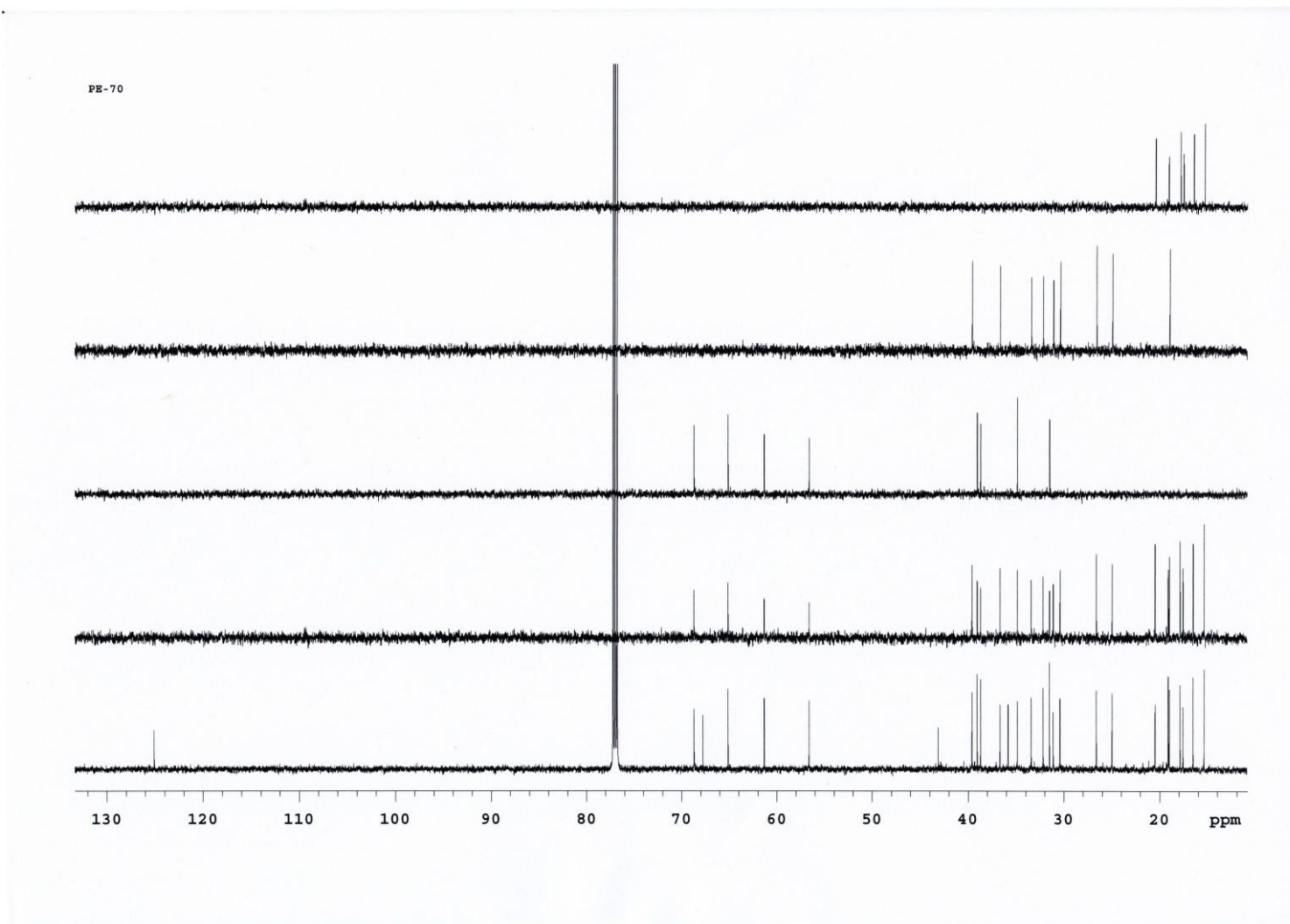


Figure S11. HSQC spectrum of compound 2.

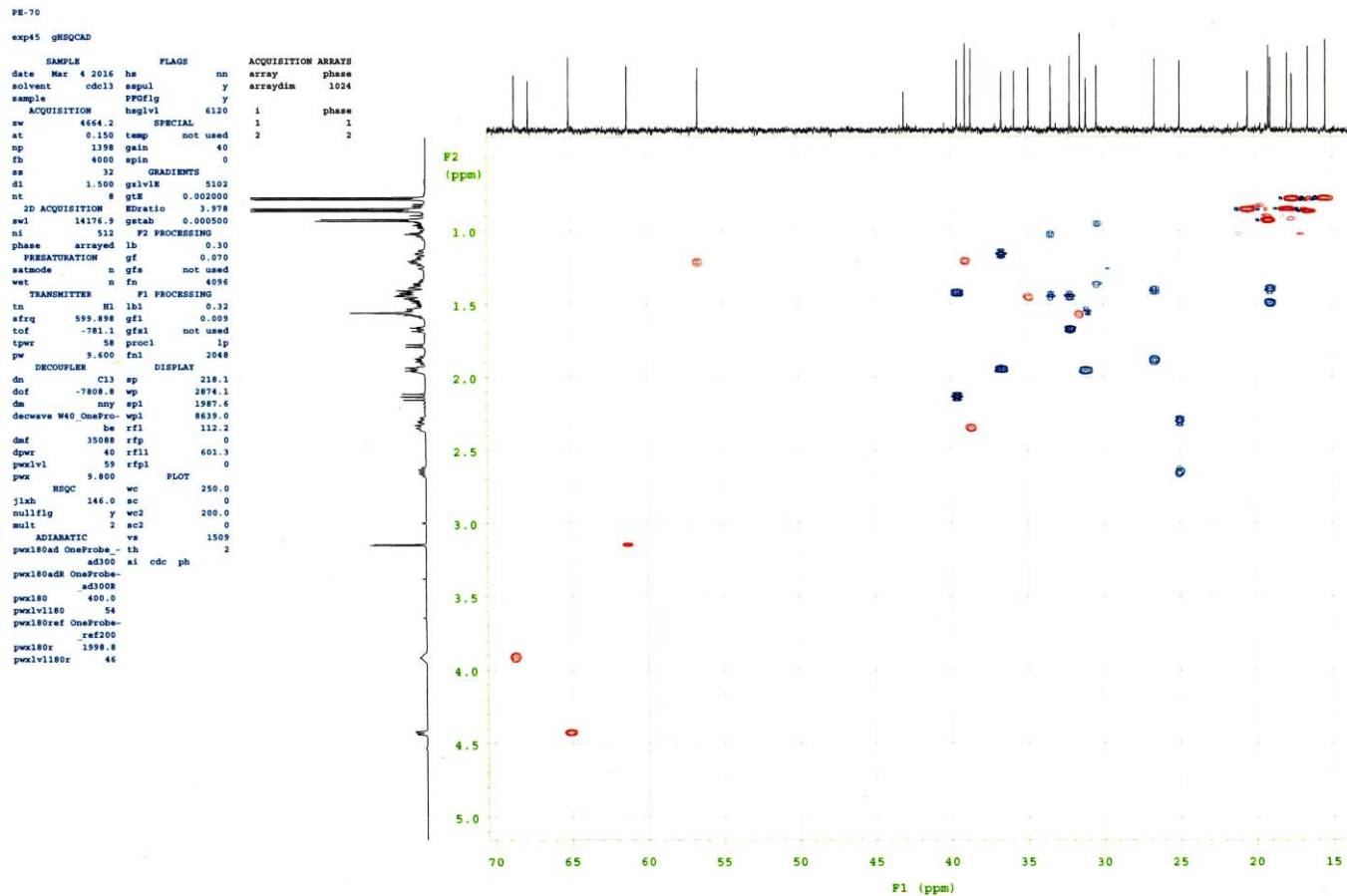


Figure S12. HMBC spectrum of compound 2.

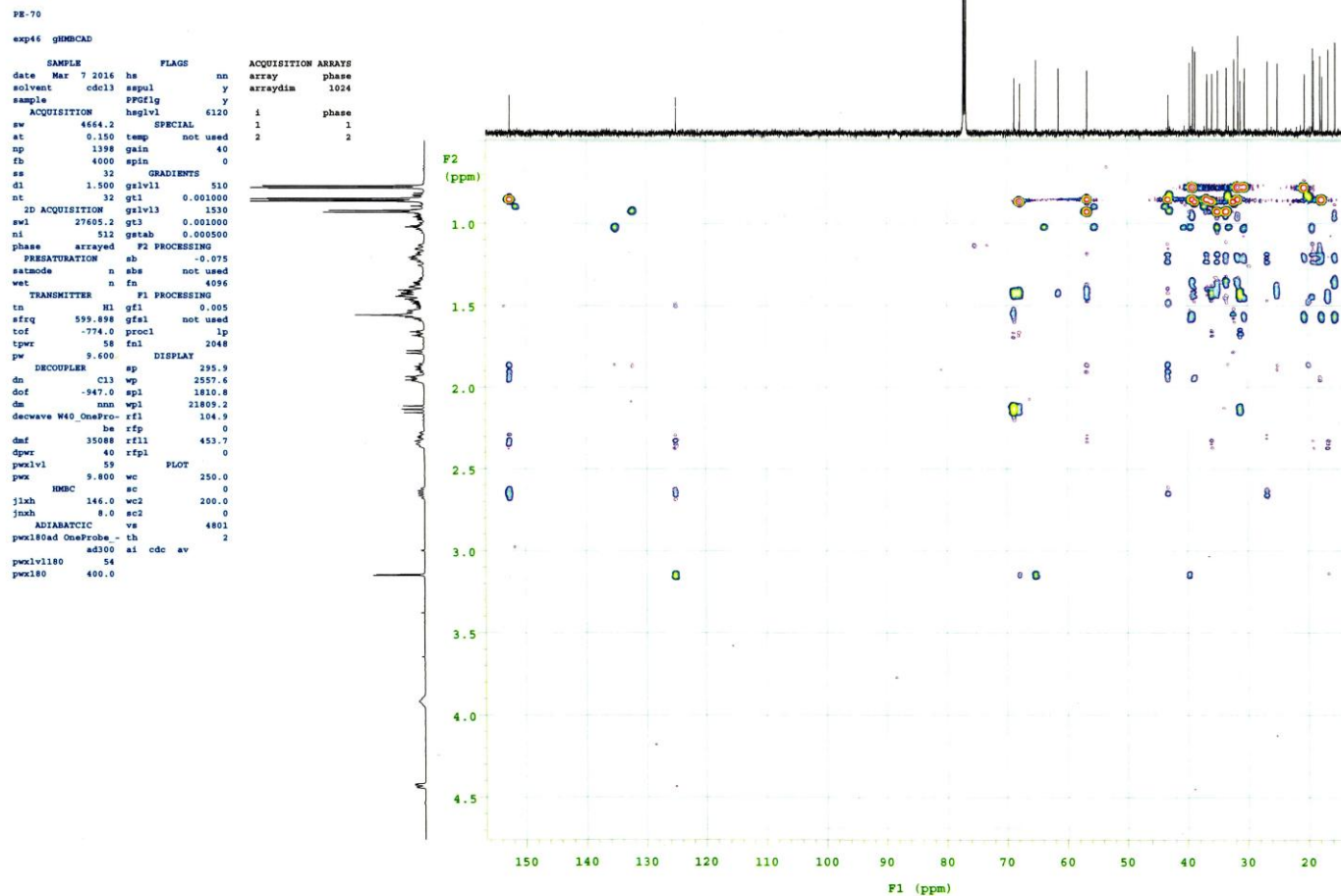


Figure S13. ^1H - ^1H COSY spectrum of compound 2.

```
PE-70
exp43 gCOSY
SAMPLE          FLAGS
date Mar 3 2016 hs nn
solvent cdcl3  sspul y
sample         hsglvl 6120
ACQUISITION     SPECIAL
aw 4595.6 temp not used
at 0.150 gain 44
ap 1378 spin 0
fb 4000 f2 PROCESSING 0
ss 32 ab -0.075
dl 1.000 abs not used
nt 8 fn 2048
2D ACQUISITION F1 PROCESSING
aw1 4595.6 sb1 -0.028
ni 256 sbel not used
d2 0 procl lp
PRESATURATION  fnl 2048
satmode n DISPLAY
wet n sp 269.7
TRANSMITTER wp 2562.6
tn H1 spl 269.7
rfq 599.898 wpl 2562.6
tof -788.2 rfl 84.8
tpwr 58 rfp 0
pw 9.600 rfl1 84.8
GRADIENTS rfp1 0
gslvie 5102 PLOT
gtE 0.001000 wc 200.0
EDratio 1.000 sc 0
gstab 0.000500 wc2 200.0
DECOUPLER sc2 0
dn C13 vs 268
da nnn th 2
a1 edc av
```

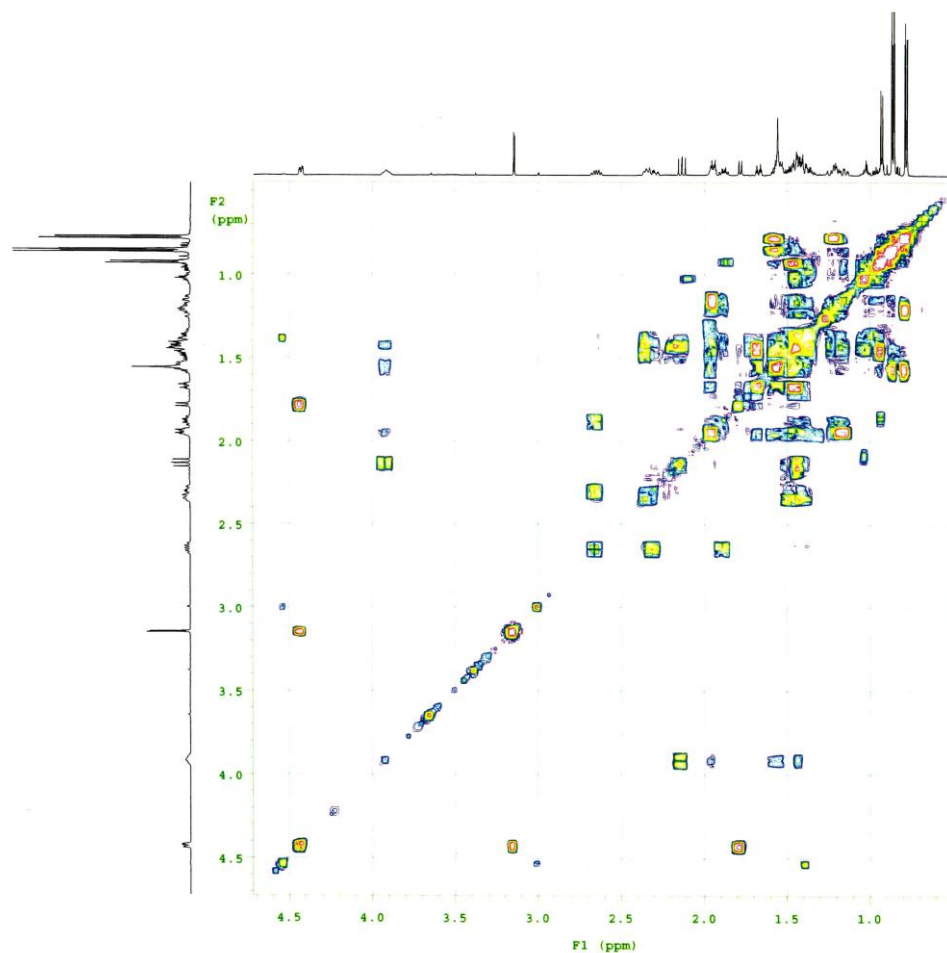


Figure S14. NOESY spectrum of compound 2.

```
PE-70
exp44 NOESY
SAMPLE          FLAGS
date Mar 3 2016 ha      nn
solvent cdc13  sepul    y
sample         PPG13g   y
ACQUISITION    hsgiv1   6120
sw 4664.2      SPECIAL
at 0.150 temp  not used
np 1400 gain   44
fb 4000 spin   0
ss 32         F2 PROCESSING
d1 1.300 gf    0.060
nt 16         not used
2D ACQUISITION fn 2048
sw1 4664.2    F1 PROCESSING
n1 256 gf1    0.030
TRANSMITTER    gfs1    not used
tn H1 procl   lp
efrq 599.898  fn1 2048
tof -781.1    DISPLAY
tpwr 58 sp    266.0
pw 9.600 wp   2559.8
NOESY         spl 266.0
mixM 0.800 wpl 2559.8
PRESATURATION rfl 112.0
satmode n rfp 0
wet n rfl1 112.0
DECOUPLER     rfp1 0
dn C13        PLOT
dm nnn wc    200.0
sc 0
wc2 200.0
sc2 0
vs 268
th 2
a1 cdc ph
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