

Supplementary Materials

Altercrasins A–E, decalin derivatives, from a sea-urchin-derived *Alternaria* sp.: Isolation and structural analysis including stereochemistry

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Table S0 NMR spectral data of **1** in acetone-*d*₆

Position	$\delta_{\text{H}}^{\text{a}}$		J/Hz	^1H - ^1H COSY	NOESY ^b	δ_{C}	HMBC (C) ^c
1 α	1.55	dq	12.8 (1 β), 3.8 (2 α , 2 β , 10)	1 β , 2 α , 2 β , 10		25.9 (t)	2, 10
1 β	1.12	qd	12.8 (1 α , 2 α , 10), 3.8 (2 β)	1 α , 2 α , 10	3, 5, 24		
2 α	0.90	m		1 α , 1 β , 2 β , 3	4 α , 10, 23	36.0 (t)	
2 β	1.74	ddt	12.8 (2 α), 5.3 (3), 3.8 (1 α , 1 β)	1 α , 2 α	23		
3	1.48	m		2 α , 4 α , 4 β , 23	1 β , 5	33.5 (d)	
4 α	0.82	q	12.8 (3, 4 β , 5)	3, 4 β , 5	2 α , 10, 23	42.6 (t)	2, 3, 5, 6, 10, 23
4 β	1.87	ddd	12.8 (4 α), 5.5 (4), 3.2 (5)	3, 4 α , 5	6, 23		
5	1.92	br t	12.8 (4 α , 10)	4 α , 4 β , 10	1 β , 3, 24	37.4 (d)	10
6	5.55	d	11.3 (7)	7	4 β	133.2 (d)	4, 5, 7, 8, 10
7	5.70	ddd	11.3 (6), 4.8 (8), 2.5	6, 8		125.3 (d)	5, 6, 8, 13
8	2.65	ddt	11.8 (13), 4.8 (7), 1.8	7, 13	14, 24	49.9 (d)	6, 7, 9, 10, 13, 14, 24
9						52.9 (s)	
10	1.49	td	12.8 (1 β , 5), 3.8 (1 α)	1 α , 1 β , 5	2 α , 4 α , 13	38.7 (d)	5, 24
11						211.6 (s)	
12						74.0 (s)	
13	3.16	dd	11.8 (8), 9.0 (14)	8, 14	10, 15	52.8 (d)	7, 8, 12, 14, 15, 18, 22
14	5.62	ddd	15.5 (15), 9.0 (13), 1.8	13, 15	8, 16, 17, 19	124.3 (d)	8, 12, 13, 15, 16
15	5.73	dd	15.5 (14), 5.5 (16)	14, 16	13, 17	141.9 (d)	13, 14, 16, 17
16	4.21	m		15, 17, 16-OH	14	68.8 (d)	14
17	1.16	d	6.8 (16)	16	14, 15	24.2 (q)	15, 16
18						207.1 (s)	
19	3.66	d	7.0 (20)	20	14, 21	70.4 (d)	18, 20, 21, 22
20	3.99	m		19, 21, 20-OH	NH	67.8 (d)	18
21	1.25	d	6.2 (20)	20	19, NH	20.4 (q)	19, 20
22						170.7 (s)	
23	0.91	d	6.5 (3)	3	2 α , 2 β , 4 α , 4 β	22.6 (q)	2, 3, 4
24	0.95	s			1 β , 5, 8	16.0 (q)	8, 9, 10, 11
16-OH	3.79	d	5.0 (16)	16			15, 16, 17
20-OH	4.17	d	5.5 (20)	20			19
NH	8.01	br s			20, 21		

^a ^1H chemical shift values (δ ppm from SiMe₄) followed by multiplicity and then the coupling constants (J/Hz). Figures in parentheses indicate the proton coupling with that position. ^b The correlations with geminal and vicinal protons are removed. ^c Long range ^1H - ^{13}C correlations from H to C observed in the HMBC experiment.

Table S1 NMR spectral data of **2** in acetone-*d*₆

Position	$\delta_{\text{H}}^{\text{a}}$		J/Hz	^1H - ^1H COSY	NOESY ^b	δ_{C}	HMBC (C) ^c
1 α	1.52	dq	13.2 (1 β), 3.6 (2 α , 2 β , 10)	1 β , 10		25.9 (t)	10
1 β	1.13	qd	13.2 (1 α , 2 α , 10), 3.6 (2 β)	1 α	3, 5, 24		
2 α	0.90	m		2 β , 3	10, 23	36.0 (t)	
2 β	1.75	ddt	12.6 (2 α), 5.4 (3), 3.6 (1 α , 1 β)	2 α	23		
3	1.49	m		2 α , 4 α , 23	1 β , 5	33.5 (d)	
4 α	0.83	q	12.0 (3, 4 β , 5)	3, 4 β , 5	10, 23	42.7 (t)	2, 3, 5, 6, 10, 23
4 β	1.88	ddd	12.0 (4 α), 5.4 (3), 3.5 (5)	4 α , 5	6, 23		
5	1.93	m		4 α , 4 β , 10	1 β , 3, 24	37.5 (d)	3, 6, 10
6	5.54	d	10.2 (7)	7	4 β	132.9 (d)	4, 5, 7, 8, 10
7	5.69	ddd	10.2 (6), 4.8 (8), 2.4	6, 8		125.7 (d)	5, 8, 9
8	2.74	ddt	12.0 (13), 4.8 (7), 1.8	7, 13	14, 24	49.7 (d)	6, 7, 9, 10, 13, 14, 24
9						52.9 (s)	
10	1.40	td	13.2 (1 α , 5), 3.0 (1 α)	1 β , 5	2 α , 4 α , 13	39.0 (d)	1, 24
11						211.7 (s)	
12						74.2 (s)	
13	3.01	dd	12.0 (8), 9.0 (14)	8, 14	10, 15	52.5 (d)	7, 8, 12, 14, 15, 18, 22
14	5.82	ddd	15.0 (15), 9.0 (13), 1.8	13, 15	8, 16, 17, 19	125.5 (d)	8, 12, 13, 16
15	5.59	ddd	15.0 (14), 5.4 (16), 0.6	14, 16	13, 17	140.8 (d)	13, 16, 17
16	4.17	m		15, 17, 16-OH	14, 20	68.0 (d)	14, 15, 17
17	1.14	d	6.6 (16)	16	14, 15	23.9 (q)	15, 16
18						207.8 (s)	
19	3.93	d	4.2 (20)	20	21, NH	69.7 (d)	18, 20, 21, 22
20	3.98	m		19, 21	16	67.4 (d)	
21	1.27	d	6.0 (20)	20	19, NH	20.7 (q)	19, 20
22						170.2 (s)	
23	0.92	d	6.6 (3)	3	2 α , 2 β , 4 α , 4 β	22.6 (q)	2, 3, 4
24	0.99	s			1 β , 5, 8	16.1 (q)	8, 9, 10, 11
16-OH	3.47	br s		16			
20-OH	4.02	br s					
NH	8.02	br s			19, 21		

^a ^1H chemical shift values (δ ppm from SiMe₄) followed by multiplicity and then the coupling constants (J/Hz). Figures in parentheses indicate the proton coupling with that position. ^b The correlations with geminal and vicinal protons are removed. ^c Long range ^1H - ^{13}C correlations from H to C observed in the HMBC experiment.

Table S2 NMR spectral data of **3** in acetone-*d*₆

Position	$\delta_{\text{H}}^{\text{a}}$		J/Hz	^1H - ^1H COSY	NOESY ^b	δ_{C}	HMBC (C) ^c
1 α	1.80	dq	12.6 (1 β), 3.6 (2 α , 2 β , 10)	1 β , 2 α , 10		26.0 (t)	
1 β	1.20	qd	12.6 (1 α , 2 α , 10), 3.6 (2 β)	1 α , 2 α , 2 β , 10	3, 5, 24		2, 5, 10
2 α	0.87	qd	12.6 (1 β , 2 α , 3), 3.6 (1 α)	1 α , 1 β , 2 β , 3	10	36.2 (t)	1, 3, 10, 23
2 β	1.74	ddt	12.6 (2 α), 5.4 (3), 3.6 (1 α , 1 β)	1 β , 2 α			
3	1.49	m		2 α , 23	1 β , 5	33.7 (d)	23
4 α	0.79	q	12.6 (3, 4 β , 5)	4 β , 5	10, 23	43.0 (t)	2, 3, 5, 6, 10, 23
4 β	1.87	ddd	12.6 (4 α), 5.4 (3), 3.6 (5)	4 α , 5	6, 23		2, 5
5	1.95	br t	12.6 (4 α , 10)	4 α , 4 β , 10	1 β , 3, 24	37.5 (d)	4, 6
6	5.57	d	9.6 (7)	7	4 β	133.1 (d)	4, 5, 8, 10
7	5.97	ddd	9.6 (6), 4.8 (8), 3.0	6, 8	14	126.1 (d)	5, 8, 9
8	3.34	ddt	12.6 (13), 4.8 (7), 0.9	7, 13	24	45.3 (d)	6, 7, 9, 10, 13, 24
9						53.4 (s)	
10	1.35	td	12.6 (1 β , 5), 3.6 (1 α)	1 α , 1 β , 5	2 α , 4 α , 13	40.4 (d)	5, 24
11						211.3 (s)	
12						74.7 (s)	
13	2.83	ddd	12.6 (8), 5.4 (14), 2.4	8, 14	10, 17	45.5 (d)	
14	6.42	ddd	8.4 (15), 5.4 (13), 2.4	13, 15	7	133.6 (d)	8, 16
15	5.83	ddd	8.4 (14), 5.4 (16), 2.4	14, 16	17	134.3 (d)	13, 16, 17, 18
16	2.48	m		15, 17		43.7 (d)	14, 18
17	1.20	d	7.2 (16)	16	13, 15	15.3 (q)	15, 16, 18
18						81.2 (s)	
19						173.3 (d)	18, 20, 21, 22
22						177.5 (s)	
23	0.89	d	6.6 (3)	3	4 α , 4 β	22.8 (q)	2, 3, 4
24	1.05	s			1 β , 5, 8	17.3 (q)	8, 9, 10, 11

a ^1H chemical shift values (δ ppm from SiMe_4) followed by multiplicity and then the coupling constants (J/Hz). Figures in parentheses indicate the proton coupling with that position. b The correlations with geminal and vicinal protons are removed. c Long range ^1H - ^{13}C correlations from H to C observed in the HMBC experiment.

Table S3 NMR spectral data of **4** in acetone-*d*₆

Position	$\delta_{\text{H}}^{\text{a}}$		J/Hz	^1H - ^1H COSY	NOESY ^b	δ_{C}	HMBC (C) ^c
1 α	1.67	m		1 β		27.6 (t)	
1 β	1.20	qd	12.6 (1 α , 2 α , 10), 3.6 (2 β)	1 α , 2 β , 10	5, 24		
2 α	0.85	qd	12.6 (1 β , 2 β , 3), 3.6 (1 α)	2 β , 3	23	36.1 (t)	1
2 β	1.72	m		2 α	23		
3	1.49	m		2 α , 23	1 β , 5	33.5 (d)	
4 α	0.79	q	12.6 (3, 4 β , 5)	4 β , 5	10, 23	42.6 (t)	2, 3, 5, 10, 23
4 β	1.85	ddd	12.6 (4 α), 5.4 (3), 3.6 (5)	4 α	6, 23		
5	2.08	m		4 α , 10	1 β , 3, 24	39.1 (d)	
6	5.48	d	10.2 (7)	7	4 β	133.3 (d)	4, 5, 8, 10
7	6.04	dd	10.2 (6), 3.0	6	14	127.7 (d)	5, 8, 9, 10
8						141.5 (s)	
9						50.7 (s)	
10	1.70	m		1 β , 5	4 α	44.7 (d)	5, 24
11						208.4 (s)	
12						70.5 (s)	
13	3.71	d	9.6 (15)	14, 15	16, 24	43.6 (d)	8, 12, 14, 15, 16, 22
14	5.52	d	1.8	13	7, 15	124.6 (d)	7, 9, 12, 13, 15
15	5.37	ddq	16.8 (16), 9.0 (13), 1.8	13, 16	14, 17	128.4 (d)	12, 16, 17
16	5.57	dq	16.8 (15), 6.6 (17)	15, 17	13	131.0 (d)	13, 17
17	1.62	d	6.6 (16)	16	15	18.0 (q)	15, 16
18						208.4 (s)	
19	3.49	d	7.2 (20)	20	21, NH	69.9 (d)	18, 20, 21, 22
20	3.99	m		19, 21		68.1 (d)	
21	1.28	d	6.6 (20)	20	19, NH	20.2 (q)	19, 20
22						168.1 (s)	
23	0.89	d	6.6 (3)	3	2 α , 2 β , 4 α , 4 β	22.6 (q)	2, 3, 4
24	1.12	s			1 β , 5, 13	17.4 (q)	8, 9, 10, 11
20-OH	4.06	br s					
NH	7.88	br s			19, 21		

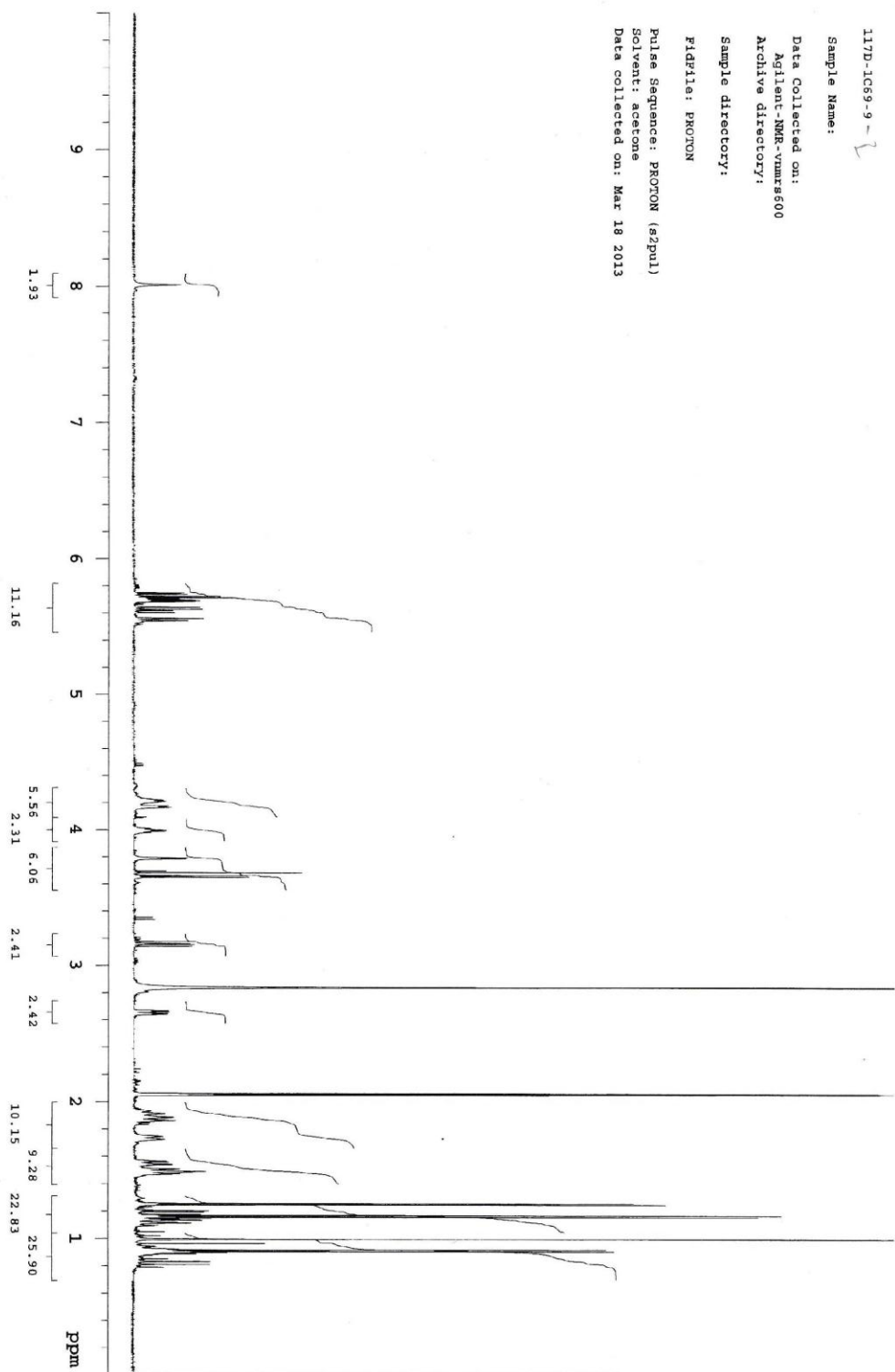
^a ^1H chemical shift values (δ ppm from SiMe₄) followed by multiplicity and then the coupling constants (J/Hz). Figures in parentheses indicate the proton coupling with that position. ^b The correlations with geminal and vicinal protons are removed. ^c Long range ^1H - ^{13}C correlations from H to C observed in the HMBC experiment.

Table S4 NMR spectral data of **5** in acetone-*d*₆

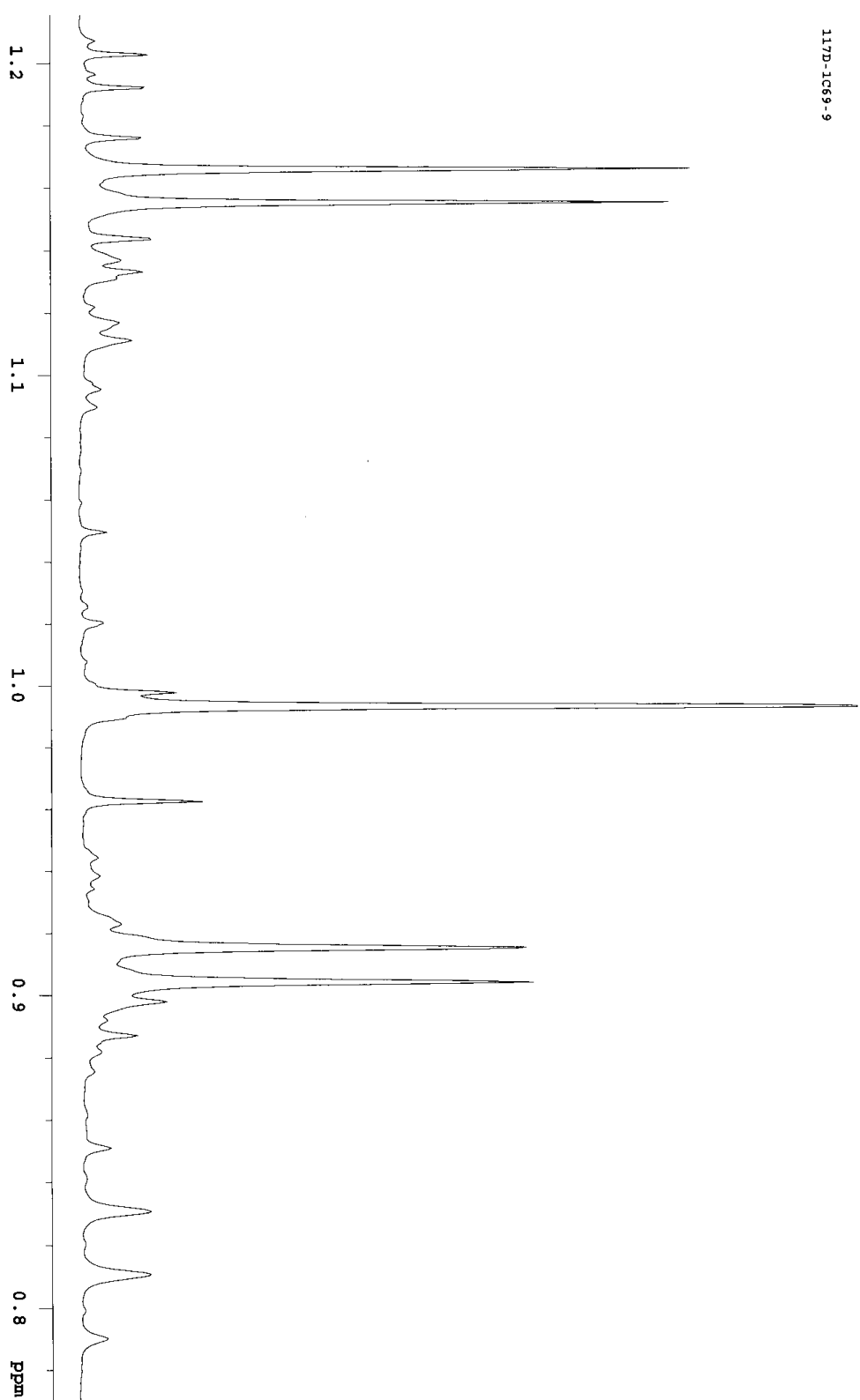
Position	$\delta_{\text{H}}^{\text{a}}$		J/Hz	^1H - ^1H COSY	NOESY ^b	δ_{C}	HMBC (C) ^c
1 α	1.91	dq	12.6 (1 β), 3.6 (2 α , 2 β , 10)	1 β		28.0 (t)	9, 10
1 β	1.20	qd	12.6 (1 α , 2 α , 10), 3.6 (2 β)	1 α	3, 5		
2 α	0.90	m		2 β	4 α	36.2 (t)	
2 β	1.73	ddt	11.4 (2 α), 5.4 (3), 3.6 (1 α , 1 β)	2 α , 3	23		
3	1.49	m		2 β , 23	1 β , 5	33.5 (d)	
4 α	0.80	q	12.0 (3, 4 β , 5)	4 β	2 α , 10, 23	42.9 (t)	2, 3, 5, 6, 10, 23
4 β	1.87	ddd	12.0 (4 α), 5.8 (3), 3.5 (5)	4 α	6, 23		
5	2.09	m		10	1 β , 3, 24	38.6 (d)	4, 6, 7
6	5.49	d	10.2 (7)	7	4 β	133.5 (d)	4, 5, 8, 10
7	6.07	dd	10.2 (6), 3.0	6	14	127.4 (d)	5, 8, 9, 14
8						140.1 (s)	
9						50.6 (s)	
10	1.37	td	12.6 (1 α , 5), 3.6 (1 α)	5	4 α	45.3 (d)	
11						205.2 (s)	
12						72.7 (s)	
13	3.96	d	9.0 (15)	14, 15	16, 24	41.5 (d)	12, 14, 15, 16, 18
14	5.70	d	1.8	13	7	126.9 (d)	7, 9, 12, 13, 15
15	5.37	ddq	16.8 (16), 9.0 (13), 1.8	13, 16	17	129.4 (d)	17
16	5.62	dq	16.8 (15), 6.6 (17)	15, 17	13	129.9 (d)	13, 17
17	1.59	d	6.6 (16)	16	15	17.9 (q)	15, 16
18						204.7 (s)	
19	3.81	d	4.8 (20)	20	21, NH	68.9 (d)	18, 20, 21, 22
20	3.90	m		19, 21		67.0 (d)	
21	1.29	d	6.0 (20)	20	19, NH	20.8 (q)	19, 20
22						170.7 (s)	
23	0.89	d	6.6 (3)	3	2 β , 4 α , 4 β	22.6 (q)	2, 3, 4
24	1.12	s			5, 13	16.6 (q)	8, 9, 10, 11
20-OH	4.02	d	6.0 (20)				
NH	7.86	br s			19, 21		

^a ^1H chemical shift values (δ ppm from SiMe₄) followed by multiplicity and then the coupling constants (J/Hz). Figures in parentheses indicate the proton coupling with that position. ^b The correlations with geminal and vicinal protons are removed. ^c Long range ^1H - ^{13}C correlations from H to C observed in the HMBC experiment.

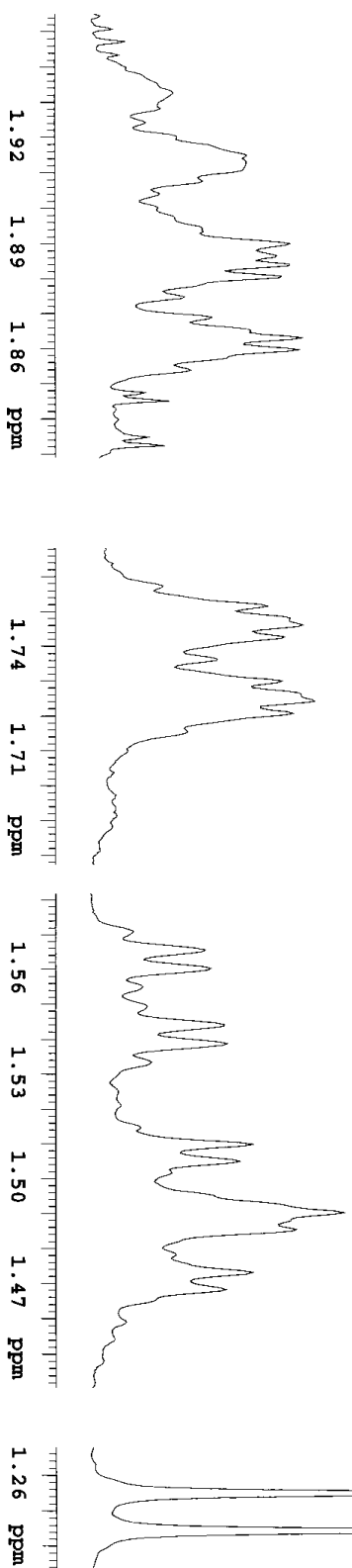
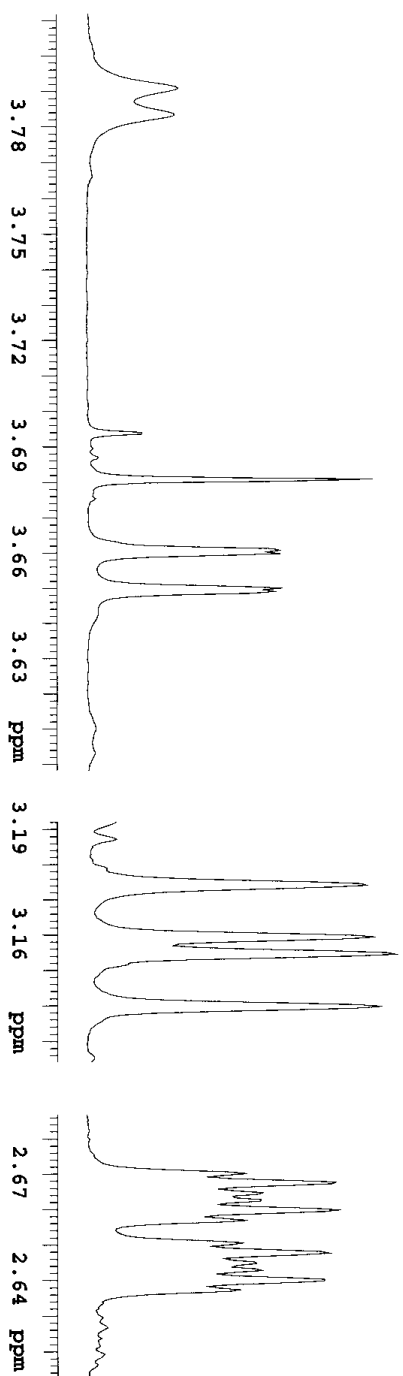
Figure S1 ^1H and ^{13}C NMR spectrum of 1 in acetone- d_6



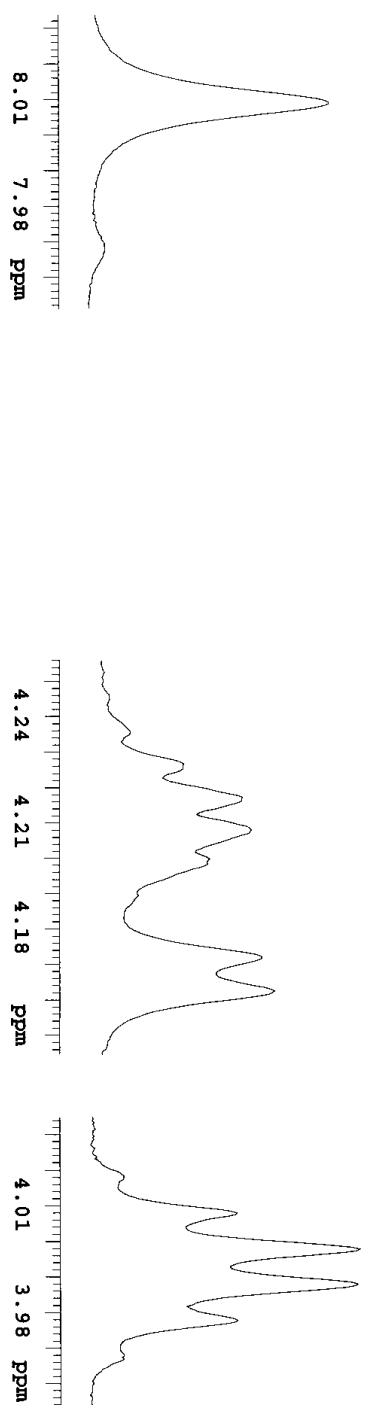
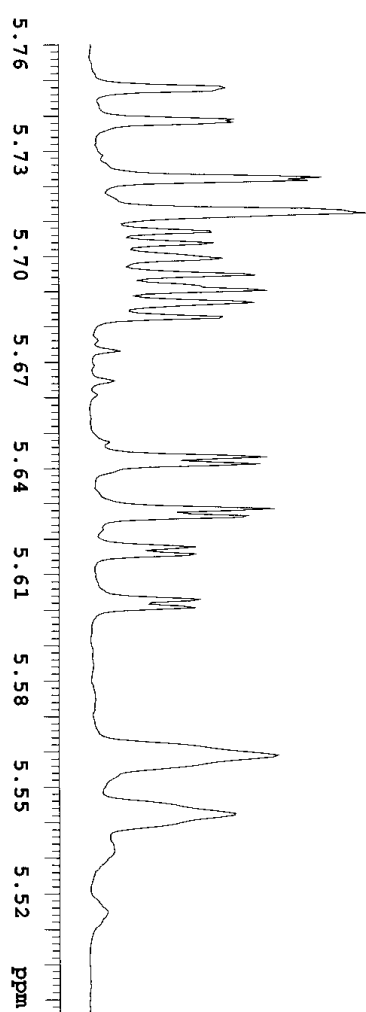
117D-1069-9



117D-1C69-9



117D-1C63-9



117D-1C89-9

Sample Name:

Data Collected on:

Agilent-NMR-vnmr600

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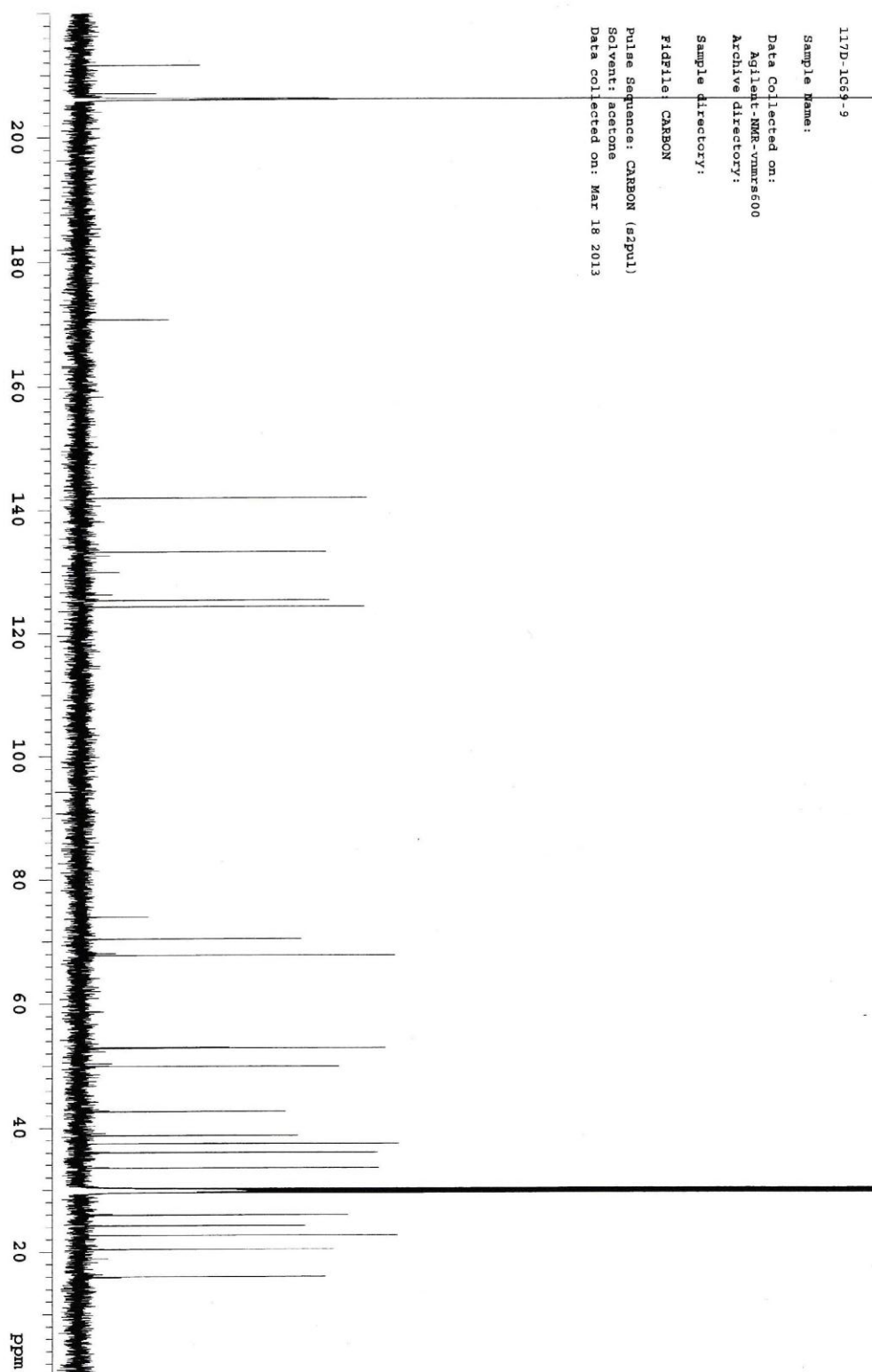
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Pulse Sequence: CARBON (s2pul)

Solvent: acetone

Data collected on: Mar 18 2013



117D-1C69-9

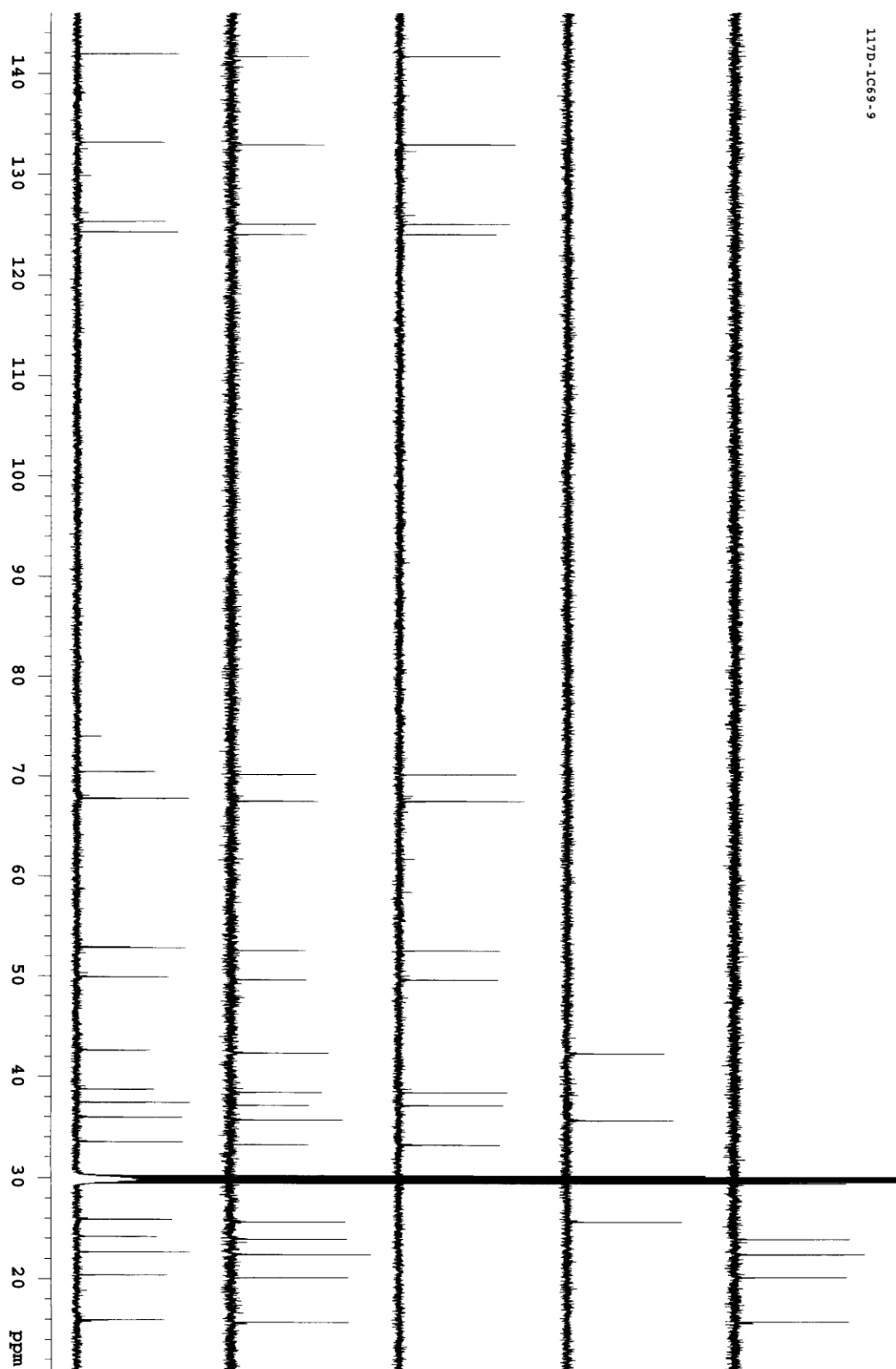
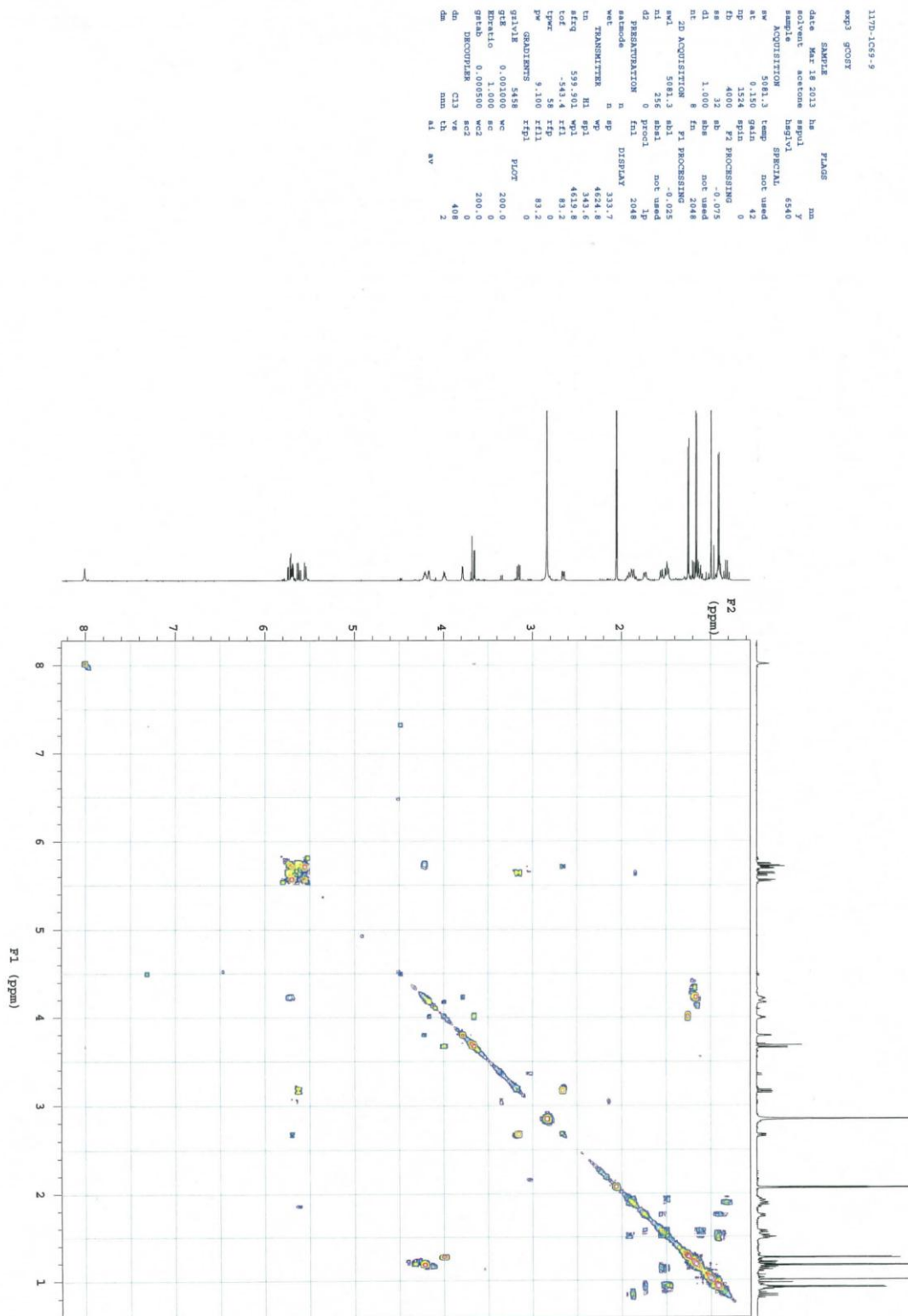


Figure S2 ^1H - ^1H COSY of 1



117D-1069-9
expt3 gcosy

SAMPLE		FLAGS	
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solvent	acetone	sepal	y
sample	bagivi	SPECIAL	6340
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at	0.150	galtb	42
ap	1524	spib	0
eb	4000	F2 PROCESSING	0
as	32	ab	-0.075
d1	1.000	abs	not used
nt	8	fn	2048
2D ACQUISITION			
sw1	5081.3	ab1	-0.025
ni	256	absl	not used
o2	PRESENTATION	0	procl
ip	2048	ip	2048
SCHEDULE			
ns	0	sp	368.4
ns	0	wp	927.9
TRANSMITTER			
tu	81	sp1	403.1
afq	599.901	wp1	903.1
tof	-543.4	rf1	83.2
lpcr	56	rfg	0
pw	9.100	rf11	83.2
gradients	5458	rfg1	0
PLOT			
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g1v1k	0.001000	mc2	200.0
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g1v1k	0.001000	mc4	200.0
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g1v1k	0.001000	mc6	200.0
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g1v1k	0.001000	mc13	200.0
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g1v1k	0.001000	mc15	200.0
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g1v1k	0.001000	mc28	200.0
g1v1k	0.001000	mc29	200.0
g1v1k	0.001000	mc30	200.0
g1v1k	0.001000	mc31	200.0
g1v1k	0.001000	mc32	200.0
g1v1k	0.001000	mc33	200.0
g1v1k	0.001000	mc34	200.0
g1v1k	0.001000	mc35	200.0
g1v1k	0.001000	mc36	200.0
g1v1k	0.001000	mc37	200.0
g1v1k	0.001000	mc38	200.0
g1v1k	0.001000	mc39	200.0
g1v1k	0.001000	mc40	200.0
g1v1k	0.001000	mc41	200.0
g1v1k	0.001000	mc42	200.0
g1v1k	0.001000	mc43	200.0
g1v1k	0.001000	mc44	200.0
g1v1k	0.001000	mc45	200.0
g1v1k	0.001000	mc46	200.0
g1v1k	0.001000	mc47	200.0
g1v1k	0.001000	mc48	200.0
g1v1k	0.001000	mc49	200.0
g1v1k	0.001000	mc50	200.0
g1v1k	0.001000	mc51	200.0
g1v1k	0.001000	mc52	200.0
g1v1k	0.001000	mc53	200.0
g1v1k	0.001000	mc54	200.0
g1v1k	0.001000	mc55	200.0
g1v1k	0.001000	mc56	200.0
g1v1k	0.001000	mc57	200.0
g1v1k	0.001000	mc58	200.0
g1v1k	0.001000	mc59	200.0
g1v1k	0.001000	mc60	200.0
g1v1k	0.001000	mc61	200.0
g1v1k	0.001000	mc62	200.0
g1v1k	0.001000	mc63	200.0
g1v1k	0.001000	mc64	200.0
g1v1k	0.001000	mc65	200.0
g1v1k	0.001000	mc66	200.0
g1v1k	0.001000	mc67	200.0
g1v1k	0.001000	mc68	200.0
g1v1k	0.001000	mc69	200.0
g1v1k	0.001000	mc70	200.0
g1v1k	0.001000	mc71	200.0
g1v1k	0.001000	mc72	200.0
g1v1k	0.001000	mc73	200.0
g1v1k	0.001000	mc74	200.0
g1v1k	0.001000	mc75	200.0
g1v1k	0.001000	mc76	200.0
g1v1k	0.001000	mc77	200.0
g1v1k	0.001000	mc78	200.0
g1v1k	0.001000	mc79	200.0
g1v1k	0.001000	mc80	200.0
g1v1k	0.001000	mc81	200.0
g1v1k	0.001000	mc82	200.0
g1v1k	0.001000	mc83	200.0
g1v1k	0.001000	mc84	200.0
g1v1k	0.001000	mc85	200.0
g1v1k	0.001000	mc86	200.0
g1v1k	0.001000	mc87	200.0
g1v1k	0.001000	mc88	200.0
g1v1k	0.001000	mc89	200.0
g1v1k	0.001000	mc90	200.0
g1v1k	0.001000	mc91	200.0
g1v1k	0.001000	mc92	200.0
g1v1k	0.001000	mc93	200.0
g1v1k	0.001000	mc94	200.0
g1v1k	0.001000	mc95	200.0
g1v1k	0.001000	mc96	200.0
g1v1k	0.001000	mc97	200.0
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g1v1k	0.001000	mc99	200.0
g1v1k	0.001000	mc100	200.0

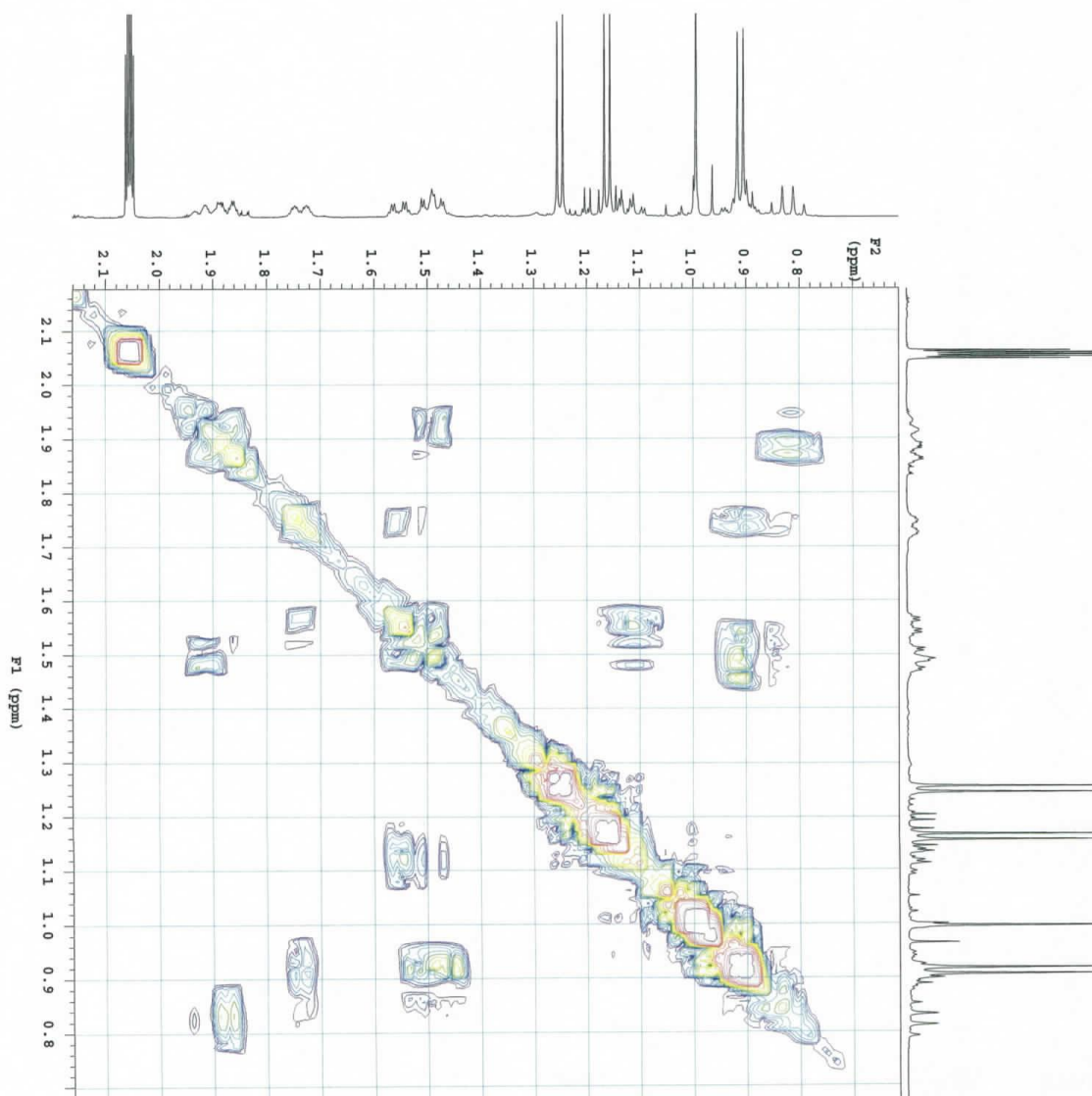
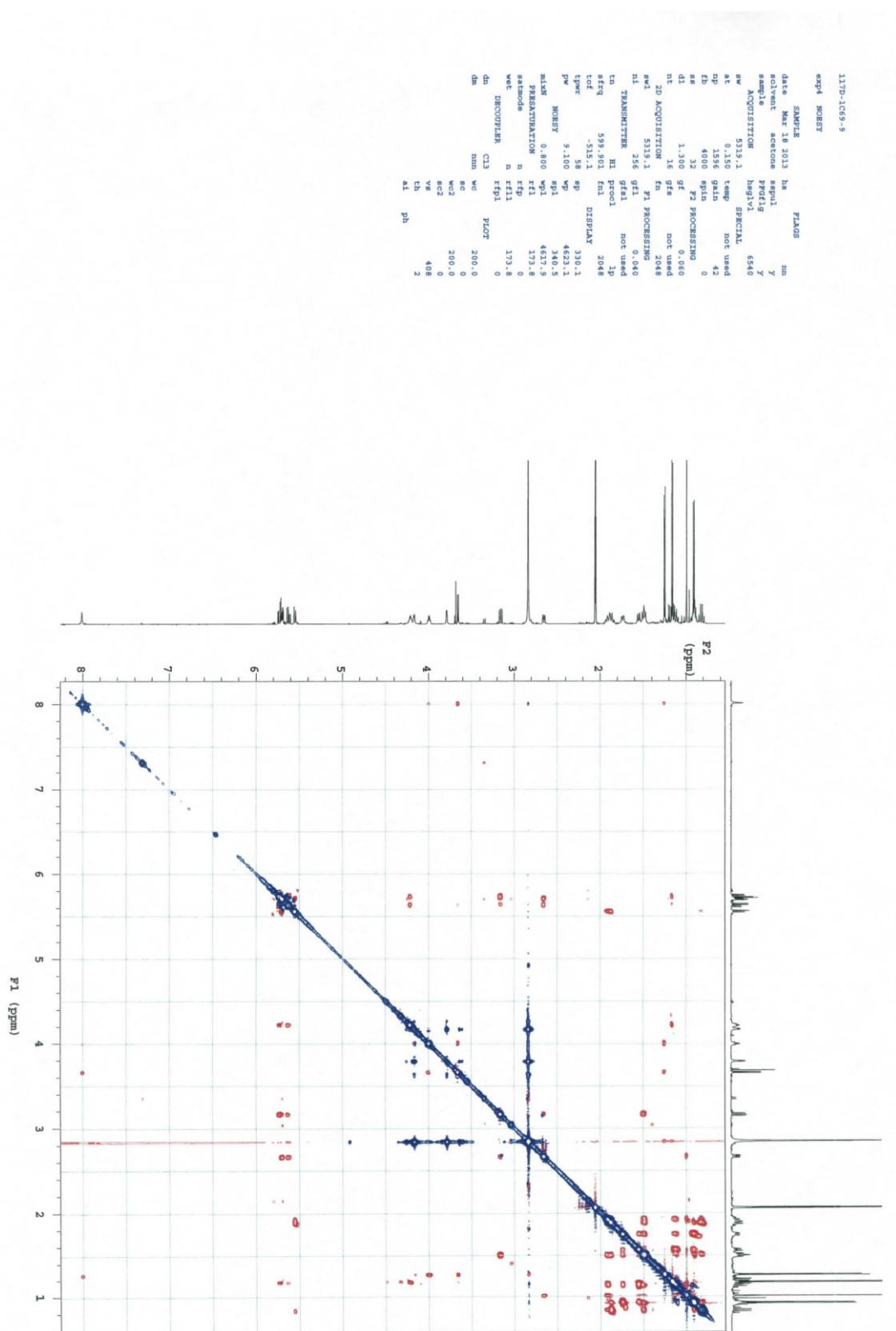


Figure S3 NOESY of 1

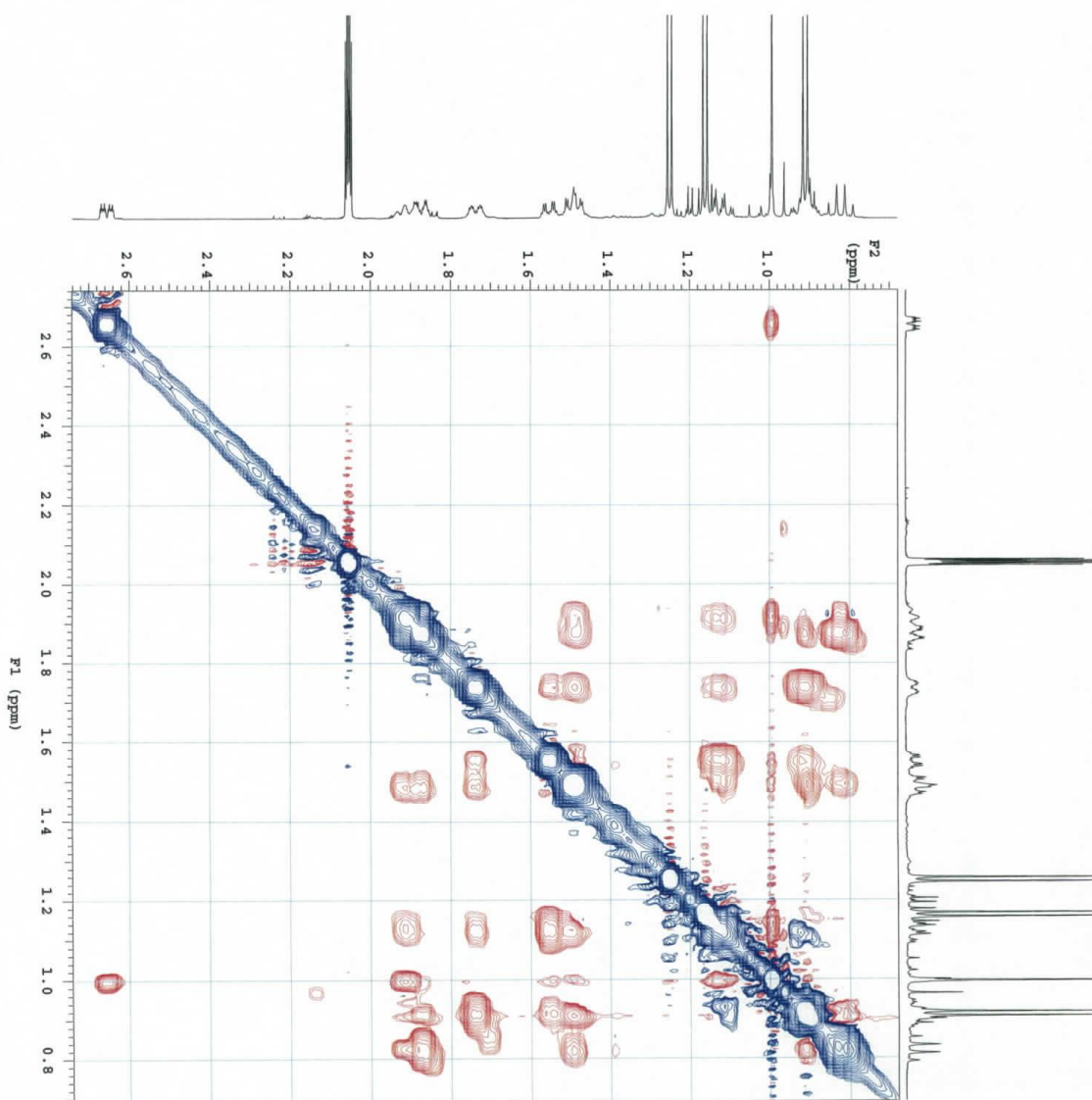



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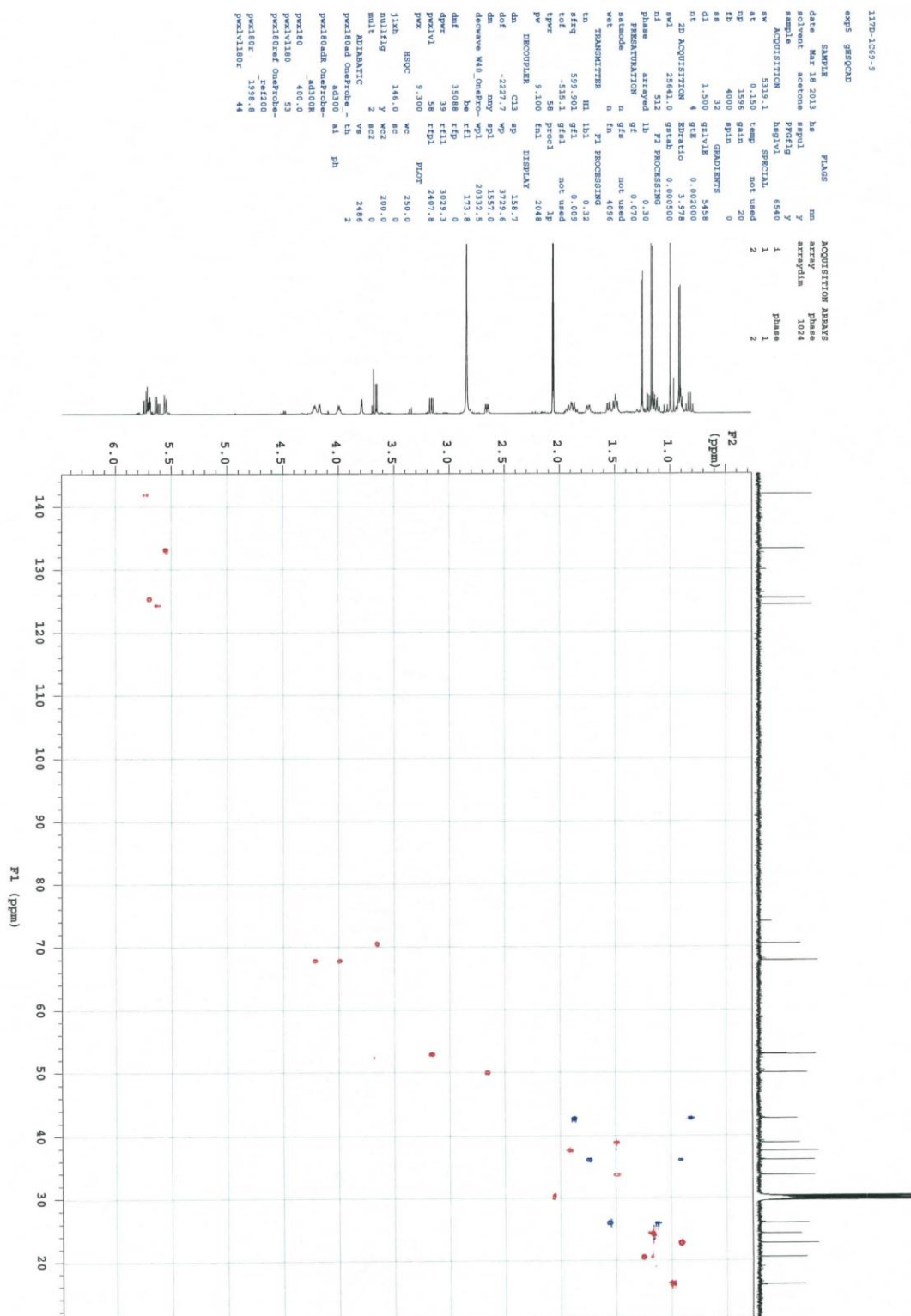
117D-1G69-9
exp4 NOESY

SAMPLE
date Mar 18 2013
solvent acetone
sample y
ACQUISITION
nu 5319.1
at 0.150 temp not used
ap 1356 gain 42
as 4032
d1 1.300 g4 not used
nt 16 gfs not used
2D ACQUISITION
sw1 5319.1 f1 PROCESSING
rl 256 gfl 0.040
tn TRANSMITTER m1 proc1 ip
rfreq 599.901 fm1
tocf -5319.1 DISPLAY 2048
tpec 58 ap 408.0
pw 9.100 p 1356.0
mlsm NOESY 0.800 wpl 433.2
PRESATURATION n rfp 1231.1
satmode n rfp 173.8
wet n rfp1 173.8
DECOUPLER C13 rfp1 0
dm nmh wc 200.0
nmh wc 200.0
sc 0
wca 200.0
vnu 0
vb 408
al ph 2

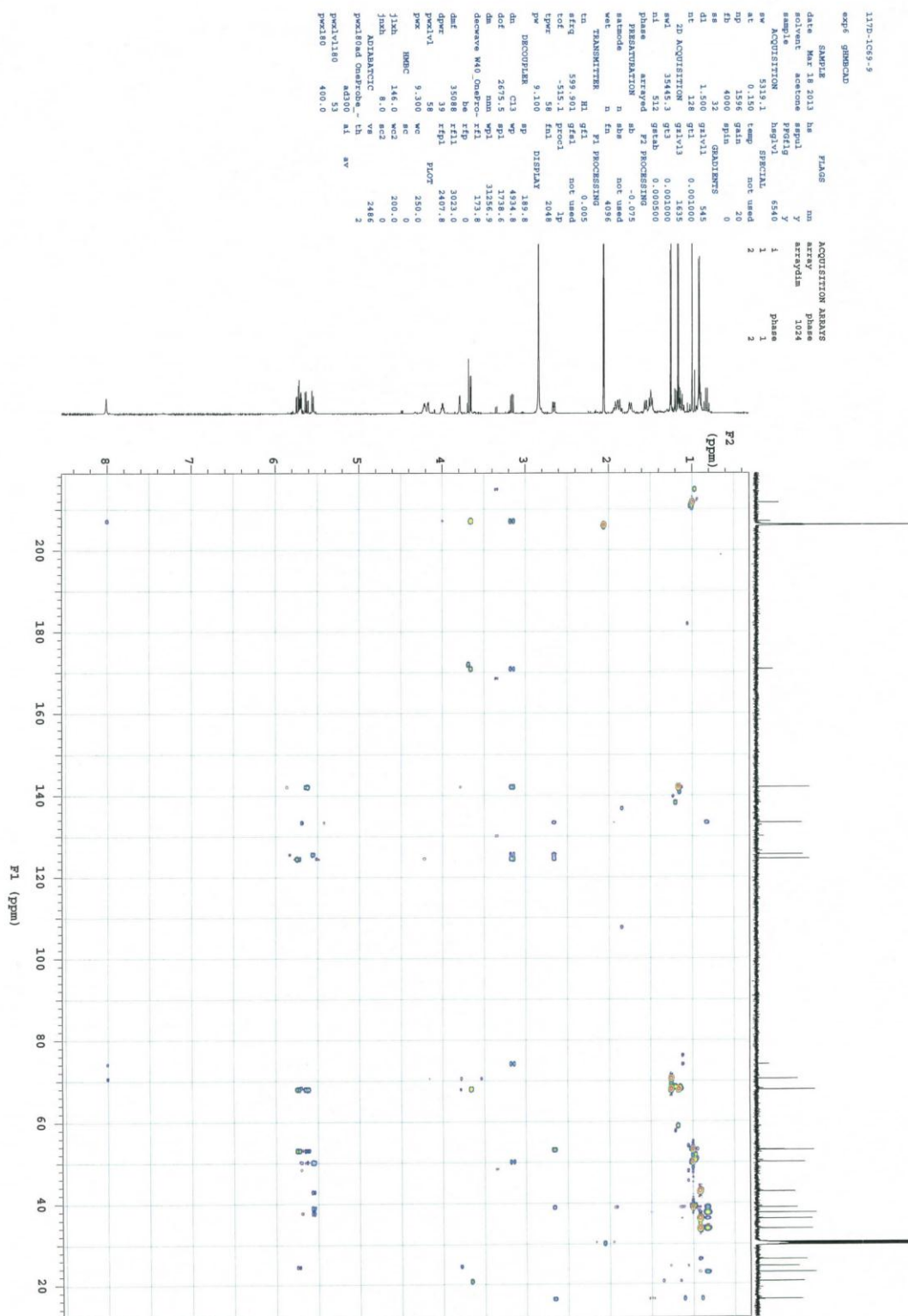
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17



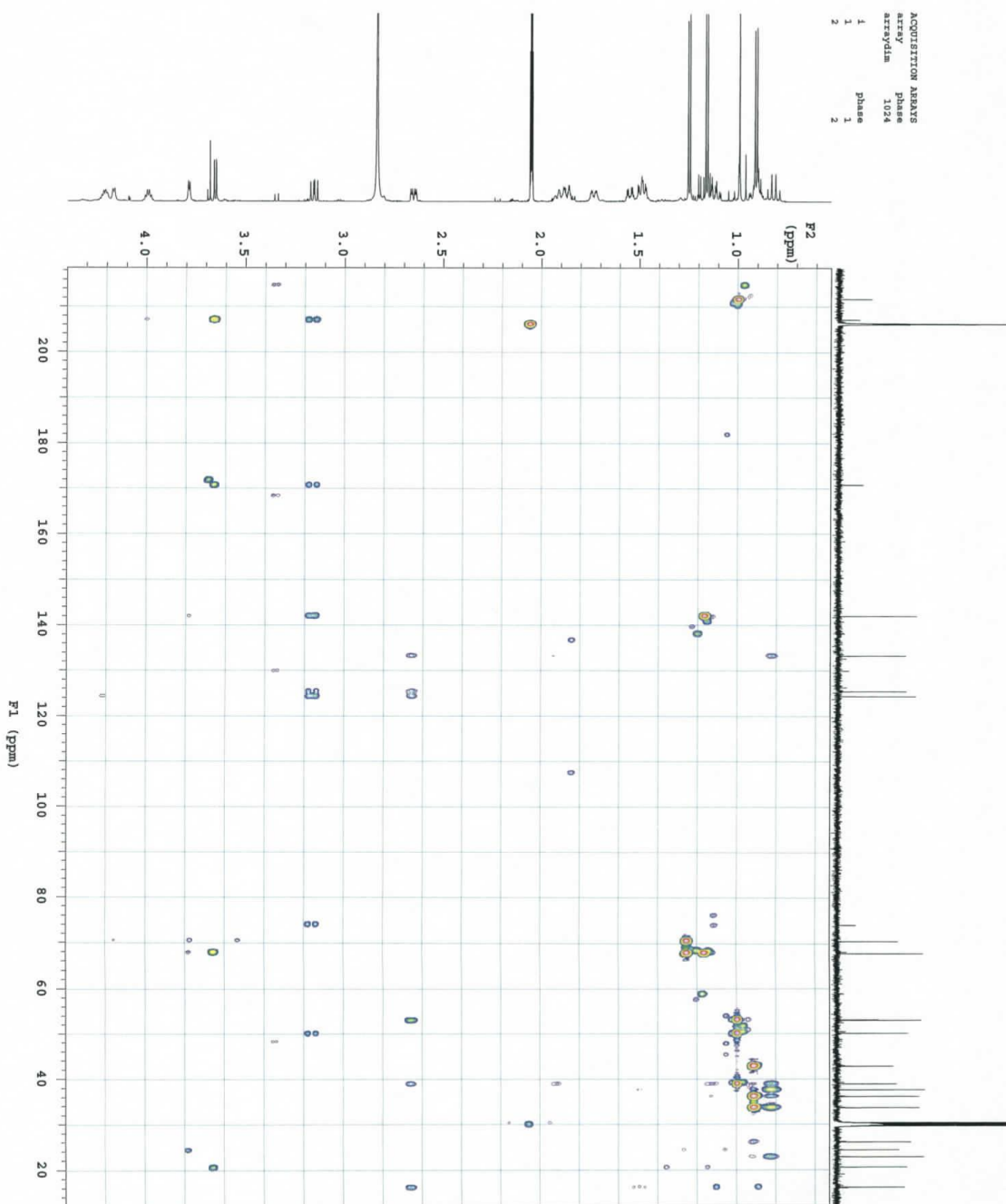
19



117D-1CS9-9

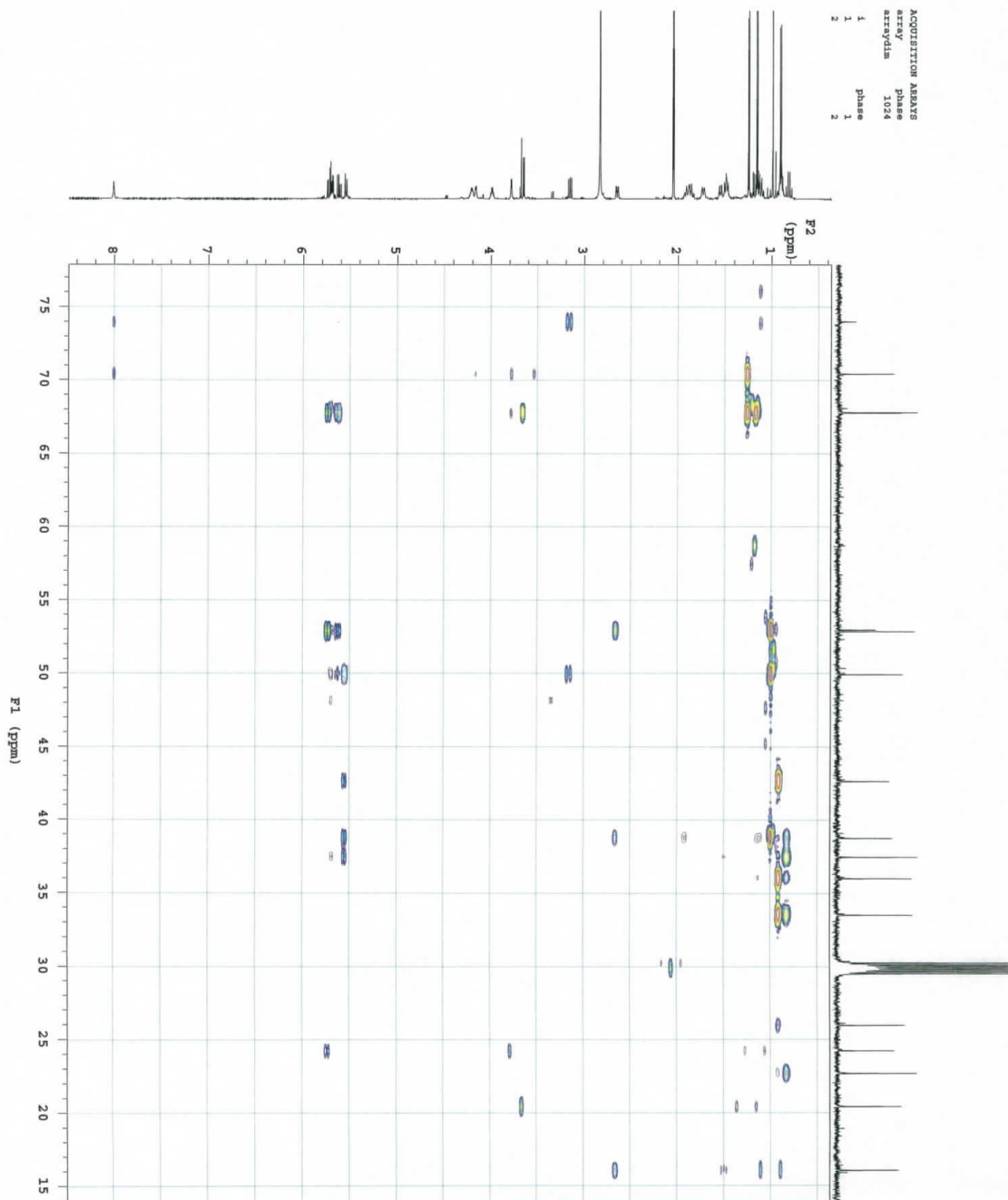
expt: gsmrcbm

SAMPLE		PLANS		ACQUISITION ARRAYS	
date	Mar 18 2013	hs	nm	array	phase
solvent	acetone	aspl1	y	arraydim	1024
sample	prof1g	hsplv1	y		
acq	5313.1	6540	1	1	1
pw	0.150	0.001000	2	2	2
at	0.150	temp	not used		
np	1596	gain	20		
fb	4000	spin	0		
as	32	GRADIENTS	0		
dl	1.500	gr1v1	545		
nt	128	gr1	0.001000		
2D ACQUISITION	gr1v13	1635			
sw1	35445.3	gr13	0.001000		
nl	512	gr1ab	0.000500		
phase	arrayed	F2 PROCESSING			
PREPARATION	AB	not used			
acqmode	h	not used			
wet	h	not used			
TRANSMITTER	h	F1 PROCESSING			
ln	599.901	gr1	0.005		
strq	-515.1	gr1	not used		
tof	58	fn1	1p		
tpwr	9.100	DISPLAY	2048		
pw	RECOUPLES	sp	317.1		
dn	CL13	wp	2321.9		
dof	2875.5	sp1	1173.2		
dm	nm	wp1	3117.7		
decave	W40	gr1	173.6		
dut	35088	rf1	3023.0		
dprc	39	rf1	2467.8		
provlv1	58	PLOT	250.0		
pxc	9.300	wc	0		
jxkh	146.0	wc2	200.0		
jxkh	8.0	mc2	0		
AUTOMATIC	vs		2486		
provlv1180	400.0	at	2		
provlv1180	400.0				



117P-1CS9-9
exp6 gbmccm

SAMPLE		FLAGS		ACQUISITION ABAYS	
date	Mar 18 2013	hs	nm	array	phase
solvent	acetone	ssol1	y	arraydim	1024
sample	Y	specifig	Y		
ACQUISITION	hsq1v1	5440	1	phase	1
ac	5119.1	SPECIAL	not used	2	2
nt	0.150	temp	not used		
fp	4000	gain	20		
fs	4000	spin	0		
as	32	GRADIENTS	545		
dl	1.500	g2v11	0.001000		
nt	128	g2v13	1635		
2D ACQUISITION	g2v13	0.001000			
sw1	35445.3	g1v3	0.001000		
nt	512	g2v1b	0.000500		
phase	arrayed	P2 PROCESSING	-0.075		
PREFATTENATION	ab	not used			
acmode	n	abn	not used		
wt	0.005	P1 PROCESSING	4096		
tn	0.005	not used			
afreq	559.401	afat	not used		
tot	-515.1	procl	1p		
tpw	58	fn1	2048		
PW	5.100	DISPLAY	221.0		
dn	CL3	wp	4867.2		
dof	2675.5	wp1	2084.7		
dm	nm	wp1	8657.5		
dacwave	W40	Qwave-ef1	173.8		
def	35000	ef1	1023.0		
dpr	38	rfp1	2407.8		
pxv1	58	PLOT	280.0		
pxw	5.300	wc	280.0		
hmc	ac	ac	0		
j1xh	146.0	wc2	200.0		
j1xh	8.0	ac2	0		
ADJMANCIC	vs		2486		
pxv180d	Qwave-ef1		2		
pxv180	ad300	at	nv		
pxv180	400.0				



117D-1C56-9

expf gbrb00d

SAMPLE		FLAGS		ACQUISITION ARRAYS	
date	Mar 18 2013	hs	nm	array	phase
solvent	acetone	aspl	y	arraydim	1024
sample	pyrid	pyrid	y		
acq1	hsplv1	SPECTRA	6540	1	1
acq2	hsplv1	SPECTRA	6540	2	2
acq3	hsplv1	SPECTRA	6540	3	3
acq4	hsplv1	SPECTRA	6540	4	4
acq5	hsplv1	SPECTRA	6540	5	5
acq6	hsplv1	SPECTRA	6540	6	6
acq7	hsplv1	SPECTRA	6540	7	7
acq8	hsplv1	SPECTRA	6540	8	8
acq9	hsplv1	SPECTRA	6540	9	9
acq10	hsplv1	SPECTRA	6540	10	10
acq11	hsplv1	SPECTRA	6540	11	11
acq12	hsplv1	SPECTRA	6540	12	12
acq13	hsplv1	SPECTRA	6540	13	13
acq14	hsplv1	SPECTRA	6540	14	14
acq15	hsplv1	SPECTRA	6540	15	15
acq16	hsplv1	SPECTRA	6540	16	16
acq17	hsplv1	SPECTRA	6540	17	17
acq18	hsplv1	SPECTRA	6540	18	18
acq19	hsplv1	SPECTRA	6540	19	19
acq20	hsplv1	SPECTRA	6540	20	20
acq21	hsplv1	SPECTRA	6540	21	21
acq22	hsplv1	SPECTRA	6540	22	22
acq23	hsplv1	SPECTRA	6540	23	23
acq24	hsplv1	SPECTRA	6540	24	24
acq25	hsplv1	SPECTRA	6540	25	25
acq26	hsplv1	SPECTRA	6540	26	26
acq27	hsplv1	SPECTRA	6540	27	27
acq28	hsplv1	SPECTRA	6540	28	28
acq29	hsplv1	SPECTRA	6540	29	29
acq30	hsplv1	SPECTRA	6540	30	30
acq31	hsplv1	SPECTRA	6540	31	31
acq32	hsplv1	SPECTRA	6540	32	32
acq33	hsplv1	SPECTRA	6540	33	33
acq34	hsplv1	SPECTRA	6540	34	34
acq35	hsplv1	SPECTRA	6540	35	35
acq36	hsplv1	SPECTRA	6540	36	36
acq37	hsplv1	SPECTRA	6540	37	37
acq38	hsplv1	SPECTRA	6540	38	38
acq39	hsplv1	SPECTRA	6540	39	39
acq40	hsplv1	SPECTRA	6540	40	40
acq41	hsplv1	SPECTRA	6540	41	41
acq42	hsplv1	SPECTRA	6540	42	42
acq43	hsplv1	SPECTRA	6540	43	43
acq44	hsplv1	SPECTRA	6540	44	44
acq45	hsplv1	SPECTRA	6540	45	45
acq46	hsplv1	SPECTRA	6540	46	46
acq47	hsplv1	SPECTRA	6540	47	47
acq48	hsplv1	SPECTRA	6540	48	48
acq49	hsplv1	SPECTRA	6540	49	49
acq50	hsplv1	SPECTRA	6540	50	50
acq51	hsplv1	SPECTRA	6540	51	51
acq52	hsplv1	SPECTRA	6540	52	52
acq53	hsplv1	SPECTRA	6540	53	53
acq54	hsplv1	SPECTRA	6540	54	54
acq55	hsplv1	SPECTRA	6540	55	55
acq56	hsplv1	SPECTRA	6540	56	56
acq57	hsplv1	SPECTRA	6540	57	57
acq58	hsplv1	SPECTRA	6540	58	58
acq59	hsplv1	SPECTRA	6540	59	59
acq60	hsplv1	SPECTRA	6540	60	60
acq61	hsplv1	SPECTRA	6540	61	61
acq62	hsplv1	SPECTRA	6540	62	62
acq63	hsplv1	SPECTRA	6540	63	63
acq64	hsplv1	SPECTRA	6540	64	64
acq65	hsplv1	SPECTRA	6540	65	65
acq66	hsplv1	SPECTRA	6540	66	66
acq67	hsplv1	SPECTRA	6540	67	67
acq68	hsplv1	SPECTRA	6540	68	68
acq69	hsplv1	SPECTRA	6540	69	69
acq70	hsplv1	SPECTRA	6540	70	70
acq71	hsplv1	SPECTRA	6540	71	71
acq72	hsplv1	SPECTRA	6540	72	72
acq73	hsplv1	SPECTRA	6540	73	73
acq74	hsplv1	SPECTRA	6540	74	74
acq75	hsplv1	SPECTRA	6540	75	75
acq76	hsplv1	SPECTRA	6540	76	76
acq77	hsplv1	SPECTRA	6540	77	77
acq78	hsplv1	SPECTRA	6540	78	78
acq79	hsplv1	SPECTRA	6540	79	79
acq80	hsplv1	SPECTRA	6540	80	80
acq81	hsplv1	SPECTRA	6540	81	81
acq82	hsplv1	SPECTRA	6540	82	82
acq83	hsplv1	SPECTRA	6540	83	83
acq84	hsplv1	SPECTRA	6540	84	84
acq85	hsplv1	SPECTRA	6540	85	85
acq86	hsplv1	SPECTRA	6540	86	86
acq87	hsplv1	SPECTRA	6540	87	87
acq88	hsplv1	SPECTRA	6540	88	88
acq89	hsplv1	SPECTRA	6540	89	89
acq90	hsplv1	SPECTRA	6540	90	90
acq91	hsplv1	SPECTRA	6540	91	91
acq92	hsplv1	SPECTRA	6540	92	92
acq93	hsplv1	SPECTRA	6540	93	93
acq94	hsplv1	SPECTRA	6540	94	94
acq95	hsplv1	SPECTRA	6540	95	95
acq96	hsplv1	SPECTRA	6540	96	96
acq97	hsplv1	SPECTRA	6540	97	97
acq98	hsplv1	SPECTRA	6540	98	98
acq99	hsplv1	SPECTRA	6540	99	99
acq100	hsplv1	SPECTRA	6540	100	100

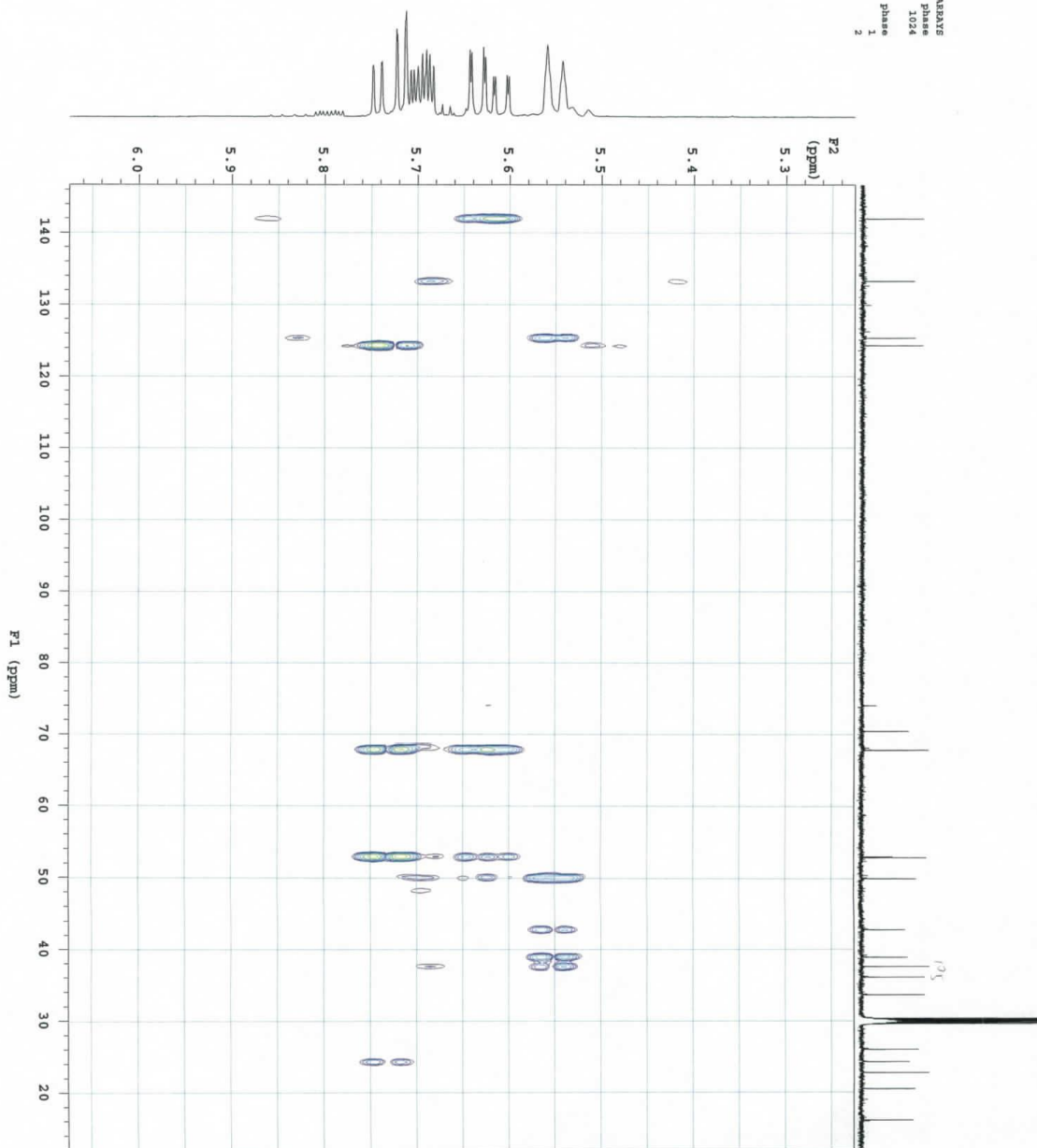


Figure S6 FABMS of 1

[Elemental Composition]
Data : 1607230 Date : 04-Aug-2016 17:33 Page: 1
Sample: 117D-1 C176-11-VI
Note : Matrix; NBA
Inlet : Direct Ion Mode : FAB+
RT : 8.07 min Scan#: (40,45)
Elements : C 30/20, H 40/30, N 5/0, O 10/0
Mass Tolerance : 20ppm, 1mmu if m/z > 50
Unsaturation (U.S.) : -1.0 - 30.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
416.2436	100.0	-0.3 / -0.1	8.5	C 24 H 34 N O 5

