

Supplementary Materials

Halosmysin A, a novel 14-membered macrodiolide isolated from the marine-alga-derived fungus *Halosphaeriaceae* sp.

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Table S1 NMR spectral data of **1** in CDCl₃^d

Position	$\delta_{\text{H}}^{\text{a}}$		J/Hz	$^1\text{H}-^1\text{H}$ COSY		NOESY ^b	δ_{C}	HMBC (C) ^c
2							165.6 (s)	
3	5.64	d	16.2 (4)	4	5 β , 9		125.3 (d)	2, 5
4	6.78	ddd	16.2 (3), 10.2 (5 β), 6.0 (5 α)	3, 5 α , 5 β	6		143.5 (d)	2, 5
5 α	2.48	ddd	13.2 (5 β), 6.0 (4), 1.2 (6)	4, 5 β	15		39.0 (t)	3, 4
5 β	2.23	ddd	13.2 (5 α), 13.2 (6), 10.2 (4)	4, 5 α , 6	3, 15			3, 4, 6, 15
6	5.30	dqd	13.2 (5 β), 6.0 (15), 1.2 (5 α)	5 β , 6-CH ₃	4		69.9 (d)	
8							168.9 (s)	
9	3.38	d	3.0 (10)	10	3, 2', 7'A, 7'B		51.9 (d)	8, 10, 11, 6'
10	4.57	d	3.0 (9)	9	13 β , 2'		51.0 (d)	8, 11, 3'
11							208.2 (s)	
12	4.55	d	7.8 (13 α)	13 α	S-CH ₃		75.6 (d)	11, 13, 14
13 α	1.96	ddd	14.4 (13 β), 7.8 (12), 3.0 (14)	12, 13 β	16		37.4 (t)	11, 12
13 β	2.64	ddd	14.4 (13 α), 12.0 (14), 1.2 (12)	13 α , 14	10, 16			14, 16
14	5.23	dqd	12.0 (13 β), 6.0 (16), 3.0 (13 α)	13 β , 14-CH ₃			65.5 (d)	
15	1.44	d	6.0 (6)	6	5 α , 5 β , 7'A		20.9 (q)	5, 6
16	1.26	d	6.0 (14)	14	13 α , 13 β		20.2 (q)	13, 14
12-OH	Not observed							
1' (NH)	5.73	s			7'A, 9'			3', 6'
2'							165.7 (s)	
3'							68.6 (s)	
4' (NH)	5.95	s			9, 10, S-CH ₃ ,			2', 6'
5'							170.9 (s)	
6'							63.7 (s)	
7'A	2.83	d	14.4 (7'B)	7'B	9, 15, 1', 9'		33.0 (t)	9, 5', 6', 8', 9'
7'B	3.88	d	14.4 (7'A)	7'A	9, 9'			5', 6', 8', 9'
8'							125.5 (s)	
9'	6.83	d	9.0 (10')	10'	5', 7'A, 7'B		131.7 (d)	7', 8', 11'
10'	7.10	d	9.0 (9')	9'	12'		115.2 (d)	8', 11'
11'							158.5 (s)	
12'	4.47	d	7.2 (13')	13'	10', 16'		64.8 (t)	11', 13', 14'
13'	5.47	br t	7.2 (12')	12'	15'		119.5 (d)	15', 16'
14'							138.4 (s)	
15'	1.79	s			13'		25.8 (q)	13', 14', 16'
16'	1.74	s			12'		18.2 (q)	13', 14', 15'
S-CH ₃	2.25	s			12, 2'		13.0 (q)	3'

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 $^1\text{H}-^{13}\text{C}$ correlations from H to C observed in the HMBC experiment. d 600 MHz (^1H NMR), 150 MHz (^{13}C NMR)

Figure S1 14-membered macrodiolides associated to halosmyin A

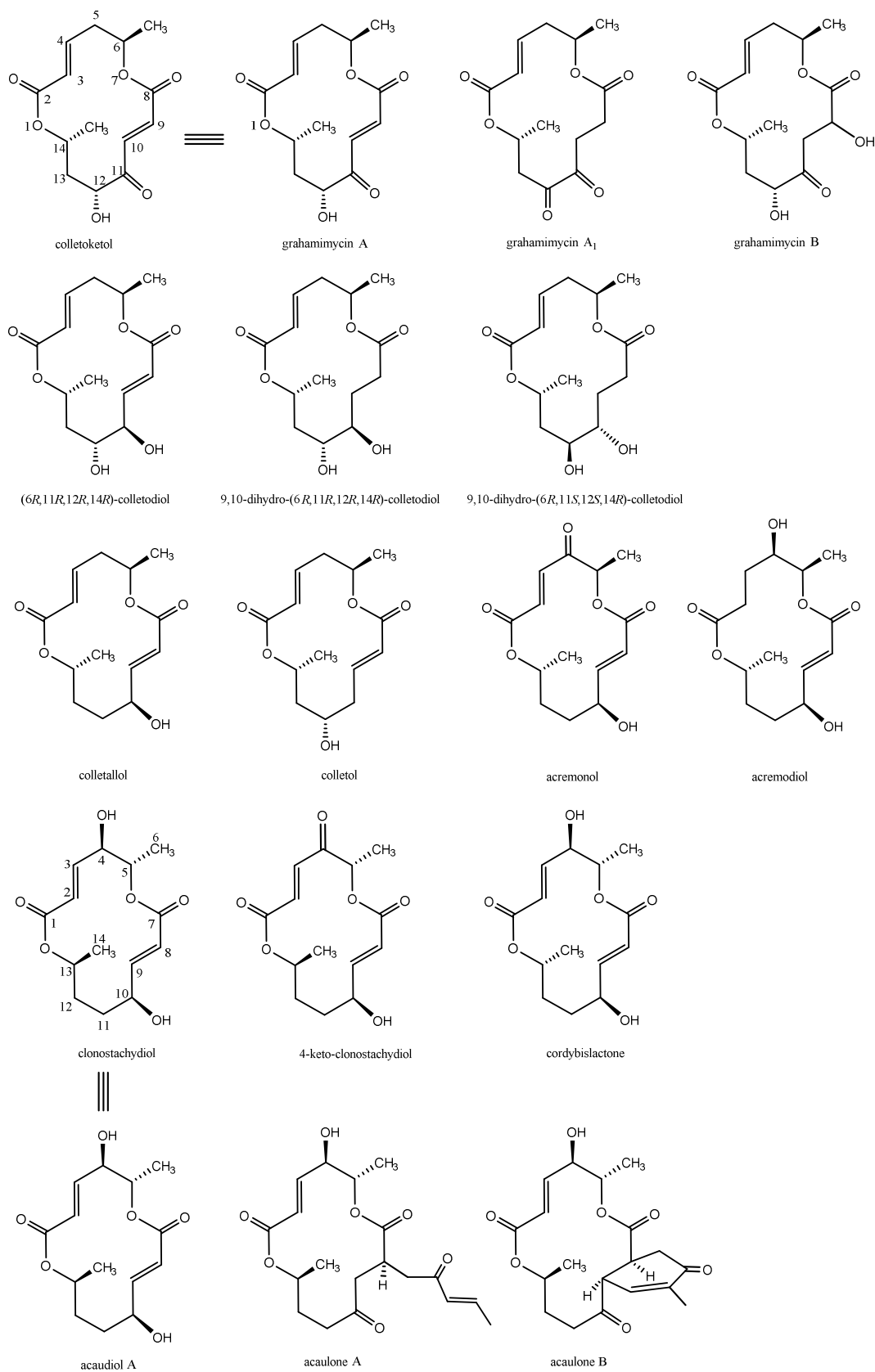
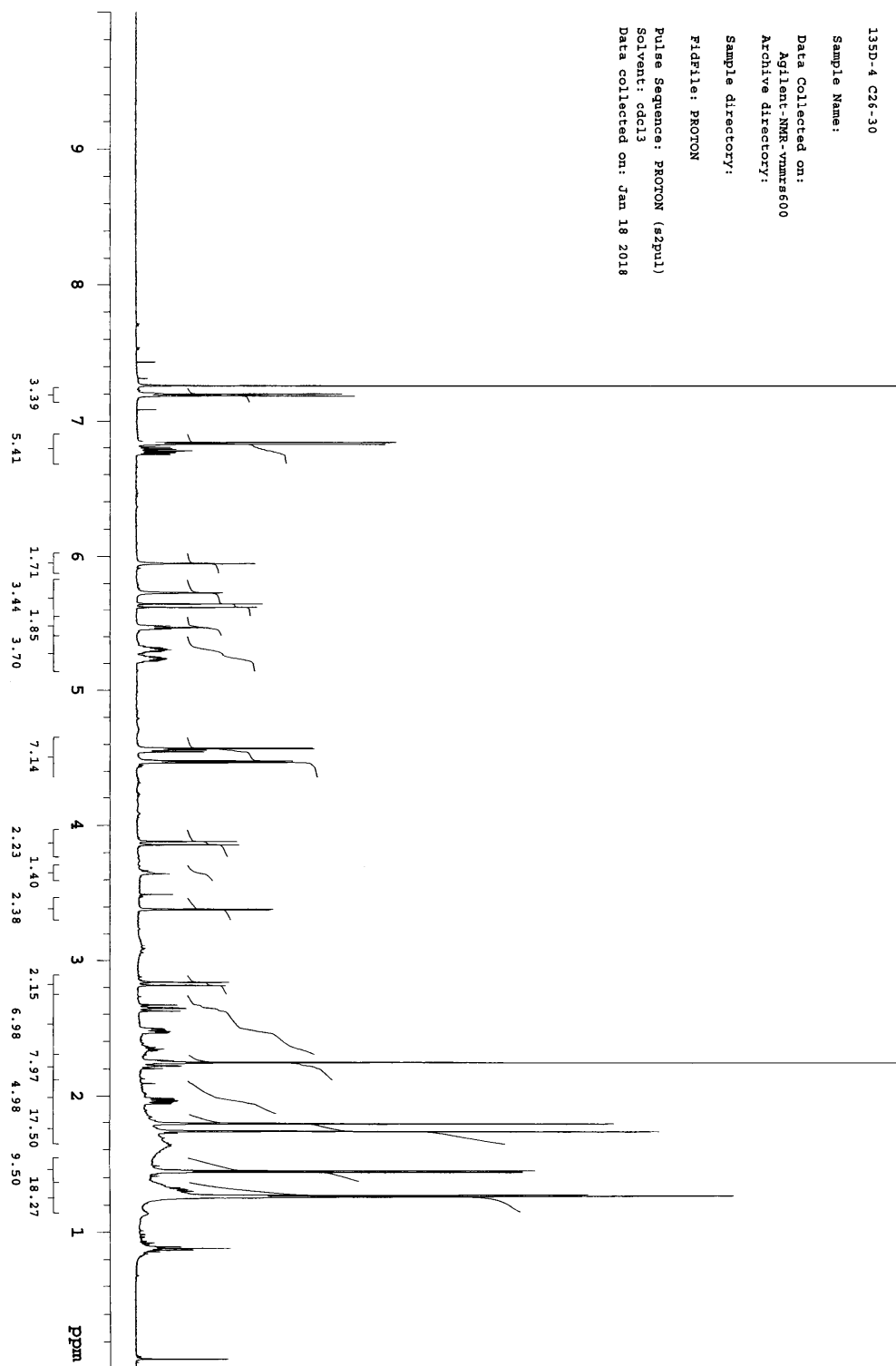
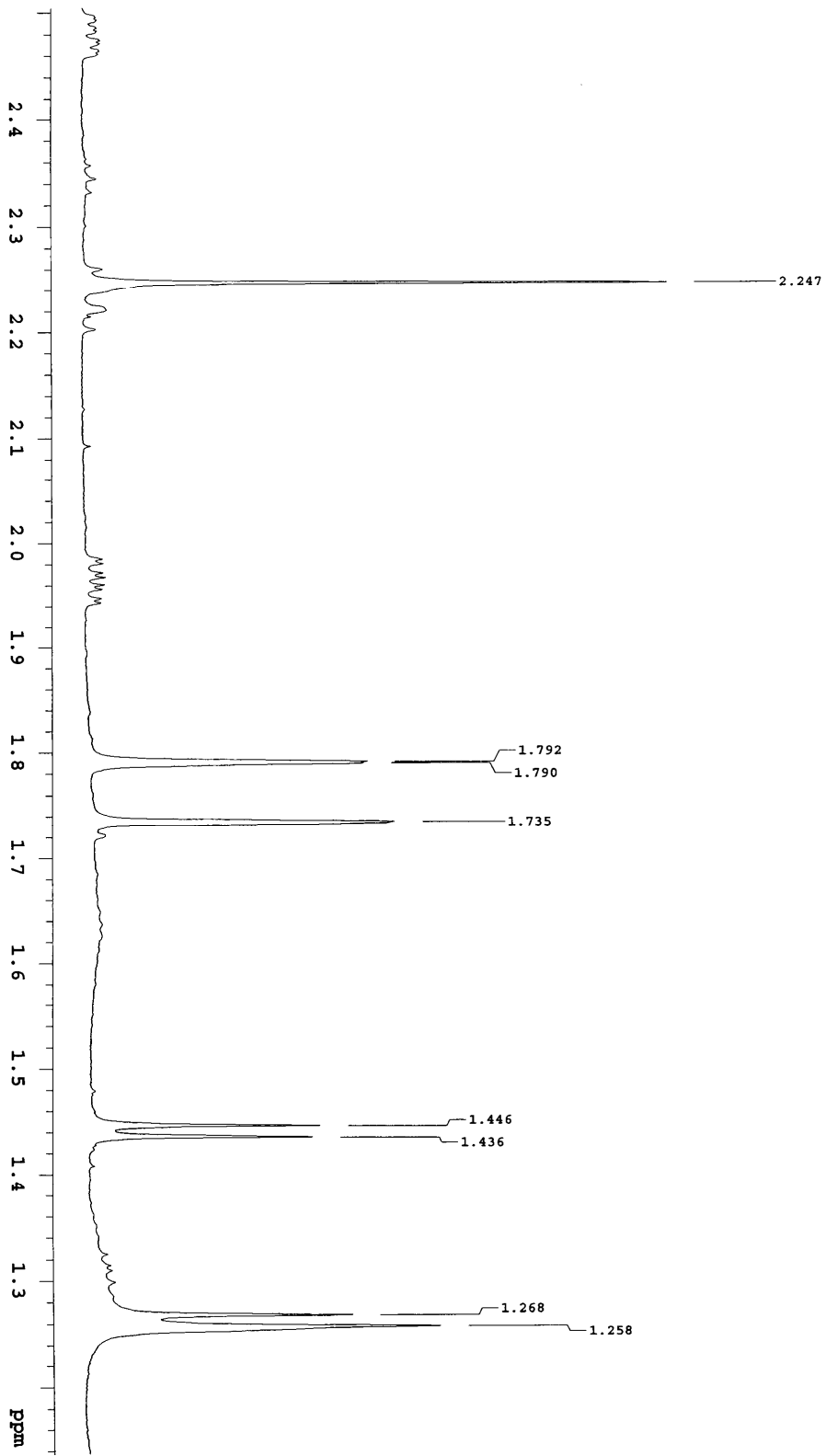


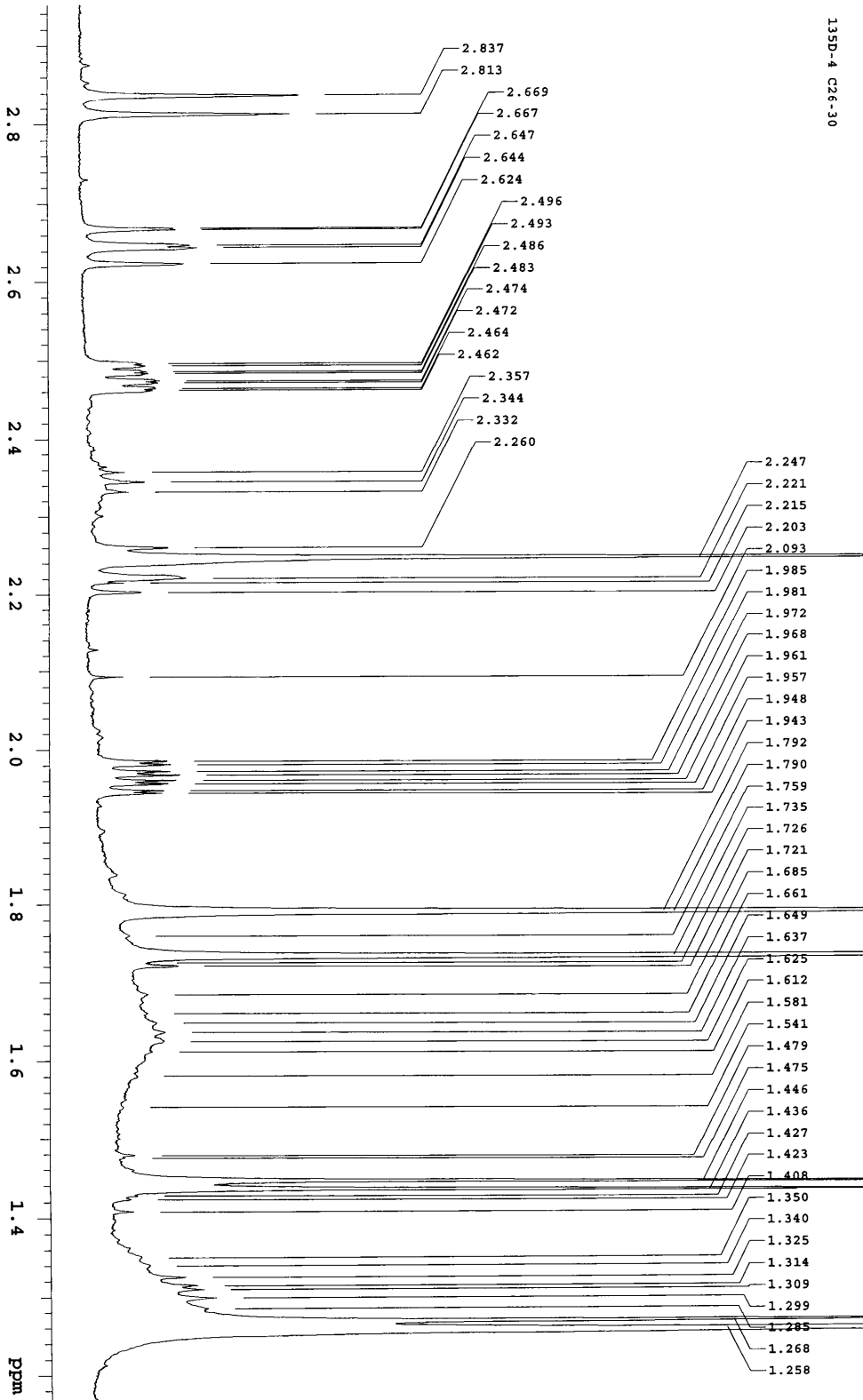
Figure S2 ¹H NMR spectrum of 1 in CDCl₃

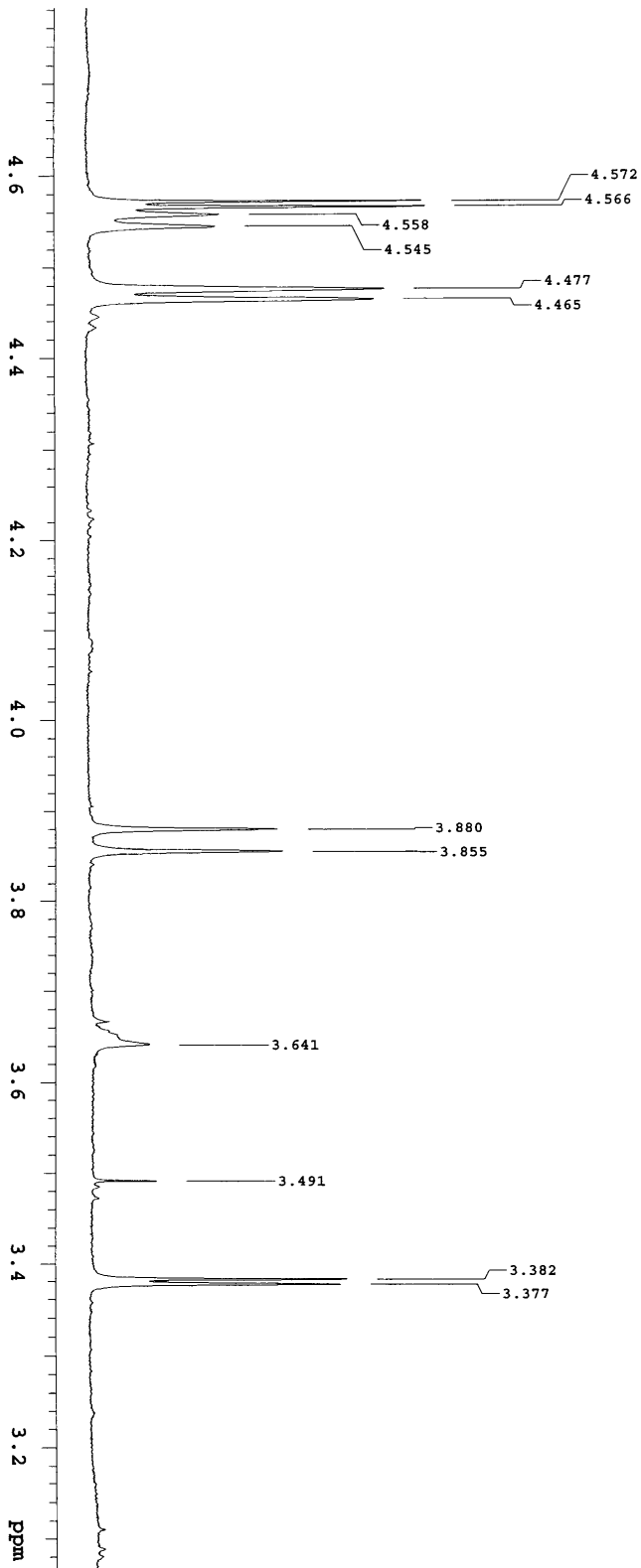


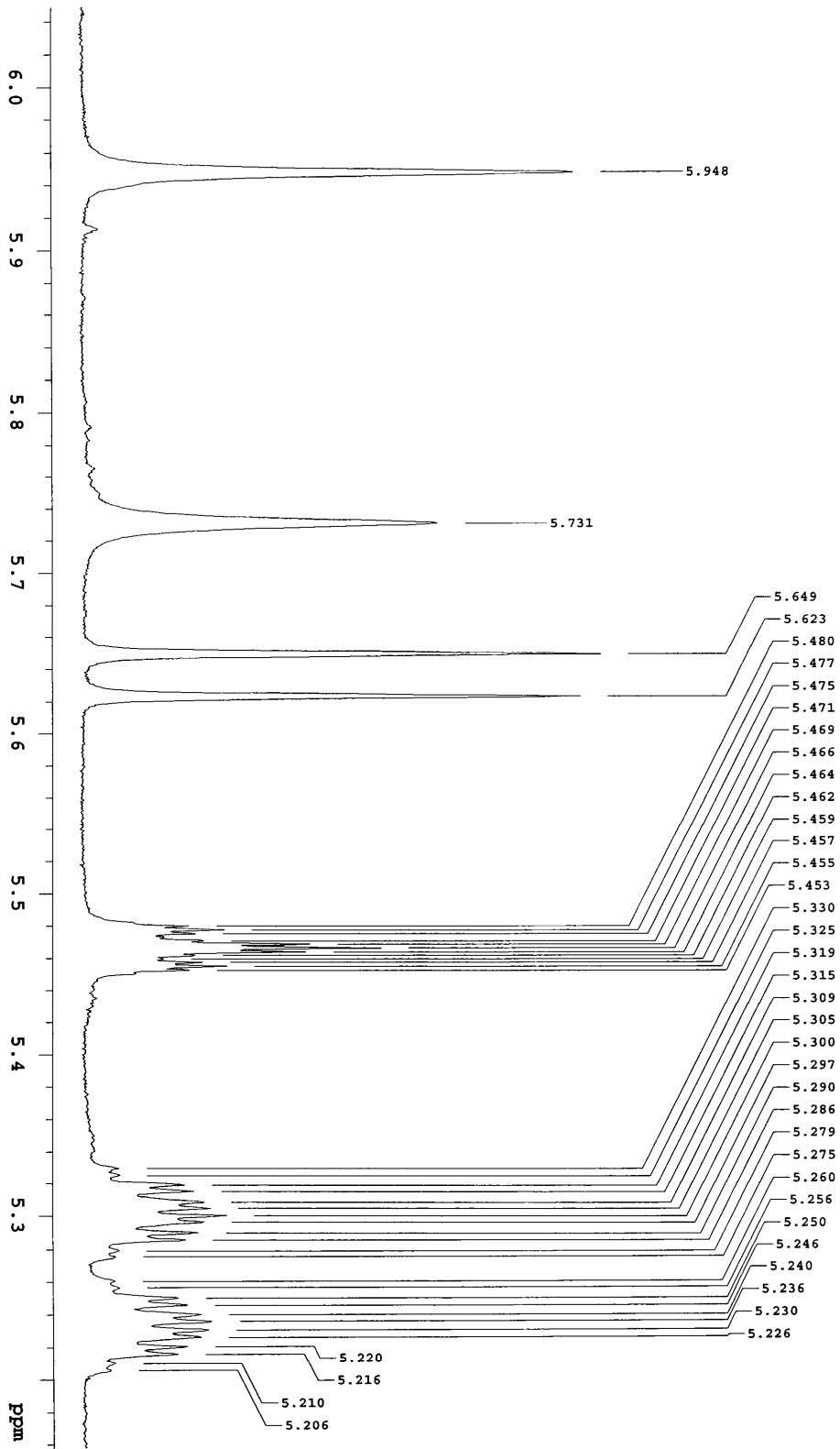
135D-4 C26-30



135D-4 C26-30







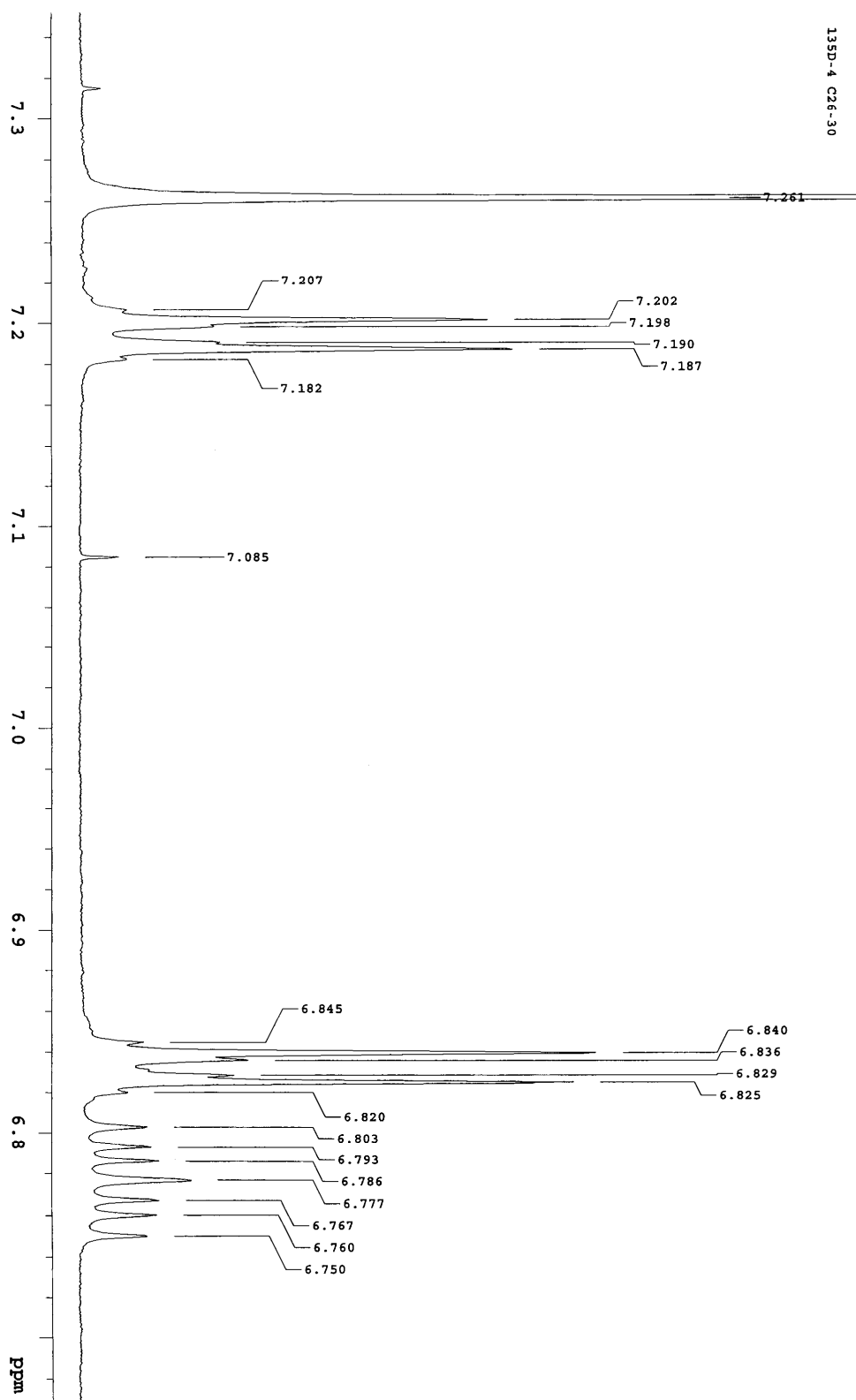
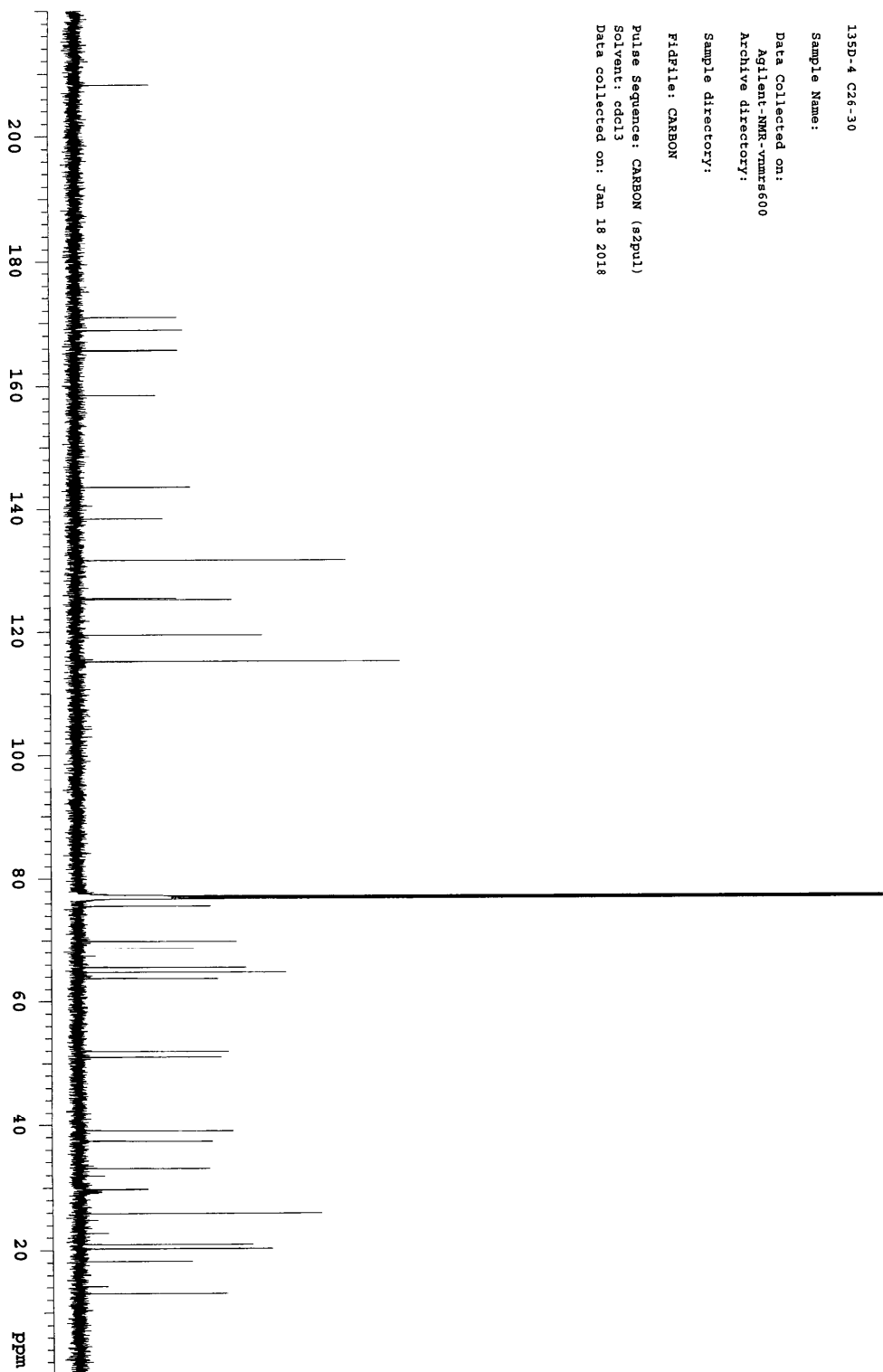


Figure S3 ^{13}C NMR spectrum of 1 in CDCl_3



135D-4 C26-30

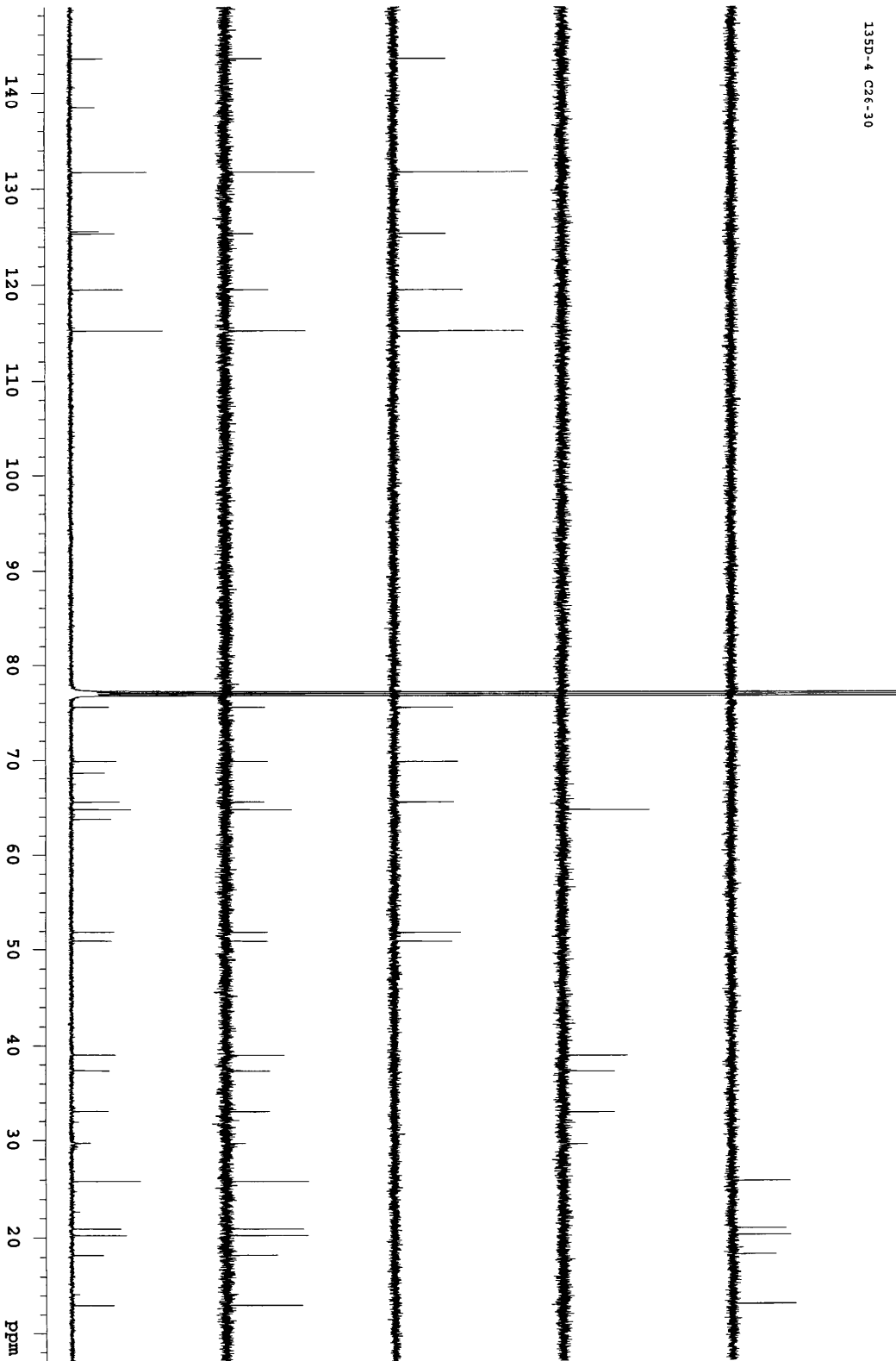


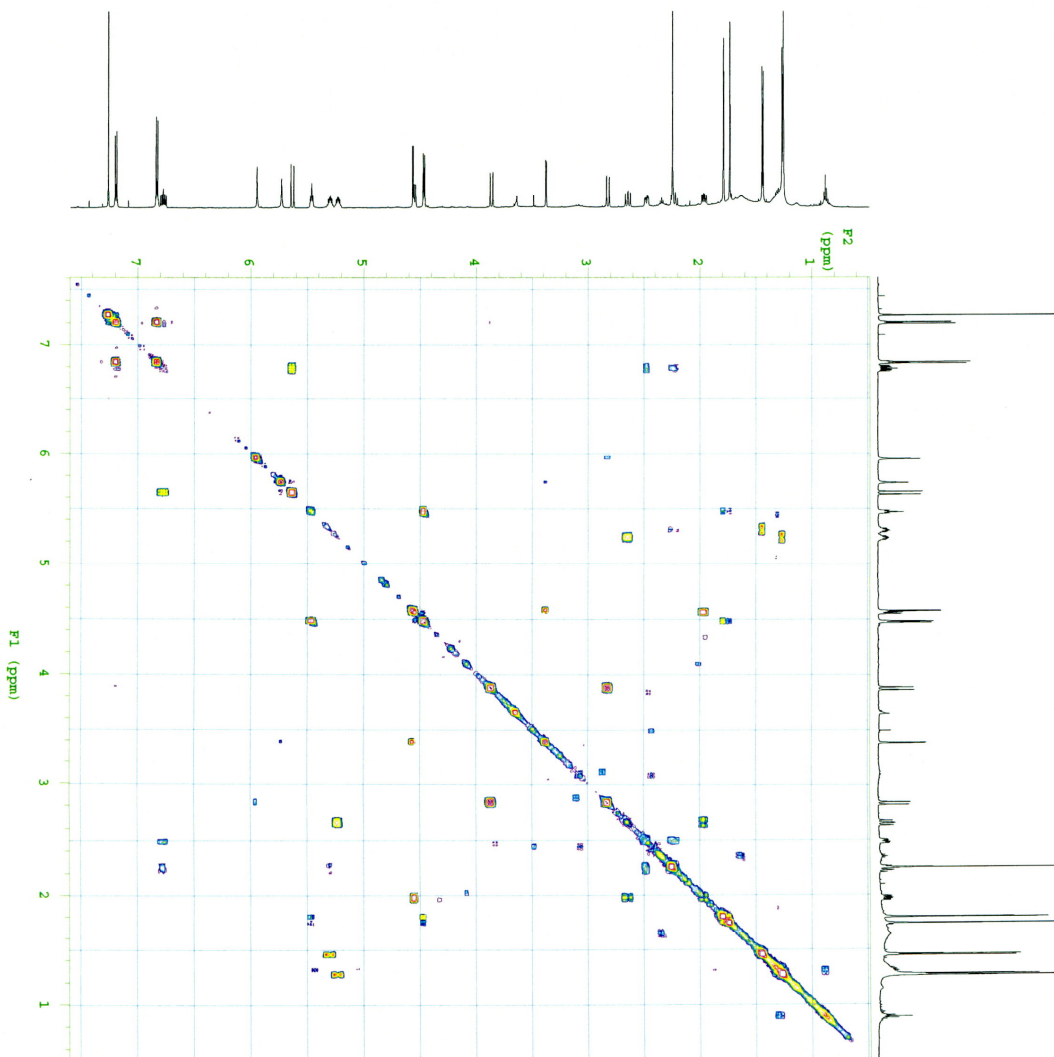
Figure S4 ^1H - ^1H COSY of 1

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13SD-4-C26-30
exp53 gcosy

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at             0.150  gain   not used
np             1454  spin    48
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n1             1.000  f2s    not used
n2             1.000  f2s    not used
2D ACQUISITION 8      F1 PROGRESSING
sw1            4845.0  sb1    not used
n1             256  sbal    not used
d2             0      prec1  1p
PREPARATION    0      Enl  DISPLAY  2048
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WEIGHT        n      wp      4267.7
UN            n1     npl     288.4
AFREQ         598.898  wpl     4272.5
COD          -681.7  fF1     103.3
UPWR         58      fF2     103.3
PW           9.600  fF1
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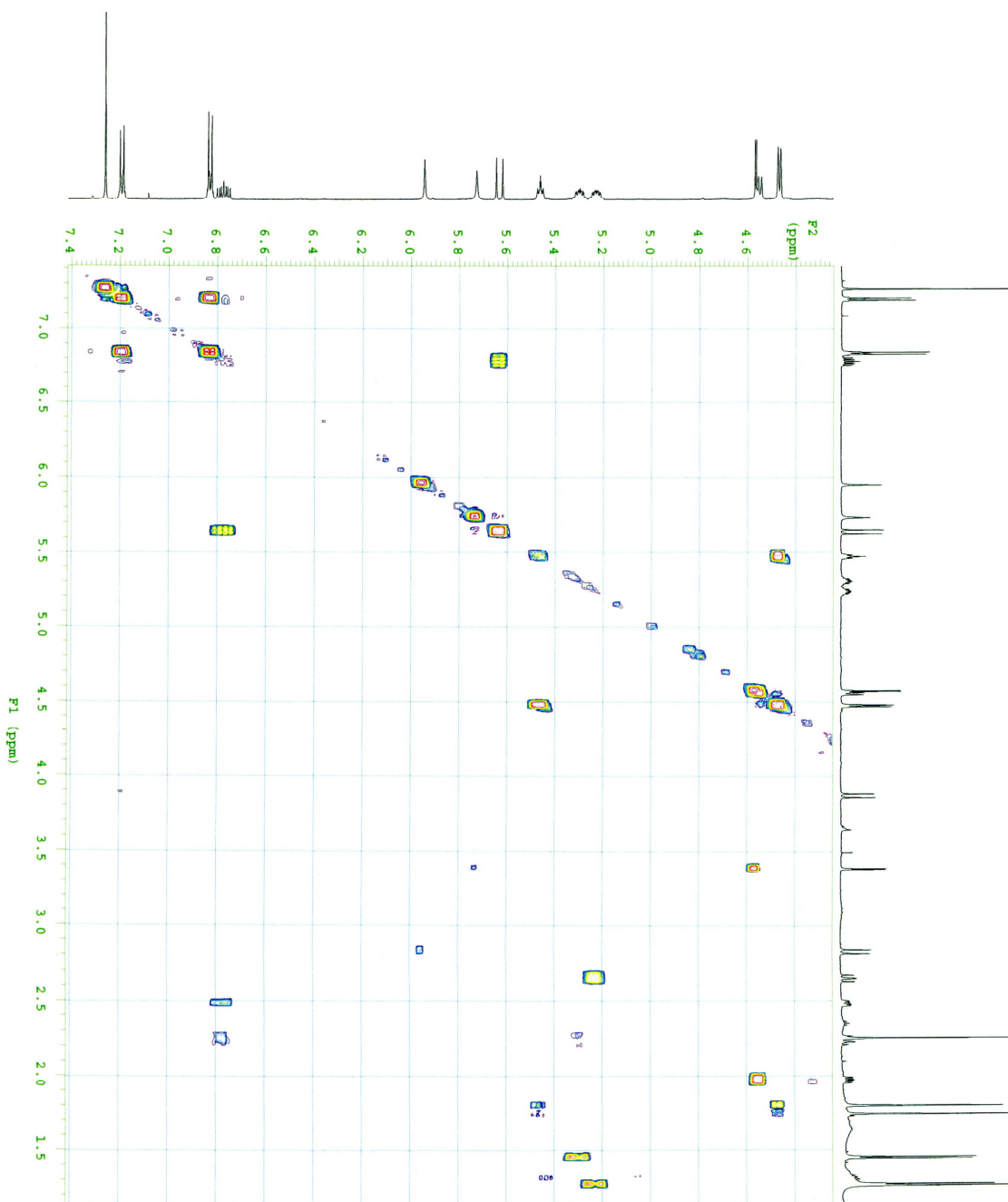
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135D-4 C6-30

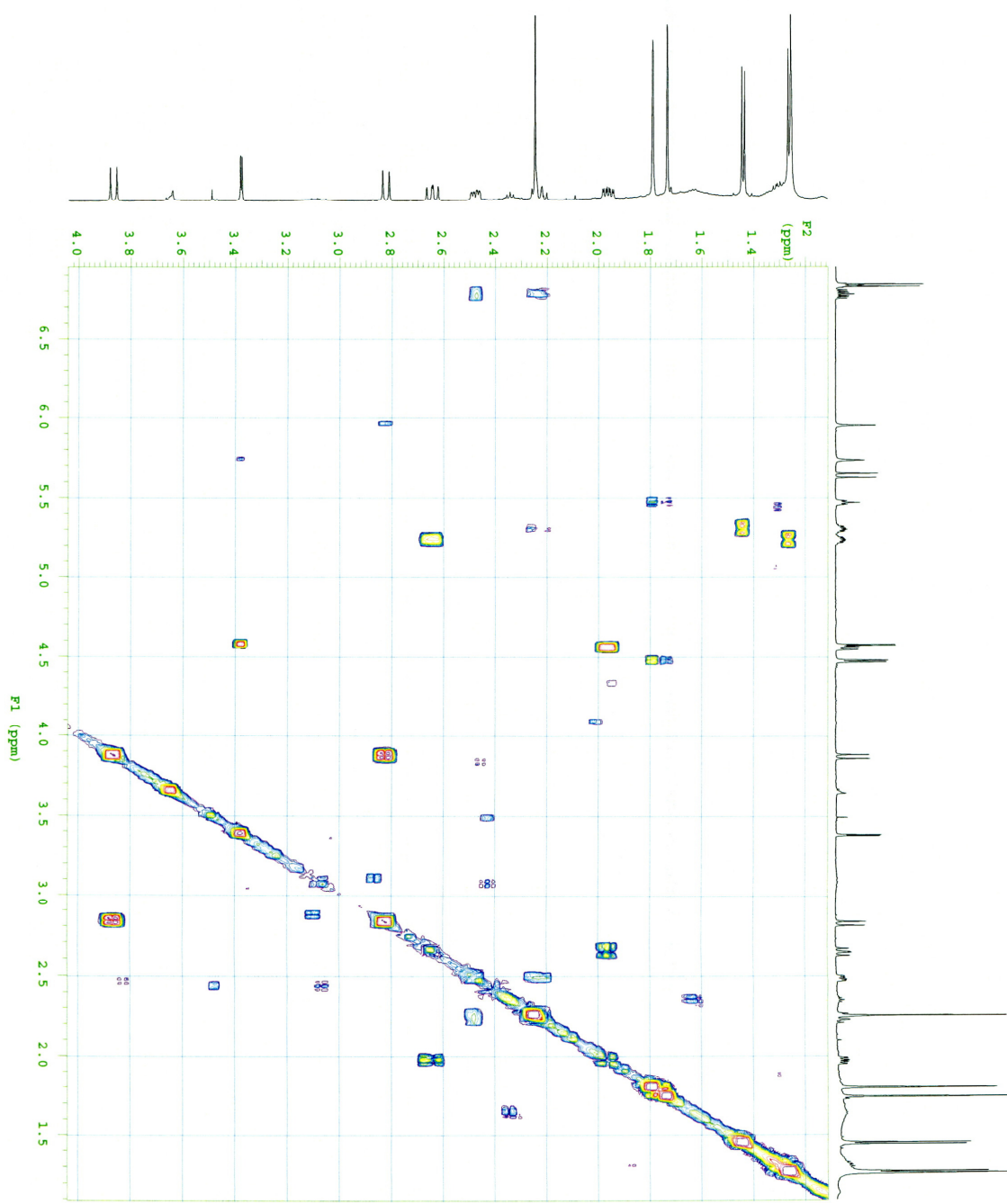
exp53 GROOSY

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fb	4000	F2 PROCESSING	
as	32	sb	-0.075
di	1.000	sbs	not used
nt	8	fn	2048
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ni	256	sb1	-0.026
d2	0	prec1	not used
d2 PRESENTATION	0	prcl	ip
acqmode	n	enl	DISPLAY 2048
wa	n	sp	DISPLAY 1546.3
wa	wp	wp	1502.0
tn	HL	api	672.7
afiq	599.896	wpi	3775.7
tof	-681.7	f1	103.3
fpwr	58	f1g	0
pw	9.600	f1l	103.3
GRADIENTS			
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PILOT			
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HzPz1e	1.000	ac	0
g1e2	0.2009500	wc2	200.0
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RECORPER	C13	vc	110
dm	mm	tb	2
at	cdc	av	



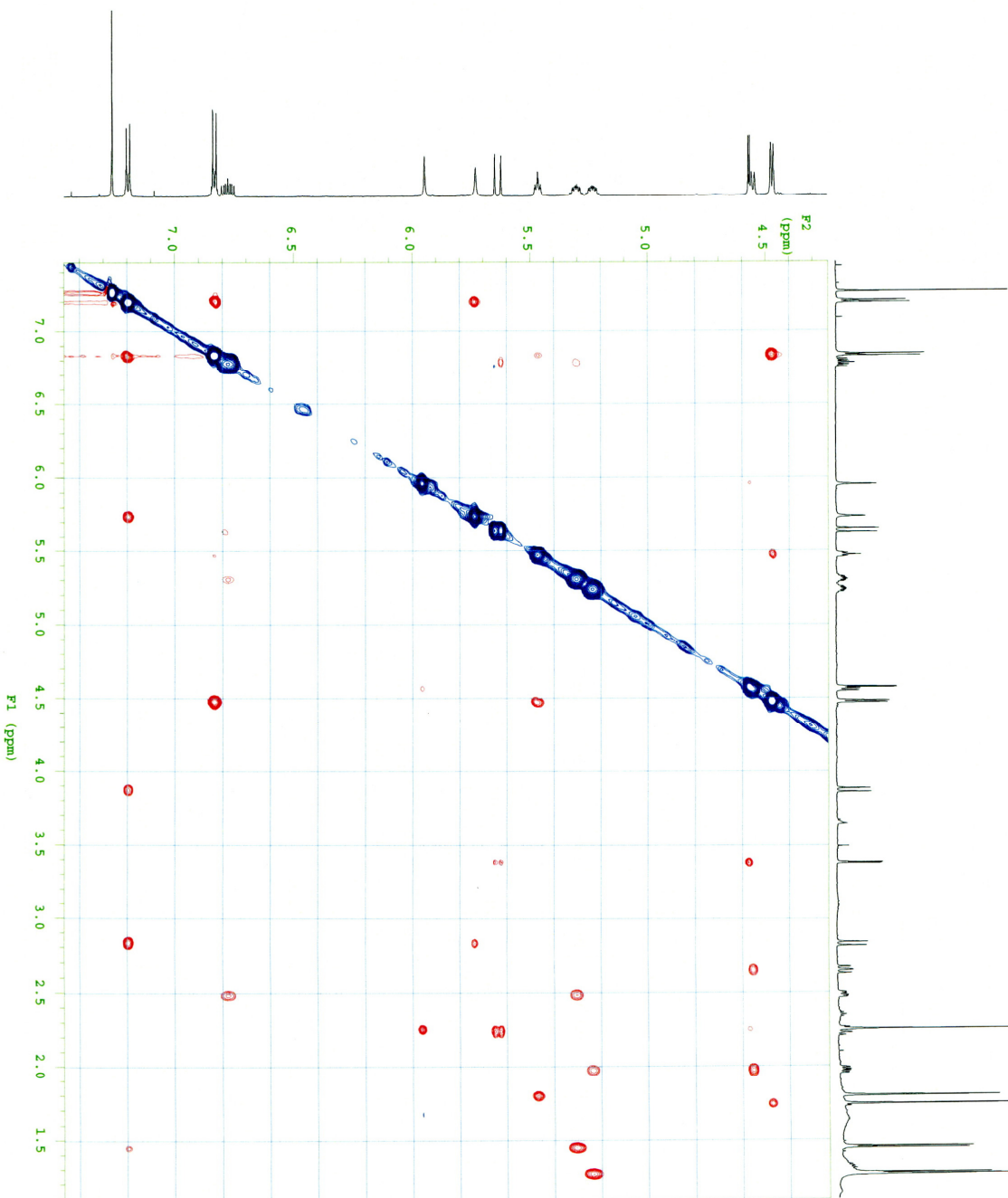
11SD-4 CDE-30
exp53 gCOSY

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solvent cdc13 sepul y
sample hsgivi SERIAL 6120
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sf 0.150 48
sp 1454 0
sb 4000 P2 PROCESSING 0
ss 32 sb -0.075
dt 1.000 sbw not used
nt 8 fn 2048
2D ACQUISITION P1 PROCESSING
sw1 4845.0 sb1 -0.026
nt1 256 sbw1 not used
d2 PREPARATION 0 prec1 Ip
spectrum n Int DISPLAY 2048
we n sp 657.9
tx TRANSMITTER HI spt 1755.4
afrc 599.896 wpt 653.7
tof -681.7 rft 3515.4
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pw 9.600 rft1 103.3
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dm mm th at cdc av 2



135D-4 C26-30
exp04 MONSIE

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SS	32	P2	PROGRESSING
DI	1.300	gf	not used
AT	16	gf	not used
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SWH	5060.7		PROGRESSING
NI	256	gf	not used
NI TRANSMITTER	256	gf	not used
EN	NI	proc	not used
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wet	n	rfl	not used
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dm	num	PILOT	not used
ac	0	250.0	not used
wc2	0	200.0	not used
wc	0	10816	not used
th	2		not used
at	cdc	ph	not used



135D-4 C26-30
exp54 NOBSY

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sample Y
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nt 16 gfs not used
2D ACQUISITION fn 2048
sw1 5060.7 F1 PROCESSING
nl 256 gfl 0.023
n1 TRANSMITTER HI proc1 not used
in 599.898 fml 2048
rfq -608.8 DISPLAY
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wet n rfp1 138.3
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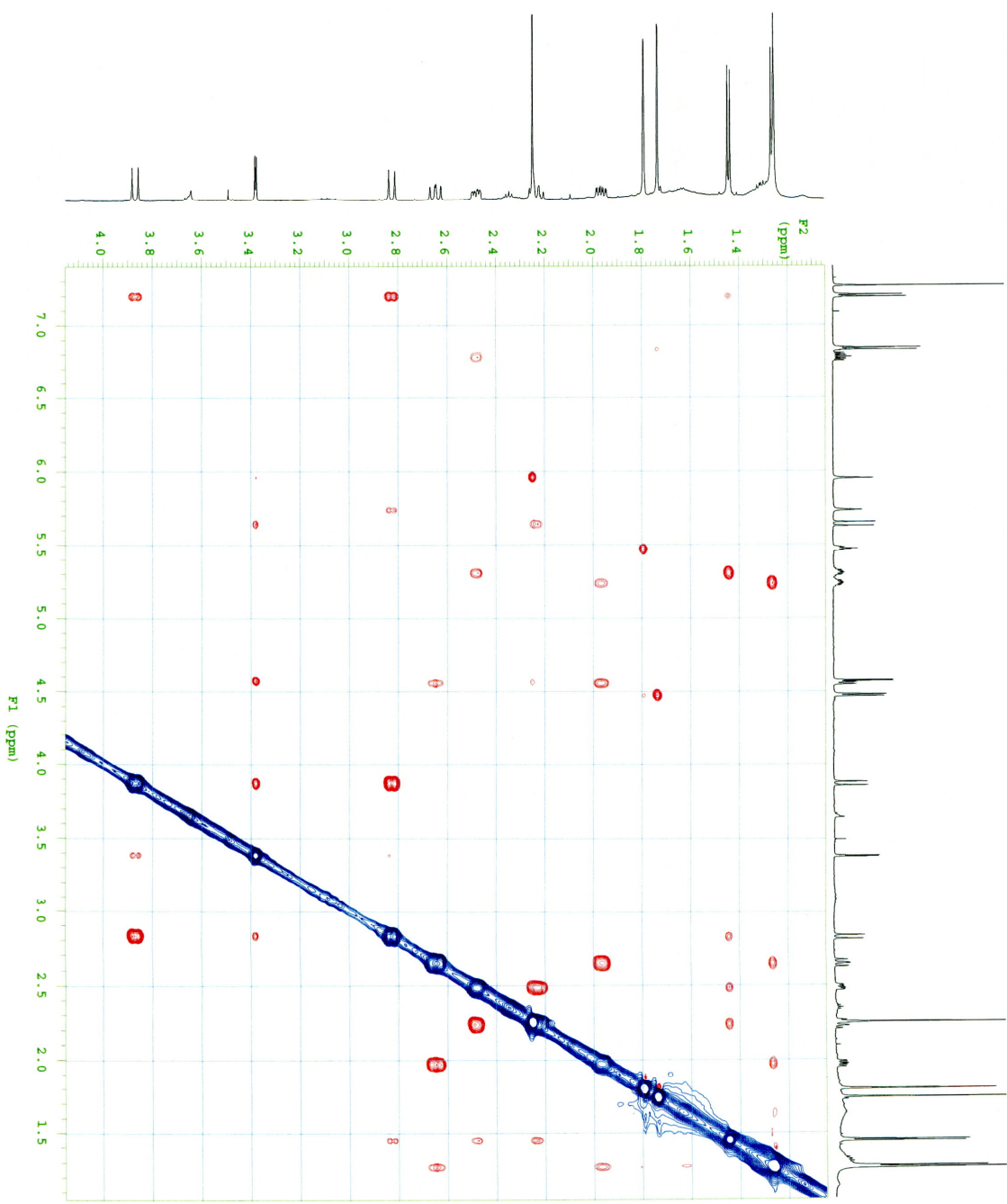
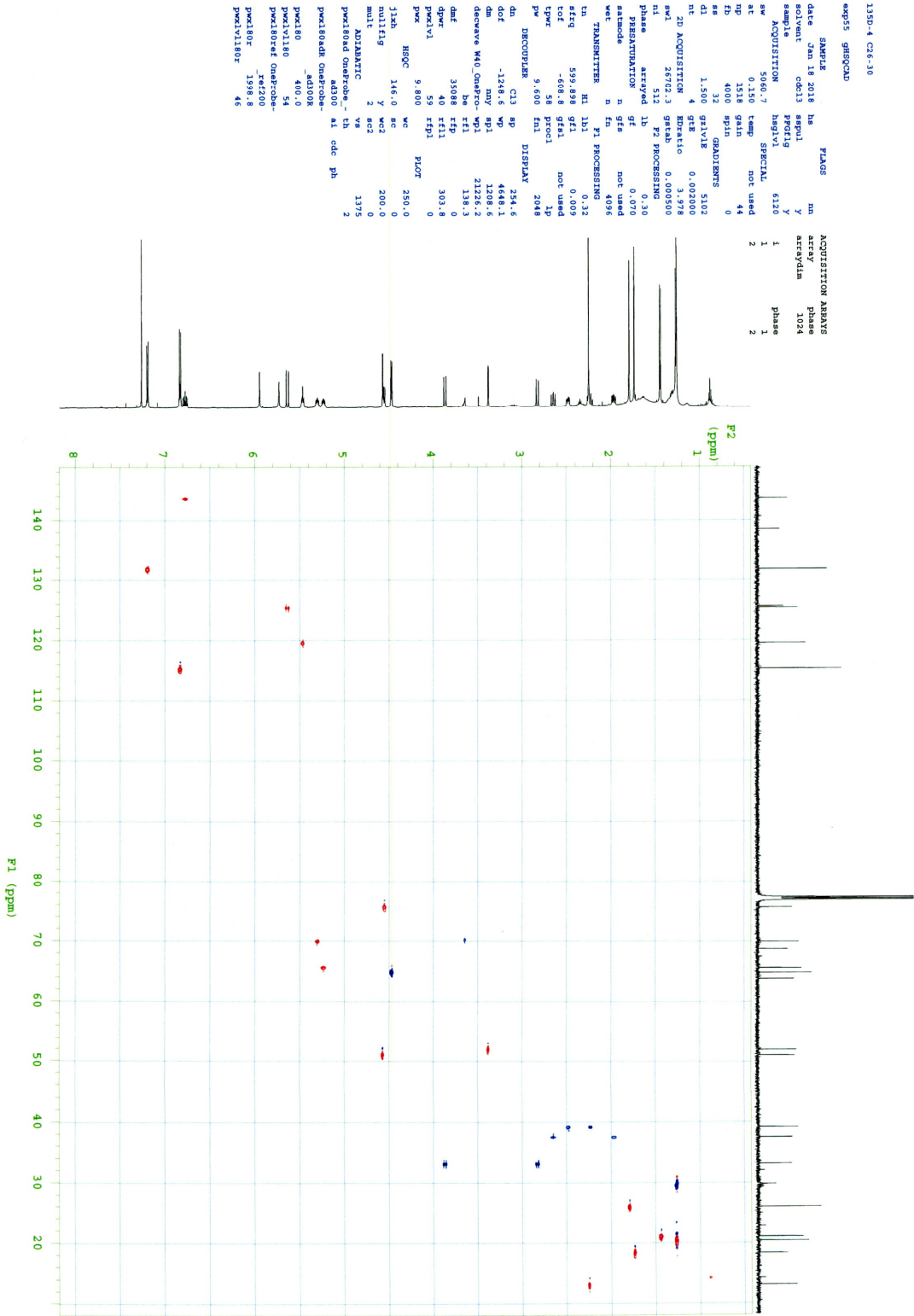
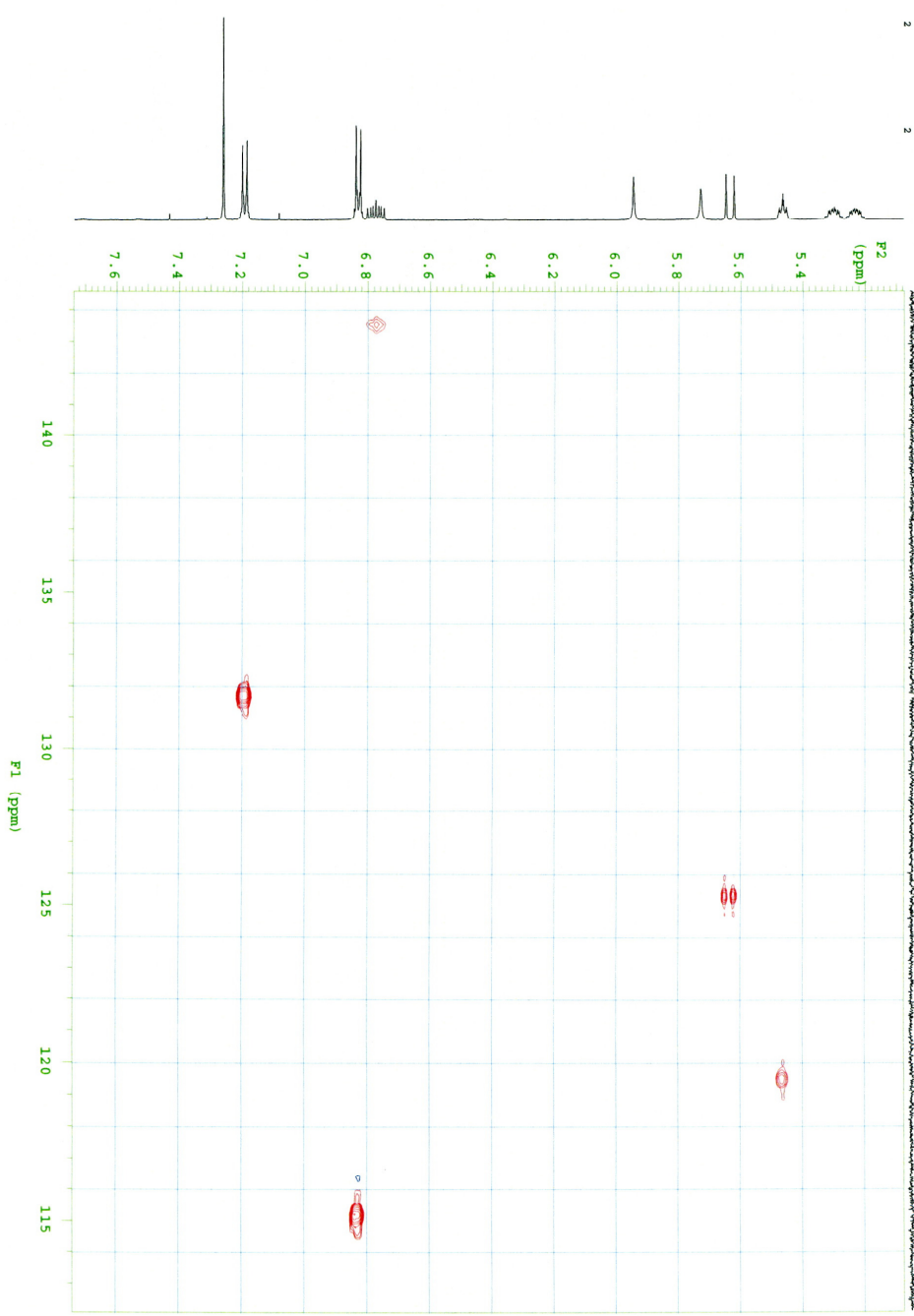


Figure S6 HMQC of 1



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 sample y
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 FD 4000 spin 0
 AS 32 GRADIENTS
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 DE 4 GE 0.002000
 2D ACQUISITION EPRatio 3.978
 SW1 26762.3 gtab 0.000500
 NI 512 P2 PROCESSING
 phase arrayed 1b 0.30
 PRESATURATION n gf 0.070
 samsode n ffs not used
 wef n ffs 0.976
 TRANSMITTER n ffs P1 PROCESSING
 tn H1 1b1 0.32
 stfg 599.896 gfl 0.009
 tot -608.8 gfl not used
 tprw 58 pfccl 1p
 pw 9.600 fml 2048
 DECOUPLER C13 sp 3044.4
 dn -1248.6 wp 1596.3
 dm may sp1 1690.6
 decoupe M40_Coupece-wp1 4922.4
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 dprw 40 rfl 303.8
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 nullfig y wc2 200.0
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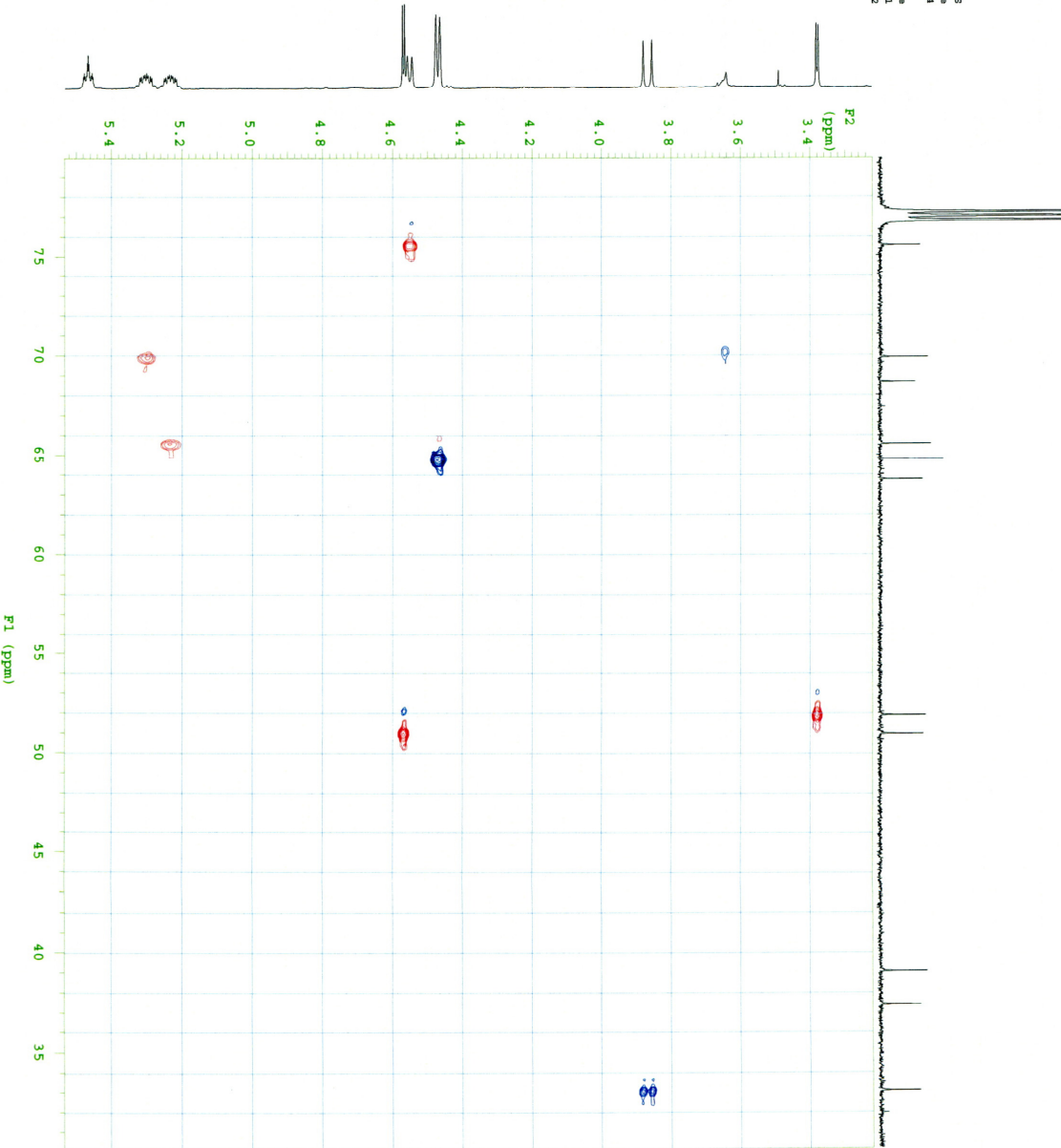
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 array phase
 arrayed 1024
 phase 1
 phase 2



exp55 ghsqcd

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sample		prctlg			phase
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nt	4	g1e	0.002000		
2D ACQUISITION		hpratio	3.978		
sw1	26702.3	grtab	0.000500		
nl	512	F2 PROCESSING	0.30		
Phase	arrayed	lb	0.30		
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wt	n	g1	not used		
we	n	g1	not used		
TRANSMITTER	n	F1 PROCESSING	4995		
tn	HL	lb1	0.32		
afq	599.898	g1	0.009		
tof	-608.8	g1eal	not used		
epwr	58	prctcl	lp		
pw	9.600	fnl	2048		

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dm		may	1386.3
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dprv1	59	rfl	0
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jkh	146.0	sc	0
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mult	2	WC2	0
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13SD-4 C26-30
exp55 ghsqcad

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sample          Y
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AQ 4 GER 0.002000
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AQ 512 F2 PROCESSING
phase arrayed 1b 0.30
PRESATURATION g1 gfe not used
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wet n fn 4096
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rot -608.8 g1v1 not used
tpwr 58 p1v1 1p
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dprv1 59 f1v1 0
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j1vh 146.0 wC 0
nullfg Y wC2 200.0
mult 2 wC2 0
ADIANATIC vs 1375
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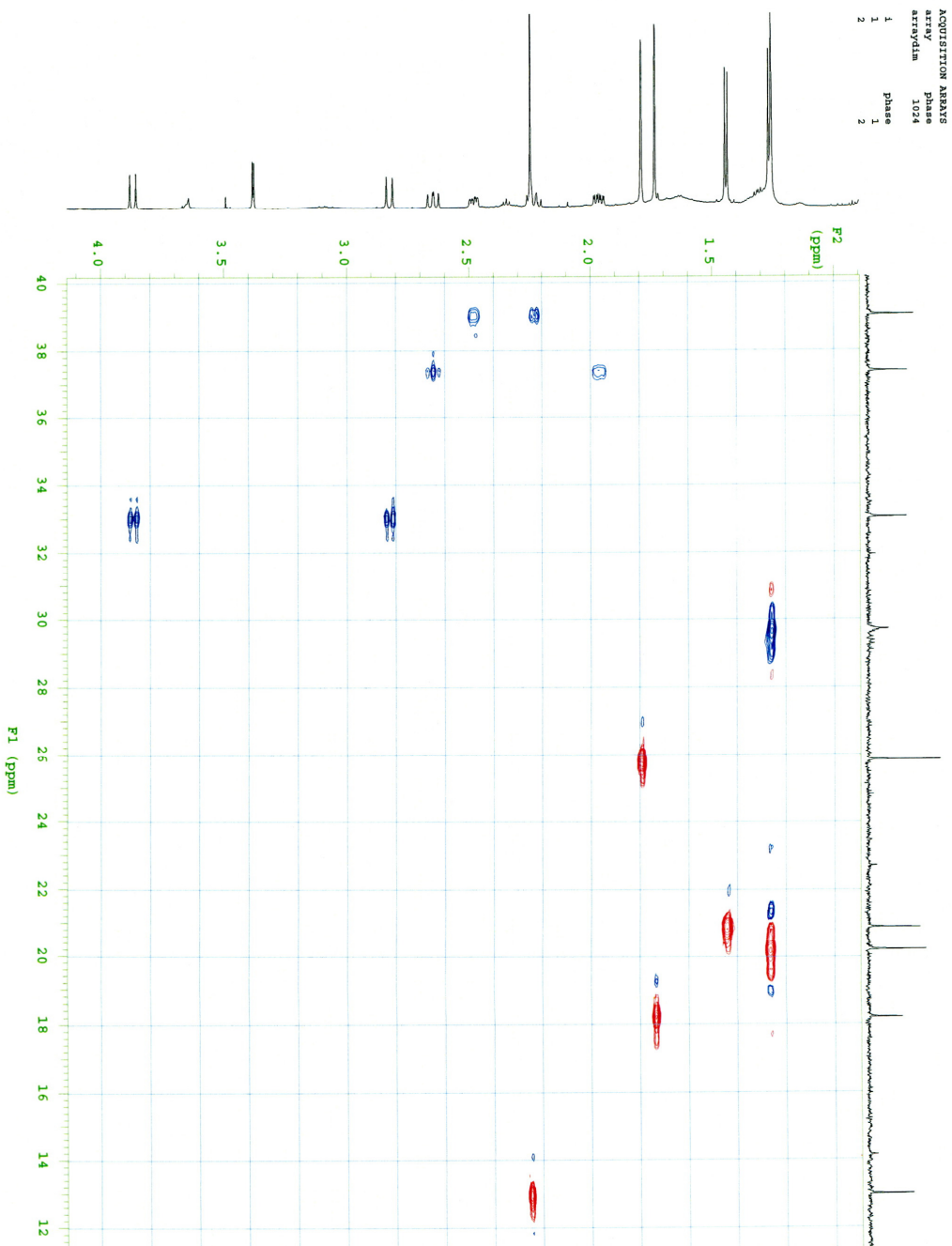
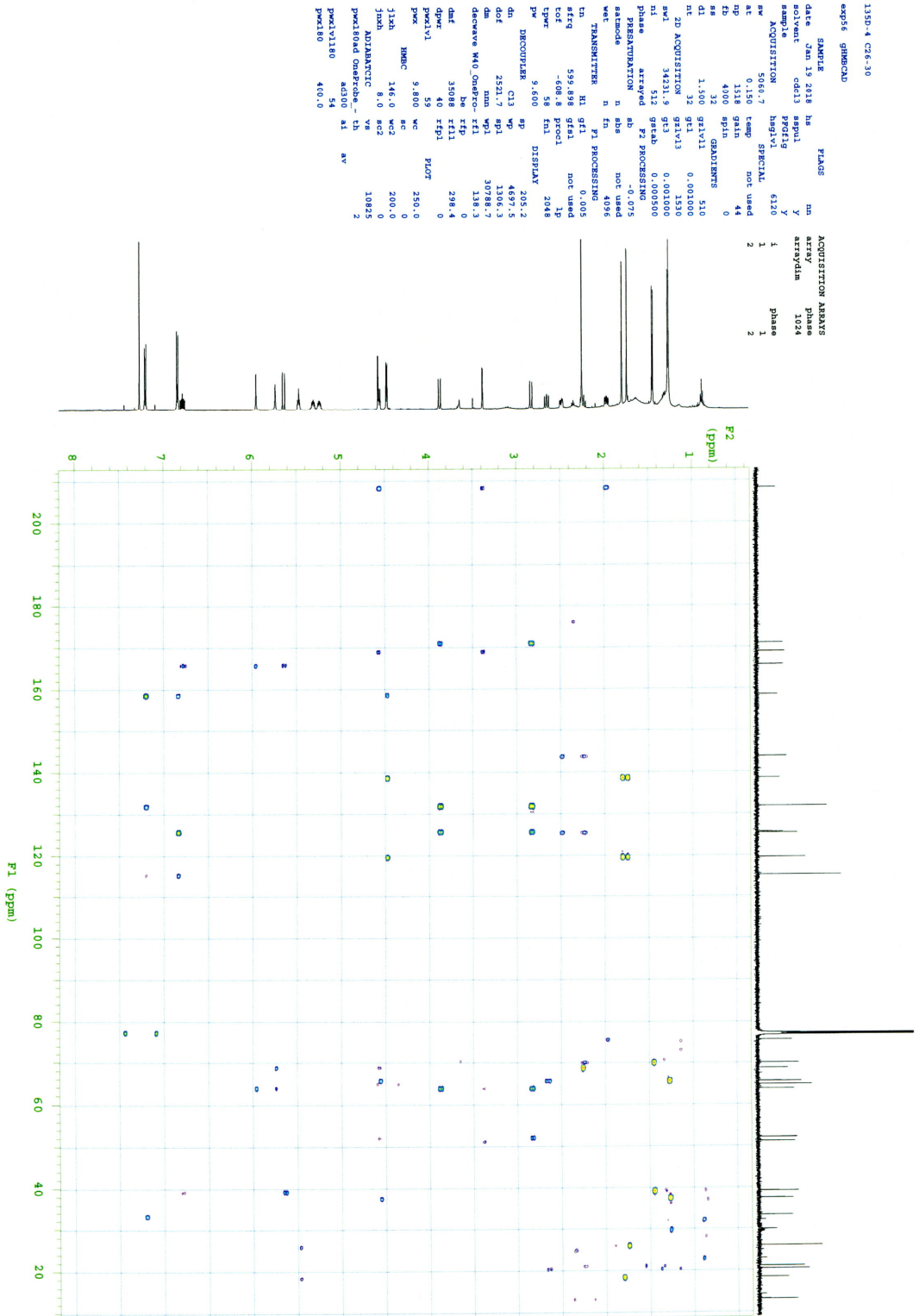
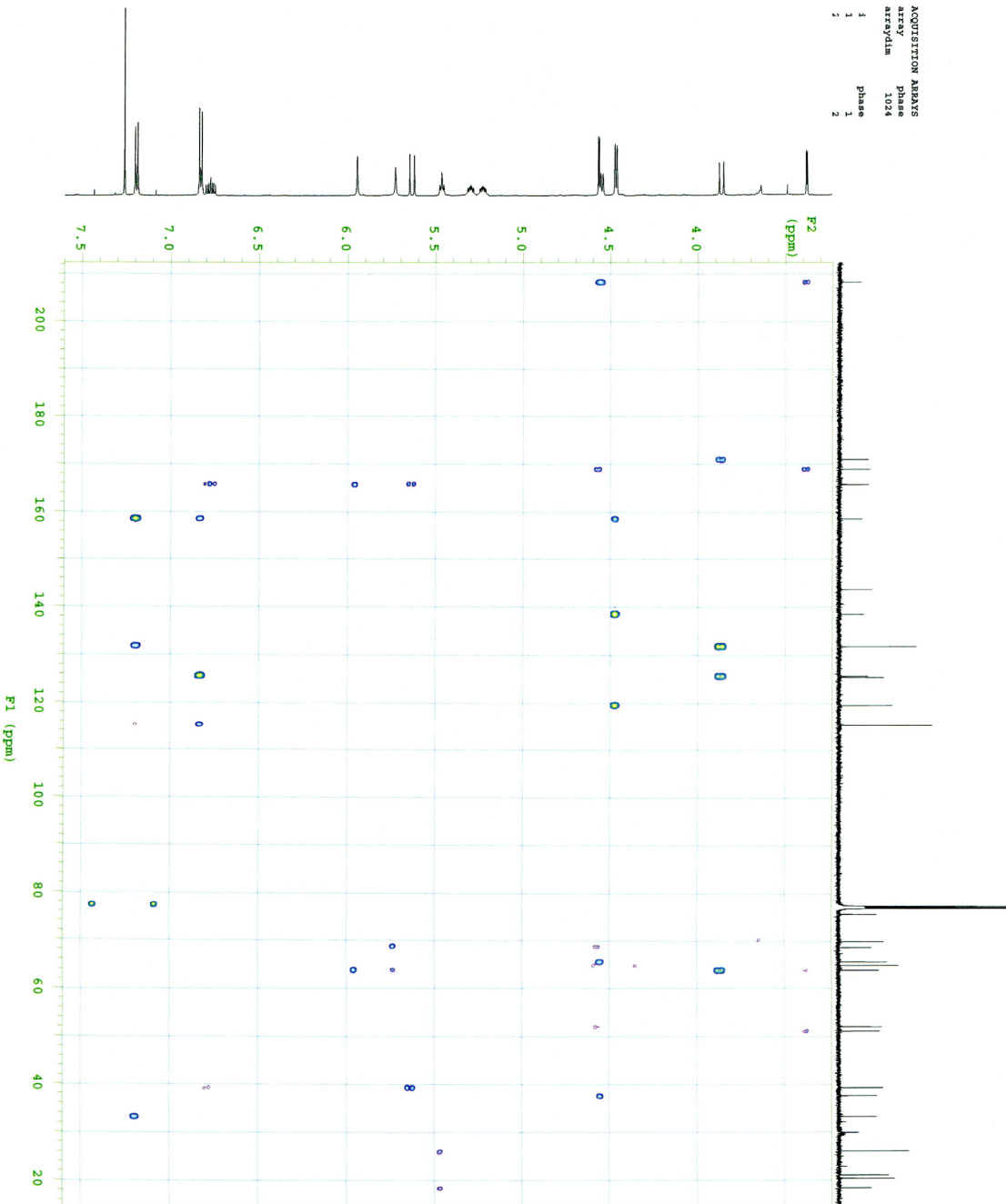


Figure S7 HMBC of 1



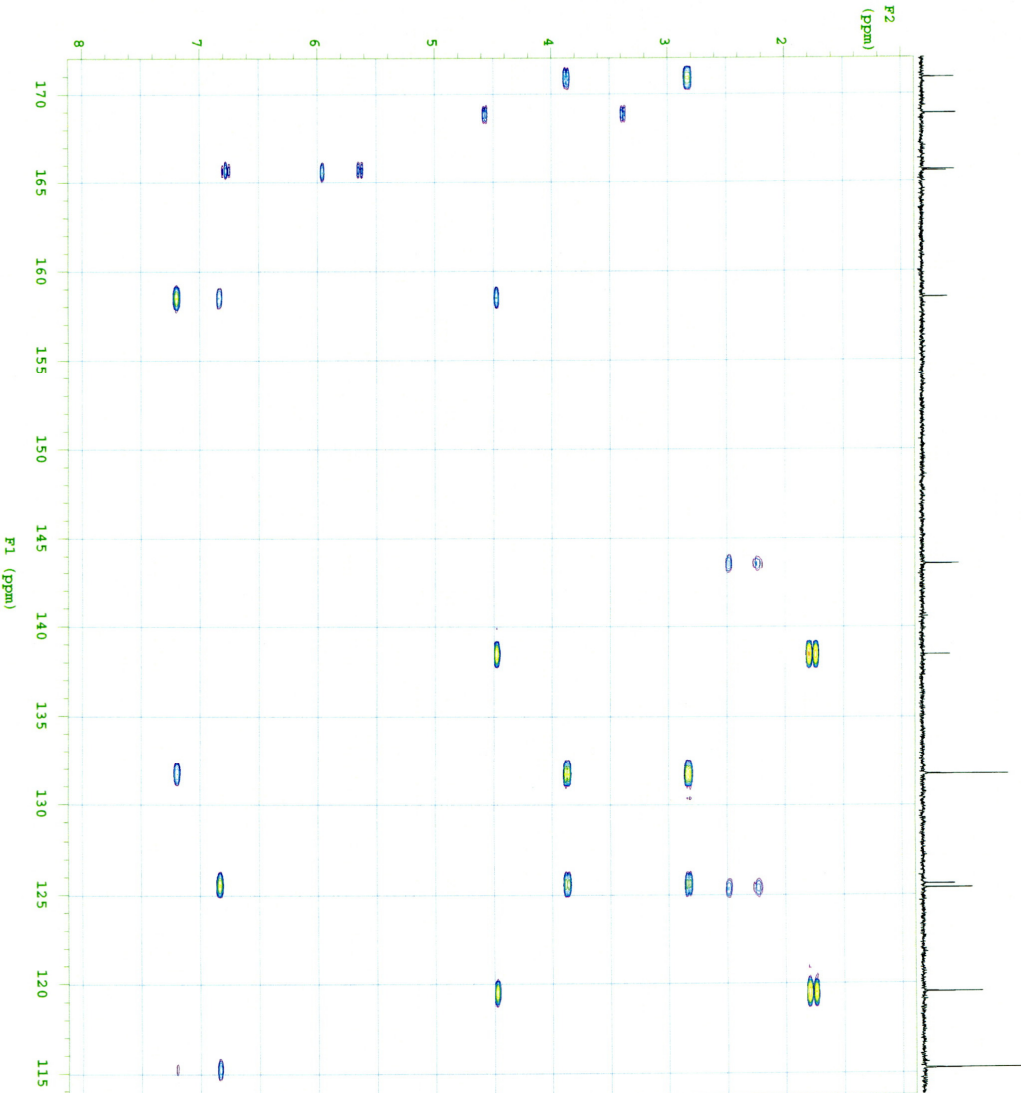
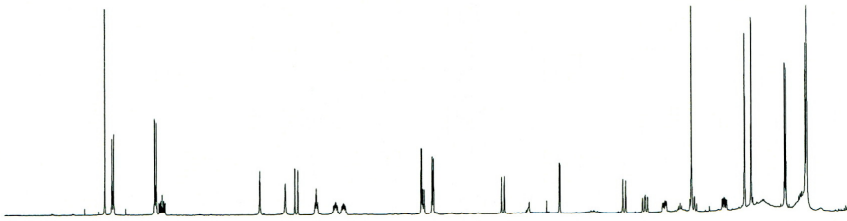
SAMPLE Jan 19 2018 hs
 solvent cdcl3 sepul
 sample 6120
 ACQUISITION 5040.7
 pw 0.150 temp not used
 nt 1518 gain 44
 tp 4000 spin 0
 ss 32 CHANNELS 510
 dt 1.500 g21v11 0.001000
 nt 32 g21 0.001000
 2D ACQUISITION g21v13 1530
 mw1 34211.9 g23 0.001000
 mw2 512 g2ab 0.000500
 phase arrayed f2 PROCESSING
 PRESENTATION n sb -0.075
 arched n sb not used
 wet n fn 4084
 TRANSMITTER n fn
 tn n gfl P1 PROCESSING
 stq 599.898 gfa1 not used
 tof -688.8 p1c01 lp
 fpr 58 fn1 2048
 pw 9.600 DISPLAY
 DECOUPLER C13 sp 1939.9
 dn C13 wp 2619.3
 dcf 2521.7 ap1 2115.4
 ds mm wp1 2952.6
 decoupr M40_Coupr be rfg 130.0
 dnt 35088 rfil 288.4
 dprv 40 rfpl
 pckv1 59 PLOT 280.0
 pck 9.800 wc
 hbnc 8c
 j1xh 146.0 wc2 200.0
 j1xh 8.0 mc2 0
 ADJAMATIC vn 10825
 pck180d Coupr08m - lh
 pck1180 48300 ai nv
 pck180 400.0

ACQUISITION ARRAYS
 array 1
 arraydim 1
 phase 2
 phase 2



exp56 ghmhcd

SAMPLE	DATE	HA	FLAG	IN	ACQUISITION ARRAYS
date	Jan 19 2018	ha		in	array
solvent	cdcl3	sepl1	Y	Y	phase
sample		prclg			arraydel
ACQUISITION		hagl1	6120	1	Phase
sw	5093.7	SERIAL		2	2
at	0.150	temp	not used		
sd	1518	gain	44		
sp	4932	spin	GRADIENTS		
dl	1.500	gr1v1	0		
nt	32	gr1	0.001000		
2D ACQUISITION	gr1v13	gr1v13	1330		
sw1	34231.9	gr3	0.001000		
nl	512	grtab	0.000500		
Phase	arrayed	F2 PROCESSING			
PRESATURATION	sb		-0.075		
balmode	n	sbs	not used		
wet	n	fn	4096		
tx	TRANSMITTER	hi	F1 PROCESSING		
freq	599.828	gr1	not used		
rof	-608.8	grcc1	lp		
tpwr	58	fn1	2048		
pw	9.600	DISPLAY			
DECOUPLER	sp	sp	533.8		
dn	Cl3	wp	4334.2		
dof	2521.7	sp1	17151.9		
dm	nmn	wp1	8792.0		
decouple	W40_OrbPtc	rfl	138.3		
dnf	De	rfl	0		
	35088	rfl1	298.4		
opw	40	rfl1	0		
ppw	5	rfl1	0		
pw	9.800	WC	250.0		
jinh	146.0	wc2	200.0		
ADJANALYTIC	vs		0		
pk180ad OnaPrbM_	th		10825		
pk180ad OnaPrbM_	al	AV	2		
pk1v1180	54				
pk180	400.0				



135D-4 C13-30
exp56 gbm60d

PARAMETER	VALUE	UNIT
date	Jan 19 2018	
solvent	cdcl3	
sample	hagl1	
ACQUISITION	hagl1	
sw	5060.7	Hz
atc	0.150	temp
rp	4318	gain
rs	4032	spn
ss	32	spn
nt	1.500	gr1v1
2D ACQUISITION	gr1v13	
sw1	34211.9	gr13
nt1	512	gr1ab
phase	arrayed	
PRESATURATION	ab	
satmode	n	
wet	n	
TRANSMITTER	n	
rf	559.838	rf1
rf2	-608.8	rf2
tpwr	58	fnl
pw	9.600	fnl
DECOUPLER	sp	
dn	C13	wp
dof	2511.7	spi
dm	nm	wpi
decayw	M40_Over-	rf1
dnc	be	rf2
dmf	35088	rf1
dmf	35088	rf2
Opn	59	zfp1
Opn	59	zfp2
pkc	9.800	wc
pkc	9.800	wc
pkc	9.800	wc
pkc	146.0	wc2
pkc	8.0	wc2
pkc	10825	wc2
pkc	4300	at
pkc	54	av
pkc	400.0	av

ACQUISITION ARRAYS	array	phase
1	arrayed	1024
2	arrayed	1024

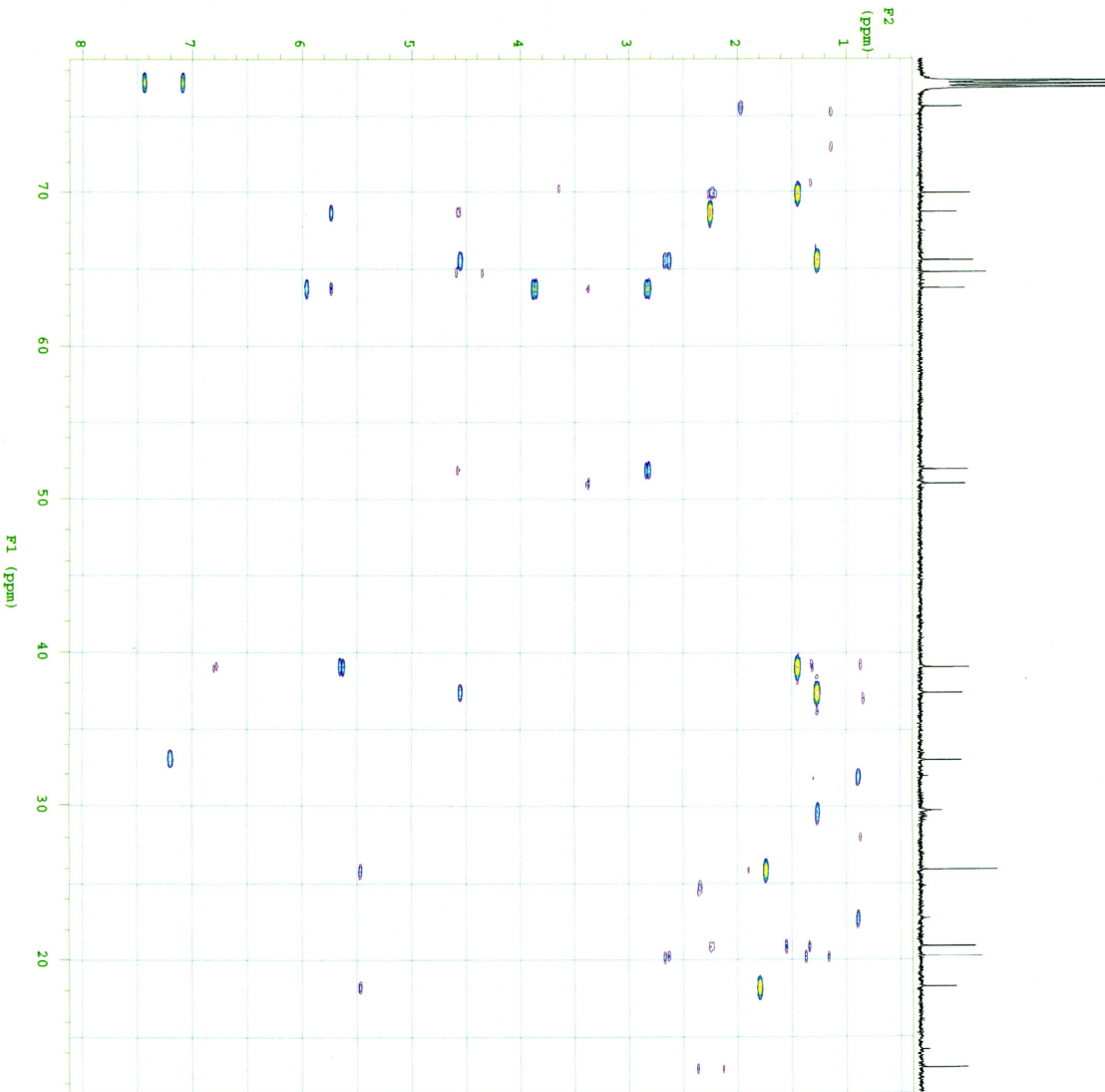
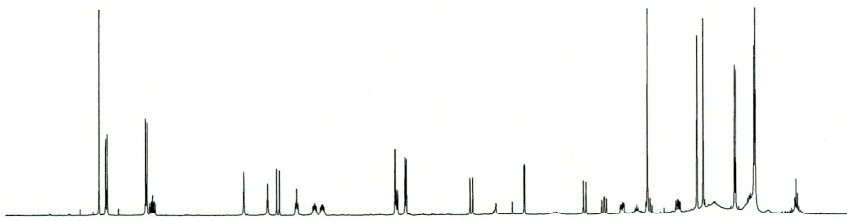
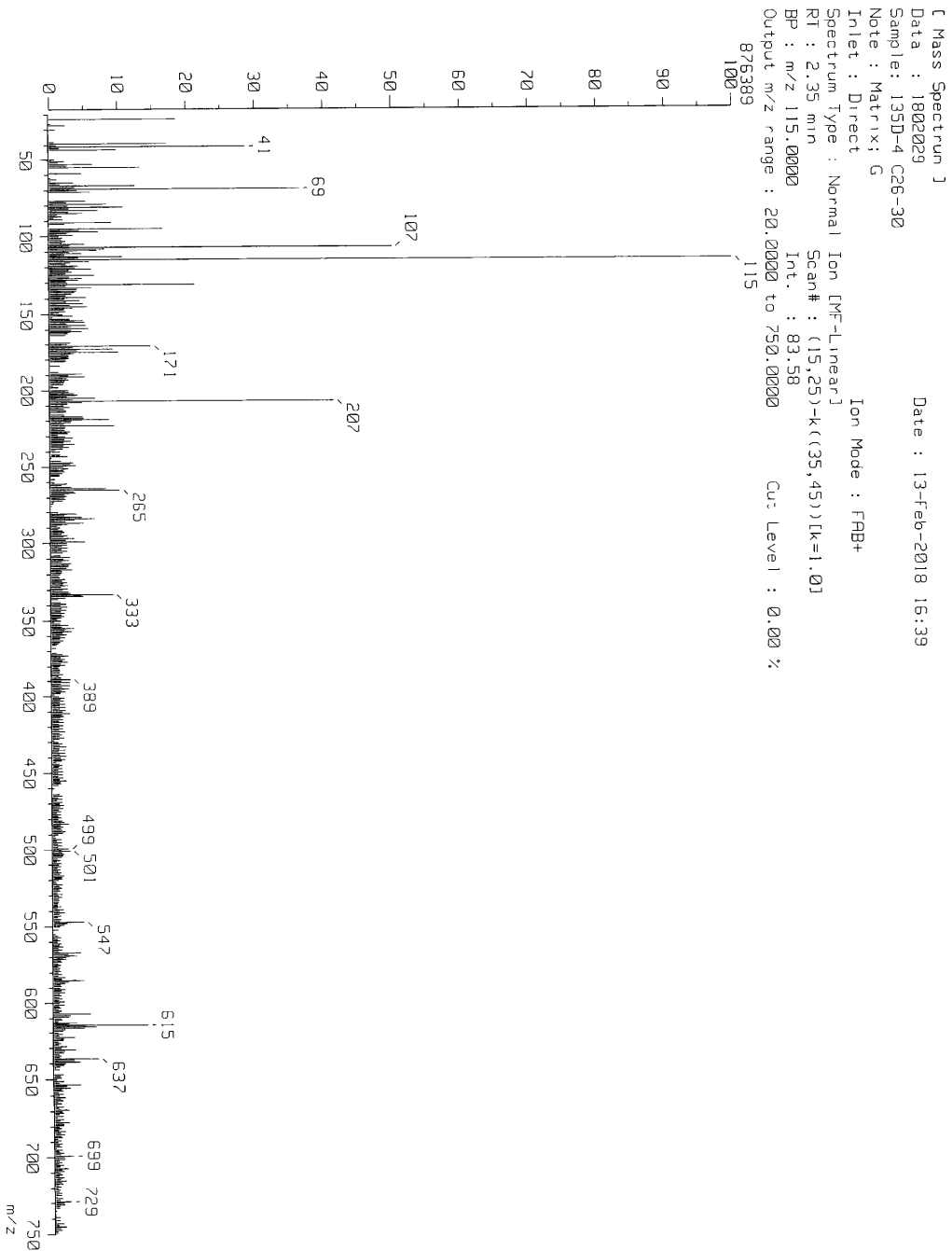


Figure S8 FABMS of 1



[Mass Spectrum]

Data : 1802029 Date : 13-Feb-2018 16:39
 Sample: 135D-4 C26-30
 Note : Matrix; G
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 2.35 min Scan# : (15,25)-k((35,45)) [k=1.0]
 BP : m/z 115.0000 Int. : 83.58
 Output m/z range : 20.0000 to 750.0000 Cut Level : 5.00 %

m/z	Int.	Norm.
23.0000	15.50	18.55
39.0000	14.38	17.20
41.0000	24.00	28.71
43.0000	8.28	9.91
53.0000	5.29	6.33
55.0000	11.09	13.26
67.0000	10.49	12.56
69.0000	30.62	36.64
71.0000	5.01	6.00
77.0000	4.49	5.37
79.0000	6.95	8.32
81.0000	9.01	10.78
83.0000	6.02	7.20
91.0000	7.60	9.09
95.0000	13.92	16.65
97.0000	5.98	7.15
105.0000	4.30	5.14
107.0000	41.92	50.16
108.0000	6.82	8.16
109.0000	5.78	6.92
113.0000	8.97	10.73
115.0000	83.58	100.00
116.0000	4.82	5.77
121.0000	5.12	6.12
125.0000	5.50	6.59
131.0000	17.81	21.31
133.0000	5.10	6.11
139.0000	4.43	5.30
145.0000	4.61	5.52
155.0000	4.26	5.10
157.0000	4.42	5.28
159.0000	4.71	5.64
171.0000	12.34	14.77
173.0000	7.68	9.19
175.0000	8.42	10.07
191.0000	4.30	5.14
205.0000	5.51	6.59
207.0000	34.68	41.49
219.0000	7.16	8.57
223.0000	7.84	9.38
264.0000	6.79	8.12
265.0000	8.44	10.10
284.0000	5.38	6.44
333.0000	7.52	9.00
607.0000	4.53	5.42
615.0000	11.56	13.83
616.0000	5.19	6.21
637.0000	5.49	6.57

[Elemental Composition]

Data : 1802049

Date : 14-Feb-2018 18:38

Page: 1

Sample: 135D-4 C26-30

Note : Matrix; G

Inlet : Direct

Ion Mode : FAB+

RT : 8.25 min

Scan#: (57,62)

Elements : C 34/28, H 45/35, N 4/0, O 11/0, S 1/0

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
615.2380	100.0	+0.7 / +0.4	14.5	C 31 H 39 N 2 O 9 S

Figure S9 IR spectrum of 1

