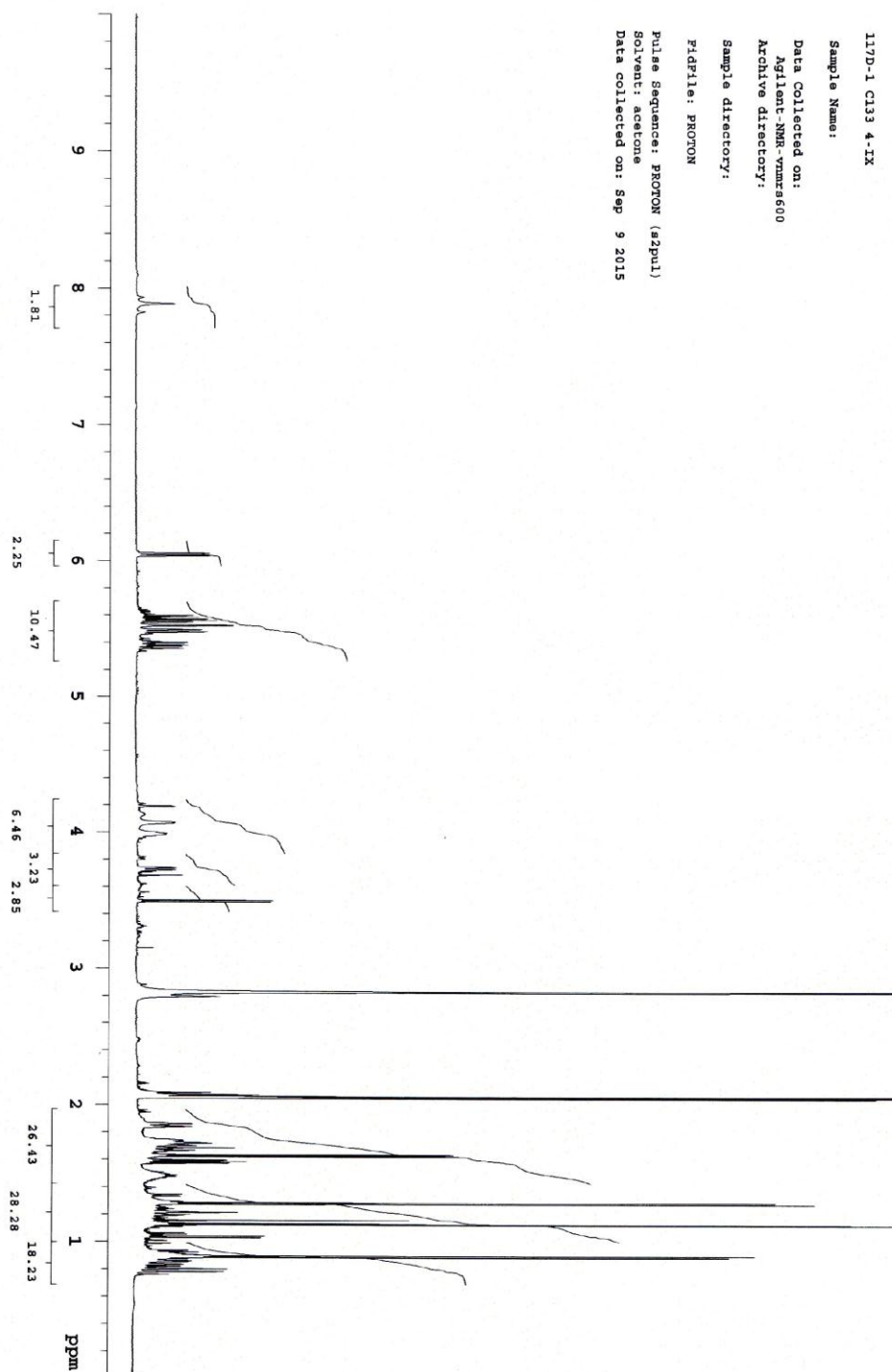
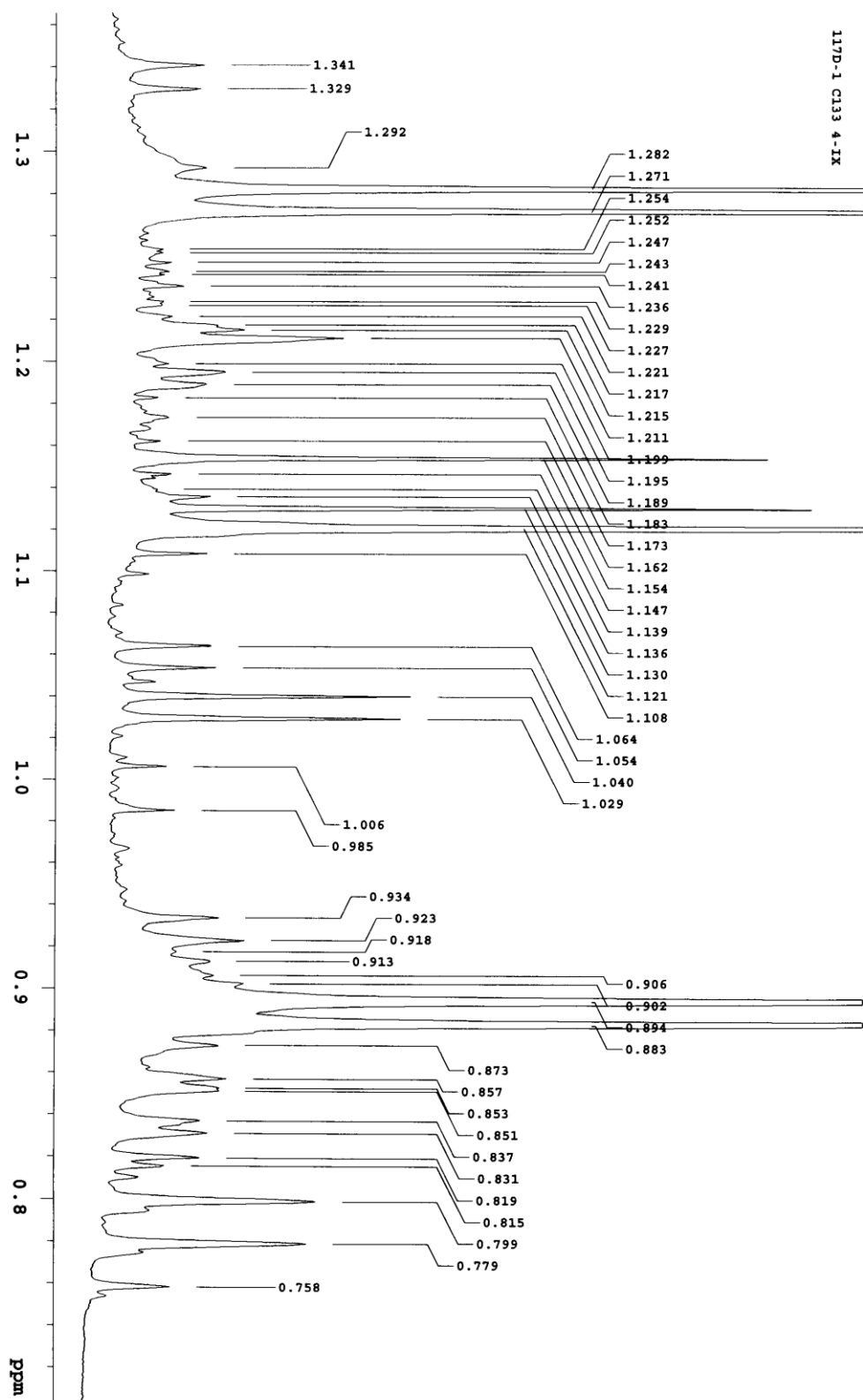
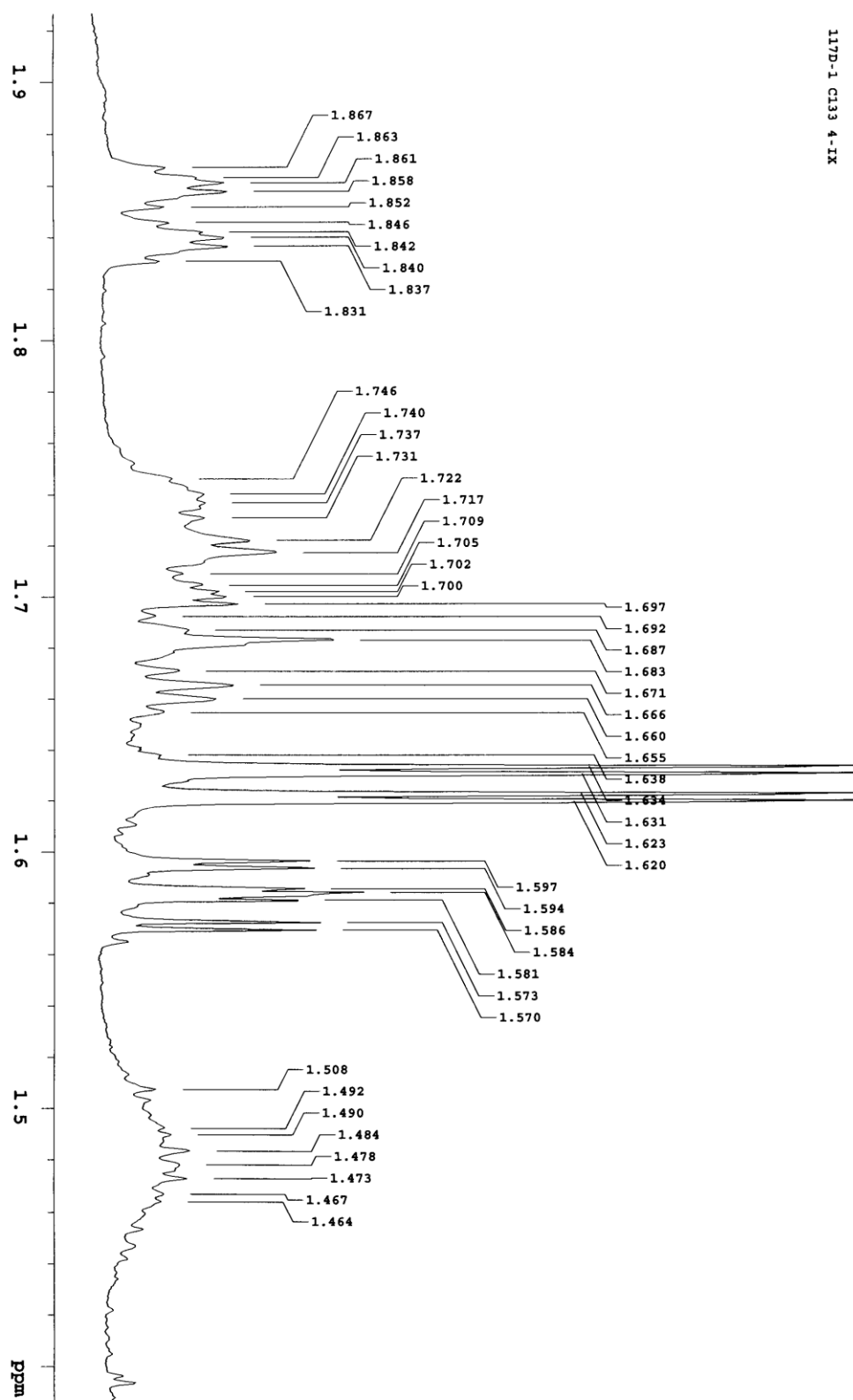
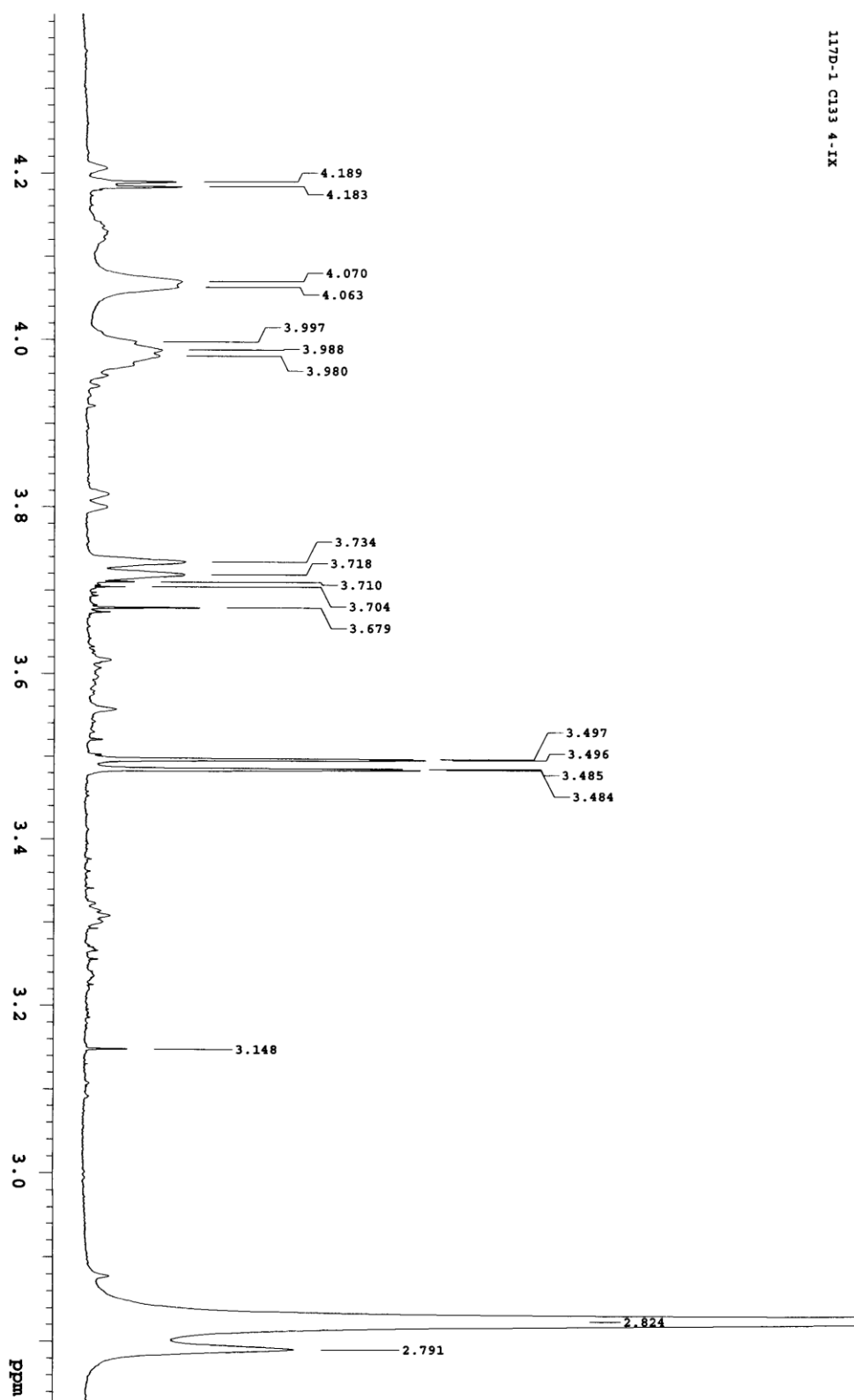


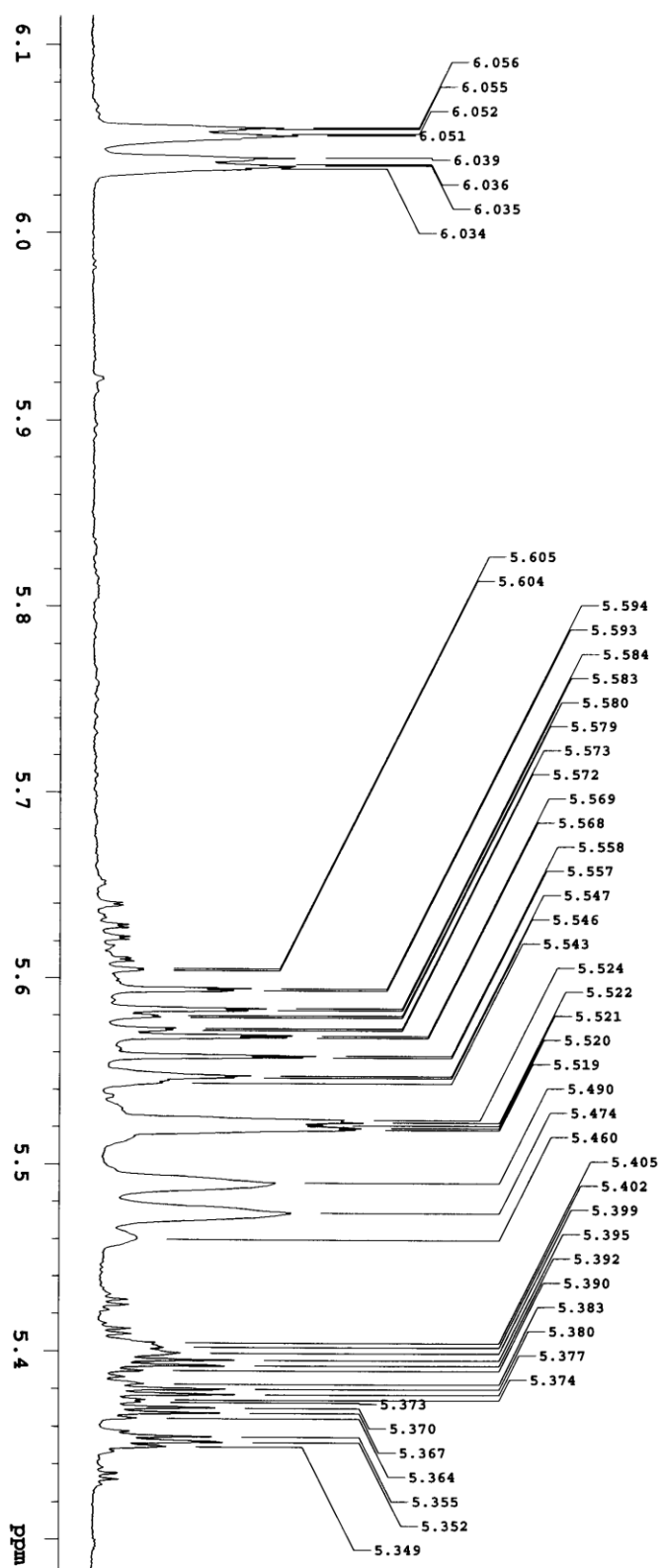
Figure S19  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra in acetone- $d_6$  of **4**

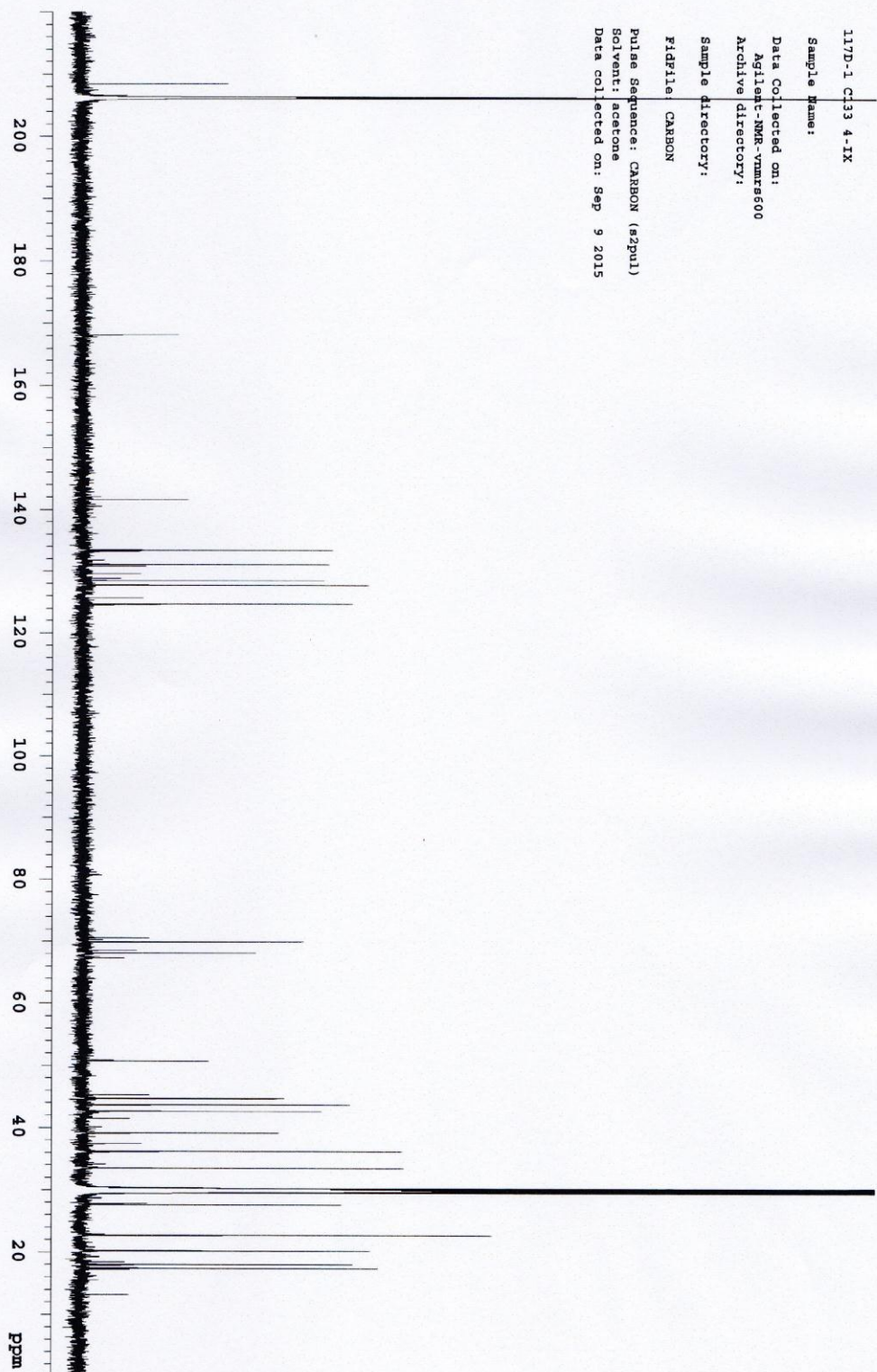




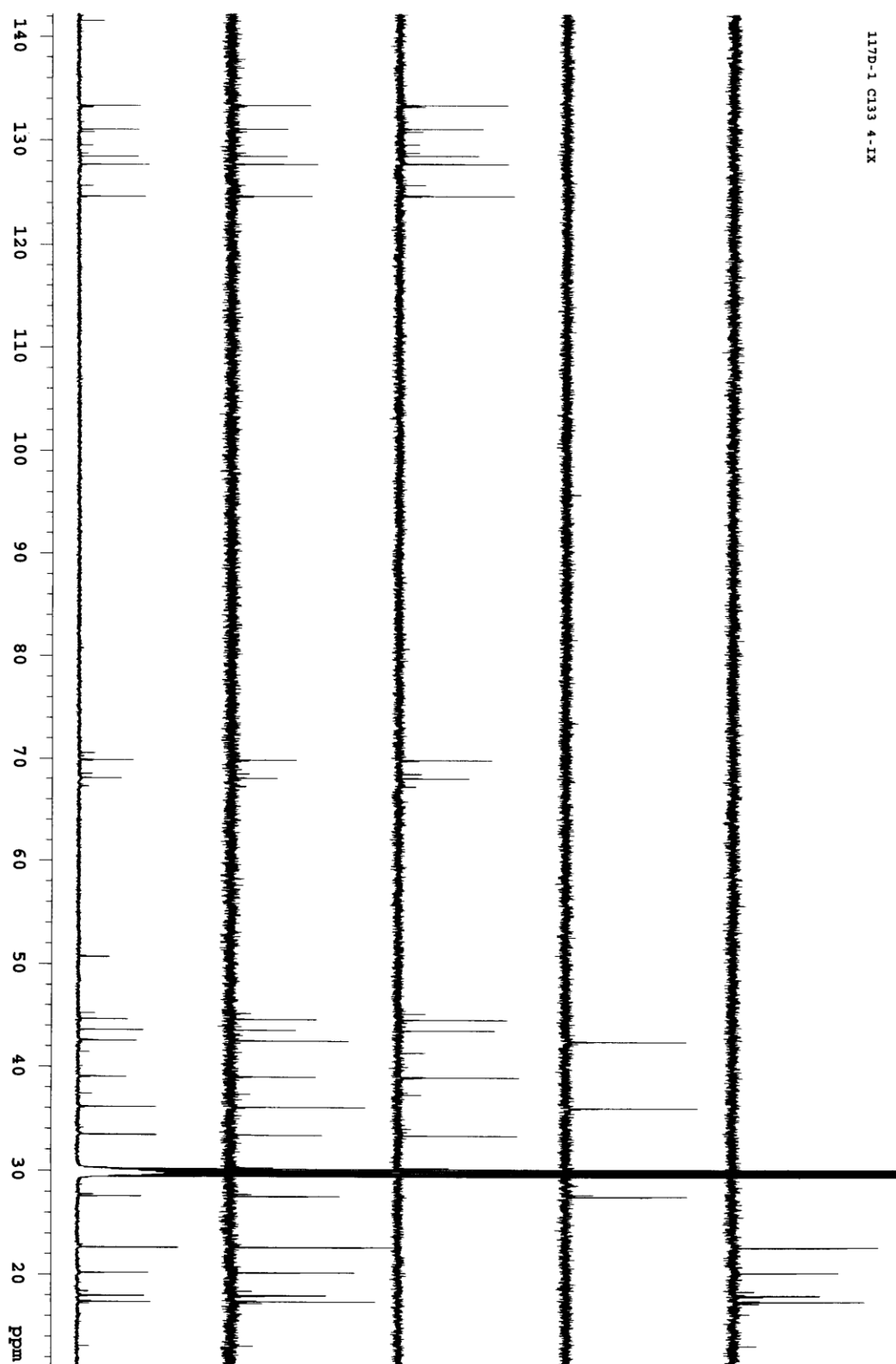




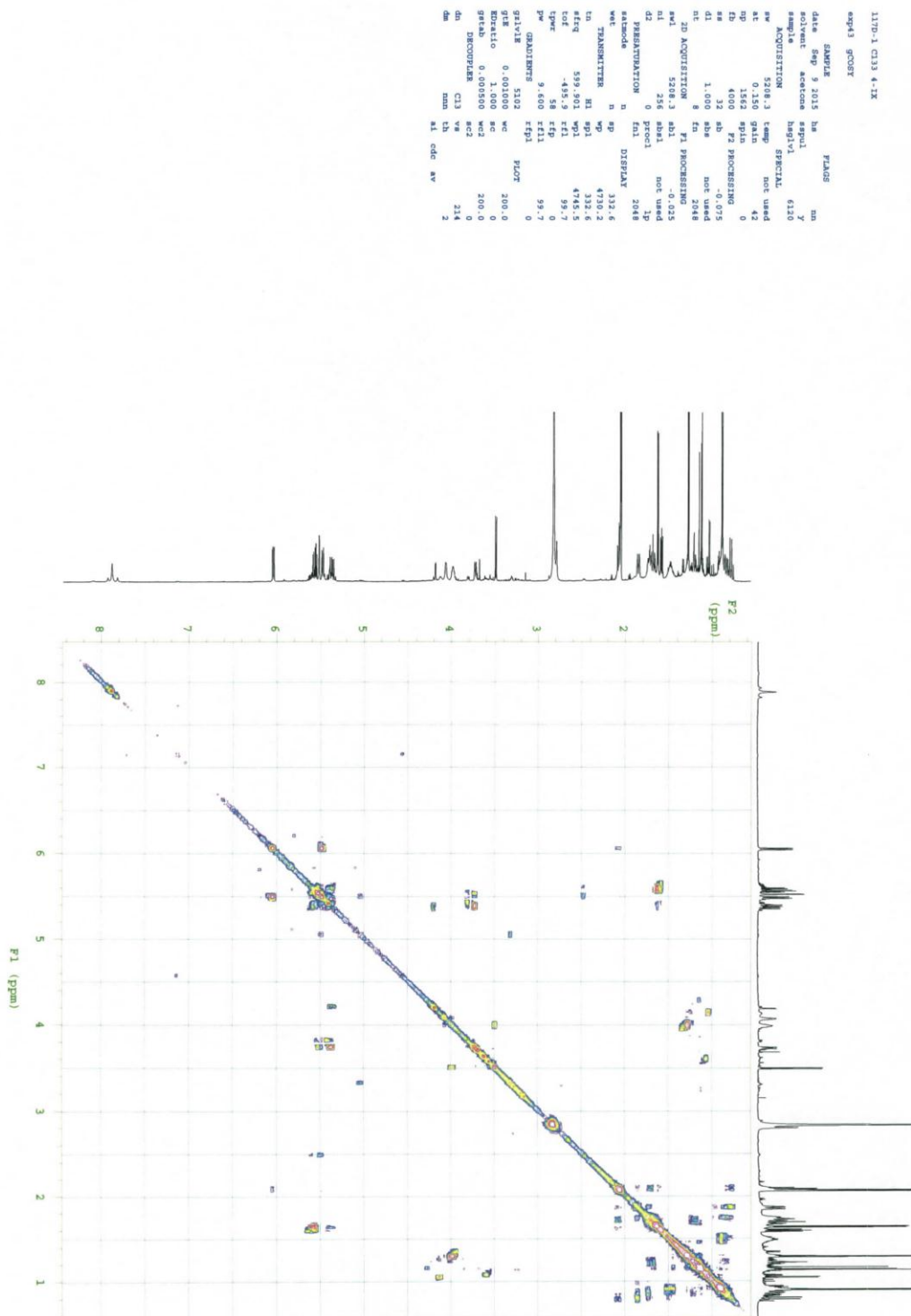




117D-1 CL33 4-IX



**Figure S20**  $^1\text{H}$ - $^1\text{H}$  COSY of **4**



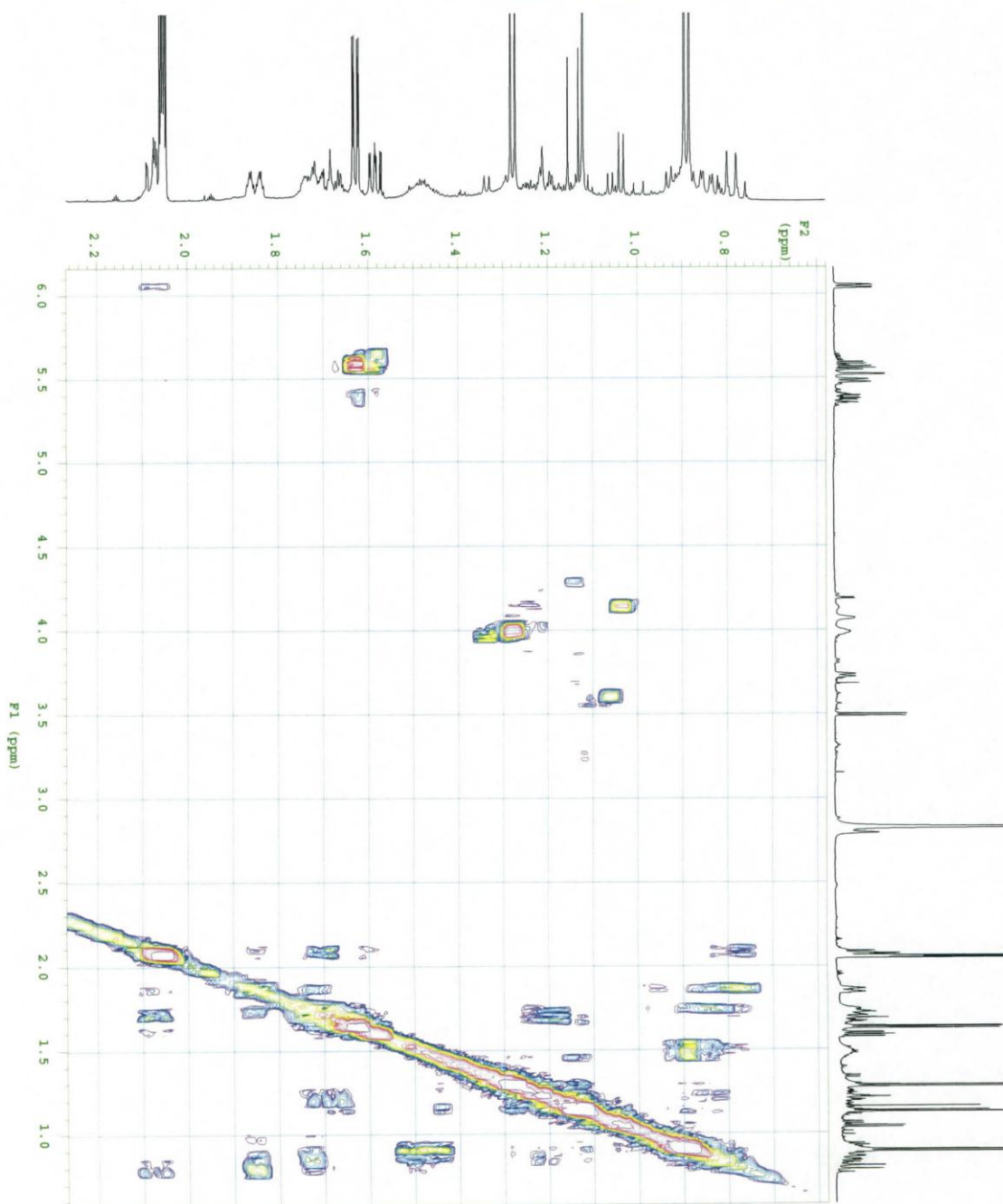


```

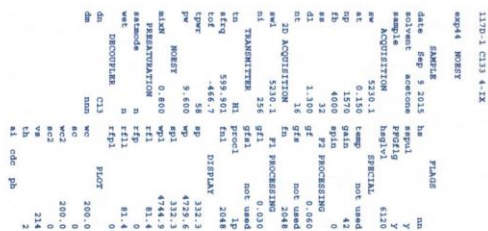
11TD-1-CL33 4-1X
exp43 300X

SAMPLE
date Sep 9 2015 ha nm
solvent acetone sepul y
sample hsg1v1 6120
ACQUISITION SPECIAL
av 5208.3 temp not used
at 0.150 gain 42
ap 1562 spin 0
fb 4000 F2 PROCESSING 0
pc 1513 ab 0.075
di 1.000 abv not used
nt 2048 fu 0
2D ACQUISITION F1 PROCESSING
av1 5208.3 ab1 -0.025
nl 256 abel not used
d1 0 p1c1 1p
PRESATURATION fml 2048
satmode n DISPLAY
wet n ap 347.8
TRANSMITTER n wp 1012.2
tu n ap1 342.8
pc n ap1 3581.9
tc n ap1 3581.9
lpc -495.8 rfi 35.7
lpcr -495.8 rfi 35.7
pw GRADIENTS 9.600 rfi 99.7
g1v1e 5102 rfi 0
g1e 0.001000 wc FLOT 250.0
g1e 1.000 ac 0
g1e 0.000500 wc2 200.0
DECOMPLER C13 va 0
dm nm th 214
at cdc mv 2

```



**Figure S21 NOESY of 4**

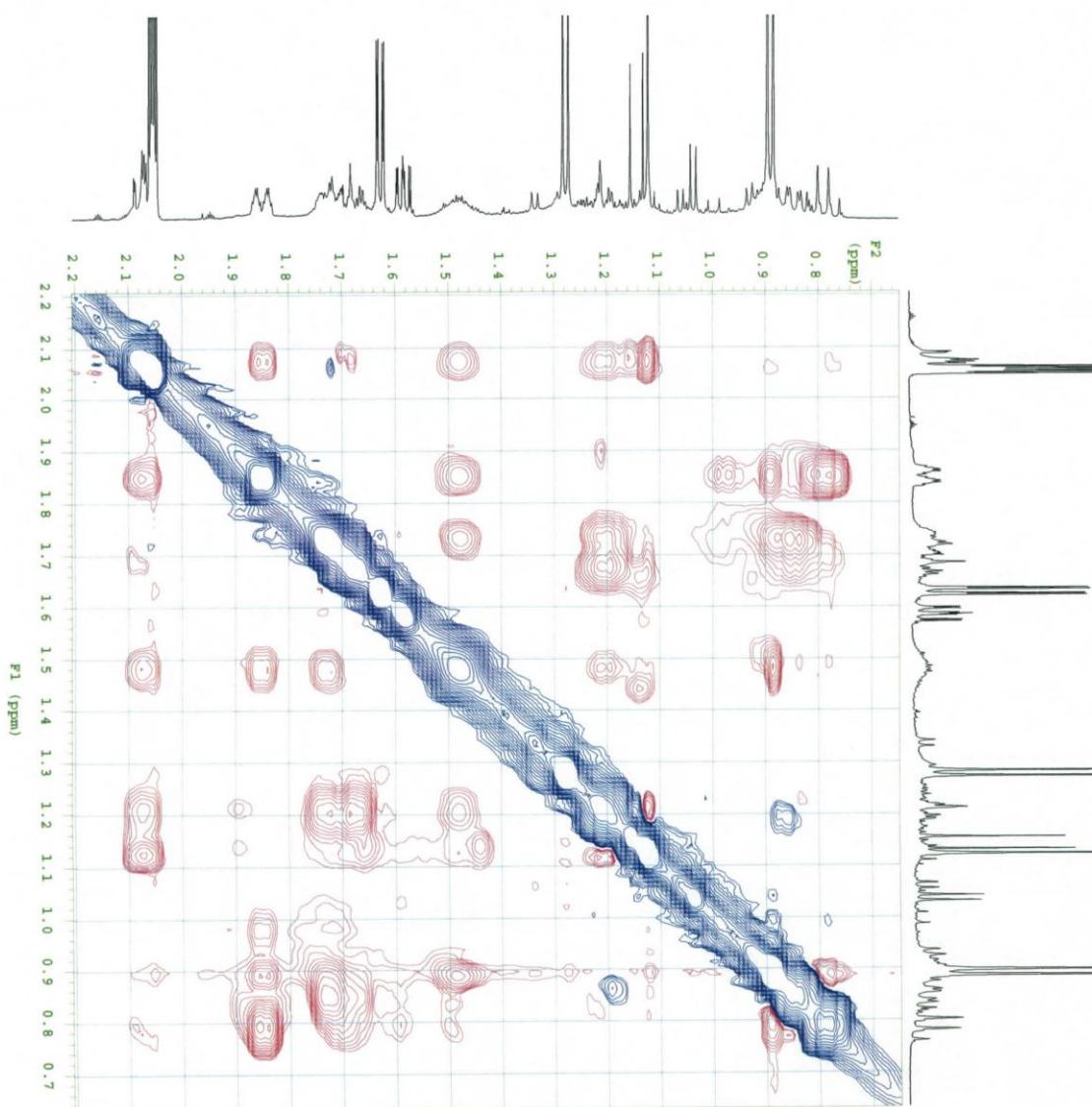


```

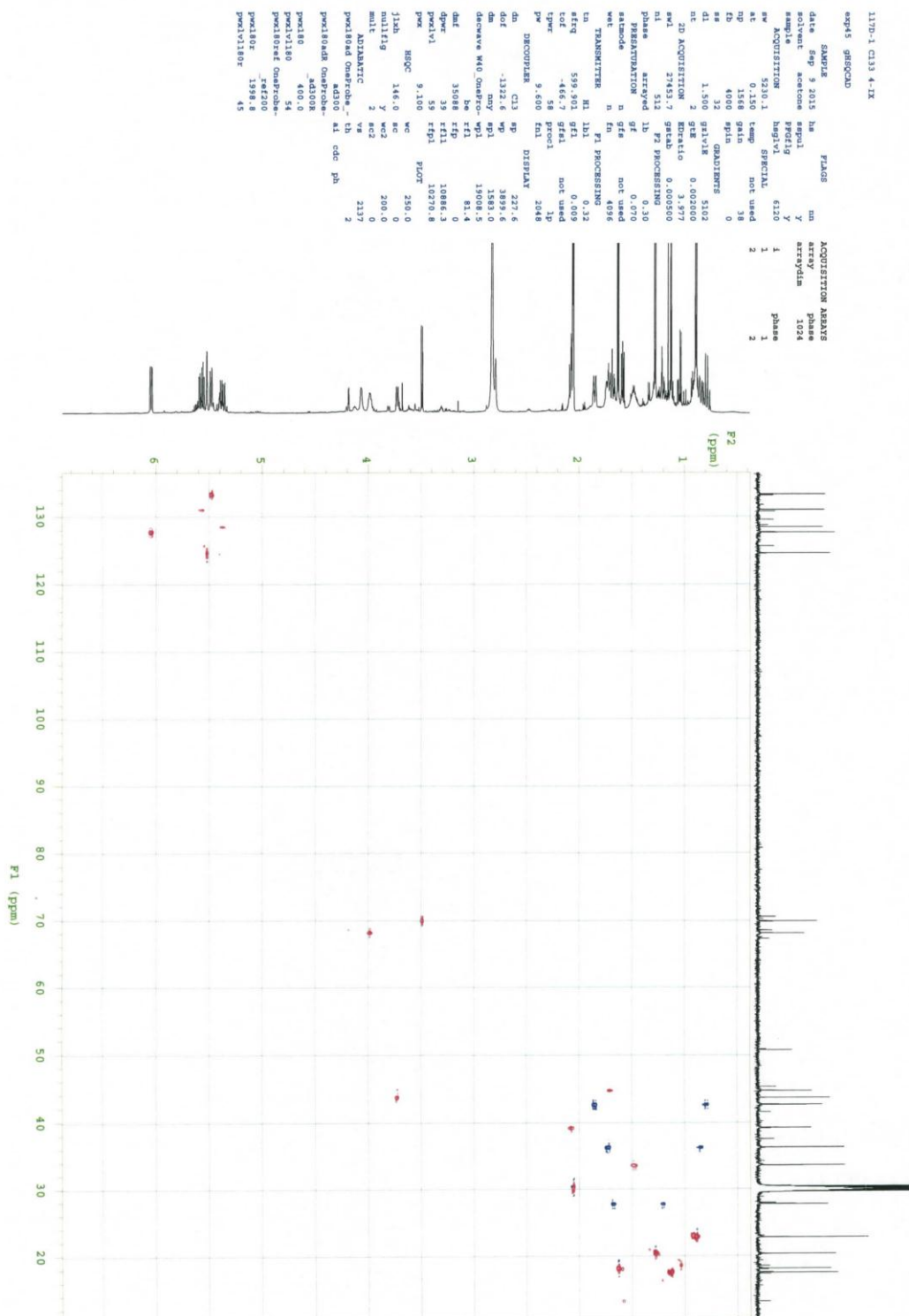
11TD-1 C133 4-IX
exp44 NOESTY

SAMPLE
date Sep 9 2015 ha
solvent acetone resol
sample y
ACQUISITION
sw 520.1 SPECIAL
at 0.150 temp not used
rp 1570 gain 42
fb 4000 spin 0
a 320 F2 PROCESSING 0
d1 1.310 gfe not used
nt 16 gfe not used
2D ACQUISITION
sw1 520.1 F1 PROCESSING
n1 256 gfe 0.030
tn TRANSMITTER n1 precl 1p
rfq 599.901 fml
lof -466.7 DISPLAY
cpw 58 ap 388.5
pw 9.600 wp 394.7
mix NOESTY 0.800 ap1 394.2
PRESATURATION n rfg 81.4
satmode n rfg 81.4
wet n rfg 81.4
DECOUPLE CL3 rfg1 0
dn nmw 200.0
wc ac 0
ac2 200.0
va ac2 0
v1 va 214
a1 cdc ph 2

```



**Figure S22** HMQC of 4



117D-1 CL33 4-1X  
exp45 gREGCMO

SAMPLE		FLAGS		ACQUISITION ANALYSIS	
date	Sep 9 2015	hs	na	array	phase
solvent	acetone	suppl	y	arraydim	1024
sample		profig	y		
ACQUISITION	hsplv1	6120		phase	1
sw	5210.1	SPECIAL			2
at	0.150	temp	not used		
mp	1268	gain	38		
sd	4093	spin	0		
as	4093	GRADIENTS	0		
dl	1.500	grv1x	5102		
nt	2	grv	0.002000		
2D ACQUISITION	2	Edratio	3.977		
sw1	27453.7	gateb	0.000500		
nl	512	F2 PROCESSING			
phase	arrayed 1b	gr	0.30		
PRESATURATION	gr	not used			
satmode	n	gr	0.070		
wet	n	fn	4096		
TRANSMITTER	h1	F1 PROCESSING	0.32		
td	1.500	grv1x	5102		
afreq	599.901	grf1	0.009		
tot	-466.7	grf1	not used		
lprc	58	procl	1p		
pw	9.600	fn1	2048		
DECOUPLER	CL3	sp	370.6		
dn	-1322.6	wp	1066.2		
da	may	sp1	1984.7		
decouwa	W40	OnaPro-	wp1	4959.9	
dec	35088	rfp	81.4		
qprc	1393	rf1	10866.3		
peakv1	59	rfp1	10270.8		
peak	9.100	wc	280.0		
nlh	146.0	sc	0		
nulling	y	wc2	200.0		
mult	2	sc2	0		
ADJANATIC	vs		2137		
peak180a	ad100	ai	cde	ph	2
peak180a	OnaPro-				
peak180	-ad100				
peakv1180	4093				
peak180a	OnaPro-				
peak180	rf1200				
peak180c	1398.8				
peakv1180c	45				

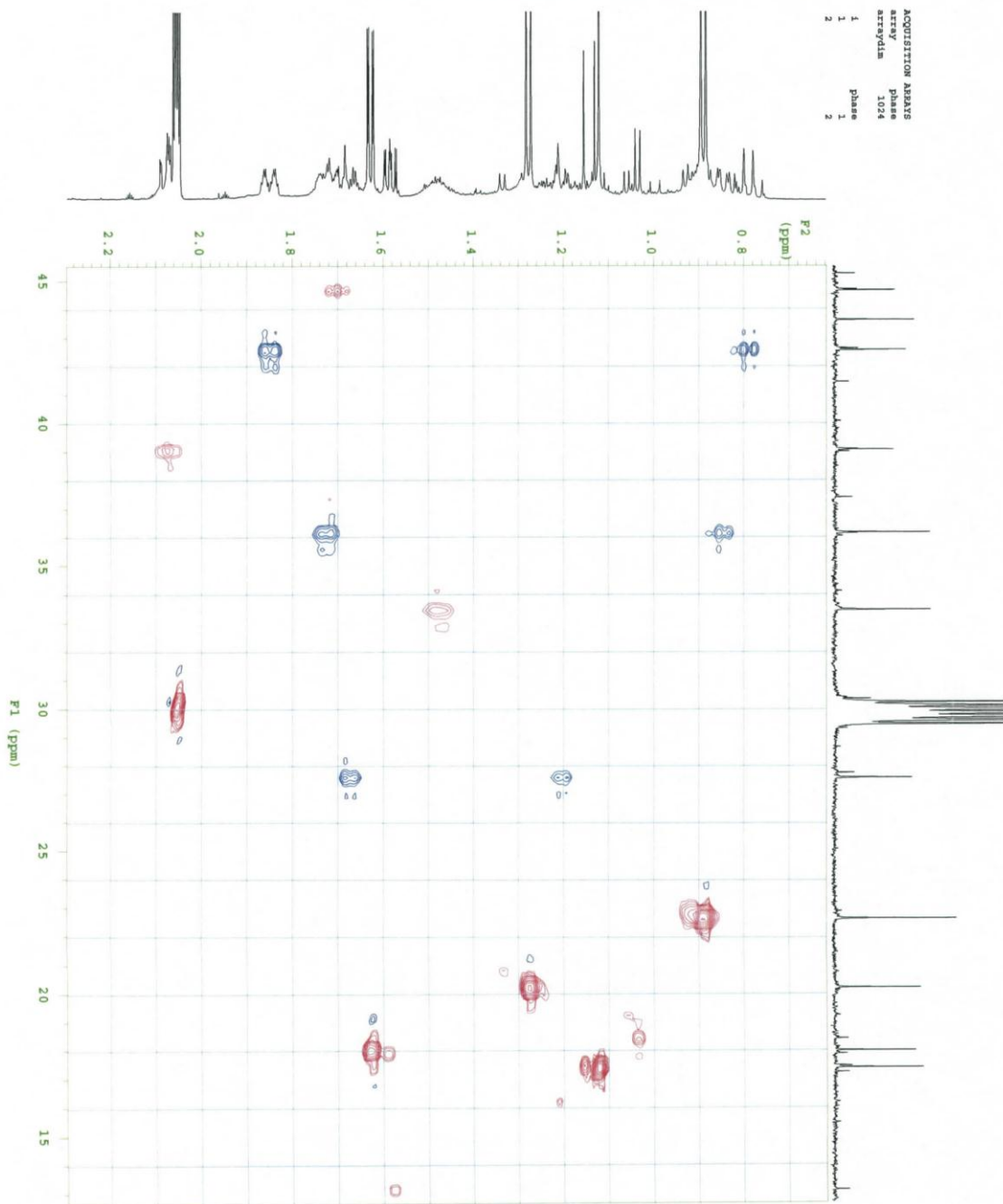
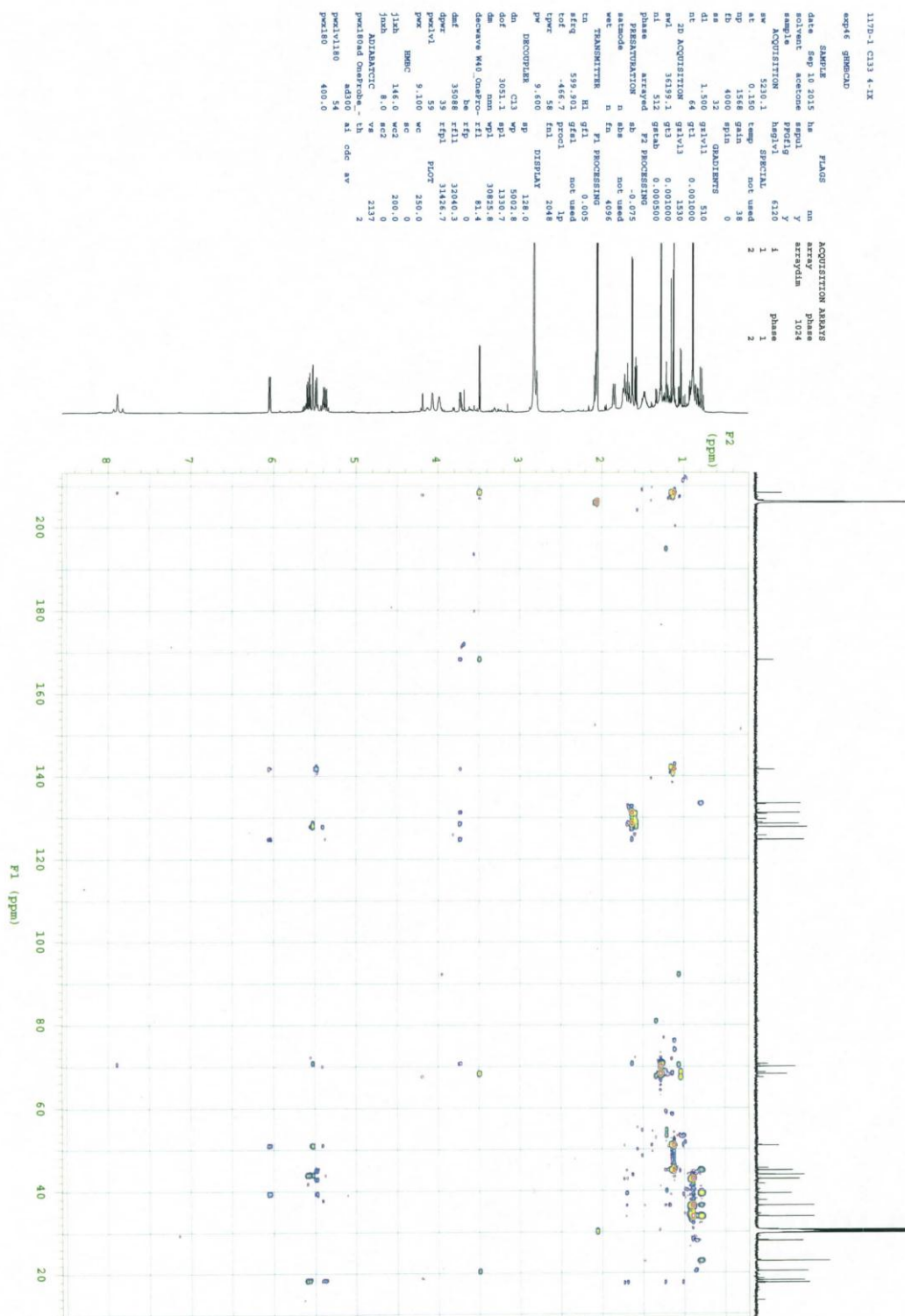




Figure S23 HMBC of 4

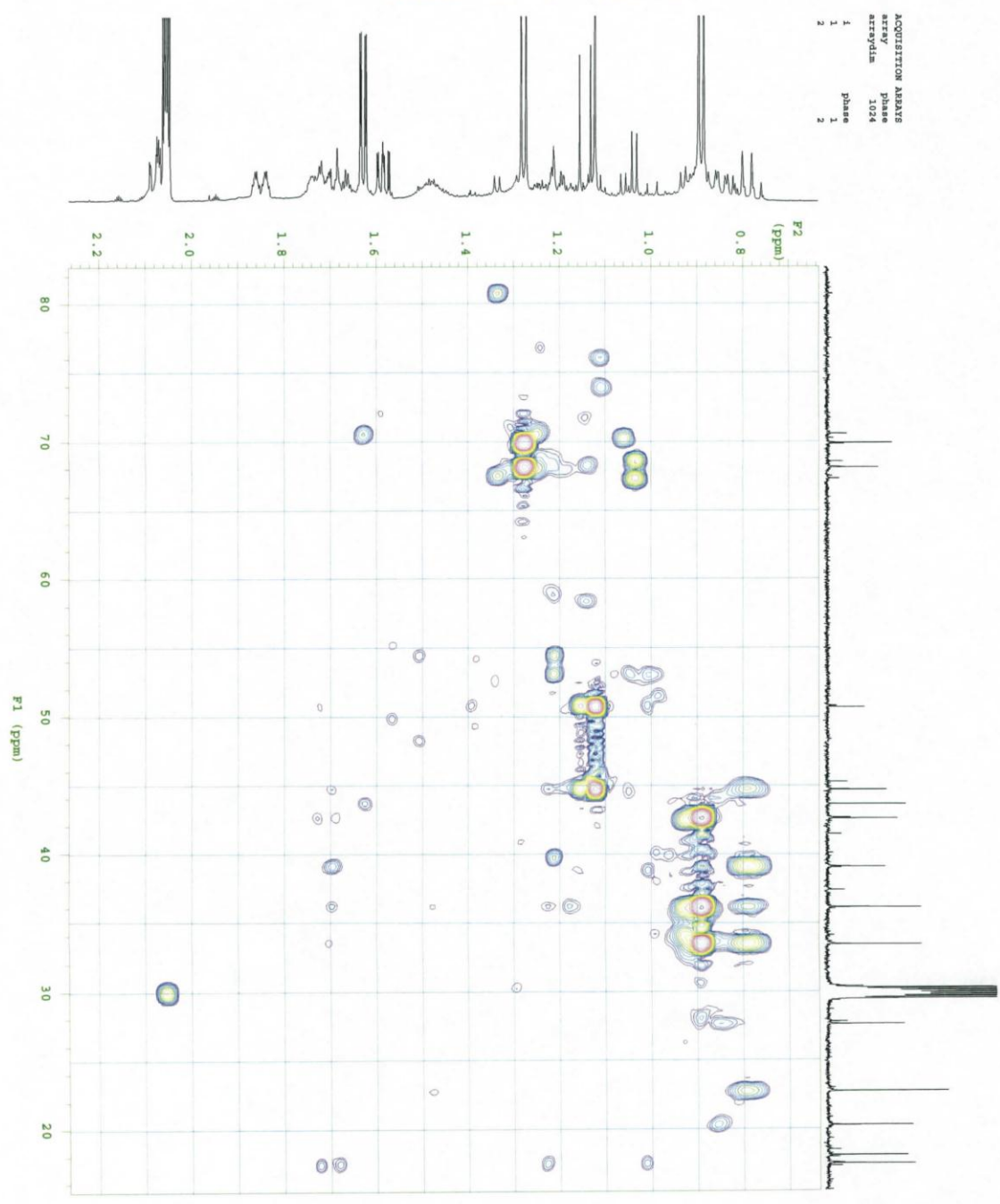


```

117D-1 C133 4-1X
exp46 gbmccao

SAMPLE          FLAGS
date Sep 10 2015   ha
solvent acetone    spul
sample            y
ACQUISITION      hsq1v1 6120
  av 5210.1 SPECIAL
  at 0.150 temp not used
  ap 1588 gain 38
  as 4083 spin 0
  ds 1.500 gtlv1 510
  nt 64 gtl 0.001000
  2D ACQUISITION gtlv13 1330
  w1 36199.1 gtl3 0.001000
  n1 512 gtlab 0.000500
  phase arrayed F2 PROCESSING
  PREPARATION ab -0.075
  astmode n ab not used
  wet n fn 4096
  1D TRANSMITTER n F1 PROCESSING
  to gtl 0.0005
  refq 599.901 gtl1 not used
  tot -466.7 pocol 1p
  lpr 58 fn1 DISPLAY 2048
  pw 9.600
  DECOUPLER sp 380.8
  dn C13 wp 978.1
  dof 3051.1 sp1 2320.5
  dn nm wp1 10145.6
  decouwa W40 OnePco-rl 81.4
  decf be rfp 32040.2
  decf 35088 rll 24466.7
  decf 35088 rfp1 24466.7
  pwk 9.100 wc FLOT 250.0
  jlab HMC 146.0 wc 200.0
  jlab ADIABATIC vs 2137
  pwk180ad OneProbe-1 ch 2
  pwk180ad ad100 at cdc av
  pwk180 400.0

```



exp46 gnmvslab

ACQUISITION ARRAYS

array	phase
arraydim	1024
phase	1
	2

F2  
(ppm)

0.8  
1.0  
1.2  
1.4  
1.6  
1.8  
2.0  
2.2



# Figure S24 FABMS of 4

[ Elemental Composition ]  
Data : 1601030  
Sample: 117D-1 C133-4-IX  
Note : Matrix; NBA  
Inlet : Direct  
RT : 7.66 min  
Elements : C 30/20, H 35/25, N 3/0, O 6/0  
Mass Tolerance : 20ppm, 1mmu if m/z > 50  
Unsaturation (U.S.) : -1.0 - 30.0

Date : 12-Jan-2016 16:47

Page: 1

Ion Mode : FAB+  
Scan#: (40,45)

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
398.2332	100.0	+0.1 / +0.0	9.5	C 24 H 32 N O 4

