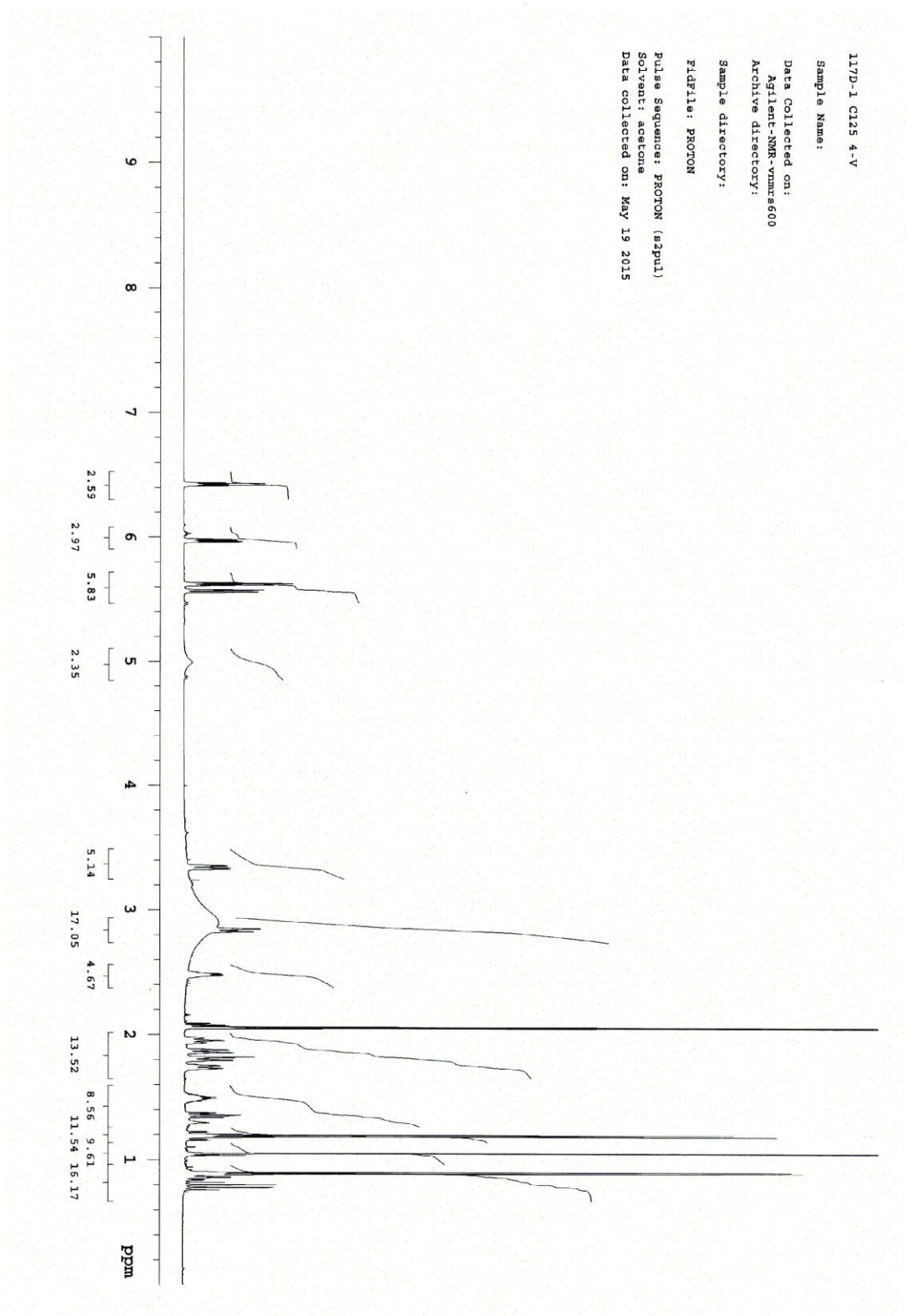
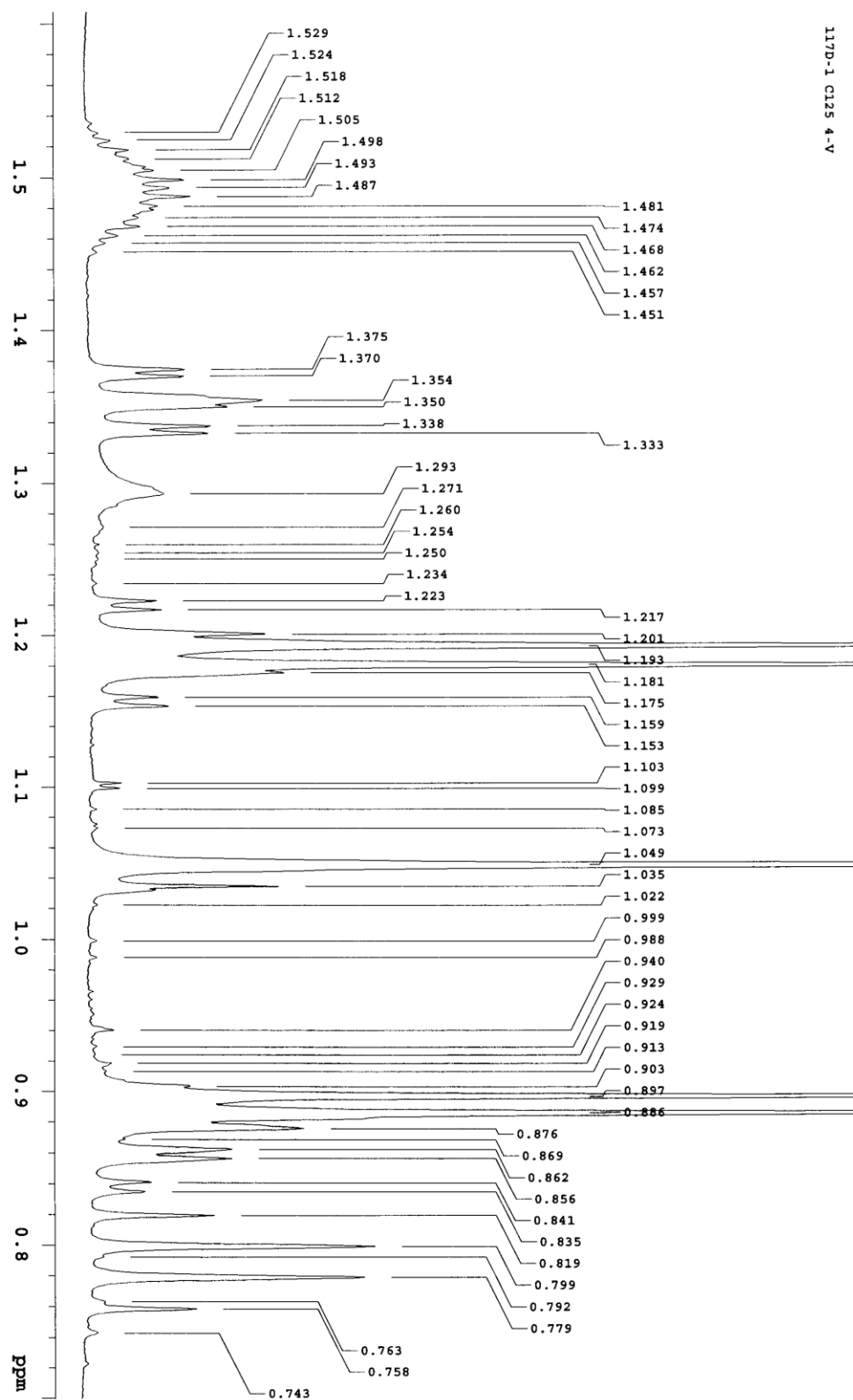
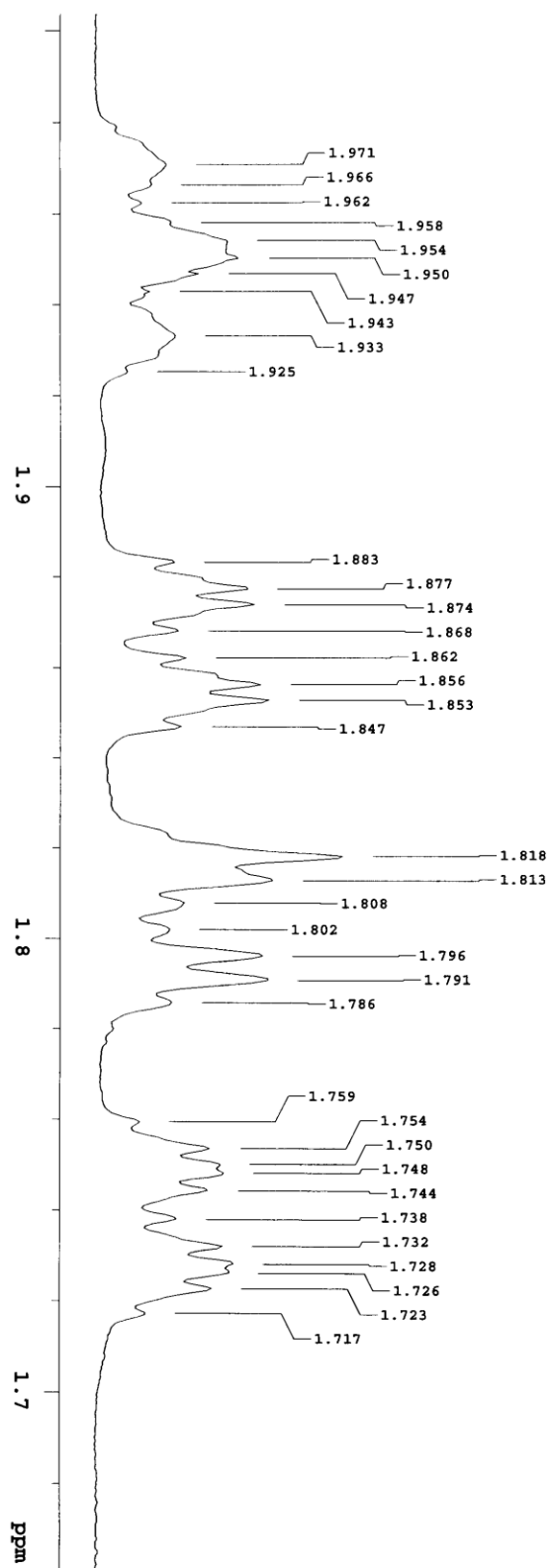
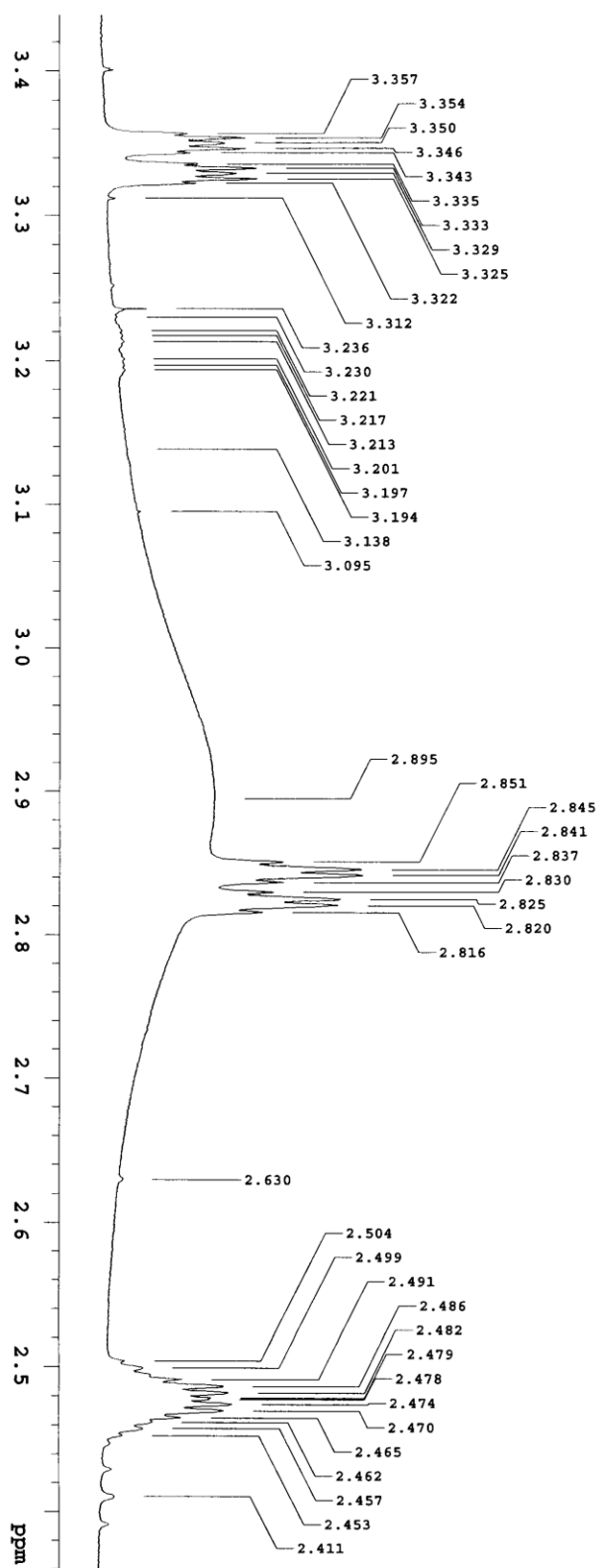


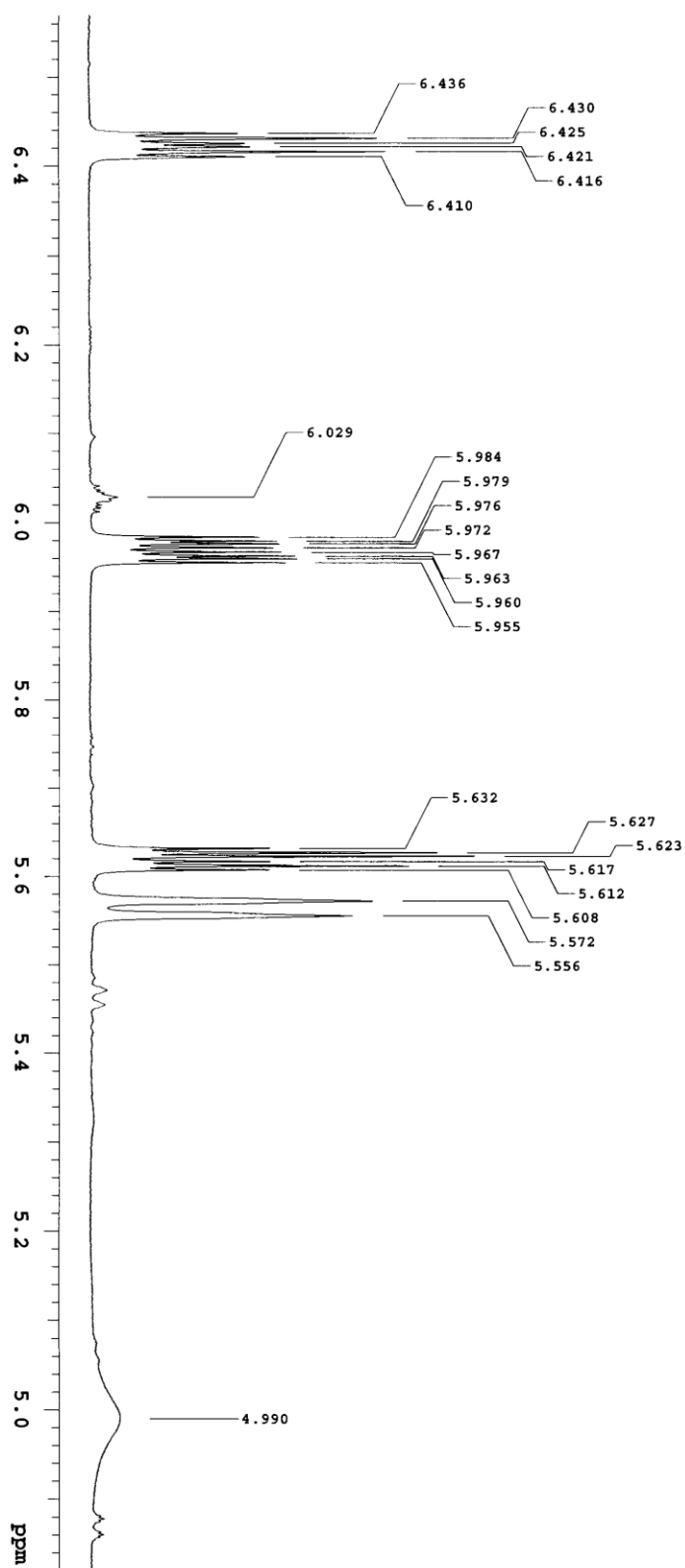
Figure S13  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra in acetone- $d_6$  of **3**











117D-1 CH25 4-V

Sample Name:

Data Collected on:

Agilent-NMR-vnmrse600

Archive directory:

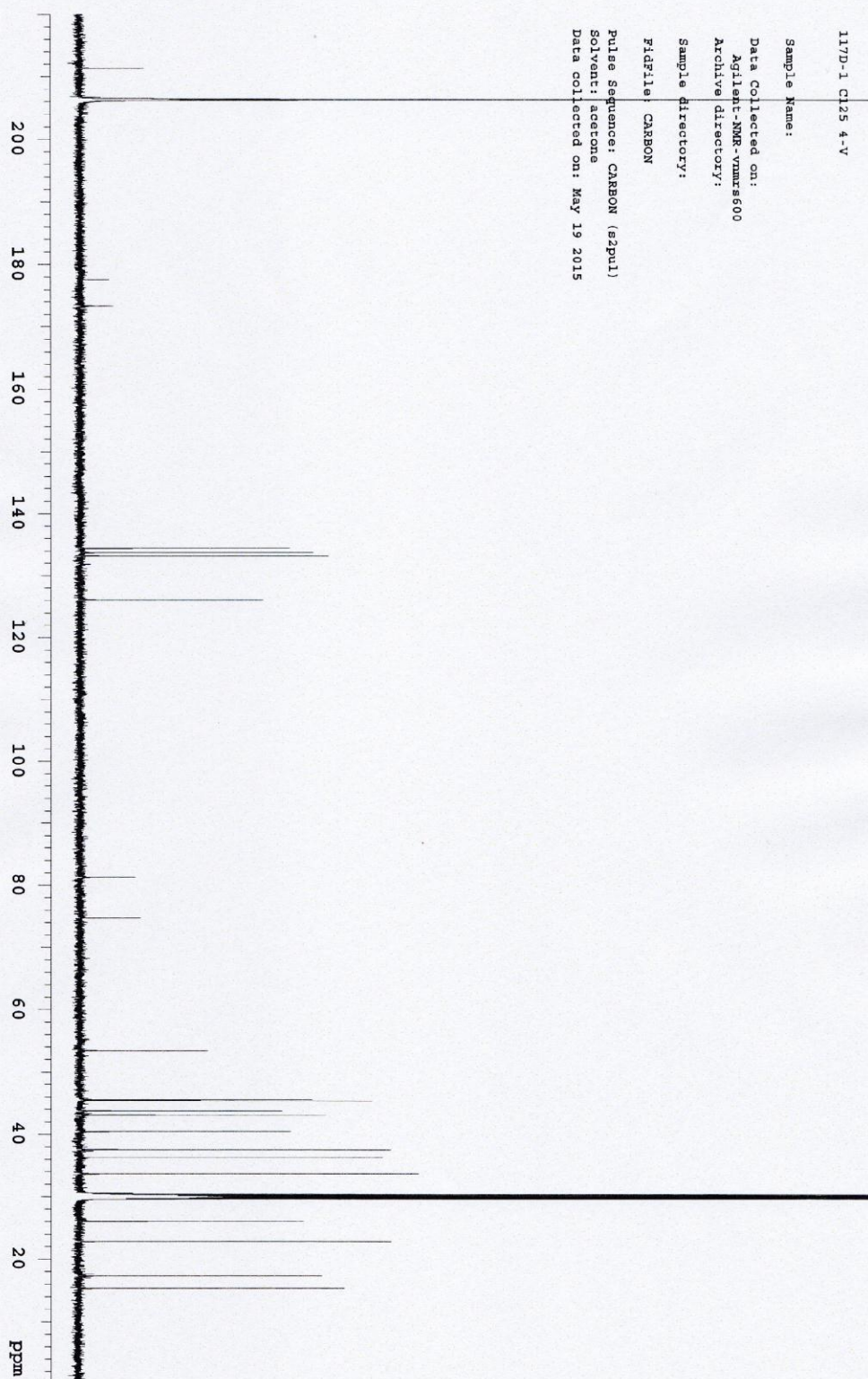
Sample directory:

F1DFile: CARBON

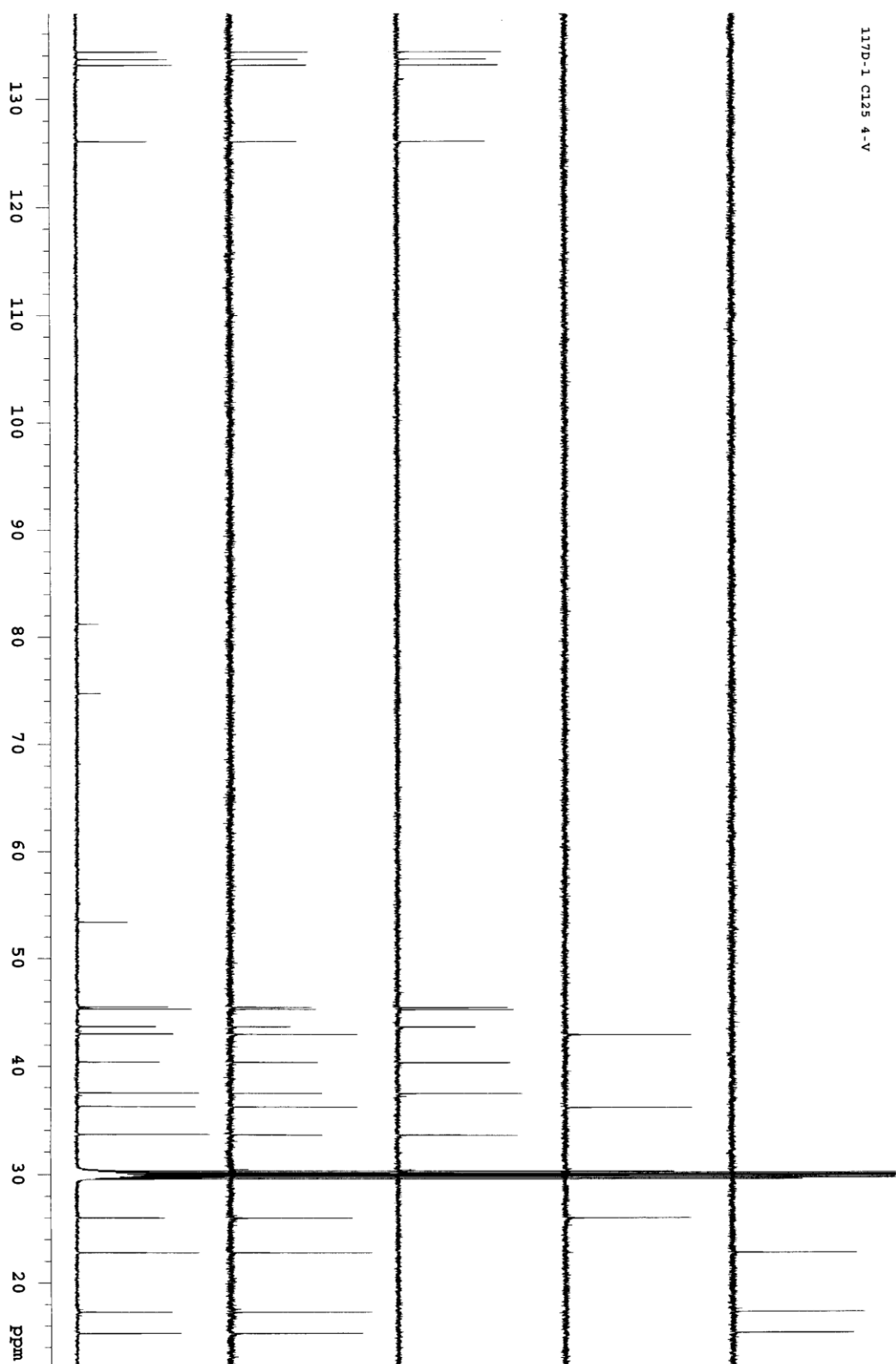
Pulse Sequence: CARBON (szpul)

Solvent: acetone

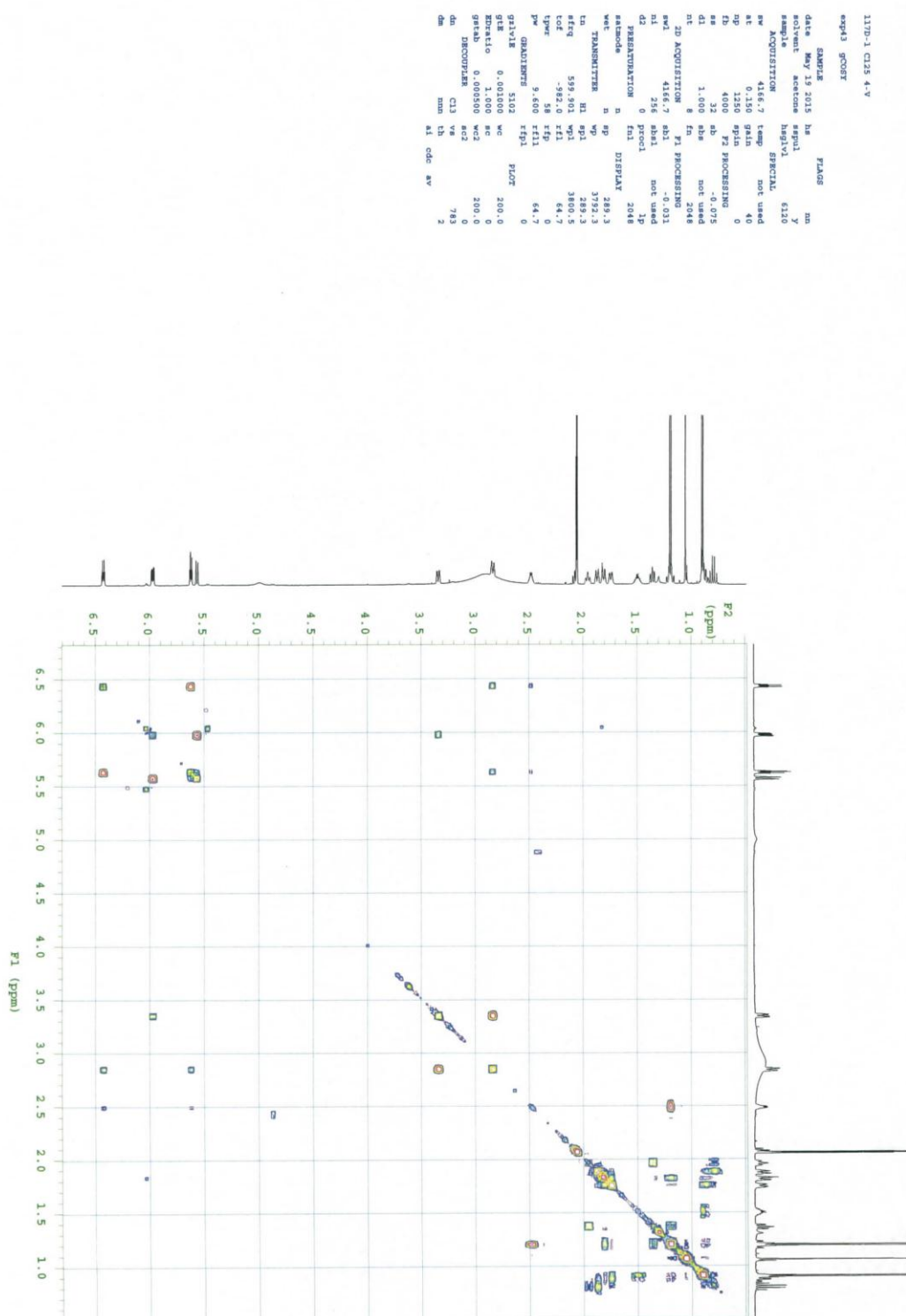
Data collected on: May 19 2015



117D-1 C125 4-V



**Figure S14**  $^1\text{H}$ - $^1\text{H}$  COSY of **3**



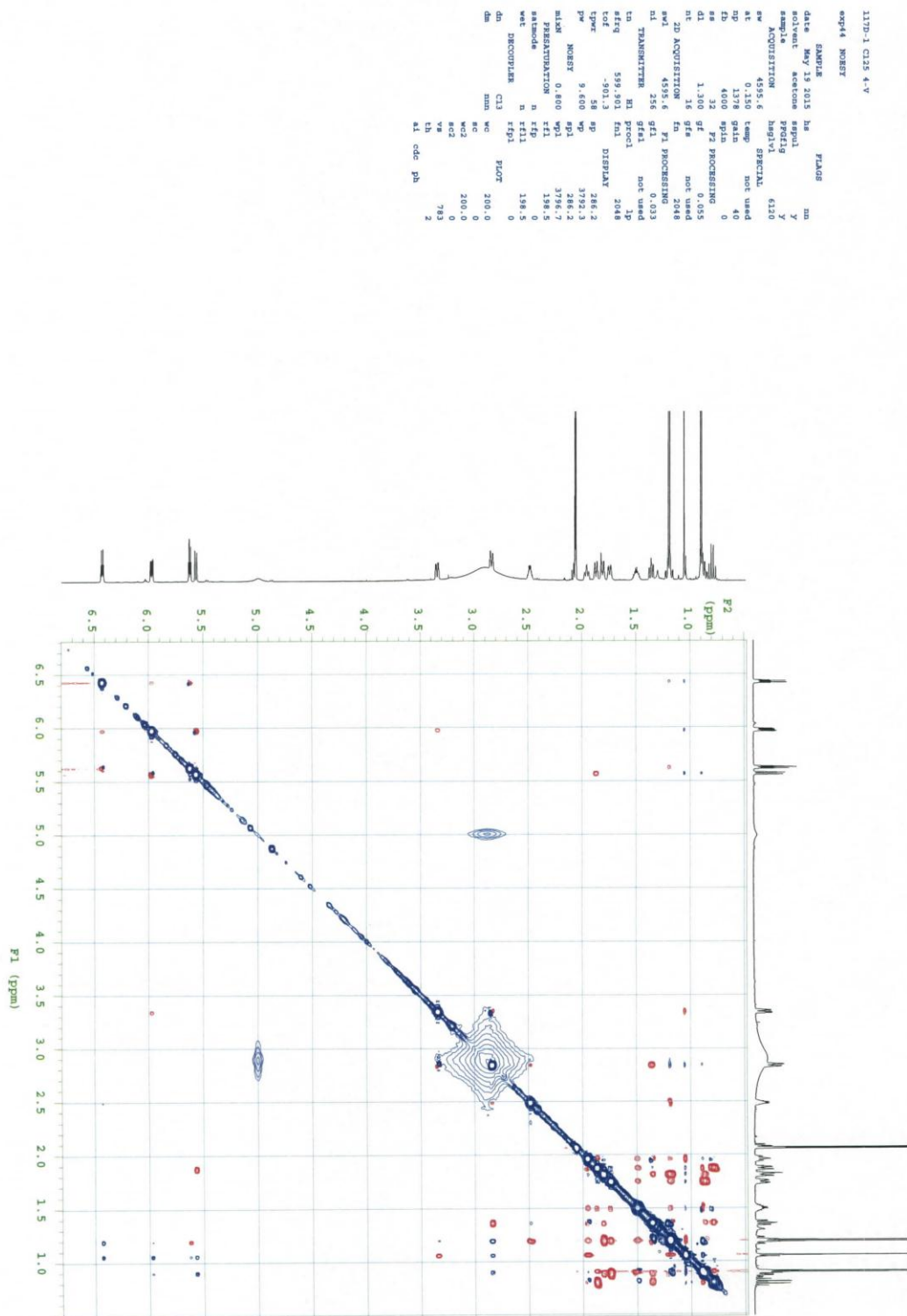


exp43 gcosy

a1 cdc av



Figure S15 NOESY of 3



117D-1 C125 4-V  
exp4 NOESY

SAMPLE		FLAGS	
date	May 19 2015	hs	mn
solvent	acetone	sepal	y
sample	pyridig	y	
sample	bag1v1	6120	
ACQUISITION			
ac	4595.6	SPECIAL	not used
at	0.150	temp	not used
az	0.125	spin	not used
fb	4000	sp12	40
ss	32	P2 PROCESSING	0
d1	1.300	gfe	0.055
nt	16	gfe	not used
2D ACQUISITION			
sw1	4595.6	F1 PROCESSING	2048
nl	256	gfe1	0.033
tl	TRANSMITTER	gfe1	not used
tr	MI	prec1	1p
efrq	599.901	fm1	DISPLAY 2048
tofr	-901.3	sp	380.5
upwr	13.545	wp1	950.0
pw	9.600	wp1	380.5
mlsm	0.800	wp1	911.0
PRESATURATION			
satmode	n	rfg	198.5
wet	n	rfg1	0
decoupler	n	rfg1	198.5
dm	C13	PLOT	200.0
dm	nm	wc	200.0
ac	0	wc2	200.0
wd	0	wd2	785
vb	2	vb	2
al	cdc	ph	

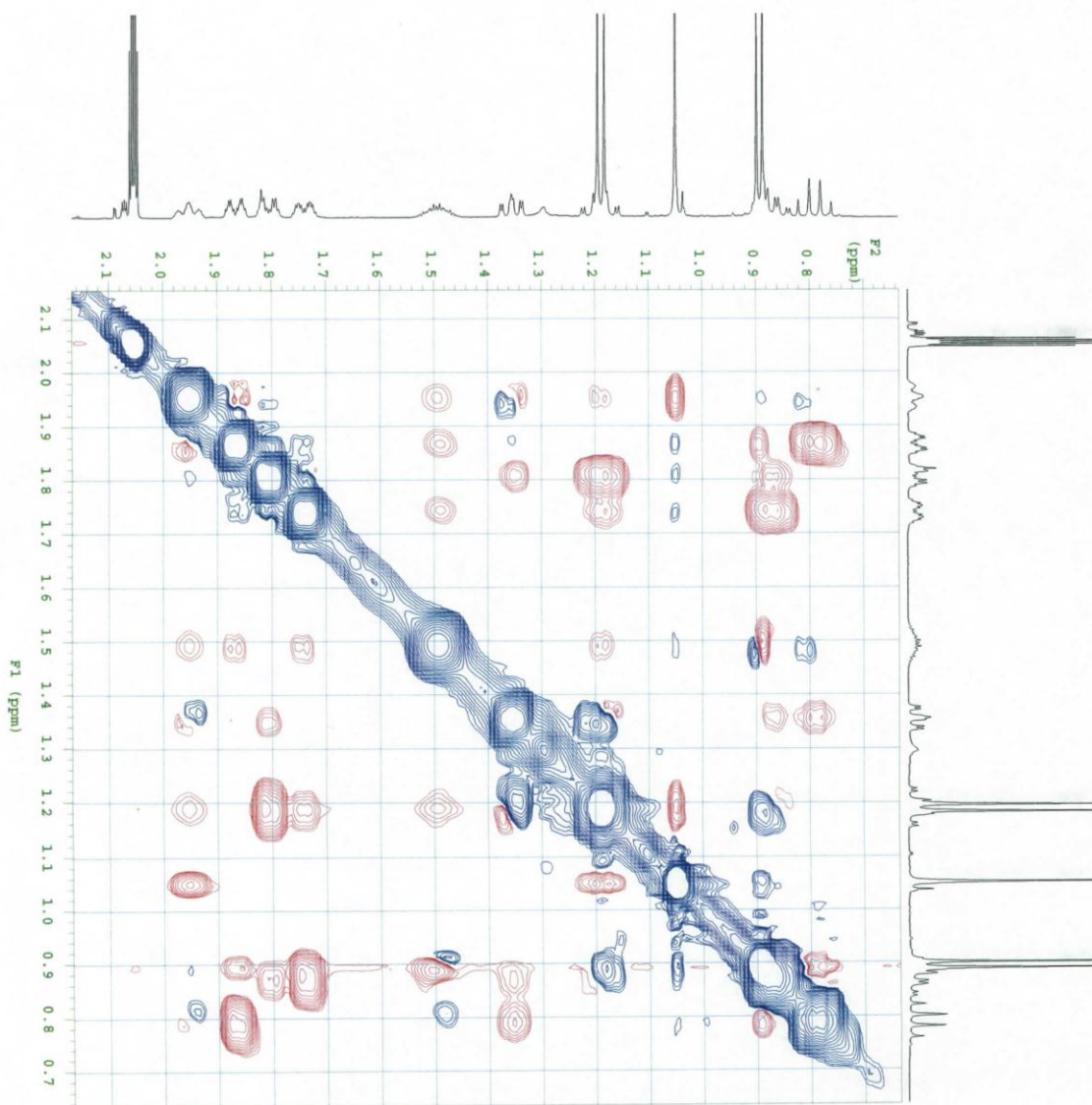
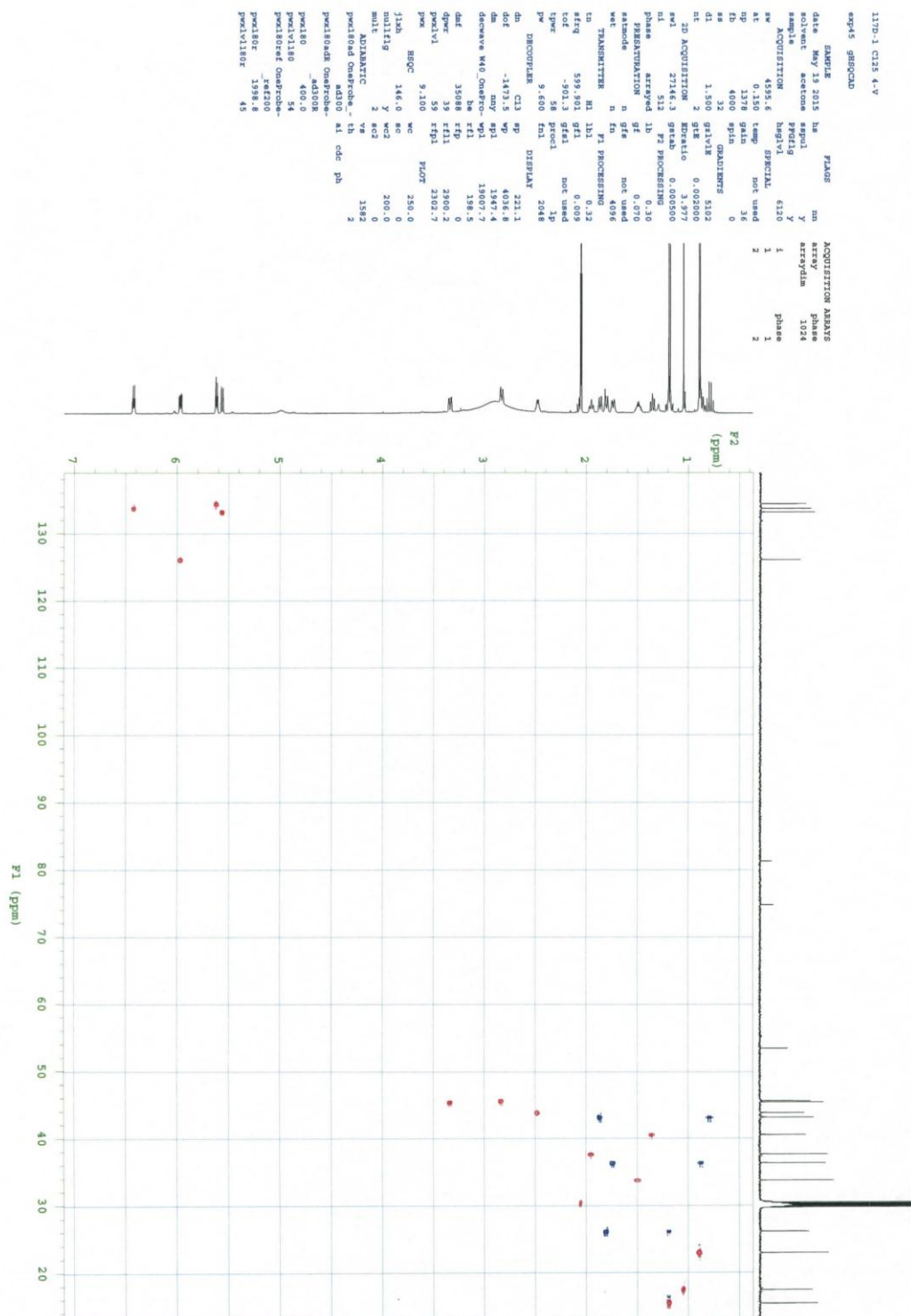
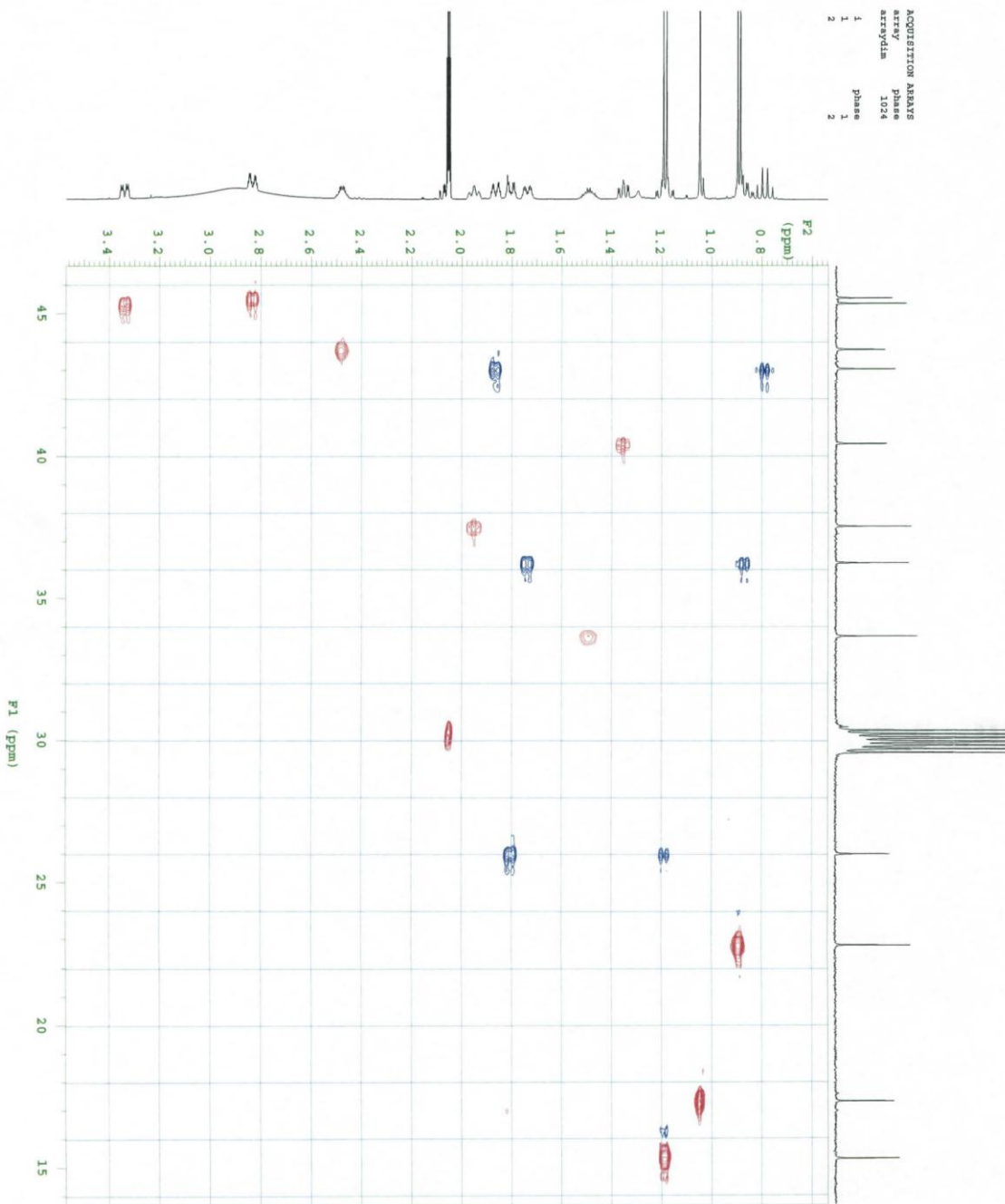


Figure S16 HMQC of 3



117D-1 C125 4-V  
exp45 ghsocld

SAMPLE		FLAGS		ACQUISITION ANALYSIS	
date	May 15 2015	hs	nm	array	phase
solvent	acetone	suppl	y	arraydim	1024
sample	pyridine	proflg	y		
ACQUISITION	hsq1v1	6120	1	phase	1
nr	4595.6	temp	not used	1	2
ac	0.150	spin	36		
dp	0.150	spin	36		
fs	4000	spin	36		
ss	32	GRADIENTS	0		
dl	1.500	gr1v1e	5102		
nt	2	gr2	0.002000		
2D ACQUISITION	Hdratio	3.977			
sv1	27146.3	gr2ab	0.000500		
nl	512	F2 PROCESSING	0.30		
phase	arrayed 1b	gr	0.070		
PRESENTATION	gr	not used			
atmode	n	gr	not used		
wt	TRANSMITTER	n	4096		
to	0.150	F1 PROCESSING	0.32		
afreq	559.901	gr1	0.009		
tot	-901.3	gr1	not used		
lpr	58	procl	1p		
pw	9.600	fn1	2048		
DECOMPOSE					
dh	C13	sp	322.1		
dof	-1473.5	wp	1819.8		
dm	any	sp1	2053.5		
decawa	W40	Qnsrco	4983.9		
def	3508.0	he	188.5		
dpr	39	ft1	2880.2		
psk1v1	55	rfp1	2382.7		
pw	9.100	wt	250.0		
HQC					
j1kh	146.0	ac	0		
nullf1g	y	wc2	200.0		
mult	2	ac2	0		
ADDITIONAL					
psk180ad	Qnsrco	th	1582		
psk180ad	Qnsrco	th	2		
psk180	400.0				
psk1v1180	54				
psk180ref	Qnsrco				
psk180c	1398.8				
psk1v1180c	45				





[illegible]







**Figure S18 FABMS of 3**

[ Elemental Composition ] <sup>22</sup>  
Data : 1506059 Date : 10-Jun-2015 15:54 Page: 1  
Sample: 117D-1 C125-4-V  
Note : Matrix; G  
Inlet : Direct Ion Mode : FAB+  
RT : 8.41 min Scan#: (27,32)  
Elements : C 30/17, H 32/22, N 3/0, O 6/0, Na 1/0  
Mass Tolerance : 20ppm, 1mmu if m/z > 50  
Unsaturation (U.S.) : -1.0 - 50.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
392.1839	37.4	+0.4 / +0.2	9.5	C 22 H 27 N O 4 Na

