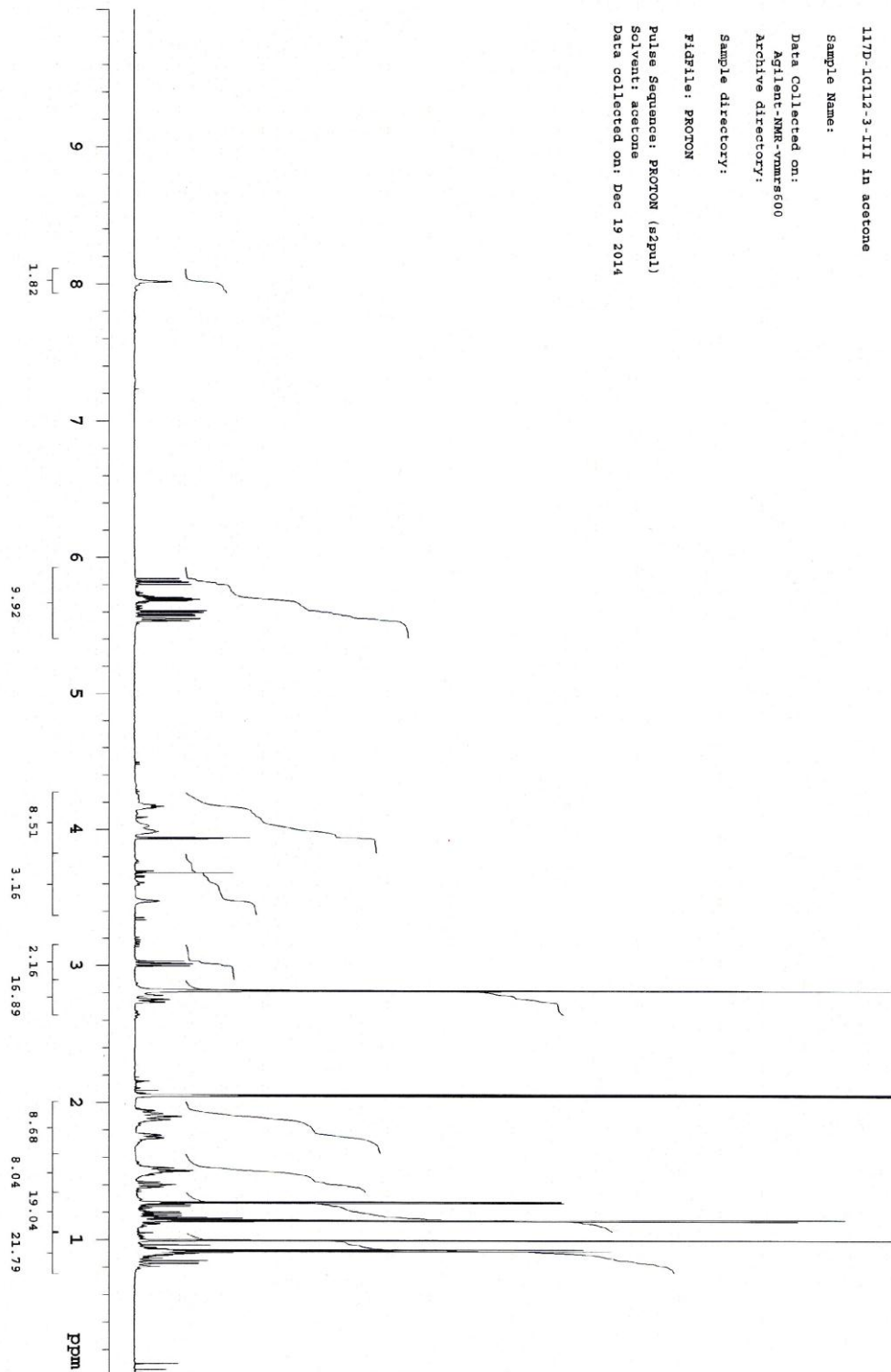
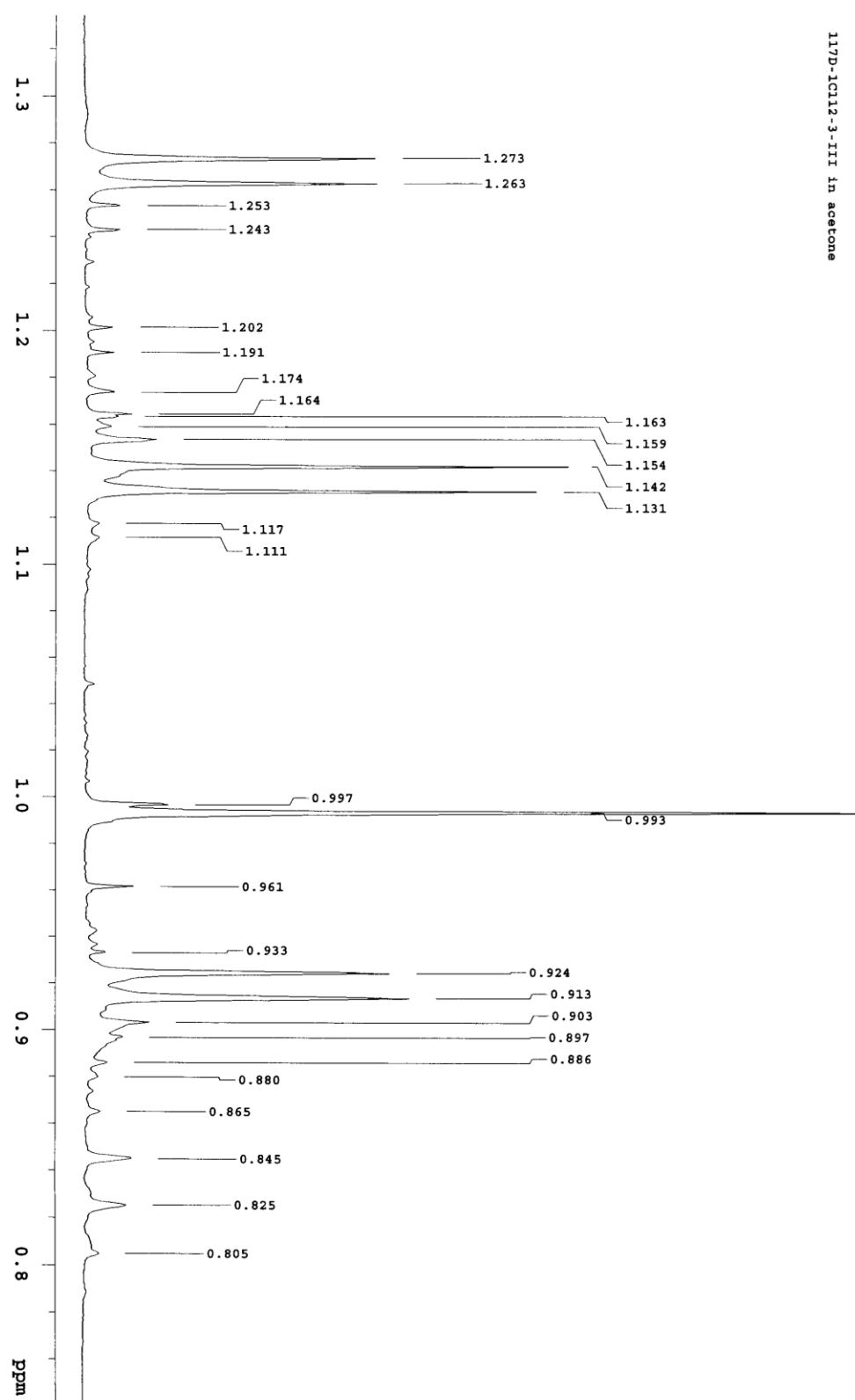
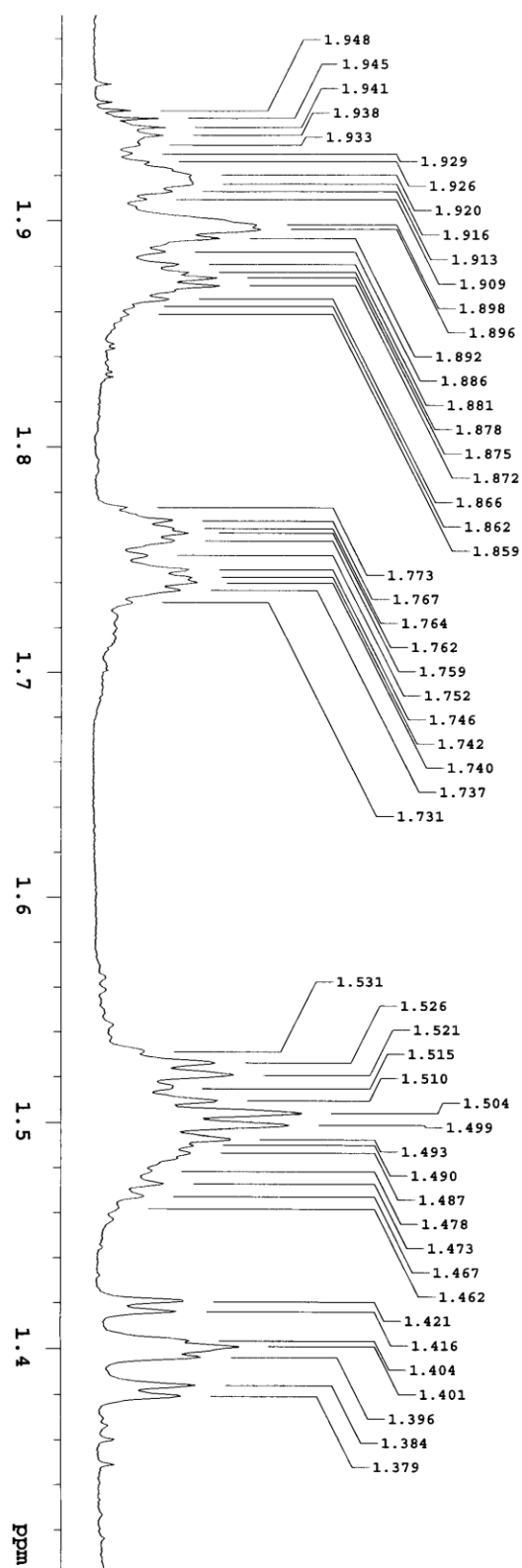
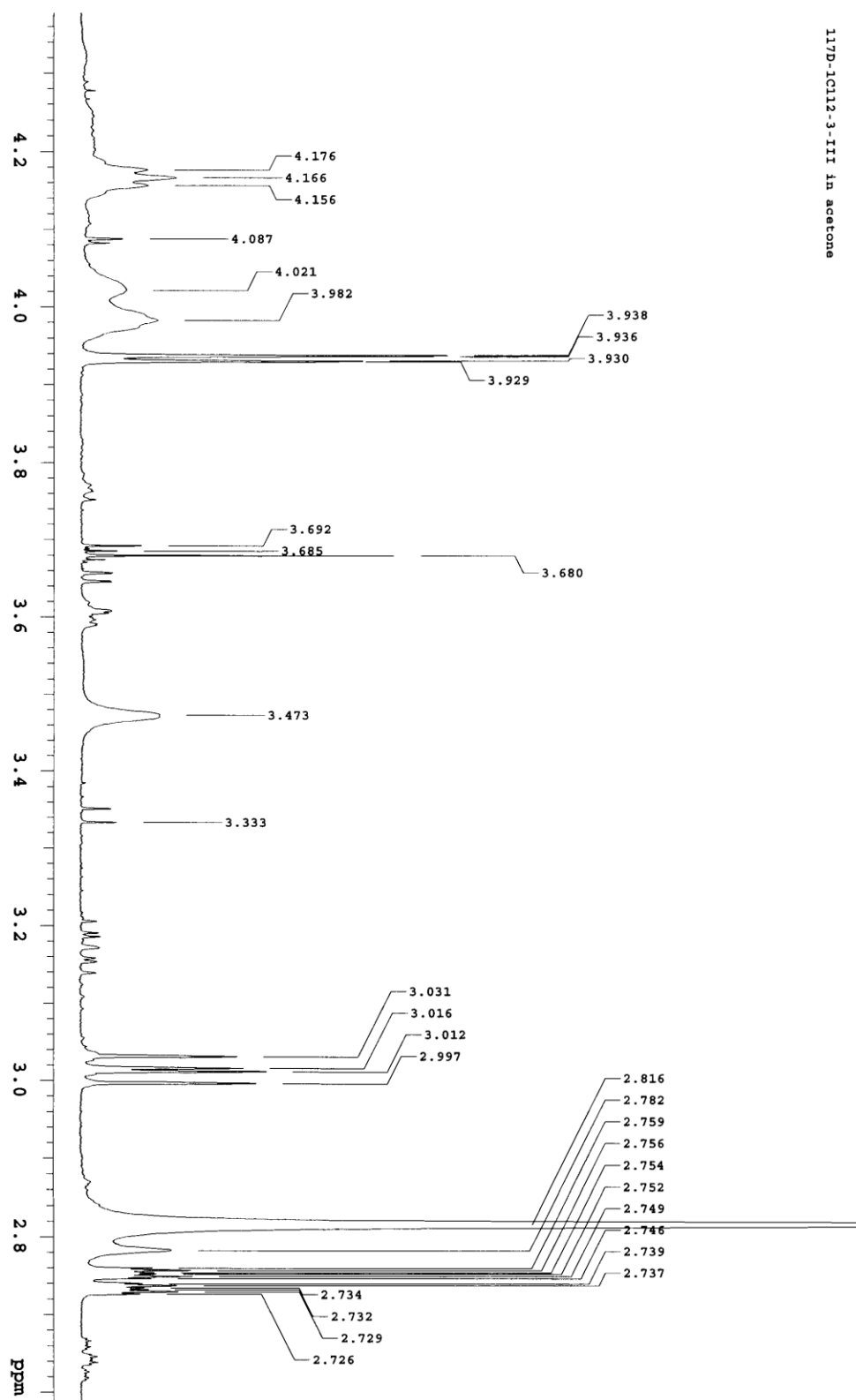


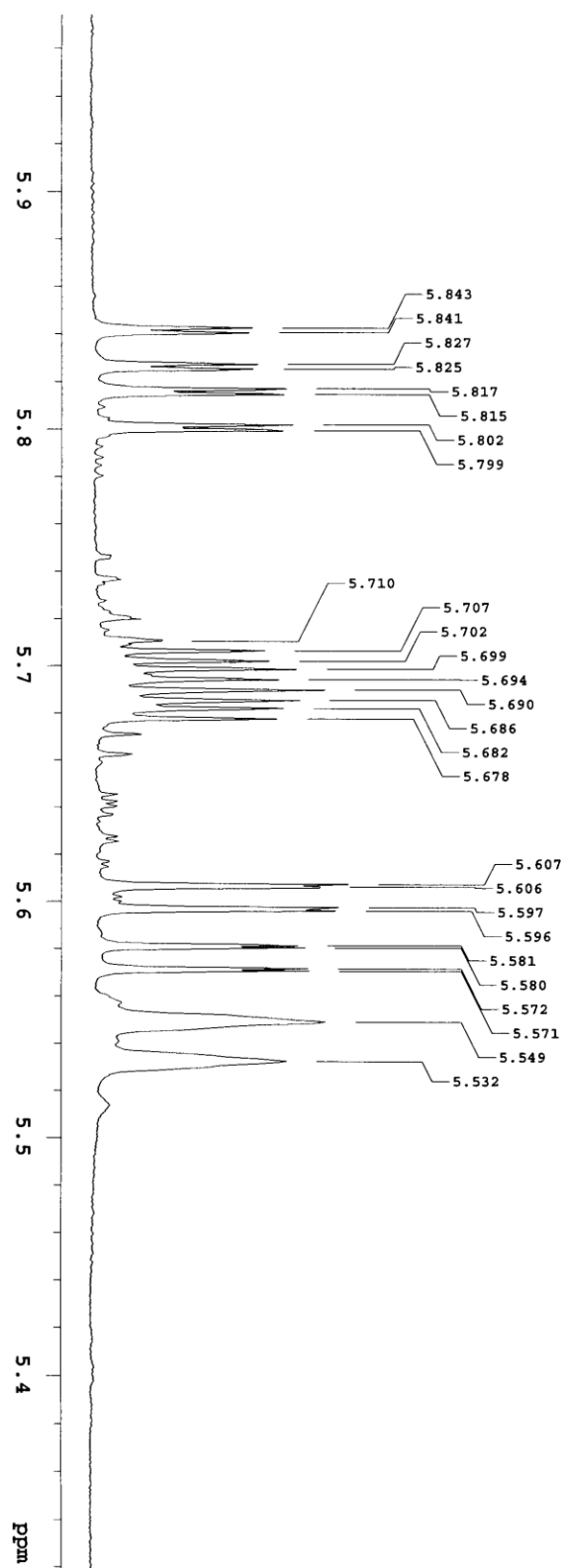
Figure S7 ^1H and ^{13}C NMR spectra in acetone- d_6 of **2**











117D-IC12-3-III

Sample Name:

Data Collected on:

Agilent-NMR-vnmr600

Archive directory:

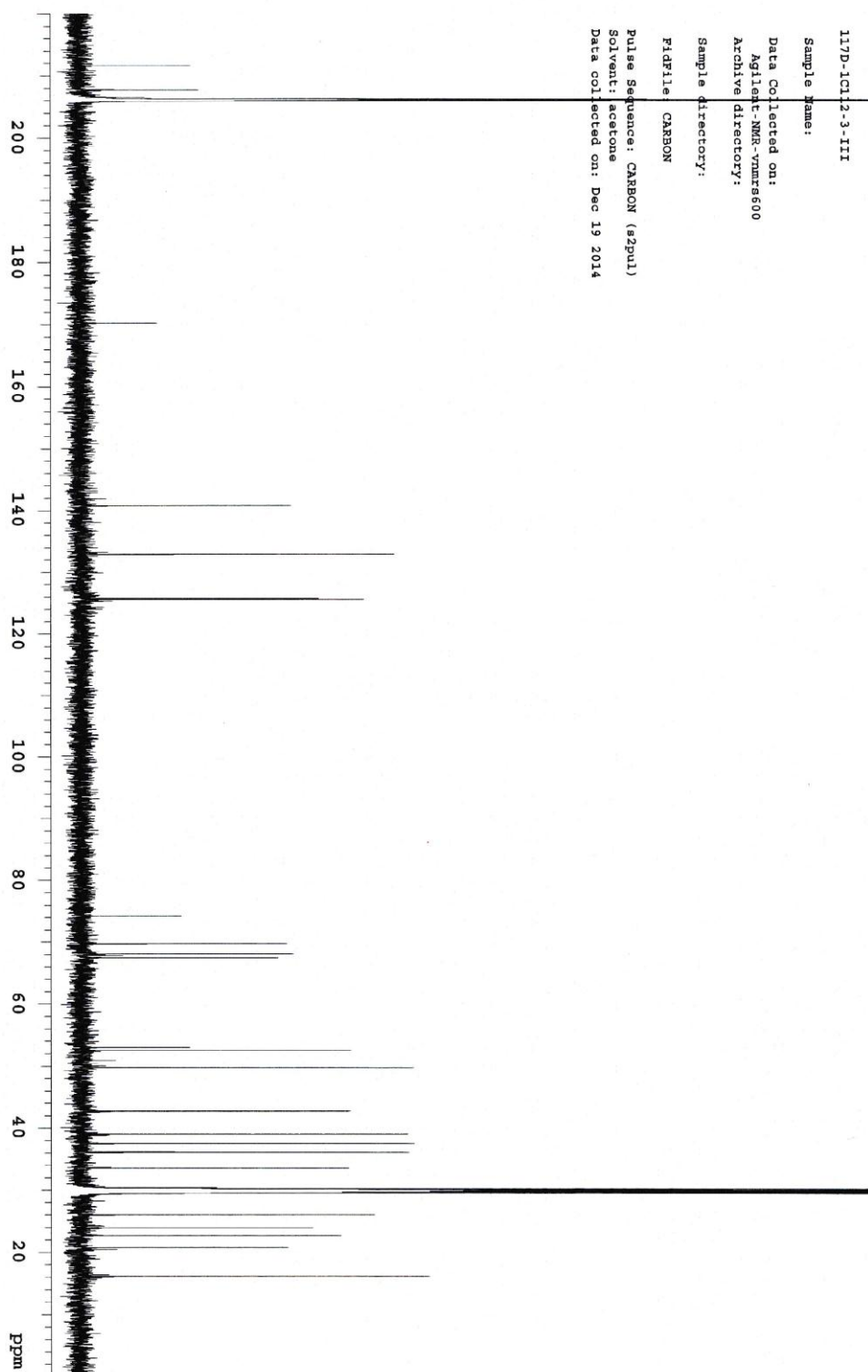
Sample directory:

F14F116 CARBON

Pulse Sequence: CARBON (s2pul1)

Solvent: acetone

Data collected on: Dec 19 2014



117D-1C112-3-III

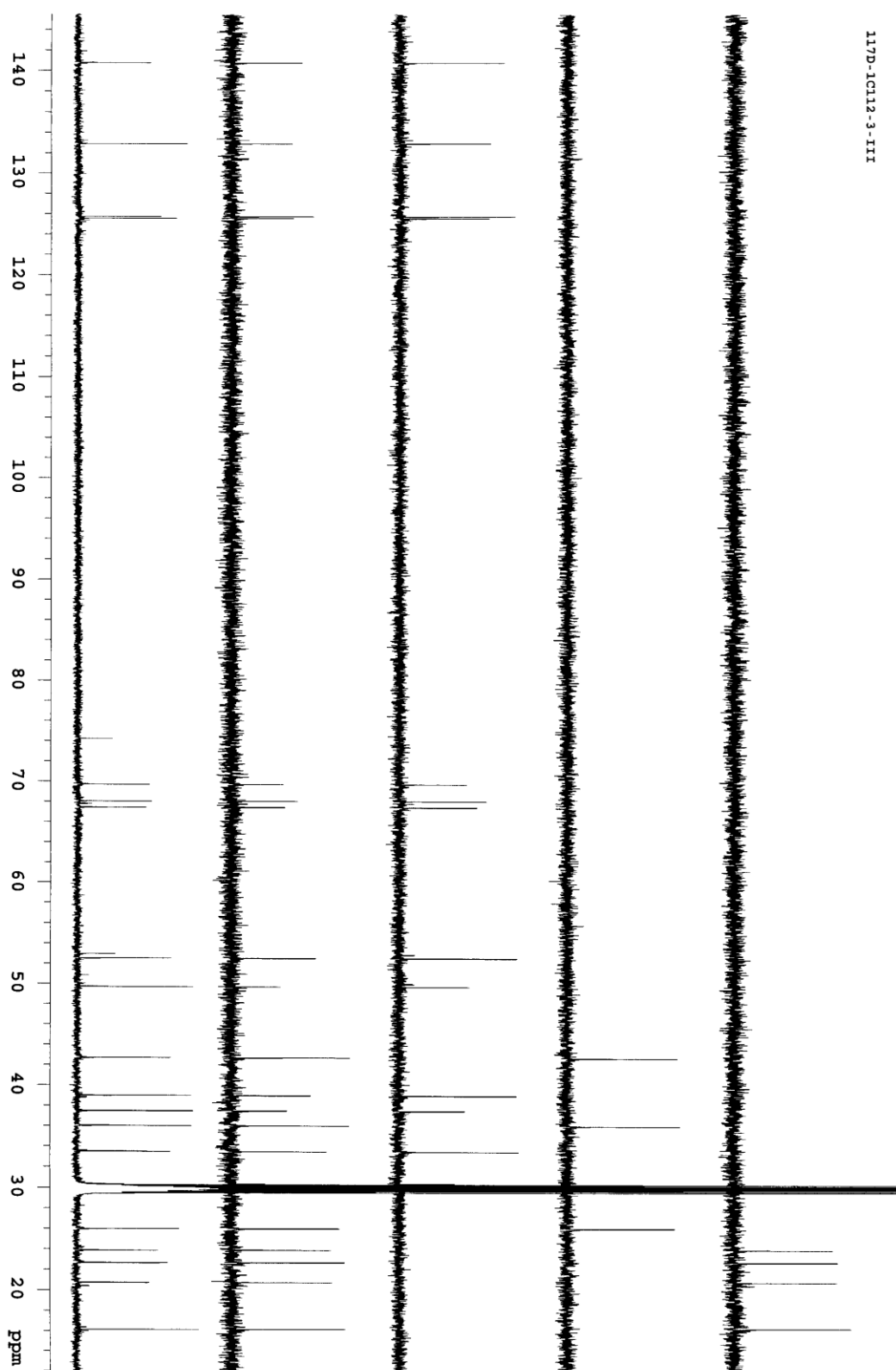
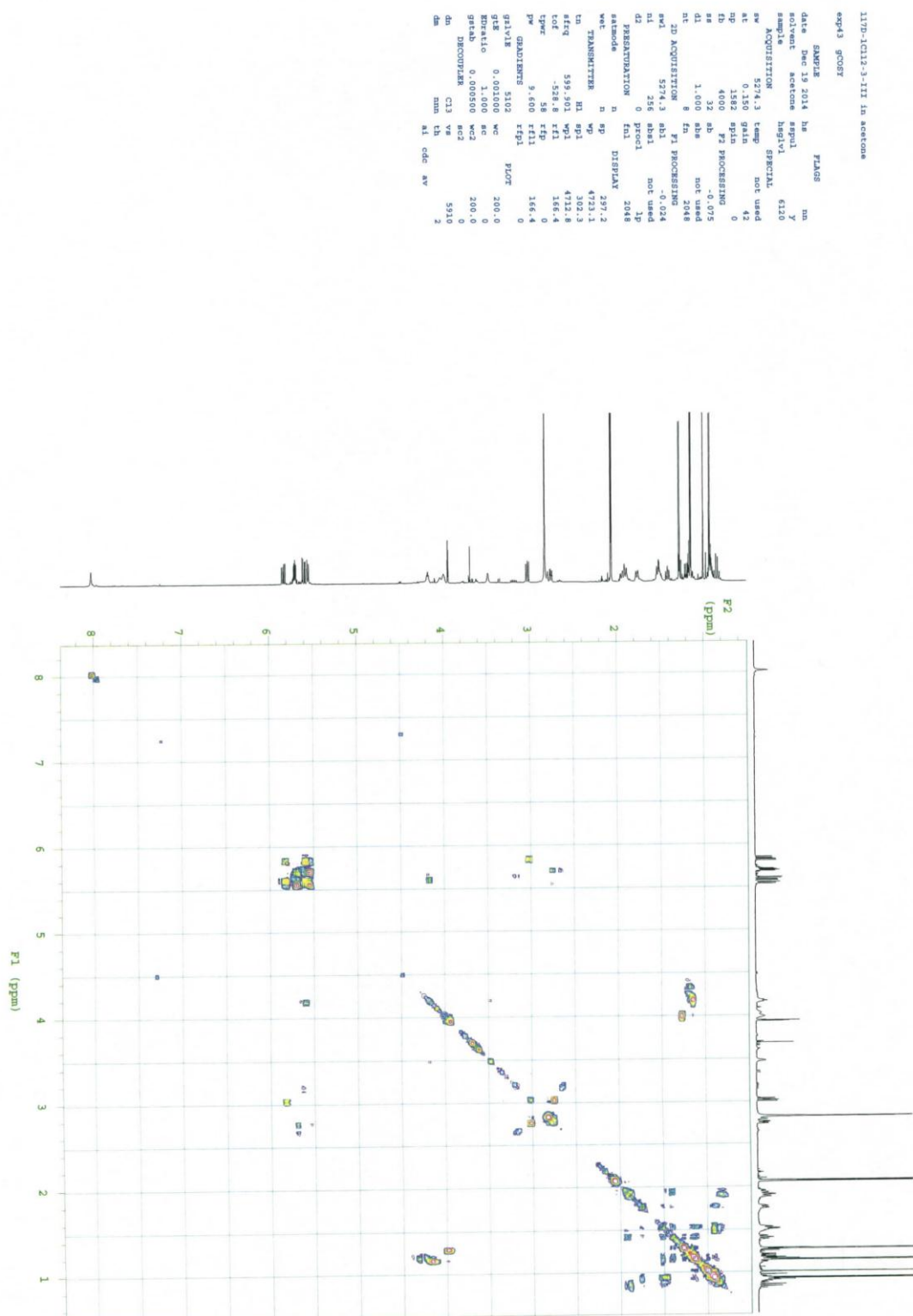


Figure S8 ^1H - ^1H COSY of 2




```

117D-1C112-3-III in acetone
exp43 gcosy

SAMPLE          FLAGS
date    Dec 19 2014   hs      mn
solvent  acetone      sepul   y
sample   hsglv1       6120
ACQUISITION SPECIAL
ac       5274.3 temp  not used
at       0.150 gain   42
ap       1582 spin    0
da       4000 f2 PROCESSING
de       1.000 ab     not used
di       1.000 sbc    2048
nt
2D ACQUISITION 8 f1 PROCESSING
sw1      5274.3 sb1   -0.024
nl       256 sbal   not used
d1       0 p1001    1p
PRESATURATION 0 fml
satmode   n      DISPLAY 2048
wet        n      369.3
tu TRANSMITTER n1 wp 1025.0
tcf4      559.8304 374.4
tcf4      -528.8 f1 202.4
tprc      9.600 rfp 166.4
pw GRADIENTS 5102 rfp1 0
gvlr      0.001000 wc PLOT 250.0
gpratio   1.000 sc 0
gprab     0.000500 wc2 200.0
DRCOMPLER C13 vs 0
da      nm th 5910 2
at cdc av

```

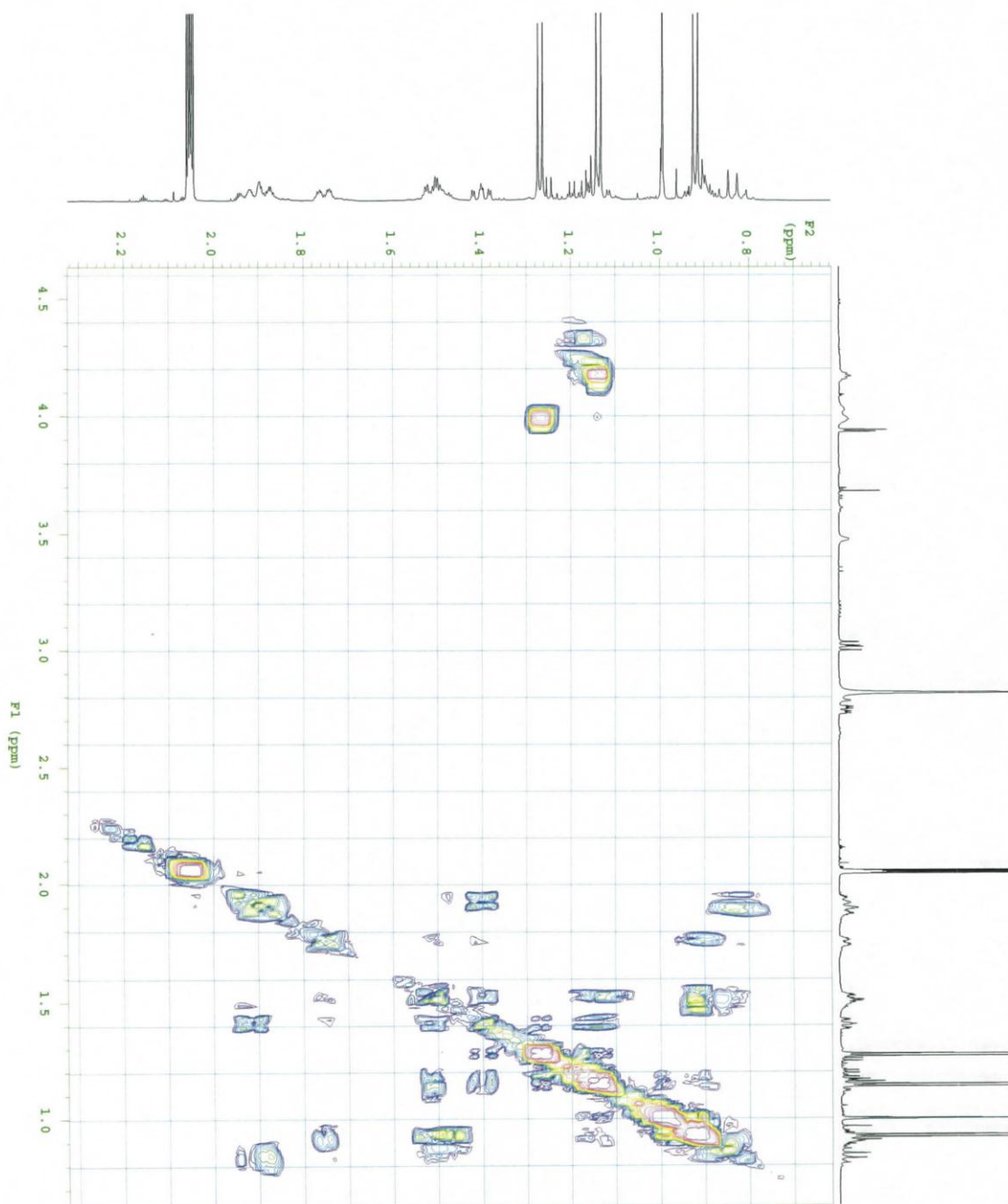
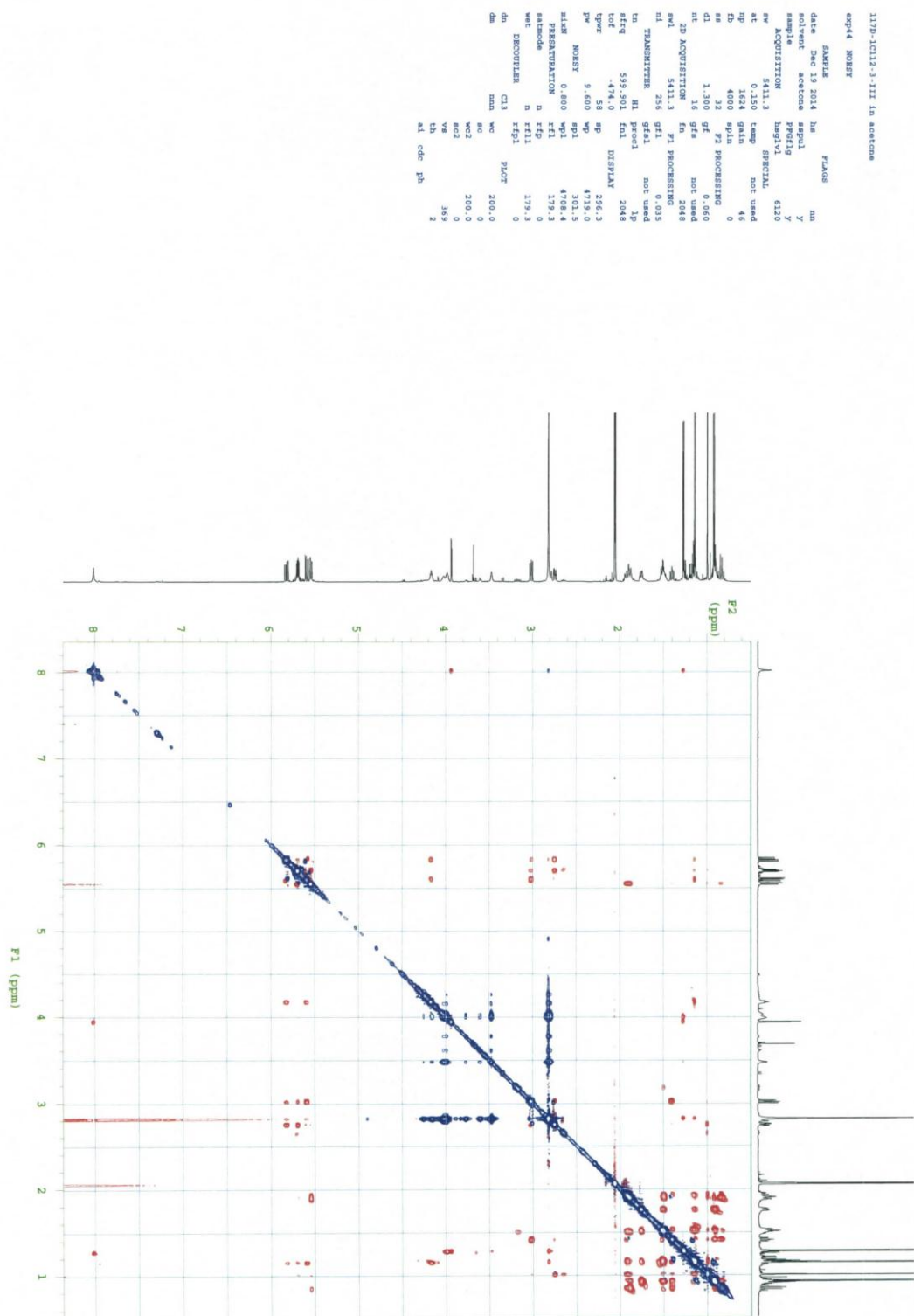


Figure S9 NOESY of **2**

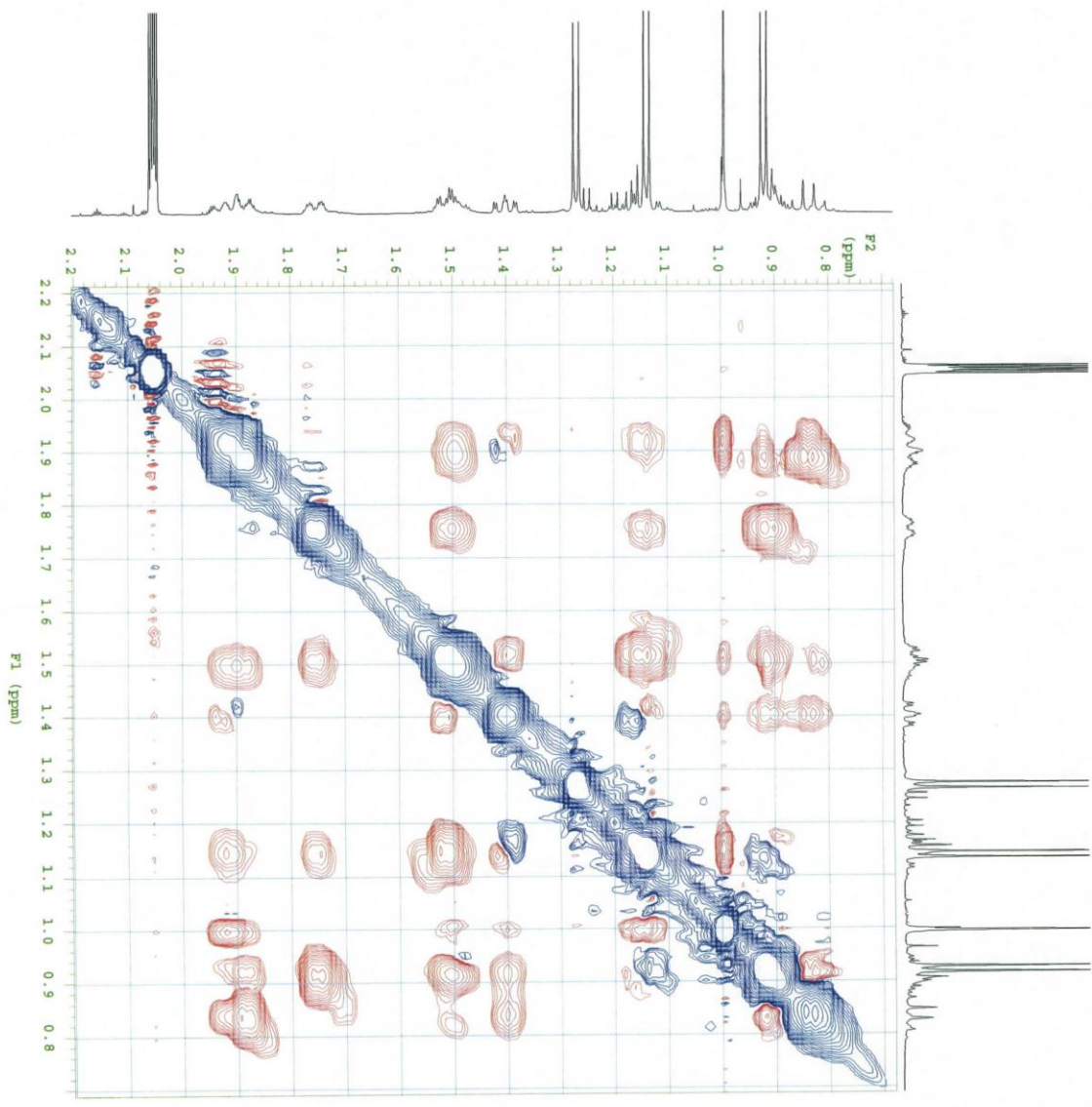


```

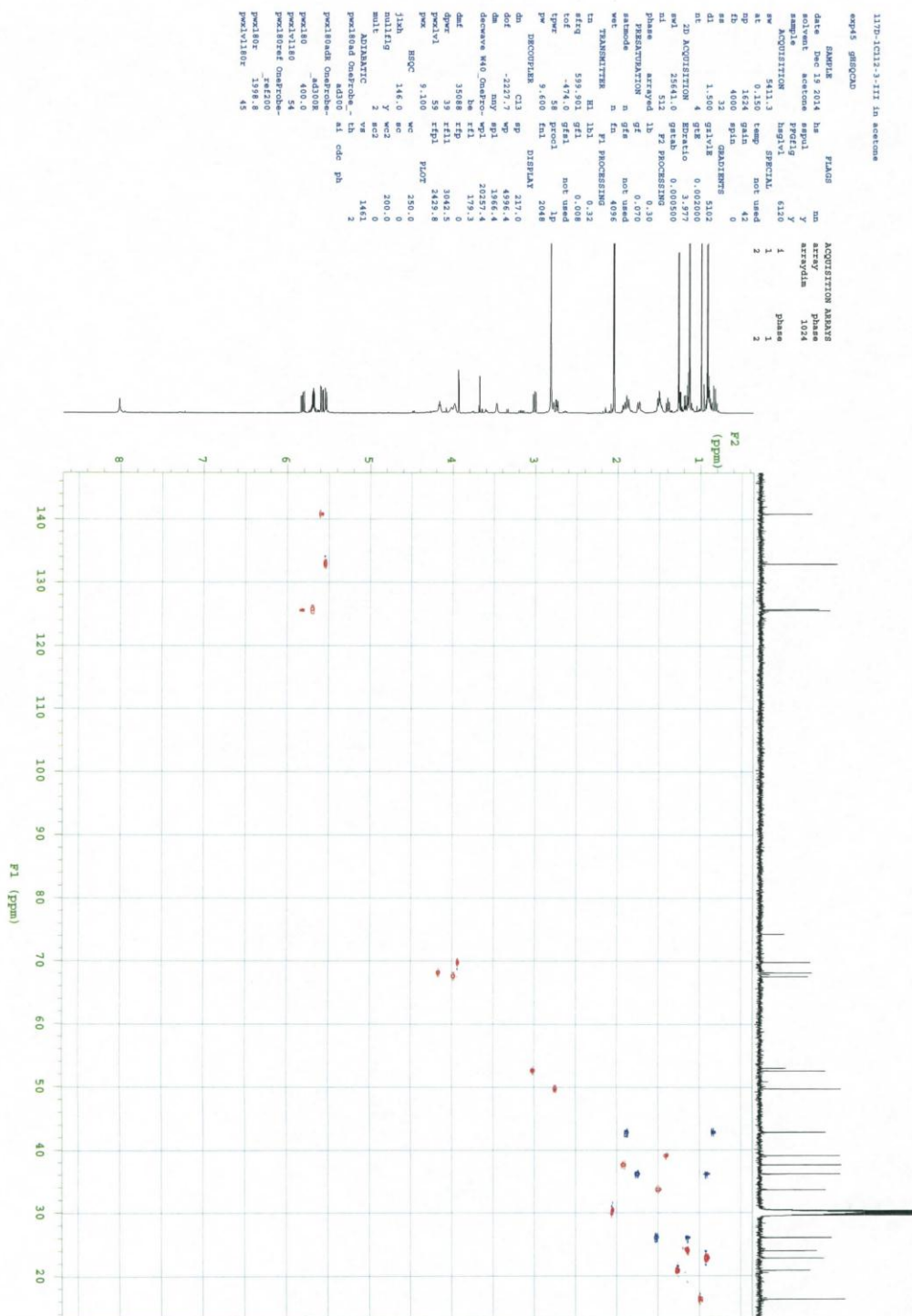
117D-1C112-3-III in acetone
exp44 NOESTY

SAMPLE
date Dec 19 2014 ha
solvent acetone sepul
sample y
PRODIG 6120
ACQUISITION
sw 5411.3 SPECIAL
at 0.150 temp not used
rp 1624 gain 46
fs 4000 spin 0
ns 32 F2 PROCESSING 0
al 1.310 gfa 0.060
nt 16 ffe not used
2D ACQUISITION f2 2048
sw1 5411.3 F1 PROCESSING
n1 256 gfa 0.035
TRANSMITTER
tn 256 gfa1 not used
rfq 599.901 fml 1p
tof -474.0 DISPLAY
tprc 58 sp 407.2
pw 9.600 wp 914.2
mz 0.800 ep1 412.5
PRESENTATION n f1 324.2
satmode n rfi 179.3
wet n rfi1 179.3
DECOMPOSE n fpl 0
dm nm PLOT 200.0
wc sc 0
sc2 200.0
vr 0
th 369
al cdc ph 2

```



36

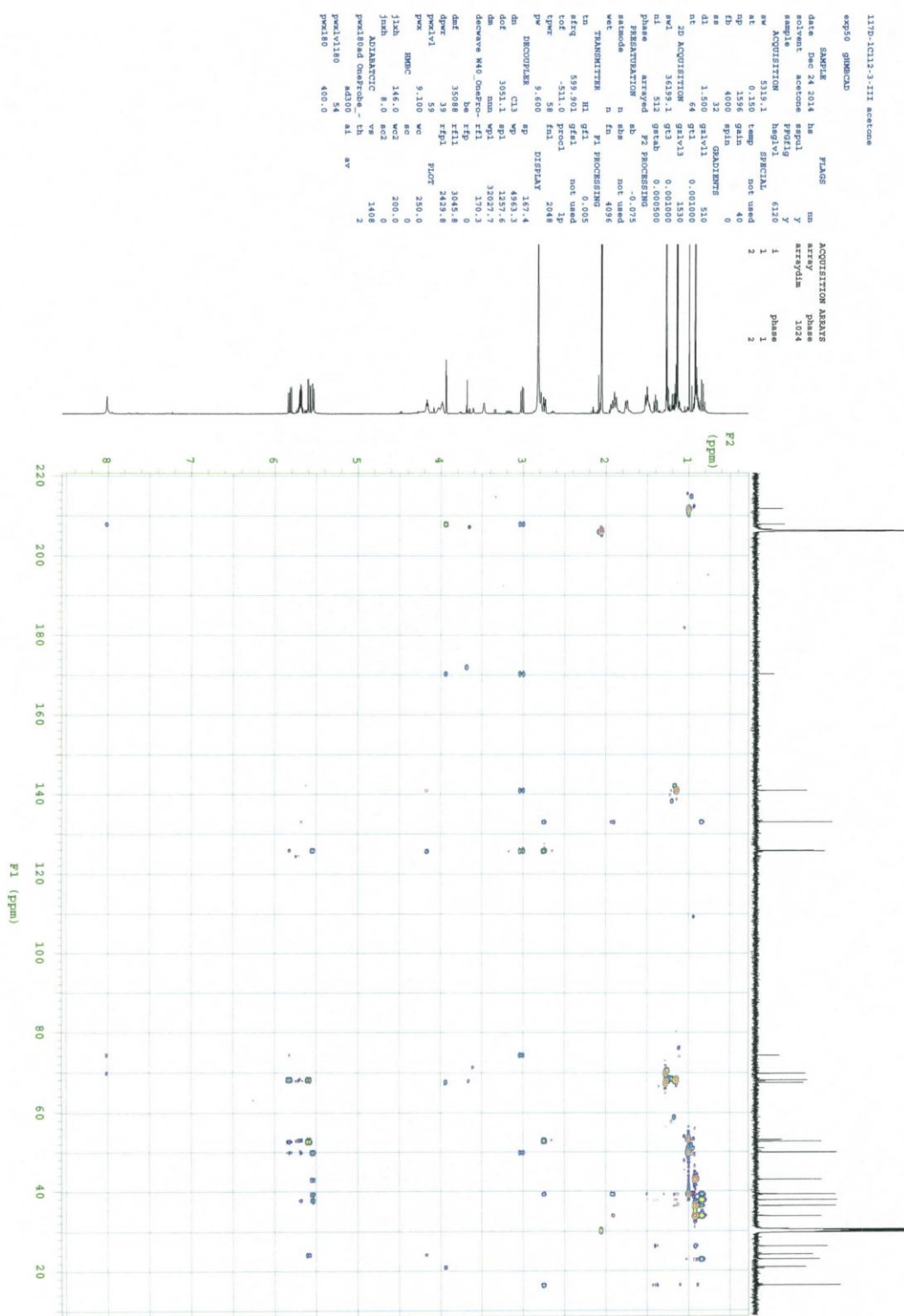


exp45 ghsqcad

pwslv1180f 45



Figure S11 HMBC of **2**



exp50 gmbcad

pxxl80 400.0



Figure S12 FABMS of 2

[Elemental Composition] ²

Page: 1

Data : 1503094 Date : 12-Mar-2015 15:41
Sample: 117D-1C112-3-III
Note : Matrix; G
Inlet : Direct Ion Mode : FAB+
RT : 6.33 min Scan#: (23,28)
Elements : C 28/20, H 38/30, N 3/0, O 7/0, 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
416.2430	80.6	-1.6 / -0.7	8.5 C 24 H 34 N O 5
		-2.2 / -0.9	10.0 C 25 H 33 N 2 O 2 Na
438.2263	59.4	+1.5 / +0.7	8.5 C 24 H 33 N O 5 Na

