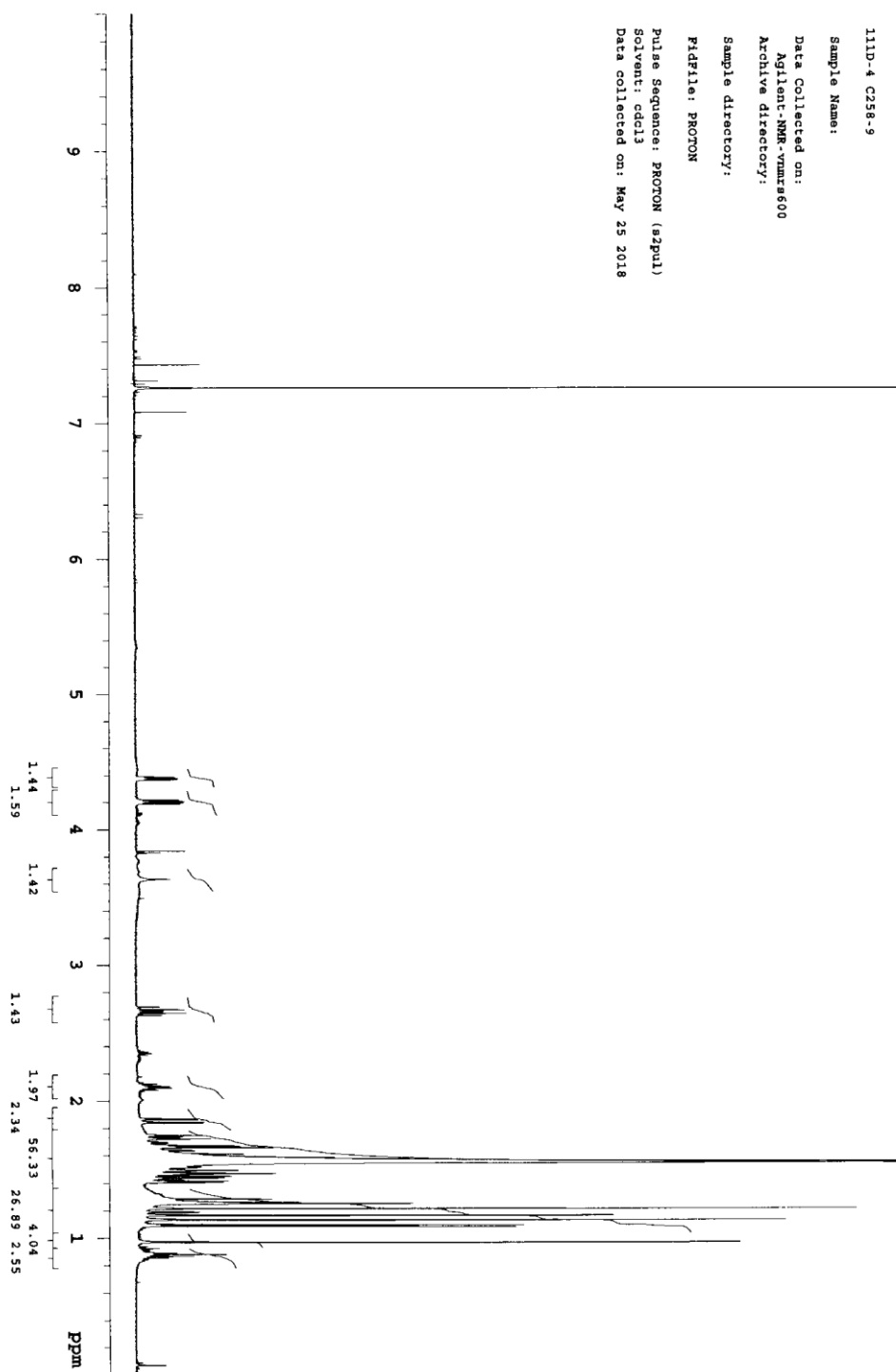
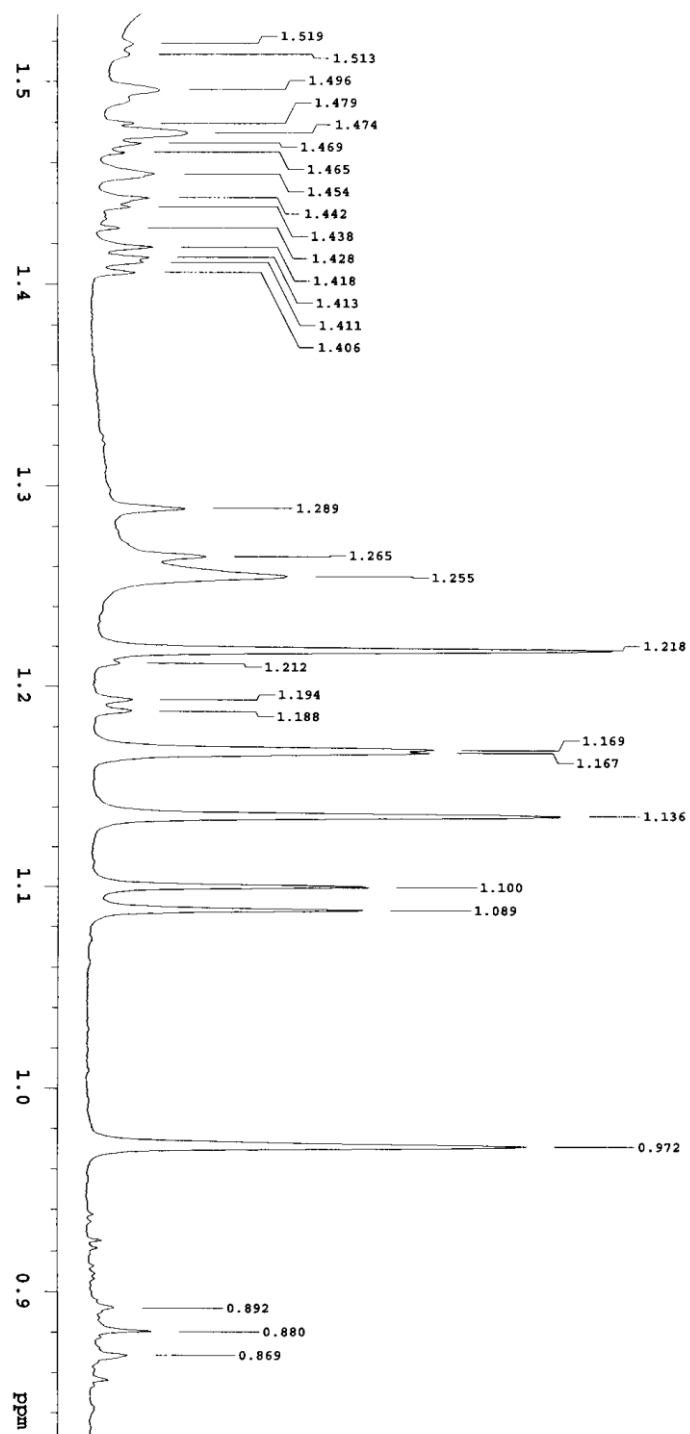
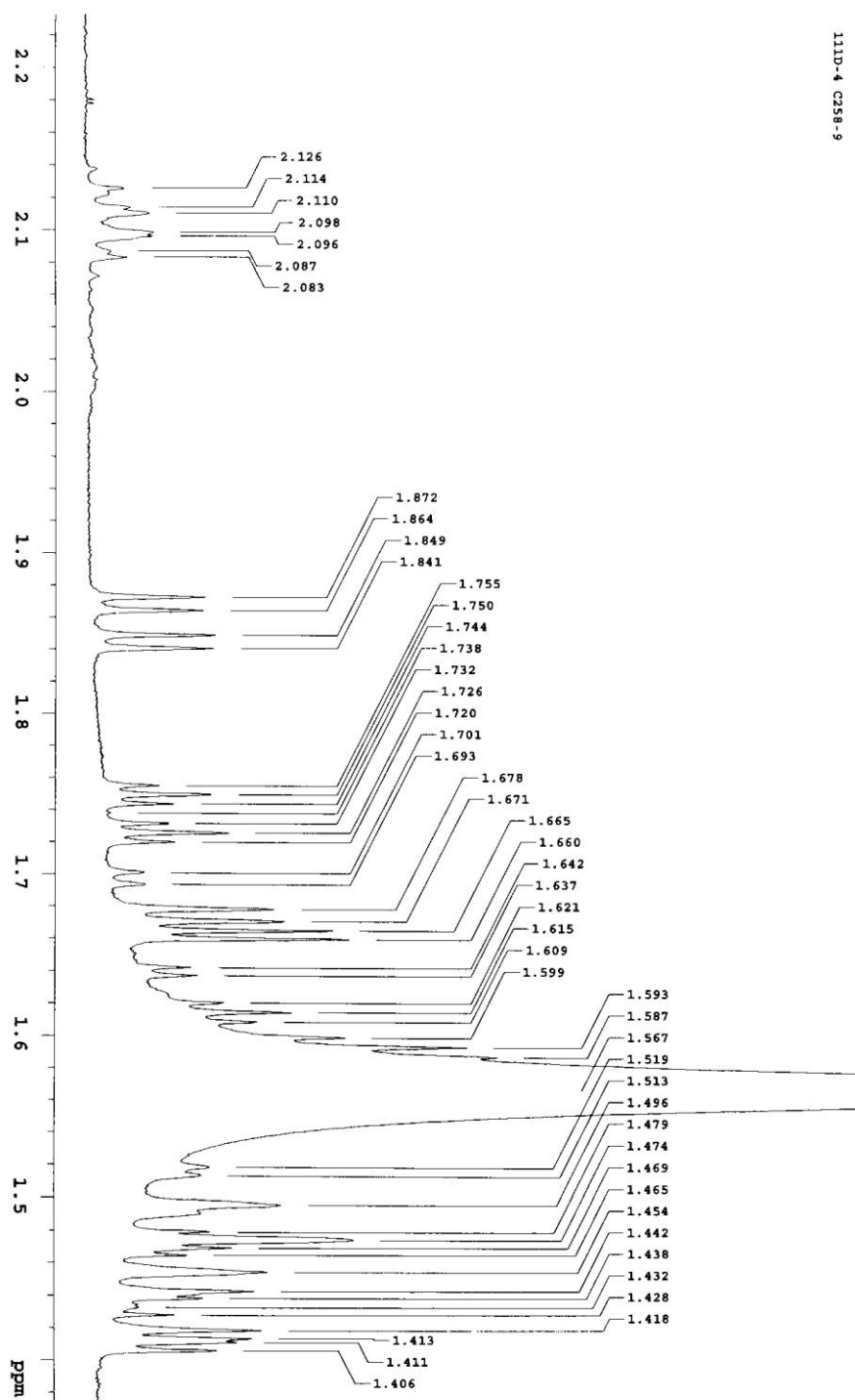


Figure S15  $^1\text{H}$  NMR spectrum of 3 in  $\text{CDCl}_3$







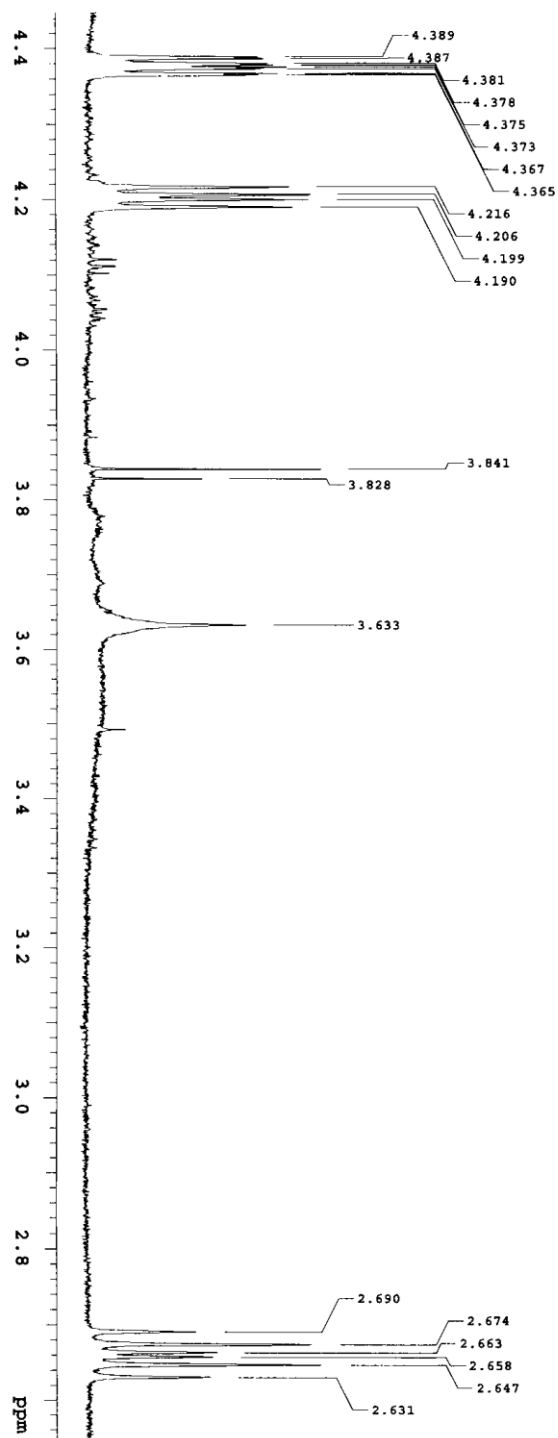
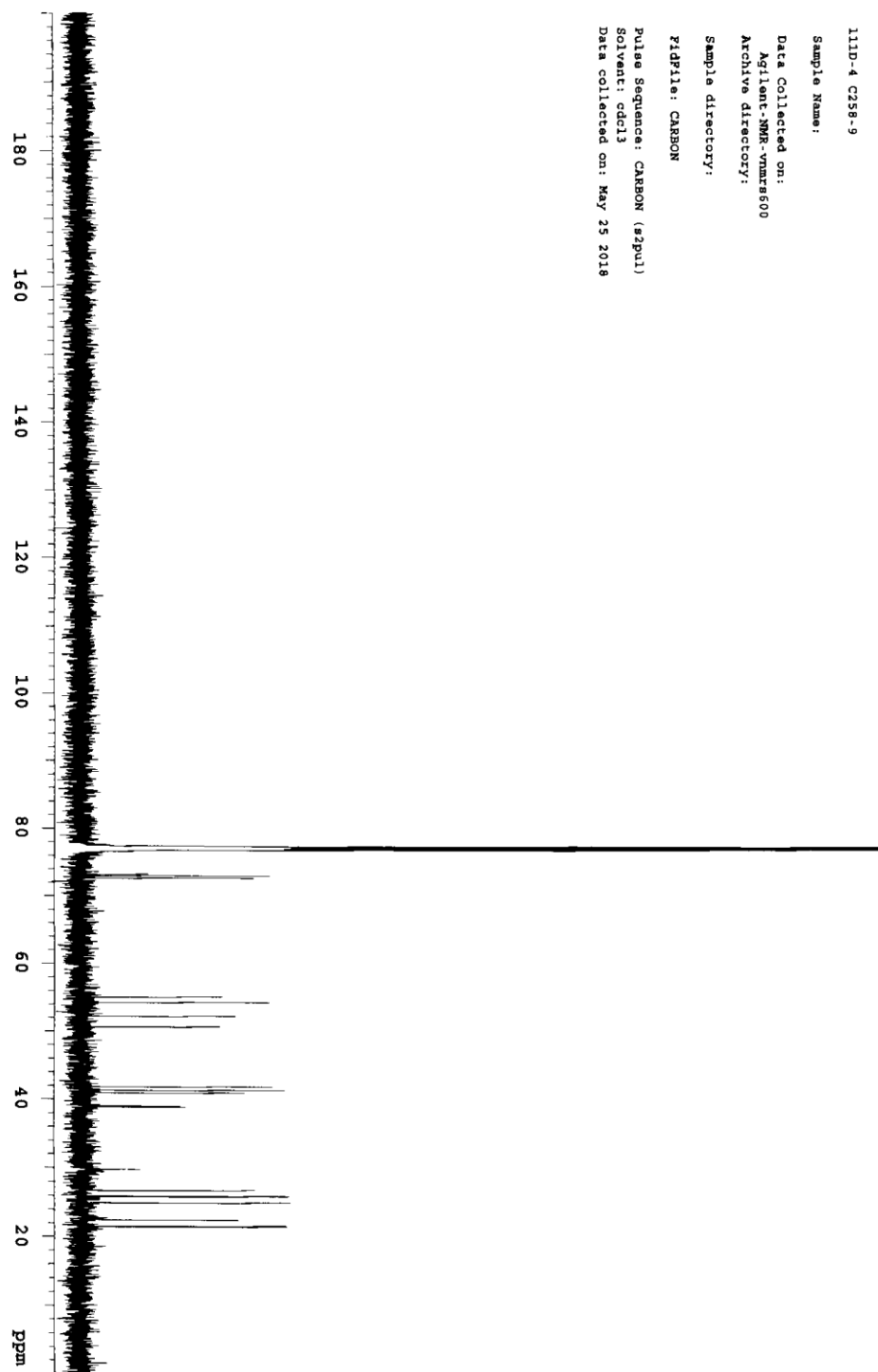
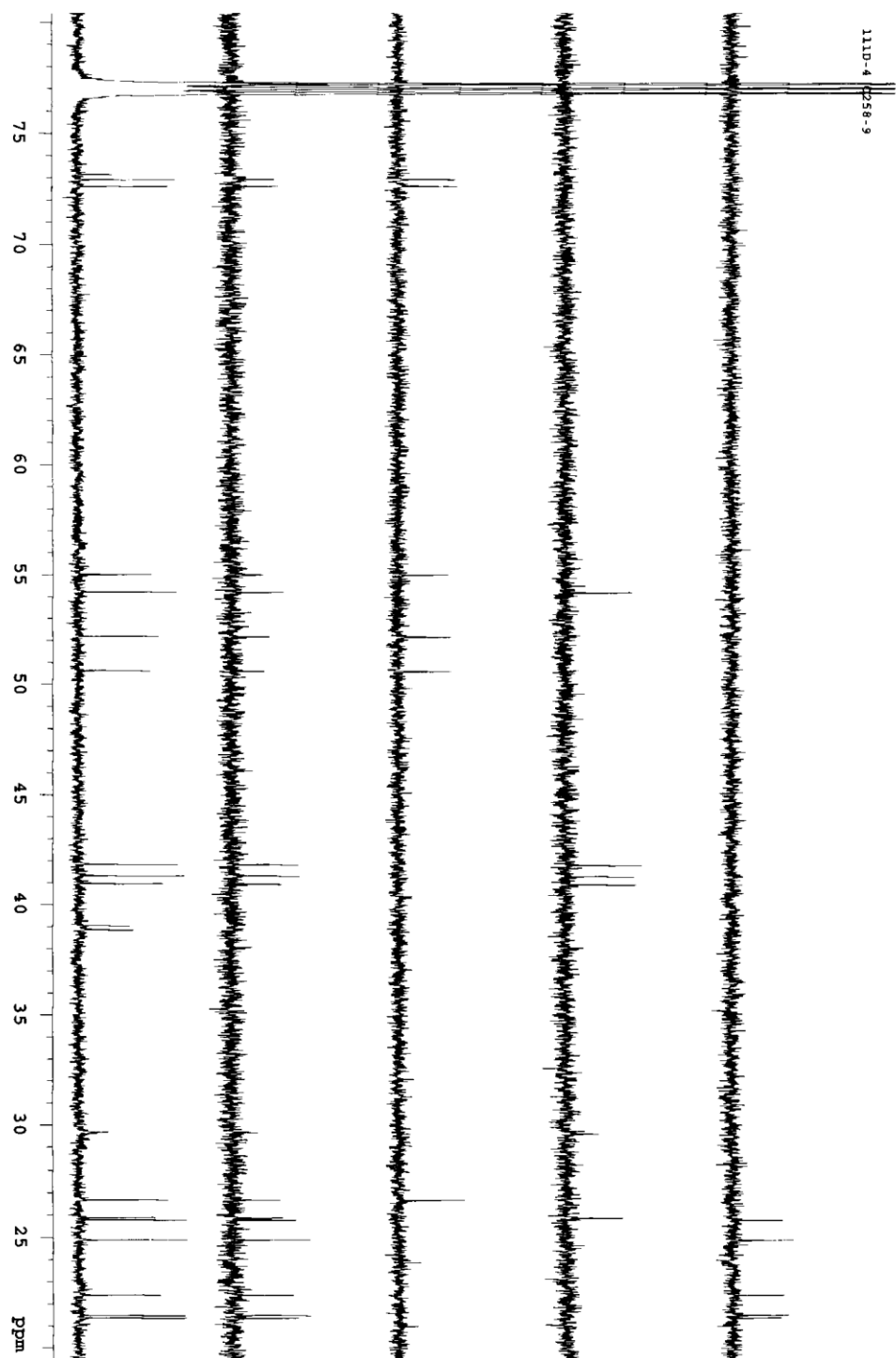


Figure S16  $^{13}\text{C}$  NMR spectrum of 3 in  $\text{CDCl}_3$



11D-4 C258-9			
INDEX	FREQUENCY	PPM	HEIGHT
1	11647.3	77.215	3007.5
2	11615.0	77.000	3101.7
3	11583.8	76.793	2743.4
4	11021.2	72.130	12.2
5	10996.5	72.900	36.5
6	10950.3	72.594	31.4
7	8299.7	55.022	27.5
8	8179.4	54.425	36.5
9	7874.3	51.201	30.0
10	7638.4	50.638	26.9
11	6309.1	41.825	37.1
12	6230.5	41.304	39.4
13	6177.3	40.952	31.7
14	5886.0	39.020	18.2
15	5862.9	38.867	18.0
16	5858.3	38.837	20.5
17	479.2	29.694	11.6
18	4026.0	26.690	33.6
19	3905.8	25.893	28.6
20	3890.8	25.794	40.3
21	3754.4	24.889	40.5
22	3739.9	24.406	30.6
23	340.0	21.479	39.6
24	3221.5	21.356	40.0



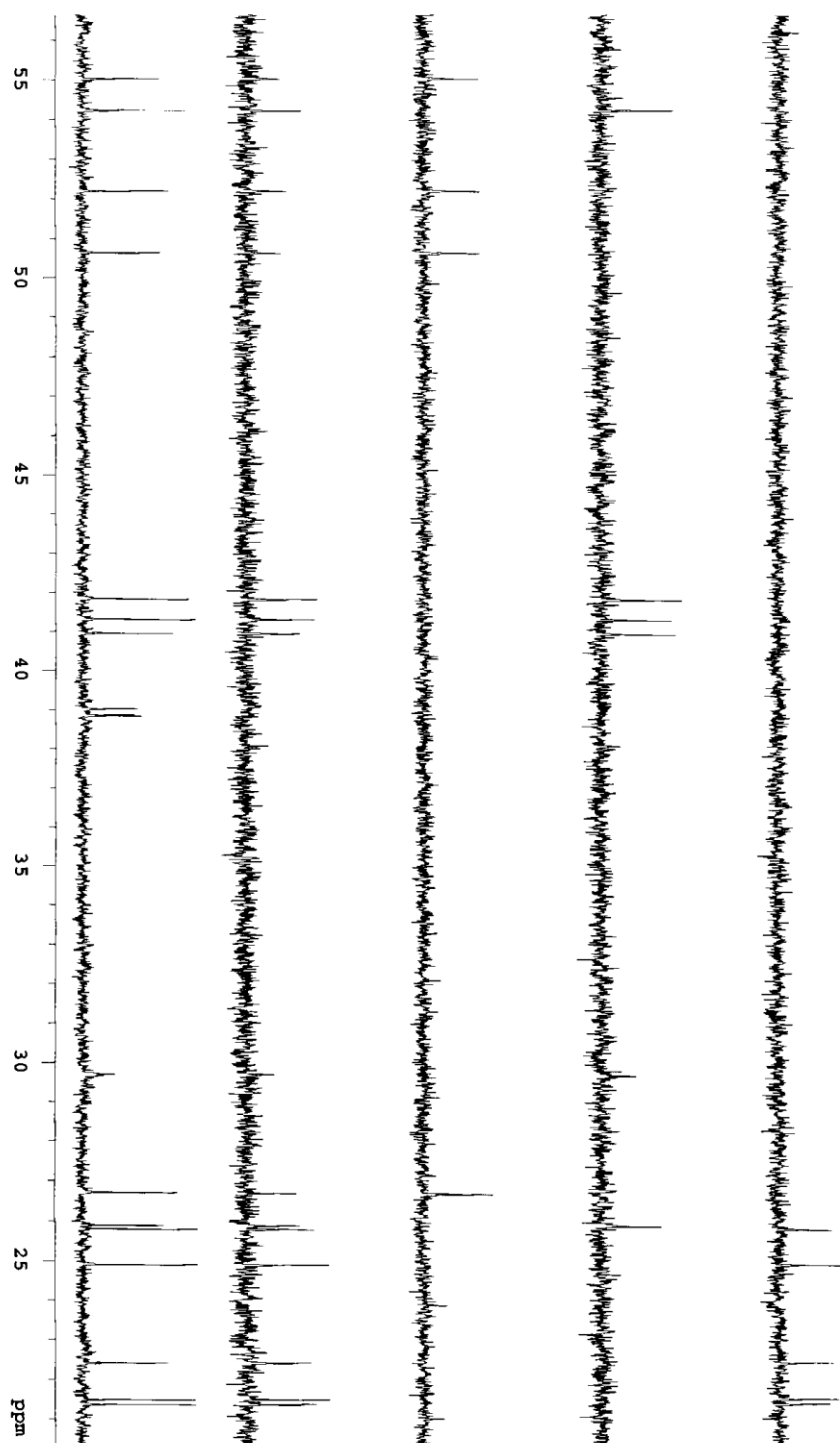
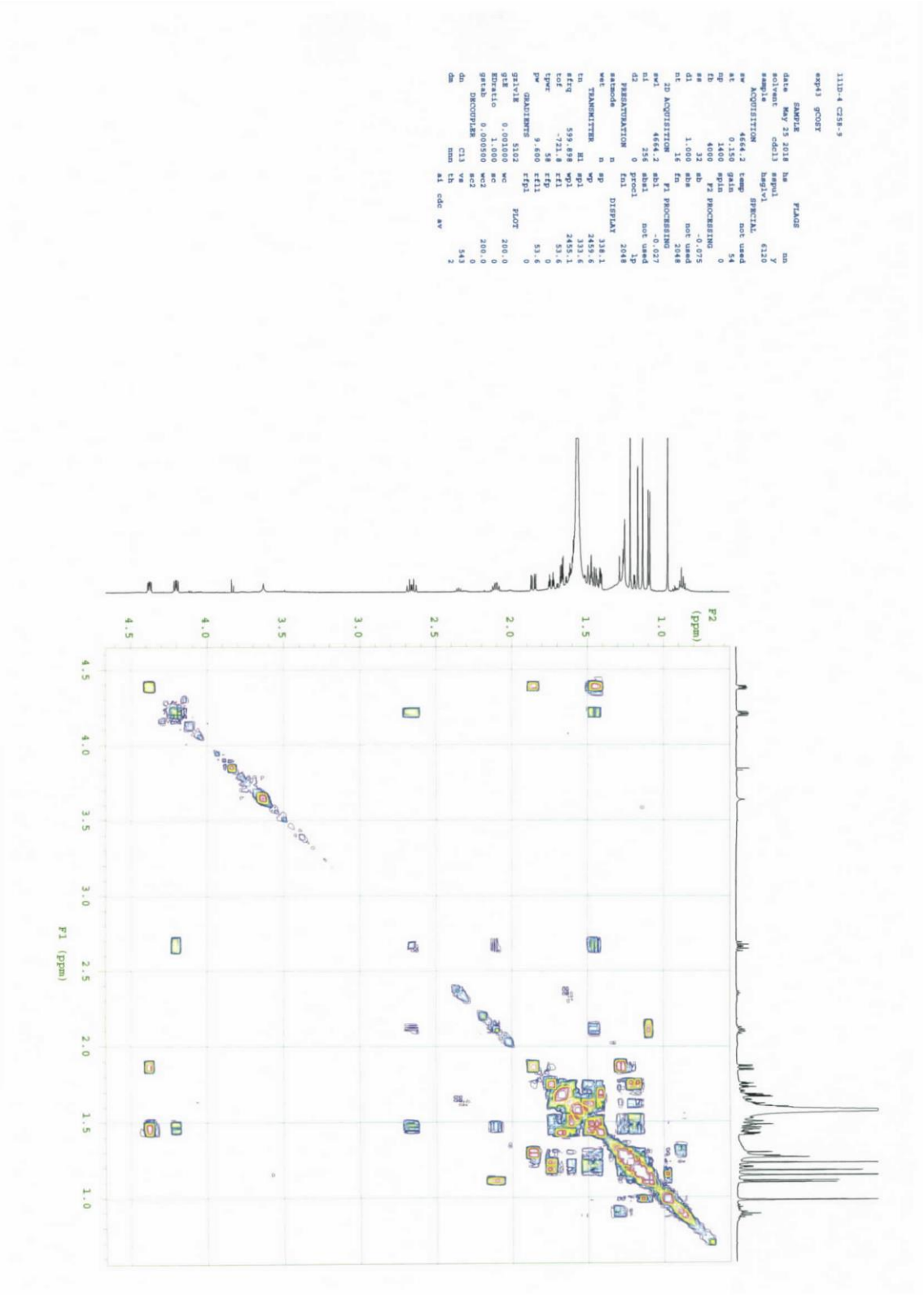




Figure S17 <sup>1</sup>H-<sup>1</sup>H COSY of 3



11D-4 C758-9		SAMPLE		FLAC	
expid	gcxref	date	May 25 2018	hs	
sample	acqref	exptent	cd13	hspl	ym
1	1664.2	temp		SERIAL	6120
2	1.000	gain		not used	
3	0.150	rate		not used	
4	1400	spin		94	
5	fb	P PROGRAMING			
6	32	2b	-0.075		
7	1.000	abs	not used		
8	1.000	abs	not used		
9	1.000	abs	not used		
10	1.000	abs	not used		
11	22	P PROGRAMING	-0.027		
12	22	P PROGRAMING			
13	22	P PROGRAMING			
14	4664.2	hbl	not used		
15	256	hbl	not used		
16	256	hbl	not used		
17	4664.2	hbl	not used		
18	256	hbl	not used		
19	4664.2	hbl	not used		
20	256	hbl	not used		
21	4664.2	hbl	not used		
22	256	hbl	not used		
23	4664.2	hbl	not used		
24	256	hbl	not used		
25	4664.2	hbl	not used		
26	256	hbl	not used		
27	4664.2	hbl	not used		
28	256	hbl	not used		
29	4664.2	hbl	not used		
30	256	hbl	not used		
31	4664.2	hbl	not used		
32	256	hbl	not used		
33	4664.2	hbl	not used		
34	256	hbl	not used		
35	4664.2	hbl	not used		
36	256	hbl	not used		
37	4664.2	hbl	not used		
38	256	hbl	not used		
39	4664.2	hbl	not used		
40	256	hbl	not used		
41	4664.2	hbl	not used		
42	256	hbl	not used		
43	4664.2	hbl	not used		
44	256	hbl	not used		
45	4664.2	hbl	not used		
46	256	hbl	not used		
47	4664.2	hbl	not used		
48	256	hbl	not used		
49	4664.2	hbl	not used		
50	256	hbl	not used		
51	4664.2	hbl	not used		
52	256	hbl	not used		
53	4664.2	hbl	not used		
54	256	hbl	not used		
55	4664.2	hbl	not used		
56	256	hbl	not used		
57	4664.2	hbl	not used		
58	256	hbl	not used		
59	4664.2	hbl	not used		
60	256	hbl	not used		
61	4664.2	hbl	not used		
62	256	hbl	not used		
63	4664.2	hbl	not used		
64	256	hbl	not used		
65	4664.2	hbl	not used		
66	256	hbl	not used		
67	4664.2	hbl	not used		
68	256	hbl	not used		
69	4664.2	hbl	not used		
70	256	hbl	not used		
71	4664.2	hbl	not used		
72	256	hbl	not used		
73	4664.2	hbl	not used		
74	256	hbl	not used		
75	4664.2	hbl	not used		
76	256	hbl	not used		
77	4664.2	hbl			

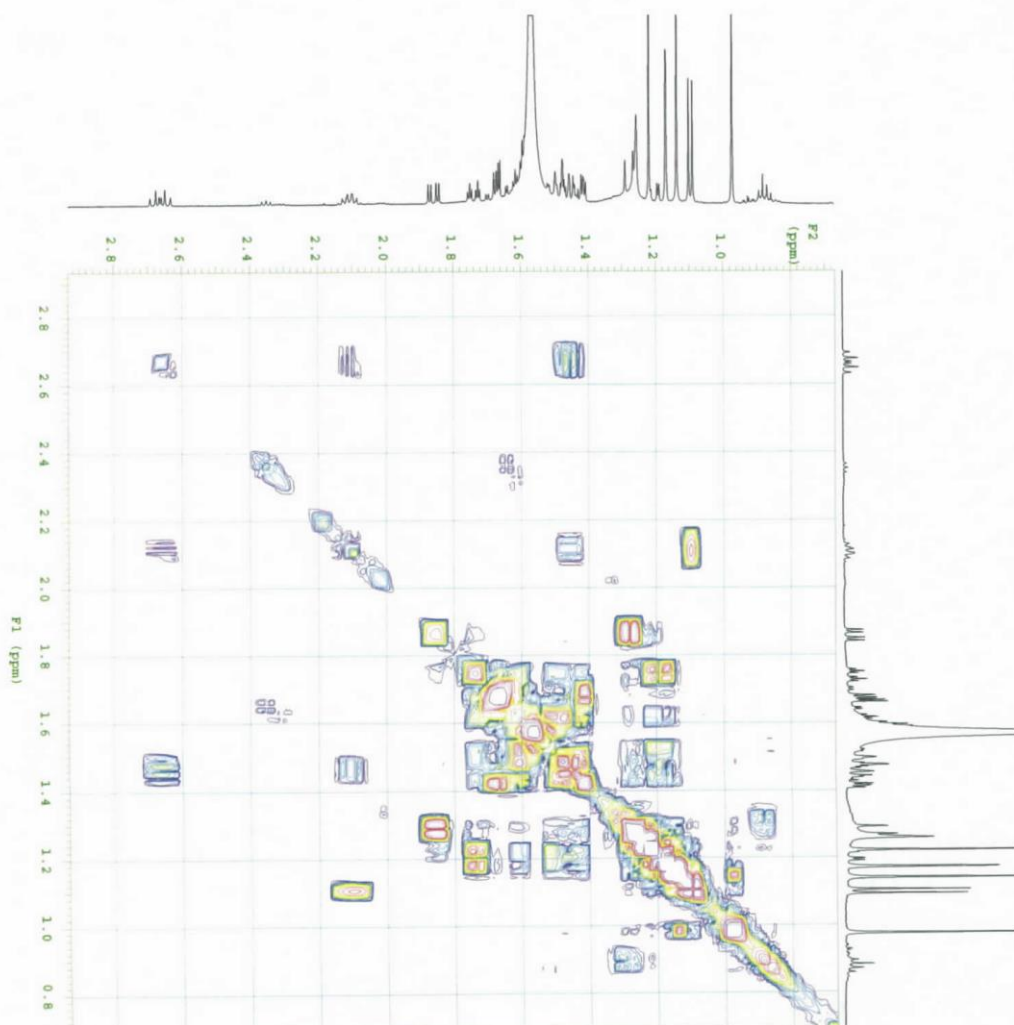
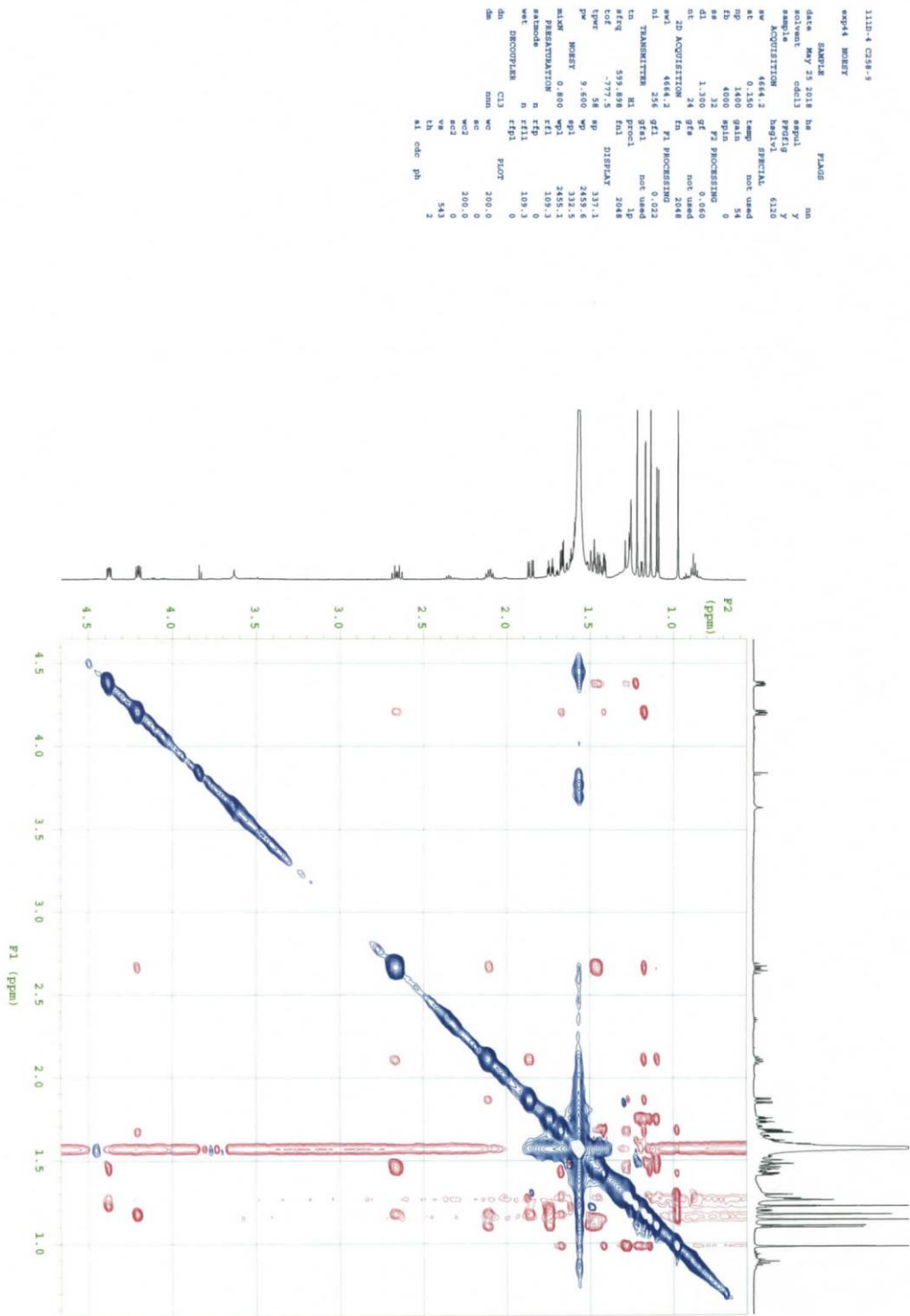


Figure S18 NOESY of 3









[illegible]



exp 6    ginnocul

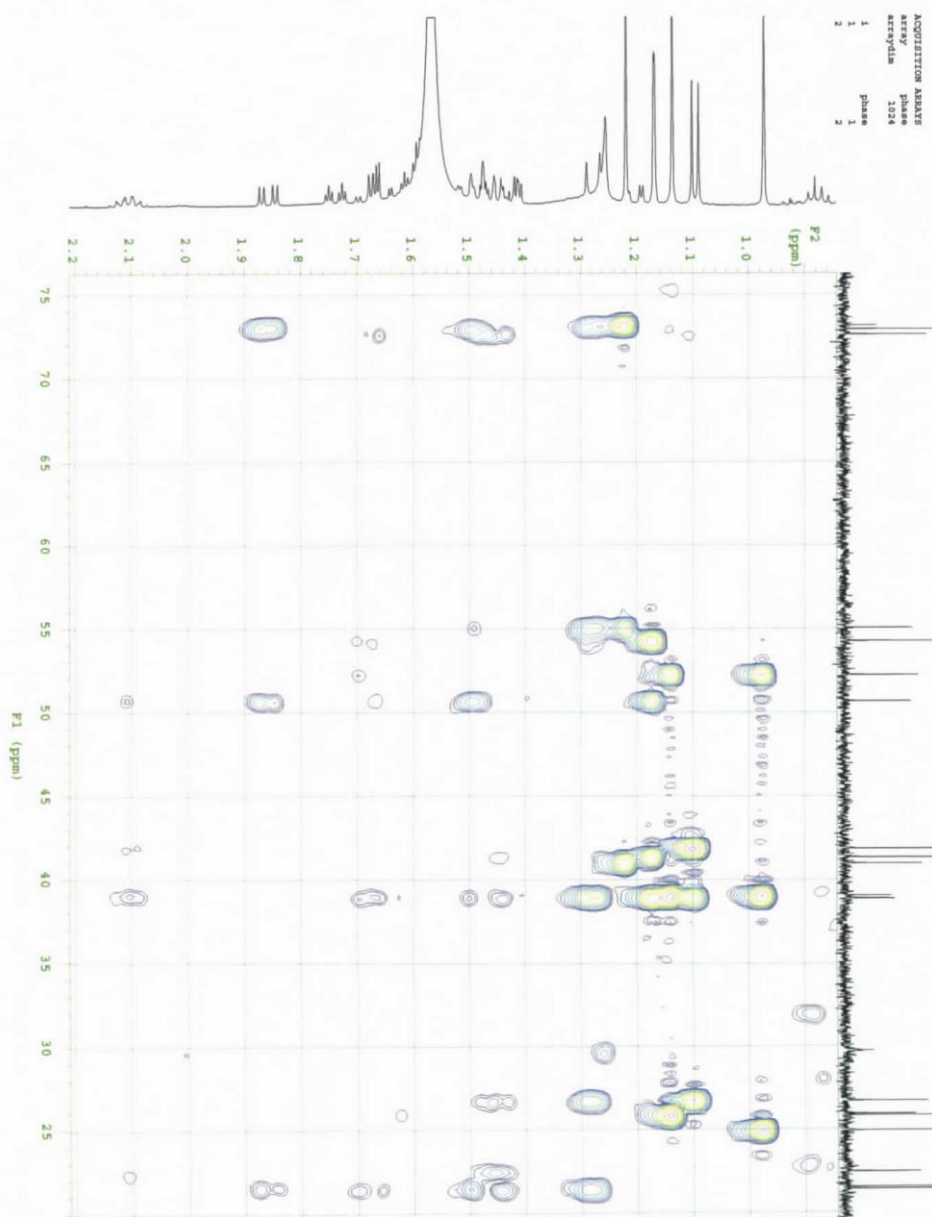
[illegible]



Figure S21 FAB/MS of 3

[ Elemental Composition ] 高分解能  
Data : 1807068 Date : 12-Jul-2018 14:41  
Sample: 111D-4 C258-9  
Note : Matrix; G  
Inlet : Direct Ion Mode : FAB+  
RT : 5.41 min Scan#: (35,40)  
Elements : C 25/15, H 40/30, O 5/0, Na 1/0  
Mass Tolerance : 20ppm, 2mmu if m/z > 100  
Unsaturation (U.S.) : -1.0 - 40.0  

Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
345.2398	100.0	-2.3 / -0.8	3.5 C 20 H 34 O 3 Na

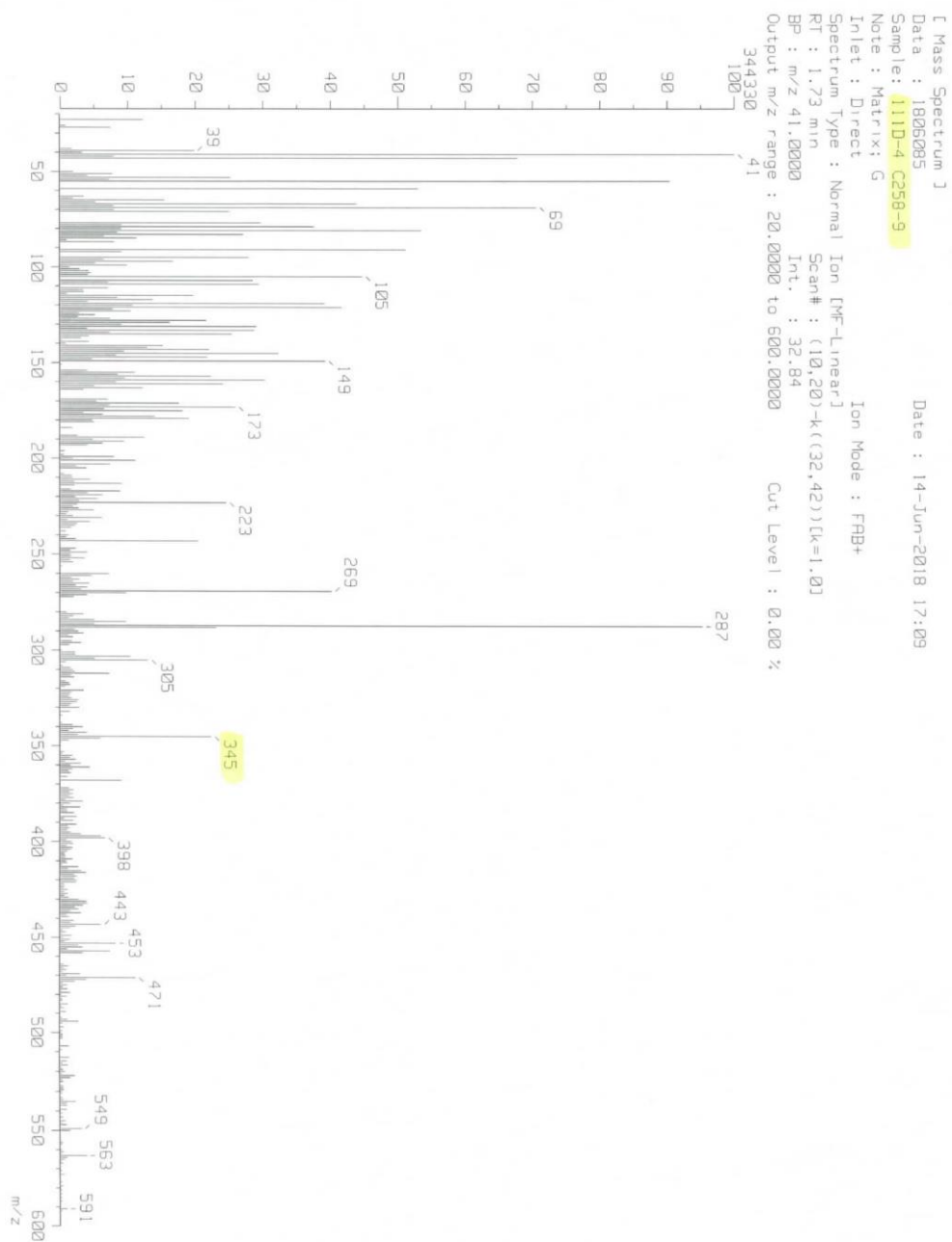
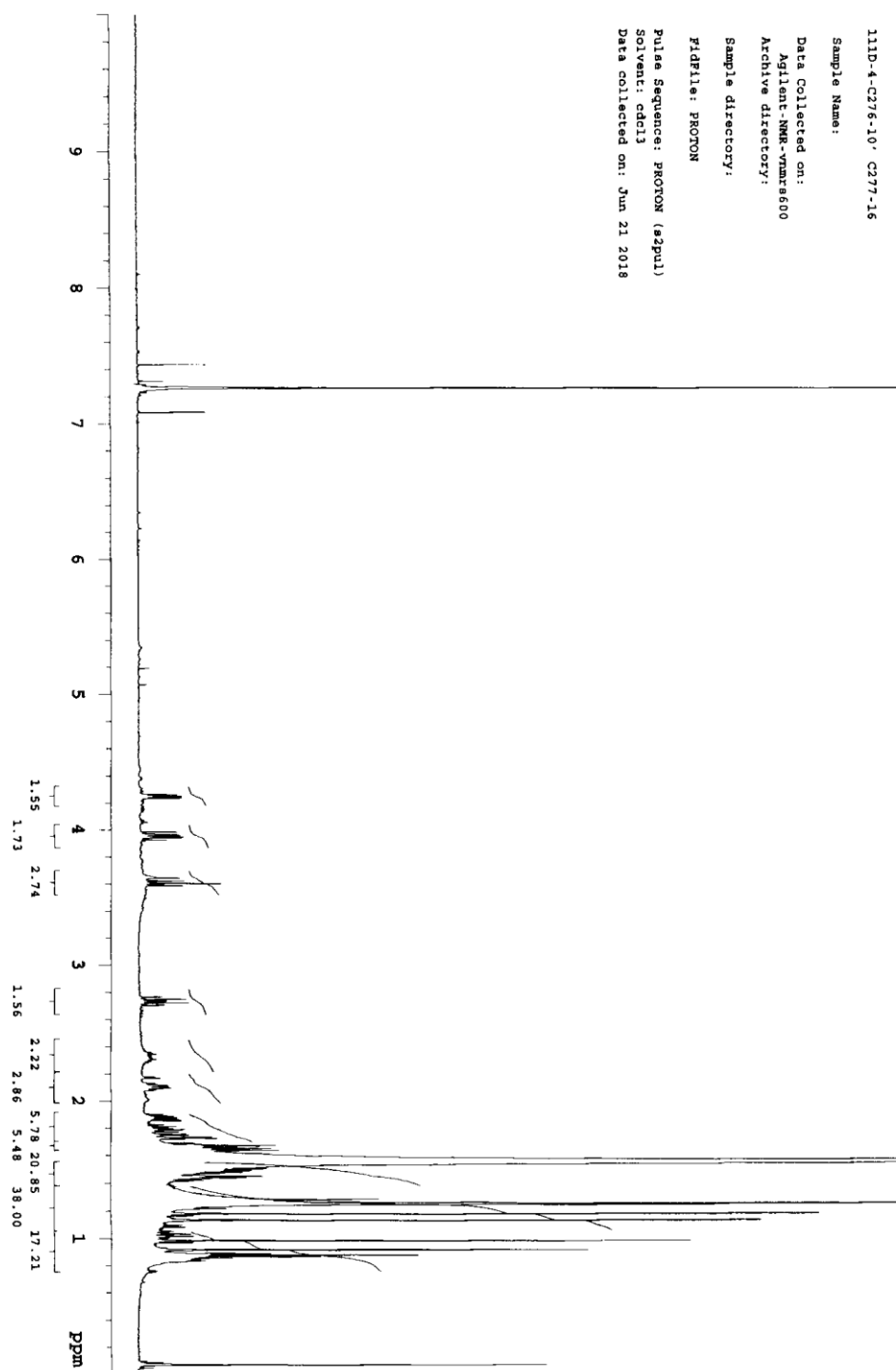
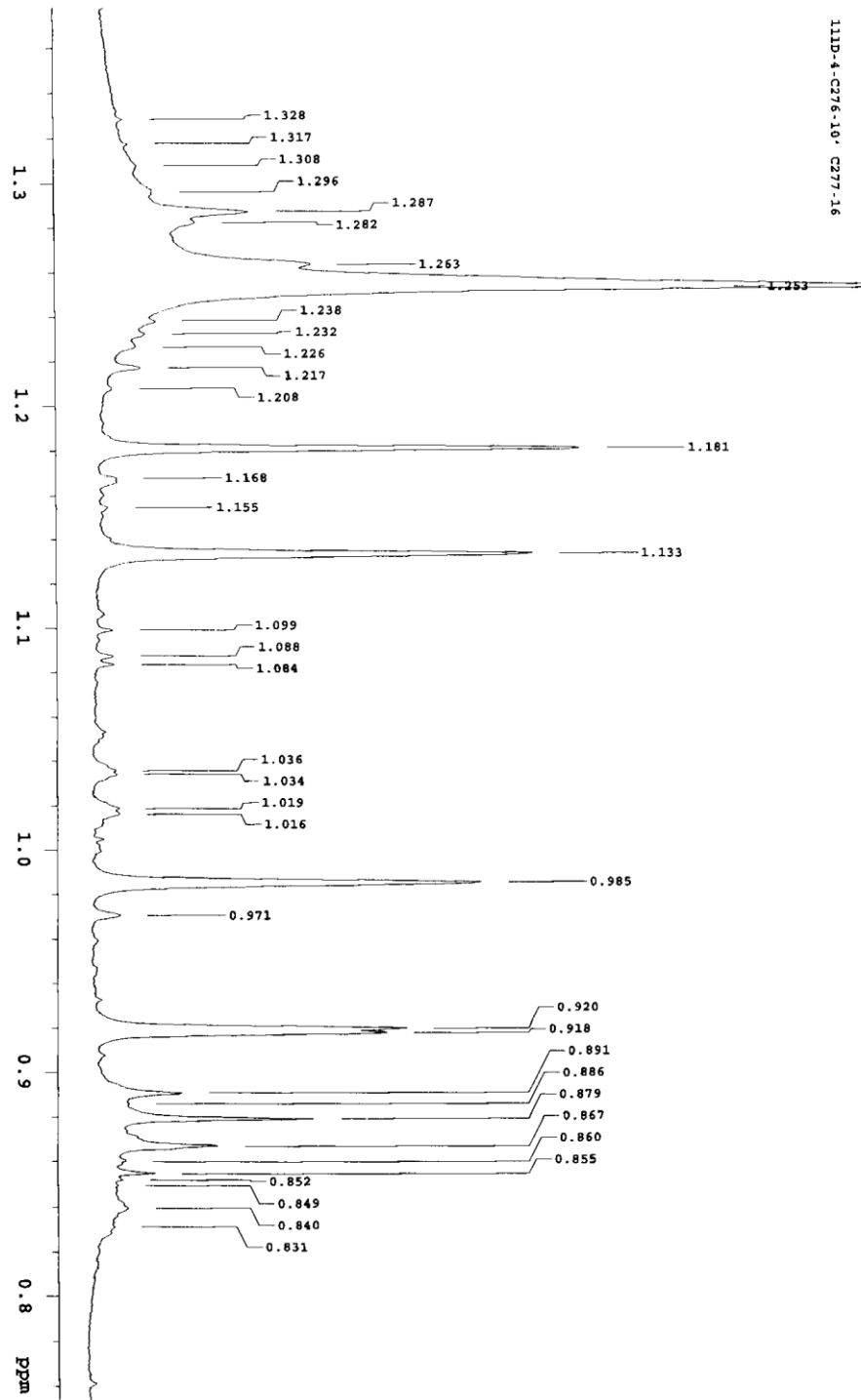
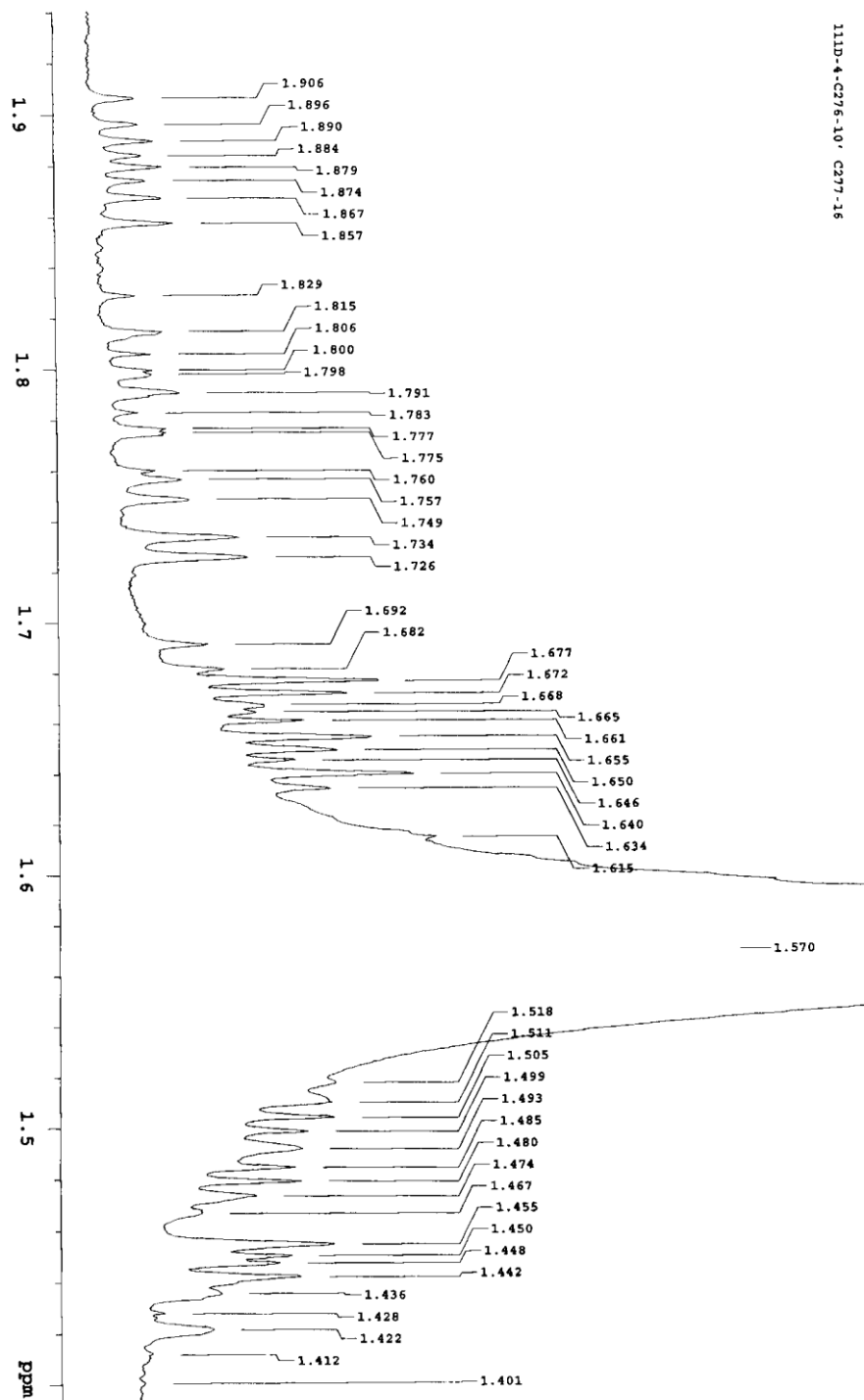
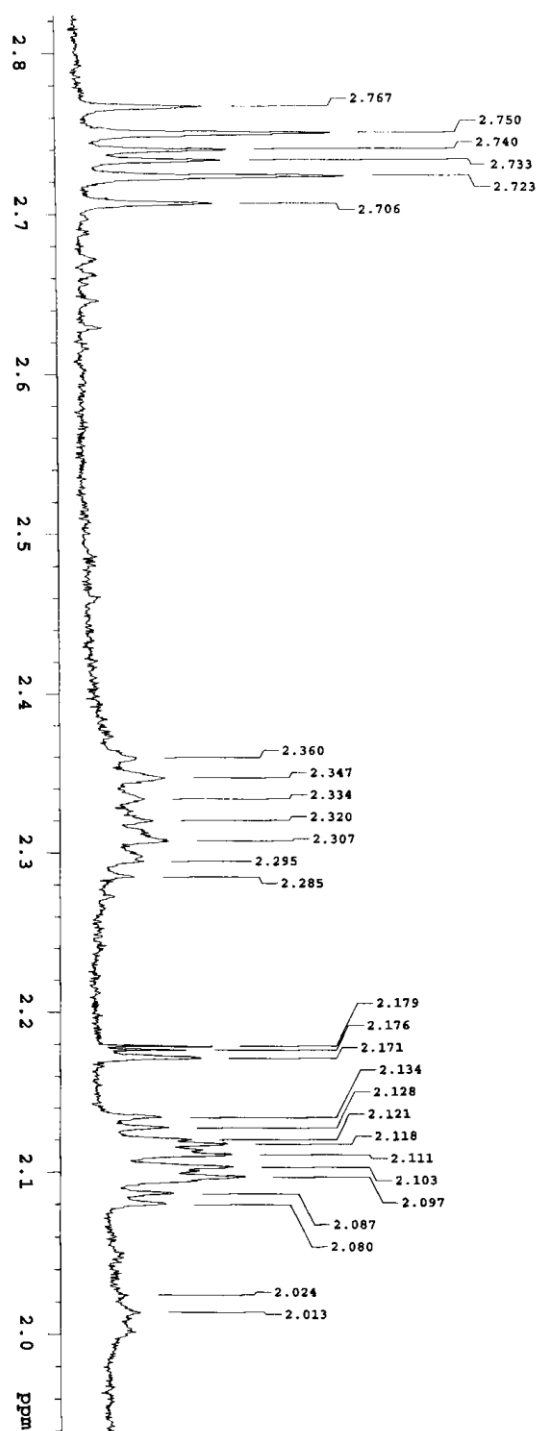


Figure S22  $^1\text{H}$  NMR spectrum of 4 in  $\text{CDCl}_3$









111D-4-C276-10' C277-16

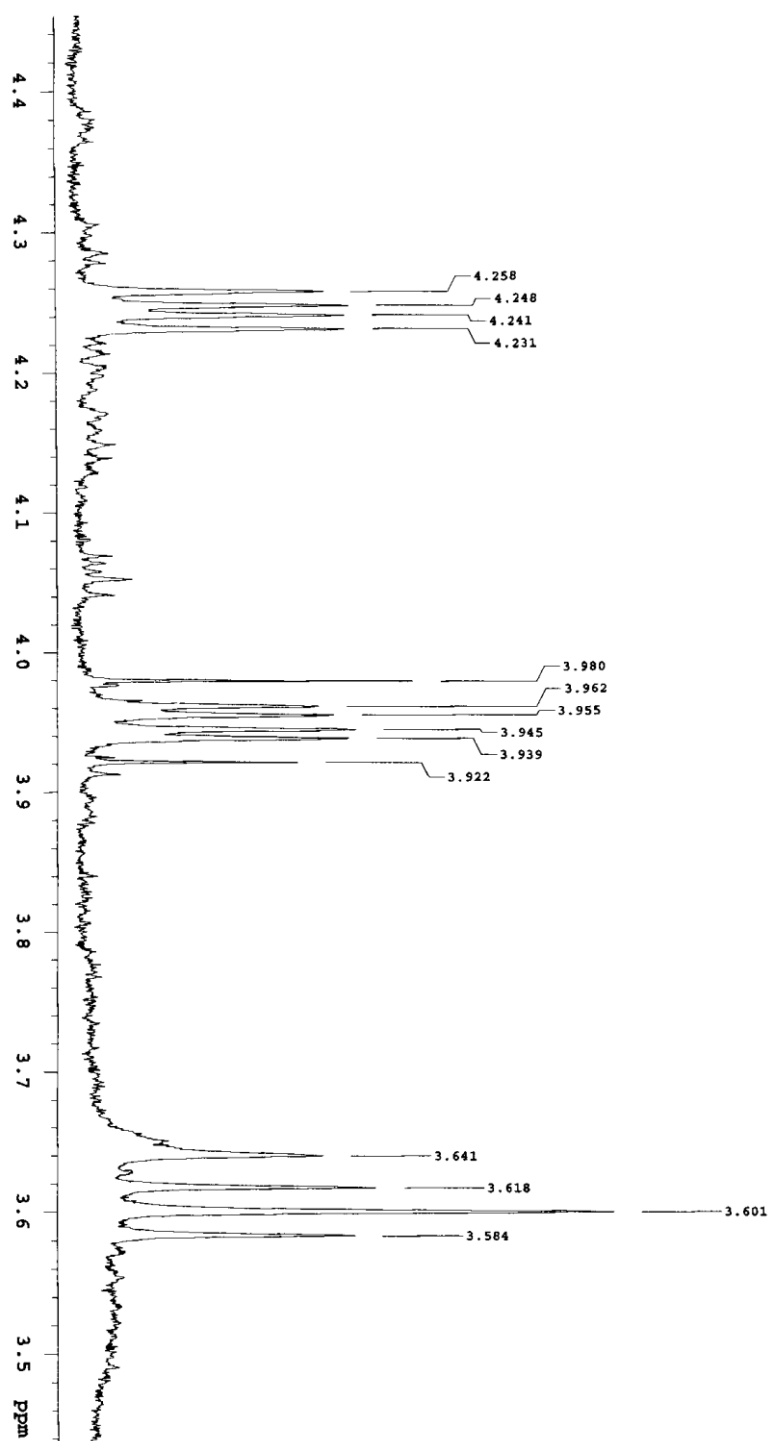
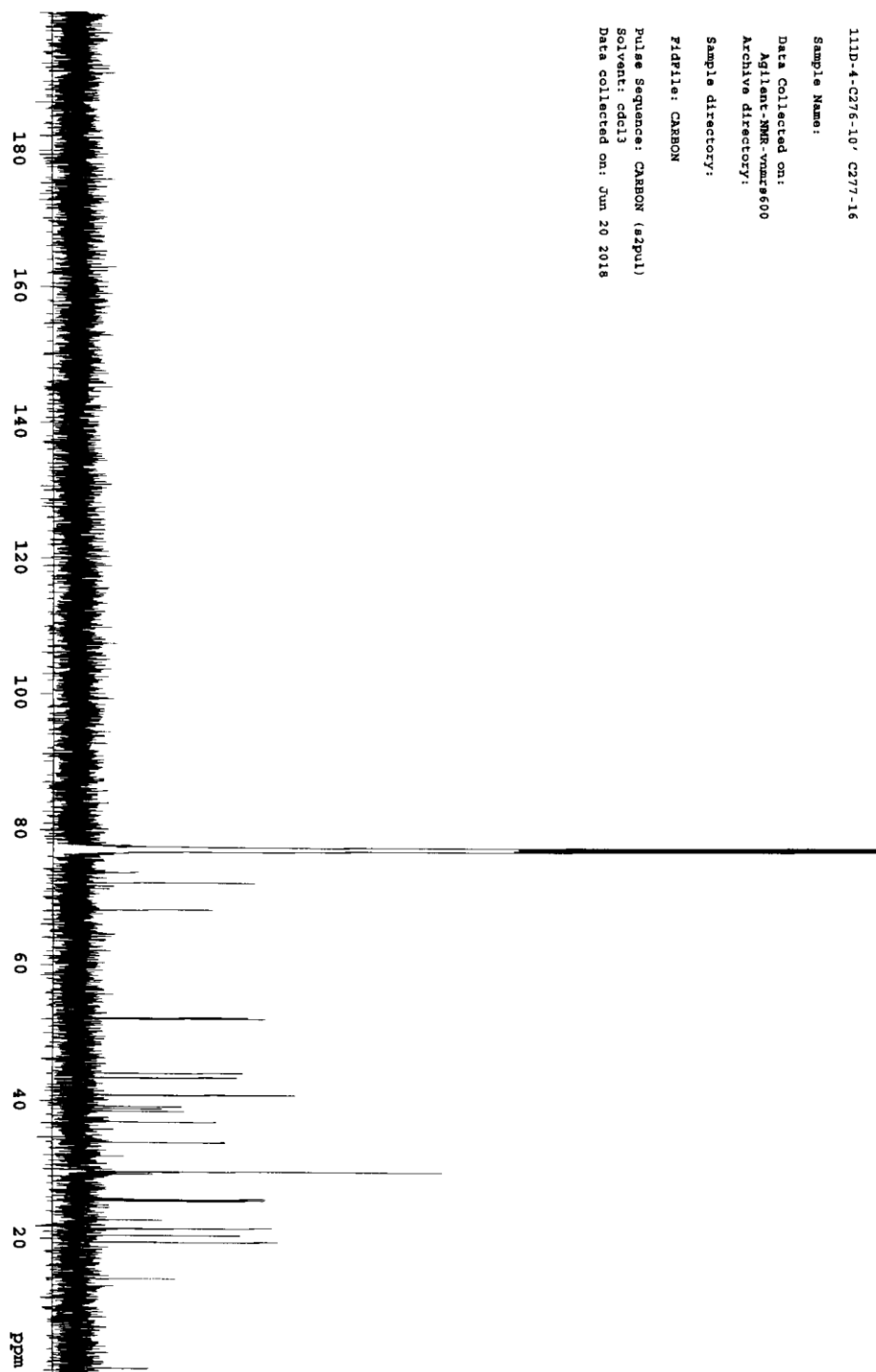
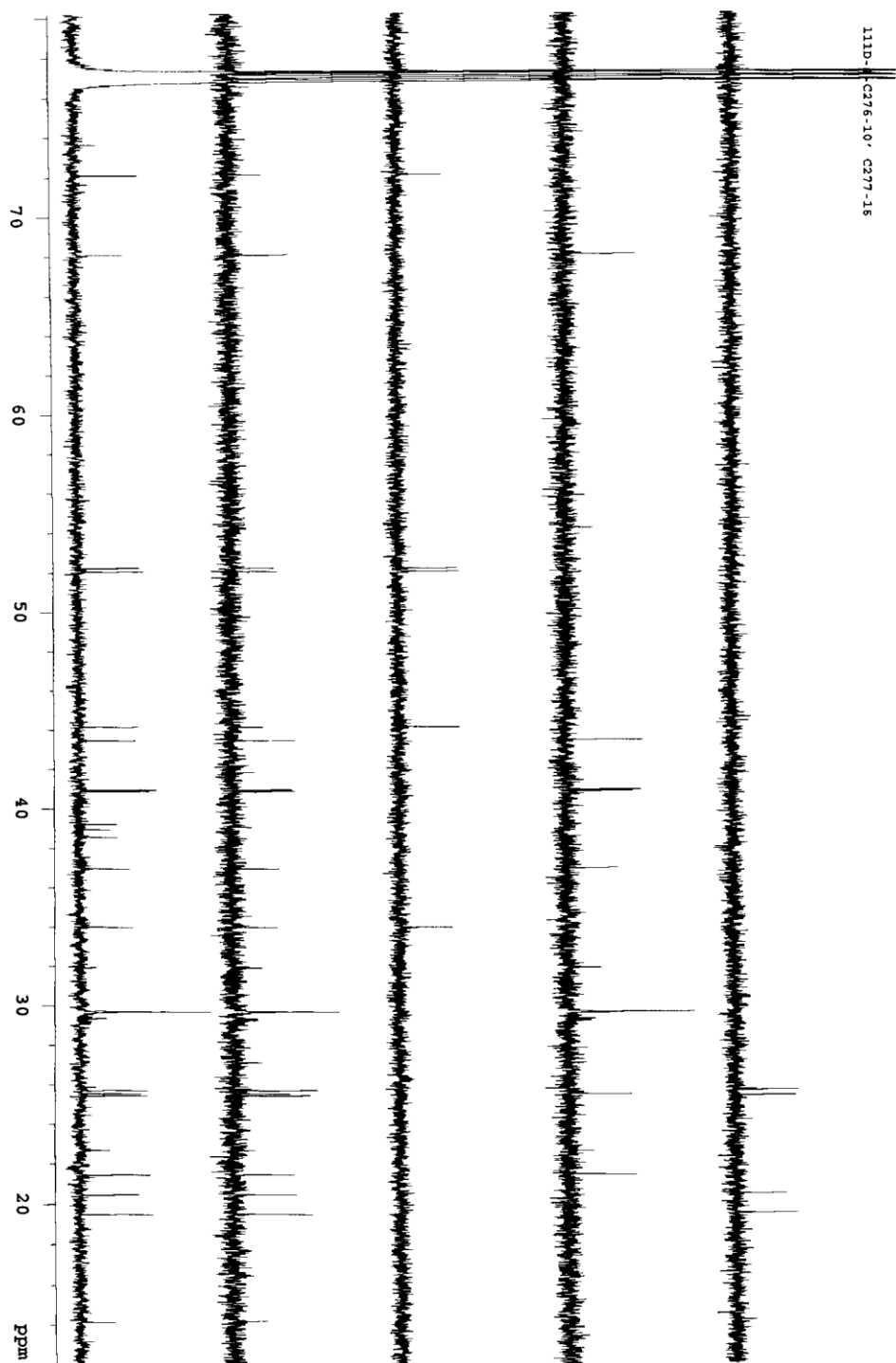


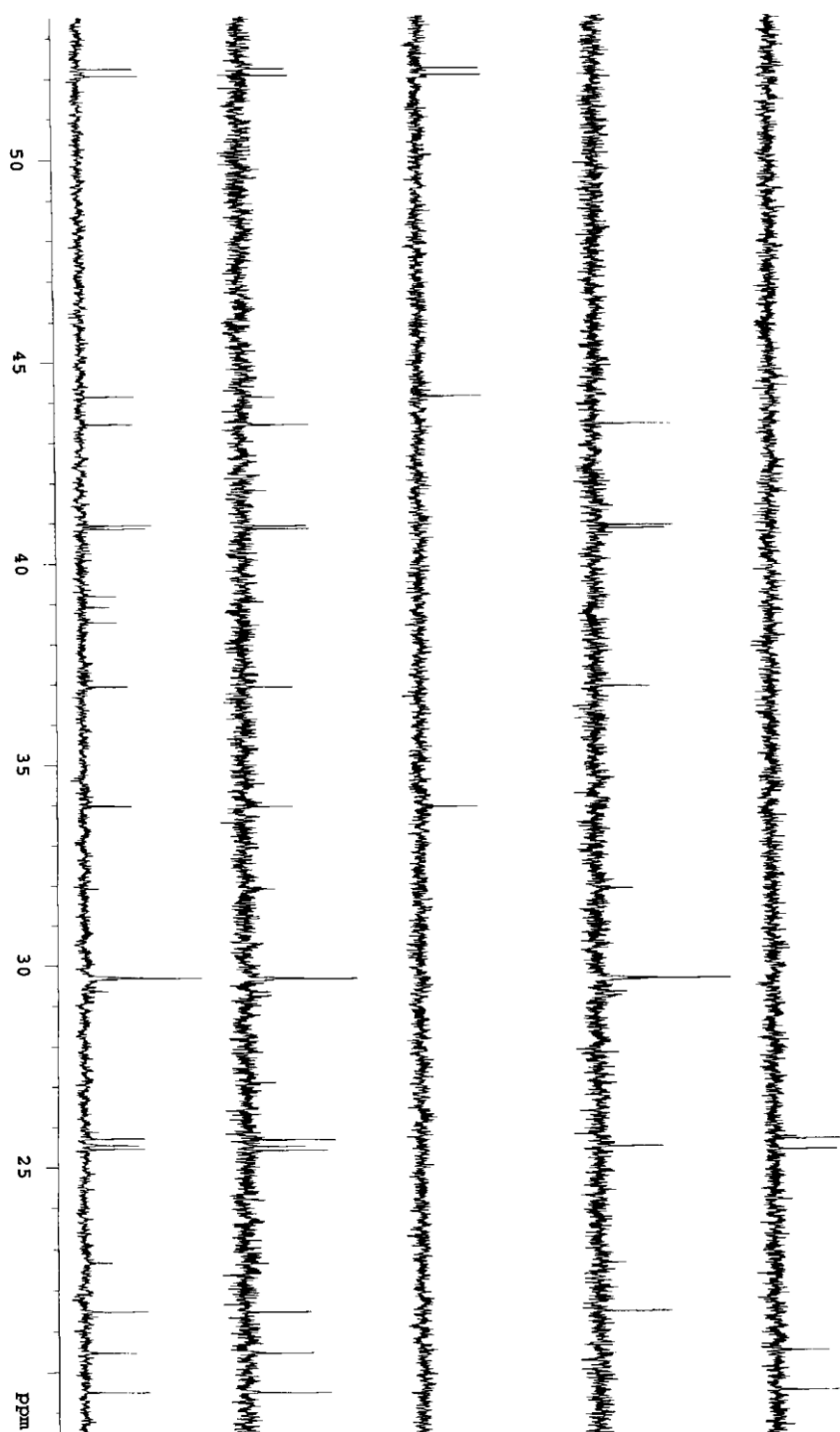
Figure S23  $^{13}\text{C}$  NMR spectrum of 4 in  $\text{CDCl}_3$





11D-4-C276-10' C277-16			
INDEX	FREQUENCY, PPM	HEIGHT	
1	28196.2	186.923	-8.6
2	11647.3	77.215	6137.4
3	11615.0	77.000	6539.4
4	11582.6	76.785	5889.2
5	11105.2	73.620	11.5
6	10872.8	72.090	33.8
7	10266.0	68.057	25.7
8	7877.7	52.224	32.6
9	7851.1	52.048	36.1
10	6658.2	44.140	31.6
11	6554.1	43.450	30.5
12	6176.1	40.944	41.7
13	6164.6	40.867	37.6
14	5913.7	39.204	19.9
15	5872.1	38.928	16.0
16	5814.3	38.545	20.4
17	5572.7	36.944	26.6
18	5217.8	34.591	-8.2
19	5124.2	33.970	28.5
20	4815.6	31.924	8.7
21	4479.2	29.694	70.3
22	4428.3	29.357	14.2
23	3905.8	25.893	8.5
24	3879.2	25.717	36.0
25	3853.8	25.548	32.5
26	3839.9	25.456	36.0
27	3421.5	22.682	16.0
28	3282.8	21.763	-8.4
29	3240.0	21.479	37.4
30	3088.6	20.475	31.2
31	2940.6	19.494	38.6
32	2127.9	14.107	18.7
33	1551.4	1.010	13.3







```

111D-4-C276-1D-C277-16
exp3 gcosy
=====
SAMPLE          PLACE
date    Sun 21 2018   hr
solvent  cdcl3      repul  Y
sample   hesyl      6120
=====
ACQUISITION
ac  2748.1  temp  not used
ad  0.000000  54
af  0.000000  54
fb  4000  f2  PROCESSING  0
as  32  ab  -0.075
dl  1.000  abs  not used
nl  ID ACQUISITION  16  fn  not used
sw1  2748.1  ab1  not used
nl  256  ab1  not used
d3  PREPARATION  0  prec1  1p
=====
PARAMETER      n  p  DISPLAY
=====
wdsolve         n  sp  1024
=====
TRANSMITTER    n  sp  1307.1
=====
rfreq  599.897  wp1  414.3
rf1q  -1447.4  rf1  1312.8
tproc  58  rf1  121.2
pwr  9.400  rf1  121.2
pw  GRANUBITS  5102  rf1  0
g1v1n  0.001000  wc  200.0
g1v1o  1.000  wc  200.0
g1v1b  0.000500  wc2  382
d3  DECOUPLER  C13  v1  2
dm  num  lb  at  av  2

```

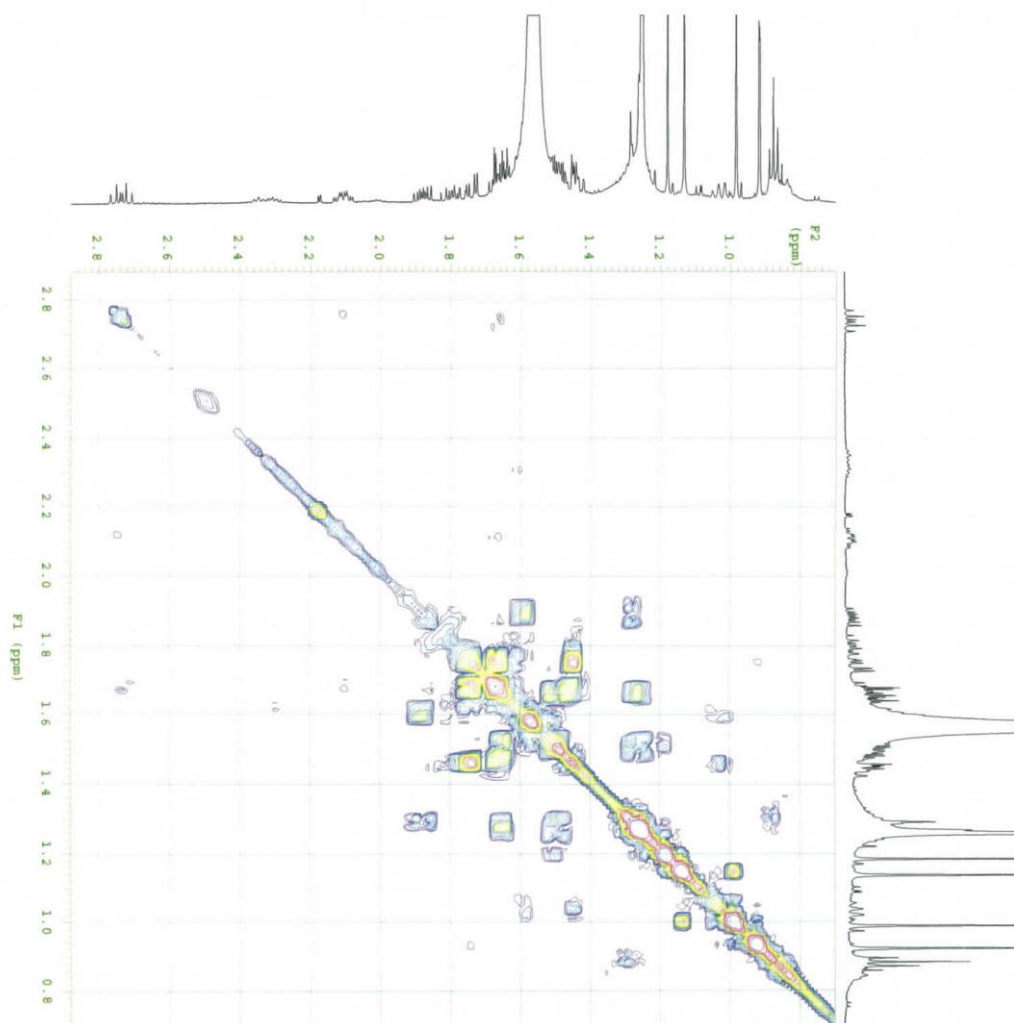
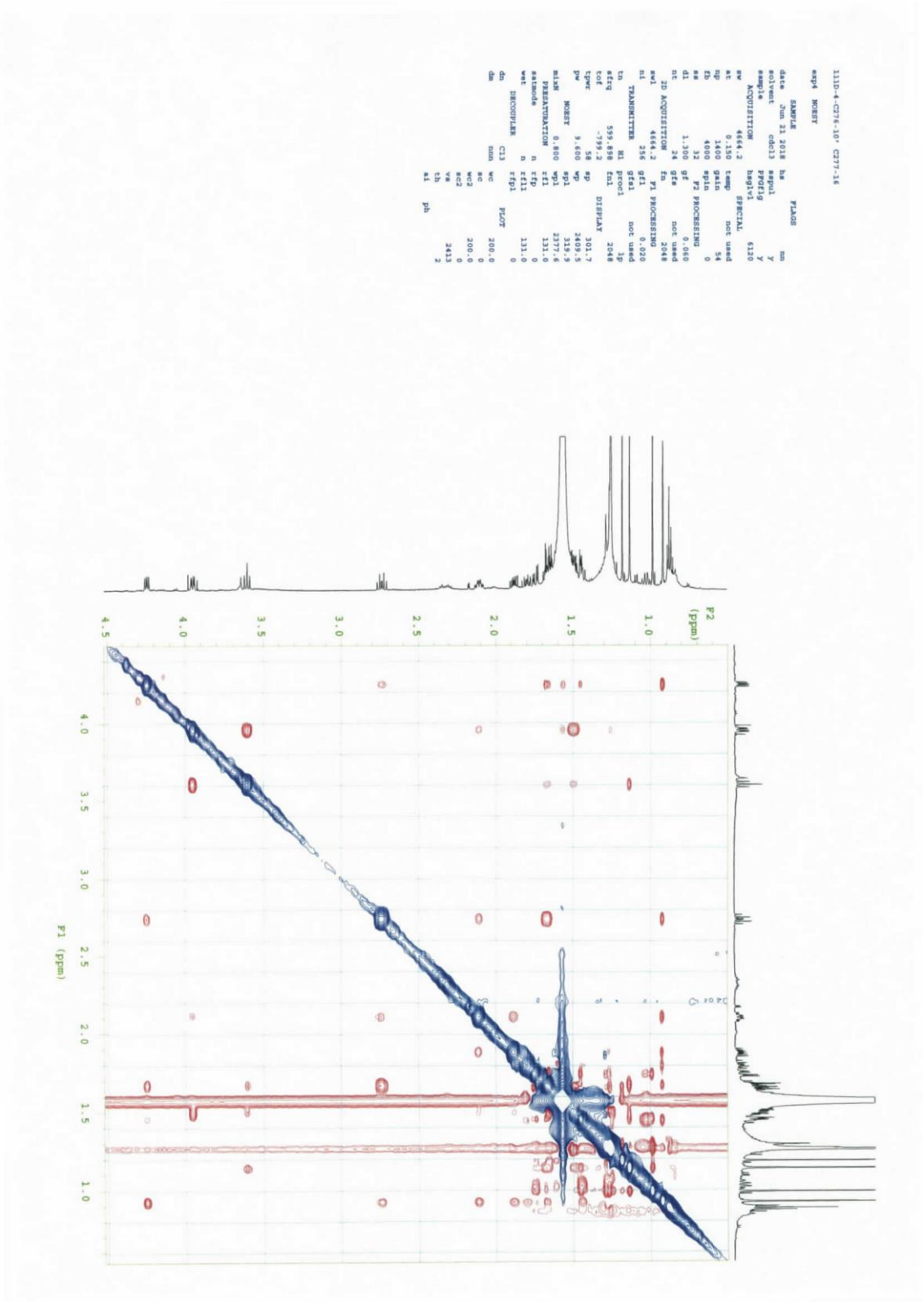
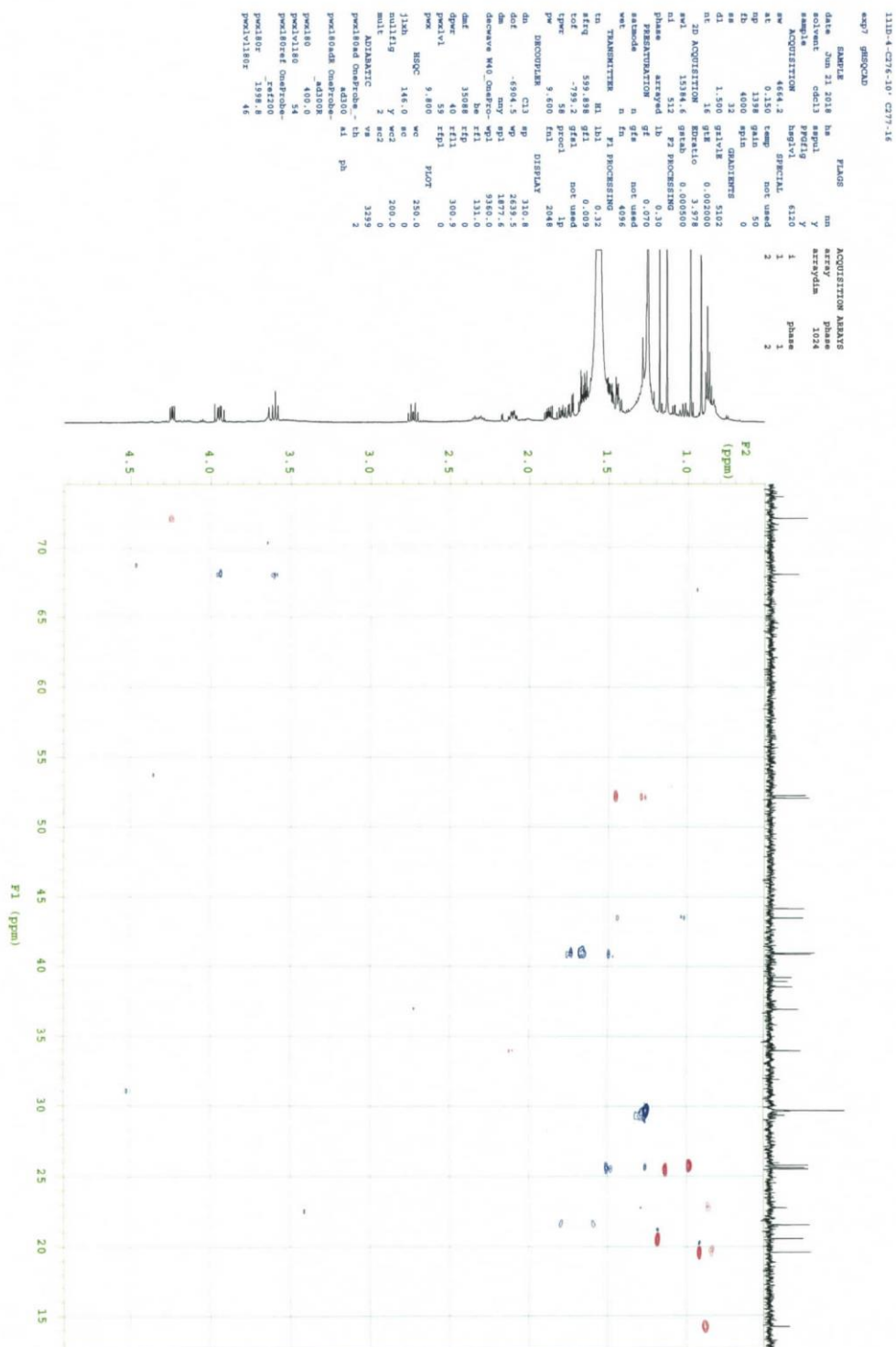


Figure S25 NOESY of 4





**Figure S26** HMQC of 4





exp7 ghsqcat

pwv1v1180r 46

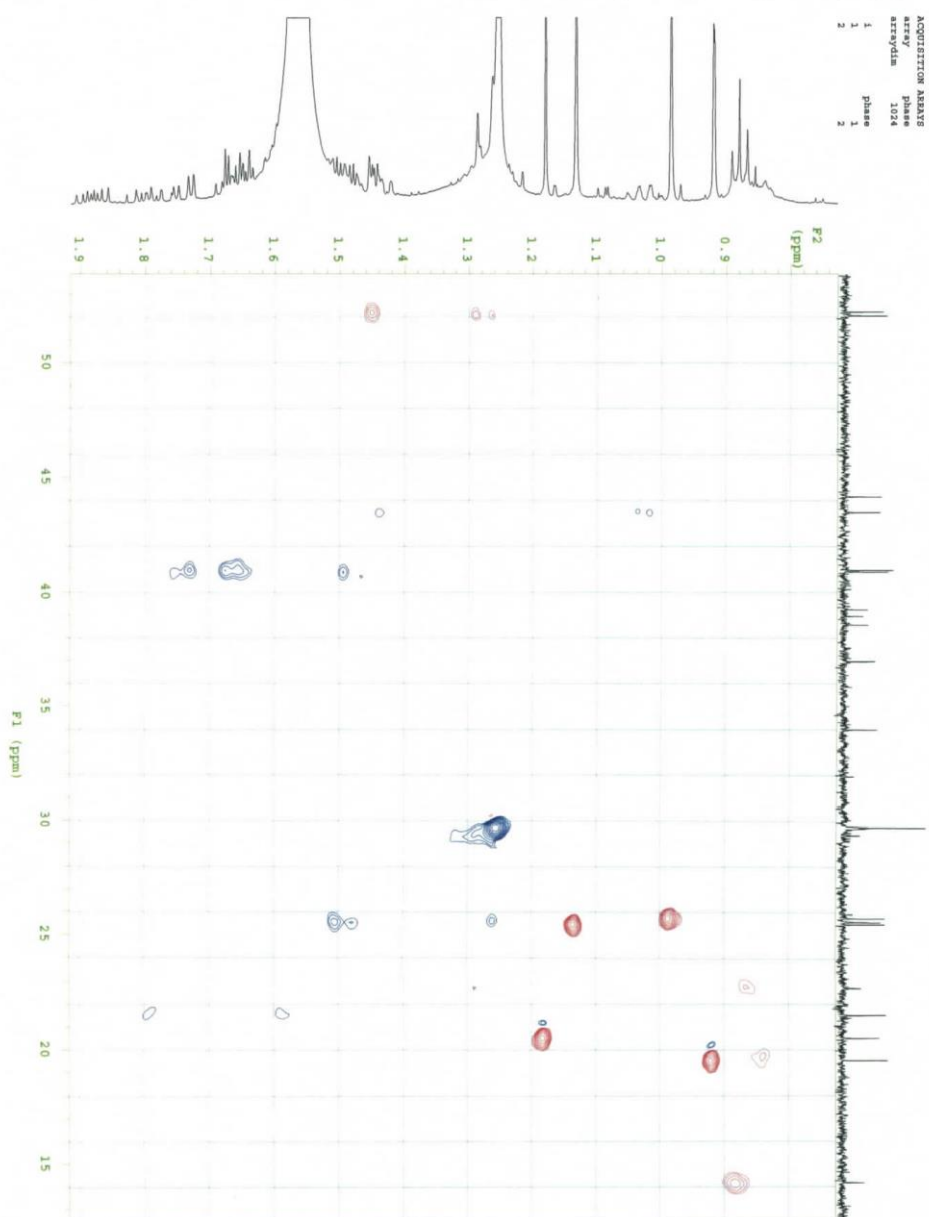
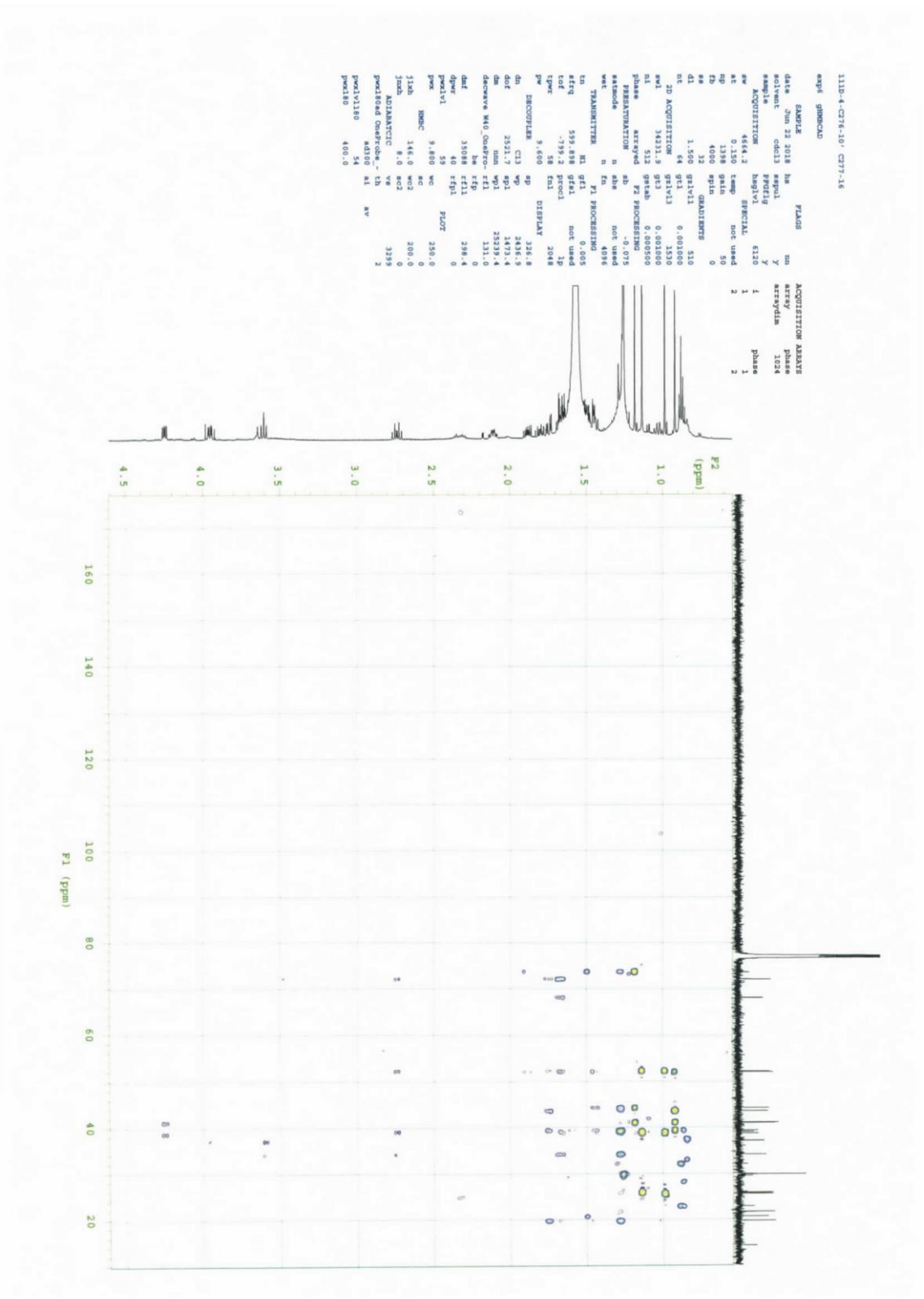


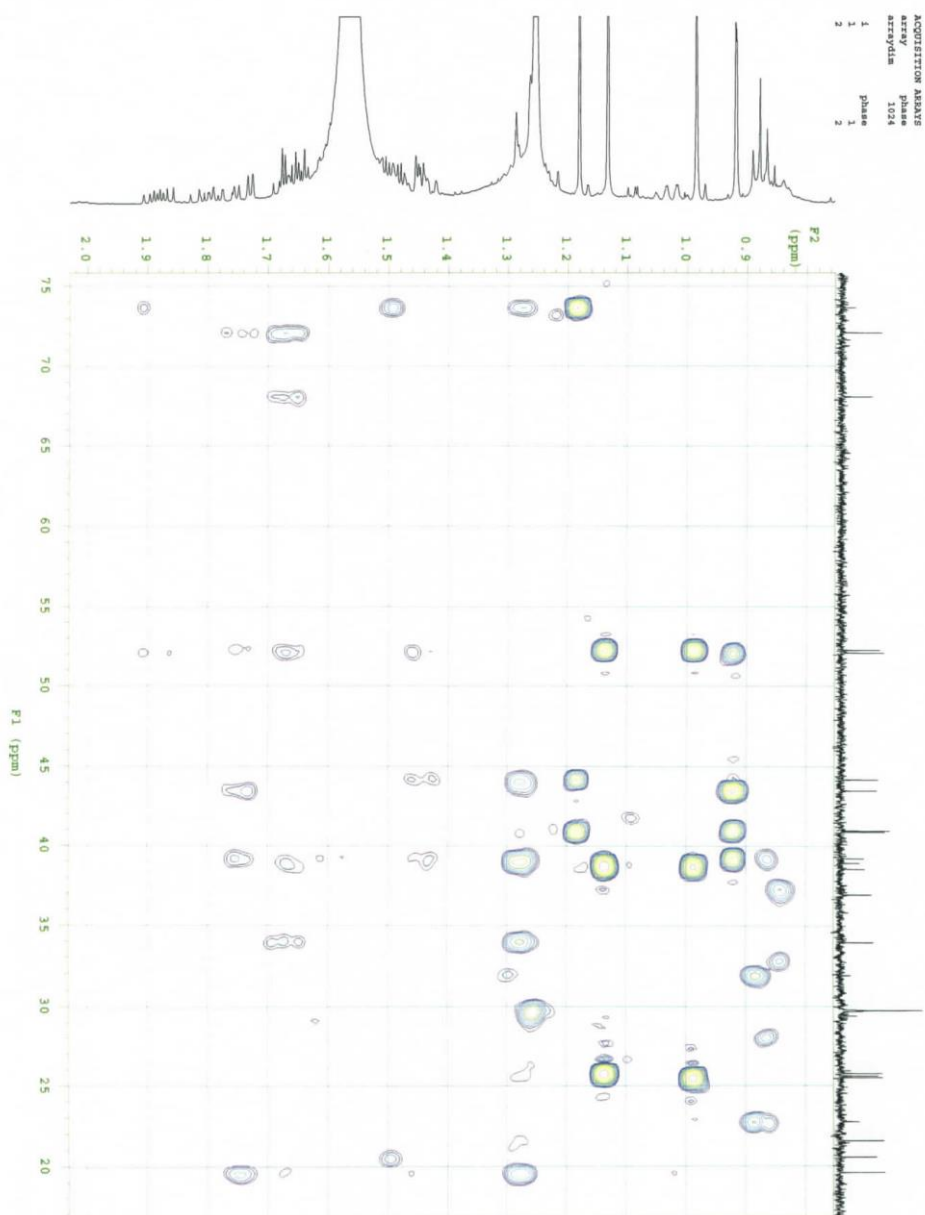
Figure S27 HMBC of 4



111D-4-C276-1D-1 C277.16

exp6 gsmcld

SAMPLE FLAG  
 date 2011.01.18 hr mn  
 solvent cdc13 acq1 y  
 sample 4664.2 proc1g 6120 y  
 ACQUISITION 4664.2 SPECIAL 6120 y  
 ac 0.138 temp not used 2  
 nu 1138 gain 40  
 zb 4600 apin 0  
 as 32 GRADIENTS 510  
 d1 1.500 gainv11 0.00100  
 ac ID ACQUISITION 64 g11v13 0.00100  
 w1 14311.9 0.00100  
 n1 512 grab 0.000500  
 phase arrayed F2 PROCESSING  
 PRESENTATION ab -0.075  
 atmode n abe not used  
 w1 TANMINITEN n f2 not used  
 tn 512 F1 PROCESSING  
 ateq 559.898 gfa1 not used  
 tot -799.2 proc1 1p  
 tpe 58 f01 DISPLAY 2048  
 pw HORIZONTAL 1.600 ap 442.0  
 dh 113 mp 765.2  
 dof 2921.7 ap1 2509.7  
 dm 8925.7  
 deconvolve 940.0 acq1 131.0  
 dnc 15688 f1f1 239.0  
 dnc 15688 f1f1 239.0  
 dnc 40 f1f1 239.0  
 pwr 59 FLOT 250.0  
 pwr 3.800 wc 250.0  
 113h 1461.0 ac 200.0  
 113h 84.0 ac 200.0  
 ADIANTIC 1399  
 postload Overload - lb 2  
 postload 400.0 at av



exp6 gibberCAD

ACQUISITION PARAMETERS  
array phase 1024  
arraybits 1  
phase 2

The figure displays a 2D NMR spectrum with 1D projections on the top and right axes. The horizontal axis (F2) is labeled in ppm and ranges from 1.9 to 0.8. The vertical axis (F1) is labeled in ppm and ranges from 1.9 to 0.8. The 1D projection on the top shows several sharp peaks, with the most prominent ones between 1.0 and 1.3 ppm. The 1D projection on the right shows a broad, noisy baseline. The 2D contour plot shows a series of peaks, with the most intense ones clustered between 1.0 and 1.3 ppm on the F2 axis and between 1.0 and 1.3 ppm on the F1 axis. The peaks are color-coded, with blue representing negative intensity and red representing positive intensity.

**Figure S28 FABMS of 4**

[ Elemental Composition ]  
Data : 1808049 Date : 07-Aug-2018 20:44 Page: 1  
Sample: 111D-4 C277-16  
Note : Matrix; G  
Inlet : Direct Ion Mode : FAB+  
RT : 4.67 min Scan#: (30,35)  
Elements : C 25/15, H 40/30, O 10/0, Na 1/0  
Mass Tolerance : 20ppm, 1mmu if m/z > 50  
Unsaturation (U.S.) : -1.0 - 40.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
345.2415	100.0	+2.7 / +0.9	3.5	C 20 H 34 O 3 Na

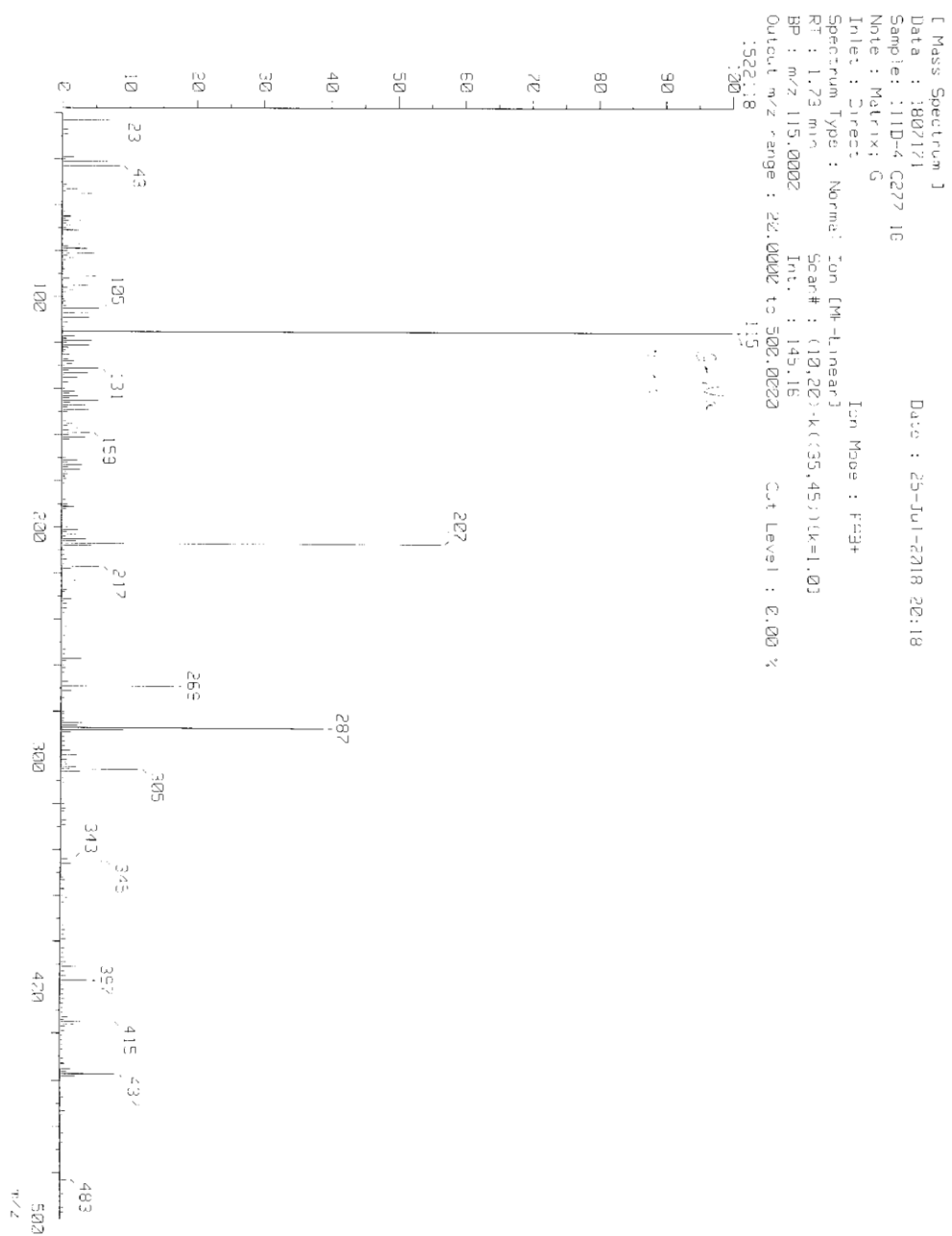
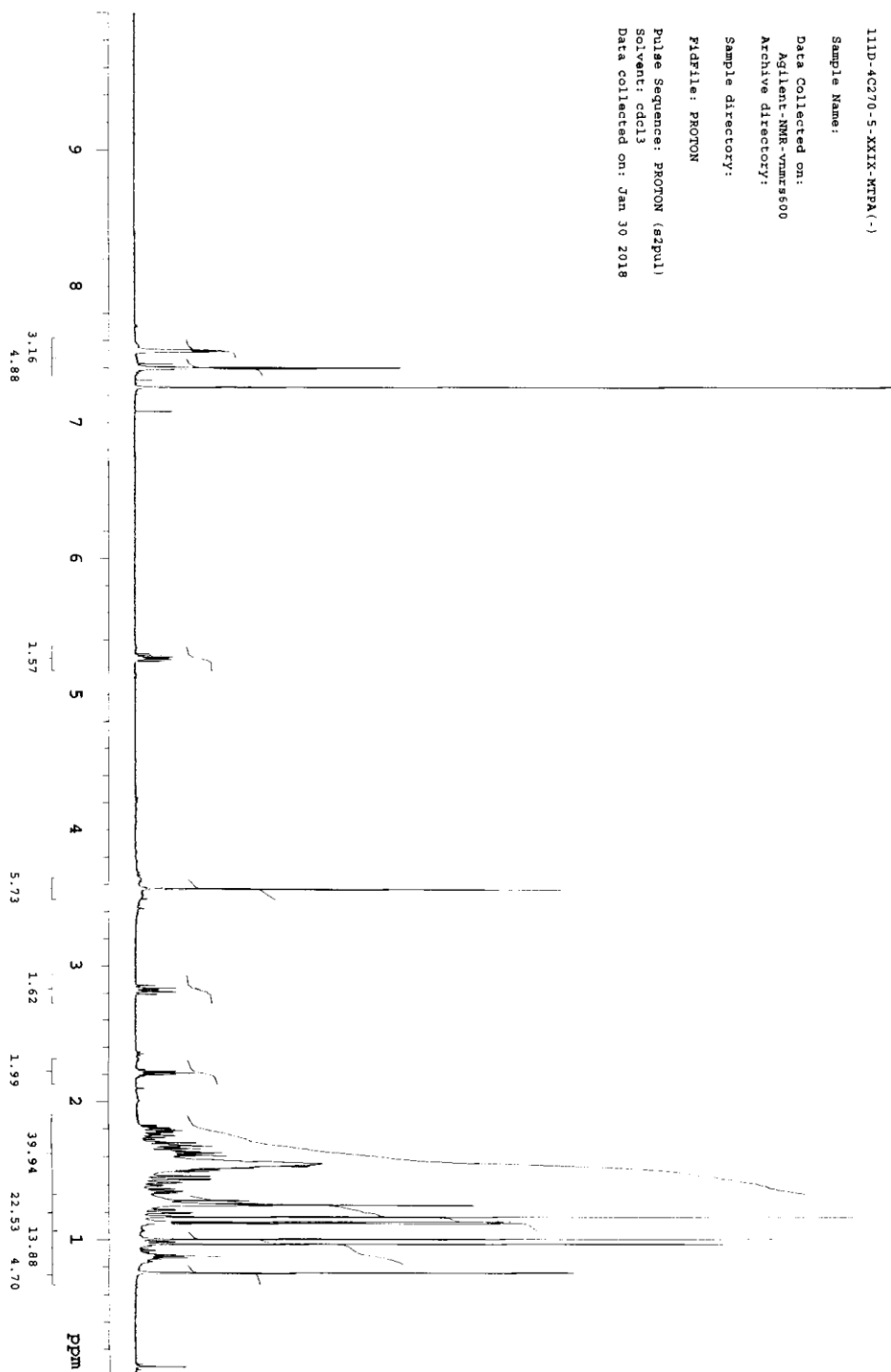
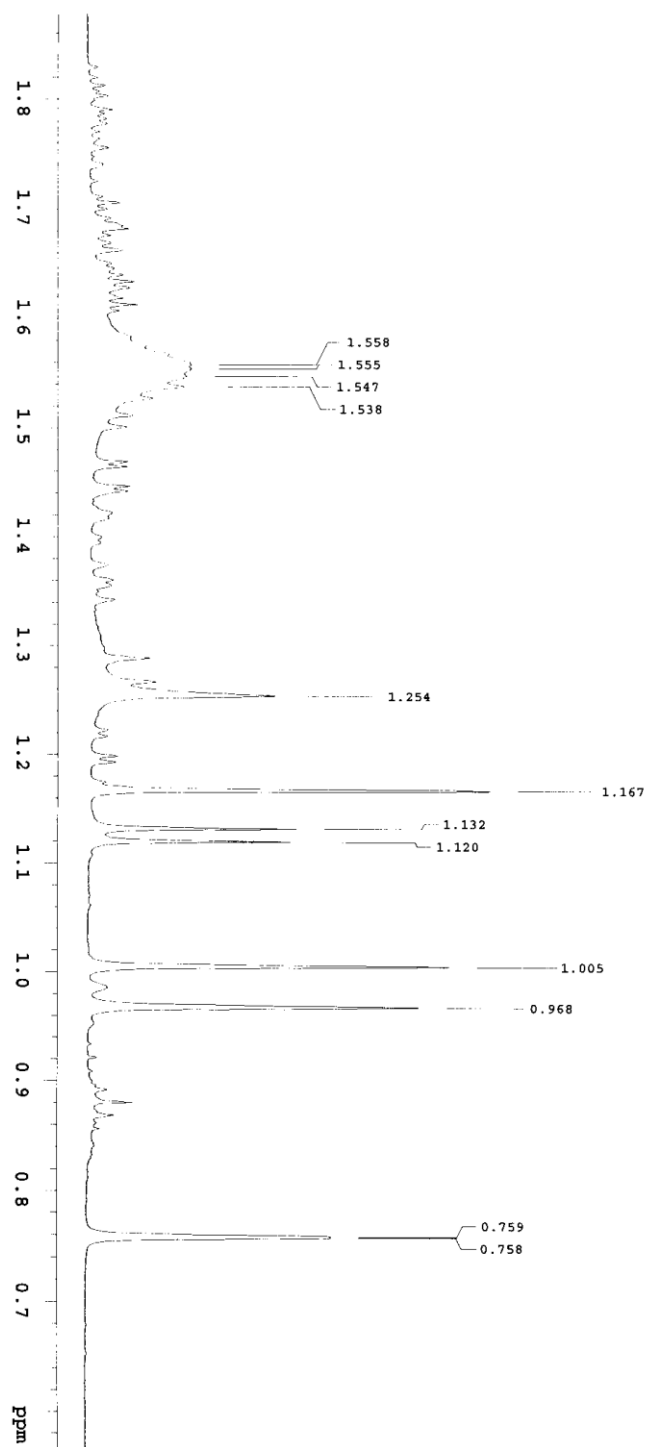


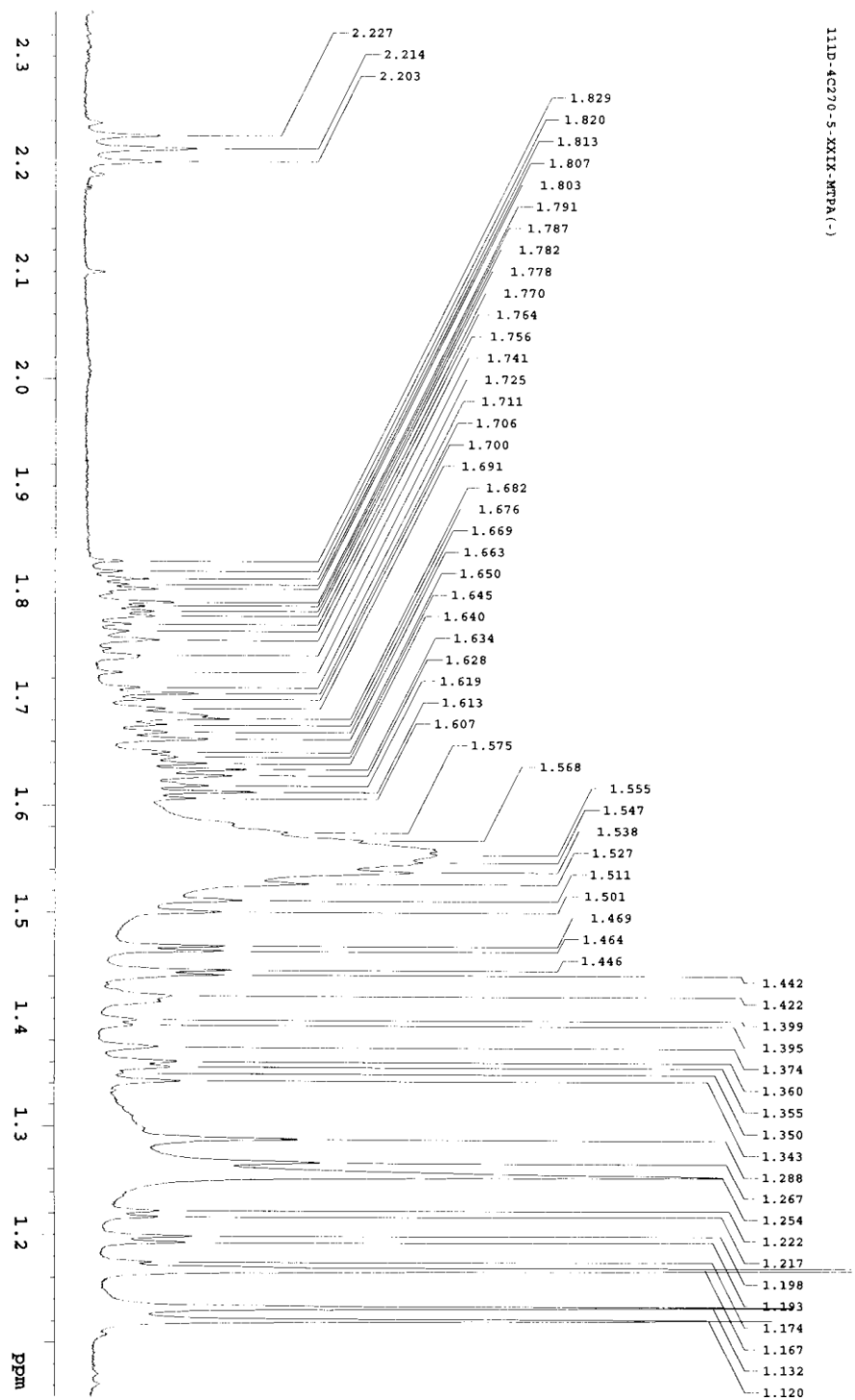
Figure S29  $^1\text{H}$  NMR spectrum of 2a in  $\text{CDCl}_3$



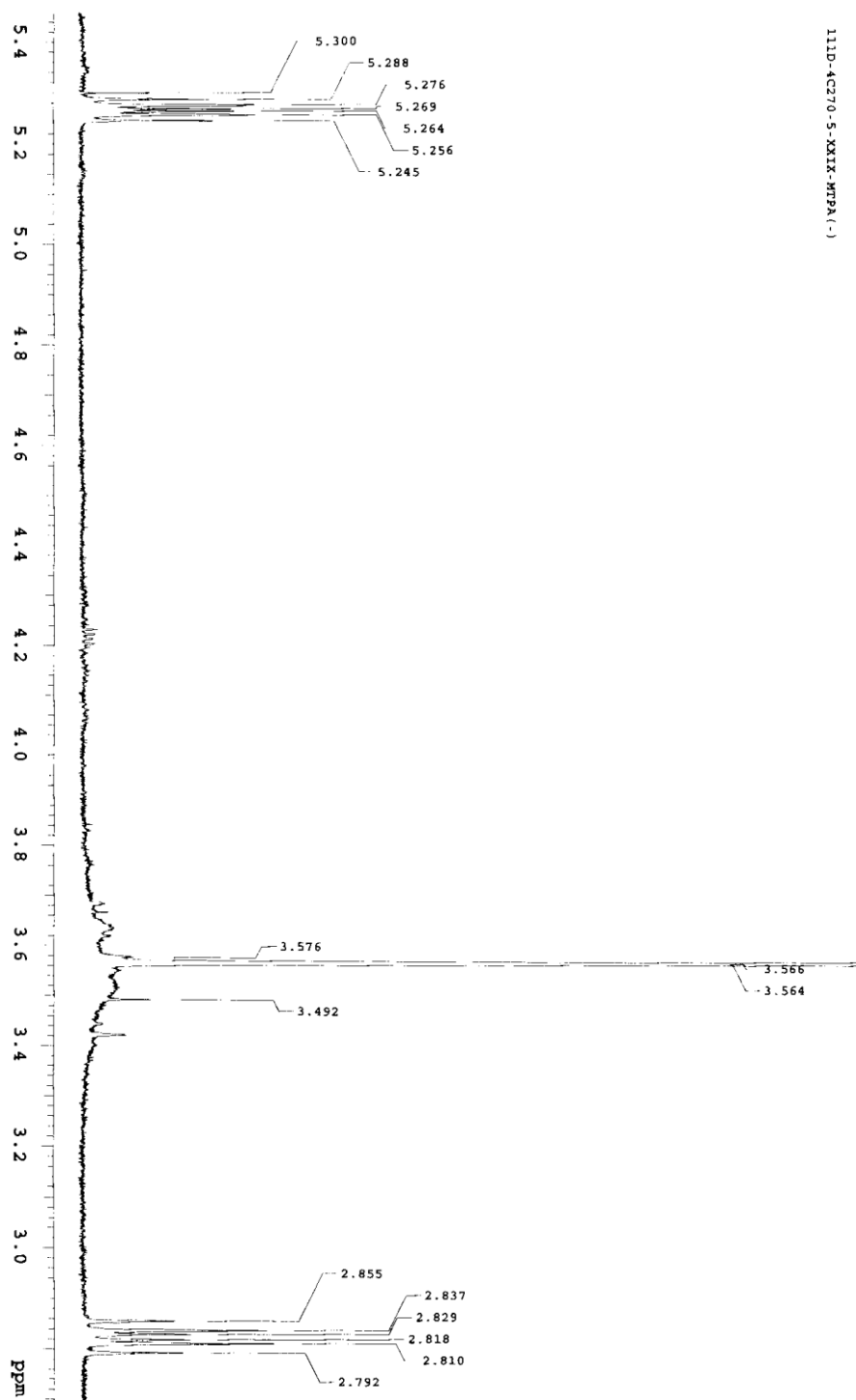
11D-4C270-5-XXIX-MTPA (-)

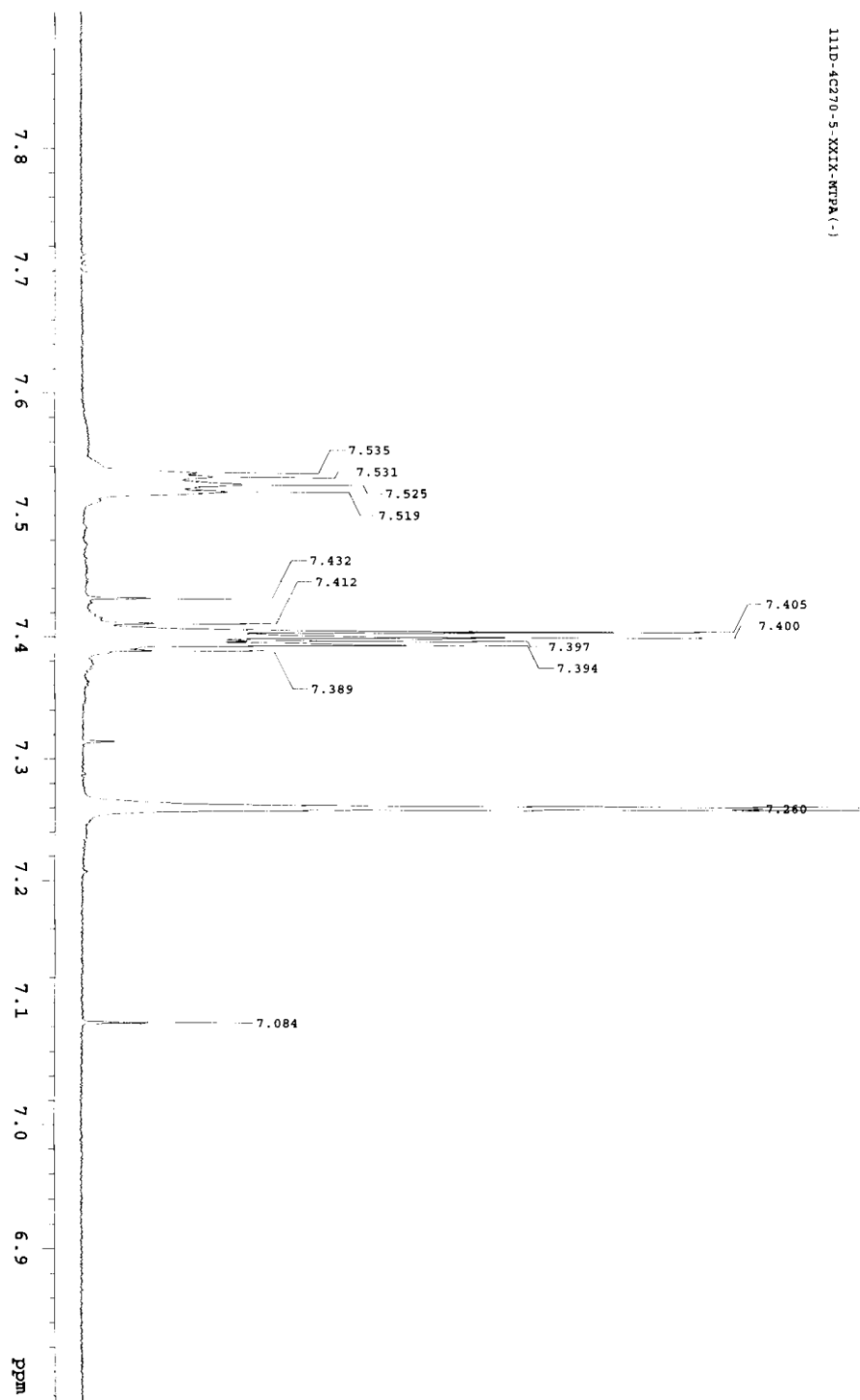




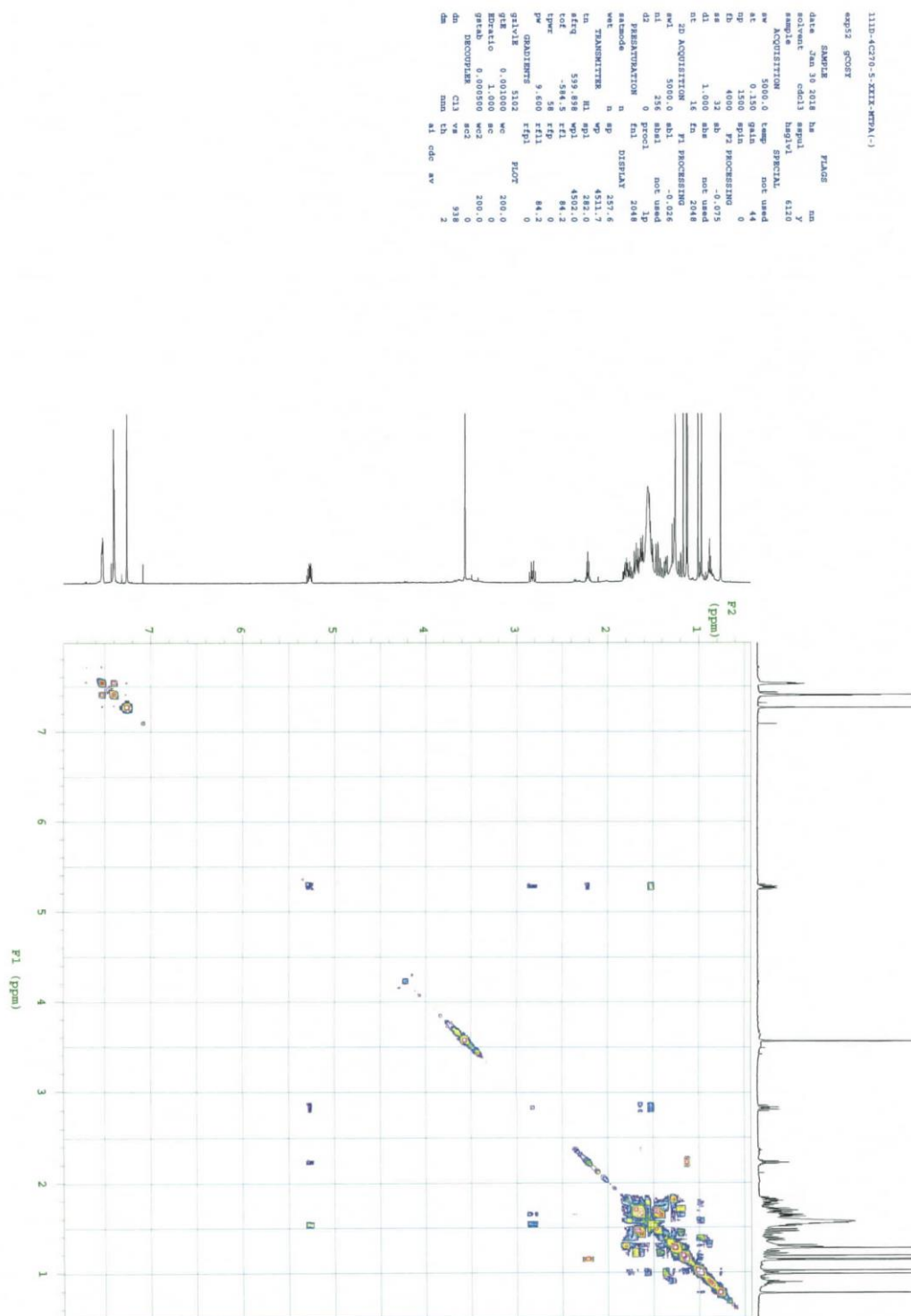


11D-4C270-5-XXIX-MPA (-)



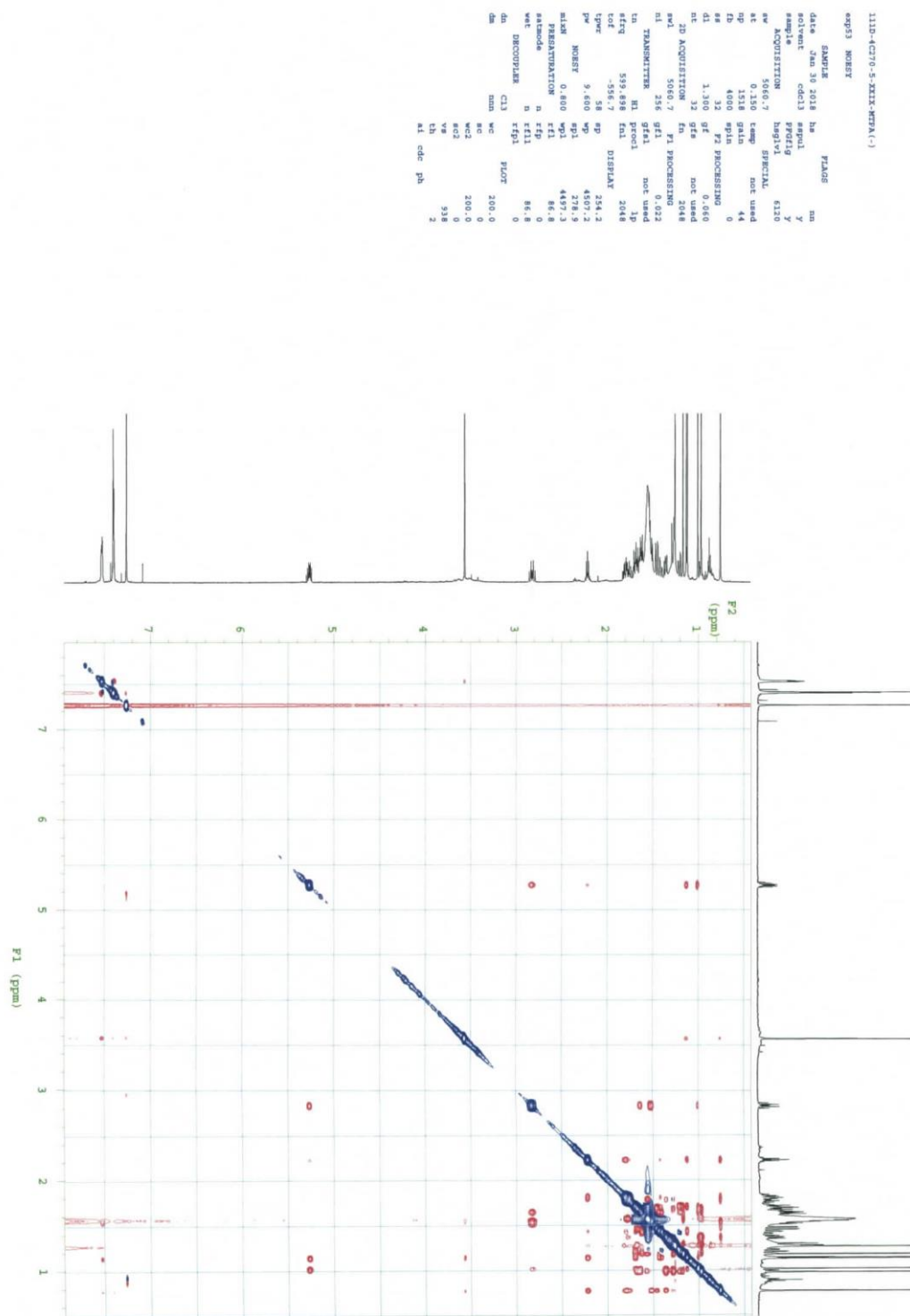


**Figure S30**  $^1\text{H}$ - $^1\text{H}$  COSY of 2a



exp52 gcost

**Figure S31 NOESY of 2a**

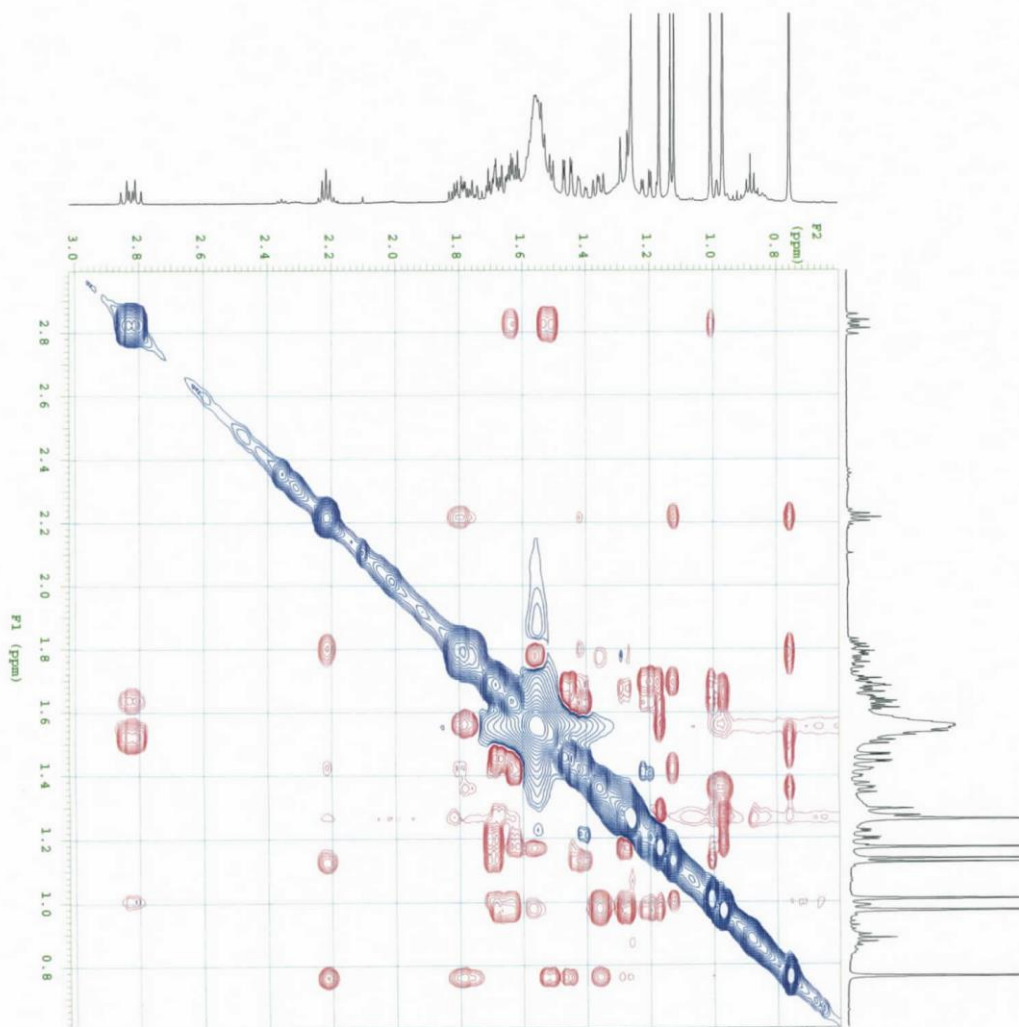


```

111D-4C70-5-KIKK-MPNA(-)
exp53 NOREY

SAMPLE
date 2013.03.18
solvent cdcl3
sample 1
ACQUISITION
aw 5506.7
at 0.130
ab 4600
al 1.300
rt 32
2D ACQUISITION
at 5506.7
ab 4600
al 1.300
rt 32
TRANSMITTEN
in 559.898
ufreq -556.7
pwr 9.600
MAIN PREPARATION
atmode n
wv 86.8
wv1 86.8
wv2 86.8
wv3 86.8
wv4 86.8
wv5 86.8
wv6 86.8
wv7 86.8
wv8 86.8
wv9 86.8
wv10 86.8
wv11 86.8
wv12 86.8
wv13 86.8
wv14 86.8
wv15 86.8
wv16 86.8
wv17 86.8
wv18 86.8
wv19 86.8
wv20 86.8
wv21 86.8
wv22 86.8
wv23 86.8
wv24 86.8
wv25 86.8
wv26 86.8
wv27 86.8
wv28 86.8
wv29 86.8
wv30 86.8
wv31 86.8
wv32 86.8
wv33 86.8
wv34 86.8
wv35 86.8
wv36 86.8
wv37 86.8
wv38 86.8
wv39 86.8
wv40 86.8
wv41 86.8
wv42 86.8
wv43 86.8
wv44 86.8
wv45 86.8
wv46 86.8
wv47 86.8
wv48 86.8
wv49 86.8
wv50 86.8
wv51 86.8
wv52 86.8
wv53 86.8
wv54 86.8
wv55 86.8
wv56 86.8
wv57 86.8
wv58 86.8
wv59 86.8
wv60 86.8
wv61 86.8
wv62 86.8
wv63 86.8
wv64 86.8
wv65 86.8
wv66 86.8
wv67 86.8
wv68 86.8
wv69 86.8
wv70 86.8
wv71 86.8
wv72 86.8
wv73 86.8
wv74 86.8
wv75 86.8
wv76 86.8
wv77 86.8
wv78 86.8
wv79 86.8
wv80 86.8
wv81 86.8
wv82 86.8
wv83 86.8
wv84 86.8
wv85 86.8
wv86 86.8
wv87 86.8
wv88 86.8
wv89 86.8
wv90 86.8
wv91 86.8
wv92 86.8
wv93 86.8
wv94 86.8
wv95 86.8
wv96 86.8
wv97 86.8
wv98 86.8
wv99 86.8
wv100 86.8

```



**Figure S32 FABMS of 2a**

[ Elemental Composition ]  
Data : 1802046 Date : 14-Feb-2018 18:14 Page: 1  
Sample: 111D-4 C271-5 MTPA(-) XXIX  
Note : Matrix; NBA+Na  
Inlet : Direct Ion Mode : FAB+  
RT : 4.77 min Scan#: (40,45)  
Elements : C 33/28, H 45/35, F 5/0, O 10/0, Na 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
545.2860	100.0	+1.0 / +0.5	8.5 C 30 H 41 F 3 O 4 Na



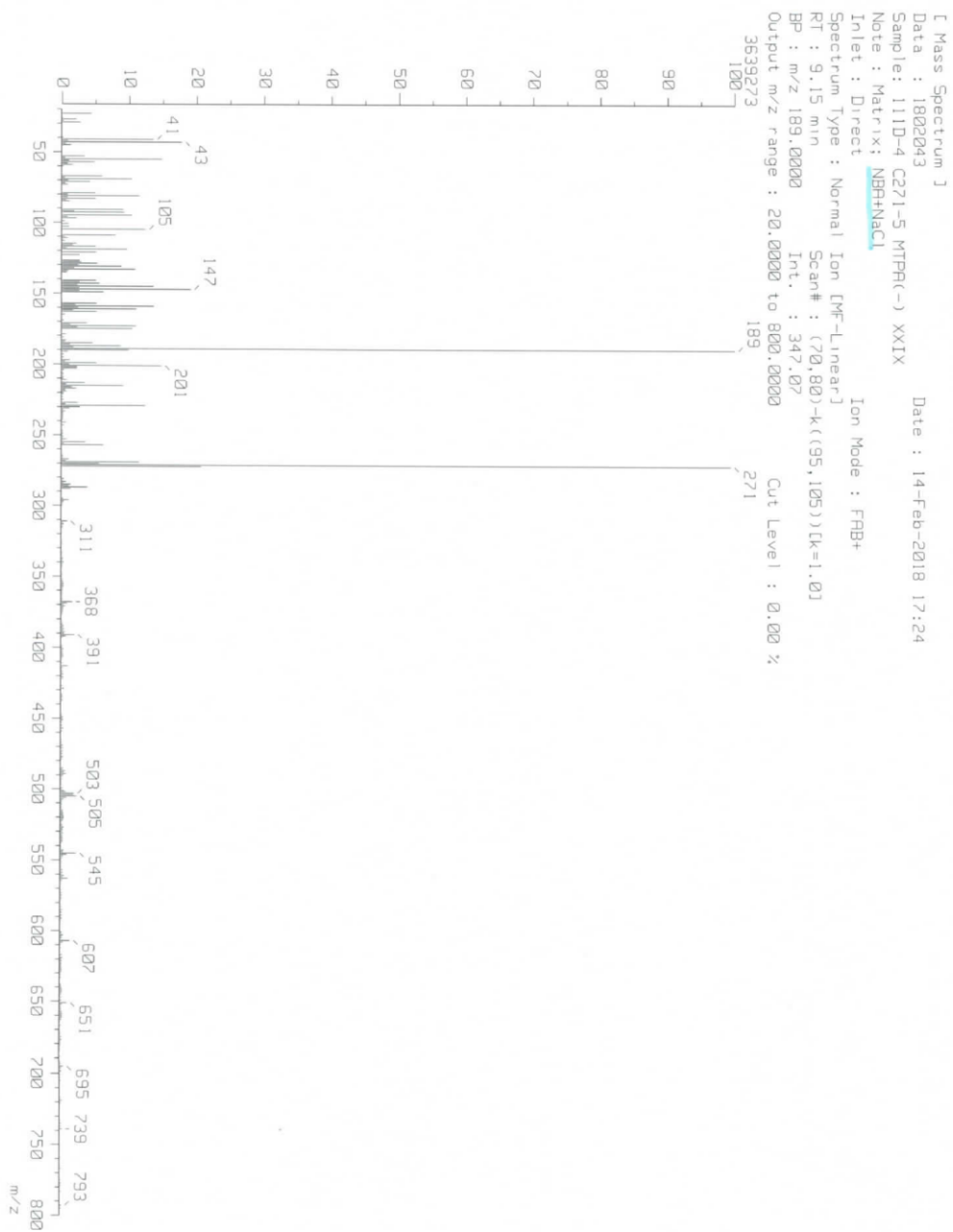
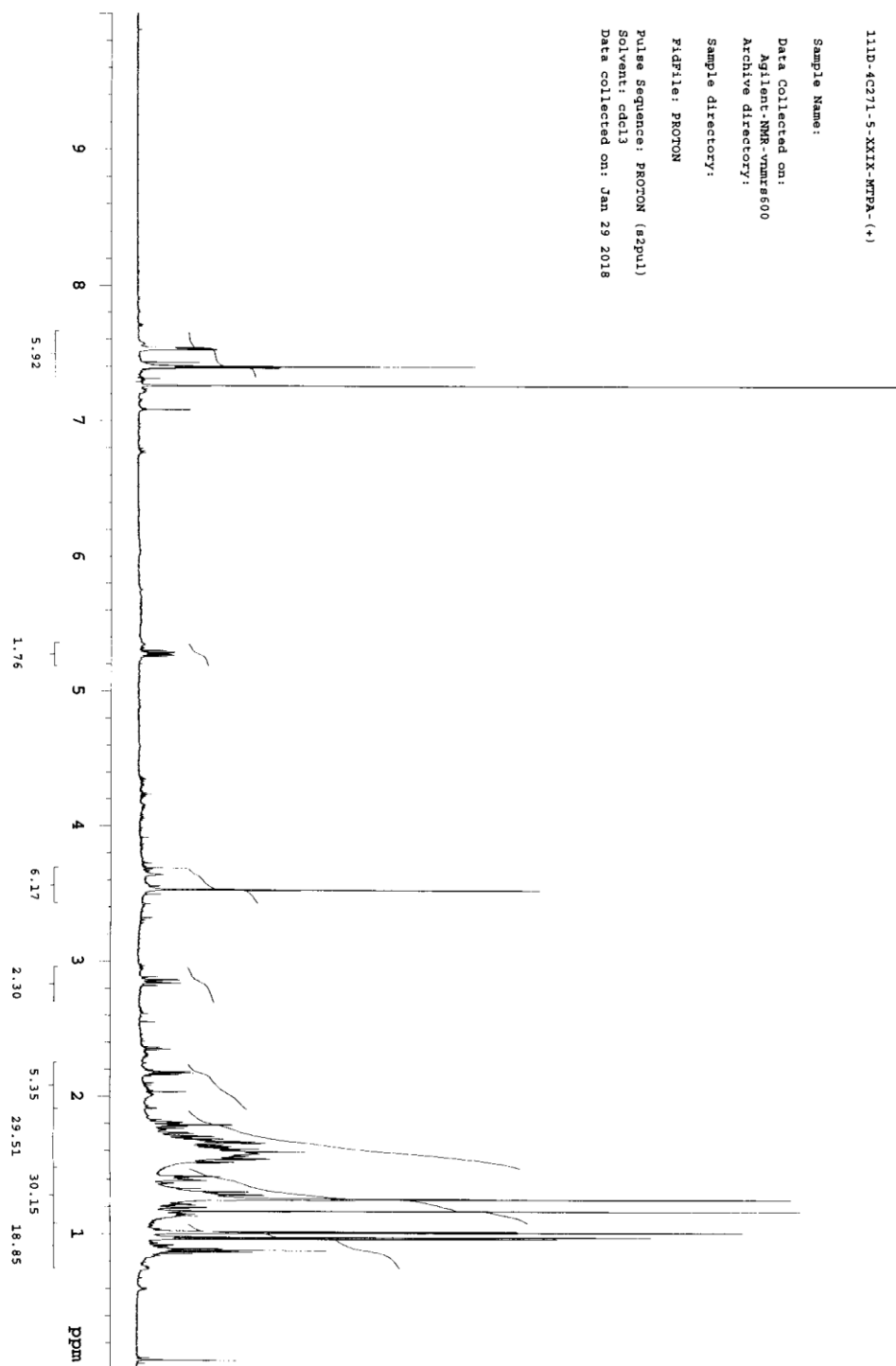
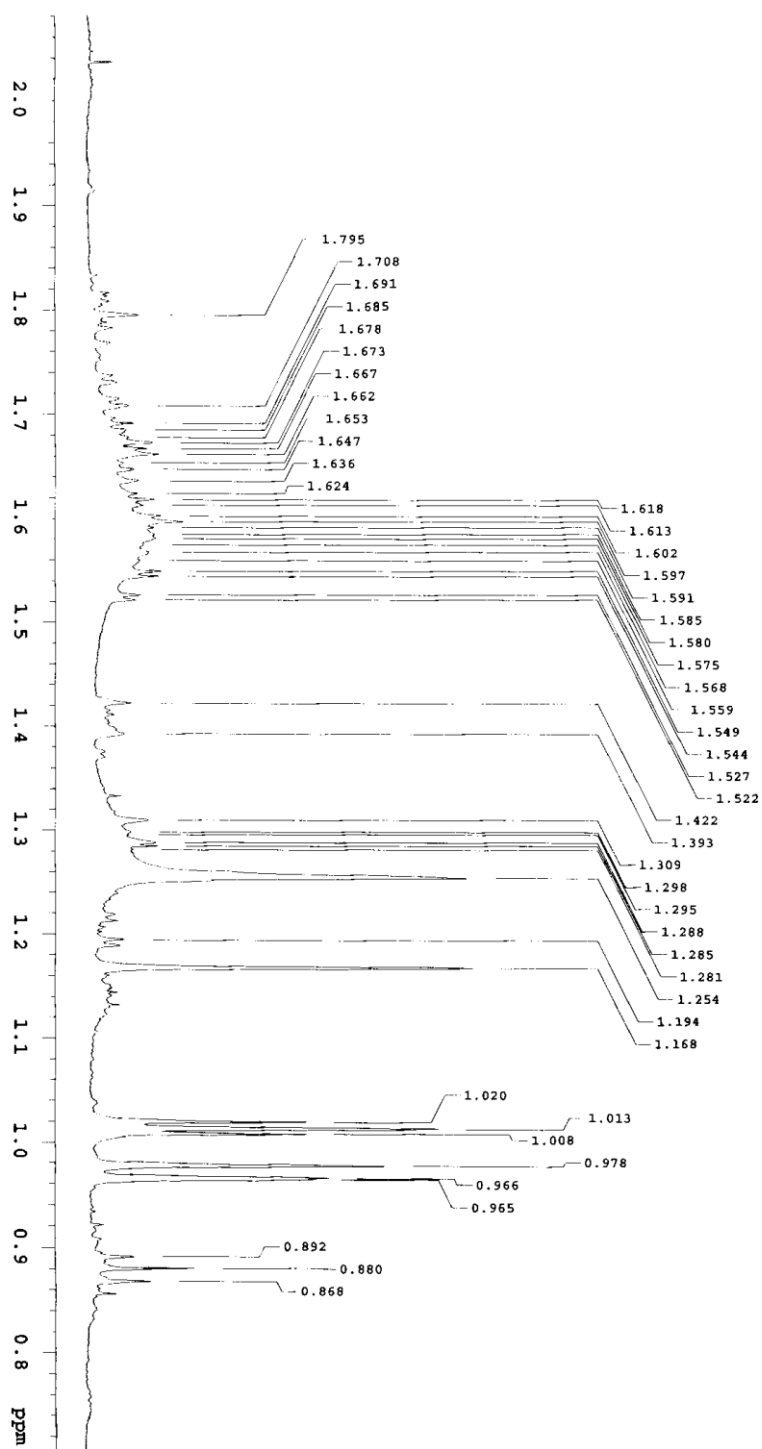
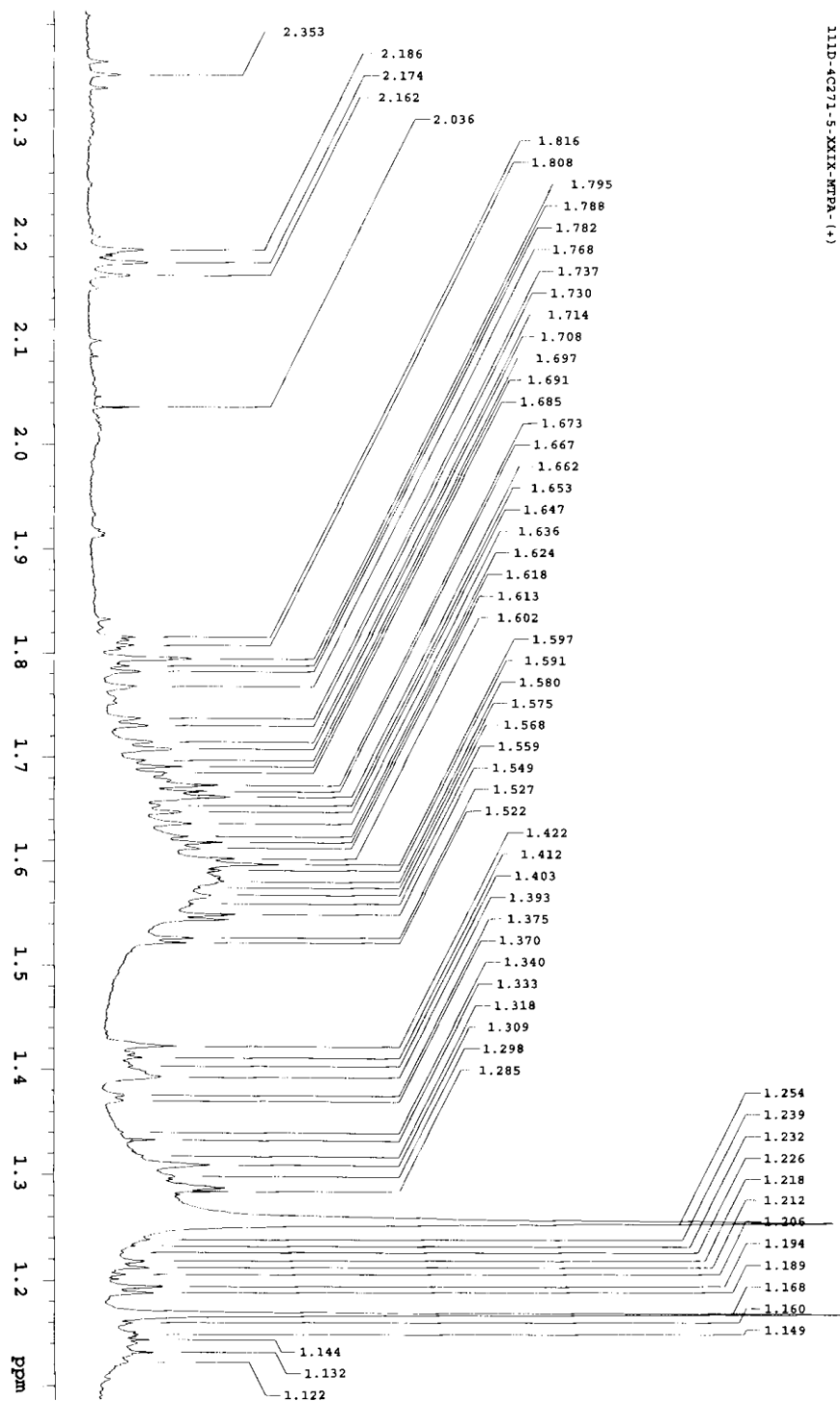


Figure S33  $^1\text{H}$  NMR spectrum of 2b in  $\text{CDCl}_3$

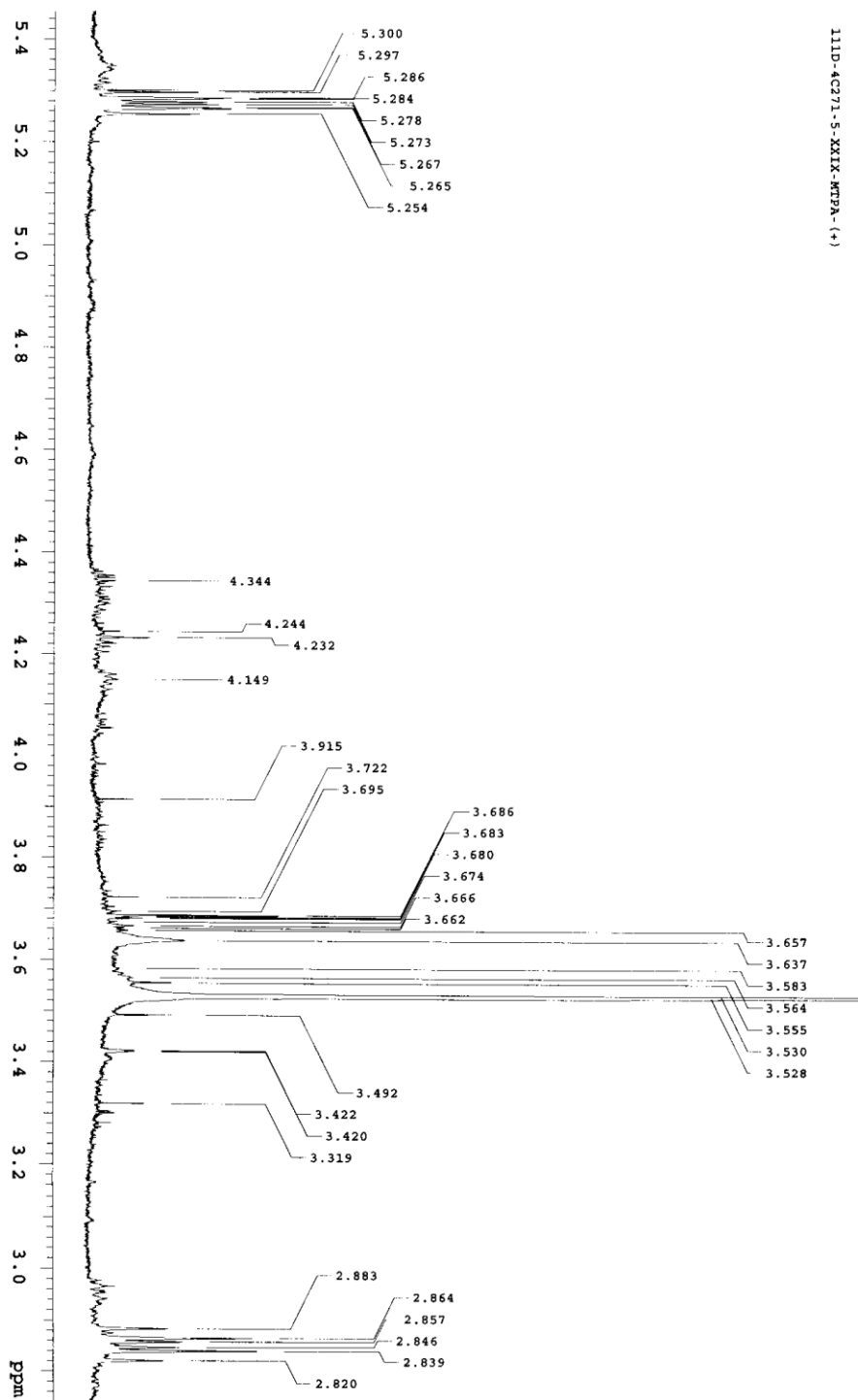


11ID-4CZ71-5-XXIX-MTPA- (+)

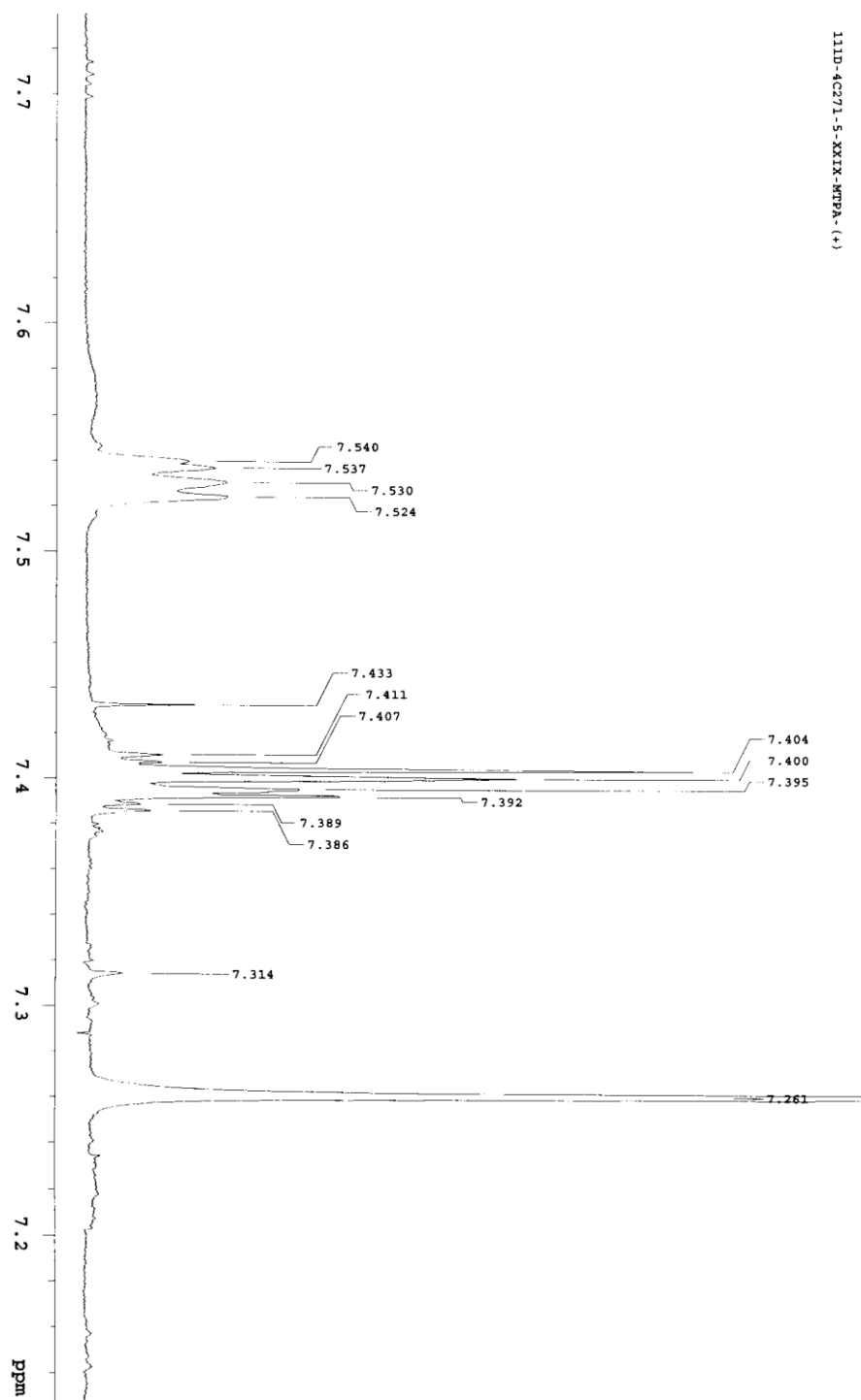


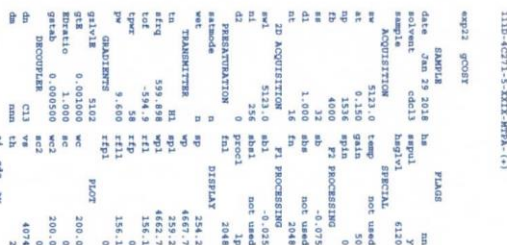


11D-4C271-5-XXIX-MTPA-(+)



11D-4C271.5-XXIX-MTPA-(+)

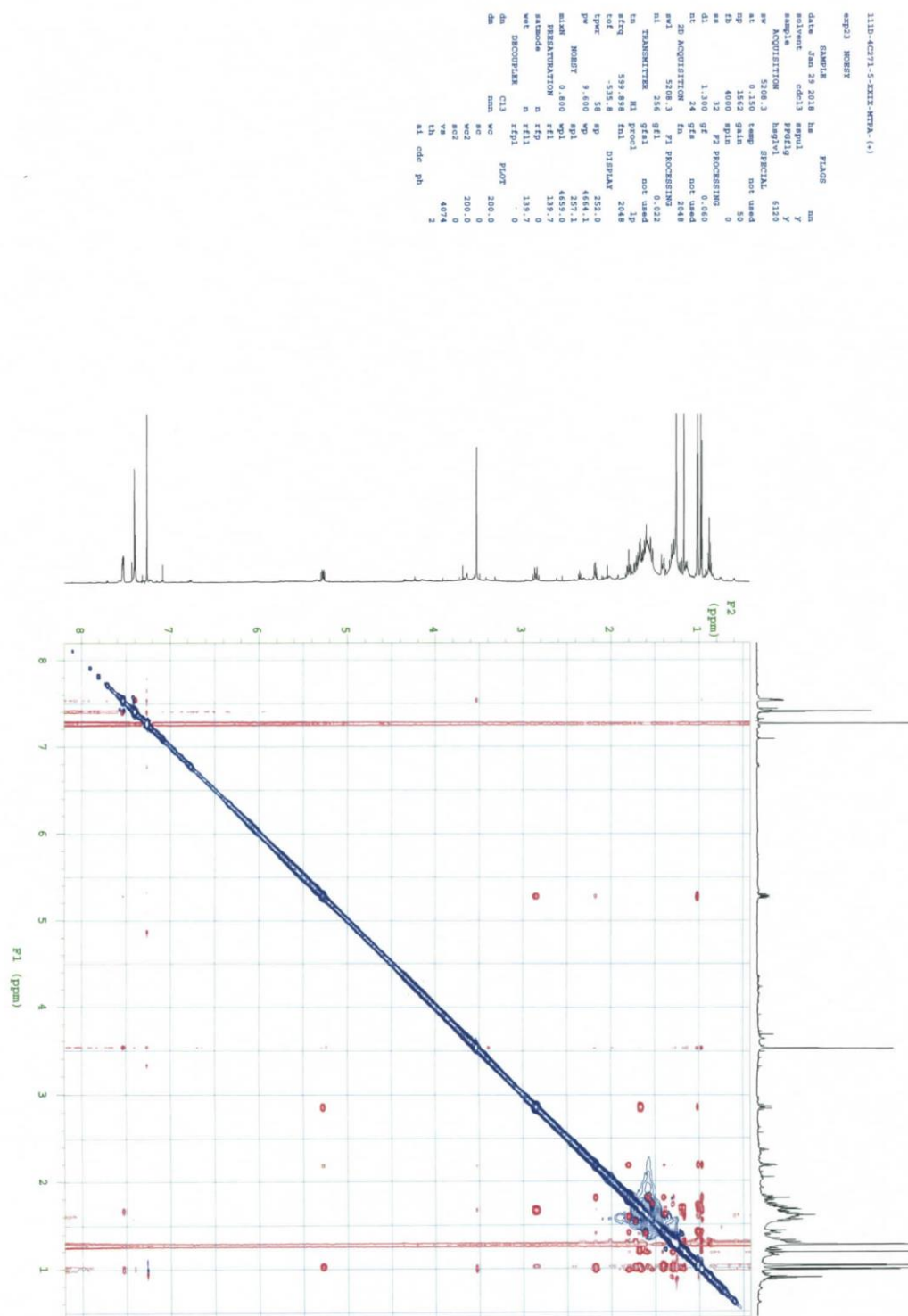




[illegible]



**Figure S35** NOESY of 2b



exp23: MOKSY

**Figure S36 FABMS of 2b**

[ Elemental Composition ]  
Data : 1802047 Date : 14-Feb-2018 18:26 Page: 1  
Sample: 111D-4 C271-5 MTPA(+) XXIX  
Note : Matrix; NBA+Na  
Inlet : Direct Ion Mode : FAB+  
RT : 5.34 min Scan#: (45,50)  
Elements : C 32/28, H 45/35, F 5/0, O 10/0, Na 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
545.2849	100.0	-1.1 / -0.6	8.5 C 30 H 41 F 3 O 4 Na

