Supplementary Information

Sterepinic acids A–C, new carboxylic acids produced by a marine alga-derived Fungus

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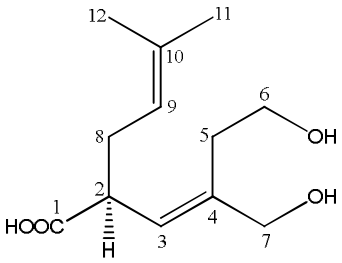
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7

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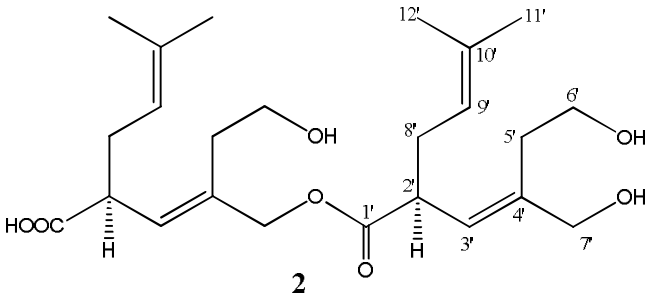
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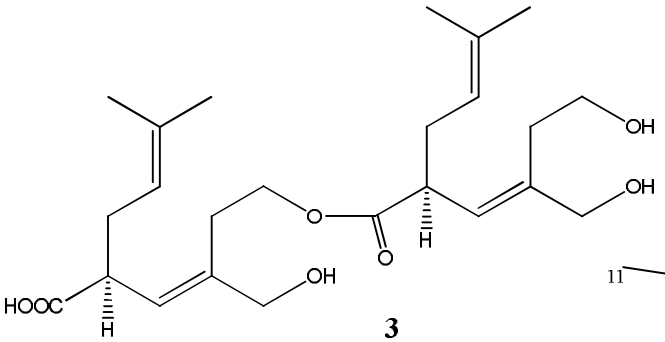
7'

2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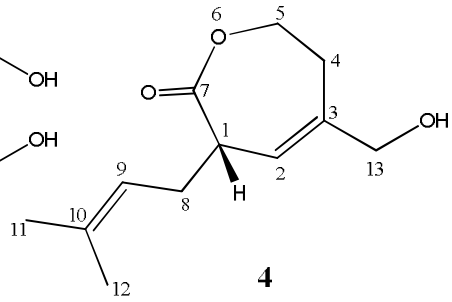
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8
10
11
12

4

Table S1 NMR spectral data of **1** in $CDCl_3$

Position	δ_H[a]		J/Hz	^1H-^1H COSY	NOESY[b]	δ_C		HMBC (C)[c]
1						177.5	(s)	
2	3.27	m		3, 8A, 8B	9, 11, 12	44.9	(d)	1, 3, 4, 8, 9
3	5.50	d	10.2 (2)	2	8A, 8B, 9, 11, 12	127.0	(d)	1, 2, 5, 7, 8
4						138.7	(s)	
5A	2.25	m		5B, 6		31.9	(t)	3, 4, 6, 7
5B	2.49	m		5A, 6				3, 4, 6, 7
6	3.68	br s		5A, 5B	11, 12	61.0	(t)	4
7	4.03	br s			3, 11, 12	66.8	(t)	3, 4, 5
8A	2.20	m		2, 8B, 9	3, 11, 12	30.9	(t)	1, 2, 3, 9, 10
8B	2.44	m		2, 8A, 9	3, 11, 12			1, 2, 3, 9, 10
9	5.04	dd	7.2 (8), 7.2 (8)	8A, 8B	2, 3, 11, 12	120.2	(d)	2, 8, 11, 12
10						134.1	(s)	
11	1.67	s			2, 3, 6, 7, 8A, 8B, 9	25.7	(q)	9, 10, 12
12	1.60	s			2, 3, 6, 7, 8A, 8B, 9	17.8	(q)	9, 10, 11

a ^1H chemical shift values (δ ppm from $SiMe_4$) 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 protones are removed. c Long range ^1H-^{13}C correlations from H to C observed in the HMBC experiment

Table S2 NMR spectral data of **2** in $CDCl_3$

Position	δ_H[a]		J/Hz	^{1}H-^{1}H COSY	NOESY[b]	δ_C	HMBC (C)[c]
1						173.5 (s)	
2	3.28	m		3, 8A, 8B	5, 9	45.4 (d)	1, 3, 4, 8, 9
3	5.49	d	10.8 (2)	2	7A, 7B, 8A, 8B	129.3 (d)	2, 5, 7, 8
4						133.9 (s)	
5A	2.18	m		5B, 6A, 6B	2	32.3 (t)	3, 4, 6, 7
5B	2.54	m		5A, 6A, 6B	2		3, 4, 6, 7
6A	3.65	br s		5A, 5B, 6B		61.4 (t)	
6B	3.72	br s		5A, 5B, 6A			
7A	4.48	d	13.2 (7B)	7B	3	67.9 (t)	1, 3, 4, 5
7B	4.62	d	13.2 (7A)	7A	3		1, 3, 4, 5
8A	2.20	m		2, 8B, 9	3, 11, 12	30.8[d1] (t)	1, 2, 3, 9, 10
8B	2.46	m		2, 8A, 9	3, 11, 12		1, 2, 3, 9, 10
9	5.03	m		8A, 8B	2, 11, 12	120.2[d2] (d)	2, 8, 11, 12
10						134.2[d3] (s)	
11	1.67	s			9	25.7 (q)	9, 10, 12
12	1.60	s			8A, 8B, 9	17.8 (q)	9, 10, 11
1'						173.5 (s)	
2'	3.28	m		3', 8'A, 8'B	5', 9'	45.4 (d)	1', 8', 9'
3'	5.52	d	10.2 (2')	2'	7', 8'A, 8'B	127.2 (d)	5', 7'
4'						139.6 (s)	
5'A	2.29	m		5'B, 6'	2'	32.3 (t)	3', 4', 6', 7'
5'B	2.54	m		5'A, 6'	2'		3', 4', 6', 7'
6'	3.72	br s		5'A, 5'B		60.5 (t)	
7'	4.05	br s			3'	67.5 (t)	3', 4', 5'
8'A	2.20	m		2', 8'B, 9'	3', 11', 12'	30.6[d1] (t)	1', 2', 3', 9', 10'
8'B	2.46	m		2', 8'A, 9'	3', 11', 12'		1', 2', 3', 9', 10'
9'	5.03	m		8'A, 8'B	2', 11', 12'	120.3[d2] (d)	2', 8', 11', 12'
10'						134.3[d3] (s)	
11'	1.67	s			9'	25.7 (q)	9', 10', 12'
12'	1.60	s			8'A, 8'B, 9'	17.8 (q)	9', 10', 11'

a 1H che+B14:L36mical shift values (d 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 protones are removed. c Long range 1H-13C correlations from H to C observed in the HMBC experiment. d1-d3 interchangeable

Table S3 NMR spectral data of **3** in $CDCl_3$

Position	δ_H[a]		J/Hz	^{1}H-^{1}H COSY	NOESY[b]	δ_C	HMBC (C)[c]
1						174.3 (s)	
2	3.28	m		3, 8A, 8B	5, 9	44.9 (d)	1, 8, 9
3	5.55	d	9.6 (2)	2	7, 9	129.3 (d)	5, 7
4						137.9 (s)	
5A	2.30	ddd	14.4 (5B), 5.4 (6), 5.4 (6)	5B, 6	2	27.7 (t)	3, 4, 6, 7
5B	2.54	ddd	14.4 (5B), 5.4 (6), 5.4 (6)	5A, 6	2		3, 4, 6, 7
6	4.20	m		5A, 5B		63.5 (t)	1', 4
7	4.07	m			3	66.5 (t)	3, 4
8A	2.20	m		2, 8B, 9	12	31.4 (t)	1, 2, 3, 9, 10
8B	2.44	m		2, 8A, 9	12		1, 2, 3, 9, 10
9	5.02[d1]	dd	7.2 (8A), 7.2 (8B)	8A, 8B	2, 3, 11	120.2[d2] (d)	2, 8, 11, 12
10						134.3 (s)	
11	1.67	s			9	25.7 (q)	9, 10, 12
12	1.59[d3]	s			8A, 8B	17.8[d4] (q)	9, 10, 11
1'						174.3 (s)	
2'	3.28	m		3', 8'A, 8'B	5', 9'	44.9 (d)	1', 3', 4', 8', 9'
3'	5.51	d	9.6 (2')	2'	7', 8'A, 8'B, 9'	127.2 (d)	1', 2', 5', 7', 8'
4'						138.7 (s)	
5'A	2.25	m		5'B, 6'A, 6'B	2'	32.2 (t)	3', 4', 6', 7'
5'B	2.51	m		5'A, 6'A, 6'B	2'		3', 4', 6', 7'
6'A	3.65	br s		5'A, 5'B, 6'B		61.1 (t)	
6'B	3.71	br s		5'A, 5'B, 6'A			
7'	4.02	m			3'	67.4 (t)	3', 4'
8'A	2.20	m		2', 8'B, 9'	12'	31.4 (t)	1', 2', 3', 9', 10'
8'B	2.44	m		2', 8'A, 9'	12'		1', 2', 3', 9', 10'
9'	5.06[d1]	dd	7.2 (8'A), 7.2 (8'B)	8'A, 8'B	2', 3', 11'	120.3[d2] (d)	11', 12'
10'						134.3 (s)	
11'	1.67	s			9'	25.7 (q)	9', 10', 12'
12'	1.61[d3]	s			8'A, 8'B	17.9[d4] (q)	9', 10', 11'

a 1H che+B23:L35mical shift values (d 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 protones are removed. c Long range 1H-13C correlations from H to C observed in the HMBC experiment. d1-d4 interchangeable

Table S4 NMR spectral data of **4** in $CDCl_3$

Position	δ_H[a]		J/Hz	^1H-^1H COSY	NOESY[b]	δ_C		HMBC (C)[c]
1	3.68	m		2, 8A, 8B	9	40.2	(d)	
2	5.36	br s		1	8A, 8B, 9,13A, 13B	121.2	(d)	4, 7, 8, 13
3						139.2	(s)	
4A	2.45	br d	19.2 (5B)	4B, 5	13A	30.3	(t)	
4B	2.59	m		5A, 5B, 6B	13B			
5α	4.68	ddd	12.6 (4B), 12.6 (5β), 1.8 (4A)	4, 5β		64.4	(t)	3, 4, 7
5β	4.33	ddd	12.6 (5α), 4.8 (4B), 2.4 (4A)	4, 5α				3, 4, 7
6								
7						174.3	(s)	
8A	2.33	ddd	14.4 (8B), 6.6 (1), 6.6 (9)	1, 8B, 9	2, 11	30.1	(t)	1, 2, 7, 9, 10
8B	2.52	ddd	14.4 (8A), 6.6 (1), 6.6 (9)	1, 8A, 9	2, 11			1, 2, 7, 9, 10
9	5.14	dd	6.6 (8A), 6.6 (8B)	8A, 8B	1, 2, 11	120.9	(d)	1, 8, 11, 12
10						134.6	(s)	
11	1.72	s			9	25.8	(q)	9, 10, 12
12	1.67	s			8A, 8B	18.0	(q)	9, 10, 12
13A	3.99	d	13.8 (13B)		2, 4	67.4	(t)	2, 3, 4
13B	4.01	d	13.8 (13A)		2, 4			

a ^1H chemical shift values (δ ppm from $SiMe_4$) 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 protones are removed. c Long range ^1H-^{13}C correlations from H to C observed in the HMBC experiment.

Figure S1 ^{1}H NMR spectrum of 1

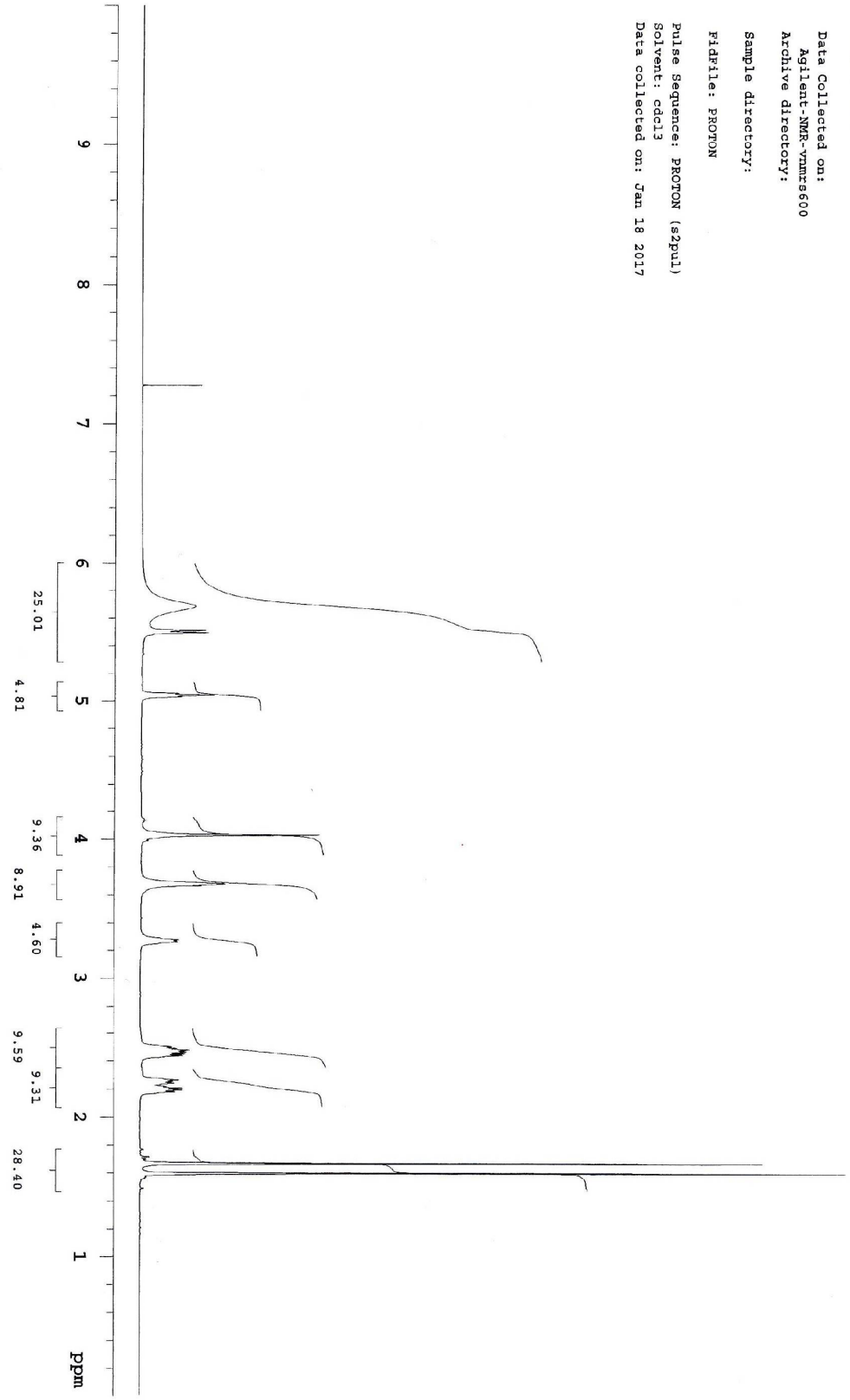

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Figure S2 ^{13}C NMR spectrum of 1 in $CDCl_3$

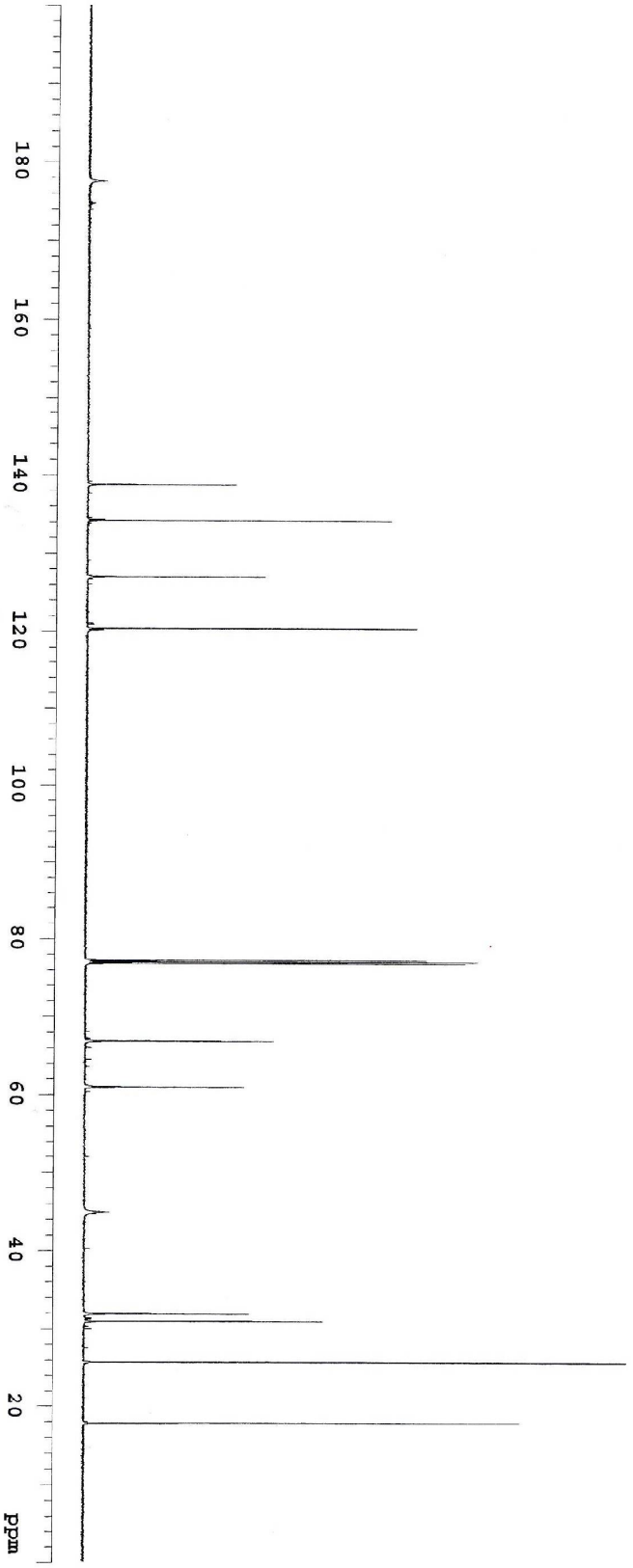
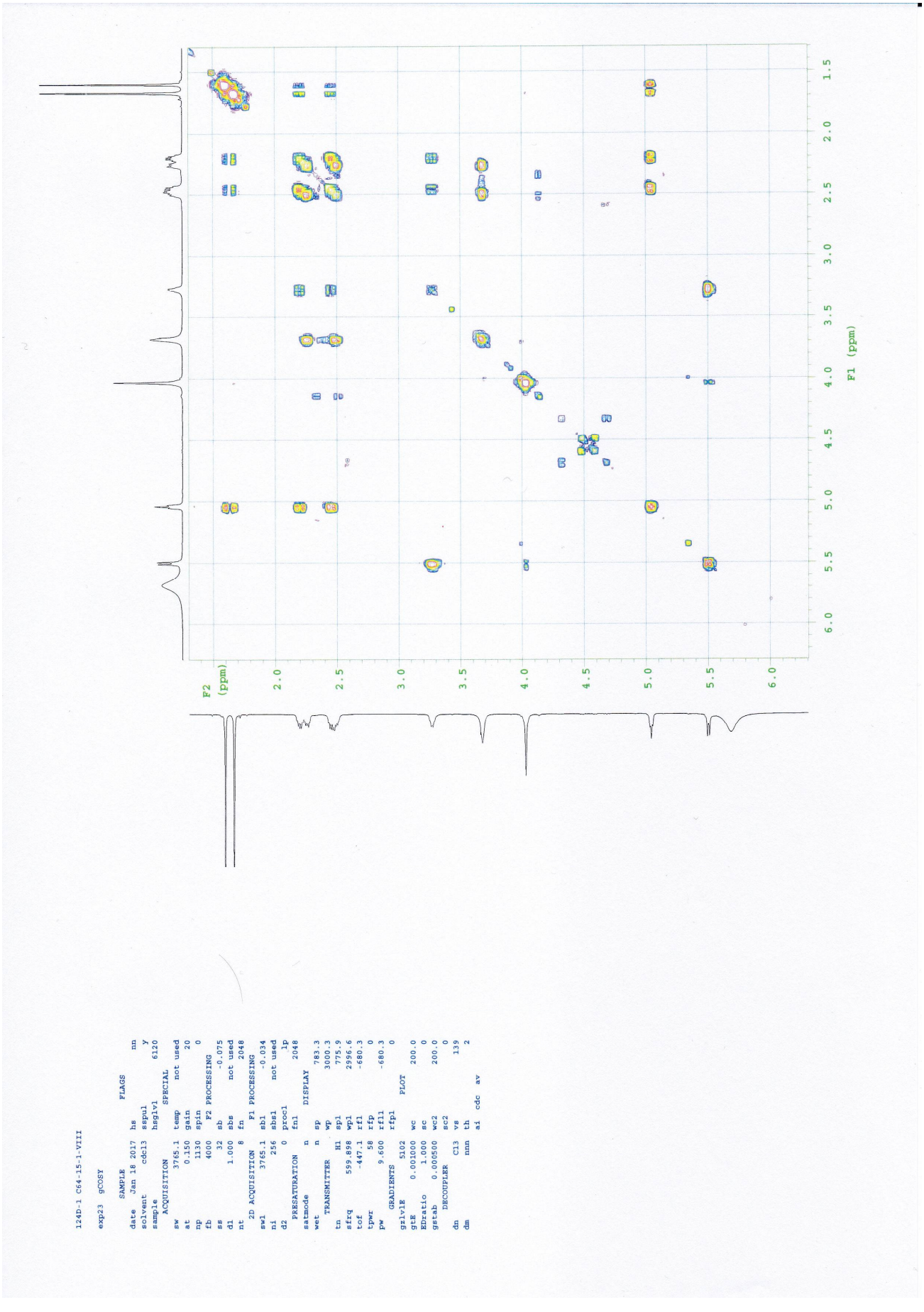


Figure S3 ^{1}H-^{1}H COSY of 1



124D-1 C64-15-1-VIII

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sample hsglvl 6120
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ss 32 sb -0.075
d1 1.000 sbs not used
nt 8 fn 2048
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ni 256 sbs1 not used
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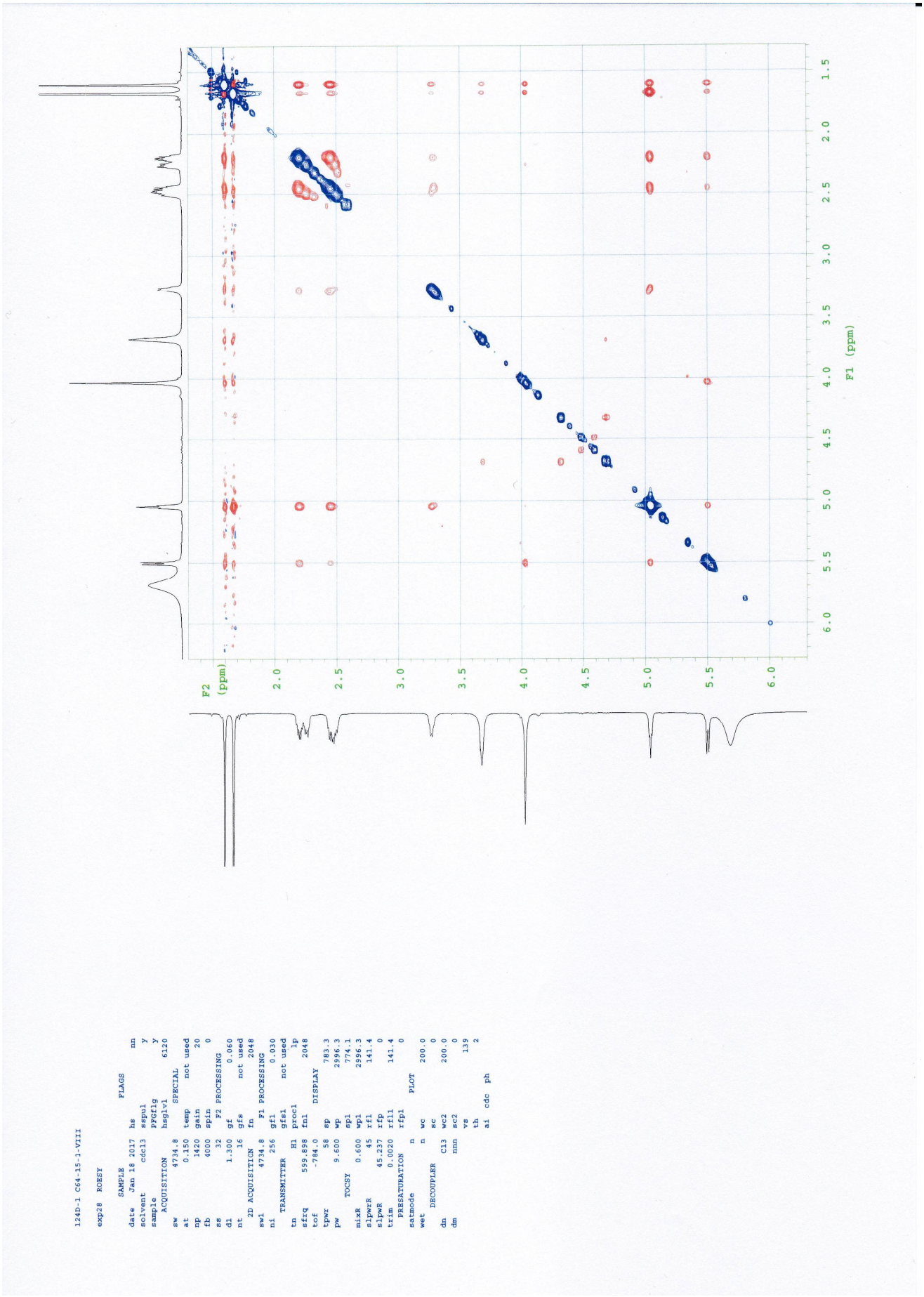
ai cdc av

Figure S4 NOESY of 1



124D-1 C64-15-1-VIII

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nt 16 gfs not used
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sw1 4734.8 F1 PROCESSING
ni 256 gf1 0.030
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th 2
ai cdc ph

Figure S5 HMQC of 1

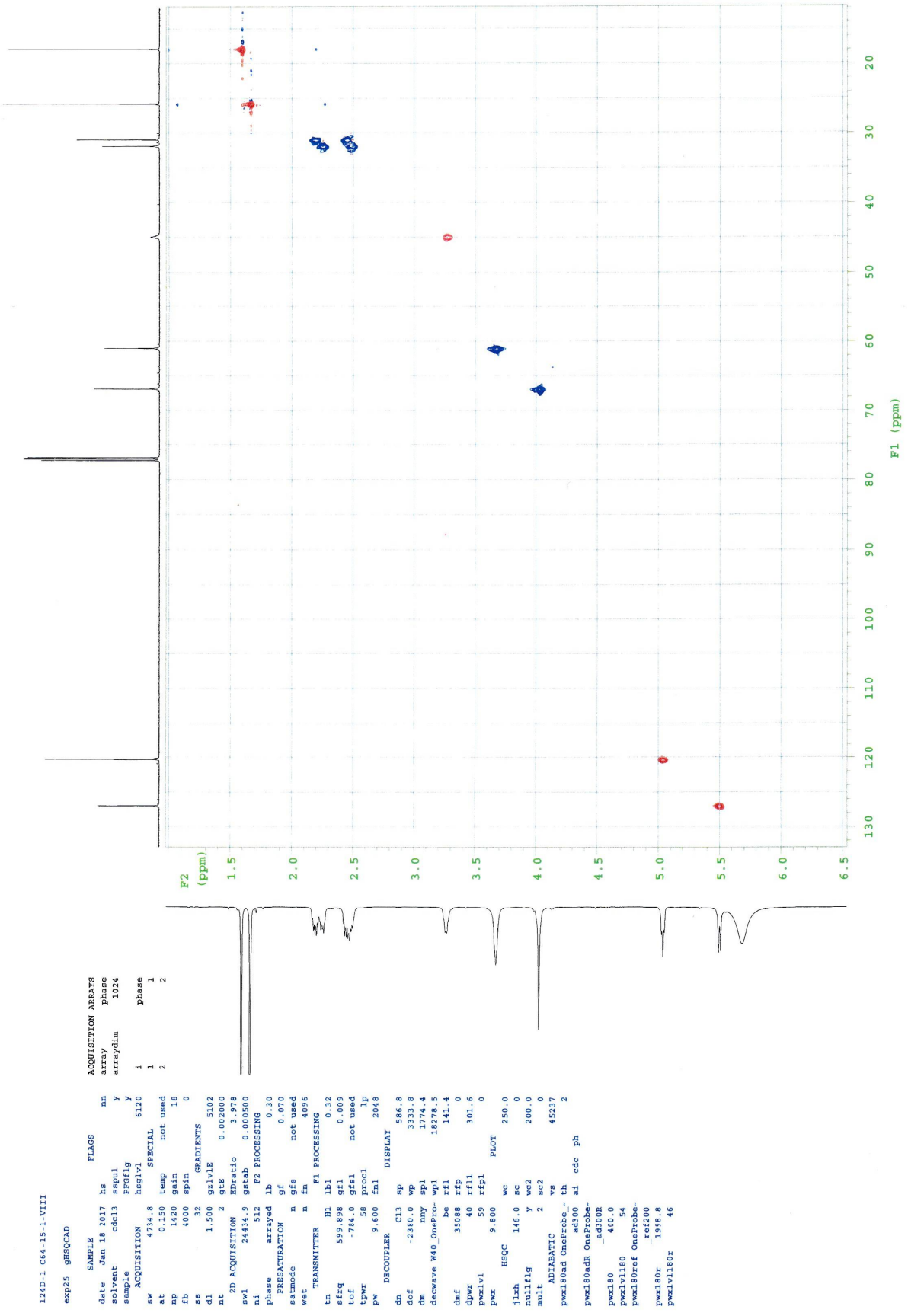


Figure S6 HMBC of 1

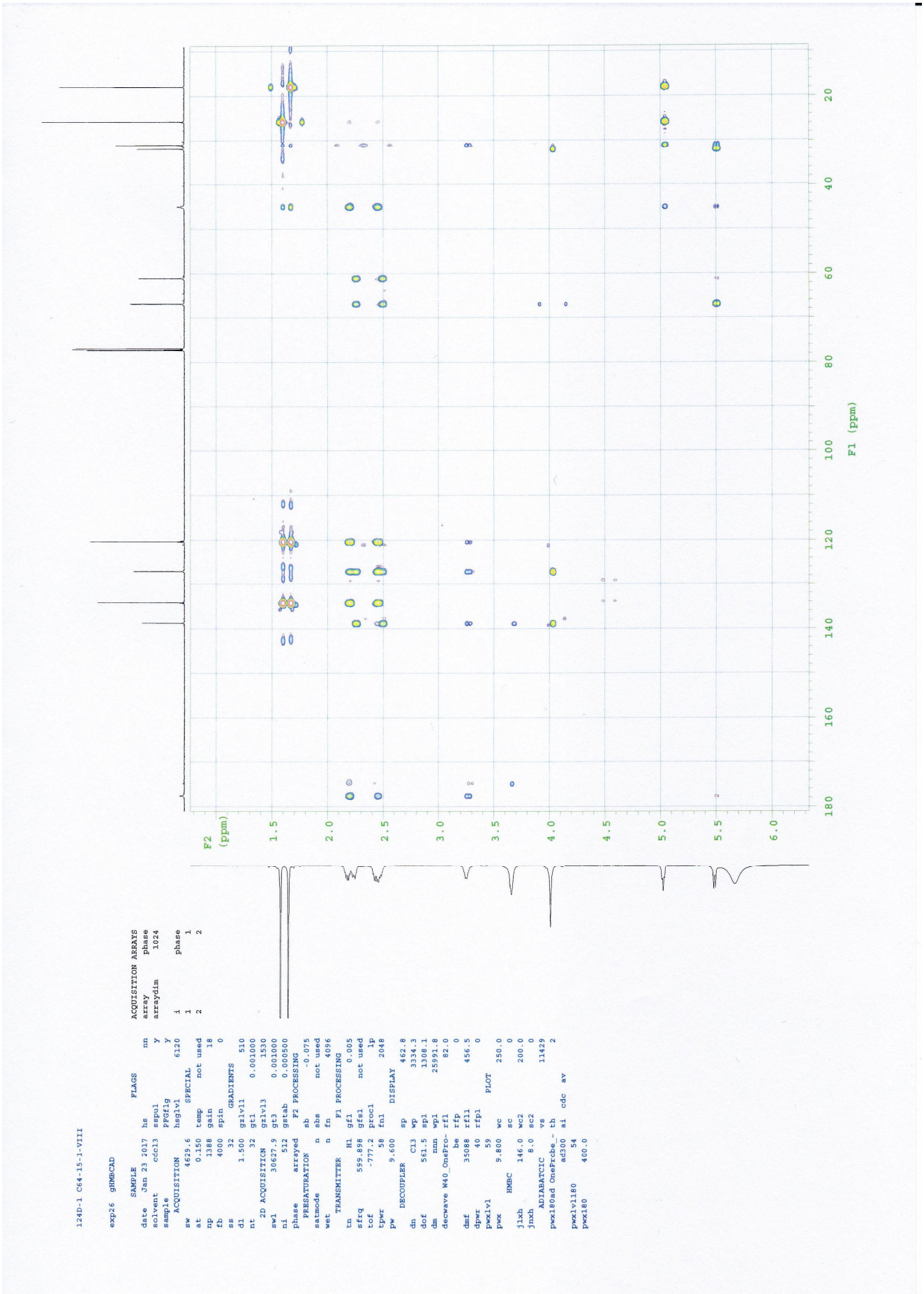


Figure S7 ^{1}H NMR spectrum of 2 in $CDCl_3$

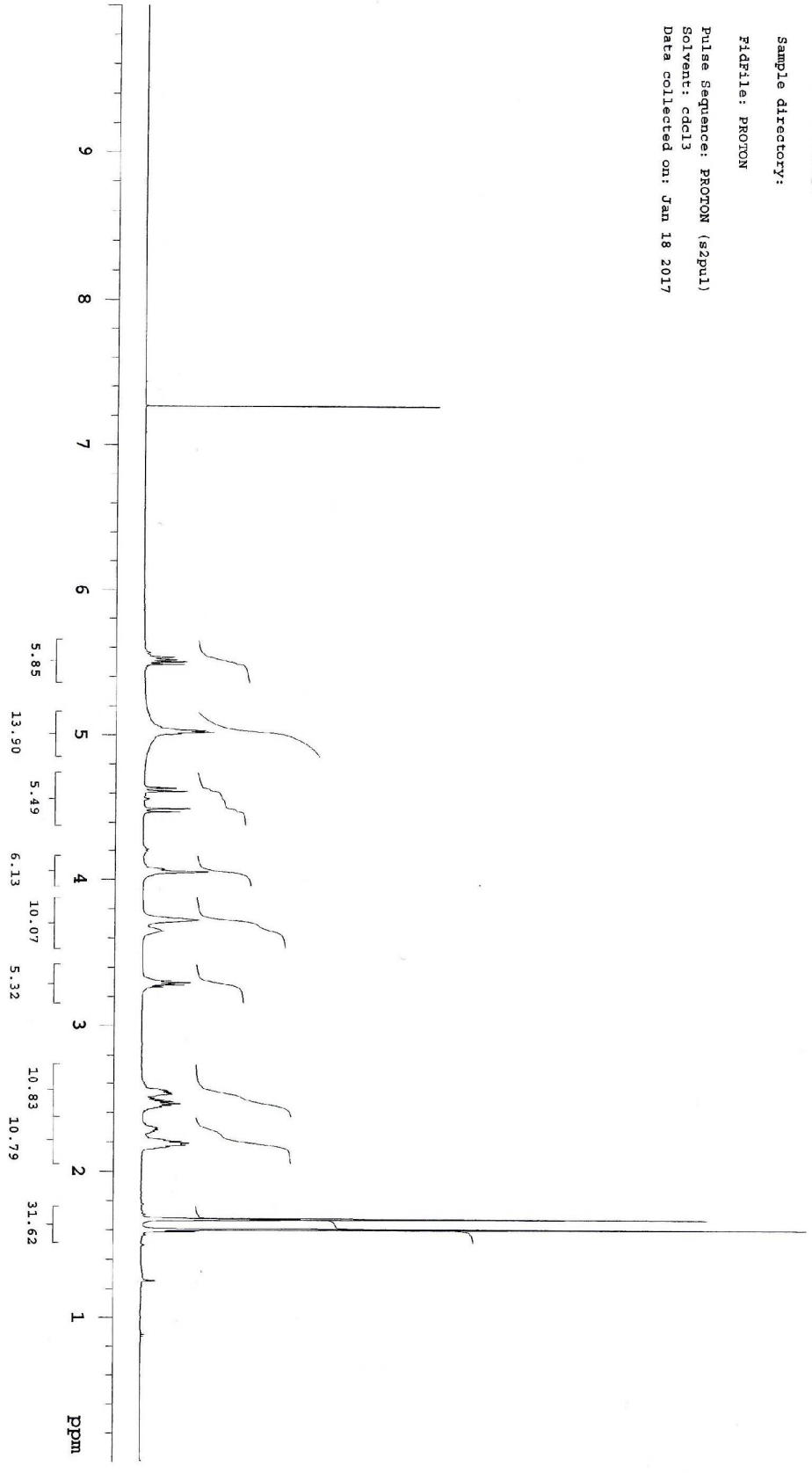


Figure S8 ^{13}C NMR spectrum of 2 in $CDCl_3$

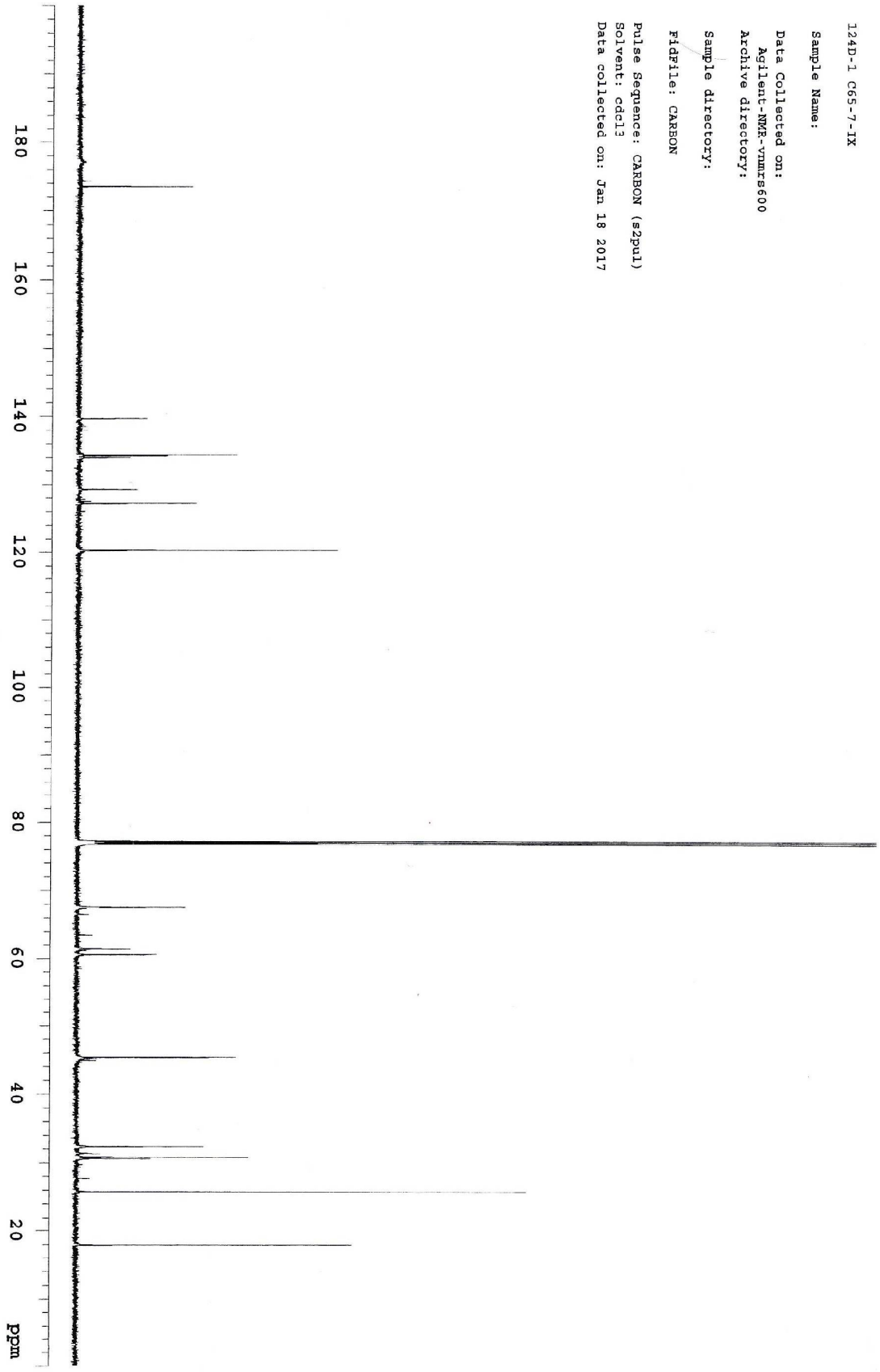


Figure S9 ^{1}H-^{1}H COSY of 2

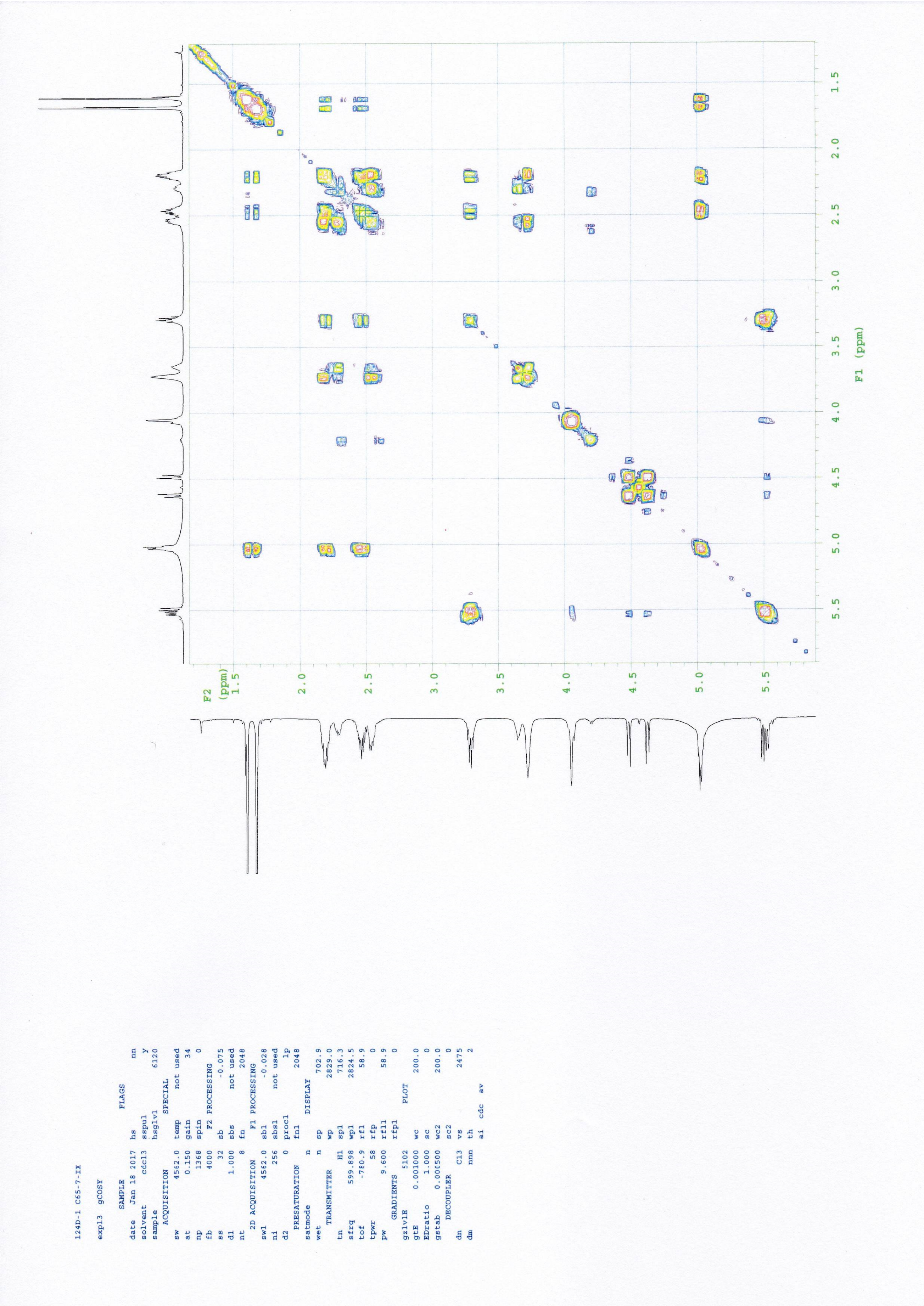


Figure S10 NOESY of 2

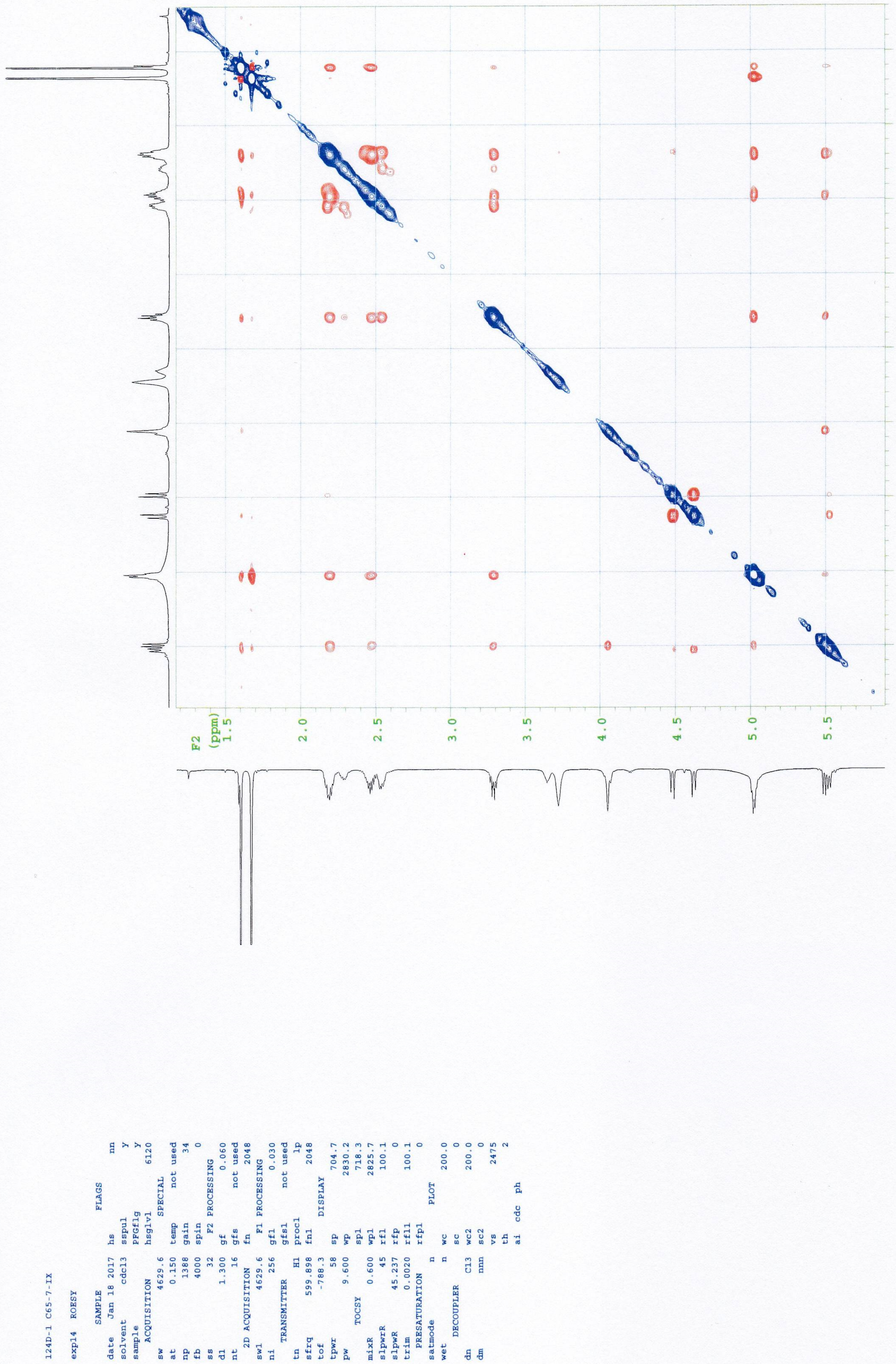


Figure S11 HMQC of 2

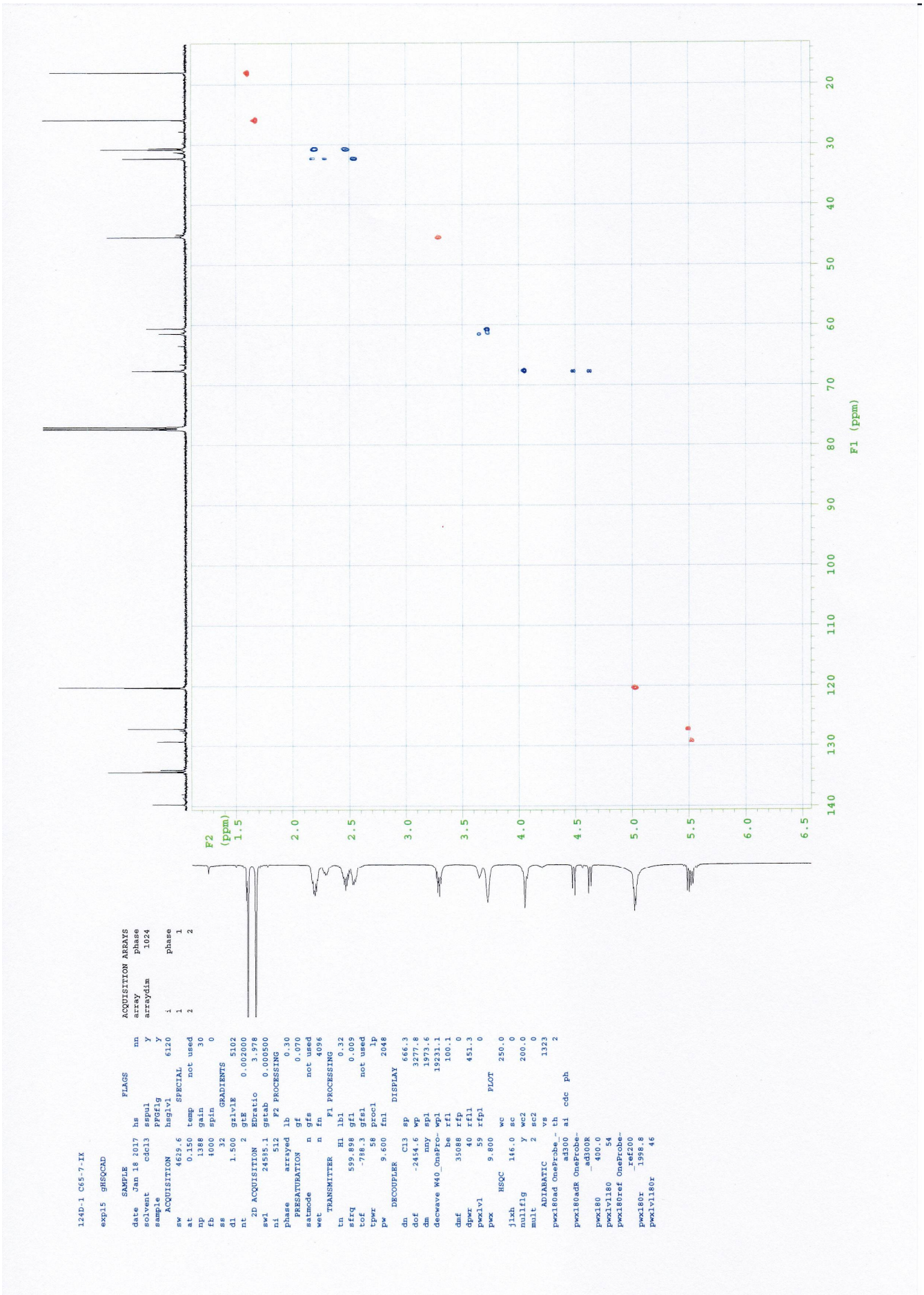


Figure S12 HMBC of 2

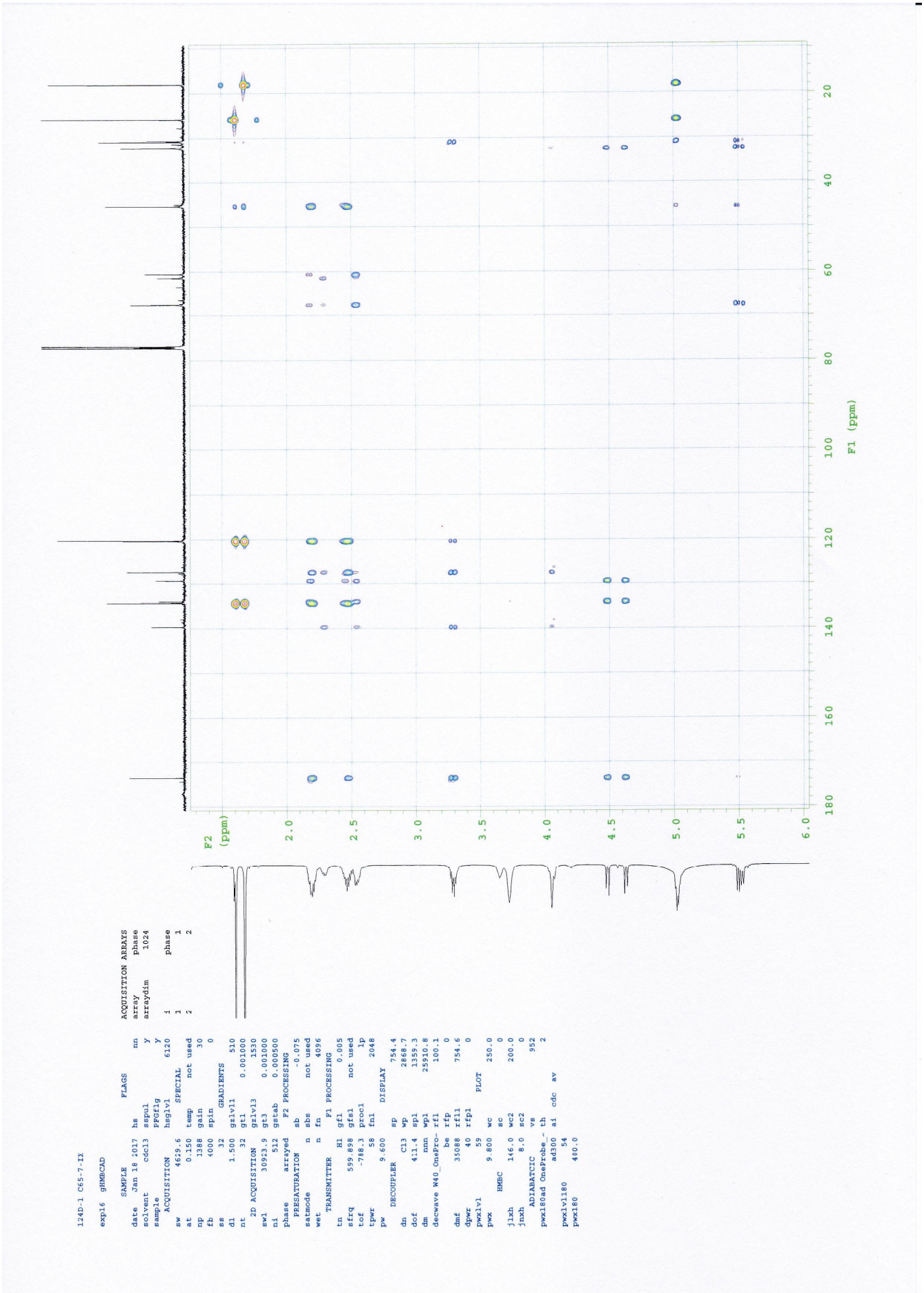


Figure S13 ^{1}H NMR spectrum of 3 in $CDCl_3$

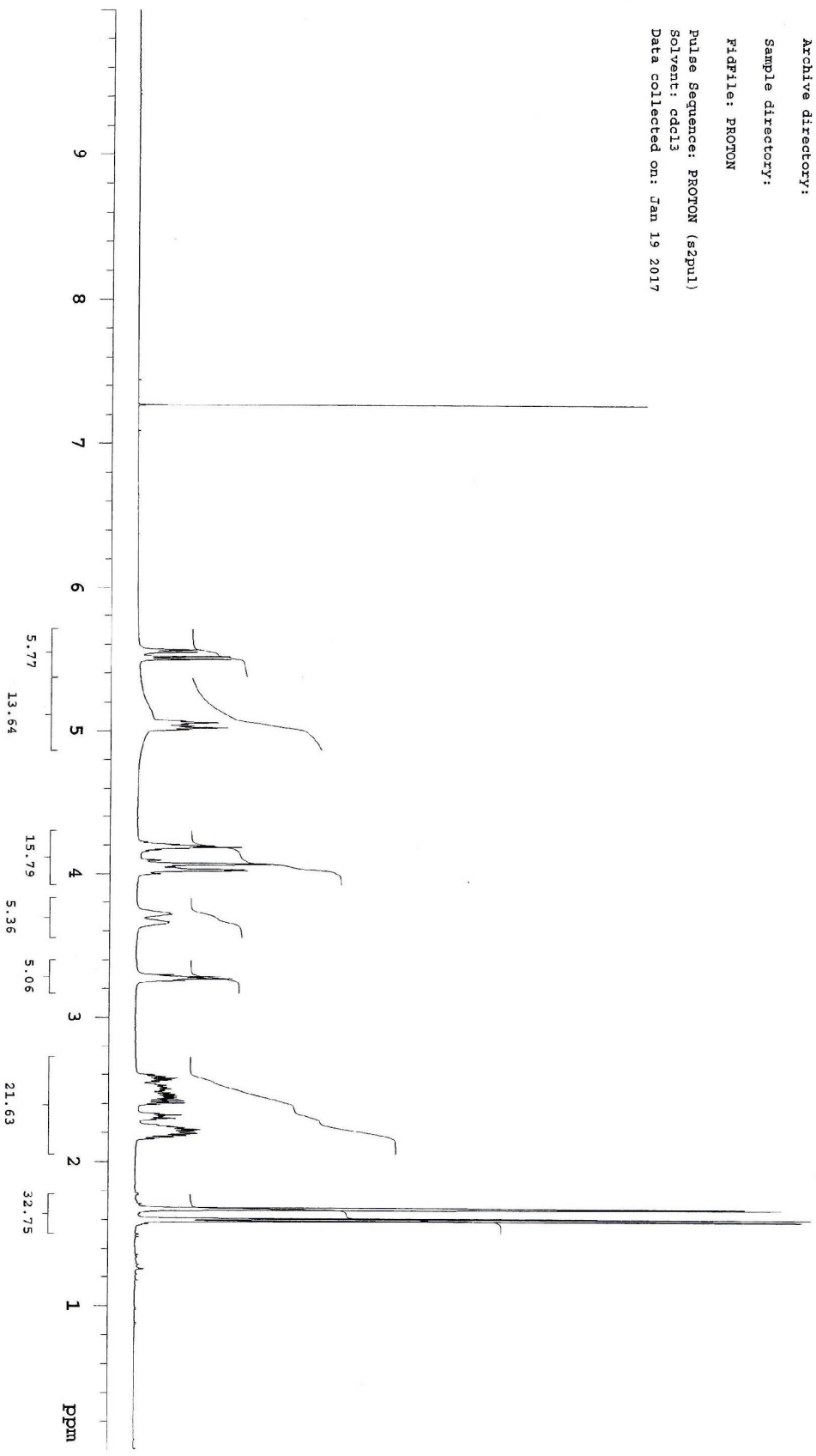


Figure S14 ^{13}C NMR spectrum of 3 in $CDCl_3$

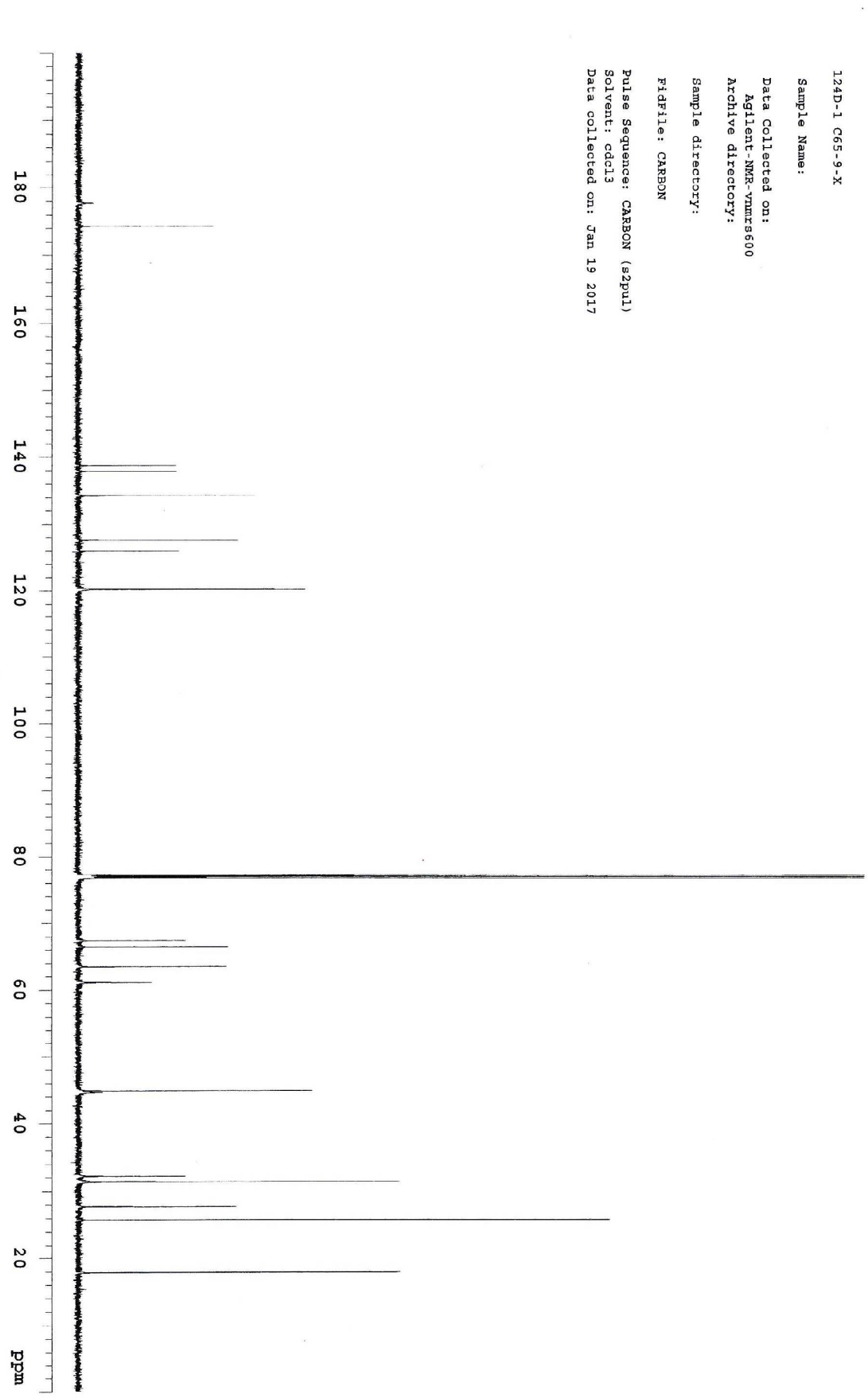
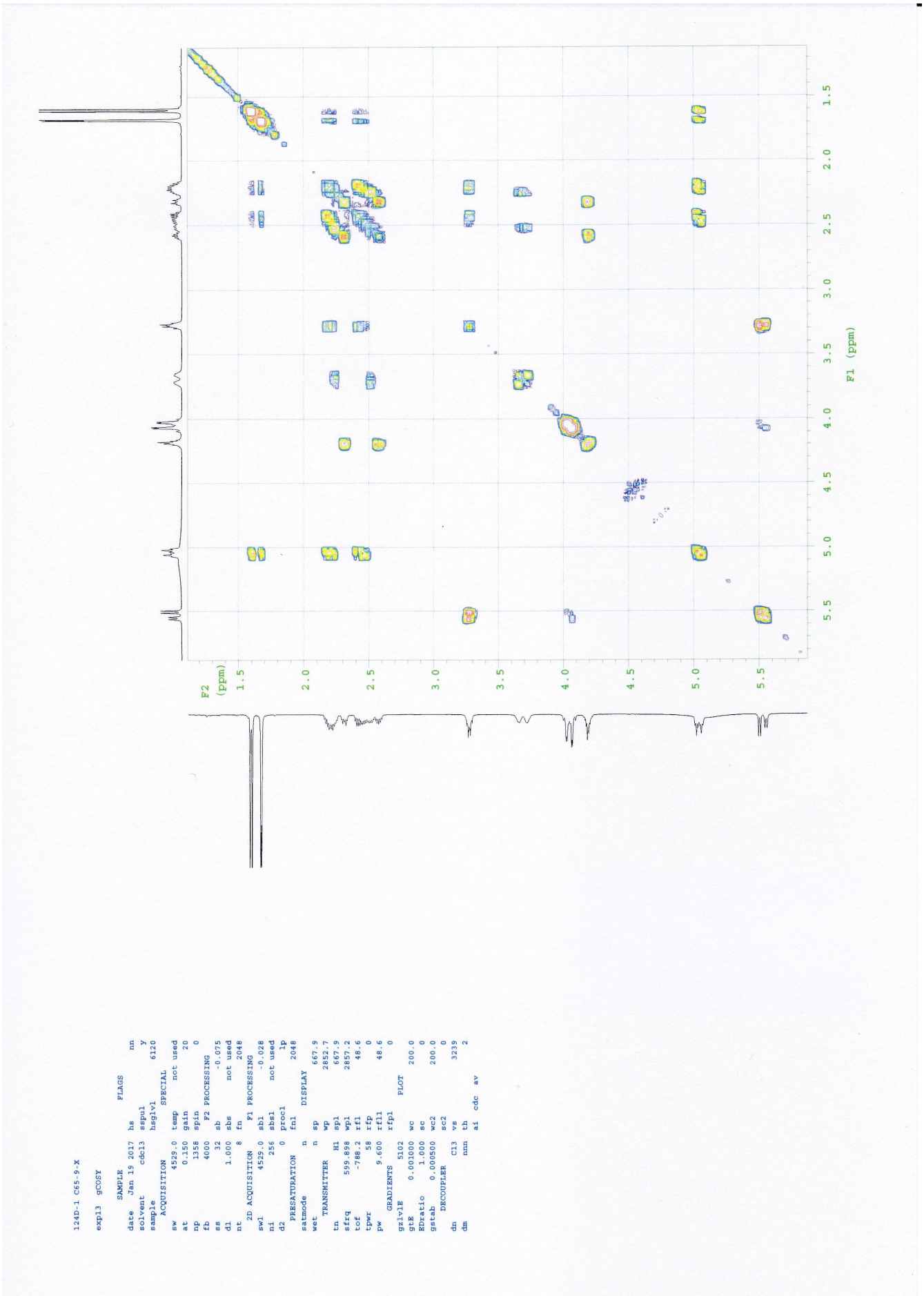


Figure S15 ^{1}H-^{1}H COSY of 3

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124D-1 C65-9-X

exp13  gCOSY

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sample                   hsglvl
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np            1358  spin                 0
fb            4000     F2 PROCESSING
ss              32  sb              -0.075
d1           1.000  sbs           not used
nt               8  fn                2048
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sw1         4529.0  sb1             -0.028
ni              256  sbs1          not used
d2                0  proc1               lp
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satmode              n          DISPLAY
wet                  n  sp          667.9
   TRANSMITTER           wp         2852.7
tn                   H1  sp1         667.9
sfrq          599.898  wp1        2857.2
tof            -788.2  rf1          48.6
tpwr               58  rfp             0
pw            9.600  rfl1          48.6
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gzlvlE          5102          PLOT
gtE          0.001000  wc          200.0
EDratio         1.000  sc              0
gstab        0.000500  wc2         200.0
   DECOUPLER           sc2               0
dn                C13  vs             3239
dm                nnn  th                2
                       ai  cdc  av
```

Figure S16 NOESY of 3

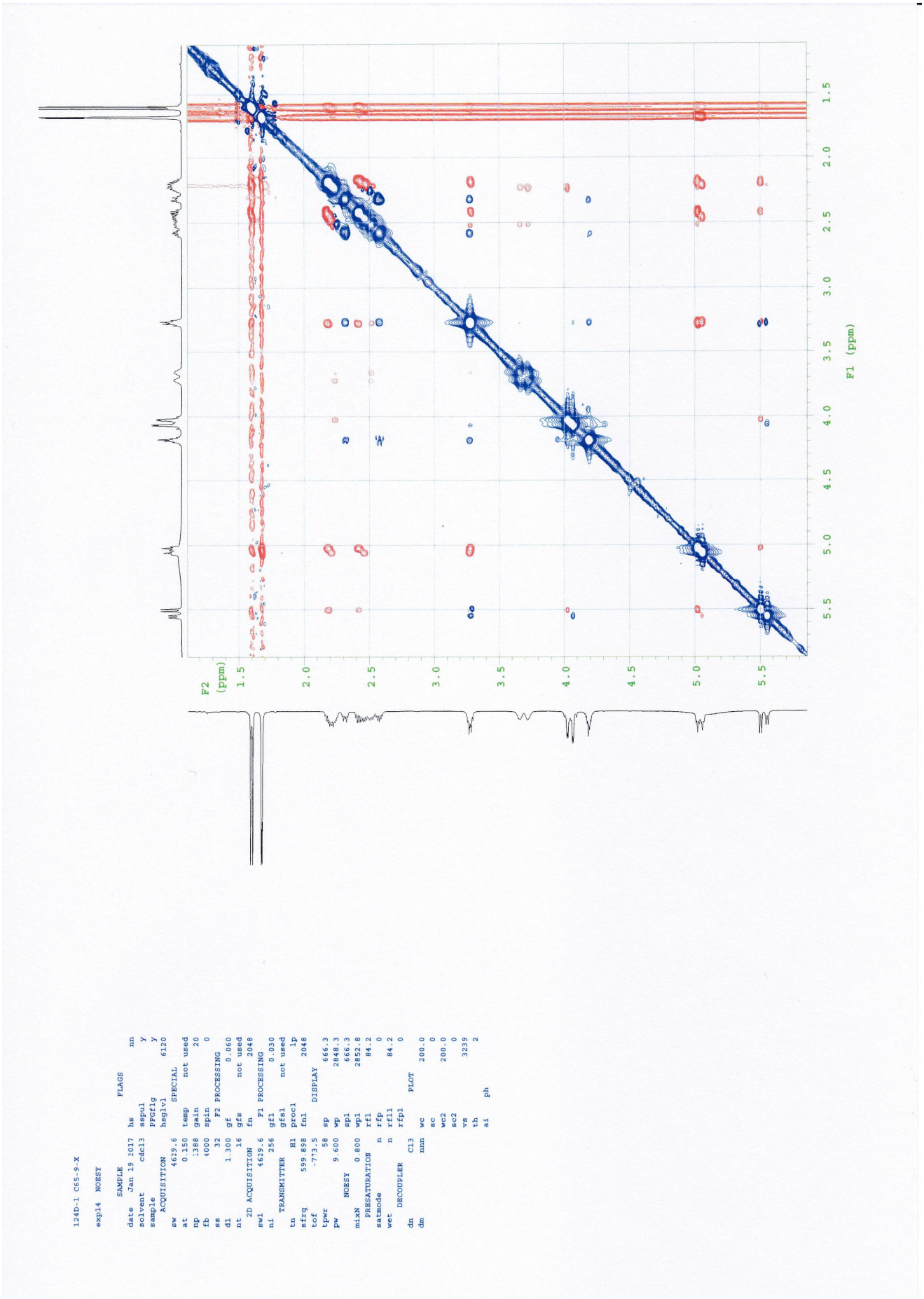


Figure S17 HMQC of 3

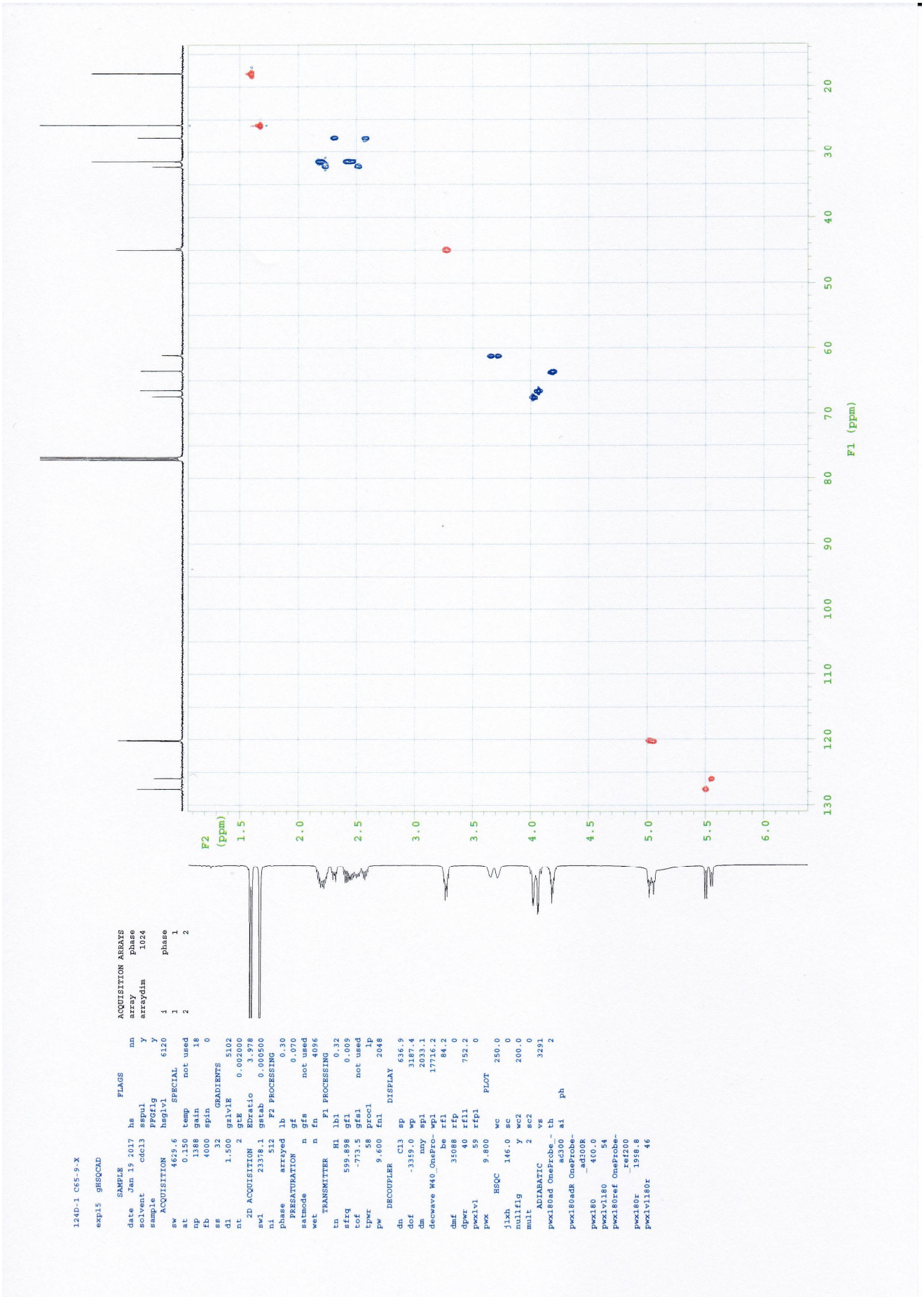


Figure S18 HMBC of 3

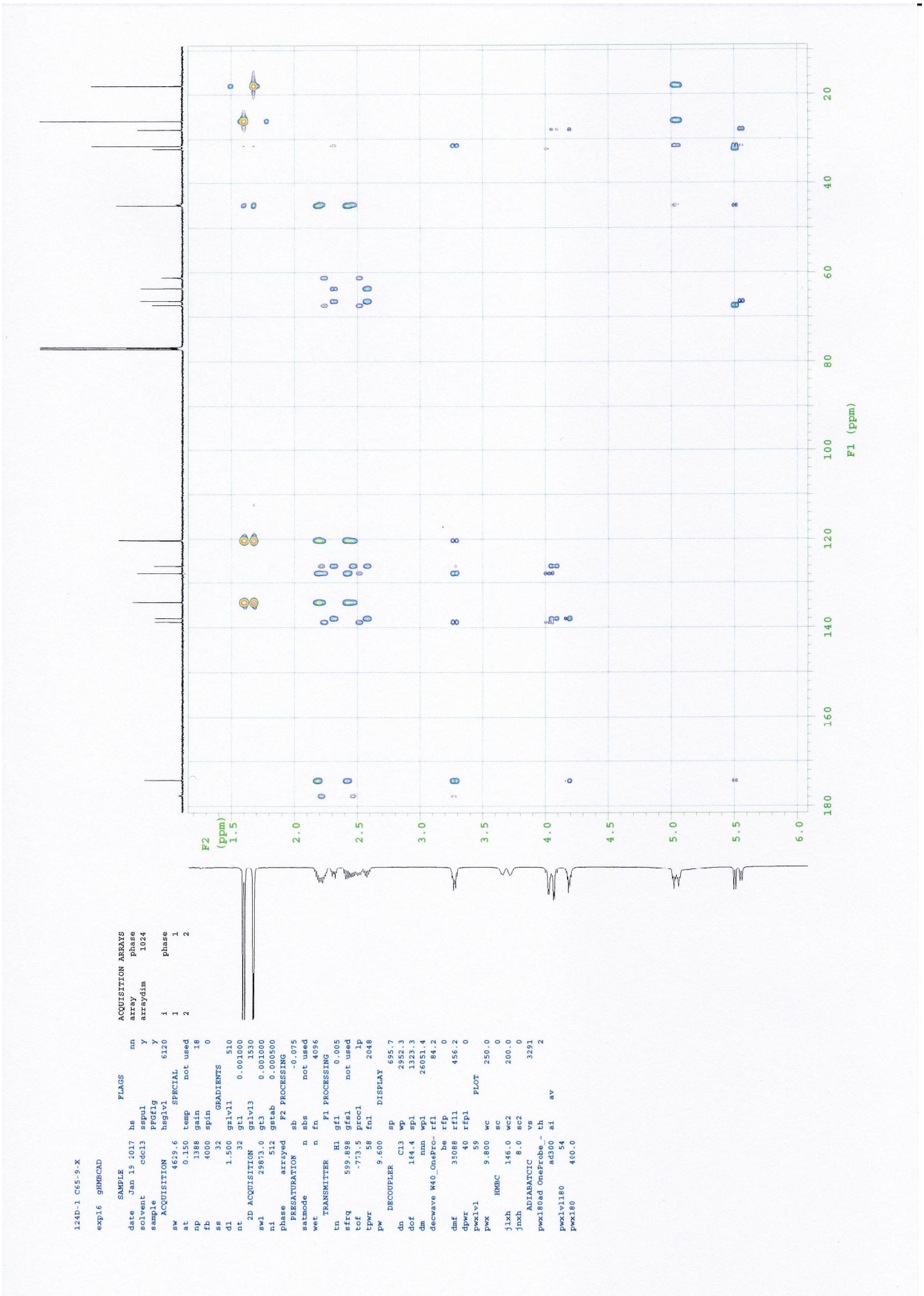


Figure S19 ^{1}H NMR spectra of 4 in $CDCl_3$

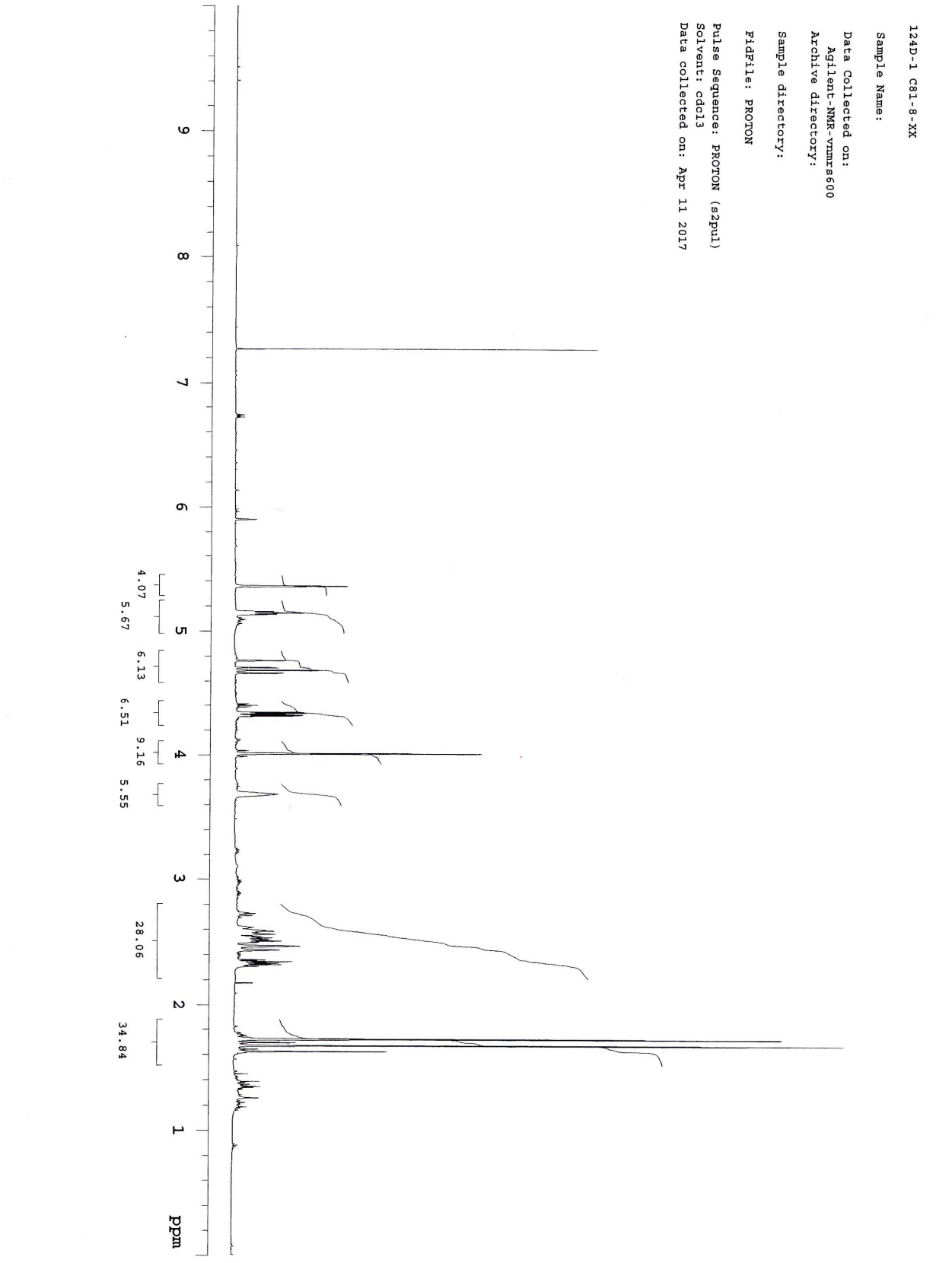


Figure S20 ^{13}C NMR spectra of 4 in $CDCl_3$

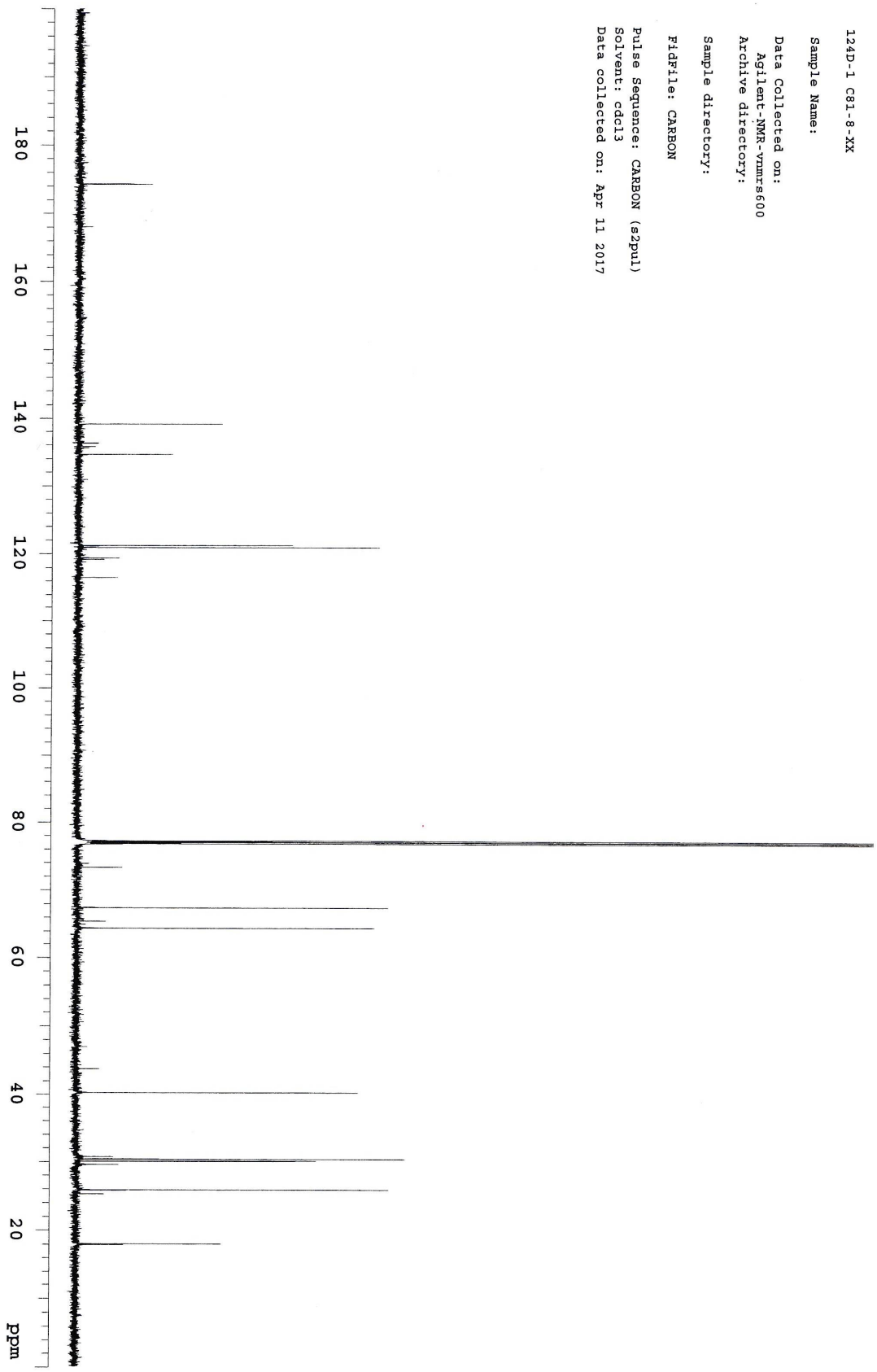
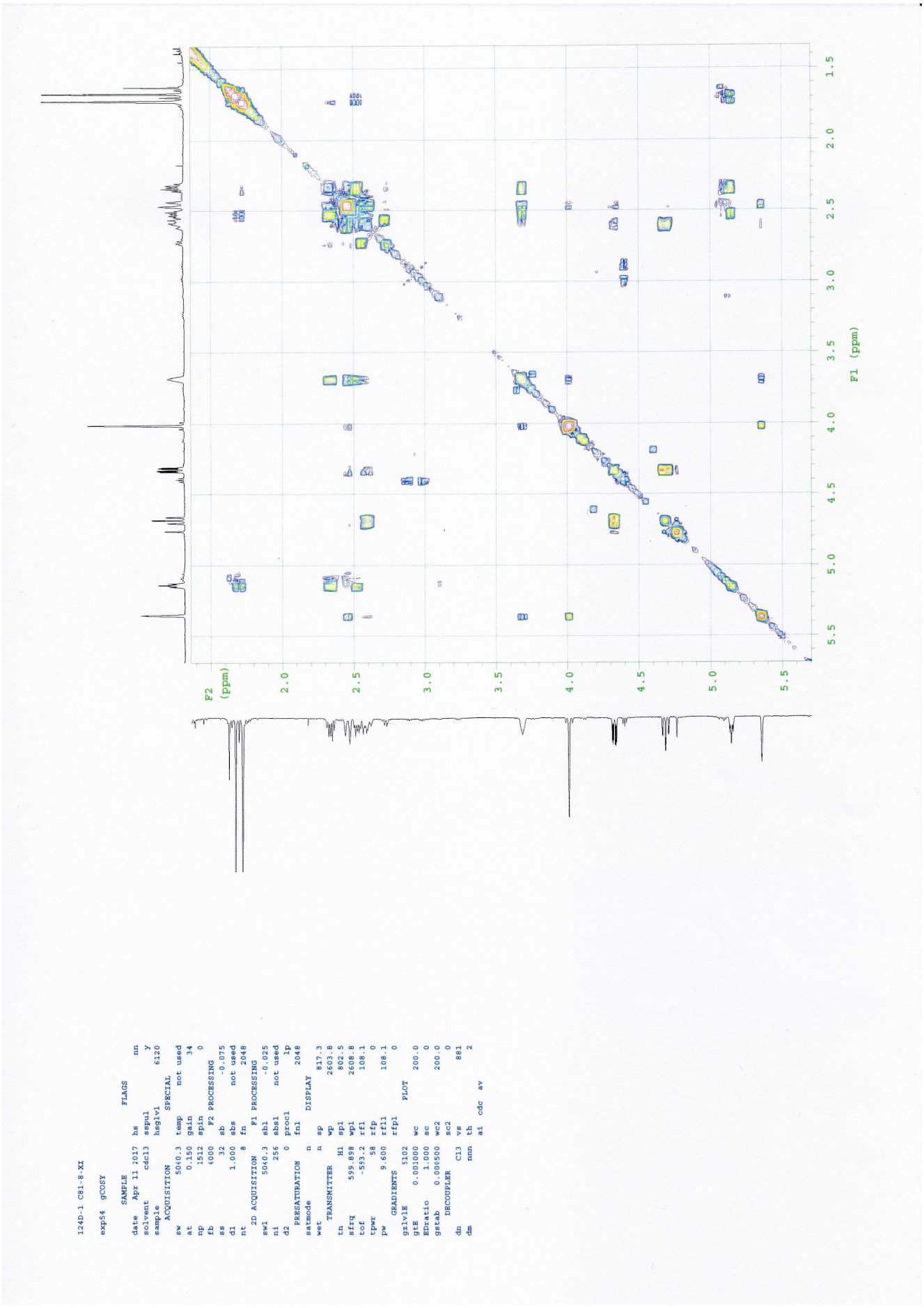


Figure S21 ^{1}H-^{1}H COSY of 4

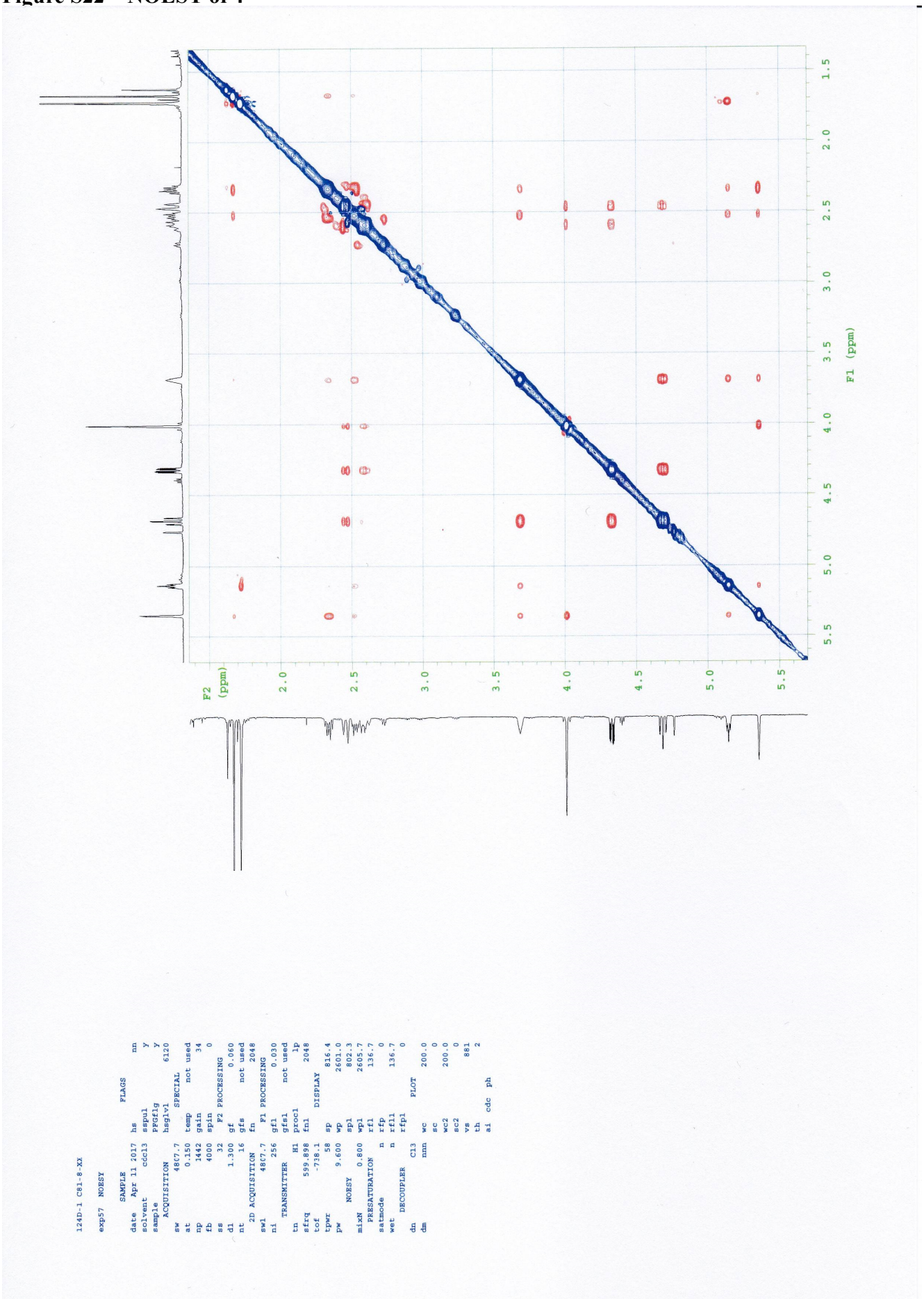


124D-1 C81-8-XX

exp54 gCOSY

SAMPLE FLAGS
date Apr 11 2017 hs nn
solvent cdcl3 sspul y
sample hsglv1 6120
ACQUISITION SPECIAL
sw 5040.3 temp not used
at 0.150 gain 34
np 1512 spin 0
fb 4000 F2 PROCESSING
ss 32 sb -0.075
d1 1.000 sbs not used
nt 8 fn 2048
2D ACQUISITION F1 PROCESSING
sw1 5040.3 sb1 -0.025
ni 256 sbs1 not used
d2 0 proc1 lp
PRESATURATION fn1 2048
satmode n DISPLAY
wet n sp 817.3
TRANSMITTER wp 2603.8
tn H1 sp1 802.5
sfrq 599.898 wp1 2608.8
tof -593.2 rf1 108.1
tpwr 58 rfp 0
pw 9.600 rf11 108.1
GRADIENTS rfp1 0
gzlvlE 5102 PLOT
gtE 0.001000 wc 200.0
EDratio 1.000 sc 0
getab 0.000500 wc2 200.0
DECOUPLER sc2 0
dn C13 vs 881
dm nnn th 2
al cdc av

Figure S22 NOESY of 4^+

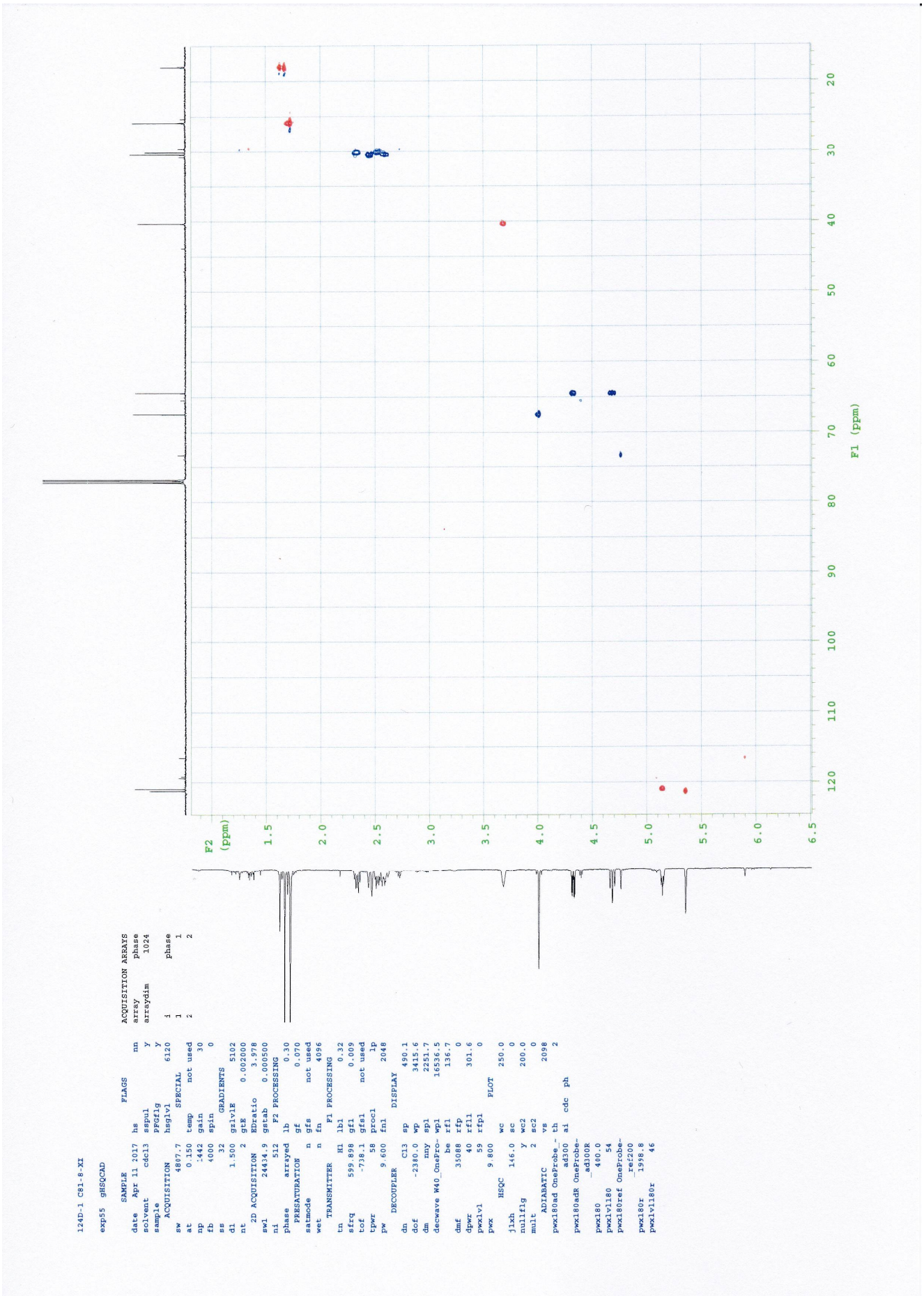



```
124D-1 C81-8-XX

exp57  NOESY

                SAMPLE                  FLAGS
        date  Apr 11 2017   hs                nn
        solvent     cdcl3   sspul             y
        sample              PFGflg            y
          ACQUISITION       hsglvl          6120
        sw        4807.7    SPECIAL
        at         0.150    temp      not used
        np          1442    gain            34
        fb          4000    spin             0
        ss            32      F2 PROCESSING
        d1         1.300    gf             0.060
        nt            16    gfs       not used
          2D ACQUISITION    fn              2048
        sw1       4807.7      F1 PROCESSING
        ni           256    gf1            0.030
          TRANSMITTER       gfs1      not used
        tn              H1  proc1             lp
        sfrq       599.898  fn1             2048
        tof         -738.1      DISPLAY
        tpwr            58  sp             816.4
        pw           9.600  wp            2601.0
              NOESY         sp1            802.3
        mixN         0.800  wp1           2605.7
          PRESATURATION     rf1            136.7
        satmode          n  rfp                0
        wet              n  rfl1           136.7
          DECOUPLER         rfp1               0
        dn              C13       PLOT
        dm              nnn   wc          200.0
                              sc                0
                              wc2         200.0
                              sc2               0
                              vs              881
                              th                2
                              ai  cdc  ph
```

Figure S23 HMQC of 4




```
124D-1 C81-8-XI

exp55  gHSQCAD

      SAMPLE                  FLAGS          nn          ACQUISITION ARRAYS
      date  Apr 11 2017       hs             array       phase
      solvent    cdcl3        ssqul          arraydim    1024
      sample                  pFGflg         y
        ACQUISITION           hsglvl         6120        i       phase
        sw          4807.7    SPECIAL                    1       1
        at           0.150    temp       not used        2       2
        np             1442   gain             30
        fb             4000   spin              0
        ss               32          GRADIENTS
        d1            1.500   gzlvlE         5102
        nt                2   gtE       0.002000
          2D ACQUISITION      EDratio      3.978
        sw1        2443.4.9   gstab     0.000500
        ni              512     F2 PROCESSING
        phase       arrayed   lb            0.30
          PRESATURATION       gf            0.070
        satmode           n   gfs        not used
        wet               n   fn            4096
          TRANSMITTER             F1 PROCESSING
        tn                H1    lb1           0.32
        sfrq         599.898    gf1           0.009
        tof             -738.1   gfs1       not used
        tpwr              58    proc1           lp
        pw              9.600   fn1           2048
          DECOUPLER               DISPLAY
        dn                C13   sp          490.1
        dof           -2380.0   wp         3415.6
        dm                nny   sp1        2251.7
        decwave W40_OnePro-     wp1       16536.5
                             be   rfl         136.7
        dmf              35088   rfp             0
        dpwr                40   rfl1        301.6
        pwx1v1              59   rfp1            0
        pwx       9.800   HSQC          PLOT
          jlxh          146.0   wc         250.0
          nullflg             y   sc             0
          mult                2   wc2        200.0
                              2   sc2            0
            ADIABATIC         vs             2098
        pwx180ad OnePrObe_-   th                2
                    ad300     ai    cdc    ph
        pwx180adR OnePrObe-
                    _ad100R
        pwx180          400.0
        pwx1v1180         54
        pwx180ref OnePrObe-
                    _ref200
        pwx180r         1998.8
        pwx1v1180r        46
```

Figure S24 HMBC of 4

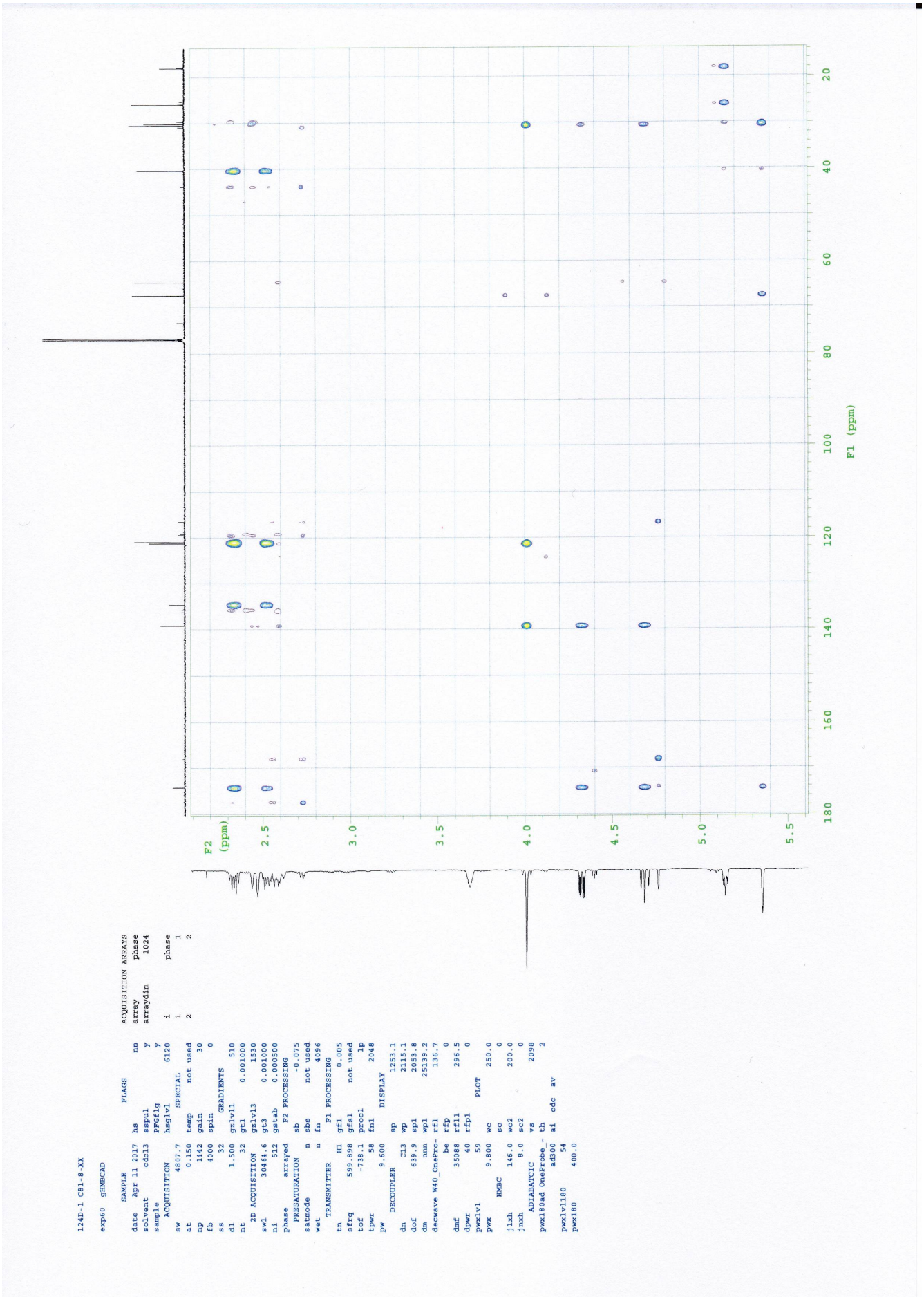
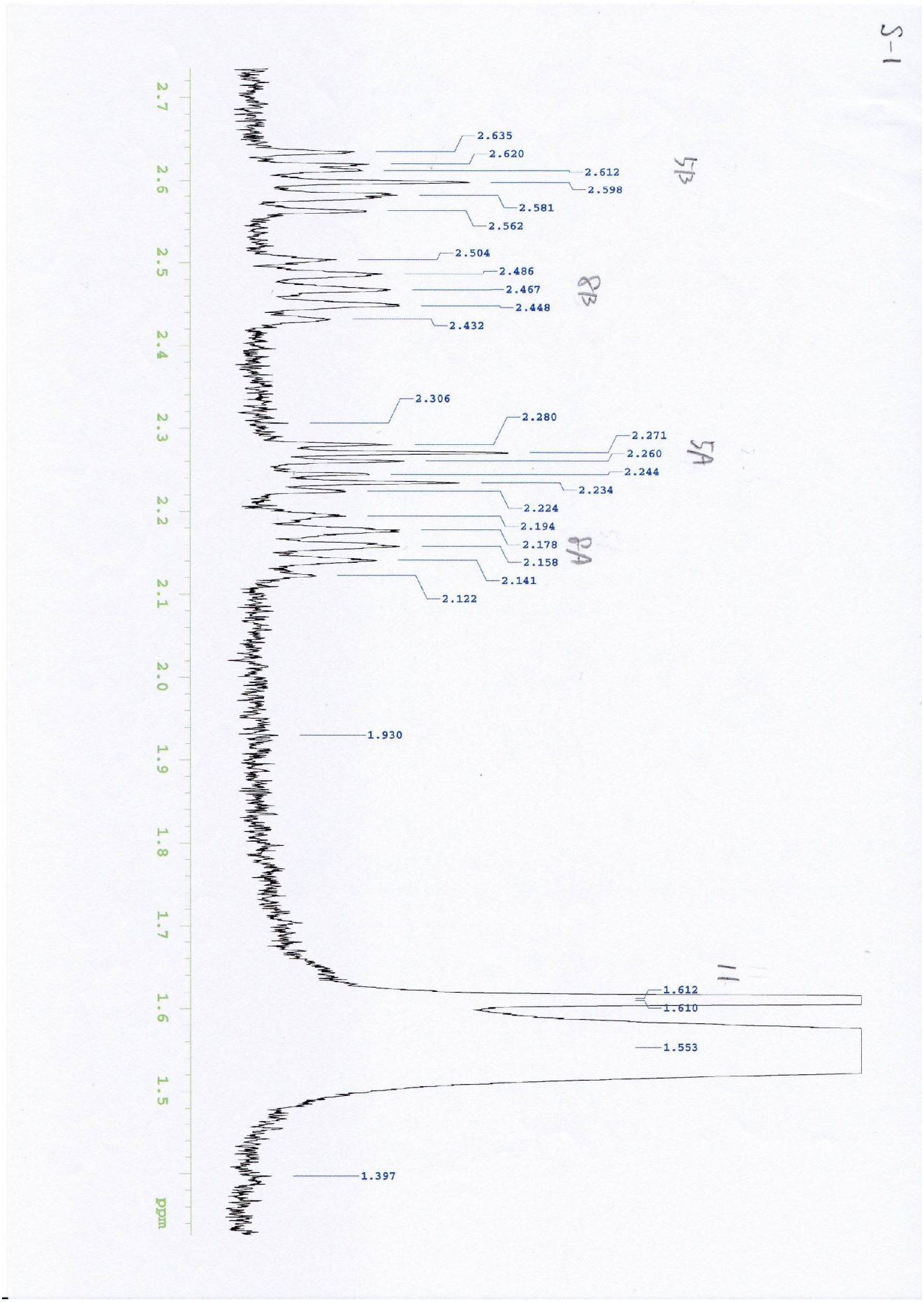
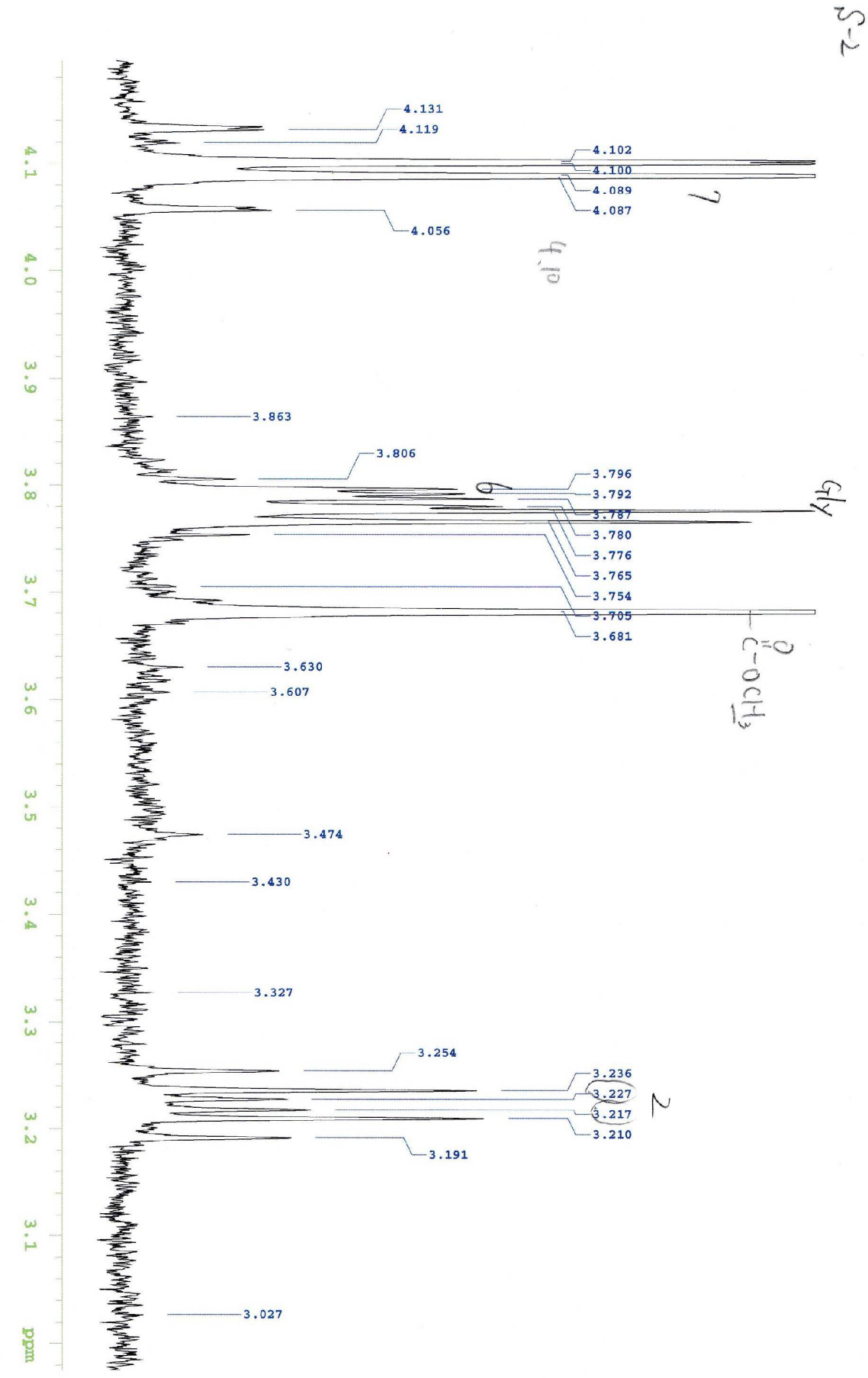
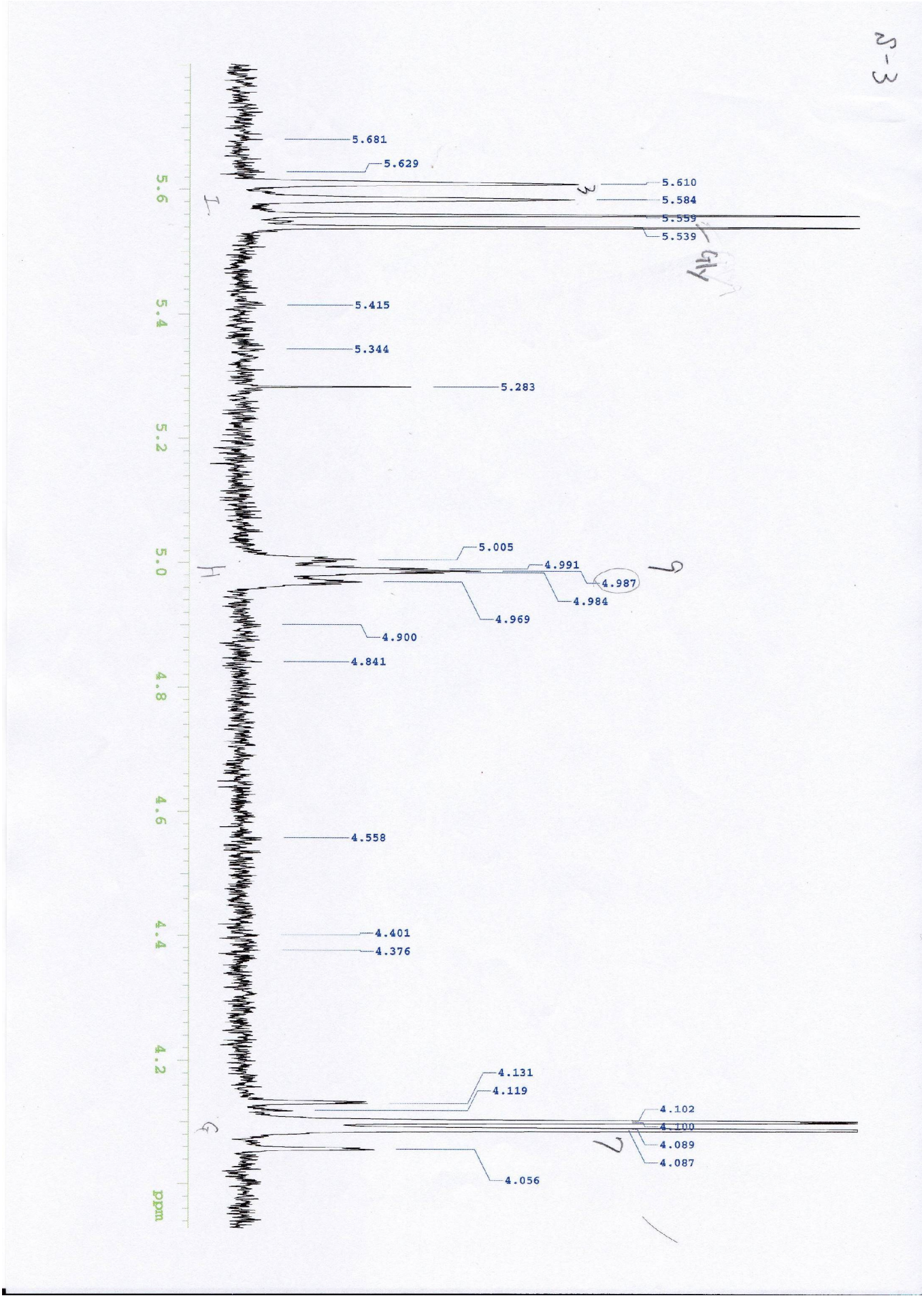


Figure S25 ^{1}H NMR spectra of 1a in $CDCl_3$




S-2
4.131
4.119
4.102
4.100
4.089
4.087
4.056
3.863
3.806
3.796
3.792
3.787
3.780
3.776
3.765
3.754
3.705
3.681
3.630
3.607
3.474
3.430
3.327
3.254
3.236
3.227
3.217
3.210
3.191
3.027
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
ppm


5.681
5.629
5.610
5.584
5.559
5.539
5.415
5.344
5.283
5.005
4.991
4.987
4.984
4.969
4.900
4.841
4.558
4.401
4.376
4.131
4.119
4.102
4.100
4.089
4.087
4.056
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
ppm

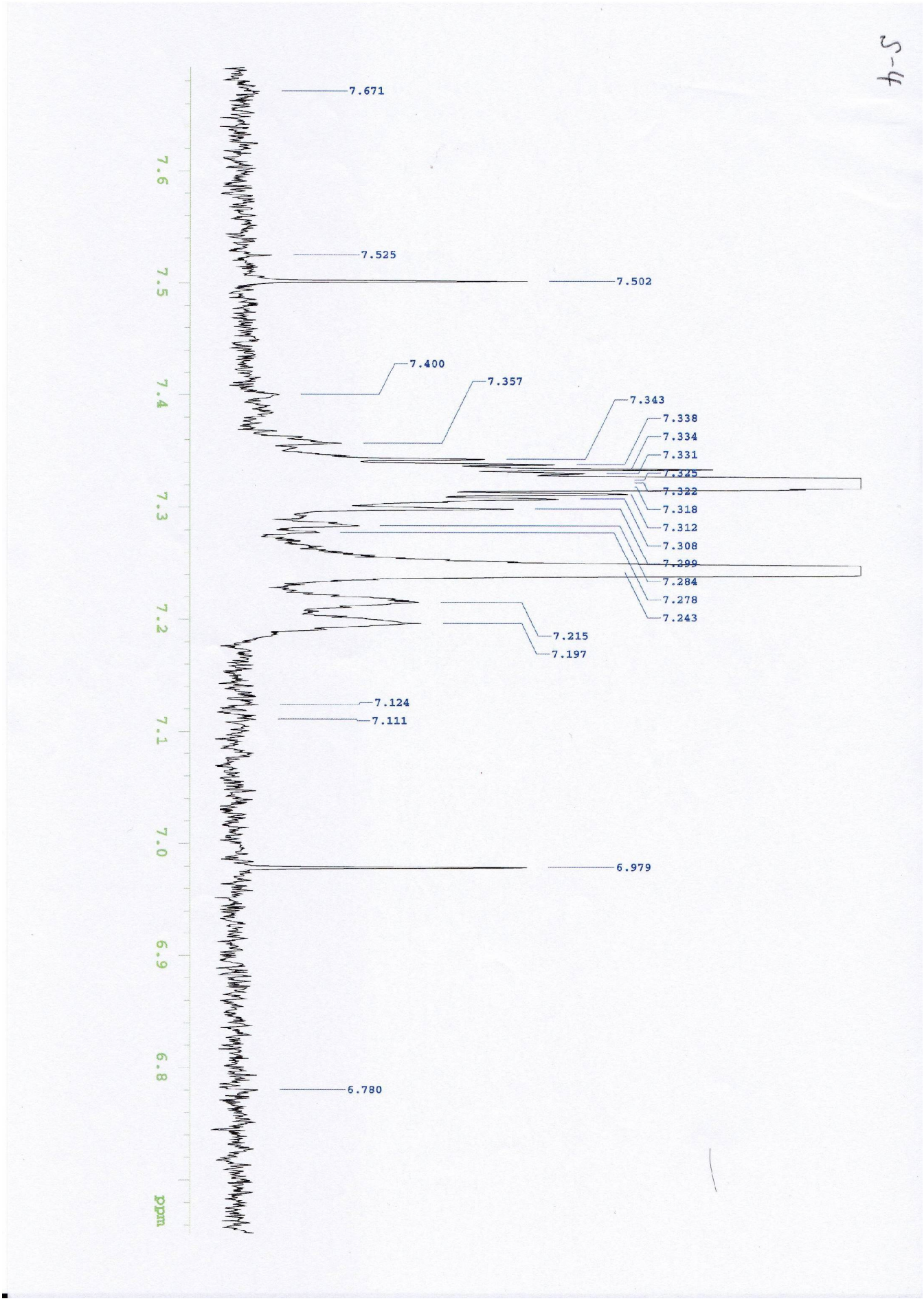
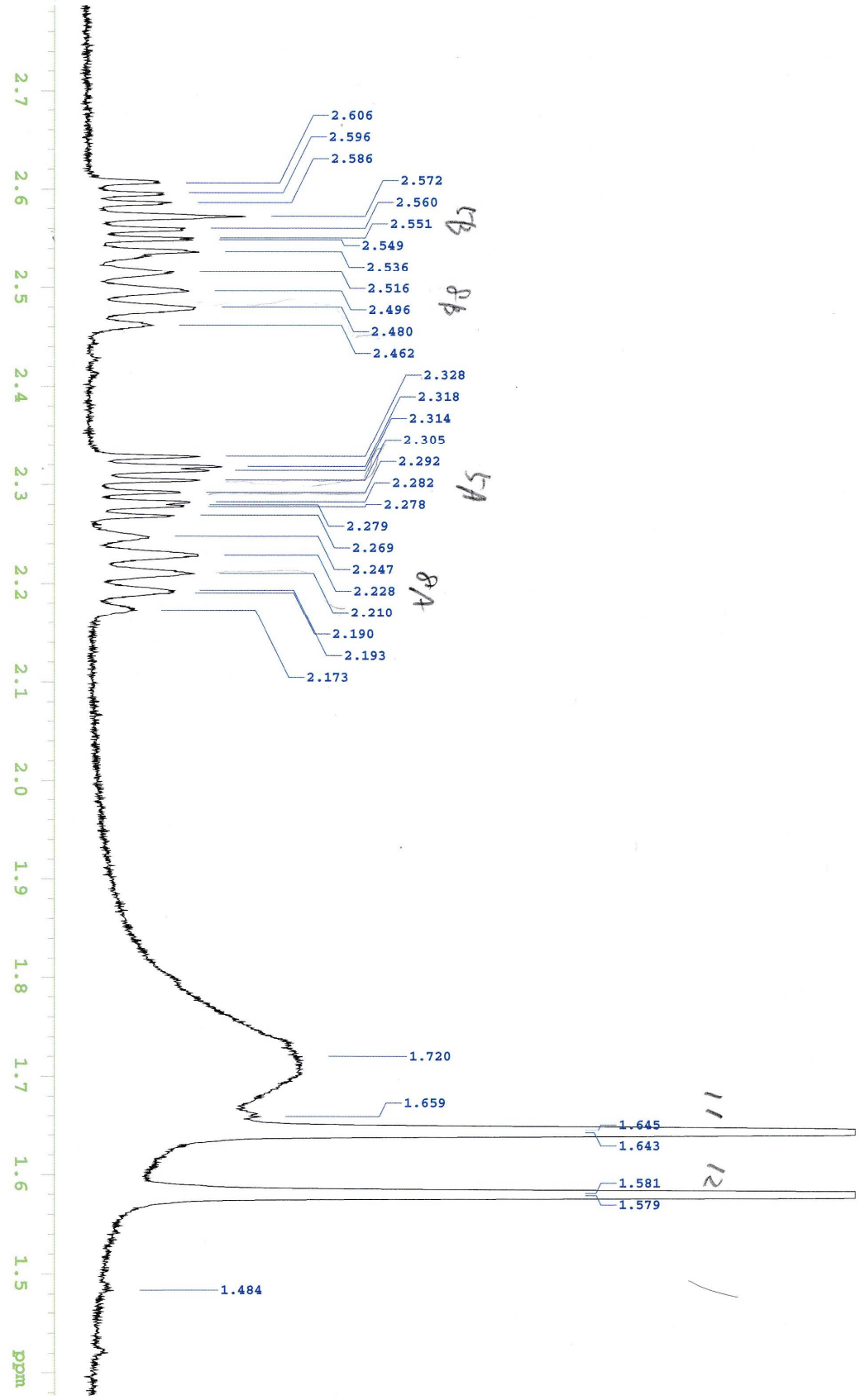
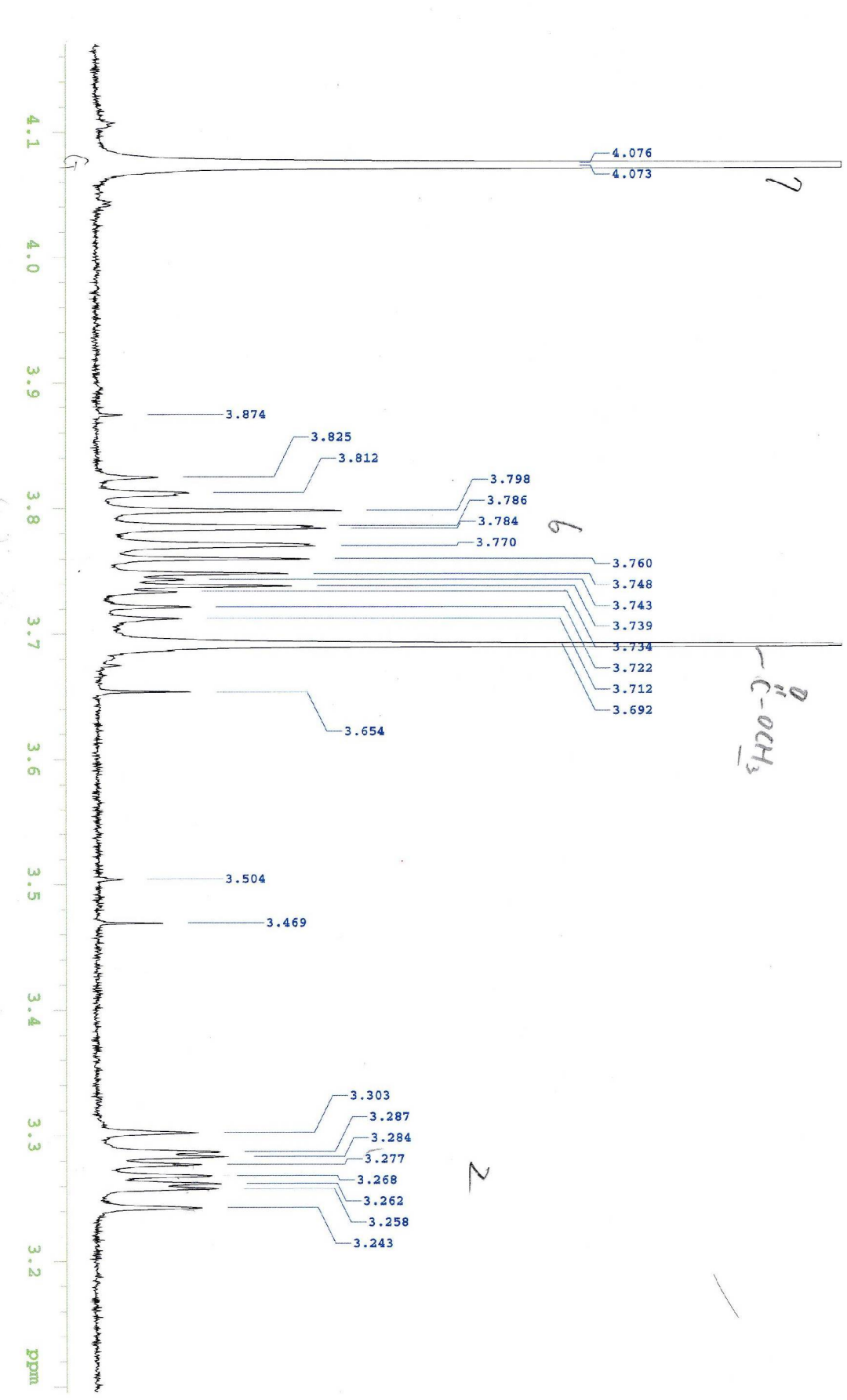

h-5
7.671
7.525
7.502
7.400
7.357
7.343
7.338
7.334
7.331
7.325
7.322
7.318
7.312
7.308
7.299
7.284
7.278
7.243
7.215
7.197
7.124
7.111
6.979
6.780
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm

Figure S26 ^{1}H NMR spectra of 2a in $CDCl_{3+}$




R-2
4.076
4.073
3.874
3.825
3.812
3.798
3.786
3.784
3.770
3.760
3.748
3.743
3.739
3.734
3.722
3.712
3.692
3.654
3.504
3.469
3.303
3.287
3.284
3.277
3.268
3.262
3.258
3.243
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
ppm

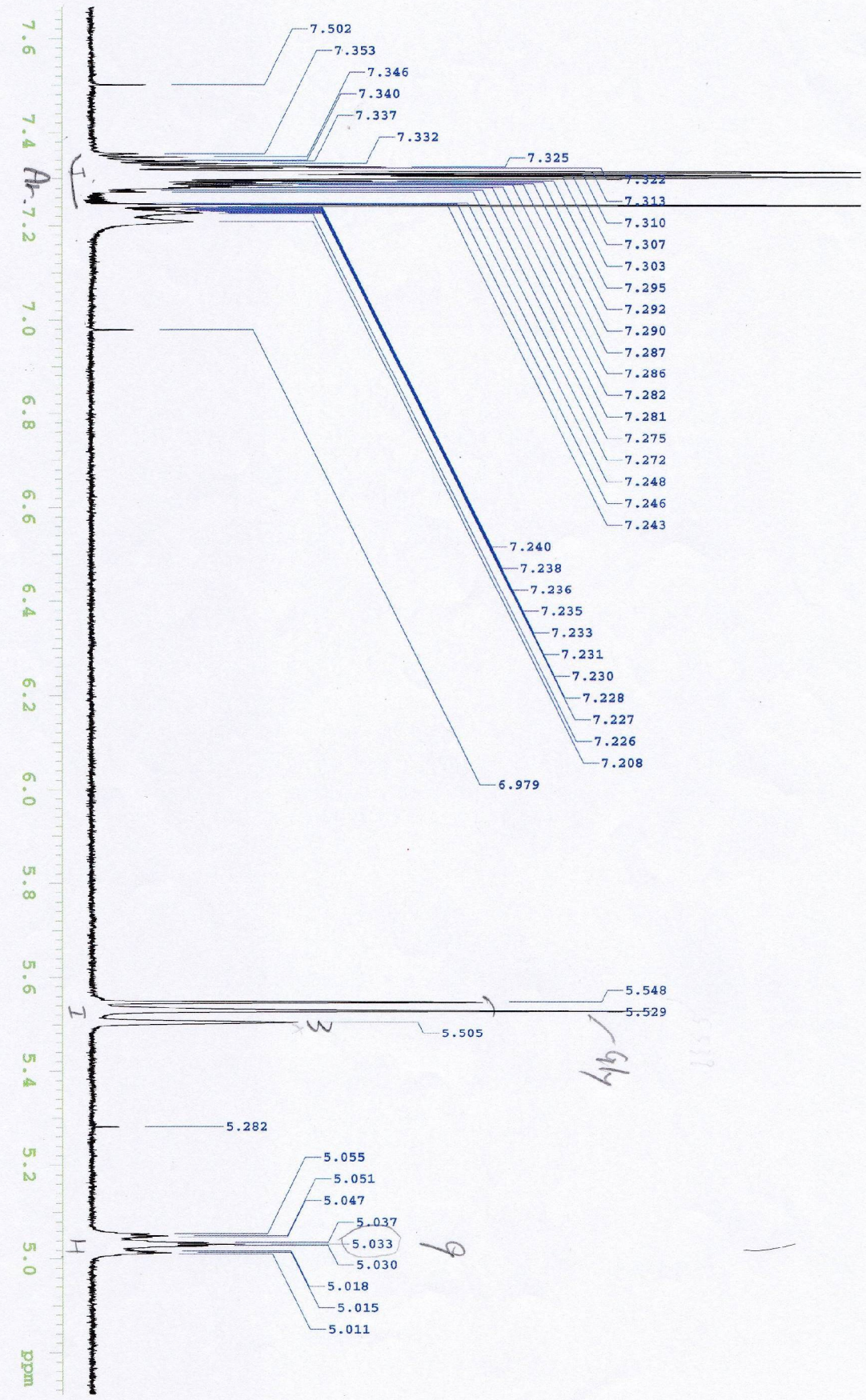

R-3
7.502
7.353
7.346
7.340
7.337
7.332
7.325
7.322
7.313
7.310
7.307
7.303
7.295
7.292
7.290
7.287
7.286
7.282
7.281
7.275
7.272
7.248
7.246
7.243
7.240
7.238
7.236
7.235
7.233
7.231
7.230
7.228
7.227
7.226
7.208
6.979
5.548
5.529
5.505
5.282
5.055
5.051
5.047
5.037
5.033
5.030
5.018
5.015
5.011
Ar
ppm

Figure S27 ^{1}H NMR spectra of 2b in $CDCl_3$