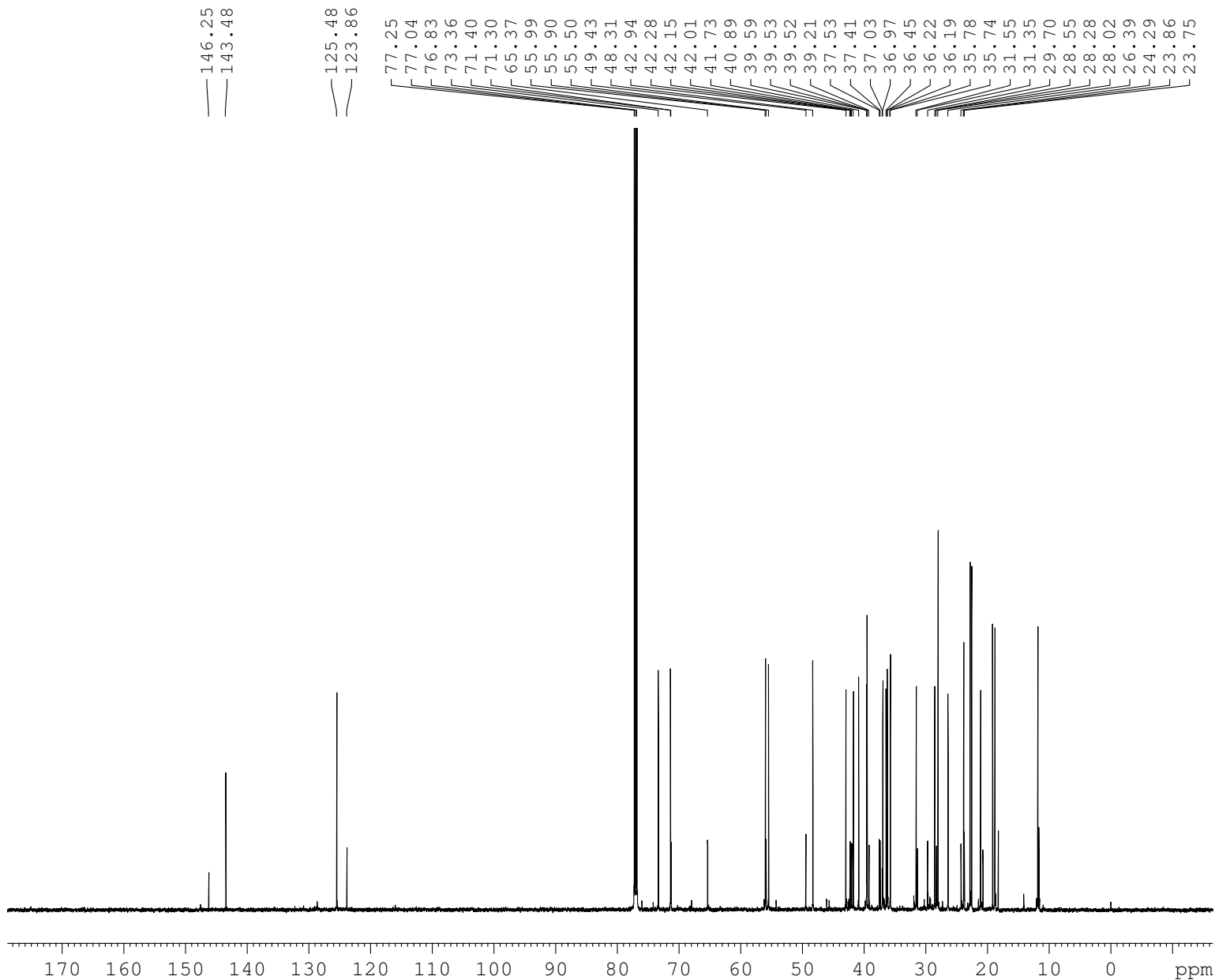


ste-1 13C

Figure S1



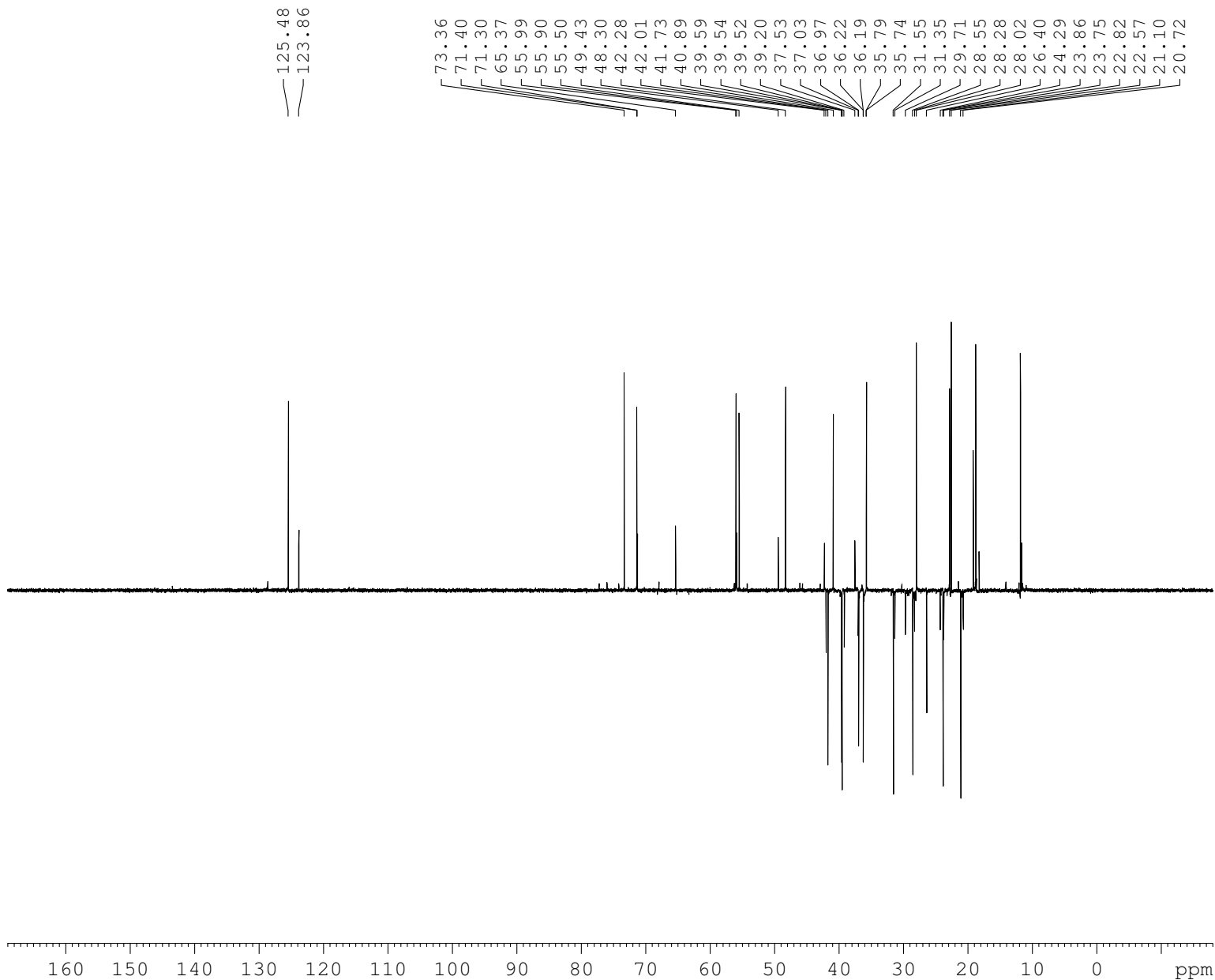
```
NAME 120380
EXPNO 2
PROCNO 1
Date_ 20120511
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1616
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
PL1 1.00 dB
PL1W 79.21191406 W
SFO1 151.0310627 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.41 dB
PL13 13.65 dB
PL2W 23.13002586 W
PL12W 0.52865964 W
PL13W 0.62976158 W
SFO2 600.5824023 MHz
SI 65536
SF 151.0159612 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
```

ste-1 DEPT

Figure S2



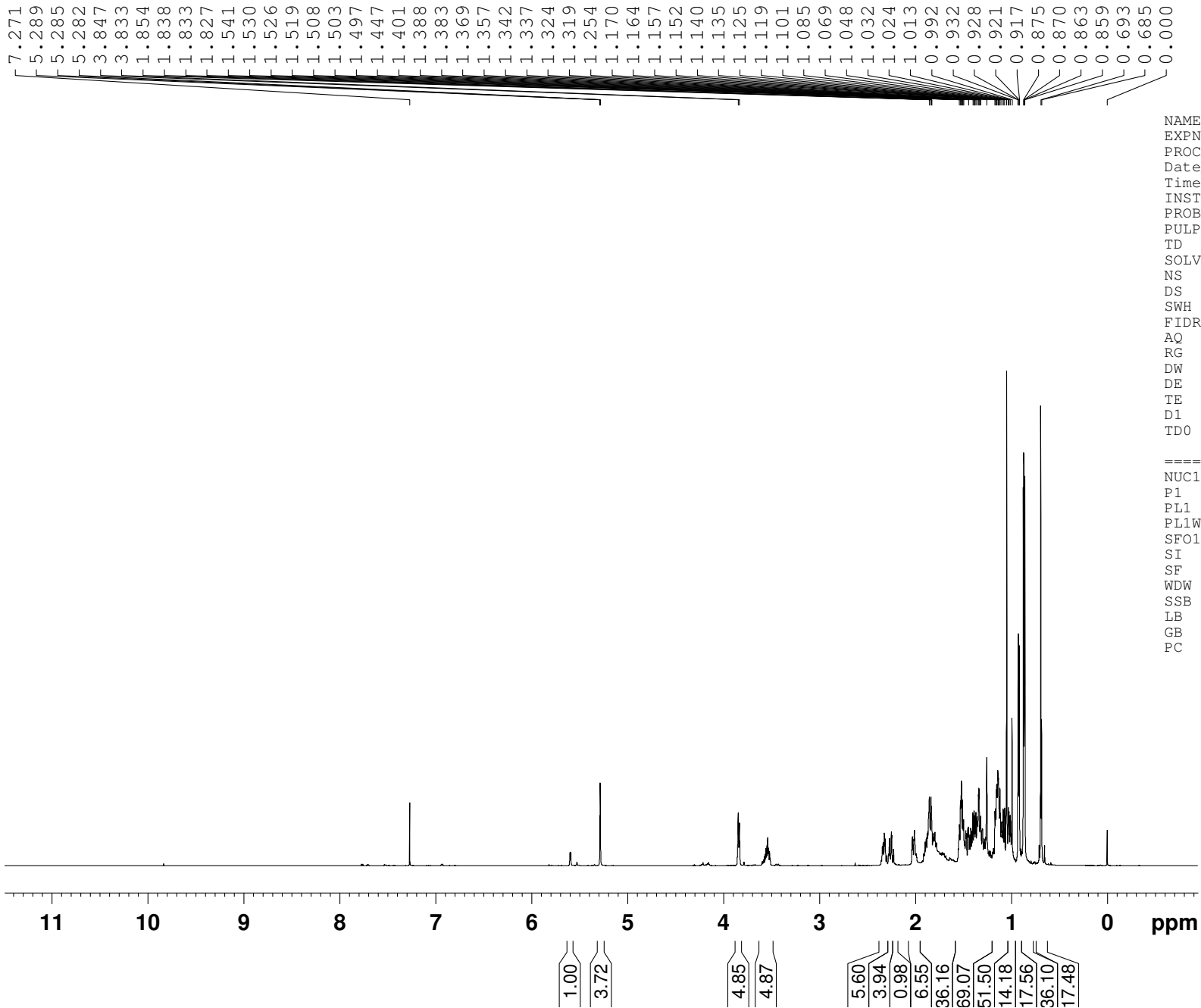
```
NAME 120380
EXPNO 3
PROCNO 1
Date_ 20120511
Time 15.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 298.0 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
P2 19.40 usec
PL1 1.00 dB
PL1W 79.21191406 W
SFO1 151.0310627 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.10 usec
P4 24.20 usec
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.41 dB
PL2W 23.13002586 W
PL12W 0.52865964 W
SFO2 600.5824023 MHz
SI 65536
SF 151.0159610 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

ste-1

Figure S3

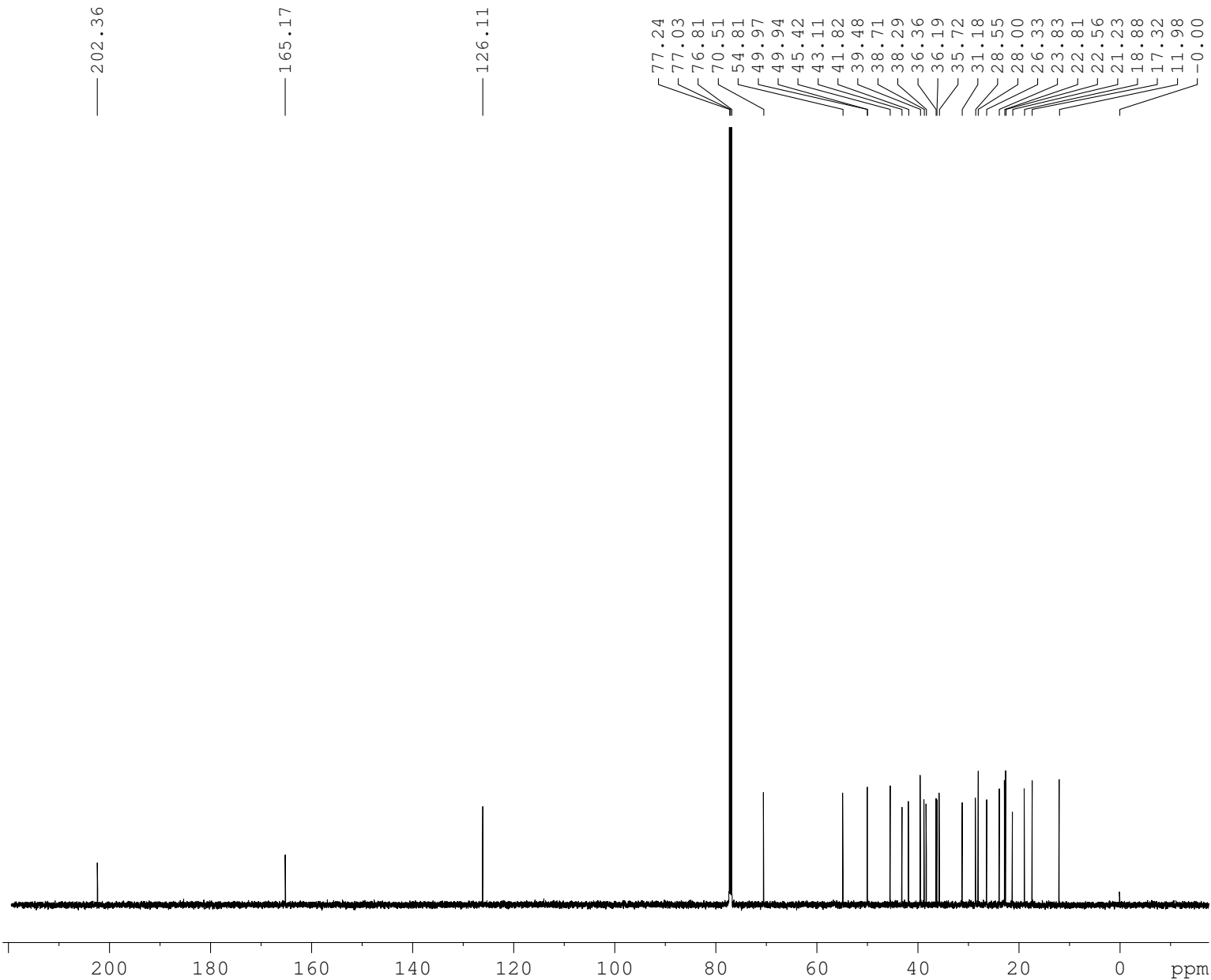


```
NAME 120380
EXPNO 1
PROCNO 1
Date_ 20120511
Time 14.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079220 sec
RG 32
DW 52.000 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.10 usec
PL1 -2.00 dB
PL1W 23.13002586 W
SFO1 600.5840839 MHz
SI 65536
SF 600.5800118 MHz
WDW EM
SSB 0
LB 0.40 Hz
GB 0
PC 1.00
```

ste-3 13C

Figure S4



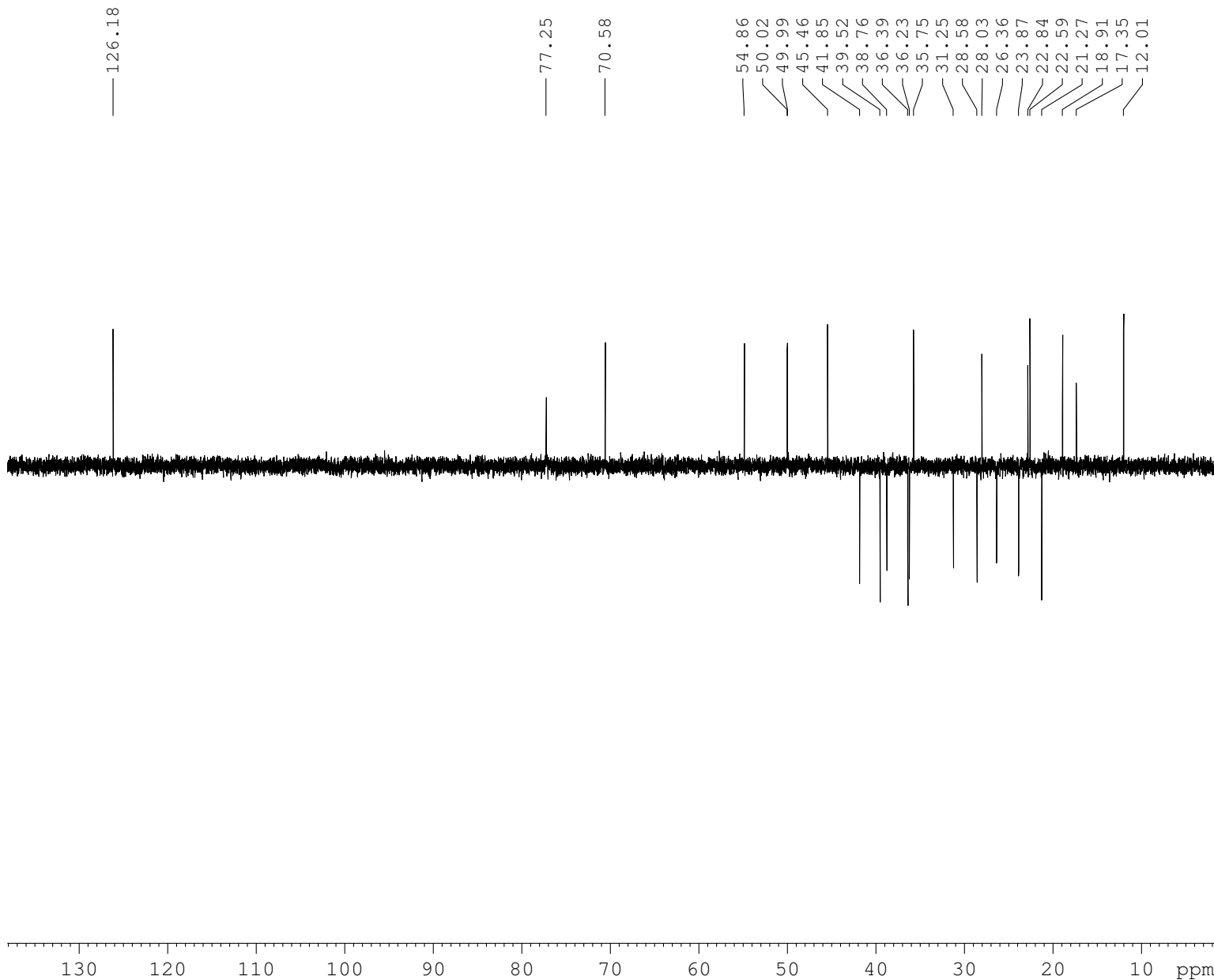
```
NAME 120709
EXPNO 2
PROCNO 1
Date_ 20121010
Time 10.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 408
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 295.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
PL1 1.00 dB
PL1W 79.21191406 W
SFO1 151.0310627 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.41 dB
PL13 13.65 dB
PL2W 23.13002586 W
PL12W 0.52865964 W
PL13W 0.62976158 W
SFO2 600.5824023 MHz
SI 65536
SF 151.0159624 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

ste-2 DEPT135

Figure S5



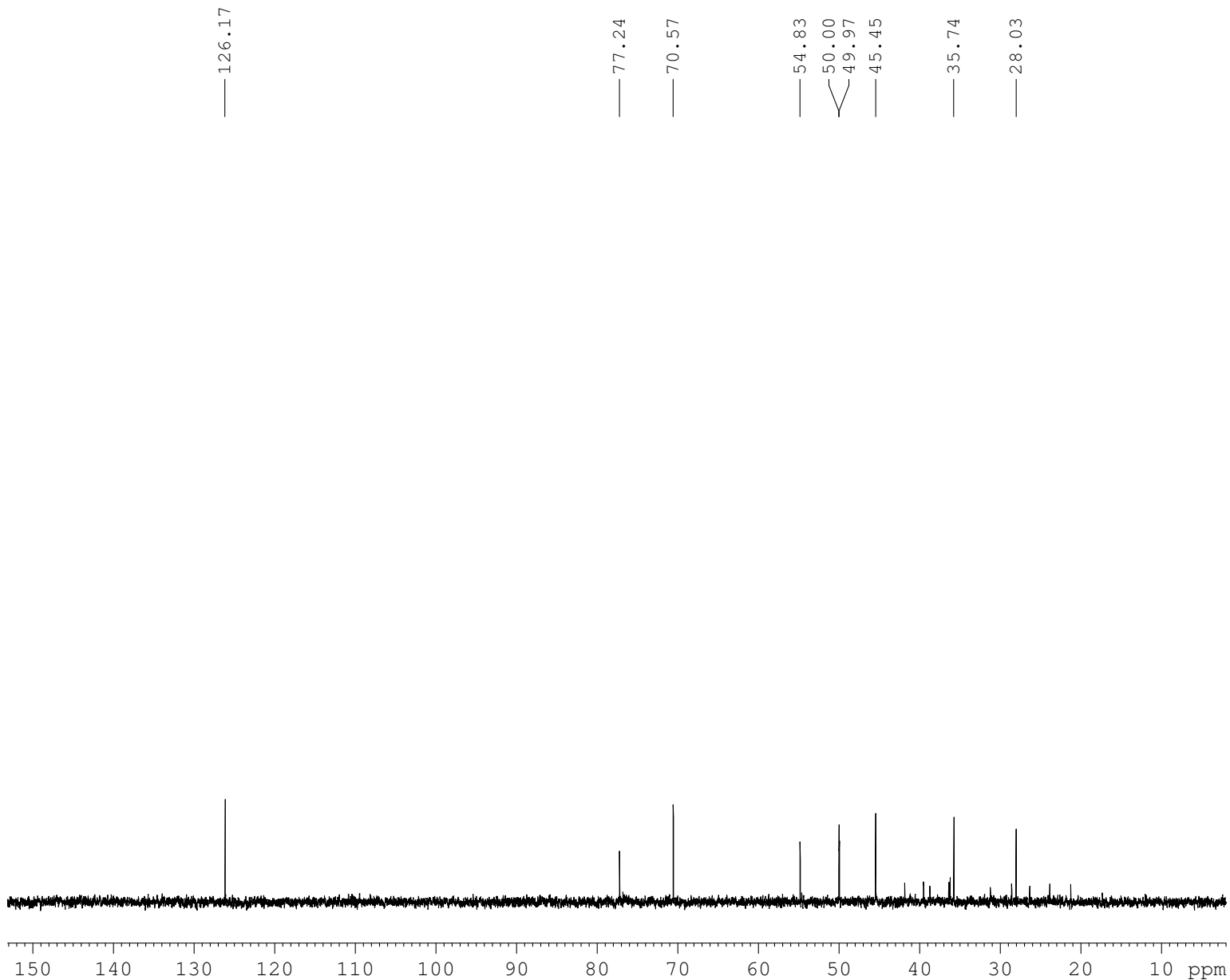
```
NAME 120503
EXPNO 3
PROCNO 1
Date_ 20120618
Time 14.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDC13
NS 1600
DS 8
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2050
DW 13.867 usec
DE 6.50 usec
TE 295.9 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
P2 19.40 usec
PL1 1.00 dB
PL1W 79.21191406 W
SFO1 151.0310626 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.10 usec
P4 24.20 usec
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.41 dB
PL2W 23.13002586 W
PL12W 0.52865964 W
SFO2 600.5824023 MHz
SI 65536
SF 151.0159570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

ste-2 DEPT90

Figure S6



```
NAME          120503
EXPNO         4
PROCNO        1
Date_         20120618
Time          12.48
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       dept90
TD            65536
SOLVENT       CDCl3
NS            1600
DS            8
SWH           36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG            2050
DW            13.867 usec
DE            6.50 usec
TE            295.8 K
CNST2         145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TDO           1
```

```
===== CHANNEL f1 =====
NUC1          13C
P1            9.70 usec
P2            19.40 usec
PL1           1.00 dB
PL1W          79.21191406 W
SFO1          151.0310627 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
P3            12.10 usec
P4            24.20 usec
PCPD2         80.00 usec
PL2           -2.00 dB
PL12          14.41 dB
PL2W          23.13002586 W
PL12W         0.52865964 W
SFO2          600.5824023 MHz
SI            32768
SF            151.0159584 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40
```

ste-3 1H

Figure S7



7.267
5.693
5.690
3.676
2.423
2.420
2.404
2.400
2.397
2.260
2.242
2.239
2.221
2.045
2.023
1.965
1.959
1.941
1.935
1.577
1.571
1.561
1.527
1.524
1.516
1.505
1.503
1.364
1.357
1.345
1.338
1.326
1.319
1.259
1.255
1.248
1.199
1.151
1.148
1.138
1.135
1.131
1.123
1.120
1.114
1.102
1.088
1.072
0.927
0.916
0.872
0.867
0.861
0.856
0.682

```
NAME 120709
EXPNO 1
PROCNO 1
Date_ 20121010
Time 10.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4079220 sec
RG 144
DW 52.000 usec
DE 6.50 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 12.10 usec
PL1 -2.00 dB
PL1W 23.13002586 W
SFO1 600.5839038 MHz
SI 65536
SF 600.5800145 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

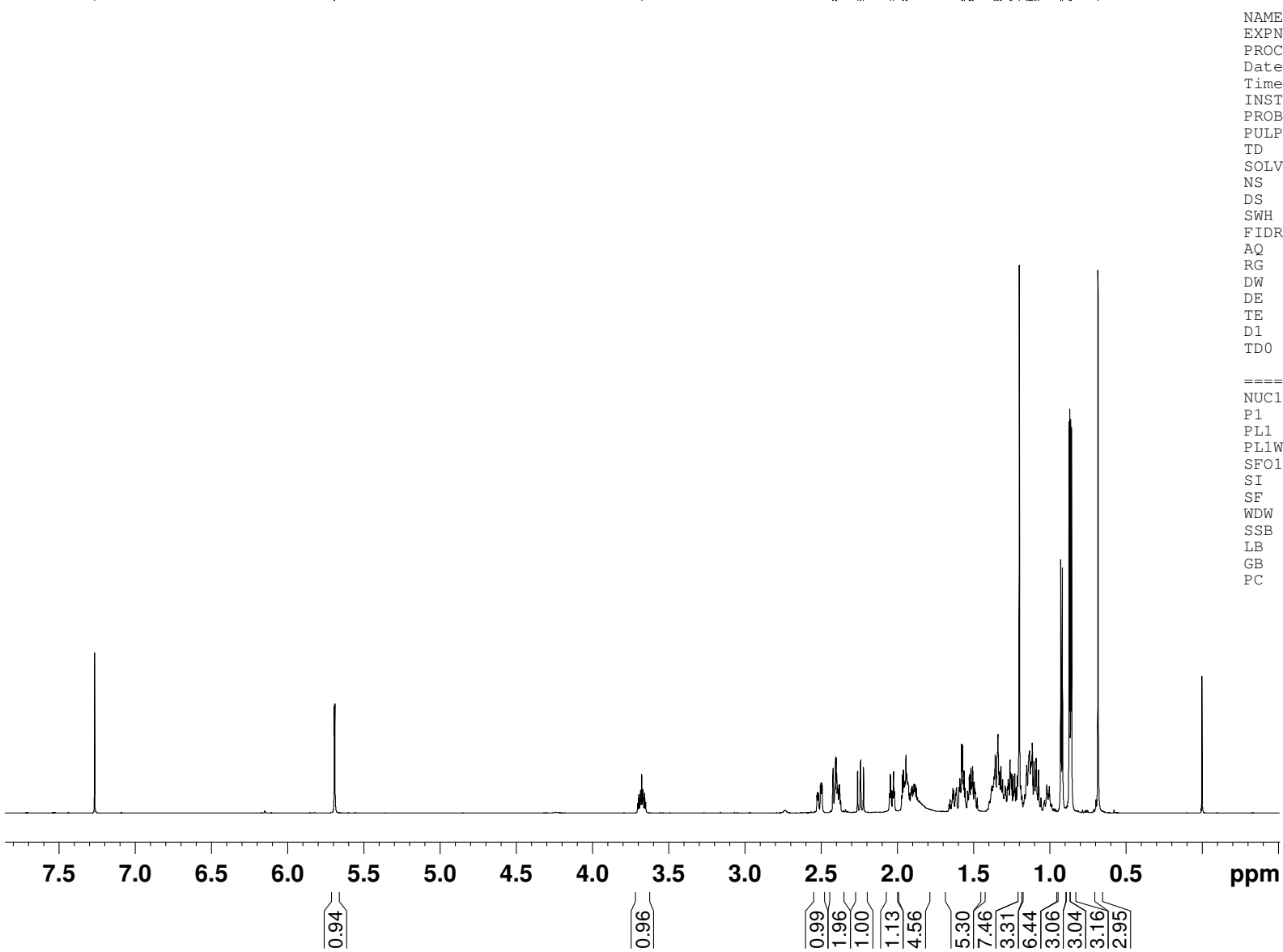
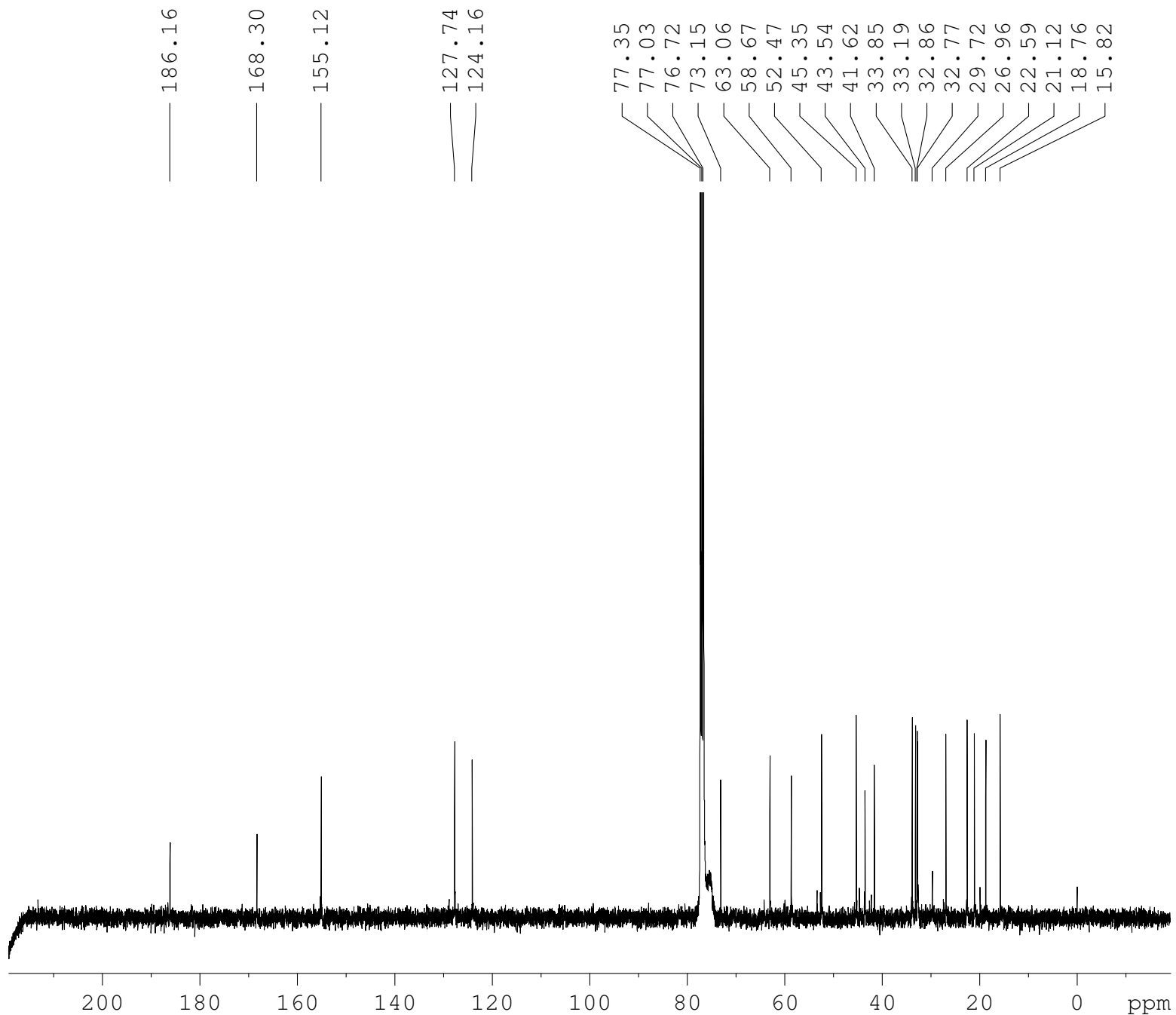


Figure S8

42-45



Current Data Parameters
NAME zhongkai
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140815
Time 18.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15194
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 300.1 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

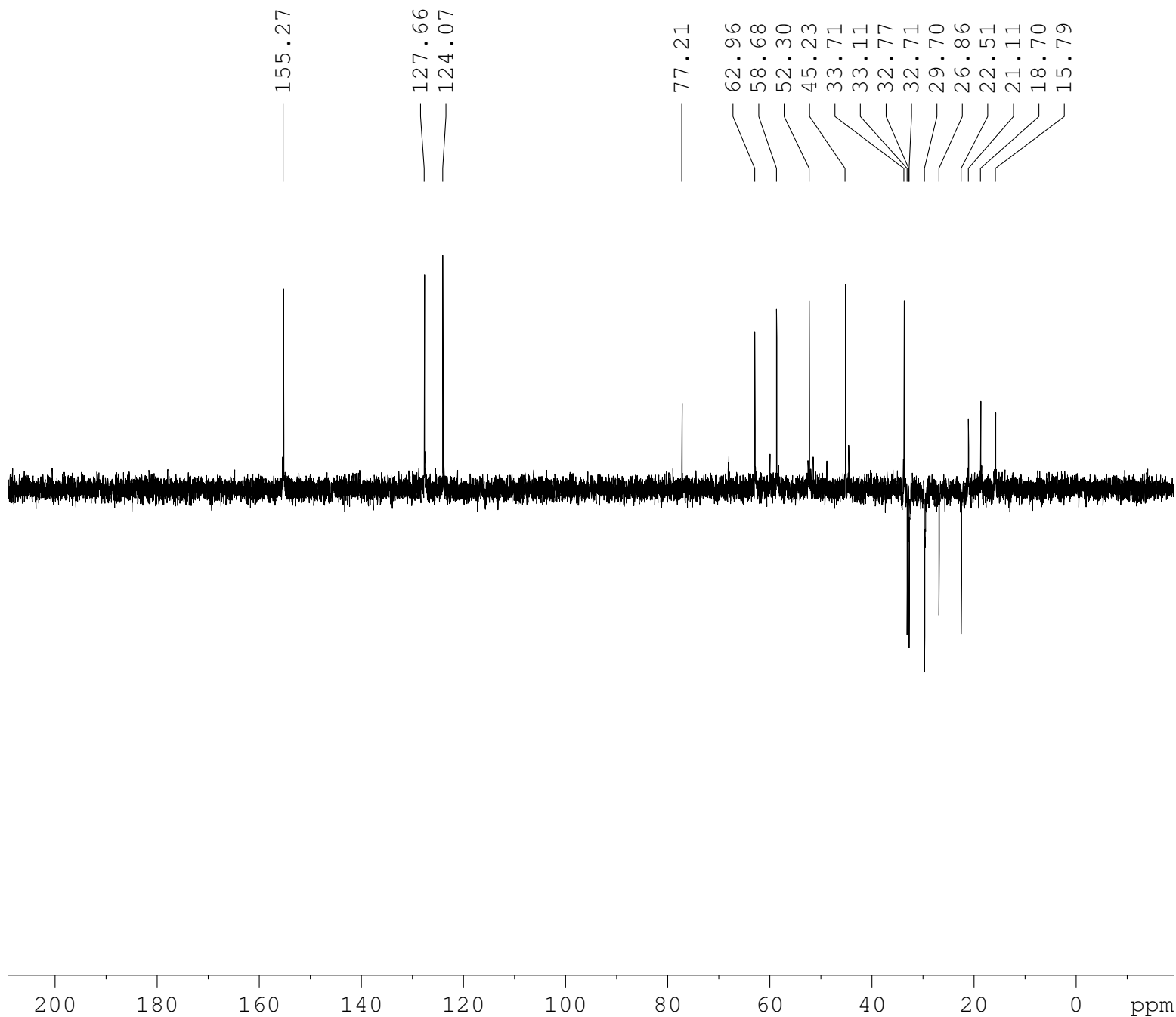
==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 1.08 dB
PL13 1.08 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127613 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S9

42-45 dept135



Current Data Parameters
NAME zhangzhibin
EXPNO 224
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141110
Time 8.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT CDC13
NS 11004
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.5 K
CNST2 145.000000
D1 2.0000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001019 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

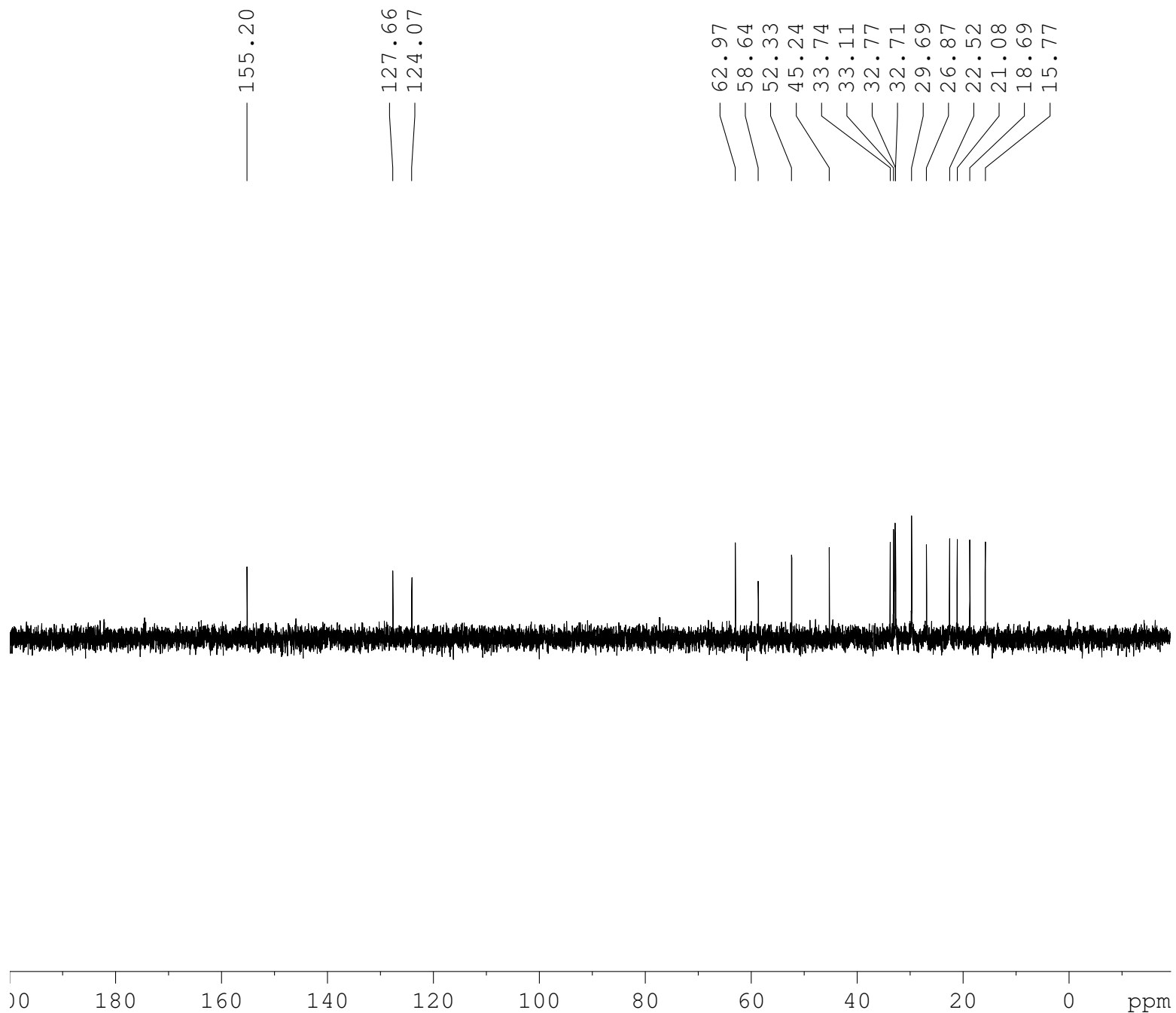
===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
p2 16.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 14.00 usec
p4 28.00 usec
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 12.14 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S10

42-45 dept90



Current Data Parameters
NAME zhongkai
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140828
Time 22.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept90
TD 65536
SOLVENT CDC13
NS 16532
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 299.3 K
CNST2 145.000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001019 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

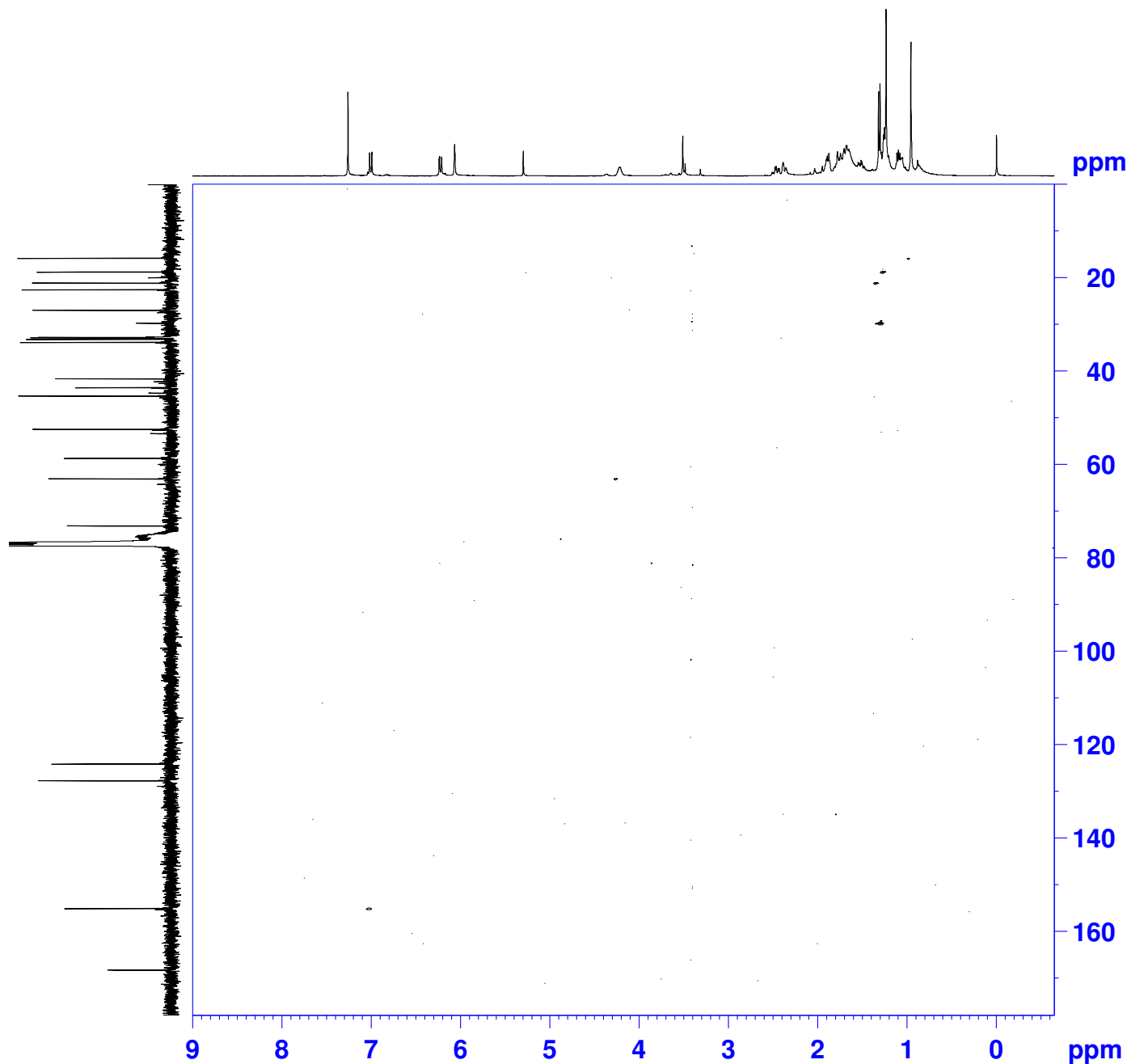
==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
p2 16.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 14.00 usec
p4 28.00 usec
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 1.08 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S11

42-45 HMQC



```

Current Data Parameters
NAME      zhangzhibin
EXPNO     212
PROCNO    1

F2 - Acquisition Parameters
Date_     20141107
Time      6.49
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   hsqcetgp
TD         1000
SOLVENT   CDCl3
NS         50
DS         16
SWH        3980.892 Hz
FIDRES     3.980892 Hz
AQ         0.1256500 sec
RG         18390.4
DW         125.600 usec
DE         6.00 usec
TE         299.5 K
CNST2     145.0000000
d0         0.00000300 sec
D1         2.00000000 sec
d4         0.00172414 sec
d11        0.03000000 sec
d13        0.00000400 sec
D16        0.00020000 sec
DELTA      0.00123400 sec
DELTA1     0.00071614 sec
IN0        0.00002550 sec
MCREST     0.00000000 sec
MCWRK     0.40000001 sec
ST1CNT     256

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
p2         28.00 usec
P28        1000.00 usec
PL1        -3.00 dB
SFO1       400.1313688 MHz

===== CHANNEL f2 =====
CPDPRG2   garp
NUC2       13C
P3         8.00 usec
p4         16.00 usec
PCPD2     80.00 usec
PL2        -2.00 dB
PL12       12.00 dB
SFO2       100.6225824 MHz

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPX1      0.00 %
GPX2      0.00 %
GPY1      0.00 %
GPY2      0.00 %
GPZ1      80.00 %
GPZ2      20.10 %
P16       1000.00 usec

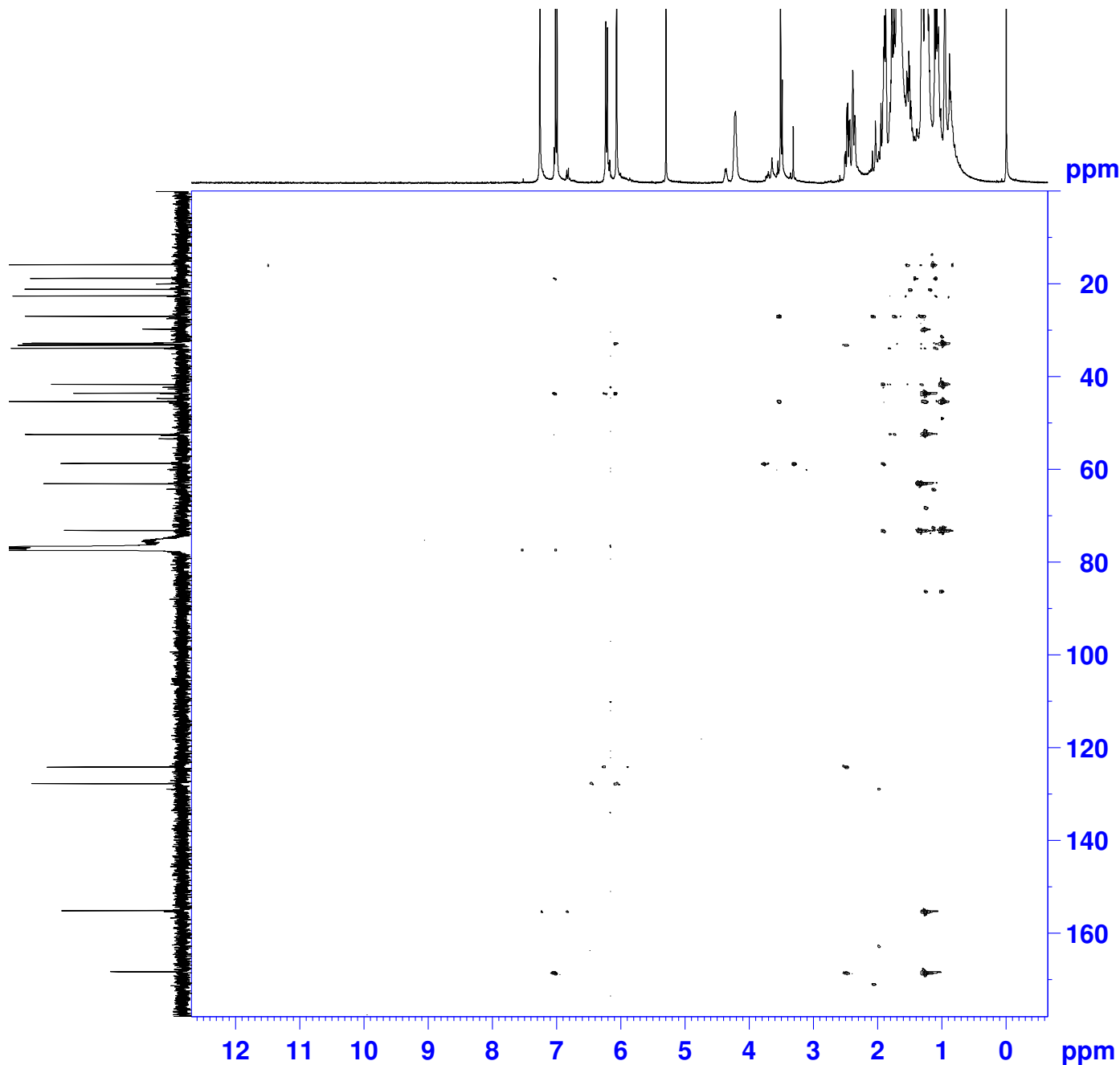
F1 - Acquisition parameters
ND0        2
TD         1093
SFO1       100.6226 MHz
FIDRES     18.105118 Hz
SW         194.865 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI         1024
SF         400.1300082 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        echo-antiecho
SF         100.6127613 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
    
```

Figure S12

42-45 HMBC



```

Current Data Parameters
NAME      zhongkai
EXPNO    26
PROCNO    1

F2 - Acquisition Parameters
Date_    20141121
Time     16.28
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  hmbcgpndqf
TD       4096
SOLVENT  CDCl3
NS       128
DS       16
SWH      4280.822 Hz
FIDRES   1.045123 Hz
AQ       0.4784628 sec
RG       26008
DW       116.800 usec
DE       6.00 usec
TE       295.6 K
CNST13   8.0000000
d0       0.00000300 sec
d1       1.50000000 sec
d6       0.06250000 sec
d16      0.00020000 sec
IN0      0.00002481 sec
MCREST   0.00000000 sec
MCWRK    1.50000000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       14.00 usec
p2       28.00 usec
PL1      -3.00 dB
SFO1     400.1324688 MHz

===== CHANNEL f2 =====
NUC2     13C
P3       8.00 usec
PL2      -2.00 dB
SFO2     100.6228298 MHz

===== GRADIENT CHANNEL =====
GPNAM1   SINE.100
GPNAM2   SINE.100
GPNAM3   SINE.100
GPX1     0.00 %
GPX2     0.00 %
GPX3     0.00 %
GPY1     0.00 %
GPY2     0.00 %
GPY3     0.00 %
GPZ1     50.00 %
GPZ2     30.00 %
GPZ3     40.10 %
P16      1000.00 usec

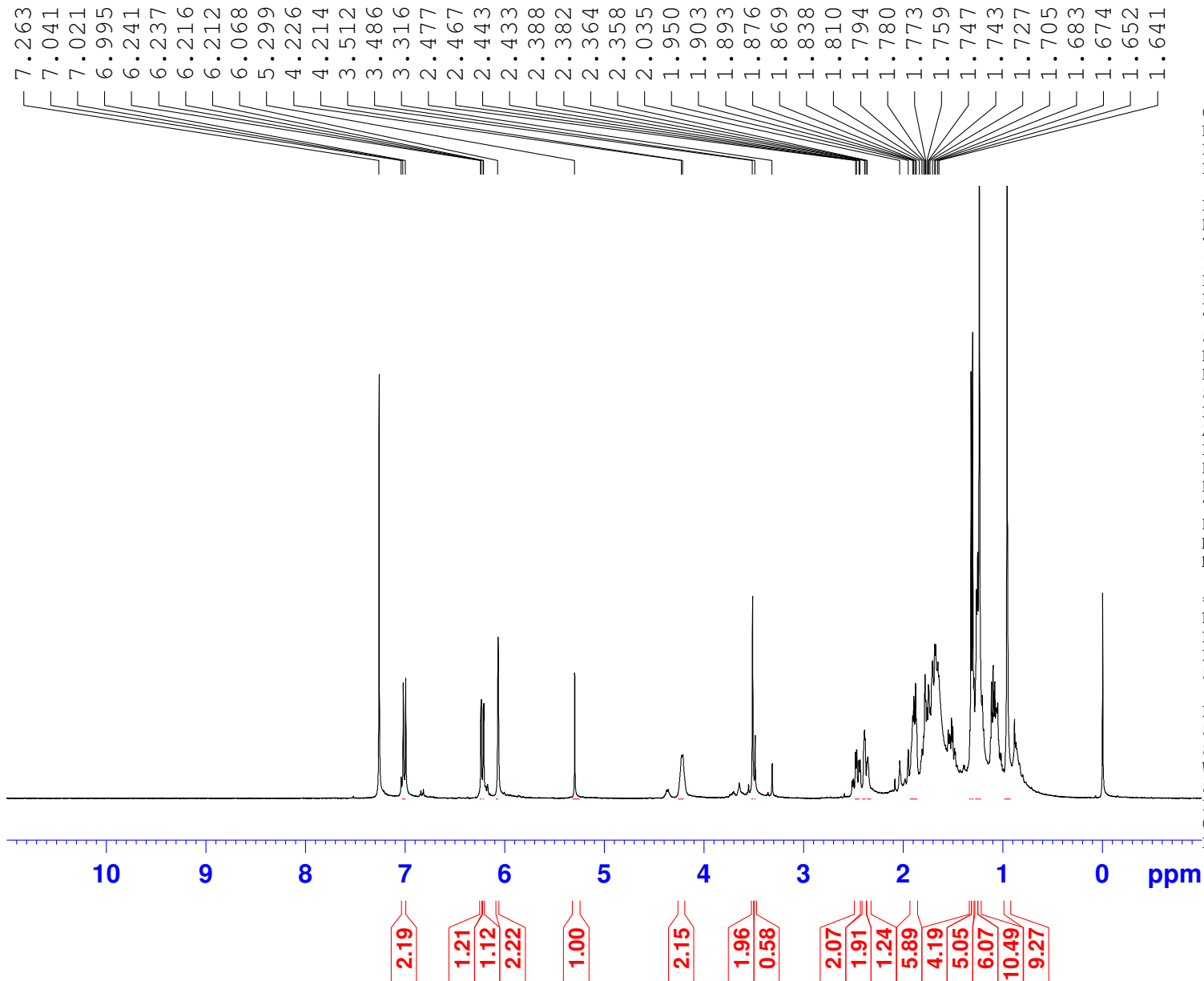
F1 - Acquisition parameters
ND0      2
TD       732
SFO1     100.6228 MHz
FIDRES   27.528872 Hz
SW       200.264 ppm
FrMODE   QF

F2 - Processing parameters
SI       1024
SF       400.1300082 MHz
WDW      SINE
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      QF
SF       100.6127613 MHz
WDW      SINE
SSB      0
LB       0.00 Hz
GB       0
    
```

Figure S13

42-45



```

Current Data Parameters
NAME                zhongkai
EXPNO                13
PROCNO              1

F2 - Acquisition Parameters
Date_                20140815
Time                 13.27
INSTRUM              spect
PROBHD               5 mm BBO BB-1H
PULPROG              zg30
TD                   65536
SOLVENT              CDC13
NS                   1528
DS                   0
SWH                  8278.146 Hz
FIDRES               0.126314 Hz
AQ                   3.9584243 sec
RG                   1625.5
DW                   60.400 usec
DE                   6.00 usec
TE                   298.1 K
D1                   1.00000000 sec
MCREST               0.00000000 sec
MCWRK               0.01500000 sec

===== CHANNEL f1 =====
NUC1                  1H
P1                    14.00 usec
PL1                   -3.00 dB
SFO1                  400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF                    400.1300082 MHz
WDW                   EM
SSB                   0
LB                    0.30 Hz
GB                   0
PC                    1.00
    
```

Figure S14: The ^1H spectral data for compound 1-3

The ^1H and ^{13}C NMR spectral data for compound **1** was as follows: ^1H NMR • (600 MHz, CDCl_3) 0.69(3H, s), 1.05(3H,s), 0.86(3H, d, J=2.4 Hz), 0.87(3H,d,J= 3.0 Hz), 0.93(3H, d, J=6.6 Hz), 1.15-1.58(26H, m), 2.05(1H, m), 2.30(1H, m), 3.54(H, m), 3.84(1H, dt, J=8.4, 2.4 Hz), 5.28(1H, t, J=2.4 Hz).

The ^1H and ^{13}C NMR spectrum data of compound **2** was as follows: ^1H NMR • (600MHz, CDCl_3) 0.68 (s, 3H) , 0.86(d, 3H, J=2.4), 0.87(d, 3H, J=3.0), 0.92 (d, 3H, J=6.6) , 1.12 (s, 3H) , 5.69 (1H, s, C-6.

The ^1H and ^{13}C NMR spectrum data of compound **3** was as follows: ^1H NMR • (400MHz, CDCl_3) , 7.01(1H, d ,J=10.4Hz), 6.22(1H, dd, J=10.4,1.6Hz), 6.06(1H, s), 4.22(1H, q, J=4.8Hz) , 3.51(1H, d, s),1.30(3H, d, J=6.4Hz), 1.23(3H, s), 0.95(3H, s); ^{13}C NMR •(100MHz, CDCl_3): 155.1 (C-1), 127.7 (C-2), 186.1 (C-3), 124.1 (C-4), 168.3 (C-5), 33.1 (C-6), 32.7 (C-7), 33.7(C-8),52.3 (C-9), 45.2 (C-10), 22.5 (C-11), 32.7 (C-12), 41.6 (C-13), 43.5 (C-14), 29.7 (C-15), 58.6 (C-16),73.1 (C-17), 15.7 (C-18), 21.1(C-19),62.9 (C-20), 18.7 (C-21).

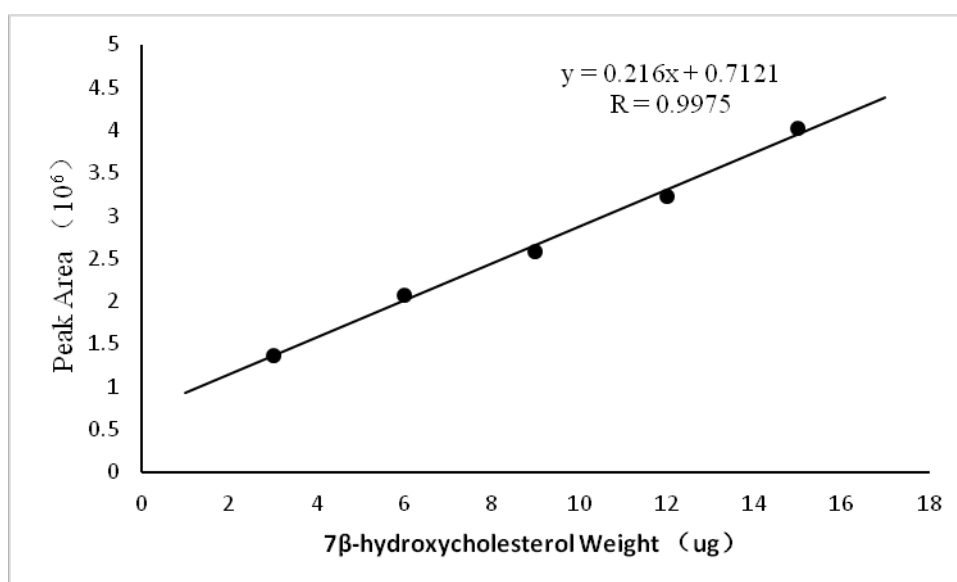
Figure S15: The ^{13}C NMR spectral data for compound 1-3

<i>C</i>	(1)	(2)	(3)	<i>cholesterol</i>
1	36.9	36.4	155.1	37.3
2	31.6	31.3	127.7	31.6
3	71.4	70.6	186.1	71.6
4	41.7	41.8	124.1	42.2
5	143.5	165.0	168.3	140.8
6	125.5	126.2	33.1	121.6
7	73.4	202.2	32.7	31.9
8	40.9	45.5	33.7	31.9
9	48.3	50.0	52.3	50.2
10	36.4	38.3	45.2	36.5
11	21.1	21.3	22.5	21.1
12	28.6	28.6	32.7	28.3
13	42.9	43.1	41.6	42.3
14	55.5	54.9	43.5	56.8
15	26.4	26.3	29.7	24.3
16	39.6	38.8	58.6	39.8
17	54.9	54.9	73.1	56.8
18	11.8	12.0	15.7	11.9
19	19.2	18.9	21.1	19.4
20	35.7	35.8	62.9	35.8
21	18.7	18.7	18.7	18.7
22	36.2	36.2		36.2
23	23.9	23.9		23.9
24	39.5	39.5		39.5
25	28.0	28.0		28.0
26	22.6	22.6		22.6
27	22.8	22.8		22.8

Figure S16

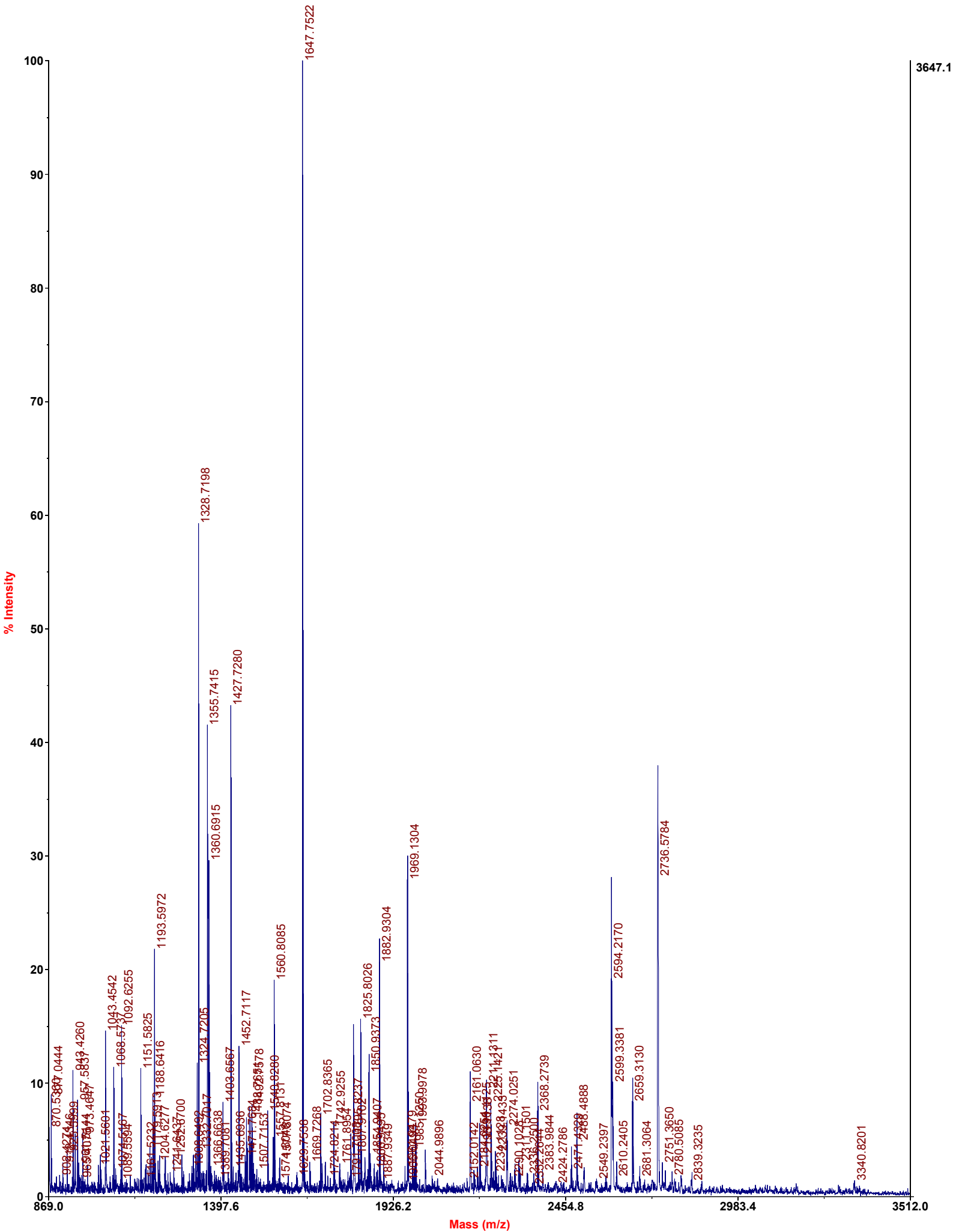
Standard concentration 7-hydroxycholesterol Preparation method

weight (ug)	Peak area (10 ⁶)
3	1.368915
6	2.070902
9	2.579276
12	3.232314
15	4.027717



Standard curve of 7-hydroxycholesterol

Figure S17



4700 MS/MS Precursor 1328.7202 Spec #1 MC[BP = 70.1, 2609]

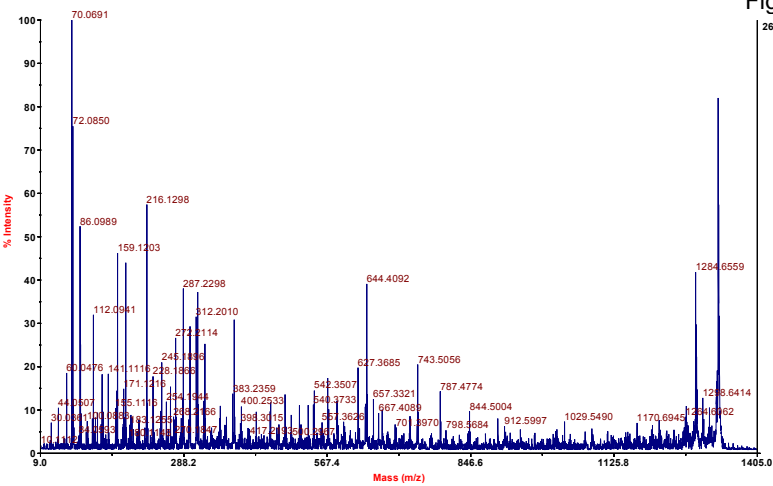
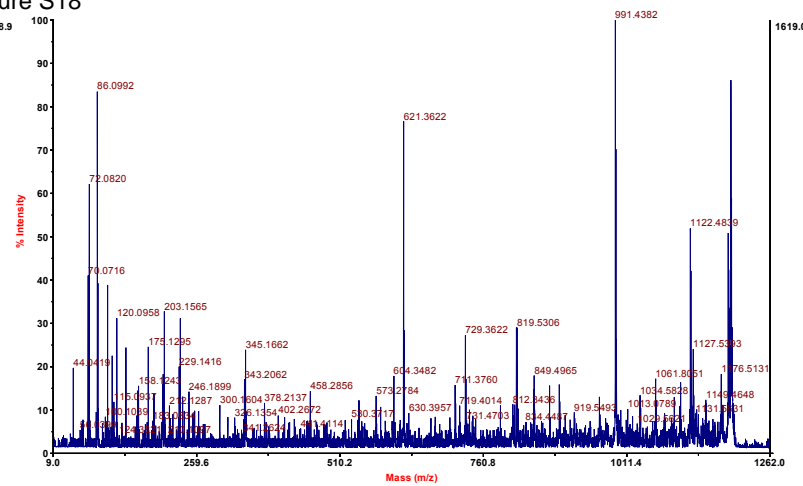
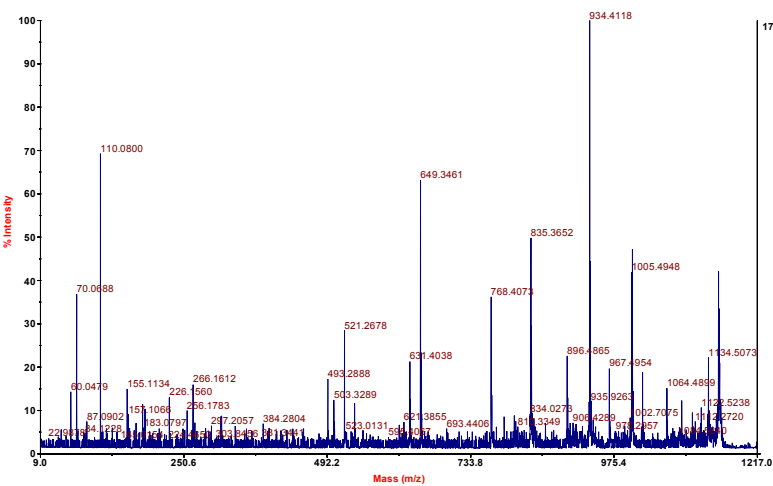


Figure S18

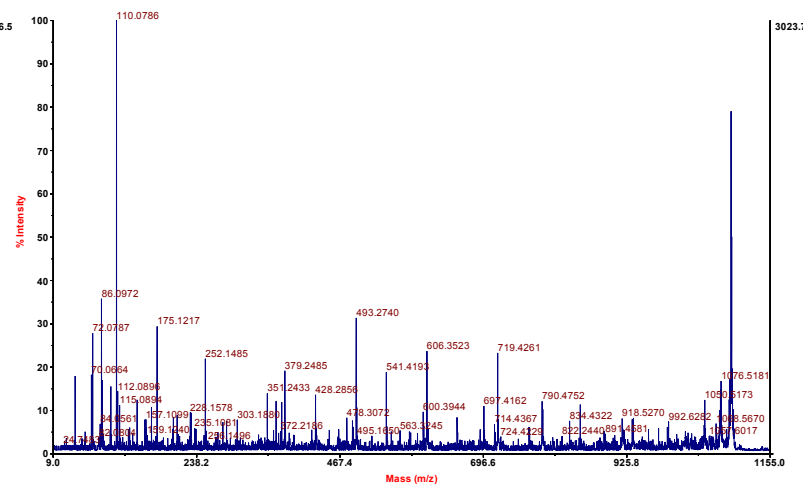
4700 MS/MS Precursor 1193.6 Spec #1 MC[BP = 991.4, 1619]



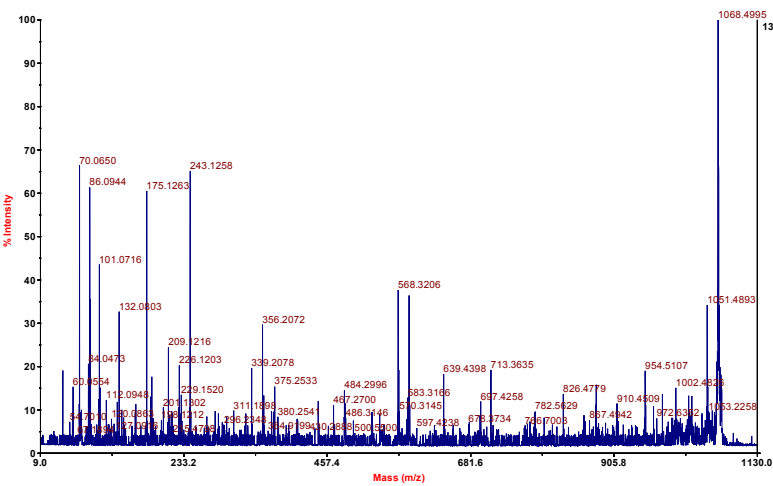
4700 MS/MS Precursor 1151.58 Spec #1 MC[BP = 934.4, 1756]



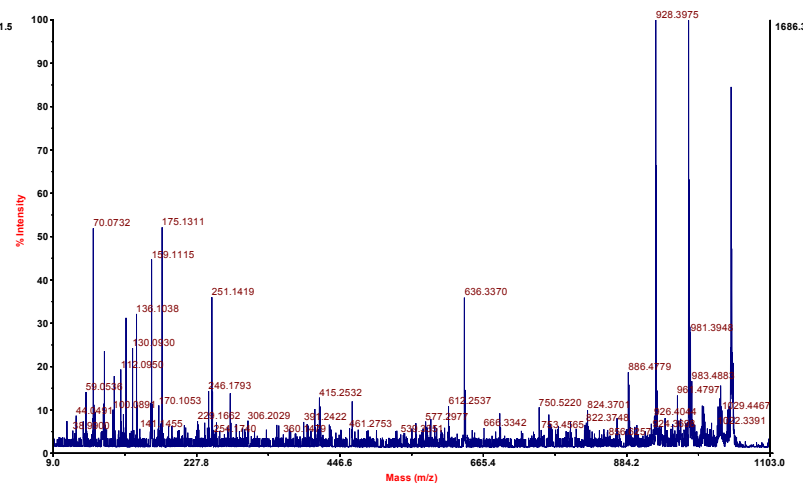
4700 MS/MS Precursor 1092.63 Spec #1 MC[BP = 110.1, 3024]



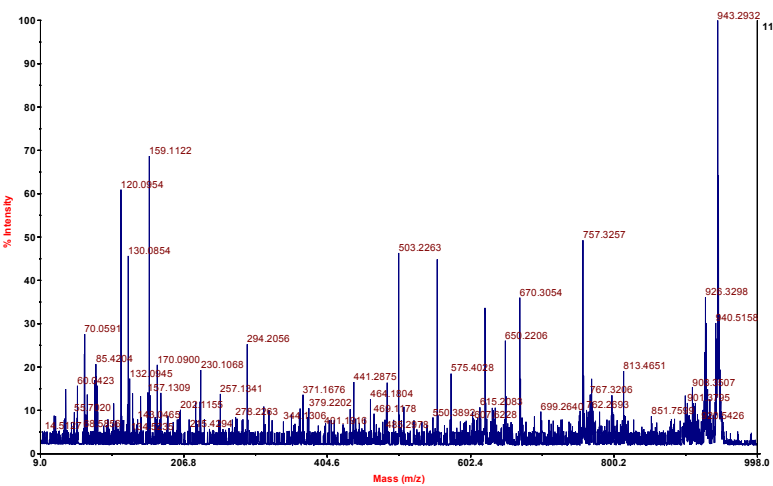
4700 MS/MS Precursor 1068.57 Spec #1 MC[BP = 1068.6, 1392]



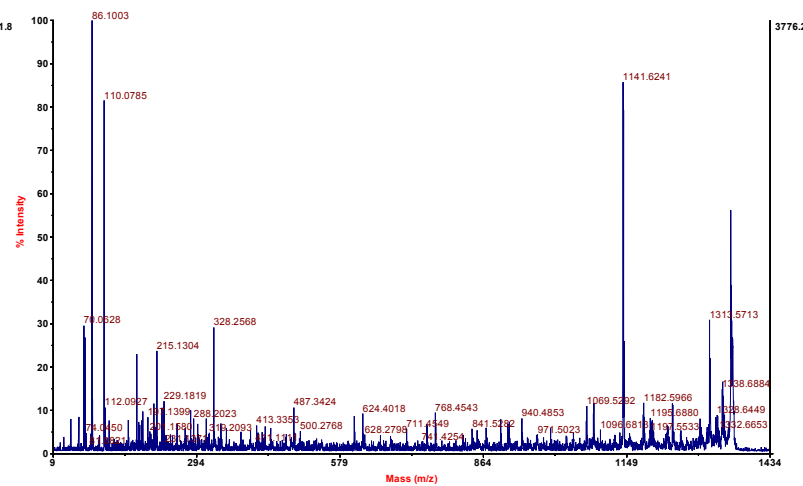
4700 MS/MS Precursor 1043.45 Spec #1 MC[BP = 928.4, 1686]



4700 MS/MS Precursor 943.427 Spec #1 MC[BP = 943.3, 1152]

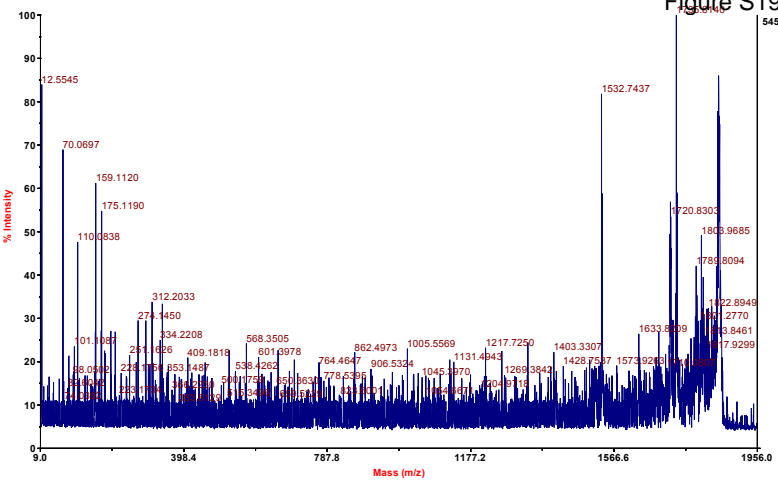


4700 MS/MS Precursor 1355.74 Spec #1 MC[BP = 86.1, 3776]



4700 MS/MS Precursor 1850.94 Spec #1 MC[BP = 1735.8, 545]

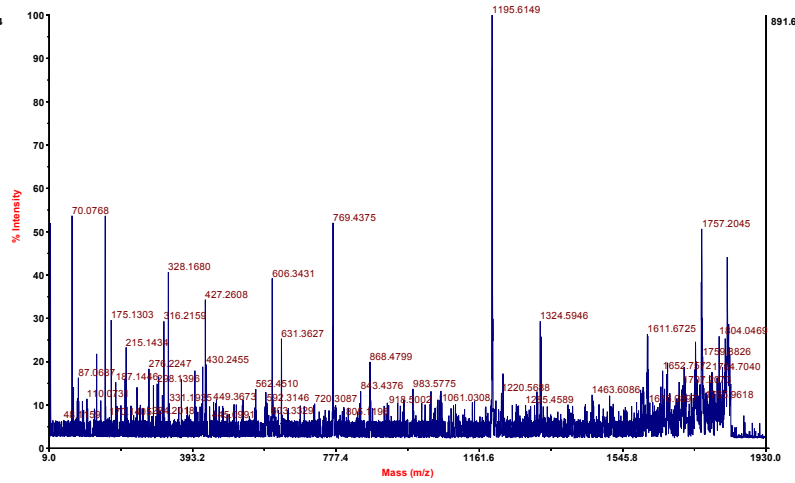
Figure S19



F:\...\J10_MSMS_1850.9360_94.t2d

Acquired:

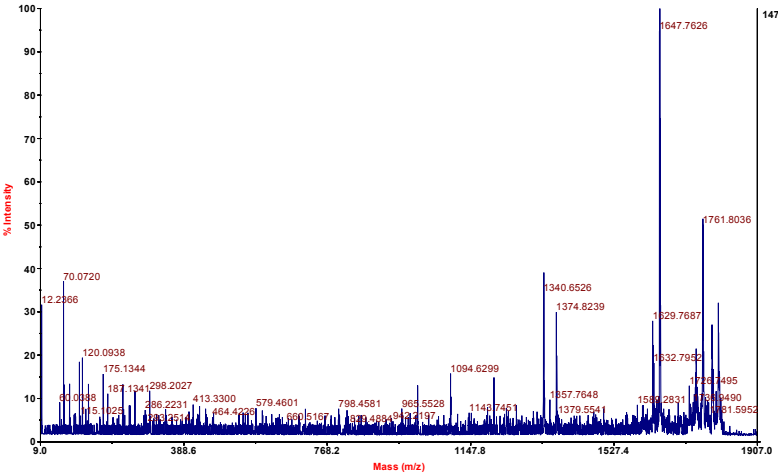
4700 MS/MS Precursor 1825.8 Spec #1 MC[BP = 1195.6, 892]



F:\...\J10_MSMS_1825.8009_101.t2d

Acquired:

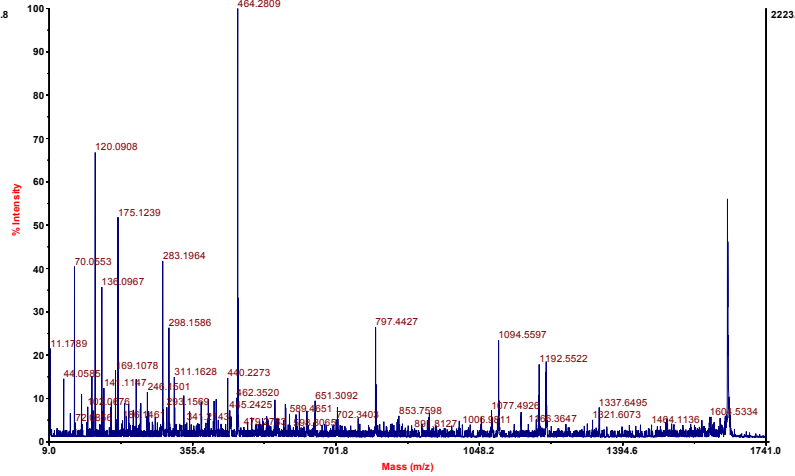
4700 MS/MS Precursor 1803.89 Spec #1 MC[BP = 1648.8, 1479]



F:\...\J10_MSMS_1803.8860_103.t2d

Acquired:

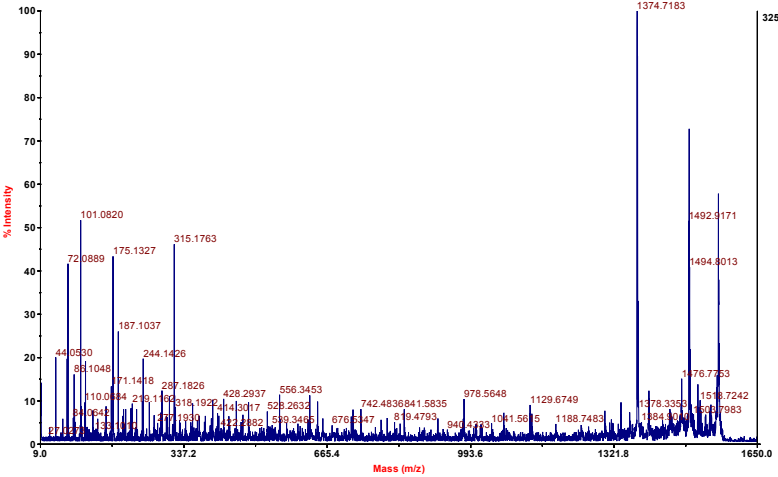
4700 MS/MS Precursor 1647.75 Spec #1 MC[BP = 464.3, 2224]



F:\...\J10_MSMS_1647.7499_111.t2d

Acquired:

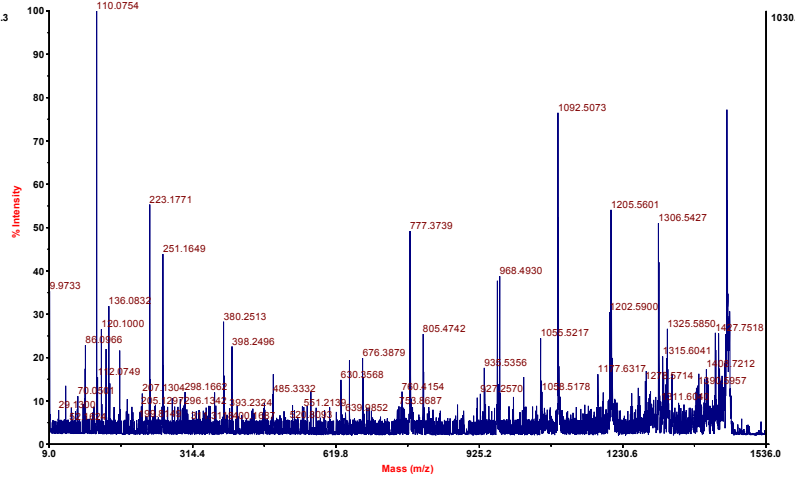
4700 MS/MS Precursor 1560.81 Spec #1 MC[BP = 1374.7, 3259]



F:\...\J10_MSMS_1560.8083_99.t2d

Acquired:

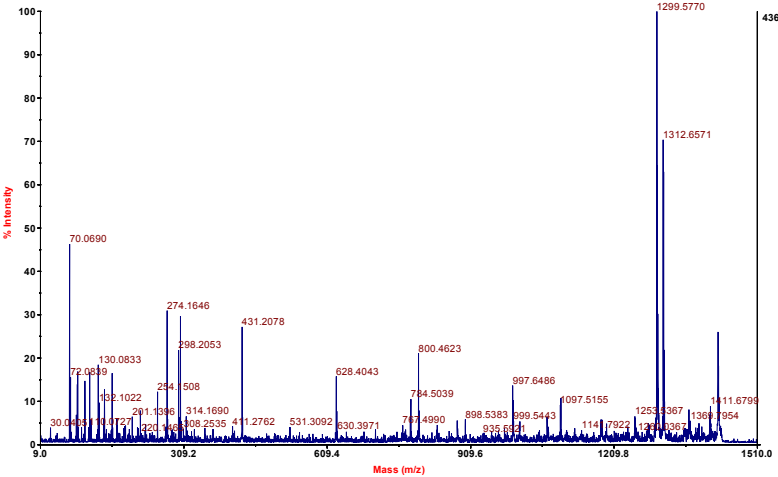
4700 MS/MS Precursor 1452.71 Spec #1 MC[BP = 110.1, 1030]



F:\...\J10_MSMS_1452.7109_96.t2d

Acquired:

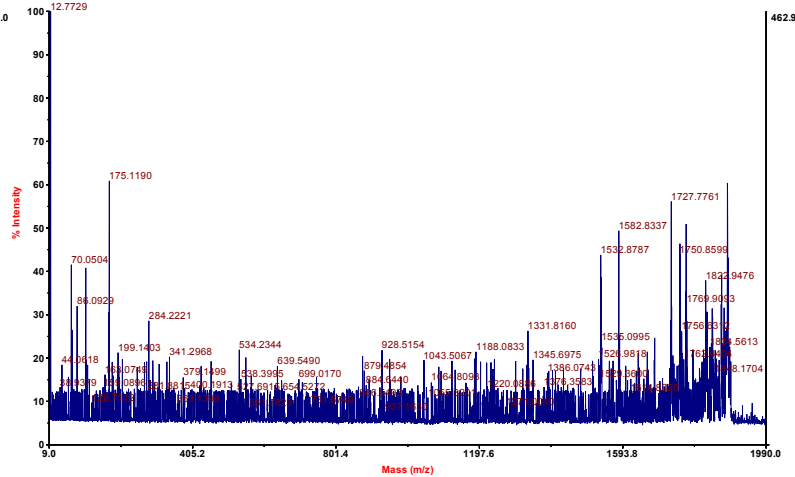
4700 MS/MS Precursor 1427.73 Spec #1 MC[BP = 1299.5, 4365]



F:\...\J10_MSMS_1427.7281_106.t2d

Acquired:

4700 MS/MS Precursor 1882.93 Spec #1 MC[BP = 12.8, 463]



F:\...\J10_MSMS_1882.9298_104.t2d

Acquired: