Supporting Information I

A Ligand-Based Drug Design, Discovery of 4-Trifluoromethyl-7,8-Pyranocoumarin as a Selective Inhibitor of Human Cytochrome P450 1A2

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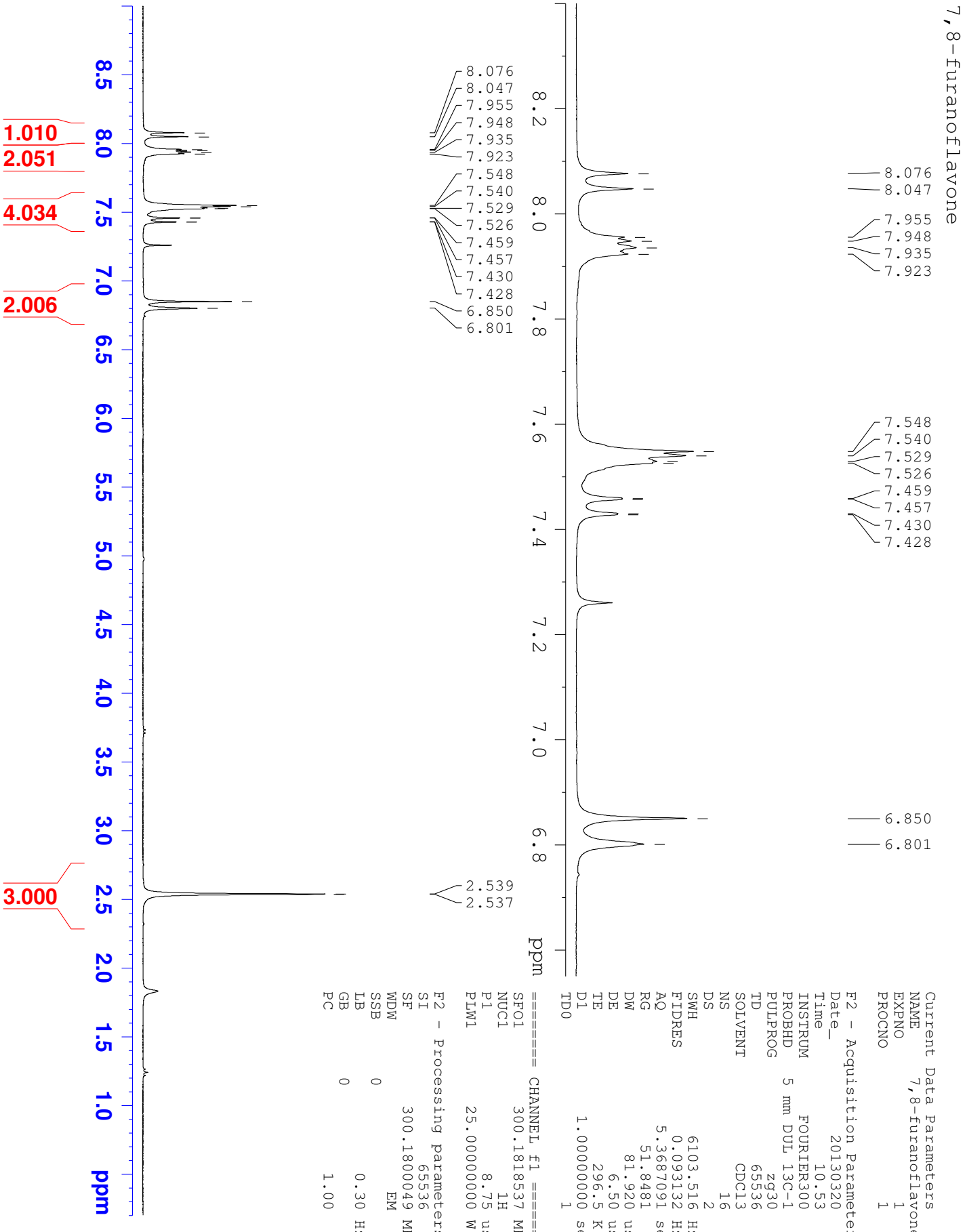
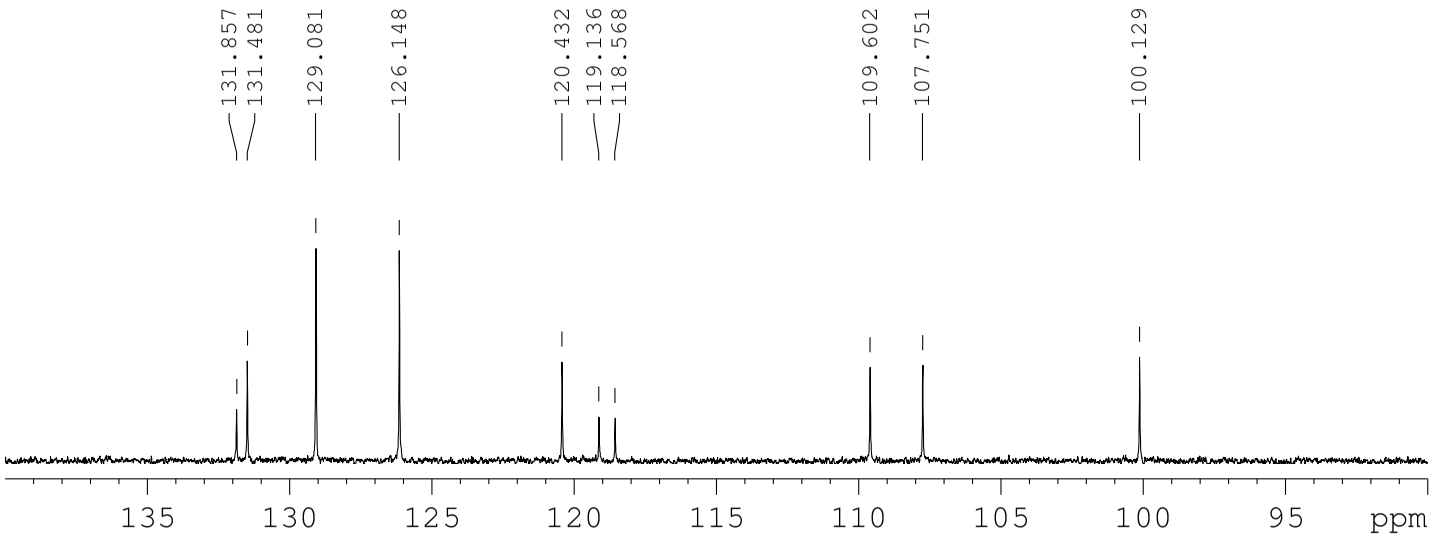
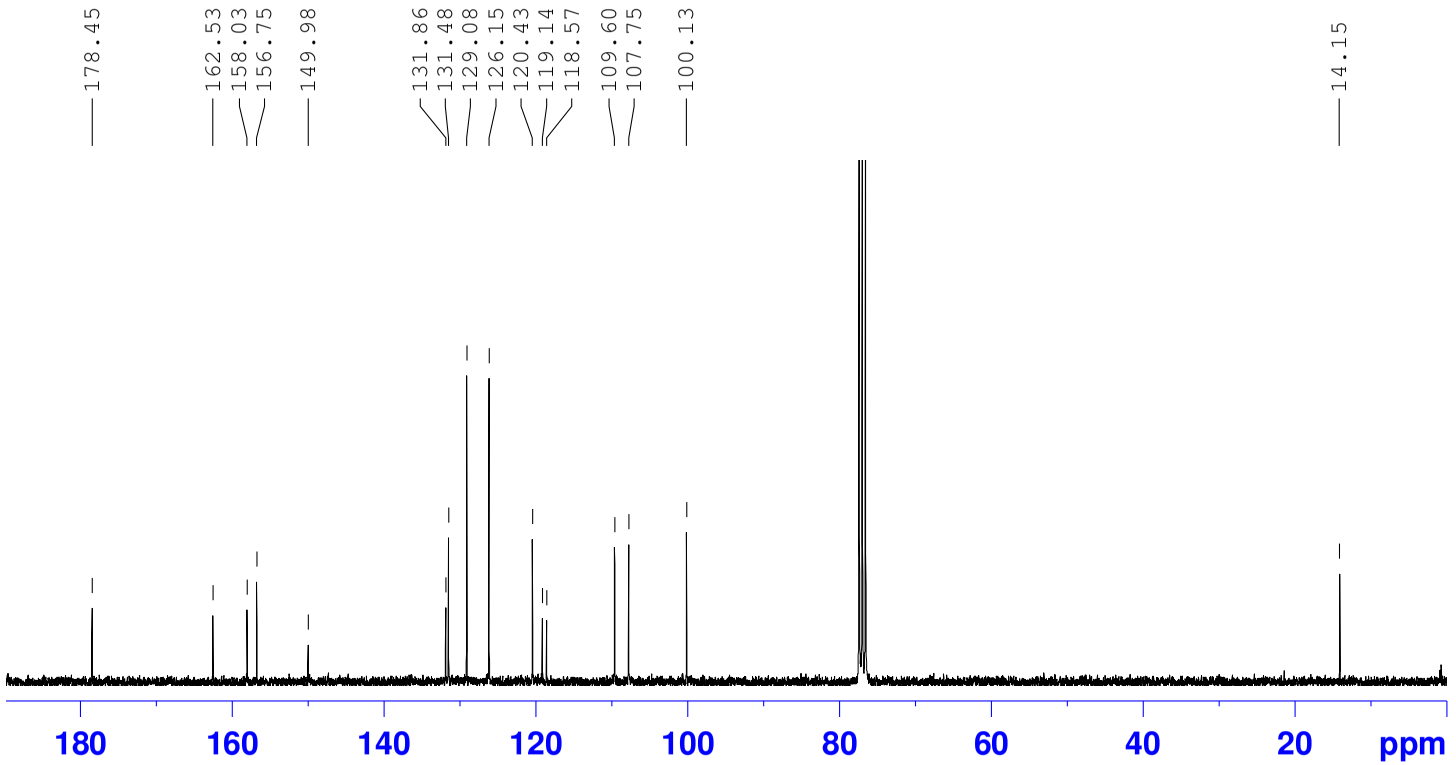
78FF (Compound 3)



7,8-furanoflavone

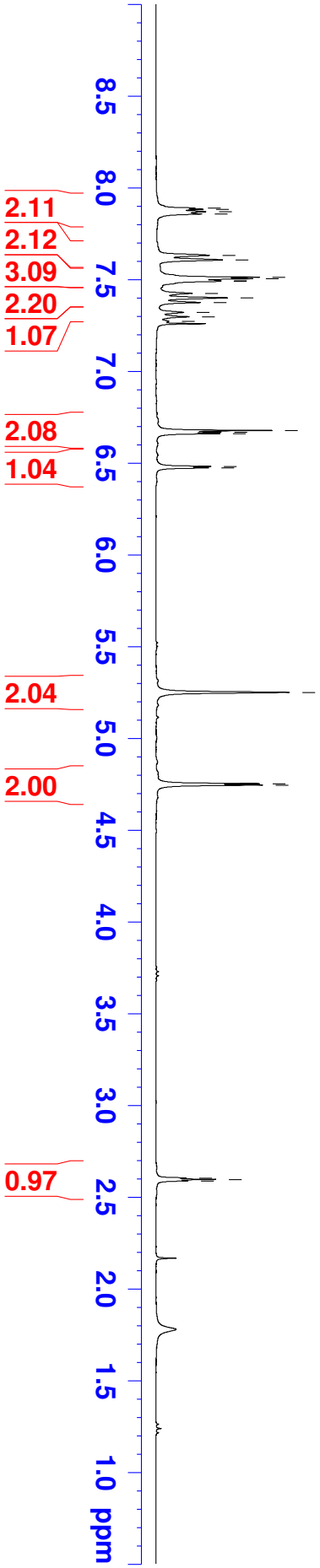


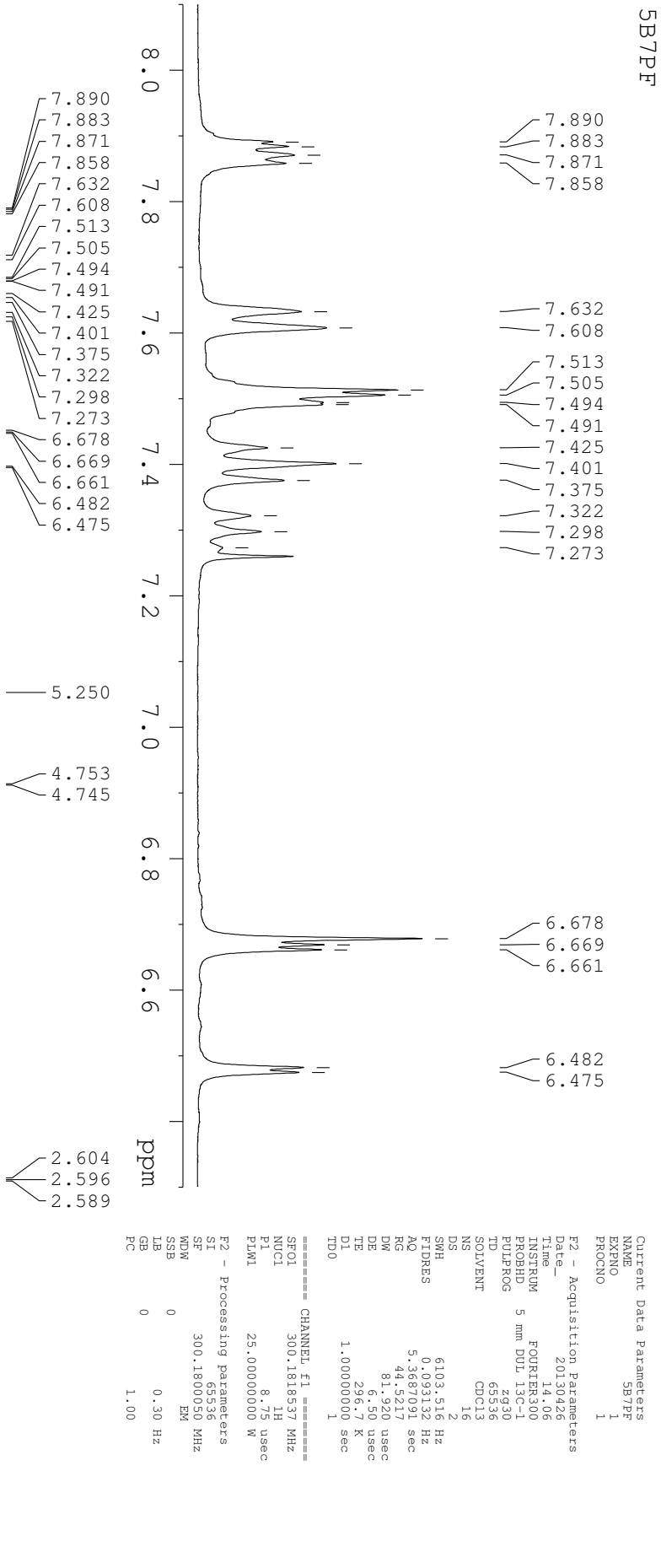


78FF (Compound 3)

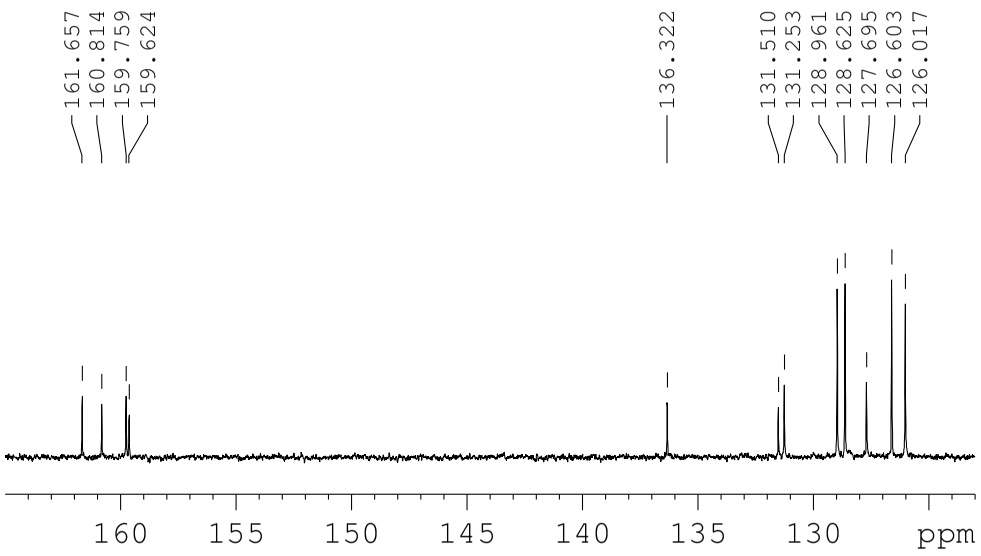
```
Current Data Parameters
NAME      7,8-furanoflavone
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20130320
Time                11.04
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1818
DS                    4
SWH           24414.063 Hz
FIDRES         0.372529 Hz
AQ            1.3421773 sec
RG              501.187
DW               20.480 usec
DE                6.50 usec
TE               296.6 K
D1            2.00000000 sec
D11           0.03000000 sec
D31           0.00001600 sec
D40           0.02432300 sec
L4                   34
L5                   49
P32              105.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1          75.4878687 MHz
NUC1                 13C
P1                16.00 usec
PLW1         60.00000000 W

======== CHANNEL f2 ========
SFO2         300.1812007 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             105.00 usec
PLW2         25.00000000 W
PLW12         0.21336000 W
PLW13         0.23522000 W

F2 - Processing parameters
SI                32768
SF           75.4803210 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

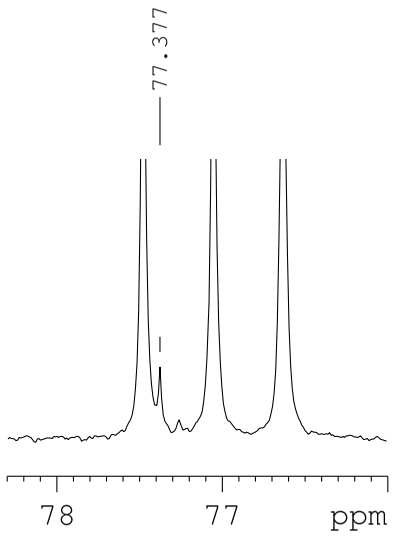
5B7PF (Compound 6)





5B7PF





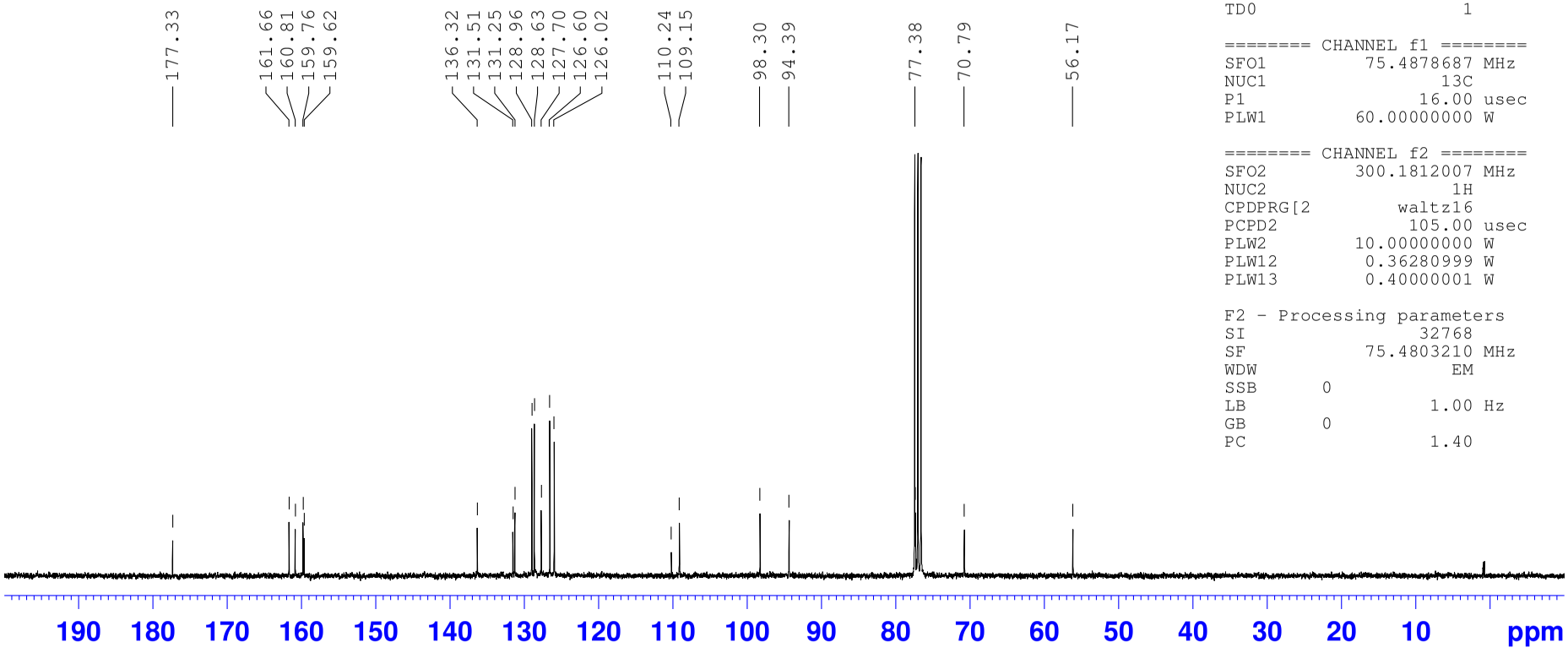
Current Data Parameters
NAME 5B7PF
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130426
Time 14.24
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001600 sec
D40 0.02432300 sec
L4 34
L5 49
P32 105.00 usec
TD0 1

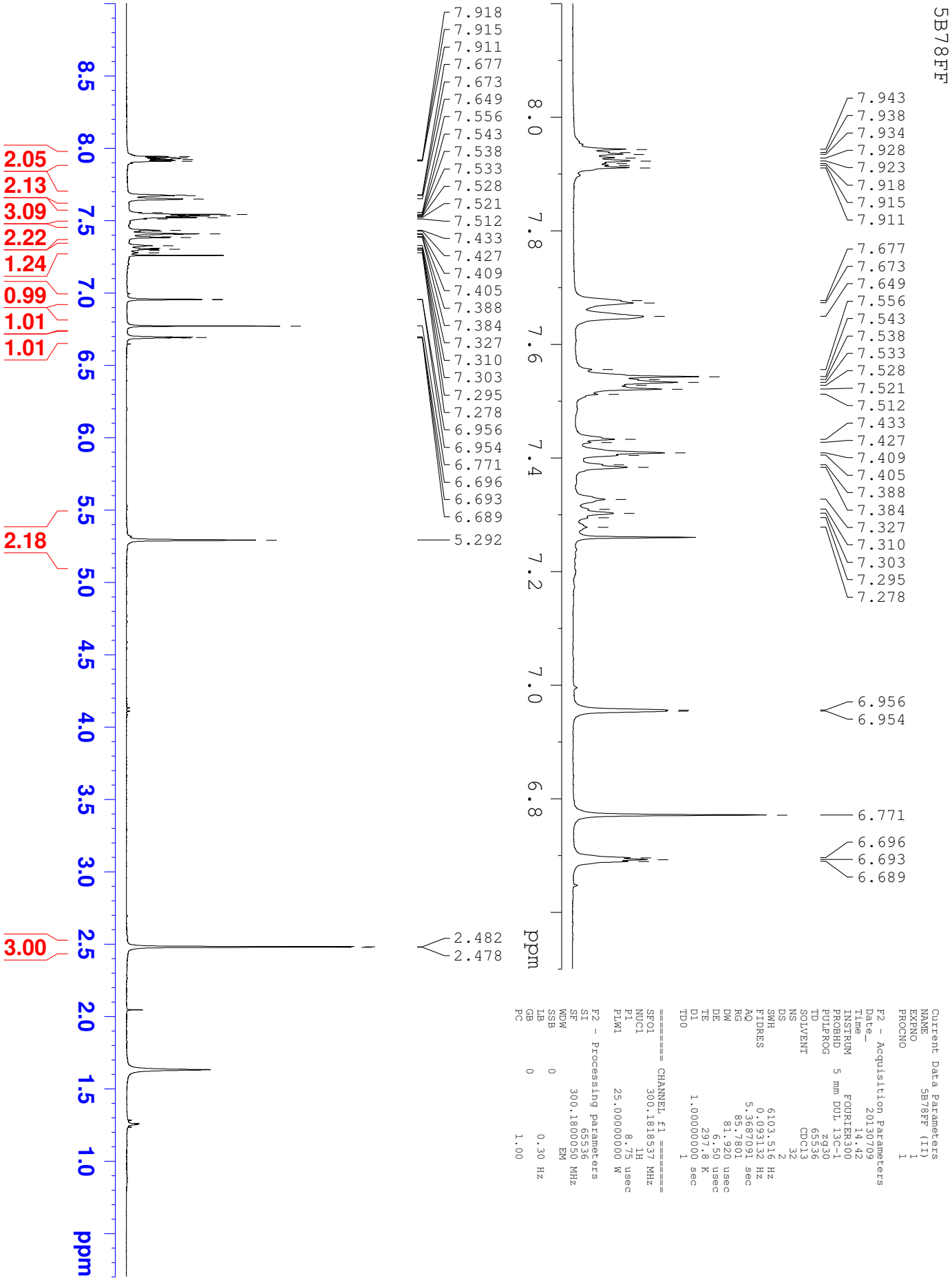
======== CHANNEL f1 ========
SFO1 75.4878687 MHz
NUC1 13C
P1 16.00 usec
PLW1 60.00000000 W

======== CHANNEL f2 ========
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 105.00 usec
PLW2 10.00000000 W
PLW12 0.36280999 W
PLW13 0.40000001 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



5B7PF (Compound 6)


5B78FF
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7.938
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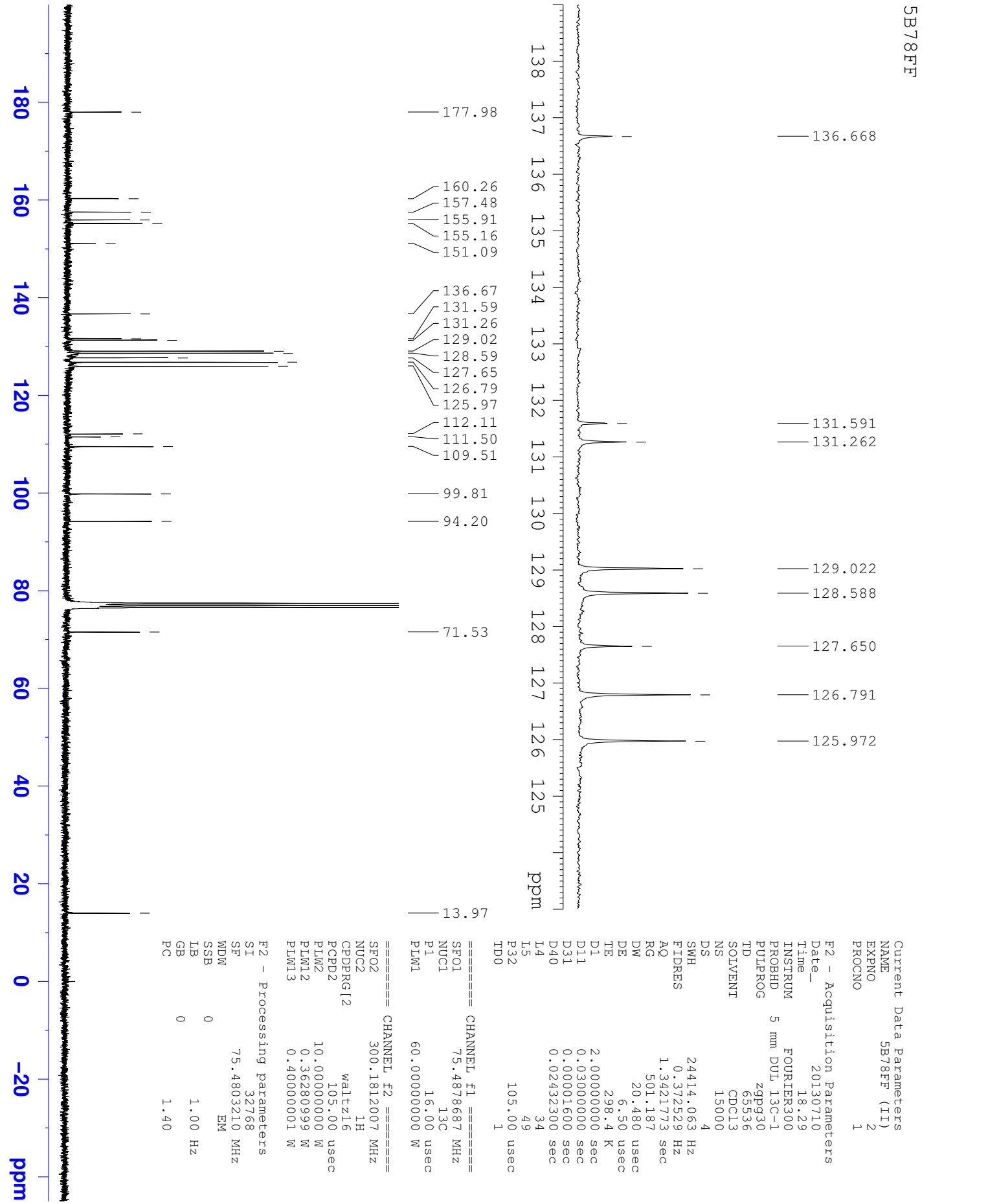
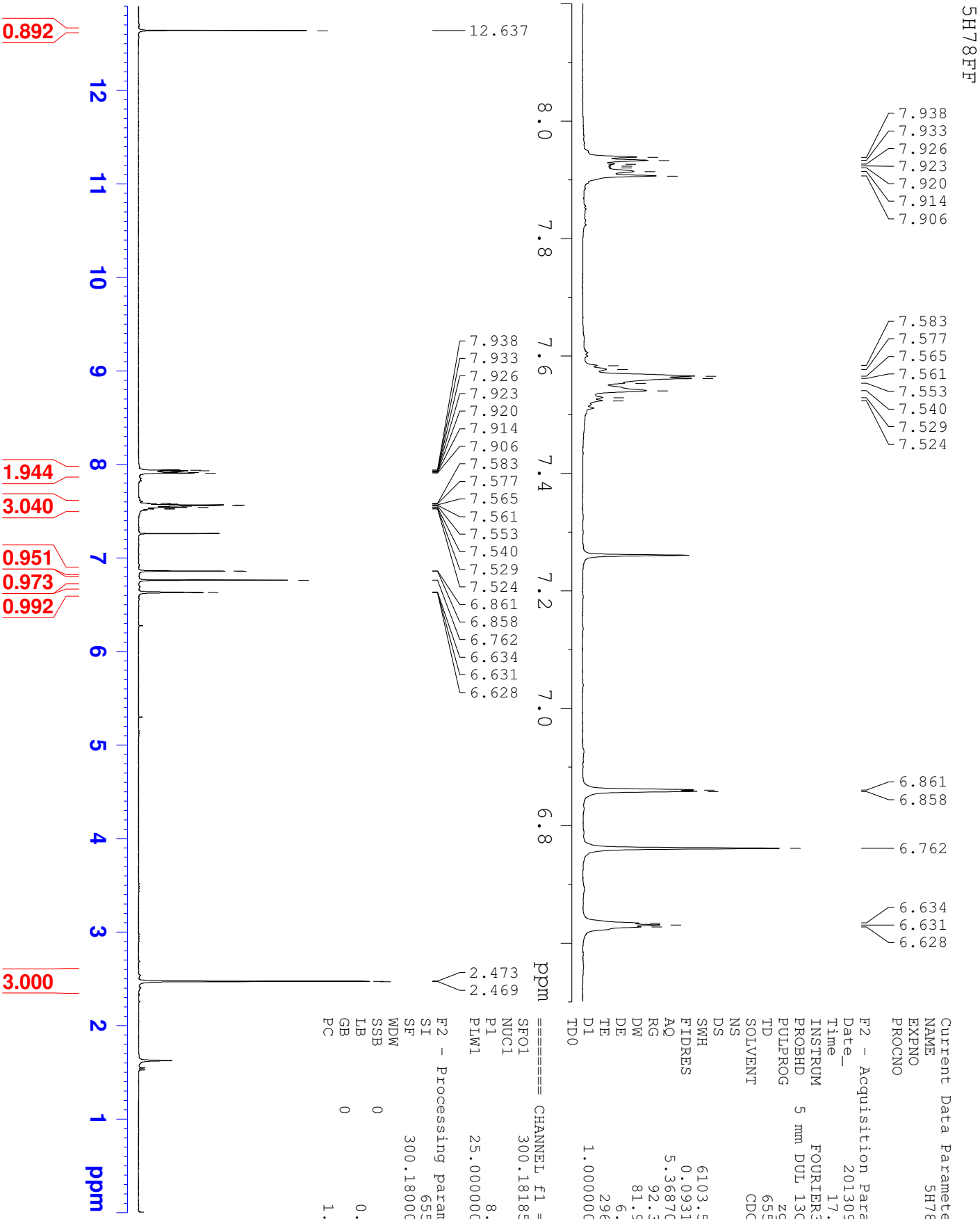
7.928
7.923
7.918
7.915
7.911
7.677
7.673
7.649
7.556
7.543
7.538
7.533
7.528
7.521
7.512
7.433
7.427
7.409
7.405
7.388
7.384
7.327
7.310
7.303
7.295
7.278
6.956
6.954
6.771
6.696
6.693
6.689
5.292
2.482
2.478
2.05
2.13
3.09
2.22
1.24
0.99
1.01
1.01
2.18
3.00
ppm
Current Data Parameters
NAME 5B78FF (II)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130709
Time 14.42
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 85.7801
DW 81.920 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

5B78FF (Compound 7)

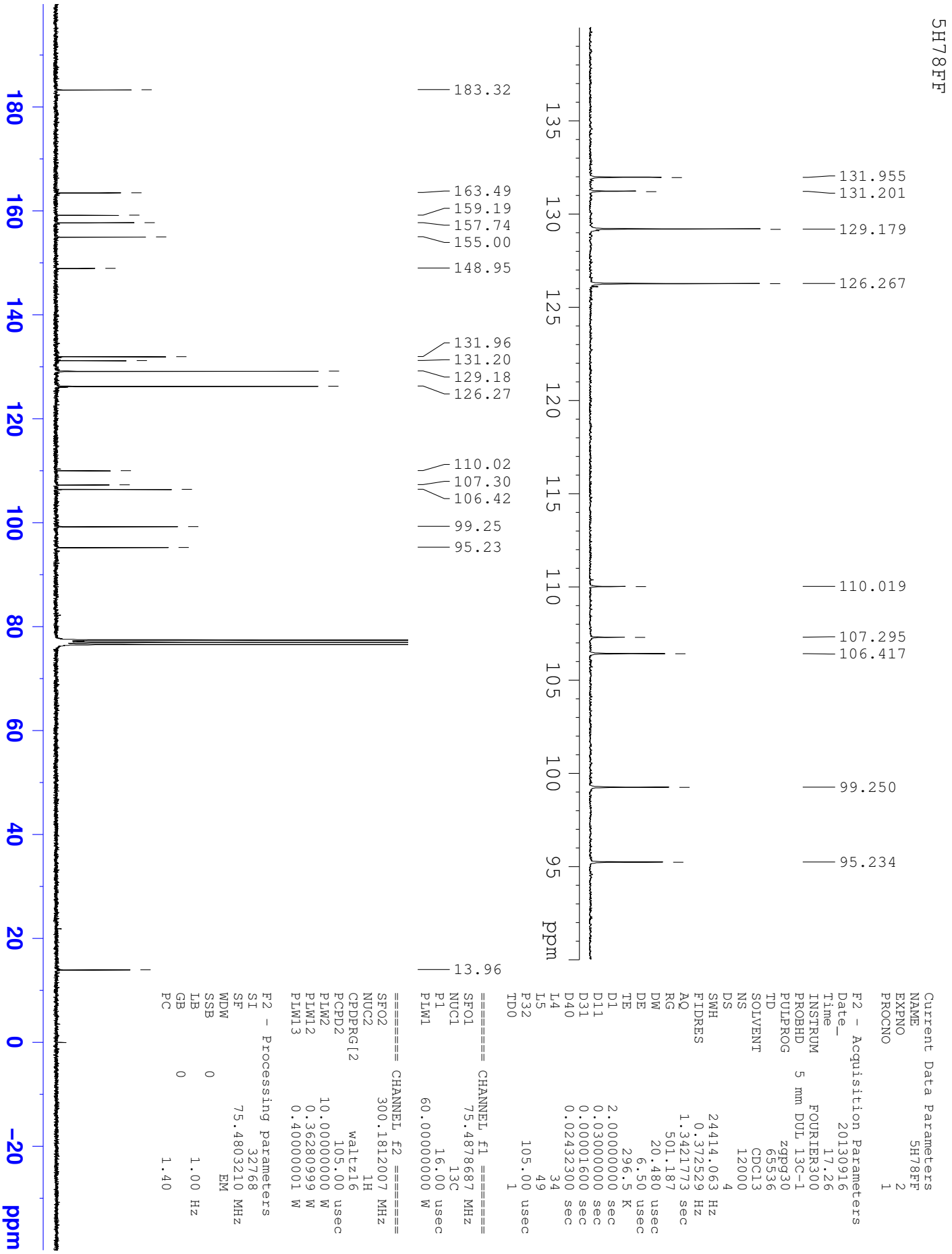



```
Current Data Parameters
NAME                  5B78FF (II)
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130710
Time                         18.29
INSTRUM                FOURIER300
PROBHD      5 mm DUL 13C-1
PULPROG                zgpg30
TD                        65536
SOLVENT                CDC13
NS                        15000
DS                            4
SWH                   24414.063 Hz
FIDRES                0.372529 Hz
AQ                    1.3421773 sec
RG                      501.187
DW                     20.480 usec
DE                      6.50 usec
TE                     298.4 K
D1                    2.00000000 sec
D11                   0.03000000 sec
D31                   0.00001600 sec
D40                   0.02432300 sec
L4                            34
L5                            49
P32                    105.00 usec
TD0                           1

========== CHANNEL f1 ========
SFO1                  75.4878687 MHz
NUC1                        13C
P1                     16.00 usec
PLW1                60.00000000 W

========== CHANNEL f2 ========
SFO2                 300.1812007 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                  105.00 usec
PLW2                10.00000000 W
PLW12                0.36280999 W
PLW13                0.40000001 W

F2 - Processing parameters
SI                        32768
SF                    75.4803210 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                        1.40
```

5H78FF (Compound 8)



5H78FF (Compound 8)



Current Data Parameters
NAME 5H78FF
EXPNO 2
PROCNO 1

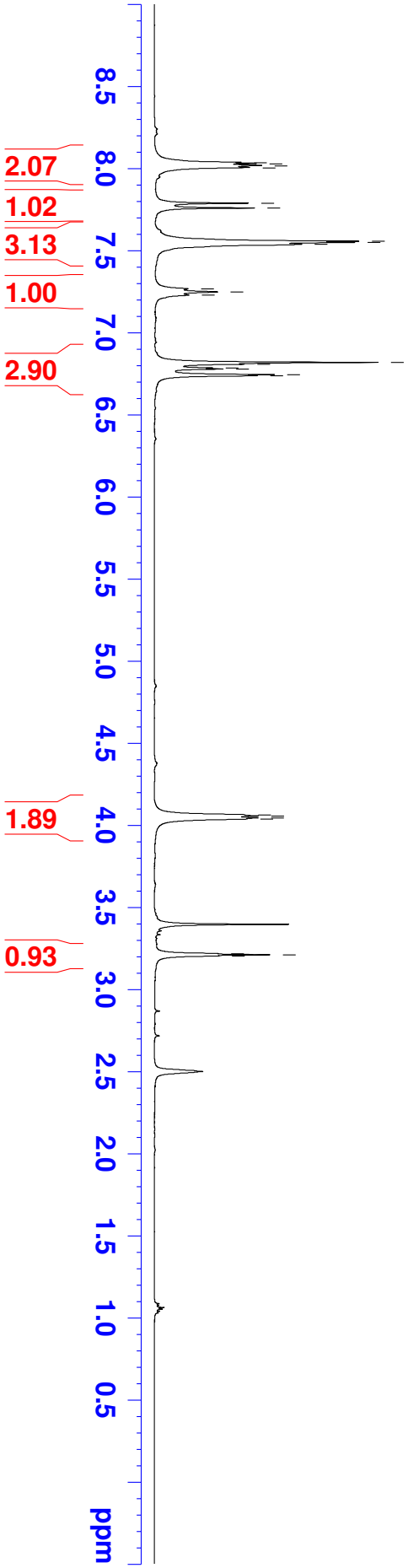
F2 - Acquisition Parameters
Date_ 20130916
Time 17.26
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12000
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001600 sec
D40 0.02432300 sec
L4 34
L5 49
P32 105.00 usec
TD0 1

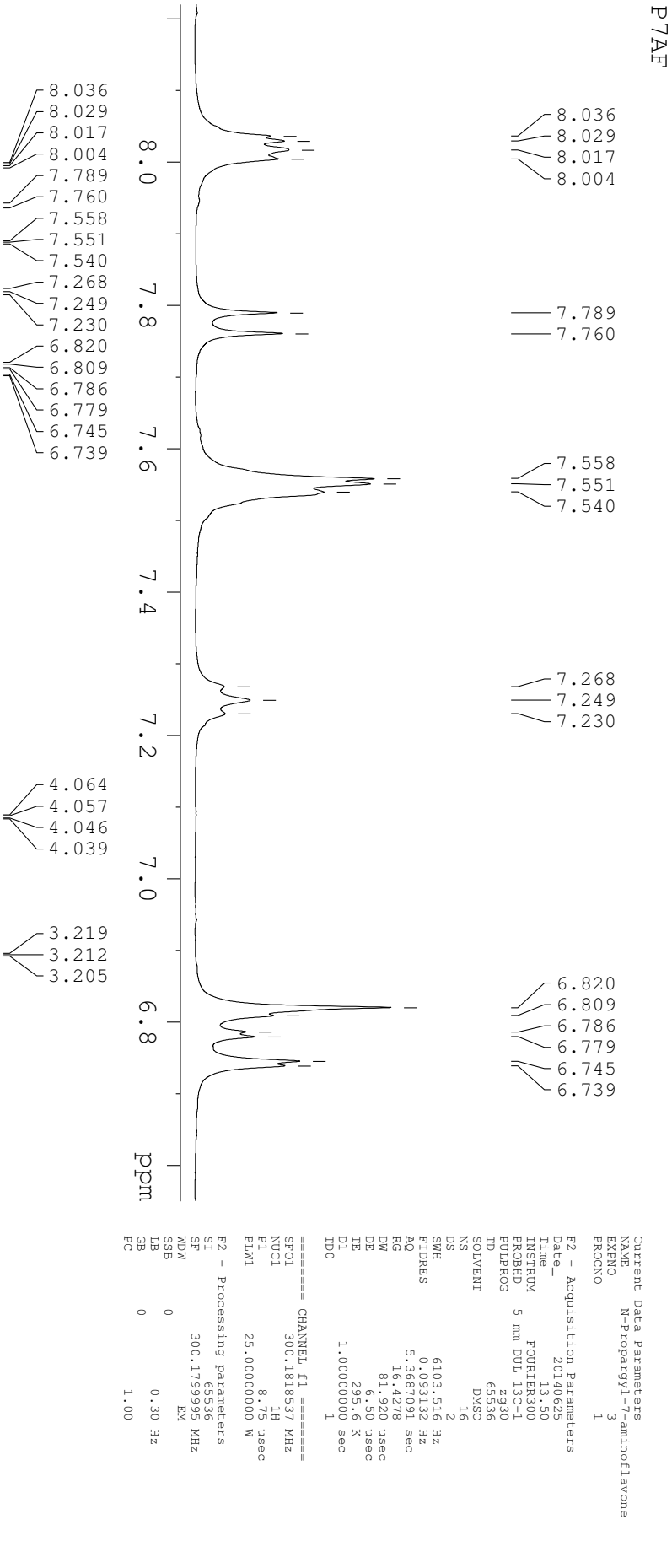
========== CHANNEL f1 ==========
SFO1 75.4878687 MHz
NUC1 13C
P1 16.00 usec
PLW1 60.00000000 W

========== CHANNEL f2 ==========
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 105.00 usec
PLW2 10.00000000 W
PLW12 0.36280999 W
PLW13 0.40000001 W

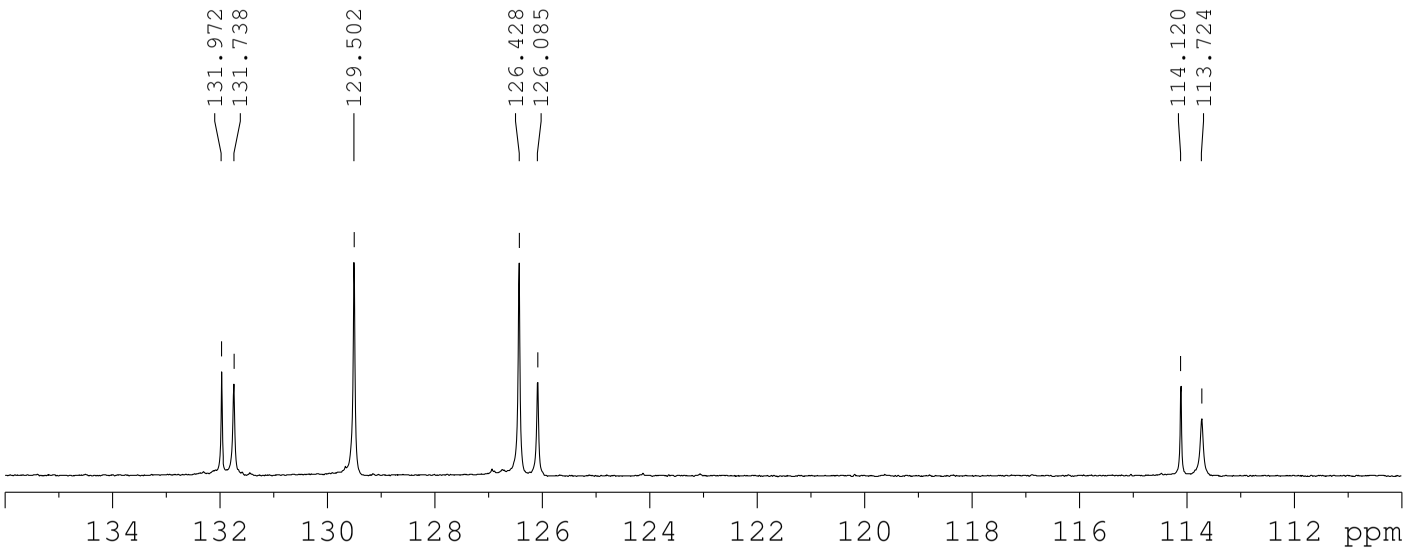
F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

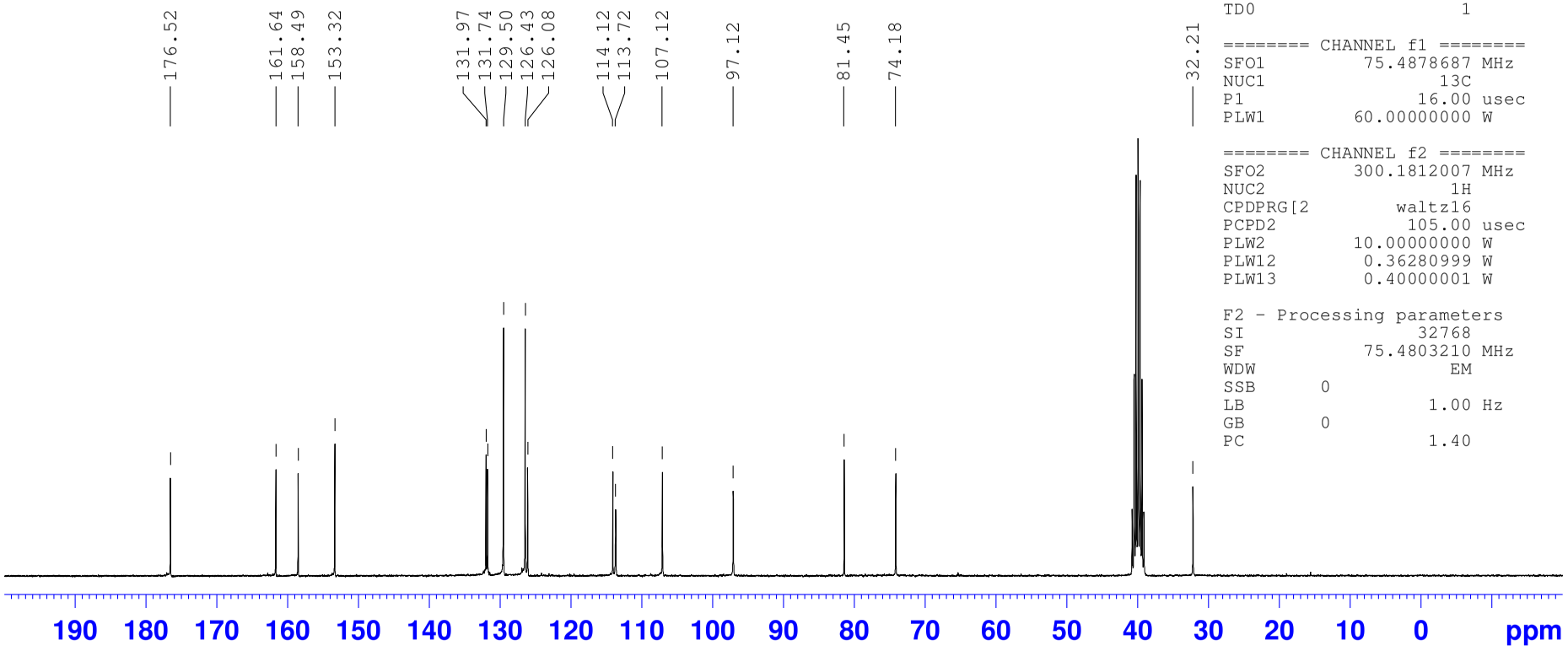
P7AF (Compound 9)





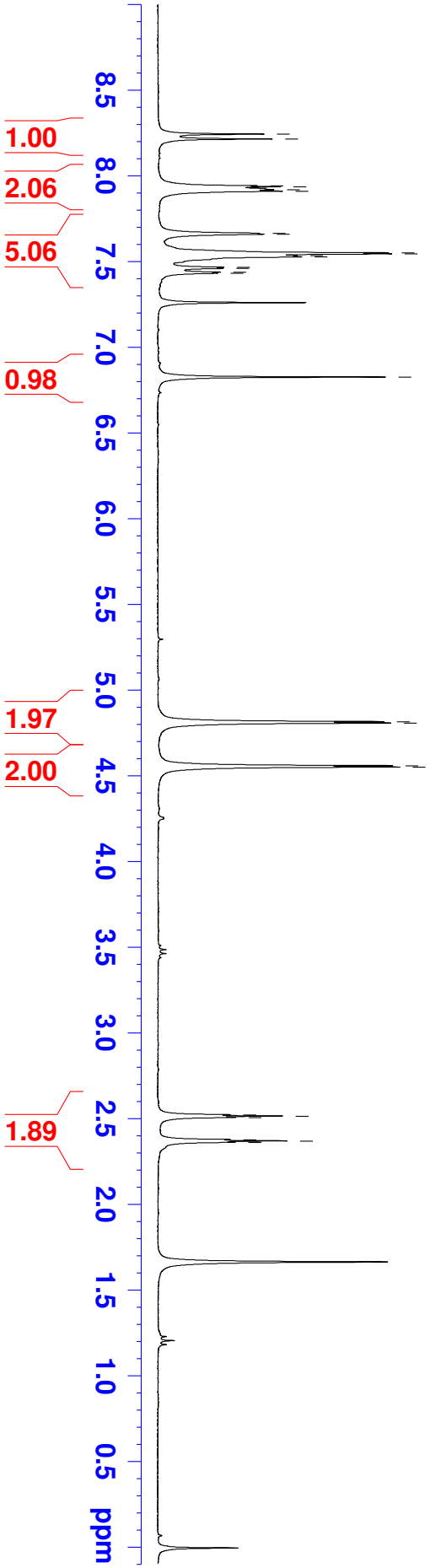
P7AF

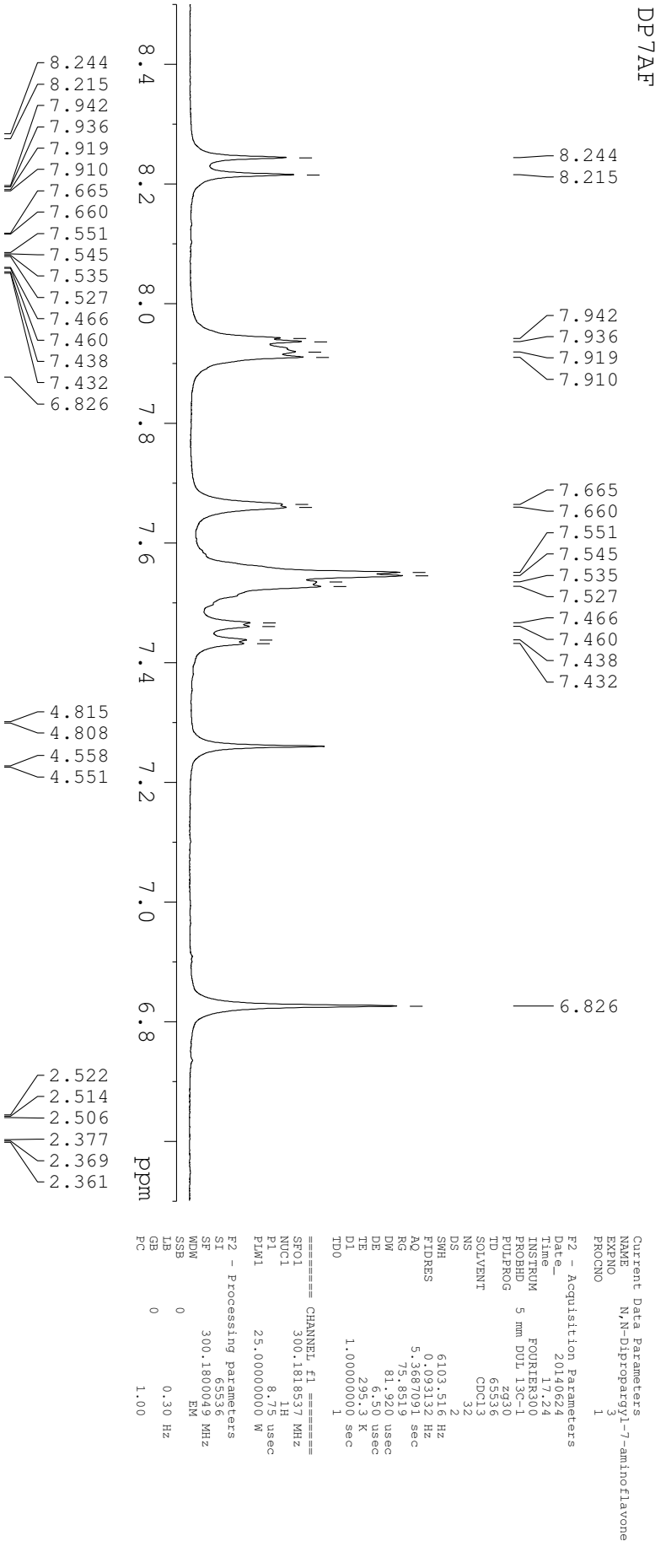




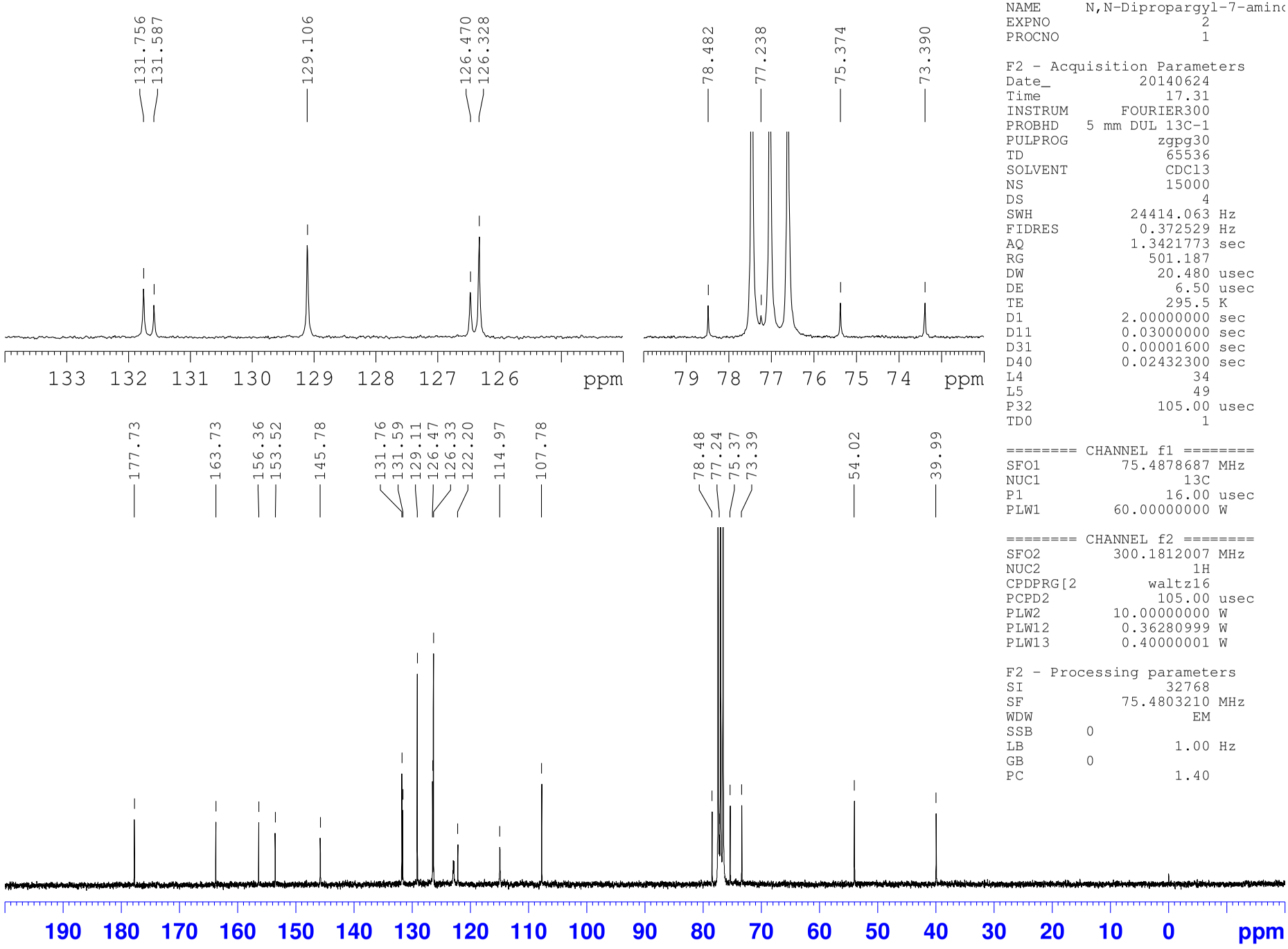

```
Current Data Parameters
NAME      N-Propargyl-7-aminoflav
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140625
Time              18.13
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG           zgpg30
TD                65536
SOLVENT             DMSO
NS                14000
DS                    4
SWH           24414.063 Hz
FIDRES         0.372529 Hz
AQ            1.3421773 sec
RG              501.187
DW               20.480 usec
DE                6.50 usec
TE               295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
D31          0.00001600 sec
D40          0.02432300 sec
L4                   34
L5                   49
P32              105.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4878687 MHz
NUC1               13C
P1               16.00 usec
PLW1        60.00000000 W

======== CHANNEL f2 ========
SFO2        300.1812007 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            105.00 usec
PLW2        10.00000000 W
PLW12        0.36280999 W
PLW13        0.40000001 W

F2 - Processing parameters
SI                32768
SF           75.4803210 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

DP7AF (Compound 10)



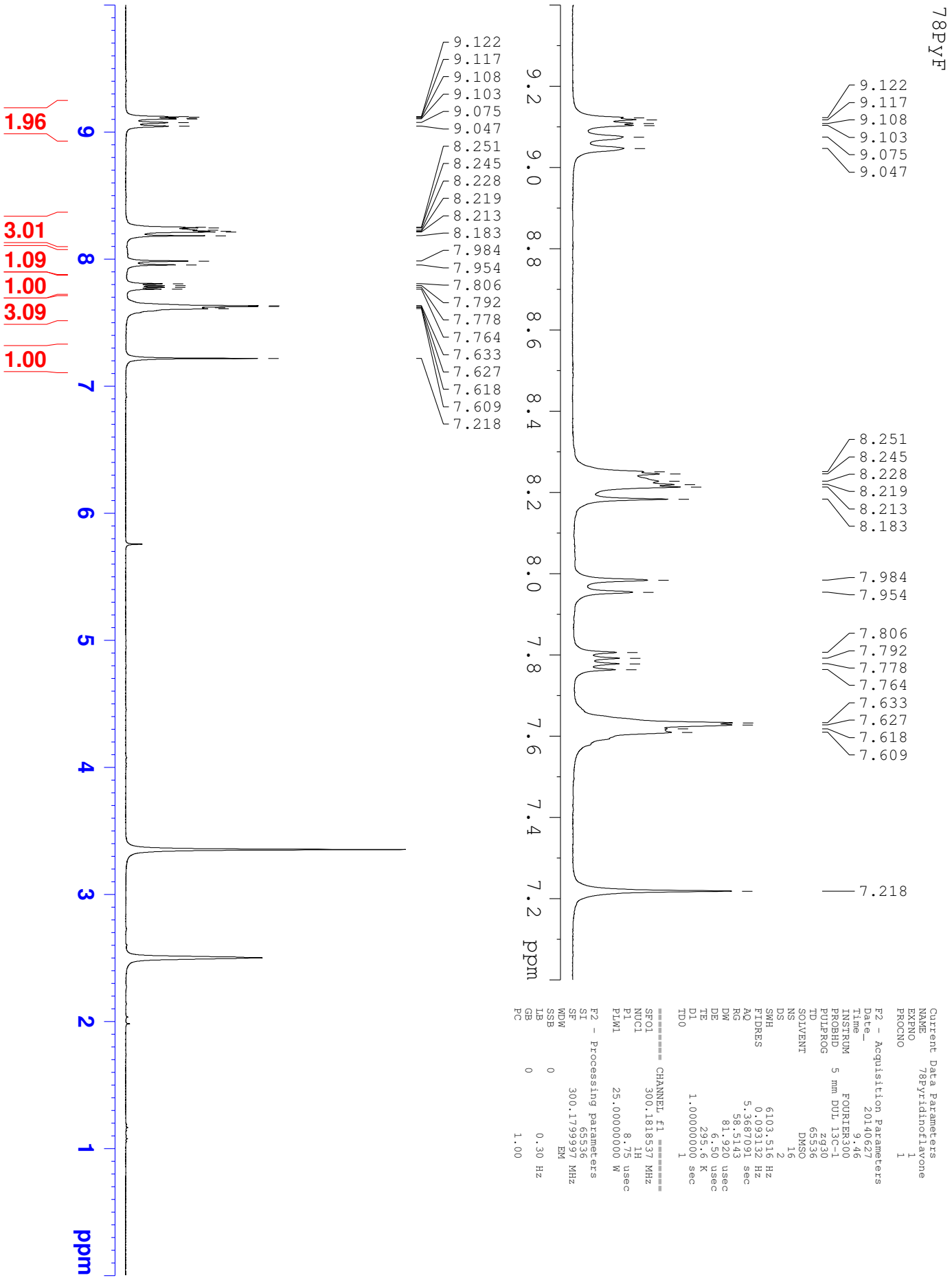


DP7AF




```
Current Data Parameters
NAME      N,N-Dipropargyl-7-amino
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140624
Time                       17.31
INSTRUM                FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                         15000
DS                             4
SWH                    24414.063 Hz
FIDRES                 0.372529 Hz
AQ                     1.3421773 sec
RG                       501.187
DW                        20.480 usec
DE                         6.50 usec
TE                        295.5 K
D1                     2.00000000 sec
D11                    0.03000000 sec
D31                    0.00001600 sec
D40                    0.02432300 sec
L4                            34
L5                            49
P32                      105.00 usec
TD0                            1

======== CHANNEL f1 ========
SFO1                 75.4878687 MHz
NUC1                        13C
P1                       16.00 usec
PLW1                60.00000000 W

======== CHANNEL f2 ========
SFO2                300.1812007 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    105.00 usec
PLW2                10.00000000 W
PLW12                0.36280999 W
PLW13                0.40000001 W

F2 - Processing parameters
SI                         32768
SF                   75.4803210 MHz
WDW                           EM
SSB       0
LB                        1.00 Hz
GB        0
PC                        1.40
```

78PyF (Compound 11)



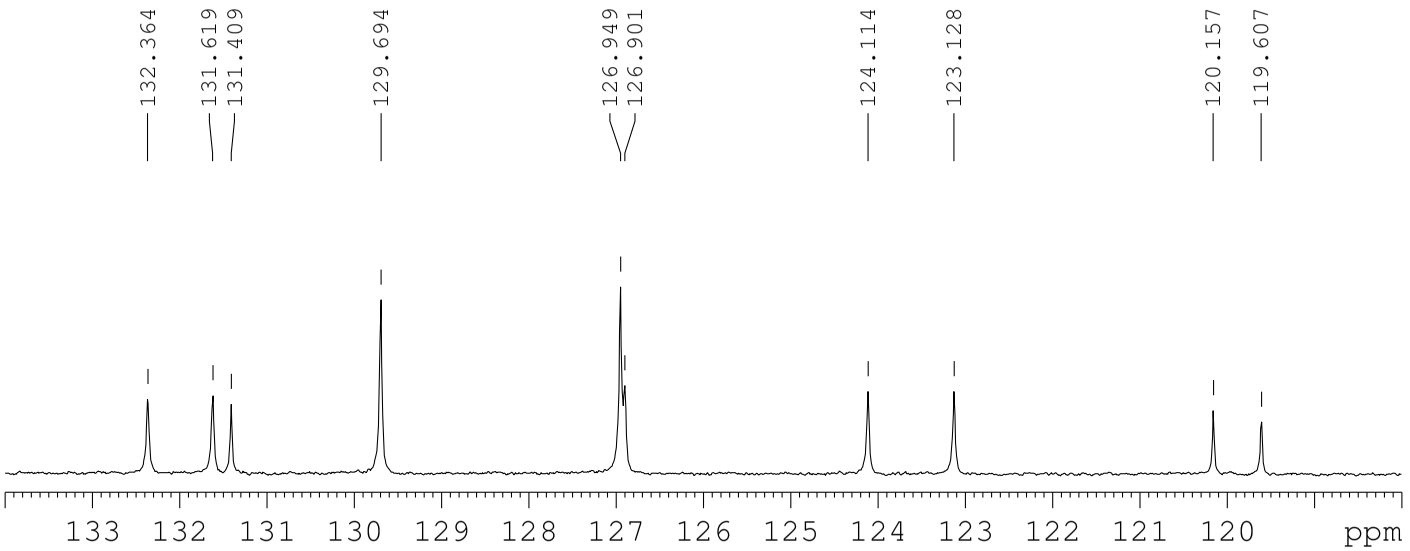
Current Data Parameters
NAME 78Pyridinoflavone
EXPNO 1
PROCNO 1

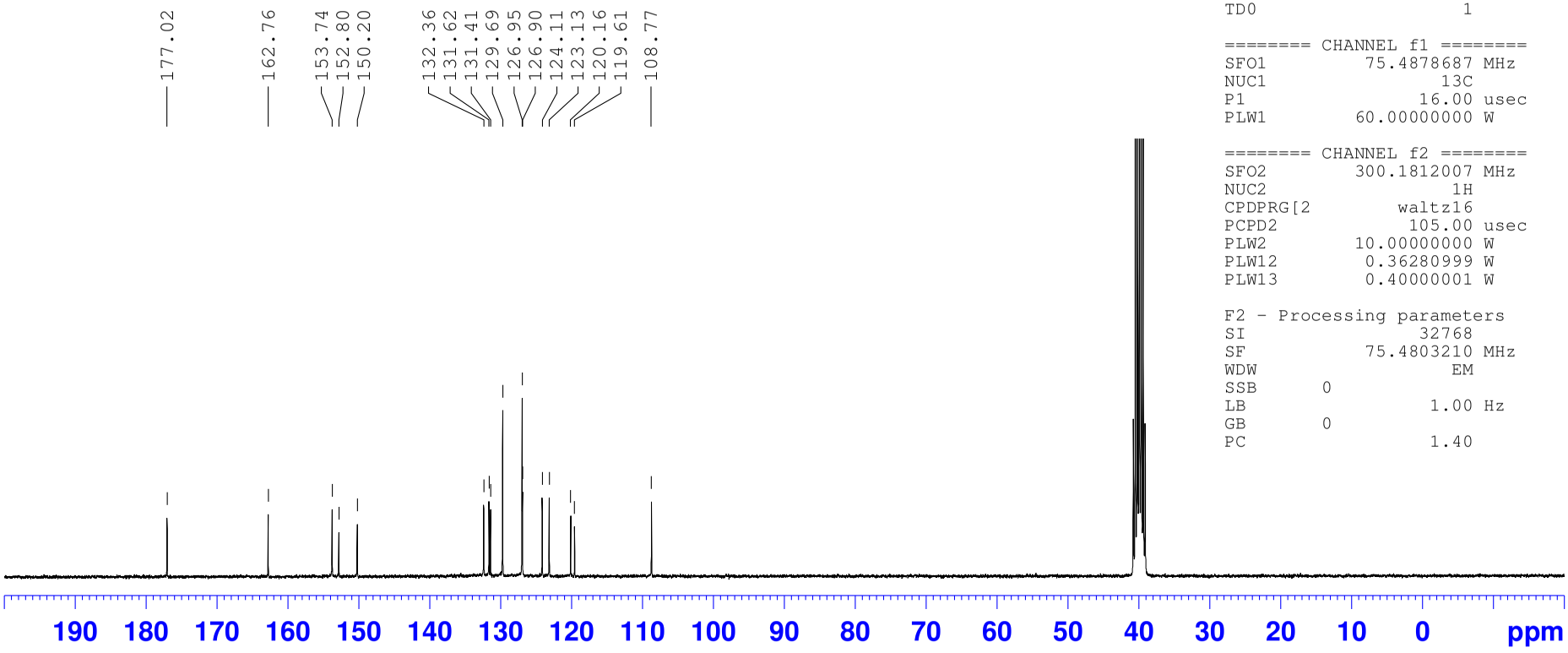
F2 - Acquisition Parameters
Date_ 20140627
Time 9.46
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 58.5143
DW 81.920 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1799997 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

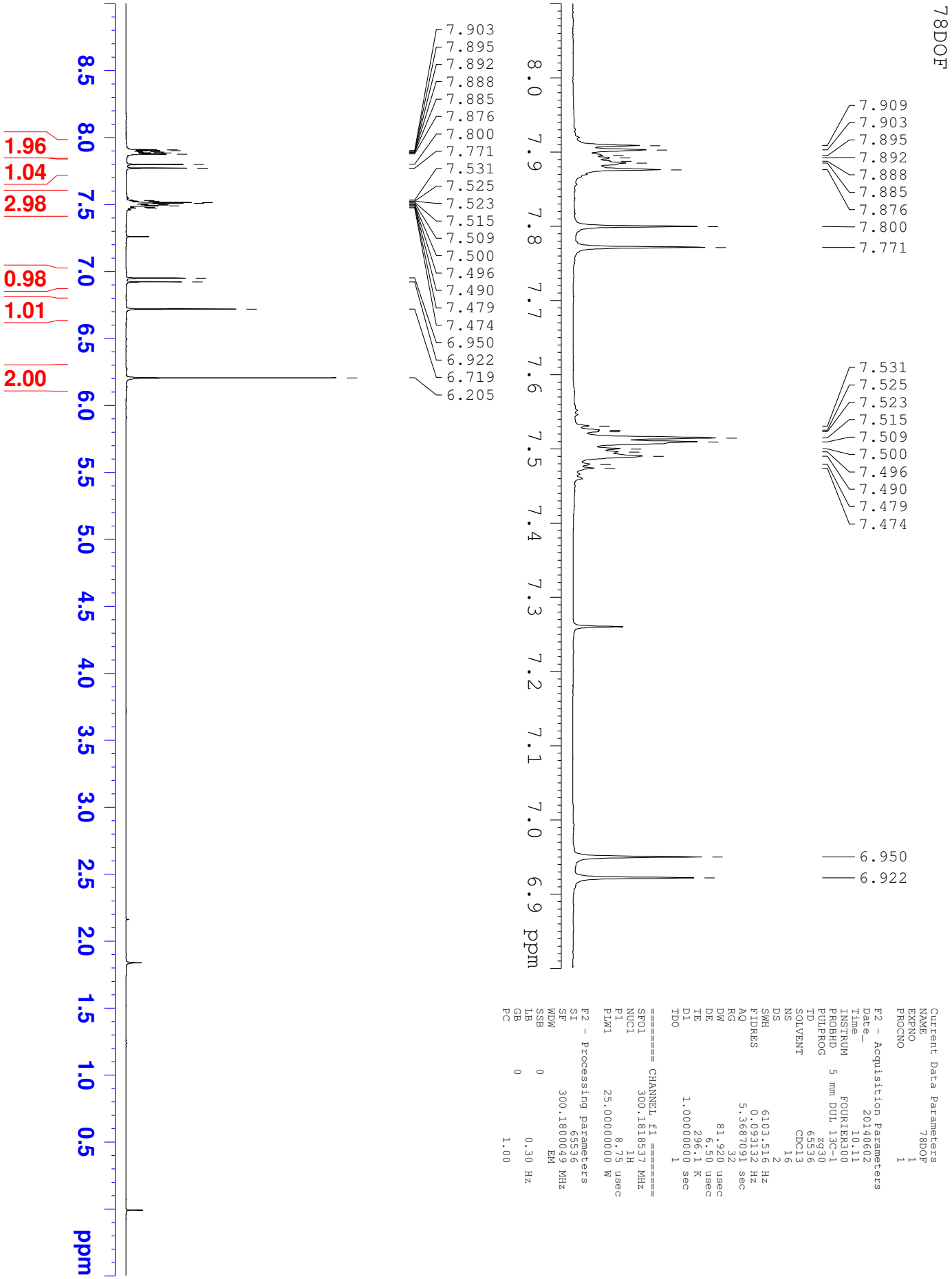
78PyF





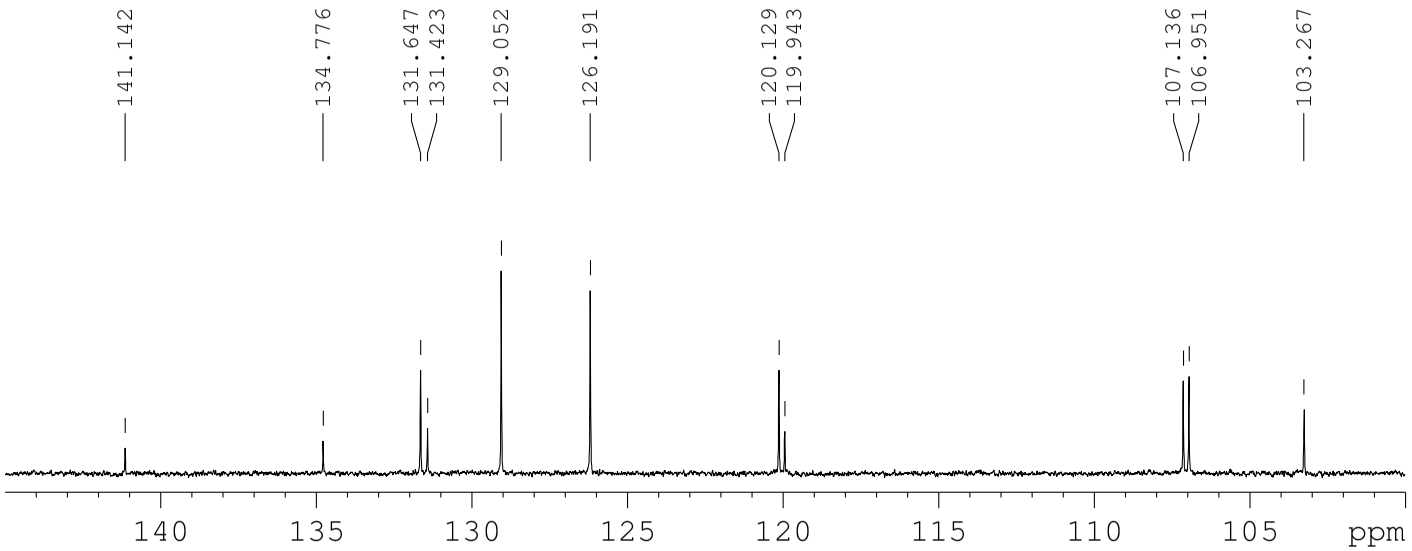

```
Current Data Parameters
NAME      78Pyridinoflavone
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20140627
Time                 18.28
INSTRUM        FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT               DMSO
NS                  20000
DS                      4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  295.7 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001600 sec
D40             0.02432300 sec
L4                      34
L5                      49
P32                105.00 usec
TD0                     1

======== CHANNEL f1 ========
SFO1           75.4878687 MHz
NUC1                  13C
P1                  16.00 usec
PLW1          60.00000000 W

======== CHANNEL f2 ========
SFO2          300.1812007 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2          10.00000000 W
PLW12          0.36280999 W
PLW13          0.40000001 W

F2 - Processing parameters
SI                    32768
SF             75.4803210 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

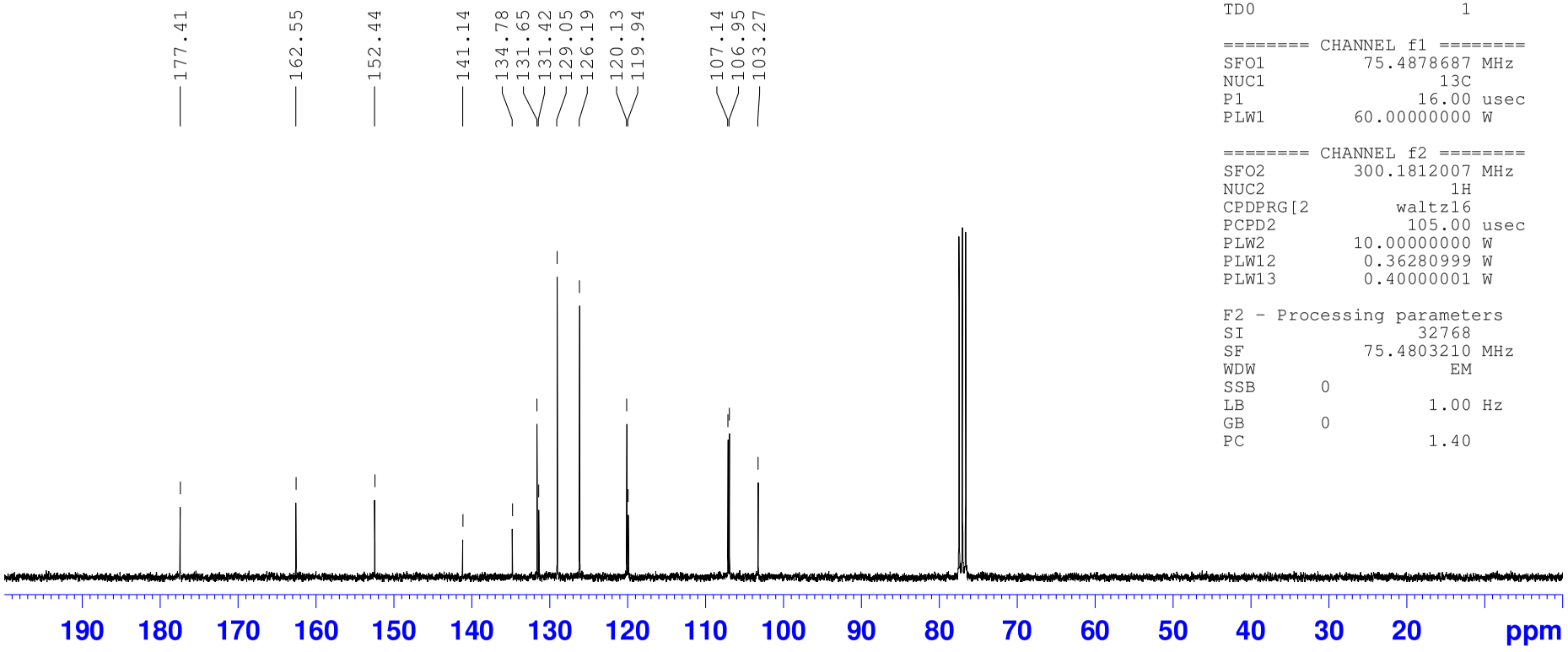
78DOF (Compound 12)




```
Current Data Parameters
NAME                  78DOF
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140602
Time               10.11
INSTRUM       FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6103.516 Hz
FIDRES        0.093132 Hz
AQ            5.3687091 sec
RG                   32
DW              81.920 usec
DE               6.50 usec
TE              296.1 K
D1              1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        300.1818537 MHz
NUC1                    1H
P1                   8.75 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                    65536
SF          300.1800049 MHz
WDW                      EM
SSB                   0
LB                    0.30 Hz
GB                    0
PC                    1.00
```

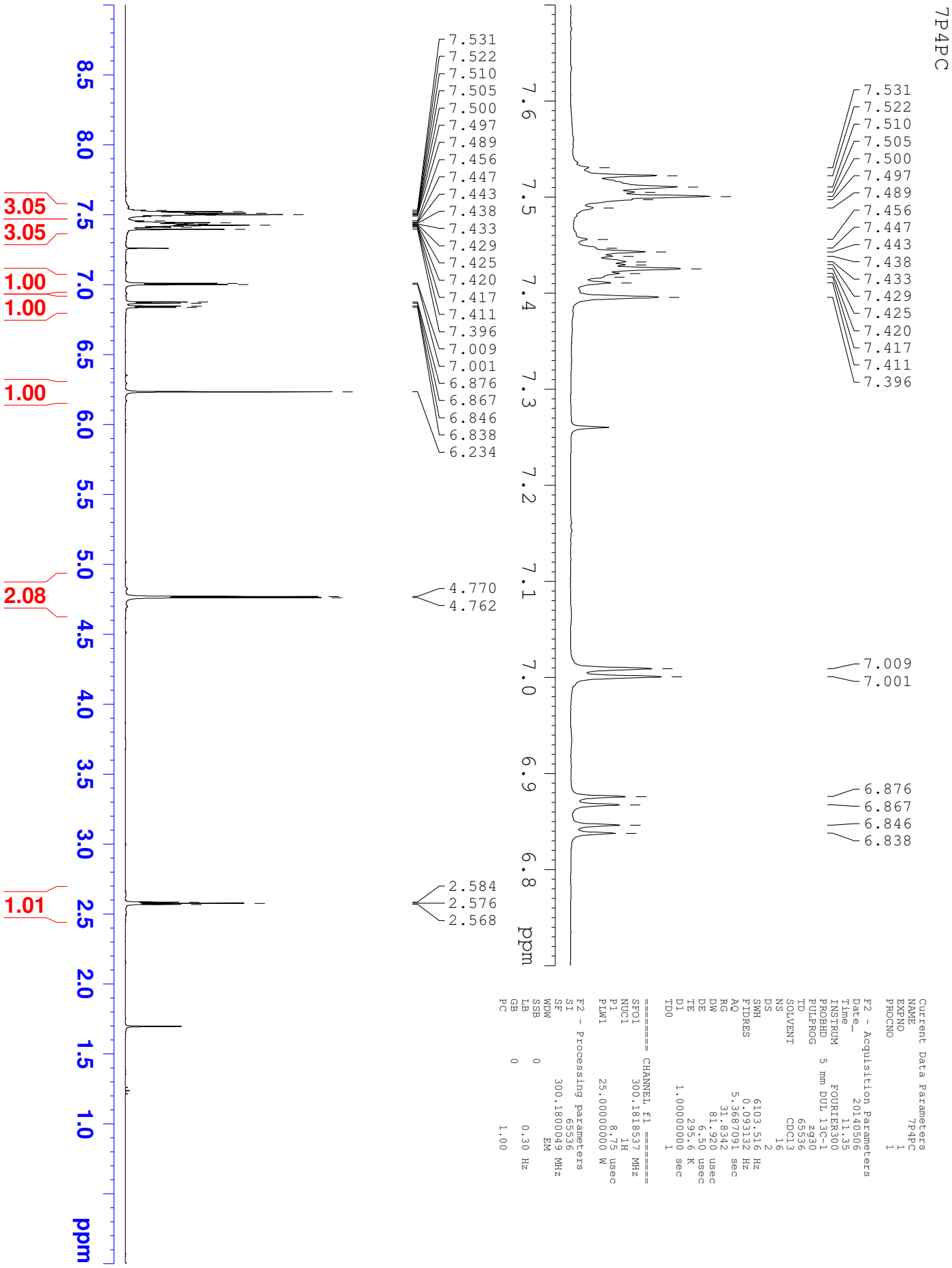
78DOF



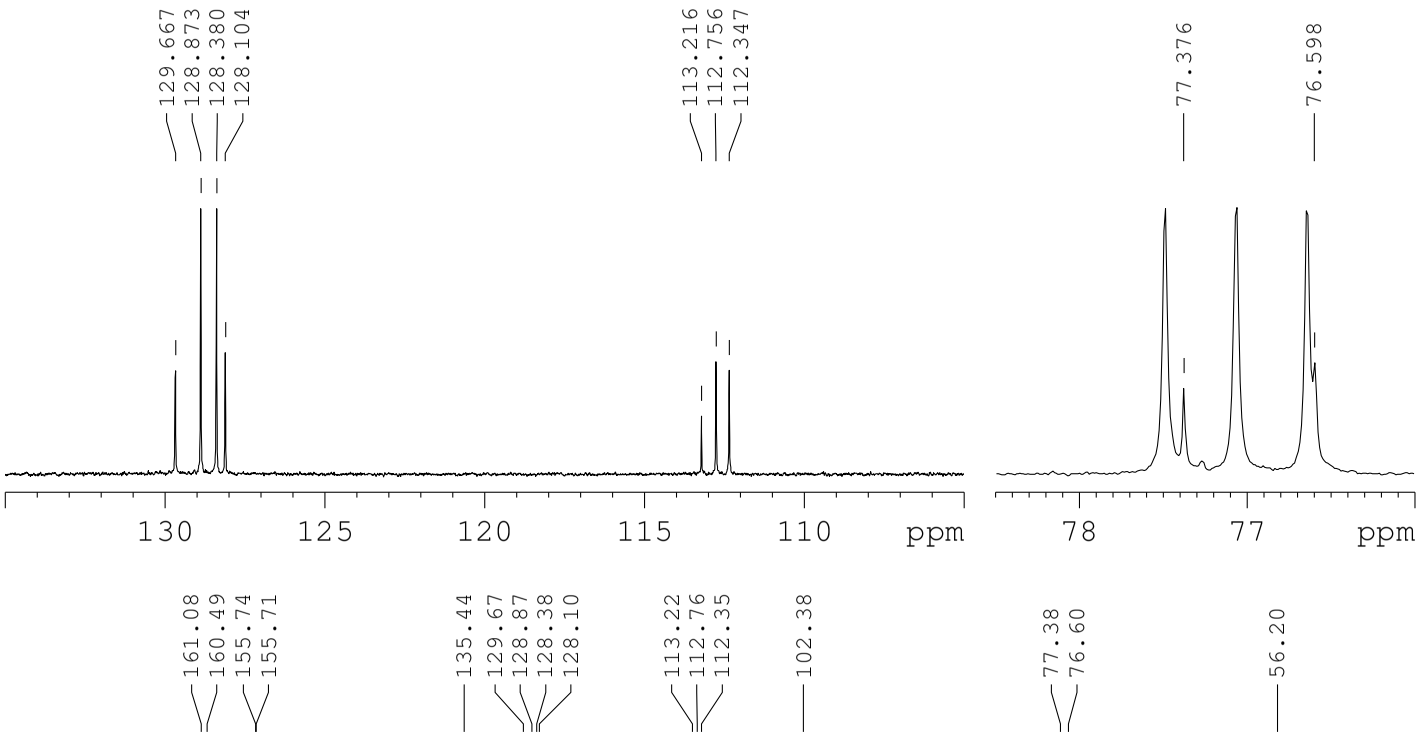


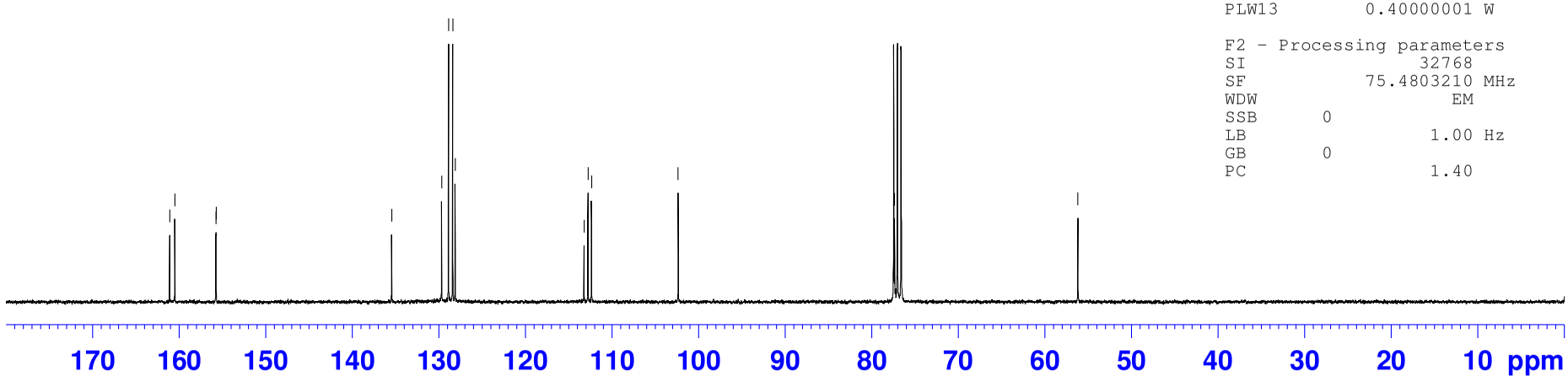
78DOF (Compound 12)

```
Current Data Parameters
NAME                  78DOF
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140602
Time                 10.17
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     626
DS                       4
SWH              24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  296.4 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001600 sec
D40             0.02432300 sec
L4                      34
L5                      49
P32                105.00 usec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                   13C
P1                  16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2               105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                     32768
SF              75.4803210 MHz
WDW                       EM
SSB         0
LB                   1.00 Hz
GB          0
PC                   1.40
```

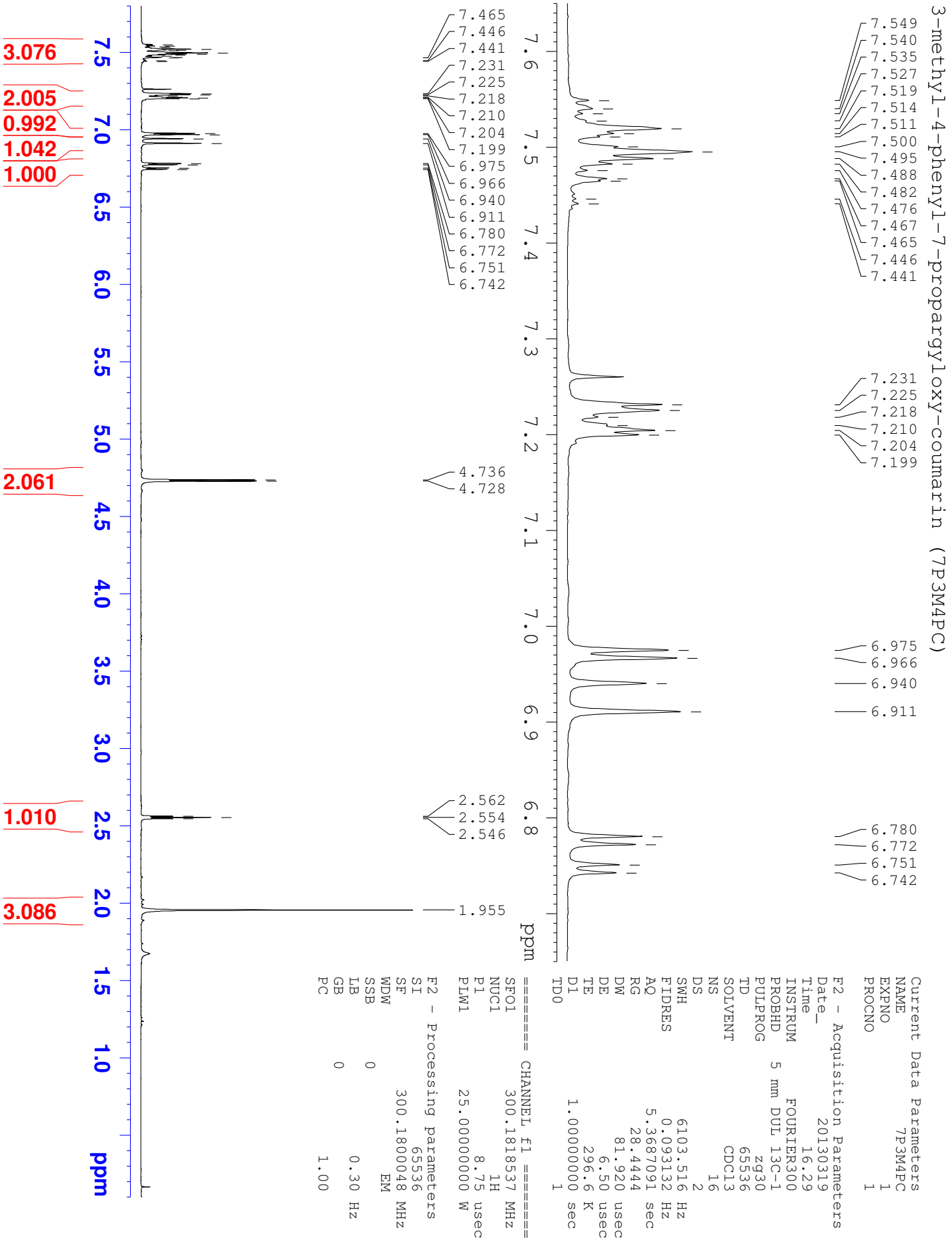

7P4PC
7.531
7.522
7.510
7.505
7.500
7.497
7.489
7.456
7.447
7.443
7.438
7.433
7.429
7.425
7.420
7.417
7.411
7.396
7.009
7.001
6.876
6.867
6.846
6.838
4.770
4.762
2.584
2.576
2.568
3.05
3.05
1.00
1.00
1.00
2.08
1.01
ppm
Current Data Parameters
NAME 7P4PC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140506
Time 11.35
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 31.8342
DW 81.920 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7P4PC

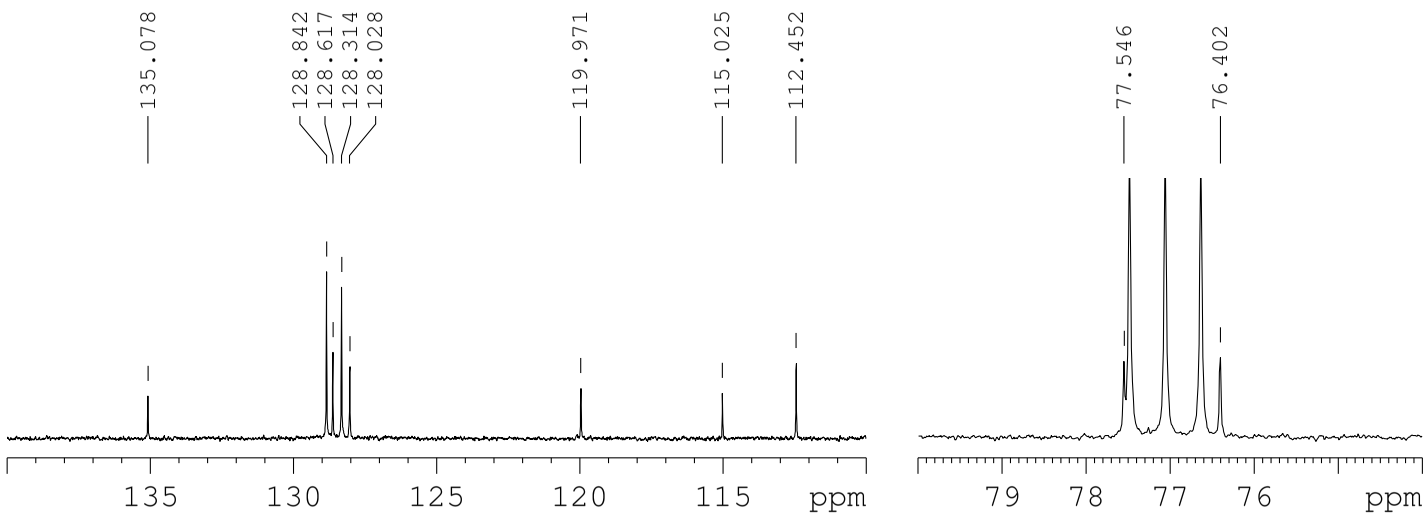


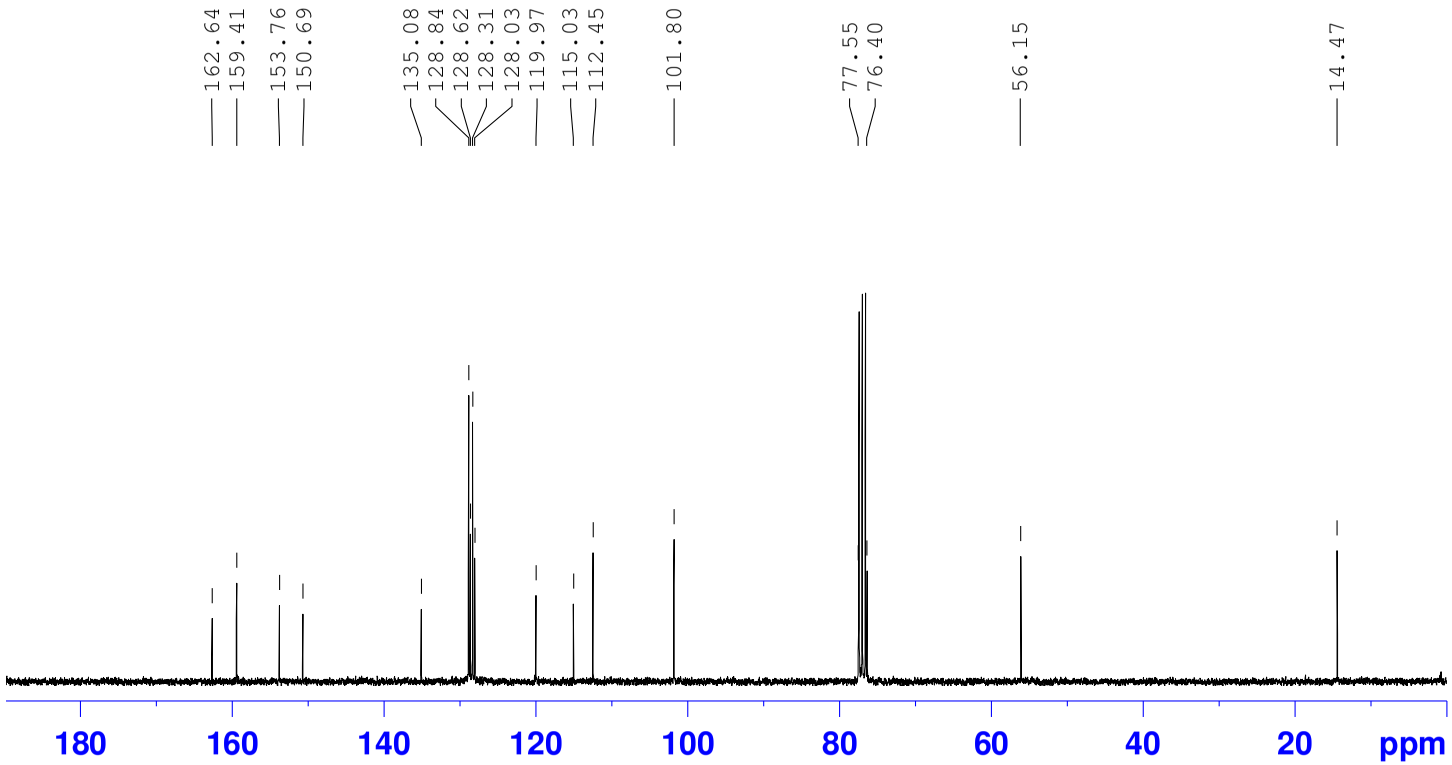



```
Current Data Parameters
NAME                  7P4PC
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140506
Time                  11.53
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2000
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   295.8 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001600 sec
D40             0.02432300 sec
L4                       34
L5                       49
P32                 105.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                    13C
P1                   16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                    32768
SF              75.4803210 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

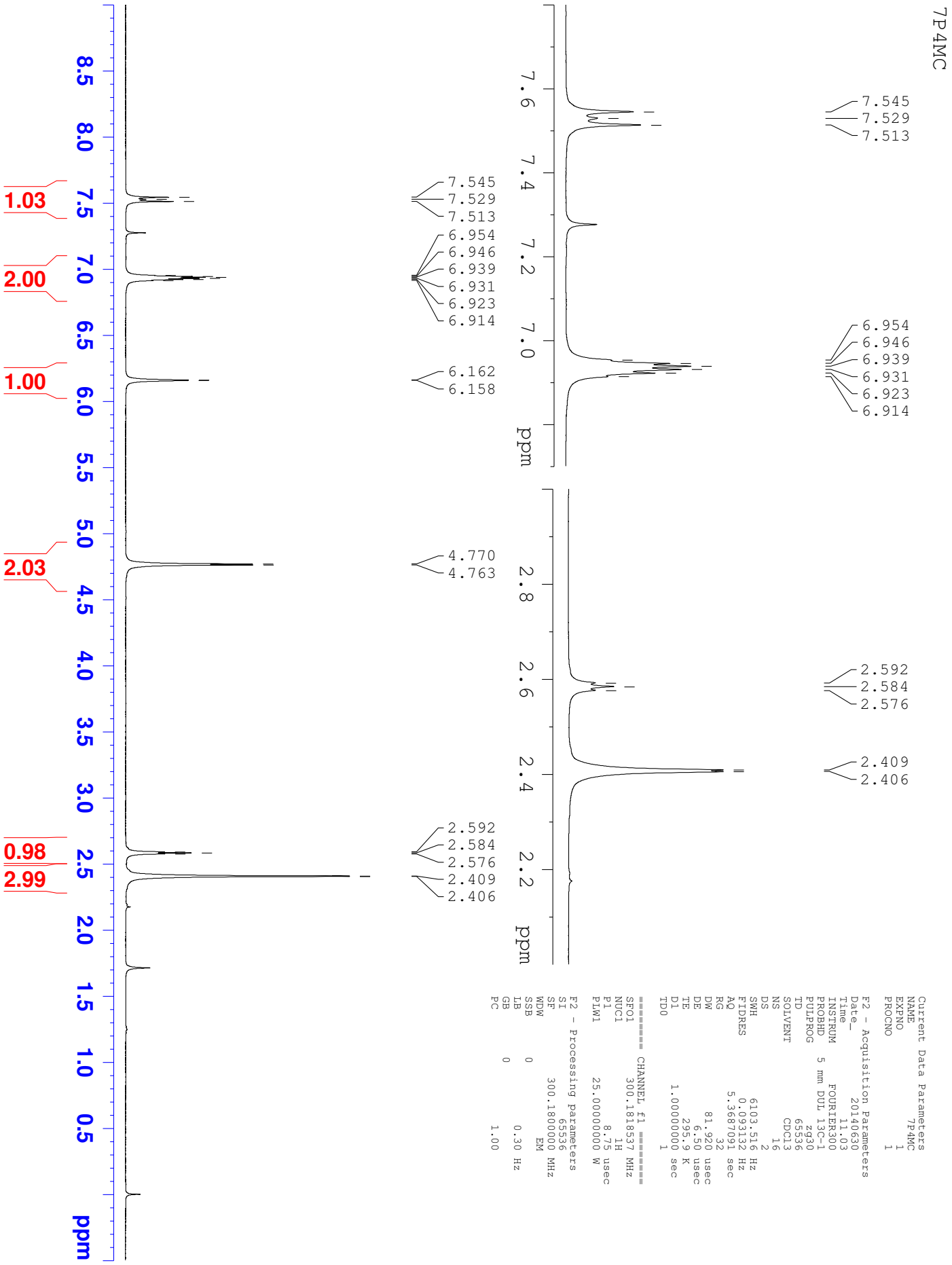

3-methyl-4-phenyl-7-propargyloxy-coumarin (7P3M4PC)
7.549
7.540
7.535
7.527
7.519
7.514
7.511
7.500
7.495
7.488
7.482
7.476
7.467
7.465
7.446
7.441
7.231
7.225
7.218
7.210
7.204
7.199
6.975
6.966
6.940
6.911
6.780
6.772
6.751
6.742
4.736
4.728
2.562
2.554
2.546
1.955
3.076
2.005
0.992
1.042
1.000
2.061
1.010
3.086
ppm
Current Data Parameters
NAME 7P3M4PC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130319
Time 16.29
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 28.4444
DW 81.920 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3-methyl-4-phenyl-7-propargyloxy-coumarin (7P3M4PC)

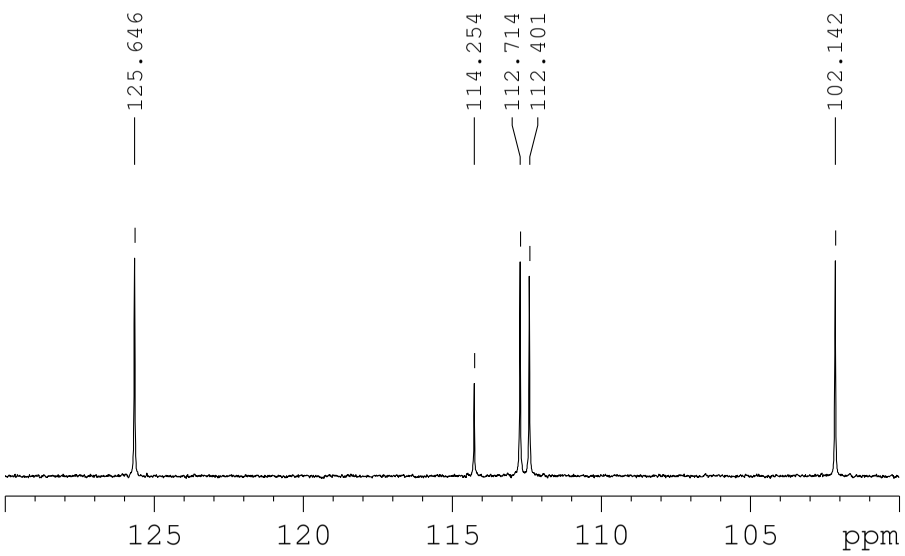


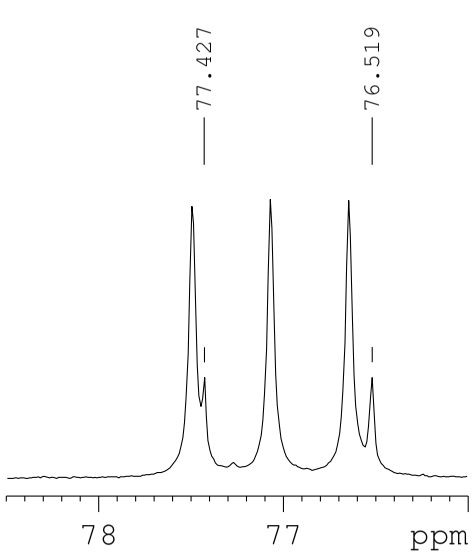


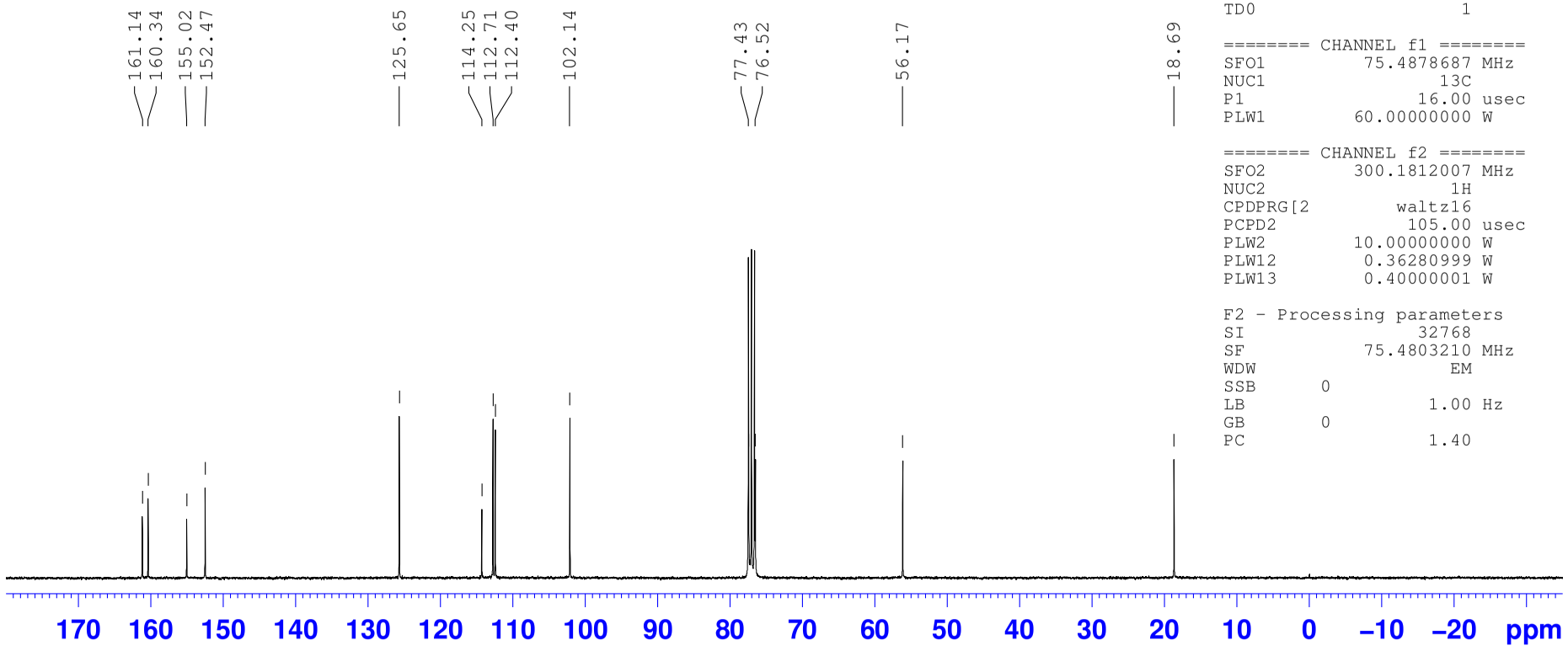

```
Current Data Parameters
NAME                  7P3M4PC
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130319
Time                  16.33
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1009
DS                        4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                 1.3421773 sec
RG                   501.187
DW                    20.480 usec
DE                     6.50 usec
TE                    296.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
D31                0.00001600 sec
D40                0.02432300 sec
L4                         34
L5                         49
P32                  105.00 usec
TD0                        1

======== CHANNEL f1 ========
SFO1              75.4878687 MHz
NUC1                     13C
P1                    16.00 usec
PLW1             60.00000000 W

======== CHANNEL f2 ========
SFO2             300.1812007 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                105.00 usec
PLW2             25.00000000 W
PLW12             0.21336000 W
PLW13             0.23522000 W

F2 - Processing parameters
SI                       32768
SF                75.4803210 MHz
WDW                         EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```


7P4MC
7.545
7.529
7.513
6.954
6.946
6.939
6.931
6.923
6.914
6.162
6.158
4.770
4.763
2.592
2.584
2.576
2.409
2.406
ppm
1.03
2.00
1.00
2.03
0.98
2.99
Current Data Parameters
NAME 7P4MC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140630
Time 11.03
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 32
DW 81.920 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7P4MC

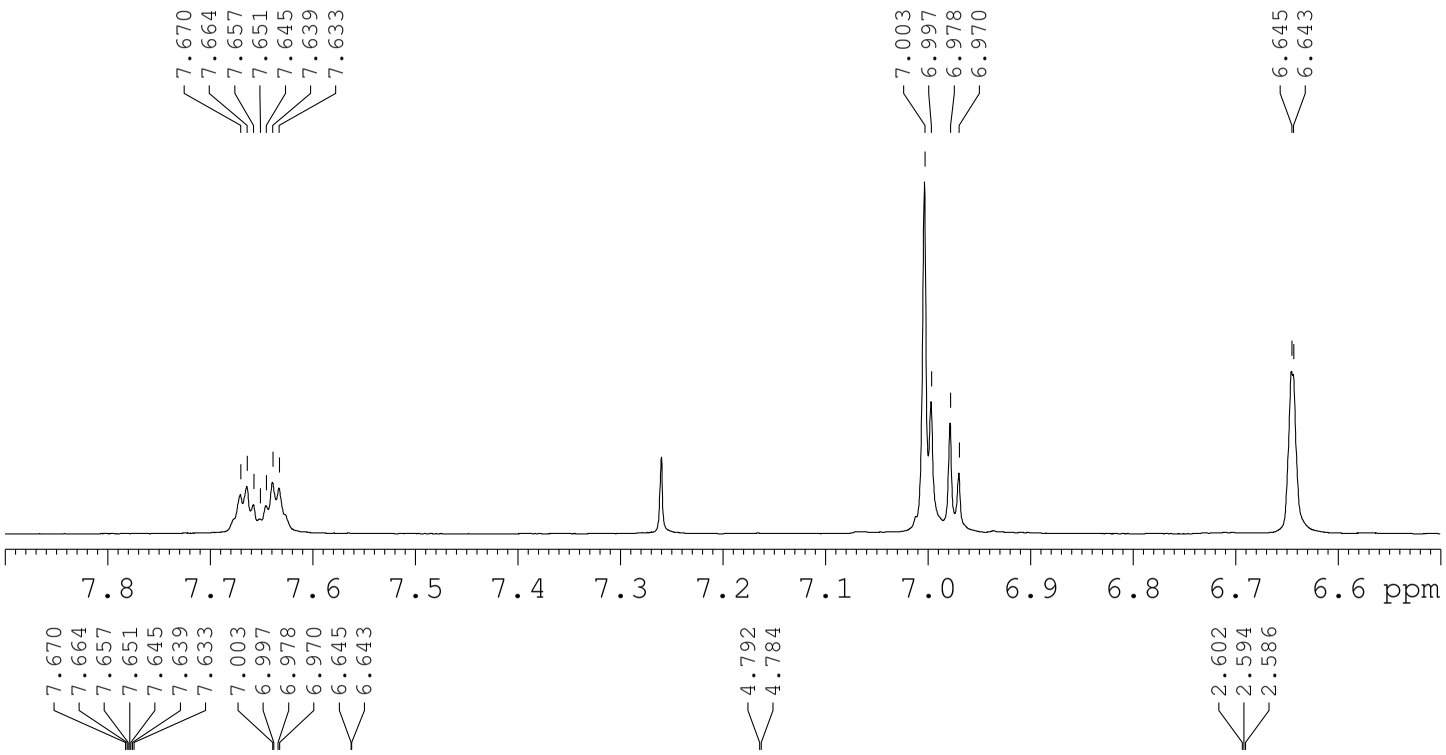






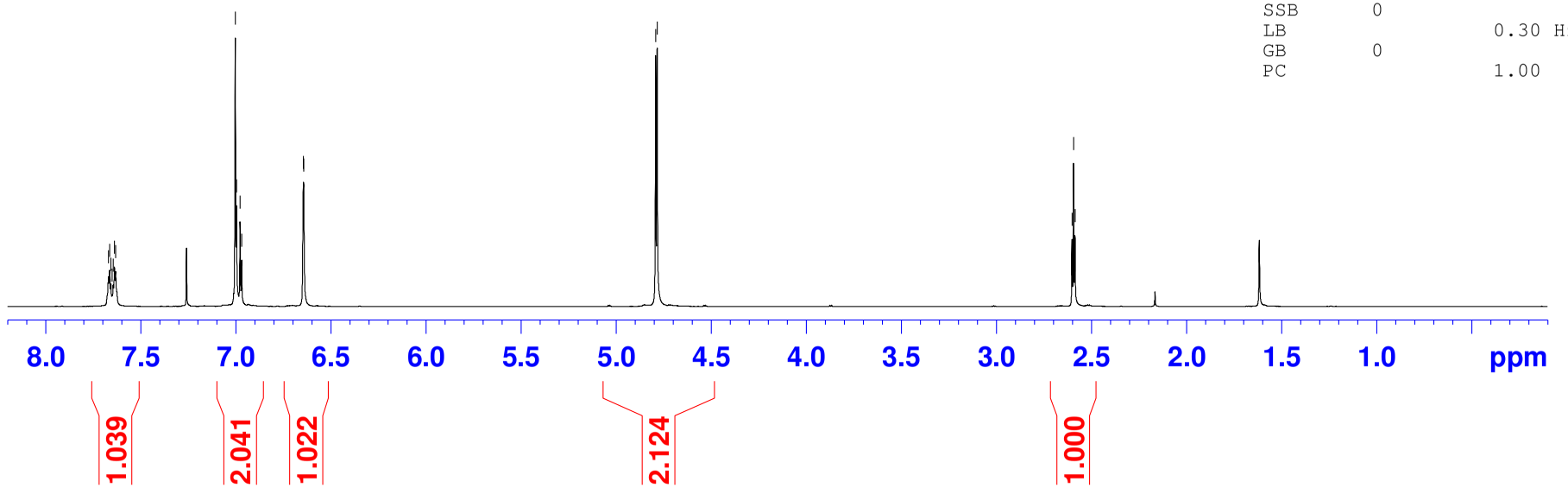

```
Current Data Parameters
NAME                  7P4MC
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140706
Time                 21.38
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   10000
DS                       4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  296.3 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001600 sec
D40             0.02432300 sec
L4                      34
L5                      49
P32                105.00 usec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4878687 MHz
NUC1                  13C
P1                  16.00 usec
PLW1          60.00000000 W

======== CHANNEL f2 ========
SFO2          300.1812007 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2          10.00000000 W
PLW12          0.36280999 W
PLW13          0.40000001 W

F2 - Processing parameters
SI                    32768
SF             75.4803210 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

7P4TFC

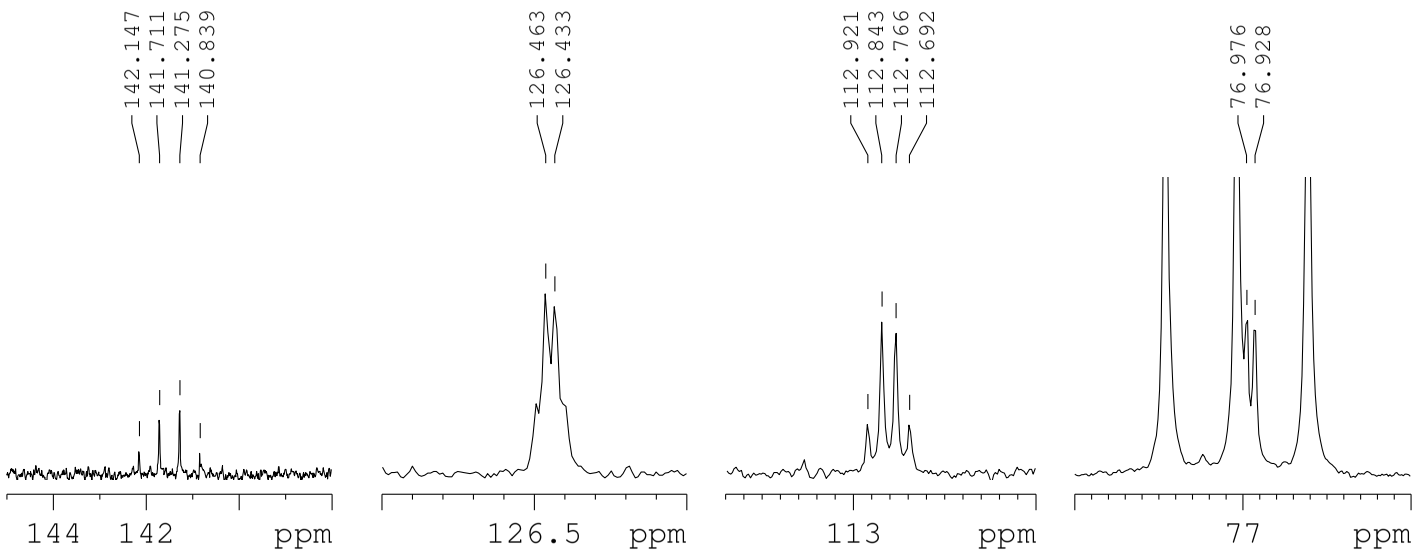


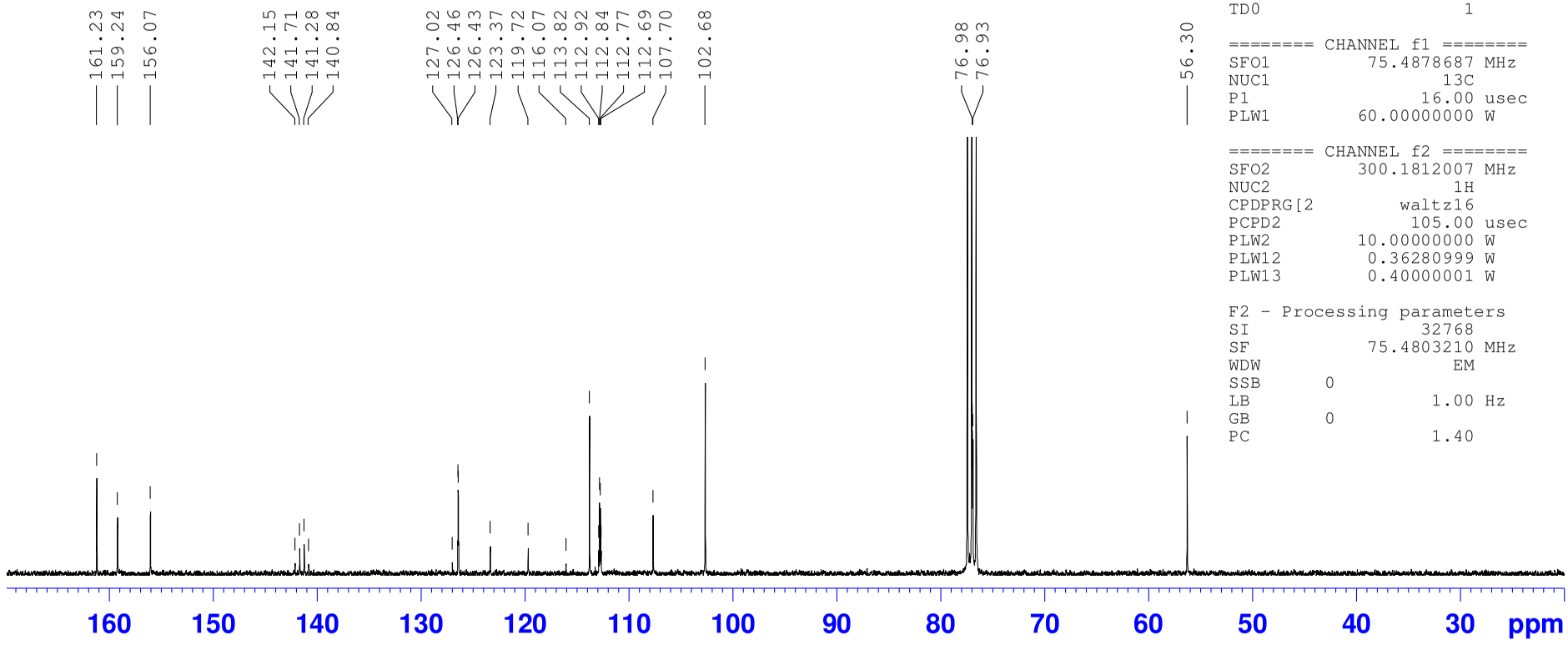

```
Current Data Parameters
NAME                  7P4TFC
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140508
Time                  11.01
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   52.2894
DW                  81.920 usec
DE                   6.50 usec
TE                  296.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1818537 MHz
NUC1                     1H
P1                    8.75 usec
PLW1           25.00000000 W

F2 - Processing parameters
SI                    65536
SF             300.1800051 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

4TF7PC (Compound 16)



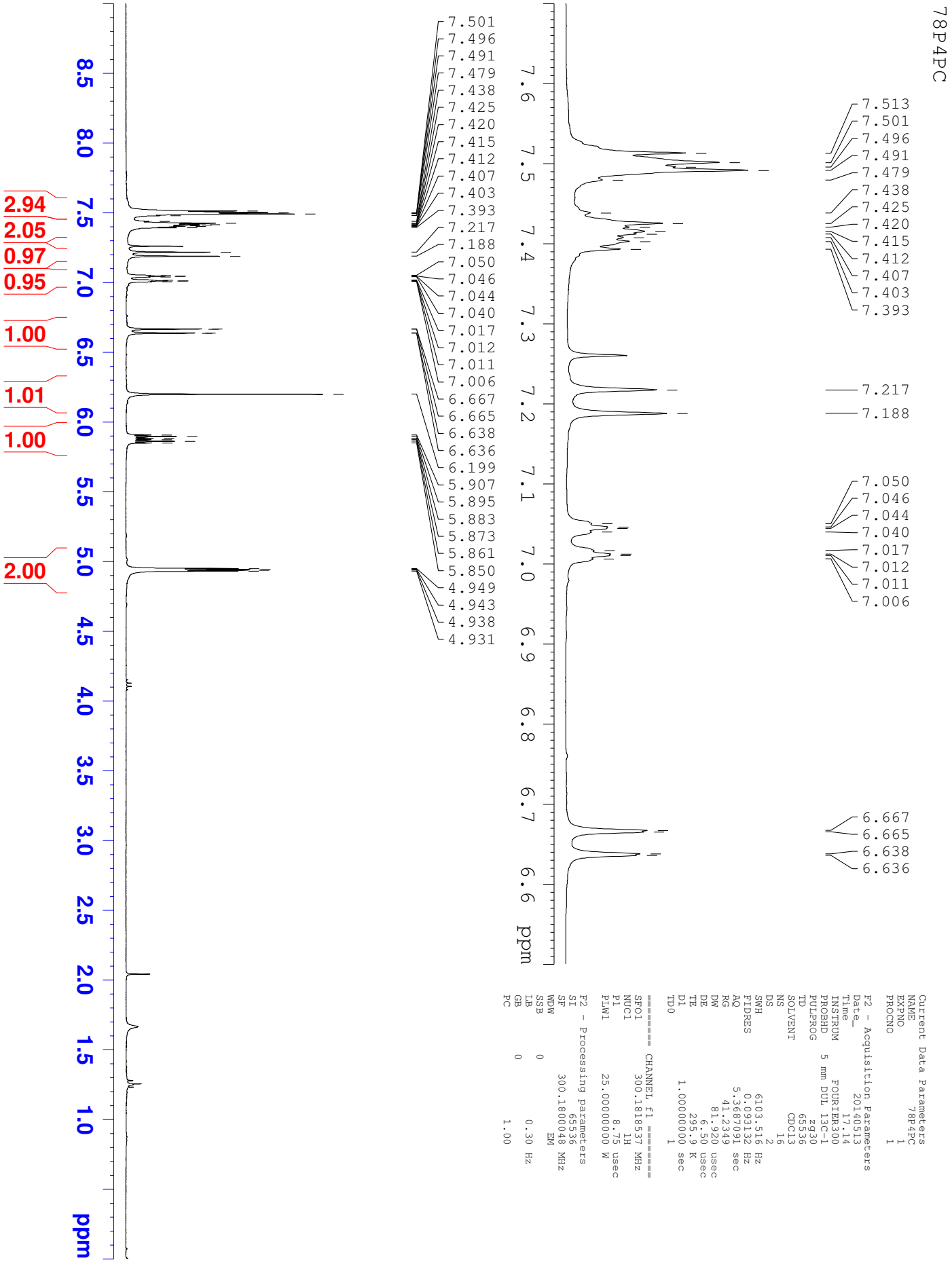
7P4TFC






```
Current Data Parameters
NAME                  7P4TFC
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140512
Time                  11.57
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2000
DS                       4
SWH              24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  296.1 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001600 sec
D40              0.02432300 sec
L4                        34
L5                        49
P32                 105.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                    13C
P1                   16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                    32768
SF              75.4803210 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

4P78PC (Compound 17)



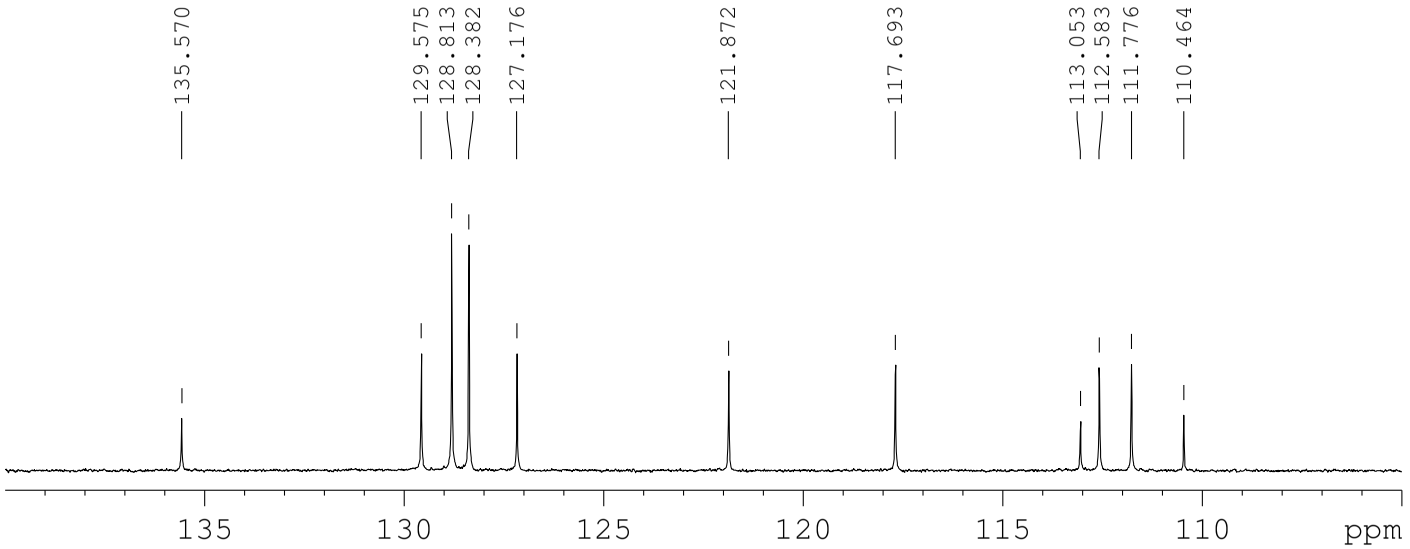
Current Data Parameters
NAME 78P4PC
EXPNO 1
PROCNO 1

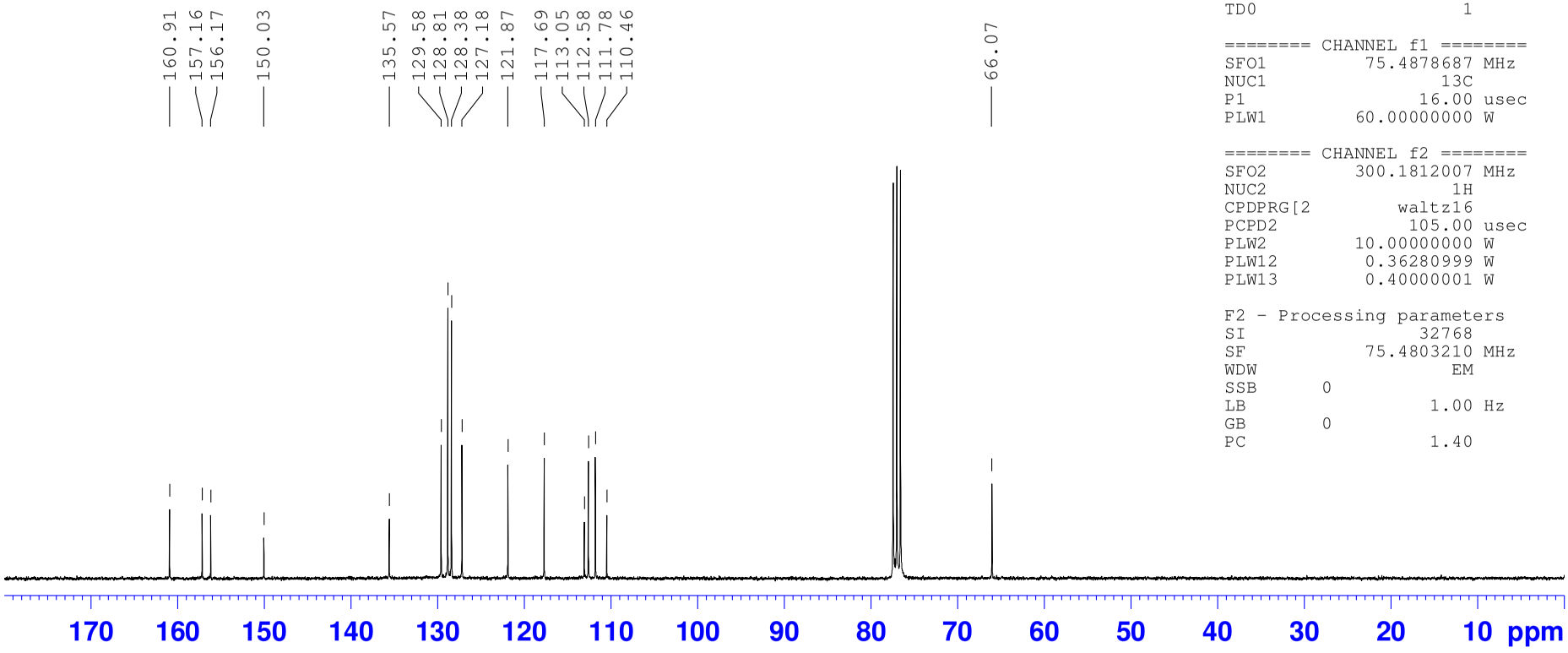
F2 - Acquisition Parameters
Date_ 20140513
Time 17.14
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 41.2349
DW 81.920 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

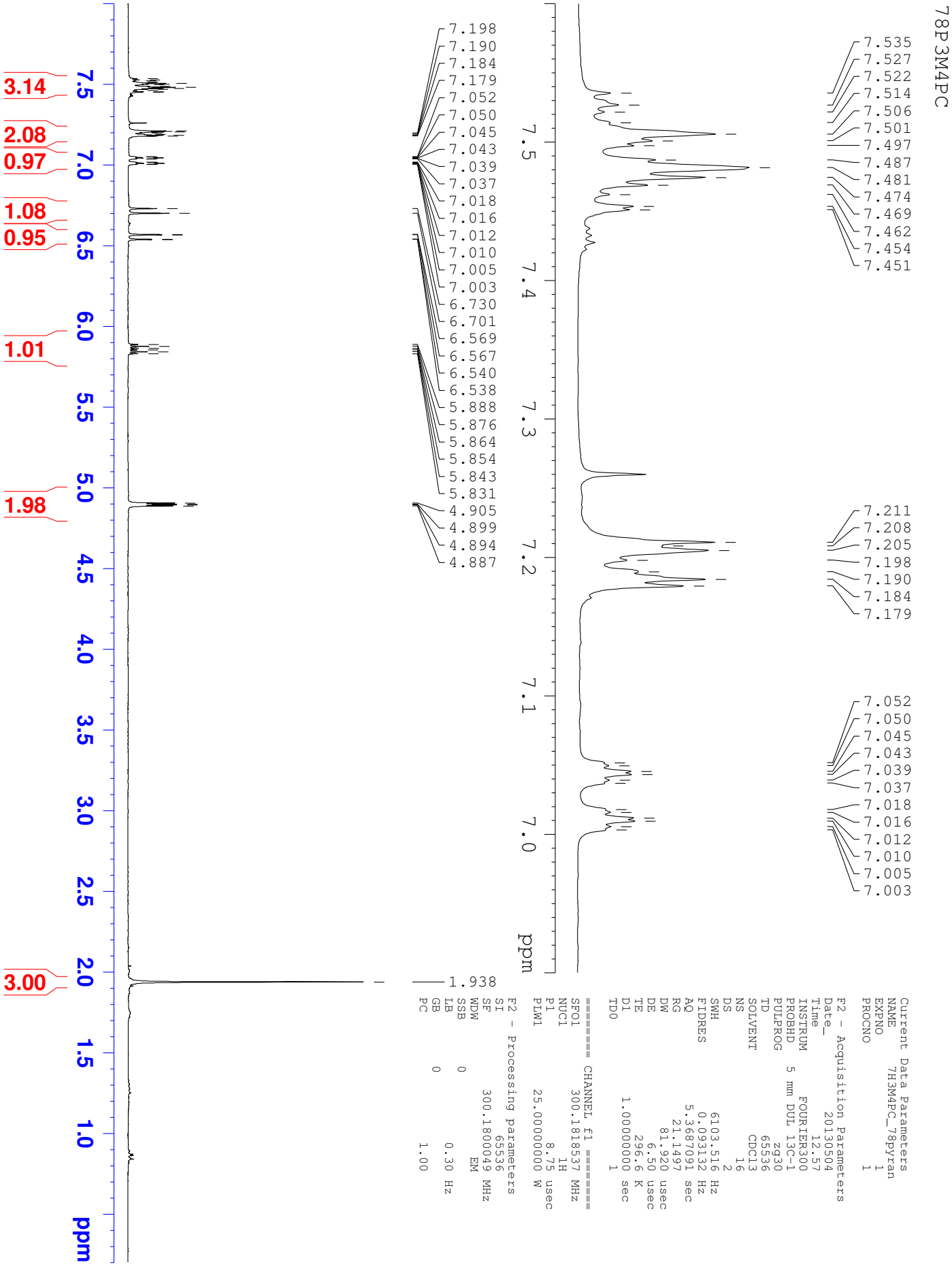
78P4PC



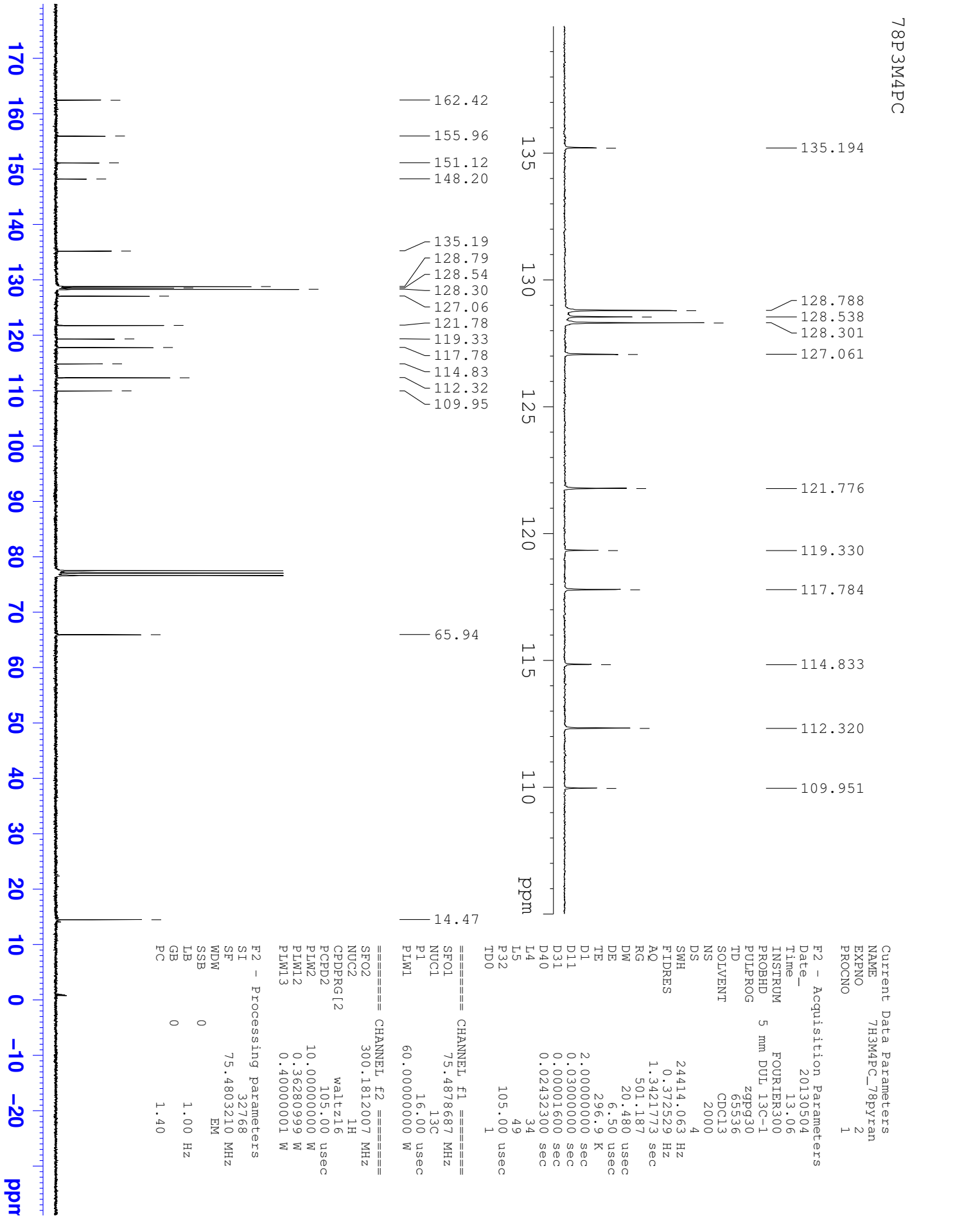


4P78PC (Compound 17)

```
Current Data Parameters
NAME                  78P4PC
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140513
Time                  17.19
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    8000
DS                       4
SWH              24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  296.1 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001600 sec
D40              0.02432300 sec
L4                        34
L5                        49
P32                 105.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                    13C
P1                   16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                     32768
SF              75.4803210 MHz
WDW                       EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```


78P3M4PC
7.535
7.527
7.522
7.514
7.506
7.501
7.497
7.487
7.481
7.474
7.469
7.462
7.454
7.451
7.211
7.208
7.205
7.198
7.190
7.184
7.179
7.052
7.050
7.045
7.043
7.039
7.037
7.018
7.016
7.012
7.010
7.005
7.003
7.198
7.190
7.184
7.179
7.052
7.050
7.045
7.043
7.039
7.037
7.018
7.016
7.012
7.010
7.005
7.003
6.730
6.701
6.569
6.567
6.540
6.538
5.888
5.876
5.864
5.854
5.843
5.831
4.905
4.899
4.894
4.887
1.938
7.5
7.4
7.3
7.2
7.1
7.0
ppm
3.14
2.08
0.97
1.08
0.95
1.01
1.98
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
Current Data Parameters
NAME 7H3M4PC_78pyran
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130504
Time 12.57
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 21.1497
DW 81.920 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
========== CHANNEL f1 ==========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3M4P78PC (Compound 18)



Current Data Parameters
NAME 7H3M4PC_78pyran
EXPNO 2
PROCNO 1

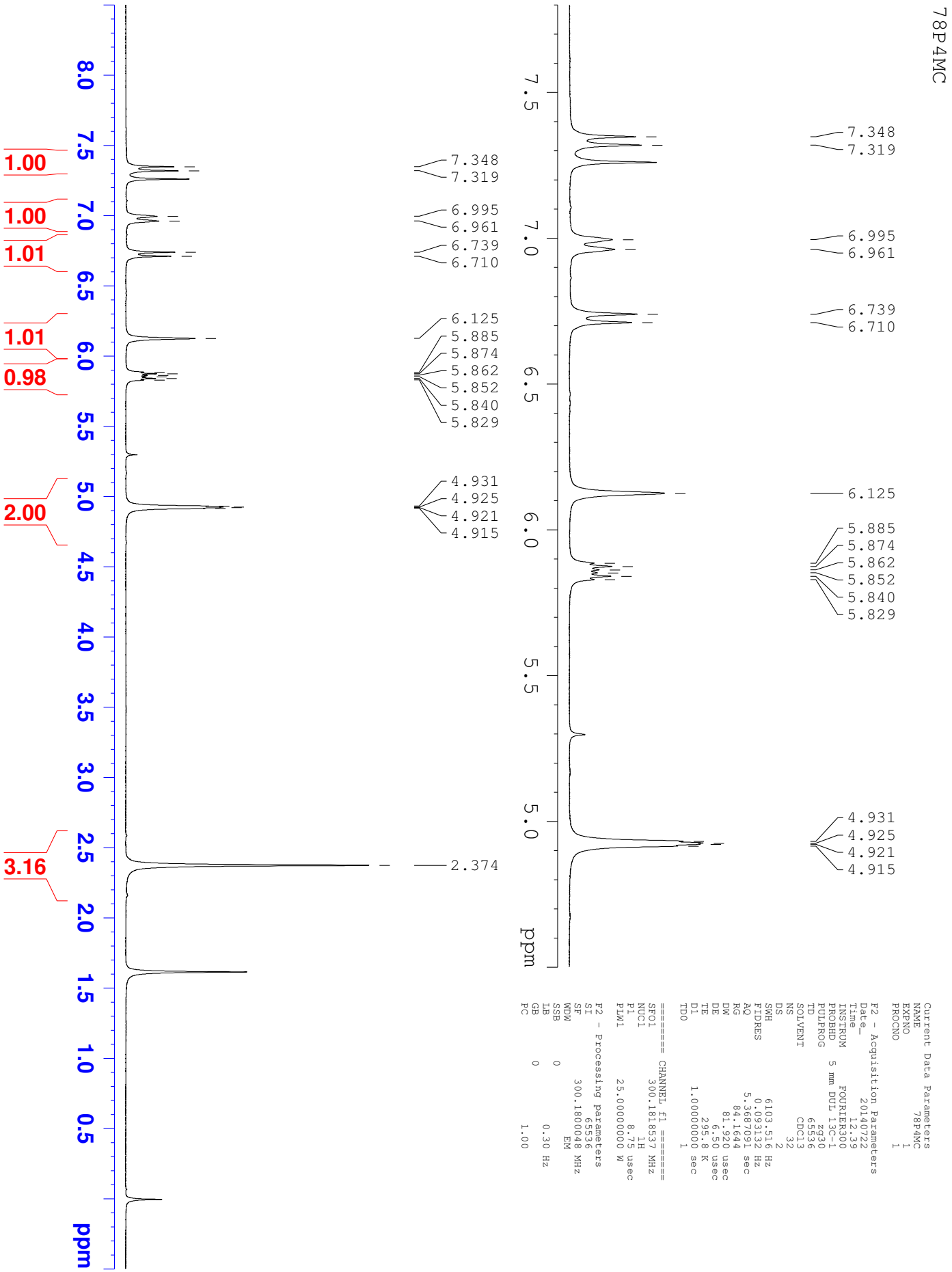
F2 - Acquisition Parameters
Date_ 20130504
Time 13.06
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2000
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001600 sec
D40 0.02432300 sec
L4 34
L5 49
P32 105.00 usec
TD0 1

========== CHANNEL f1 ==========
SFO1 75.4878687 MHz
NUC1 13C
P1 16.00 usec
PLW1 60.00000000 W

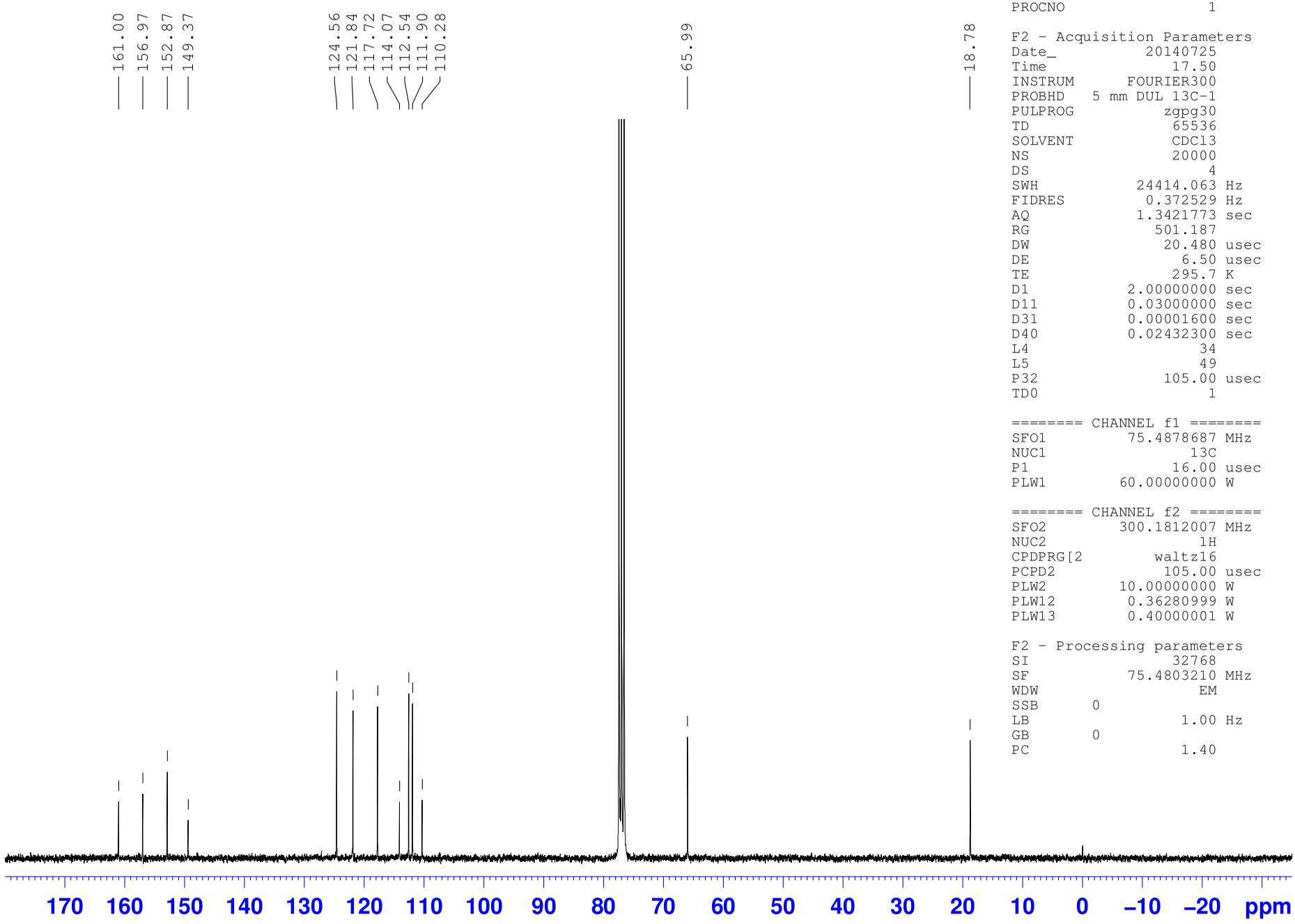
========== CHANNEL f2 ==========
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 105.00 usec
PLW2 10.00000000 W
PLW12 0.36280999 W
PLW13 0.40000001 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4M78PC (Compound 19)

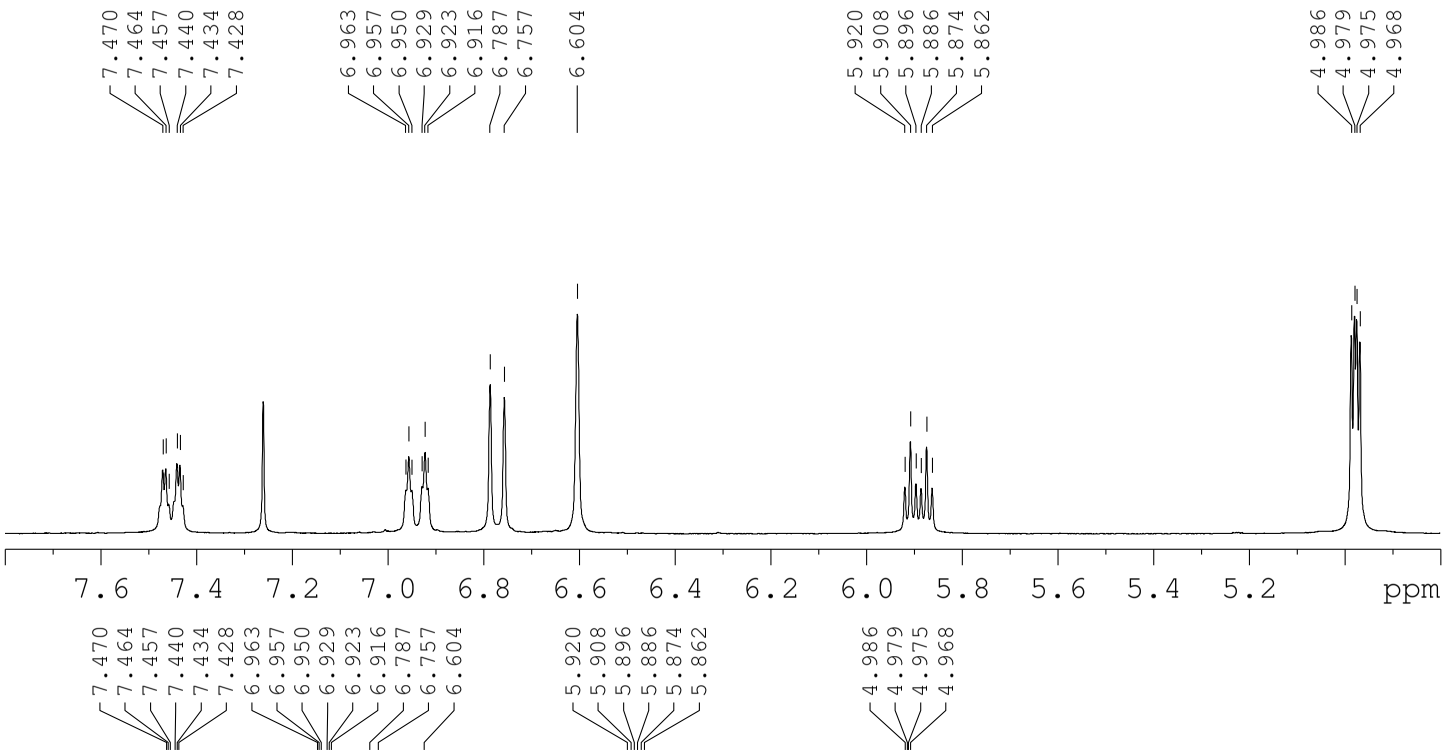


78P4MC

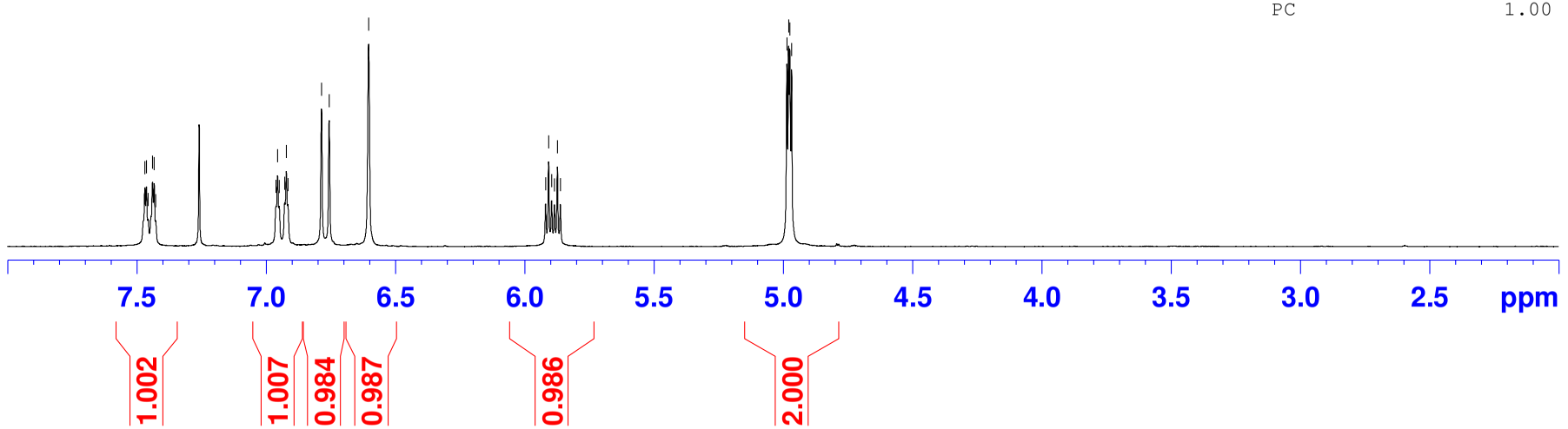



```
Current Data Parameters
NAME                 78P4MC
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140725
Time                 17.50
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   20000
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   295.7 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001600 sec
D40            0.02432300 sec
L4                       34
L5                       49
P32                 105.00 usec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4878687 MHz
NUC1                  13C
P1                  16.00 usec
PLW1          60.00000000 W

======== CHANNEL f2 ========
SFO2          300.1812007 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2          10.00000000 W
PLW12          0.36280999 W
PLW13          0.40000001 W

F2 - Processing parameters
SI                   32768
SF             75.4803210 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

78P4TFC

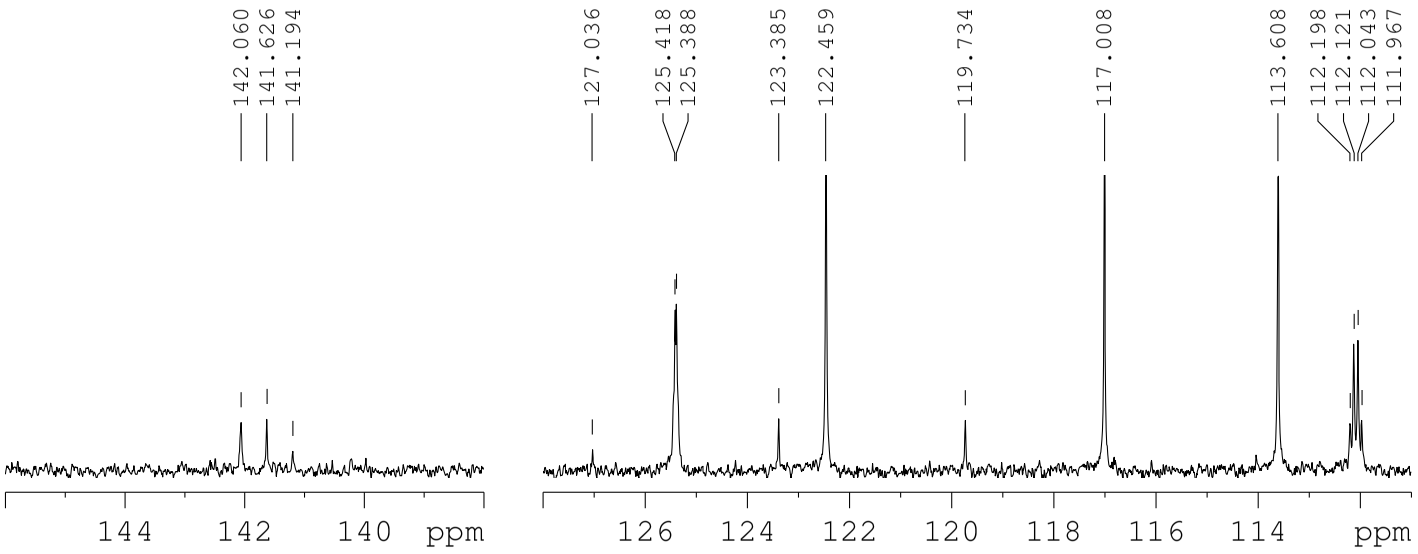


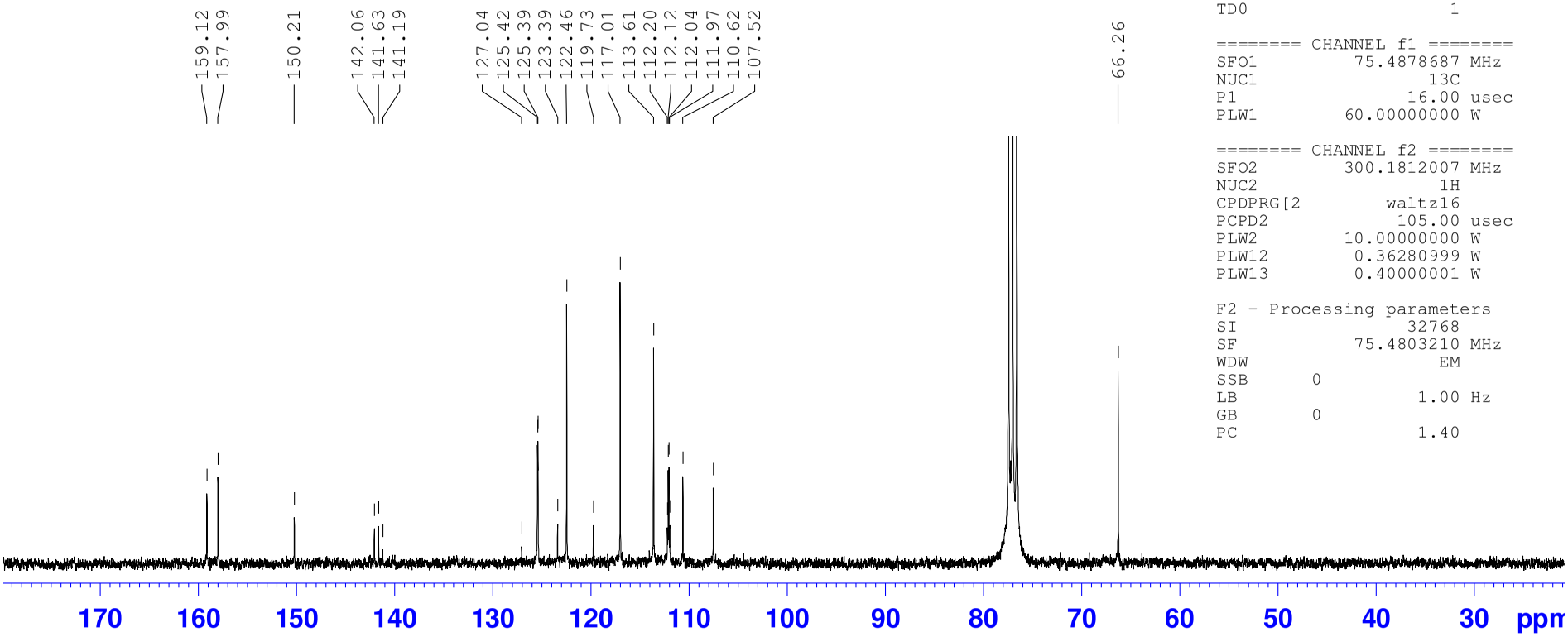

```
Current Data Parameters
NAME                  78P4TFC
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140516
Time                  11.12
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   78.0719
DW                  81.920 usec
DE                   6.50 usec
TE                  296.1 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            300.1818537 MHz
NUC1                      1H
P1                     8.75 usec
PLW1            25.00000000 W

F2 - Processing parameters
SI                    65536
SF              300.1800050 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

4TF78PC (Compound 20)

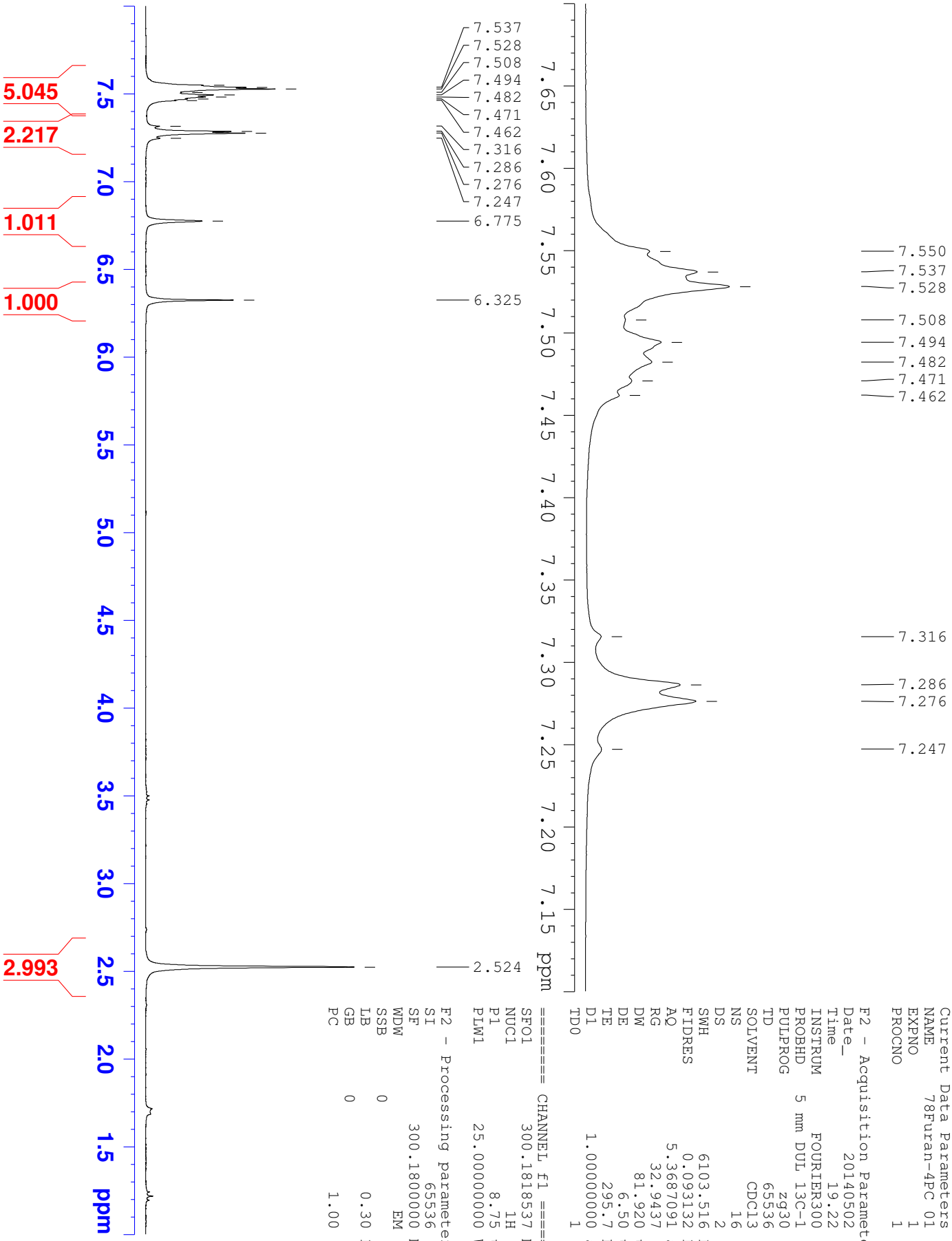
78P4TFC

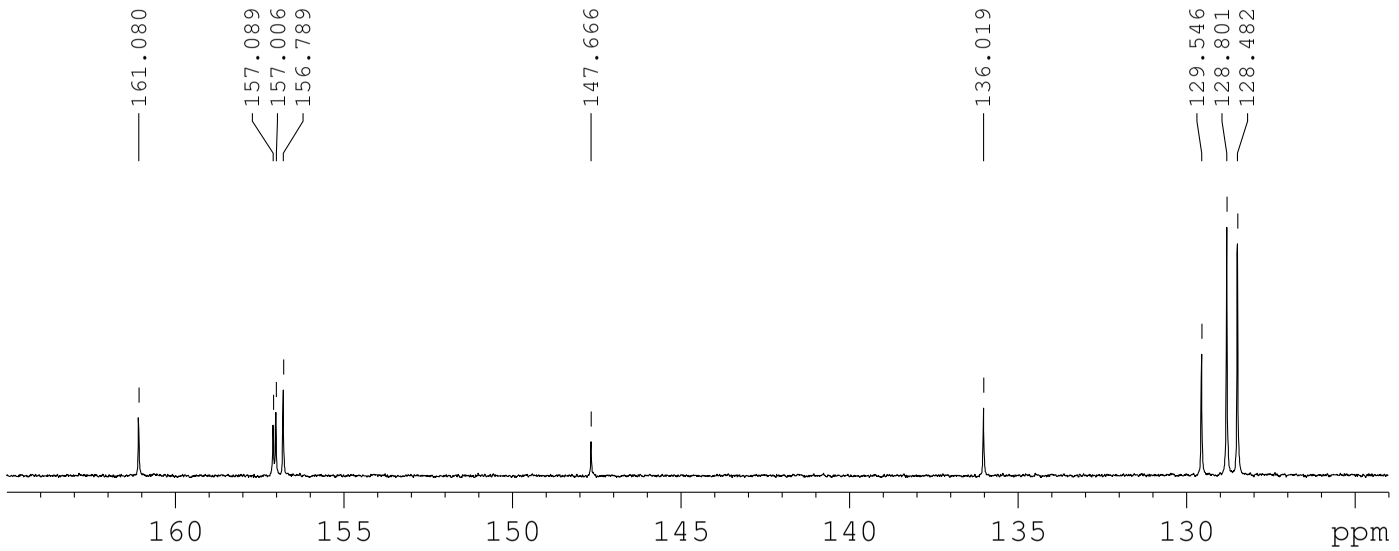


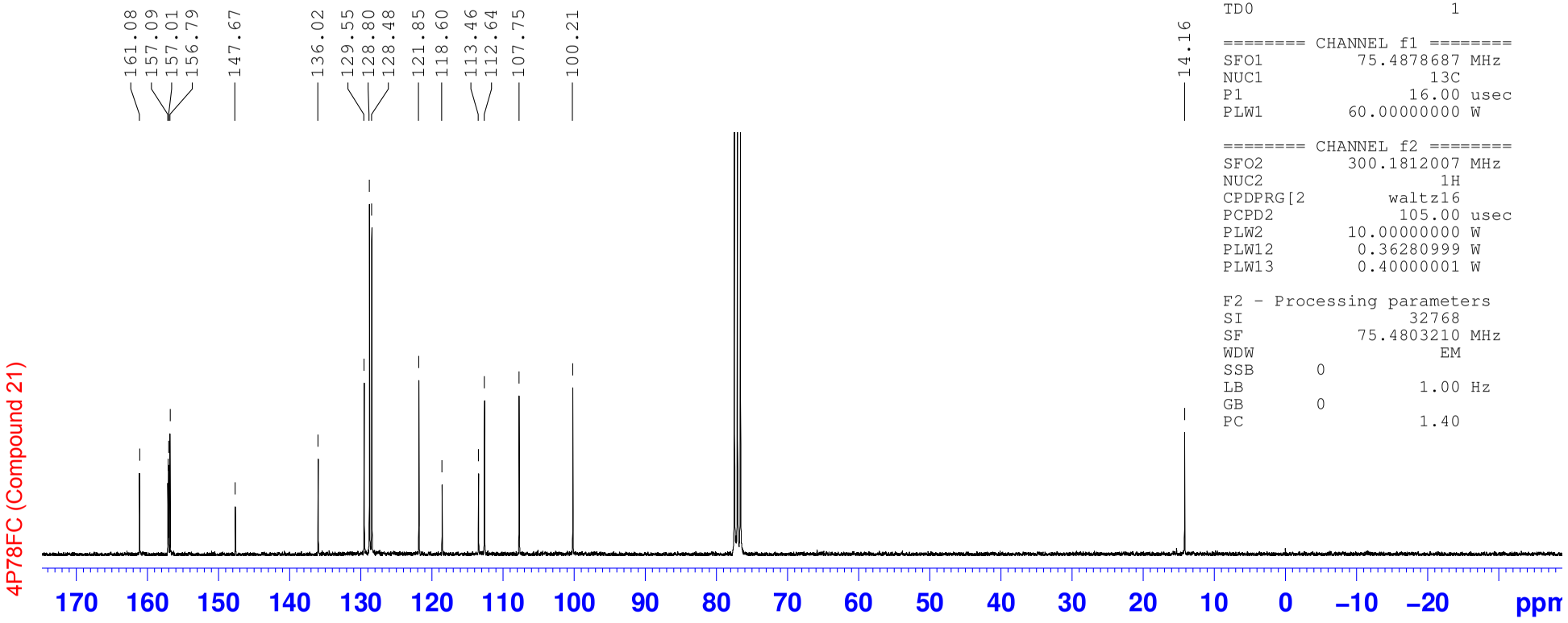



```
Current Data Parameters
NAME                  78P4TFC
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140519
Time                  17.47
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                    10000
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  296.2 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001600 sec
D40              0.02432300 sec
L4                        34
L5                        49
P32                 105.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                    13C
P1                   16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2               105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                    32768
SF              75.4803210 MHz
WDW                      EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```

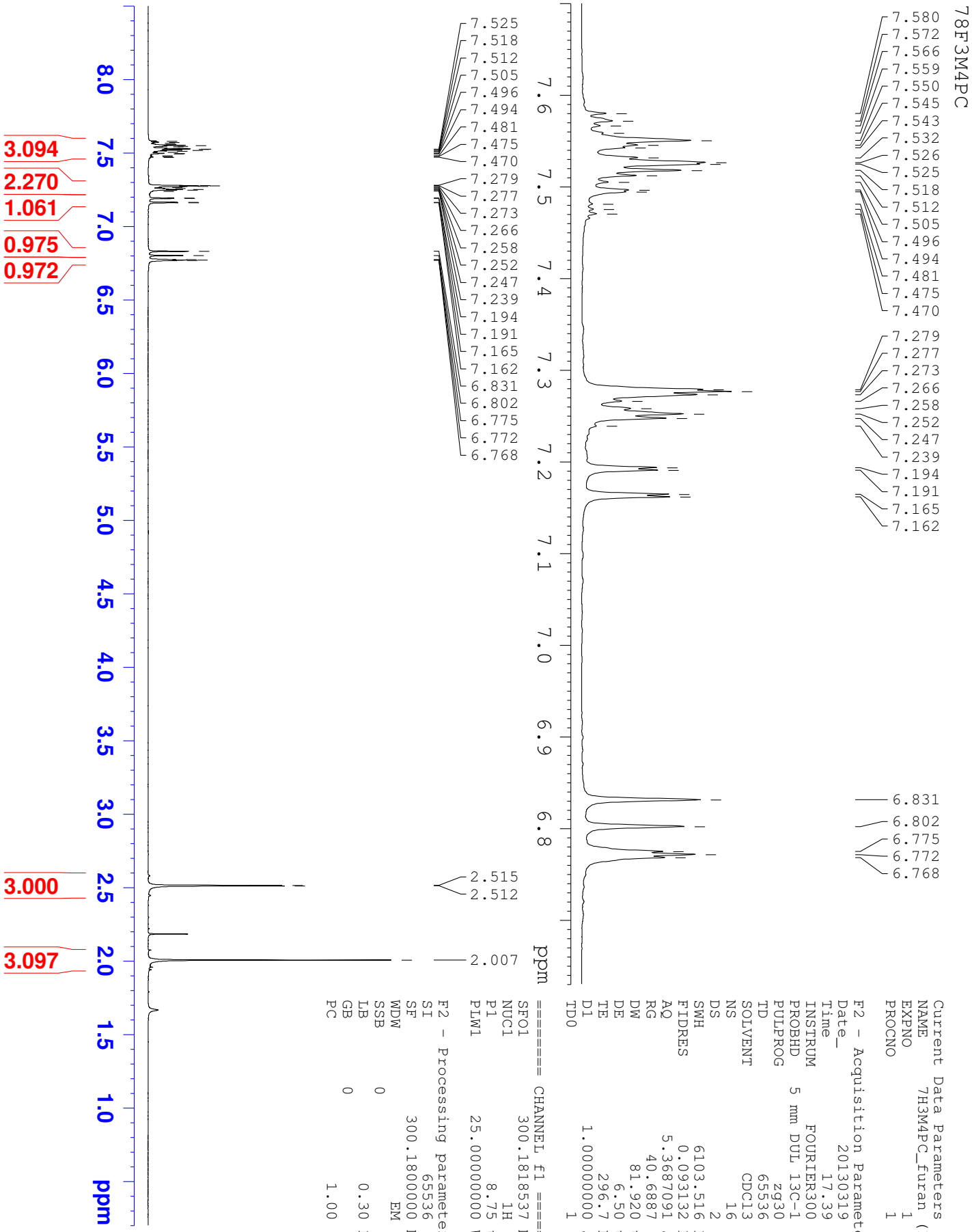
4P78FC (Compound 21)



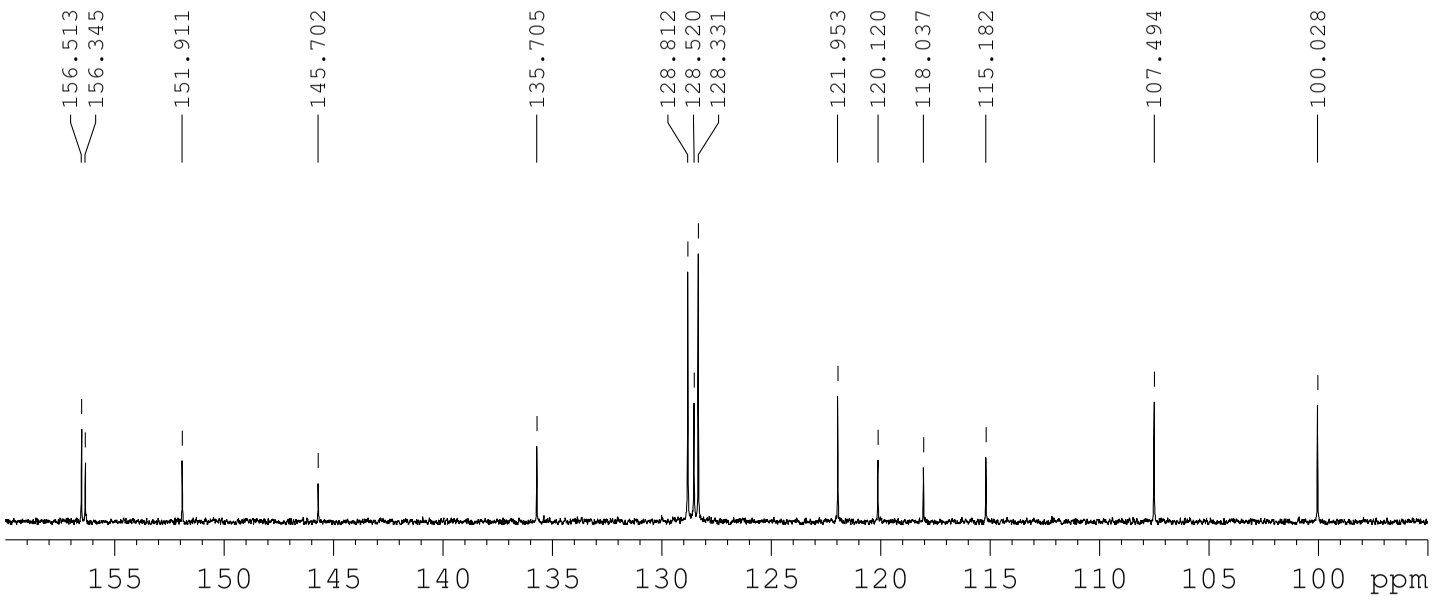


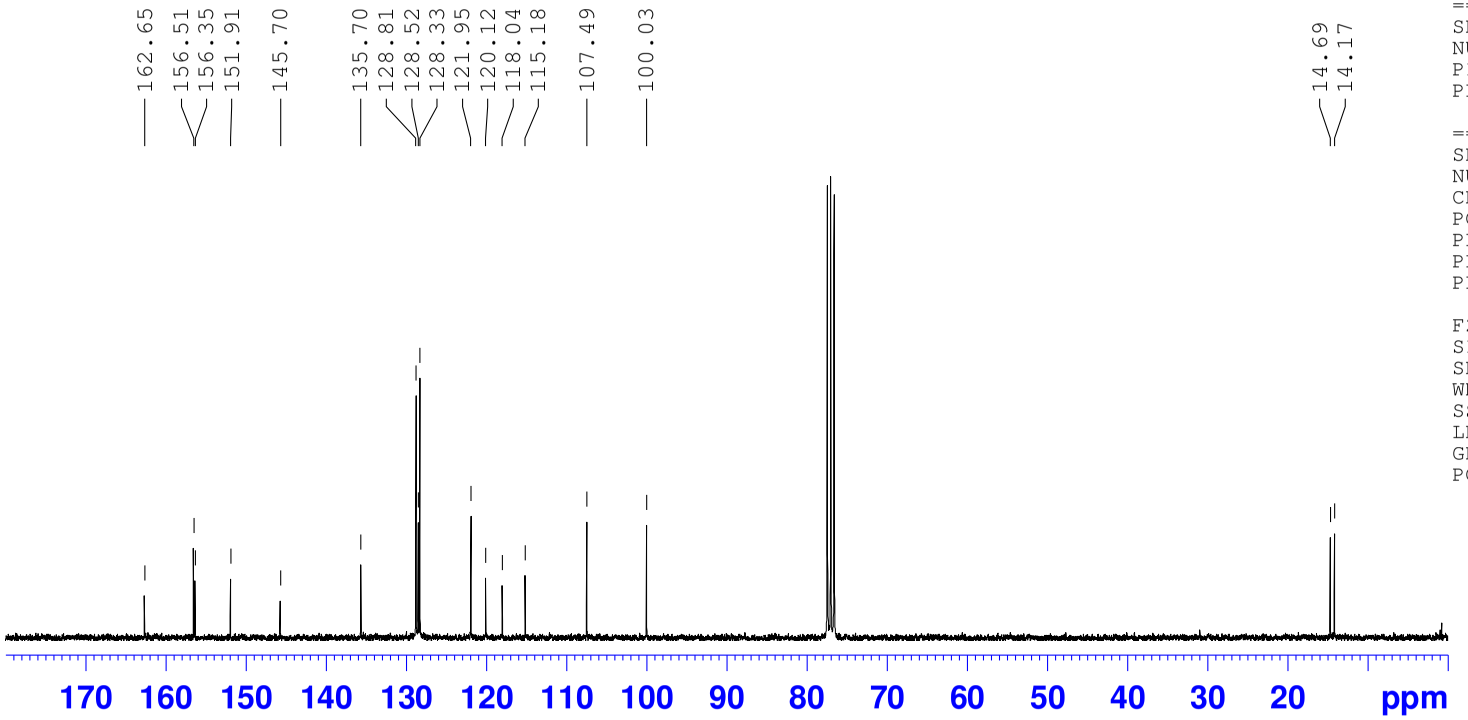



```
Current Data Parameters
NAME      78Furan-4PC 01
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20140502
Time              19.26
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 6000
DS                    4
SWH           24414.063 Hz
FIDRES         0.372529 Hz
AQ            1.3421773 sec
RG              501.187
DW               20.480 usec
DE                6.50 usec
TE               295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
D31          0.00001600 sec
D40          0.02432300 sec
L4                   34
L5                   49
P32              105.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4878687 MHz
NUC1               13C
P1               16.00 usec
PLW1        60.00000000 W

======== CHANNEL f2 ========
SFO2        300.1812007 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            105.00 usec
PLW2        10.00000000 W
PLW12        0.36280999 W
PLW13        0.40000001 W

F2 - Processing parameters
SI                32768
SF           75.4803210 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


78F3M4PC
7.580
7.572
7.566
7.559
7.550
7.545
7.543
7.532
7.526
7.525
7.518
7.512
7.505
7.496
7.494
7.481
7.475
7.470
7.279
7.277
7.273
7.266
7.258
7.252
7.247
7.239
7.194
7.191
7.165
7.162
6.831
6.802
6.775
6.772
6.768
2.515
2.512
2.007
3.094
2.270
1.061
0.975
0.972
3.000
3.097
ppm
Current Data Parameters
NAME 7H3M4PC_furan (III)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130319
Time 17.39
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 40.6887
DW 81.920 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

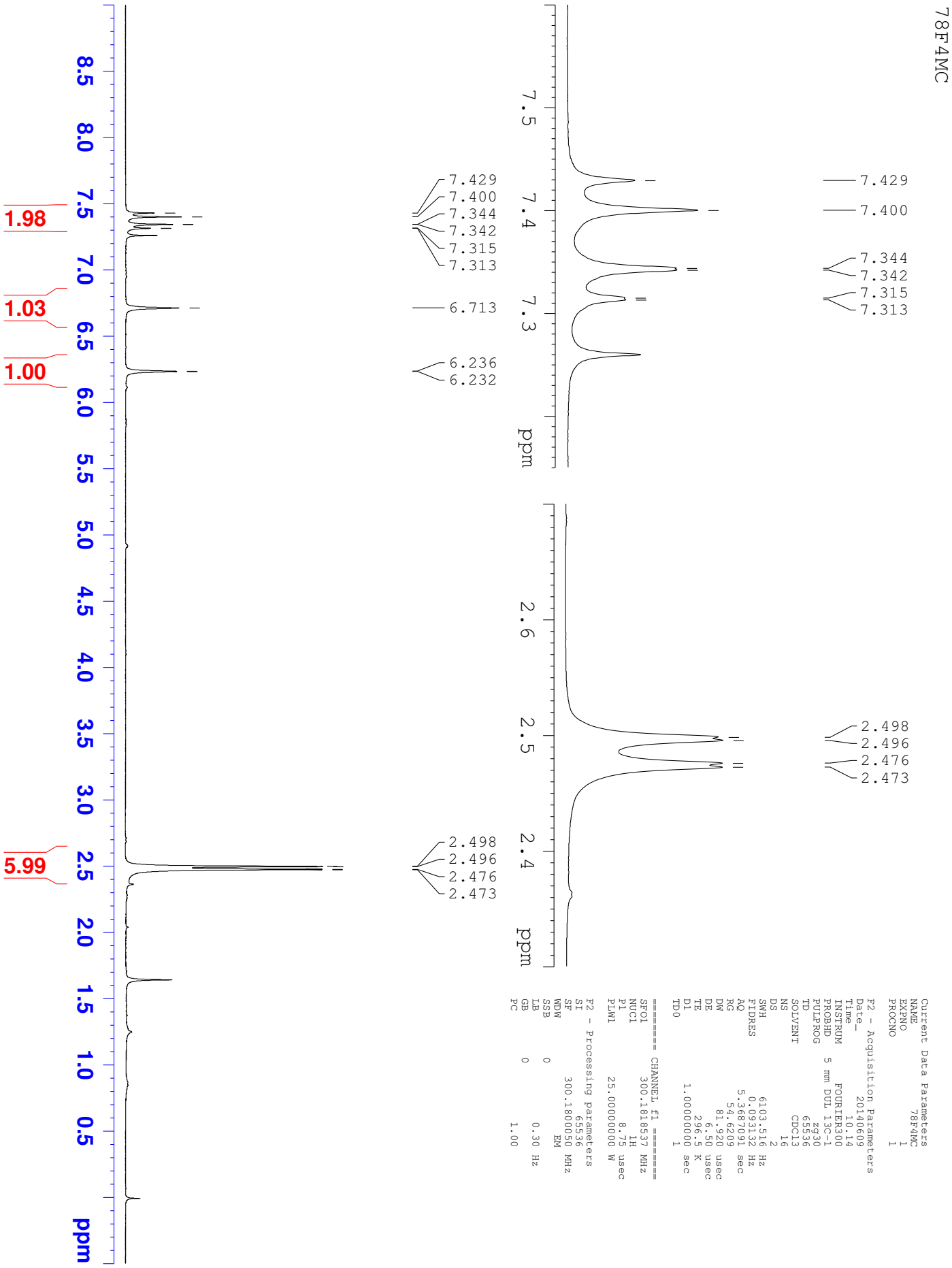
78F3M4PC



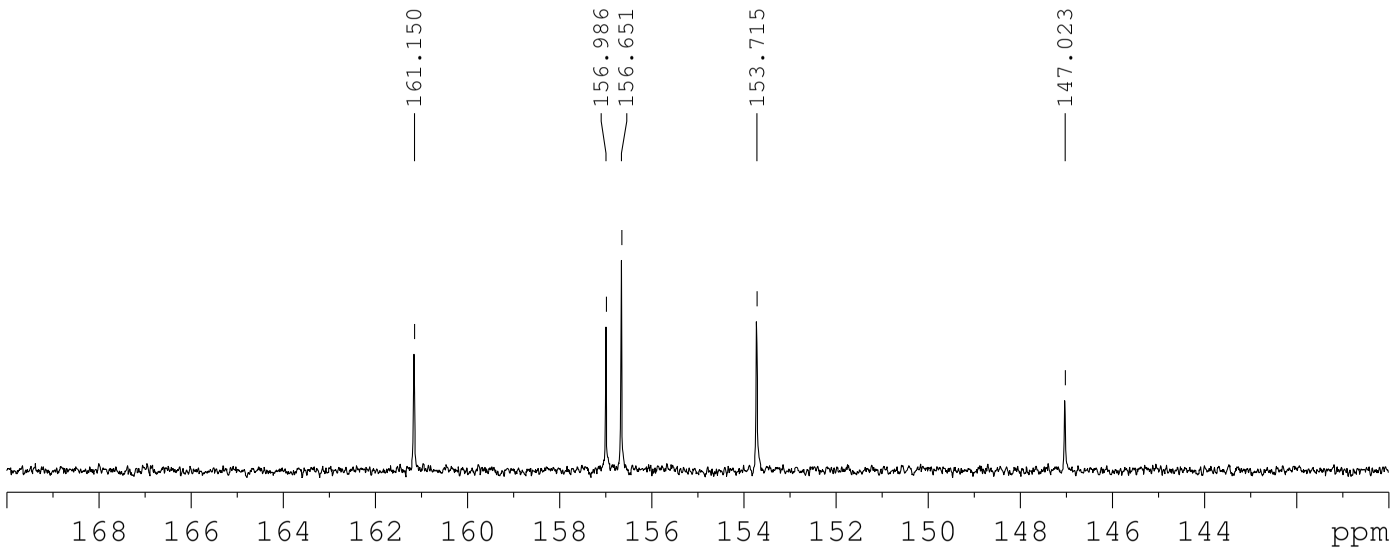


3M4P78FC (Compound 22)

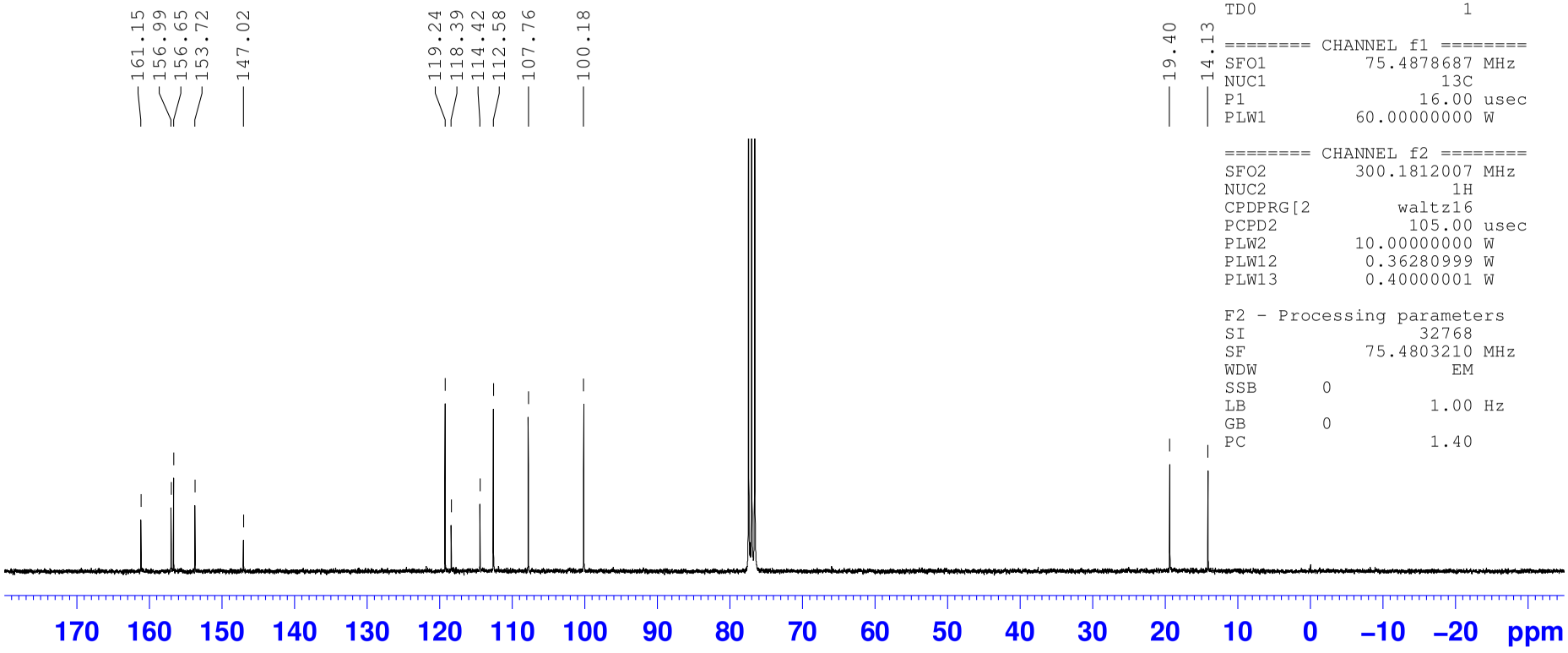
```
Current Data Parameters
NAME      7H3M4PC_furan (III)
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_           20130319
Time               17.52
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1759
DS                    4
SWH           24414.063 Hz
FIDRES         0.372529 Hz
AQ            1.3421773 sec
RG              501.187
DW               20.480 usec
DE                6.50 usec
TE               296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
D31          0.00001600 sec
D40          0.02432300 sec
L4                   34
L5                   49
P32              105.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4878687 MHz
NUC1               13C
P1               16.00 usec
PLW1        60.00000000 W

======== CHANNEL f2 ========
SFO2        300.1812007 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            105.00 usec
PLW2        25.00000000 W
PLW12        0.21336000 W
PLW13        0.23522000 W

F2 - Processing parameters
SI                32768
SF           75.4803210 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

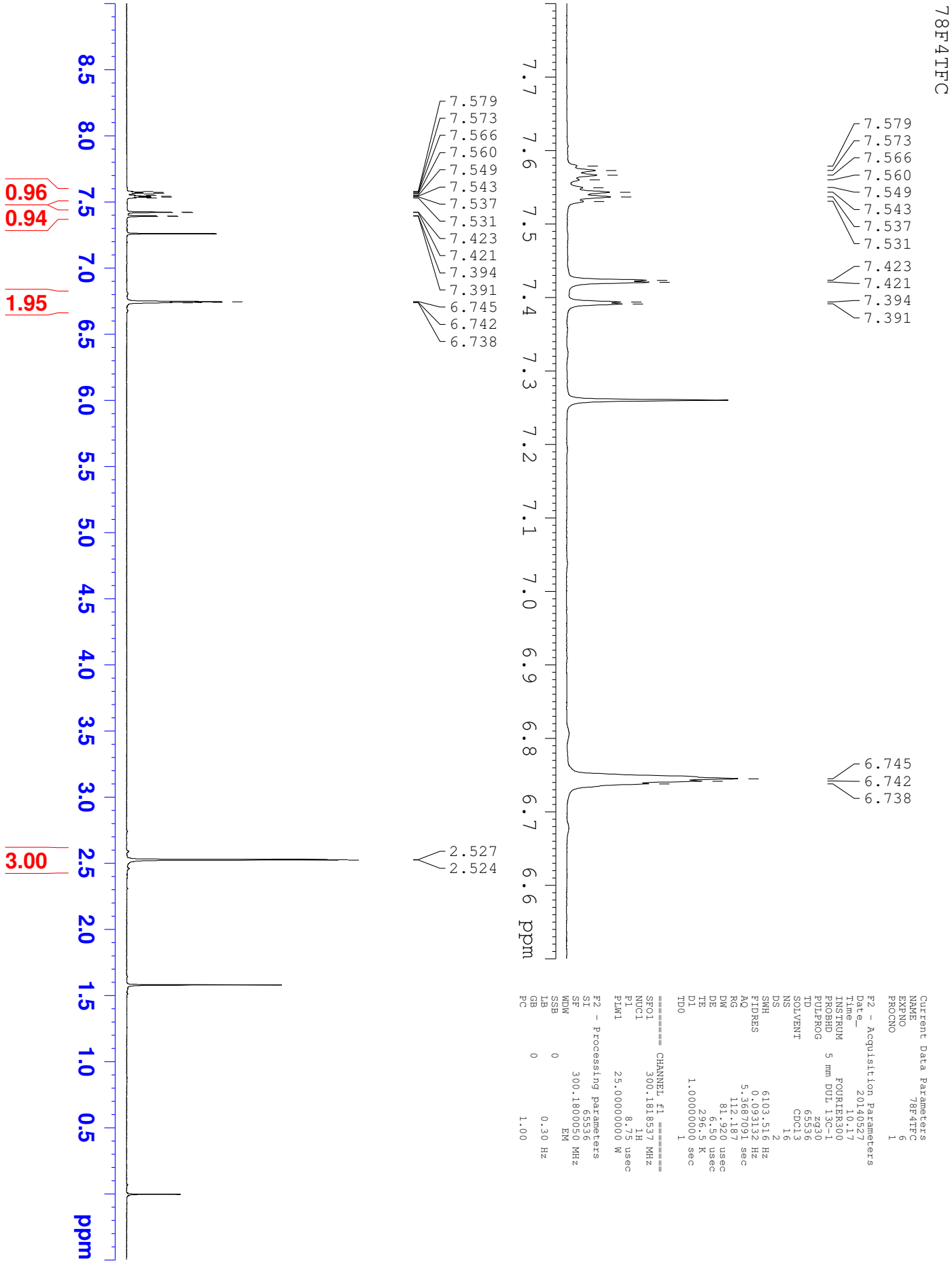

78F4MC
7.429
7.400
7.344
7.342
7.315
7.313
6.713
6.236
6.232
2.498
2.496
2.476
2.473
1.98
1.03
1.00
5.99
ppm
Current Data Parameters
NAME 78F4MC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140609
Time 10.14
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 54.6209
DW 81.920 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

78F4MC

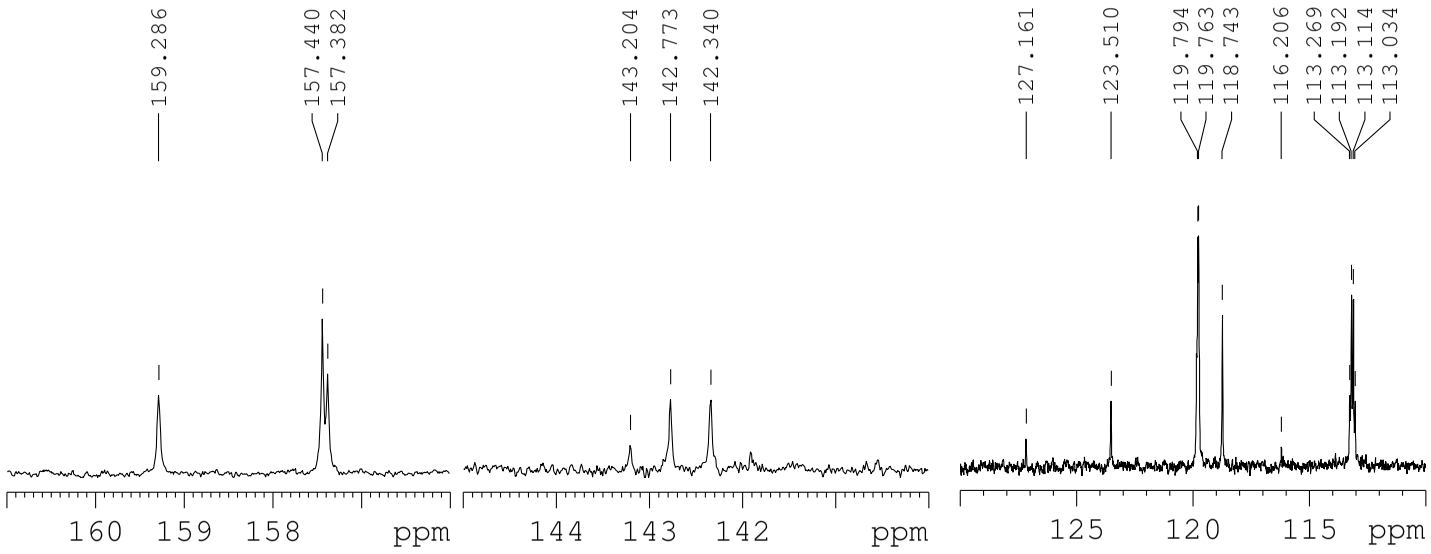


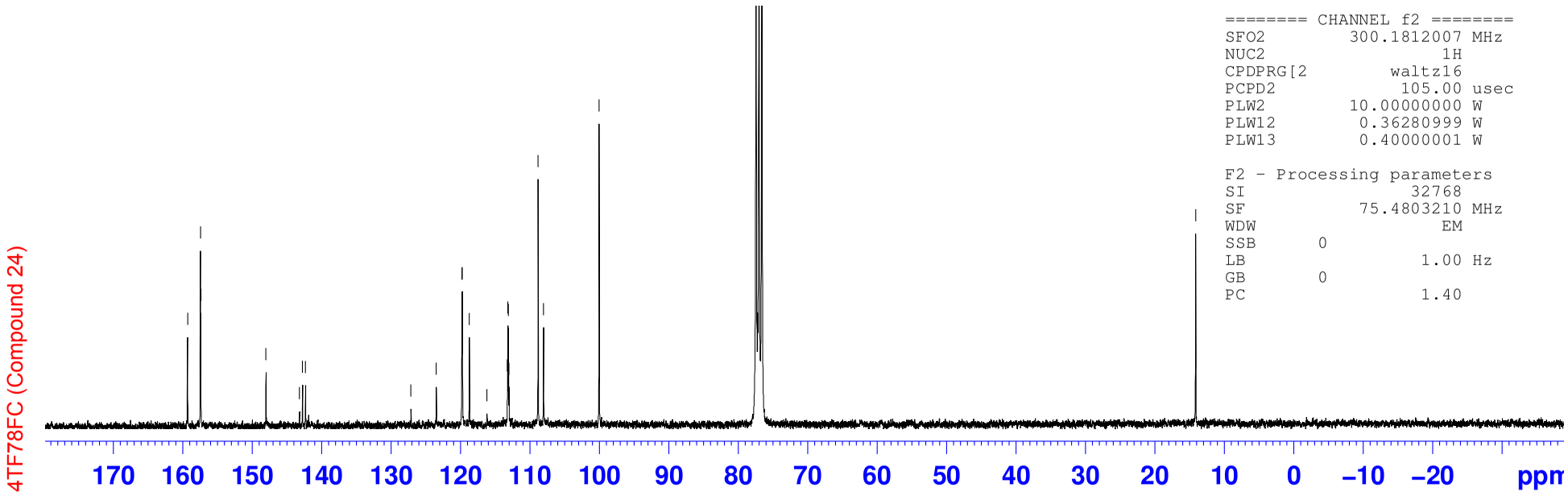

```
Current Data Parameters
NAME                 78F4MC
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140609
Time                 17.24
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  10000
DS                      4
SWH             24414.063 Hz
FIDRES          0.372529 Hz
AQ              1.3421773 sec
RG                501.187
DW                20.480 usec
DE                 6.50 usec
TE                297.5 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001600 sec
D40             0.02432300 sec
L4                       34
L5                       49
P32                105.00 usec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4878687 MHz
NUC1                   13C
P1                  16.00 usec
PLW1          60.00000000 W

======== CHANNEL f2 ========
SFO2          300.1812007 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2          10.00000000 W
PLW12          0.36280999 W
PLW13          0.40000001 W

F2 - Processing parameters
SI                    32768
SF             75.4803210 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



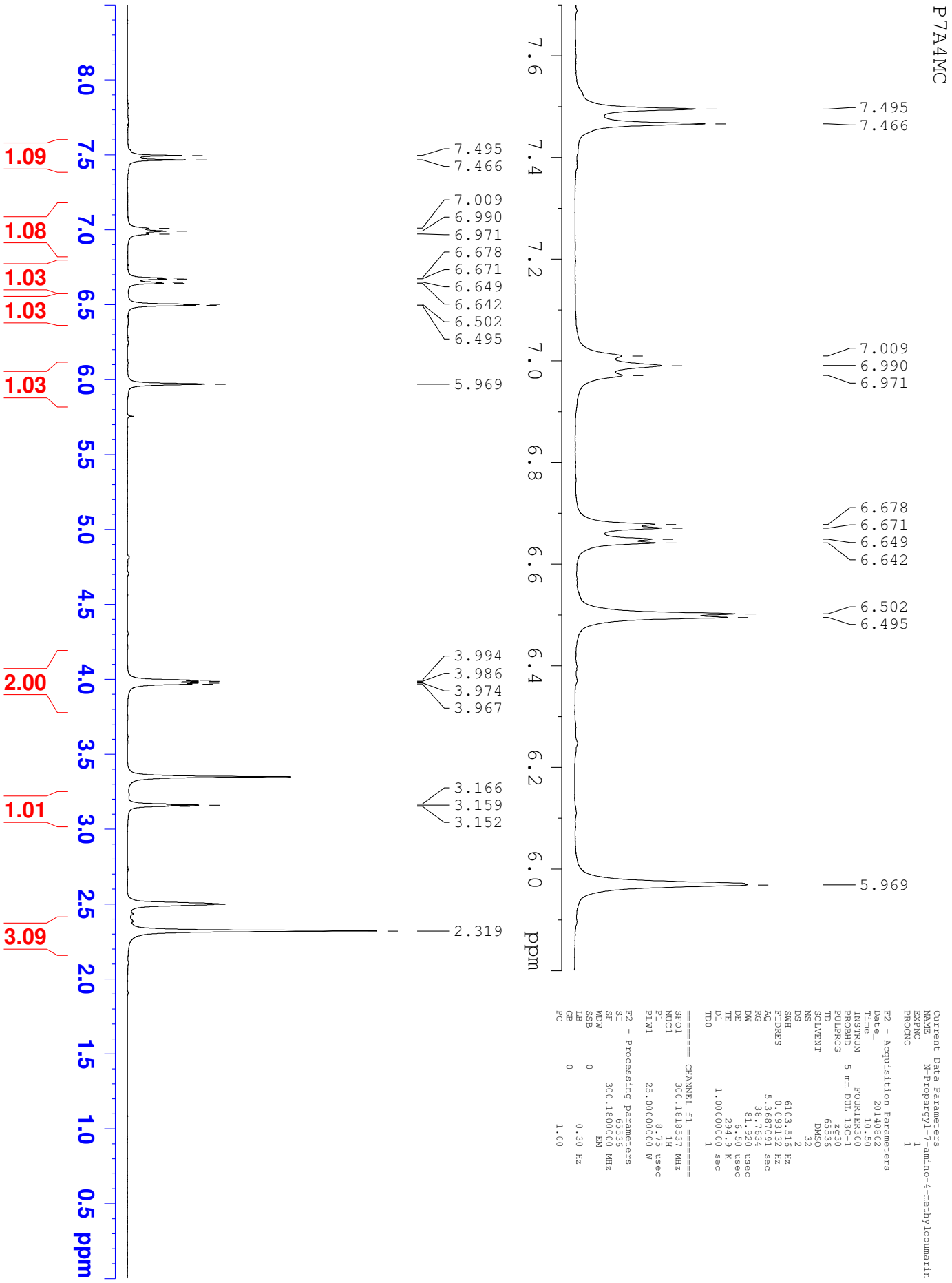

78F4TFC
7.579
7.573
7.566
7.560
7.549
7.543
7.537
7.531
7.423
7.421
7.394
7.391
6.745
6.742
6.738
2.527
2.524
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm
Current Data Parameters
NAME 78F4TFC
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140527
Time 10.17
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 112.187
DW 81.920 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
========== CHANNEL f1 ==========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.96
0.94
1.95
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

78F4TFC

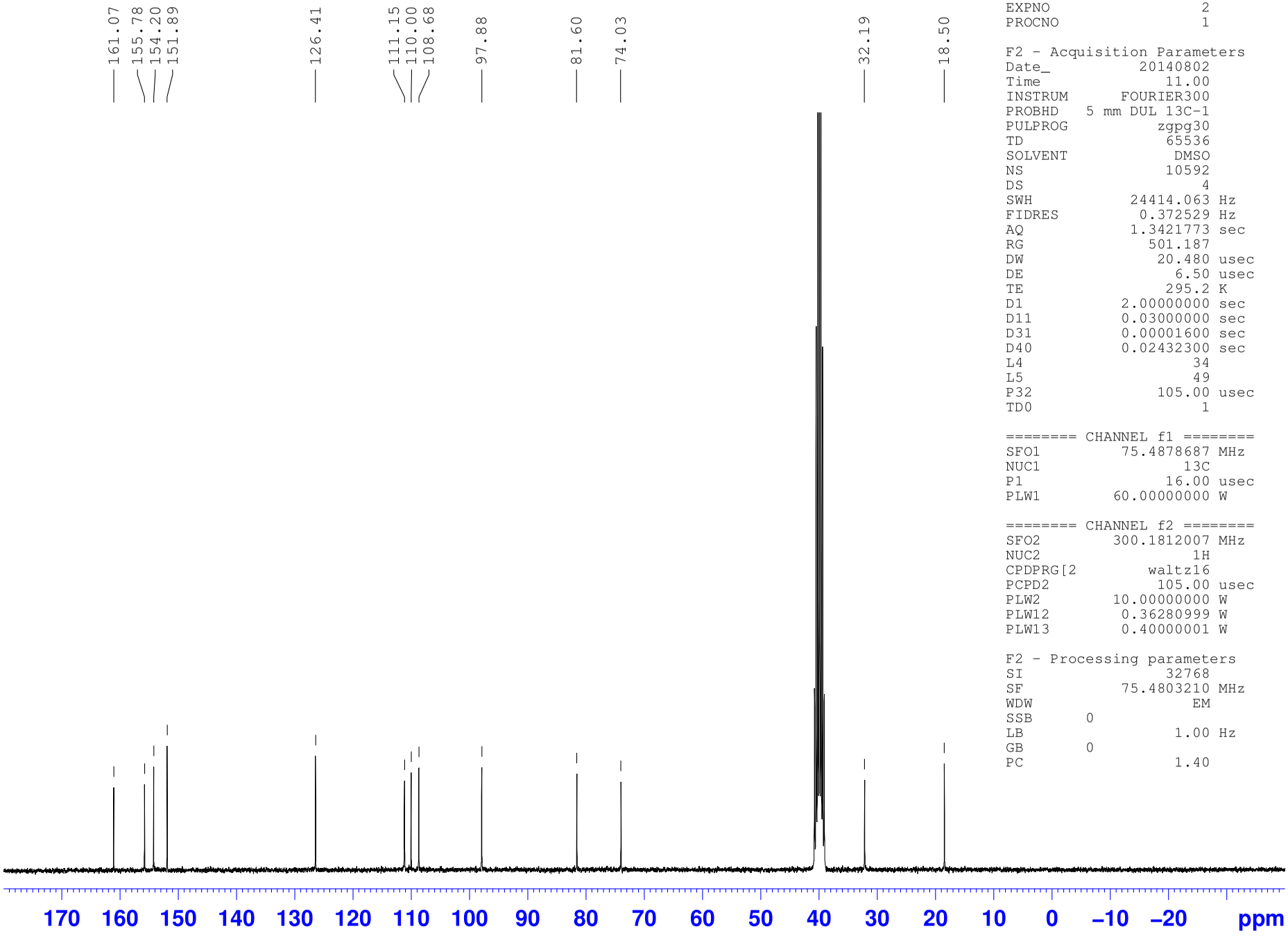




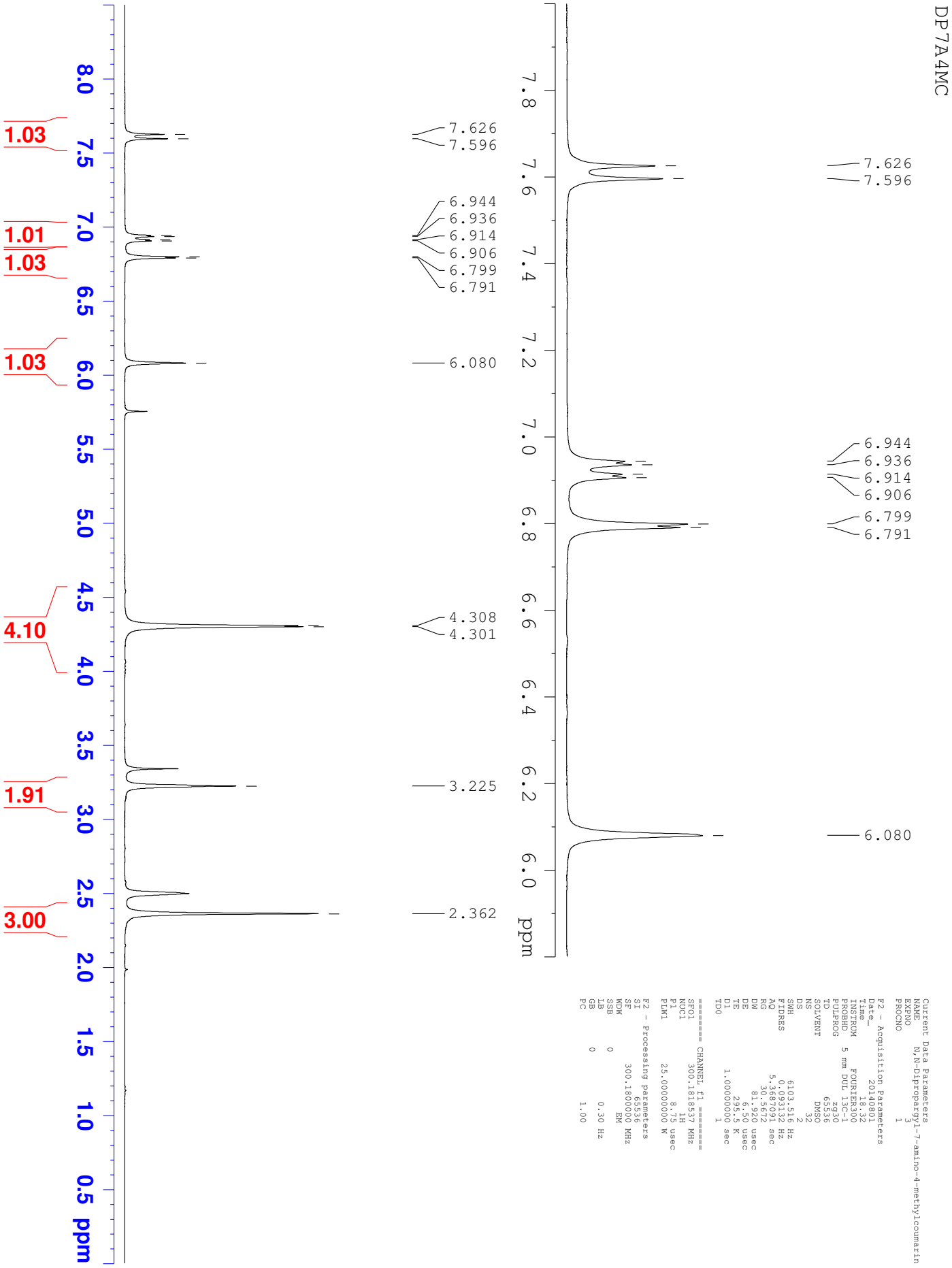

```
Current Data Parameters
NAME                  78F4TFC
EXPNO                       9
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140607
Time                 18.01
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                   35000
DS                       4
SWH              24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  296.2 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001600 sec
D40              0.02432300 sec
L4                       34
L5                       49
P32                 105.00 usec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                   13C
P1                  16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2               105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                    32768
SF              75.4803210 MHz
WDW                      EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```


P7A4MC
7.495
7.466
7.009
6.990
6.971
6.678
6.671
6.649
6.642
6.502
6.495
5.969
3.994
3.986
3.974
3.967
3.166
3.159
3.152
2.319
1.09
1.08
1.03
1.03
1.03
2.00
1.01
3.09
ppm
Current Data Parameters
NAME N-Propargyl-7-amino-4-methylcoumarin
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140802
Time 10.50
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 38.7634
DW 81.920 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

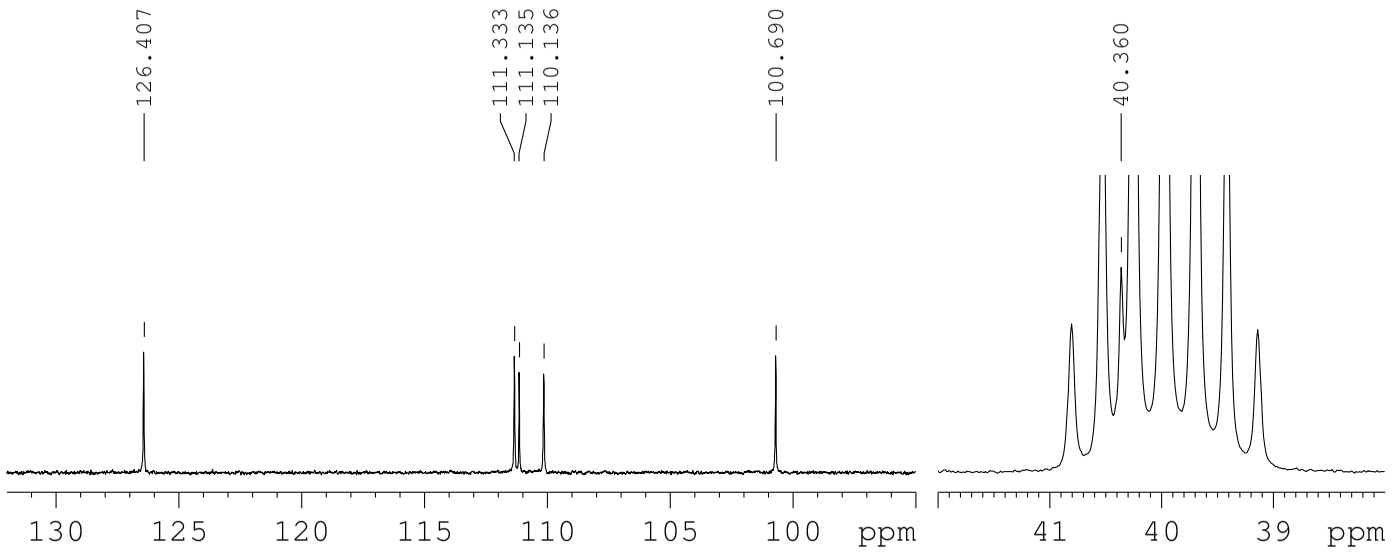
P7A4MC




```
Current Data Parameters
NAME      N-Propargyl-7-amino-4-r
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_               20140802
Time                   11.00
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                  65536
SOLVENT               DMSO
NS                    10592
DS                        4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   295.2 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001600 sec
D40             0.02432300 sec
L4                        34
L5                        49
P32                  105.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                   13C
P1                   16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2                105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                    32768
SF              75.4803210 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


DP7A4MC
7.626
7.596
6.944
6.936
6.914
6.906
6.799
6.791
6.080
4.308
4.301
3.225
2.362
1.03
1.01
1.03
1.03
4.10
1.91
3.00
ppm
Current Data Parameters
NAME N,N-Dipropargyl-7-amino-4-methylcoumarin
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140801
Time 18.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 30.5672
DW 81.920 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

DP7A4MC




```
Current Data Parameters
NAME      N,N-Dipropargyl-7-amino
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140801
Time              18.41
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG           zgpg30
TD                65536
SOLVENT             DMSO
NS                12000
DS                    4
SWH           24414.063 Hz
FIDRES         0.372529 Hz
AQ            1.3421773 sec
RG              501.187
DW               20.480 usec
DE                6.50 usec
TE               295.7 K
D1           2.00000000 sec
D11          0.03000000 sec
D31          0.00001600 sec
D40          0.02432300 sec
L4                   34
L5                   49
P32              105.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4878687 MHz
NUC1               13C
P1               16.00 usec
PLW1        60.00000000 W

======== CHANNEL f2 ========
SFO2        300.1812007 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             105.00 usec
PLW2        10.00000000 W
PLW12        0.36280999 W
PLW13        0.40000001 W

F2 - Processing parameters
SI                32768
SF           75.4803210 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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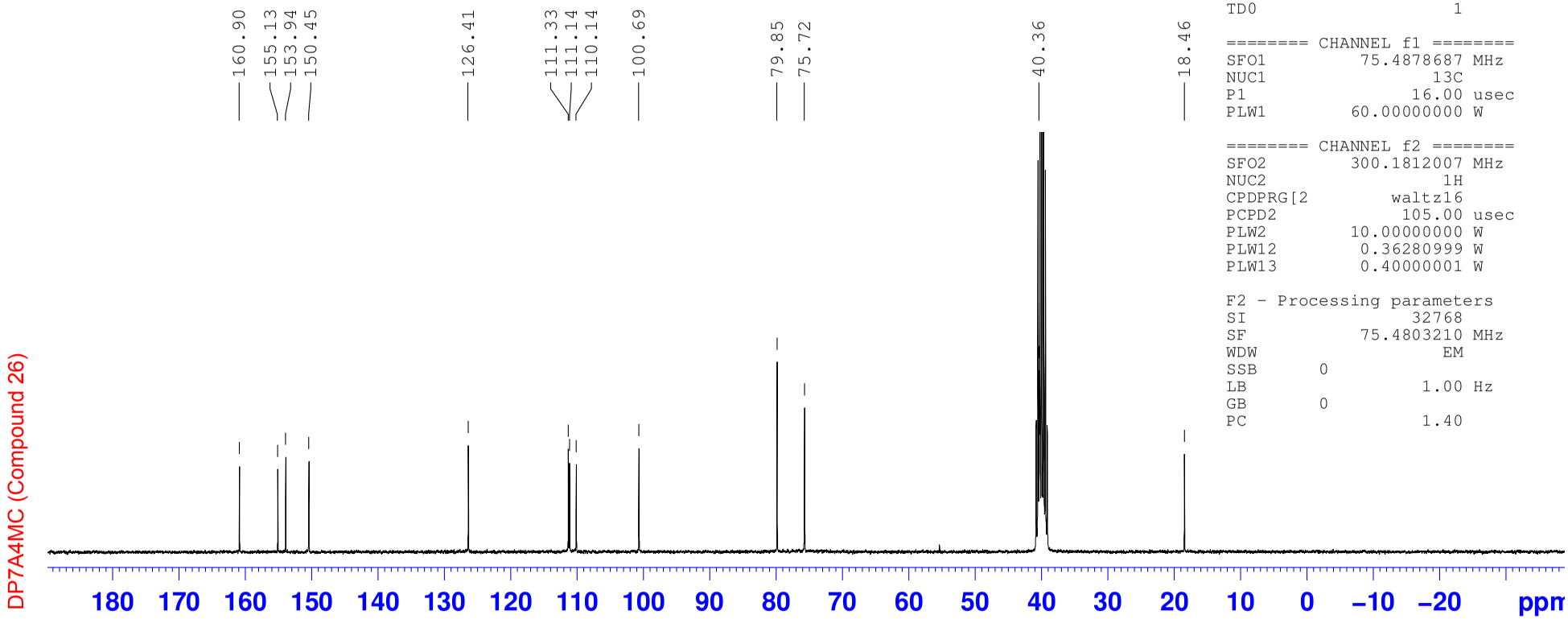
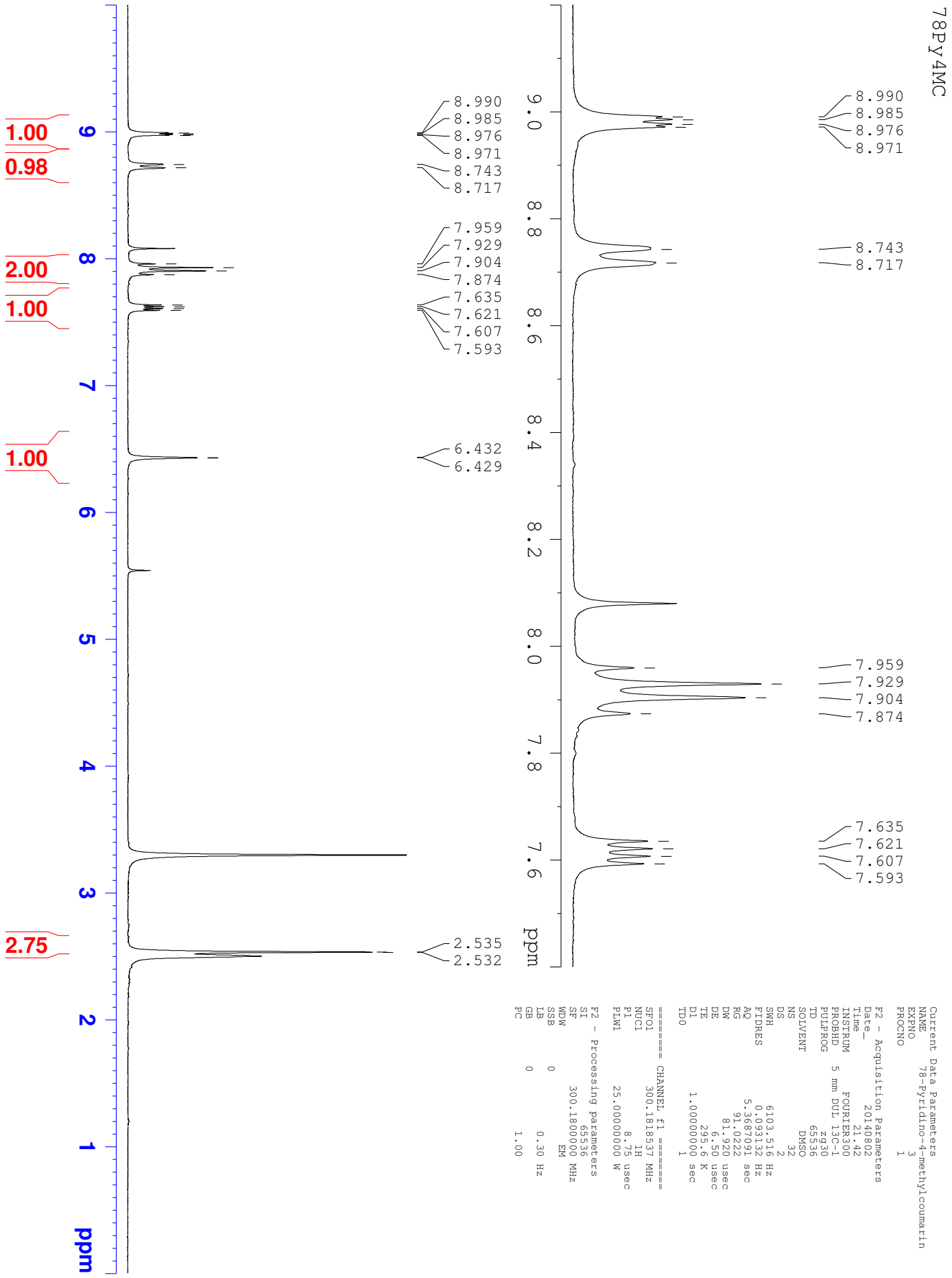
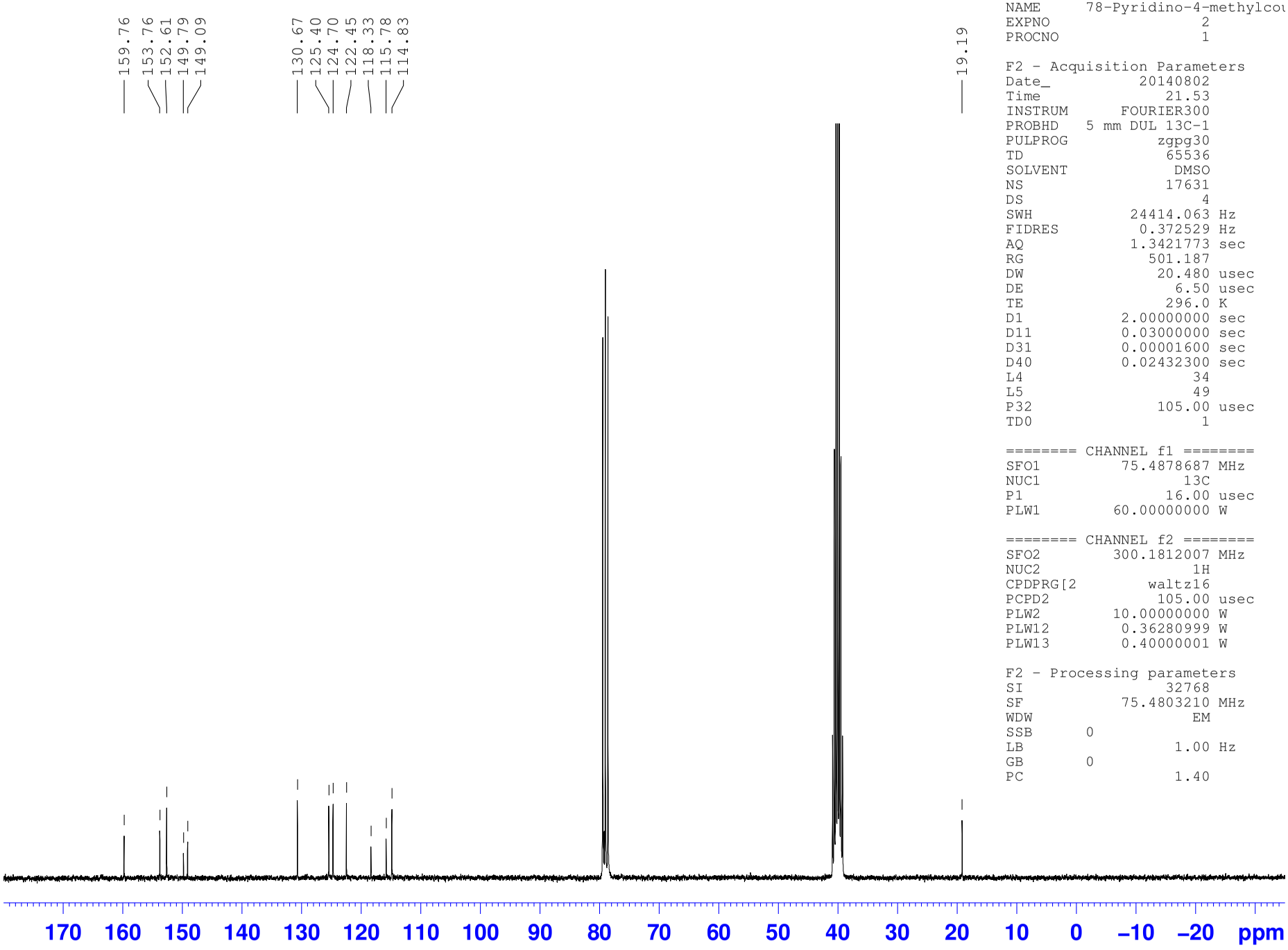



78Py4MC
8.990
8.985
8.976
8.971
8.743
8.717
7.959
7.929
7.904
7.874
7.635
7.621
7.607
7.593
6.432
6.429
2.535
2.532
1.00
0.98
2.00
1.00
1.00
2.75
ppm
Current Data Parameters
NAME 78-Pyridino-4-methylcoumarin
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140802
Time 21.42
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 91.0222
DW 81.920 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

78Py4MC

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Current Data Parameters
NAME      78-Pyridino-4-methylcou
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20140802
Time                 21.53
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                   17631
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  296.0 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001600 sec
D40             0.02432300 sec
L4                       34
L5                       49
P32                 105.00 usec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                   13C
P1                  16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2               105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                   32768
SF              75.4803210 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
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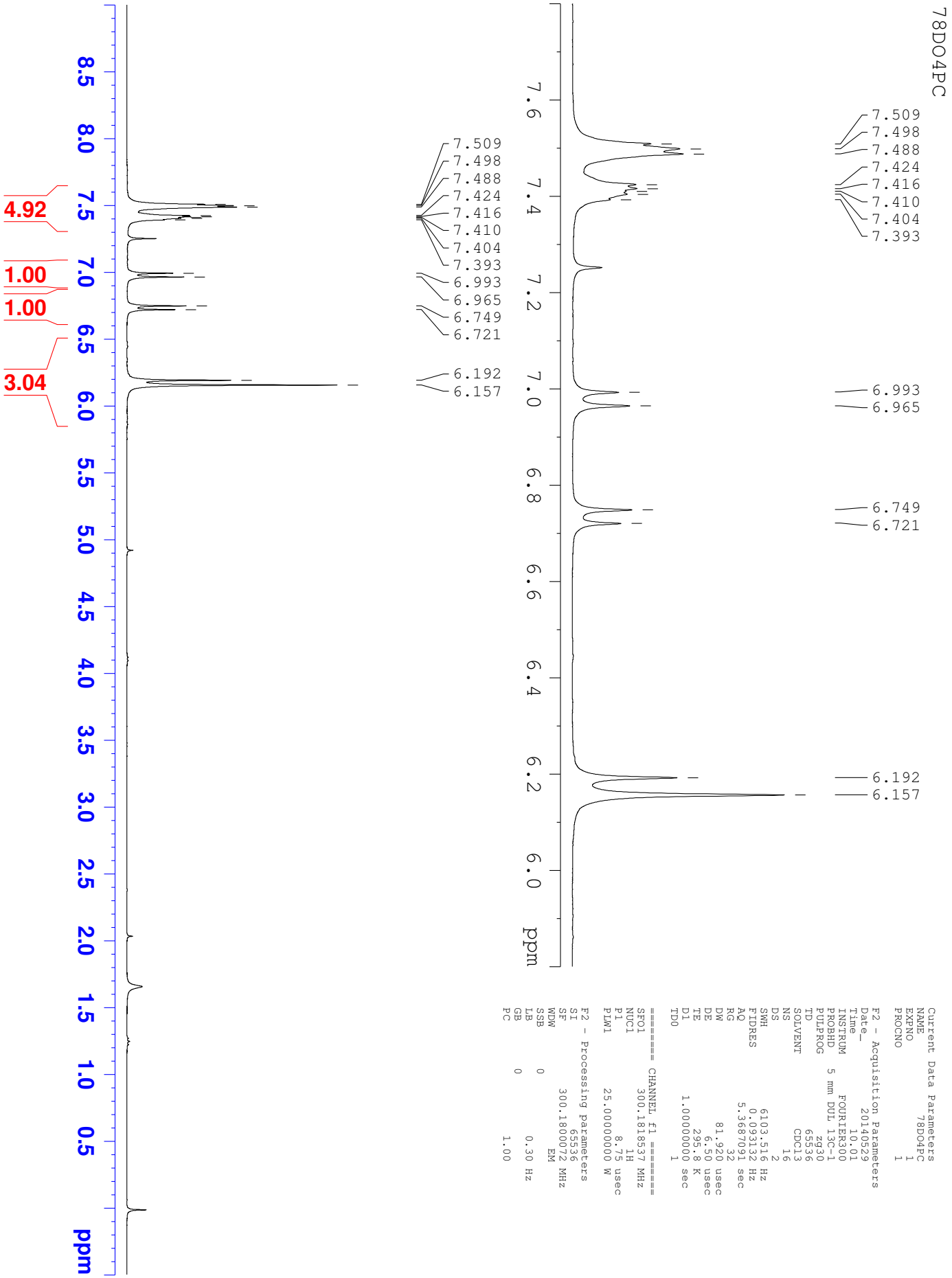
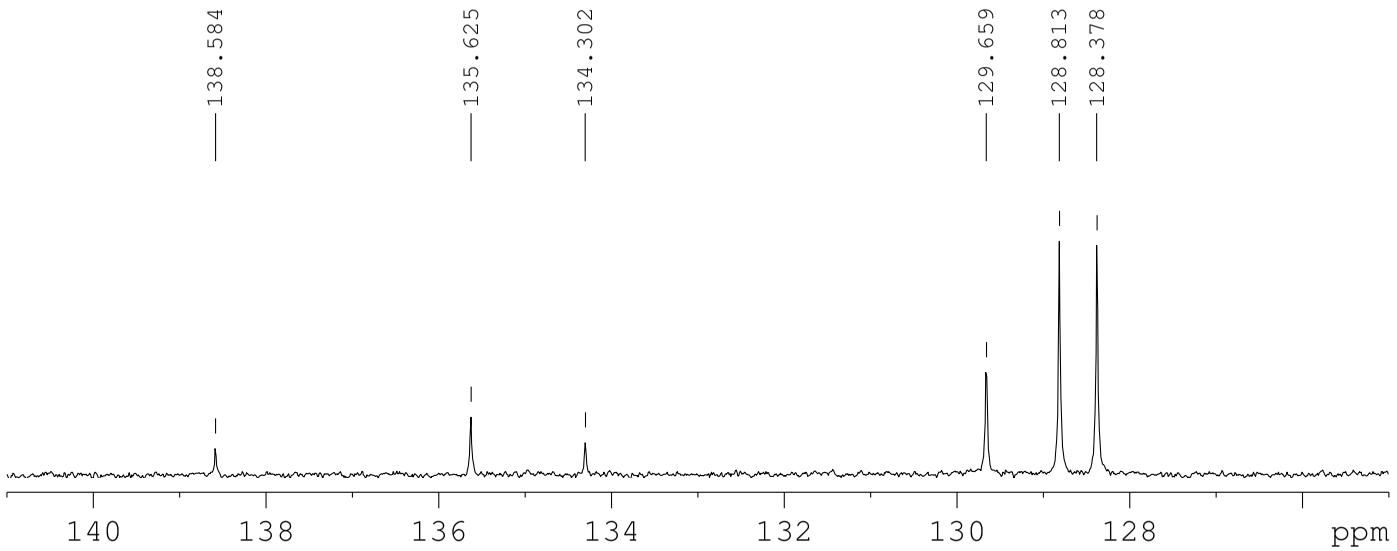
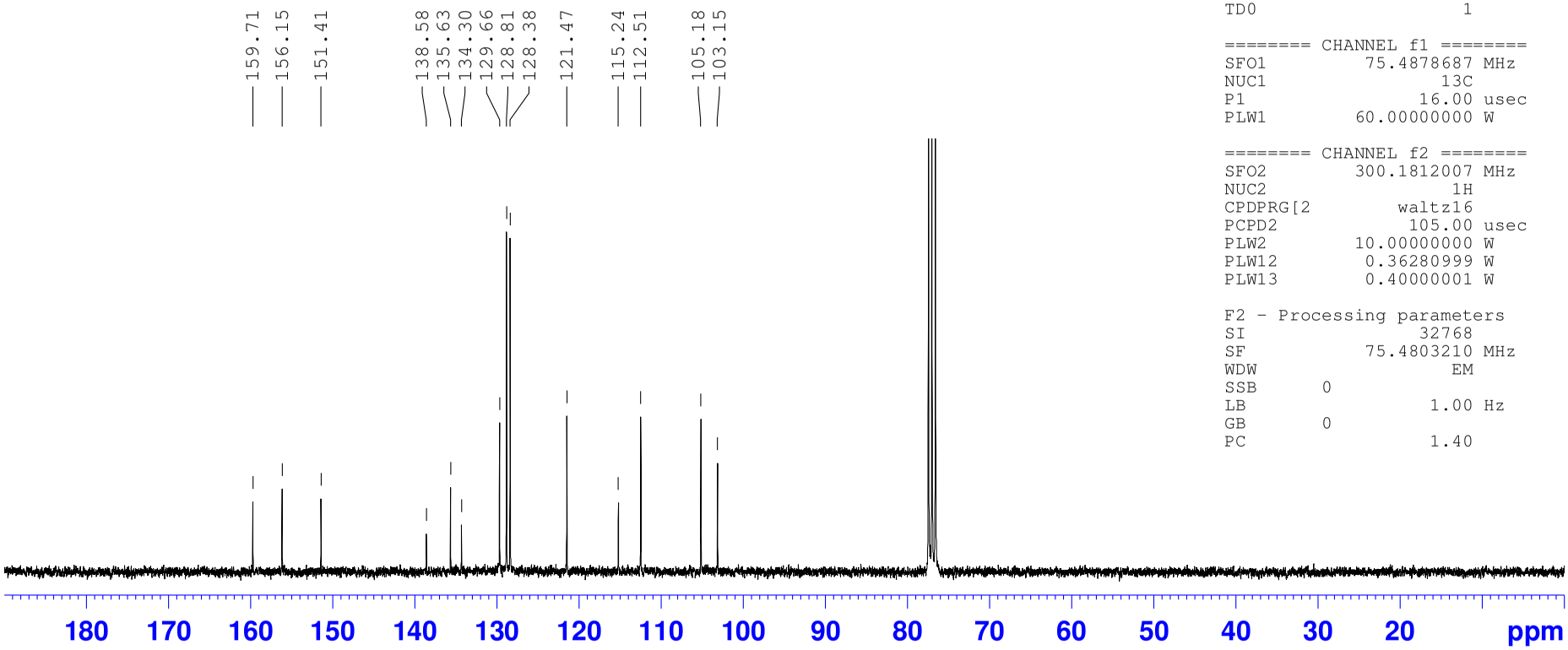
4P78DOC (Compound 28)



78DO4PC



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Current Data Parameters
NAME                 78DO4PC
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140529
Time                 10.09
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2000
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   296.1 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001600 sec
D40              0.02432300 sec
L4                        34
L5                        49
P32                  105.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4878687 MHz
NUC1                    13C
P1                   16.00 usec
PLW1           60.00000000 W

======== CHANNEL f2 ========
SFO2           300.1812007 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                105.00 usec
PLW2           10.00000000 W
PLW12           0.36280999 W
PLW13           0.40000001 W

F2 - Processing parameters
SI                      32768
SF              75.4803210 MHz
WDW                        EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```

Atlantic Microlab, Inc.

Sample No. 78FF

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Company/School Xavier University of Louisiana
Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 08/19/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	78.25	78.05	77.95
H	4.38	4.48	4.41

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
Include Email Address or FAX # Below
mforooze@xula.edu

Date Received AUG 25 P.M. Date Completed AUG 26 2014
Remarks:

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Sample No. 5H78FF

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Name Jiawang Liu Date 08/19/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	73.97	73.42	73.47
H	4.14	4.14	4.22

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Name Jiawang Liu Date 08/19/2014
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Element	Theory	Found	
C	79.11	77.73	77.82
H	4.06	4.37	4.29
N	5.13	4.98	4.91

Single ☐ Duplicate ☒
Elements Present: C, H, O, N
Analyze for: C, H, N
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Remarks:

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Name Jiawang Liu Date 08/19/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	72.18	71.92	71.97
H	3.79	3.87	3.85

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Name Jiawang Liu Date 08/19/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	78.25	78.23	78.11
H	4.38	4.48	4.43

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Sample No. 3M4P78PC

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Name Jiawang Liu Date 08/19/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	78.61	77.07	77.12
H	4.86	5.03	5.08

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Name Jiawang Liu Date 08/19/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	72.89	72.61	72.62
H	4.71	4.74	4.67

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Date Received AUG 25 P.M.
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Date Completed AUG 26 2014

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Name Jiawang Liu Date 08/19/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	58.22	57.99	57.96
H	2.63	2.47	2.46
F	21.25	21.12	21.12

Single ☐ Duplicate ☒
Elements Present: C, H, O, F
Analyze for: C, H, F
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Address 1 Drexel Dr
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Name Jiawang Liu Date 08/28/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	78.25	77.76	77.64
H	4.38	4.49	4.54

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 08/28/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	78.61	78.24	78.31
H	4.86	5.14	5.17

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 08/28/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	72.89	72.51	72.63
H	4.71	4.96	5.03

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Remarks:

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Name Jiawang Liu Date 08/28/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	58.22	58.17	58.14
H	2.63	2.51	2.64
F	21.25	21.48	21.42

Single ☐ Duplicate ☒
Elements Present: C, H, O, F
Analyze for: C, H, F
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 08/28/2014
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	73.92	71.44	71.58
H	4.29	4.44	4.50
N	6.63	6.31	6.23

Single ☐ Duplicate ☒
Elements Present: C, H, O, N
Analyze for: C, H, N
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
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Date Received SEP 22 P.M. Date Completed SEP 23 2014
Remarks:

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Sample No. 4P78DOC

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Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 08/28/2014
Phone (504) 638-4036

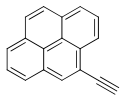
Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0050279

Element	Theory	Found	
C	72.18	72.11	71.97
H	3.79	4.01	3.91

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
Include Email Address or FAX # Below
mforooze@xula.edu

Date Received SEP 22 P.M. Date Completed SEP 23 2014
Remarks:

Structures of P450 1A2 Inhibitors Used for Alignment Study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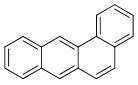
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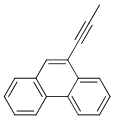
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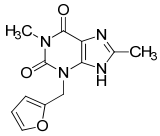
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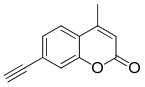
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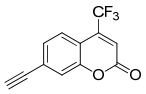
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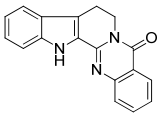
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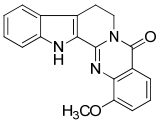
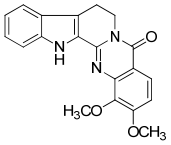
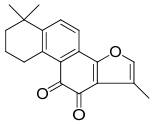
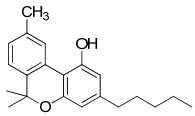
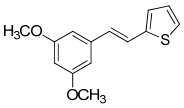

Rutaecarpine derivative 5


Rutaecarpine derivative 8


Tanshinone IIA


CBN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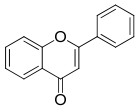
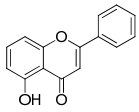
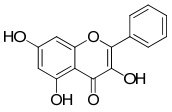
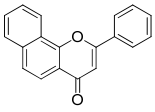
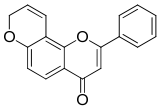
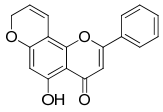

Flavone


5-Hydroxyflavone (5HF)


3,5,7-Trihydroxyflavone


a-Naphthoflavone


7,8-Pyranoflavone


5-Hydroxy-7,8-pyranoflavone

Alamar Blue Cell Viability Assay

HepG2 cells were plated onto 96-well plates in 100 µL/well at 1.2×10^5 cell/mL in DMEM with 10% FBS, and grew until they reached confluency for 72 h. The media was replaced with 100 µL of serum-free media for another 24 h. After that, 10 µL of Alamar Blue Dye (Invitrogen, cat#DAL1180) were added to each well of 96-well plates and incubated for 2 h at 37 ℃ in CO_2-incubator, and fluorescence 560Ex/590Em base reading was taken using Synergy H1 multiplate deader (BioTeck). Then, the media was removed, and 1 µL of the compound solution in DMSO were added to 100 µL of free serum-free media for each well. After 72 h, another Alamar Blue Dye florescence reading was taken. If the ratio of the second reading to the base reading for untreated cells was equal to 1 (within 10% error), the assay was considered valid, and calculations to normalize the toxicity of compounds were made. Figure S1 shows twice independent cell viability assay data. The results indicate that up to 10^{-5} M compound 4TF78PC is not toxic to HepG2 cells.