

Supporting Information I

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

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7,8-furanoflavone

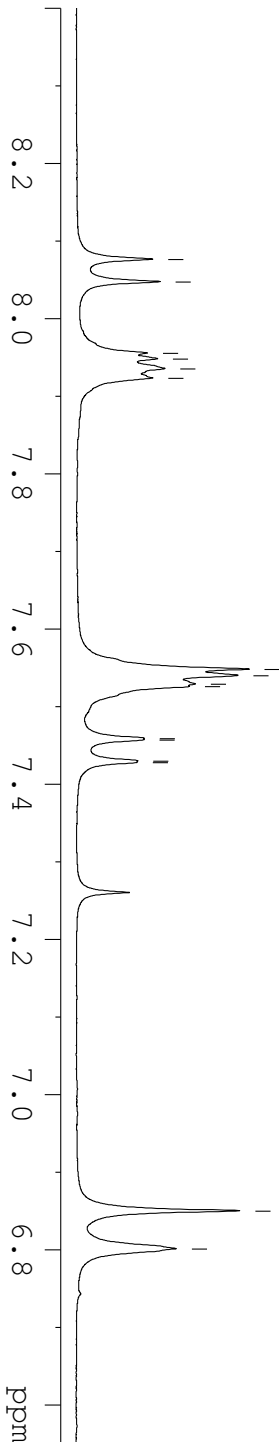
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7.923

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7.529
7.526
7.459
7.457
7.430
7.428

6.850
6.801

8.076
8.047
7.955
7.948
7.935
7.923
7.548
7.540
7.529
7.526
7.459
7.457
7.430
7.428
6.850
6.801

2.539
2.537



1.010

2.051

4.034

2.006

3.000

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
ppm

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

F2 - Acquisition Parameters

Date_ 20130320
Time 10.53
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 51.8481
DW 81.920 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 300.1818537 MHz
NUC1 1H
P1 8.75 usec
PLW1 25.00000000 W

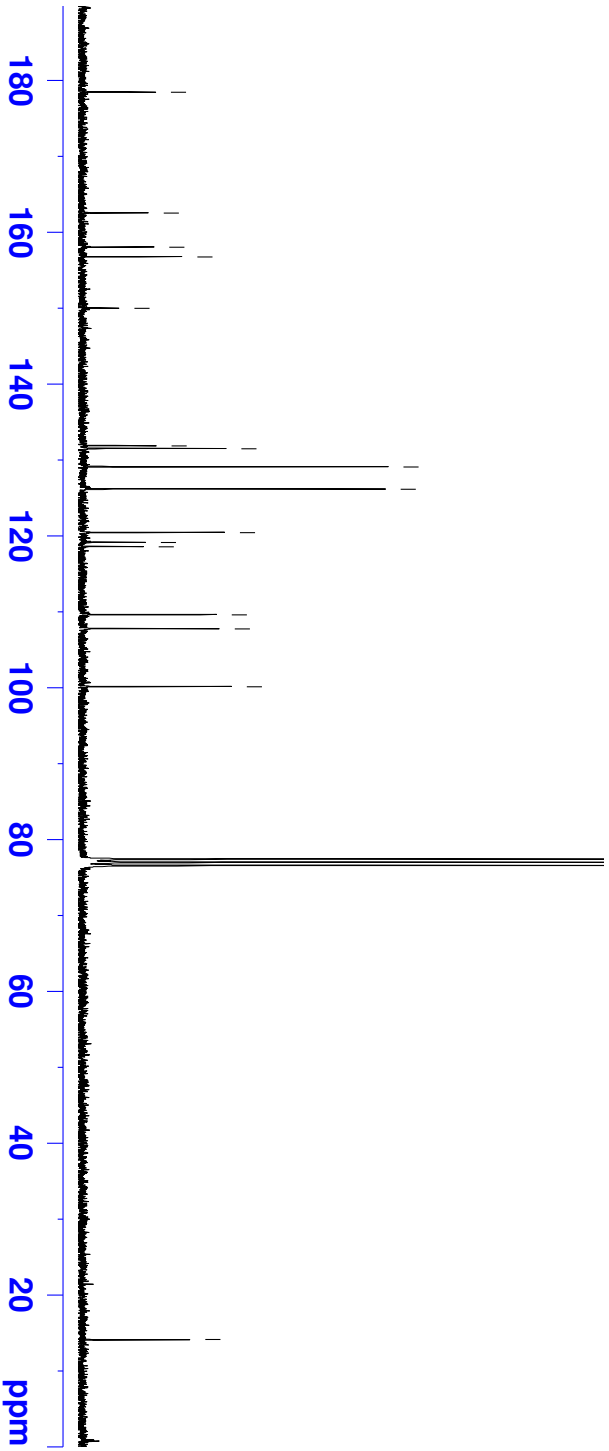
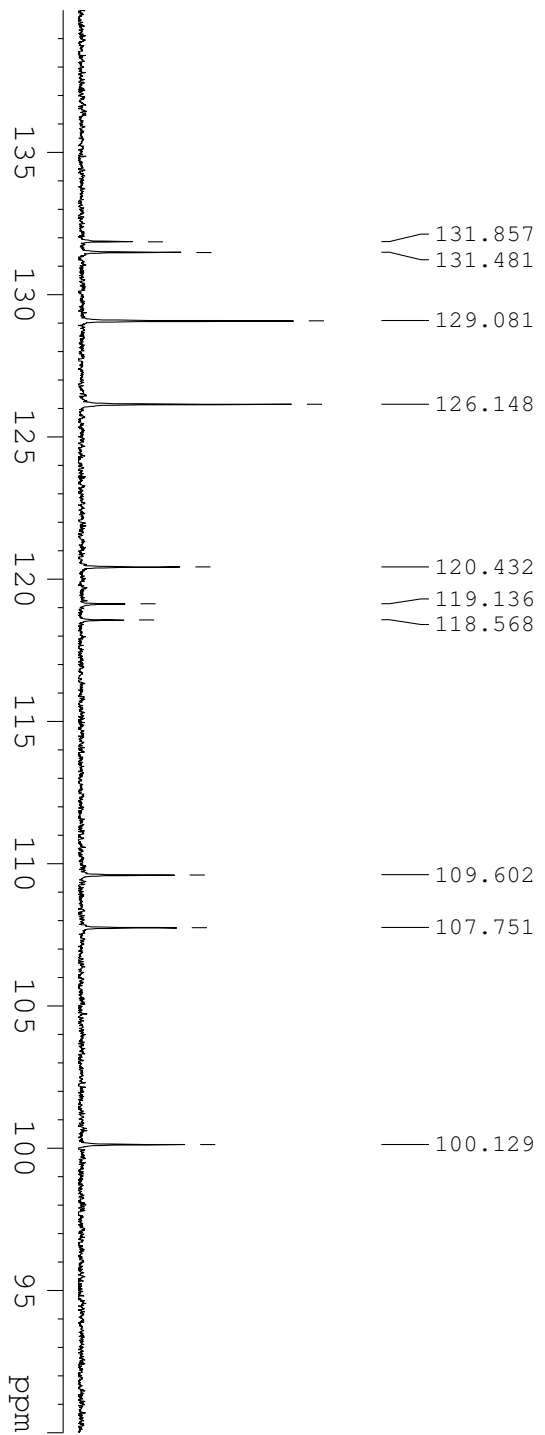
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7,8-Furanoflavone

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

F2 - Acquisition Parameters

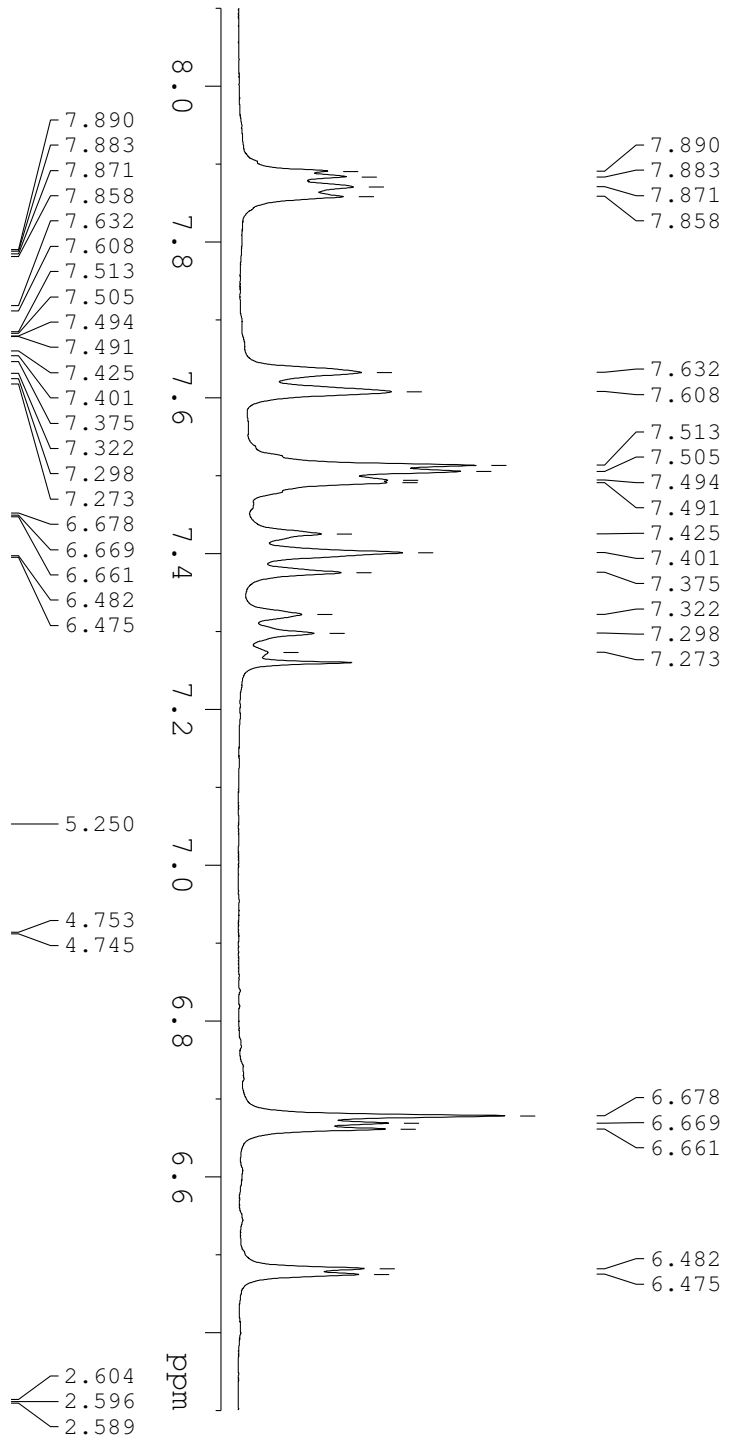
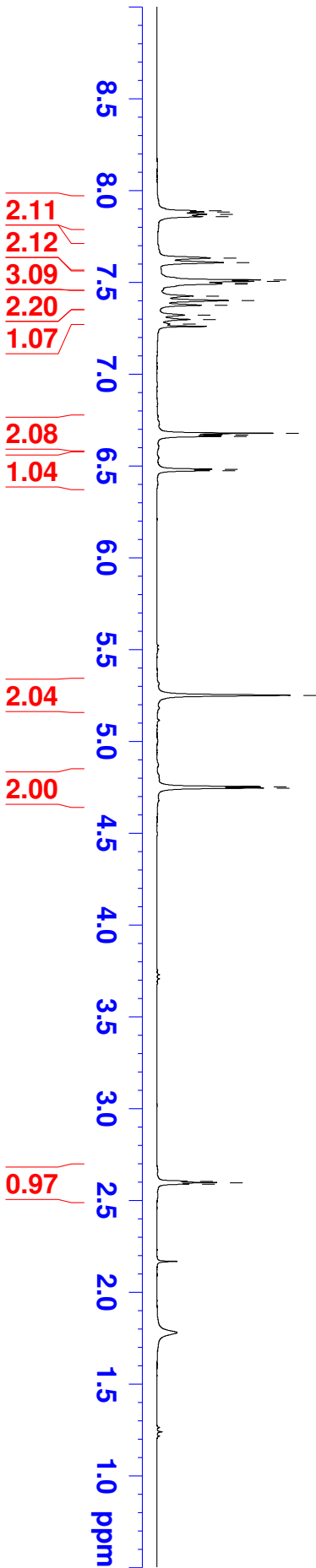


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 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 25.00000000 W
 PLW12 0.21336000 W
 PLW13 0.23522000 W

F2 - Processing parameters
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 SF 75.4803210 MHz
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5B7PF (Compound 6)

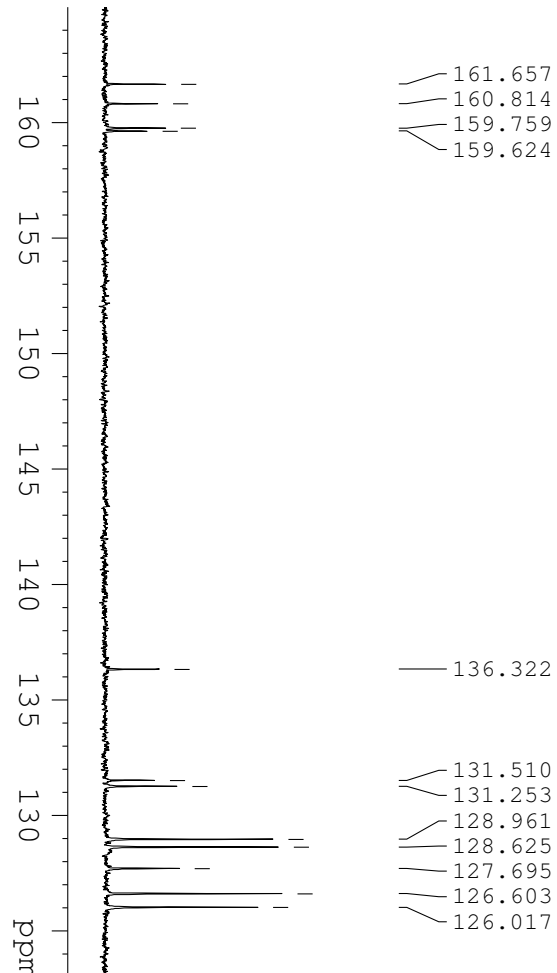
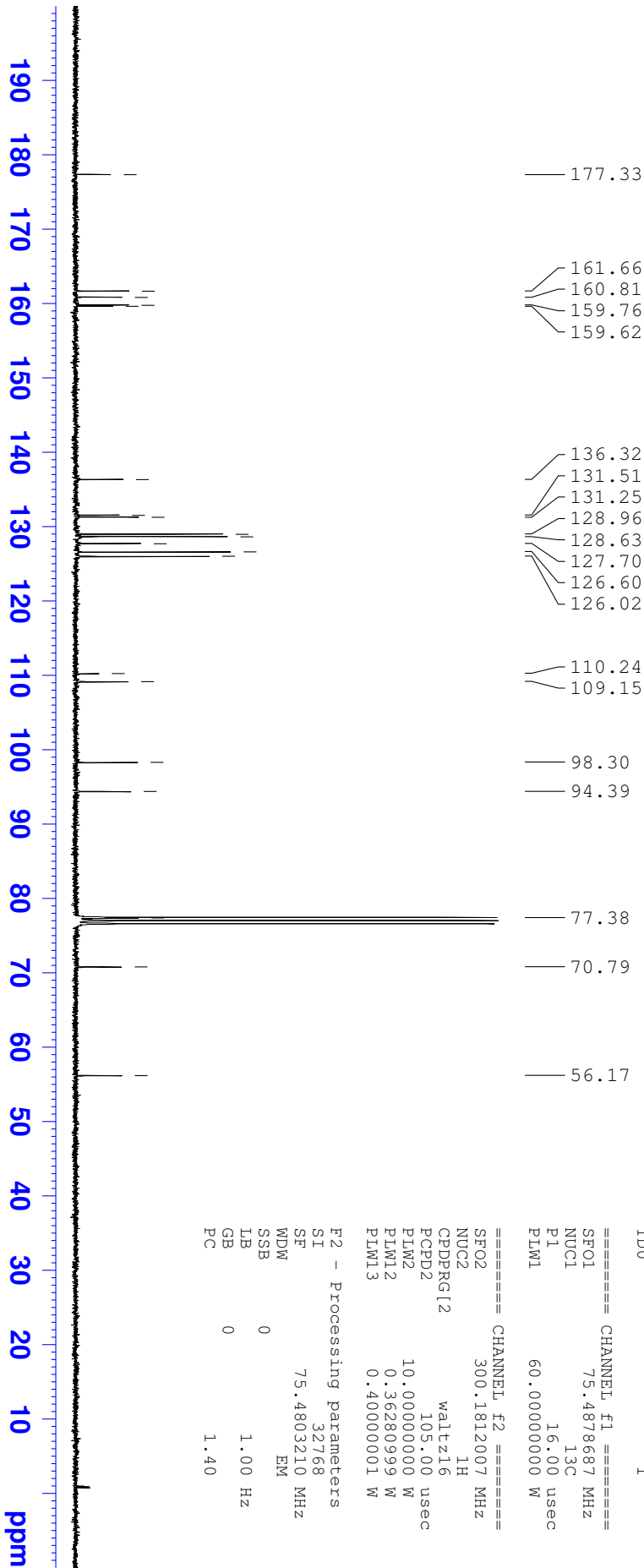


Current Data Parameters
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 PROCNO 1
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 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 44.5217
 DW 81.920 usec
 DE 6.50 usec
 TE 296.7 K
 D1 1.00000000 sec
 TDO 1
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 SFOL 300.1818537 MHz
 NUCL1 1H
 P1 8.75 usec
 PLWL 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

5B7PF

5B7PF (Compound 6)

5B7PF



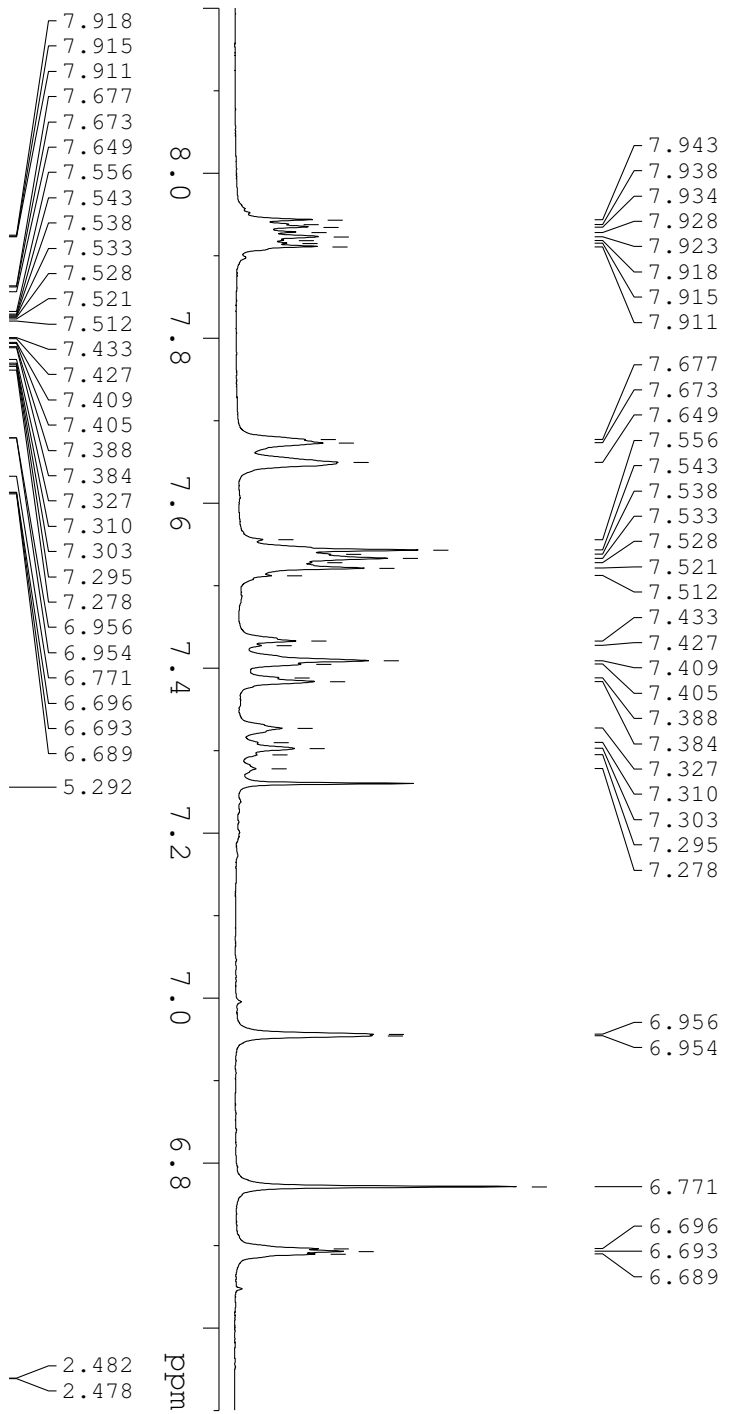
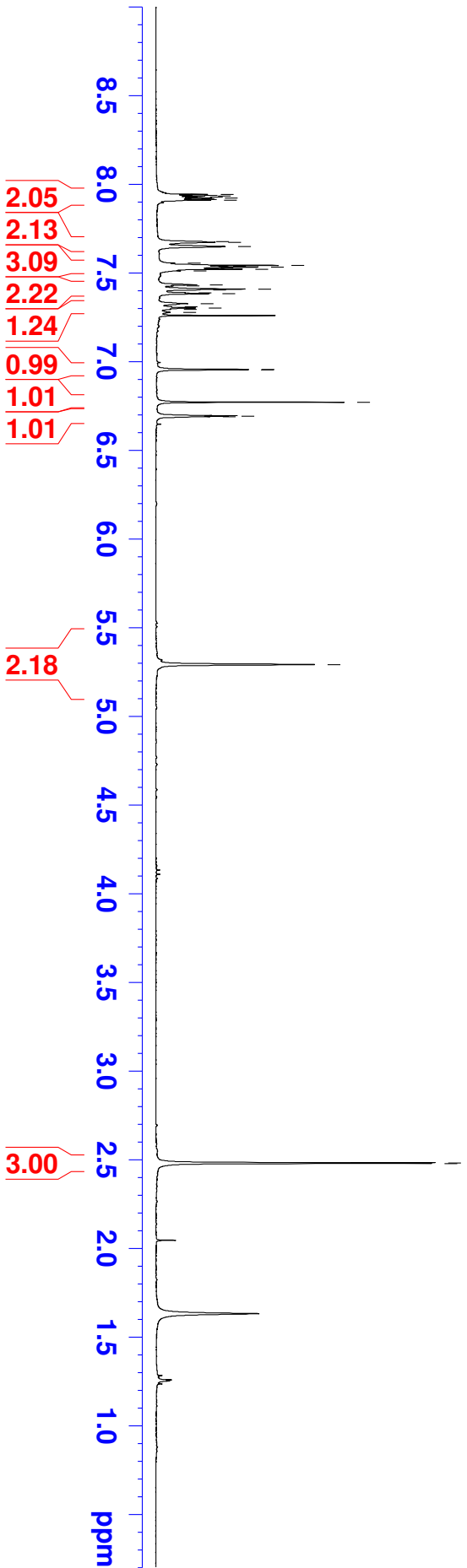
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130426
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 INSTRUM FOURIER300
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 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
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.400000001 W

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

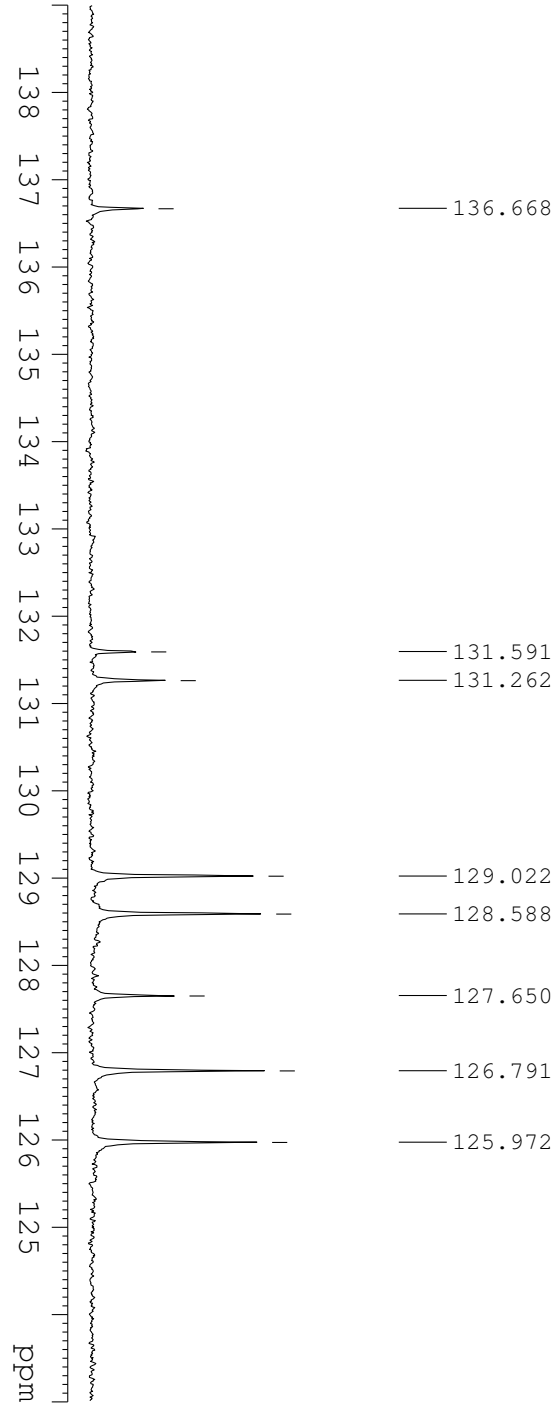
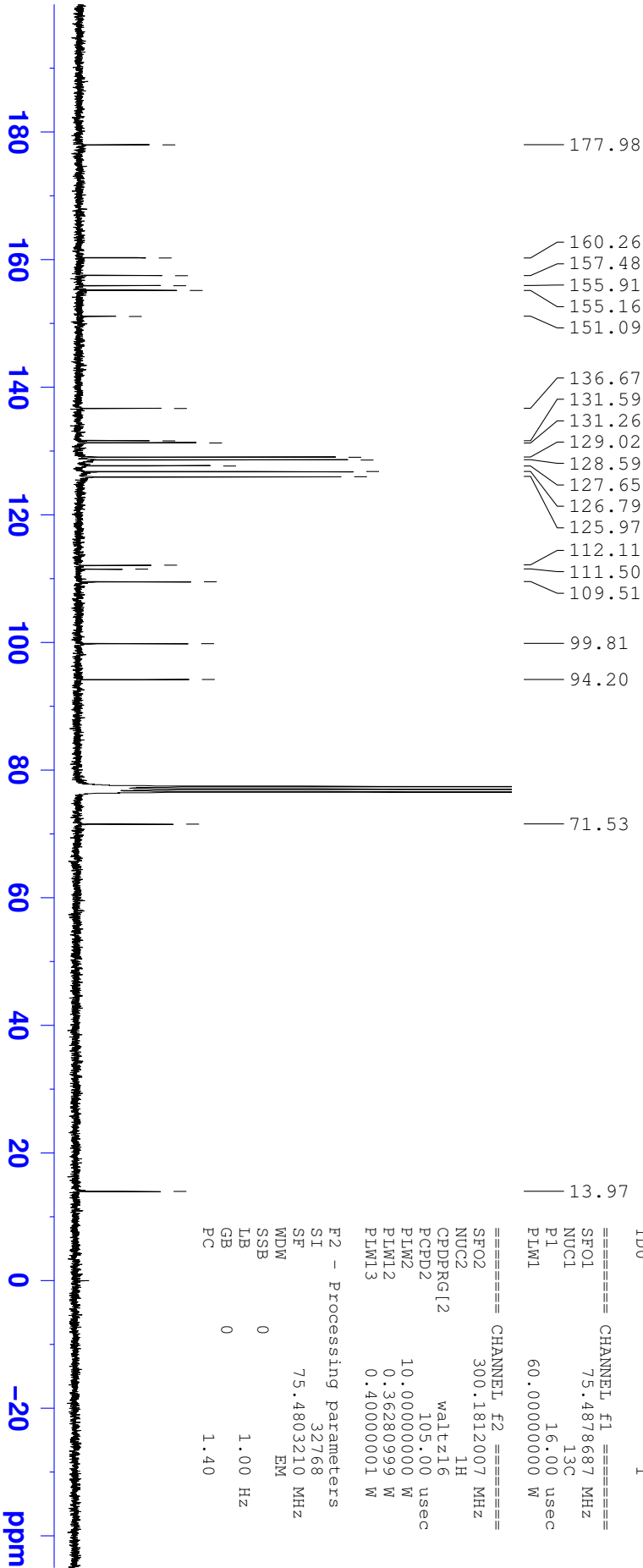


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 PROCNO 1

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 INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SMH 6103.516 Hz
 FIDRES 0.093132 Hz
 AO 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
 NUCL1 1H
 P1 8.75 usec
 PLWL 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



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

F2 - Acquisition Parameters
 Date_ 20130710
 Time 18.29
 INSTRUM FOURIER300
 PROBD 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 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.400000001 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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7.914
7.906

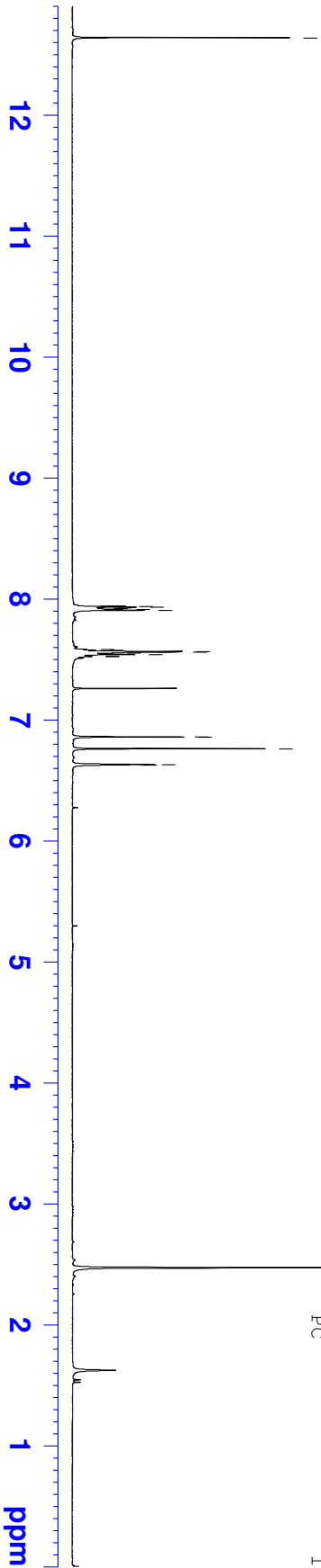
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6.762
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6.628

12.637
7.938
7.933
7.926
7.923
7.920
7.914
7.906
7.583
7.577
7.565
7.561
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6.628
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ppm



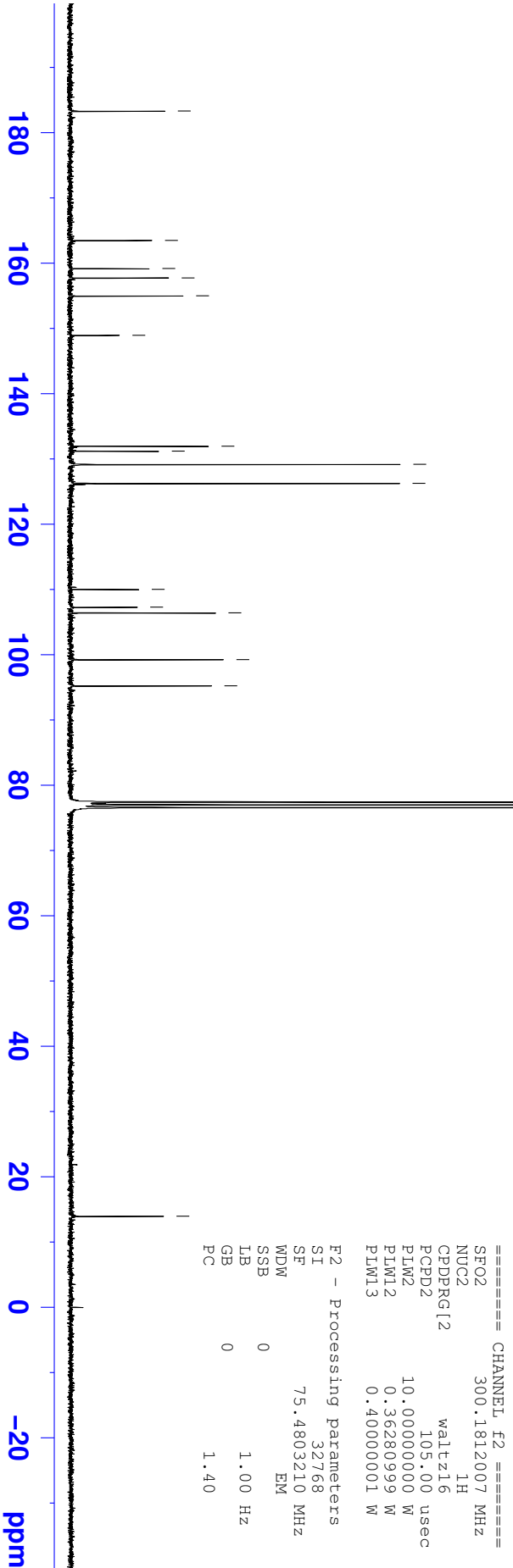
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

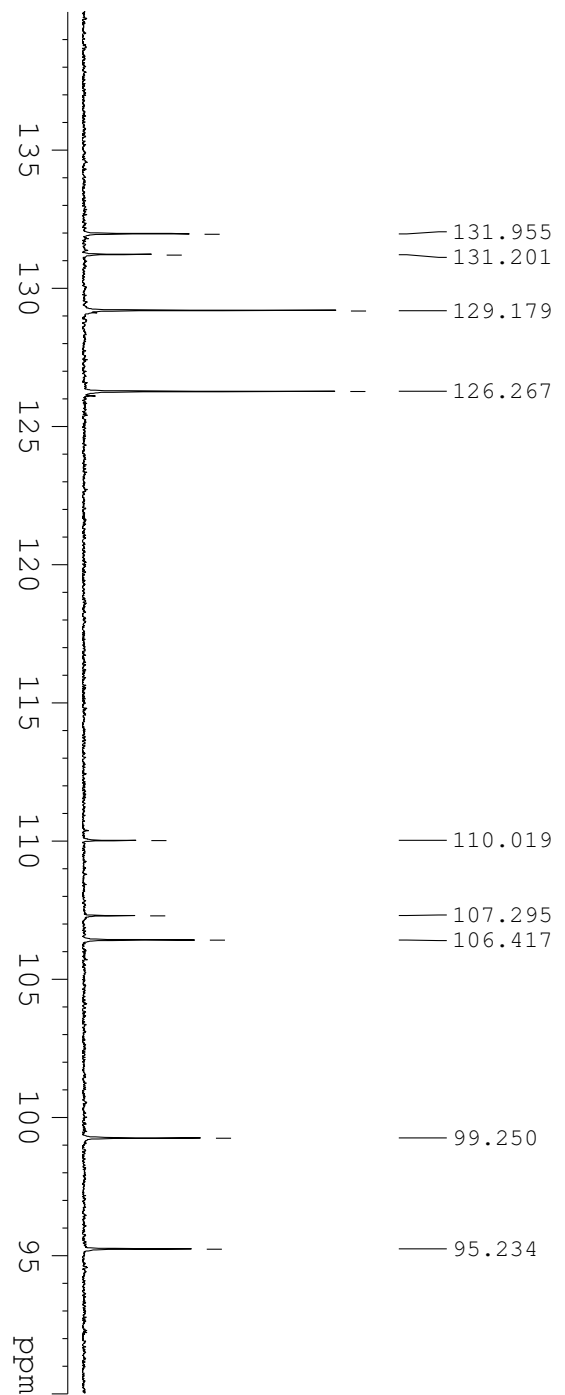
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Time 17.18
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 92.391
DW 81.920 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 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



- 183.32
- 163.49
- 159.19
- 157.74
- 155.00
- 148.95
- 131.96
- 131.20
- 129.18
- 126.27
- 110.02
- 107.30
- 106.42
- 99.25
- 95.23



- 131.955
- 131.201
- 129.179
- 126.267
- 110.019
- 107.295
- 106.417
- 99.250
- 95.234

Current Data Parameters
 NAME 5H78FF
 EXPNO 2
 PROCNO 1

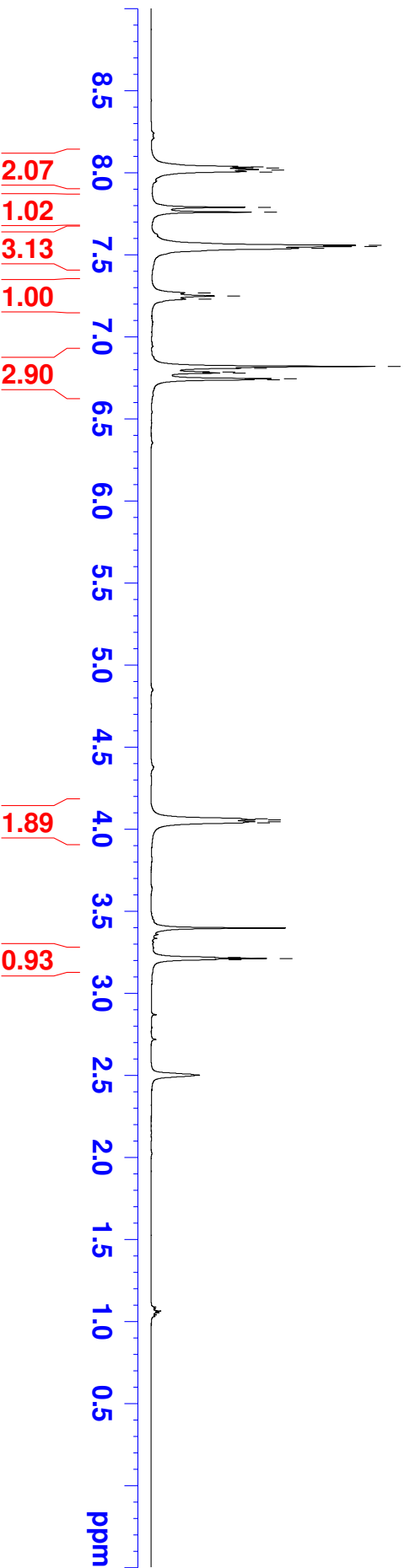
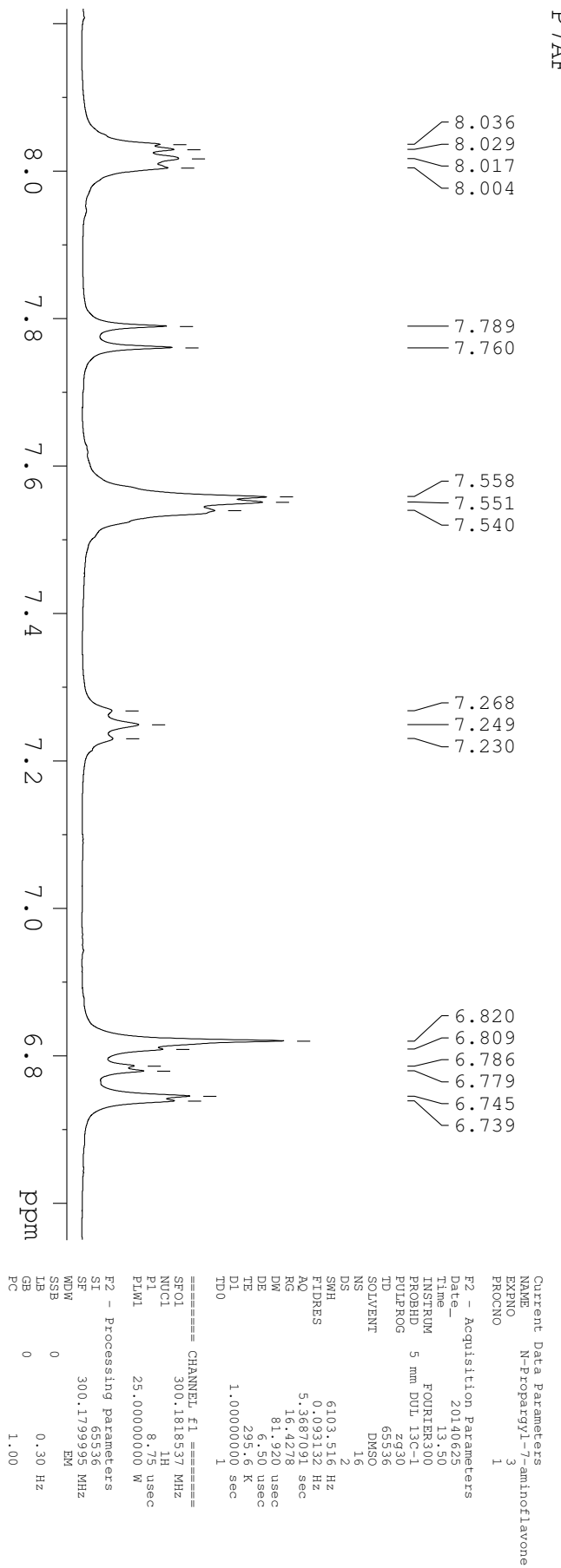
F2 - Acquisition Parameters

Date_ 20130916
 Time 17.26
 INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 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

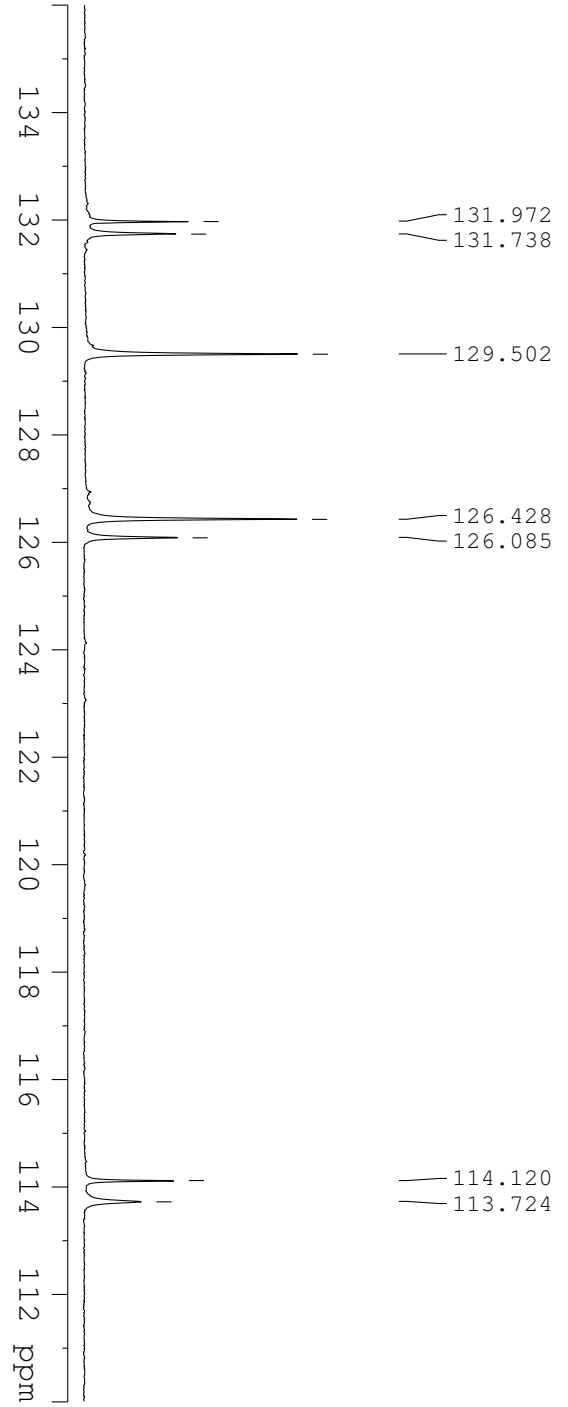
==== CHANNEL F2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.40000001 W

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



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

F2 - Acquisition Parameters



==== CHANNEL F1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.40000001 W

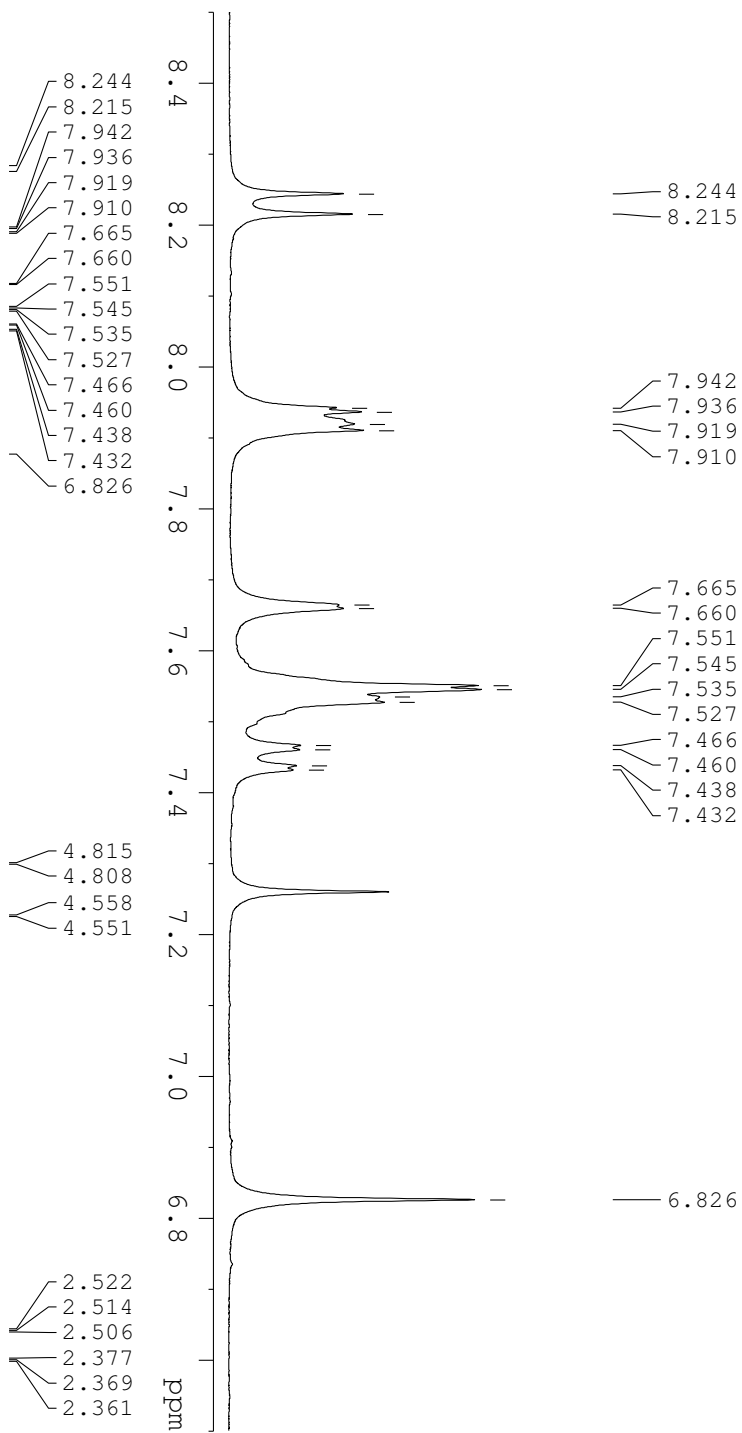
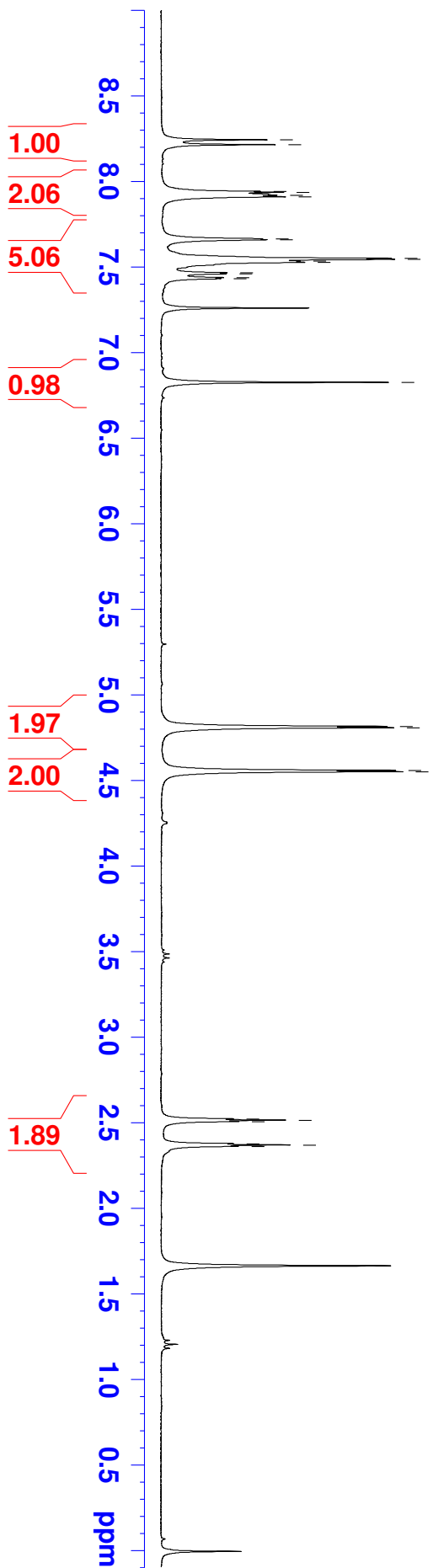
F2 - Processing parameters

SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



DP7AF (Compound 10)

DP7AF



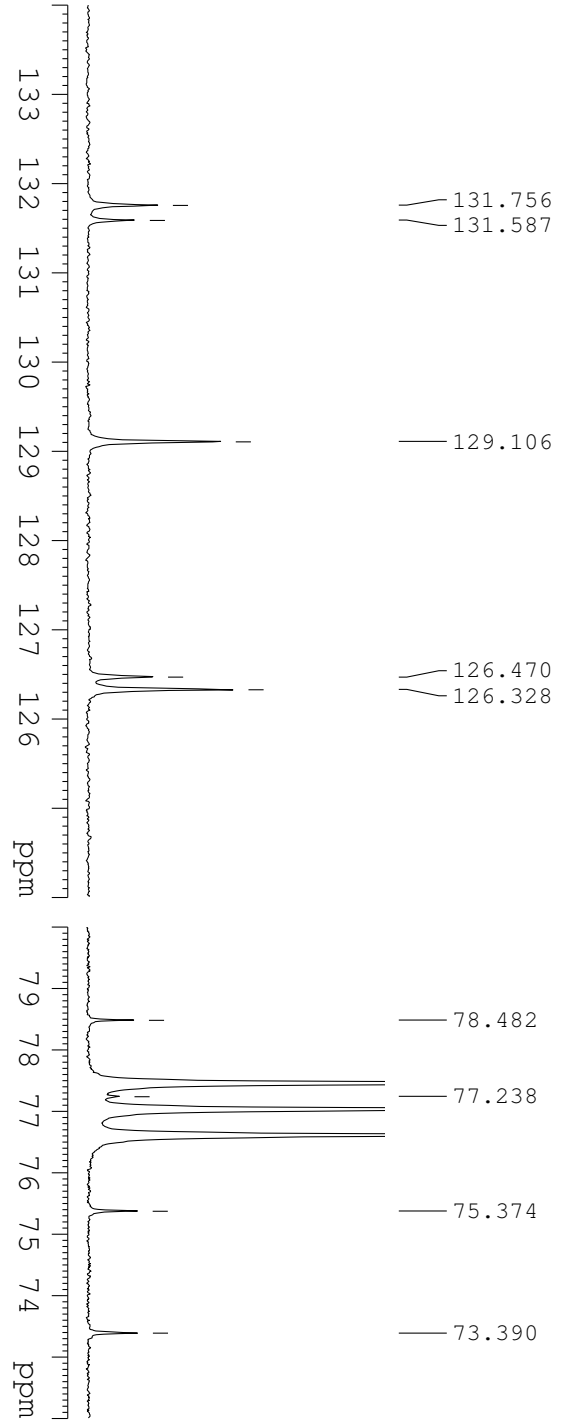
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 NAME N,N-Dipropargyl-7-aminoflavone
 EXPNO 3
 PROCNO 1

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 Time 17.24
 INSTRUM PULPROG
 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 75.8519
 DW 81.920 usec
 DE 6.50 usec
 TE 295.3 K
 D1 1.00000000 sec
 IDU 1

==== CHANNEL f1 =====
 SF01 300.1818537 MHz
 NUC1 13C
 P1 8.15 usec
 F1 25.00000000 W
 FWHM 25.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800049 MHz
 MWDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.00

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



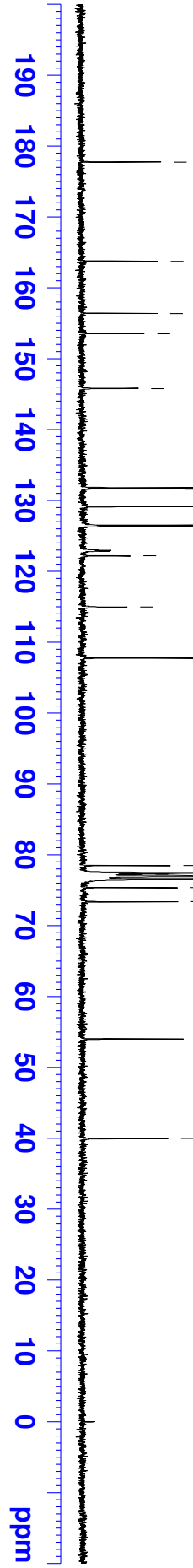
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 Date_ 20140624
 Time 17.31
 INSTRUM FOURIER300
 PROBHID 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 15000
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 295.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001600 sec
 D40 0.02432300 sec
 L4 34
 L5 49
 P32 105.00 usec
 TD0 1

177.73
 163.73
 156.36
 153.52
 145.78
 131.76
 131.59
 129.11
 126.47
 126.33
 122.20
 114.97
 107.78
 78.48
 77.24
 75.37
 73.39
 54.02
 39.99

==== CHANNEL F1 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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

Current Data Parameters
 NAME 78Pyridinoflavone
 EXPNO 1
 PROCNO 1

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

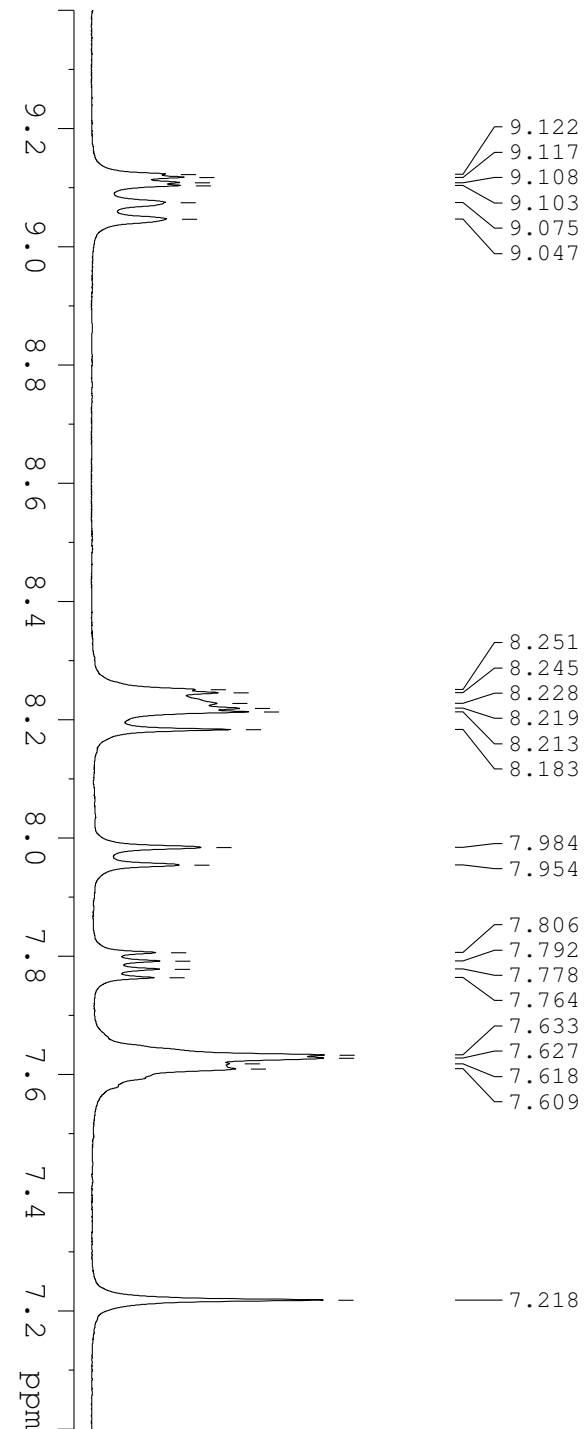
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7.609

7.218

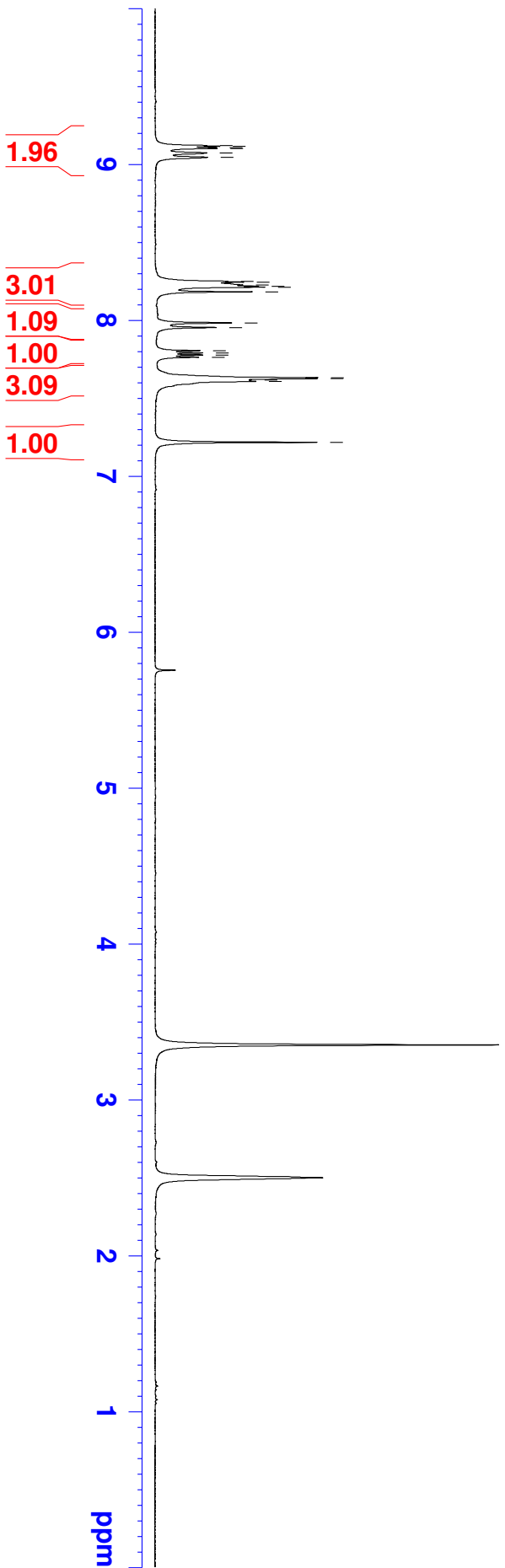


==== CHANNEL f1 =====
 SFOL 300.1818537 MHz
 NUC1 1H
 P1 8.75 usec
 PLWL 25.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.179997 MHz
 MDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.122
9.117
9.108
9.103
9.075
9.047
8.251
8.245
8.228
8.219
8.213
8.183
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7.954
7.806
7.792
7.778
7.764
7.633
7.627
7.618
7.609
7.218

78PyF (Compound 11)



78PyF

Current Data Parameters
 NAME 78Pyridinoflavone
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140627
 Time 18.28

INSTRUM FOURIER300
 PROBD 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

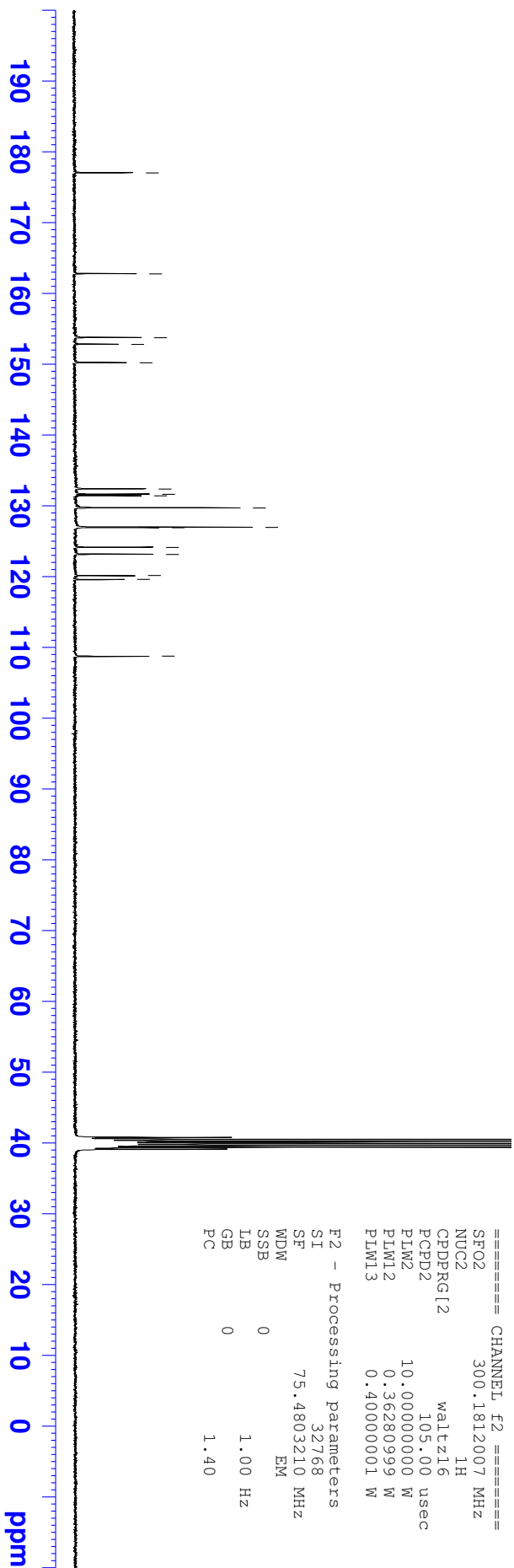
P32 105.00 usec
 TD0 1

==== CHANNEL F1 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.400000001 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)



78DOF

Current Data Parameters
 NAME 78DOF
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140602
 Time_ 10.11
 INSTRUM FOURIER30
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 ID 65336
 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
 NUCL1 1H
 P1 8.75 usec
 PLW1 25.00000000 W

F2 - Processing parameters

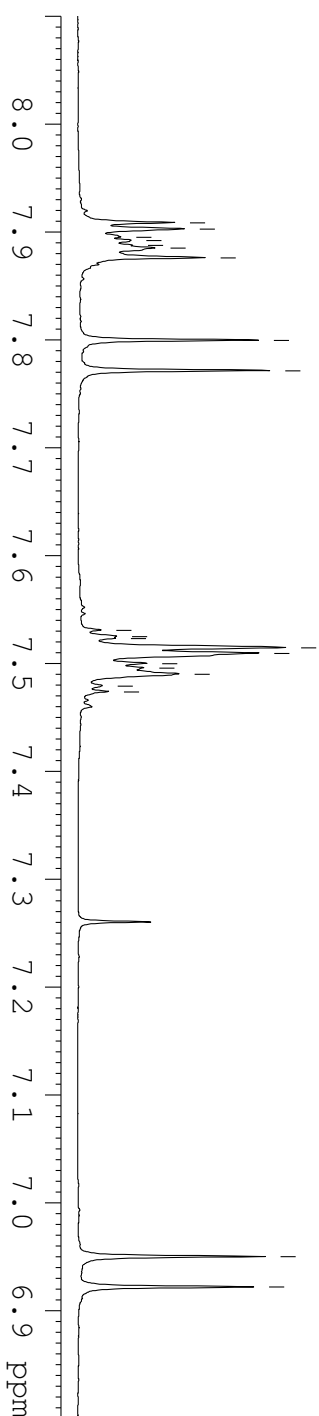
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 SF 300.1800049 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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7.771

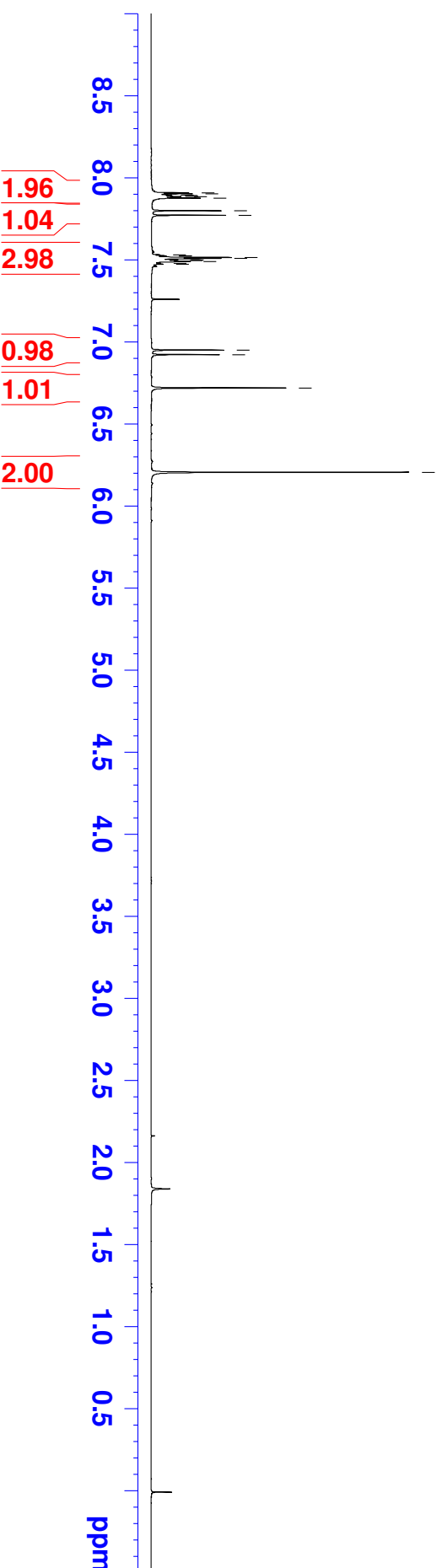
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6.950
6.922

7.903
7.895
7.892
7.888
7.885
7.876
7.800
7.771
7.531
7.525
7.523
7.515
7.509
7.500
7.496
7.490
7.479
7.474
6.950
6.922
6.719
6.205



78DOF (Compound 12)



Current Data Parameters
 NAME 78DOF
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140602
 Time 10.17
 INSTRUM FOURIER300
 PROBHID 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 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 =====

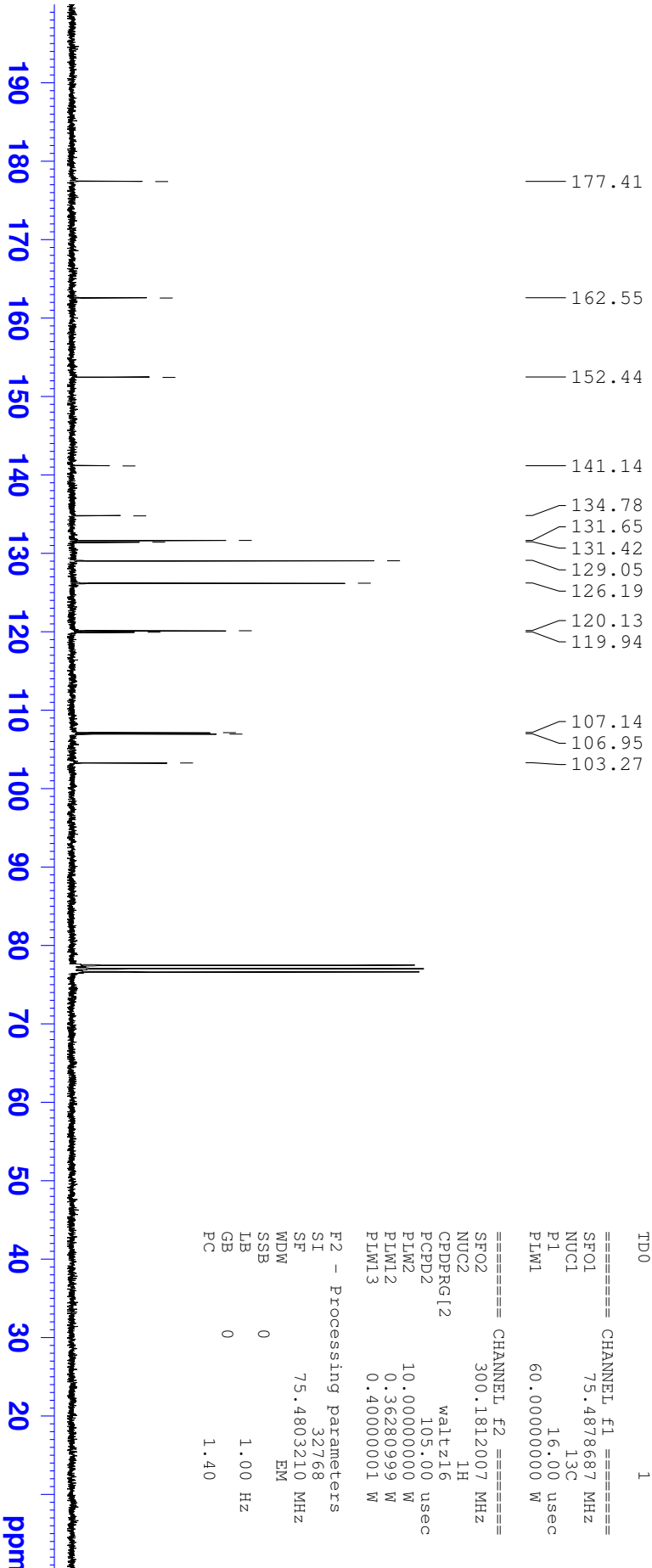
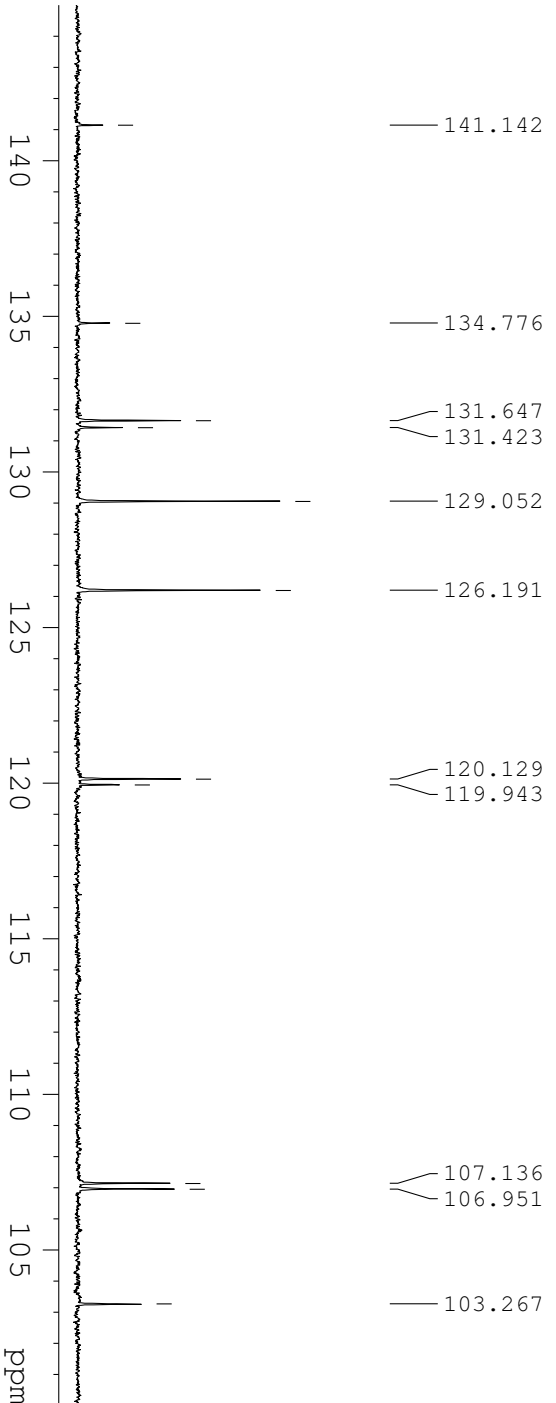
SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====

SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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



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

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

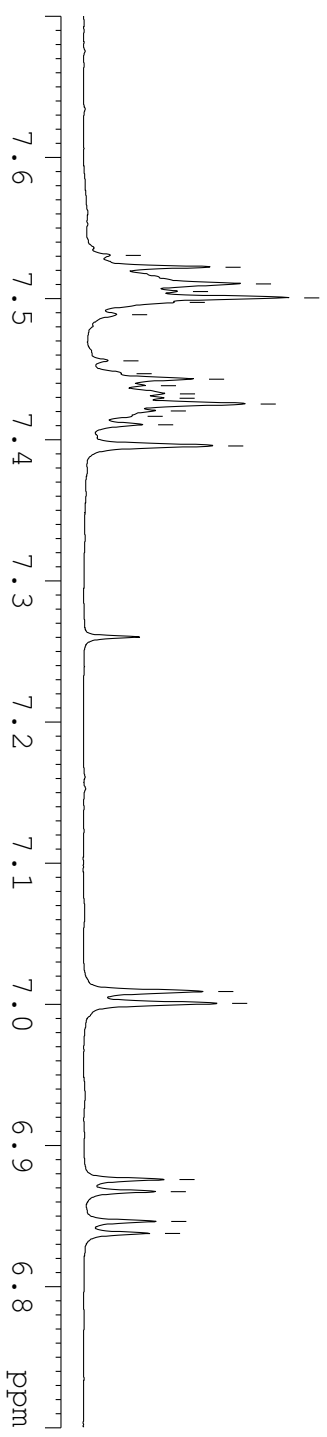
```

Current Data Parameters
NAME       7P4PC
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     2014096
Time     11.35
INSTRUM  FOURIER200
PROBHD   5 mm DUL 13C-1
PULPROG  zg30
ID       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 =====
SF01     300.1818537 MHz
NUC1     1H
P1       8.75 usec
PL1     25.00000000 W
PIWL

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



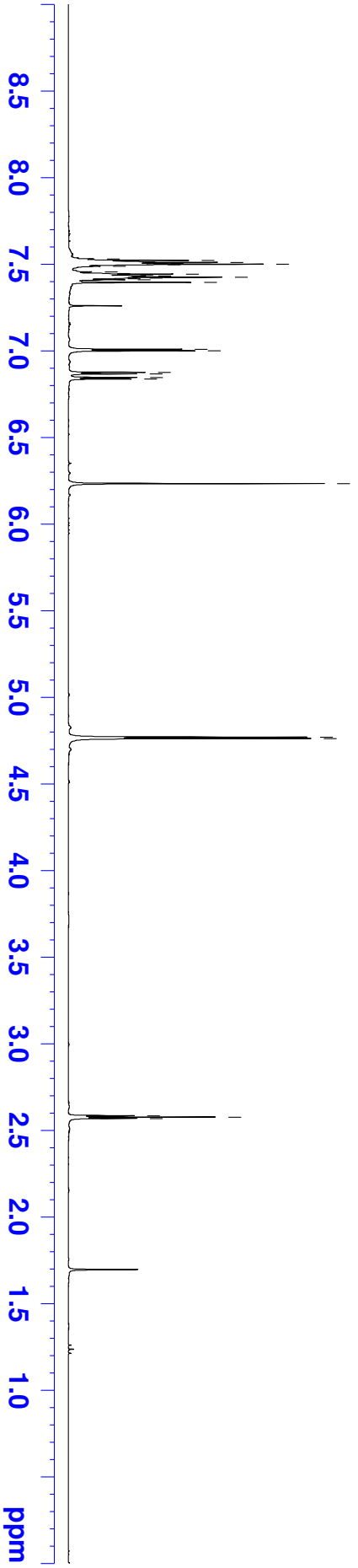
3.05
3.05

1.00
1.00

1.00

2.08

1.01



Current Data Parameters
 NAME 7P4PC
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140506
 Time 11.53

INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2000
 DS 4

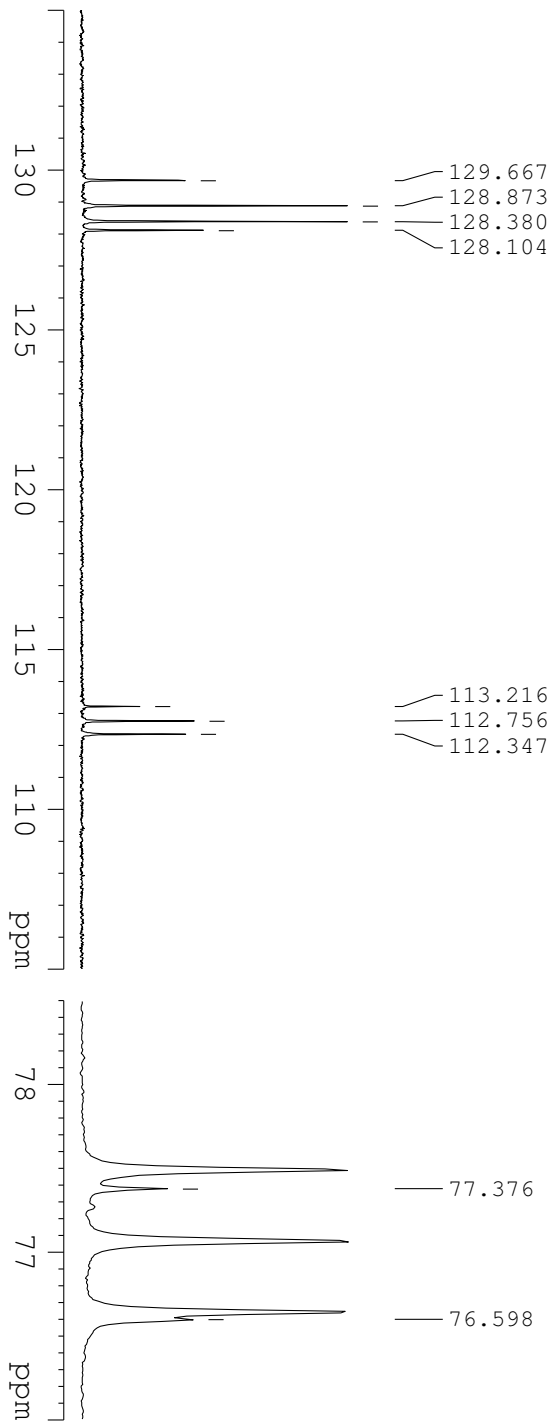
SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 295.8 K

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
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.400000001 W

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



161.08
 160.49
 155.74
 155.71

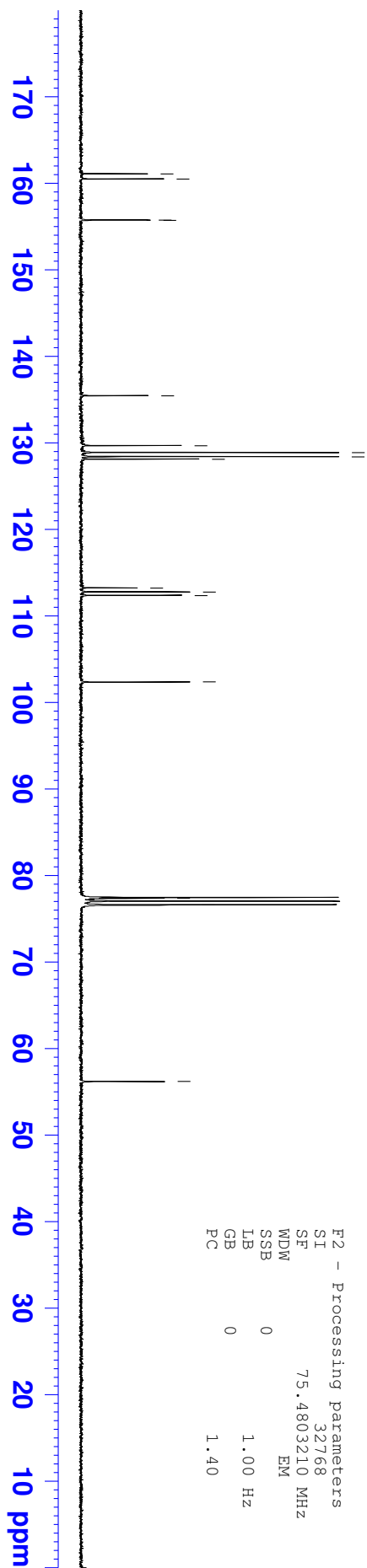
135.44
 129.67
 128.87
 128.38
 128.10

113.22
 112.76
 112.35

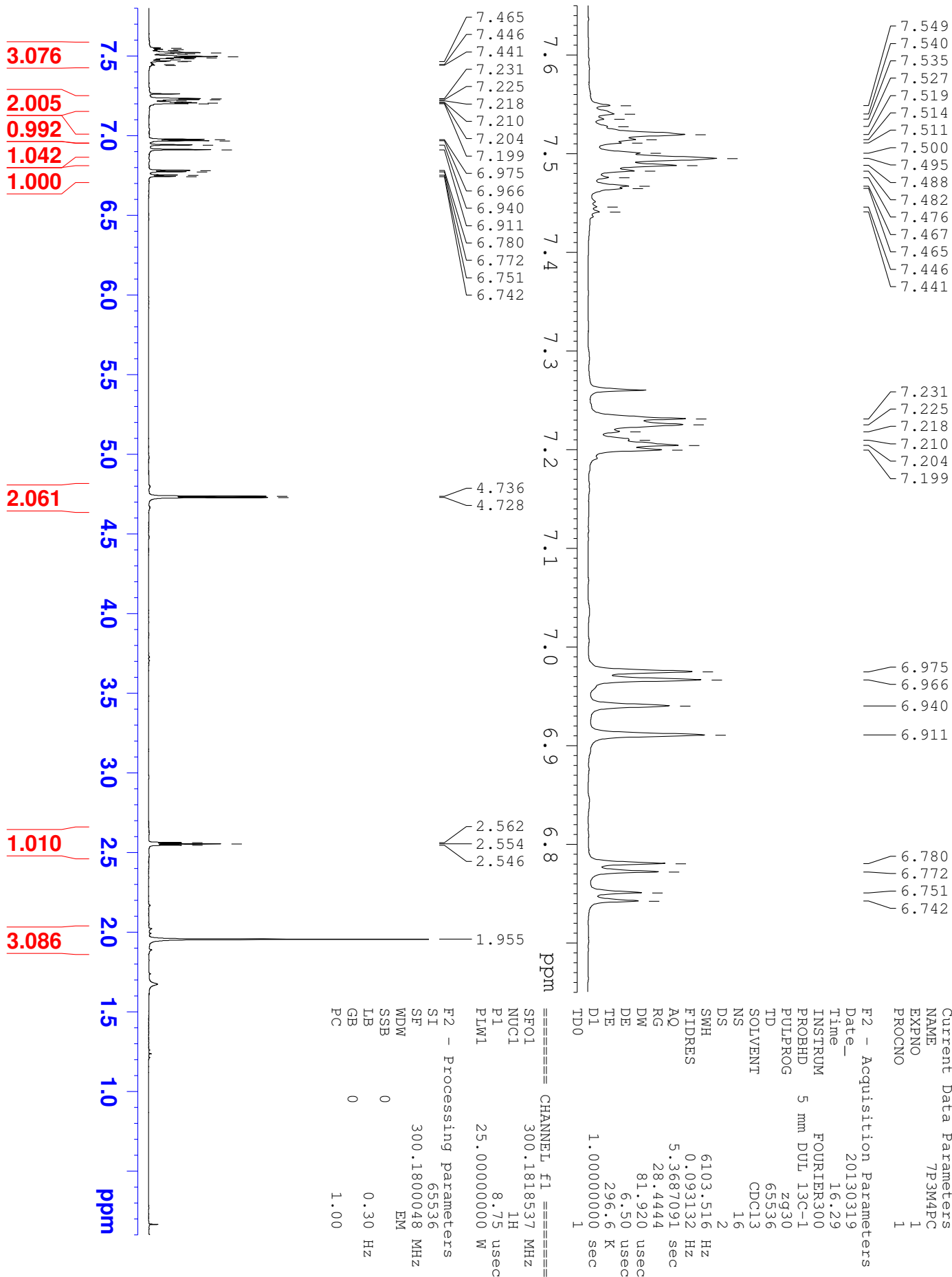
102.38

77.38
 76.60

56.20



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



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
 SMH 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 =====
 SF01 300.1818537 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 25.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800048 MHz
 WDM 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
 PROBDH 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1009
 DS 4

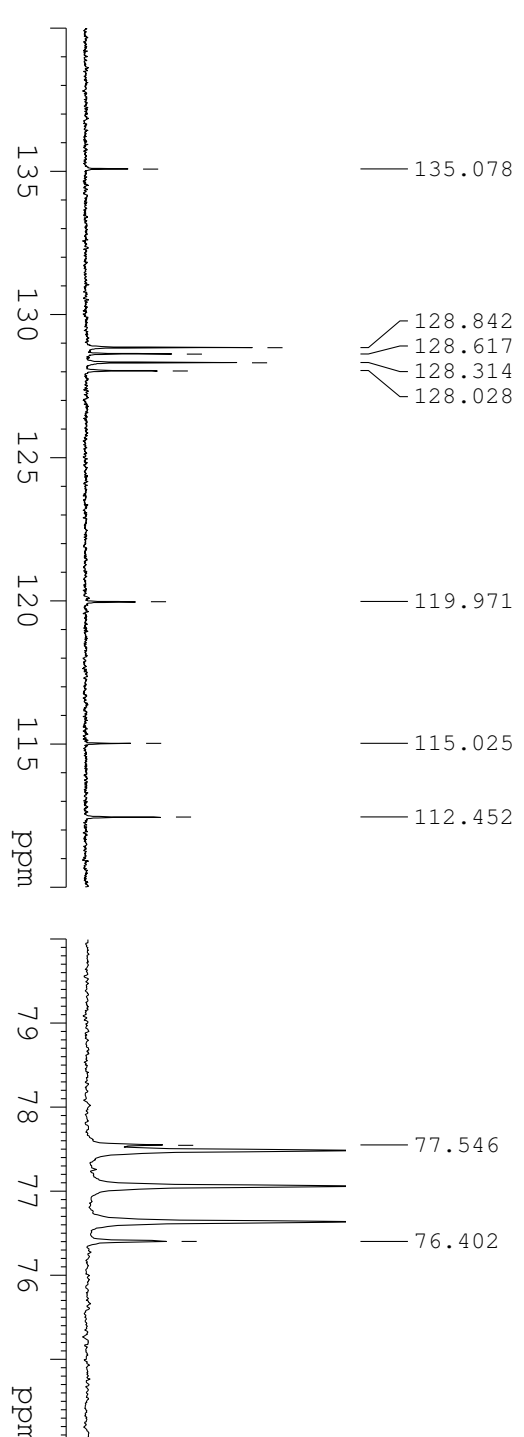
SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 296.8 K

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

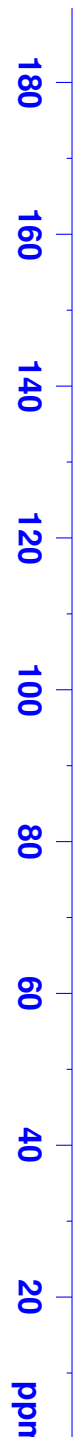
==== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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



- 162.64
- 159.41
- 153.76
- 150.69
- 135.08
- 128.84
- 128.62
- 128.31
- 128.03
- 119.97
- 115.03
- 112.45
- 101.80
- 77.55
- 76.40
- 56.15
- 14.47



3M4P7PC (Compound 14)

7.545
7.529
7.513

6.954
6.946
6.939
6.931
6.923
6.914

2.592
2.584
2.576

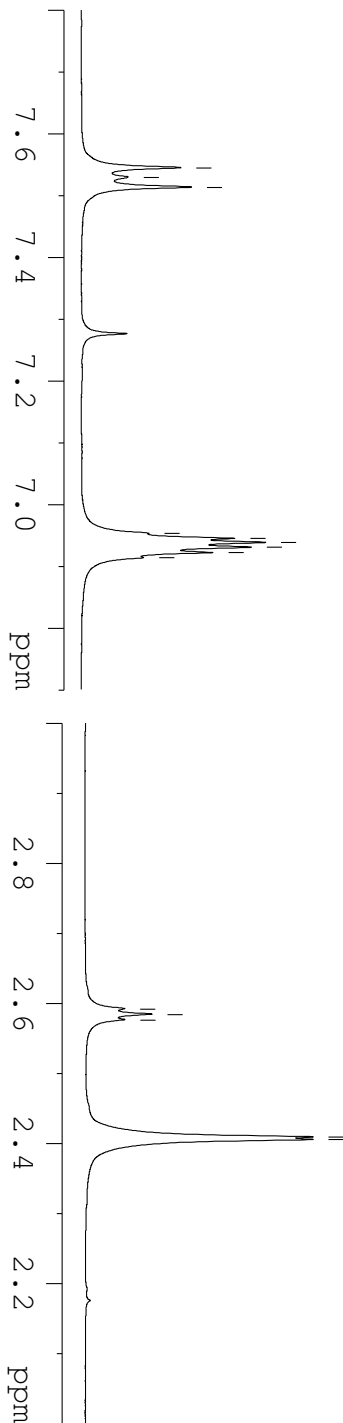
2.409
2.406

7.545
7.529
7.513
6.954
6.946
6.939
6.931
6.923
6.914

6.162
6.158

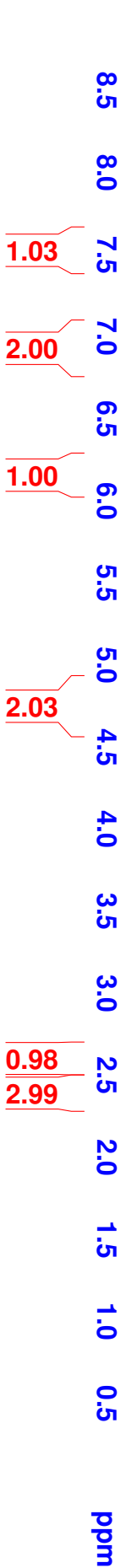
4.770
4.763

2.592
2.584
2.576
2.409
2.406



```

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
PLM1         25.00000000 W
F2 - Processing parameters
SI            65536
SF           300.180000 MHz
WDW           EM
SSB           0
GB            0
PC            1.00
  
```



Current Data Parameters
 NAME 7P4MC
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140706
 Time 21.38

INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 10000
 DS 4

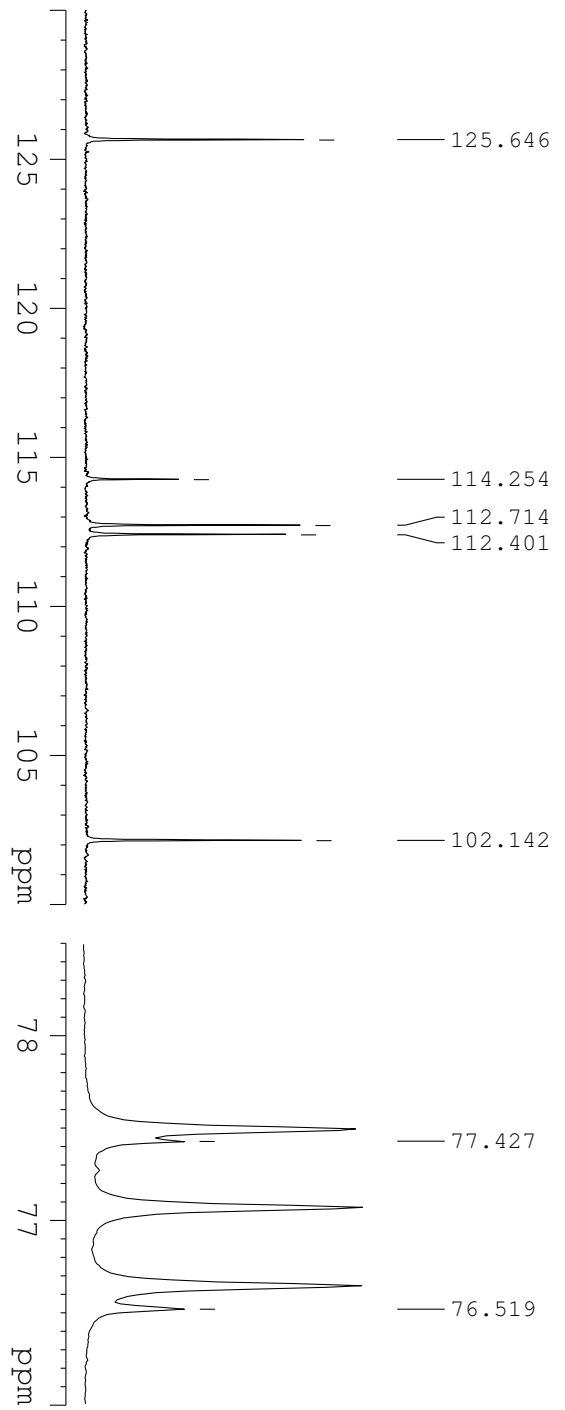
SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 296.3 K

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

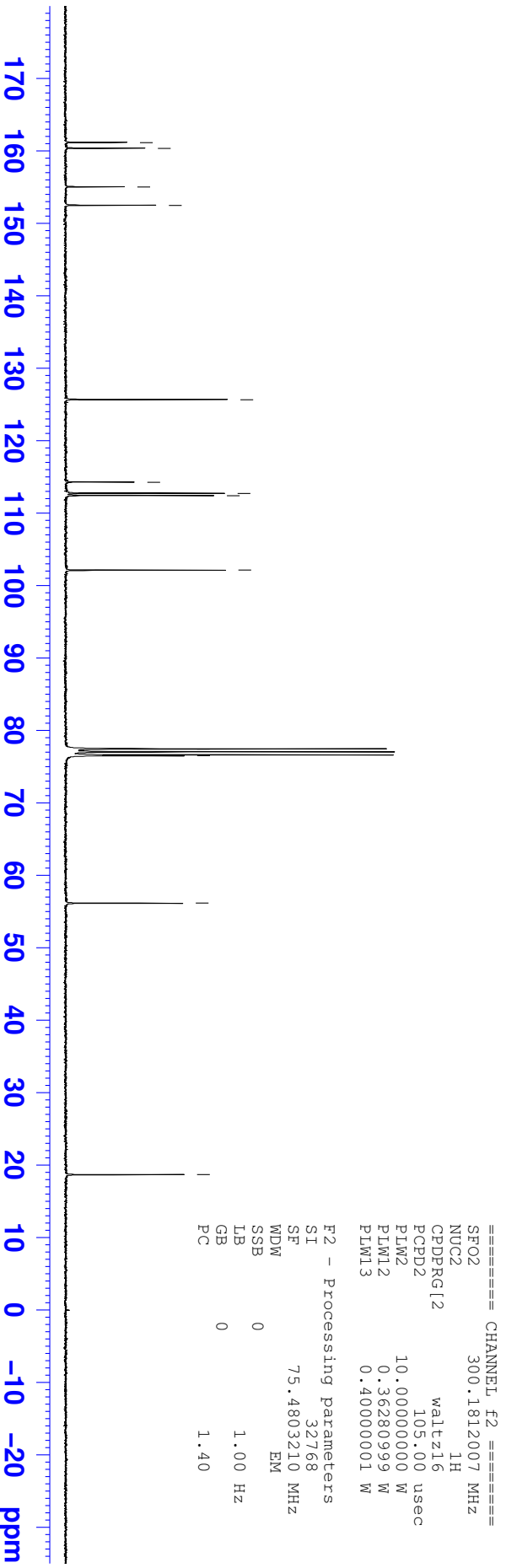
==== CHANNEL f1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL f2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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



161.14
 160.34
 155.02
 152.47
 125.65
 114.25
 112.71
 112.40
 102.14
 77.43
 76.52



7.670
7.664
7.657
7.651
7.645
7.639
7.633

7.003
6.997
6.978
6.970

7.003
6.997
6.978
6.970

6.645
6.643

7.8 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

7.670
7.664
7.657
7.651
7.645
7.639
7.633
7.003
6.997
6.978
6.970
6.645
6.643

4.792
4.784

2.602
2.594
2.586

Current Data Parameters
NAME 7P4TFC
EXPNO 1
PROCNO 1

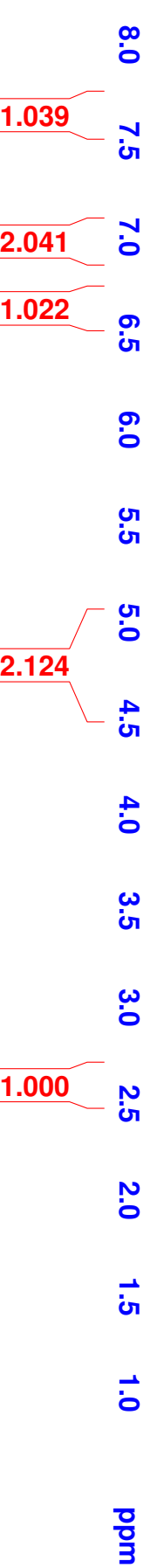
F2 - Acquisition Parameters

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 =====
SF01 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)



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 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 296.1 K

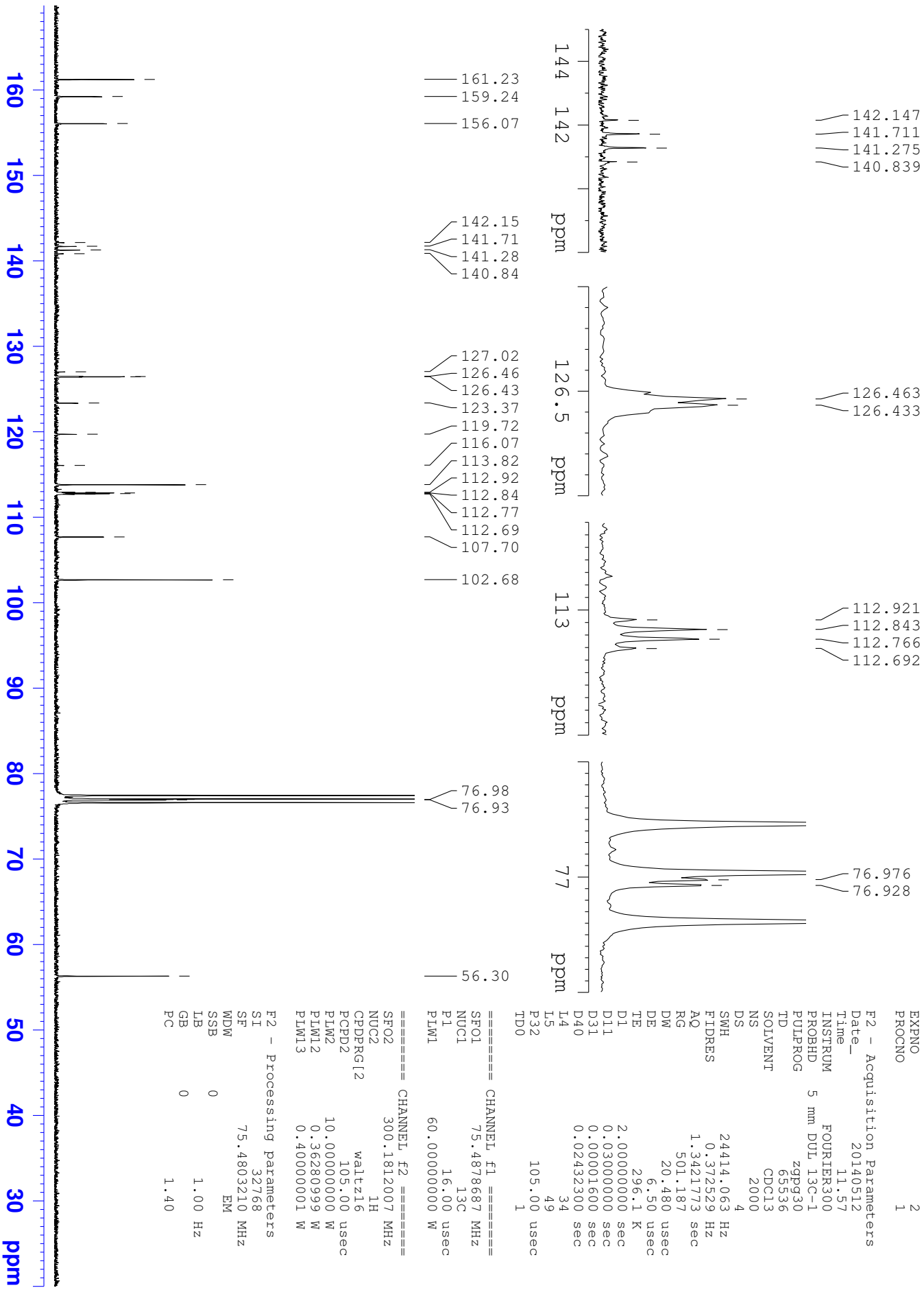
D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001600 sec
 D40 0.02432300 sec
 L4 34
 L5 49
 P32 105.00 usec
 TD0 1

==== CHANNEL F1 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.400000001 W

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

4TF7PC (Compound 16)

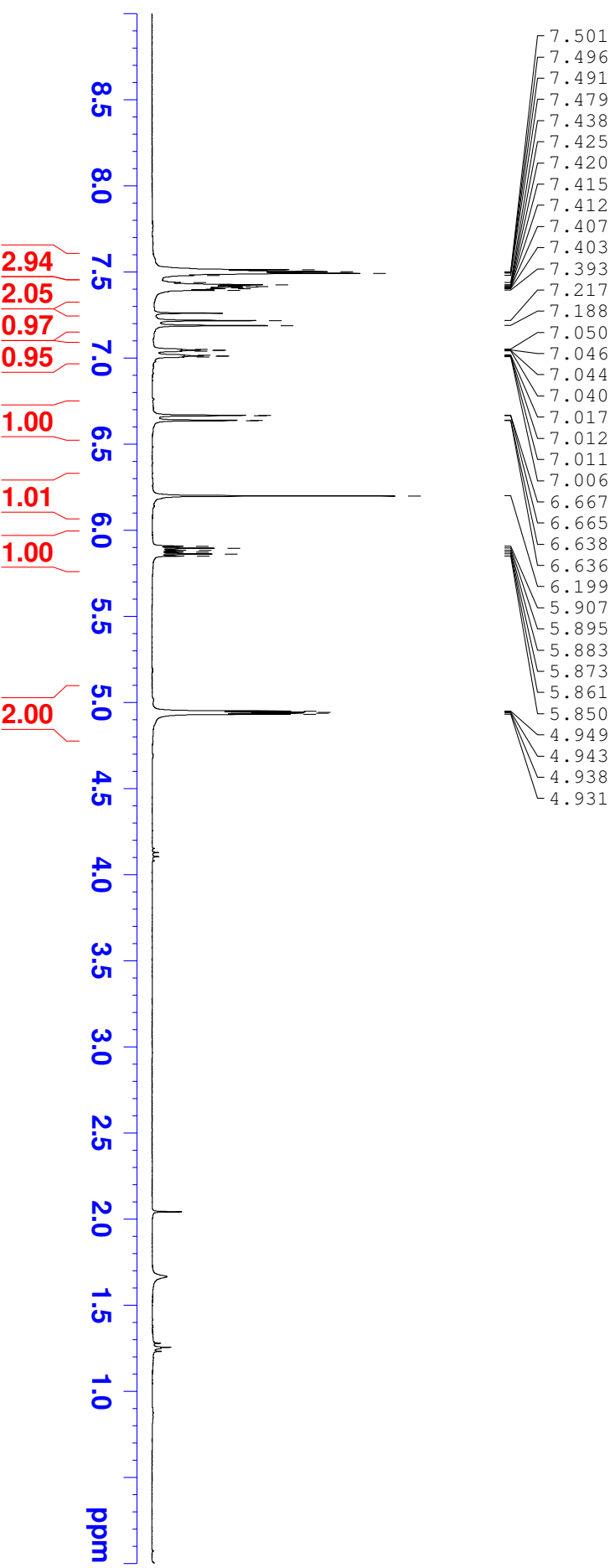
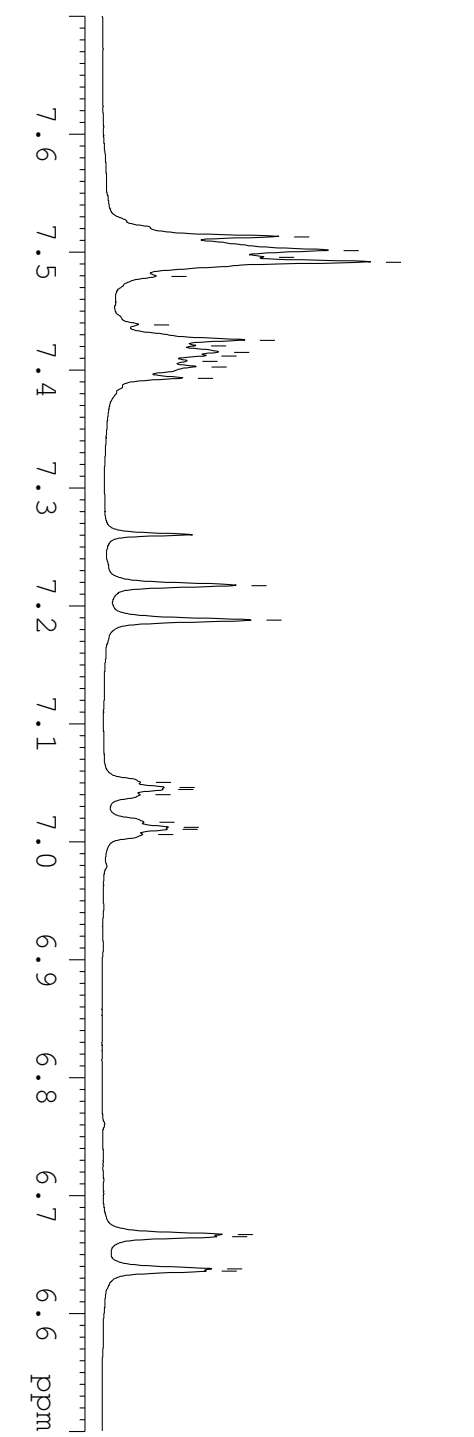


Current Data Parameters
 NAME 78p4pc
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140513
 Time_ 17.14
 INSTRUM FOURIER300
 PROBD 5 mm PUL 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 300.181537 MHz
 NUC1 1H
 P1 8.75 usec
 FWH1 25.00000000 W

F2 - Processing parameters
 SI 300.180048 MHz
 SF 500.137566 MHz
 NDM 0
 NSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00



Current Data Parameters
 NAME 78P4PC
 EXPNO 2
 PROCNO 1

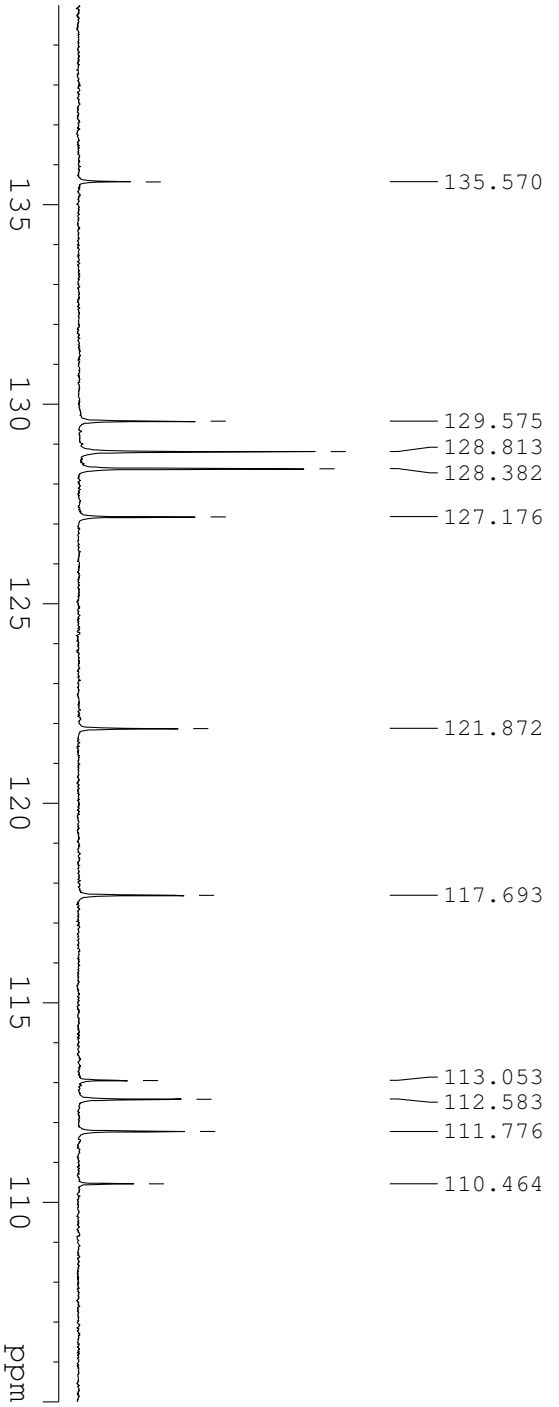
F2 - Acquisition Parameters

Date_ 20140513
 Time 17.19
 INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 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

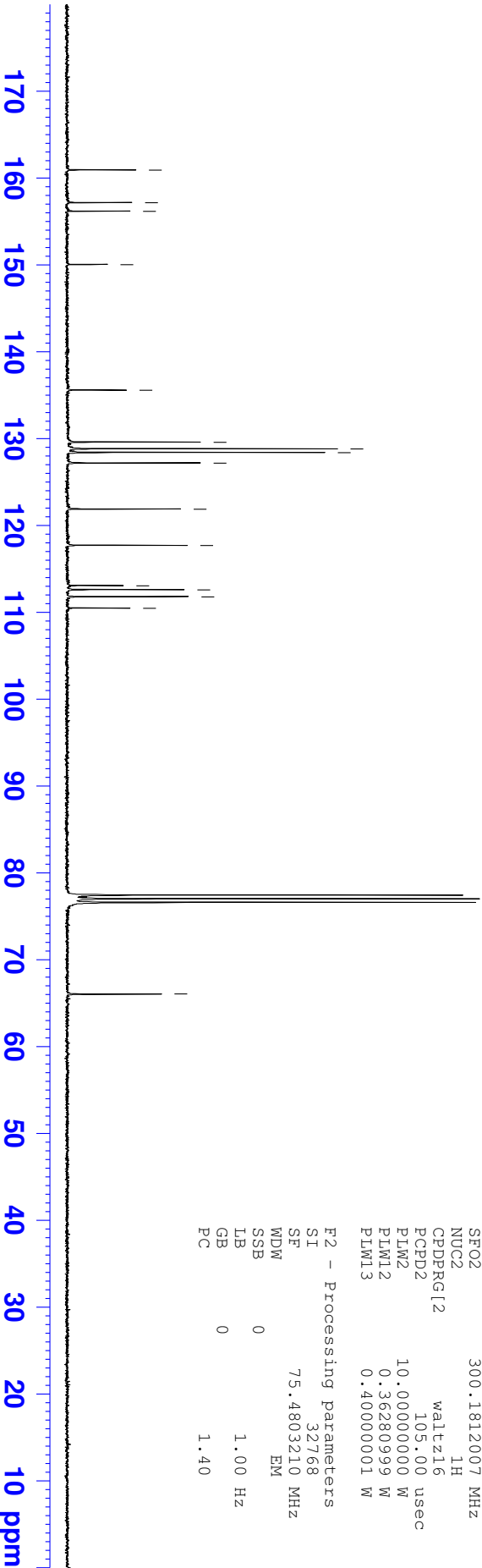
==== CHANNEL F1 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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
 WDDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



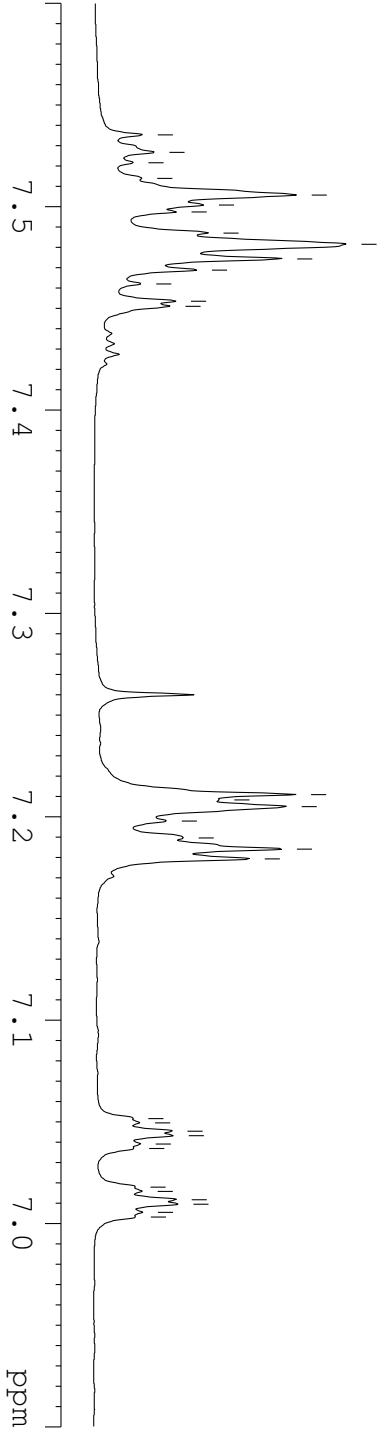
160.91
 157.16
 156.17
 150.03
 135.57
 129.58
 128.81
 128.38
 127.18
 121.87
 117.69
 113.05
 112.58
 111.78
 110.46



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

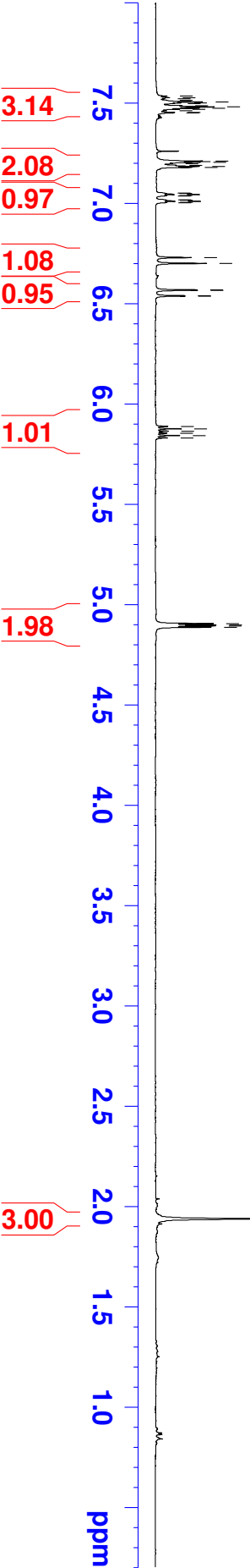
```

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
DE         81.920 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

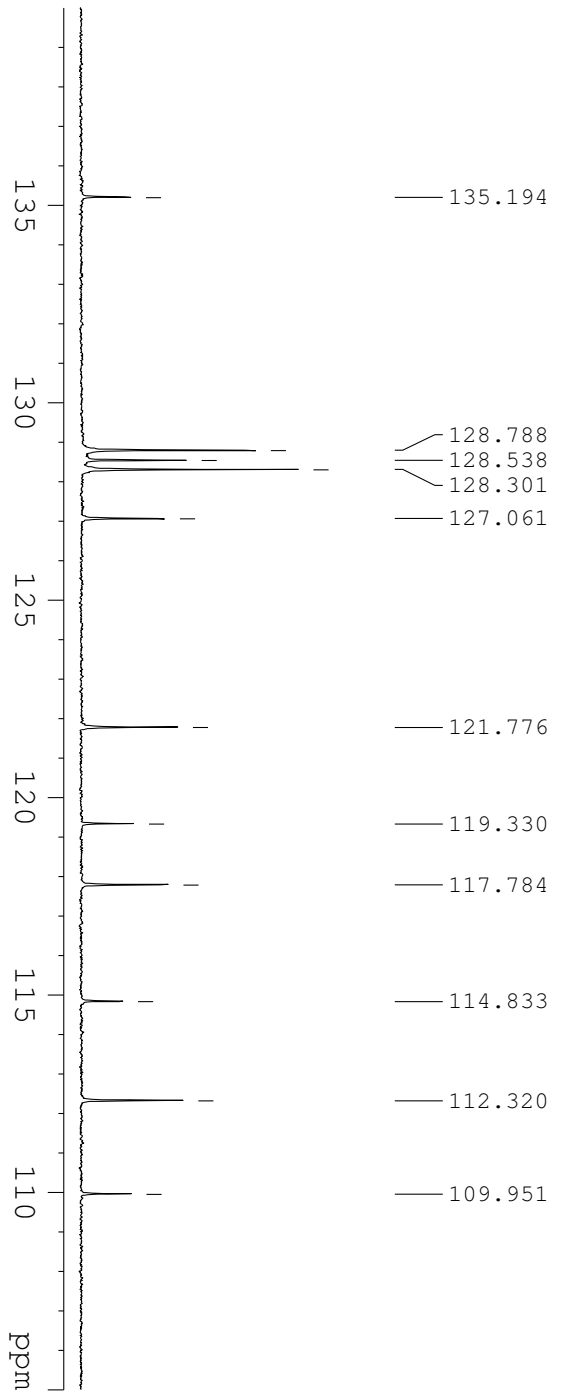
F2 - Processing parameters
SI         65536
SF         300.1800049 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



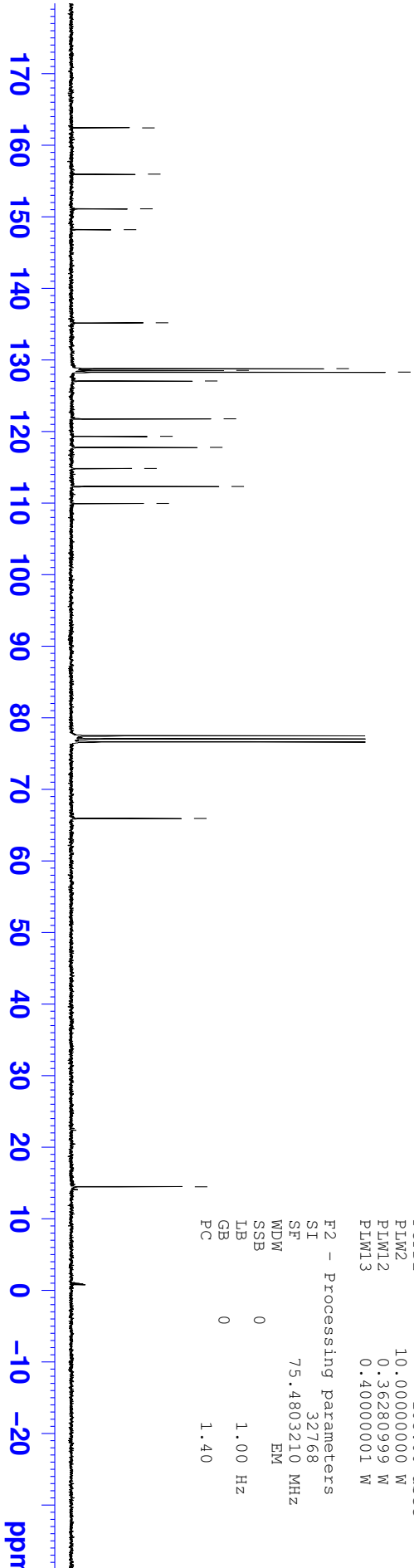
3.14
2.08
0.97
1.08
0.95
1.01
1.98
3.00

78P3M4PC

Current Data Parameters
 NAME 7H3M4PC_78pyran
 EXPNO 2
 PROCNO 1



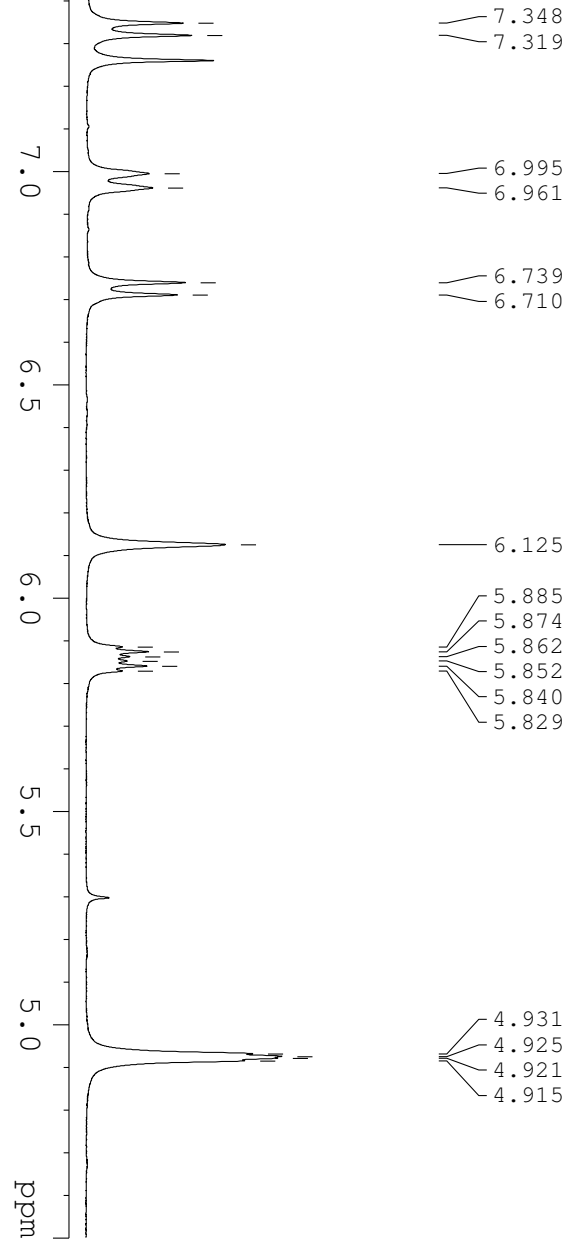
162.42
 155.96
 151.12
 148.20
 135.19
 128.79
 128.54
 128.30
 127.06
 121.78
 119.33
 117.78
 114.83
 112.32
 109.95



==== CHANNEL F1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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

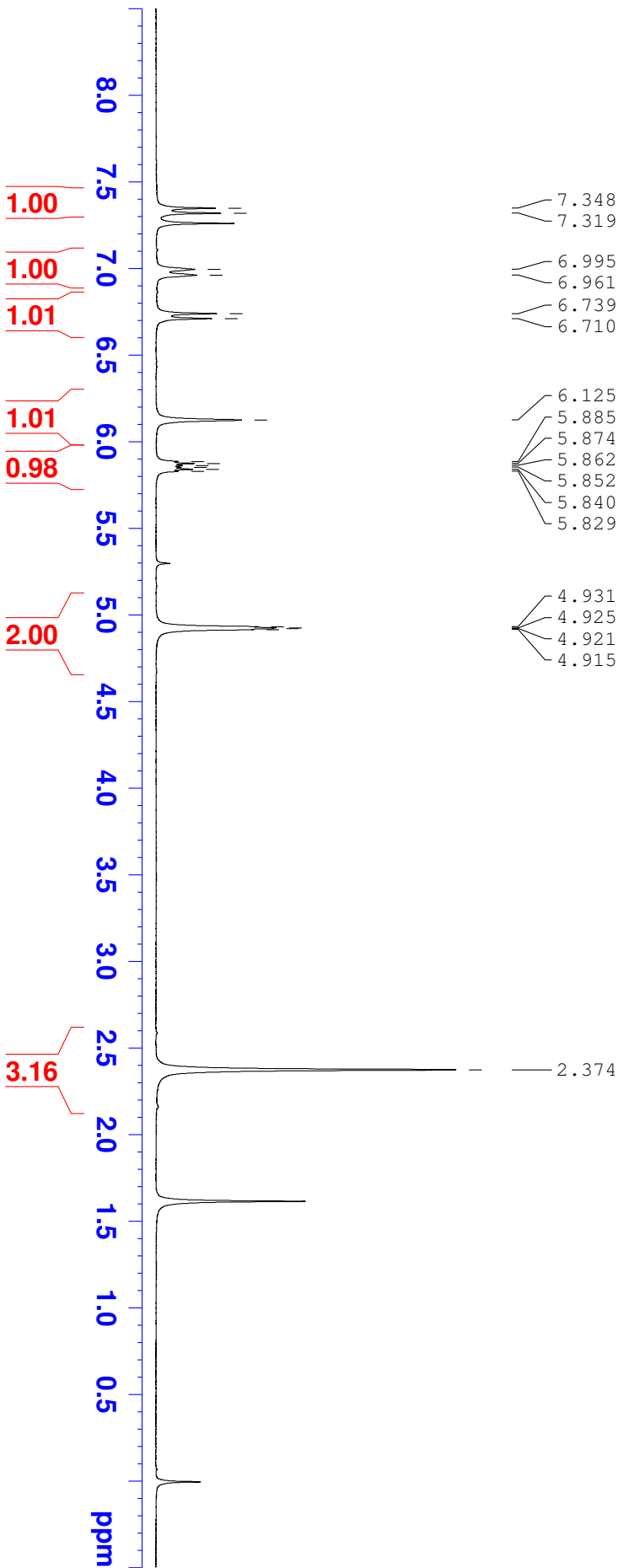


Current Data Parameters
 NAME 78P4MC
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140722
 Time 12.39
 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 841.1644
 DW 81.920 usec
 DE 6.50 usec
 TE 295.8 K
 D1 1.00000000 sec
 IDU 1

==== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUC1 13C
 P1 8.15 usec
 F1 25.00000000 W
 FLM1 W

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



Current Data Parameters
 NAME 78P4MC
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140725
 Time 17.50

INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30

TD 65536
 SOLVENT CDC13
 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
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.40000001 W

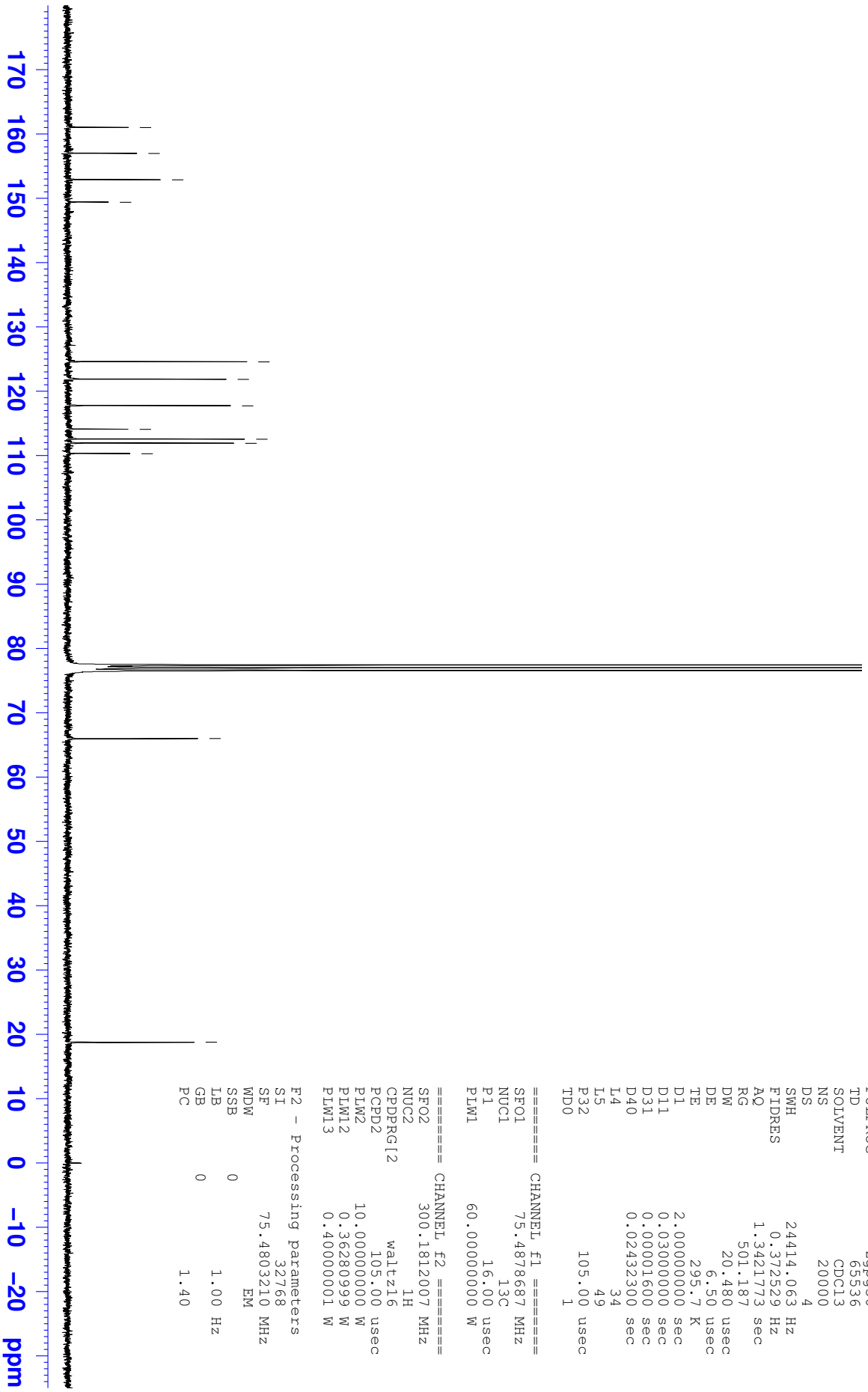
F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

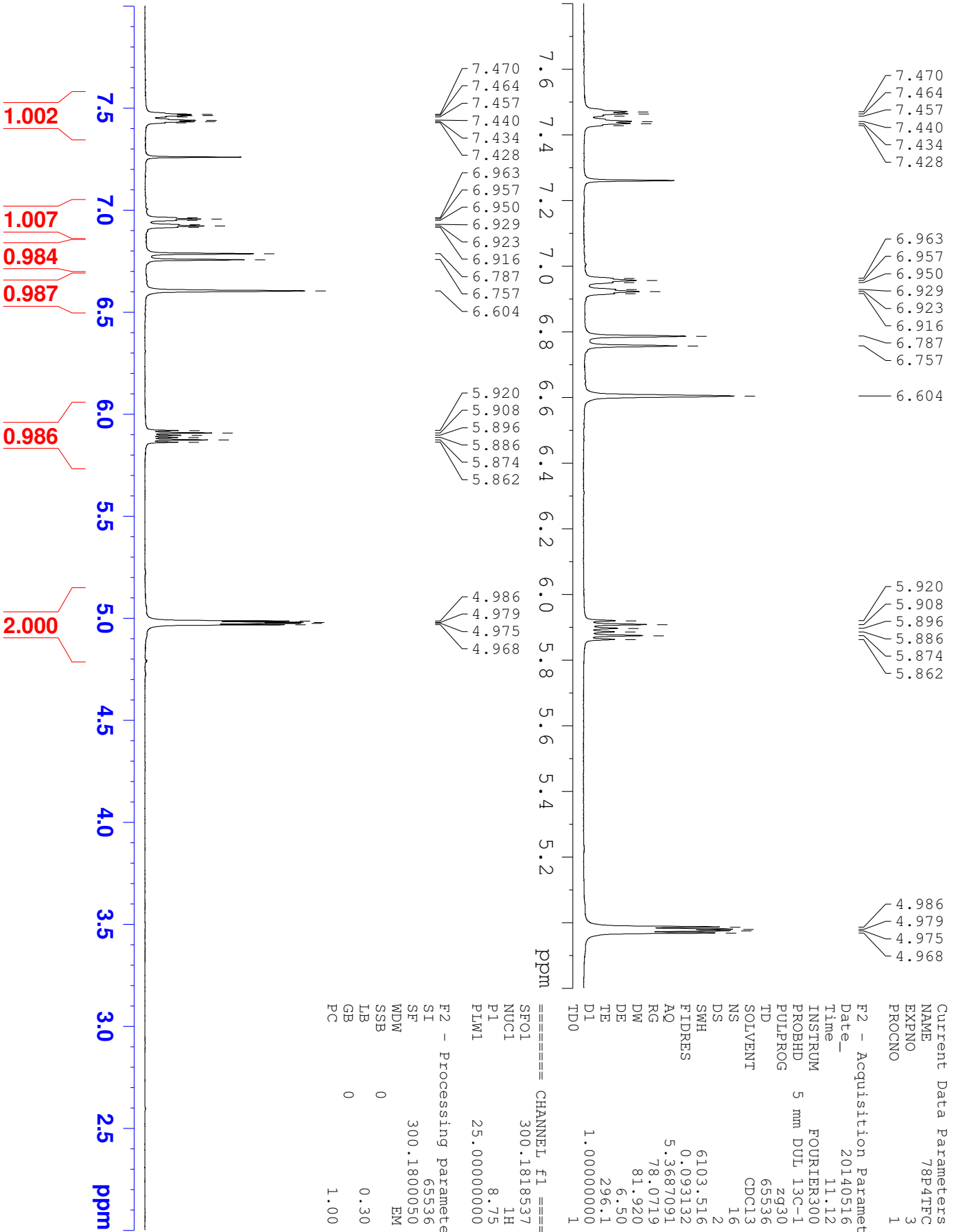
- 161.00
- 156.97
- 152.87
- 149.37
- 124.56
- 121.84
- 117.72
- 114.07
- 112.54
- 111.90
- 110.28

65.99

18.78

4M78PC (Compound 19)





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
 SMH 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 =====
 SF01 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

Current Data Parameters
 NAME 78P4TFC
 EXPNO 2
 PROCNO 1

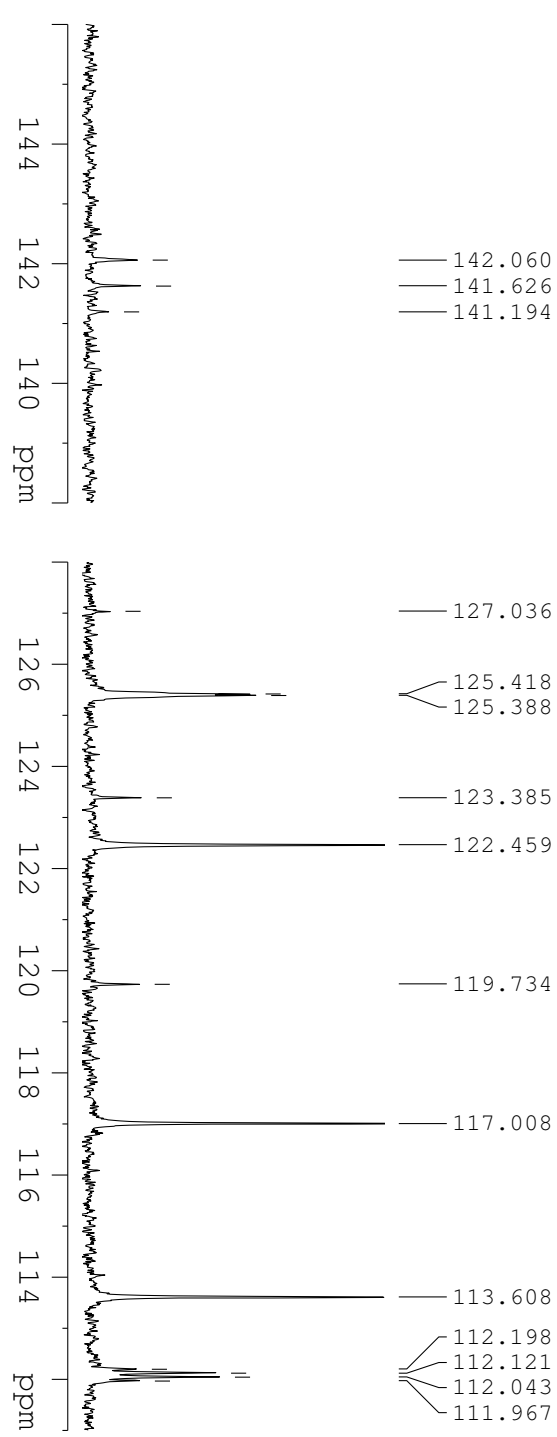
F2 - Acquisition Parameters

Date_ 20140519
 Time 17.47
 INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 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

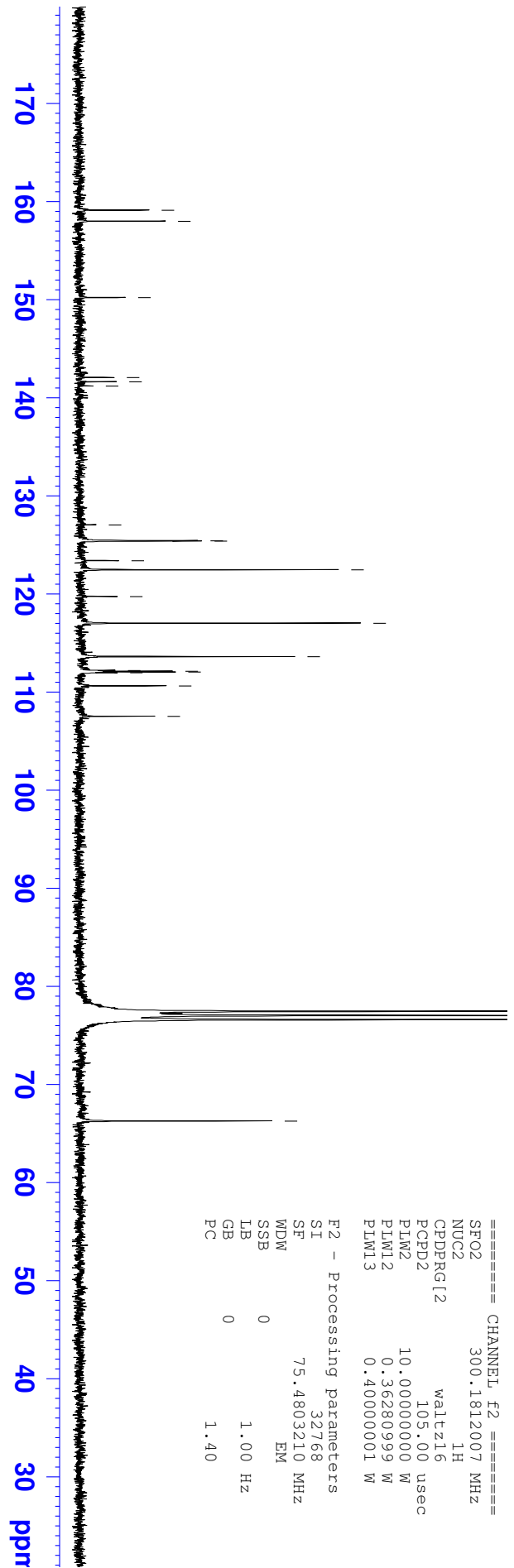
==== CHANNEL F1 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.40000001 W

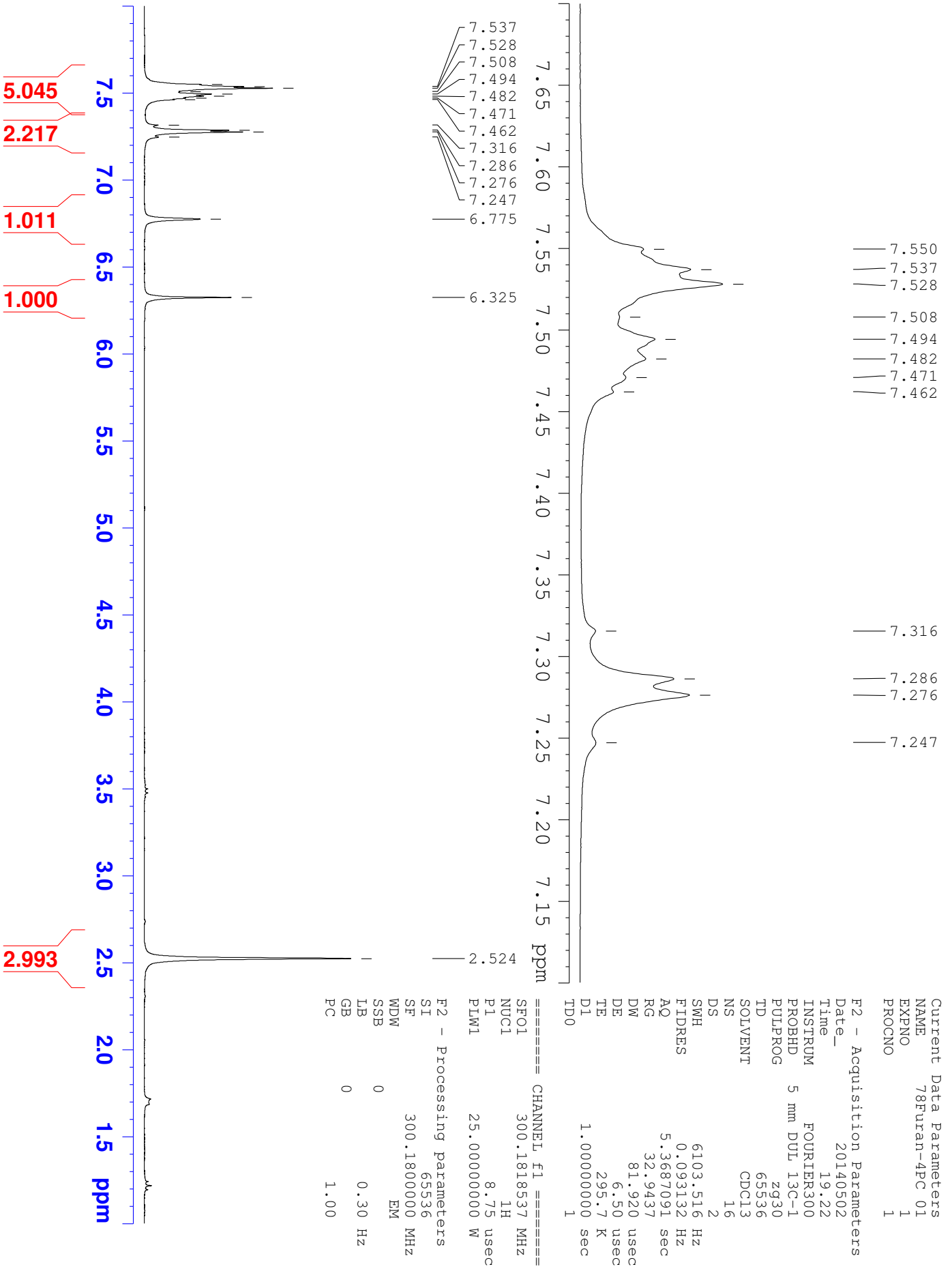
F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



159.12
 157.99
 150.21
 142.06
 141.63
 141.19
 127.04
 125.42
 125.39
 123.39
 122.46
 119.73
 117.01
 113.61
 112.20
 112.12
 112.04
 111.97
 110.62
 107.52
 66.26



4P78FC (Compound 21)



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

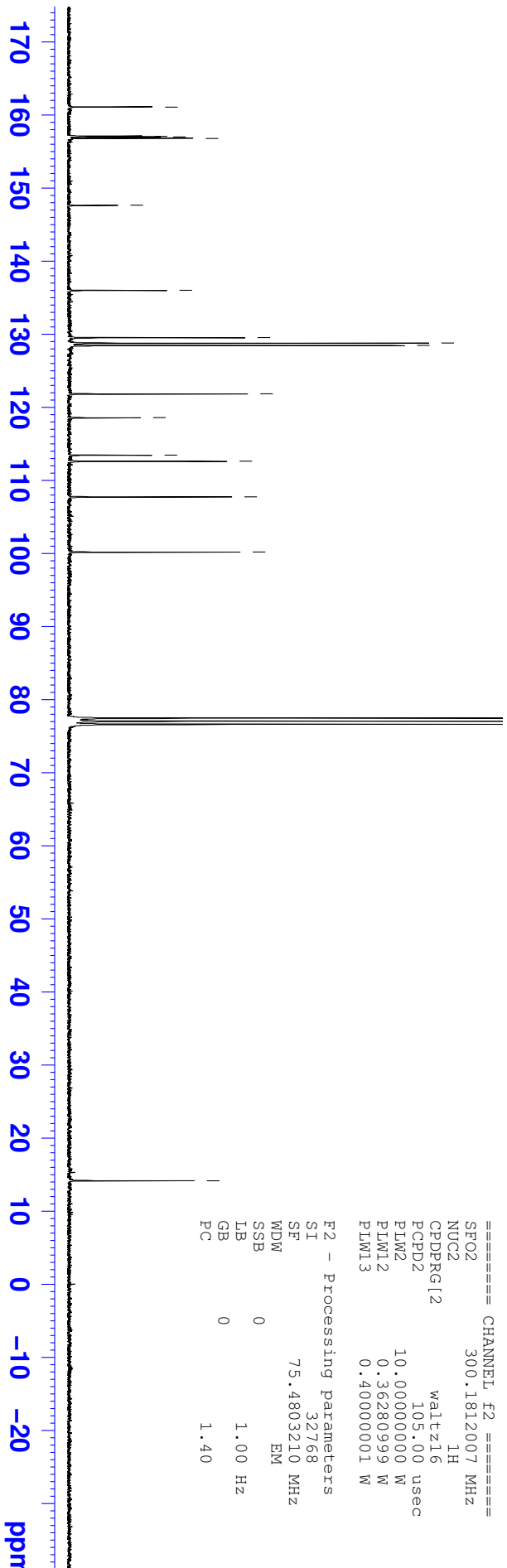
F2 - Acquisition Parameters

Date_ 20140502
 Time 19.22
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 32.9437
 DW 81.920 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.00000000 sec
 TD0 1

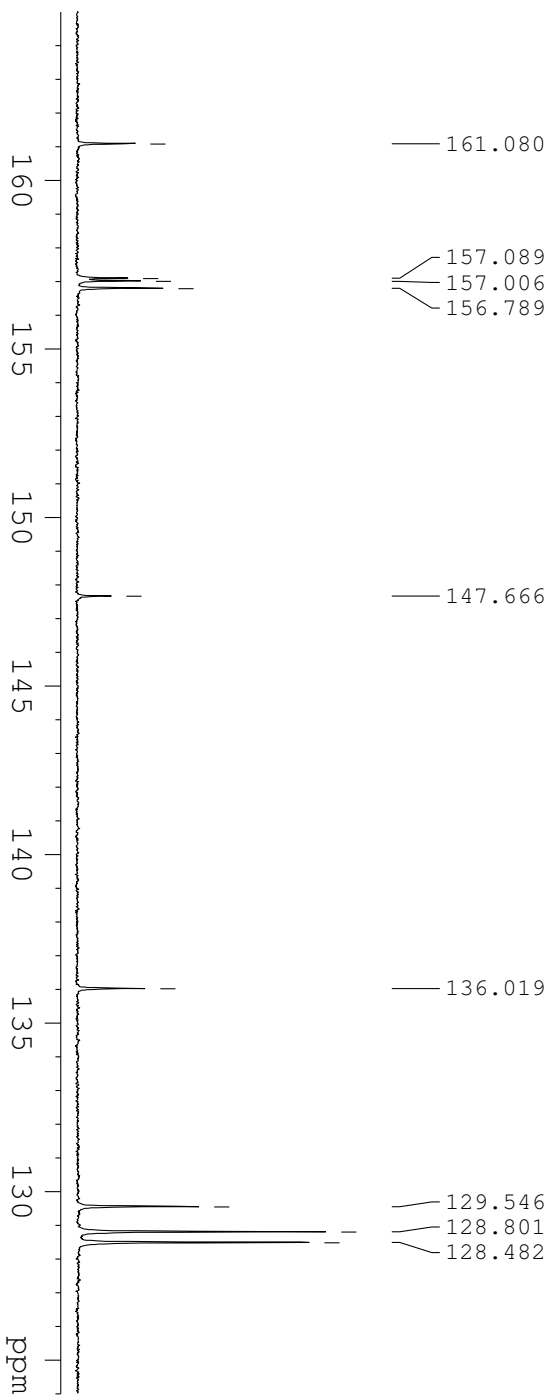
==== CHANNEL f1 =====
 SF01 300.1818537 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 25.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

4P78FC (Compound 21)



161.08
 157.09
 157.01
 156.79
 147.67
 136.02
 129.55
 128.80
 128.48
 121.85
 118.60
 113.46
 112.64
 107.75
 100.21
 14.16



161.080
 157.089
 157.006
 156.789
 147.666
 136.019
 129.546
 128.801
 128.482
 14.16

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

F2 - Acquisition Parameters
 Date_ 20140502
 Time 19.26

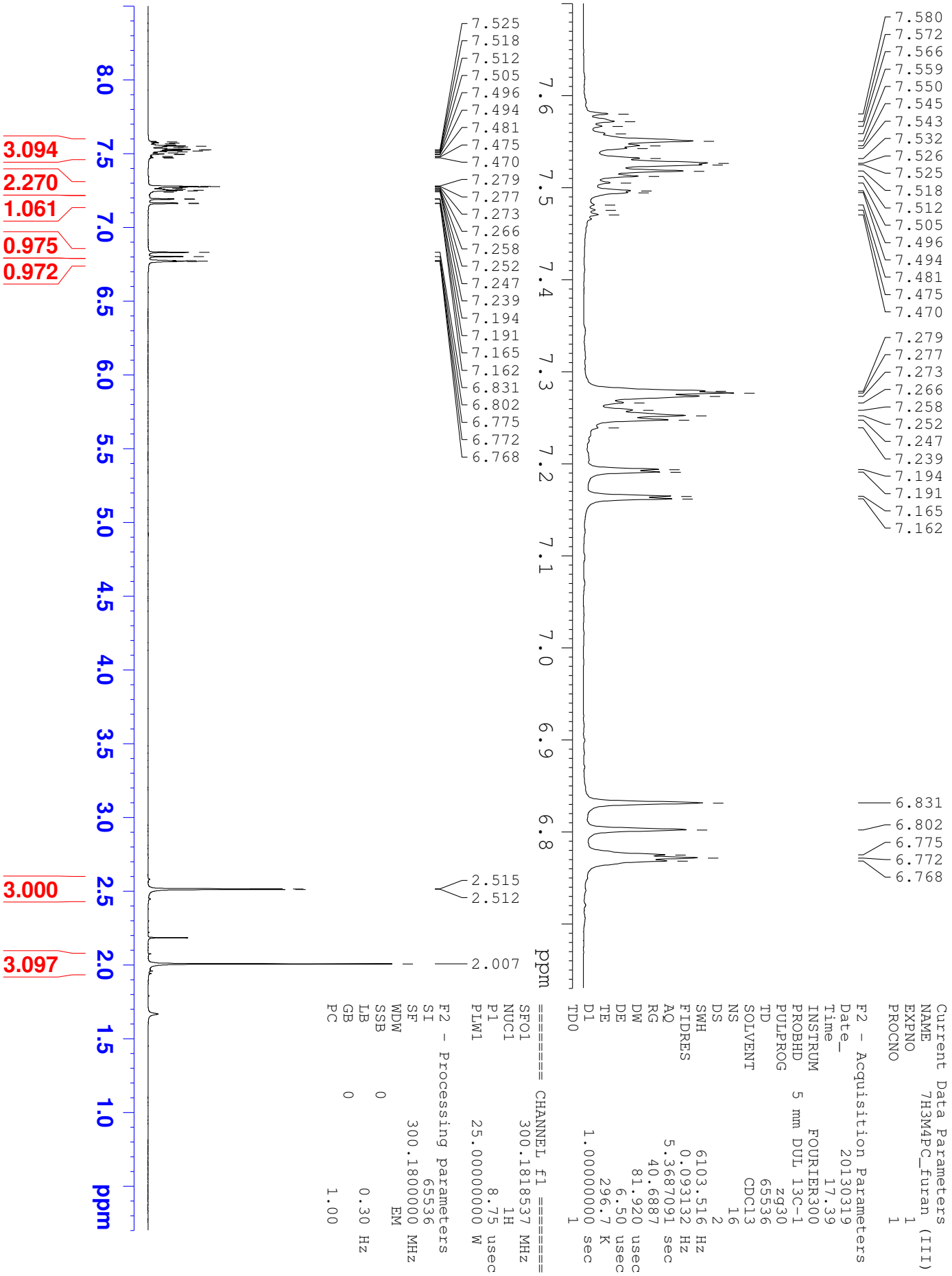
INSTRUM FOURIER300
 PROBDH 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 6000
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 295.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00001600 sec
 D40 0.02432300 sec
 L4 34
 L5 49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

==== CHANNEL F1 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

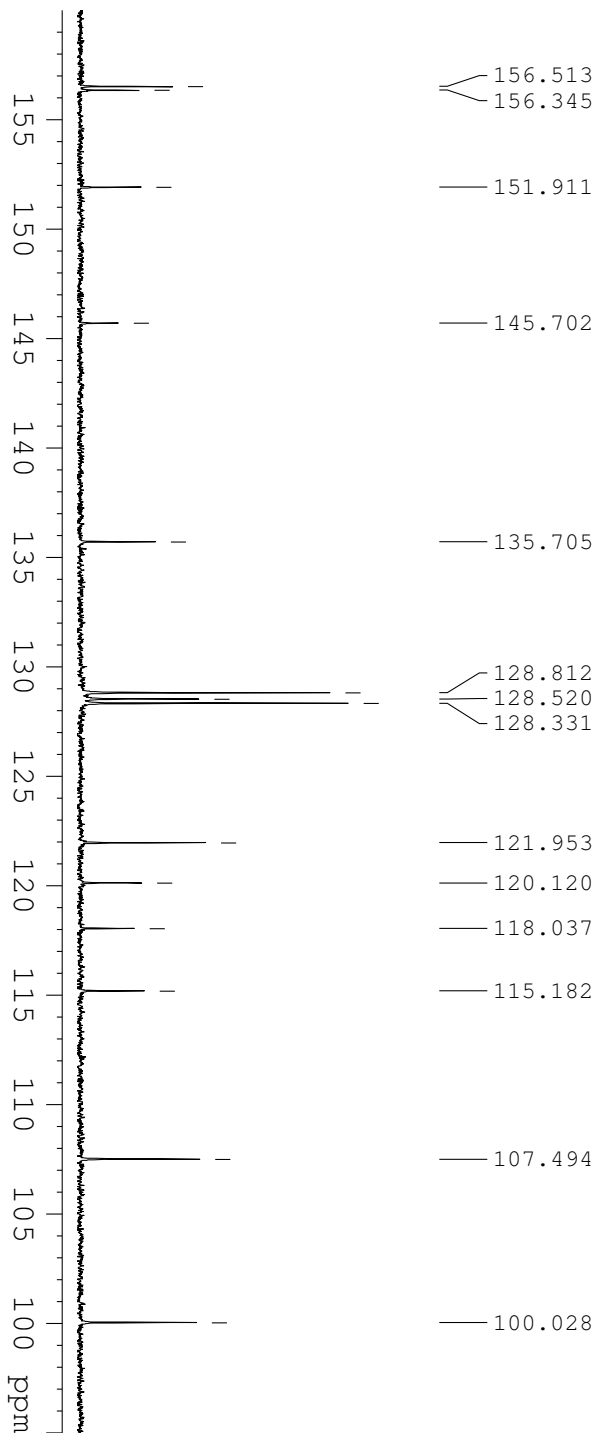
==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.400000001 W

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

78F3M4PC



78F3M4PC



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

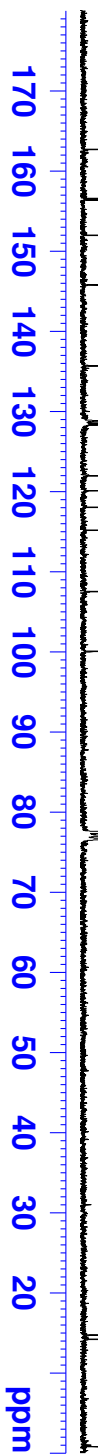
162.65
 156.51
 156.35
 151.91
 145.70
 135.70
 128.81
 128.52
 128.33
 121.95
 120.12
 118.04
 115.18
 107.49
 100.03

99.14
 97.14
 94.14

==== CHANNEL F1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

 ===== CHANNEL F2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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



Current Data Parameters
 NAME 78F4MC
 EXPNO 1
 PROCNO 1

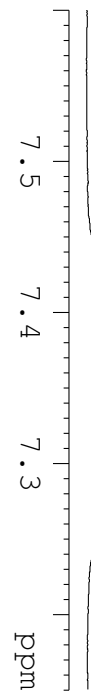
7.429
 7.400
 7.344
 7.342
 7.315
 7.313

2.498
 2.496
 2.476
 2.473

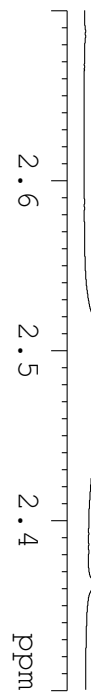
F2 - Acquisition Parameters
 Date_ 20140609
 Time 10.14
 INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 6103.516 Hz
 FIDRES 0.093132 Hz
 AQ 5.3687091 sec
 RG 54.6209
 DW 81.920 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 300.1818537 MHz
 NUCL1 1H
 P1 8.75 usec
 PLWL 25.00000000 W

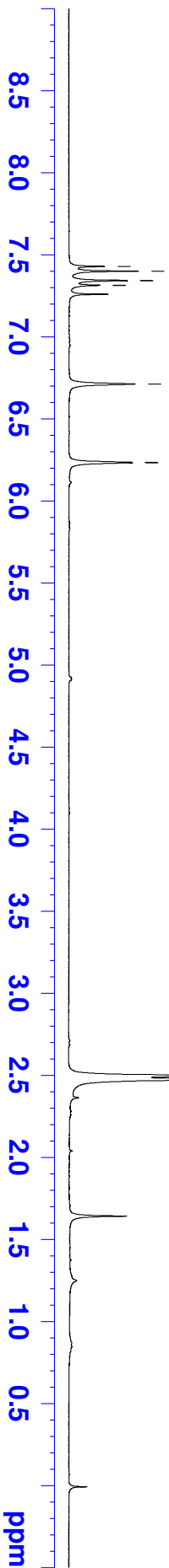
F2 - Processing parameters
 SI 65536
 SF 300.1800050 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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

Current Data Parameters
 NAME 78F4MC
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140609
 Time 17.24
 INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 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

161.15
 156.99
 156.65
 153.72
 147.02

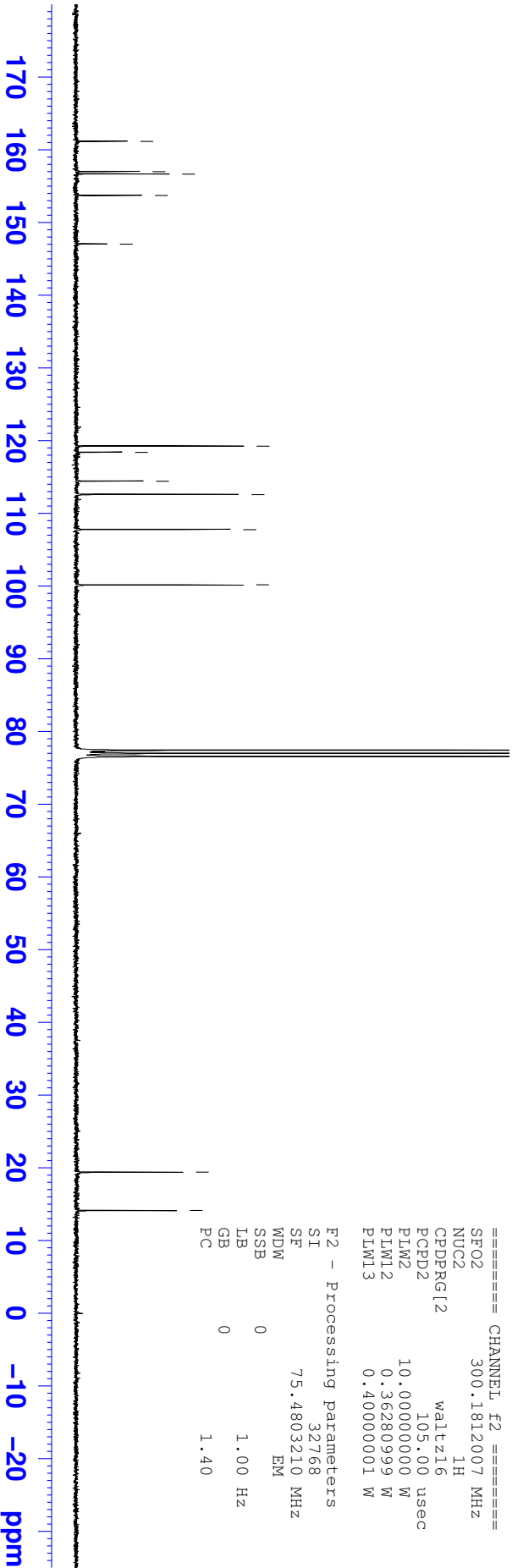
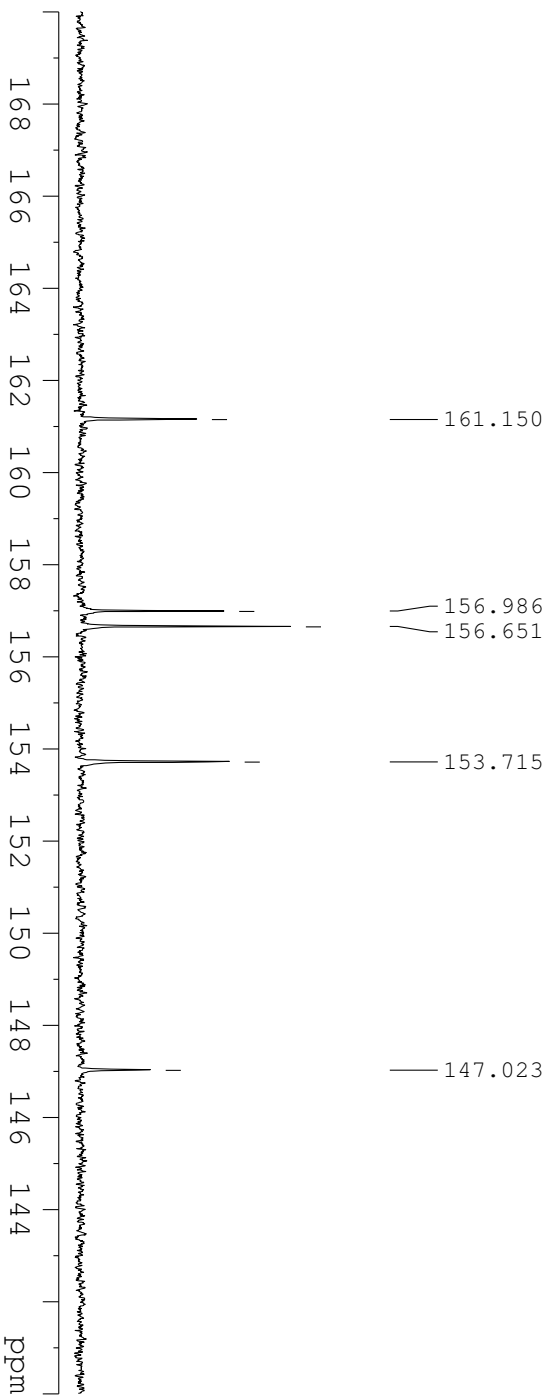
119.24
 118.39
 114.42
 112.58
 107.76
 100.18

19.40
 14.13

==== CHANNEL F1 =====
 SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
 SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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

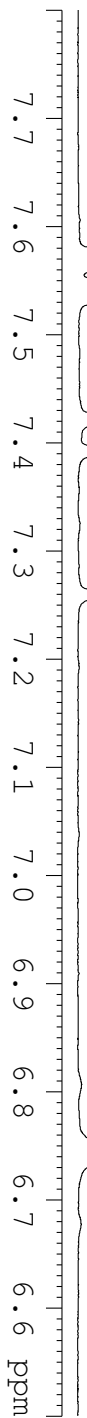


7.579
7.573
7.566
7.560
7.549
7.543
7.537
7.531
7.423
7.421
7.394
7.391

6.745
6.742
6.738

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



```

Current Data Parameters
NAME      78F4TFC
EXPNO    6
PROCNO   1

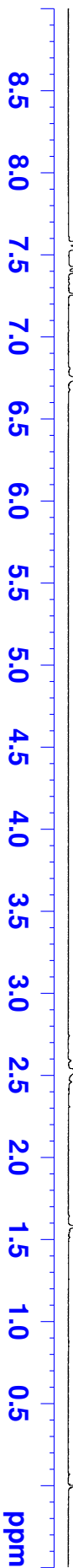
F2 - Acquisition Parameters
Date_    20140527
Time     10.17
INSTRUM  PULPROG
PROBHD   5 mm DUL 13C-1
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       6103.516 Hz
FIDRES    0.093132 Hz
AQ        5.3687091 sec
RG        112.187
DE        81.920 usec
DM        6.50 usec
TE        296.5 K
D1        1.00000000 sec
IDU       1

===== CHANNEL f1 =====
SFO1     300.1818537 MHz
NUC1     13C
P1        8.15 usec
PL1       0.00000000 W
F2 - Processing parameters
SI        300.1800050 MHz
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



Current Data Parameters
 NAME 78F4TFC
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140607
 Time 18.01

INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 35000
 DS 4

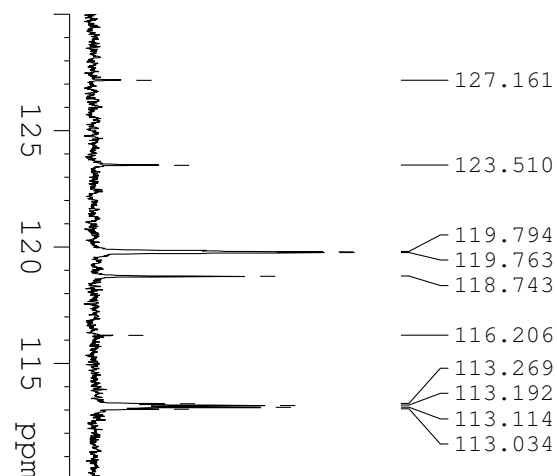
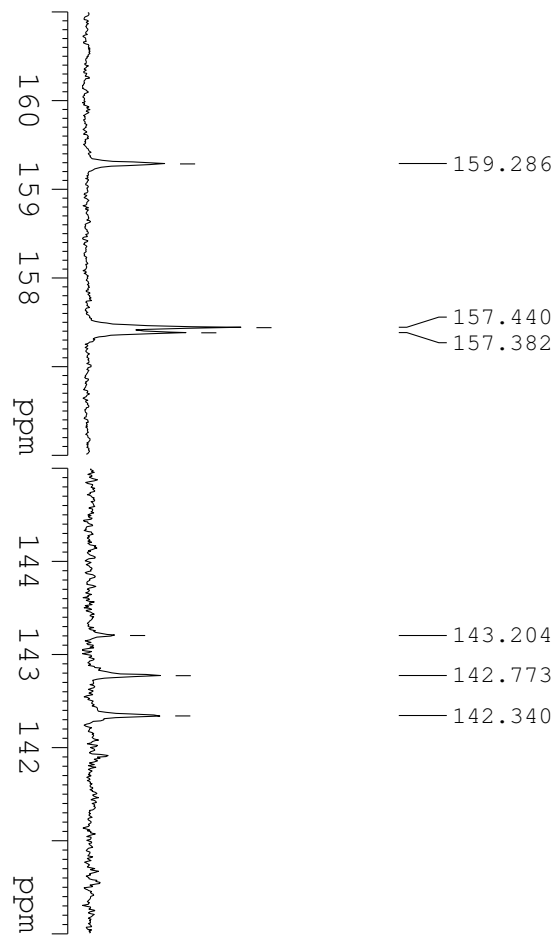
SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 296.2 K

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

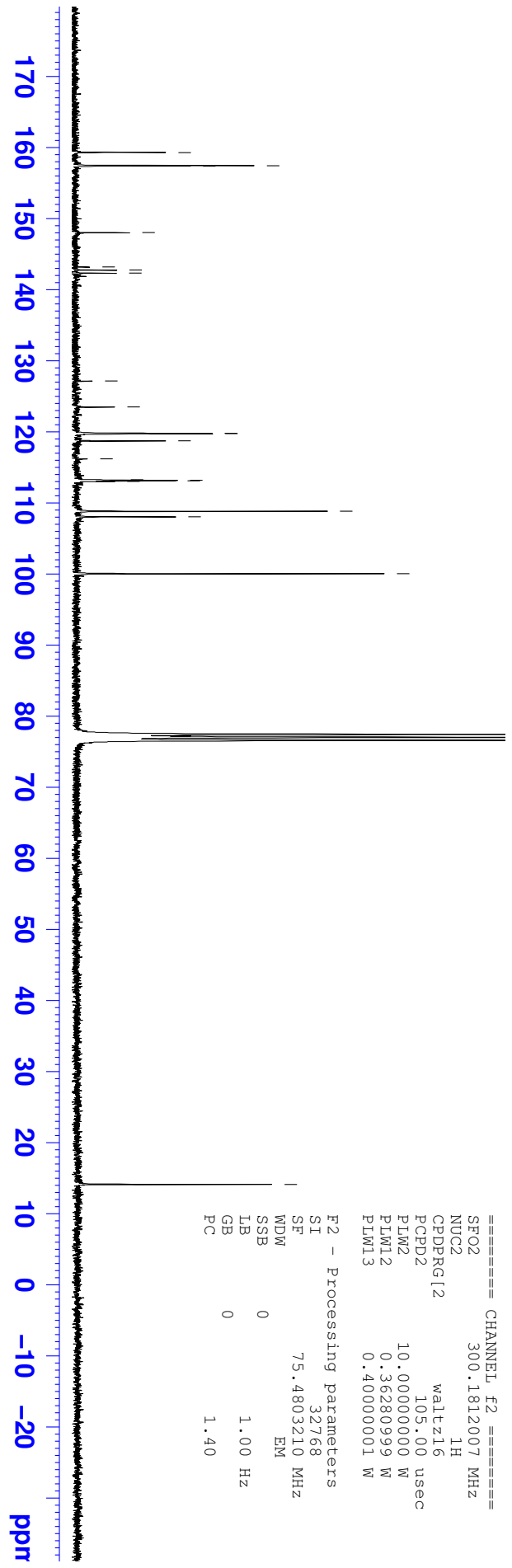
==== CHANNEL F1 =====
 SF01 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

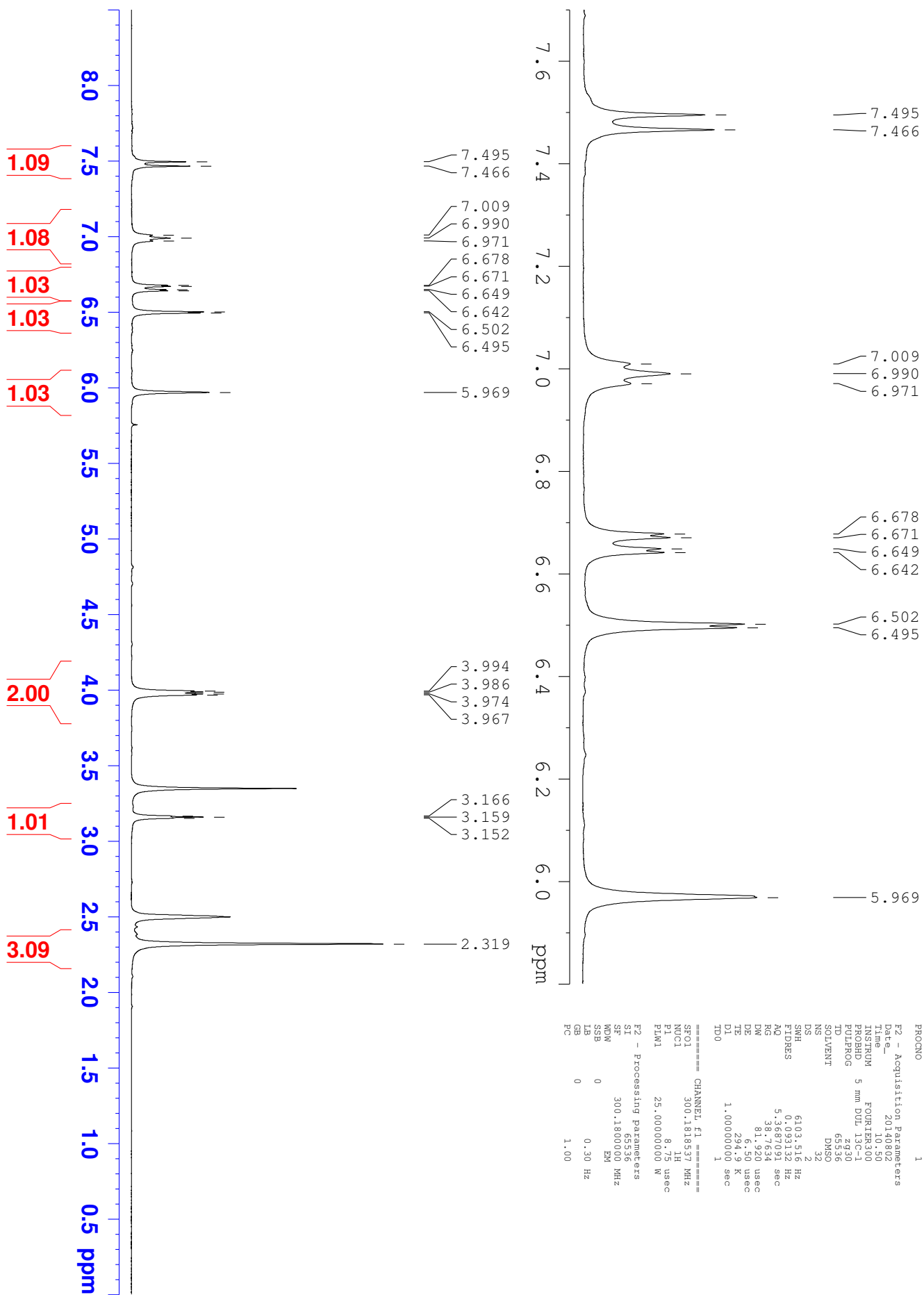
==== CHANNEL F2 =====
 SF02 300.1812007 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.40000001 W

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



- 159.29
- 157.44
- 157.38
- 148.04
- 143.20
- 142.77
- 142.34
- 127.16
- 123.51
- 119.79
- 119.76
- 118.74
- 116.21
- 113.27
- 113.19
- 113.11
- 113.03
- 108.84
- 108.05
- 100.05





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

161.07
 155.78
 154.20
 151.89

126.41

111.15
 110.00
 108.68

97.88

81.60

74.03

32.19

18.50

F2 - Acquisition Parameters

Date_ 20140802
 Time 11.00
 INSTRUM FOURIER300
 PROBD 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

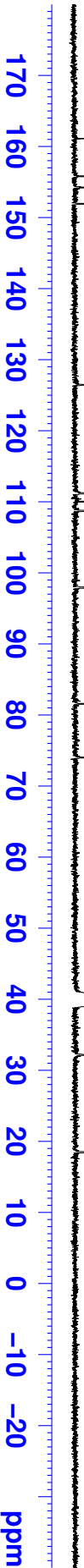
SFO1 75.4878687 MHz
 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

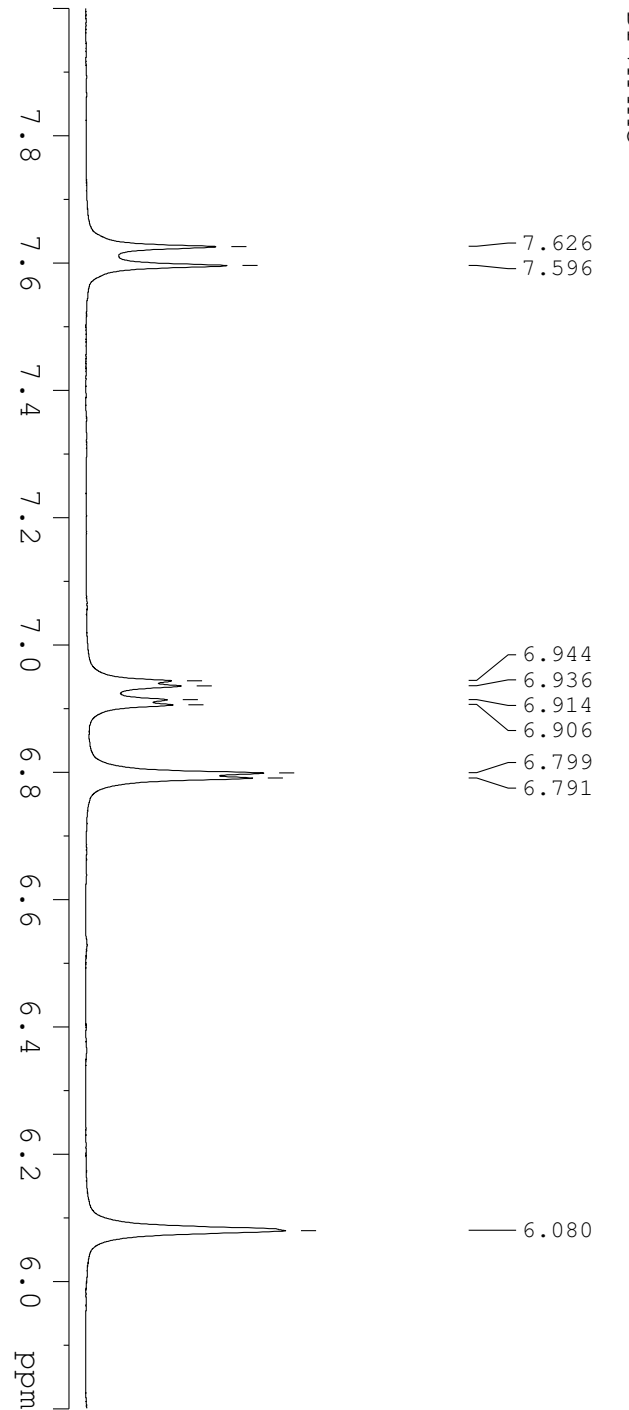
CHANNEL F2

SFO2 300.1812007 MHz
 NUC2 1H
 CPDPRG12 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

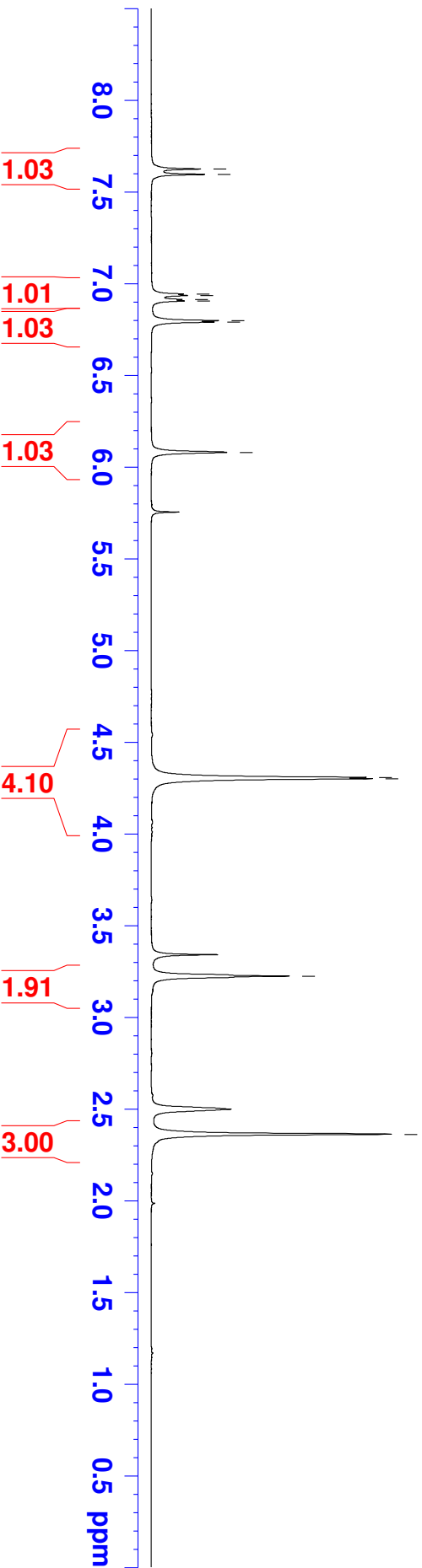




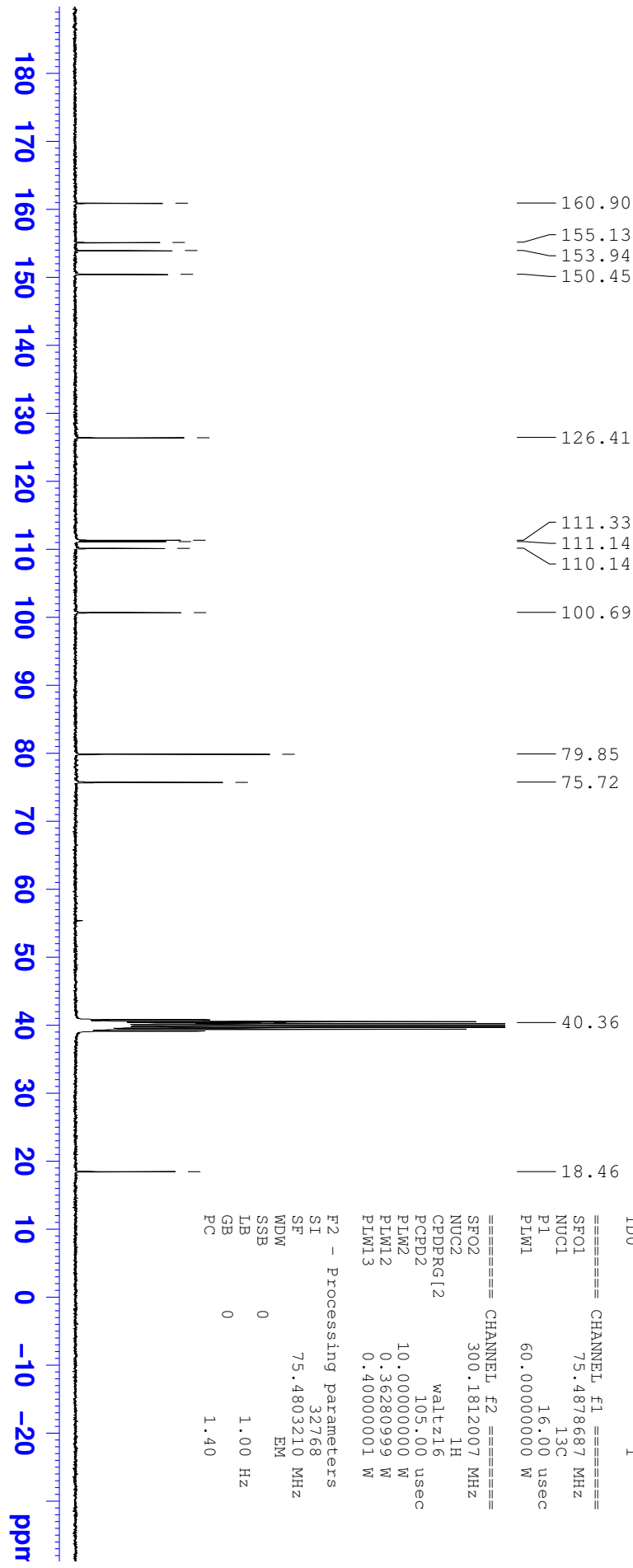
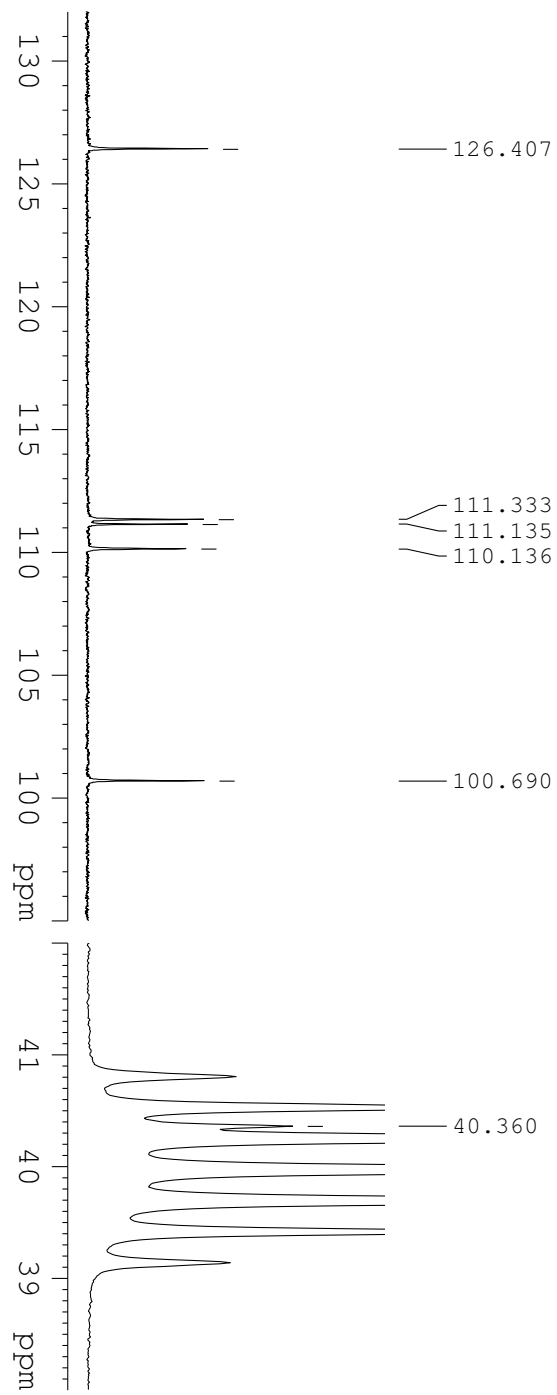
Current Data Parameters
 NAME N,N-Dipropargyl-7-amino-4-methylcoumarin
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140801
 Time 18.32
 INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SFO 125.760
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 6103.516 Hz
 FWHM 0.402116 Hz
 AQ 5.3687091 sec
 RG 30.5672
 DW 81.920 usec
 DE 6.50 usec
 TE 295.2 K
 D1 1.0000000 sec
 TDO 1

CHANNEL f1
 SFO1 300.1818537 MHz
 PULPROG zgpg30
 TD 65536
 SFO 125.7600000 MHz
 P1 8.75 usec
 P1M1 25.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.180000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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



F2 - Acquisition Parameters

Date_ 20140801
 Time 18.41
 INSTRUM FOURIER300
 PROBDH 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
 CPDPRG12 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

78Py4MC

Current Data Parameters
 NAME 78-Pyridino-4-methylcoumarin
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140802
 Time_ 21.42

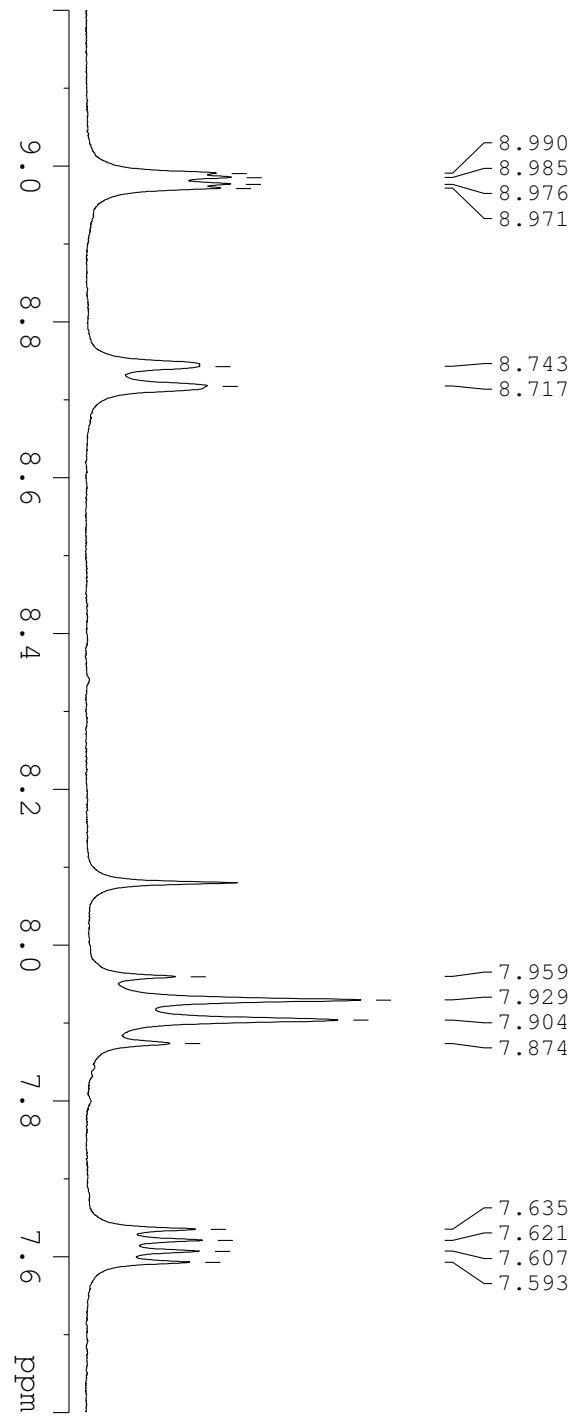
INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32

DS 2
 SMH 6103.516 Hz
 FIDRES 0.093132 Hz
 AO 5.3687091 sec
 RG 91.0222

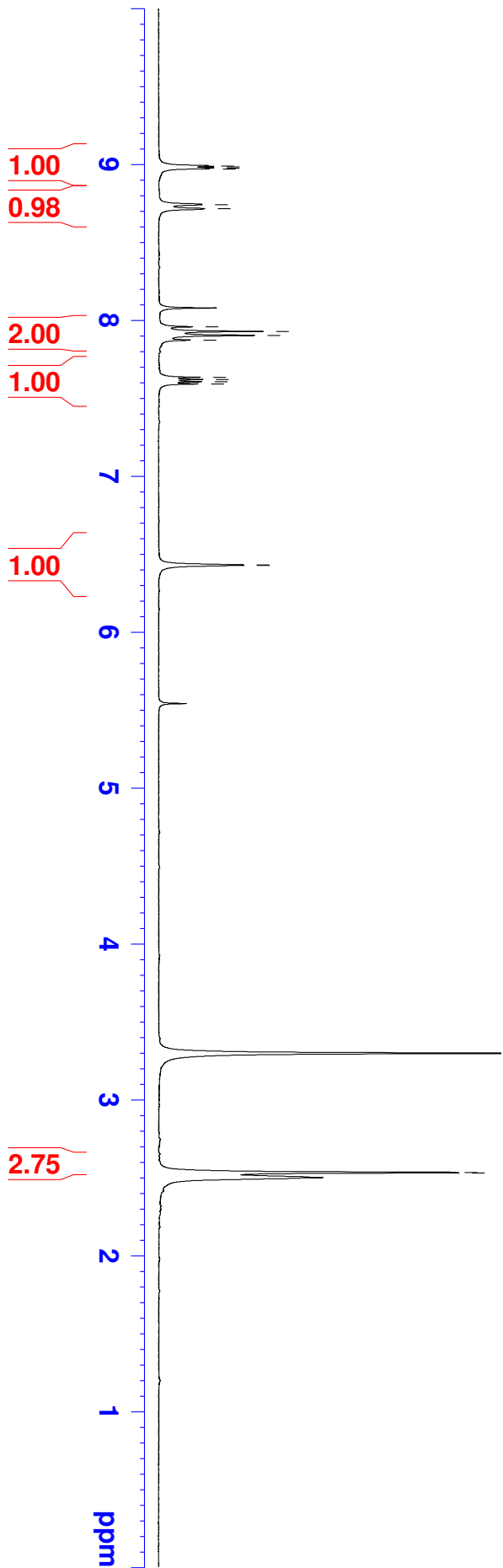
DW 81.920 usec
 DE 6.50 usec
 TE 295.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFOL 300.1818537 MHz
 NUCL1 1H
 P1 8.75 usec
 PLWL 25.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 MDM 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



4M78PyC (Compound 27)



Current Data Parameters
 NAME 78-PyrIdino-4-methylcol
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140802
 Time 21.53
 INSTRUM FOURIER300
 PROBD 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
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.40000001 W

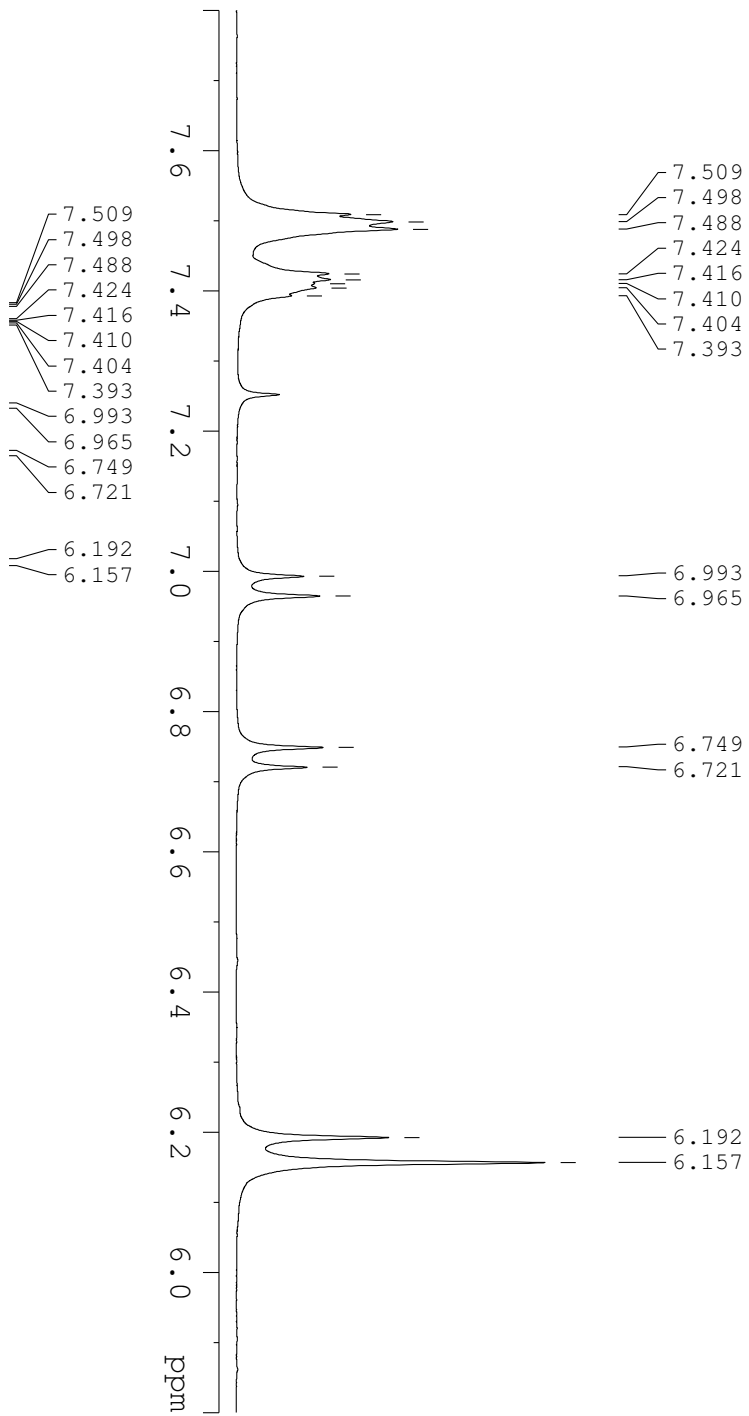
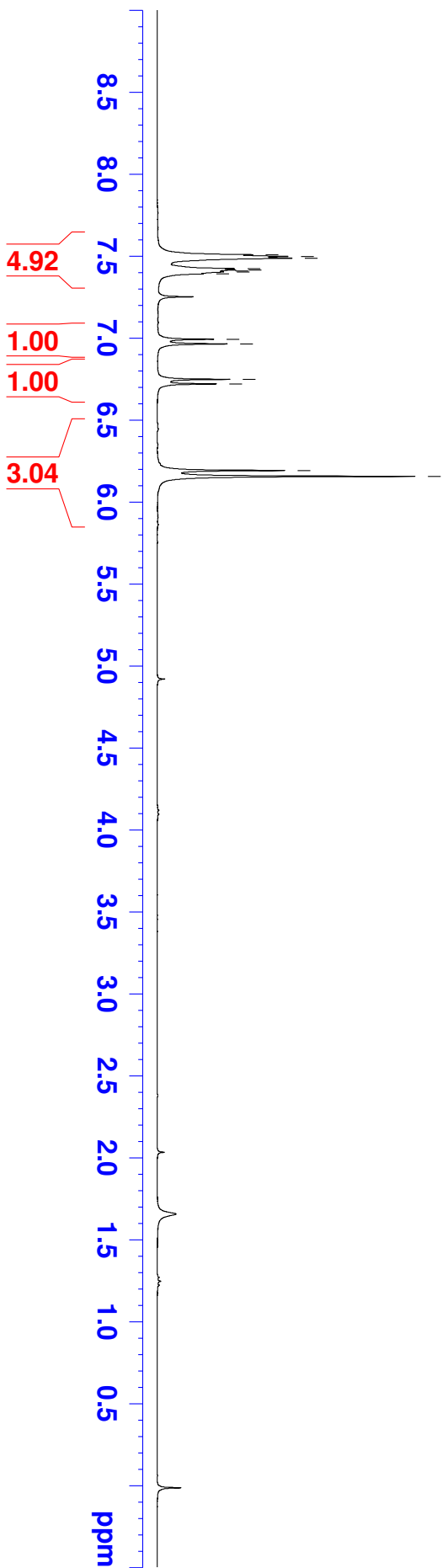
F2 - Processing parameters

SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

- 159.76
- 153.76
- 152.61
- 149.79
- 149.09
- 130.67
- 125.40
- 124.70
- 122.45
- 118.33
- 115.78
- 114.83
- 19.19



78DO4PC



```

Current Data Parameters
NAME          78DO4PC
EXPNO        1
PROCNO       1
F2 - Acquisition Parameters
Date_        20140529
Time         10:01
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           32
DW           81.920 usec
DE           6.50 usec
TE           295.8 K
D1           1.00000000 sec
TD0          1

===== CHANNEL f1 =====
SFO1        300.1818537 MHz
NUC1         1H
P1           8.75 usec
PLM1        25.00000000 W

F2 - Processing parameters
SI           65536
SF           300.1800072 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
    
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Current Data Parameters
 NAME 78DO4PC
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140529
 Time 10.09

INSTRUM FOURIER300
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2000
 DS 4

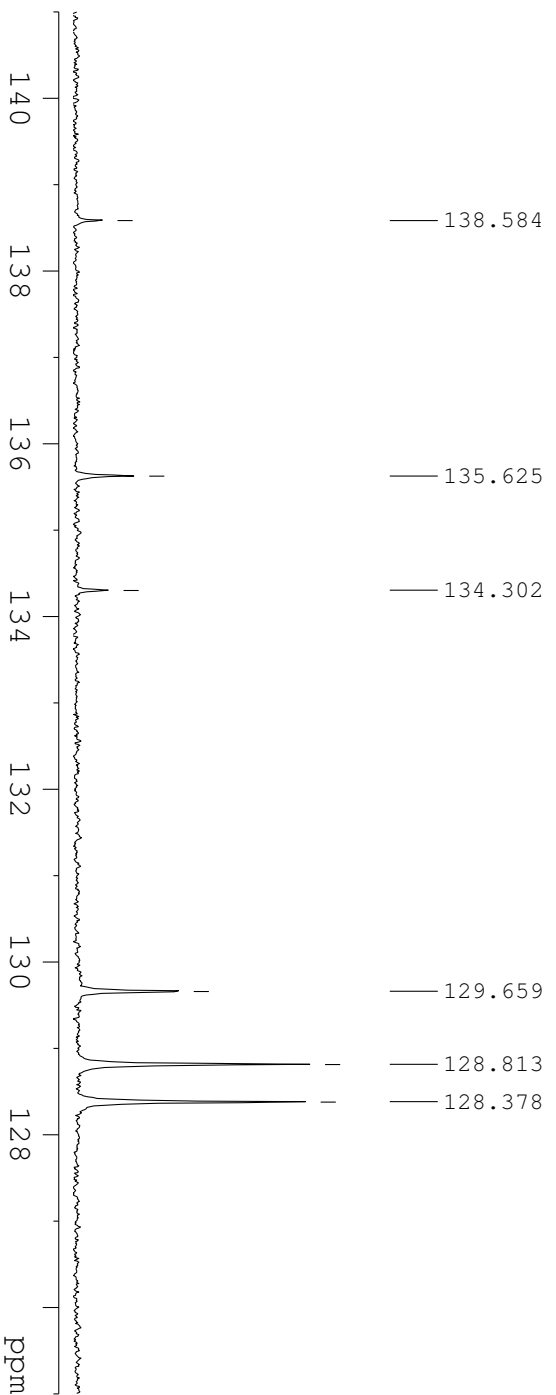
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 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 296.1 K

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

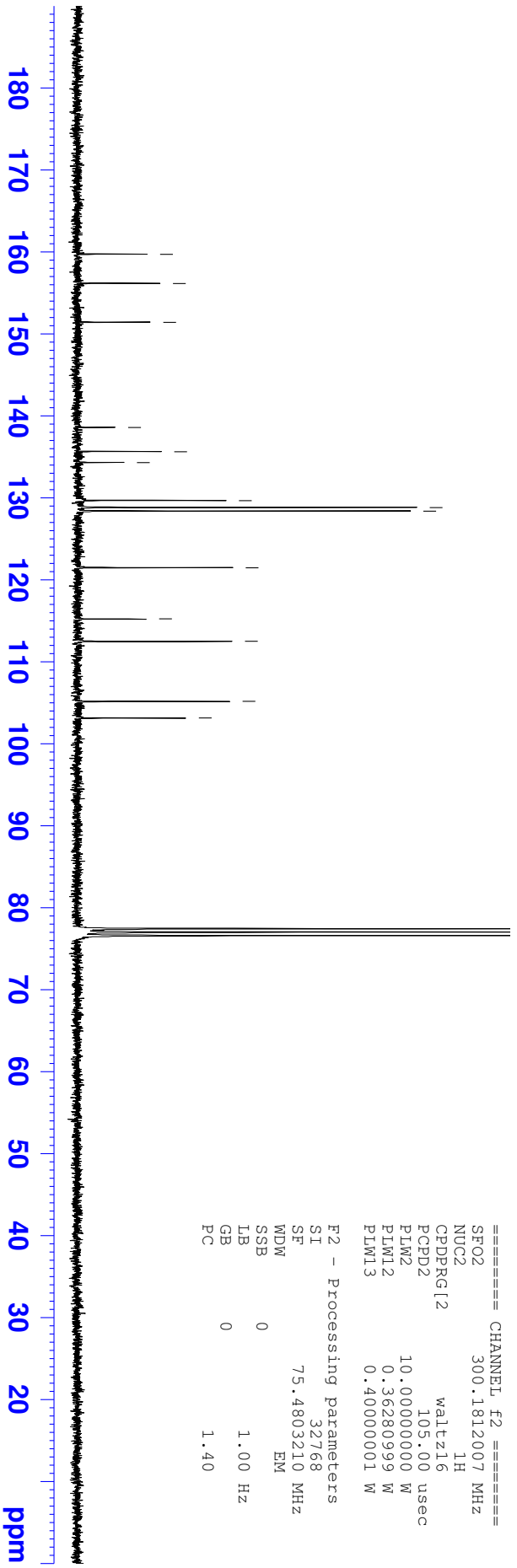
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 NUC1 13C
 P1 16.00 usec
 PLW1 60.00000000 W

==== CHANNEL F2 =====
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 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 105.00 usec
 PLW2 10.00000000 W
 PLW12 0.36280999 W
 PLW13 0.400000001 W

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



- 159.71
- 156.15
- 151.41
- 138.58
- 135.63
- 134.30
- 129.66
- 128.81
- 128.38
- 121.47
- 115.24
- 112.51
- 105.18
- 103.15



Atlantic Microlab, Inc.

Sample No. 78FF
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
 www.atlanticmicrolab.com

Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125

Professor/Supervisor: Dr Maryam Foroozesh Name Jiawang Liu Date 08/19/2014
 PO# / CC# P0050279 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/>	Duplicate <input checked="" type="checkbox"/>
C	78.25	78.05	77.95	Elements Present: C, H, O Analyze for: C, H Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. _____ B.P. _____ To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/> Temp. _____ Vac. _____ Time _____ Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small> Include Email Address or FAX # Below mforooze@xula.edu	
H	4.38	4.48	4.41		

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

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Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125

Professor/Supervisor: Dr Maryam Foroozesh Name Jiawang Liu Date 08/19/2014
 PO# / CC# P0050279 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/>	Duplicate <input checked="" type="checkbox"/>
C	73.77	73.42	73.47	Elements Present: C, H, O Analyze for: C, H Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. _____ B.P. _____ To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/> Temp. _____ Vac. _____ Time _____ Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small> Include Email Address or FAX # Below mforooze@xula.edu	
H	4.14	4.14	4.22		

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 Remarks: _____

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 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh Name Jiawang Liu Date 08/29/2014
 PO# / CC# P0050279 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/>	
				Elements Present:	Analyze for:
C	79.11	77.73	77.82	C, H, O, N	
H	4.06	4.37	4.29	C, H, N	
N	5.13	4.98	4.91	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below	
				mforooze@xula.edu	

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

Remarks:

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Sample No. 78DOF
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 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh Name Jiawang Liu Date 08/19/2014
 PO# / CC# P0050279 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/>	
				Elements Present:	Analyze for:
C	72.18	71.92	71.97	C, H, O	
H	3.79	3.87	3.85	C, H	
				Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below	
				mforooze@xula.edu	

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Remarks:

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Sample No. 4P78PC
 6180 Atlantic Blvd. Suite M
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Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125

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

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

Element	Theory	Found		Single <input type="checkbox"/>	Duplicate <input checked="" type="checkbox"/>
				Elements Present: C, H, O	
C	78.25	78.23	78.11	Analyze for: C, H	
H	4.38	4.48	4.43	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below mforooze@xula.edu	

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Sample No. 3M4P78PC
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Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125

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

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

Element	Theory	Found		Single <input type="checkbox"/>	Duplicate <input checked="" type="checkbox"/>
				Elements Present: C, H, O	
C	78.61	77.07	77.12	Analyze for: C, H	
H	4.86	5.03	5.08	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below mforooze@xula.edu	

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 Remarks:

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Sample No. 4M78PC
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Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125

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

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

Element	Theory	Found		Single <input type="checkbox"/>	Duplicate <input checked="" type="checkbox"/>
				Elements Present: C, H, O	
C	72.89	72.61	72.62	Analyze for: C, H	
H	4.71	4.74	4.67	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below	
				mforooze@xula.edu	

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 Remarks: _____

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Sample No. 4TF78PC
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 Norcross, GA 30071
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Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125

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

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

Element	Theory	Found		Single <input type="checkbox"/>	Duplicate <input checked="" type="checkbox"/>
				Elements Present: C, H, O, F	
C	58.22	57.99	57.96	Analyze for: C, H, F	
H	2.63	2.47	2.46	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
F	21.25	21.12	21.12	M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below	
				mforooze@xula.edu	

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 Remarks: _____

Atlantic Microlab, Inc.

Sample No. 4P78FC
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 Norcross, GA 30071
 www.atlanticmicrolab.com
 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh
 PO# / CC# P0050279
 Name Jlawang Liu Date 08/28/2014
 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/> Elements Present: <u>C, H, O</u> Analyze for: <u>C, H</u> Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. _____ B.P. _____ To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/> Temp. _____ Vac. _____ Time _____ Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small> Include Email Address or FAX # Below mforooze@xula.edu
C	78.25	77.76	77.64	
H	4.38	4.49	4.54	

Date Received SEP 2 2 P.M. Date Completed SEP 2 3 2014
 Remarks: _____

Atlantic Microlab, Inc.

Sample No. 3M4P78FC
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
 www.atlanticmicrolab.com
 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh
 PO# / CC# P0050279
 Name Jlawang Liu Date 08/28/2014
 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/> Elements Present: <u>C, H, O</u> Analyze for: <u>C, H</u> Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/> M.P. _____ B.P. _____ To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/> Temp. _____ Vac. _____ Time _____ Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small> Include Email Address or FAX # Below mforooze@xula.edu
C	78.61	78.24	78.31	
H	4.86	5.14	5.17	

Date Received SEP 2 2 P.M. Date Completed SEP 2 3 2014
 Remarks: _____

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Sample No. 4M78FC
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 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh Name Jiawang Liu Date 08/28/2014
 PO# / CC# P0050279 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/>	
				Elements Present:	Analyze for:
C	72.89	72.51	72.63	C, H, O	
H	4.71	4.96	5.03	C, H	
				Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below	
				mforooze@xula.edu	
Date Received		SEP 22 P.M.		Date Completed	
Remarks:				SEP 23 2014	

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Sample No. 4TF78FC
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 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh Name Jiawang Liu Date 08/28/2014
 PO# / CC# P0050279 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/>	
				Elements Present:	Analyze for:
C	58.22	58.17	58.14	C, H, O, F	
H	2.63	2.51	2.64	C, H, F	
F	21.25	21.48	21.42	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below	
				mforooze@xula.edu	
Date Received		SEP 22 P.M.		Date Completed	
Remarks:				SEP 23 2014	

Atlantic Microlab, Inc.

Sample No. 4M78PyC
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
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 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh Name Jlawang Liu Date 08/28/2014
 PO# / CC# P0050279 Phone (504) 638-4036

Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/>	
				Elements Present:	Analyze for:
C	73.92	71.44	71.58	C, H, O, N	
H	4.29	4.44	4.50	C, H, N	
N	6.63	6.31	6.23	Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below mforooze@xula.edu	

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

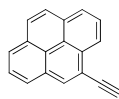
Atlantic Microlab, Inc.

Sample No. 4P78DOC
 6180 Atlantic Blvd. Suite M
 Norcross, GA 30071
 www.atlanticmicrolab.com
 Company/School Xavier University of Louisiana
 Dept. Chemistry
 Address 1 Drexel Dr
 City, State, Zip New Orleans, LA 70125
 Professor/Supervisor: Dr Maryam Foroozesh Name Jlawang Liu Date 08/28/2014
 PO# / CC# P0050279 Phone (504) 638-4036

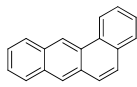
Element	Theory	Found		Single <input type="checkbox"/> Duplicate <input checked="" type="checkbox"/>	
				Elements Present:	Analyze for:
C	72.18	72.11	71.97	C, H, O	
H	3.79	4.01	3.91	C, H	
				Hygroscopic <input type="checkbox"/> Explosive <input type="checkbox"/>	
				M.P. _____ B.P. _____	
				To be dried: Yes <input type="checkbox"/> No <input checked="" type="checkbox"/>	
				Temp. _____ Vac. _____ Time _____	
				Rush Service <input type="checkbox"/> <small>Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.</small>	
				Include Email Address or FAX # Below mforooze@xula.edu	

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

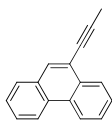
Structures of P450 1A2 Inhibitors Used for Alignment Study



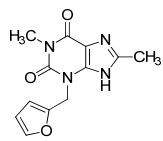
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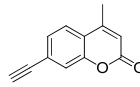
Benz[a]anthracene



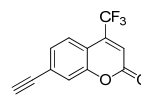
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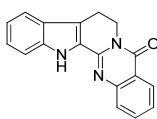
Furafylline



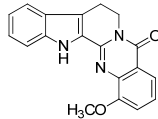
7E4MC



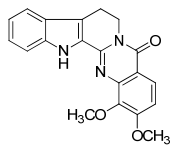
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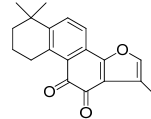
Rutacarpine



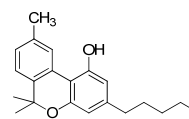
Rutacarpine derivative 5



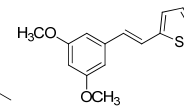
Rutacarpine derivative 8



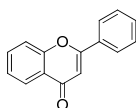
Tanshinone IIA



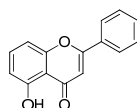
CBN



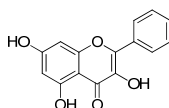
DMPVT



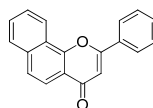
Flavone



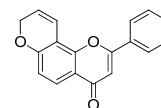
5-Hydroxyflavone (5HF)



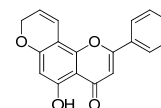
3,5,7-Trihydroxyflavone



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 $^{\circ}\text{C}$ in CO_2 -incubator, and fluorescence 560Ex/590Em base reading was taken using Synergy H1 multiplate reader (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 fluorescence 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.

