

Synthesis and Antiproliferative Activity of (Z)-1-Glycosyl-3-(5-oxo-2-thioxoimidazolidin-4-ylidene)indolin-2-ones and (Z)-3-(2-Glycosylsulfanyl-4-oxo-4,5-dihydro-thiazol-5-ylidene)indolin-2-ones

Friedrich Erben^a, Dirk Michalik^{a,b}, Holger Feist^a, Dennis Kleeblatt^a, Martin Hein^a, Abdul Matin,^c Jamshed Iqbal,^d Peter Langer^{*a,b}

^a Institut für Chemie, Universität Rostock, Albert-Einstein-Str. 3a, 18059 Rostock, Germany
Fax: +49 (381)4986412, E-mail: peter.langer@uni-rostock.de

^b Leibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Str. 29a, 18059 Rostock, Germany

^c Institute of Biomedical and Genetic Engineering, PO Box: 2891, Sector: G-9/1, Islamabad, 44000, Pakistan

^d Department of Pharmaceutical Sciences, COMSATS Institute of Information Technology, Abbottabad, Postal Code 22060, Pakistan

Supporting Information

Contents:

Copies of NMR Spectra

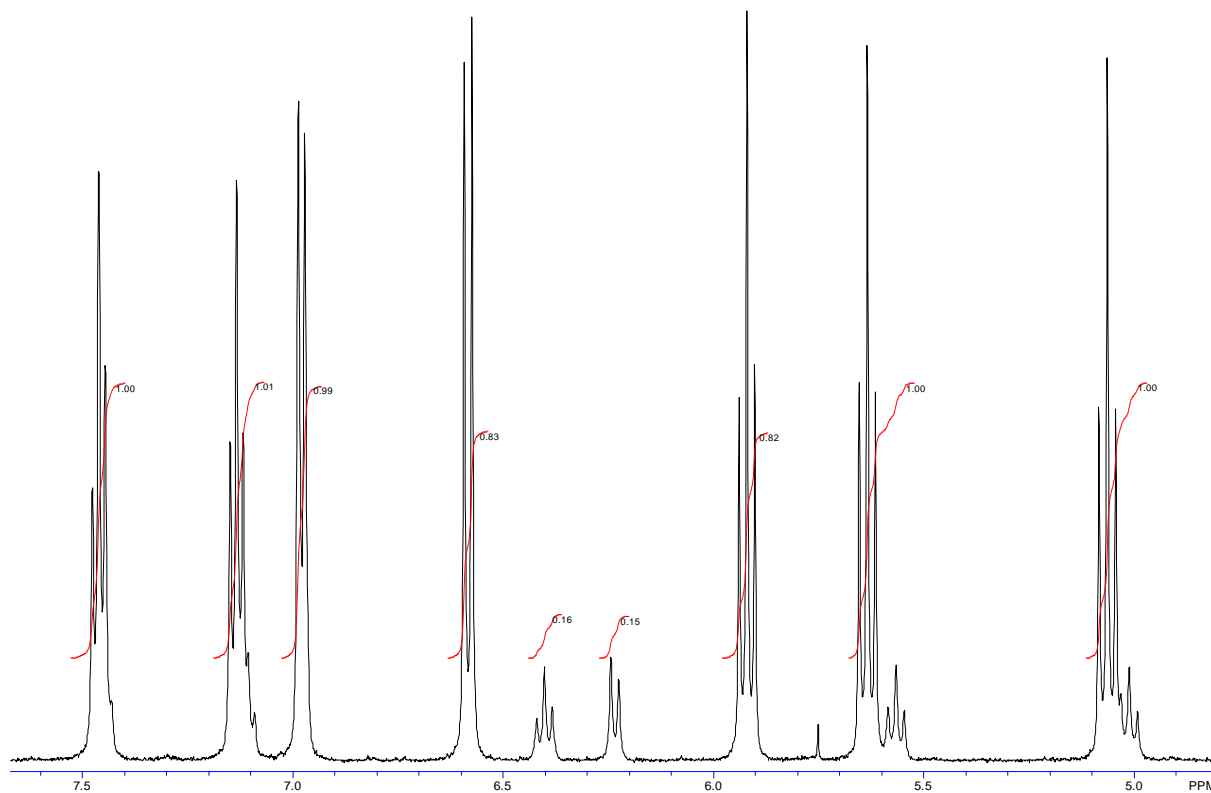
NMR Spectra of **12a** at elevated temperature

Fig. 1: ¹H-NMR-Spectrum of **12a** in DMSO-d₆ at 20 °C.

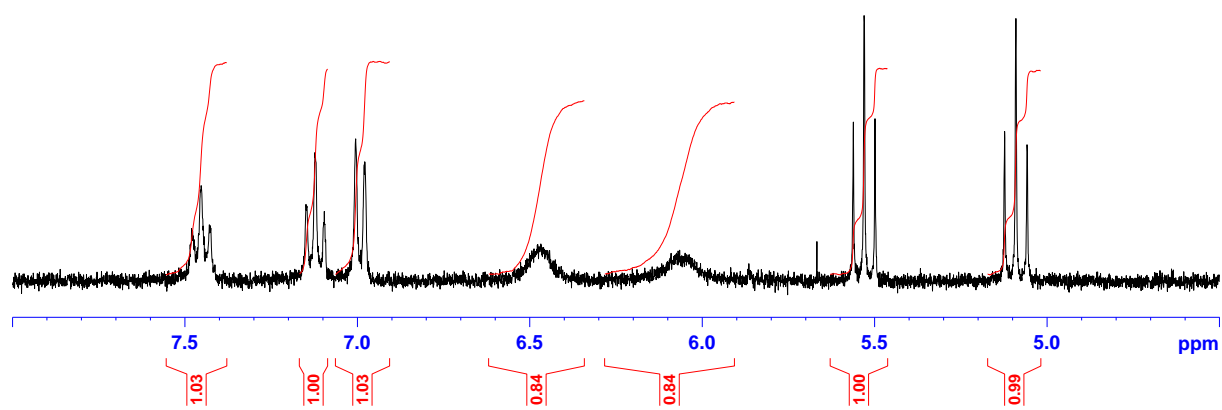


Fig. 2: ¹H-NMR-Spectrum of **12a** in DMSO-d₆ at 90 °C.

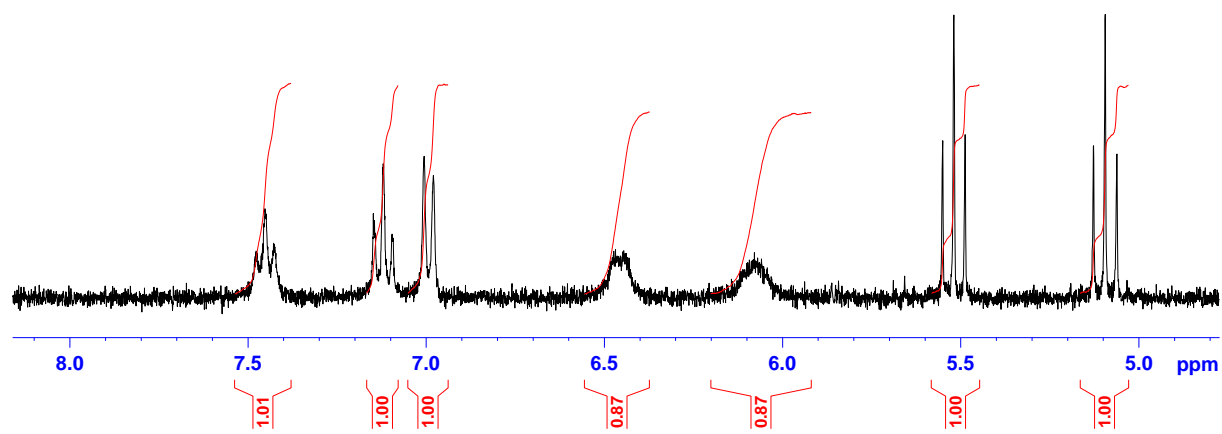


Fig. 3: ¹H-NMR-Spectrum of **12a** in DMSO-d₆ at 100 °C.

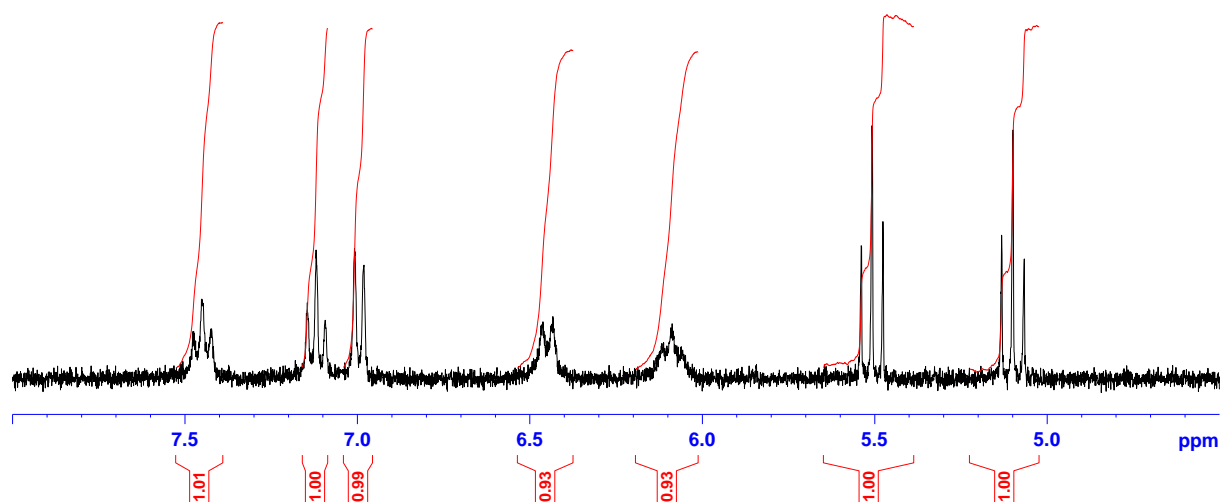


Fig. 4: $^1\text{H-NMR}$ -Spectrum of **12a** in DMSO-d_6 at $110\text{ }^\circ\text{C}$.

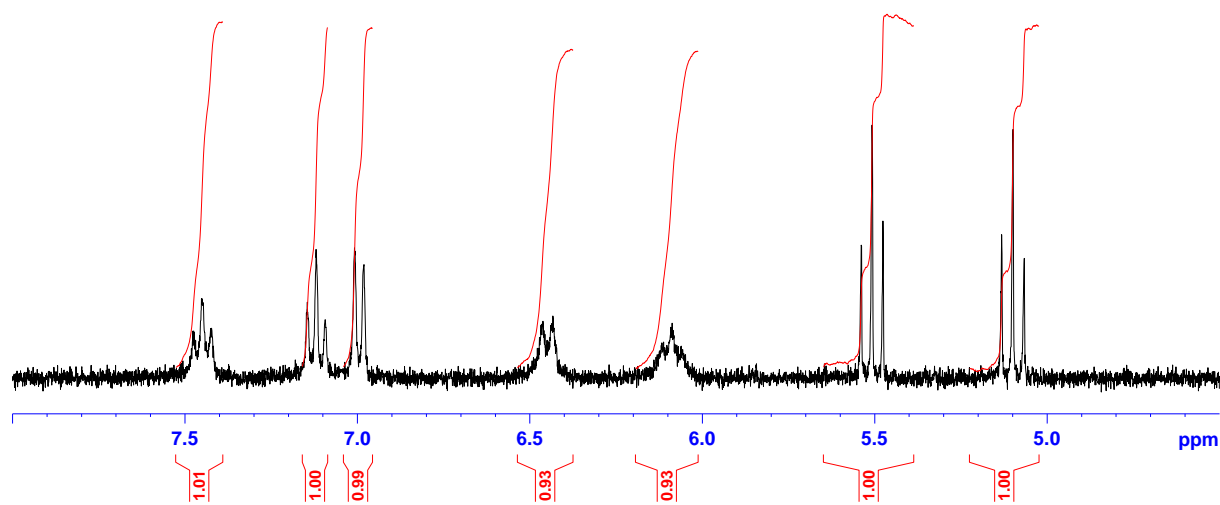


Fig. 5: $^1\text{H-NMR}$ -Spectrum of **12a** in DMSO-d_6 at $120\text{ }^\circ\text{C}$.

Erben 1H in CDC13

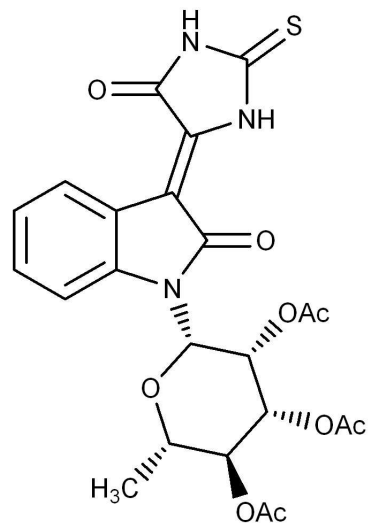


— 11.163

9.275
8.617
8.602
7.540
7.524
7.310
7.309
7.294
7.279
7.278
7.077
7.062
7.046
5.923
5.921
5.591
5.589
5.585
5.582
5.327
5.320
5.307
5.300
5.251
5.232
5.212

2.102
1.986
1.808
1.387
1.375

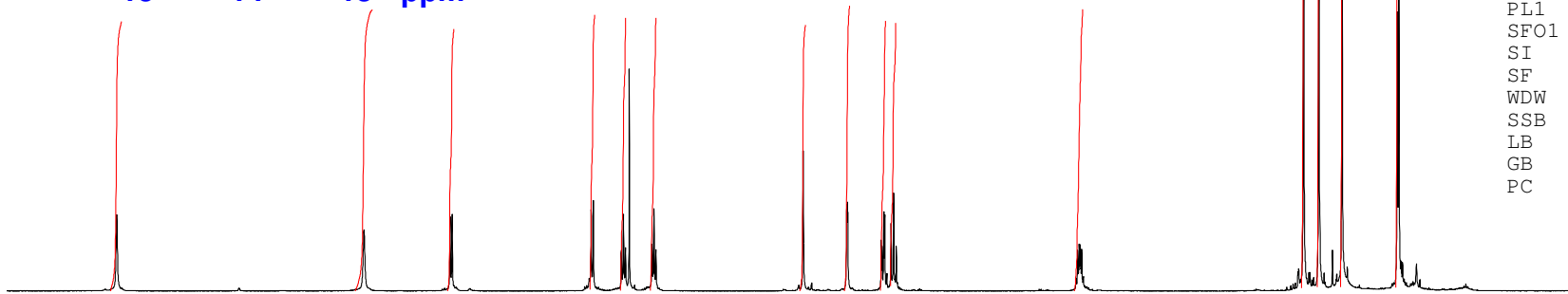
5a



NAME 101112.503
EXPNO 10
PROCNO 1
Date_ 20101114
Time 3.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 15015.015 Hz
FIDRES 0.229111 Hz
AQ 2.1824322 sec
RG 101.6
DW 33.300 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1350013 MHz
SI 32768
SF 500.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

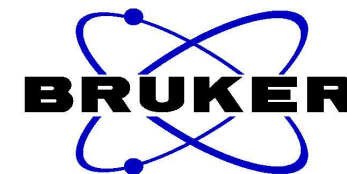
15 14 13 ppm



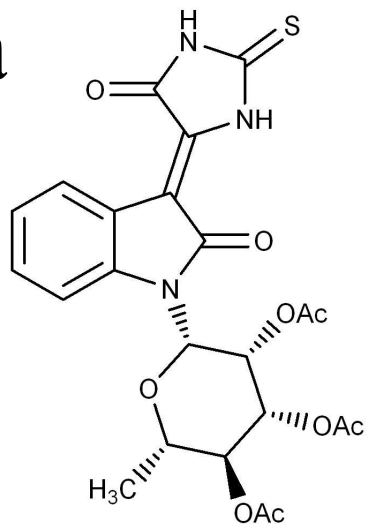
11 10 9 8 7 6 5 4 3 2 1 ppm

1.03 1.07 1.00 1.05 1.04 1.04 1.02 1.09 1.03 1.02 1.08 3.06 3.05 3.02 3.08

Erben ¹³C in CDCl₃



5a

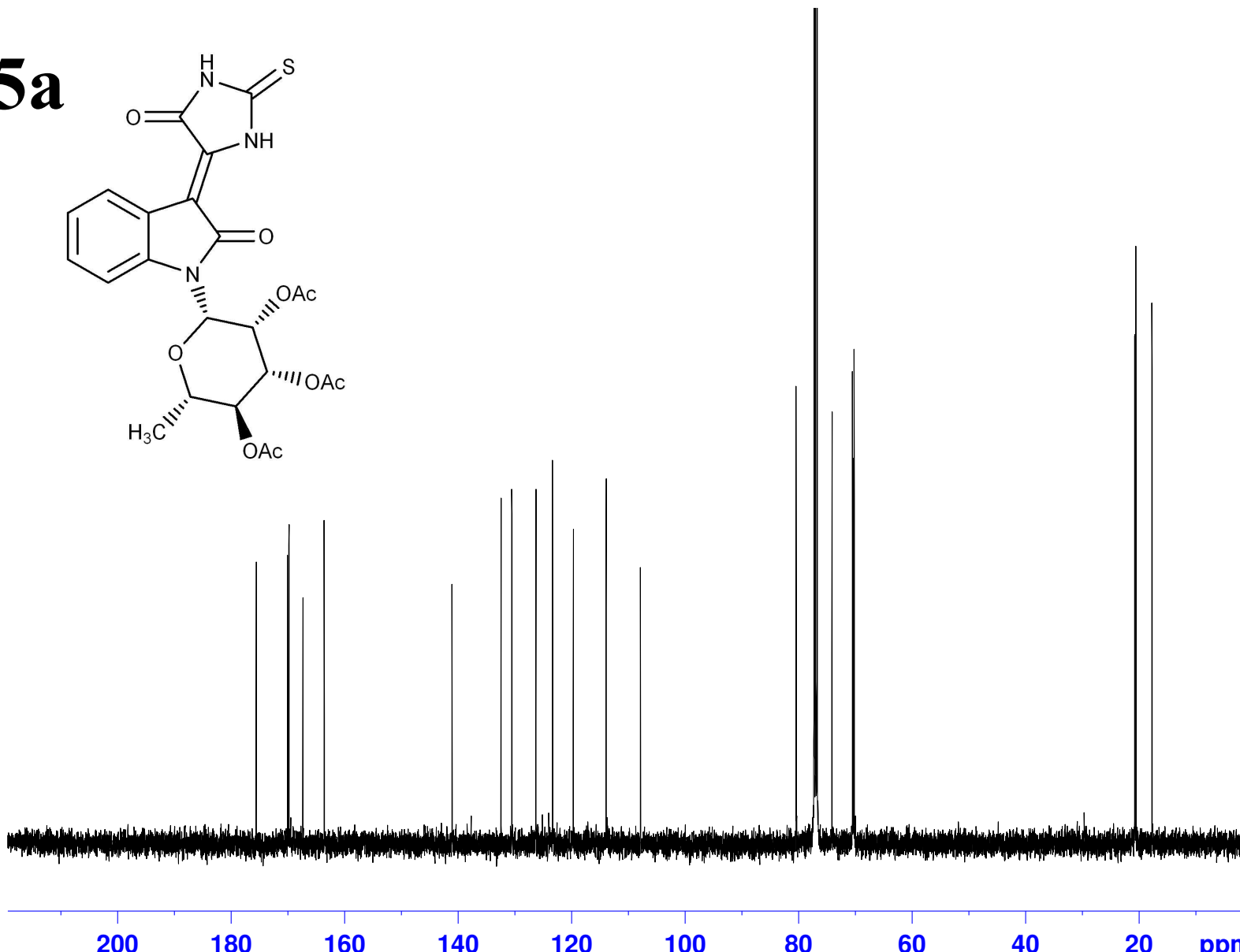


175.60
170.07
169.88
169.83
167.38
163.61

141.08
132.44
130.55
126.31
123.37
119.71
113.93
107.89

80.44
74.12
70.51
70.27
70.20

20.78
20.74
20.55
17.71

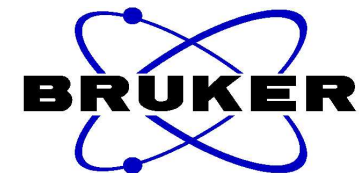


NAME 101112.503
EXPNO 17
PROCNO 1
Date_ 20101114
Time 13.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 128
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

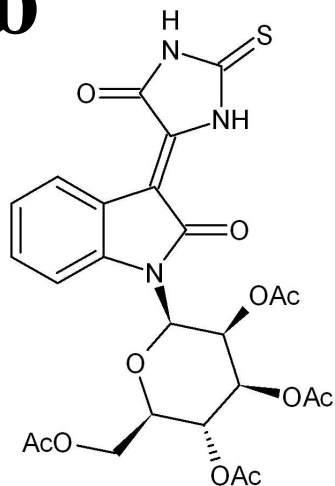
==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577934 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

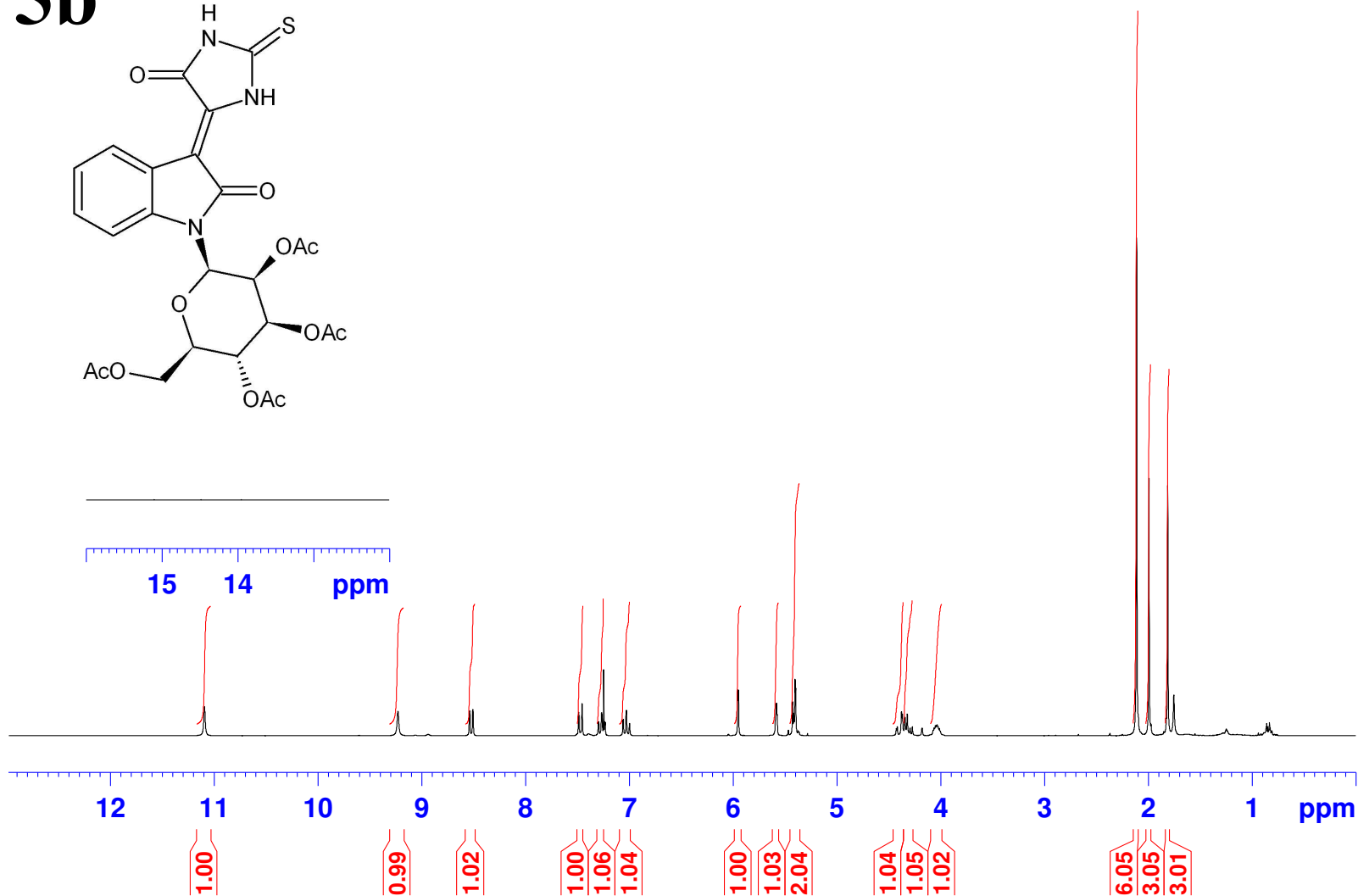
Erben 1H CDC13



5b



11.092
9.232
8.543
8.540
8.511
8.509
7.490
7.458
7.302
7.297
7.271
7.267
7.239
7.234
7.064
7.060
7.033
7.029
7.002
6.998
5.957
5.951
5.594
5.589
5.583
5.578
4.430
4.420
4.380
4.371
4.346
4.324
4.297
4.275
2.114
1.994
1.813



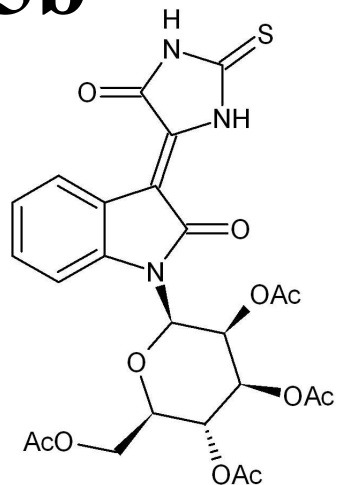
NAME 110609.217
EXPNO 10
PROCNO 1
Date_ 20110609
Time 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 724
DW 96.800 usec
DE 10.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.1300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C CDC13



5b

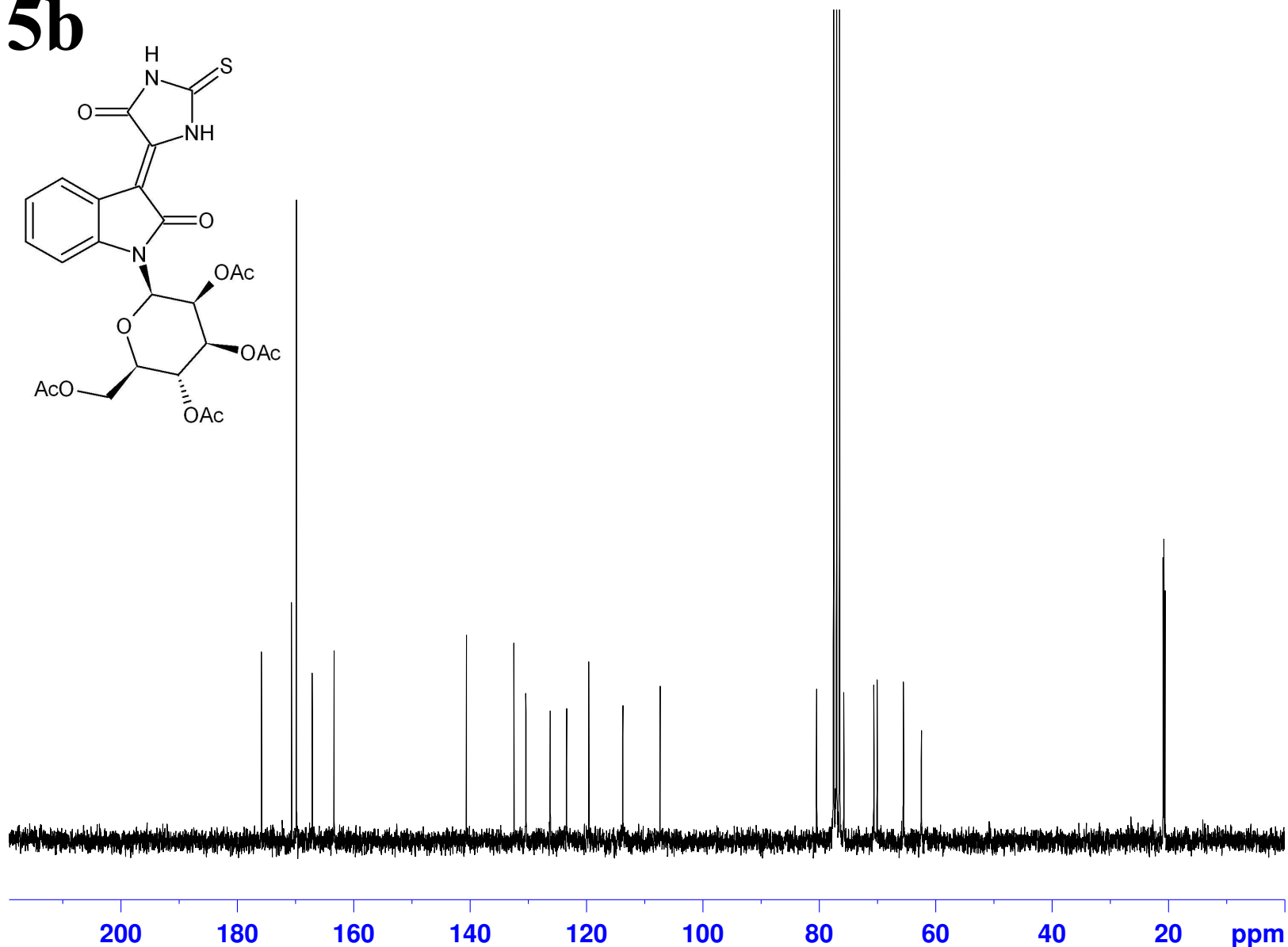


175.86
170.69
169.85
167.11
163.36

140.62
132.45
130.40
126.23
123.40
119.61
113.74
107.33

80.43
75.76
70.59
70.03
65.50
62.42

20.87
20.74
20.71
20.53

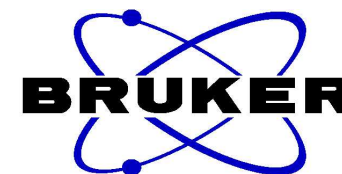


NAME 110610.208
EXPNO 10
PROCNO 1
Date_ 20110611
Time 1.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

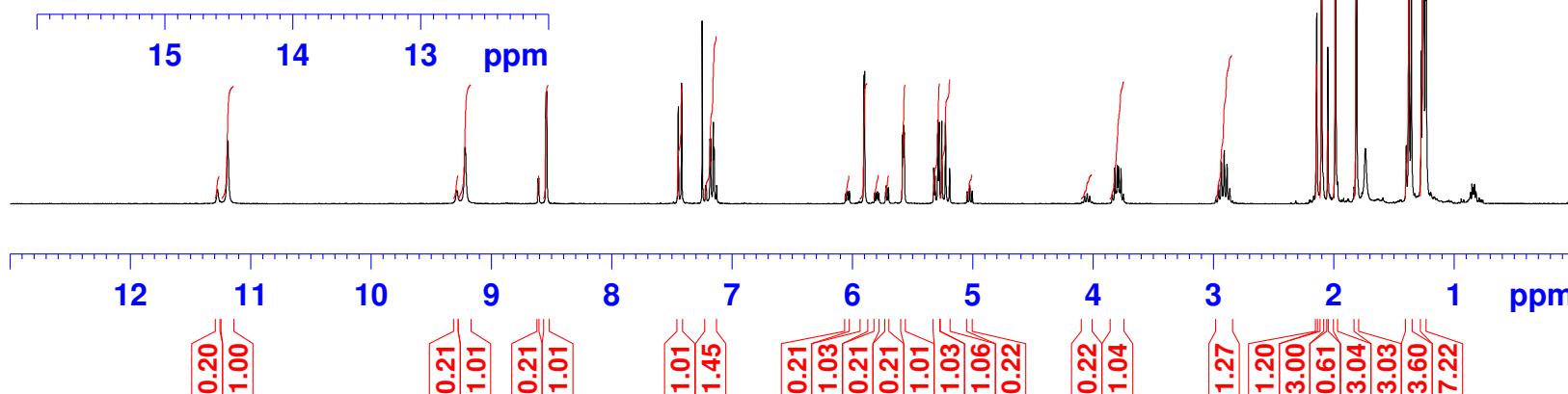
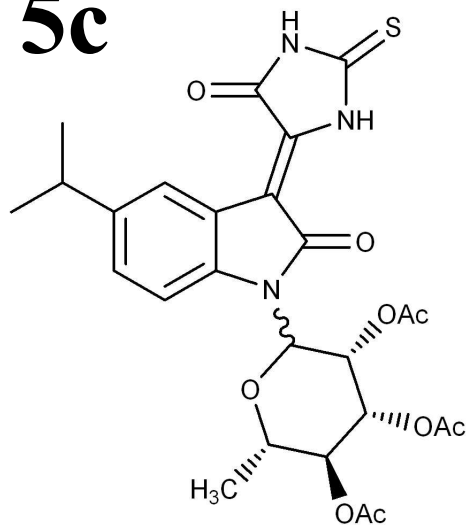
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952402 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H CDC13



11.192
9.220
8.613
8.608
8.547
8.541
7.449
7.421
7.221
7.216
7.185
7.179
7.157
7.151
7.130
5.904
5.900
5.722
5.585
5.580
5.574
5.570
5.325
5.314
5.291
5.280
5.258
5.227
5.194
5.026
2.957
2.934
2.911
2.888
2.145
2.141
2.101
2.050
1.985
1.812
1.398
1.376
1.356
1.274
1.262
1.255
1.239
1.232

5c

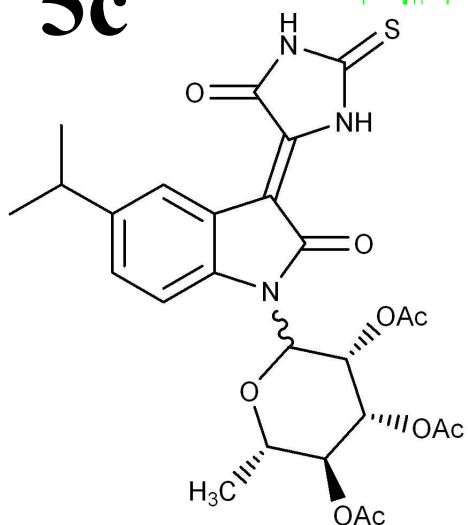


NAME 110621.u317
EXPNO 10
PROCNO 1
Date_ 20110621
Time 14.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



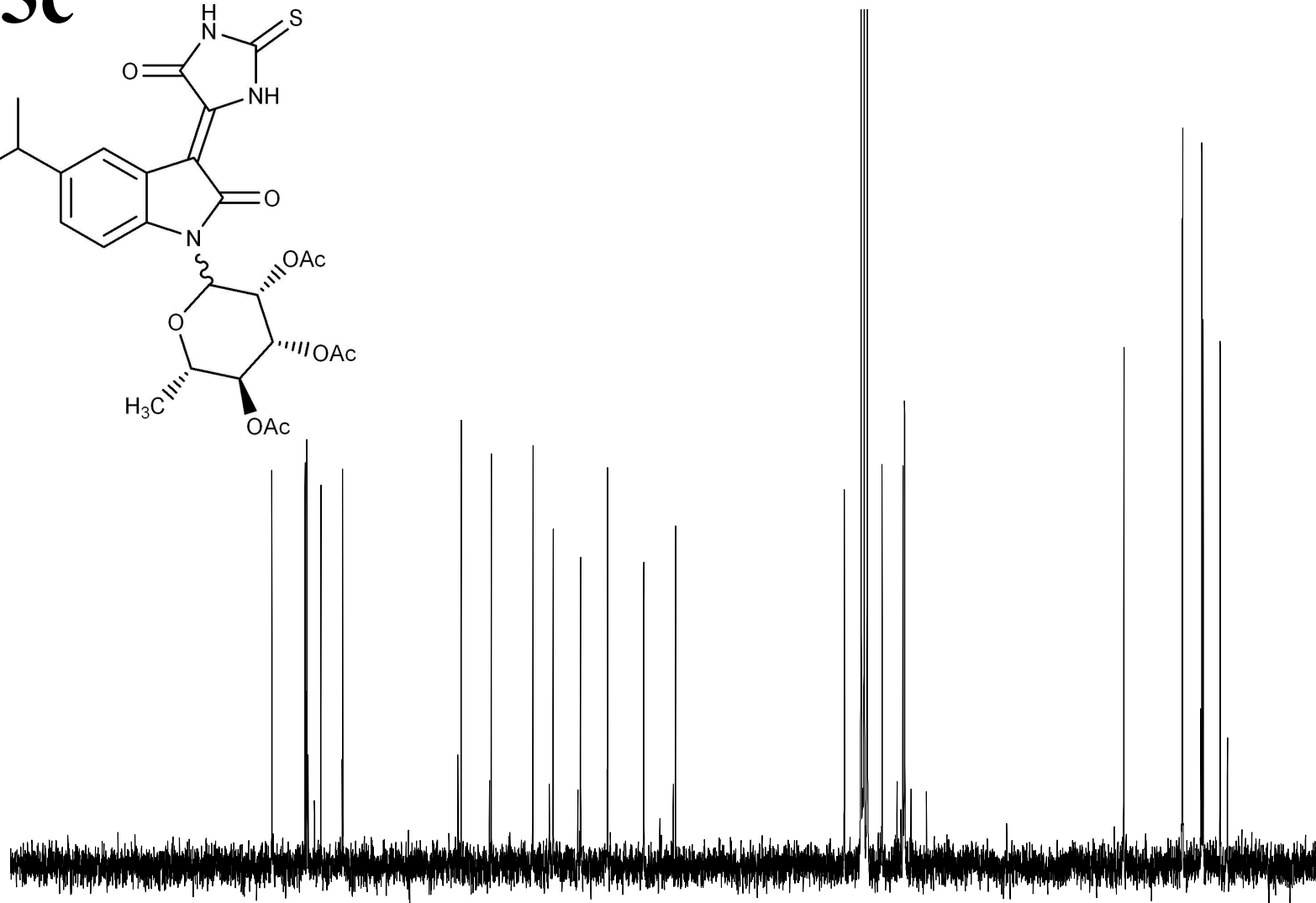
5c



175.71
175.67
170.14
169.90
169.88
169.84
169.79
169.63
168.57
167.52
163.97
163.88
144.68
144.14
139.43
139.11
132.25
132.18
129.48
128.82
124.71
124.25
119.82
119.74
113.74
108.82
108.43

80.31
74.03
71.54
70.92
70.55
70.29
70.25
69.20
66.65

33.81
33.74
24.04
23.96
20.92
20.78
20.75
20.54
17.70
16.49



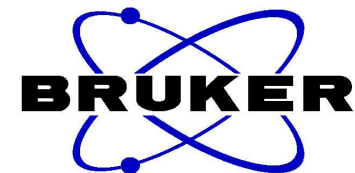
NAME 110622.205
EXPNO 10
PROCNO 1
Date_ 20110622
Time 20.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 use
DE 10.00 use
TE 300.3 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 use
PL1 -1.00 dB
SFO1 62.9015280 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 use
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952409 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

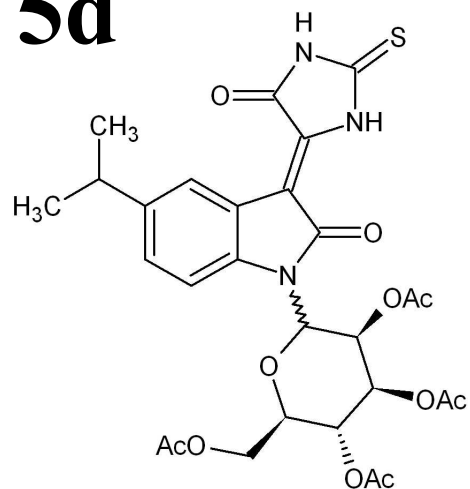
200 180 160 140 120 100 80 60 40 20 ppm

Erben 1H CDC13

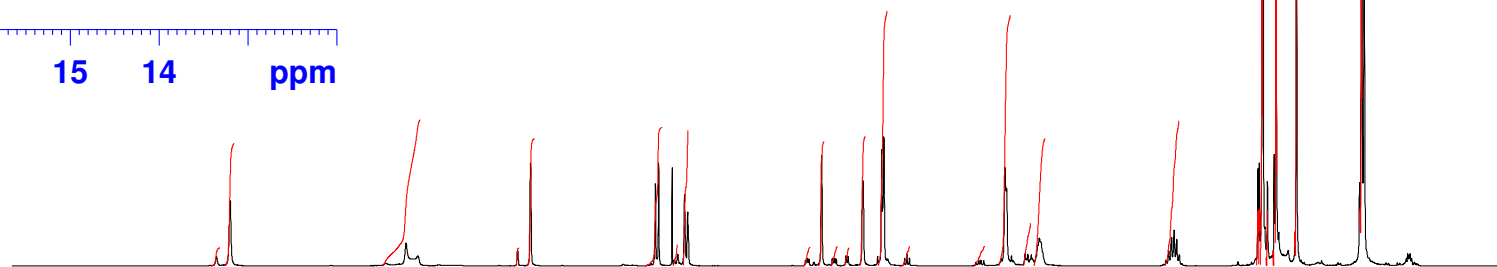


11.219
11.099
9.568
9.464
8.596
8.484
7.434
7.395
7.368
7.229
7.202
7.142
7.114
6.088
6.071
6.058
5.948
5.855
5.843
5.832
5.820
5.735
5.718
5.590
5.226
5.205
5.183
4.604
4.578
4.561
4.535
2.947
2.924
2.900
2.877
2.854
2.832
2.147
2.135
2.107
2.064
2.005
1.988
1.811

5d



15 14 ppm



12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.15
0.98
1.17
0.15
1.02
1.11
0.17
1.09
0.15
1.00
0.16
0.15
1.04
2.05
0.16
0.16
2.01
0.34
1.02
1.17
0.44
0.46
6.01
0.45
0.46
3.02
3.01
6.91

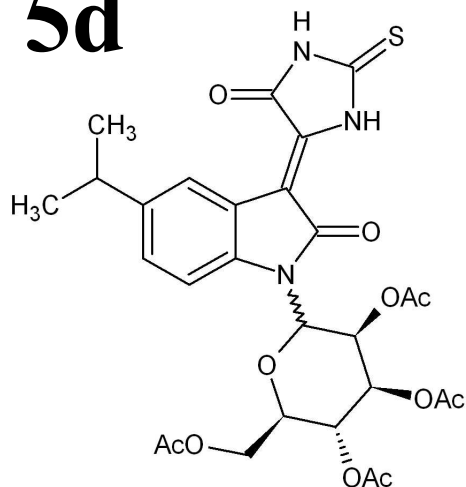
NAME 110616.u331
EXPNO 10
PROCNO 1
Date_ 20110616
Time 18.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 80.6
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C CDC13



5d

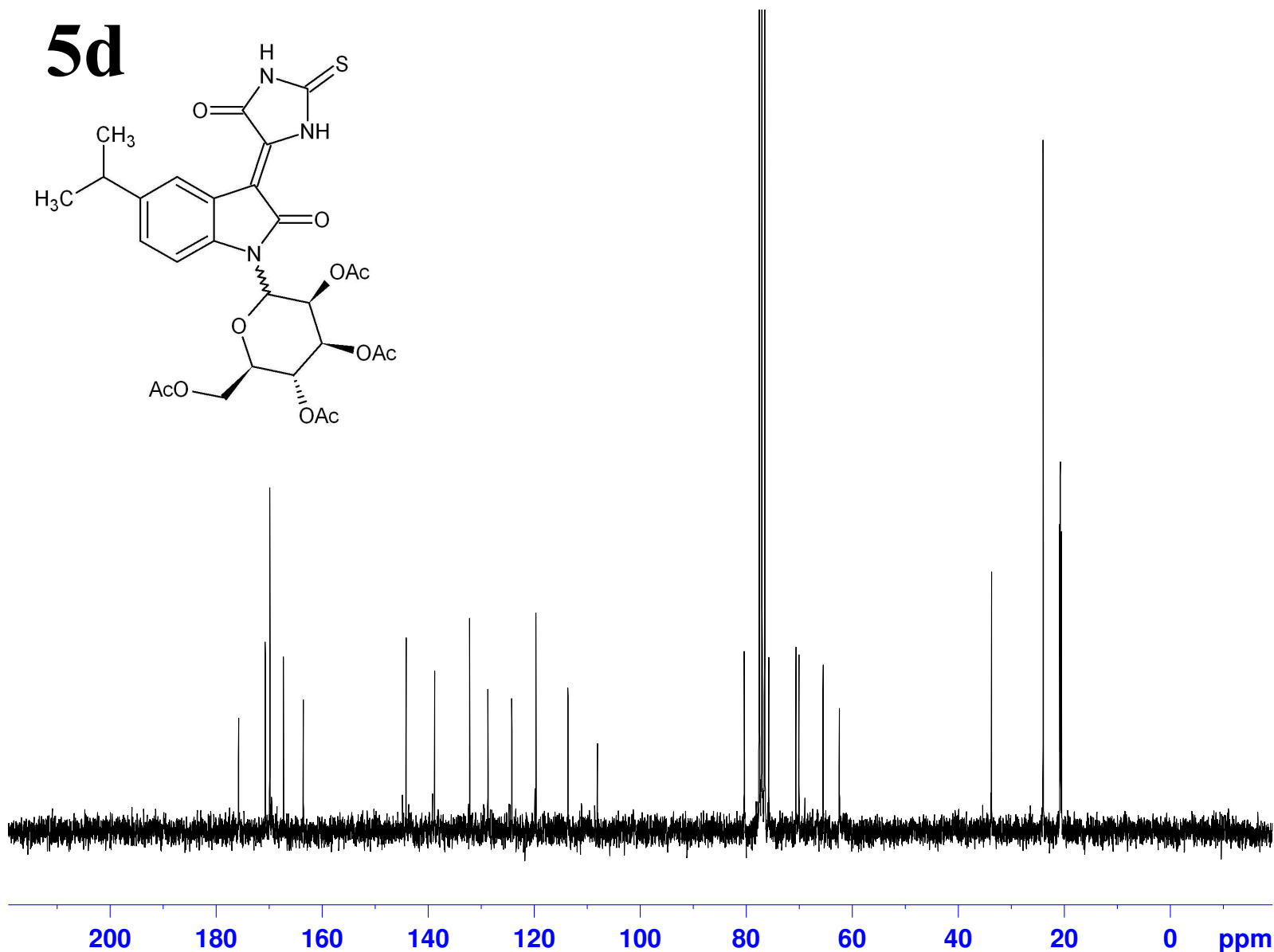


175.74
170.70
169.83
167.27
163.53

144.13
138.74
132.14
128.70
124.19
119.65
113.60
108.03

80.35
75.72
70.59
70.02
65.47
62.41

33.70
23.96
20.85
20.74
20.71
20.53



NAME 110615.206
EXPNO 10
PROCNO 1
Date_ 20110615
Time 18.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.4 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952407 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H in CDCL3

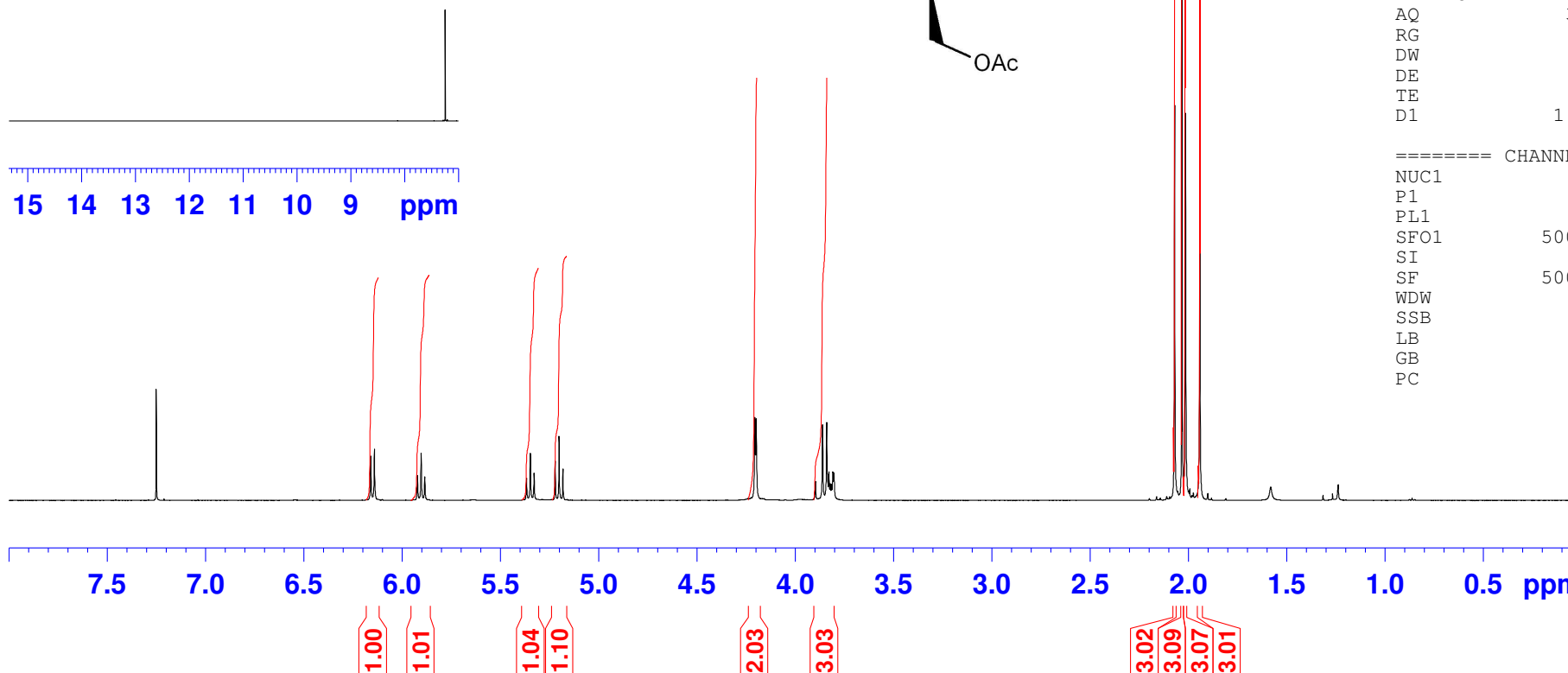
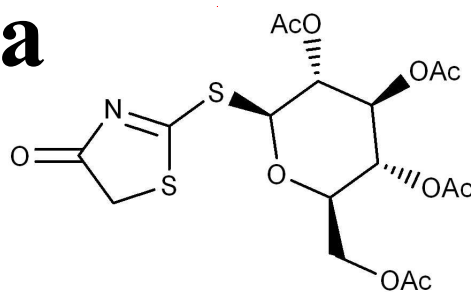


6.548
6.161
6.142
5.923
5.905
5.886
5.632
5.368
5.349
5.330
5.222
5.203
5.183

4.207
4.200
3.898
3.862
3.841
3.809
3.805

2.071
2.033
2.015
1.942

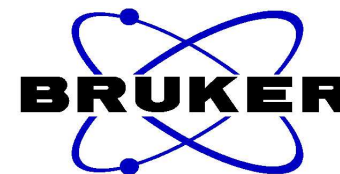
10a



NAME 100709.503
EXPNO 10
PROCNO 1
Date_ 20100709
Time 15.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 143.7
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300182 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C in CDCL3



201.46

172.00
170.56
170.02
169.91
169.34

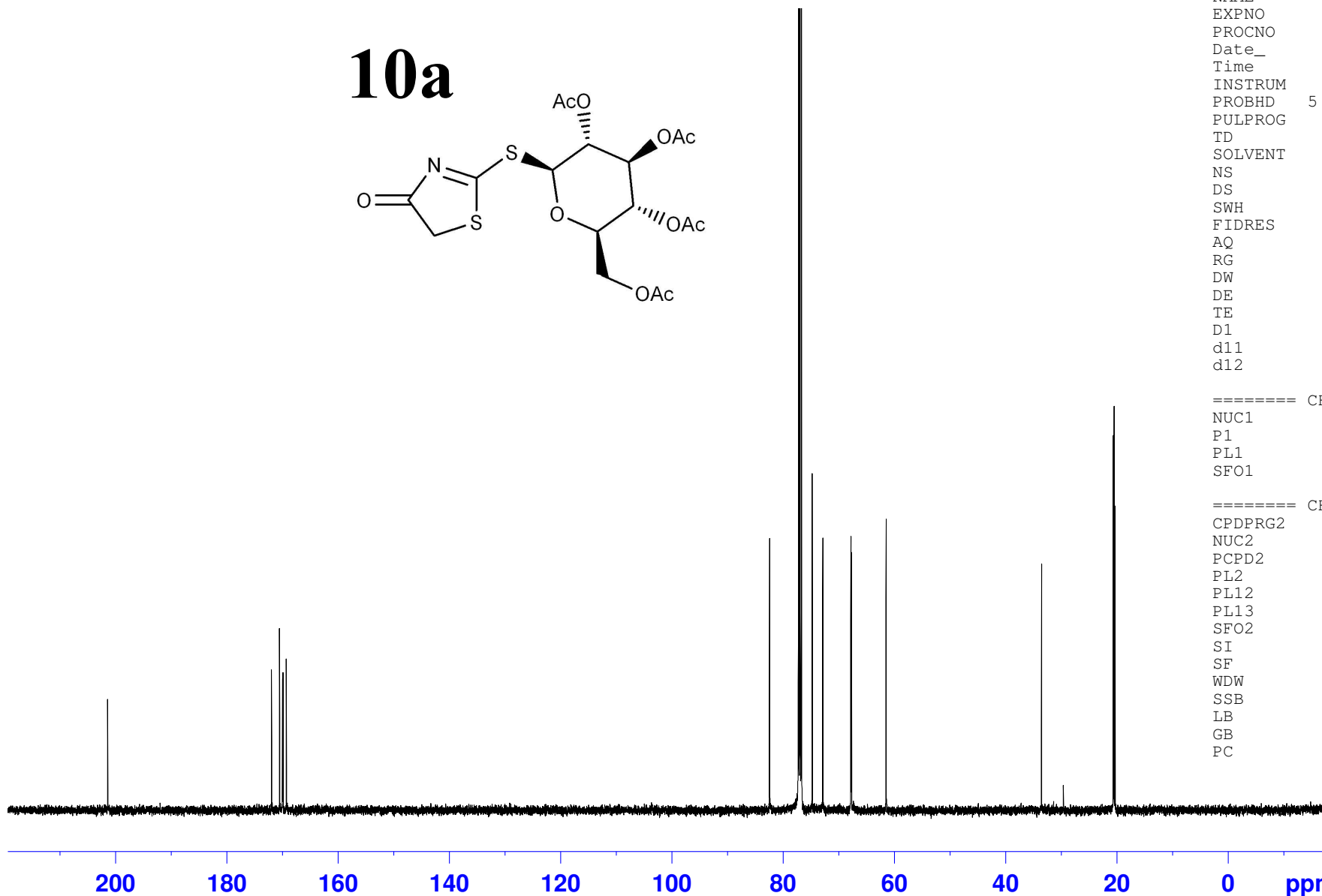
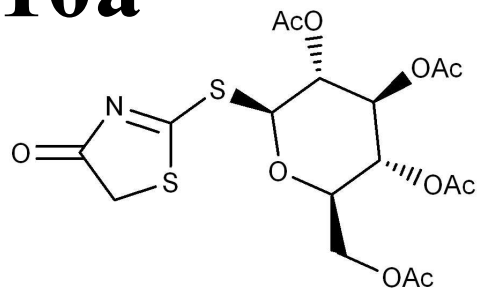
82.46

74.79
72.90
67.85
67.73
61.51

33.56

20.68
20.54
20.52
20.35

10a

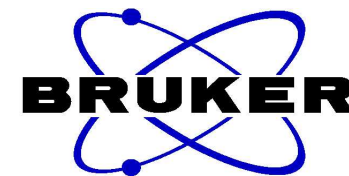


NAME 100709.503
EXPNO 16
PROCNO 1
Date_ 20100710
Time 4.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577910 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

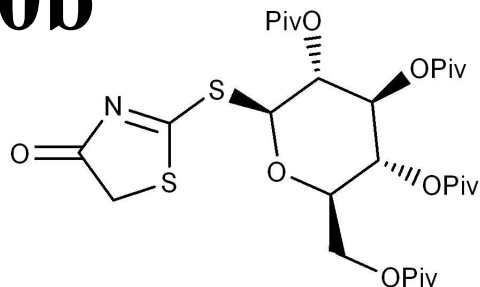
Erben 1H CDC13



6.601
6.565
6.529
6.186
6.149
5.974
5.937
5.900
5.696
5.659
5.509
5.471
5.434
5.328
5.288
5.249
5.181
5.142
5.104
4.864
4.655
4.615
4.308
4.301
4.258
4.251
4.074
4.057
4.024
4.007

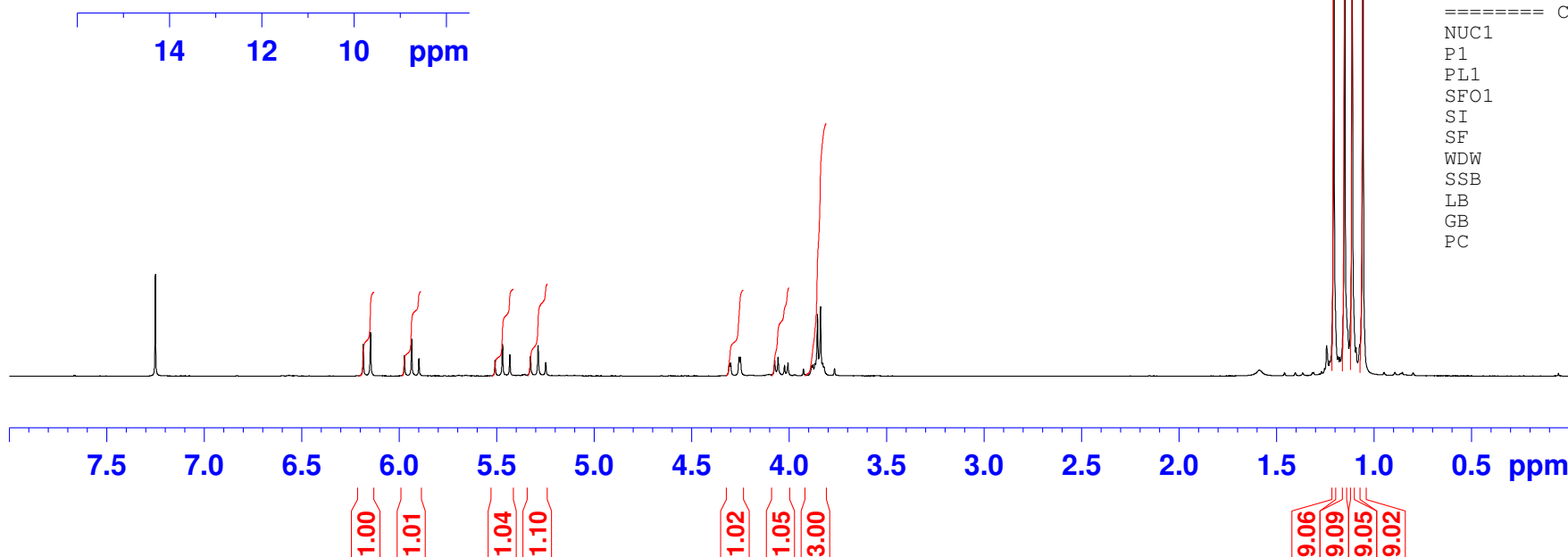
1.206
1.150
1.112
1.056

10b

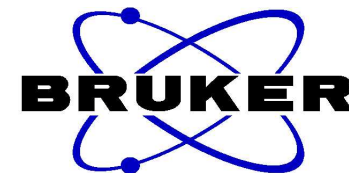


NAME 100709.212
EXPNO 10
PROCNO 1
Date_ 20100709
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 645
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

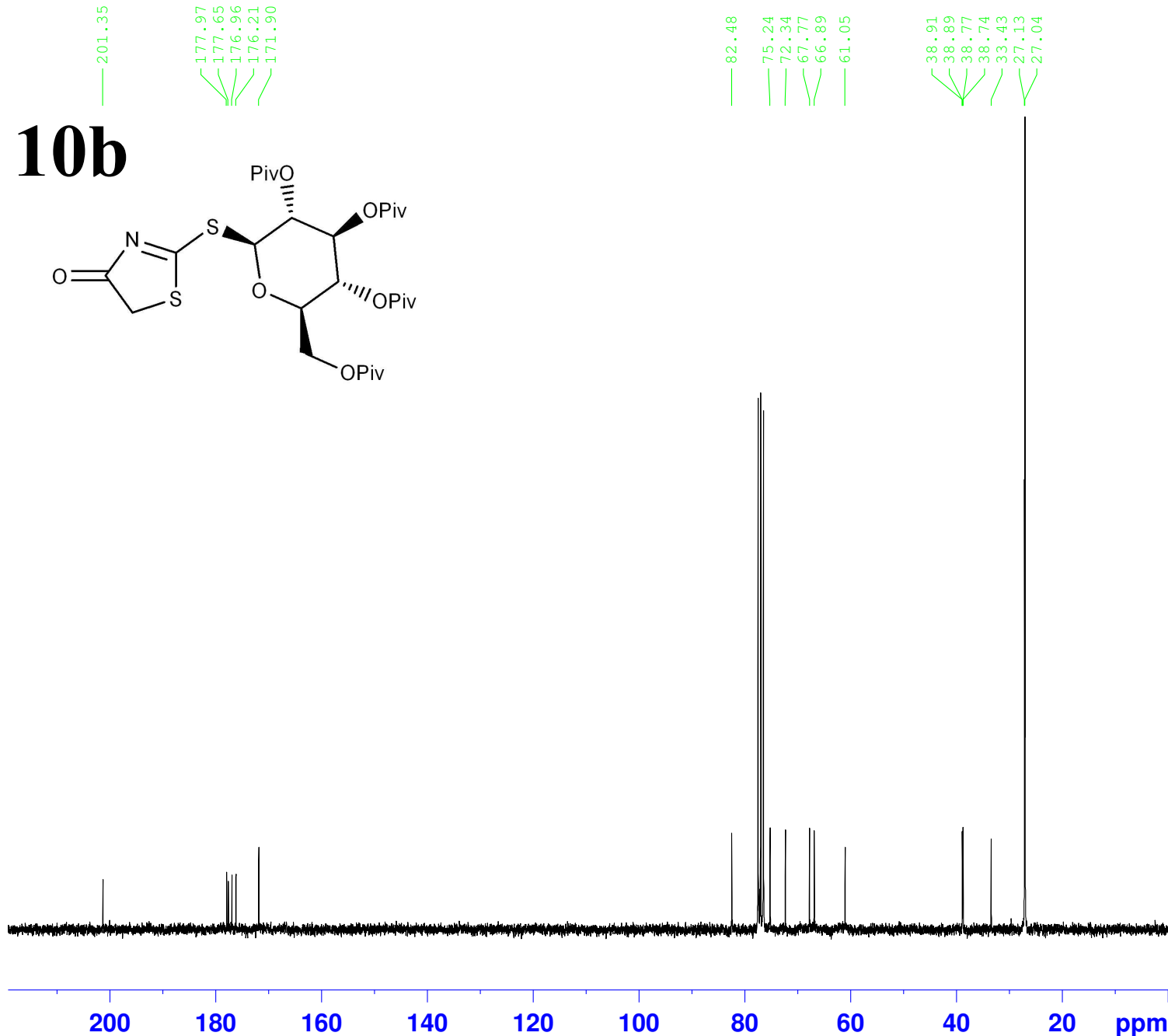
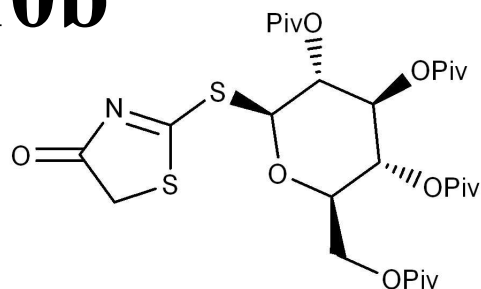
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.1300031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Erben 13C CDC13



10b



```
NAME 100709.213
EXPNO 10
PROCNO 1
Date_ 20100709
Time 17.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 300.6 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1
```

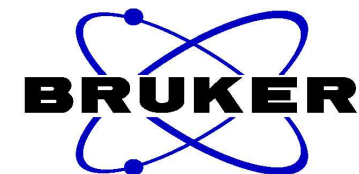
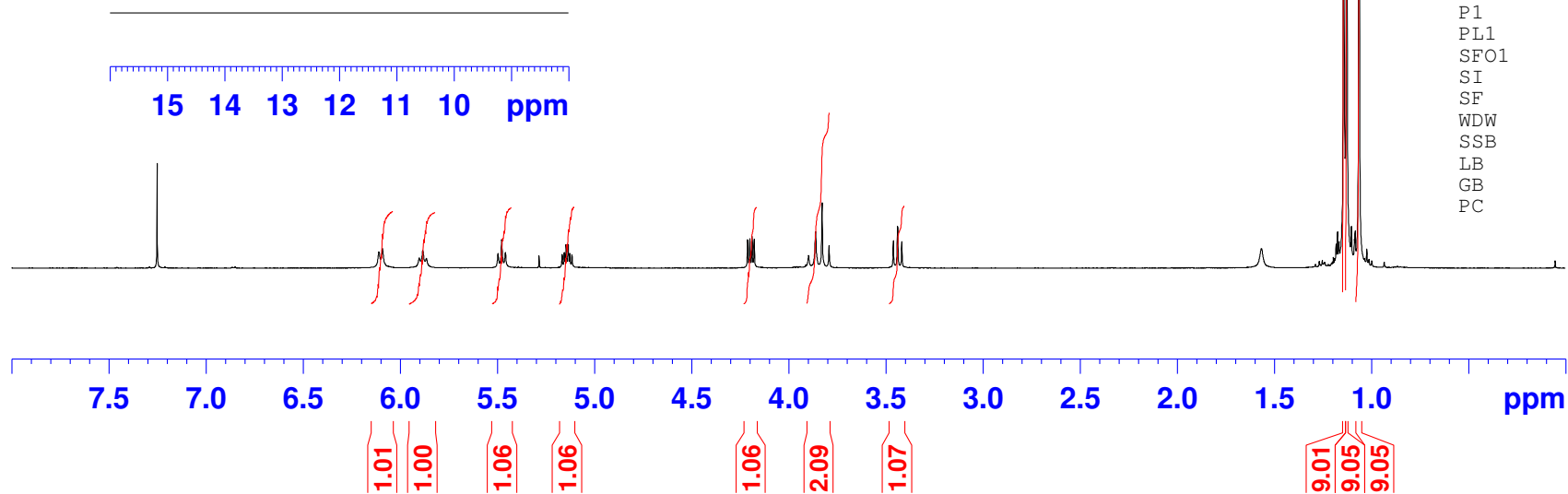
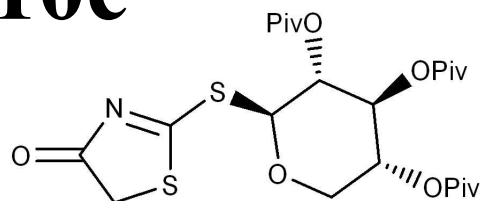
```
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952384 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```


Erben 1H in CDCl3

6.108
6.090
5.903
5.885
5.866
5.497
5.478
5.459
5.167
5.156
5.147
5.136
5.127
5.116
4.212
4.201
4.189
4.178
3.898
3.862
3.829
3.793
3.462
3.440
3.418

10c



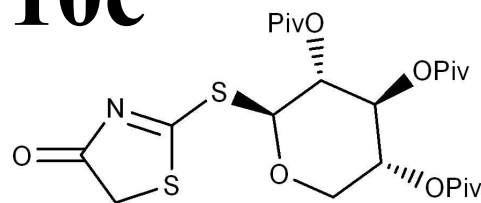
NAME 101008.501
EXPNO 10
PROCNO 1
Date_ 20101008
Time 9.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12531.328 Hz
FIDRES 0.191213 Hz
AQ 2.6149764 sec
RG 128
DW 39.900 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1340010 MHz
SI 32768
SF 500.1300181 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C in CDCl3



10c



201.32

177.75

177.08

176.91

172.32

83.14

71.90

68.33

67.71

65.63

38.91

38.78

38.74

33.43

27.11

27.06

27.05

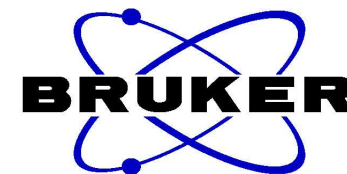
```
NAME 101008.501
EXPNO 16
PROCNO 1
Date_ 20101010
Time 23.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 25600
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 71.8
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz
```

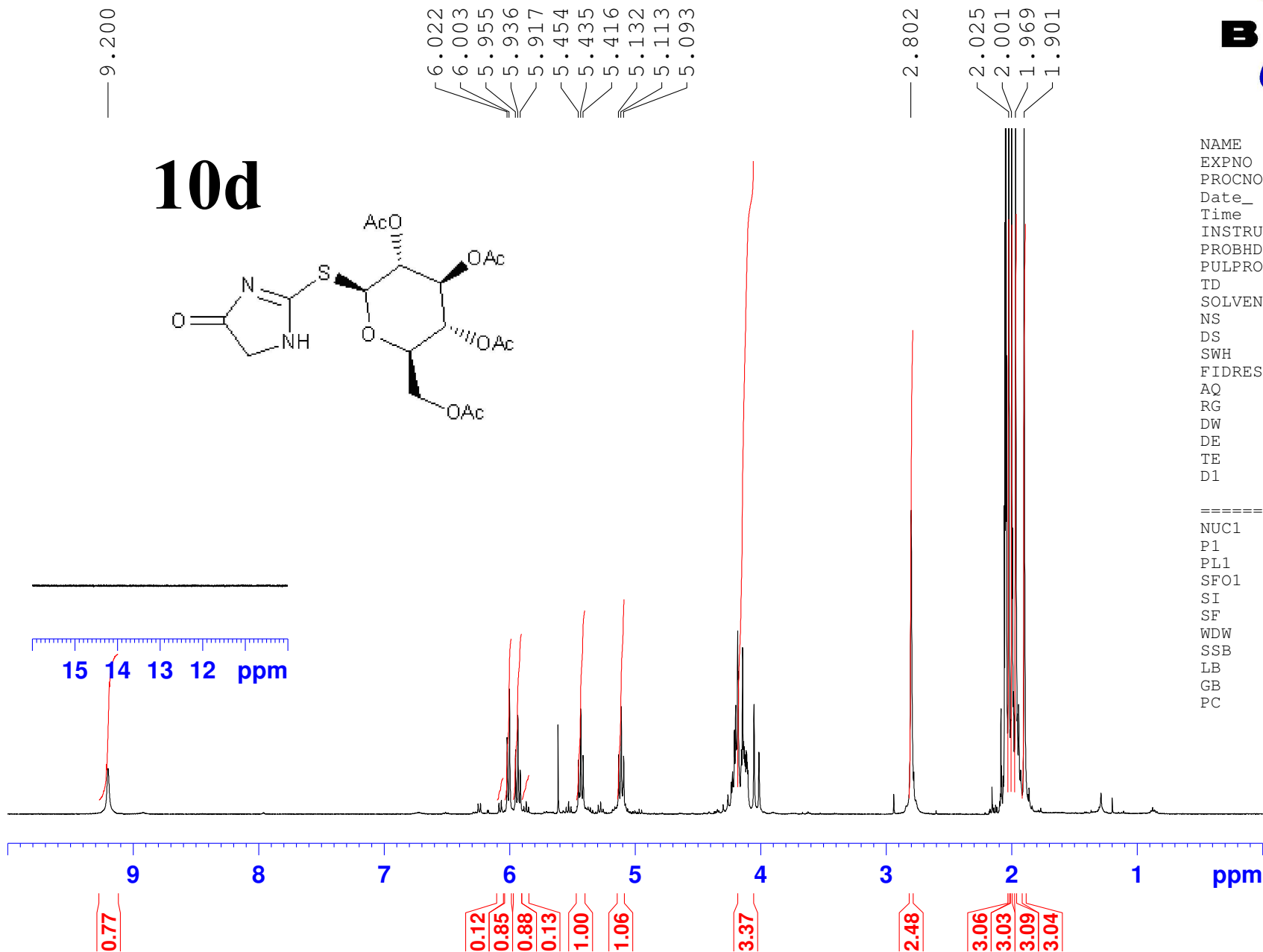
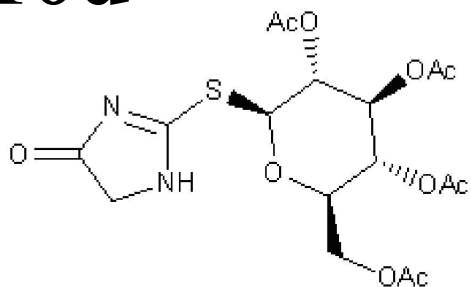
```
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577914 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```



Erben 1H in Aceton-d6



10d



NAME 100923.501
EXPNO 10
PROCNO 1
Date_ 20100923
Time 10.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 12531.328 Hz
FIDRES 0.191213 Hz
AQ 2.6149764 sec
RG 181
DW 39.900 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

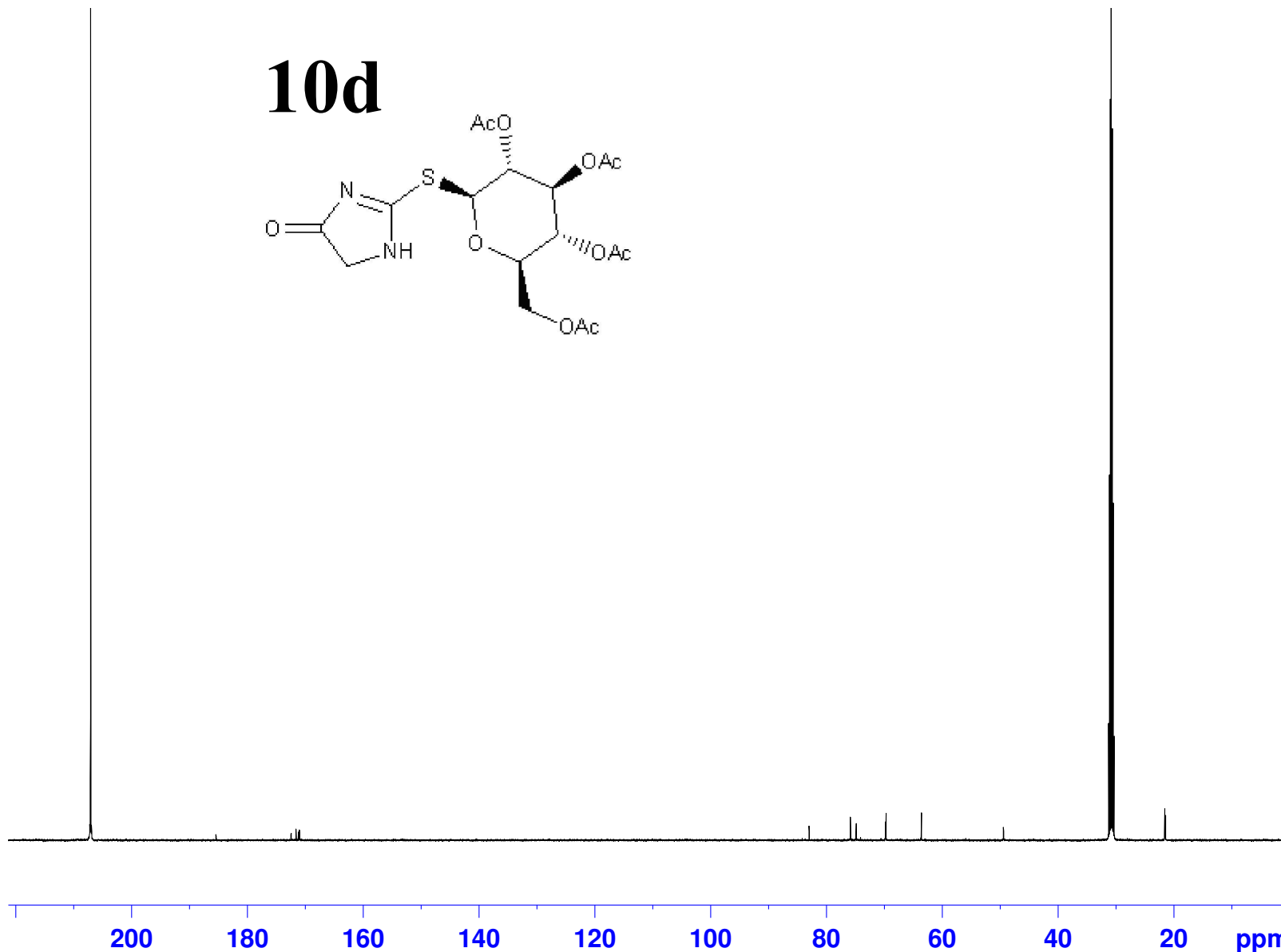
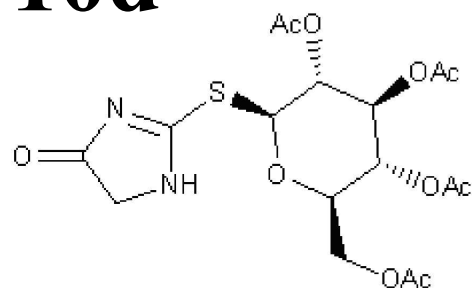
===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1340010 MHz
SI 32768
SF 500.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C in Aceton-d6



185.46
172.50
171.65
171.22
171.08
171.03
83.01
75.88
74.90
69.81
69.75
63.62
49.45
21.62
21.59
21.52
21.48

10d



NAME 100923.501
EXPNO 12
PROCNO 1
Date_ 20100923
Time 12.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2048
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 80.6
DW 16.650 use
DE 6.00 use
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 use
PL1 4.80 dB
SFO1 125.7703643 MHz

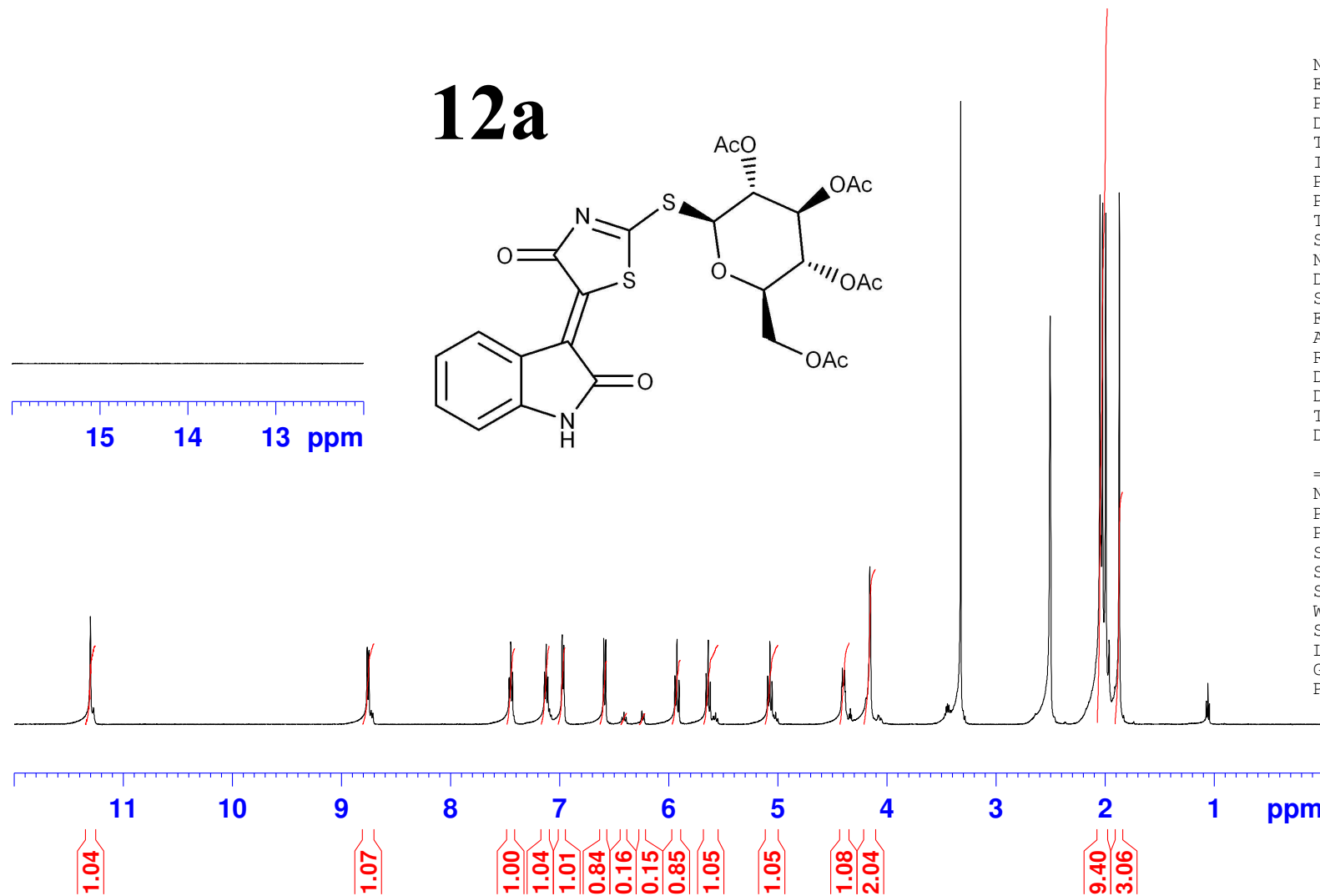
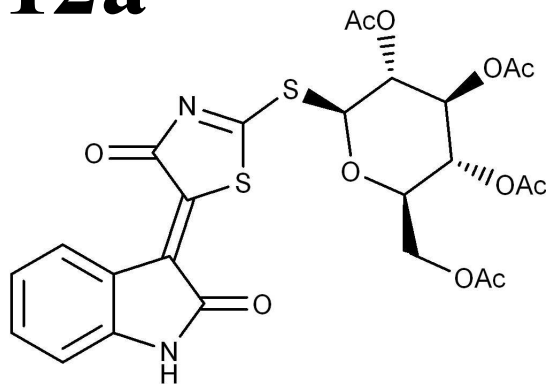
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7575504 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H in DMSO, 300 K



11.300
11.270
8.767
8.751
8.730
8.714
7.465
7.450
7.434
7.141
7.125
7.110
7.095
7.079
6.979
6.964
6.597
6.579
6.430
6.411
6.392
6.247
6.228
5.944
5.926
5.907
5.659
5.639
5.620
5.591
5.572
5.553
5.094
5.074
5.054
5.041
5.021
5.002
4.410
4.390
4.158
2.048
2.024
1.994
1.870

12a



NAME 100527.503
EXPNO 20
PROCNO 1
Date_ 20100528
Time 14.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 90.5
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.04

1.07

1.00

1.04

1.01

0.84

0.16

0.15

0.85

1.05

1.05

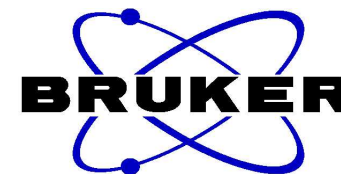
1.08

2.04

9.40

3.06

Erben 13C in DMSO, 300 K

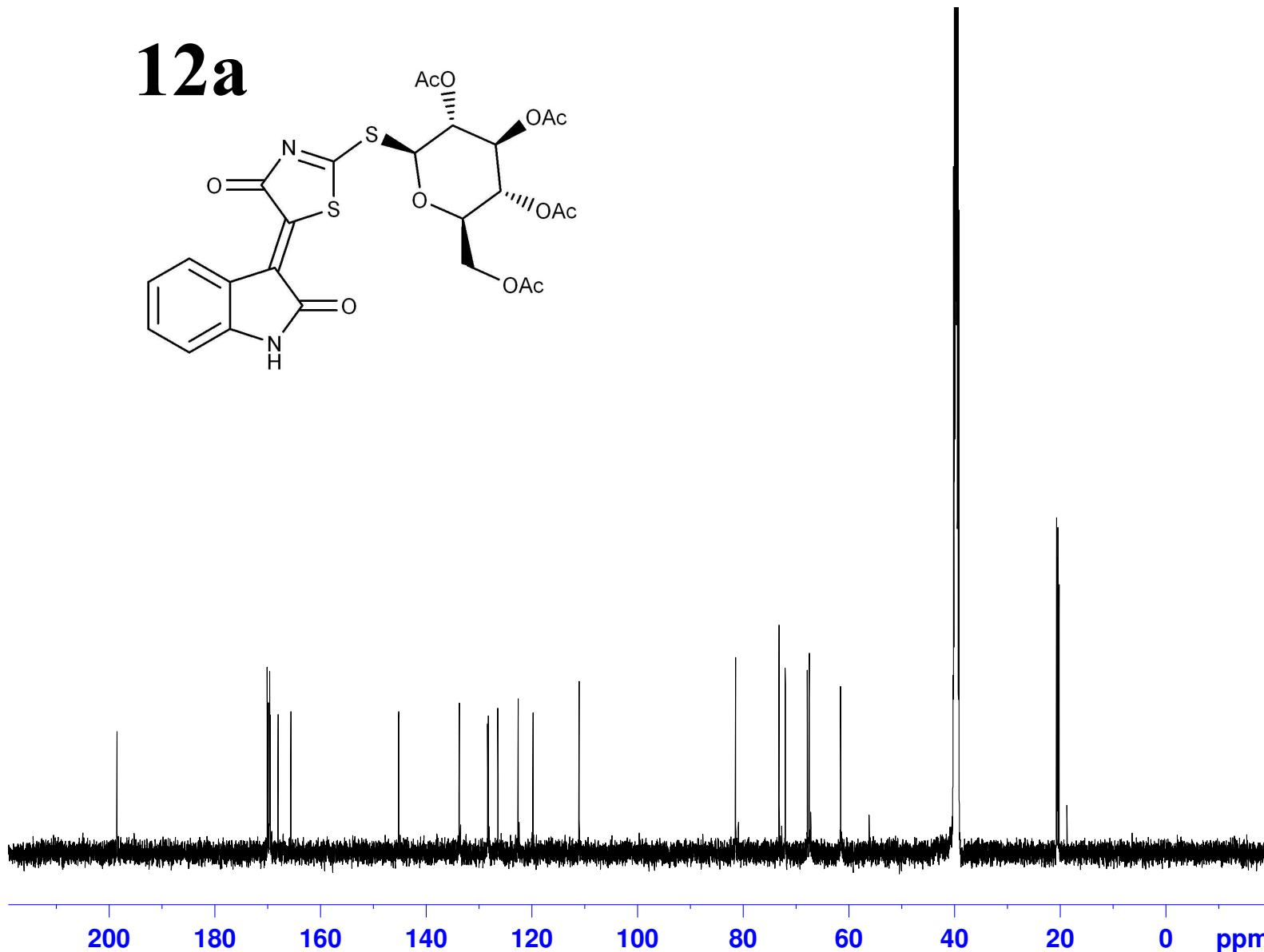
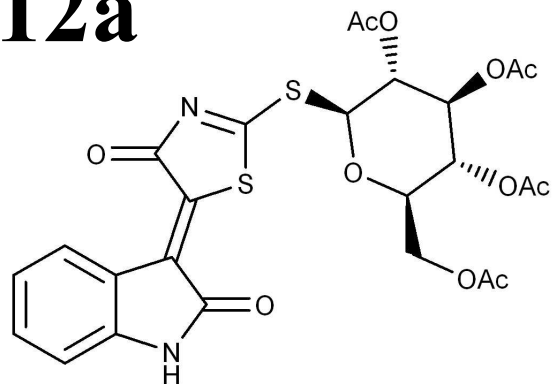


198.54
170.11
169.90
169.63
169.57
168.10
168.05
165.66
145.25
133.77
133.54
128.39
128.27
128.10
126.45
122.62
122.42
119.82
111.07

81.46
80.92
73.21
72.73
72.05
67.87
67.53
67.28
67.22
61.58

20.70
20.55
20.45
20.24

12a



NAME 100527.503
EXPNO 22
PROCNO 1
Date_ 20100528
Time 15.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 287.4
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

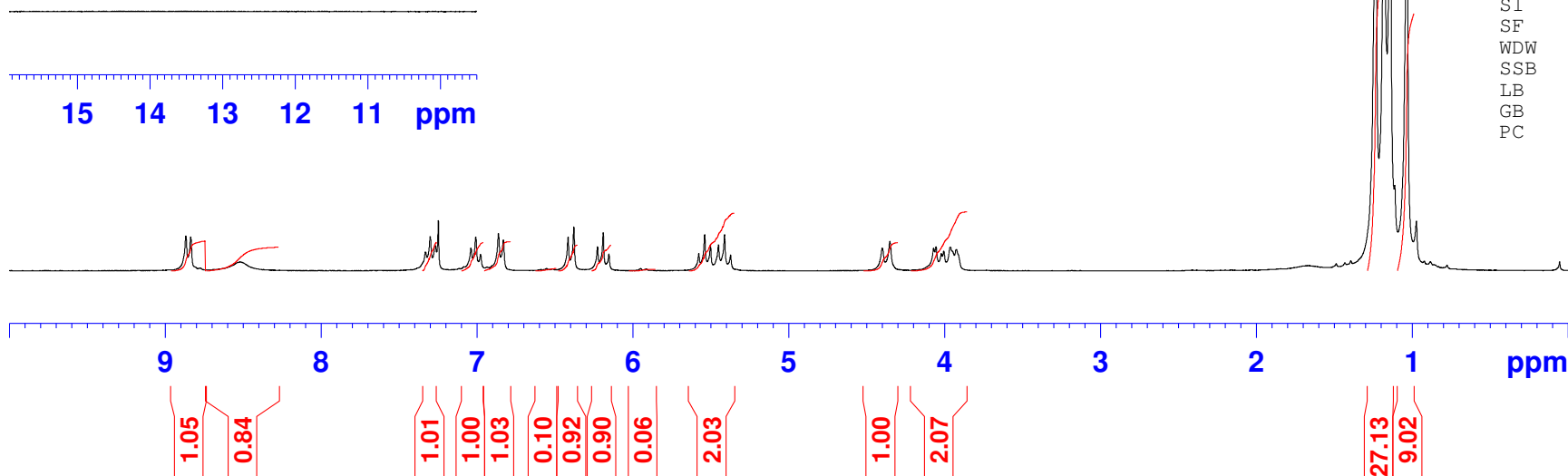
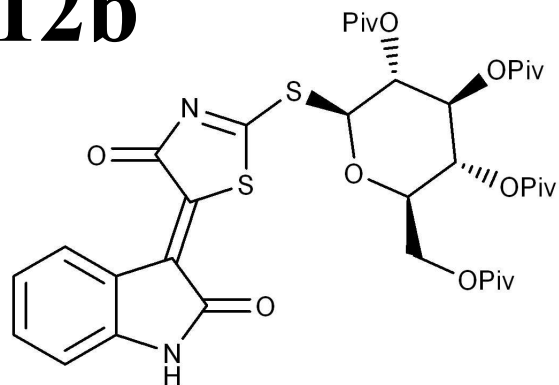
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7578272 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H CDC13



8.867
8.836
8.521
7.333
7.303
7.271
7.118
7.086
7.041
7.010
6.979
6.937
6.864
6.833
6.592
6.556
6.520
6.417
6.380
6.229
6.192
6.155
5.952
5.914
5.578
5.541
5.503
5.452
5.413
5.374
4.402
4.353
4.072
4.056
4.022
4.006
3.964
3.926

12b



1.235
1.179
1.141
1.034

NAME 100630.204
EXPNO 10
PROCNO 1
Date_ 20100630
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 512
DW 96.800 use
DE 10.00 use
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 use
PL1 -2.50 dB
SFO1 250.1315447 MHz
SI 32768
SF 250.130026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C CDC13

197.72

178.13

177.87

177.05

176.29

168.09

165.35

143.33

132.91

129.50

129.31

125.94

123.19

120.16

110.34

82.00

75.25

72.47

67.97

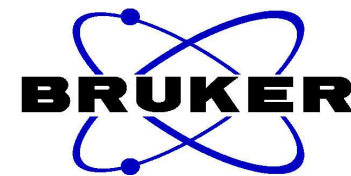
66.95

61.06

38.93

27.17

27.08

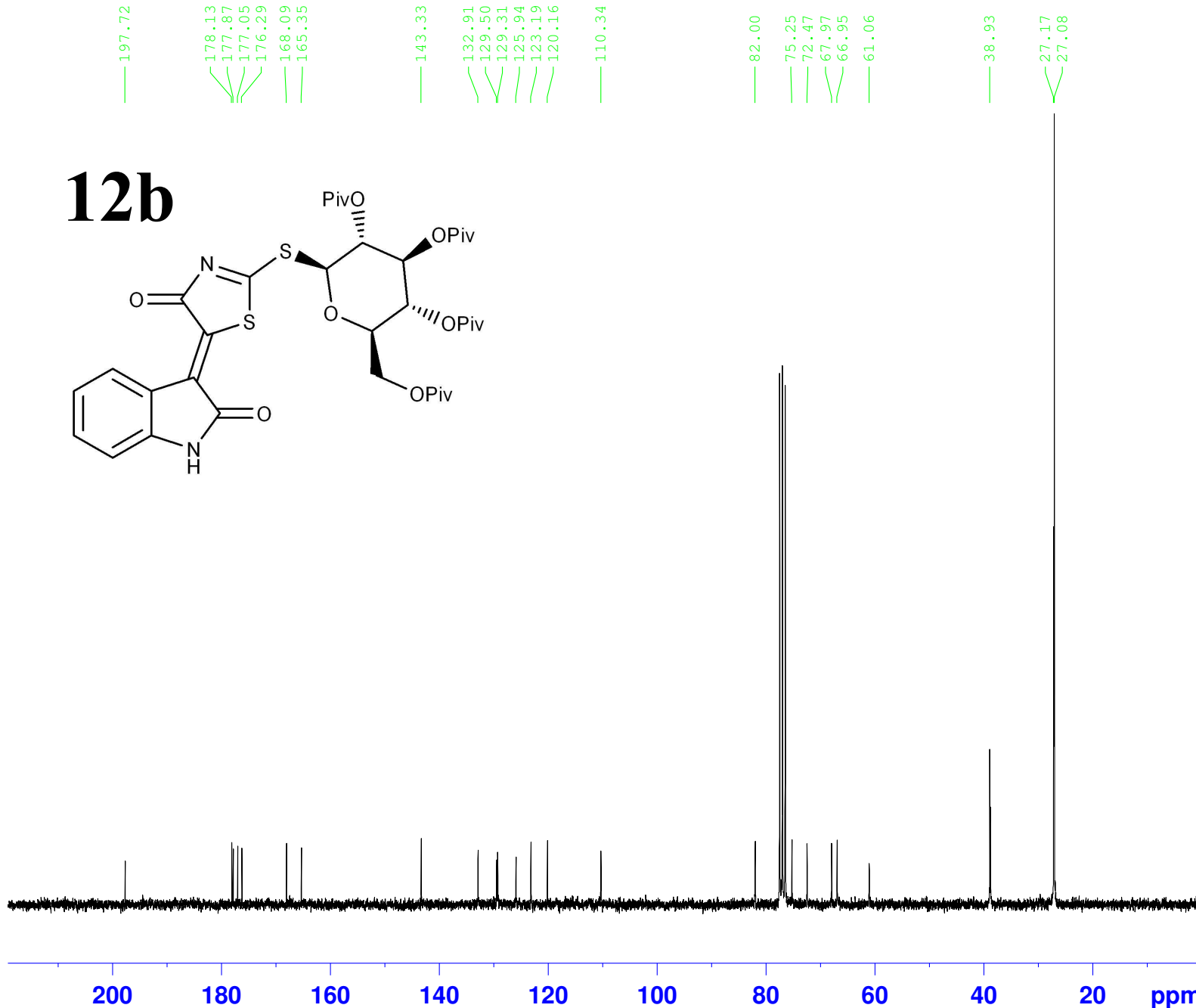
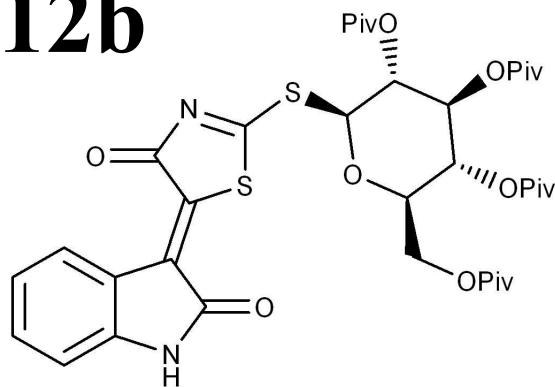


NAME 100630.211
EXPNO 10
PROCNO 1
Date_ 20100630
Time 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.7 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952394 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

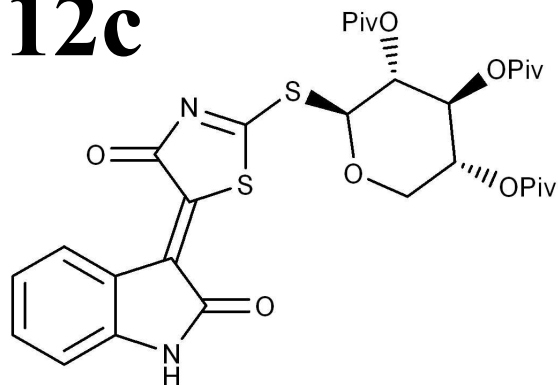
12b



Erben 1H CDC13

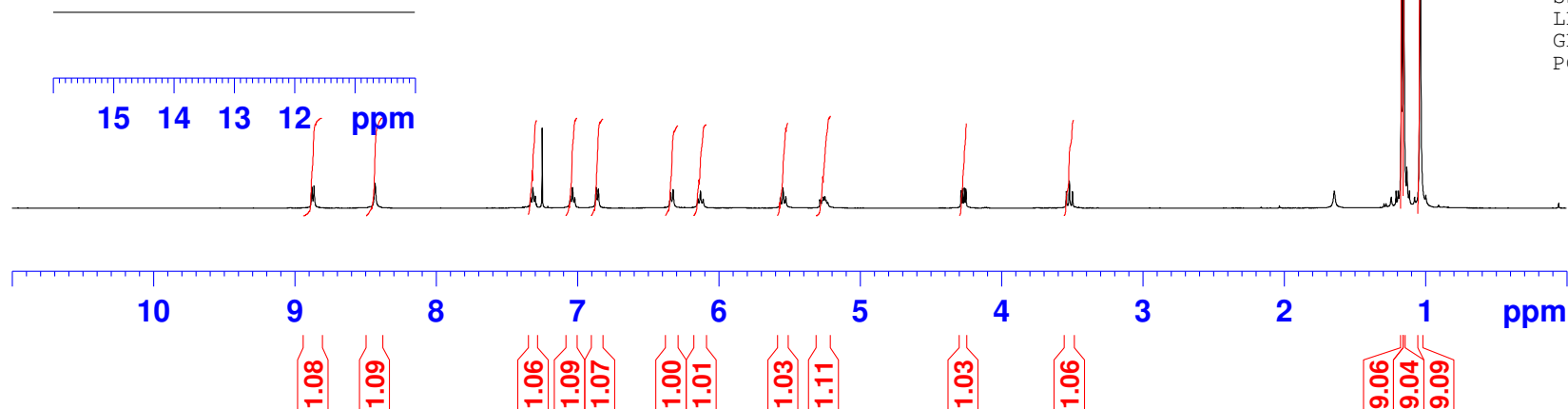


12c



8.920
8.905
8.880
8.864
8.473
8.431
7.389
7.370
7.350
7.330
7.315
7.300
7.050
7.035
7.020
6.868
6.852
6.342
6.323
6.148
6.129
6.111
5.564
5.545
5.526
4.285
4.274
4.262
4.251
3.540
3.519
3.497

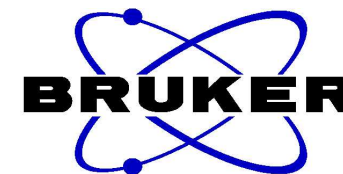
1.167
1.152
1.036



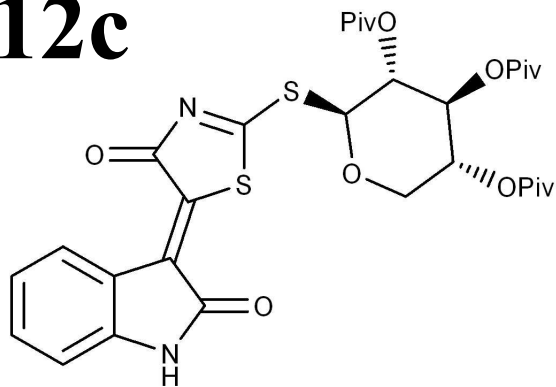
```
NAME 101005.502
EXPNO 10
PROCNO 1
Date_ 20101005
Time 15.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 15015.015 Hz
FIDRES 0.229111 Hz
AQ 2.1824322 sec
RG 101.6
DW 33.300 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1350013 MHz
SI 32768
SF 500.1300181 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

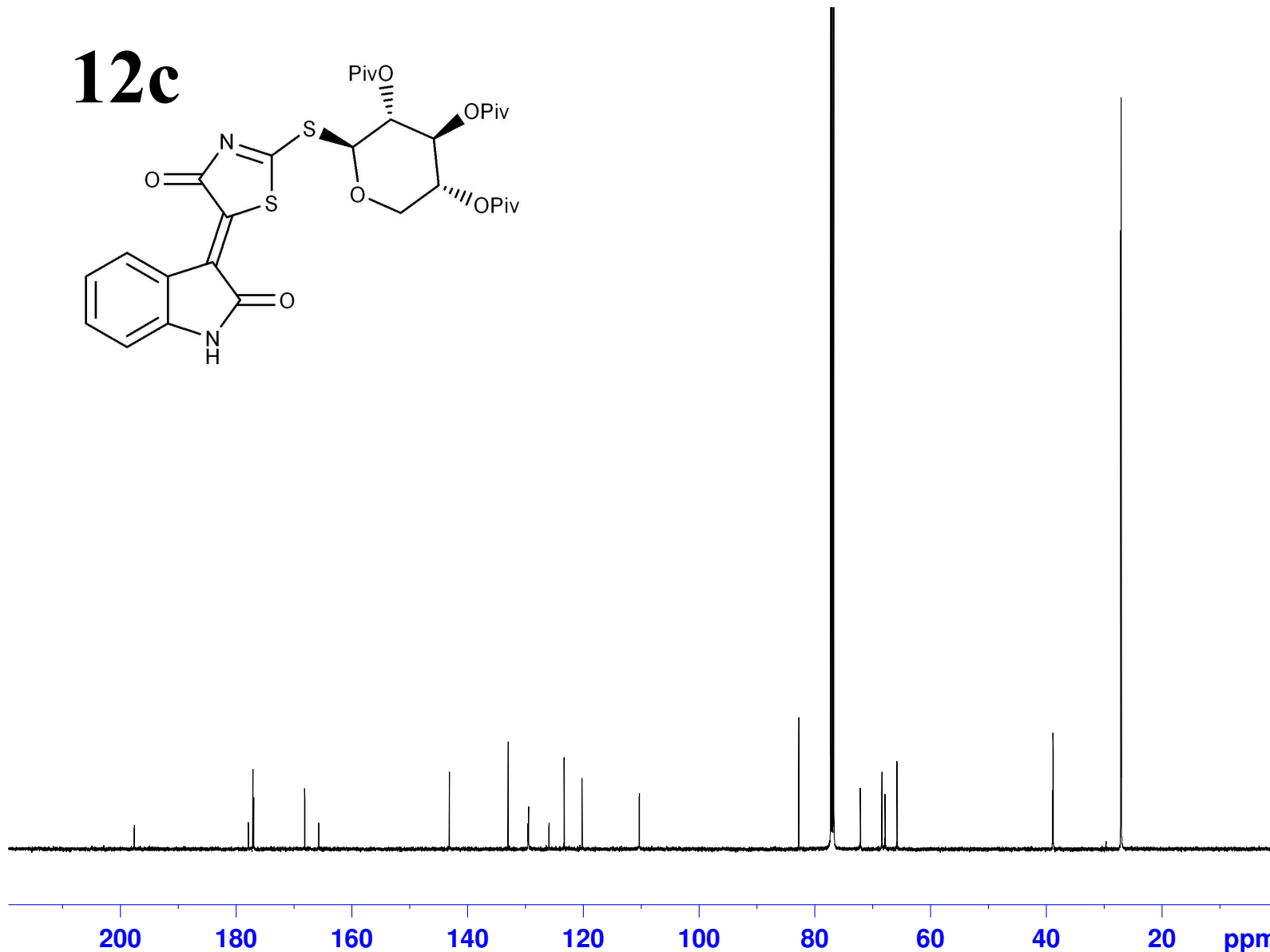
Erben 13C CDCl3



12c



197.63
177.90
177.15
176.98
168.18
165.74
143.18
133.02
129.59
129.49
125.96
123.34
120.24
110.34
82.78
72.13
68.41
67.88
65.81
38.93
38.82
38.78
27.15
27.07



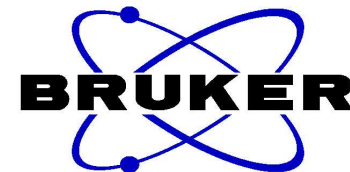
NAME 101005.502
EXPNO 18
PROCNO 1
Date_ 20101006
Time 12.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5120
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

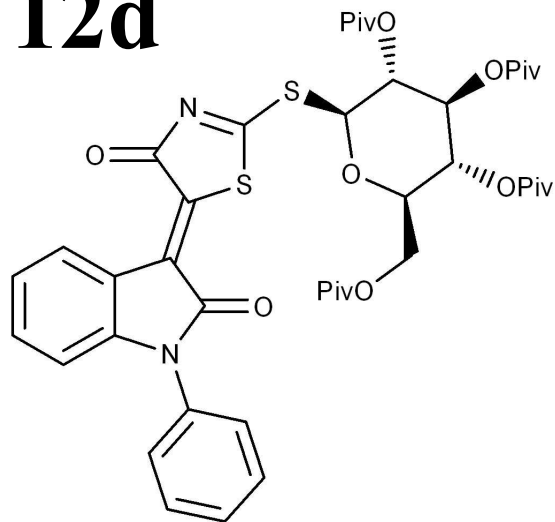
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577919 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H CDC13

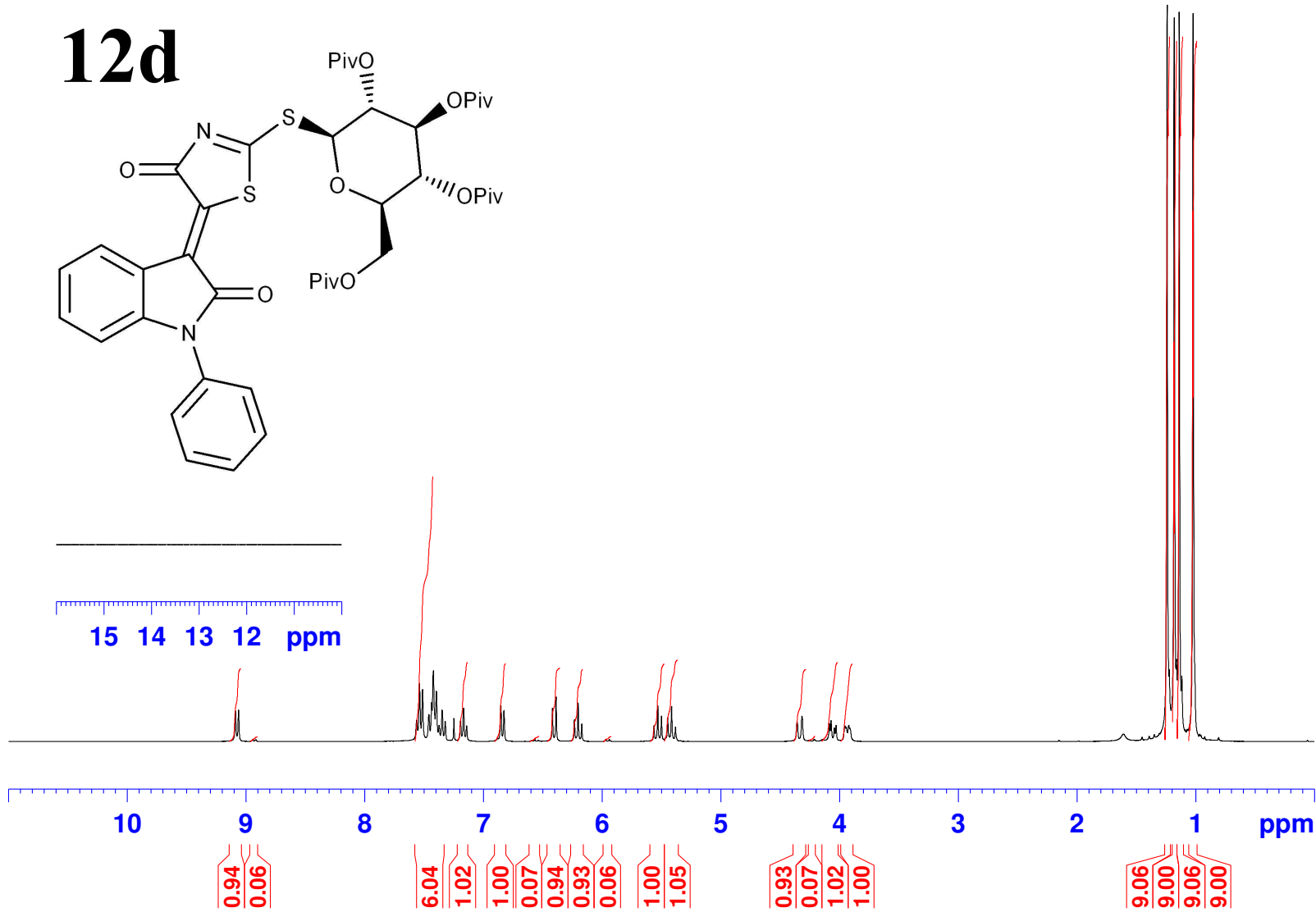
9.091
9.065
8.944
8.920
7.195
7.169
7.144
6.855
6.828
6.599
6.569
6.538
6.420
6.389
6.235
6.204
6.173
5.972
5.941
5.565
5.533
5.502
5.449
5.417
5.384
4.358
4.319
4.254
4.212
4.087
4.073
4.045
4.031
1.242
1.226
1.182
1.164
1.140
1.120
1.023
1.010



12d



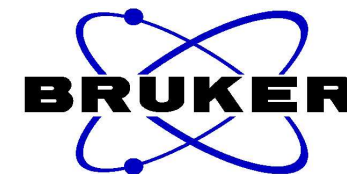
15 14 13 12 ppm



NAME 110628.u330
EXPNO 12
PROCNO 1
Date_ 20110628
Time 23.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 71.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

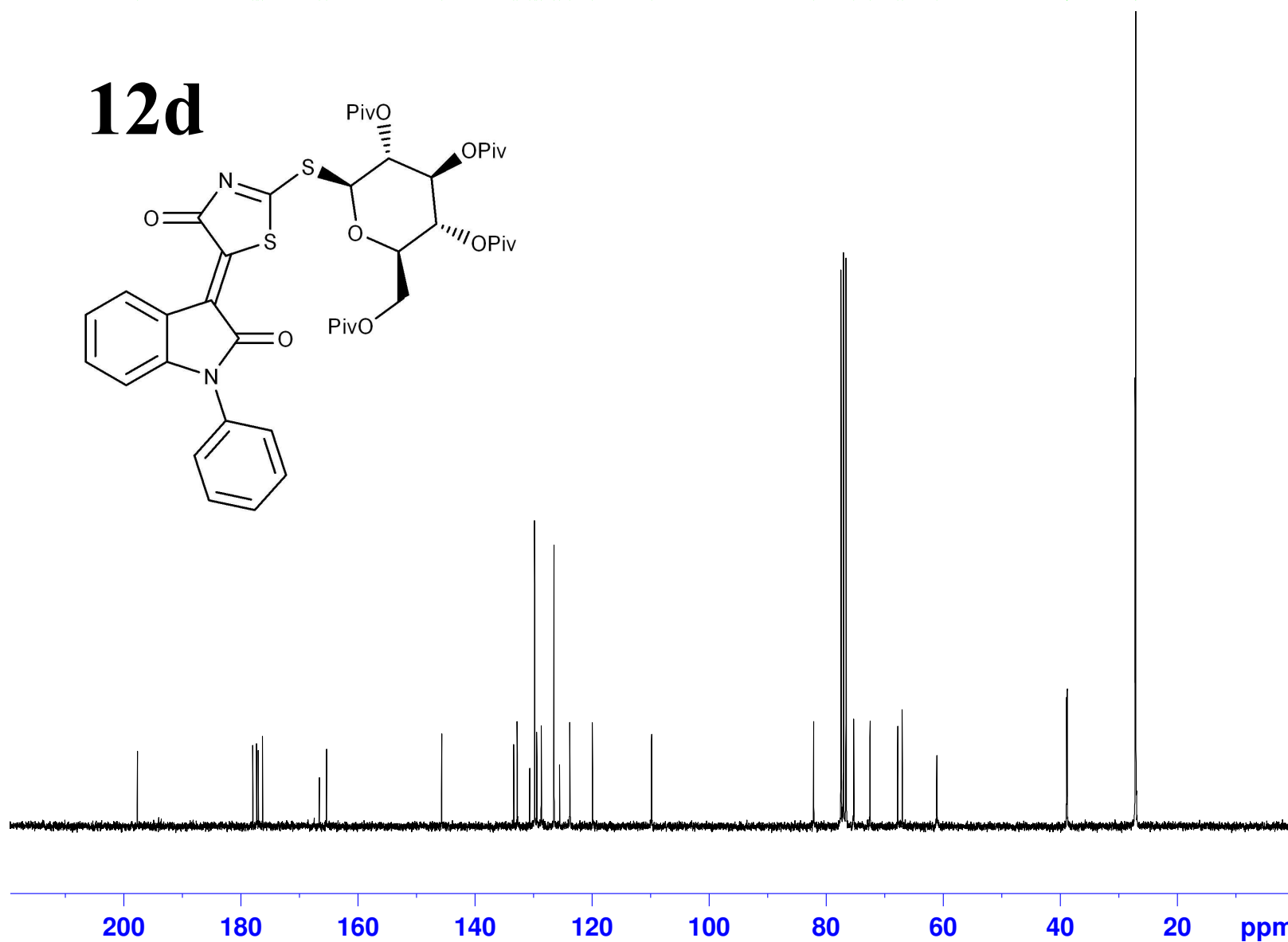
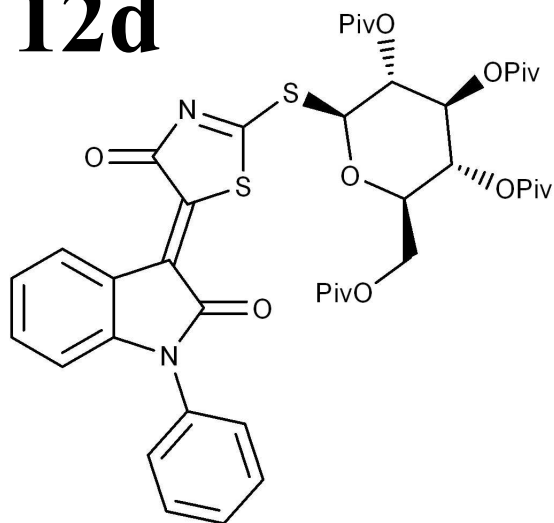
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C CDCl3



197.67
 177.94
 177.30
 177.01
 176.28
 166.58
 165.36
 145.68
 133.36
 132.77
 130.63
 129.78
 129.43
 128.65
 126.49
 125.52
 123.78
 119.91
 109.81
 82.11
 75.26
 72.48
 67.74
 66.97
 61.06
 38.91
 38.85
 38.81
 38.77
 27.16
 27.07

12d



```

NAME      110628.u330
EXPNO     10
PROCNO    1
Date_     20110628
Time      23.36
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         1024
DS         4
SWH        18028.846 Hz
FIDRES     0.275098 Hz
AQ         1.8175818 sec
RG         2050
DW         27.733 usec
DE         10.00 usec
TE         299.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1      13C
P1         10.00 usec
PL1        -0.50 dB
PL1W       33.25691986 W
SFO1       75.4752953 MHz

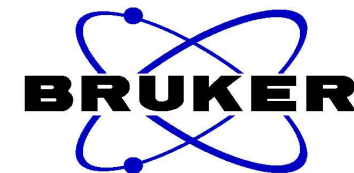
```

```

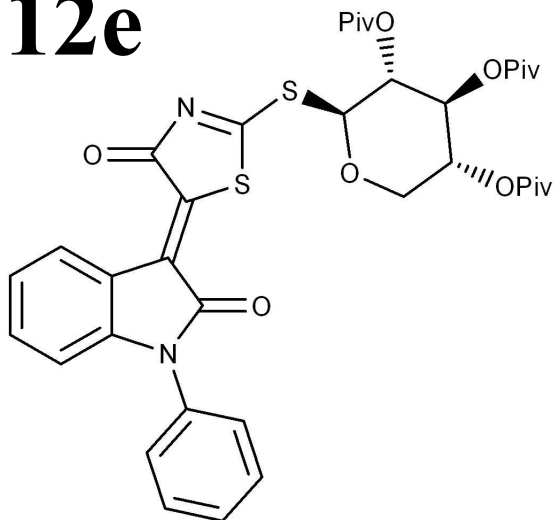
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      72.00 usec
PL2         0.00 dB
PL12        17.00 dB
PL13        17.00 dB
PL2W       11.25325108 W
PL12W       0.22453187 W
PL13W       0.22453187 W
SFO2       300.1312005 MHz
SI          32768
SF          75.4677522 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

```

Erben 1H CDC13



12e

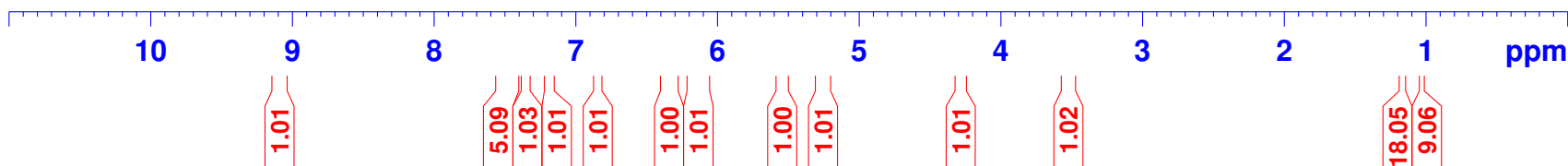


9.104
9.078
7.379
7.376
7.354
7.351
7.328
7.324
7.211
7.185
7.159
6.856
6.830
6.354
6.323
6.162
6.132
6.101
5.574
5.542
5.510
4.310
4.291
4.272
4.253
3.557
3.521
3.485
1.172
1.153
1.025

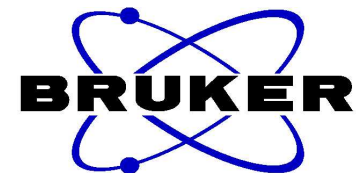
NAME 110728.u316
EXPNO 10
PROCNO 1
Date_ 20110728
Time 14.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

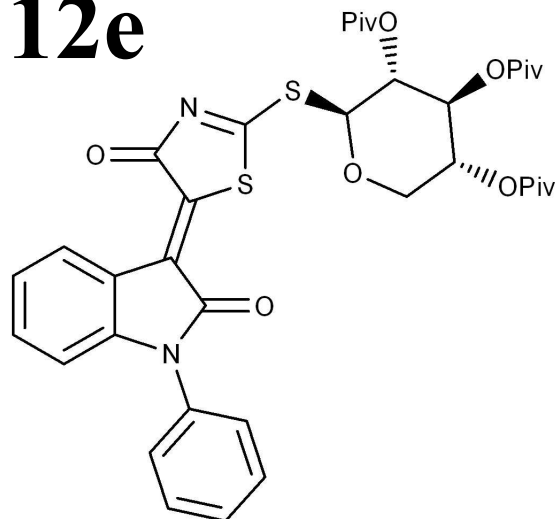
15 14 13 12 ppm



Erben 13C CDCl3



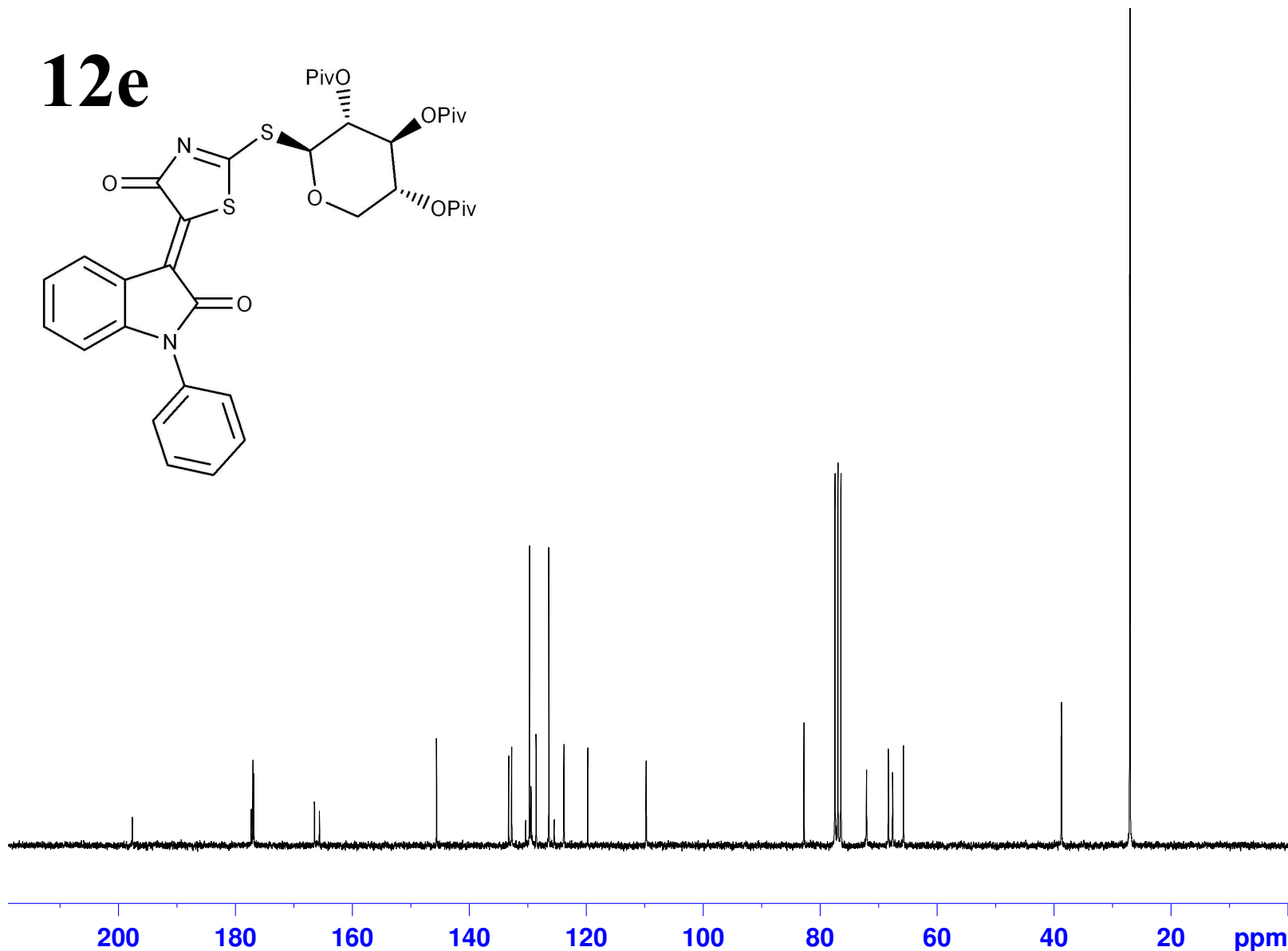
12e



197.60
177.33
177.06
176.91
166.52
165.67
145.64
133.30
132.80
130.41
129.73
129.48
128.60
126.43
125.52
123.86
119.79
109.79

82.80
72.09
68.37
67.65
65.79

38.81
38.76
38.72
27.10
27.03



NAME 110728.207
EXPNO 10
PROCNO 1
Date_ 20110728
Time 21.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

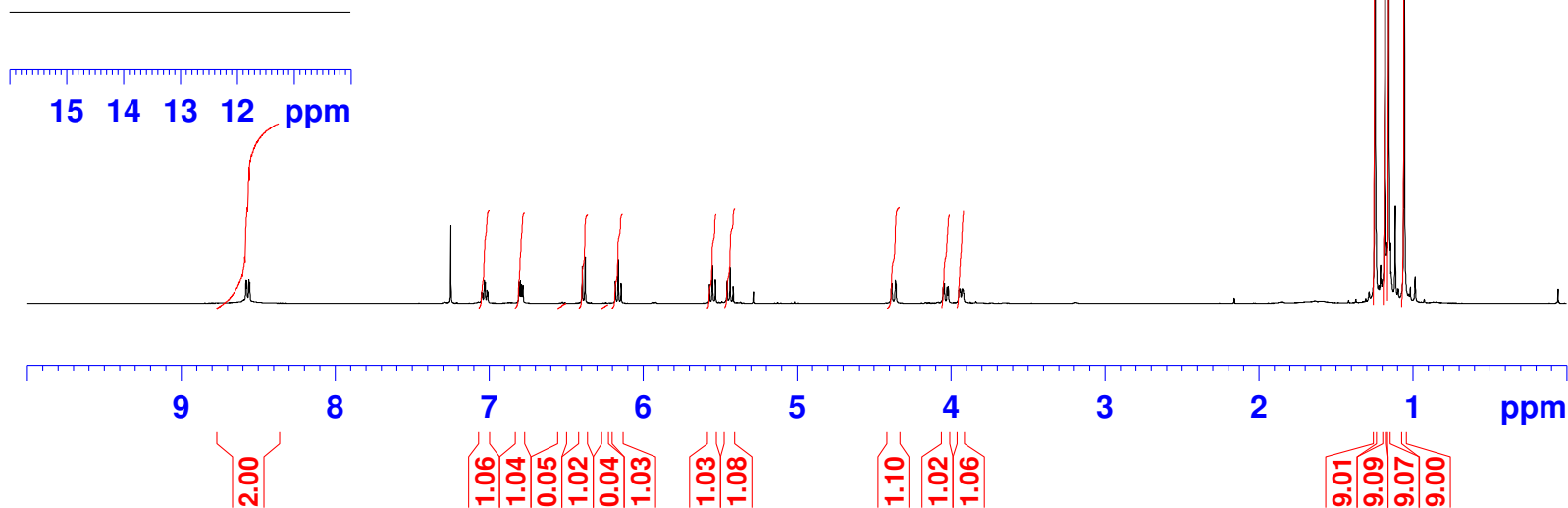
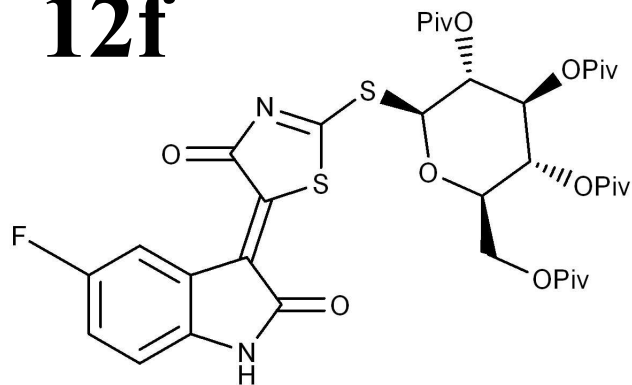
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952421 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H CDC13

8.581
8.576
8.562
8.557
7.049
7.044
7.032
7.027
7.015
7.010
6.807
6.798
6.790
6.781
6.526
6.396
6.378
6.181
6.162
6.144
5.569
5.550
5.531
5.456
5.436
5.416
4.386
4.383
4.361
4.358
4.051
4.043
4.026
4.018
3.949
3.945
3.942
3.938
3.929
3.925
3.922
3.918
1.245
1.180
1.156
1.056



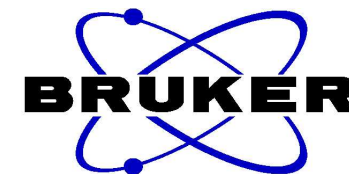
12f



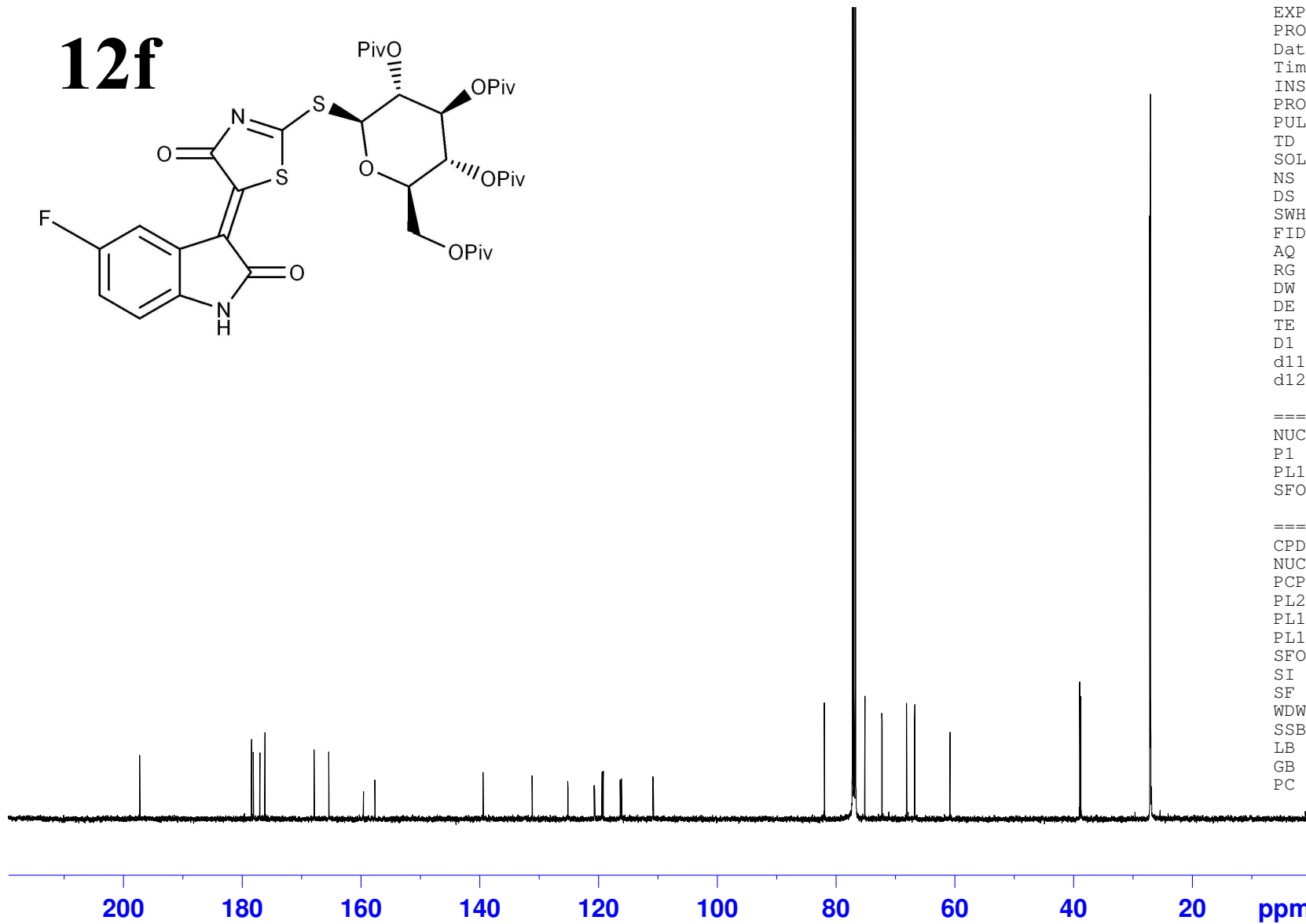
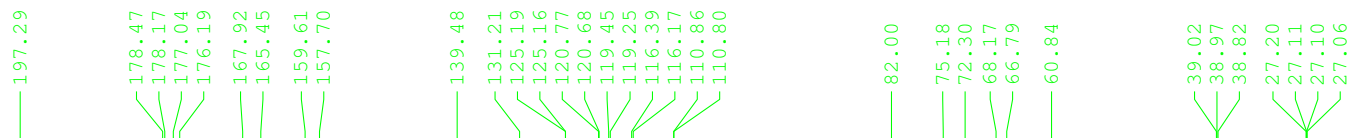
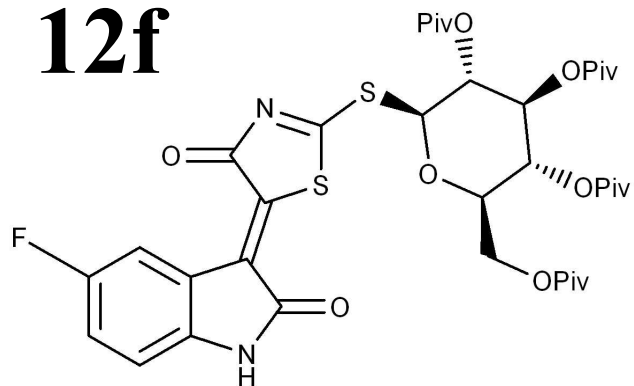
NAME 101022.501
EXPNO 20
PROCNO 1
Date_ 20101023
Time 11.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 101.6
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300180 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 1H CDC13



12f



NAME 101022.501
EXPNO 26
PROCNO 1
Date_ 20101024
Time 2.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 5120
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 101.6
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577911 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

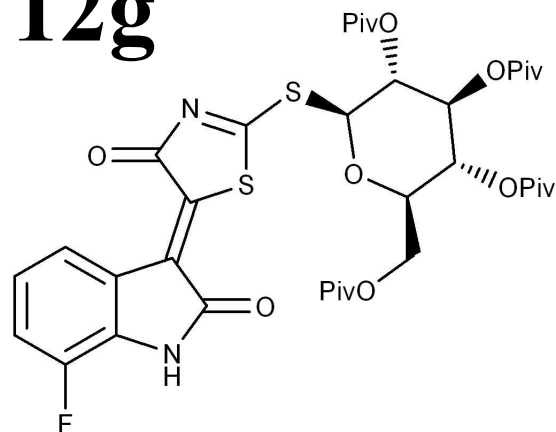
Erben 1H CDC13



8.723
8.721
8.697
8.695
8.615
8.589
7.138
7.109
7.080
6.547
6.516
6.485
6.396
6.365
6.203
6.172
6.141
5.935
5.904
5.570
5.538
5.507
5.430
5.397
5.365
4.362
4.357
4.320
4.316
4.075
4.060
4.033
4.019

1.219
1.176
1.160
1.135
1.112
1.023
0.970

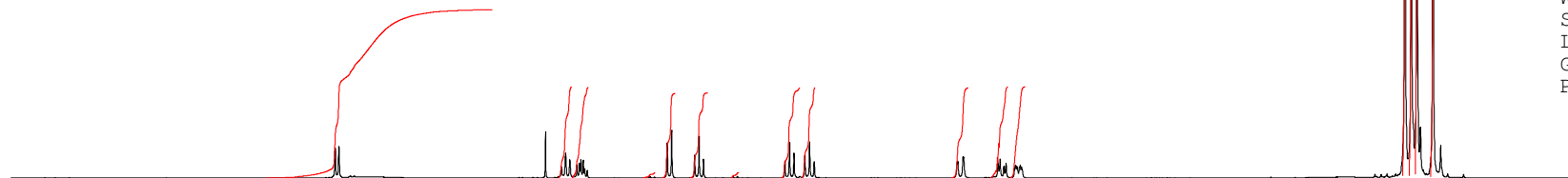
12g



NAME 110622.u311
EXPNO 10
PROCNO 1
Date_ 20110622
Time 12.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 101
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

15 14 13 12 11 ppm



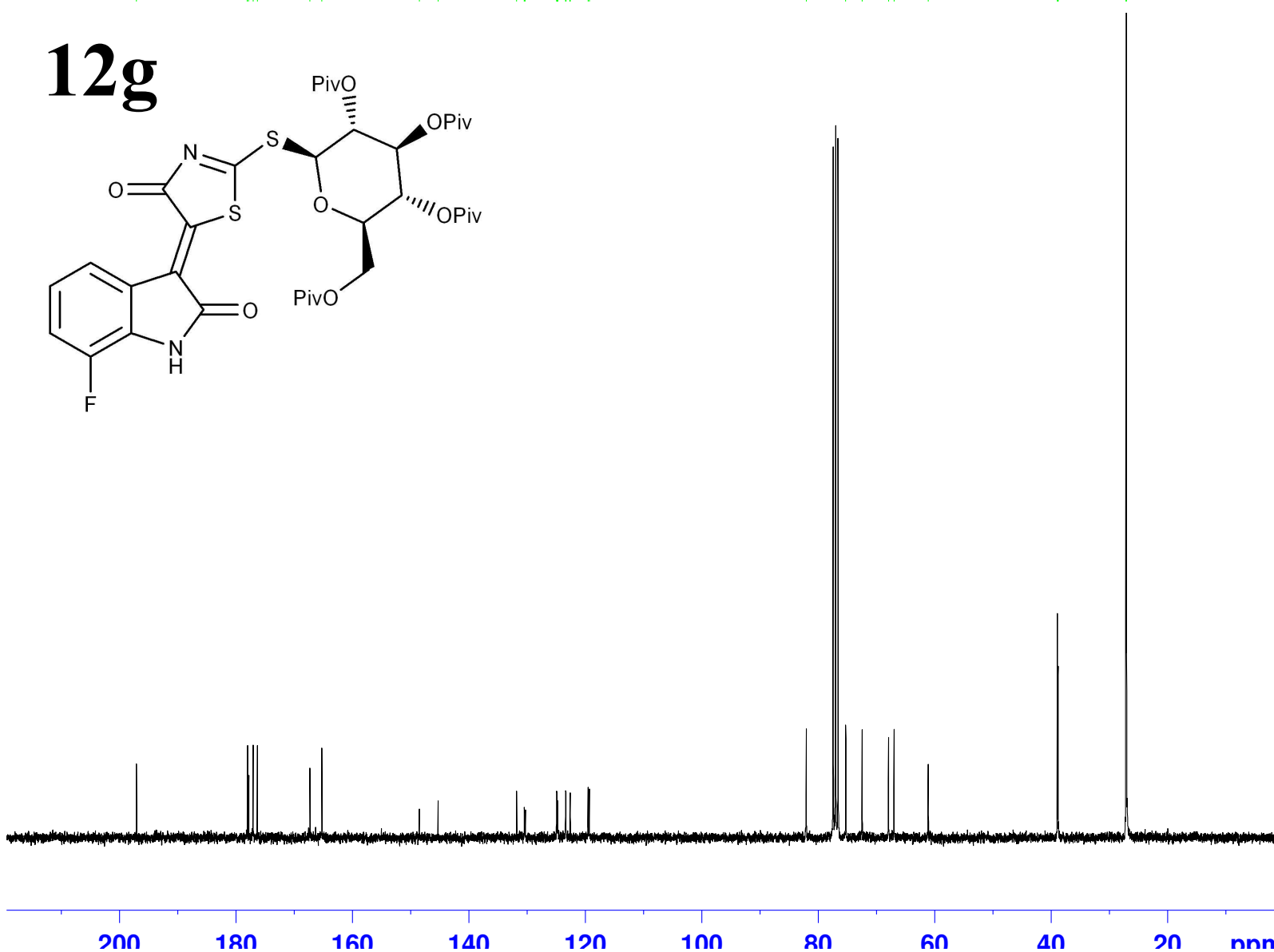
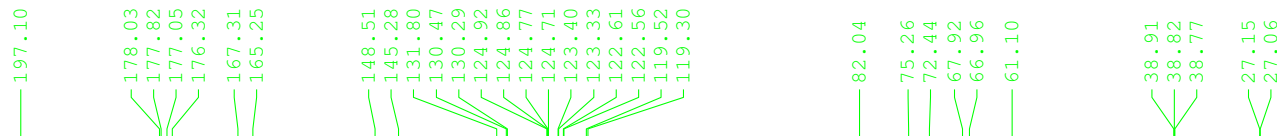
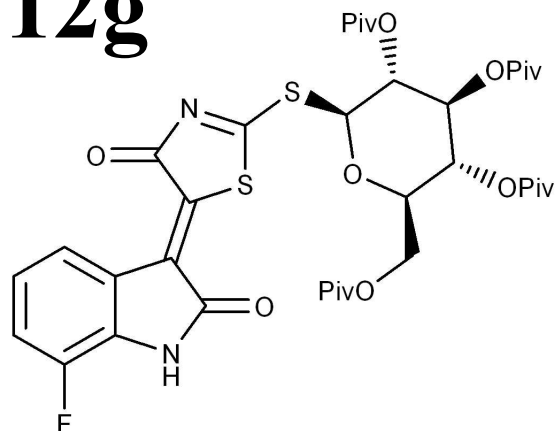
10 9 8 7 6 5 4 3 2 1 ppm

1.86
1.01
1.00
0.06
0.94
0.94
0.06
1.00
1.00
1.00
1.00
1.01
1.01
9.06
9.06
9.03
9.01

Erben 13C CDCl3



12g

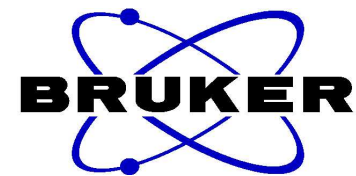


NAME 110622.u311
EXPNO 12
PROCNO 1
Date_ 20110622
Time 17.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 299.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

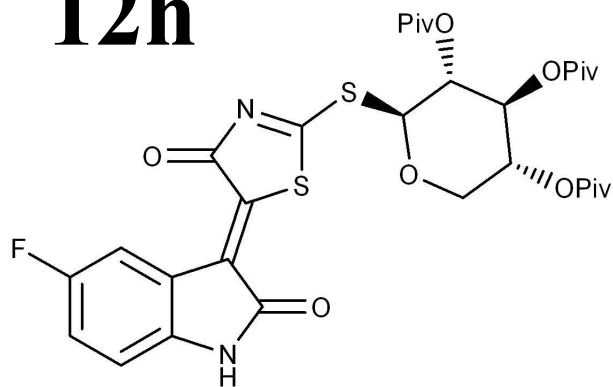
==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677515 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H CDC13



12h

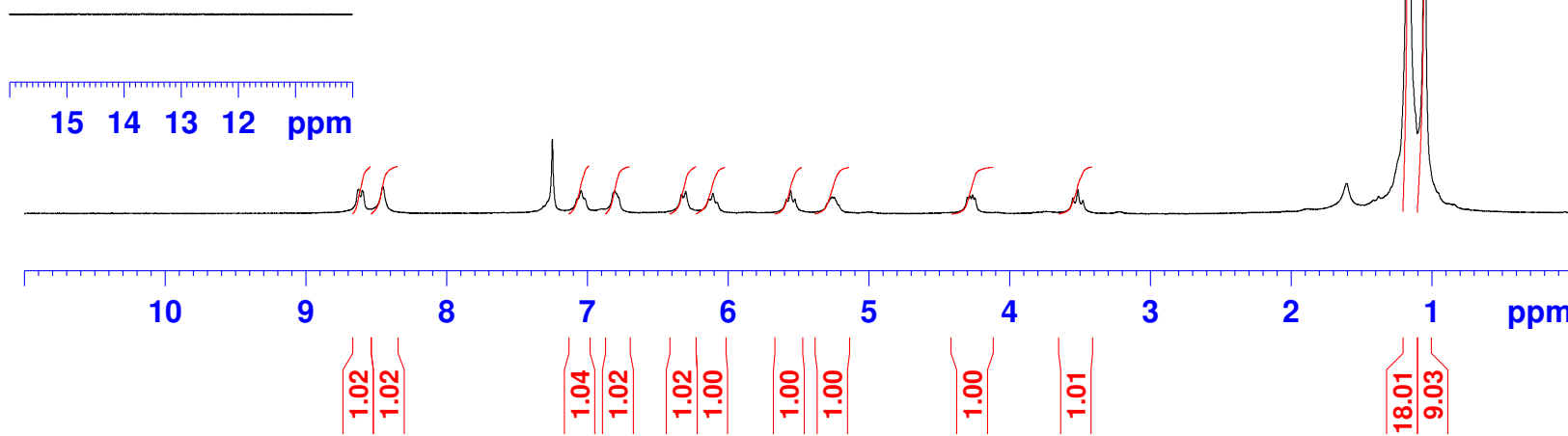


8.624
8.599
8.454

6.331
6.303
6.138
6.109
6.078
5.587
5.558
5.525

4.301
4.283
4.263
4.247
3.552
3.515
3.479

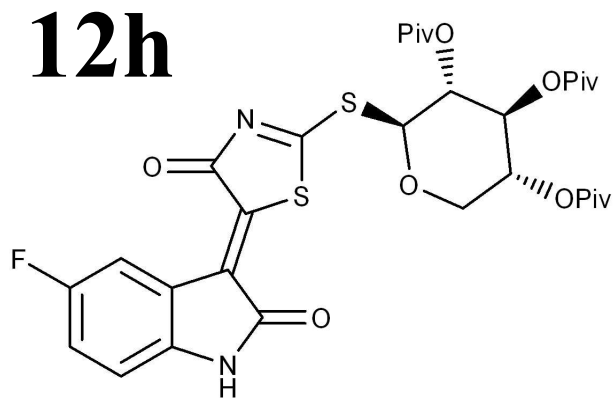
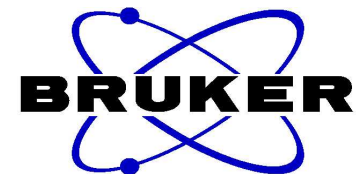
1.168
1.053



NAME 110720.u330
EXPNO 10
PROCNO 1
Date_ 20110720
Time 12.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 use
DE 10.00 use
TE 298.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 use
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300170 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C CDCl3



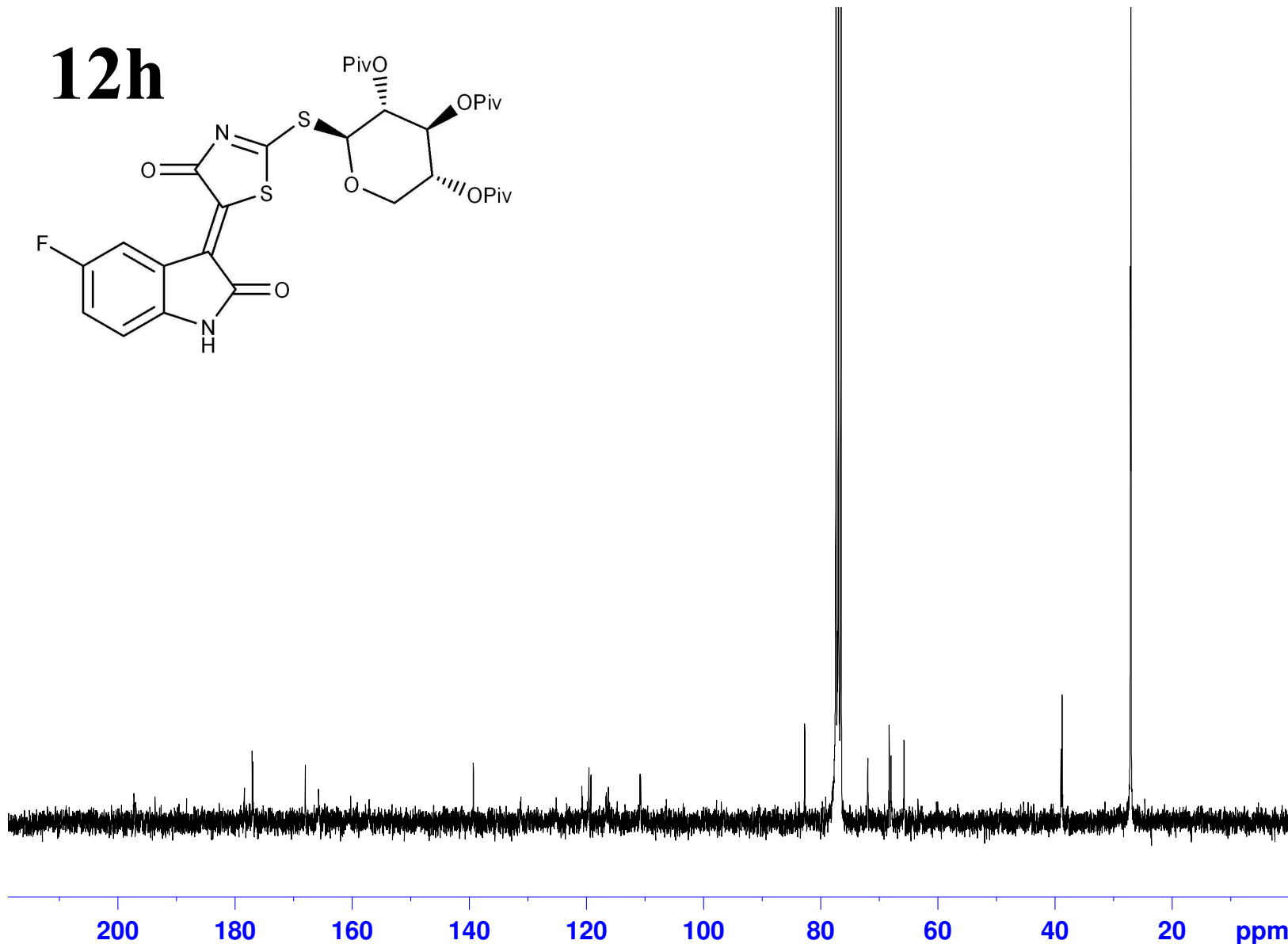
197.23
178.43
177.10
176.97
168.03
165.78
160.30
157.17
139.36
131.24
125.21
125.18
120.82
120.70
119.60
119.28
116.63
116.30
110.90
110.79

82.77

71.99
68.35
68.04
65.81

39.01
38.82

27.15
27.08



NAME 110721.u326
EXPNO 10
PROCNO 1
Date_ 20110721
Time 20.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.7 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

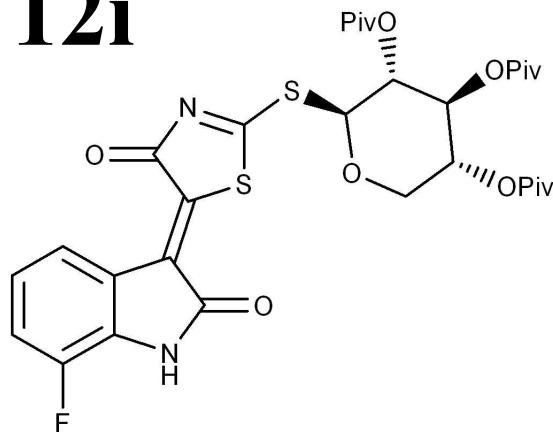
==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677515 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

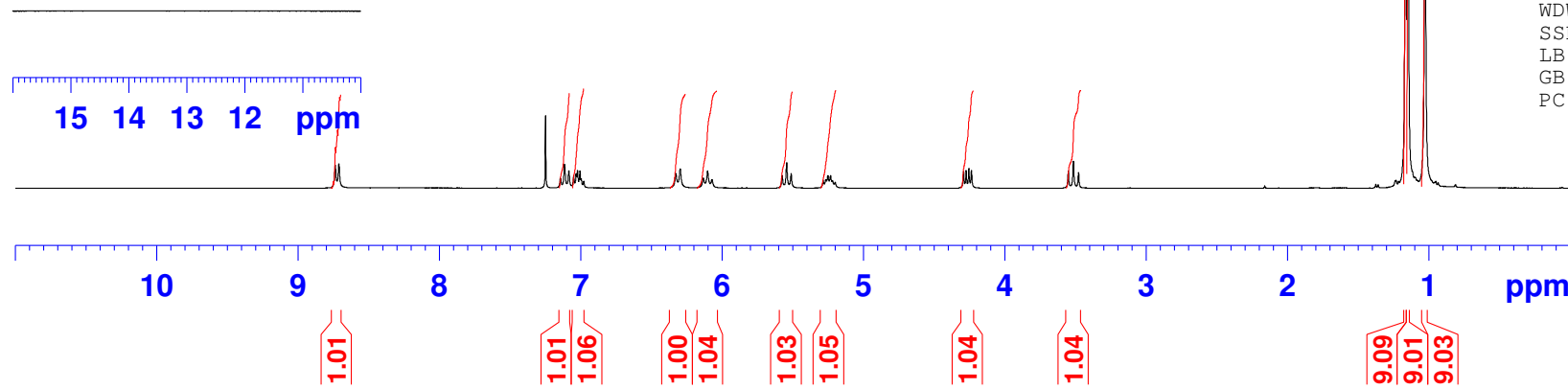
Erben 1H CDC13



12i



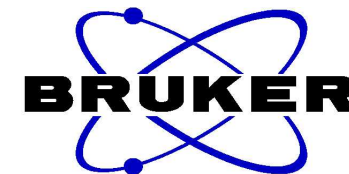
8.738
8.712
7.145
7.116
7.086
6.328
6.298
6.134
6.103
6.072
5.576
5.544
5.513
4.293
4.274
4.255
4.236
3.551
3.515
3.479
1.165
1.148
1.027



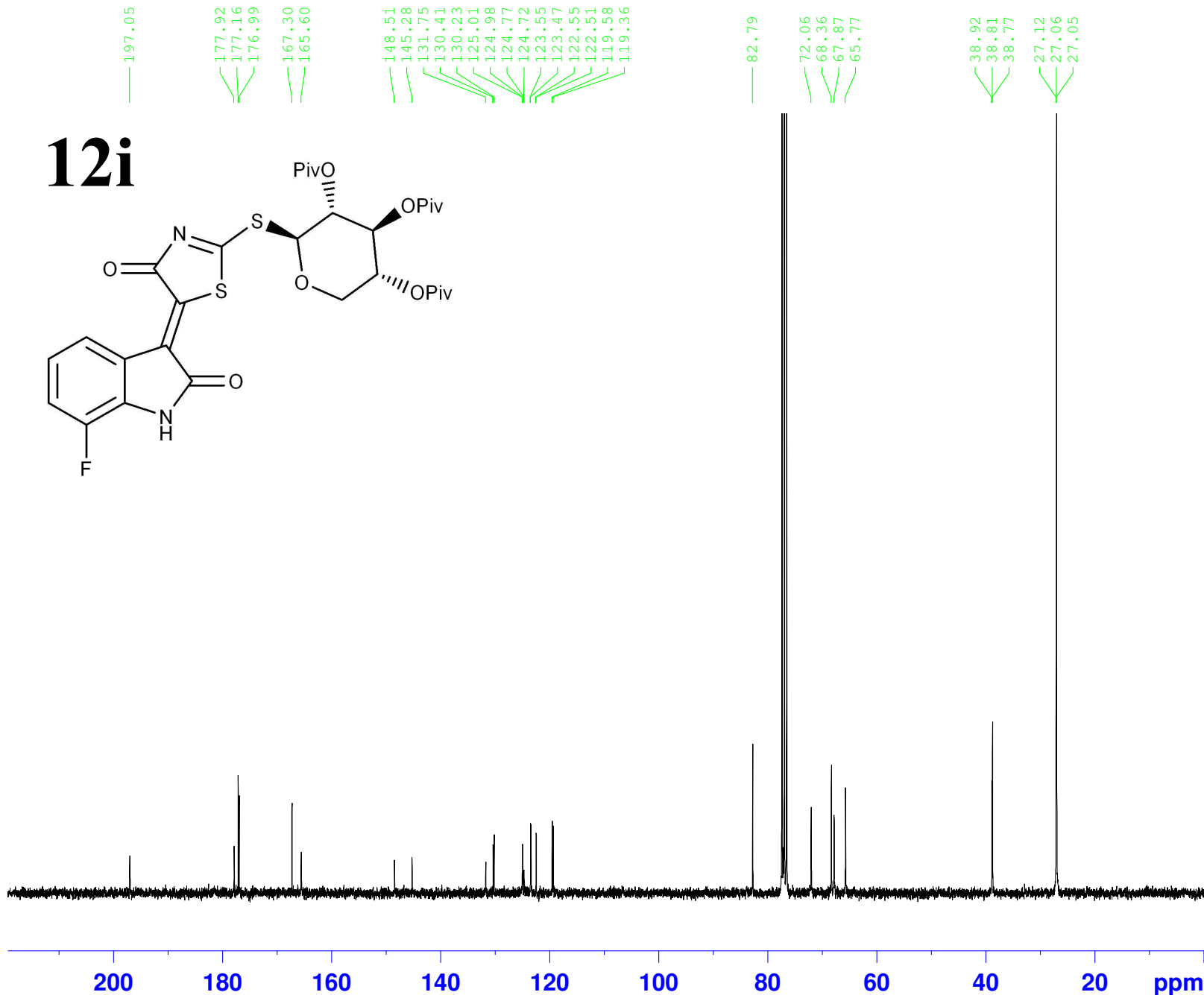
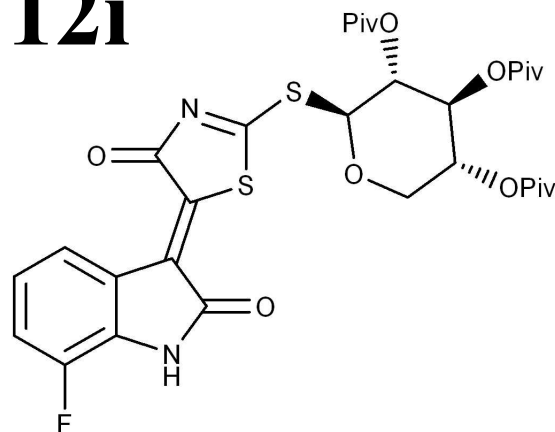
```
NAME 110701.u314
EXPNO 10
PROCNO 1
Date_ 20110701
Time 12.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

Erben 13C CDCl3



12i

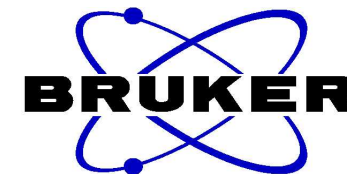


```
NAME          110707.u326
EXPNO          10
PROCNO         1
Date_          20110707
Time           20.23
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        CDC13
NS             2048
DS             4
SWH            18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG             2050
DW            27.733 usec
DE            10.00 usec
TE            298.3 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0            1
```

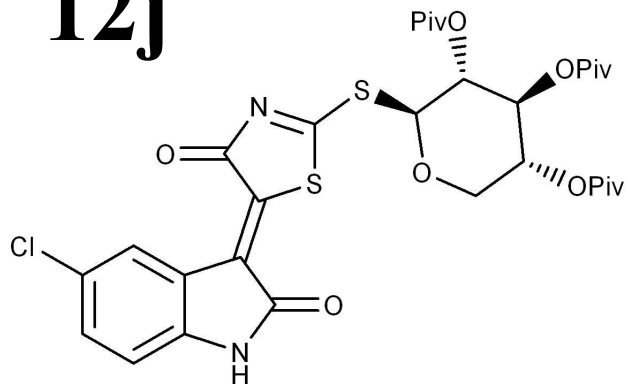
```
===== CHANNEL f1 =====
NUC1           13C
P1             10.00 usec
PL1            -0.50 dB
PL1W          33.25691986 W
SFO1           75.4752953 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2            1H
PCPD2          72.00 usec
PL2            0.00 dB
PL12           17.00 dB
PL13           17.00 dB
PL2W          11.25325108 W
PL12W          0.22453187 W
PL13W          0.22453187 W
SFO2          300.1312005 MHz
SI             32768
SF            75.4677516 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
```

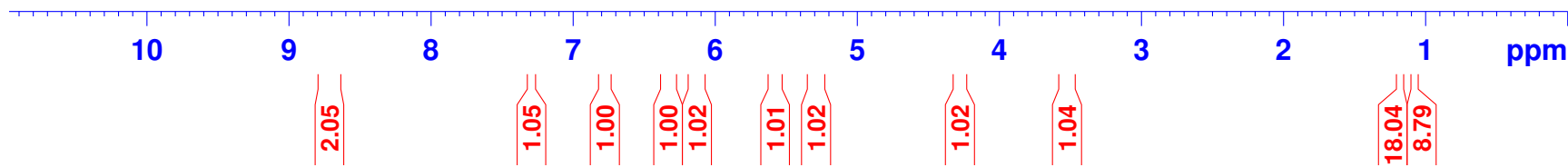
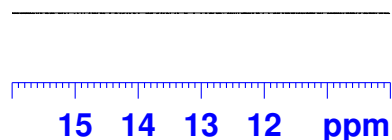
Erben 1H CDC13



12j



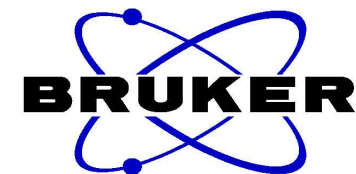
8.710
7.308
7.302
7.280
7.274
6.785
6.758
6.341
6.310
6.152
6.121
6.090
5.604
5.572
5.540
4.301
4.283
4.263
4.245
3.556
3.520
3.483
1.182
1.173
1.078



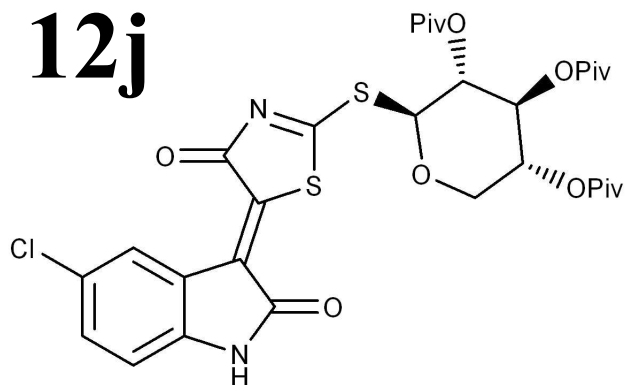
NAME 110715.u334
EXPNO 10
PROCNO 1
Date_ 20110716
Time 1.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 144
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C CDCl3



12j



197.24

179.33

177.09

176.93

167.55

165.73

141.84

132.43

131.08

128.83

128.25

124.49

120.61

111.37

82.67

71.92

68.31

68.26

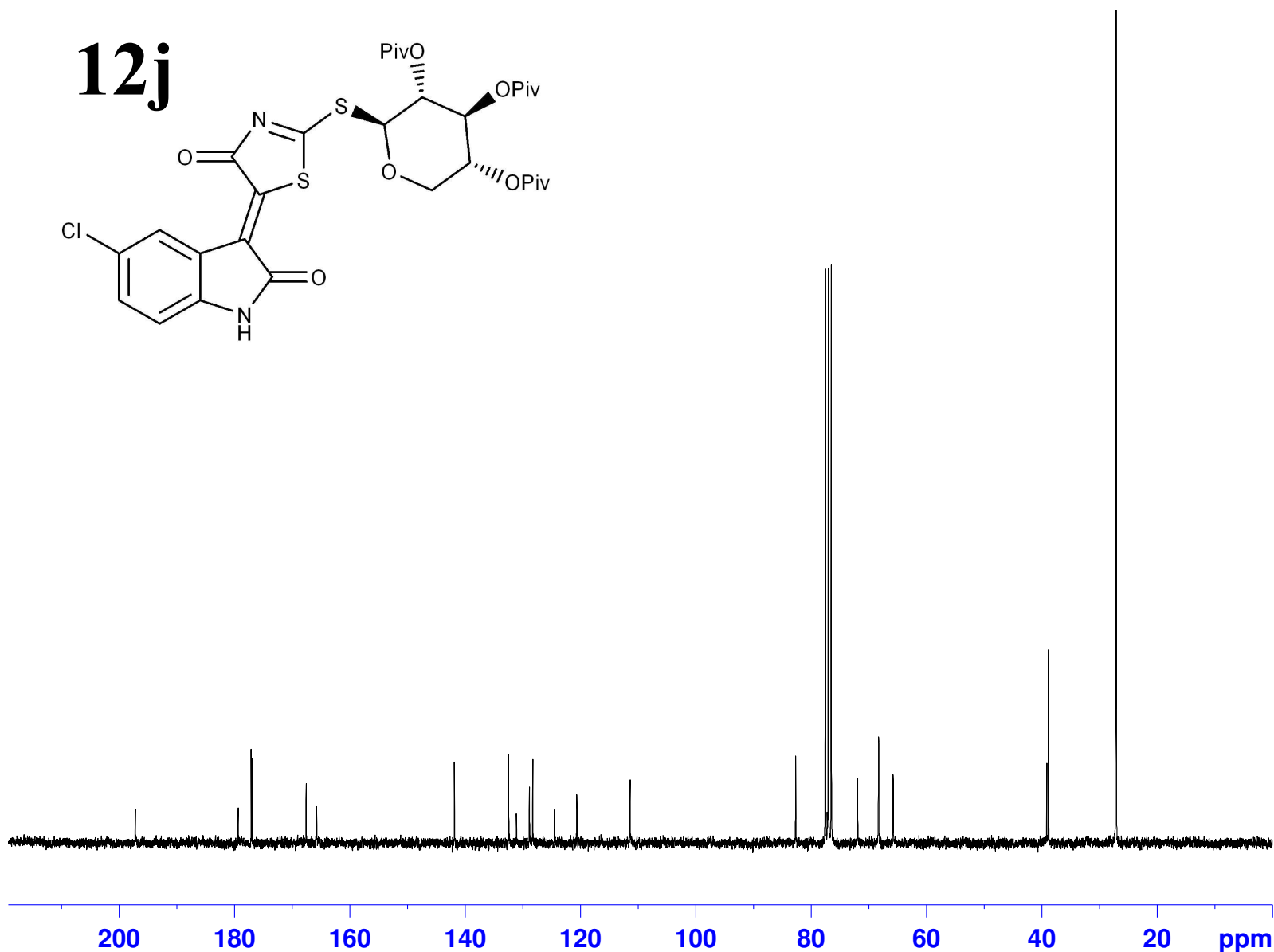
65.76

39.11

38.81

27.16

27.08

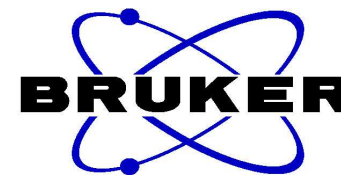


NAME 110713.202
EXPNO 10
PROCNO 1
Date_ 20110713
Time 18.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

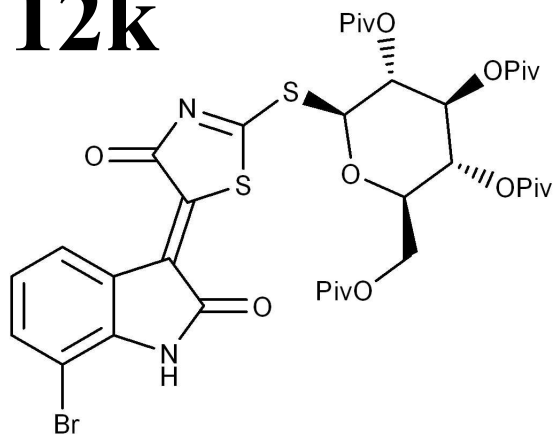
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952395 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H CDC13



8.912
8.886
8.792
8.766
8.389
7.514
7.487
7.463
7.436
6.998
6.971
6.944
6.545
6.515
6.484
6.390
6.359
6.197
6.166
6.135
5.936
5.905
5.563
5.531
5.500
5.425
5.392
5.359
4.351
4.346
4.309
4.305
4.237
4.076
4.062
4.035
4.020
1.219
1.175
1.157
1.131
1.111
1.020
0.972

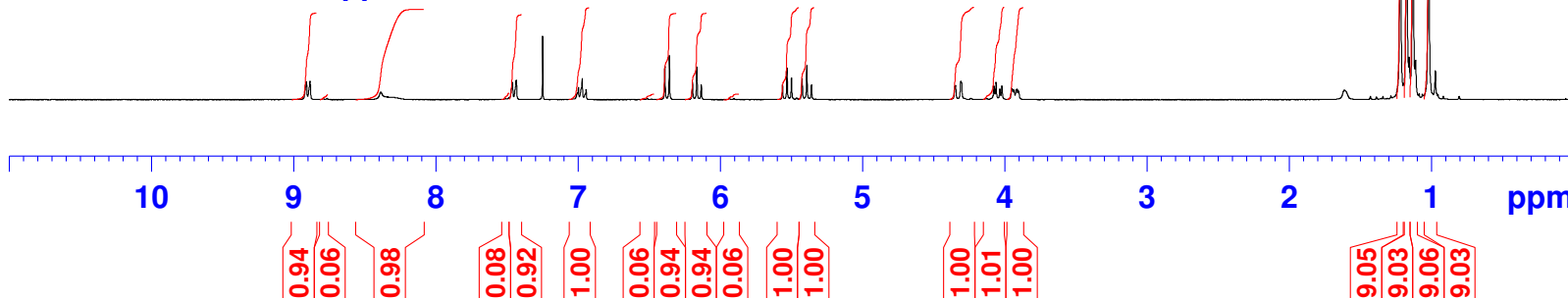
12k



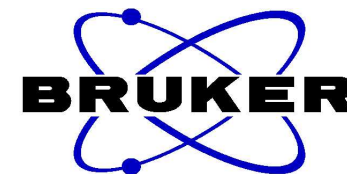
NAME 110623.u317
EXPNO 10
PROCNO 1
Date_ 20110623
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 128
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

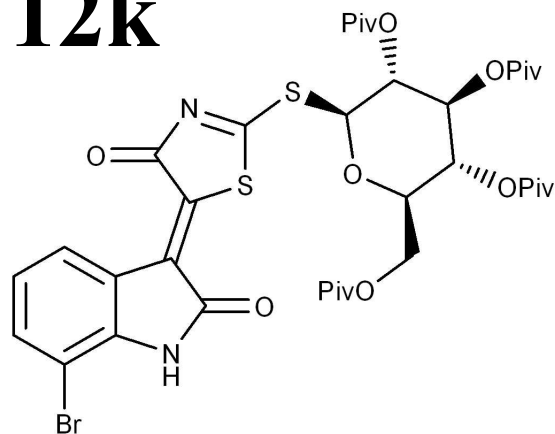
15 14 13 12 ppm



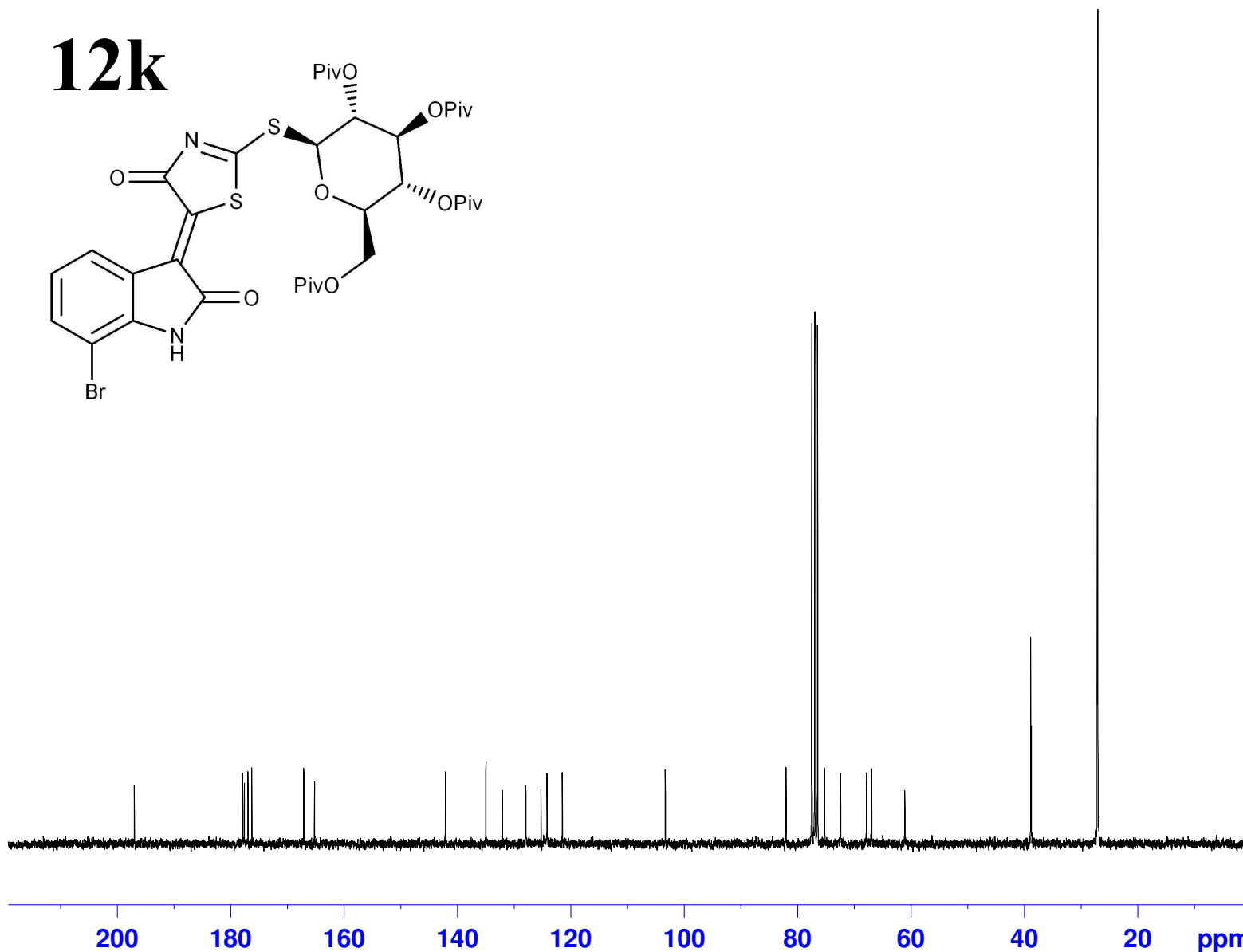
Erben 13C CDCl3



12k



197.05
177.94
177.65
176.98
176.32
167.15
165.24
142.12
135.01
132.10
127.97
125.28
124.23
121.52
103.35
82.06
75.26
72.44
67.86
66.96
61.11
38.90
38.82
38.77
27.15
27.07



NAME 110624.204
EXPNO 10
PROCNO 1
Date_ 20110626
Time 1.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

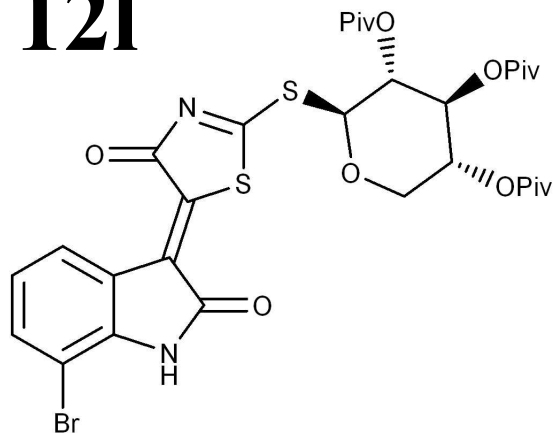
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

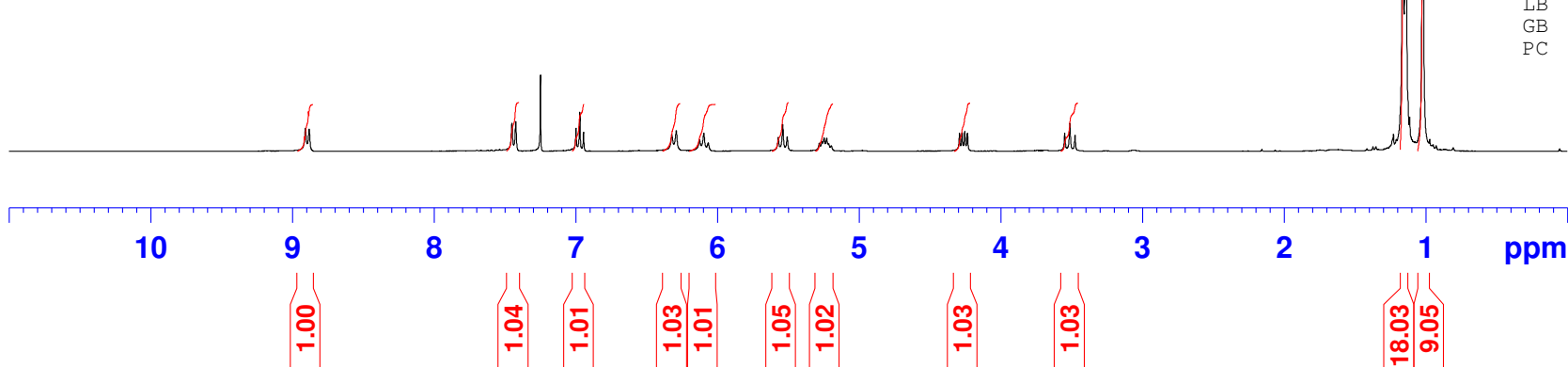
Erben 1H CDC13

8.909
8.883
7.699
7.696
7.672
7.668
7.451
7.424
6.999
6.972
6.946
6.581
6.555
6.529
6.322
6.292
6.128
6.097
6.066
5.571
5.540
5.508
4.292
4.274
4.254
4.236
3.549
3.513
3.476

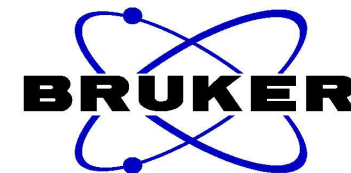
121



15 14 13 12 ppm



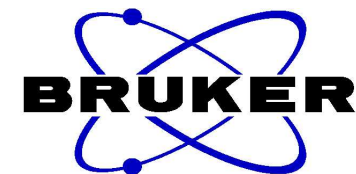
1.163
1.142
1.022



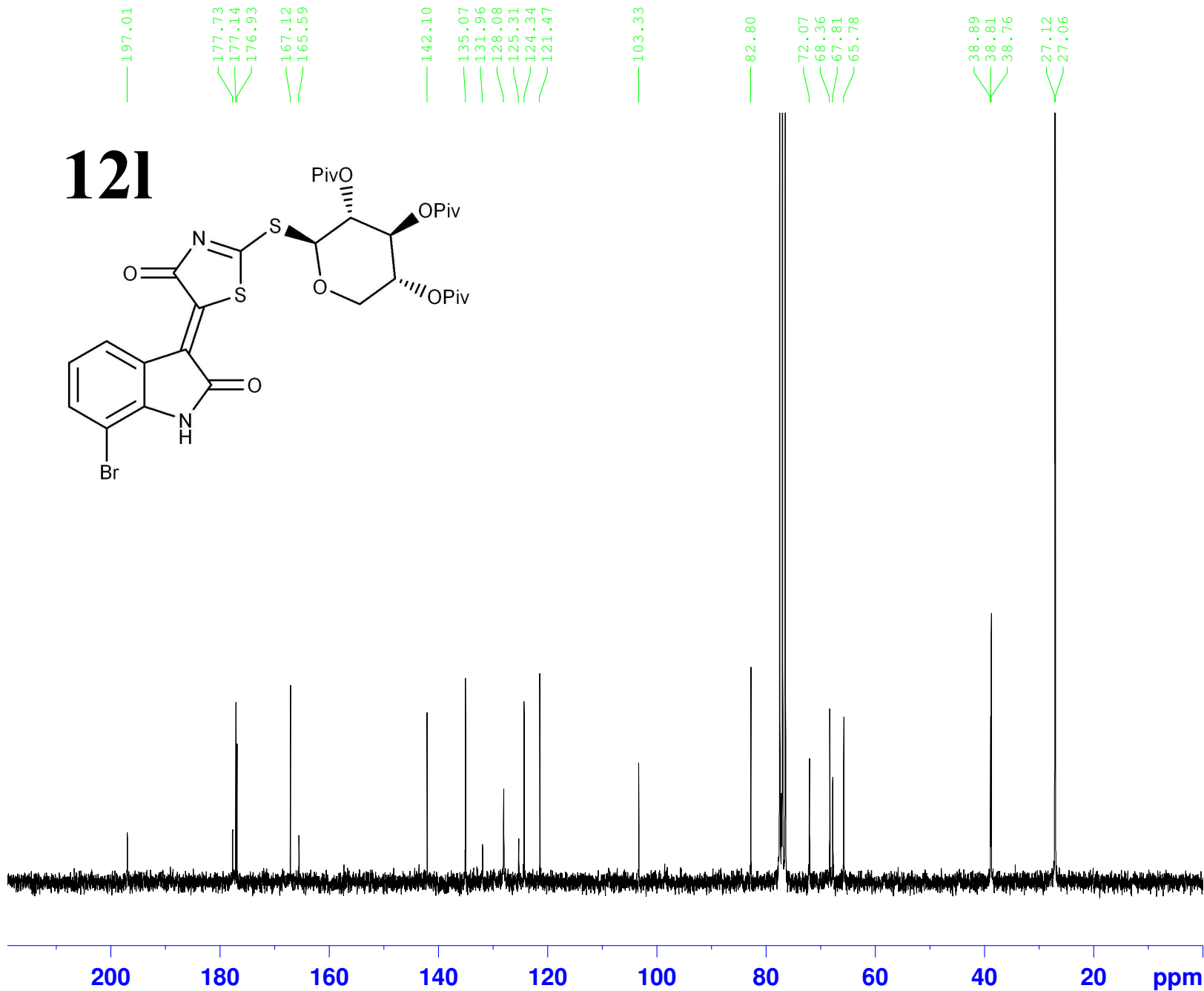
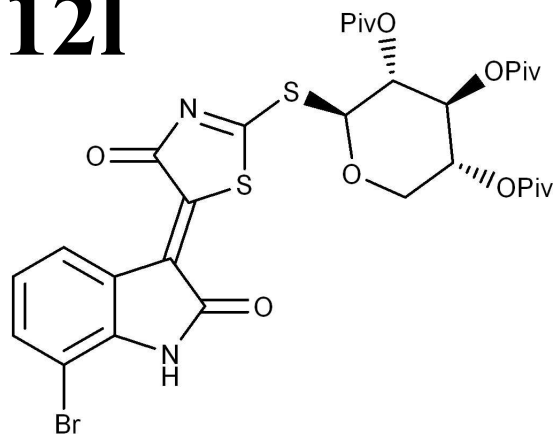
NAME 110630.u322
EXPNO 10
PROCNO 1
Date_ 20110630
Time 12.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 114
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Erben 13C CDCl3



121

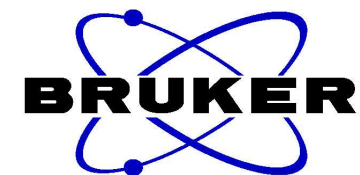


NAME 110705.202
EXPNO 10
PROCNO 1
Date_ 20110705
Time 14.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

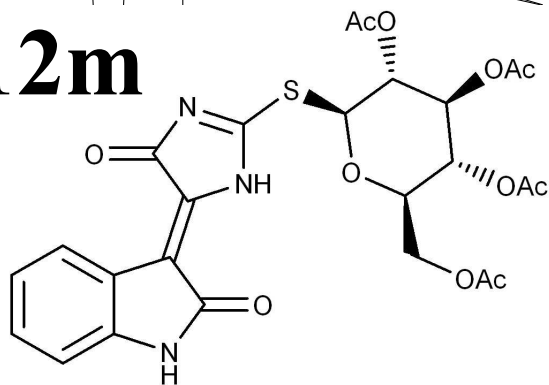
==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz
SI 32768
SF 62.8952393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Erben 1H, DMSO



12m

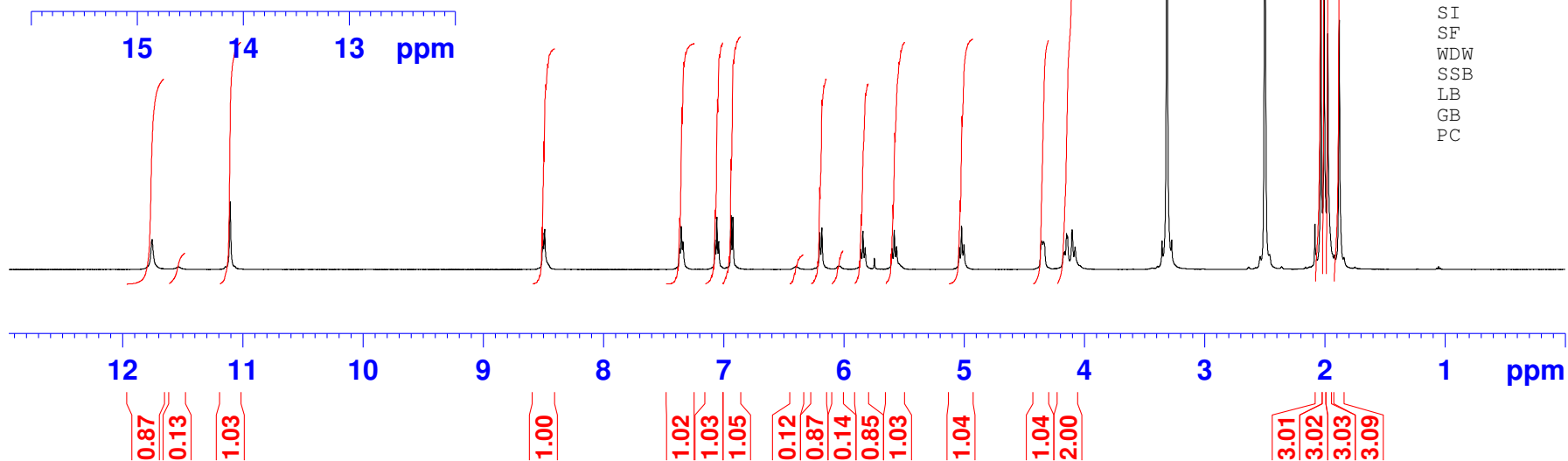


11.758
11.537
11.108

8.507
8.492
7.370
7.355
7.340
7.074
7.059
7.044
6.941
6.926
6.402
6.204
6.185
6.050
6.034
5.862
5.844
5.825
5.602
5.583
5.564
5.043
5.023
5.003
4.176
4.166
4.150
4.142
4.103
4.080
2.034
2.007
1.977
1.882

NAME 100928.502
EXPNO 10
PROCNO 1
Date_ 20100928
Time 17.03
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 15015.015 Hz
FIDRES 0.229111 Hz
AQ 2.1824322 sec
RG 161.3
DW 33.300 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

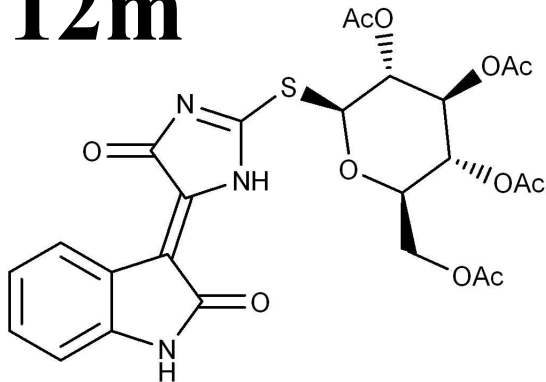
===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 -3.00 dB
SFO1 500.1350013 MHz
SI 32768
SF 500.1300046 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Erben 13C DMSO



12m



176.23
170.13
169.69
169.67
169.53
169.18
162.22

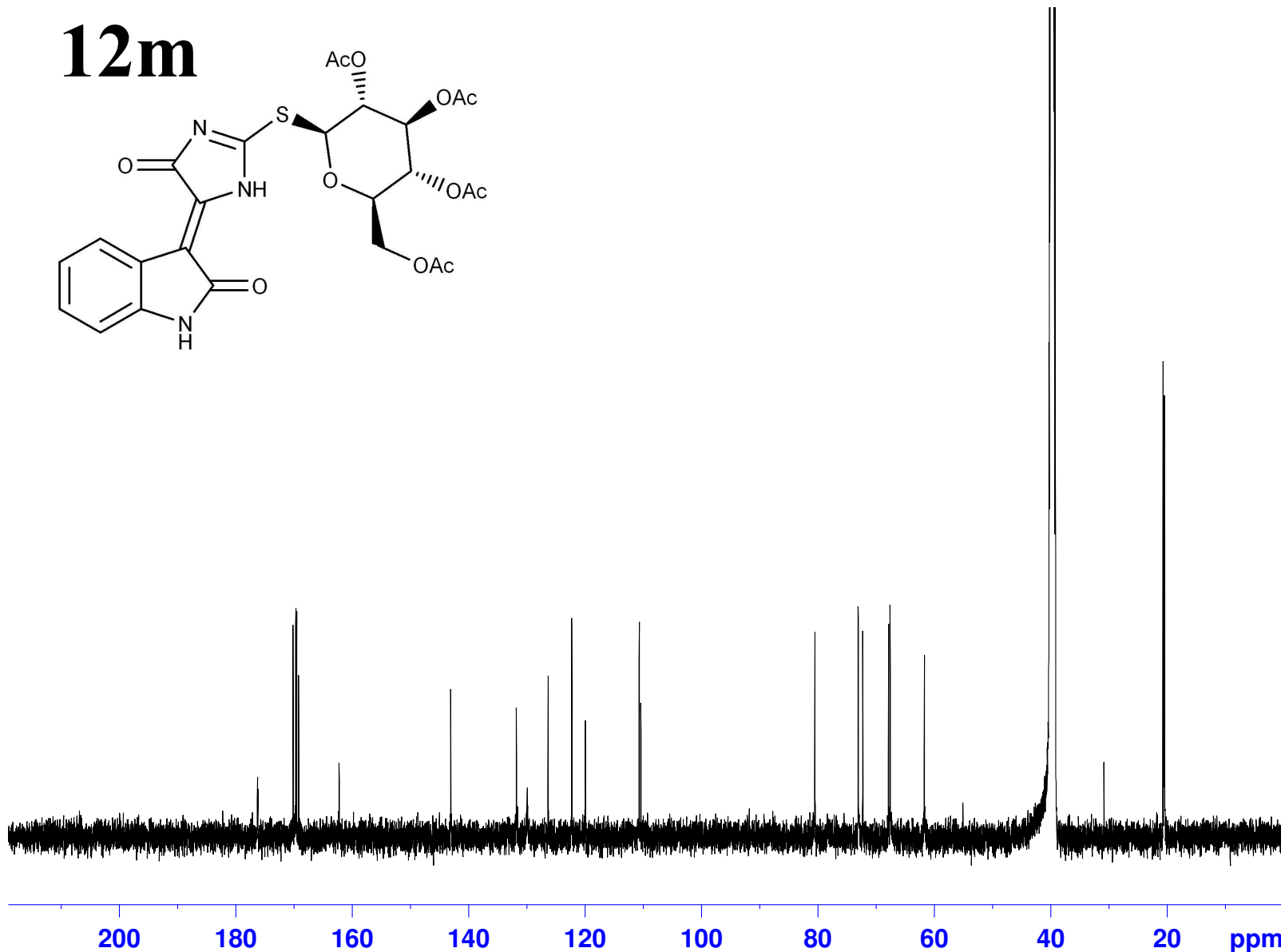
143.06

131.78
129.90
126.31
122.26
119.92

110.67
110.39

80.49
73.05
72.27
67.84
67.57
61.69

20.70
20.55
20.45
20.39



NAME 100928.502
EXPNO 16
PROCNO 1
Date_ 20100929
Time 9.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10240
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 4.80 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.50 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7578277 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40