Supporting Information

The Design, Synthesis and Evaluation of Coumarin Ring Derivatives of the Novobiocin Scaffold that Exhibit Anti-proliferative Activity

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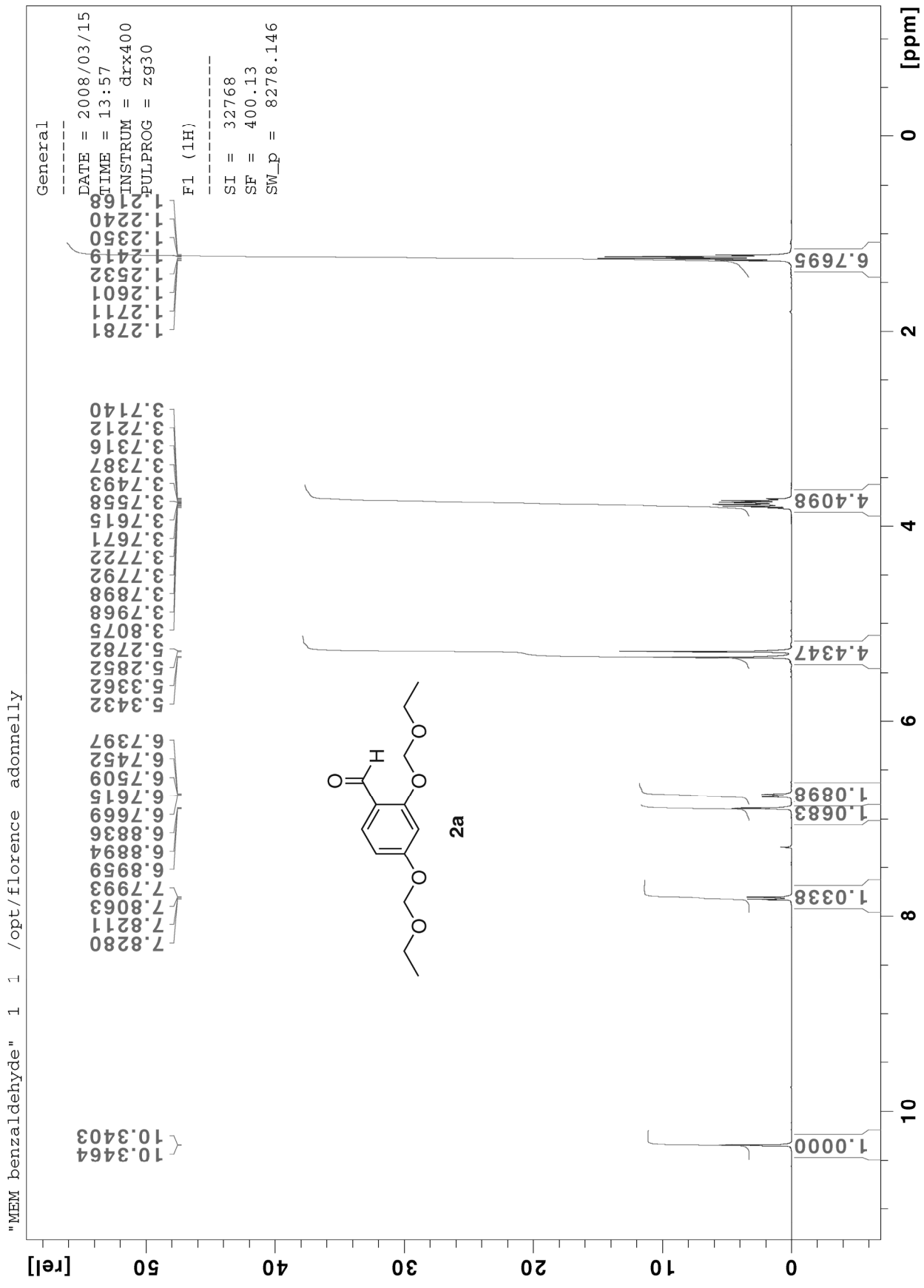
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6.7615
6.7509
6.7452
6.7397
5.3432
5.3362
5.2852
5.2782
3.8075
3.7968
3.7898
3.7792
3.7722
3.7671
3.7615
3.7558
3.7493
3.7387
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3.7212
3.7140
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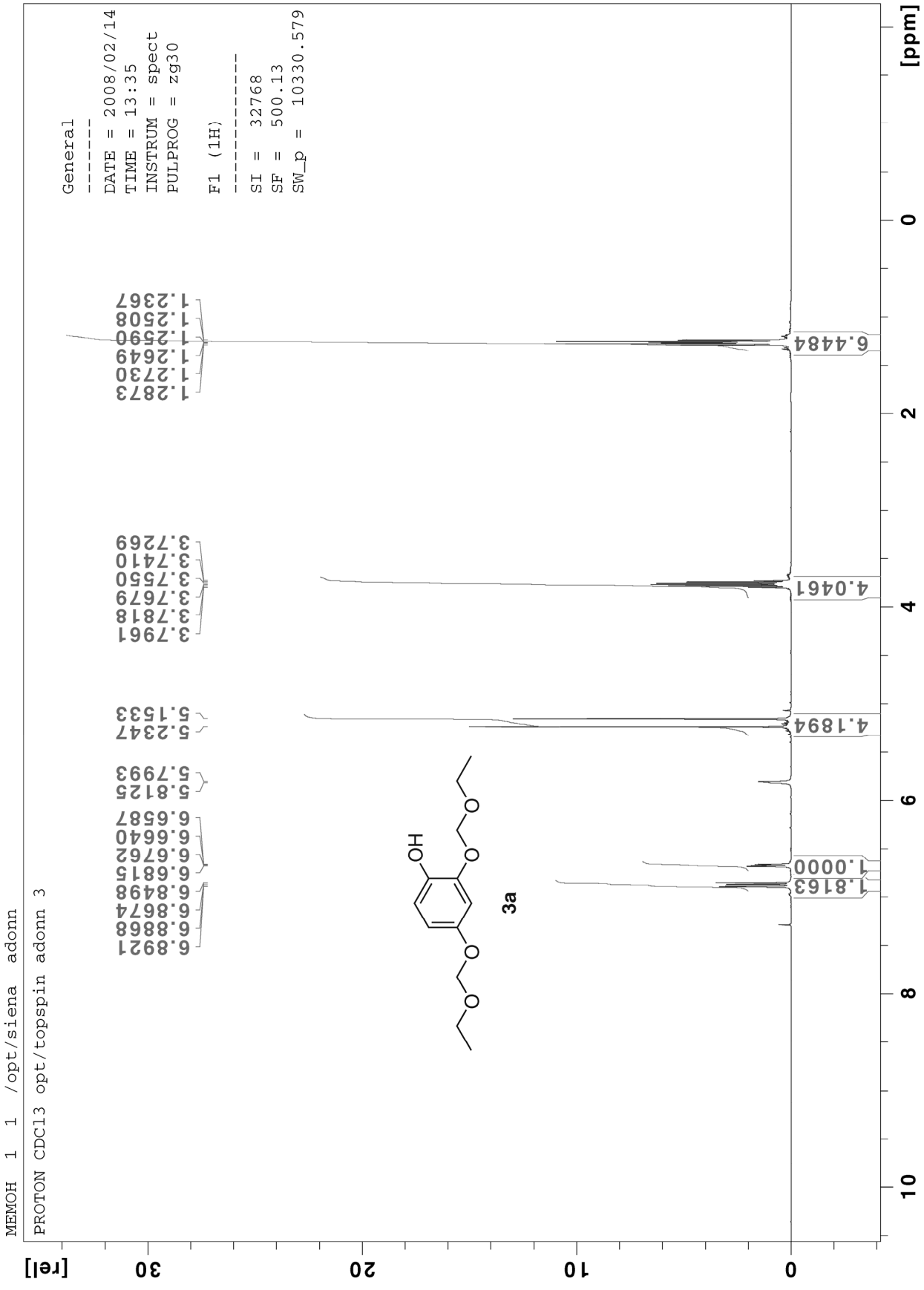
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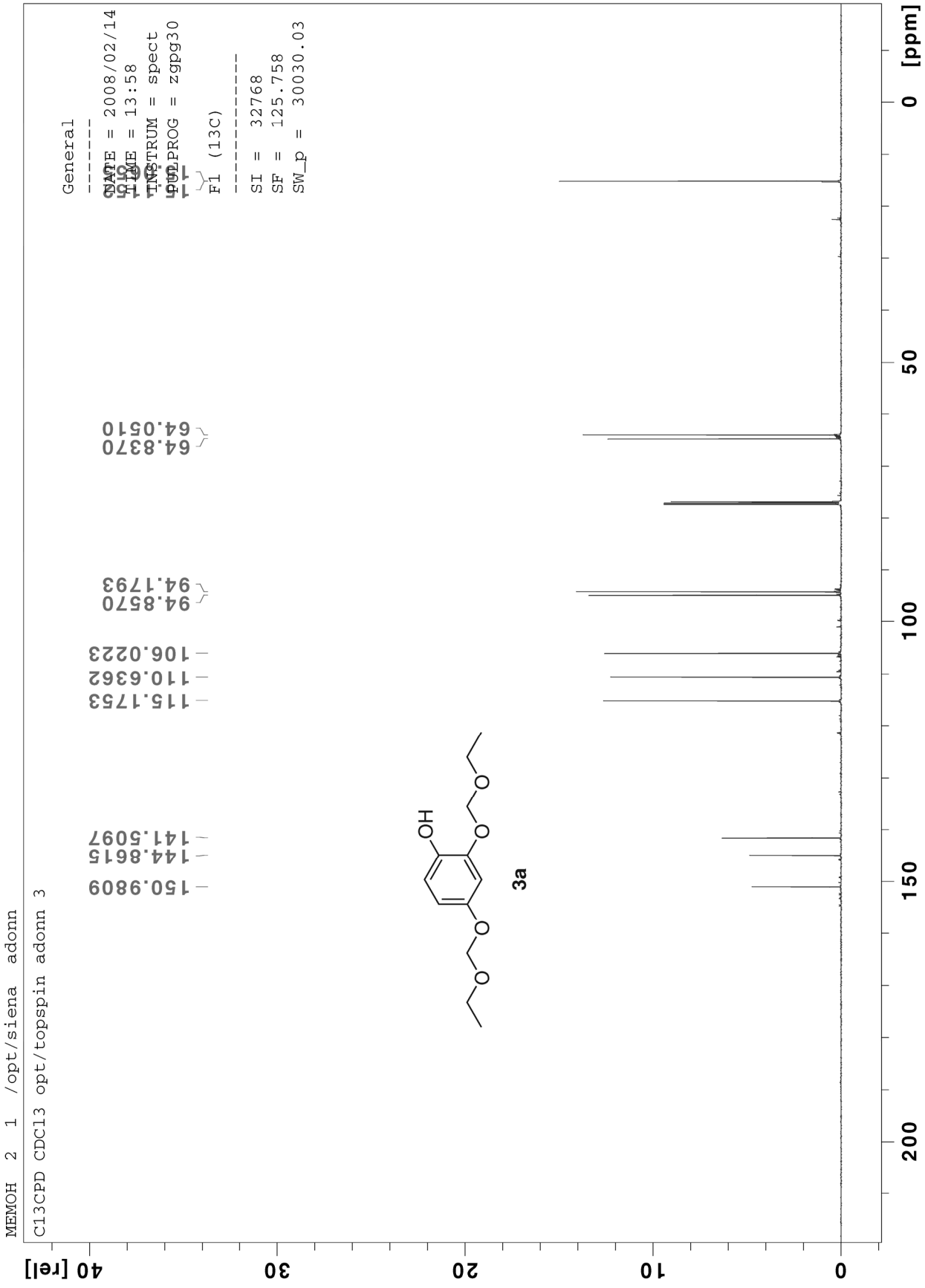
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30
20
10
0
200
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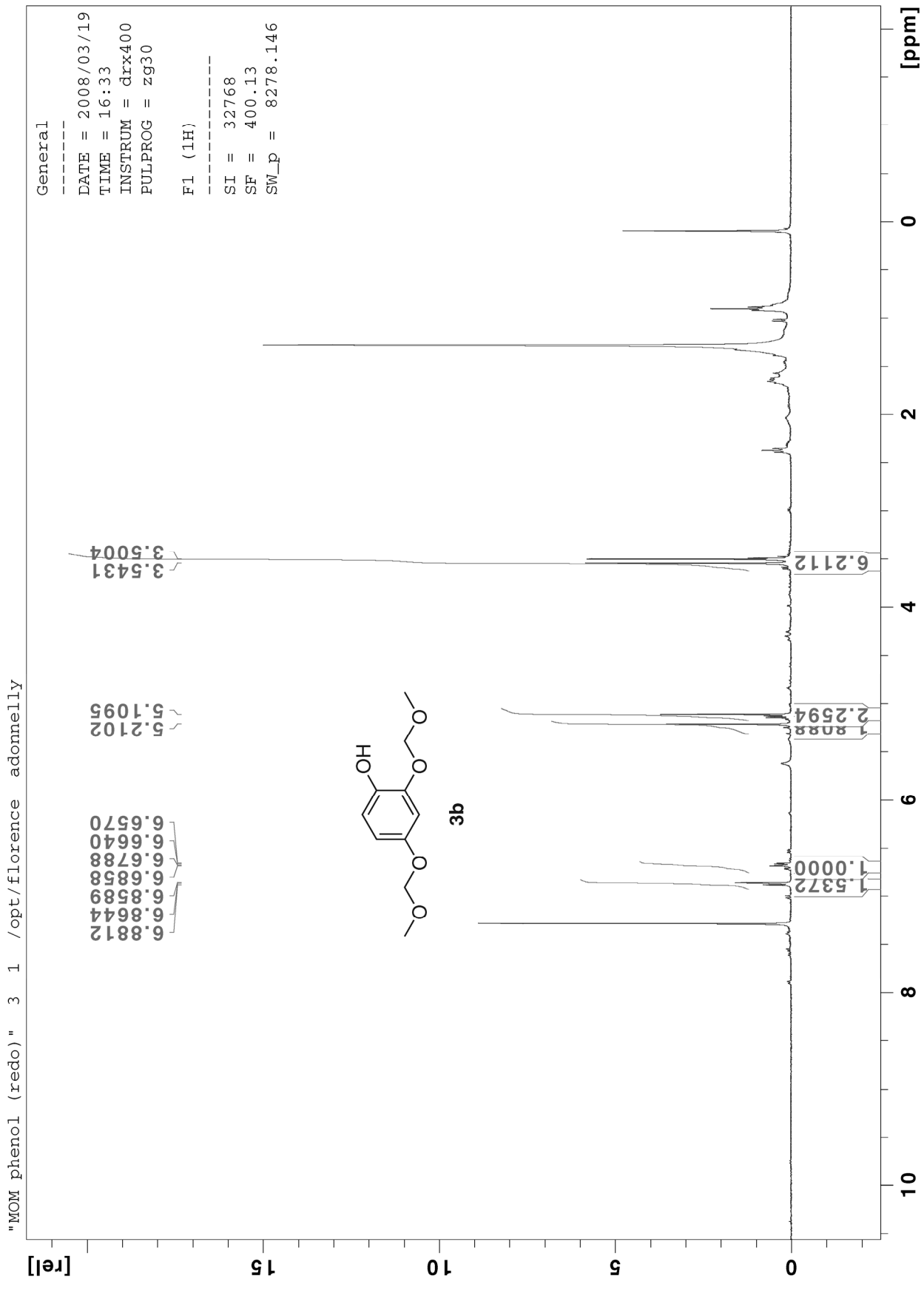
50
0 [ppm]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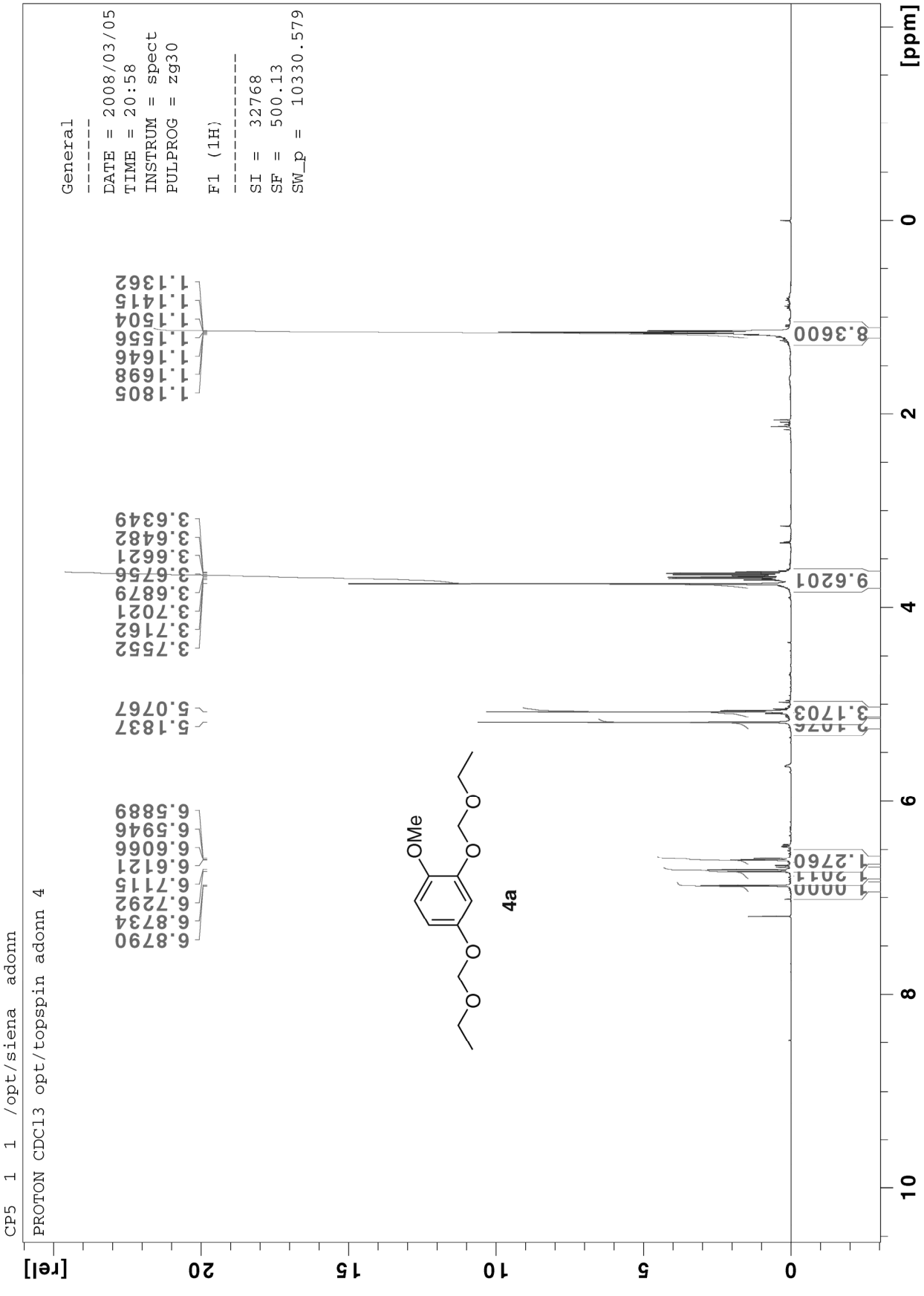
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3.7021
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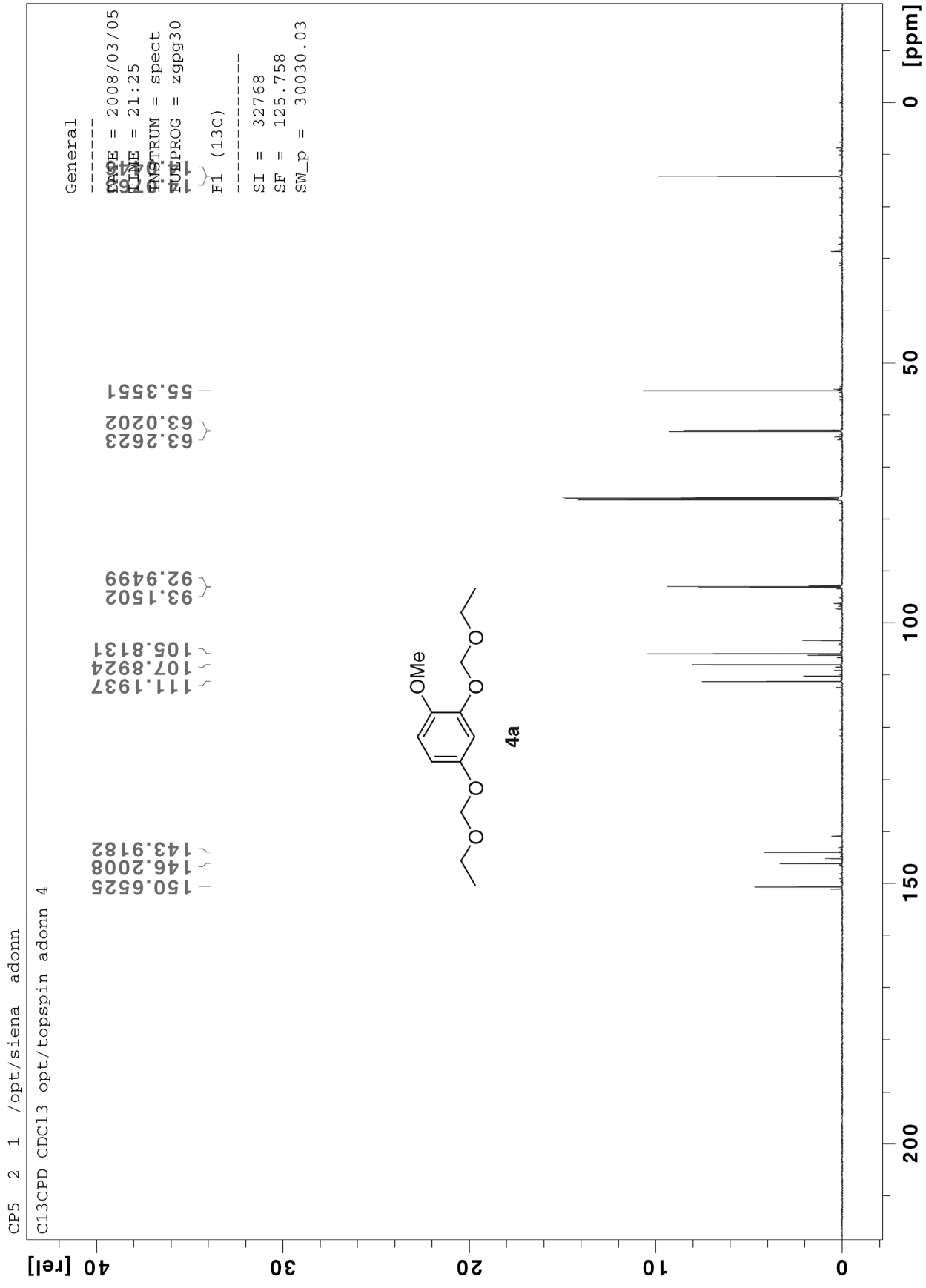
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20
10
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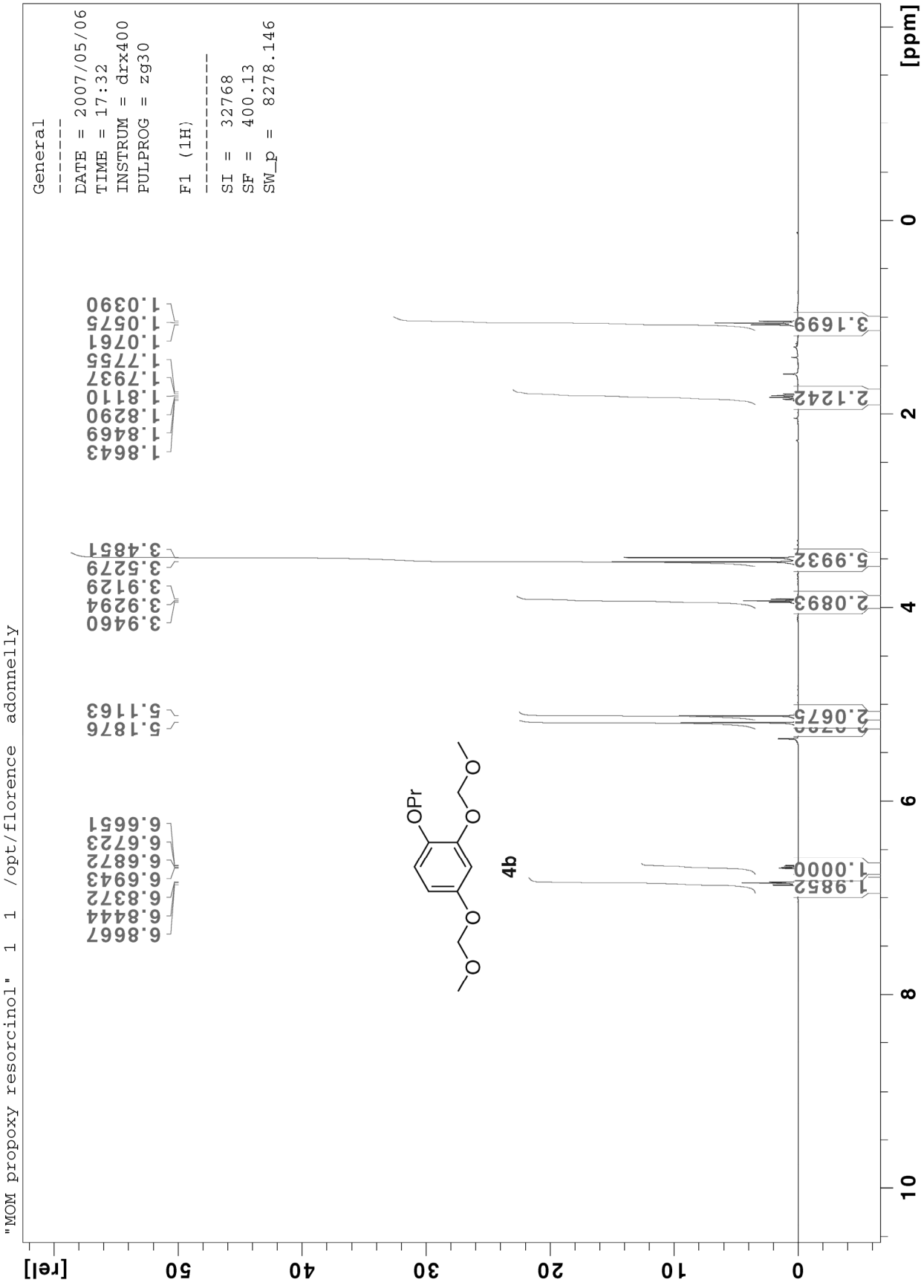
200
150
100
50
0
[ppm]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SI = 32768
SF = 400.13
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6.8444
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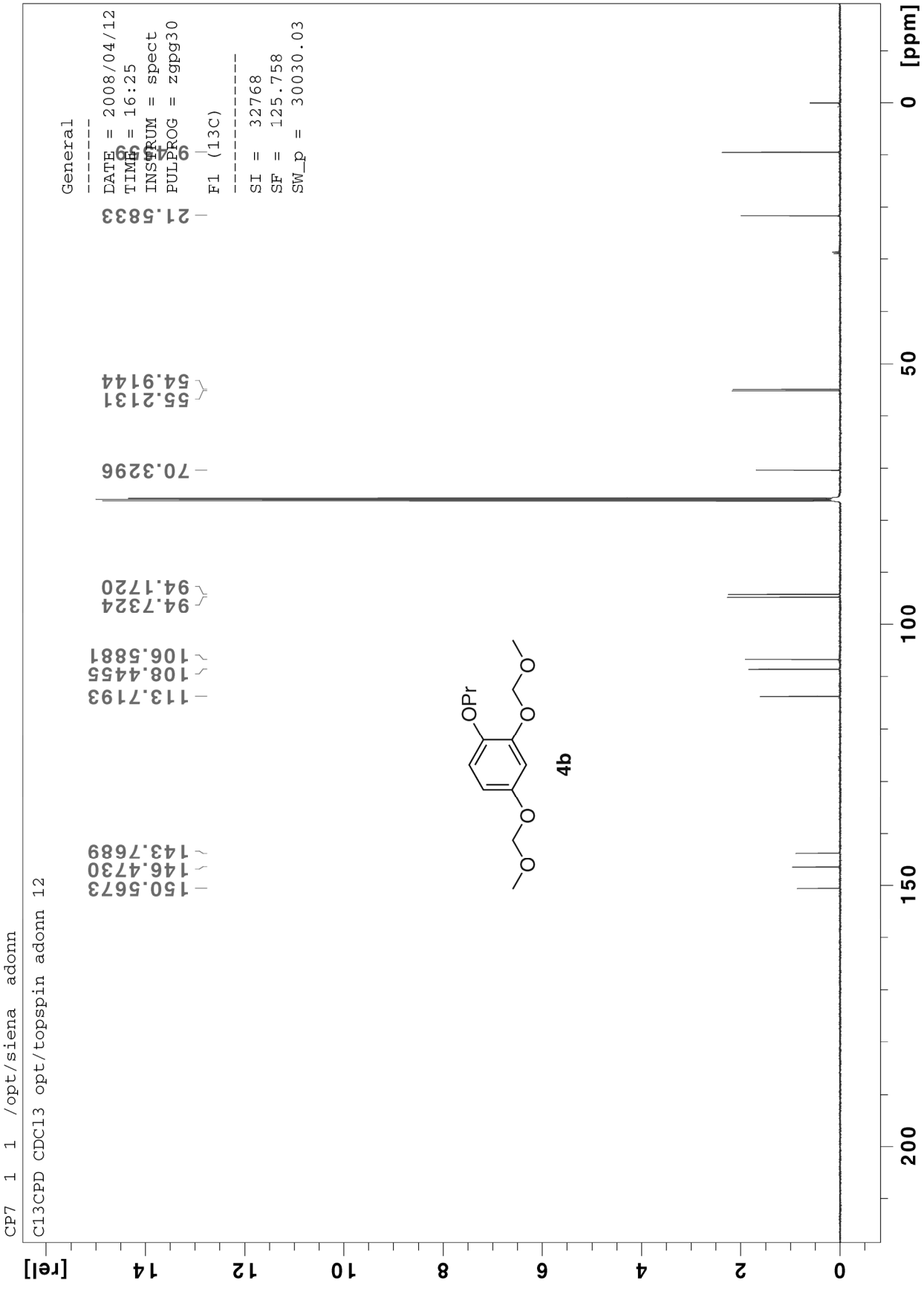
[ppm]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SI = 32768
SF = 125.758
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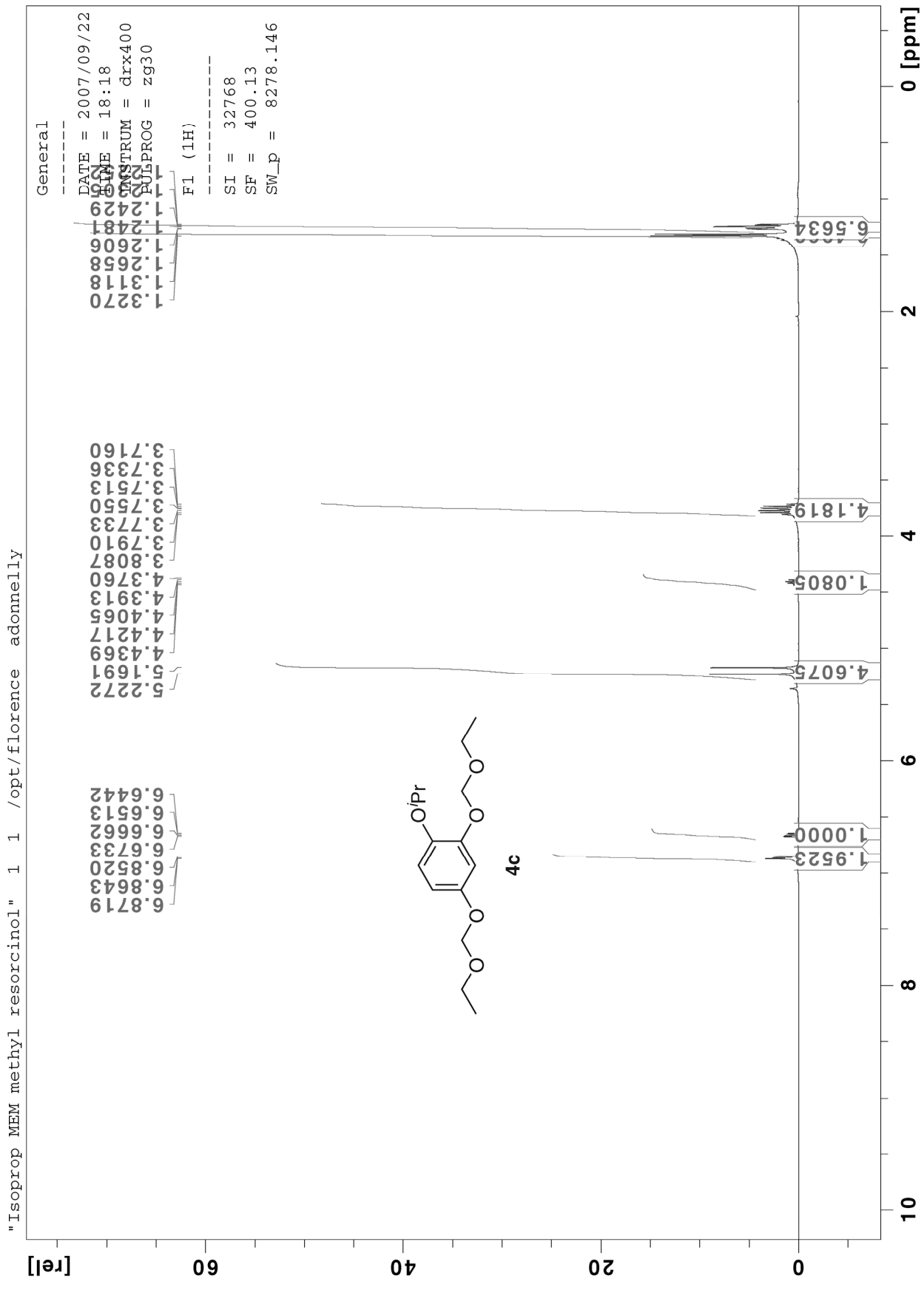
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1.2429
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4.3760
3.8087
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3.7733
3.7550
3.7513
3.7336
3.7160
6.8719
6.8643
6.8520
6.6733
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6.5634
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4.6075
1.0805
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OiPr
4c
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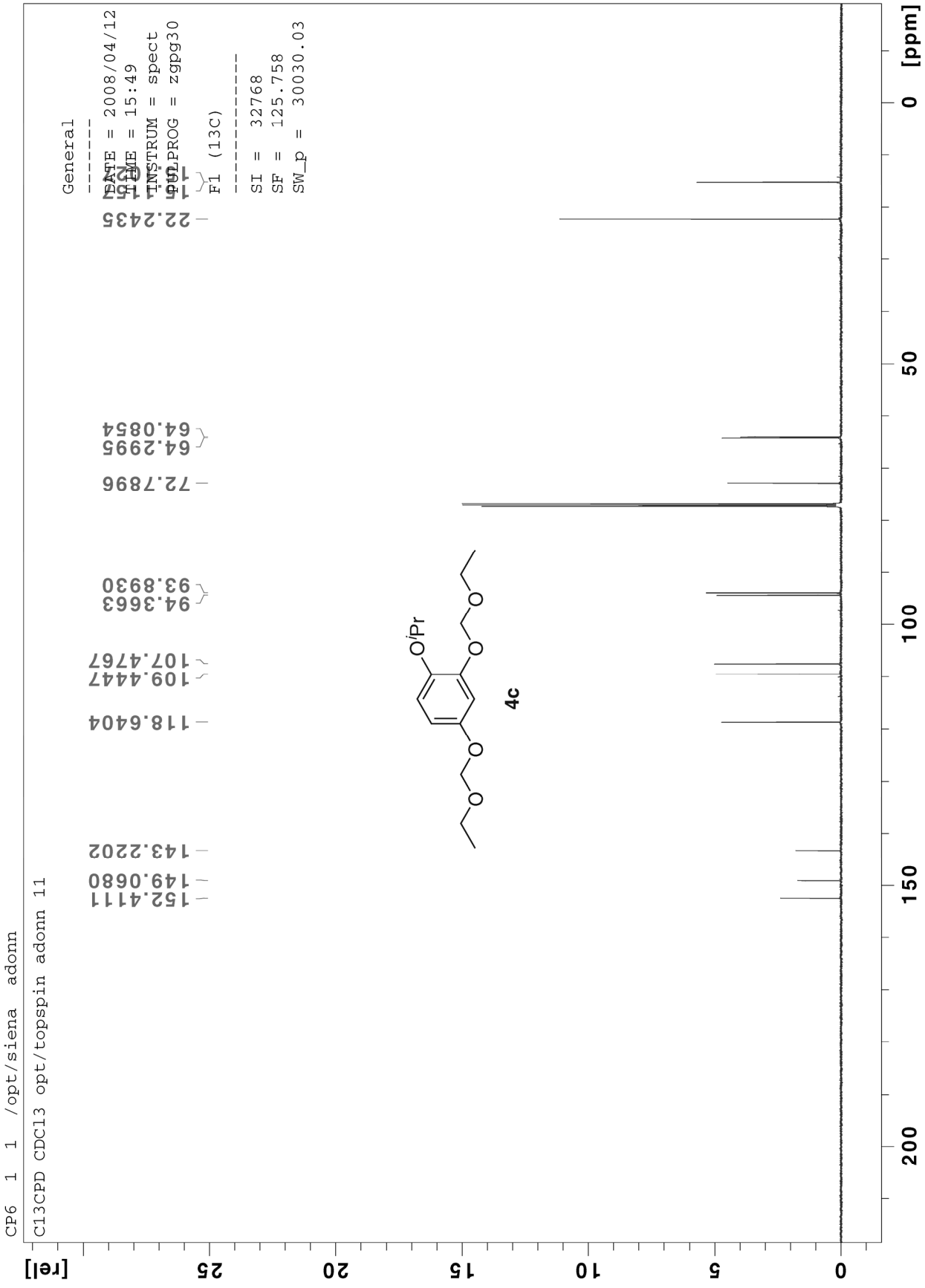
20
40
60
0 [ppm]
2
4
6
8
10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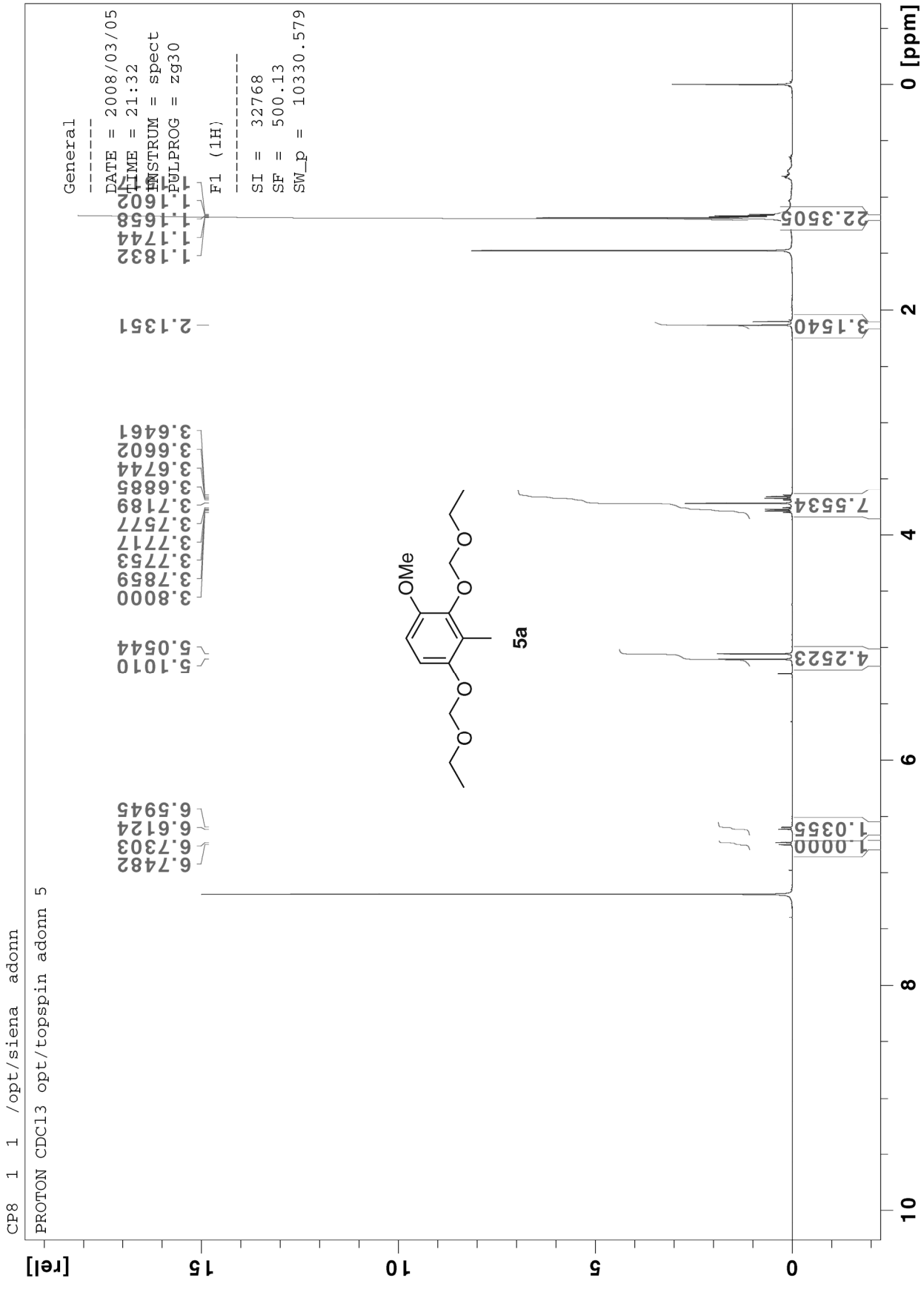
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SI = 32768
SF = 500.13
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1.1602
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4.2523
7.5534
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5
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10
8
6
4
2
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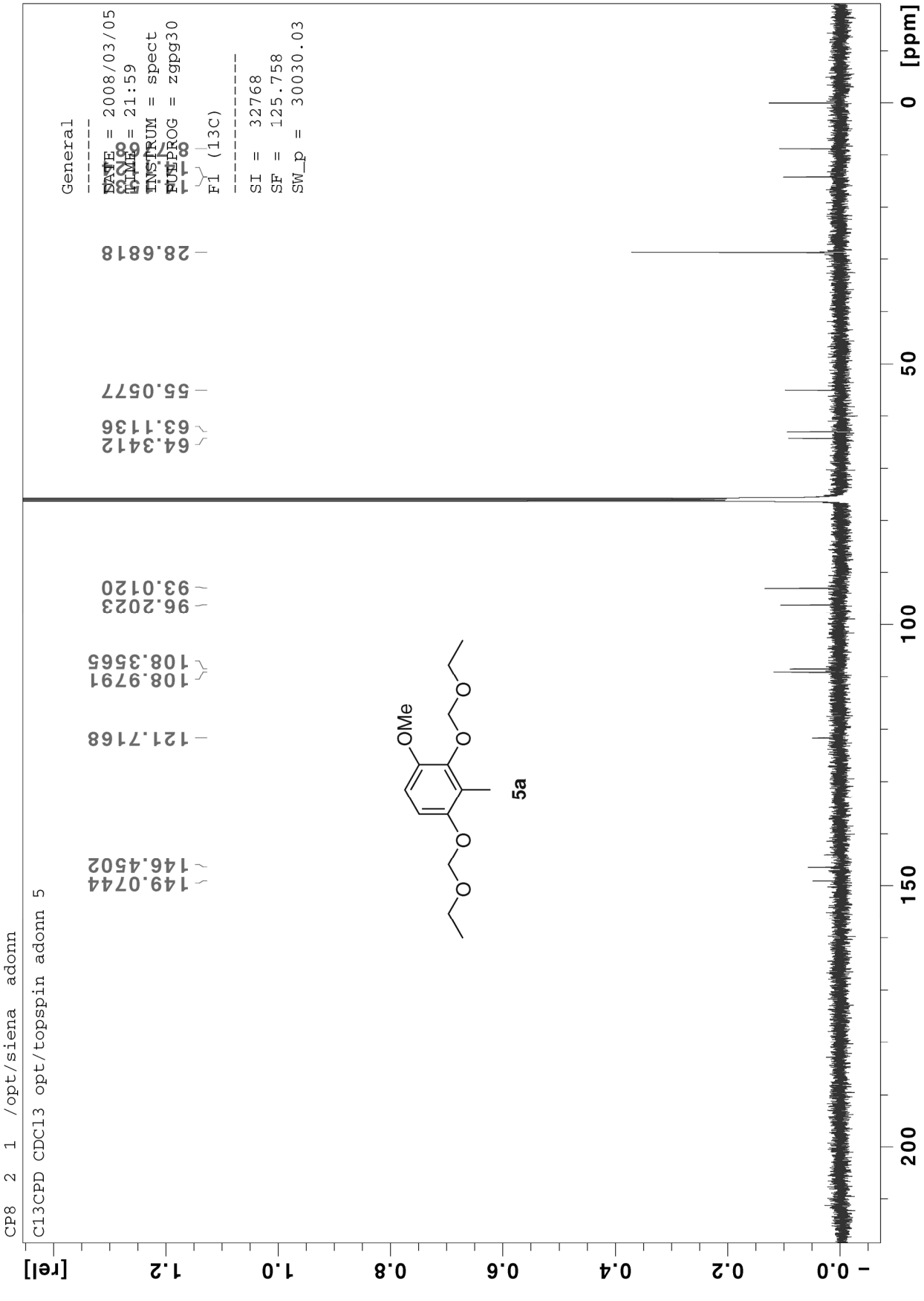
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28.6818
55.0577
63.1136
64.3412
93.0120
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149.0744
OMe
5a
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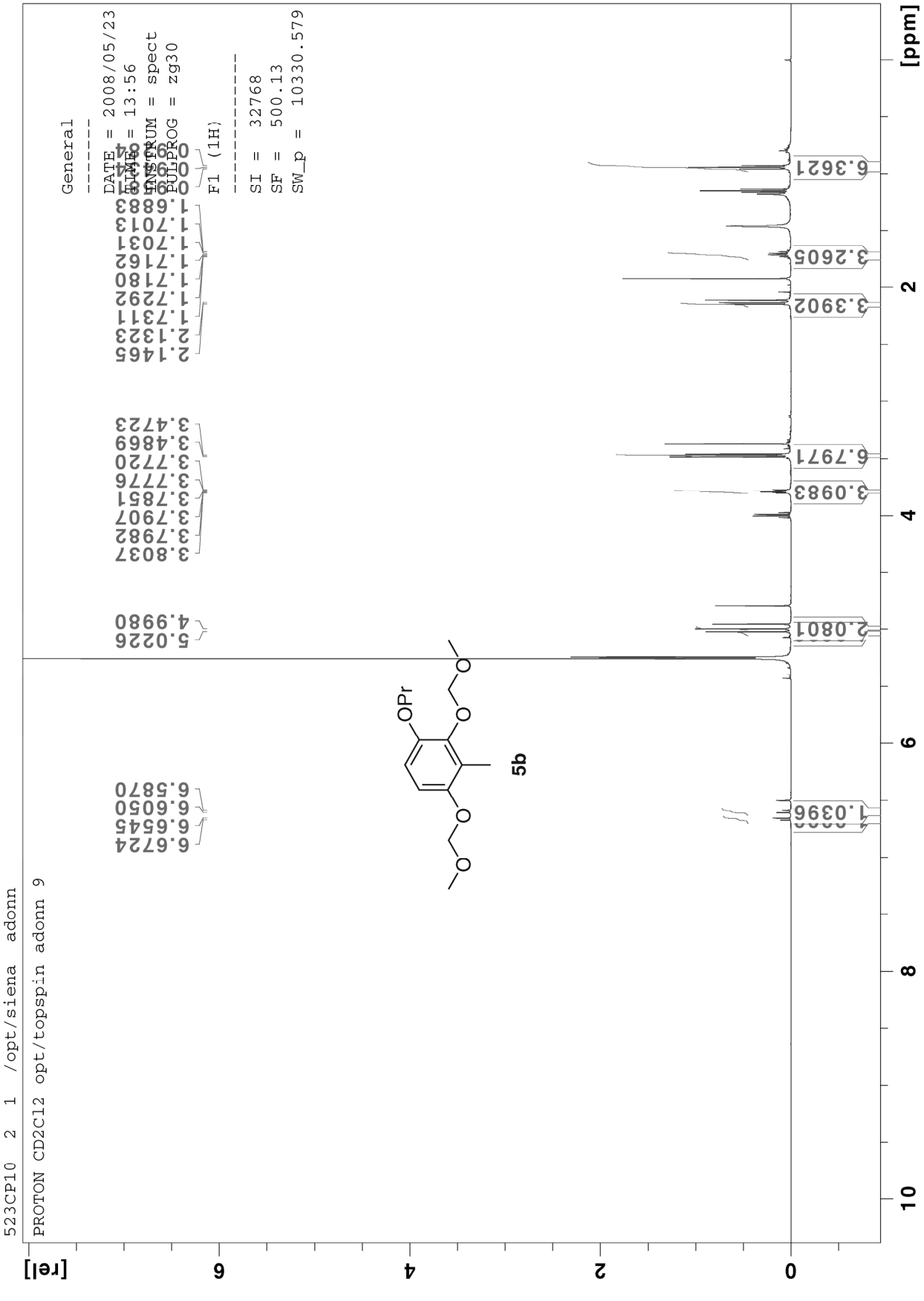
[ppm]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F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
6.6724
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6.6050
6.5870
5.0226
4.9980
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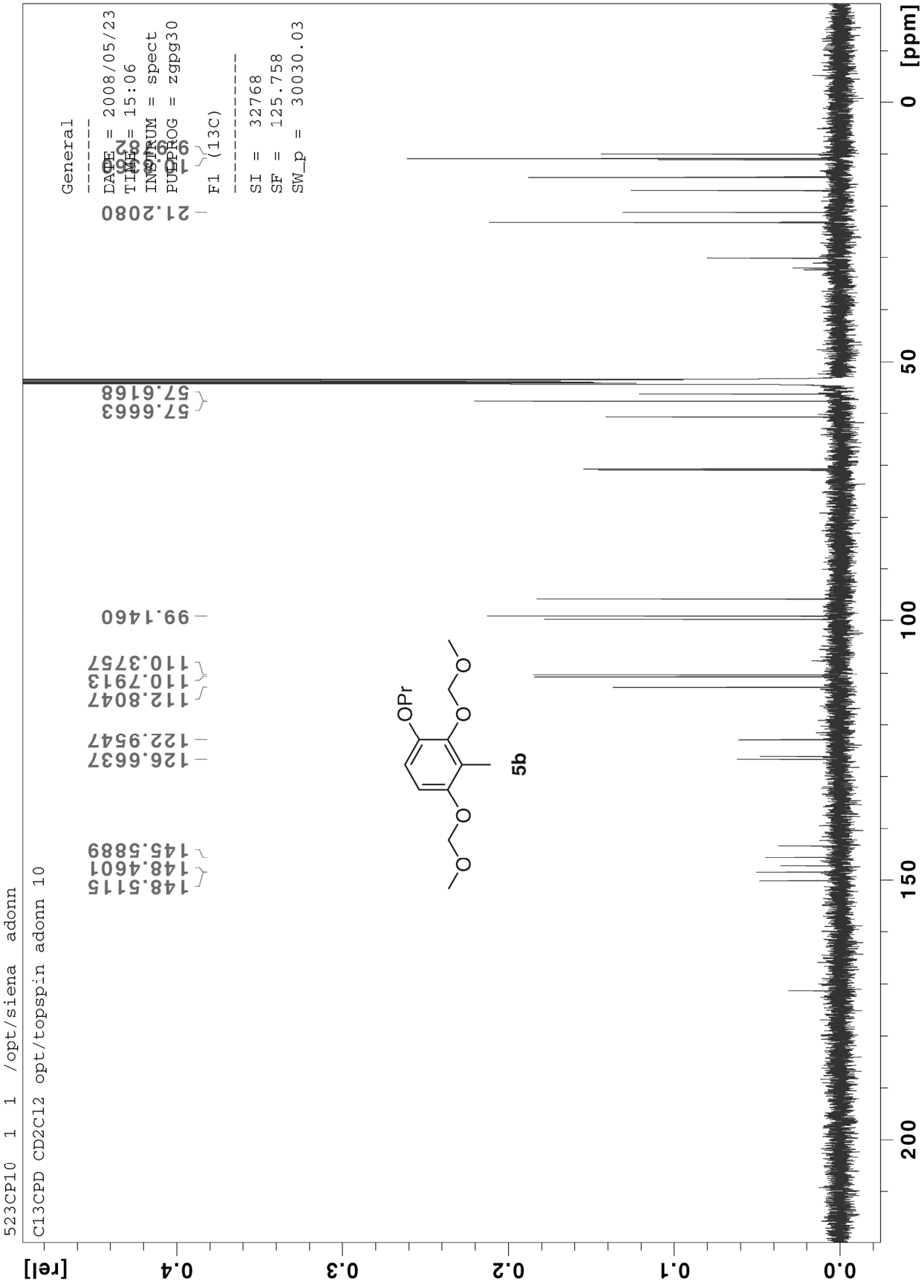
[ppm]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SI = 32768
SF = 125.758
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21.2080
57.6168
57.6663
99.1460
110.3757
110.7913
112.8047
122.9547
126.6637
145.5889
148.4601
148.5115
OPr
5b
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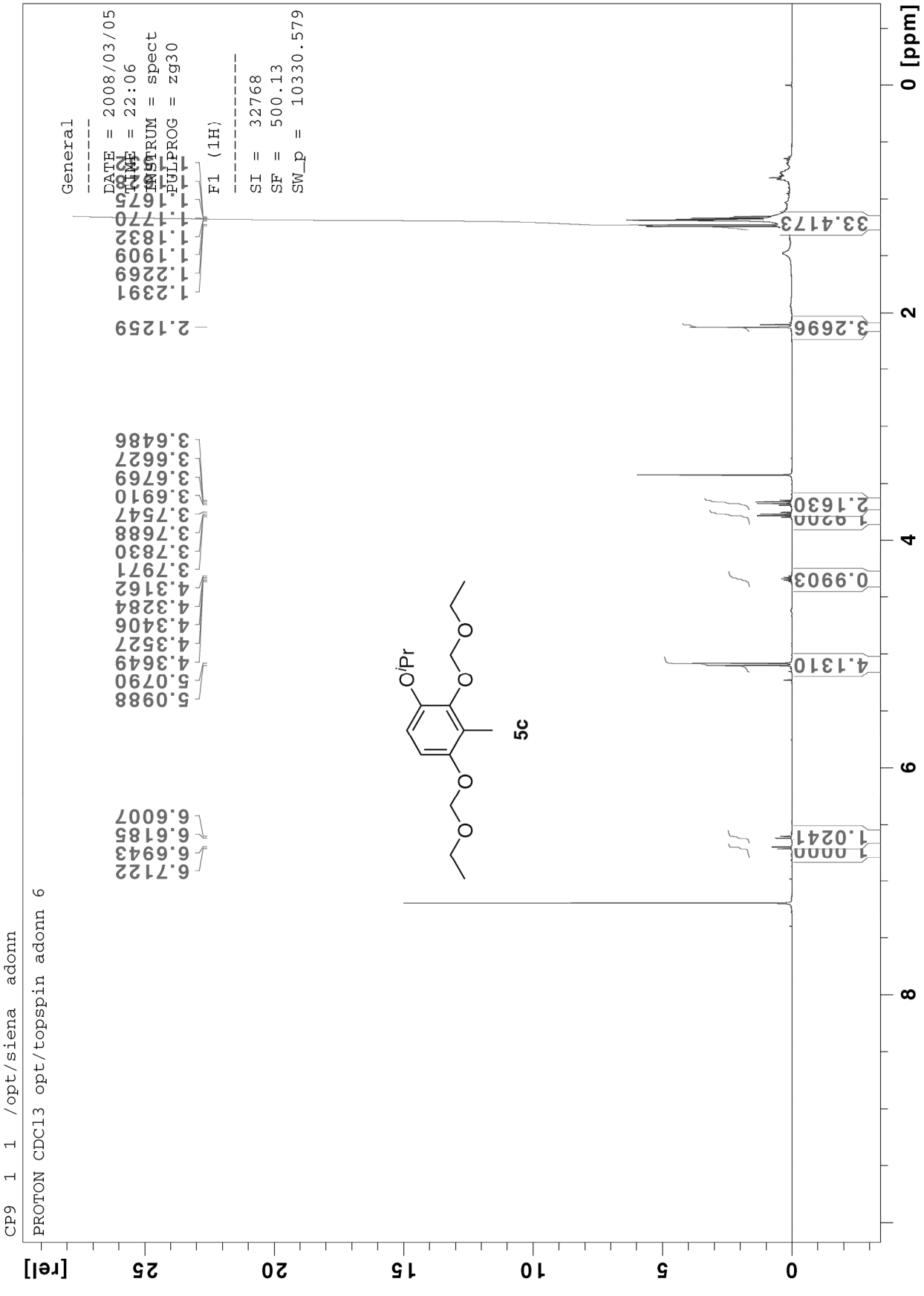
200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SI = 32768
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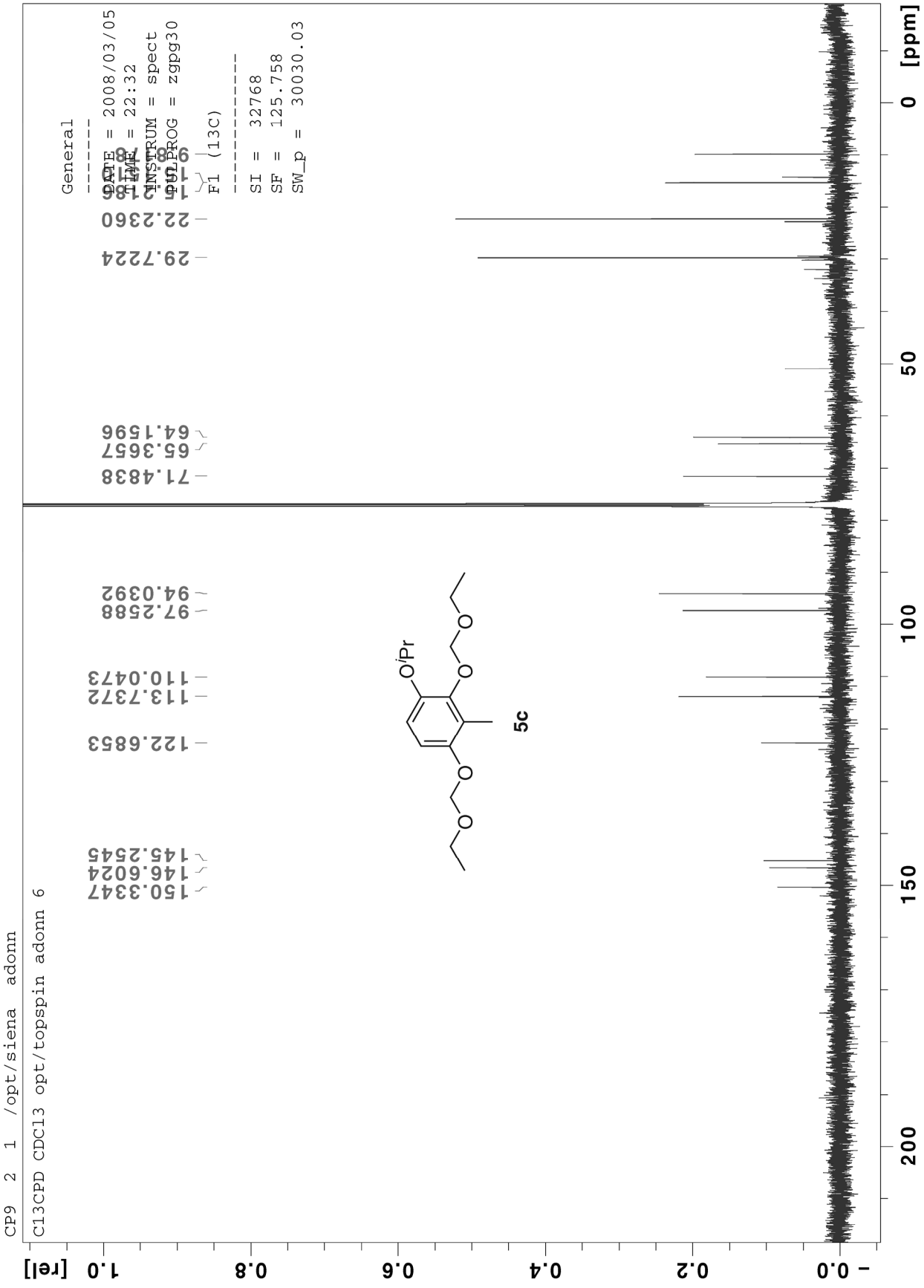
5c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SI = 32768
SF = 125.758
SW_p = 30030.03
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146.6024
145.2545
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113.7372
110.0473
97.2588
94.0392
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65.3657
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29.7224
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[ppm]
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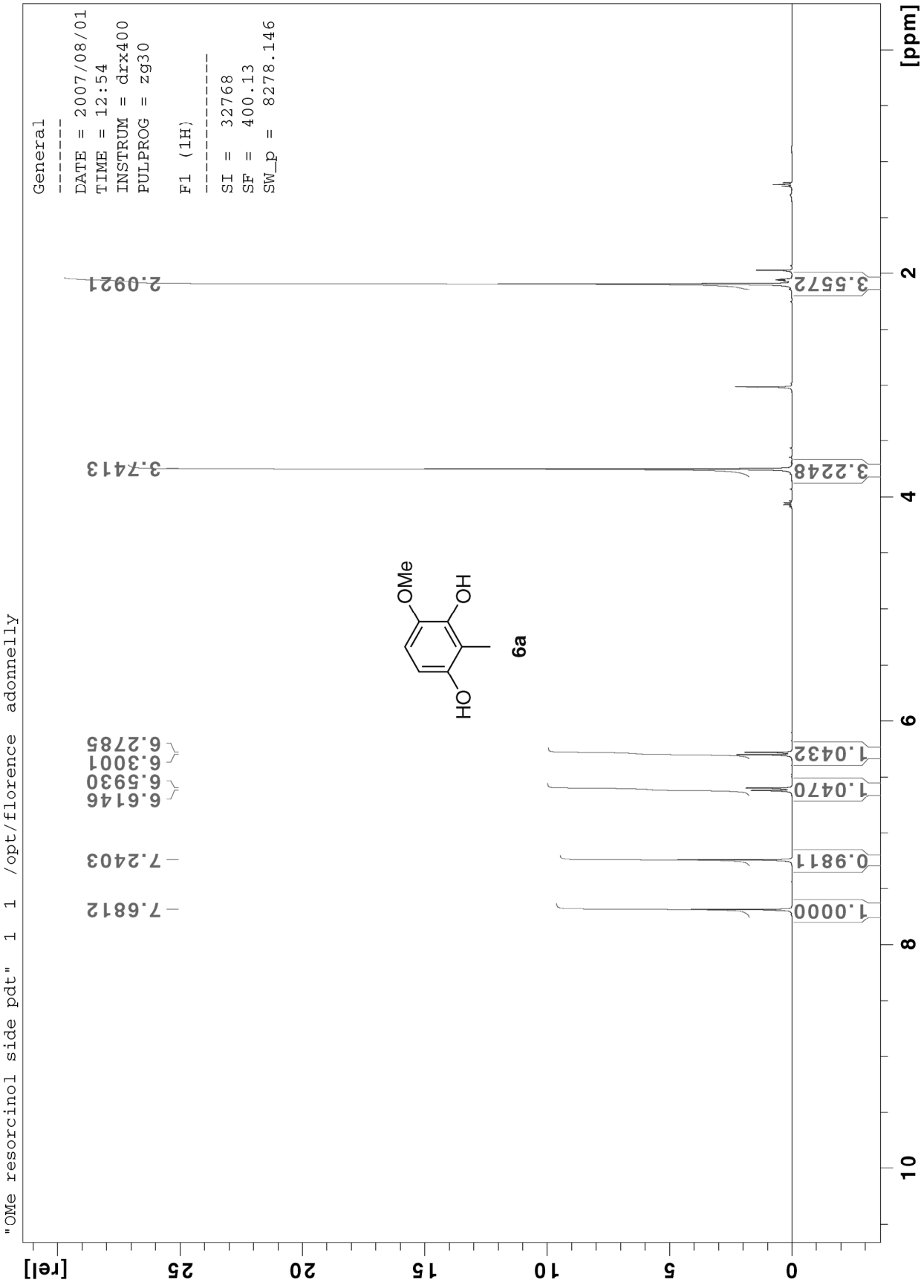
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SI = 32768
SF = 400.13
SW_p = 8278.146
2.0921
3.7413
3.5572
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1.0470
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1.0000
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OMe
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HO
6a
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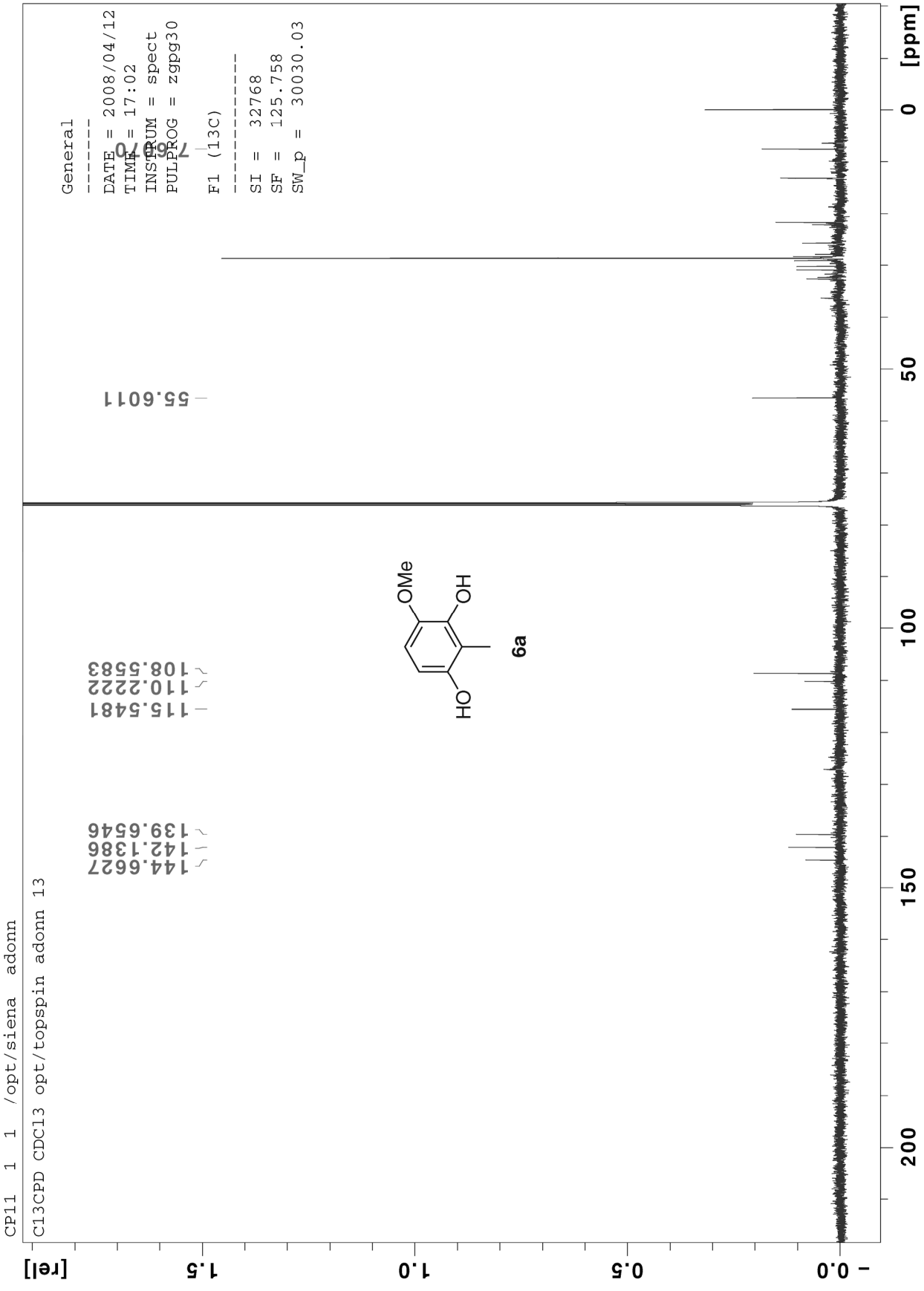
[ppm]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SI = 32768
SF = 125.758
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77.0770
55.6011
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108.5583
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139.6546
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OH
HO
6a
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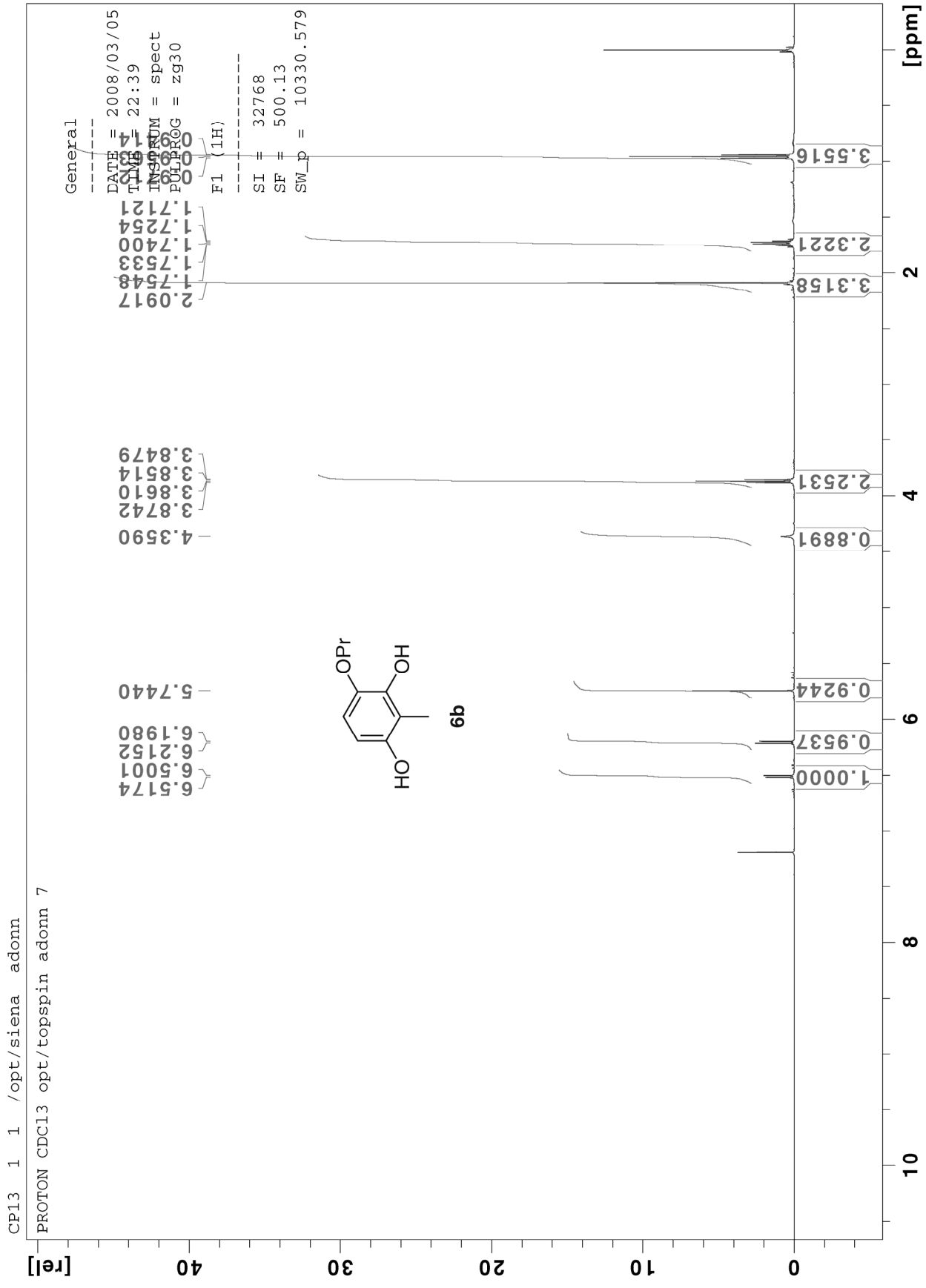
[ppm]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SF = 500.13
SW_p = 10330.579
[rel]
[ppm]
OPr
OH
HO
6b
3.5516
2.3221
3.3158
2.2531
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0.9244
0.9537
1.0000
2.0917
1.7548
1.7533
1.7400
1.7254
1.7121
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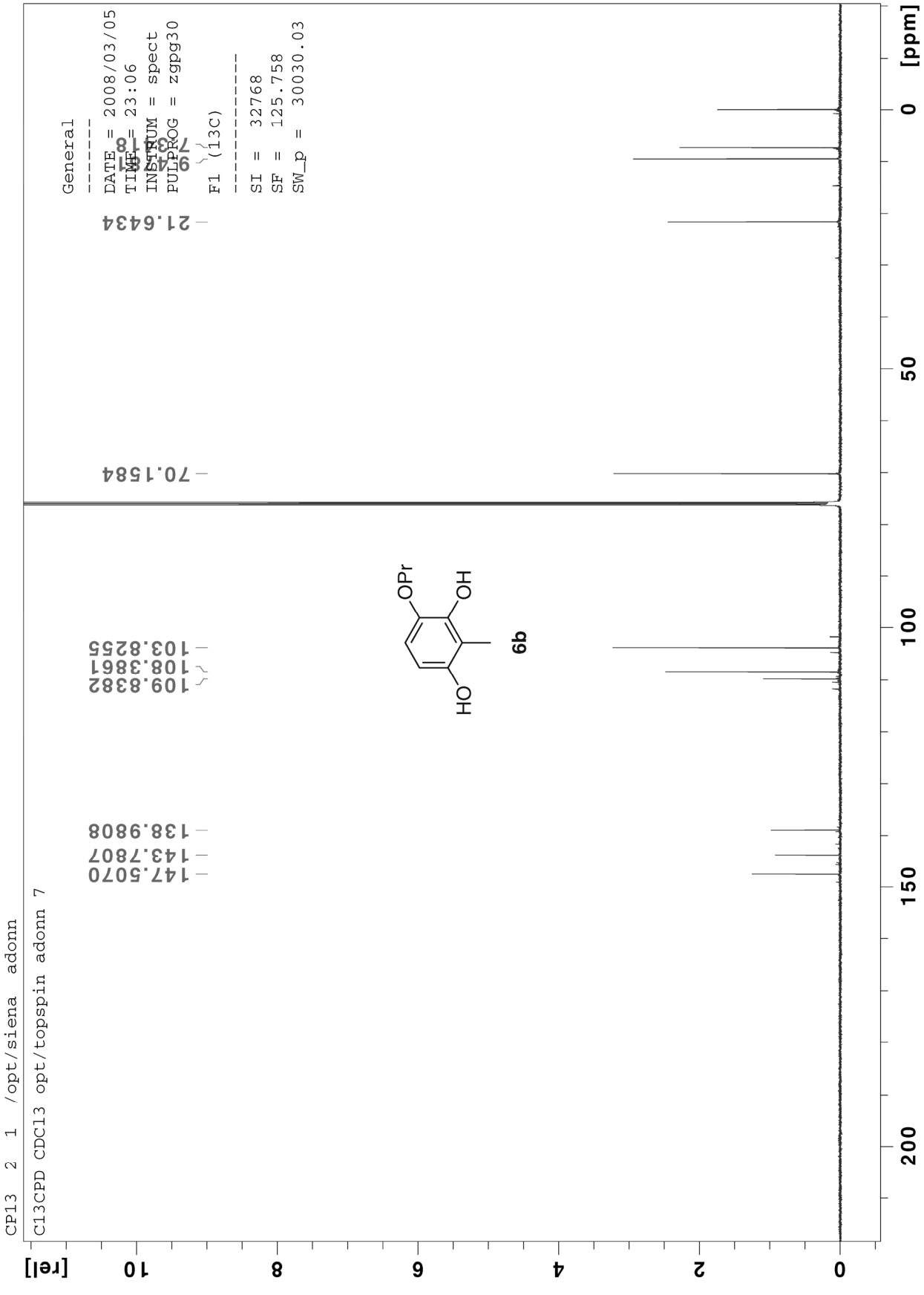
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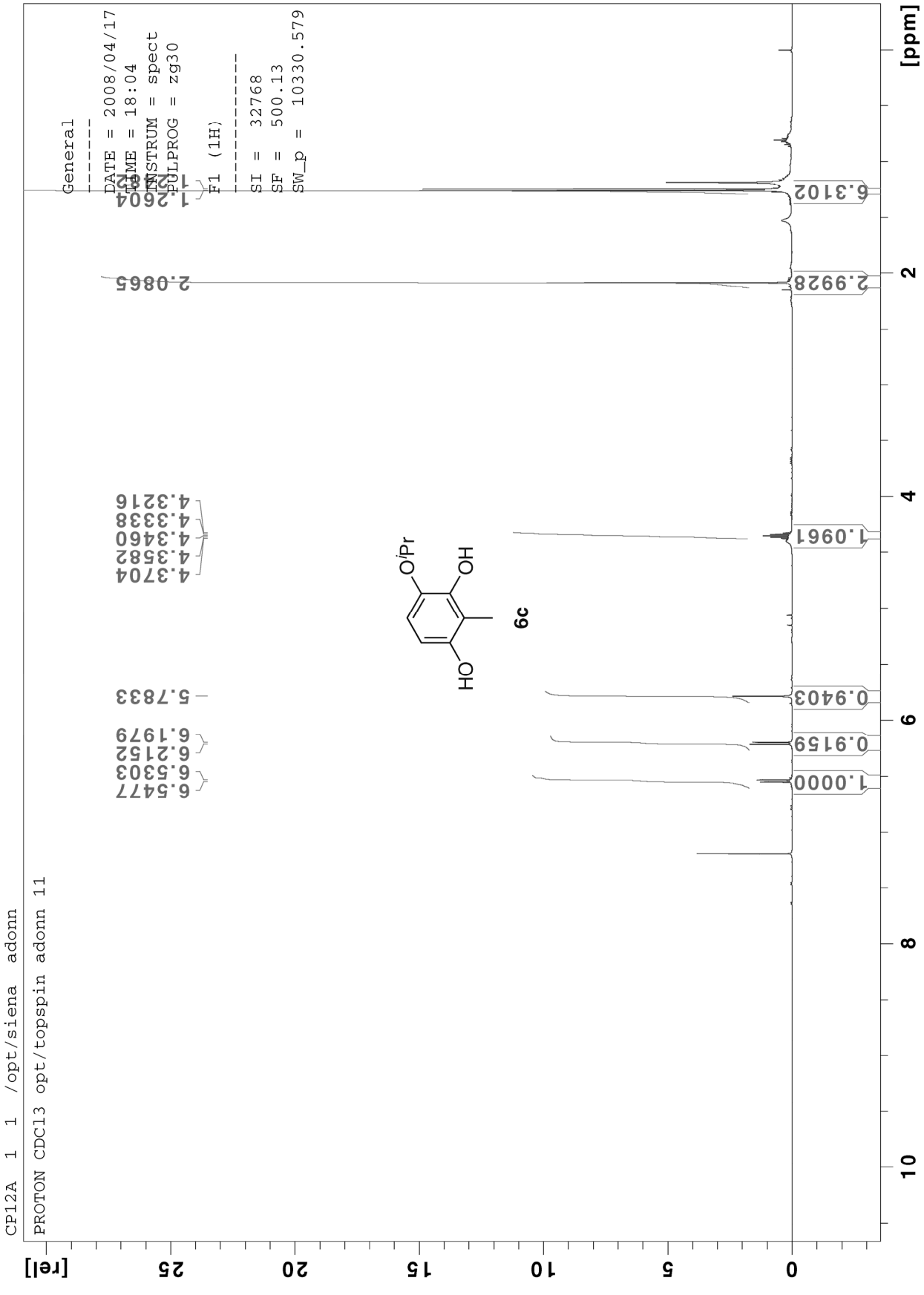
SI = 32768
SF = 125.758
SW_p = 30030.03
147.5070
143.7807
138.9808
109.8382
108.3861
103.8255
70.1584
21.6434
OPr
OH
HO
6b
[rel]
[ppm]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SI = 32768
SF = 500.13
SW_p = 10330.579
1.2604
2.0865
4.3216
4.3338
4.3460
4.3582
4.3704
5.7833
6.1979
6.2152
6.5303
6.5477
6.3102
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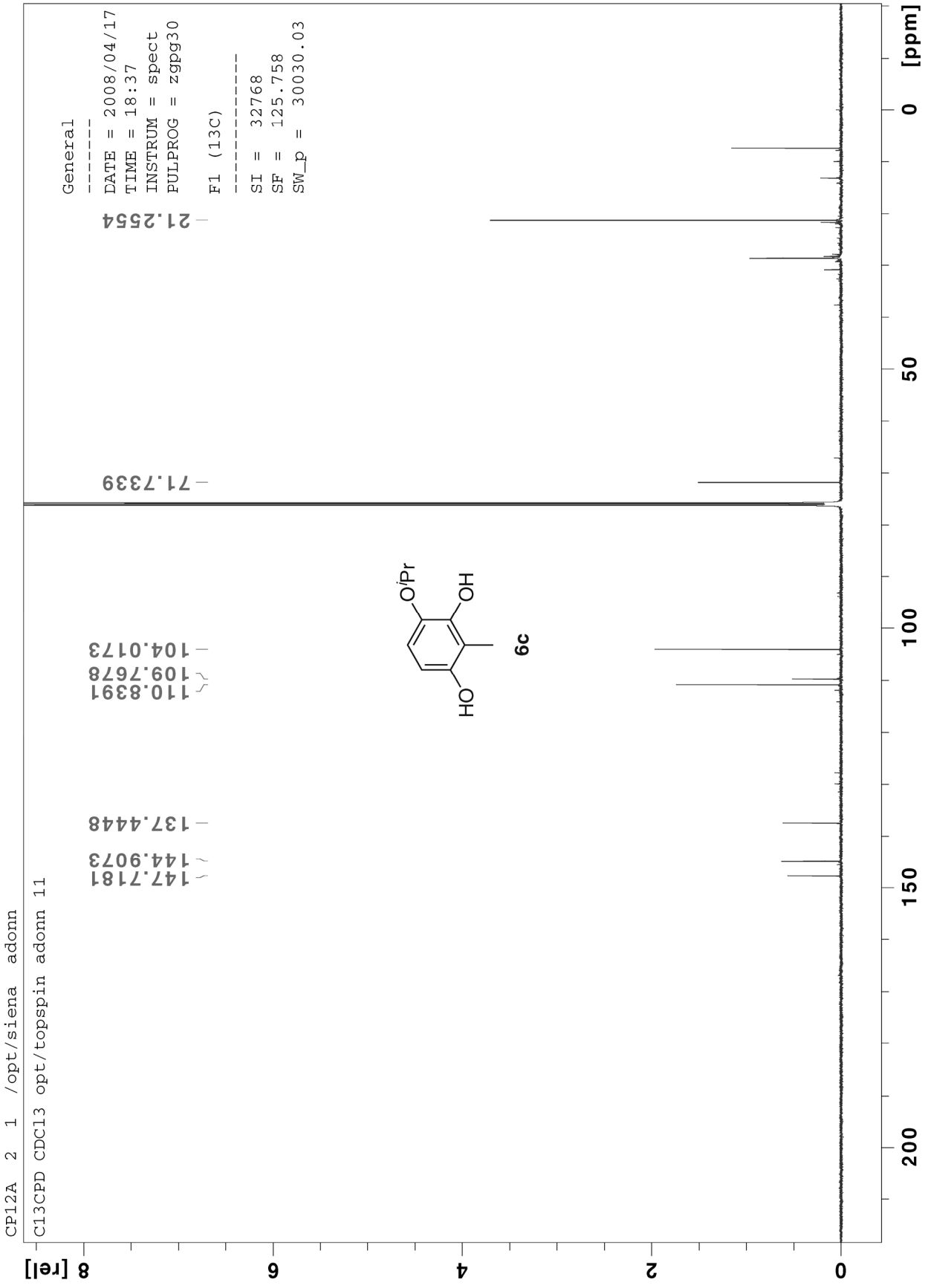
1.0961
0.9403
0.9159
1.0000
O^{i}Pr
OH
HO
6c
[rel]
[ppm]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TIME = 18:37
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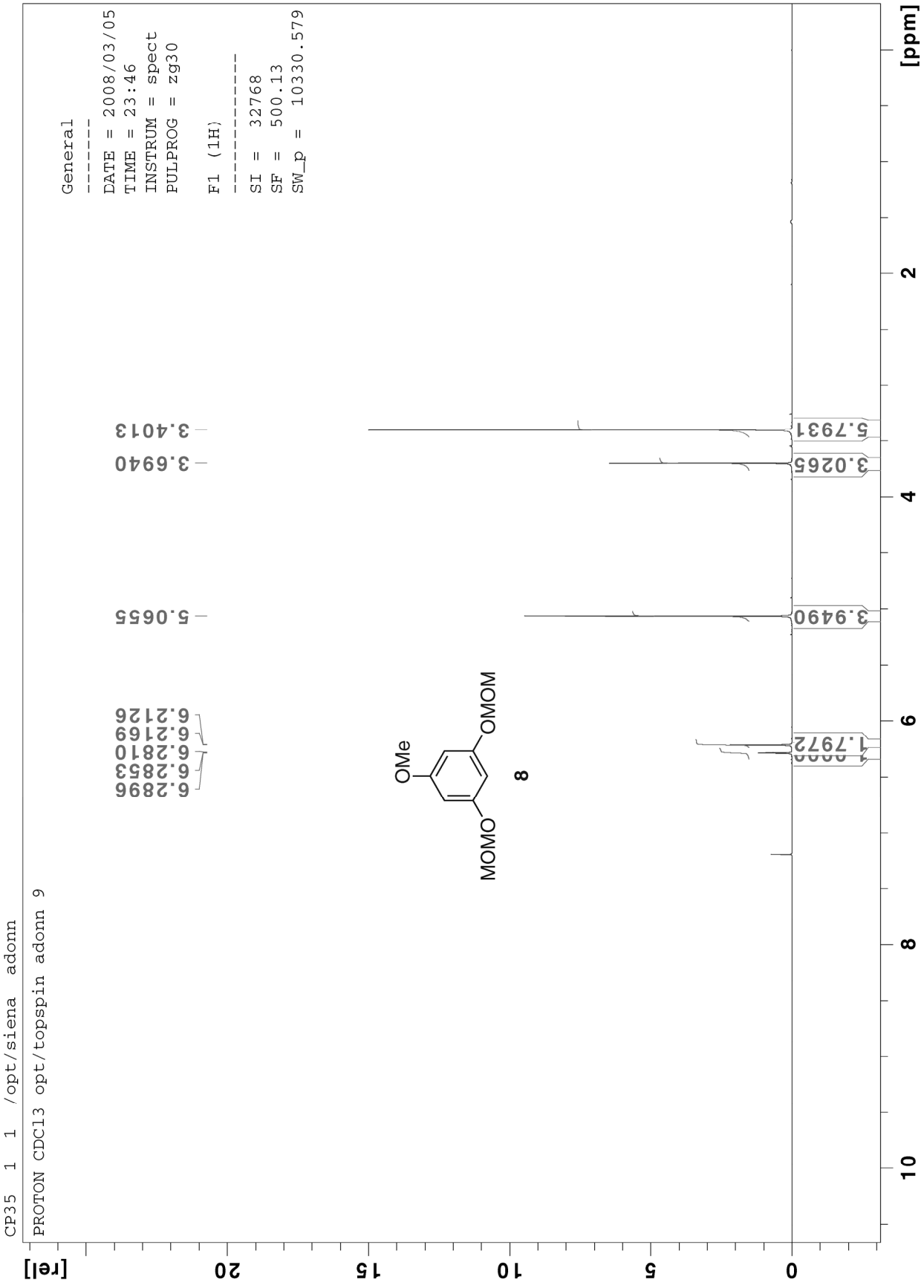
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
147.7181
144.9073
137.4448
110.8391
109.7678
104.0173
71.7339
21.2554
O^{i}Pr
OH
HO
6c
[rel]
[ppm]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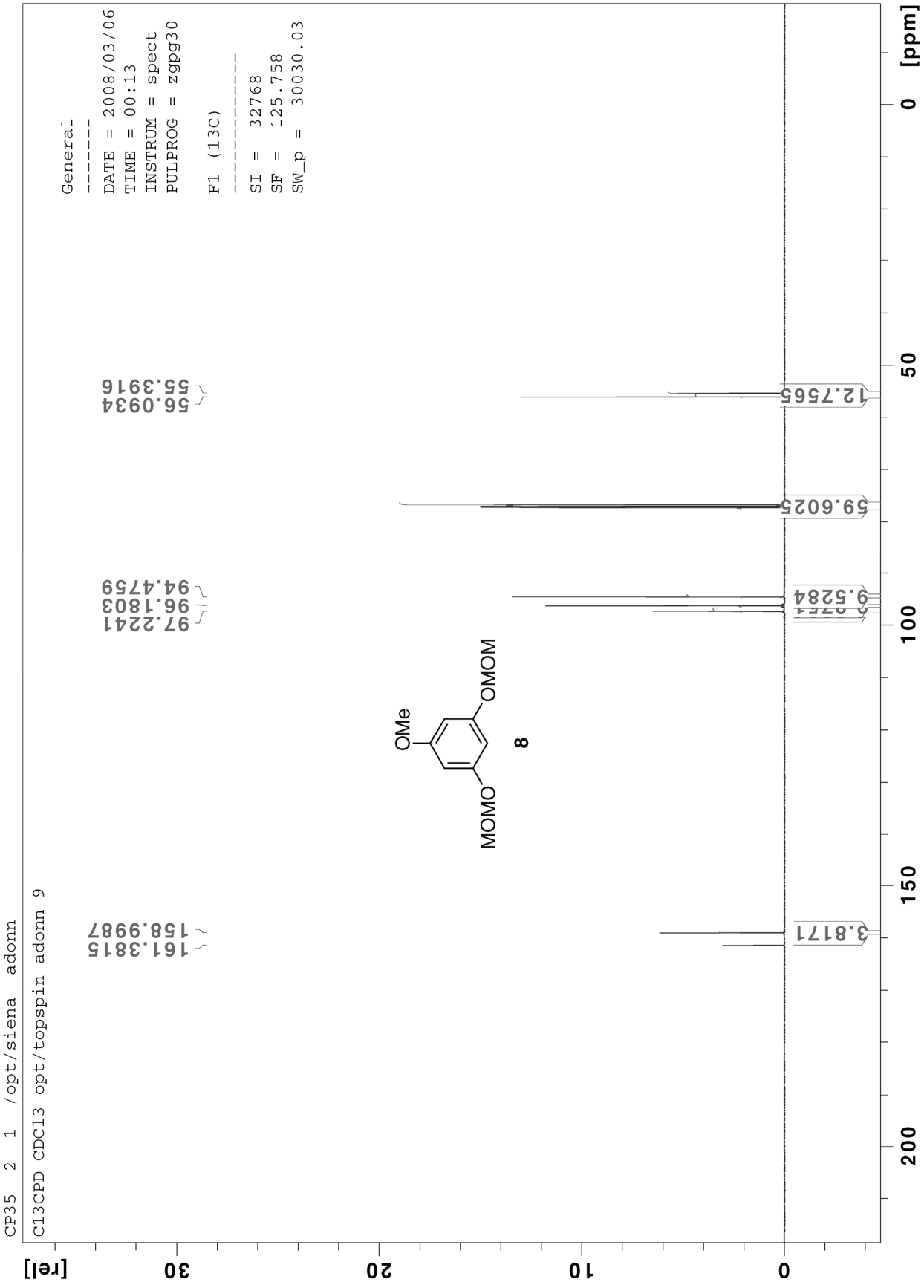
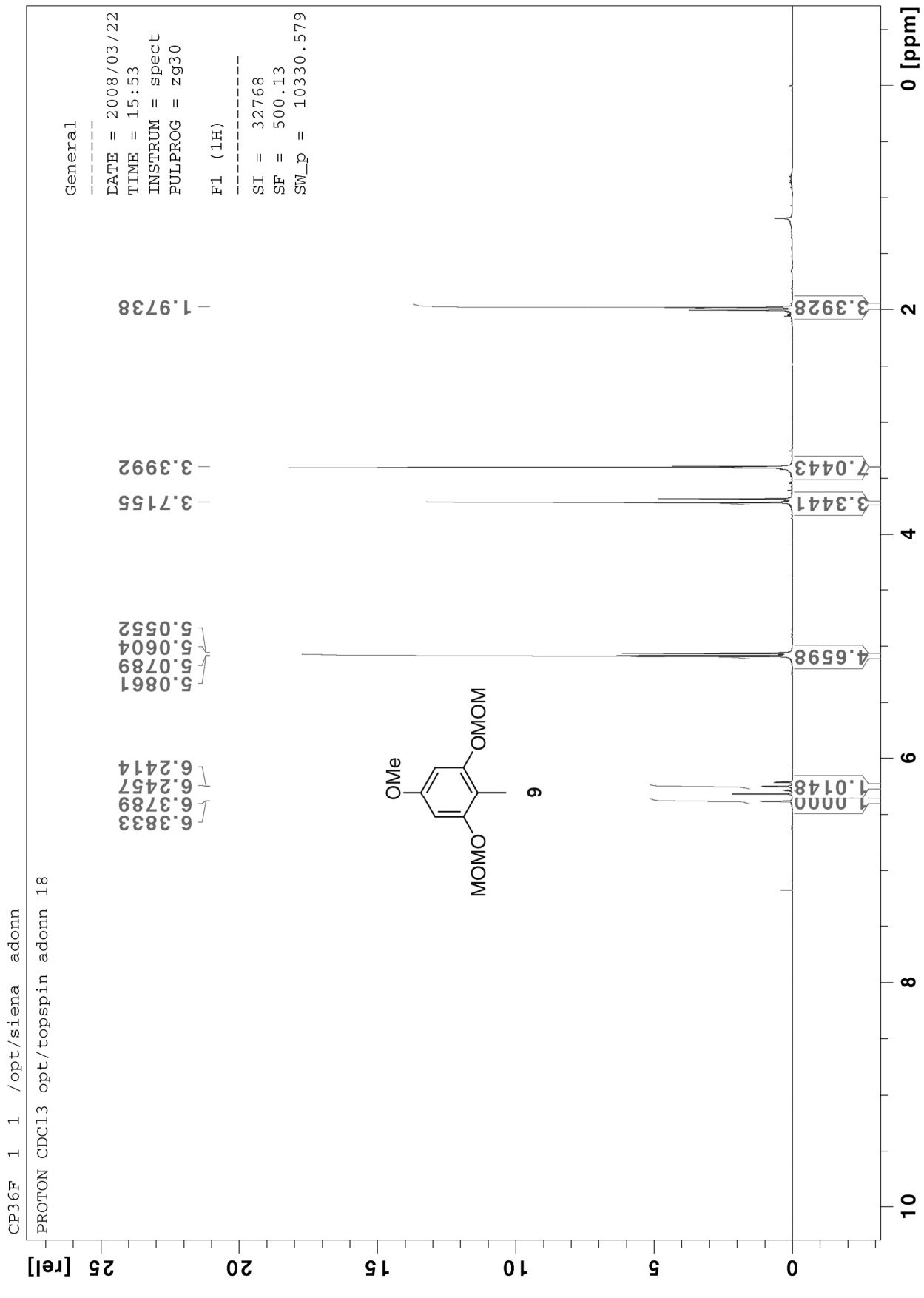
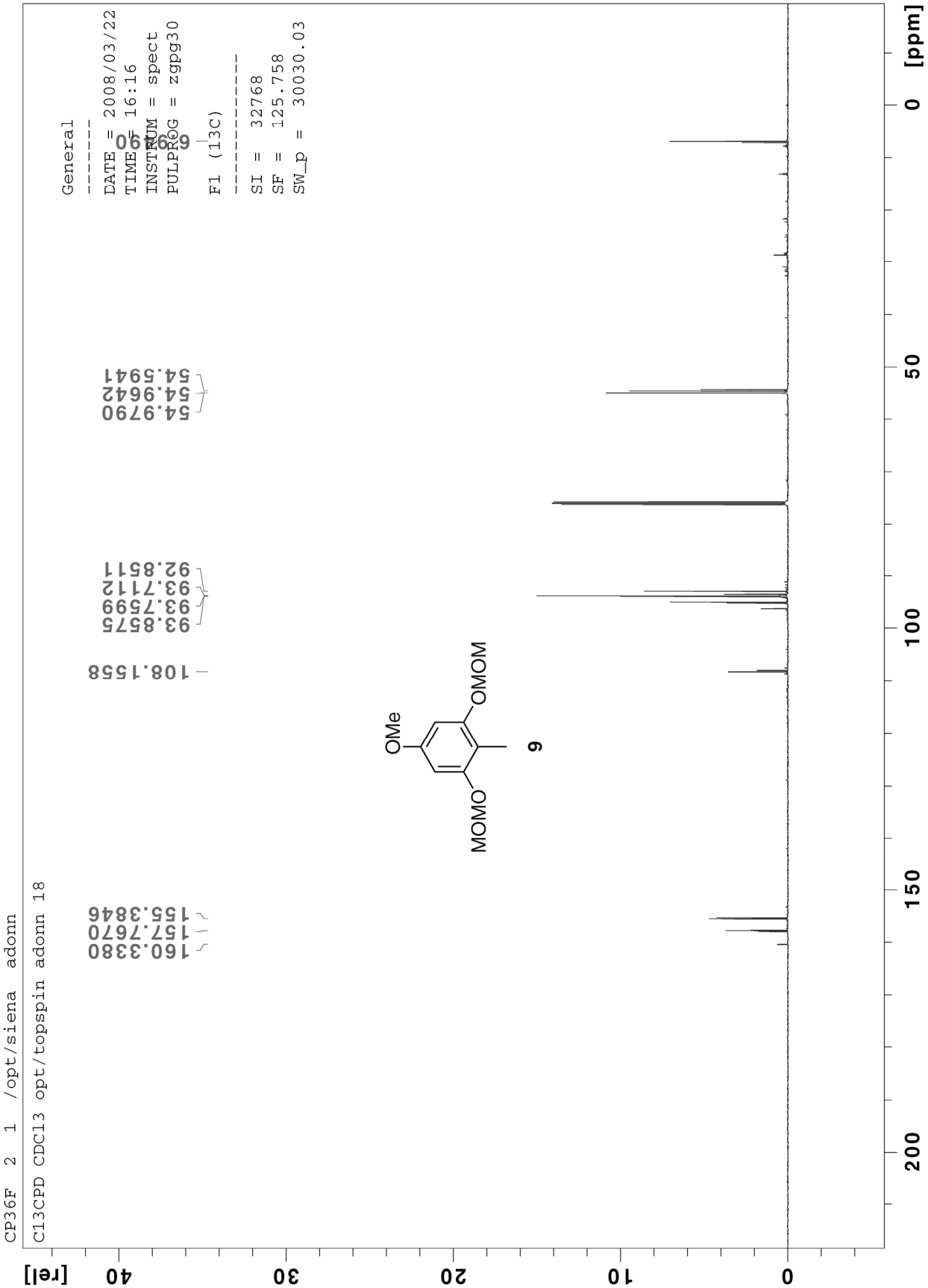
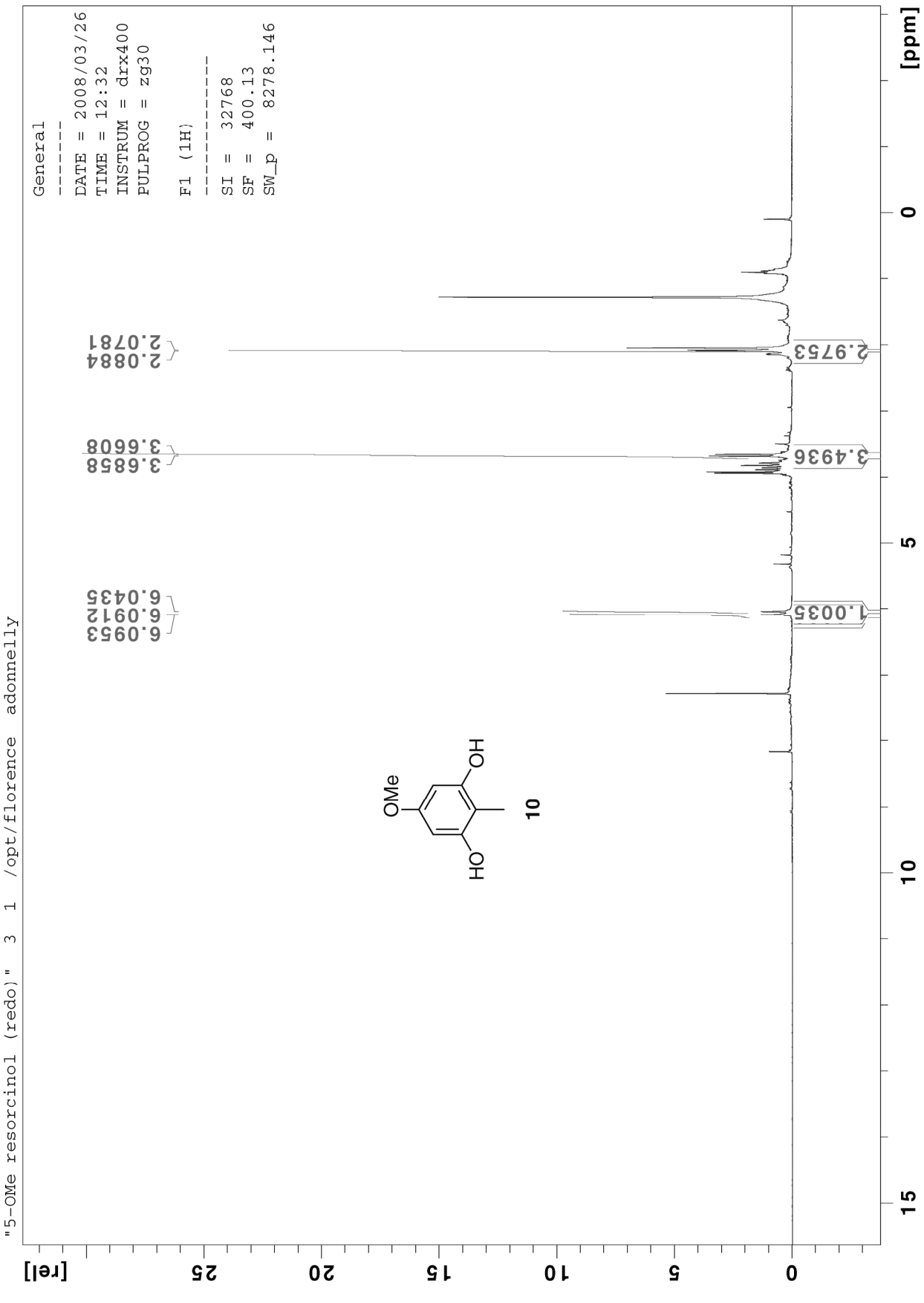
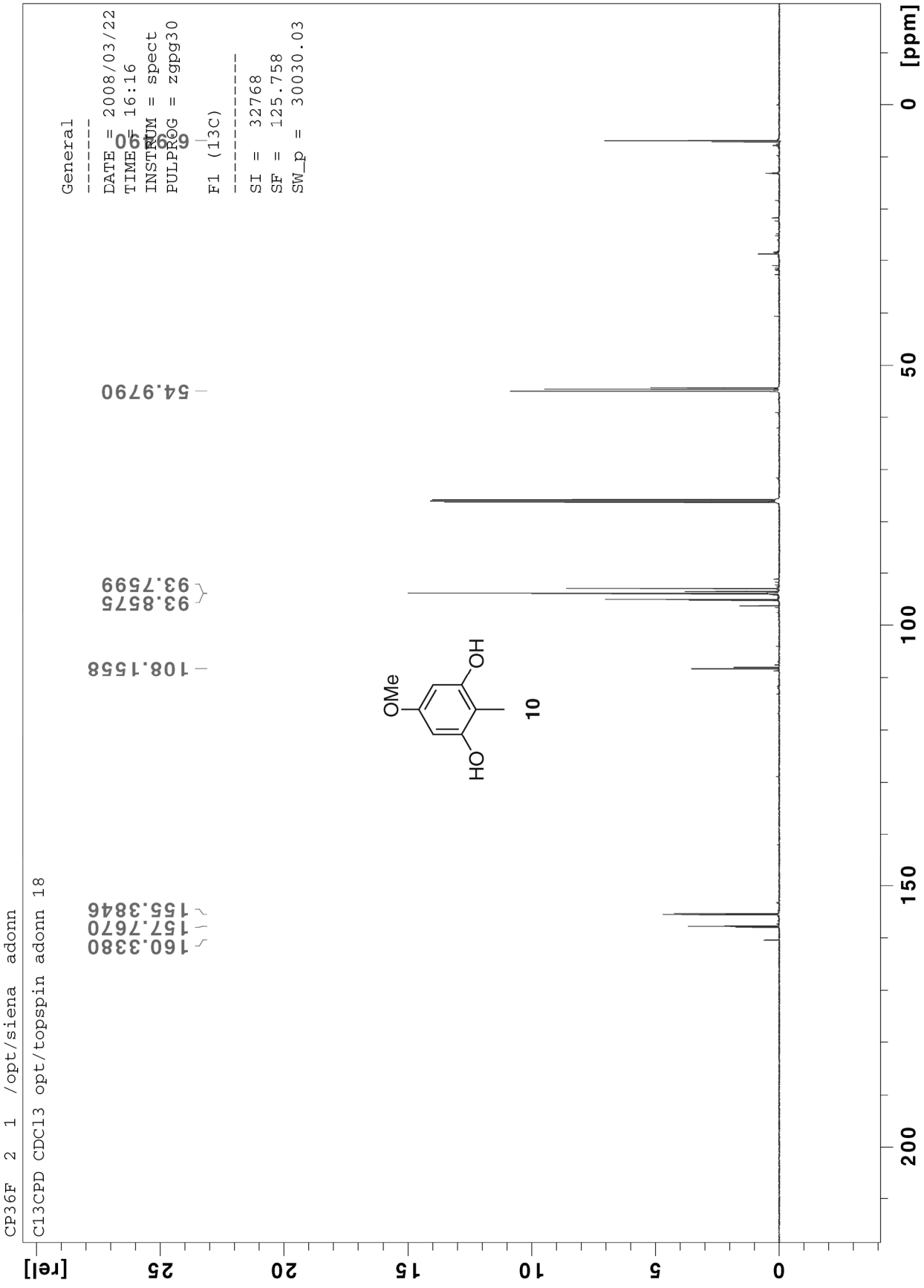
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
3.4013
3.6940
5.0655
6.2126
6.2169
6.2810
6.2853
6.2896
5.7931
3.0265
3.9490
1.7972
OMe
OMOM
MOMO
8
[rel]
[ppm]

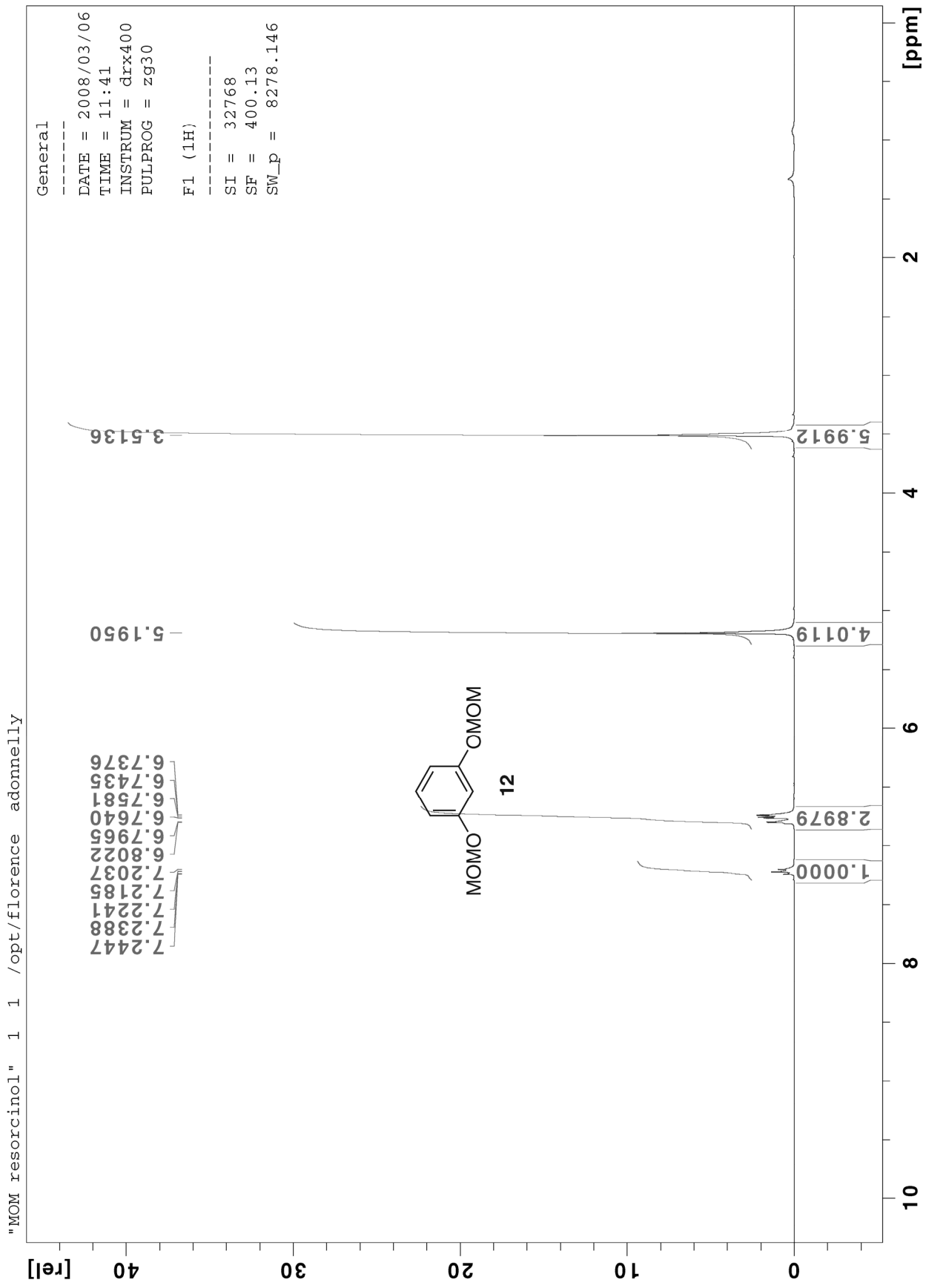

CP35 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 9
General
DATE = 2008/03/06
TIME = 00:13
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
161.3815
158.9987
97.2241
96.1803
94.4759
56.0934
55.3916
3.8171
9.5284
59.6025
12.7565
OMe
OMOM
MOMO
8
[rel]
[ppm]

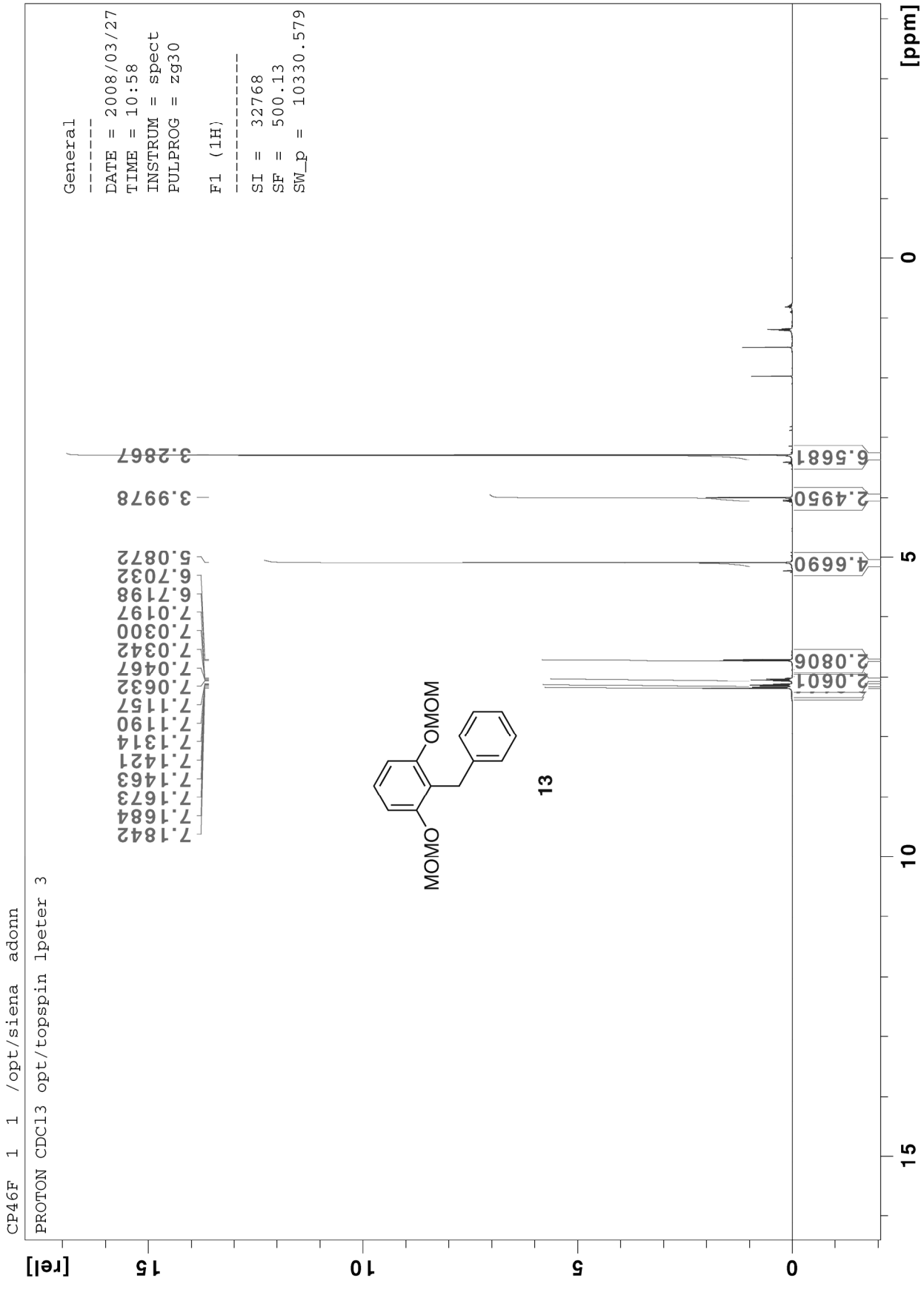

CP36F 1 1 /opt/siena adonn
PROTON CDCl3 opt/topspin adonn 18
General
DATE = 2008/03/22
TIME = 15:53
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
1.9738
3.3992
3.7155
5.0552
5.0604
5.0789
5.0861
6.2414
6.2457
6.3789
6.3833
1.0000
1.0148
4.6598
7.0443
3.3441
3.3928
OMe
OMOM
MOMO
9
[rel]
0 [ppm]

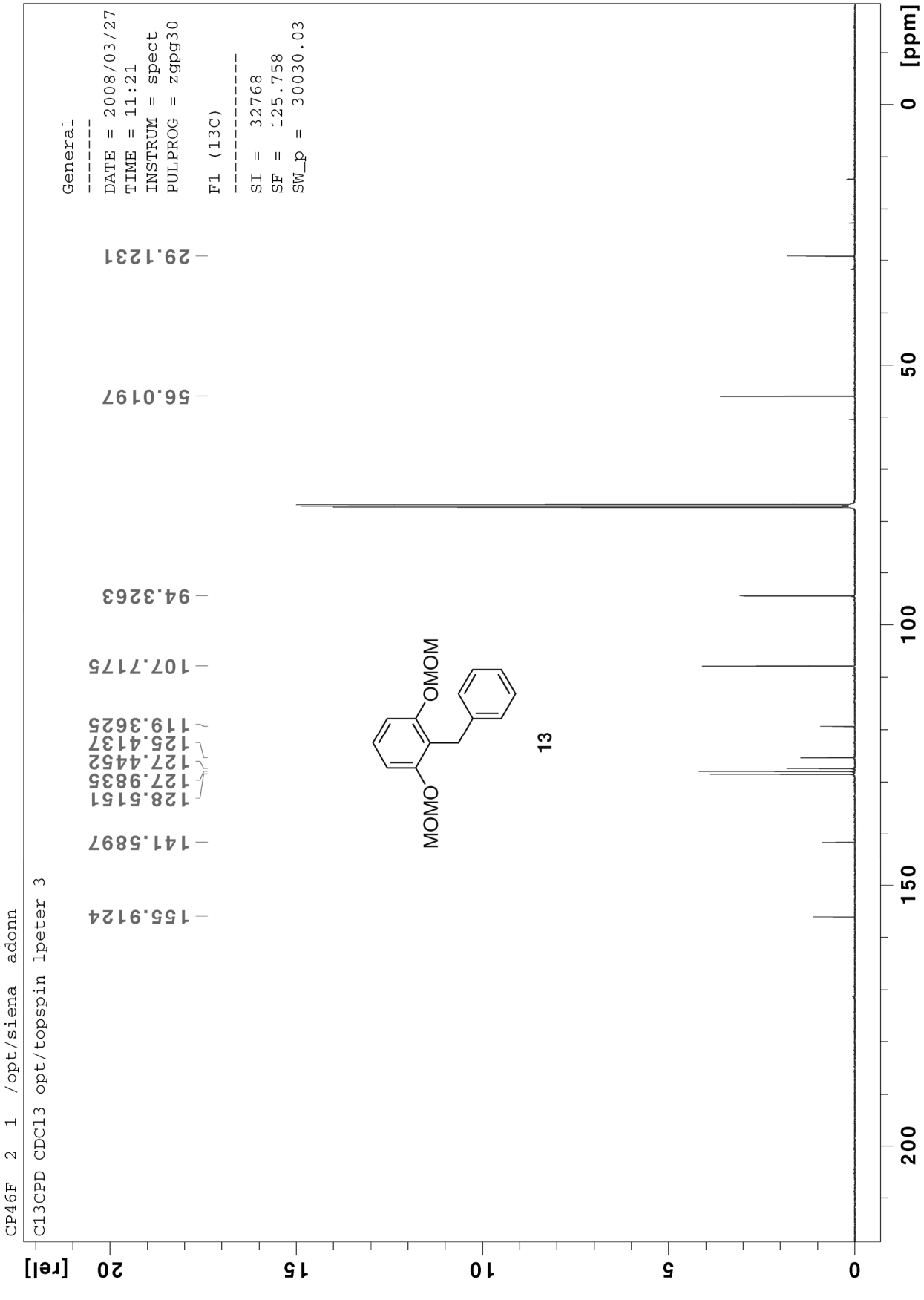

CP36F 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 18
General
DATE = 2008/03/22
TIME = 16:16
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
160.3380
157.7670
155.3846
108.1558
93.8575
93.7599
93.7112
92.8511
56.0690
54.9790
54.9642
54.5941
OMe
OMOM
MOMO
9
[rel]
40
30
20
10
0
200
150
100
50
0 [ppm]

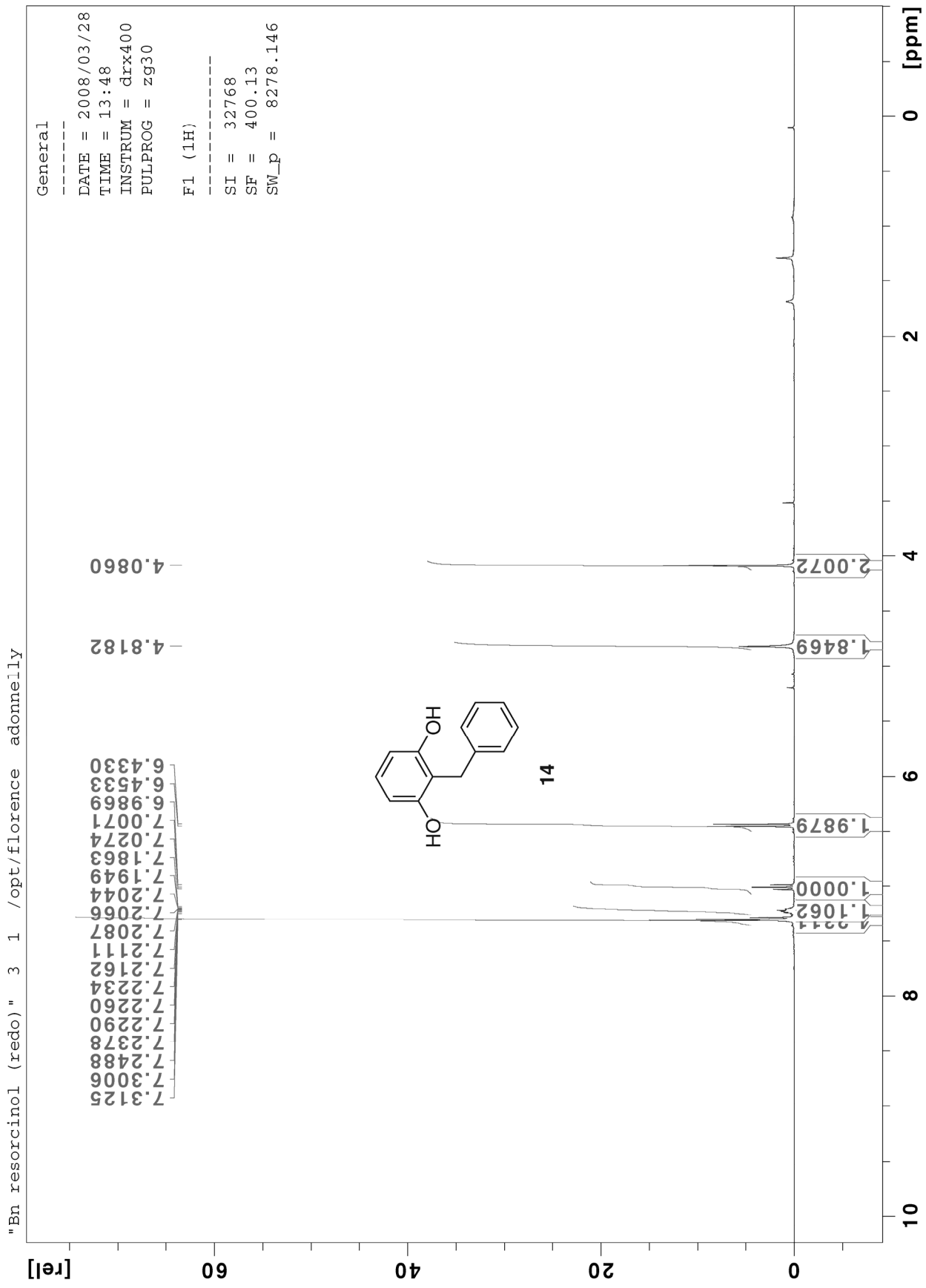

"5-OMe resorcinol (redo)" 3 1 /opt/florence adonnelly
General
DATE = 2008/03/26
TIME = 12:32
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
2.0884
2.0781
3.6858
3.6608
6.0953
6.0912
6.0435
2.9753
3.4936
1.0035
OMe
OH
HO
10
[rel]
[ppm]

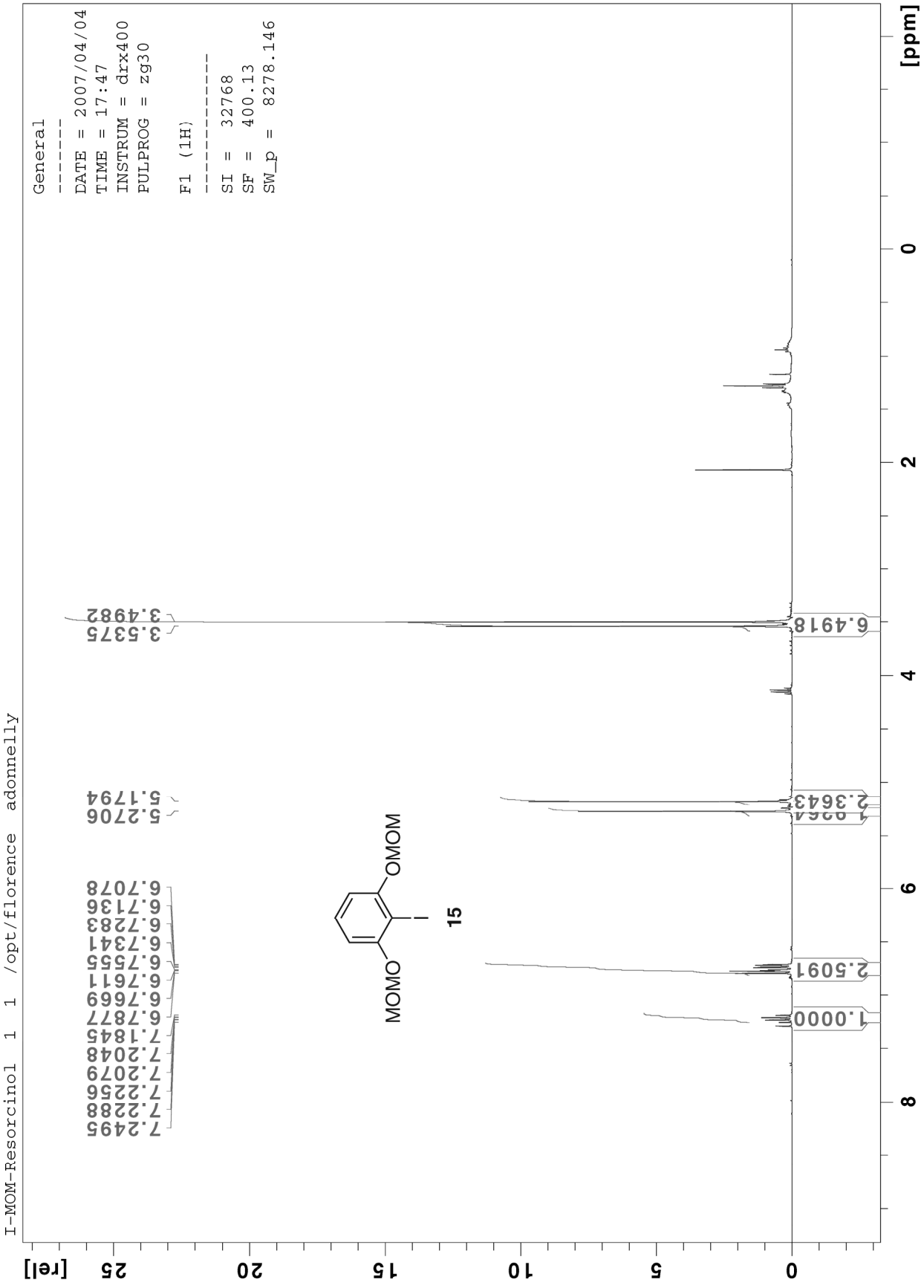

CP36F 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 18
General
DATE = 2008/03/22
TIME = 16:16
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
160.3380
157.7670
155.3846
108.1558
93.8575
93.7599
54.9790
OMe
OH
HO
10
[rel]
[ppm]

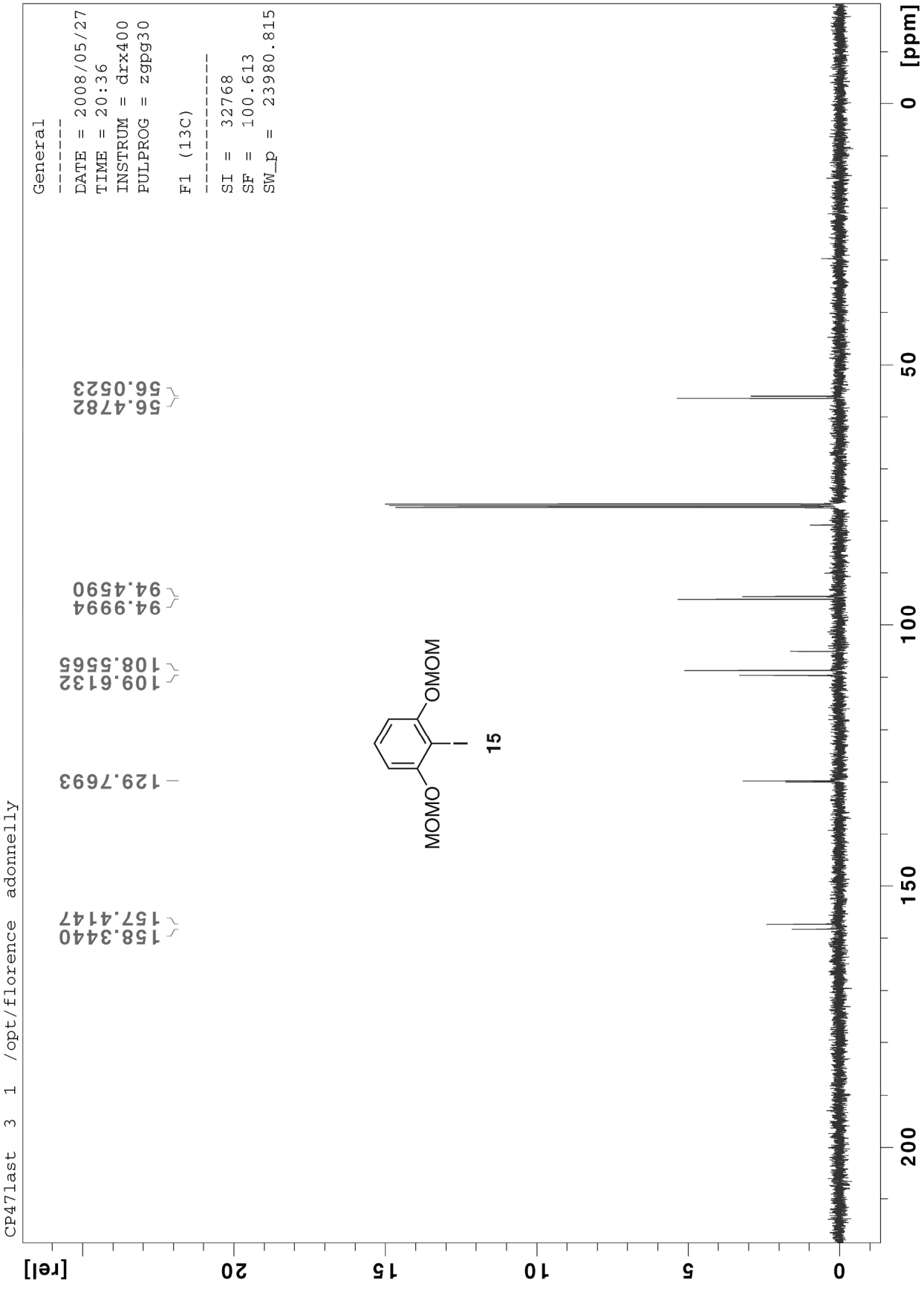

"MOM resorcinol" 1 1 /opt/florence adonnelly
General
DATE = 2008/03/06
TIME = 11:41
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
3.5136
5.1950
6.7376
6.7435
6.7581
6.7640
6.7965
6.8022
7.2037
7.2185
7.2241
7.2388
7.2447
5.9912
4.0119
2.8979
1.0000
OMOM
MOMO
12
[rel]
[ppm]

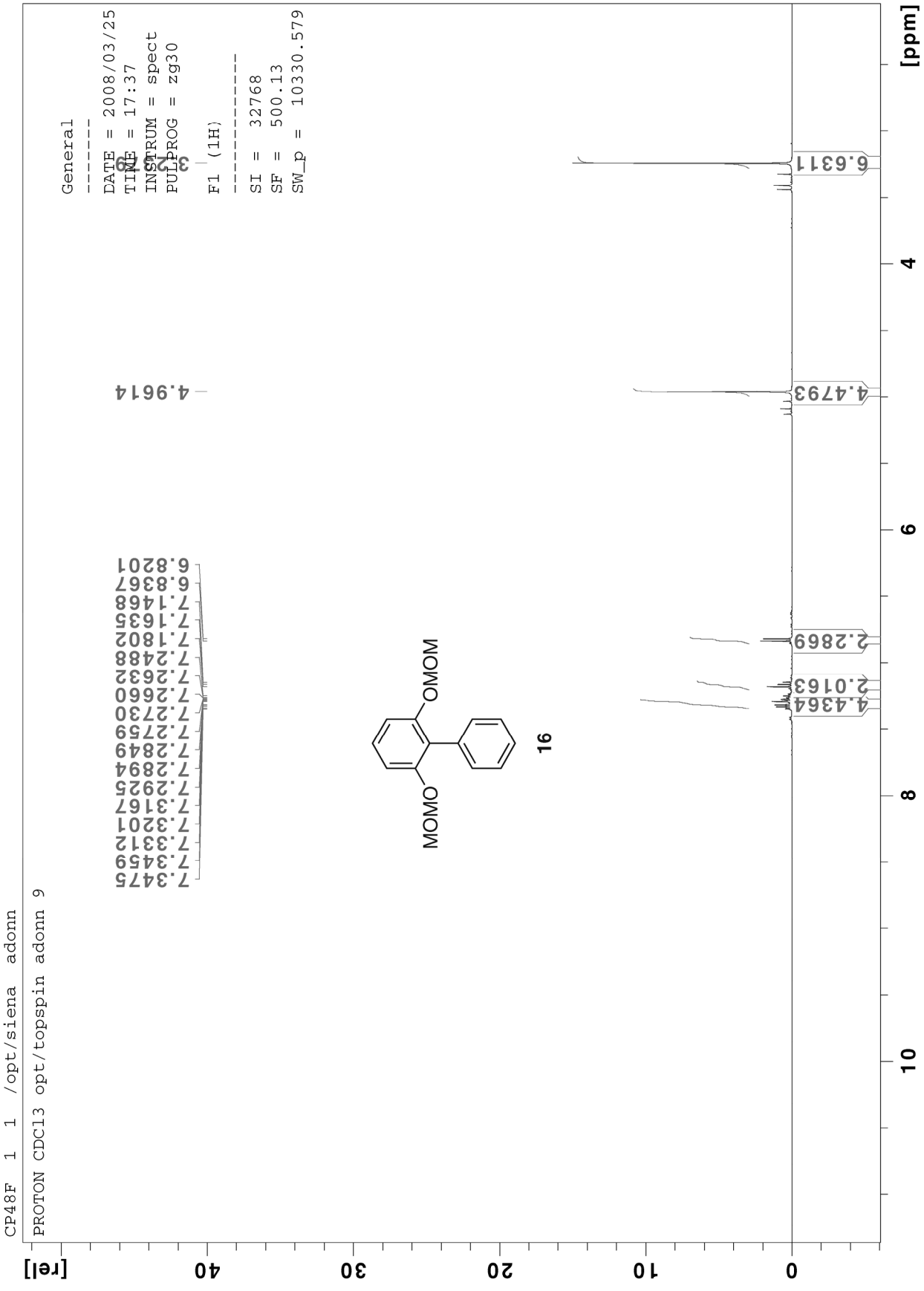

CP46F 1 1 /opt/siena adonn
PROTON CDC13 opt/topspin lpeter 3
General
DATE = 2008/03/27
TIME = 10:58
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
7.1842
7.1684
7.1673
7.1463
7.1421
7.1314
7.1190
7.1157
7.0632
7.0467
7.0342
7.0300
7.0197
6.7198
6.7032
5.0872
3.9978
3.2867
6.5681
2.4950
4.6690
2.0806
2.0601
MOMO
OMOM
13
[rel]
[ppm]

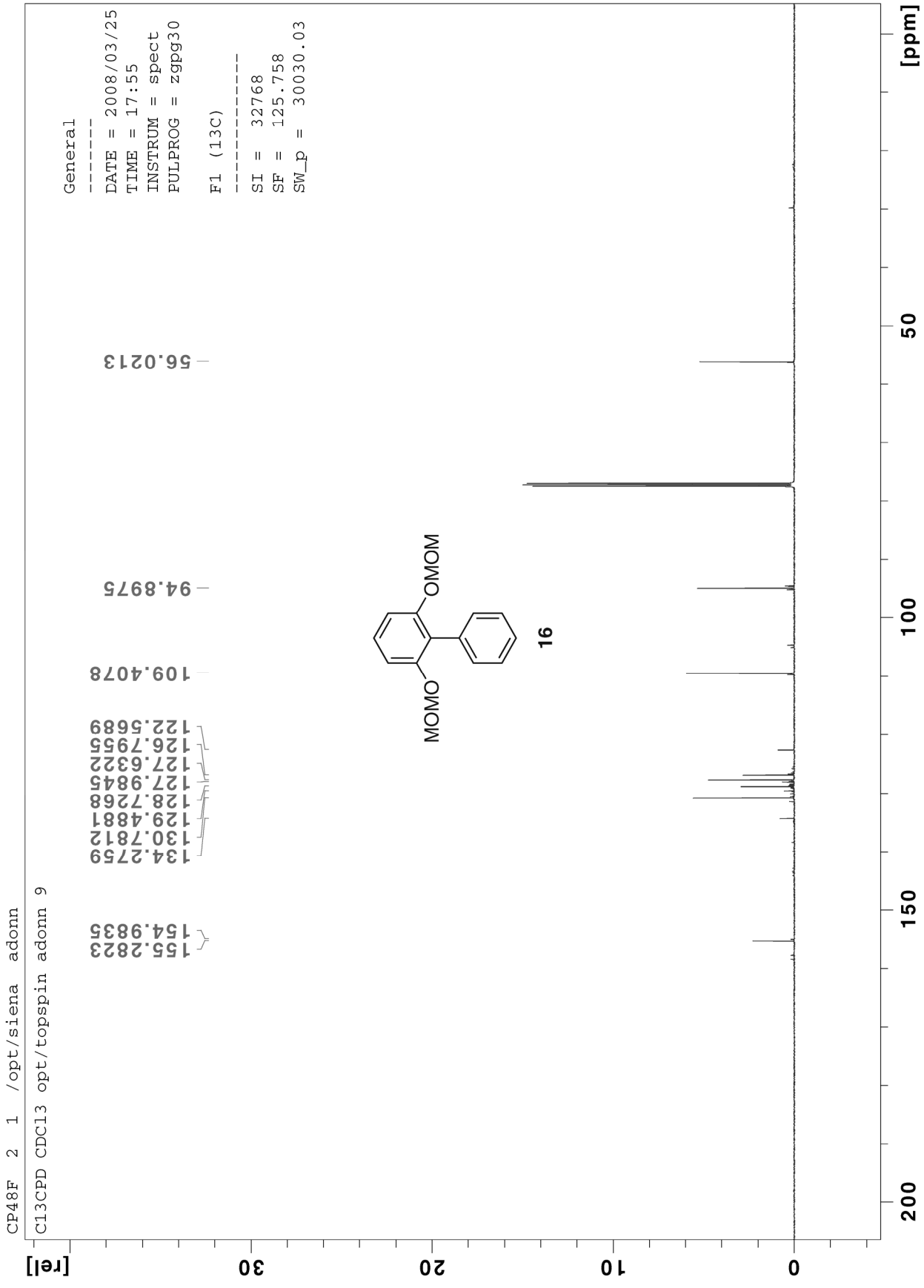

CP46F 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin lpeter 3
General
DATE = 2008/03/27
TIME = 11:21
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
155.9124
141.5897
128.5151
127.9835
127.4452
125.4137
119.3625
107.7175
94.3263
56.0197
29.1231
OMOM
MOMO
13
[rel]
[ppm]

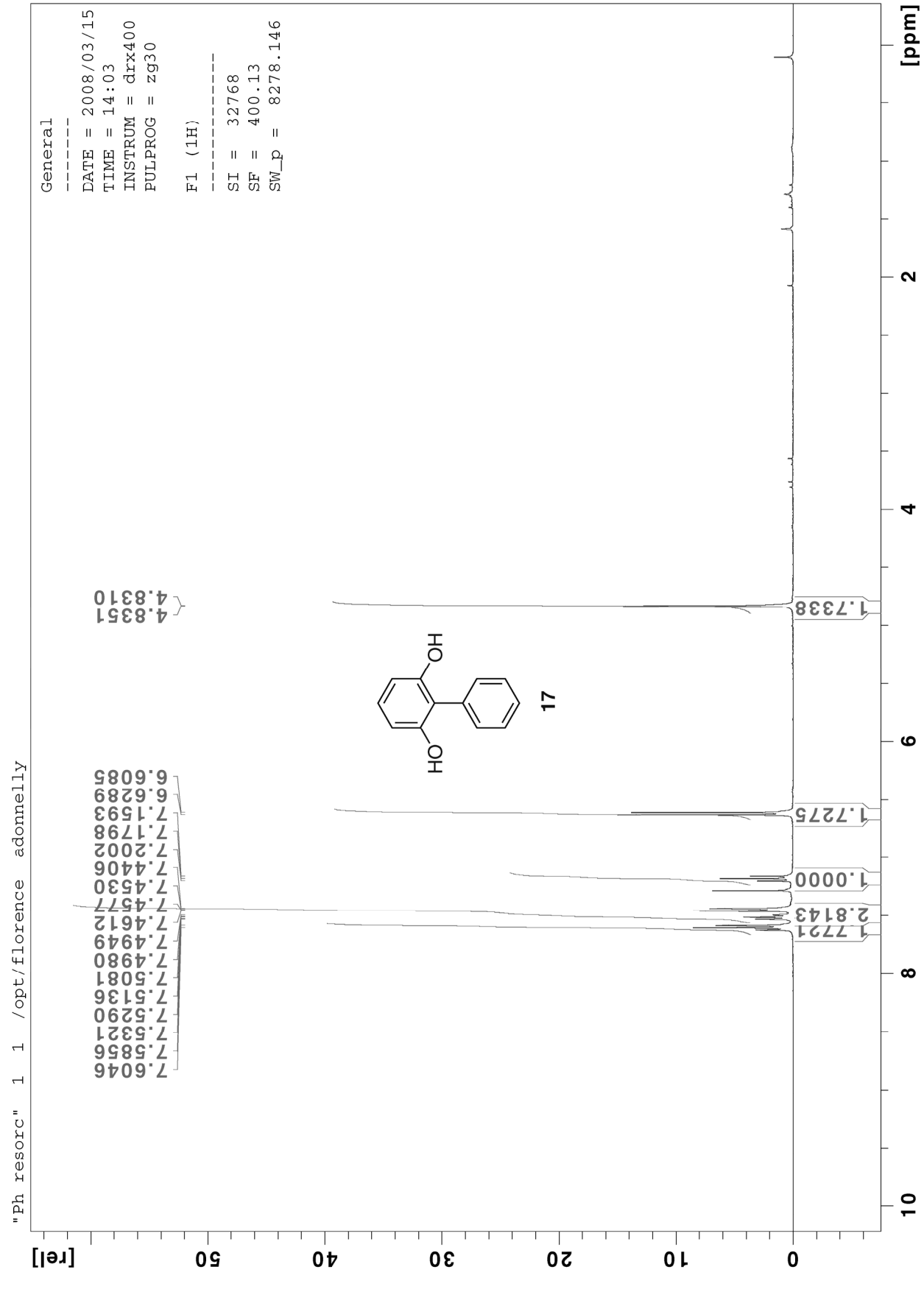

"Bn resorcinol (redo)" 3 1 /opt/florence adonnelly
General
DATE = 2008/03/28
TIME = 13:48
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
7.3125
7.3006
7.2488
7.2378
7.2290
7.2260
7.2234
7.2162
7.2111
7.2087
7.2066
7.2044
7.1949
7.1863
7.0274
7.0071
6.9869
6.4533
6.4330
4.8182
4.0860
OH
HO
14
2.0072
1.8469
1.9879
1.0000
1.1062
[rel]
[ppm]

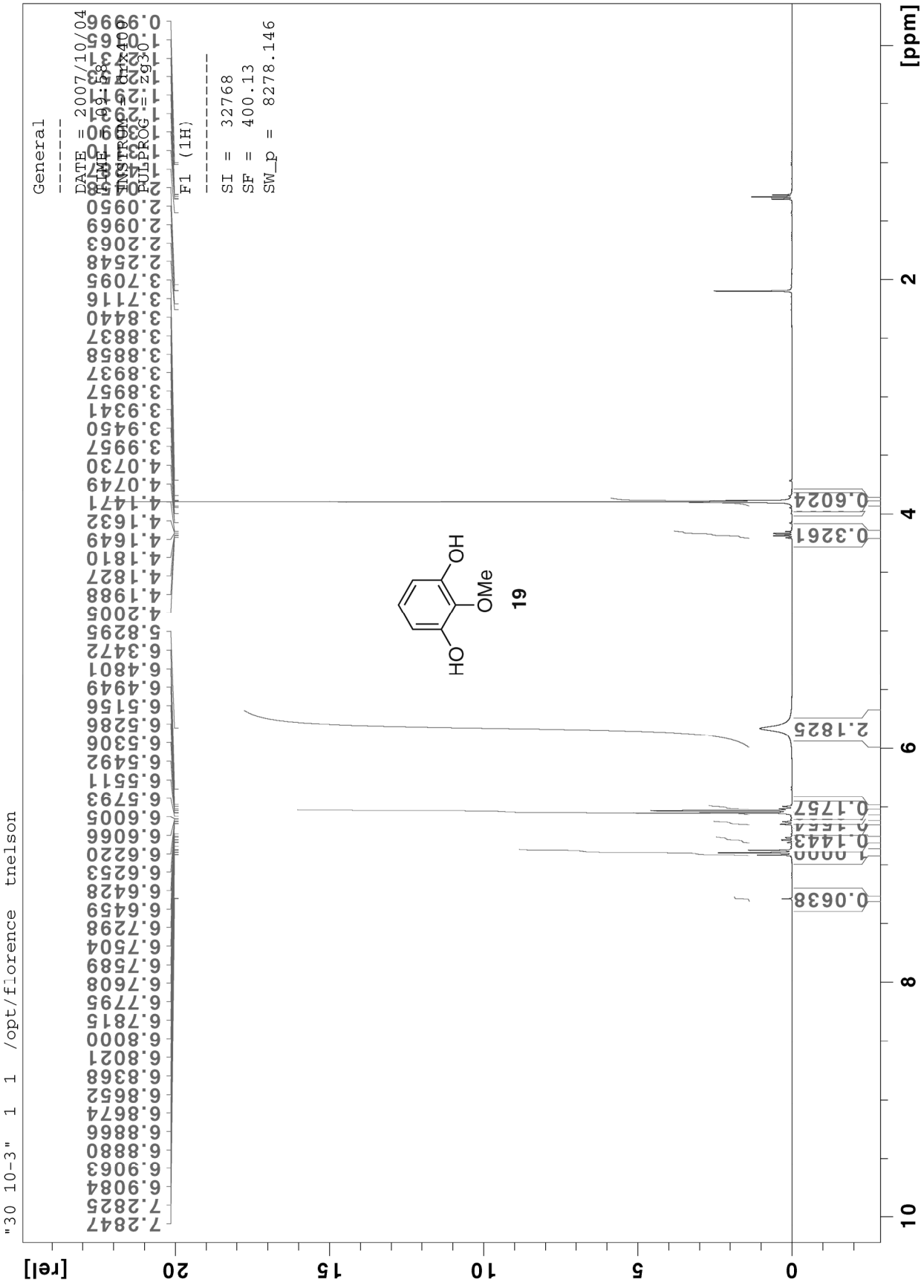

I-MOM-Resorcinol 1 1 /opt/florence adonnelly
General
DATE = 2007/04/04
TIME = 17:47
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
[rel]
[ppm]
OMOM
MOMO
15
7.2495
7.2288
7.2256
7.2079
7.2048
7.1845
6.7877
6.7669
6.7611
6.7555
6.7341
6.7283
6.7136
6.7078
5.2706
5.1794
3.5375
3.4982
6.4918
2.3643
2.5091
1.0000

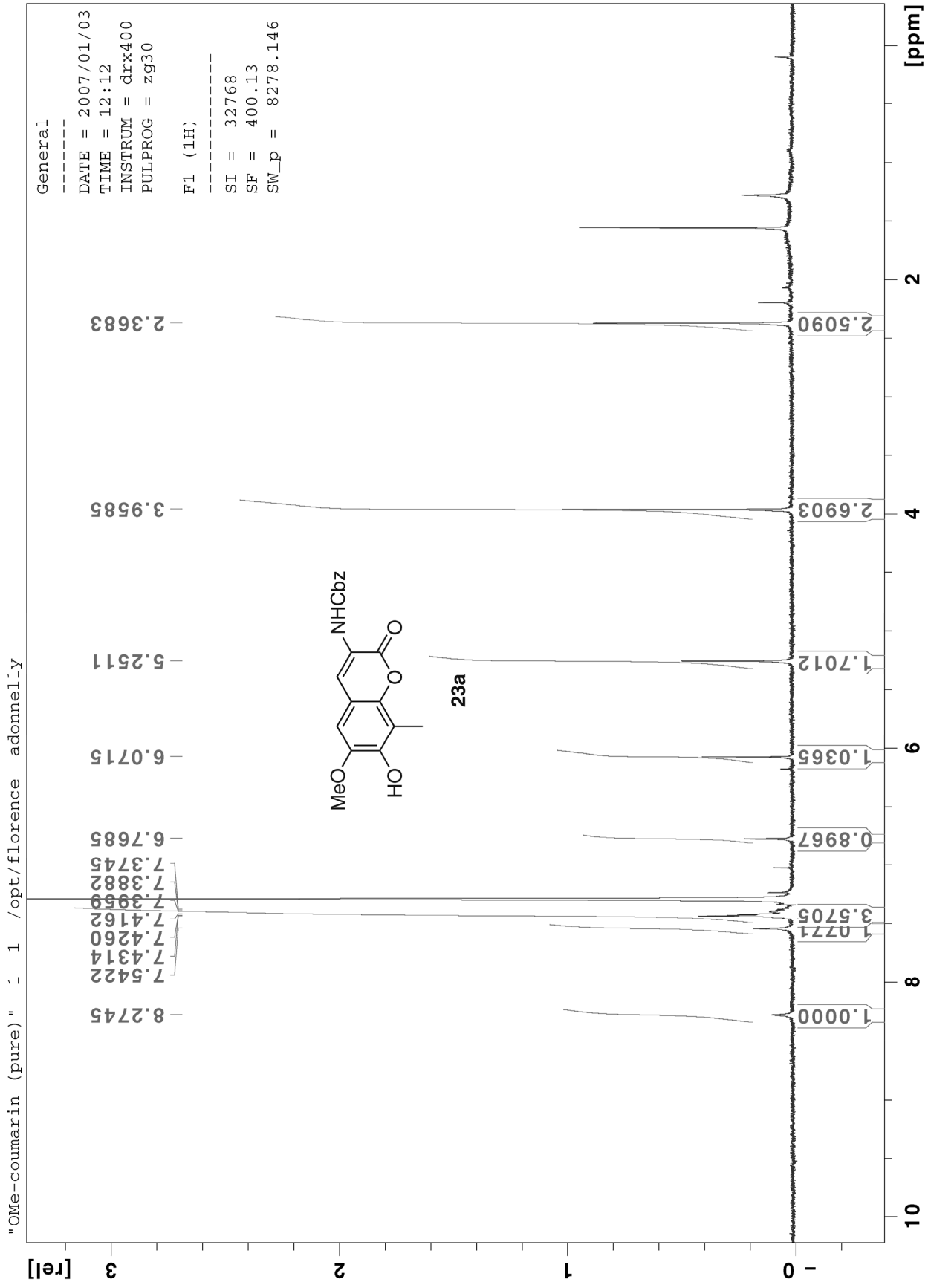

CP47last 3 1 /opt/florence adonnelly
General
DATE = 2008/05/27
TIME = 20:36
INSTRUM = drx400
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 23980.815
158.3440
157.4147
129.7693
109.6132
108.5565
94.9994
94.4590
56.4782
56.0523
OMOM
MOMO
I
15
[rel]
[ppm]

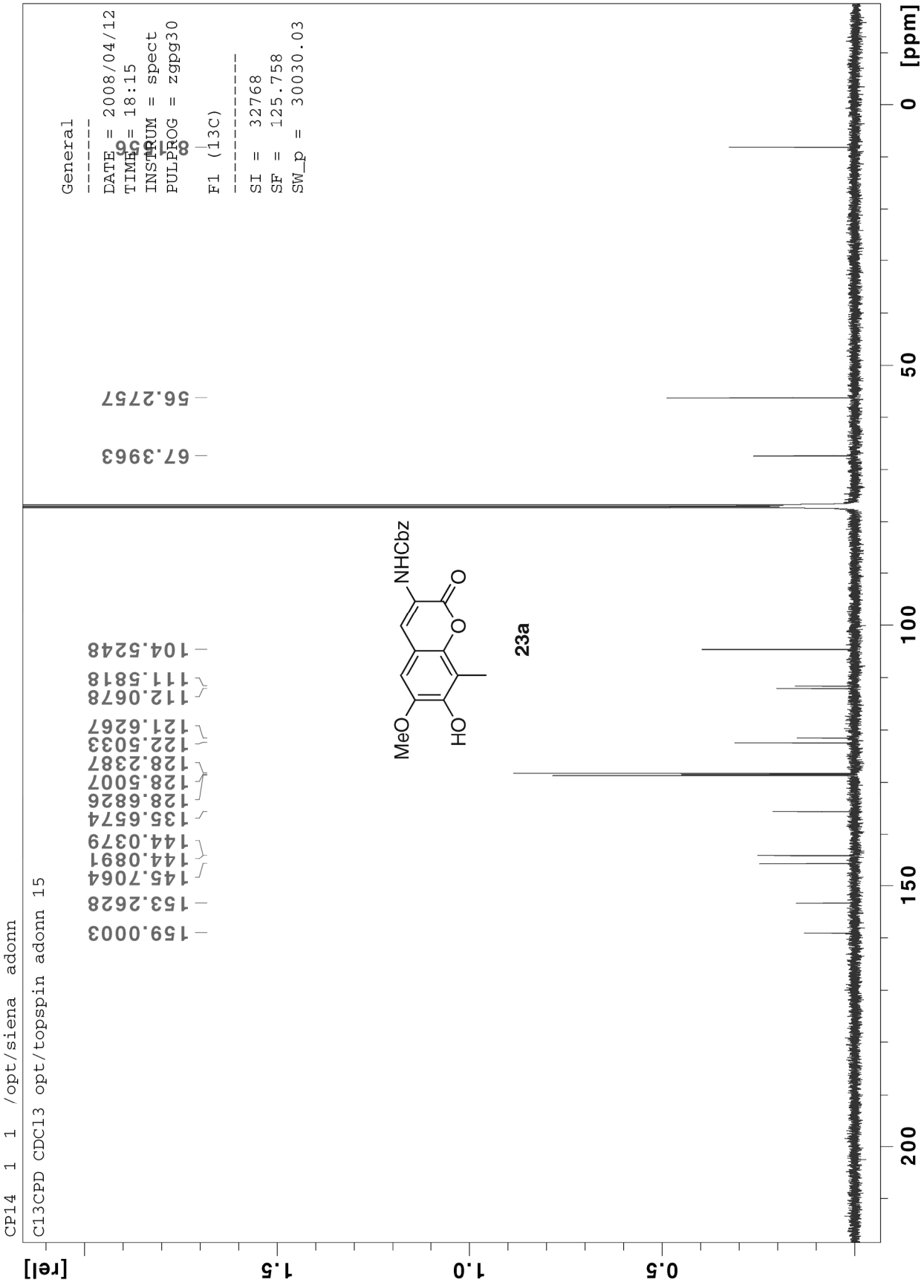

CP48F 1 1 /opt/siena adonn
PROTON CDCl3 opt/topspin adonn 9
General
DATE = 2008/03/25
TIME = 17:37
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
6.6311
4.4793
4.4364
2.0163
2.2869
7.3475
7.3459
7.3312
7.3201
7.3167
7.2925
7.2894
7.2849
7.2759
7.2730
7.2660
7.2632
7.2488
7.1802
7.1635
7.1468
6.8367
6.8201
OMOM
MOMO
16
[rel]
[ppm]

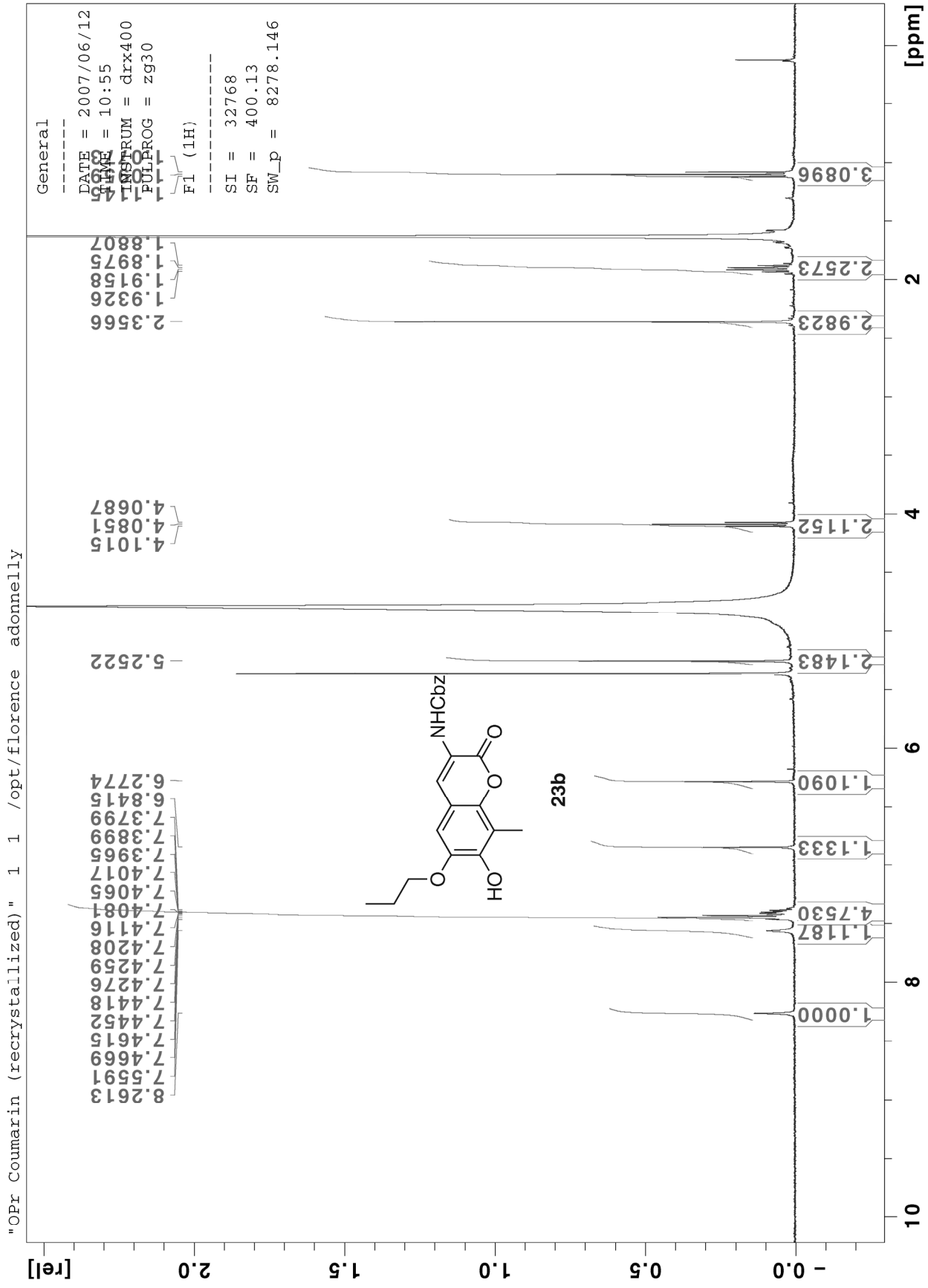

CP48F 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 9
General
DATE = 2008/03/25
TIME = 17:55
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
56.0213
94.8975
109.4078
122.5689
126.7955
127.6322
127.9845
128.7268
129.4881
130.7812
134.2759
154.9835
155.2823
OMOM
MOMO
16
[rel]
[ppm]

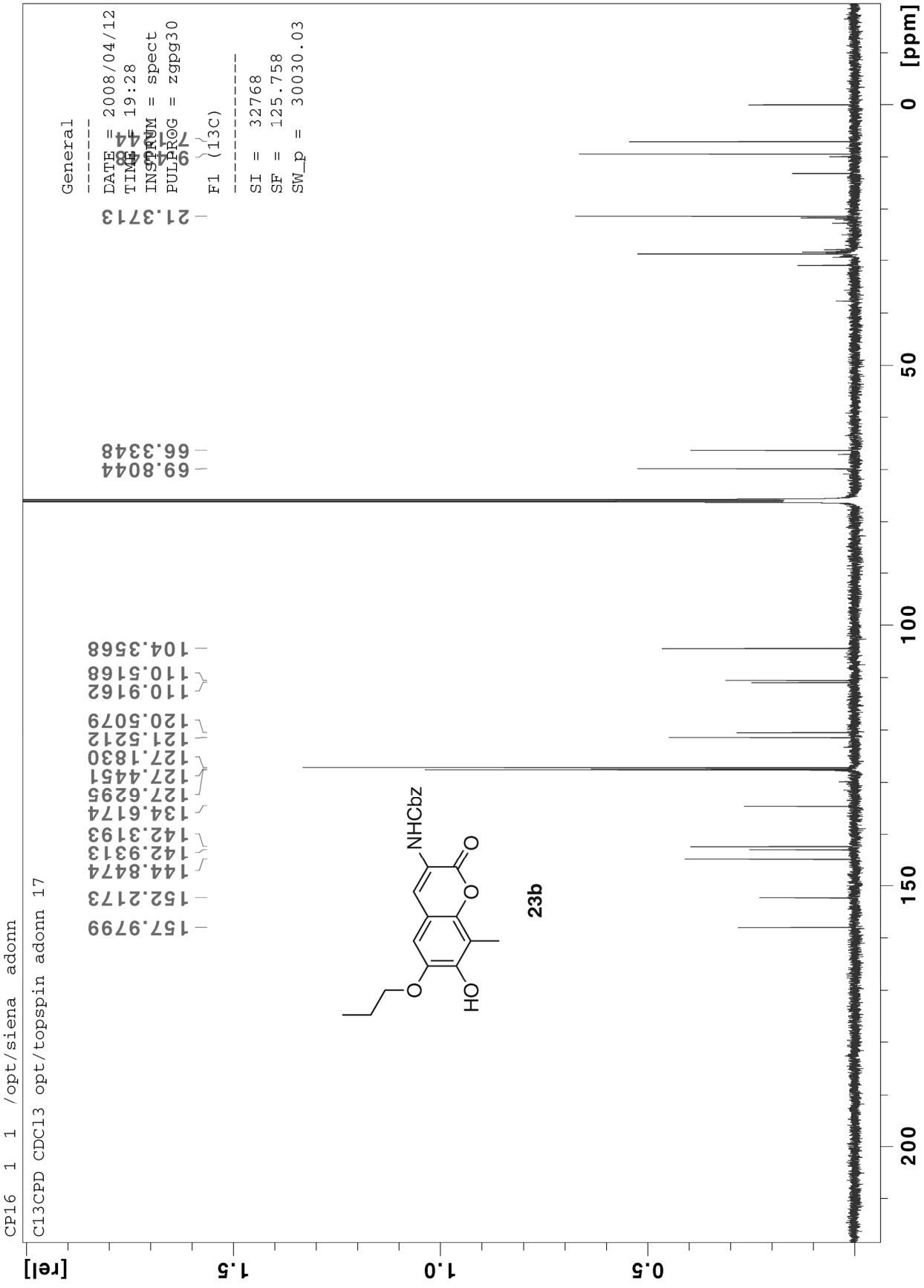

"Ph resorc" 1 1 /opt/florence adonnelly
General
DATE = 2008/03/15
TIME = 14:03
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
4.8351
4.8310
7.6046
7.5856
7.5321
7.5290
7.5136
7.5081
7.4980
7.4949
7.4612
7.4577
7.4530
7.4406
7.2002
7.1798
7.1593
6.6289
6.6085
1.7338
1.7275
1.0000
2.8143
1.7721
OH
HO
17
[rel]
[ppm]

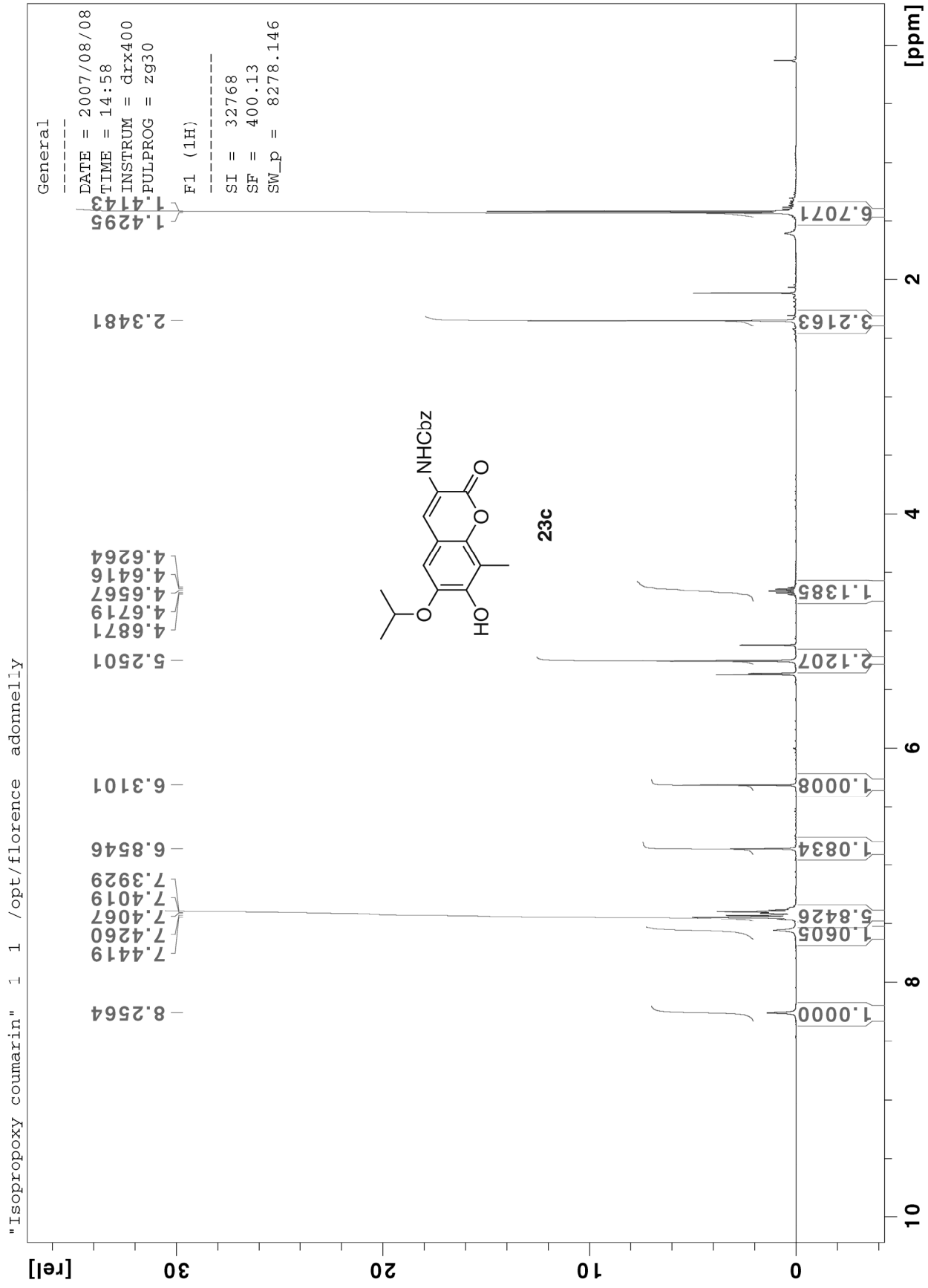

"30 10-3" 1 1 /opt/florence tnelson
General
DATE = 2007/10/04
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
OH
OMe
HO
19
0.6024
0.3261
2.1825
0.1757
0.1443
0.0638
[rel]
[ppm]

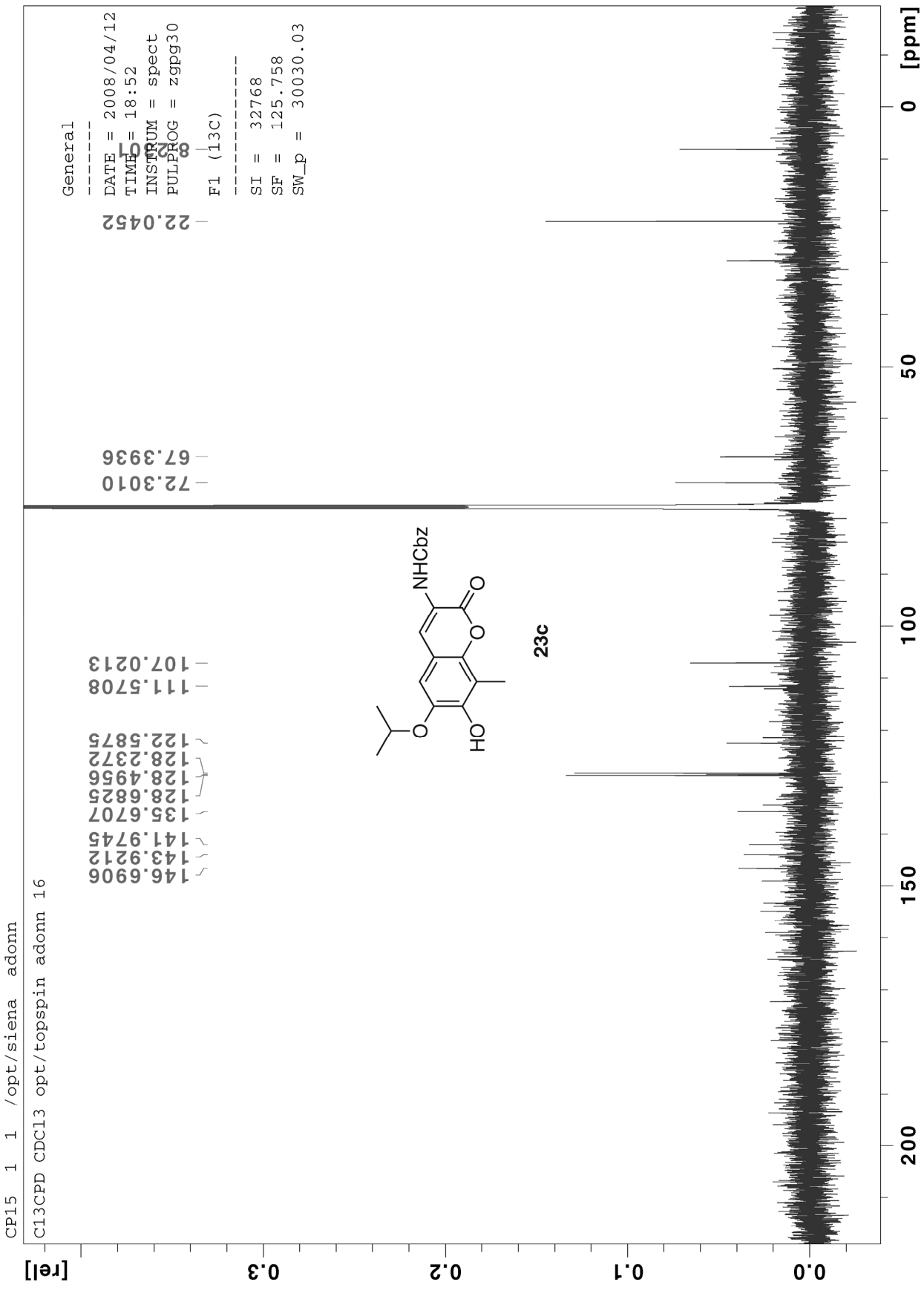

"OMe-coumarin (pure)" 1 1 /opt/florence adonnelly
General
DATE = 2007/01/03
TIME = 12:12
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
MeO
HO
23a
8.2745
7.5422
7.4314
7.4260
7.4162
7.3959
7.3882
7.3745
6.7685
6.0715
5.2511
3.9585
2.3683
1.0000
1.0221
3.5705
0.8967
1.0365
1.7012
2.6903
2.5090
[rel]
[ppm]

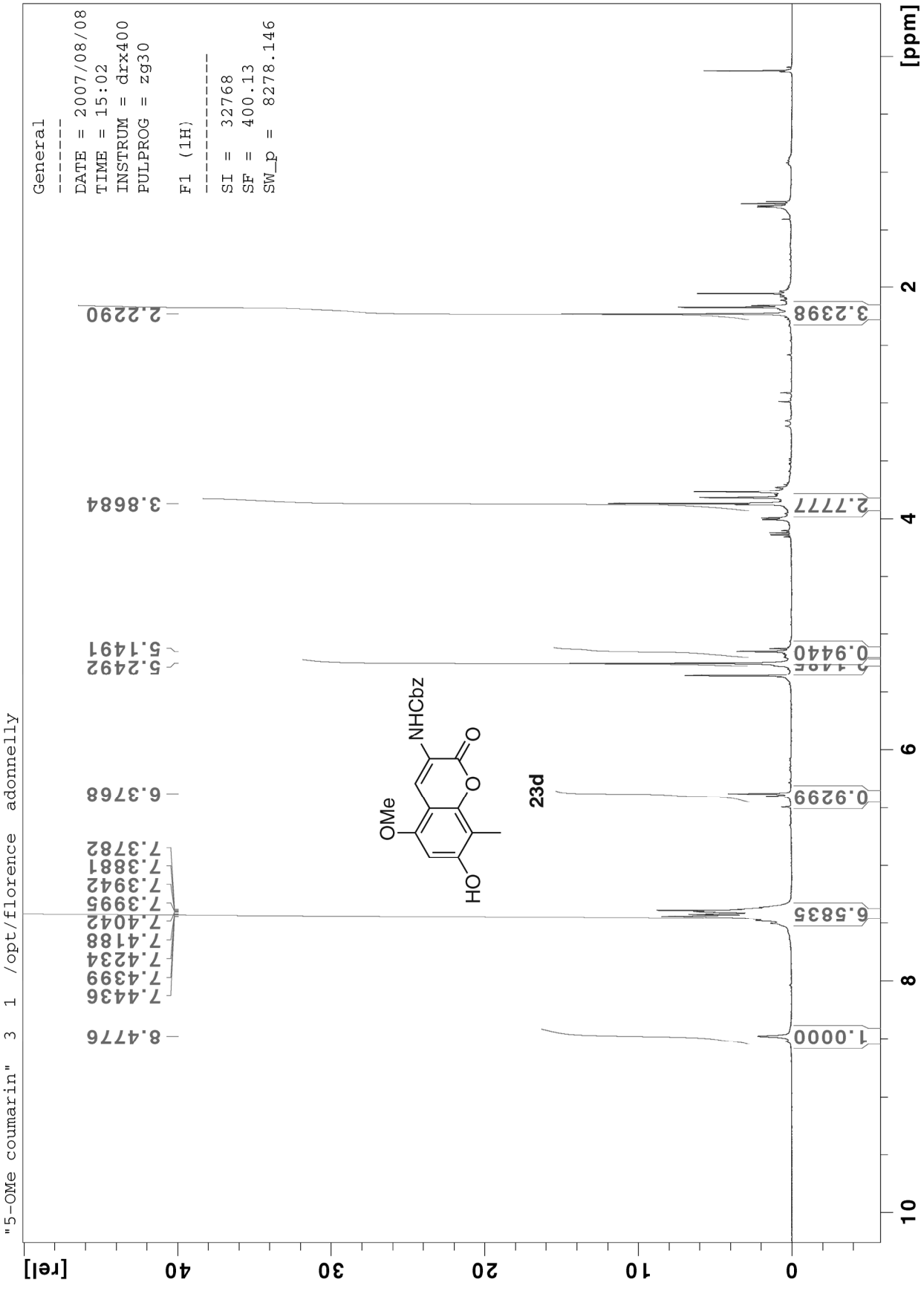

CP14 1 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 15
General
DATE = 2008/04/12
TIME = 18:15
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
159.0003
153.2628
145.7064
144.0891
144.0379
135.6574
128.6826
128.5007
128.2387
122.5033
121.6267
112.0678
111.5818
104.5248
67.3963
56.2757
NHCbz
MeO
HO
23a
[rel]
[ppm]

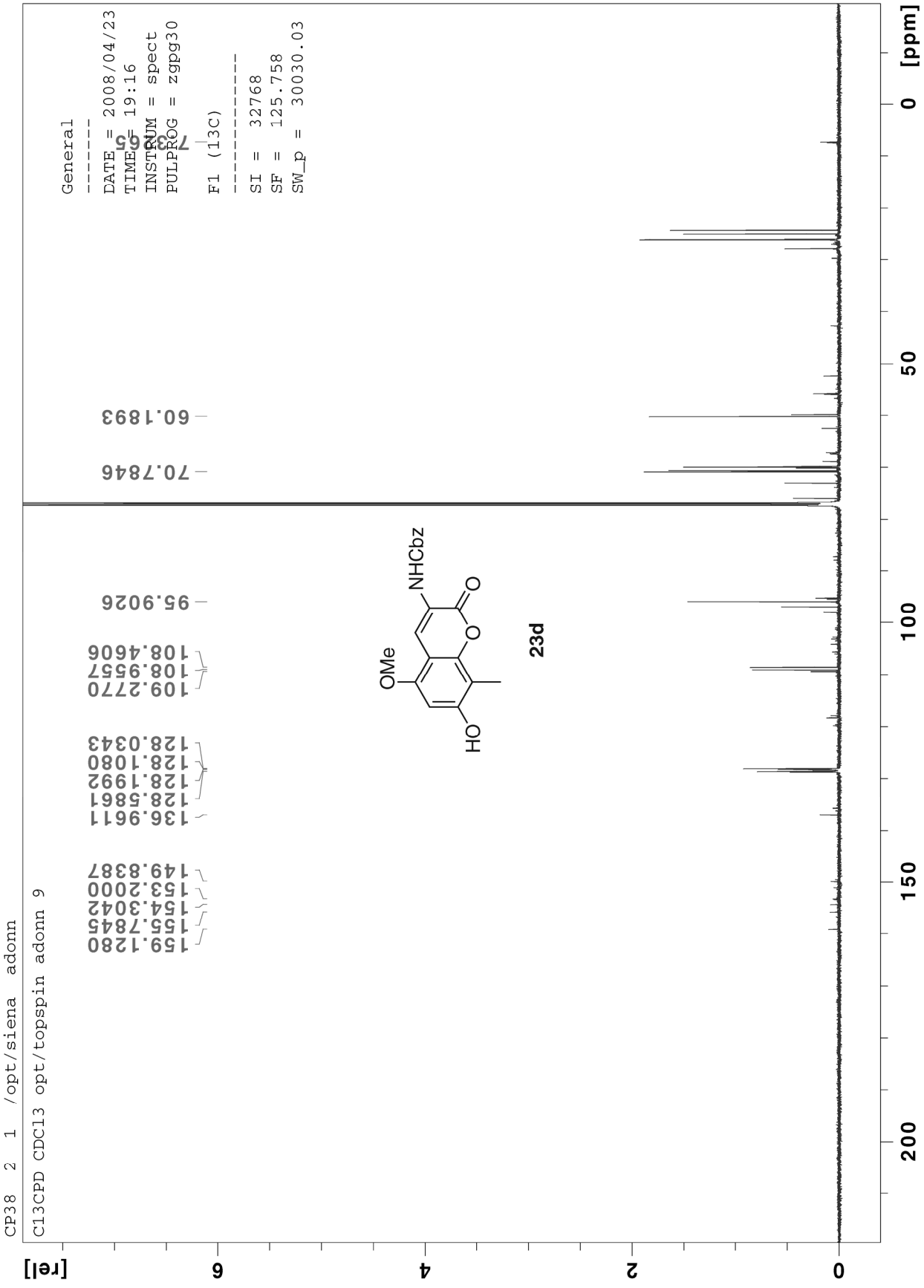

"OPr Coumarin (recrystallized)" 1 1 /opt/florence adonnelly
General
DATE = 2007/06/12
TIME = 10:55
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
O
O
O
HO
23b
8.2613
7.5591
7.4669
7.4615
7.4452
7.4418
7.4276
7.4259
7.4208
7.4116
7.4081
7.4065
7.4017
7.3965
7.3899
7.3799
6.8415
6.2774
5.2522
4.1015
4.0851
4.0687
2.3566
1.9326
1.9158
1.8975
1.8807
3.0896
2.2573
2.9823
2.1152
2.1483
1.1090
1.1333
4.7530
1.1187
1.0000
[rel]
[ppm]

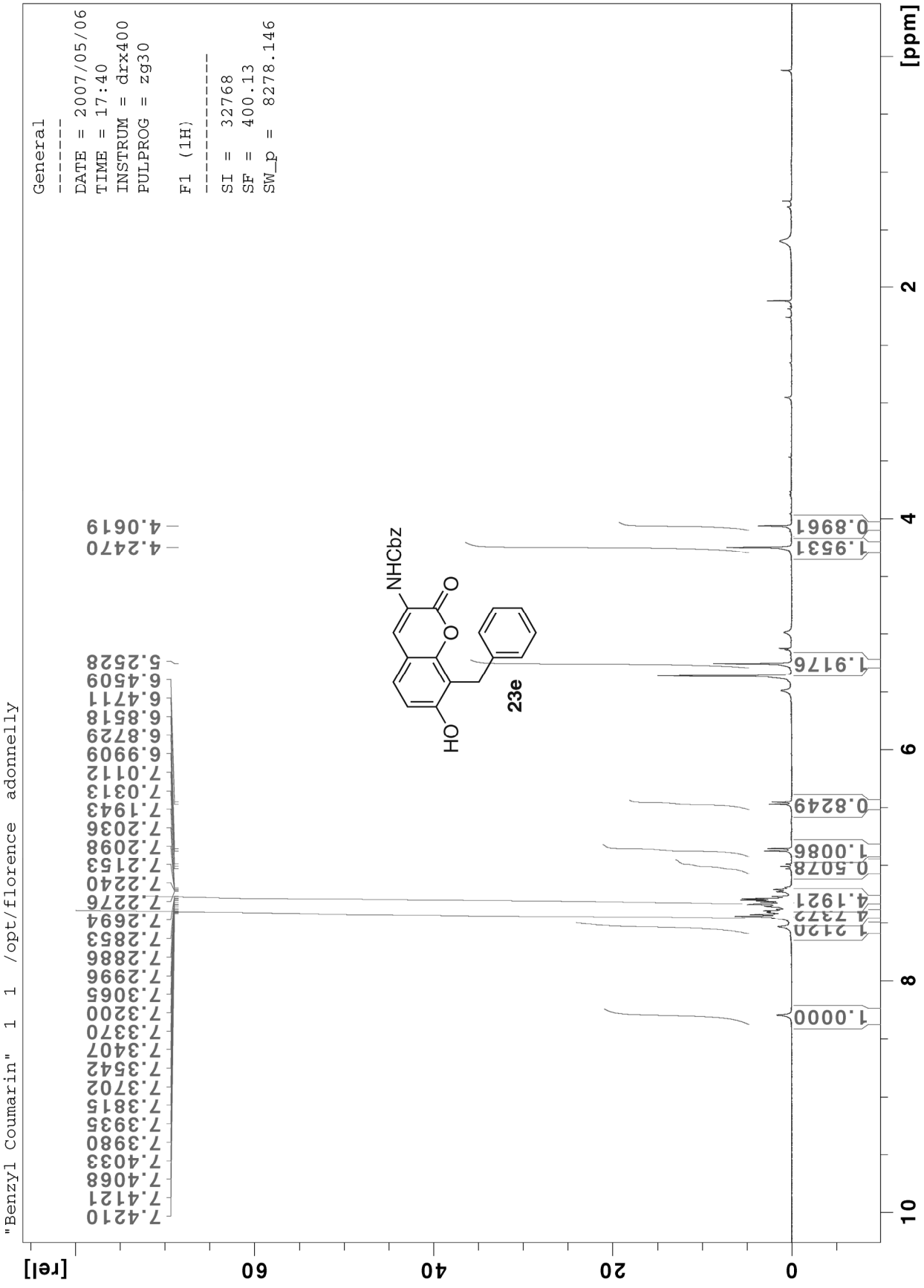

CP16 1 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 17
General
DATE = 2008/04/12
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
21.3713
66.3348
69.8044
104.3568
110.5168
110.9162
120.5079
121.5212
127.1830
127.4451
127.6295
134.6174
142.3193
142.9313
144.8474
152.2173
157.9799
NHCbz
O
O
O
HO
23b
[rel]
1.5
1.0
0.5
200
150
100
50
0
[ppm]

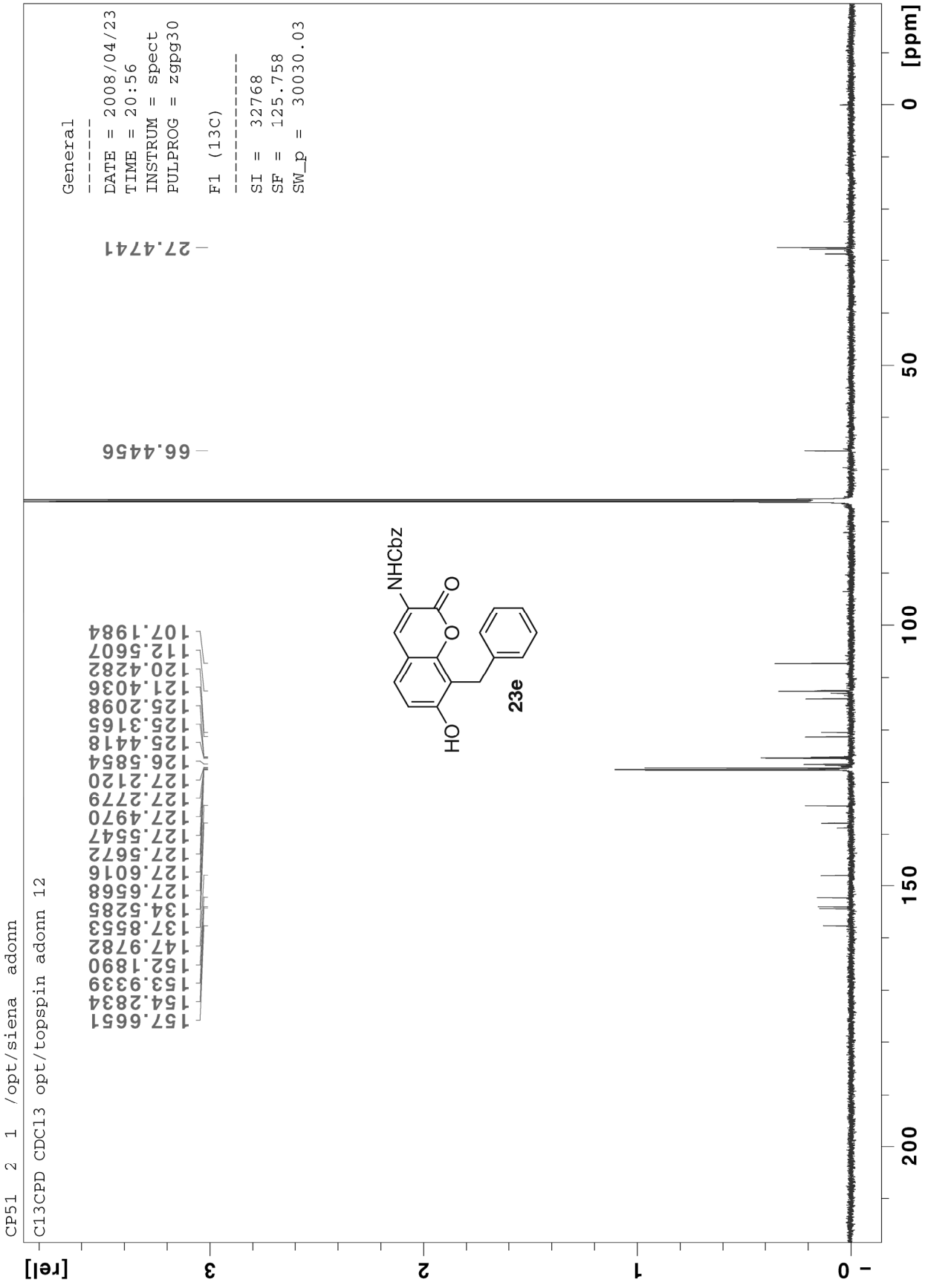

"Isopropoxy coumarin" 1 1 /opt/florence adonnelly
General
DATE = 2007/08/08
TIME = 14:58
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
O
O
O
HO
23c
[rel]
[ppm]
1.4143
1.4295
2.3481
4.6264
4.6416
4.6567
4.6719
4.6871
5.2501
6.3101
6.8546
7.3929
7.4019
7.4067
7.4260
7.4419
8.2564
6.7071
3.2163
1.1385
2.1207
1.0008
1.0834
1.0605
5.8426
1.0000

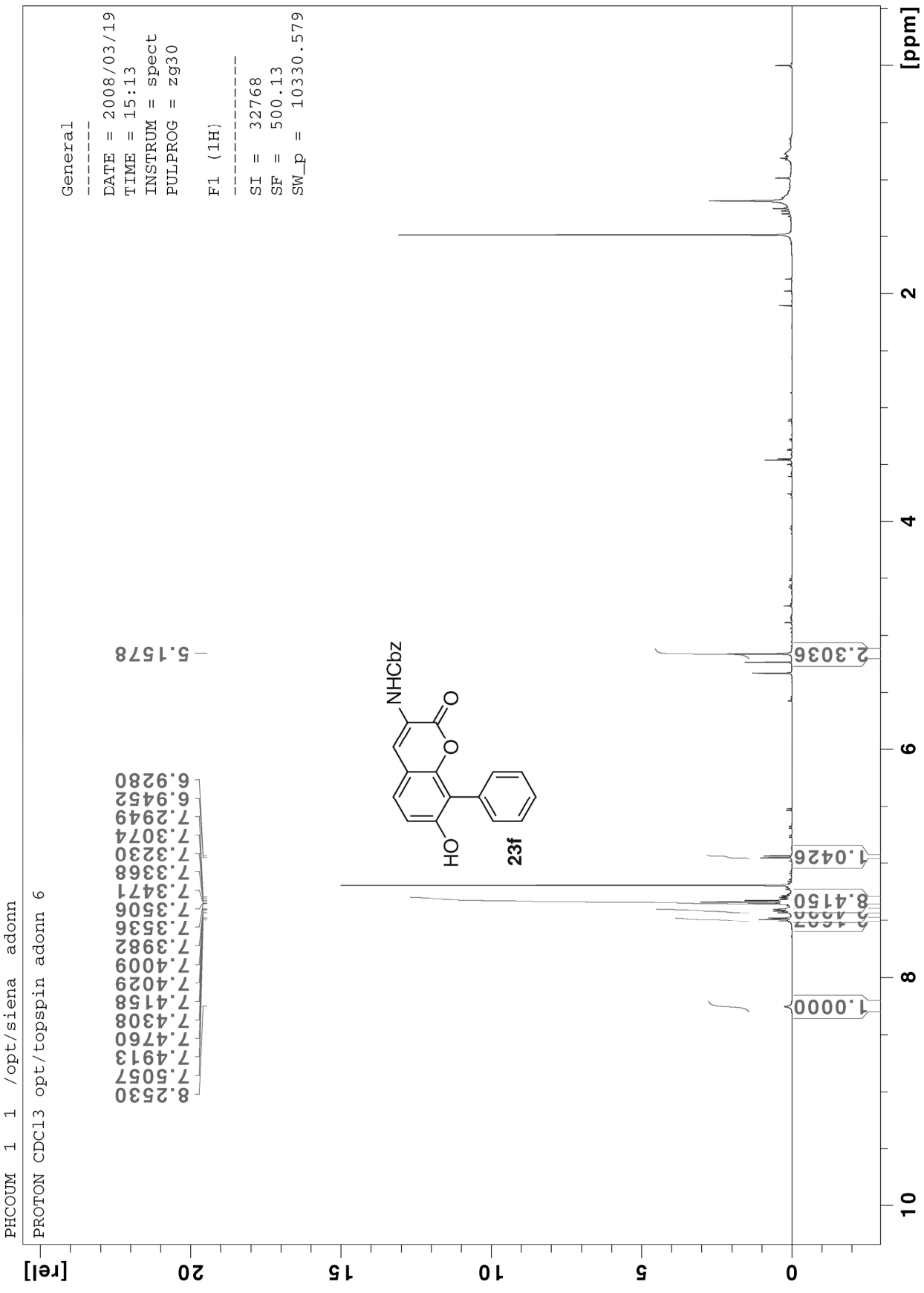

CP15 1 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 16
General
DATE = 2008/04/12
TIME = 18:52
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
146.6906
143.9212
141.9745
135.6707
128.6825
128.4956
128.2372
122.5875
111.5708
107.0213
72.3010
67.3936
22.0452
NHCbz
O
O
O
HO
23c
[rel]
0.0
0.1
0.2
0.3
200
150
100
50
0 [ppm]

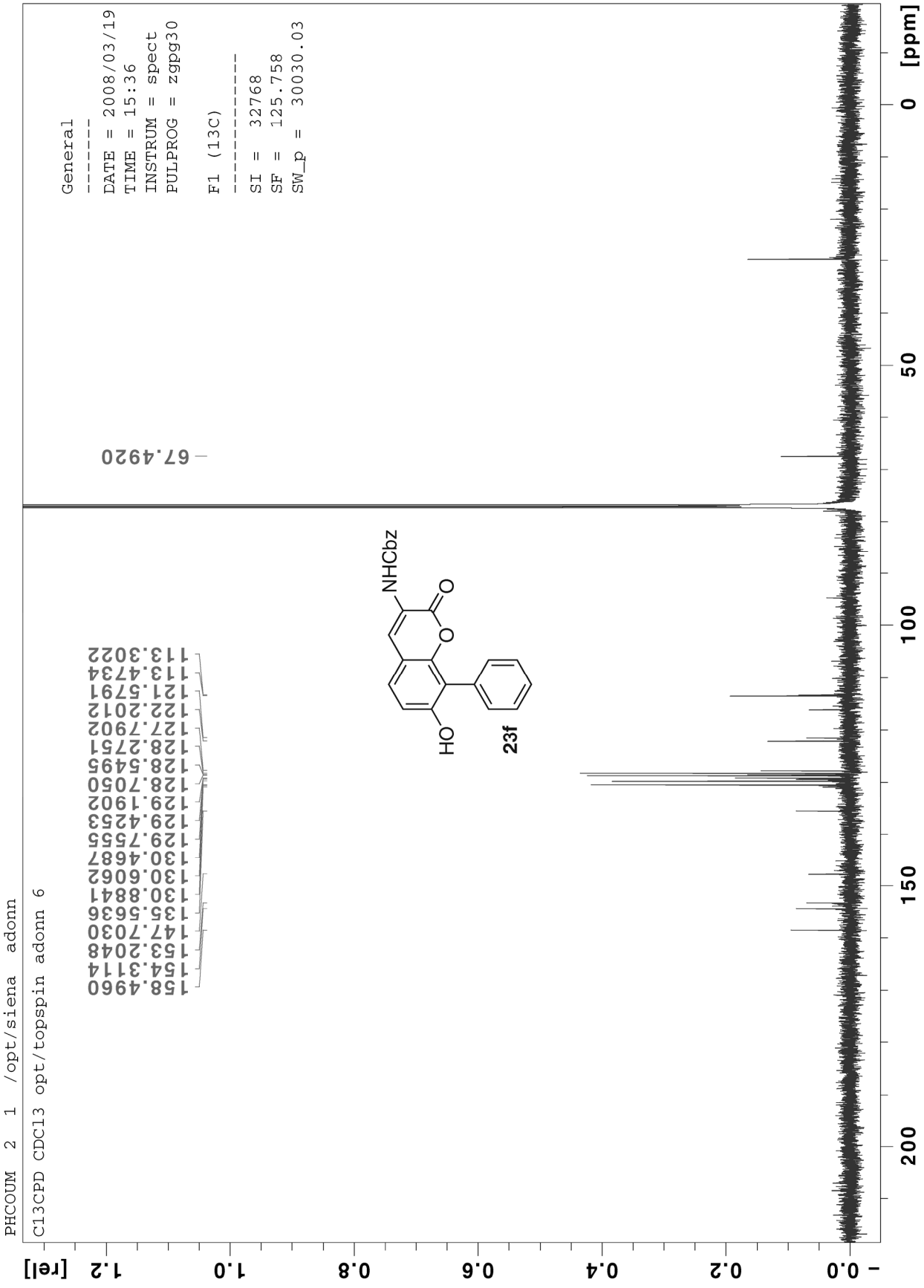

"5-OMe coumarin" 3 1 /opt/florence adonnelly
General
DATE = 2007/08/08
TIME = 15:02
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
8.4776
7.4436
7.4399
7.4234
7.4188
7.4042
7.3995
7.3942
7.3881
7.3782
6.3768
5.2492
5.1491
3.8684
2.2290
1.0000
6.5835
0.9299
0.9440
2.7777
3.2398
NHCbz
OMe
HO
23d
[rel]
[ppm]

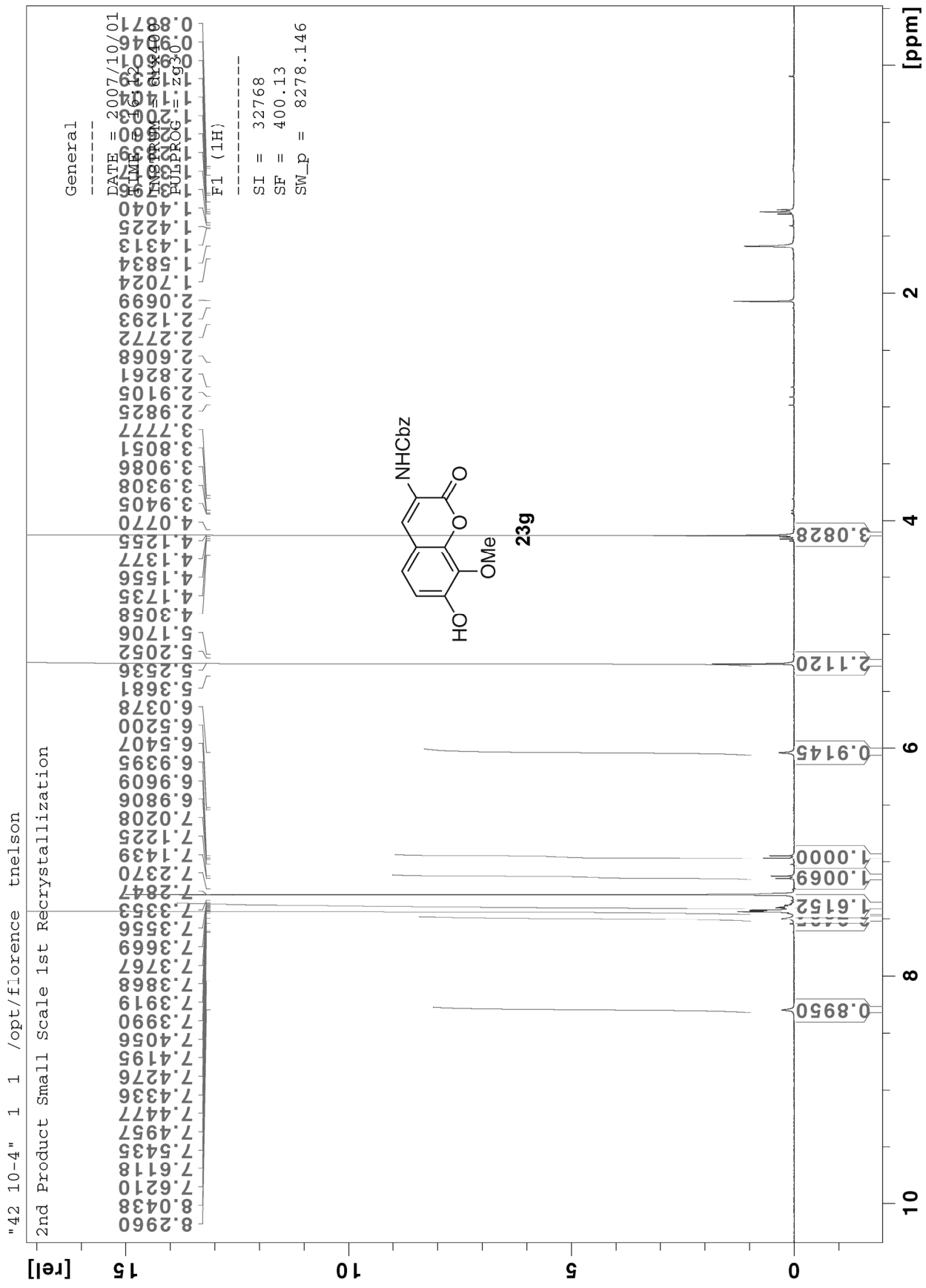

CP38 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 9
General
DATE = 2008/04/23
TIME = 19:16
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
159.1280
155.7845
154.3042
153.2000
149.8387
136.9611
128.5861
128.1992
128.1080
128.0343
109.2770
108.9557
108.4606
95.9026
70.7846
60.1893
OMe
NHCbz
OH
23d
[rel]
[ppm]

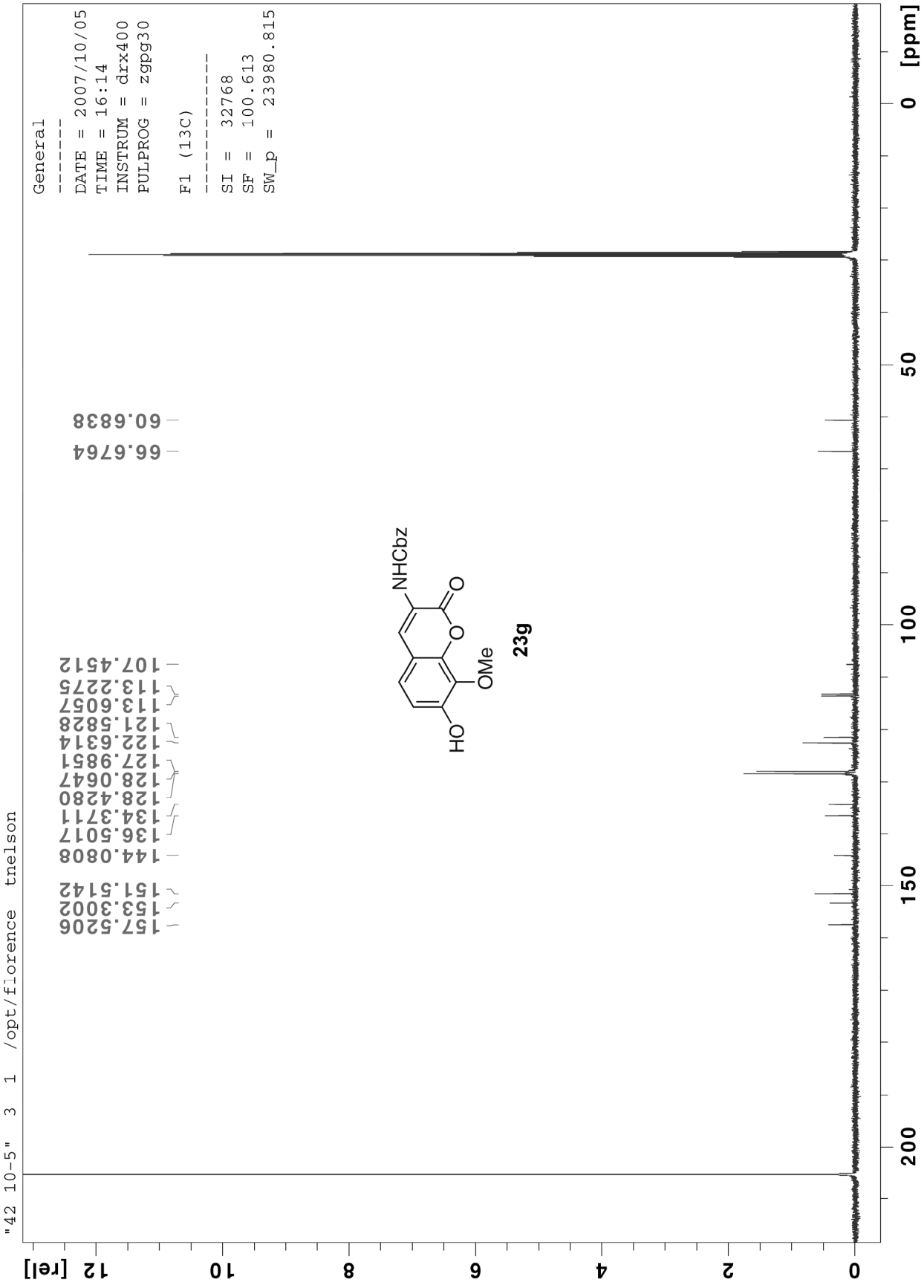

"Benzyl Coumarin" 1 1 /opt/florence adonnelly
General
DATE = 2007/05/06
TIME = 17:40
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
O
O
HO
23e
[rel]
[ppm]
1.0000
1.2120
4.7372
4.1921
0.5078
1.0086
0.8249
1.9176
0.8961
1.9531
4.2470
4.0619
7.4210
7.4121
7.4068
7.4033
7.3980
7.3935
7.3815
7.3702
7.3542
7.3407
7.3370
7.3200
7.3065
7.2996
7.2886
7.2853
7.2694
7.2276
7.2240
7.2153
7.2098
7.2036
7.1943
7.0313
7.0112
6.9909
6.8729
6.8518
6.4711
6.4509
5.2528

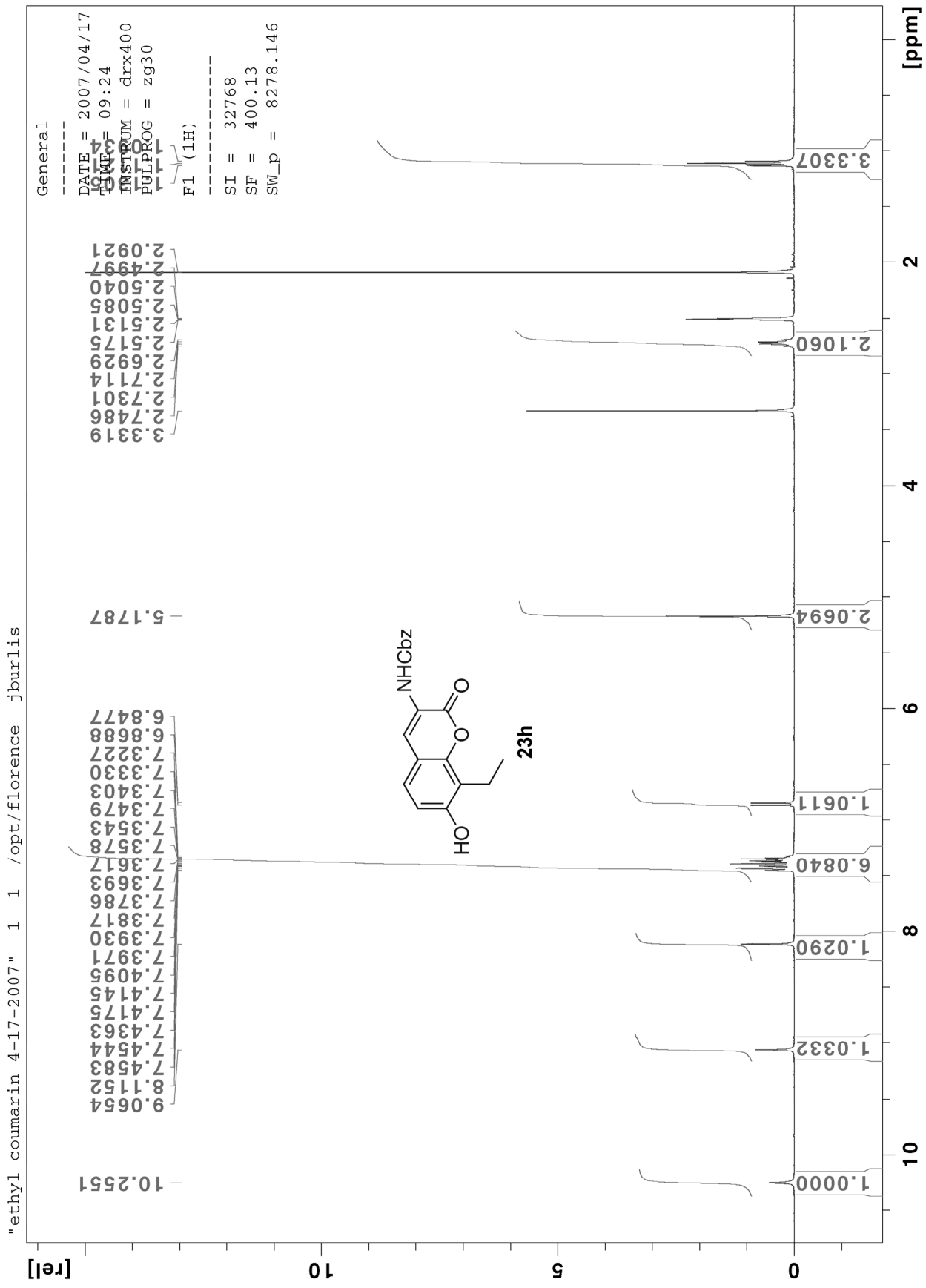

CP51 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 12
General
DATE = 2008/04/23
TIME = 20:56
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
27.4741
66.4456
157.6651
154.2834
153.9339
152.1890
147.9782
137.8553
134.5285
127.6568
127.6016
127.5672
127.5547
127.4970
127.2779
127.2120
126.5854
125.4418
125.3165
125.2098
121.4036
120.4282
112.5607
107.1984
NHCbz
O
O
HO
23e
[rel]
3
2
1
0
200
150
100
50
0 [ppm]

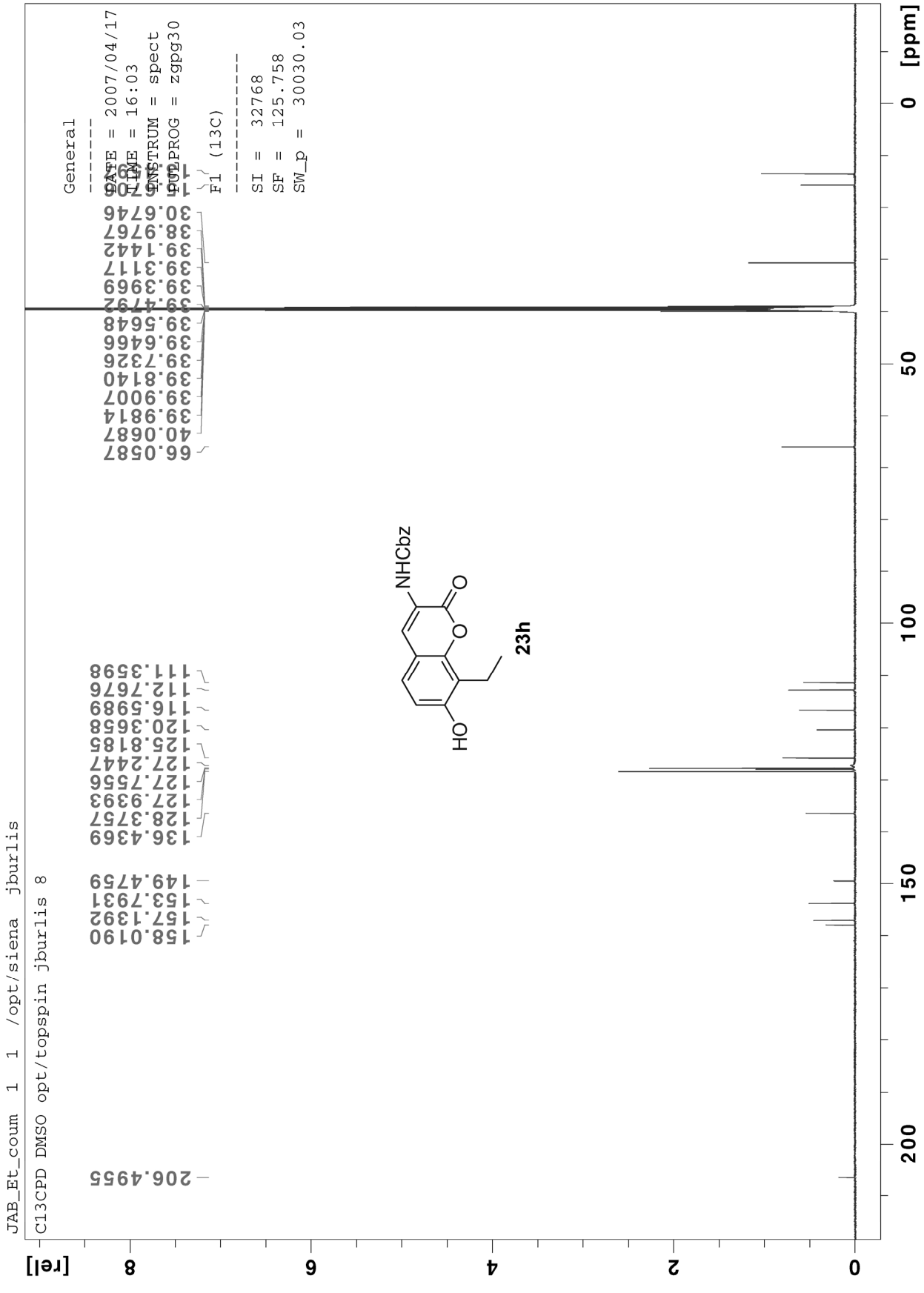

PHCOUM 1 1 /opt/siena adonn
PROTON CDCl3 opt/topspin adonn 6
General
DATE = 2008/03/19
TIME = 15:13
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
8.2530
7.5057
7.4913
7.4760
7.4308
7.4158
7.4029
7.4009
7.3982
7.3536
7.3506
7.3471
7.3368
7.3230
7.3074
7.2949
6.9452
6.9280
5.1578
NHCbz
O
O
HO
23f
1.0000
8.4150
1.0426
2.3036
[rel]
[ppm]

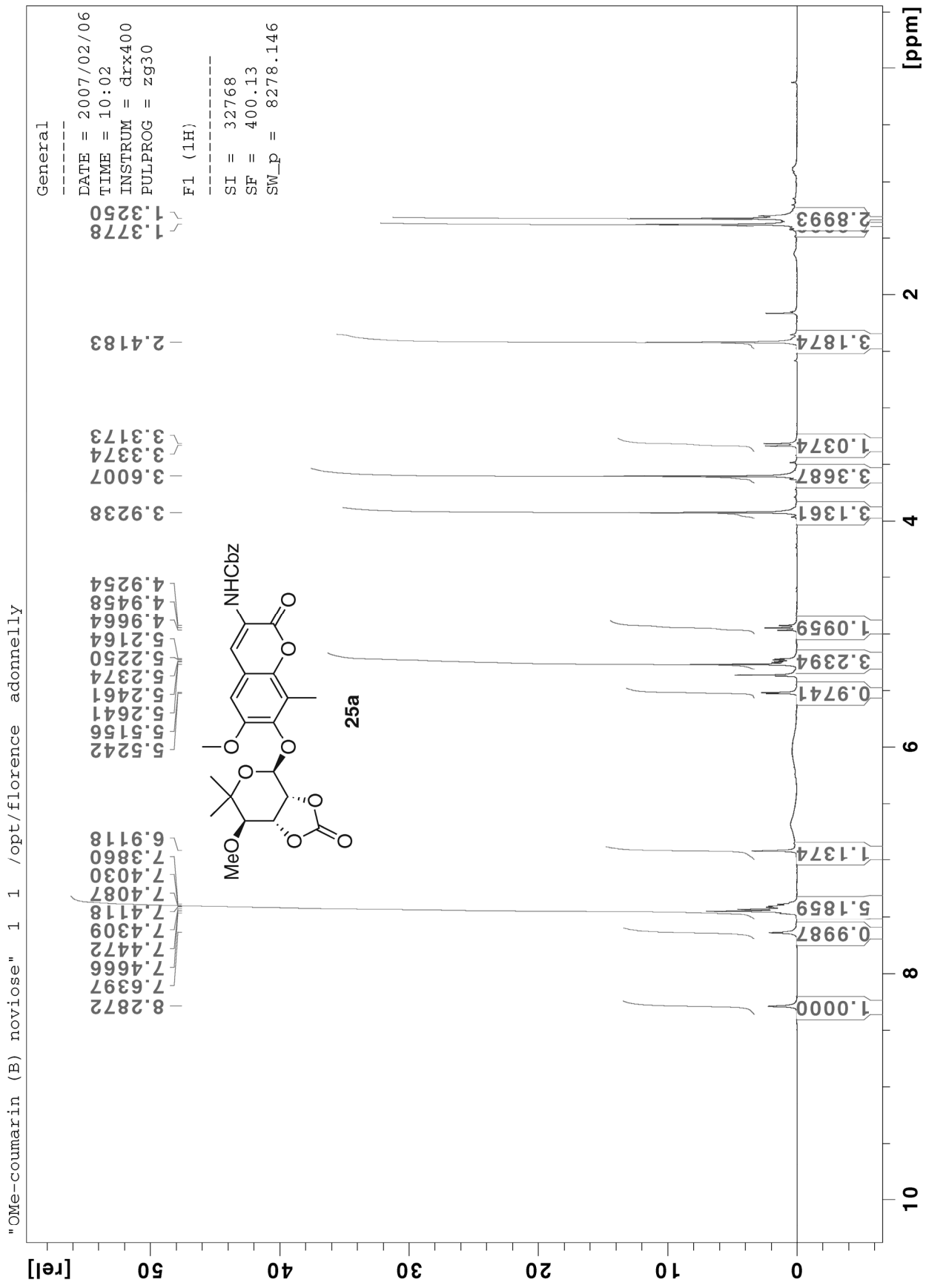

PHCOUM 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 6
General
DATE = 2008/03/19
TIME = 15:36
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
67.4920
158.4960
154.3114
153.2048
147.7030
135.5636
130.8841
130.6062
130.4687
129.7555
129.4253
129.1902
128.7050
128.5495
128.2751
127.7902
122.2012
121.5791
113.4734
113.3022
NHCbz
HO
23f
[rel]
[ppm]

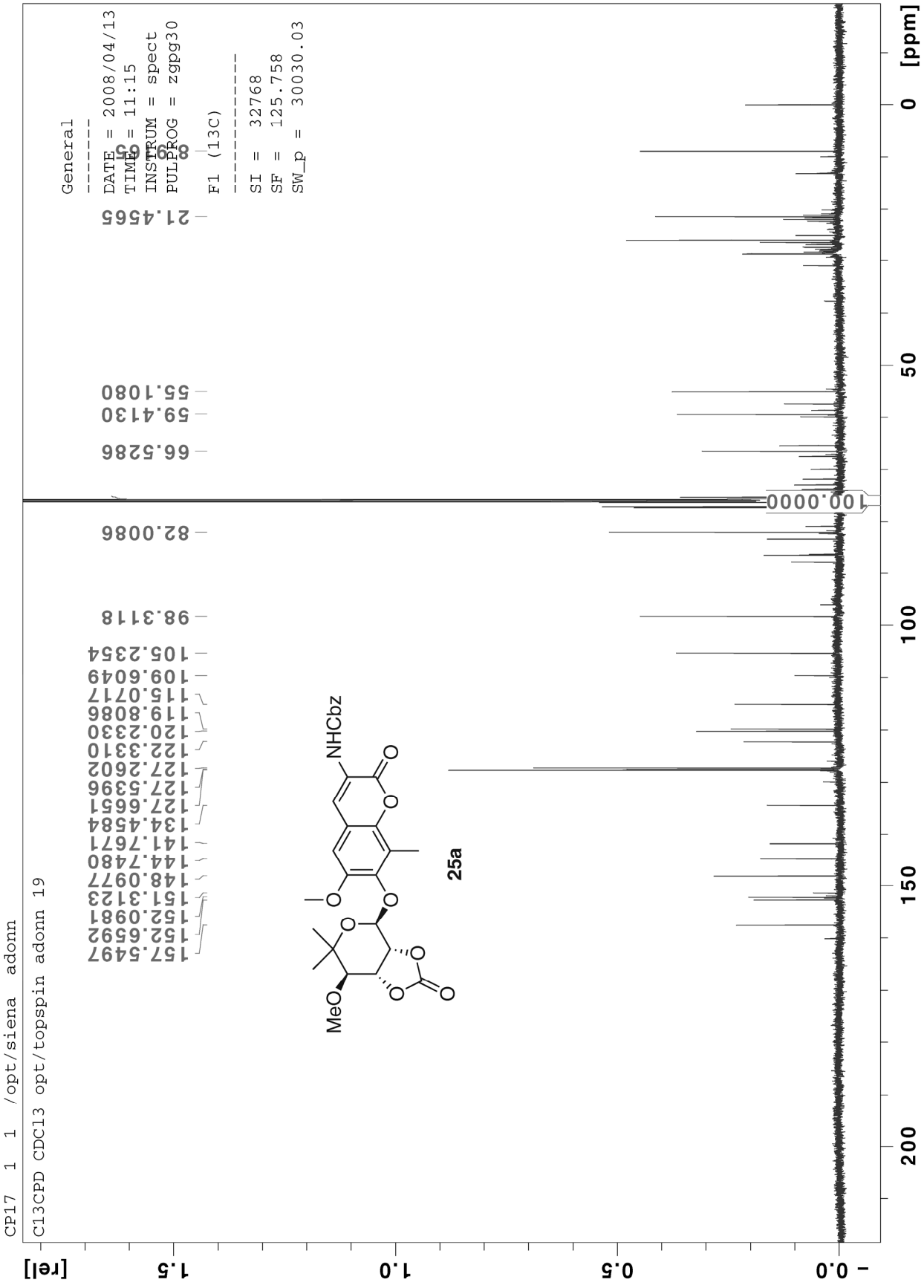

"42 10-4" 1 1 /opt/florence tnelson
2nd Product Small Scale 1st Recrystallization
General
DATE = 2007/10/01
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
OMe
HO
23g
3.0828
2.1120
0.9145
1.0000
1.0069
1.6152
0.8950
[rel]
[ppm]

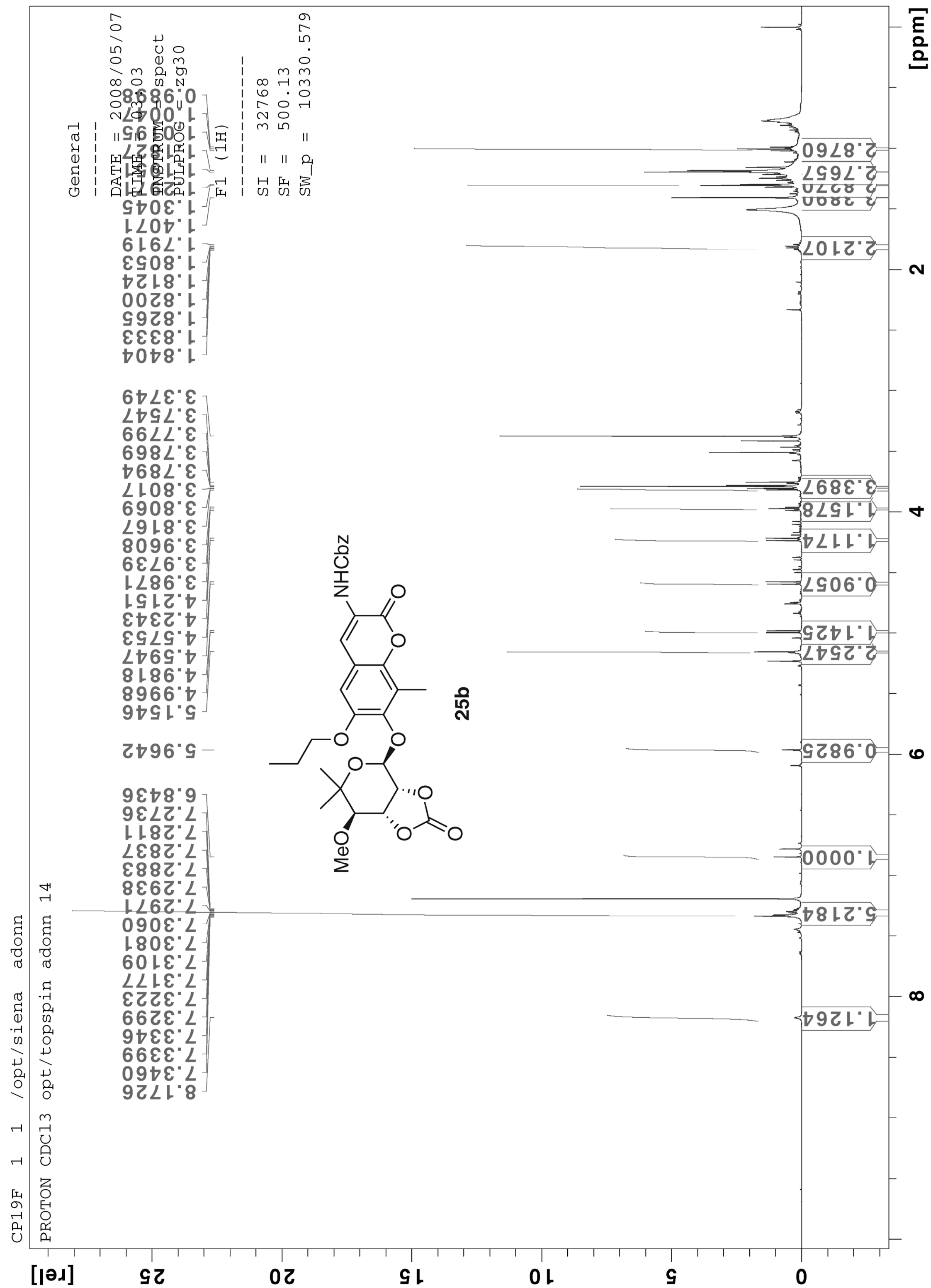

"42 10-5" 3 1 /opt/florence tnelson
General
DATE = 2007/10/05
TIME = 16:14
INSTRUM = drx400
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 23980.815
60.6838
66.6764
107.4512
113.2275
113.6057
121.5828
122.6314
127.9851
128.0647
128.4280
134.3711
136.5017
144.0808
151.5142
153.3002
157.5206
NHCbz
OMe
HO
23g
[rel]
[ppm]

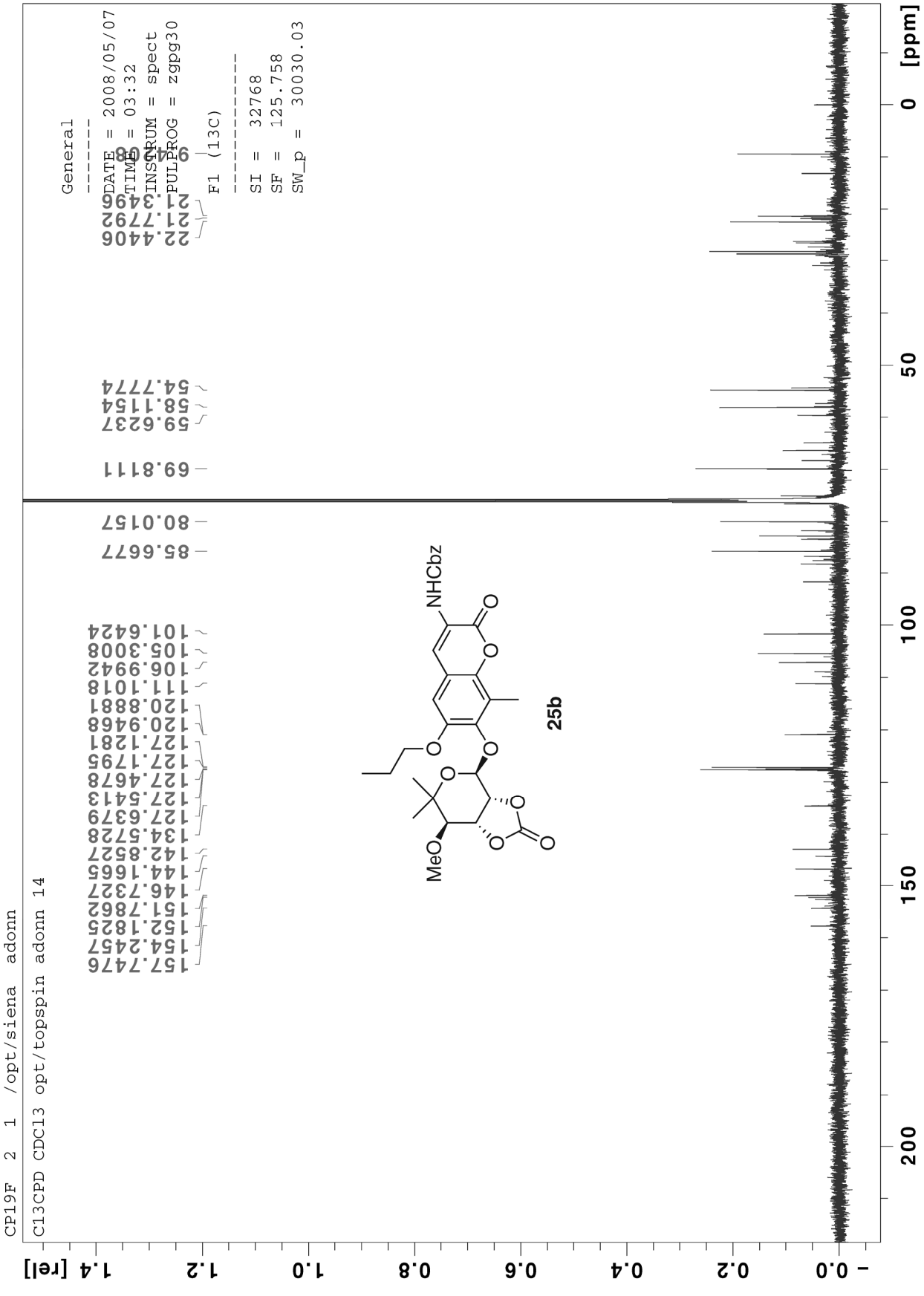

"ethyl coumarin 4-17-2007" 1 1 /opt/florence jburlis
General
DATE = 2007/04/17
TIME = 09:24
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
O
O
HO
23h
10.2551
9.0654
8.1152
7.4583
7.4544
7.4363
7.4175
7.4145
7.4095
7.3971
7.3930
7.3817
7.3786
7.3693
7.3617
7.3578
7.3543
7.3479
7.3403
7.3330
7.3227
6.8688
6.8477
5.1787
3.3319
2.7486
2.7301
2.7114
2.6929
2.5175
2.5131
2.5085
2.5040
2.4997
2.0921
1.0000
1.0332
1.0290
6.0840
1.0611
2.0694
2.1060
3.3307
[rel]
10
5
0
[ppm]
10
8
6
4
2

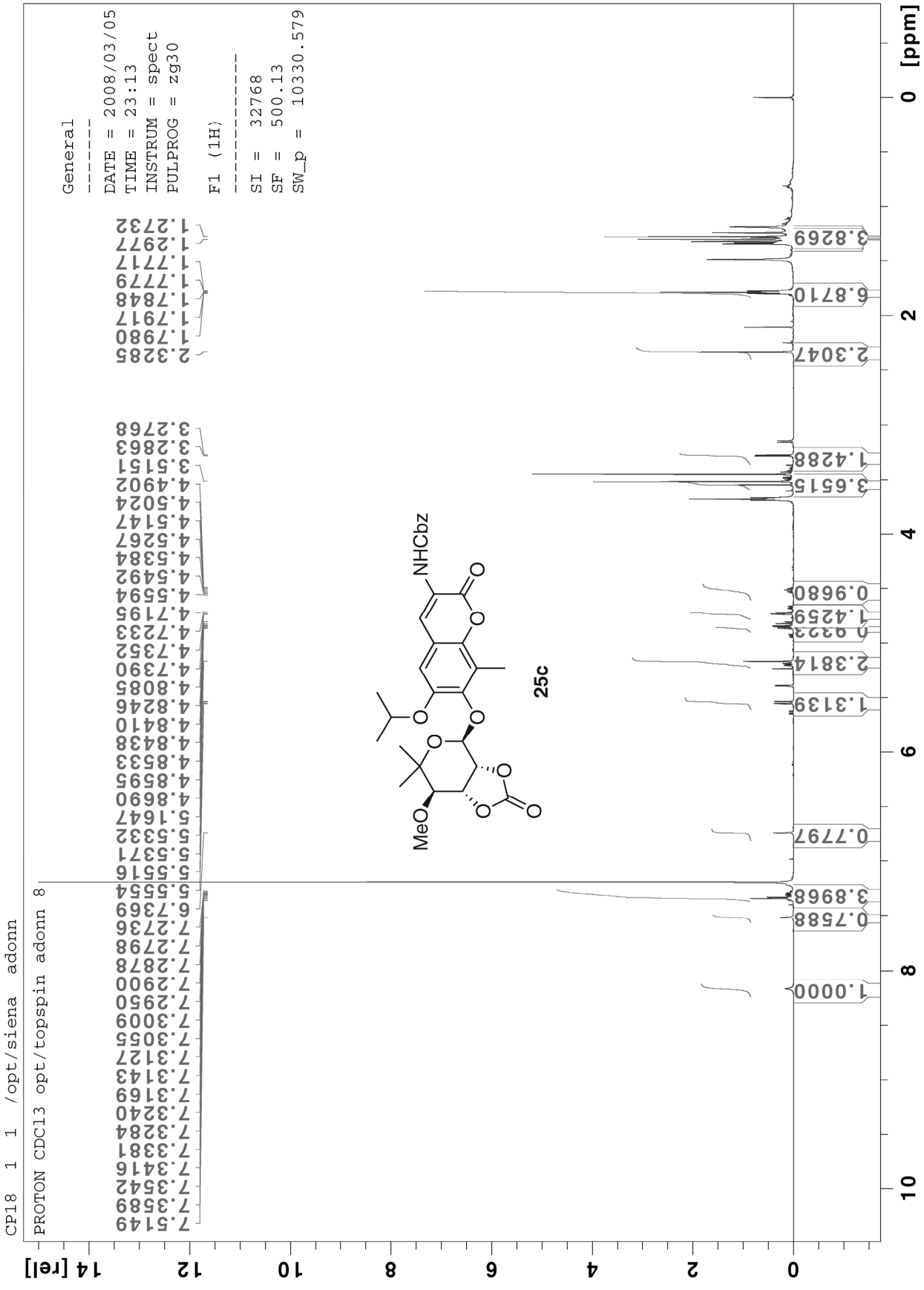

JAB_Et_coum 1 1 /opt/siena jburlis
C13CPD DMSO opt/topspin jburlis 8
General
DATE = 2007/04/17
TIME = 16:03
SPECTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
206.4955
158.0190
157.1392
153.7931
149.4759
136.4369
128.3757
127.9393
127.7556
127.2447
125.8185
120.3658
116.5989
112.7676
111.3598
66.0587
40.0687
39.9814
39.9007
39.8140
39.7326
39.6466
39.5648
39.4792
39.3969
39.3117
39.1442
38.9767
30.6746
NHCbz
O
O
HO
23h
[rel]
8
6
4
2
0
200
150
100
50
0 [ppm]

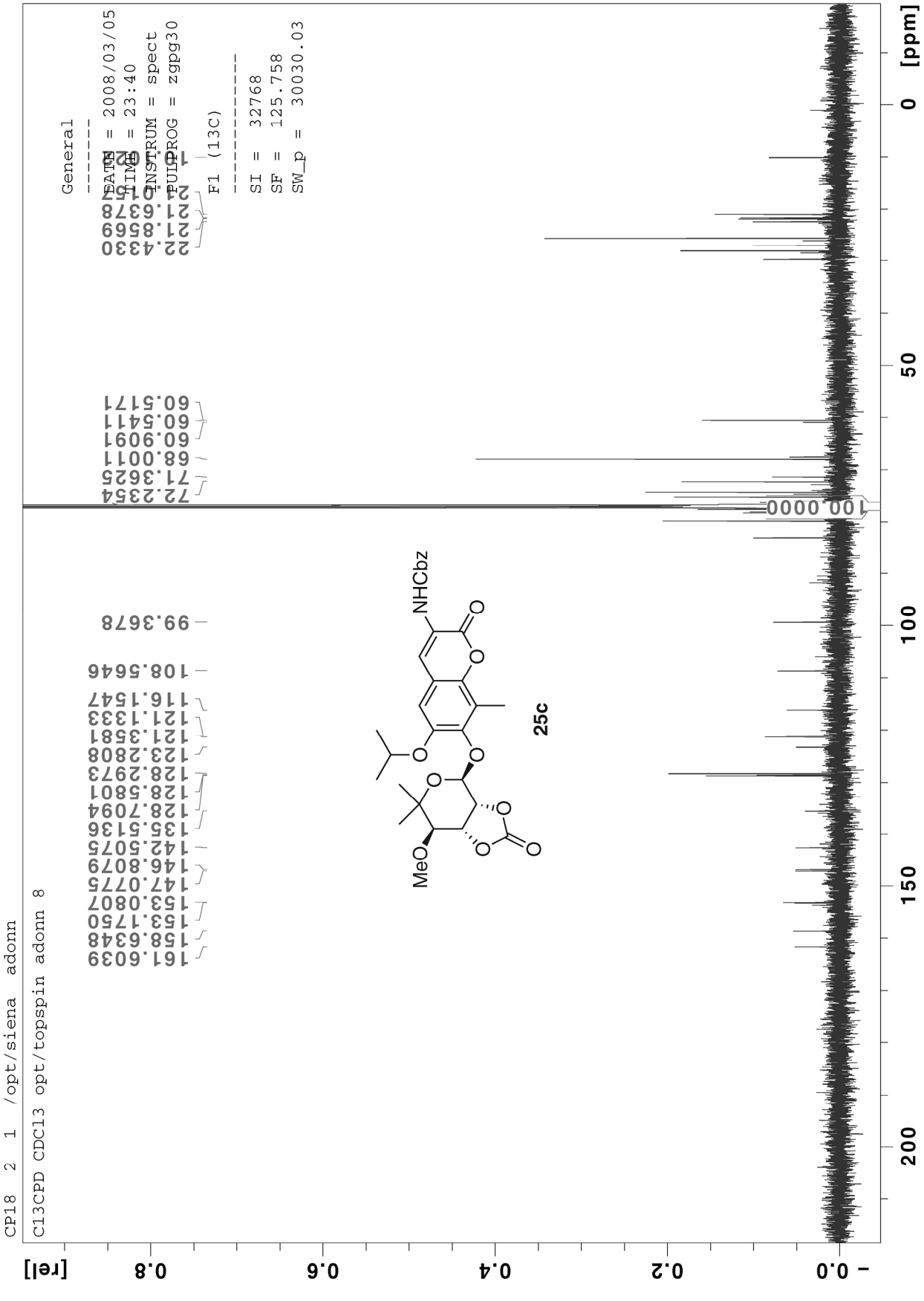

"OMe-coumarin (B) noviose" 1 1 /opt/florence adonnelly
General
DATE = 2007/02/06
TIME = 10:02
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
MeO
25a
[rel]
[ppm]

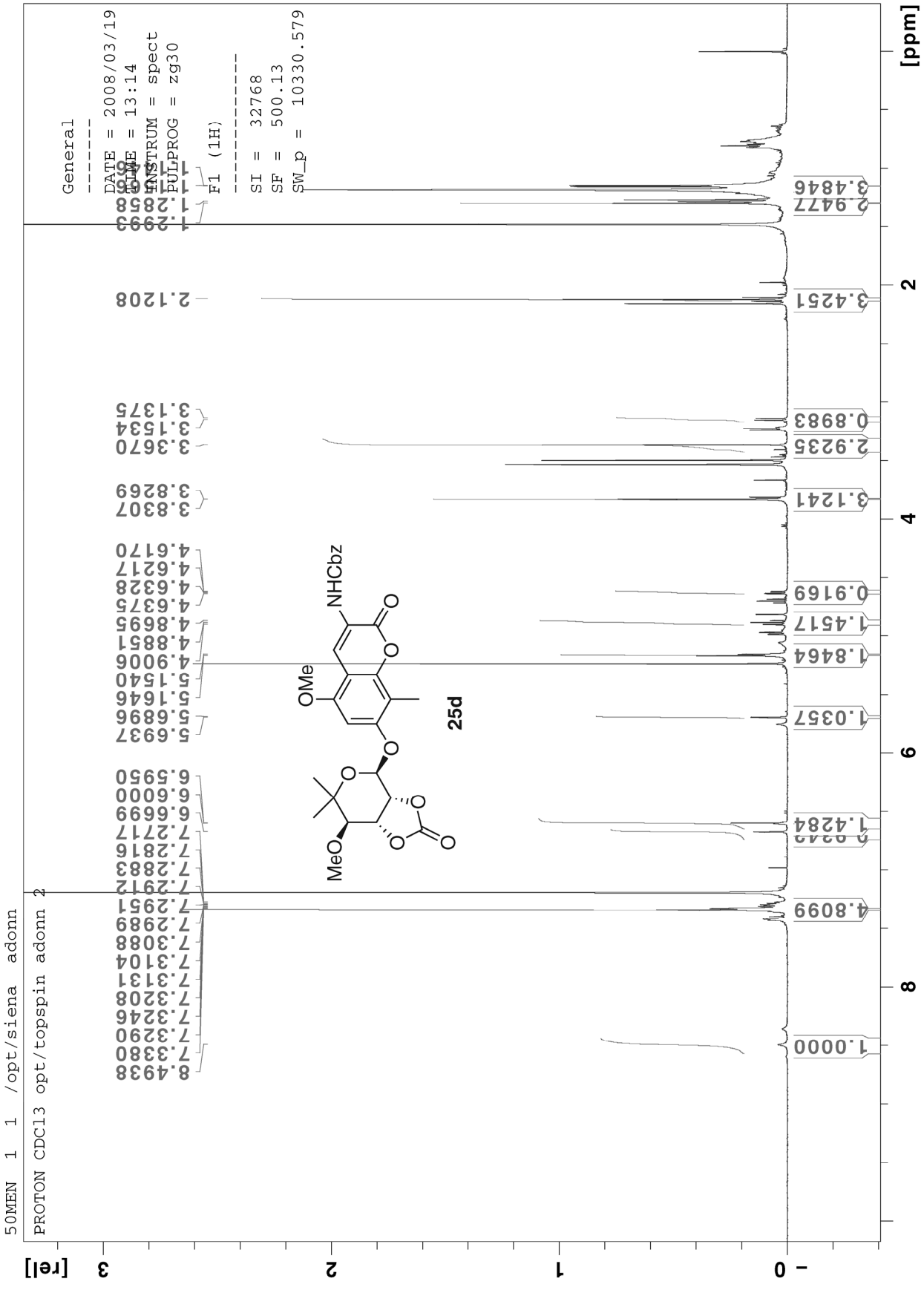

CP17 1 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 19
General
DATE = 2008/04/13
TIME = 11:15
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
21.4565
55.1080
59.4130
66.5286
82.0086
98.3118
105.2354
109.6049
115.0717
119.8086
120.2330
122.3310
127.2602
127.5396
127.6651
134.4584
141.7671
144.7480
148.0977
151.3123
152.0981
152.6592
157.5497
100.0000
NHCbz
MeO
25a
[rel]
1.5
1.0
0.5
0.0
[ppm]
0
50
100
150
200

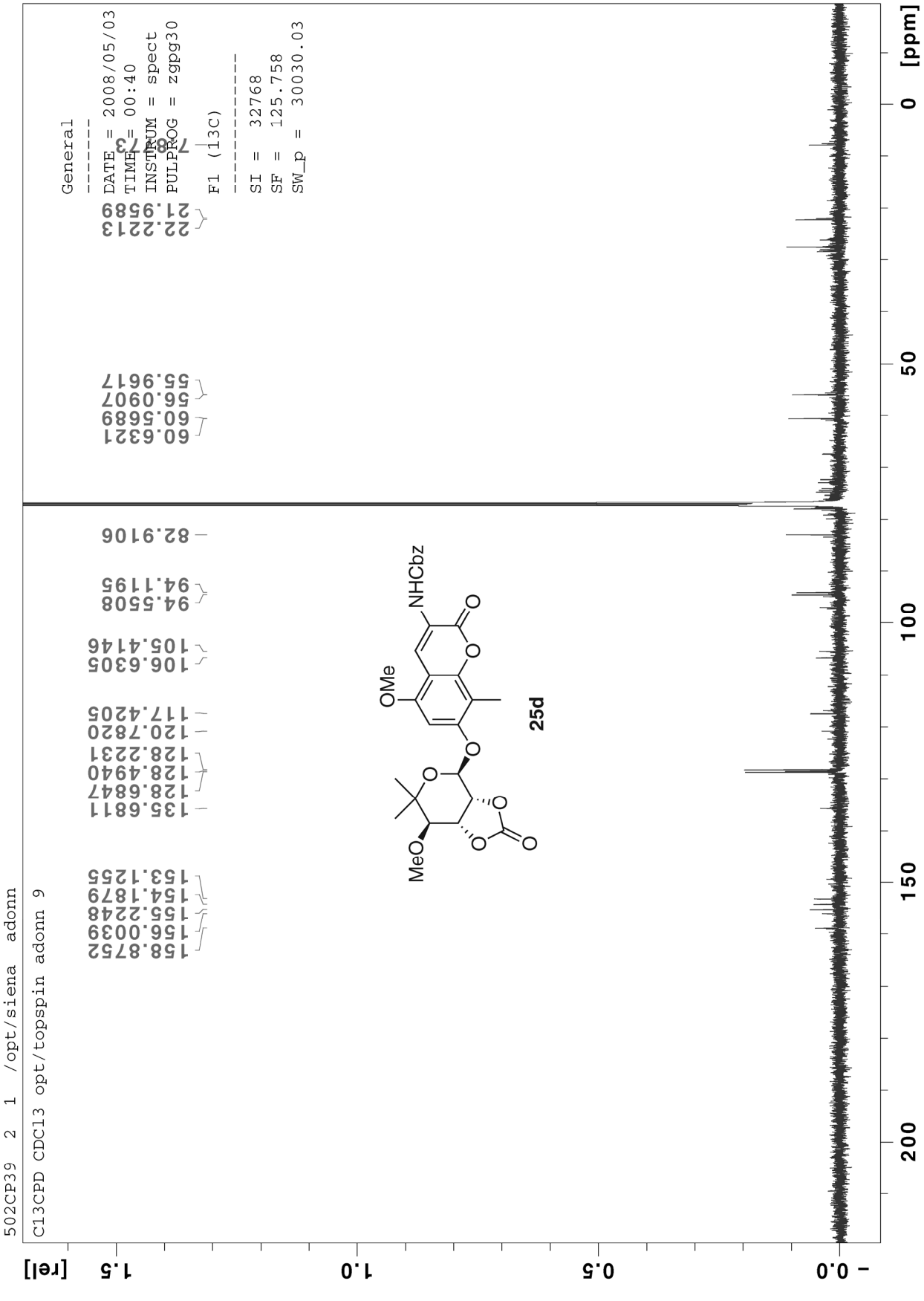

CP19F 1 1 /opt/siena adonn
PROTON CDCl3 opt/topspin adonn 14
General
DATE = 2008/05/07
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
8.1726
7.3460
7.3399
7.3346
7.3299
7.3223
7.3177
7.3109
7.3081
7.3060
7.2971
7.2938
7.2883
7.2837
7.2811
7.2736
6.8436
5.9642
5.1546
4.9968
4.9818
4.5947
4.5753
4.2343
4.2151
3.9871
3.9739
3.9608
3.8167
3.8069
3.8017
3.7894
3.7869
3.7799
3.7547
3.3749
1.8404
1.8333
1.8265
1.8200
1.8124
1.8053
1.7919
1.4071
1.3045
0.9888
1.1264
5.2184
1.0000
0.9825
2.2547
1.1425
0.9057
1.1174
1.1578
3.3897
2.2107
2.7657
2.8760
NHCbz
MeO
25b
[ppm]
[rel]

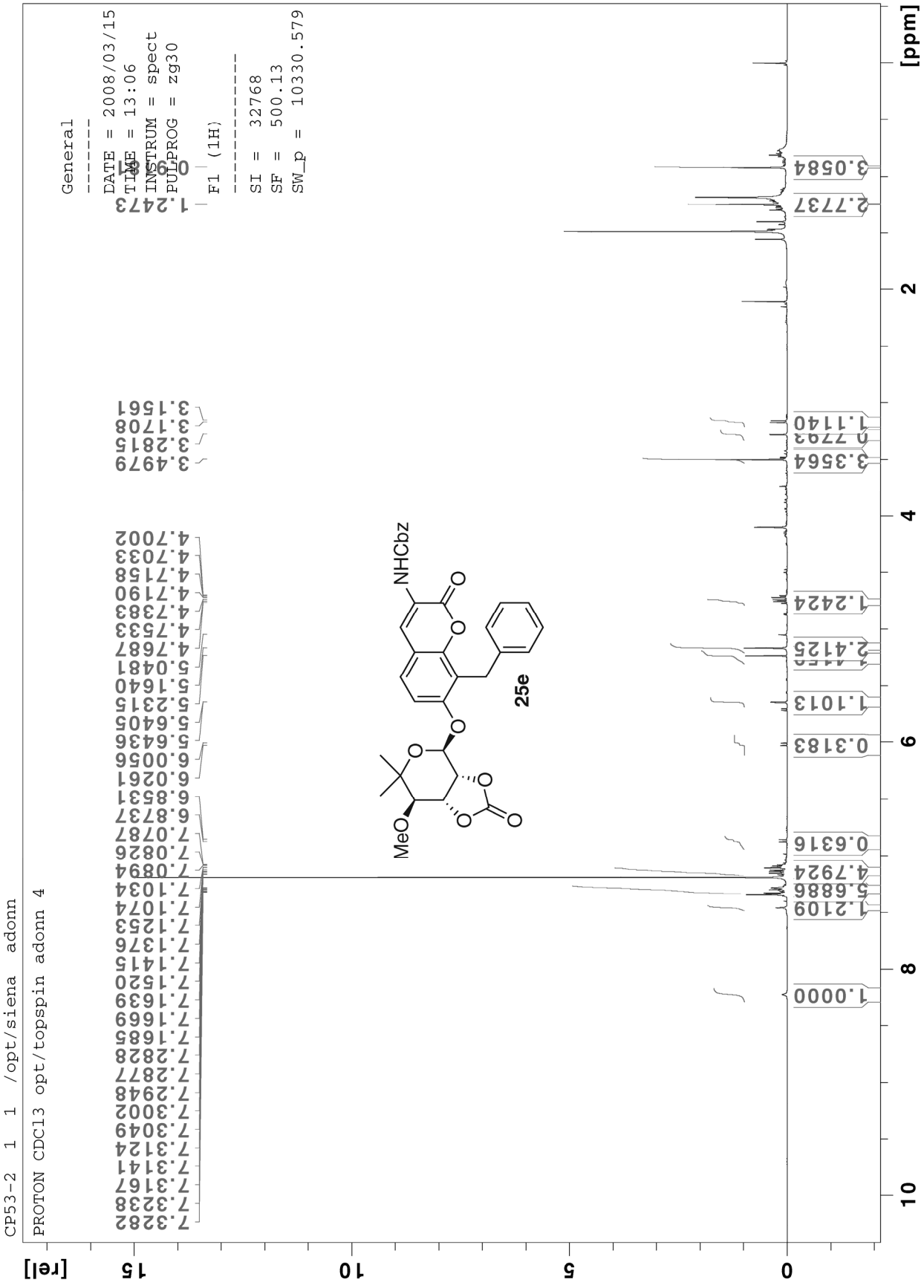

CP19F 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 14
General
DATE = 2008/05/07
TIME = 03:32
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
157.7476
154.2457
152.1825
151.7862
146.7327
144.1665
142.8527
134.5728
127.6379
127.5413
127.4678
127.1795
127.1281
120.9468
120.8881
111.1018
106.9942
105.3008
101.6424
85.6677
80.0157
69.8111
59.6237
58.1154
54.7774
22.4406
21.7792
21.3496
NHCbz
MeO
25b
[rel]
[ppm]

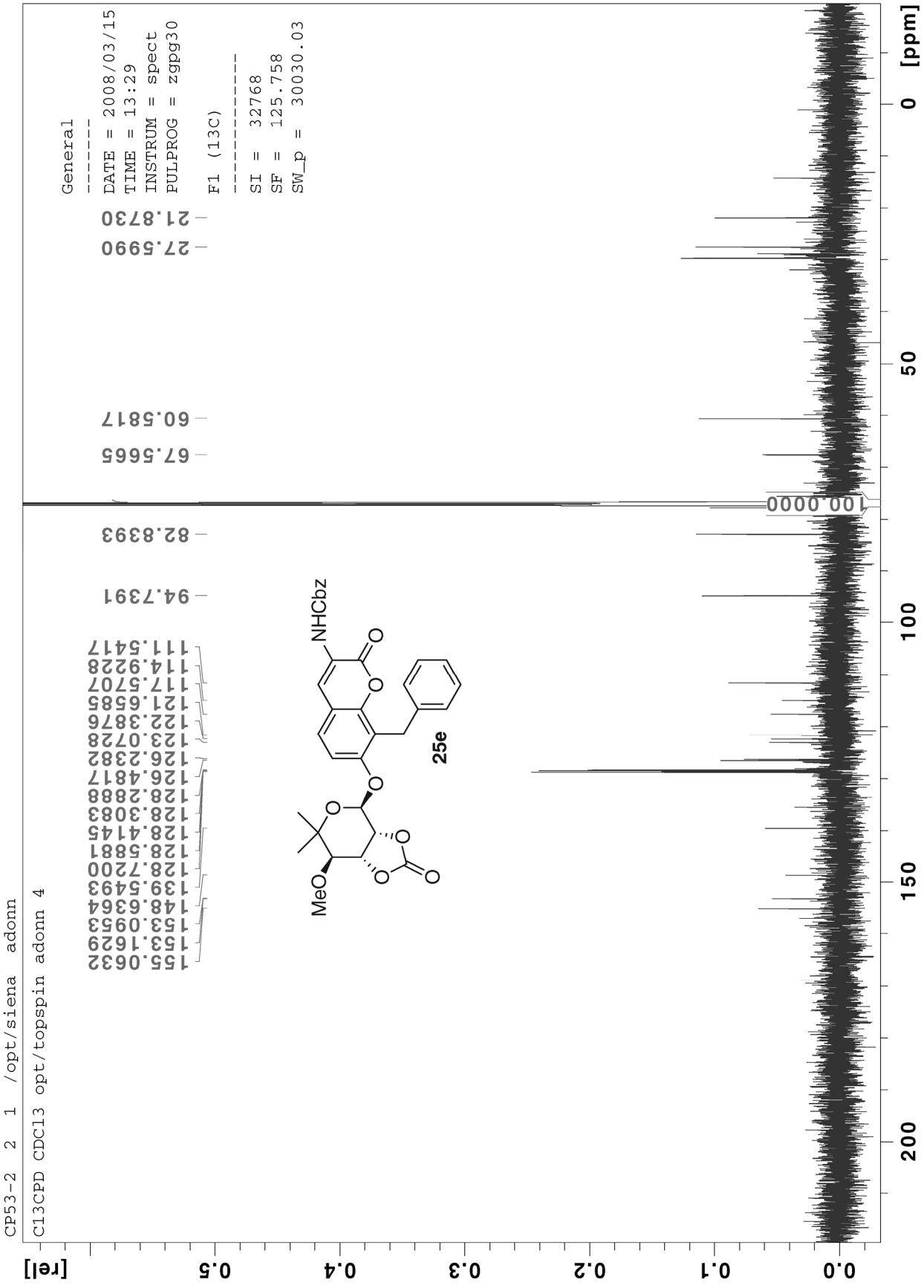

CP18 1 1 /opt/siena adonn
PROTON CDCl3 opt/topspin adonn 8
General
DATE = 2008/03/05
TIME = 23:13
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
NHCbz
MeO
25c
[rel]
[ppm]

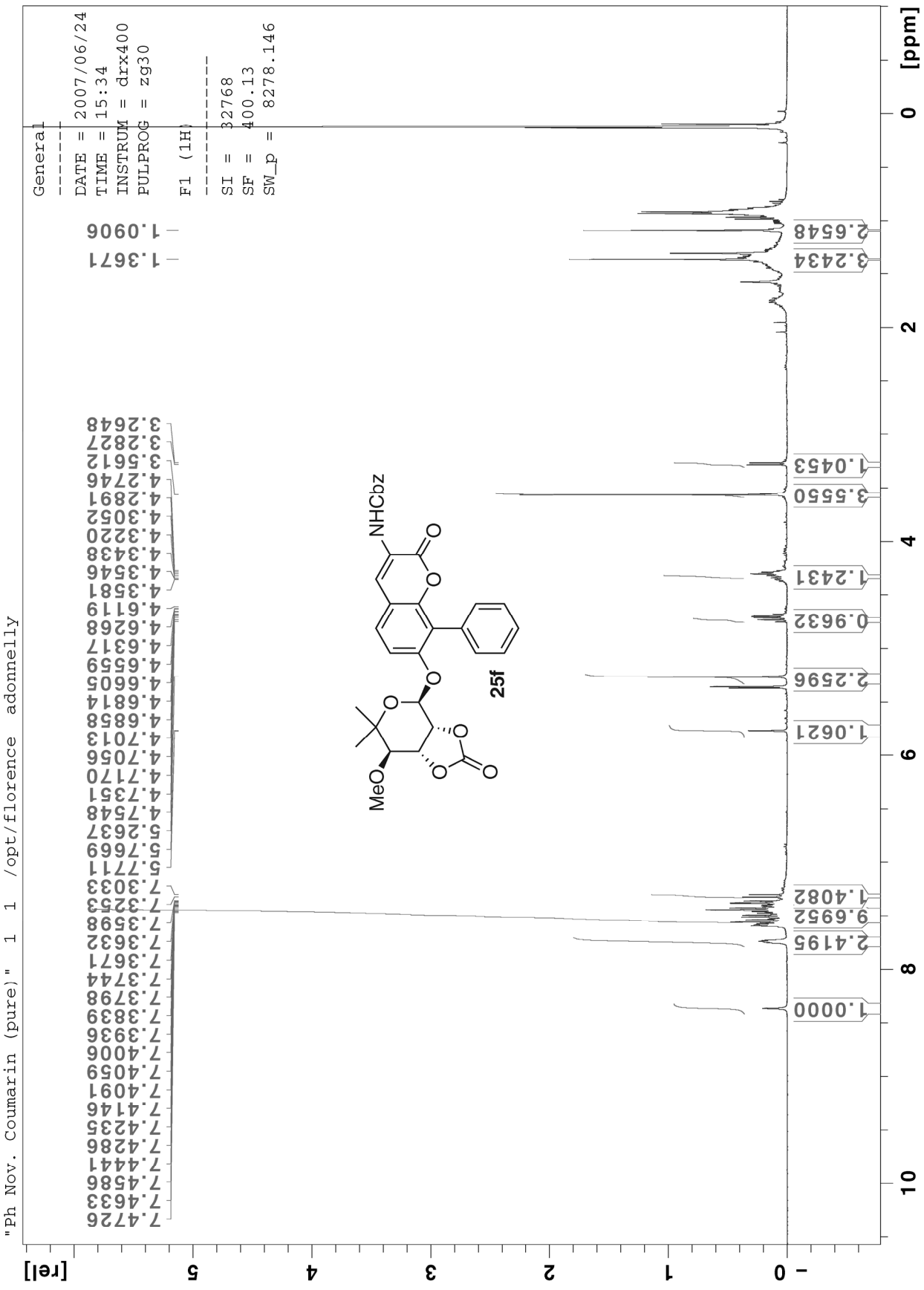

CP18 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 8
General
DATA = 2008/03/05
TIME = 23:40
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
22.4330
21.8569
21.6378
21.0157
72.2354
71.3625
68.0011
60.9091
60.5411
60.5171
99.3678
108.5646
116.1547
121.1333
121.3581
123.2808
128.2973
128.5801
128.7094
135.5136
142.5075
146.8079
147.0775
153.0807
153.1750
158.6348
161.6039
100.0000
NHCbz
MeO
25c
[rel]
0.8
0.6
0.4
0.2
0.0
200
150
100
50
0
[ppm]

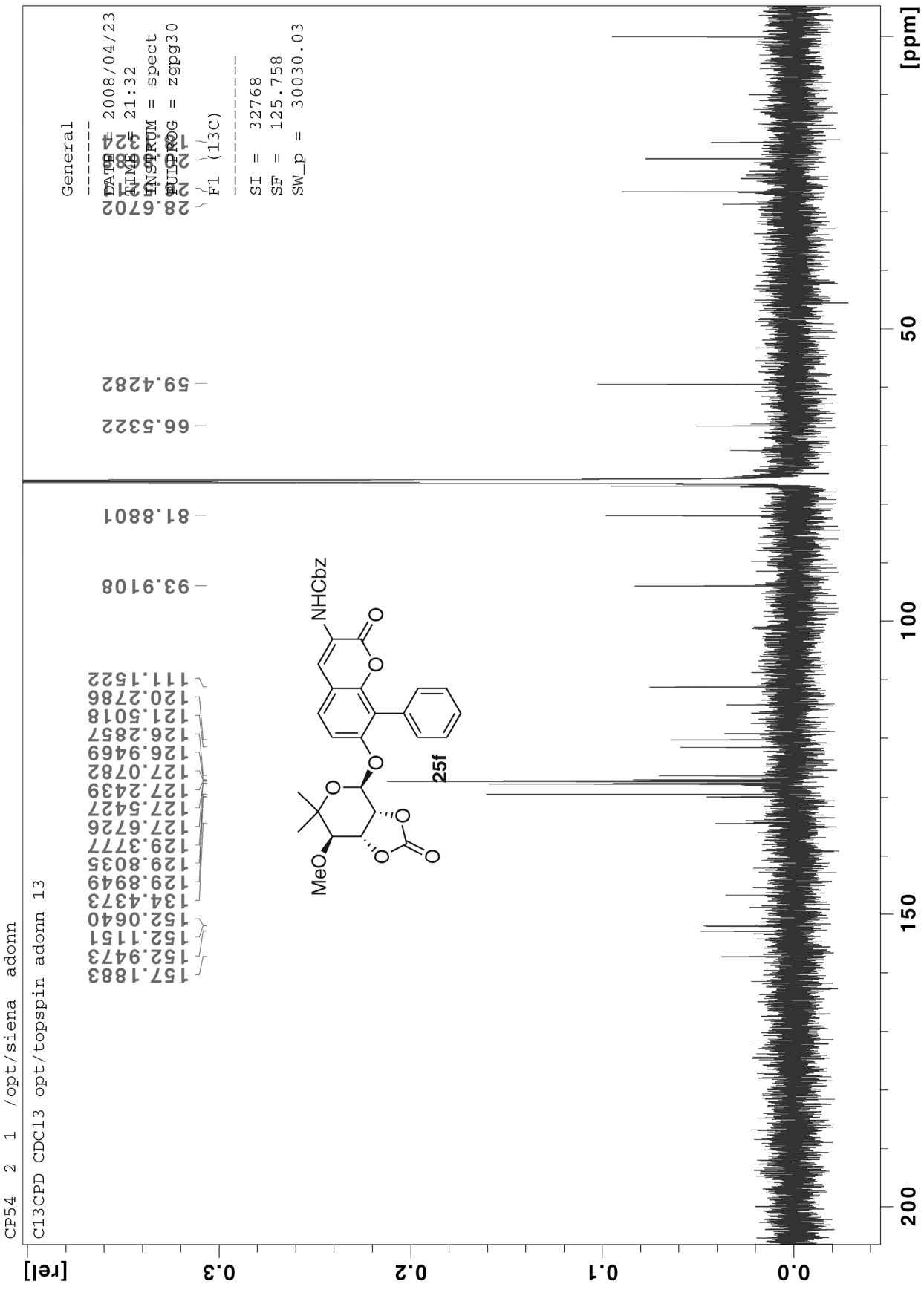

50MEN 1 1 /opt/siena adonn
PROTON CDC13 opt/topspin adonn 2
General
DATE = 2008/03/19
TIME = 13:14
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
NHCbz
OMe
MeO
25d
[rel]
[ppm]

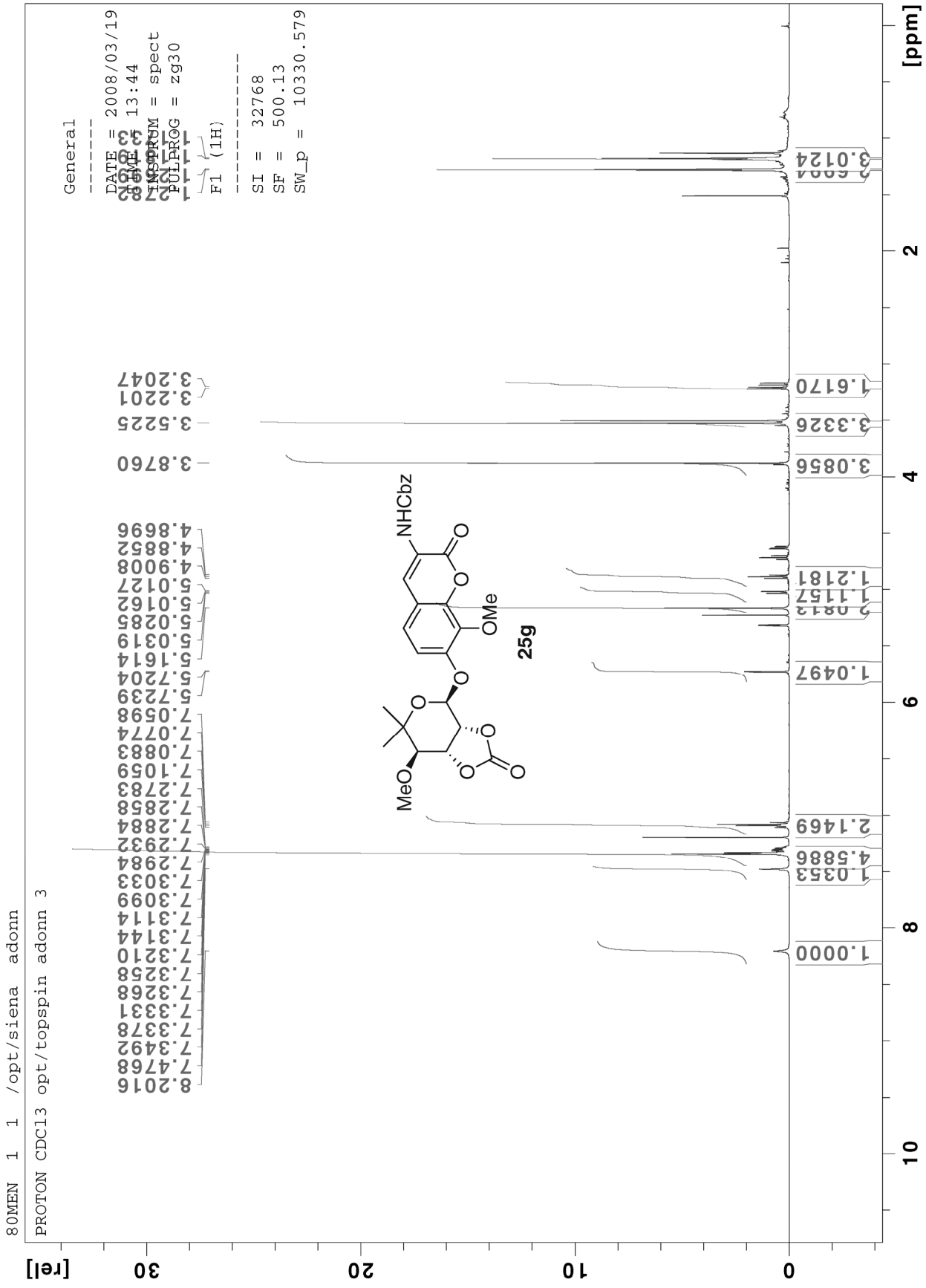

502CP39 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 9
General
DATE = 2008/05/03
TIME = 00:40
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
158.8752
156.0039
155.2248
154.1879
153.1255
135.6811
128.6847
128.4940
128.2231
120.7820
117.4205
106.6305
105.4146
94.5508
94.1195
82.9106
77.3
76.8
60.6321
60.5689
56.0907
55.9617
22.2213
21.9589
NHCbz
OMe
MeO
25d
[rel]
1.5
1.0
0.5
0.0
200
150
100
50
0 [ppm]

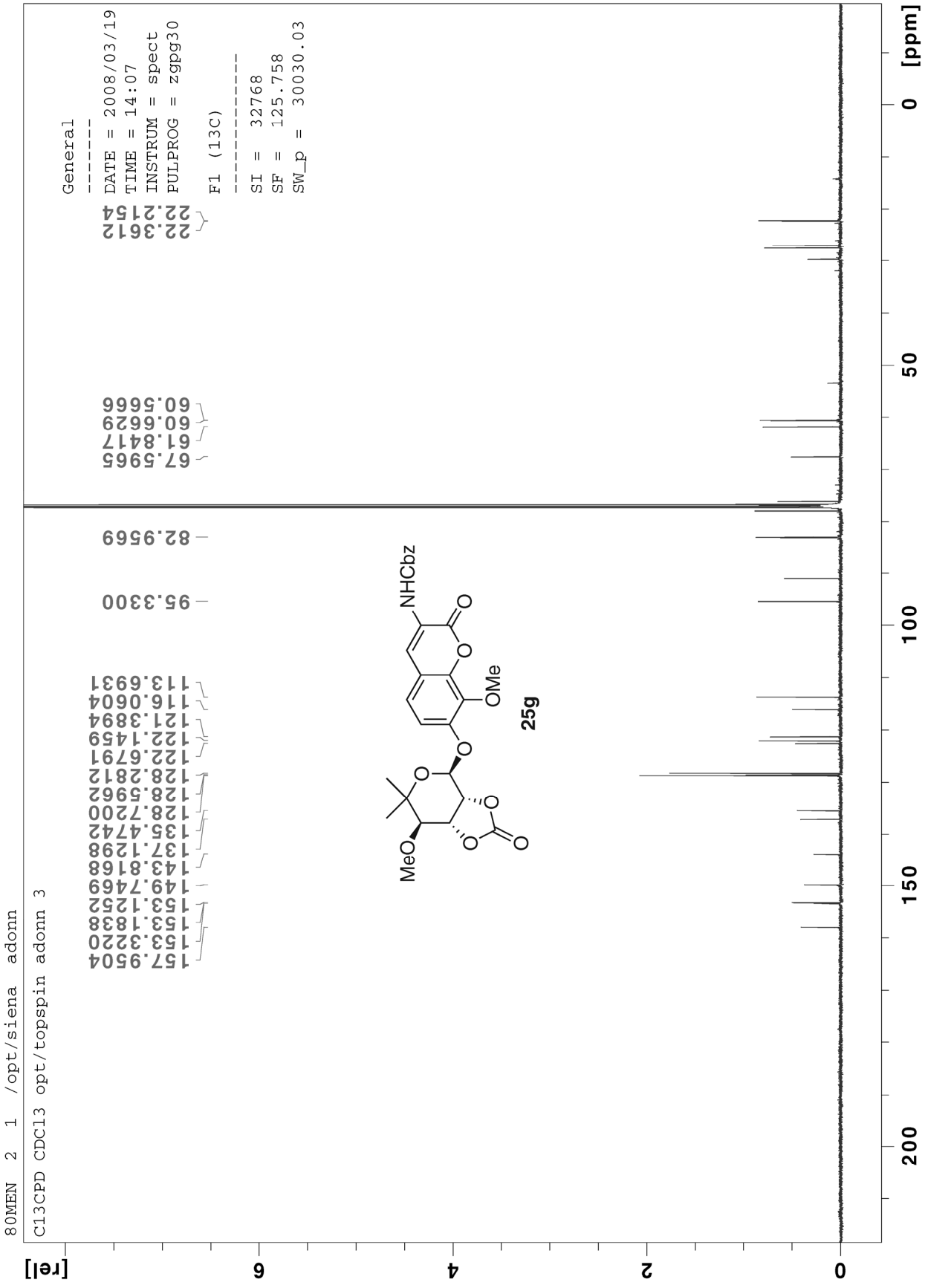

CP53-2 1 1 /opt/siena adonn
PROTON CDCl3 opt/topspin adonn 4
General
DATE = 2008/03/15
TIME = 13:06
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
NHCbz
MeO
25e
[rel]
[ppm]

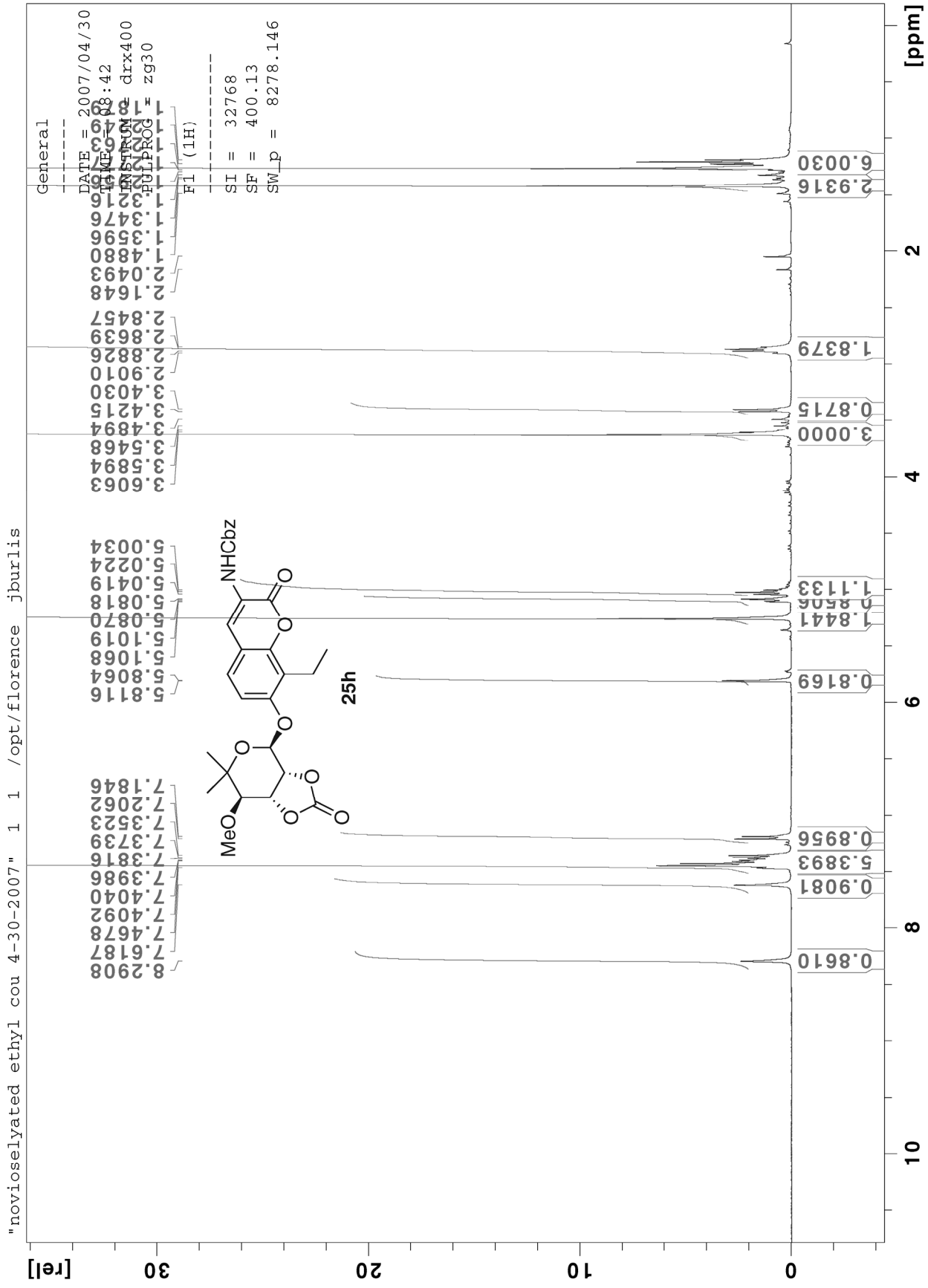

CP53-2 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 4
General
DATE = 2008/03/15
TIME = 13:29
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
155.0632
153.1629
153.0953
148.6364
139.5493
128.7200
128.5881
128.4145
128.3083
128.2888
126.4817
126.2382
123.0728
122.3876
121.6585
117.5707
114.9228
111.5417
94.7391
82.8393
67.5665
60.5817
27.5990
21.8730
100.0000
NHCbz
MeO
25e
[rel]
0.0
0.1
0.2
0.3
0.4
0.5
200
150
100
50
0
[ppm]

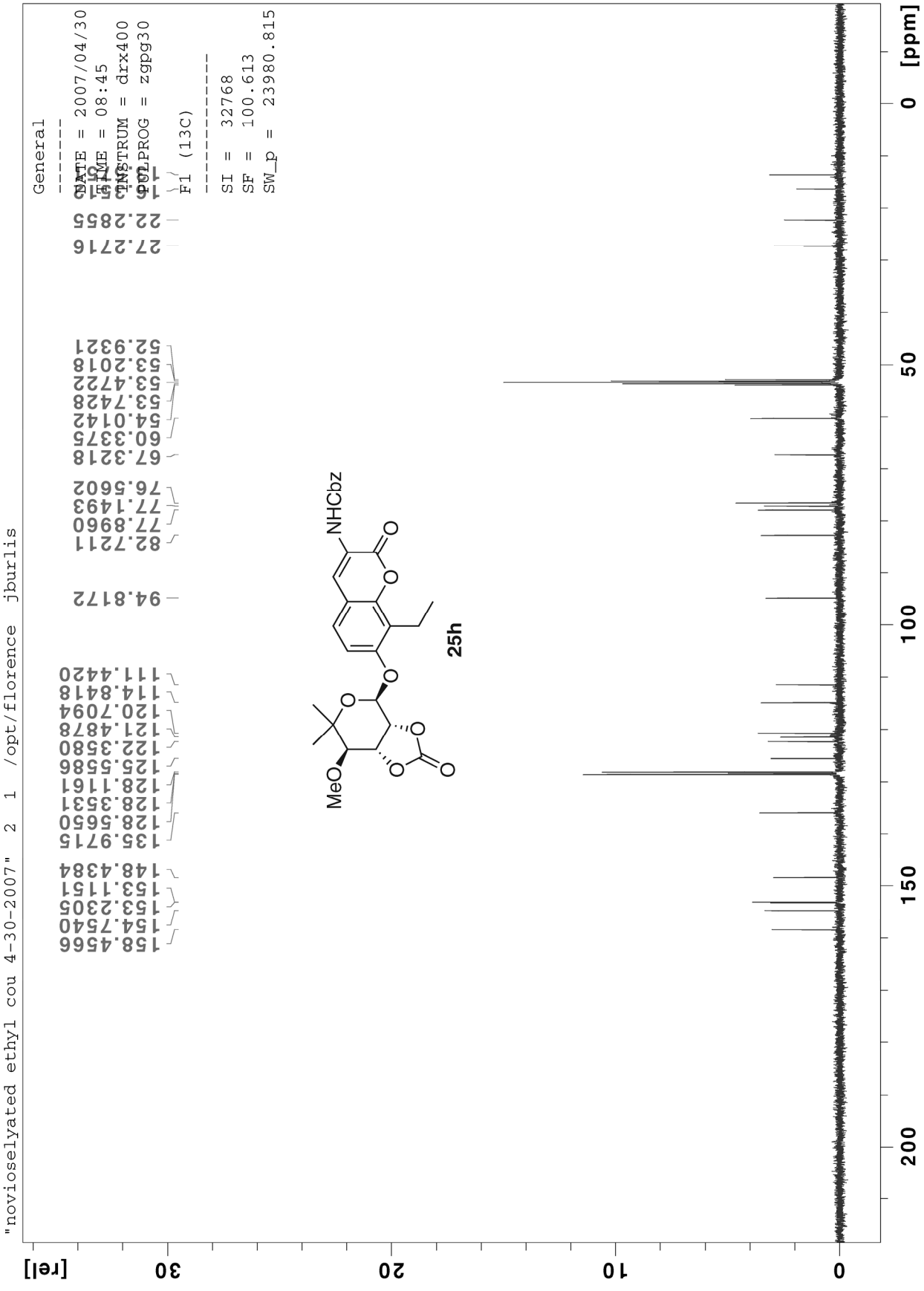

"Ph Nov. Coumarin (pure)" 1 1 /opt/florence adonnelly
General
DATE = 2007/06/24
TIME = 15:34
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
MeO
25f
[rel]
[ppm]
1.0000
2.4195
9.6952
1.4082
2.2596
0.9632
1.2431
3.5550
1.0453
3.2434
2.6548
1.0621
1.0906
1.3671

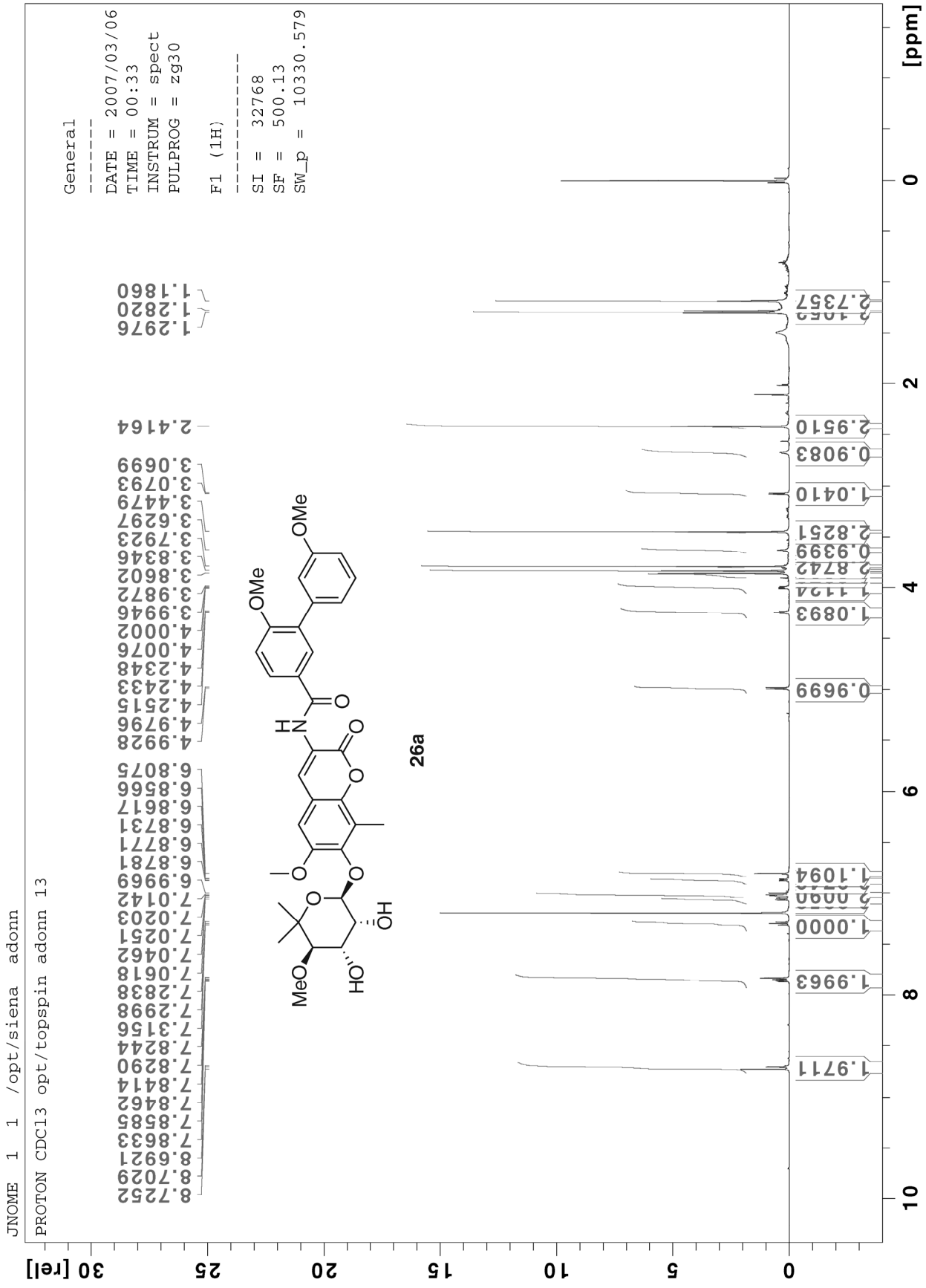

CP54 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 13
General
SI = 32768
SF = 125.758
SW_p = 30030.03
NHCbz
MeO
25f
[rel]
[ppm]
0.0
0.1
0.2
0.3
50
100
150
200

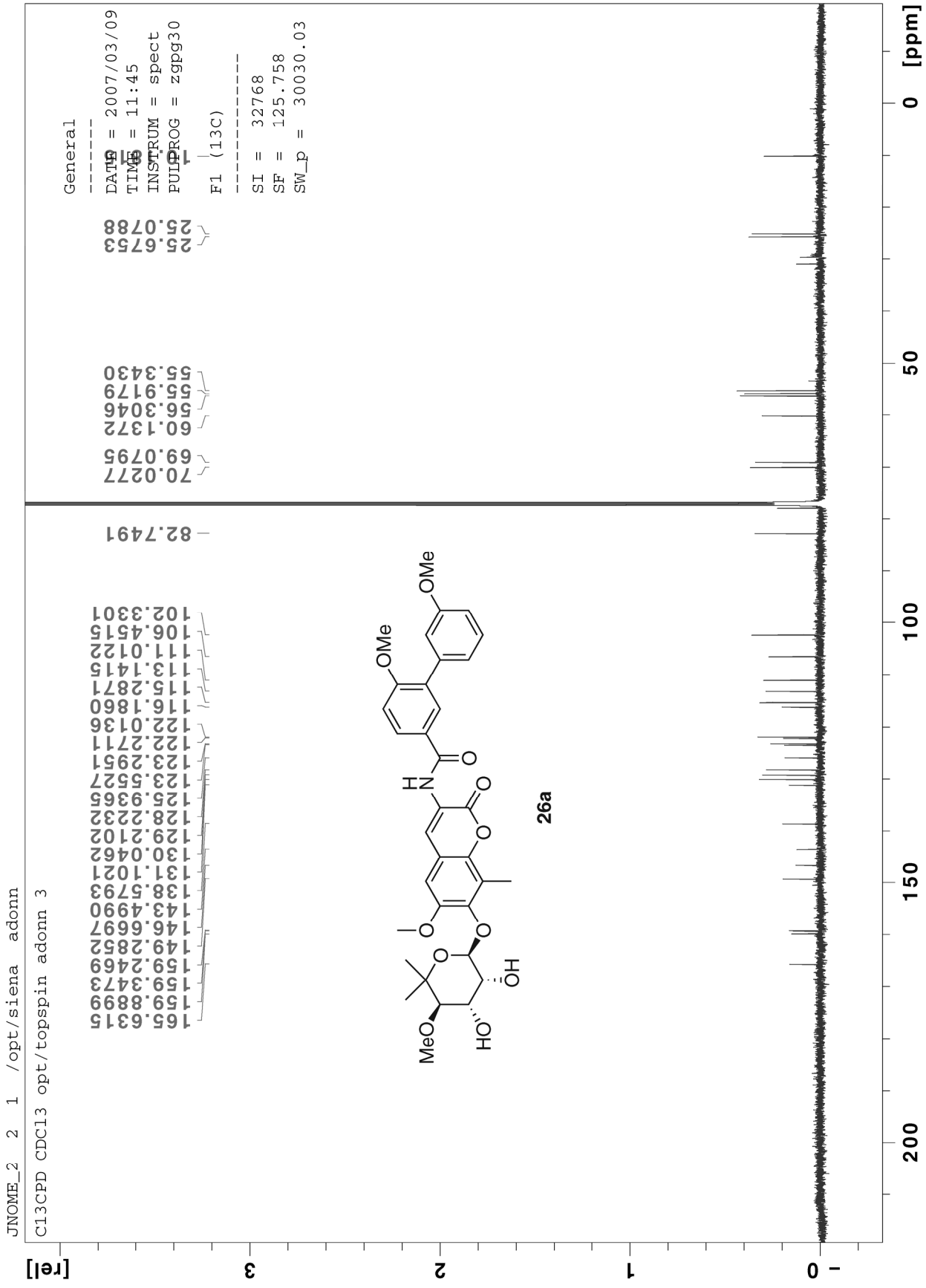

80MEN 1 1 /opt/siena adonn
PROTON CDC13 opt/topspin adonn 3
General
DATE = 2008/03/19
TIME = 13:44
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
NHCbz
OMe
MeO
25g
[rel]
[ppm]

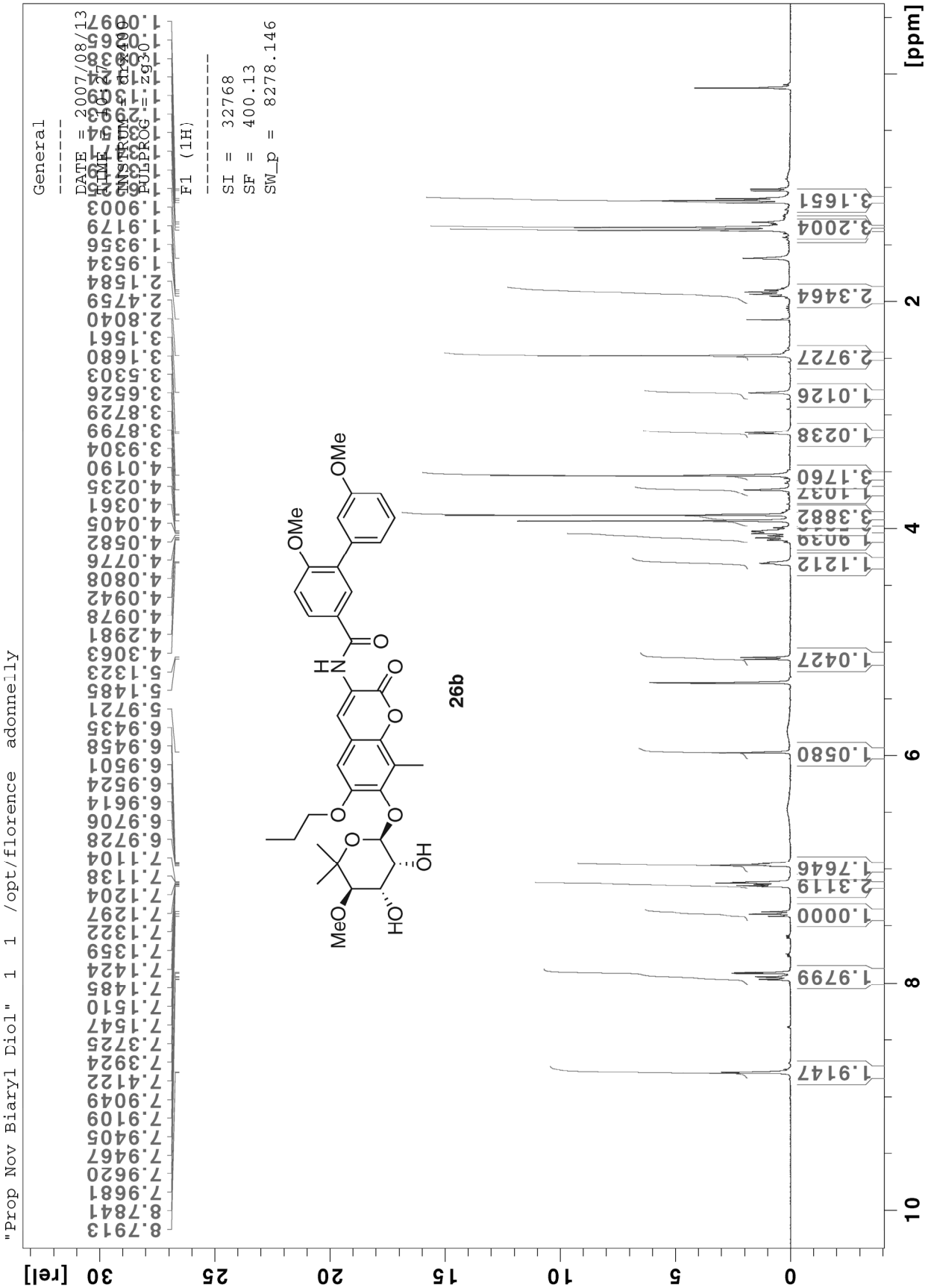

80MEN 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 3
General
DATE = 2008/03/19
TIME = 14:07
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
22.3612
22.2154
67.5965
61.8417
60.6629
60.5666
82.9569
95.3300
113.6931
116.0604
121.3894
122.1459
122.6791
128.2812
128.5962
128.7200
135.4742
137.1298
143.8168
149.7469
153.1252
153.1838
153.3220
157.9504
NHCbz
OMe
MeO
25g
[rel]
0
2
4
6
200
150
100
50
0
[ppm]

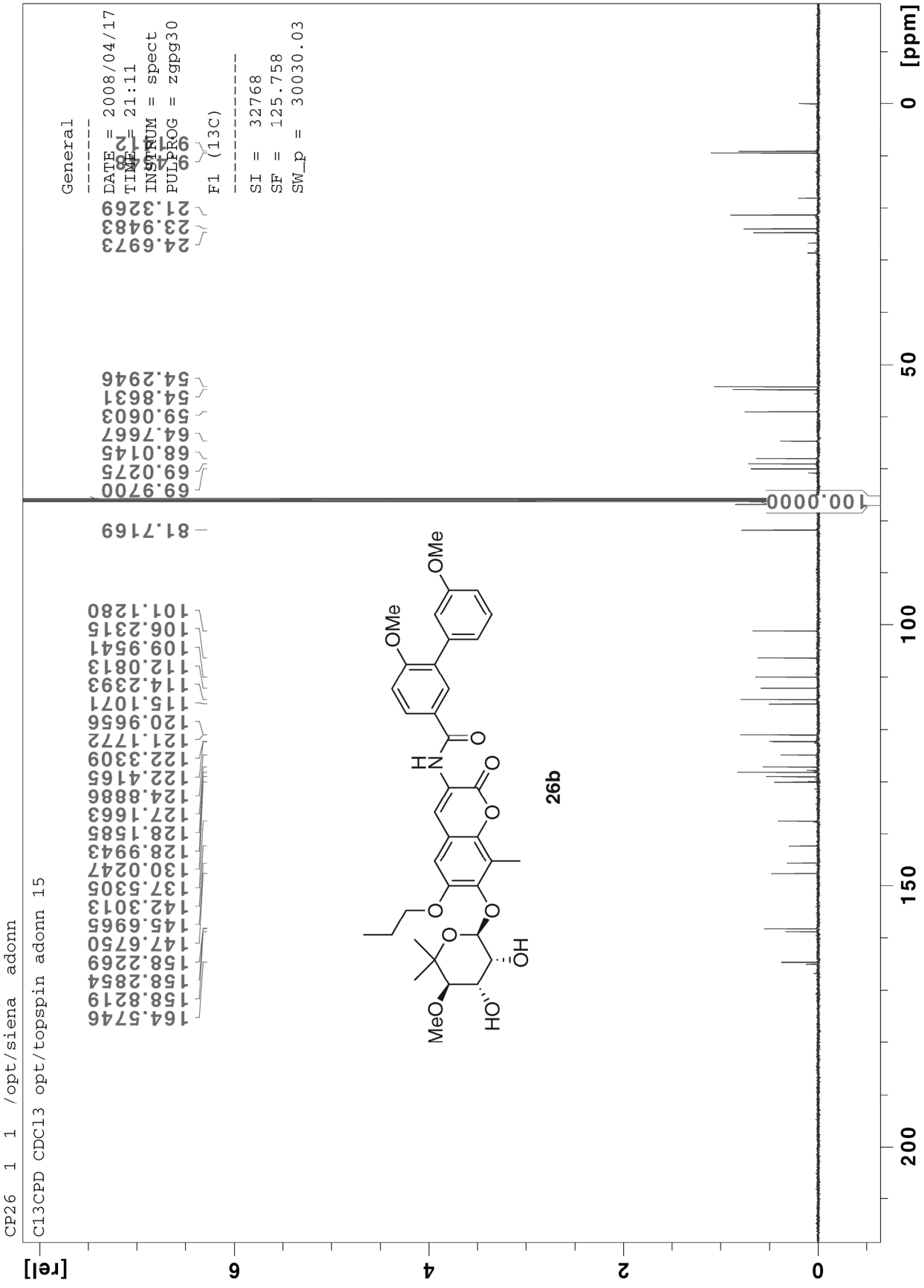

"noviosel yated ethyl cou 4-30-2007" 1 1 /opt/florence jburlis
General
DATE = 2007/04/30
TIME = 08:42
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
NHCbz
MeO
25h
[rel]
[ppm]
6.0030
2.9316
1.8379
0.8715
3.0000
1.1133
1.8441
0.8169
0.8956
5.3893
0.9081
0.8610

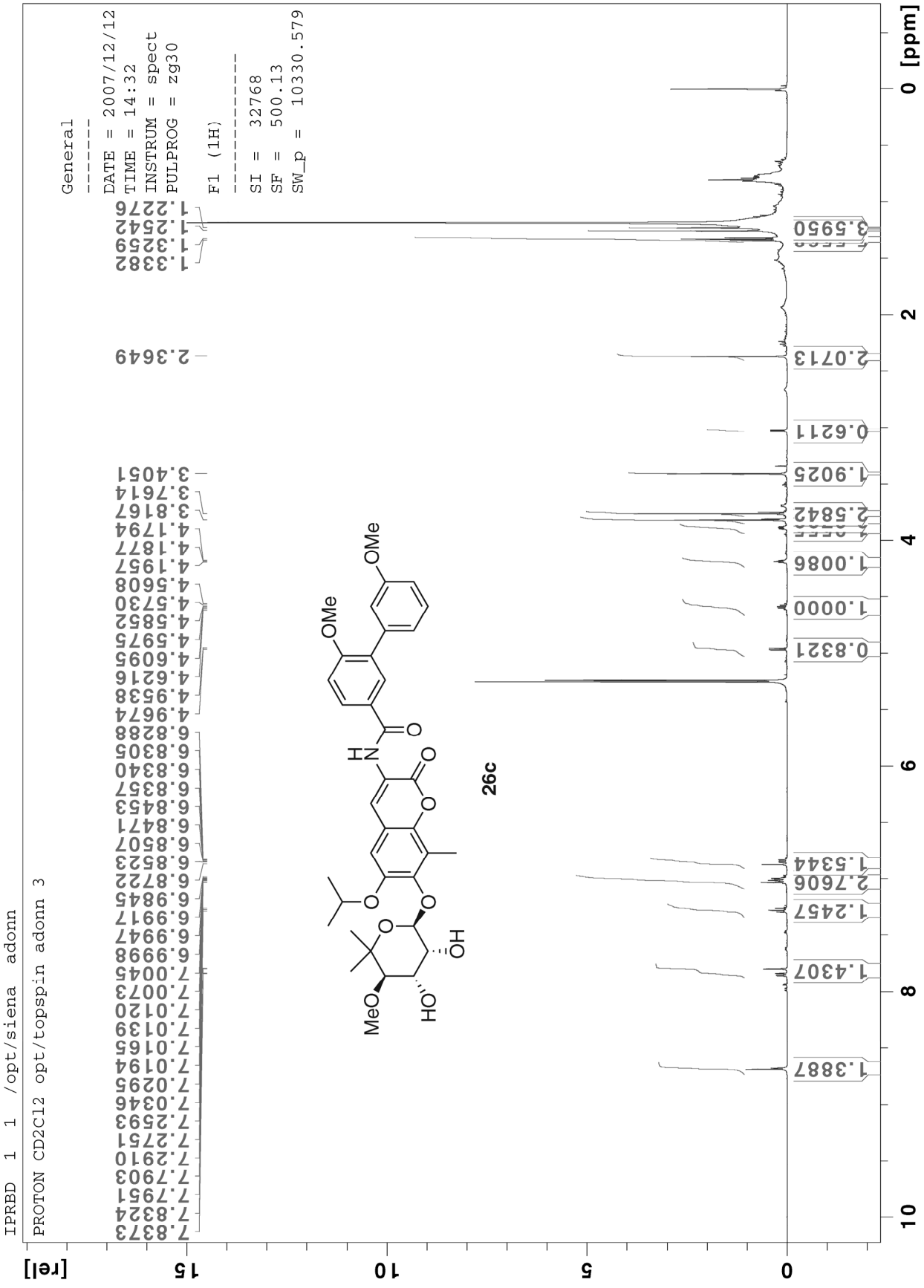

"novioselyated ethyl cou 4-30-2007" 2 1 /opt/florence jburlis
General
DATE = 2007/04/30
TIME = 08:45
INSTRUM = drx400
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 100.613
SW_p = 23980.815
158.4566
154.7540
153.2305
153.1151
148.4384
135.9715
128.5650
128.3531
128.1161
125.5586
122.3580
121.4878
120.7094
114.8418
111.4420
94.8172
82.7211
77.8960
77.1493
76.5602
67.3218
60.3375
54.0142
53.7428
53.4722
53.2018
52.9321
27.2716
22.2855
15.3551
NHCbz
MeO
25h
[rel]
30
20
10
0
200
150
100
50
0 [ppm]

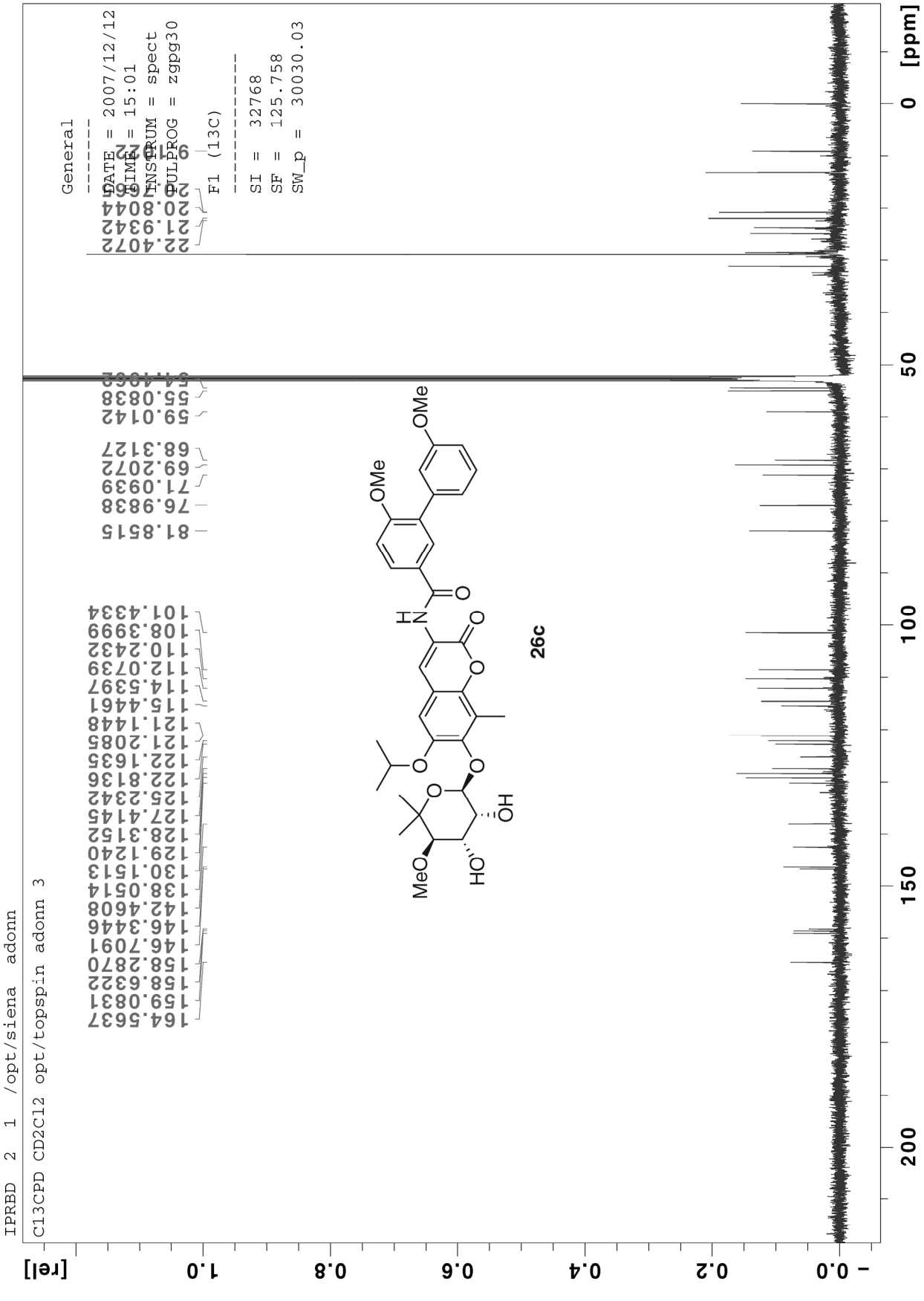

JNOME 1 1 /opt/siena adonn
PROTON CDCl3 opt/topspin adonn 13
General
DATE = 2007/03/06
TIME = 00:33
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
26a
OMe
OMe
MeO
HO
OH
[rel]
[ppm]

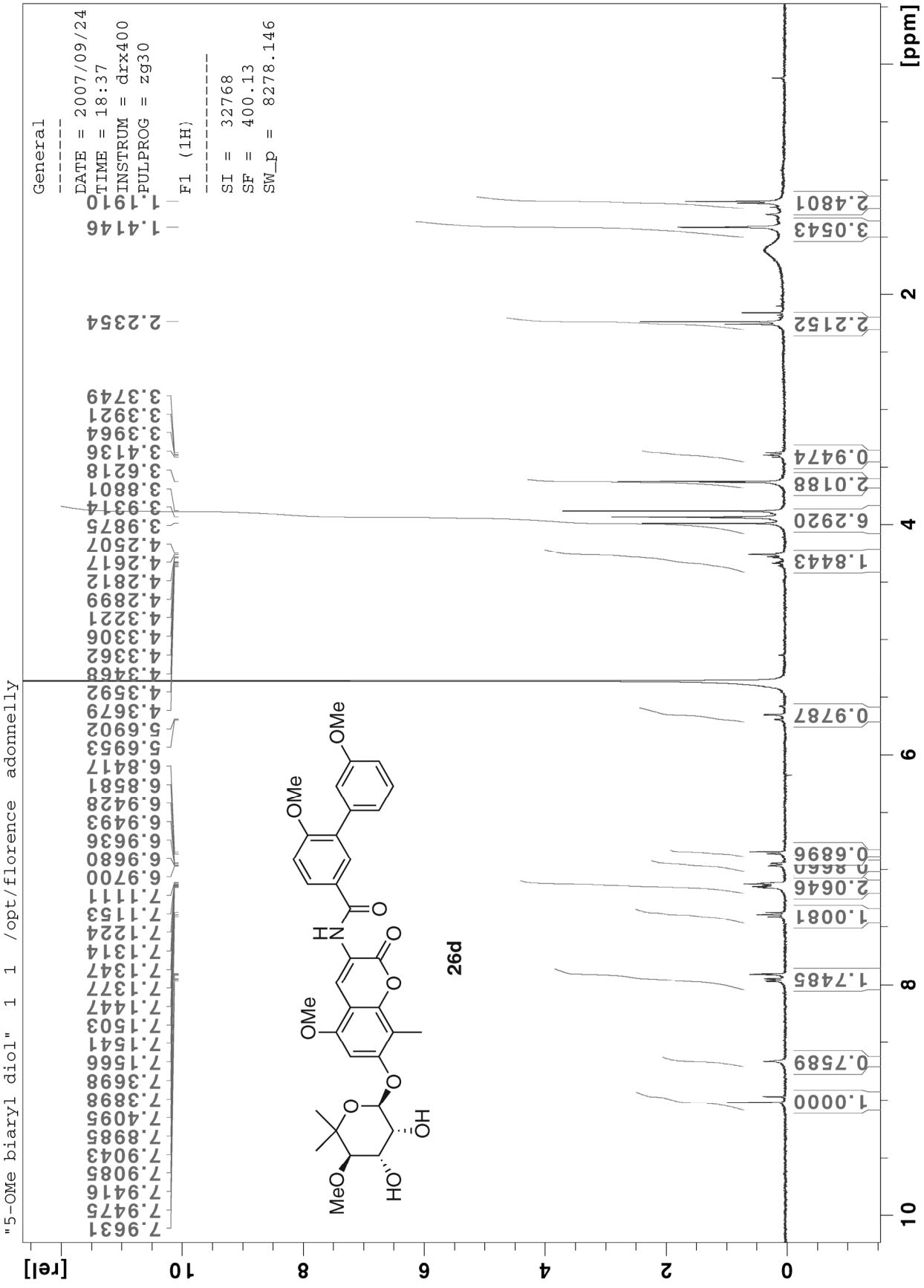

JNOME_2 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 3
General
DATE = 2007/03/09
TIME = 11:45
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
25.0788
25.6753
55.3430
55.9179
56.3046
60.1372
69.0795
70.0277
82.7491
102.3301
106.4515
111.0122
113.1415
115.2871
116.1860
122.0136
122.2711
123.2951
123.5527
125.9365
128.2232
129.2102
130.0462
131.1021
138.5793
143.4990
146.6697
149.2852
159.2469
159.3473
159.8899
165.6315
OMe
OMe
N
H
O
O
O
O
O
O
MeO
HO
OH
26a
[rel]
3
2
1
0
200
150
100
50
0 [ppm]

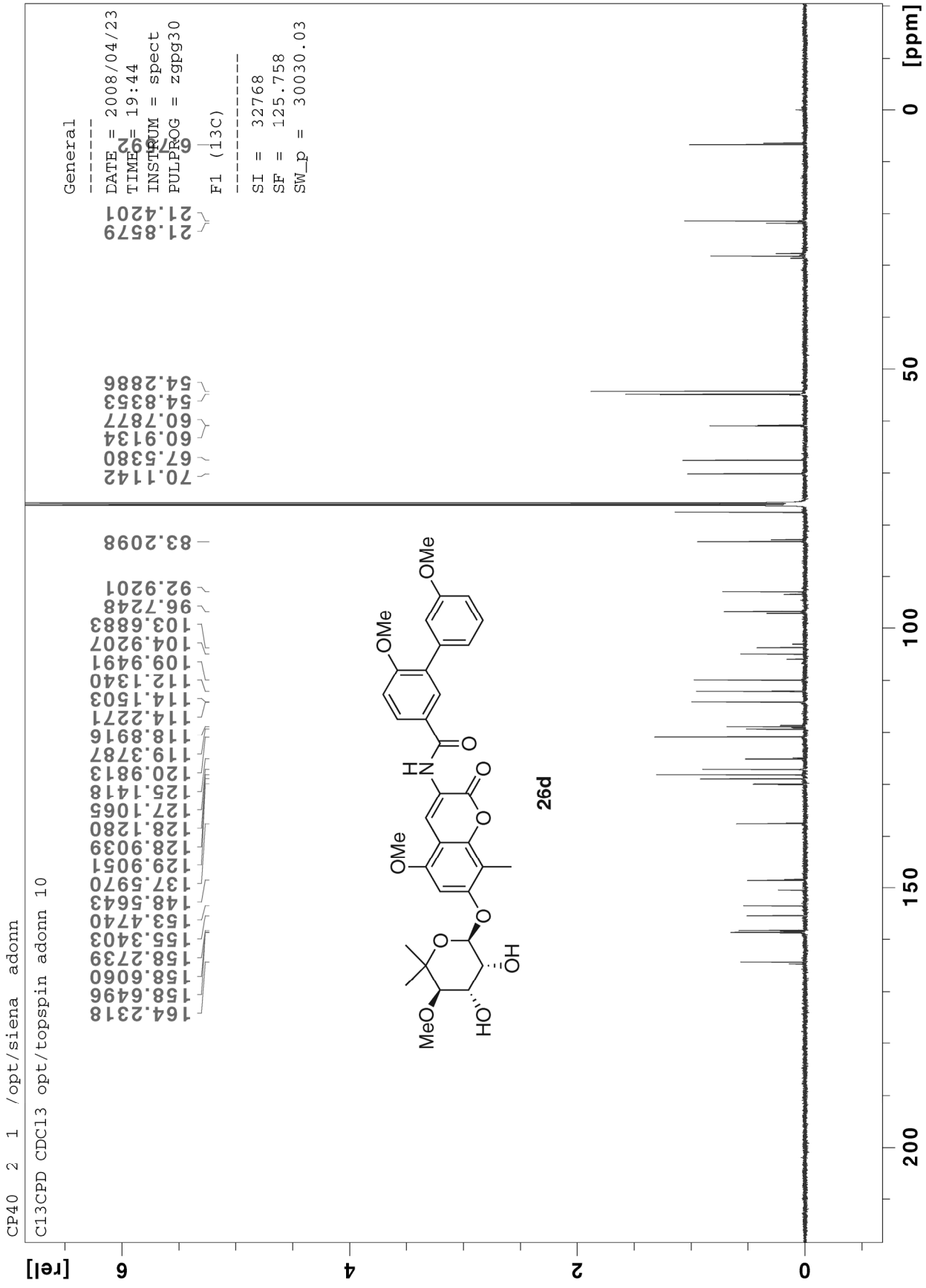

"Prop Nov Biaryl Diol" 1 1 /opt/florence adonnelly
General
DATE = 2007/08/13
SI = 32768
SF = 400.13
SW_p = 8278.146
F1 (1H)
26b
OMe
OMe
MeO
OH
OH
[rel]
[ppm]
1.9147
1.9799
1.0000
2.3119
1.7646
1.0580
1.0427
1.1212
3.3882
3.1760
1.0238
1.0126
2.9727
2.3464
3.2004
3.1651

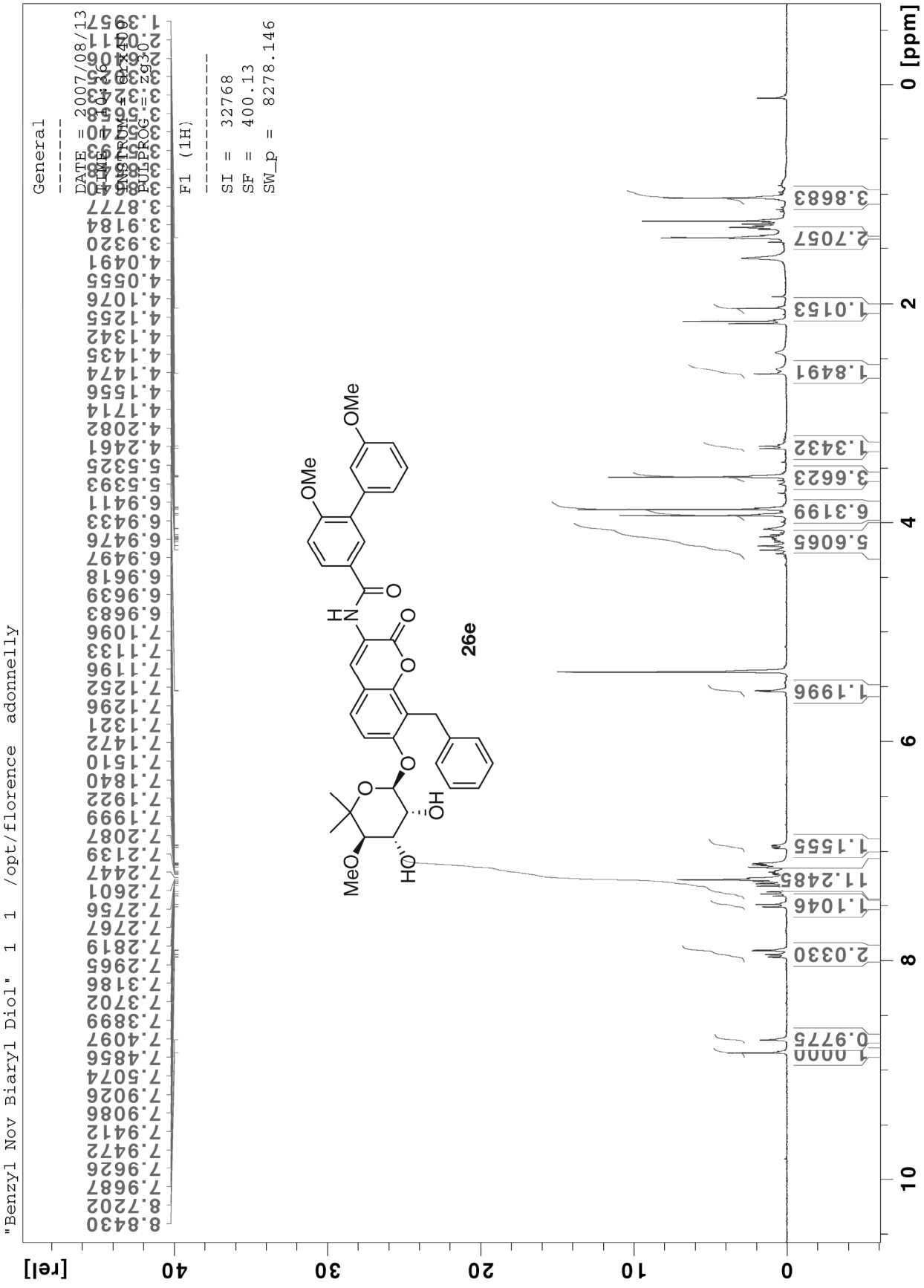

CP26 1 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 15
General
DATE = 2008/04/17
TIME = 21:11
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
164.5746
158.8219
158.2854
158.2269
147.6750
145.6965
142.3013
137.5305
130.0247
128.9943
128.1585
127.1663
124.8886
122.4165
122.3309
121.1772
120.9656
115.1071
114.2393
112.0813
109.9541
106.2315
101.1280
81.7169
69.9700
69.0275
68.0145
64.7667
59.0603
54.8631
54.2946
24.6973
23.9483
21.3269
100.0000
OMe
OMe
HN
O
O
O
O
O
O
MeO
HO
HO
26b
[rel]
6
4
2
0
200
150
100
50
0
[ppm]

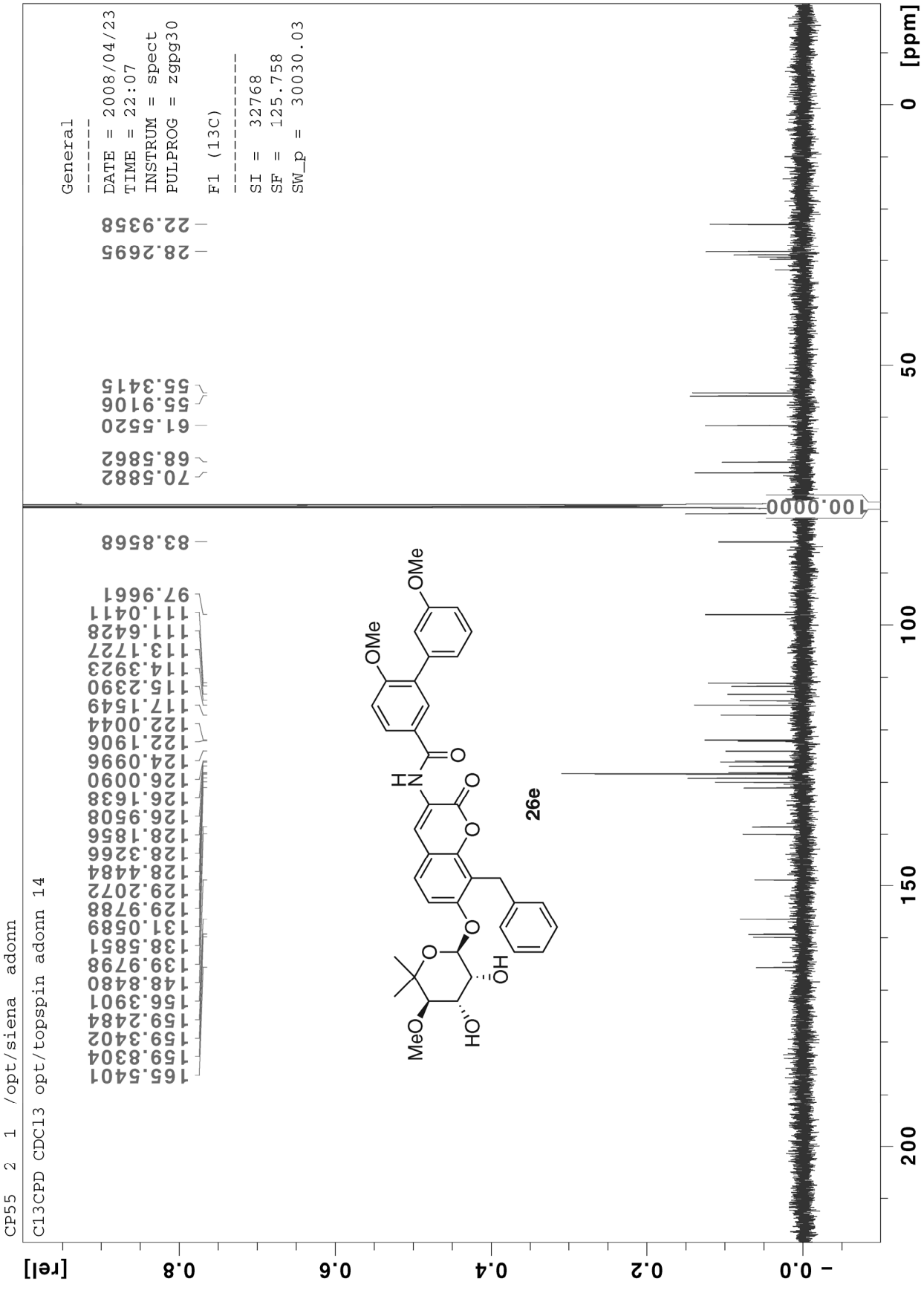

IPRBD 1 1 /opt/siena adonn
PROTON CD2Cl2 opt/topspin adonn 3
General
DATE = 2007/12/12
TIME = 14:32
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
26c
OMe
OMe
MeO
HO
OH
[rel]
[ppm]

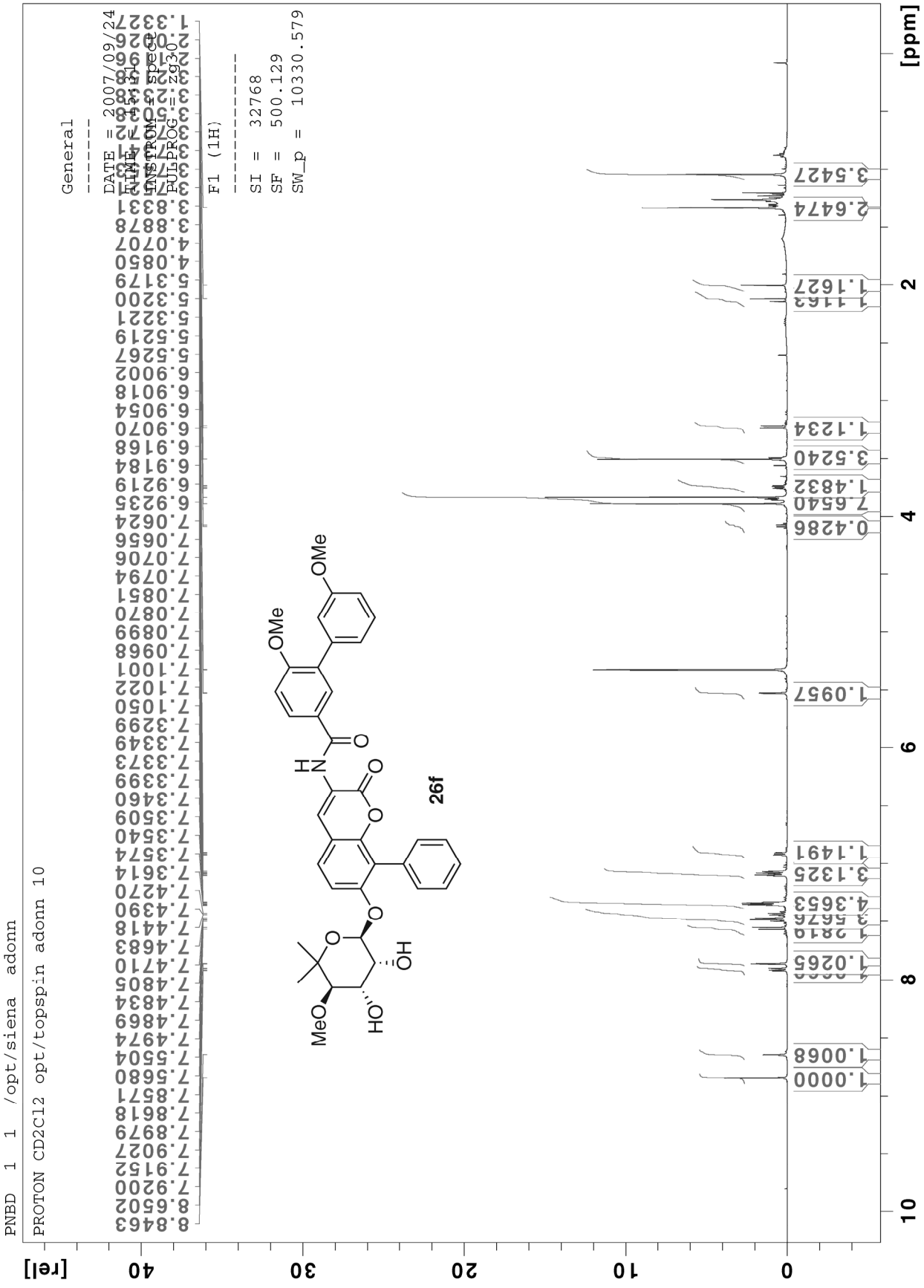

IPRBD 2 1 /opt/siena adonn
C13CPD CD2C12 opt/topspin adonn 3
General
DATE = 2007/12/12
TIME = 15:01
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
22.4072
21.9342
20.8044
59.0142
55.0838
68.3127
69.2072
71.0939
76.9838
81.8515
101.4334
108.3999
110.2432
112.0739
114.5397
115.4461
121.1448
121.2085
122.1635
122.8136
125.2342
127.4145
128.3152
129.1240
130.1513
138.0514
142.4608
146.3446
146.7091
158.2870
158.6322
159.0831
164.5637
OMe
OMe
O
N
H
O
O
O
O
O
MeO
HO
OH
26c
[rel]
1.0
0.8
0.6
0.4
0.2
0.0
200
150
100
50
0 [ppm]

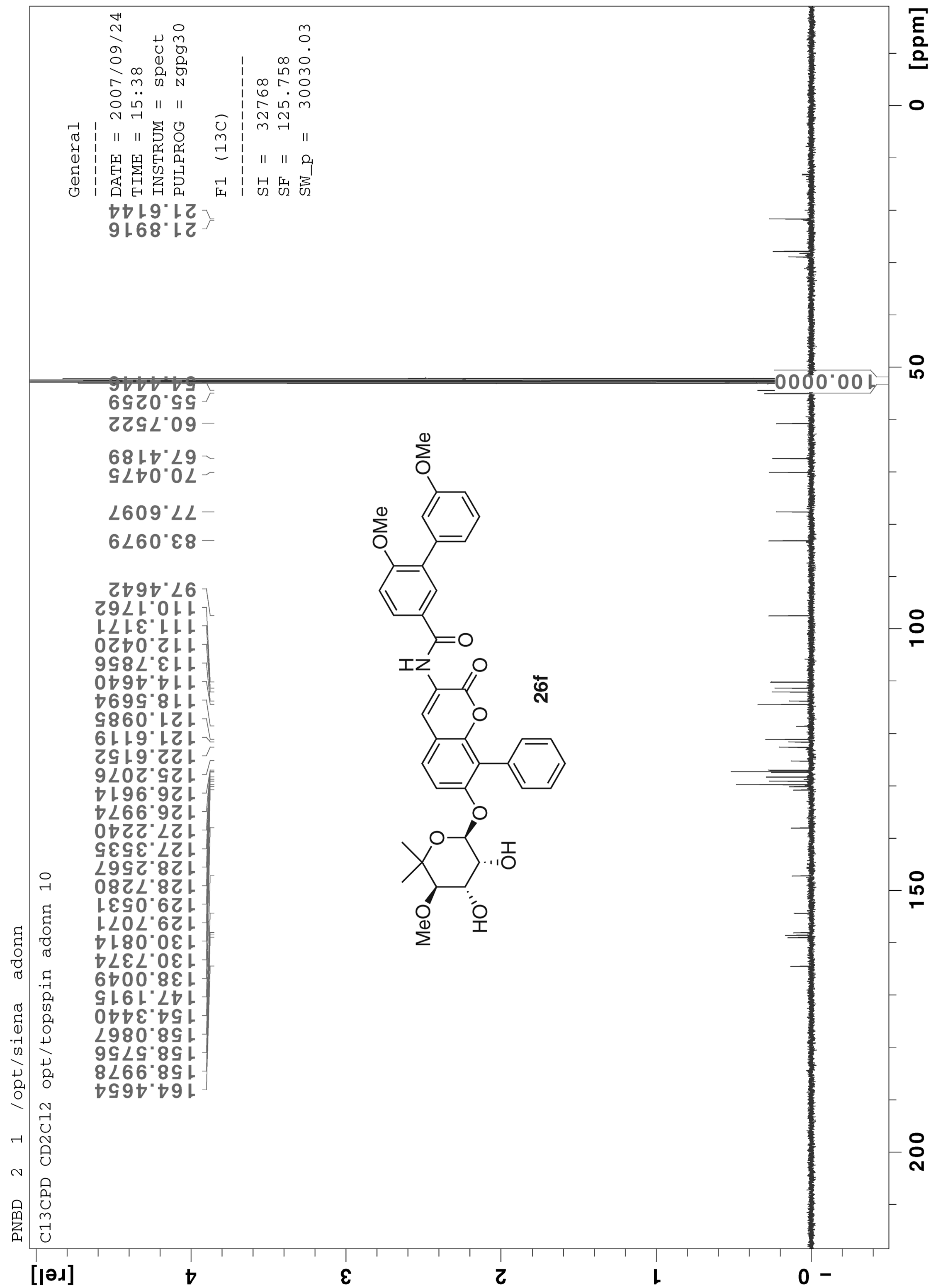

"5-OMe biaryl diol" 1 1 /opt/florence adonnelly
General
DATE = 2007/09/24
TIME = 18:37
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
26d
[rel]
[ppm]

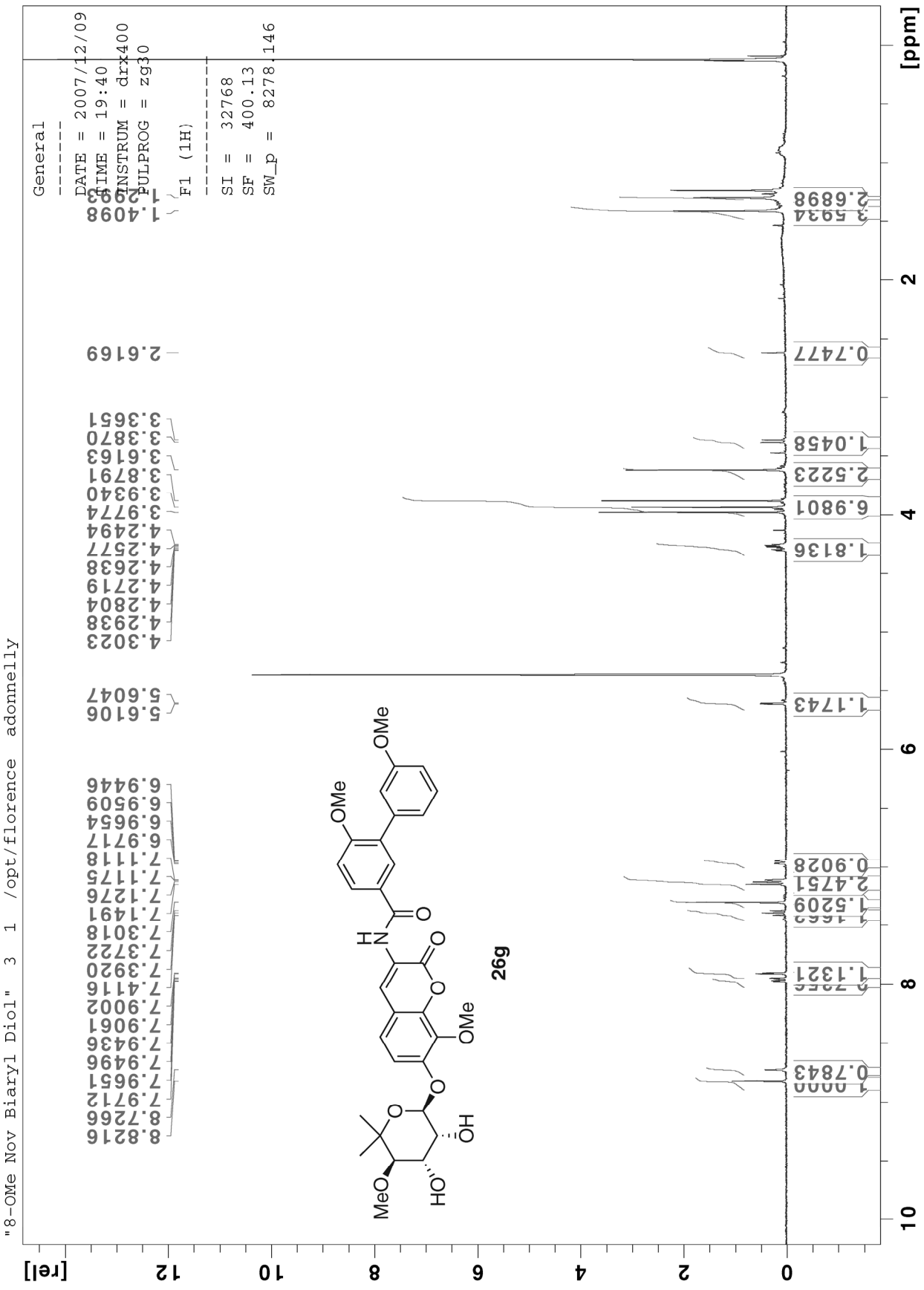

CP40 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 10
General
DATE = 2008/04/23
TIME = 19:44
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
26d
[rel]
[ppm]

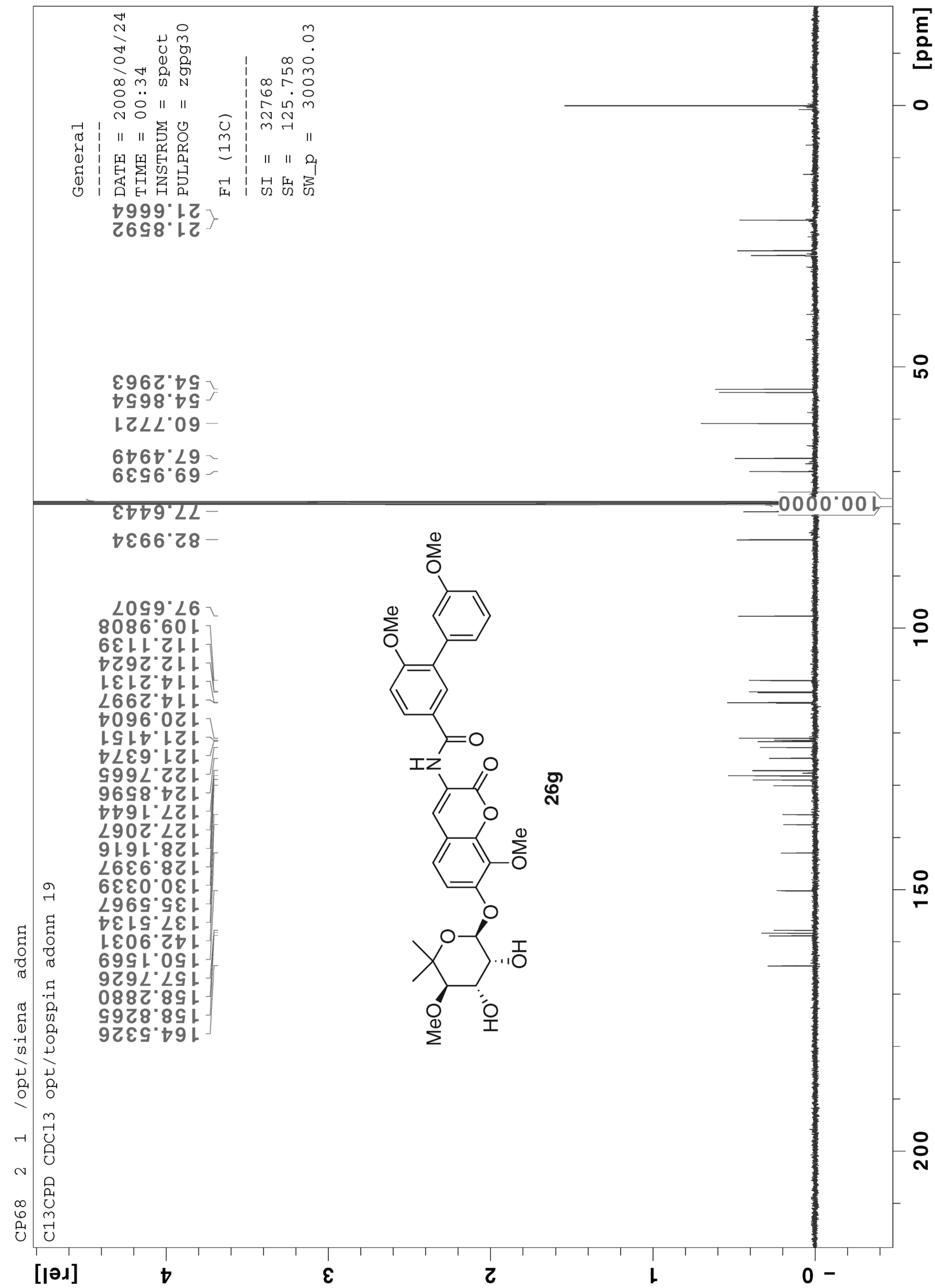

"Benzyl Nov Biaryl Diol" 1 1 /opt/florence adonnelly
General
DATE = 2007/08/13
SI = 32768
SF = 400.13
SW_p = 8278.146
F1 (1H)
26e
OMe
OMe
MeO
HO
OH
[rel]
0 [ppm]
1.0000
0.9775
2.0330
1.1046
11.2485
1.1555
1.1996
5.6065
6.3199
3.6623
1.3432
1.8491
1.0153
2.7057
3.8683

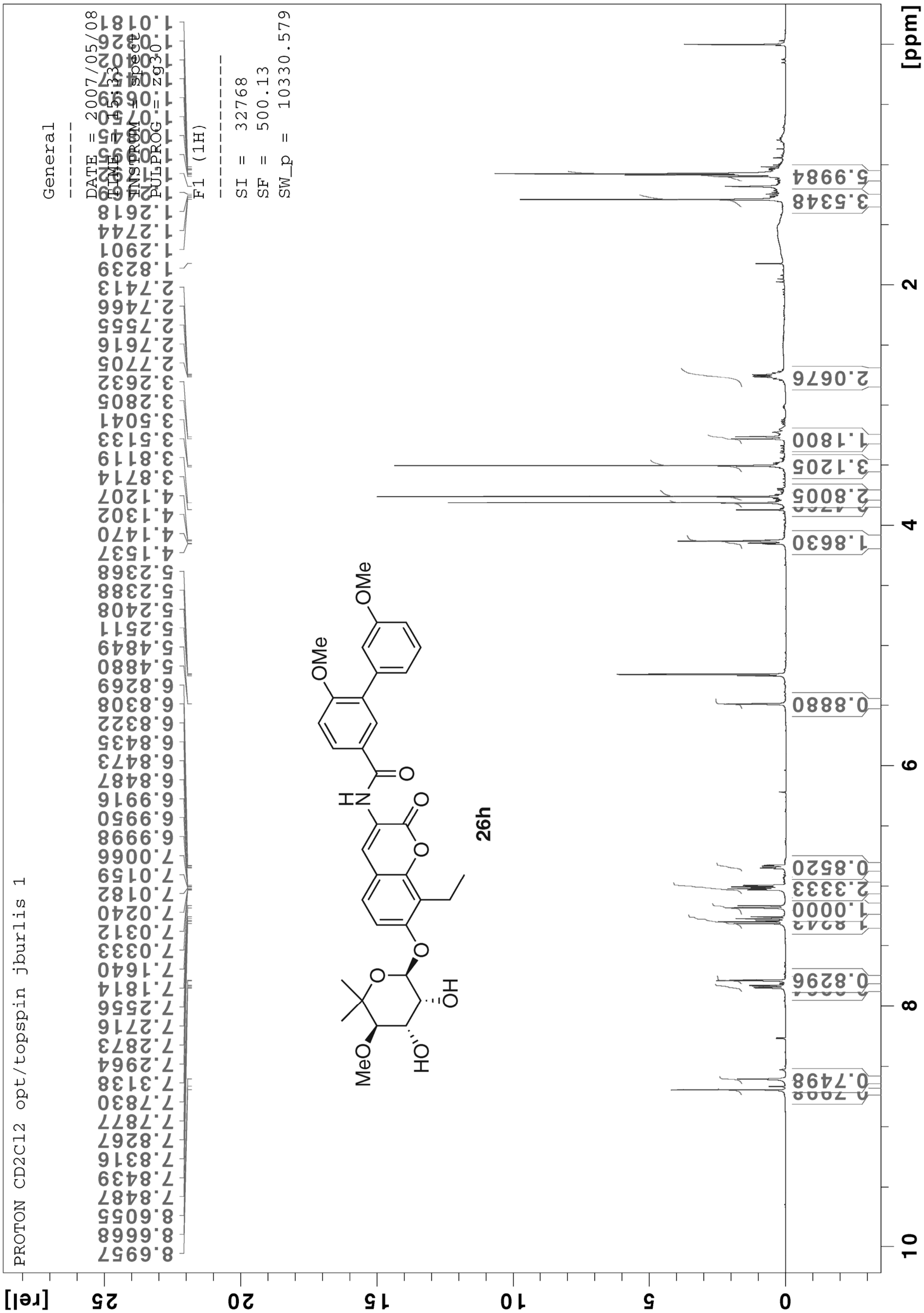

CP55 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 14
General
DATE = 2008/04/23
TIME = 22:07
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
22.9358
28.2695
55.3415
55.9106
61.5520
68.5862
70.5882
83.8568
97.9661
111.0411
111.6428
113.1727
114.3923
115.2390
117.1549
122.0044
122.1906
124.0996
126.0090
126.1638
126.9508
128.1856
128.3266
128.4484
129.2072
129.9788
131.0589
138.5851
139.9798
148.8480
156.3901
159.2484
159.3402
159.8304
165.5401
100.0000
OMe
OMe
HN
O
O
O
O
O
MeO
HO
OH
26e
[rel]
0.8
0.6
0.4
0.2
0.0
200
150
100
50
0 [ppm]

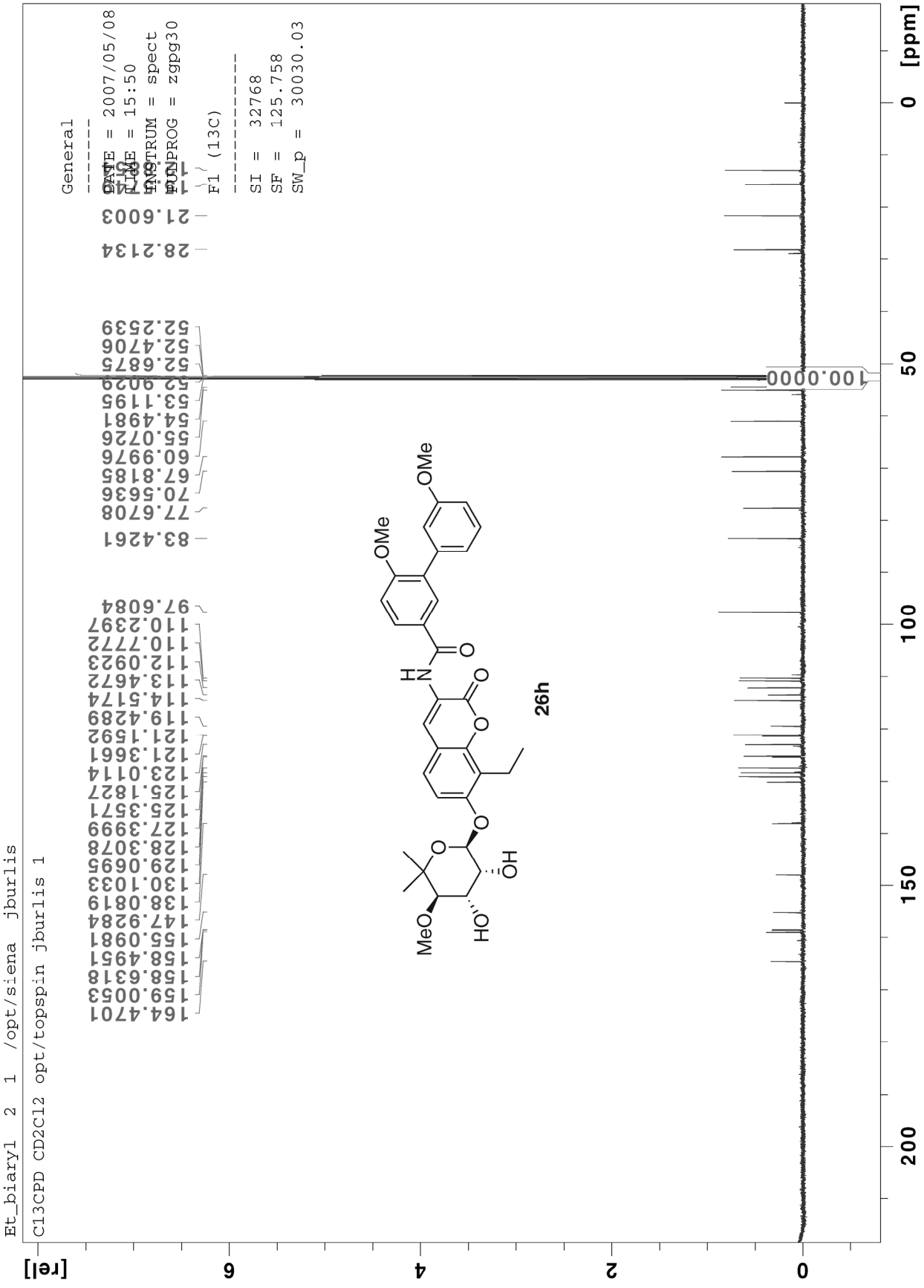

PNBD 1 1 /opt/siena adonn
PROTON CD2Cl2 opt/topspin adonn 10
General
DATE = 2007/09/24
F1 (1H)
SI = 32768
SF = 500.129
SW_p = 10330.579
26f
OMe
OMe
MeO
HO
OH
[rel]
[ppm]
1.0000
1.0068
1.0265
1.1491
3.1325
4.3653
1.0957
0.4286
7.6540
1.4832
3.5240
1.1234
2.6474
3.5427

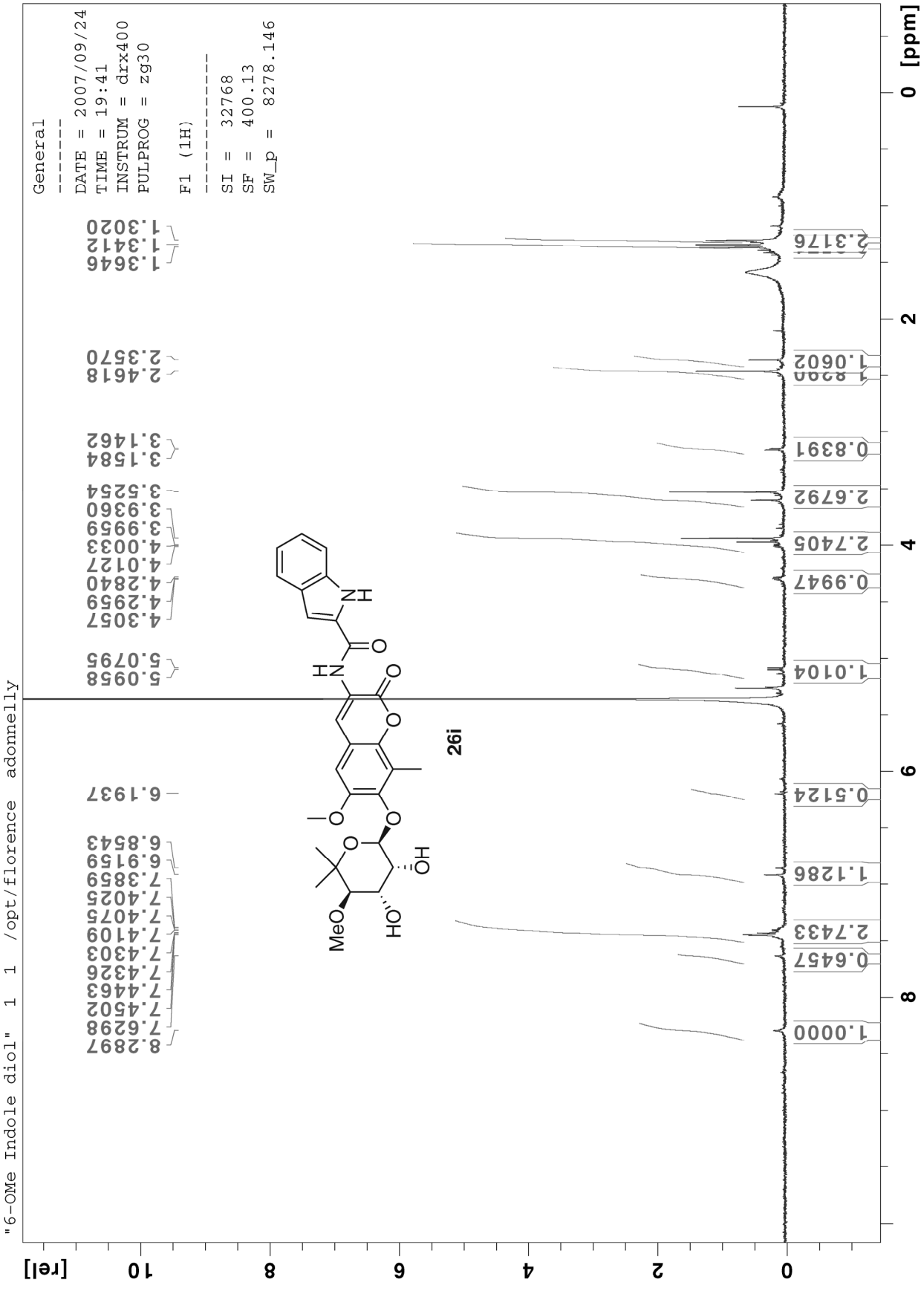

PNBD 2 1 /opt/siena adonn
C13CPD CD2Cl2 opt/topspin adonn 10
General
DATE = 2007/09/24
TIME = 15:38
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
164.4654
158.9978
158.5756
158.0867
154.3440
147.1915
138.0049
130.7374
130.0814
129.7071
129.0531
128.7280
128.2567
127.3535
127.2240
126.9974
126.9614
125.2076
122.6152
121.6119
121.0985
118.5694
114.4640
113.7856
112.0420
111.3171
110.1762
97.4642
83.0979
77.6097
70.0475
67.4189
60.7522
55.0259
54.4446
21.8916
21.6144
100.0000
MeO
HO
HO
OMe
OMe
26f
[rel]
[ppm]

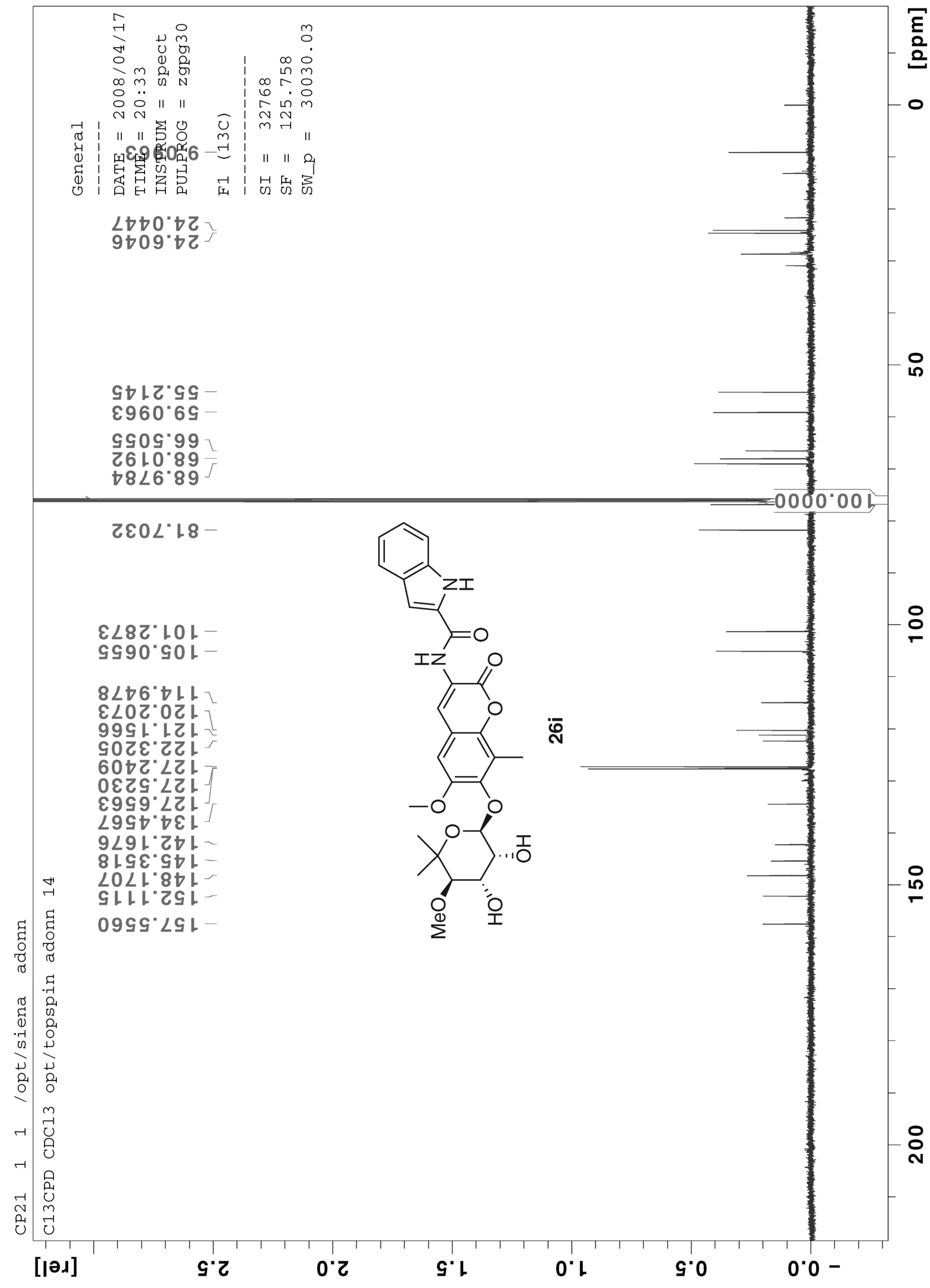

"8-OMe Nov Biaryl Diol" 3 1 /opt/florence adonnelly
General
DATE = 2007/12/09
TIME = 19:40
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
1.29923
1.40980
2.61690
3.36510
3.38700
3.61630
3.87910
3.93400
3.97740
4.24940
4.25770
4.26380
4.27190
4.28040
4.29380
4.30230
5.60470
5.61060
6.94460
6.95090
6.96540
6.97170
7.11180
7.11750
7.12760
7.14910
7.30180
7.37220
7.39200
7.41160
7.90020
7.90610
7.94360
7.94960
7.96510
7.97120
8.72660
8.82160
0.78430
1.13210
1.52090
2.47510
0.90280
0.74770
1.04580
2.52230
6.98010
1.81360
1.17430
2.68980
OMe
OMe
OMe
H
N
O
O
O
O
OH
HO
MeO
26g
[rel]
[ppm]

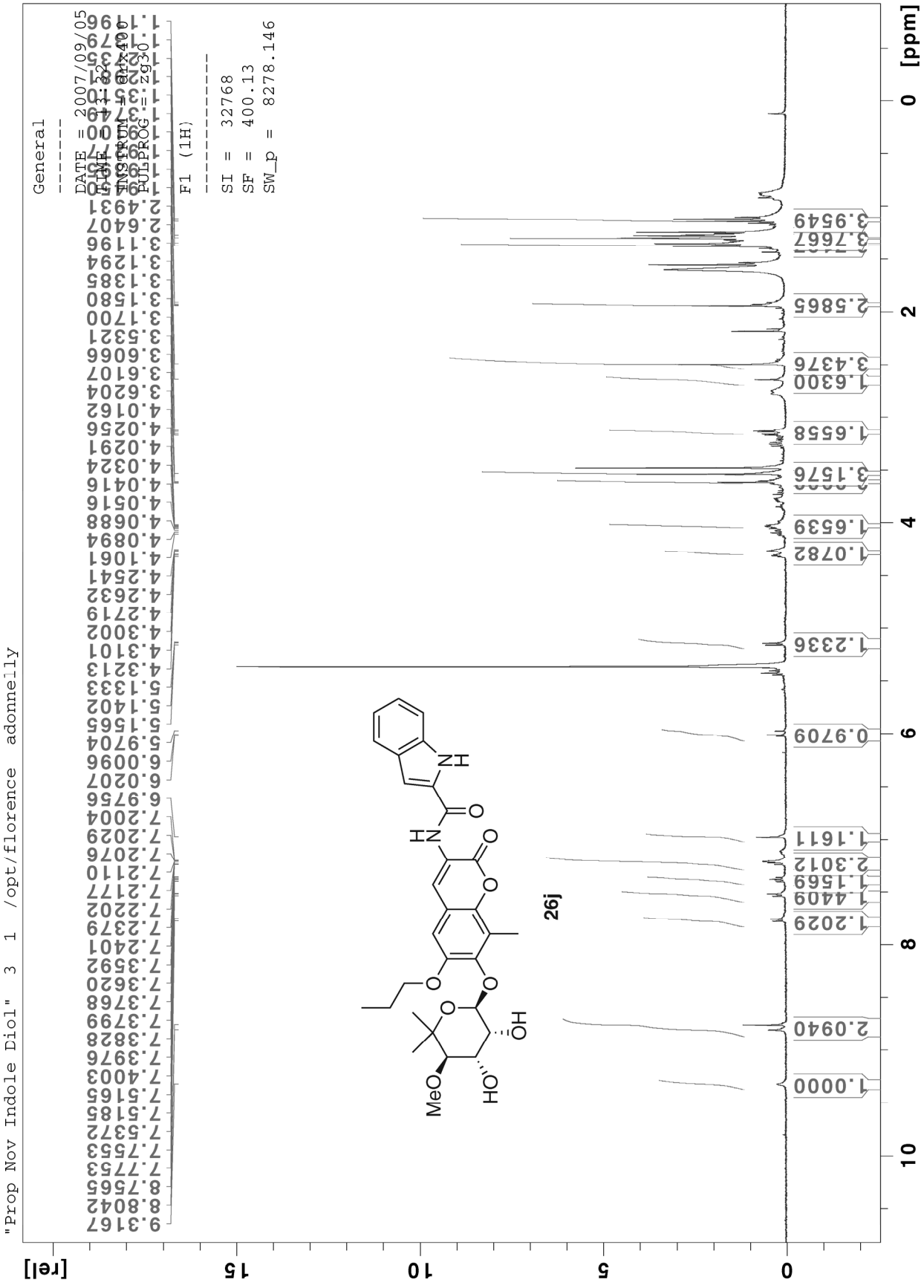

CP68 2 1 /opt/siena adonn
C13CPD CDCl3 opt/topspin adonn 19
General
DATE = 2008/04/24
TIME = 00:34
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
21.6664
21.8592
54.2963
54.8654
60.7721
67.4949
69.9539
77.6443
82.9934
97.6507
109.9808
112.1139
112.2624
114.2131
114.2997
120.9604
121.4151
121.6374
122.7665
124.8596
127.1644
127.2067
128.1616
128.9397
130.0339
135.5967
137.5134
142.9031
150.1569
157.7626
158.2880
158.8265
164.5326
100.0000
MeO
HO
OH
O
OMe
O
O
H
N
OMe
OMe
26g
[ppm]
[rel]

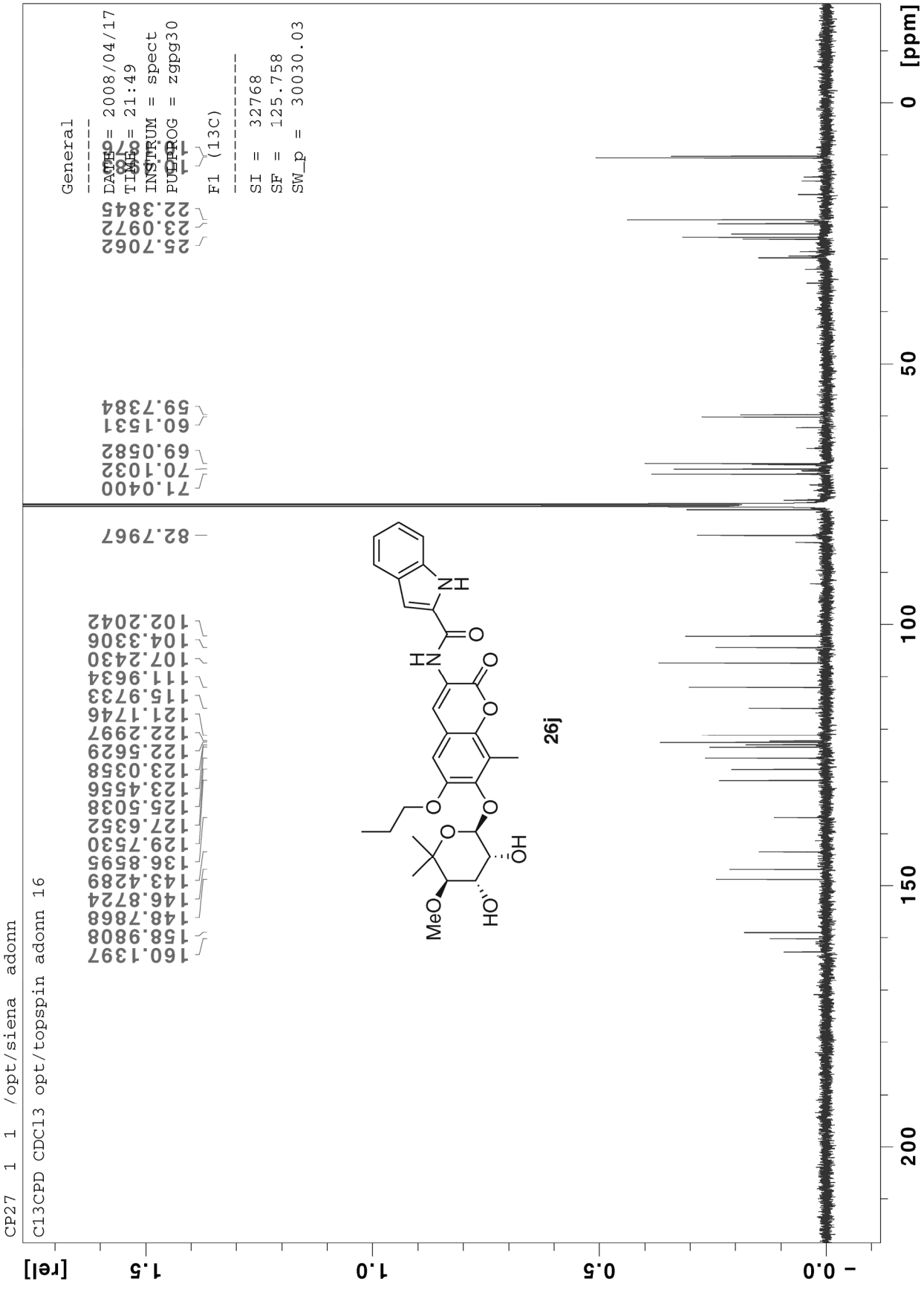

Et_biaryl 1 1 /opt/siena jburlis
PROTON CD2Cl2 opt/topspin jburlis 1
General
DATE = 2007/05/08
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
26h
[ppm]
[rel]

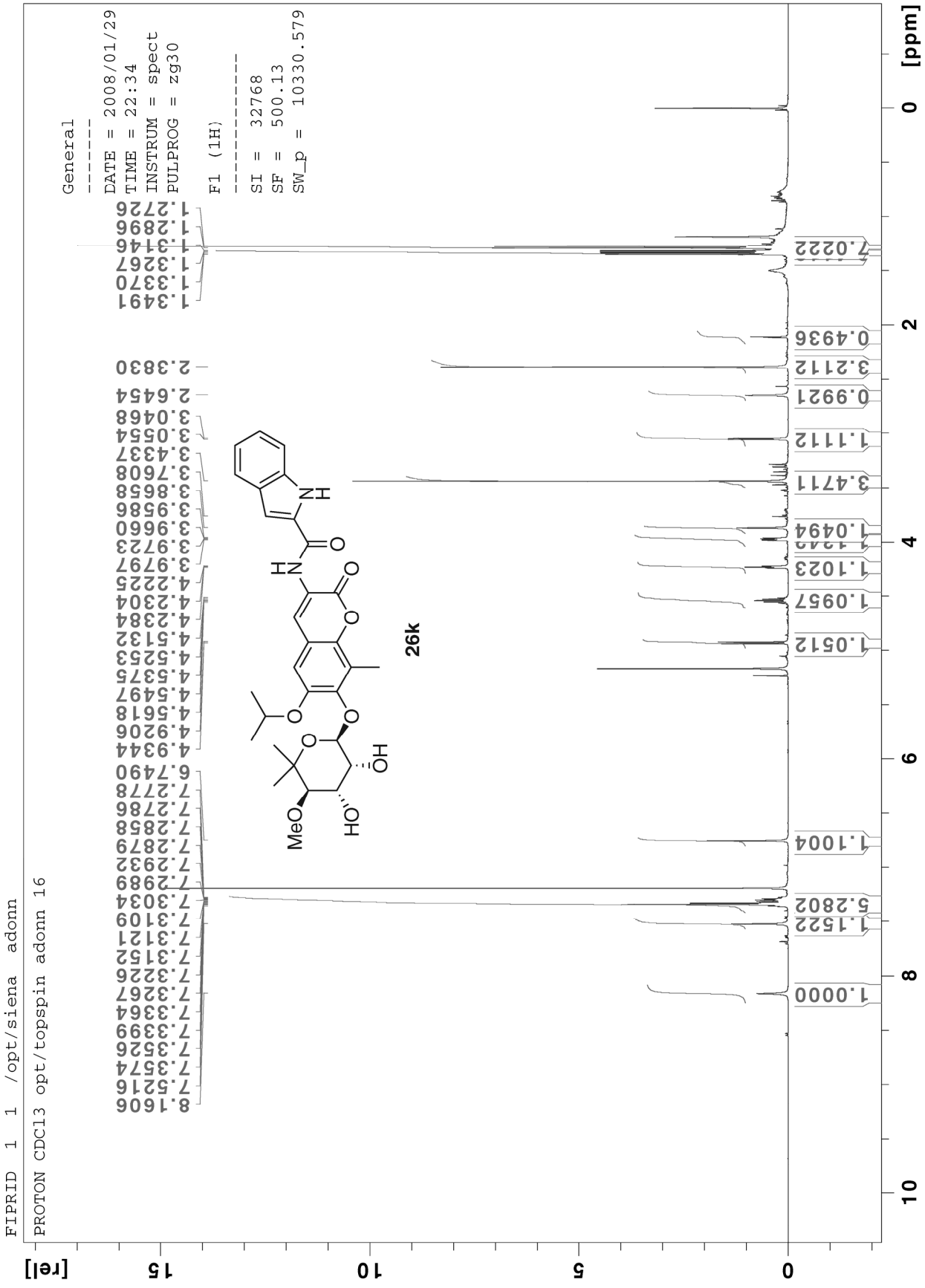

Et_biaryl 2 1 /opt/siena jburlis
C13CPD CD2C12 opt/topspin jburlis 1
General
DATE = 2007/05/08
TIME = 15:50
SPECTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
[rel]
[ppm]
26h
OMe
OMe
MeO
HO
OH
O
N
H

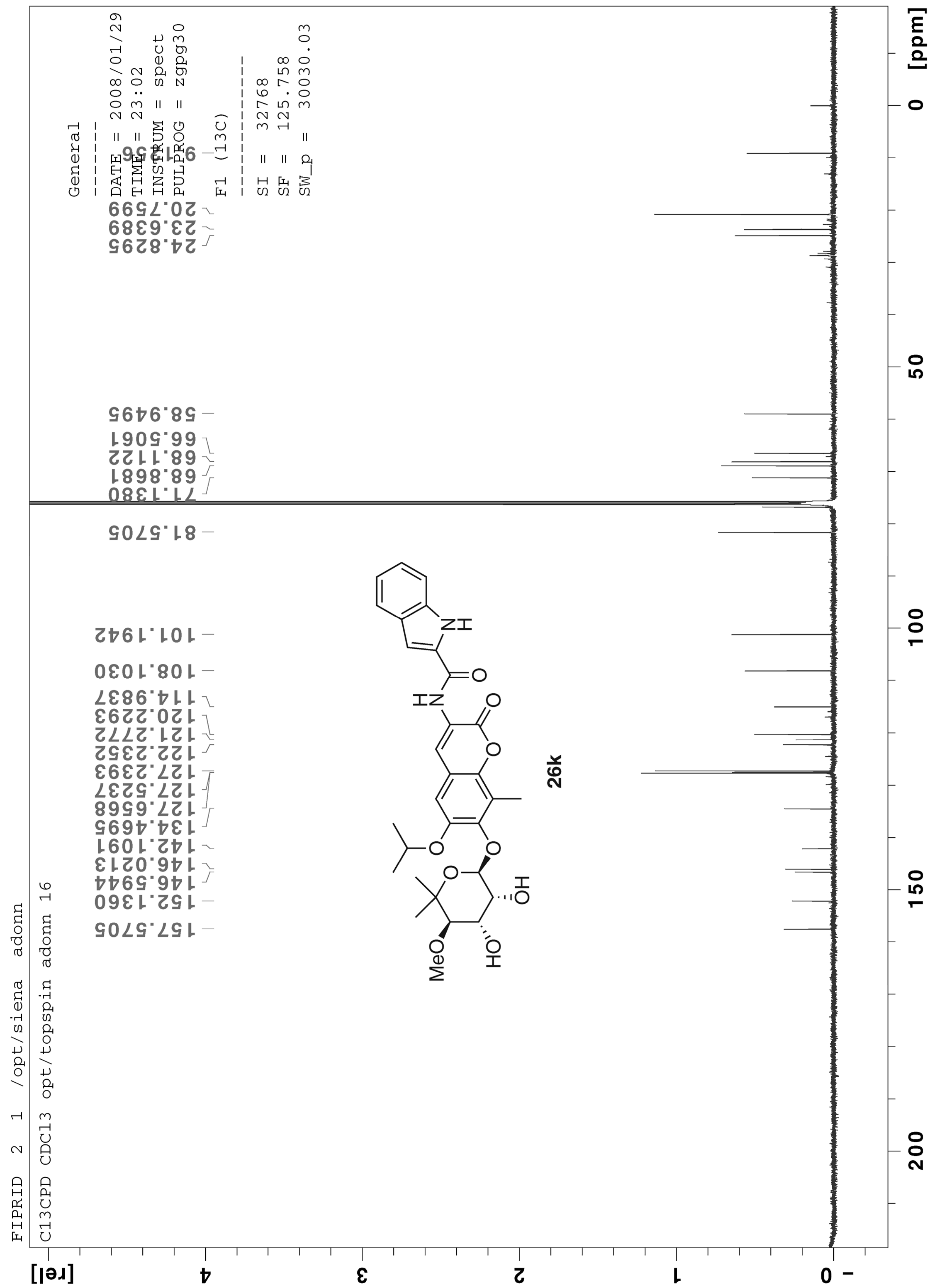

"6-OMe Indole diol" 1 1 /opt/florence adonnelly
General
DATE = 2007/09/24
TIME = 19:41
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
26i
MeO
HO
OH
[rel]
[ppm]

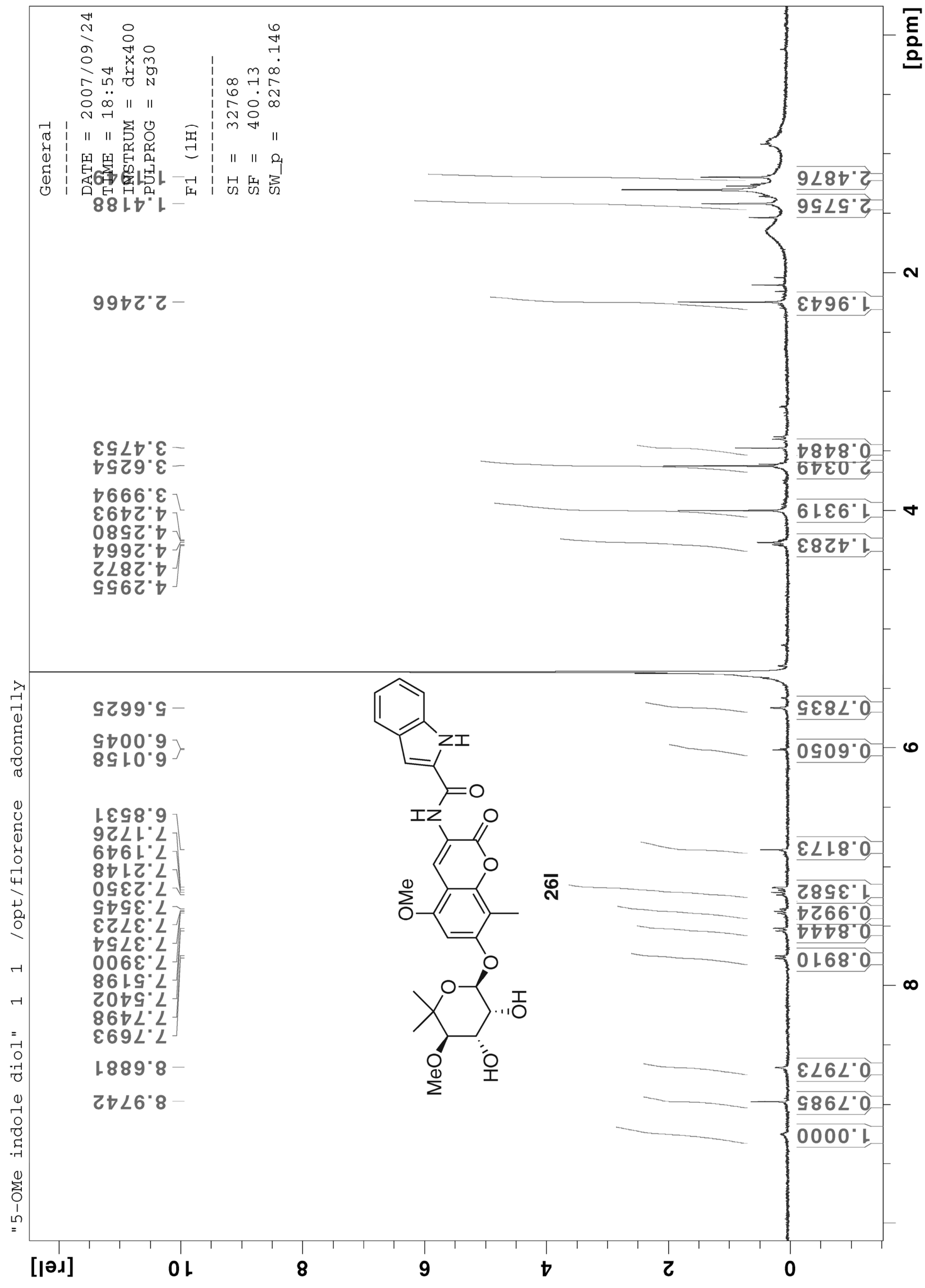

CP21 1 1 /opt/siena adonn
C13CPD CDCl3 opt/topspin adonn 14
General
DATE = 2008/04/17
TIME = 20:33
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
157.5560
152.1115
148.1707
145.3518
142.1676
134.4567
127.6563
127.5230
127.2409
122.3205
121.1566
120.2073
114.9478
105.0655
101.2873
81.7032
100.0000
68.9784
68.0192
66.5055
59.0963
55.2145
24.6046
24.0447
MeO
HO
HO
NH
NH
26i
[ppm]
[rel]

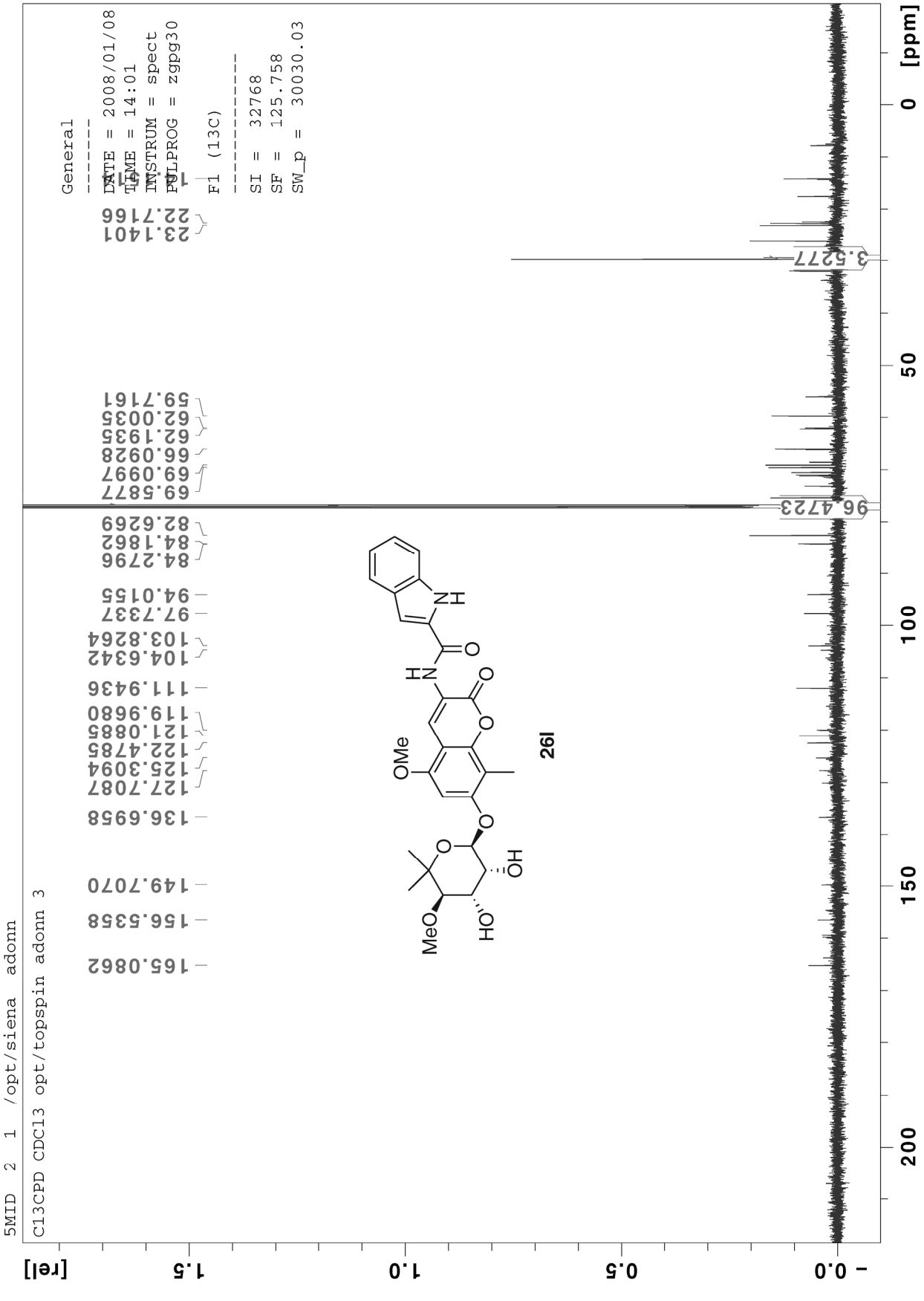

"Prop Nov Indole Diol" 3 1 /opt/florence adonnelly
General
DATE = 2007/09/05
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
26j
1.0000
2.0940
1.2029
1.4409
1.1569
2.3012
1.1611
0.9709
1.2336
1.0782
1.6539
3.1576
1.6558
1.6300
3.4376
2.5865
3.7667
3.9549
[rel]
[ppm]

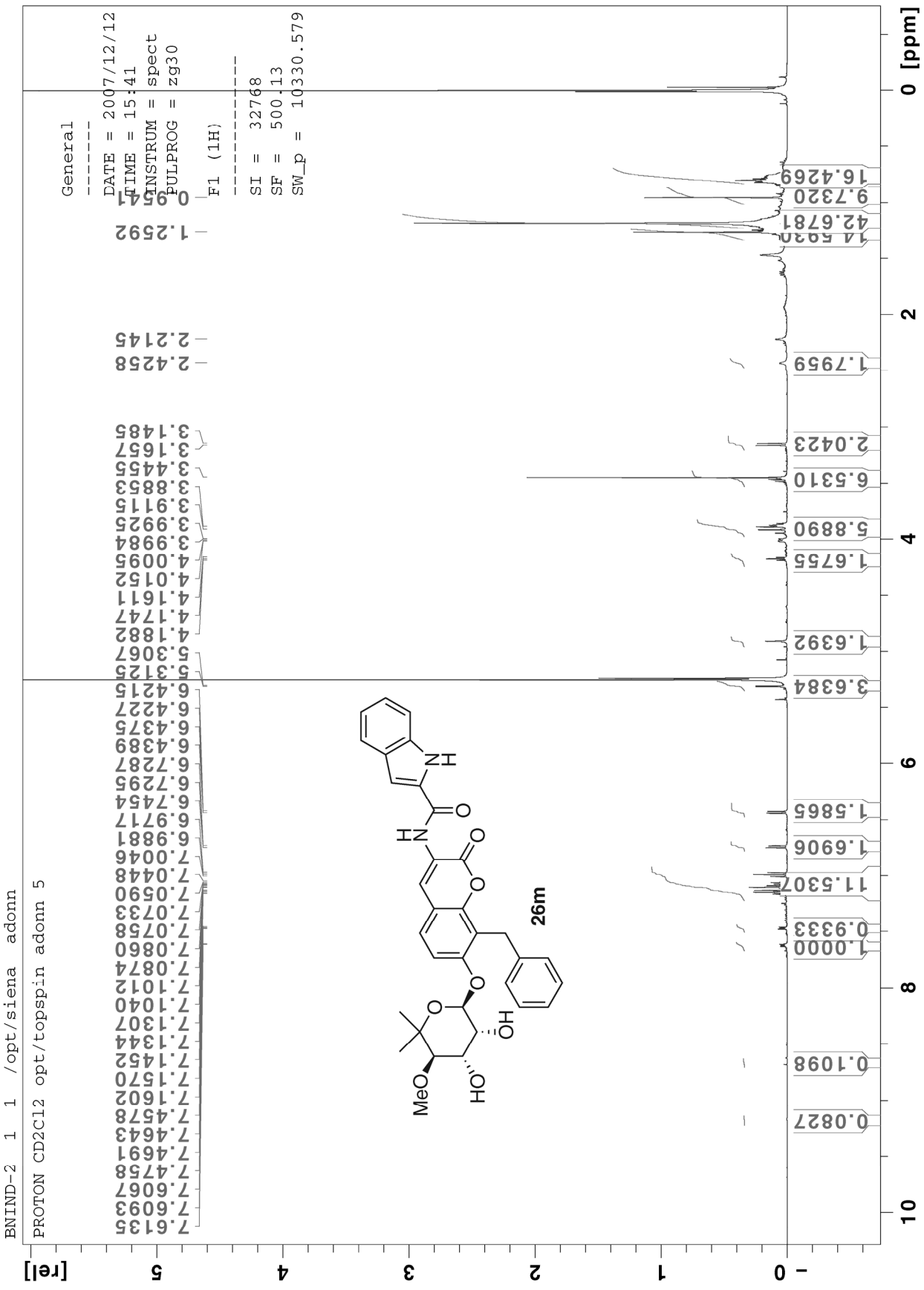

CP27 1 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 16
General
DATE = 2008/04/17
TIME = 21:49
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
160.1397
158.9808
148.7868
146.8724
143.4289
136.8595
129.7530
127.6352
125.5038
123.4556
123.0358
122.5629
122.2997
121.1746
115.9733
111.9634
107.2430
104.3306
102.2042
82.7967
71.0400
70.1032
69.0582
60.1531
59.7384
25.7062
23.0972
22.3845
MeO
HO
OH
26j
[rel]
1.5
1.0
0.5
0.0
200
150
100
50
0 [ppm]

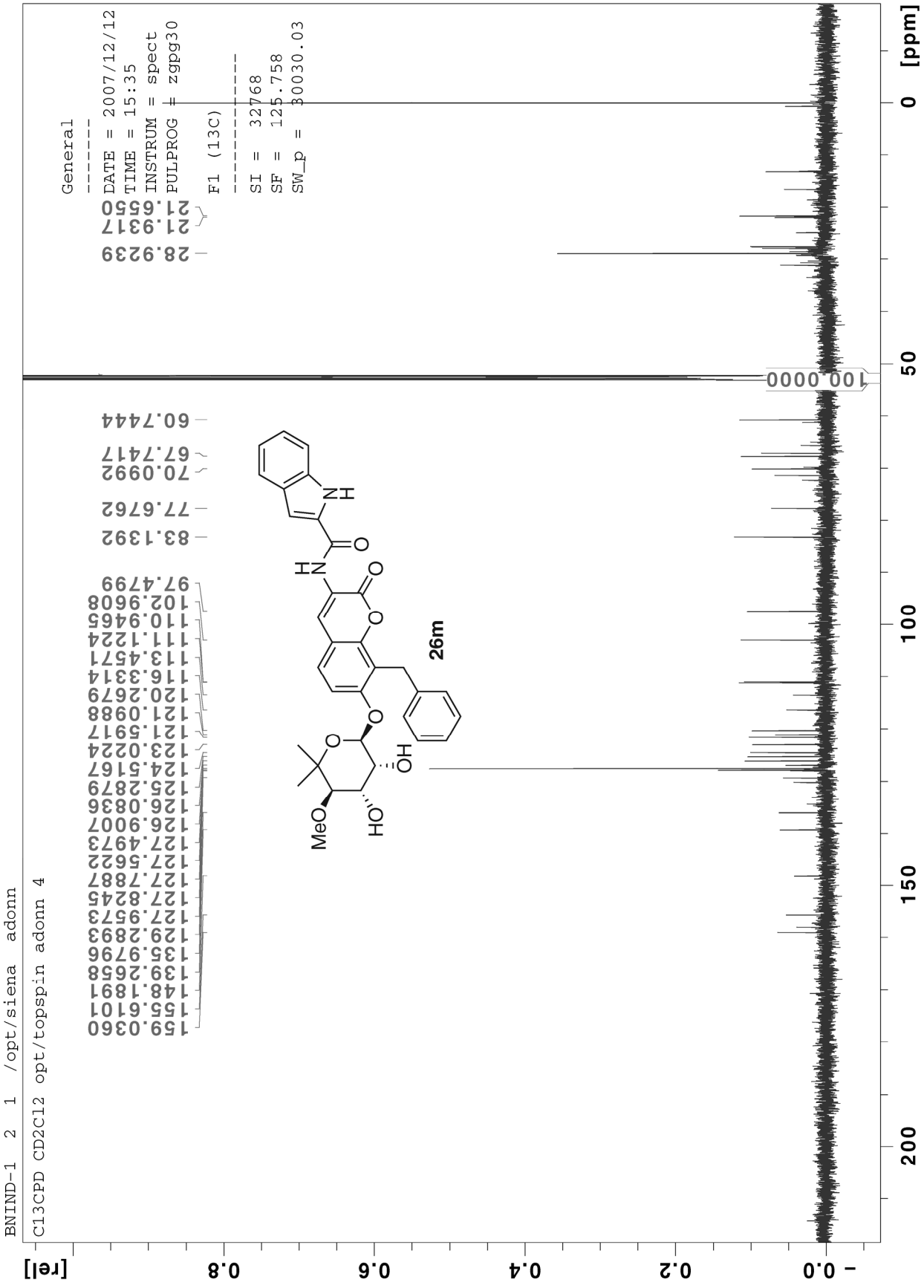

FIPRID 1 1 /opt/siena adonn
PROTON CDC13 opt/topspin adonn 16
General
DATE = 2008/01/29
TIME = 22:34
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
26k
MeO
HO
OH
[rel]
[ppm]

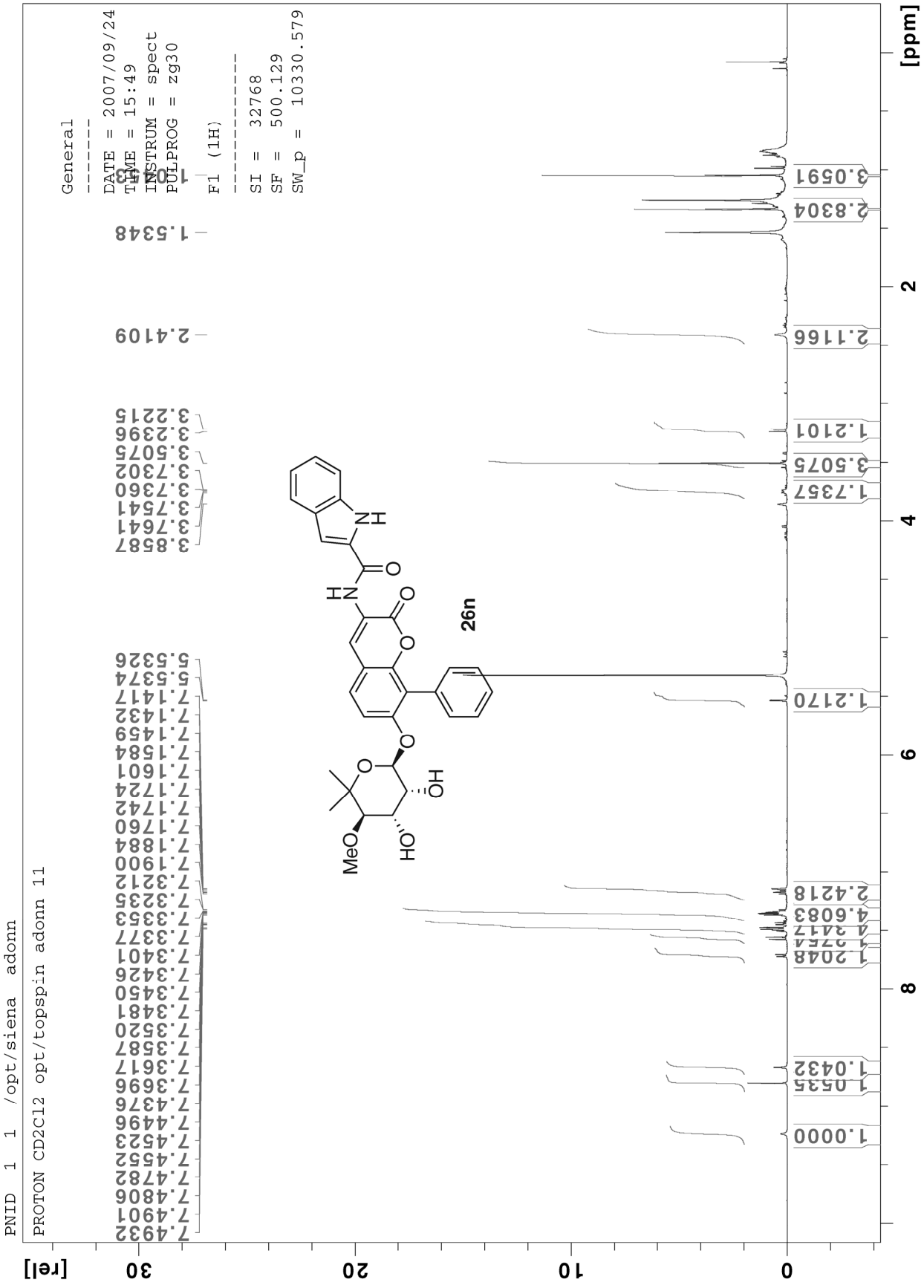

FIPRID 2 1 /opt/siena adonn
C13CPD CDCl3 opt/topspin adonn 16
General
DATE = 2008/01/29
TIME = 23:02
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
20.7599
23.6389
24.8295
58.9495
66.5061
68.1122
68.8681
71.1380
81.5705
101.1942
108.1030
114.9837
120.2293
121.2772
122.2352
127.2393
127.5237
127.6568
134.4695
142.1091
146.0213
146.5944
152.1360
157.5705
MeO
HO
OH
O
NH
26k
[ppm]
[rel]

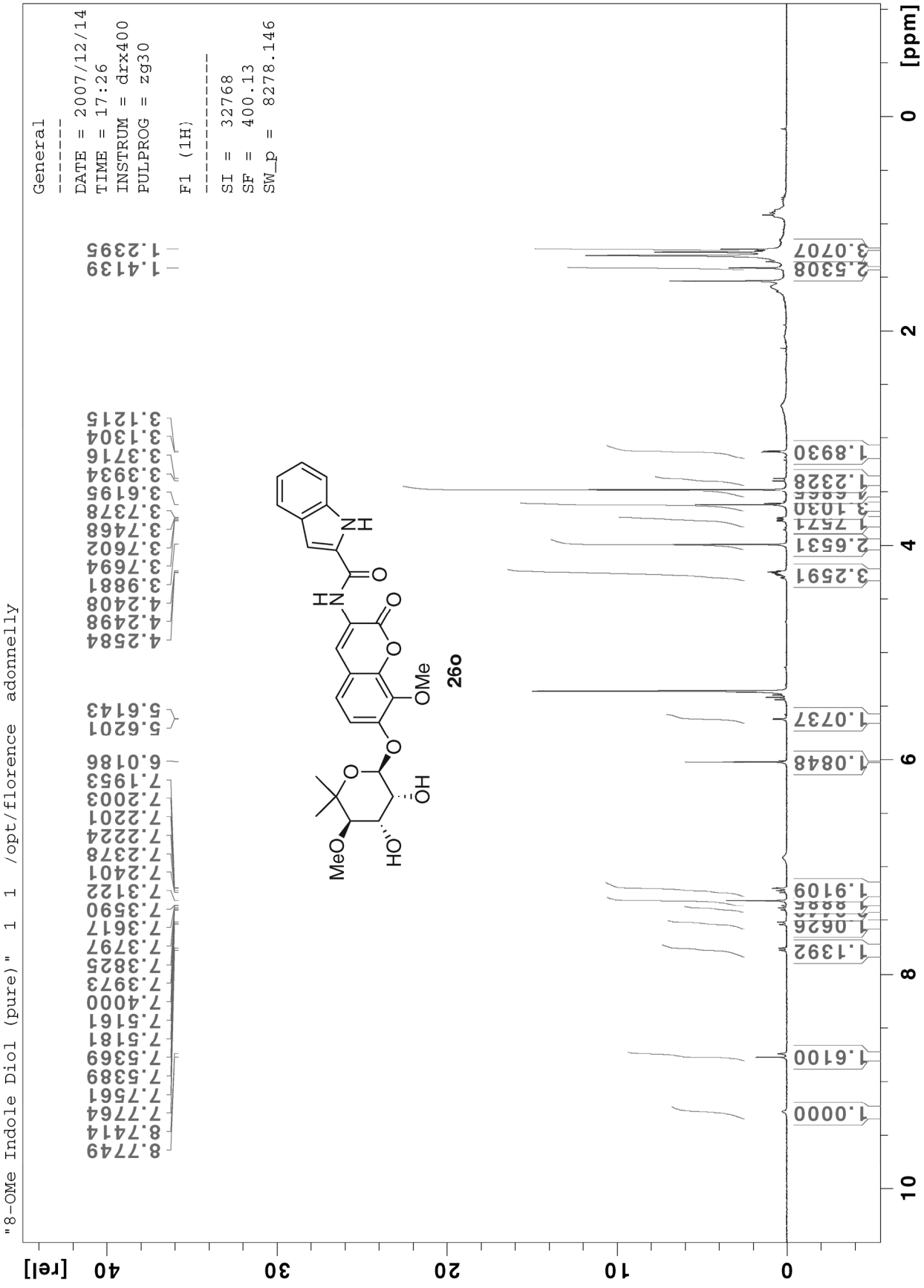

"5-OMe indole diol" 1 1 /opt/florence adonnelly
General
DATE = 2007/09/24
TIME = 18:54
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
26l
[ppm]
[rel]

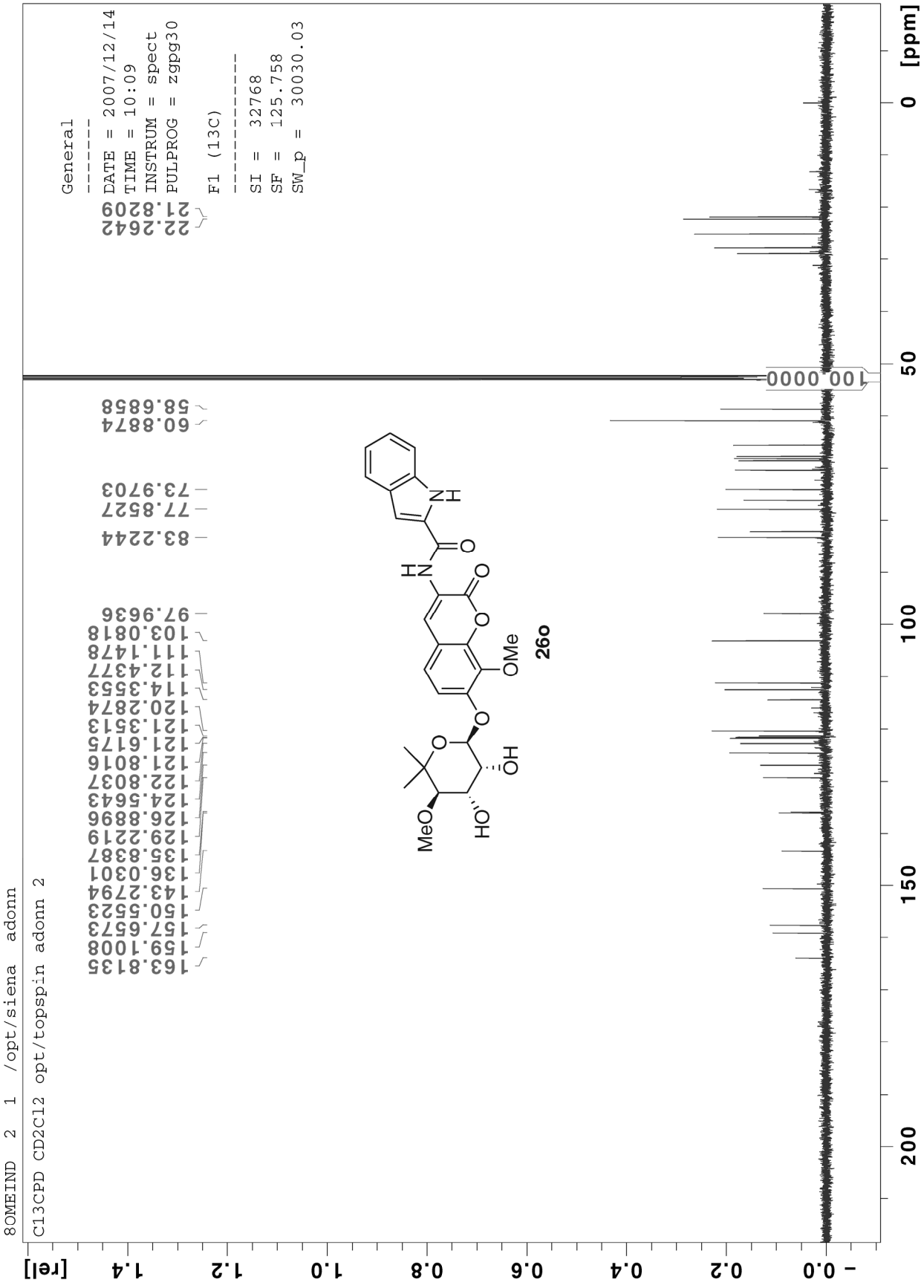

5MID 2 1 /opt/siena adonn
C13CPD CDC13 opt/topspin adonn 3
General
DATE = 2008/01/08
TIME = 14:01
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
[rel]
[ppm]
26l

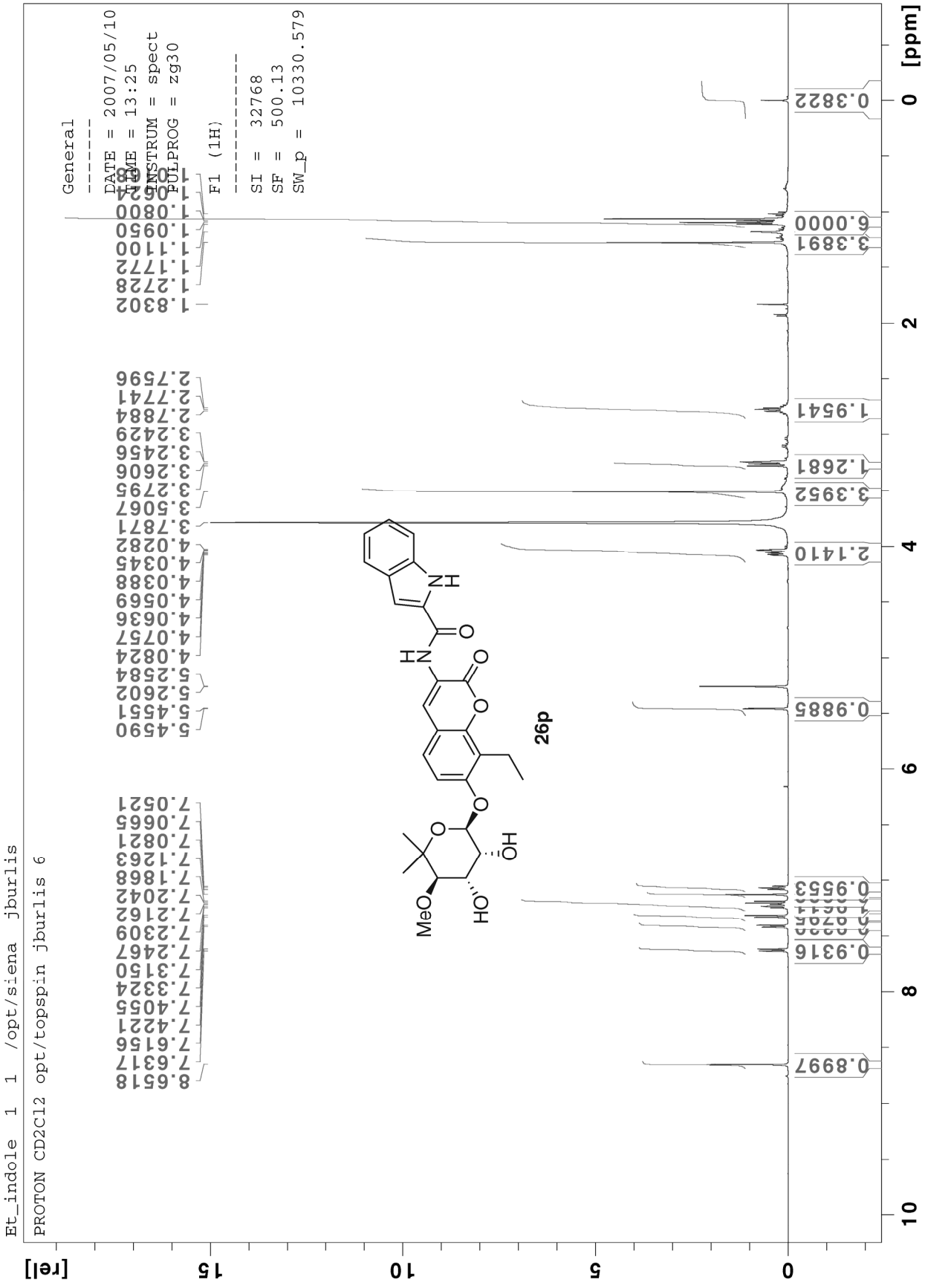

BNIND-2 1 1 /opt/siena adonn
PROTON CD2C12 opt/topspin adonn 5
General
DATE = 2007/12/12
TIME = 15:41
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
26m
MeO
OH
HO
[rel]
[ppm]

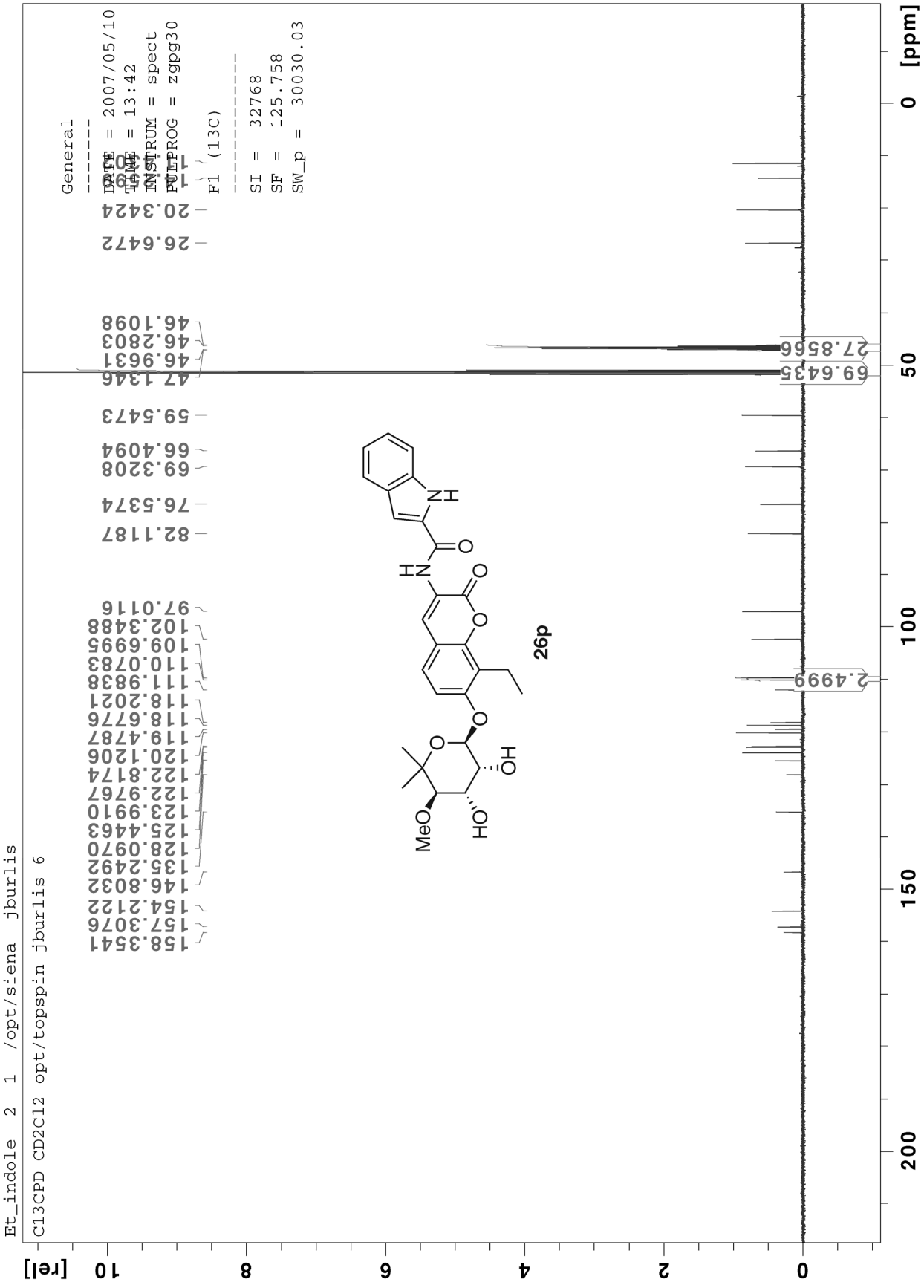

BNIND-1 2 1 /opt/siena adonn
C13CPD CD2C12 opt/topspin adonn 4
General
DATE = 2007/12/12
TIME = 15:35
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
21.6550
21.9317
28.9239
60.7444
67.7417
70.0992
77.6762
83.1392
97.4799
102.9608
110.9465
111.1224
113.4571
116.3314
120.2679
121.0988
121.5917
123.0224
124.5167
125.2879
126.0836
126.9007
127.4973
127.5622
127.7887
127.8245
127.9573
129.2893
135.9796
139.2658
148.1891
155.6101
159.0360
100.0000
26m
MeO
HO
OH
[rel]
0.0
0.2
0.4
0.6
0.8
200
150
100
50
0
[ppm]

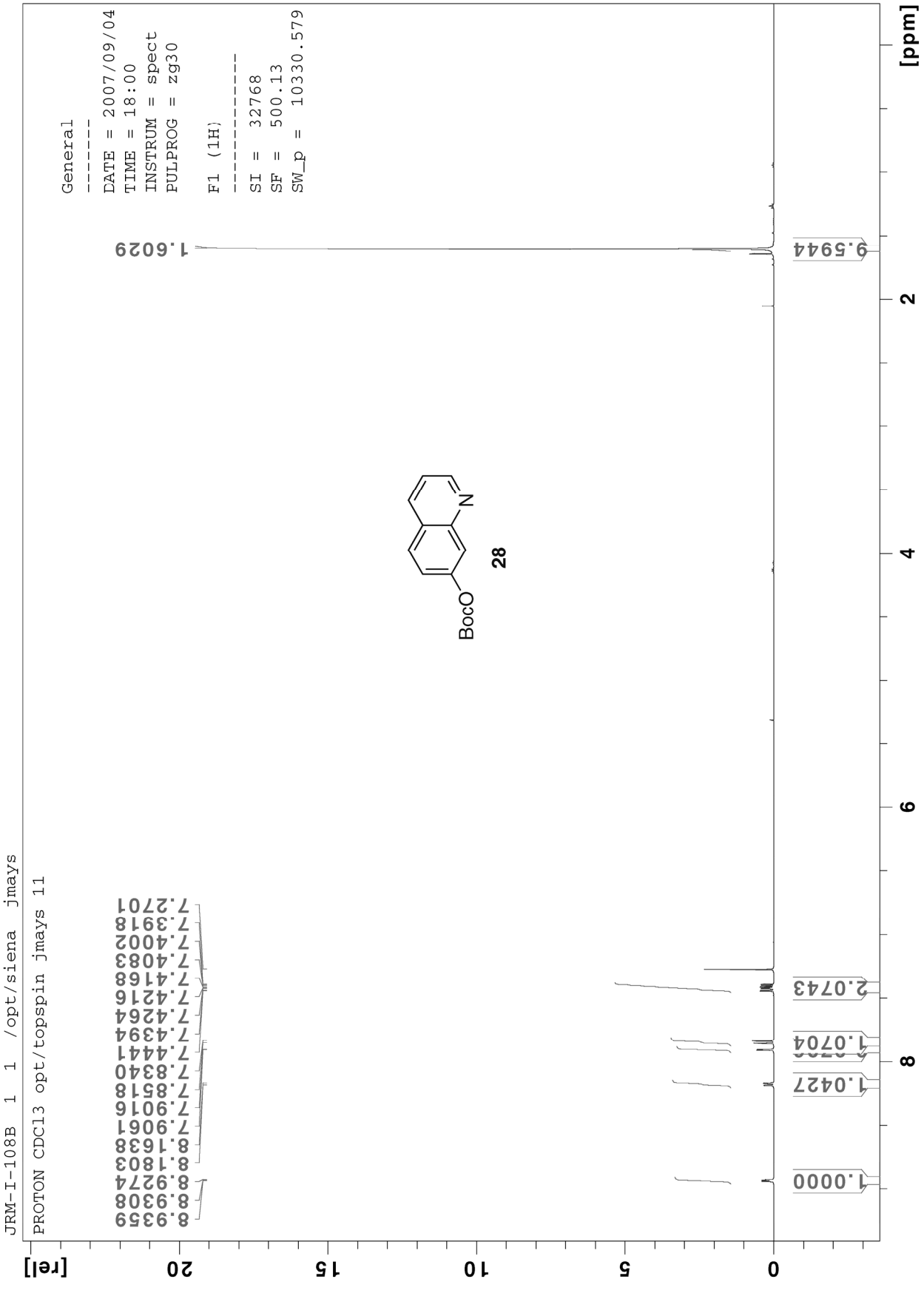

PNID 1 1 /opt/siena adonn
PROTON CD2C12 opt/topspin adonn 11
General
DATE = 2007/09/24
TIME = 15:49
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.129
SW_p = 10330.579
26n
MeO
HO
OH
[rel]
[ppm]

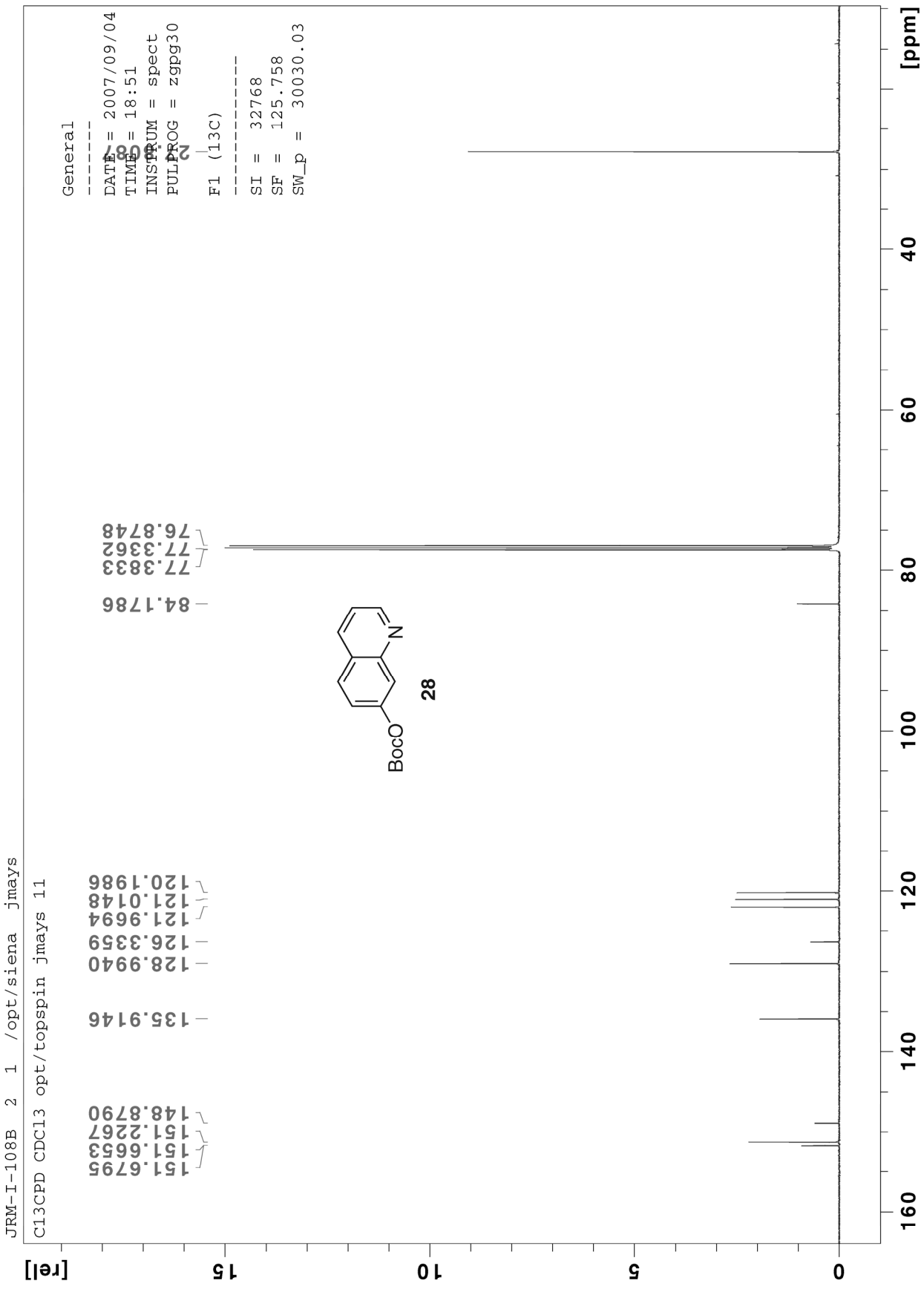

"8-OMe Indole Diol (pure)" 1 1 /opt/florence adonnelly
General
DATE = 2007/12/14
TIME = 17:26
INSTRUM = drx400
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 400.13
SW_p = 8278.146
26o
[rel]
[ppm]

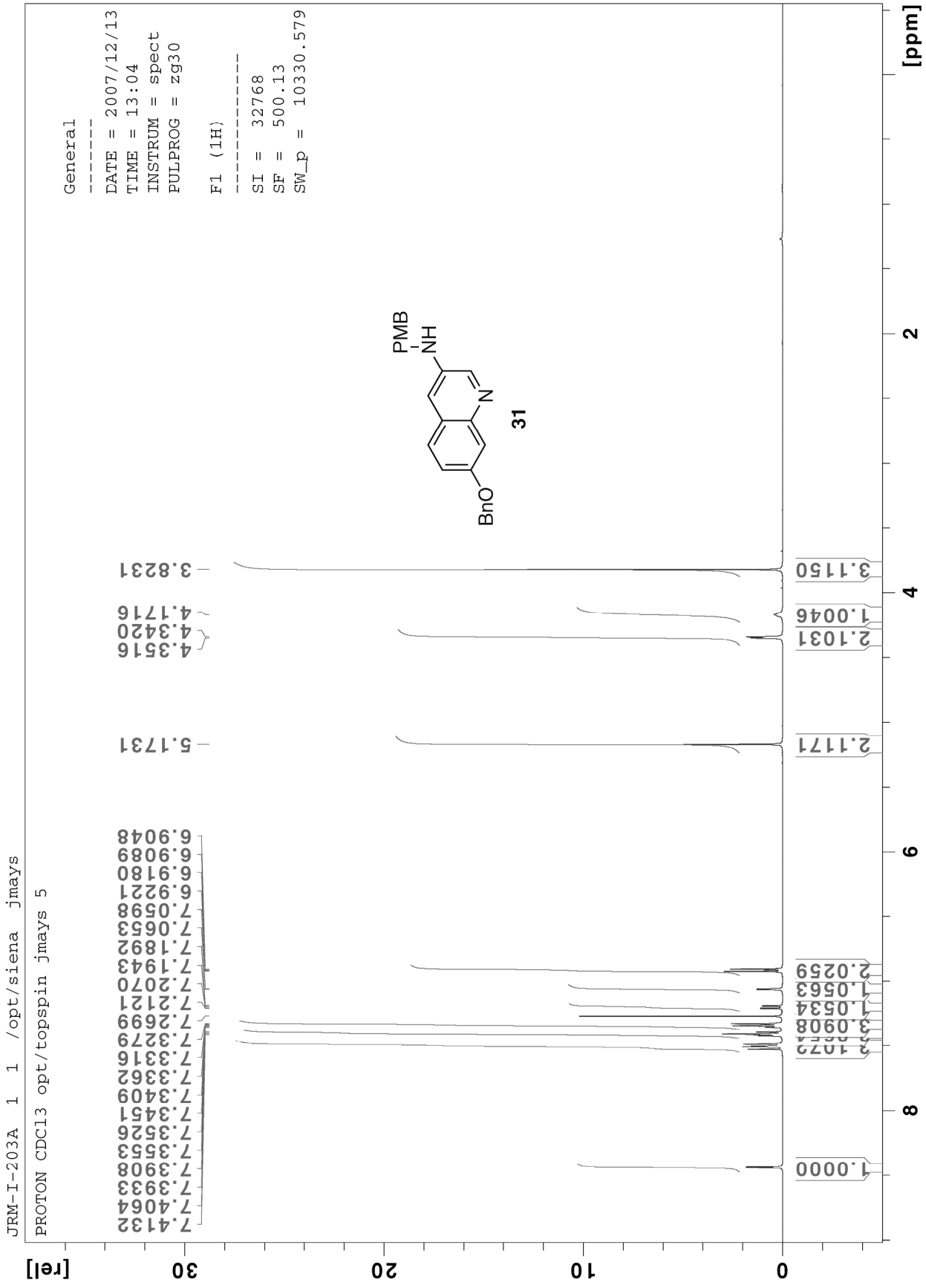

8OMEIND 2 1 /opt/siena adonn
C13CPD CD2C12 opt/topspin adonn 2
General
DATE = 2007/12/14
TIME = 10:09
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
22.2642
21.8209
163.8135
159.1008
157.6573
150.5523
143.2794
136.0301
135.8387
129.2219
126.8896
124.5643
122.8037
121.8016
121.6175
121.3513
120.2874
114.3553
112.4377
111.1478
103.0818
97.9636
83.2244
77.8527
73.9703
60.8874
58.6858
100.0000
MeO
HO
OH
OMe
26o
[rel]
[ppm]

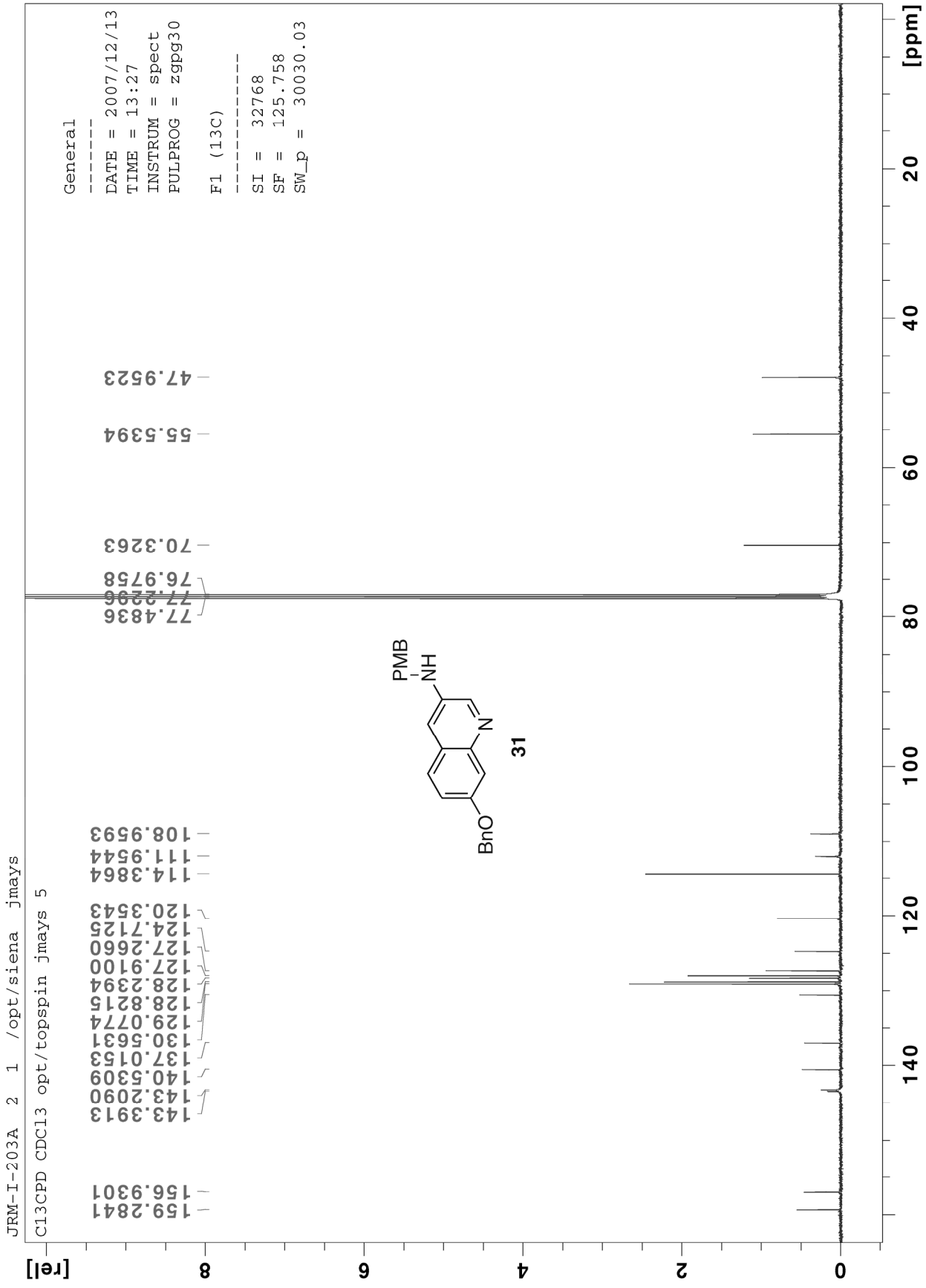

Et_indole 1 1 /opt/siena jburlis
PROTON CD2Cl2 opt/topspin jburlis 6
General
DATE = 2007/05/10
TIME = 13:25
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
26p
MeO
HO
HO
[rel]
[ppm]

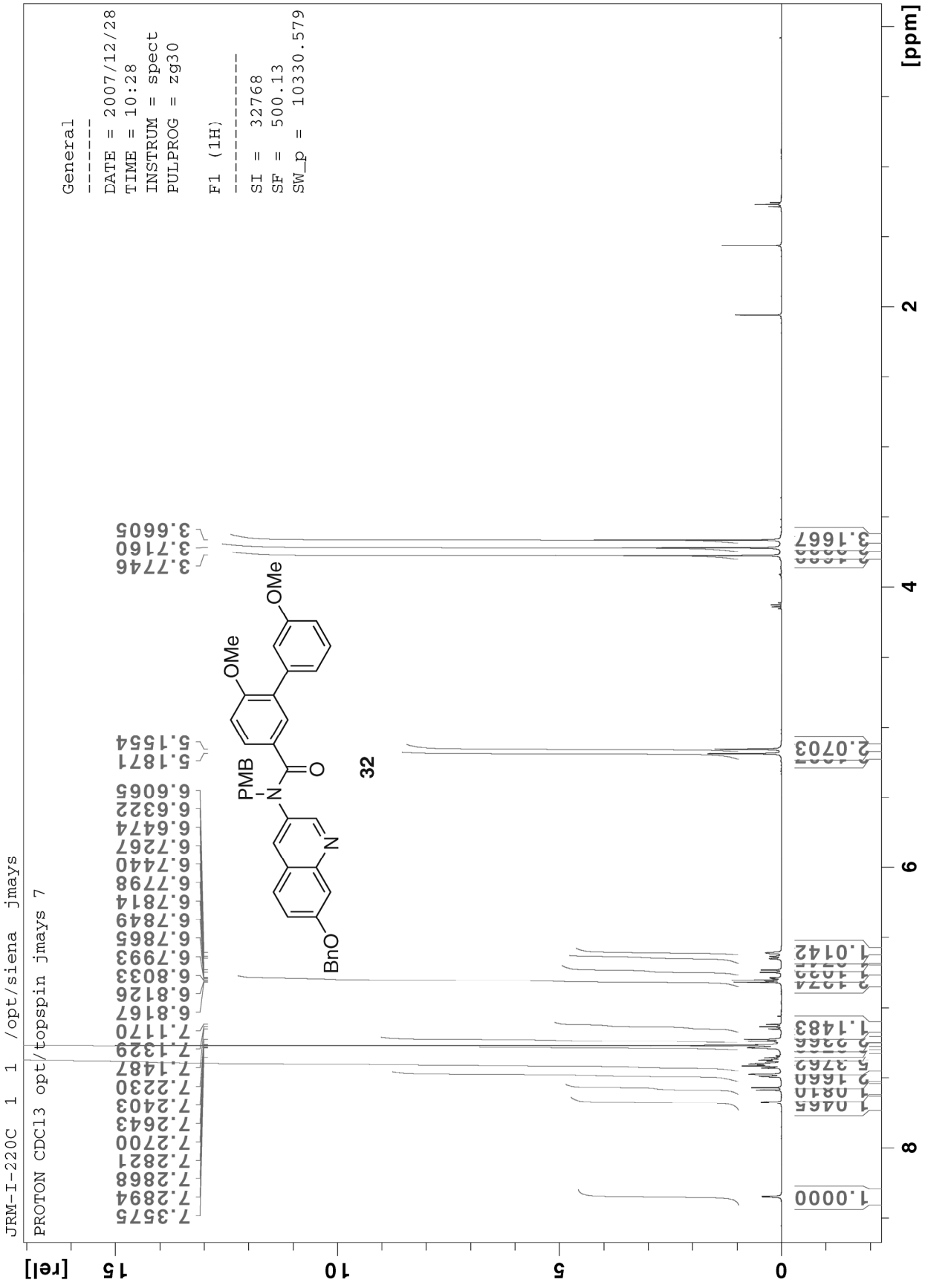

Et_indole 2 1 /opt/siena jburlis
C13CPD CD2Cl2 opt/topspin jburlis 6
General
DATE = 2007/05/10
TIME = 13:42
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
158.3541
157.3076
154.2122
146.8032
135.2492
128.0970
125.4463
123.9910
122.9767
122.8174
120.1206
119.4787
118.6776
118.2021
111.9838
110.0783
109.6995
102.3488
97.0116
82.1187
76.5374
69.3208
66.4094
59.5473
47.1346
46.9631
46.2803
46.1098
26.6472
20.3424
27.8566
69.6435
2.4999
26p
MeO
HO
OH
[rel]
[ppm]

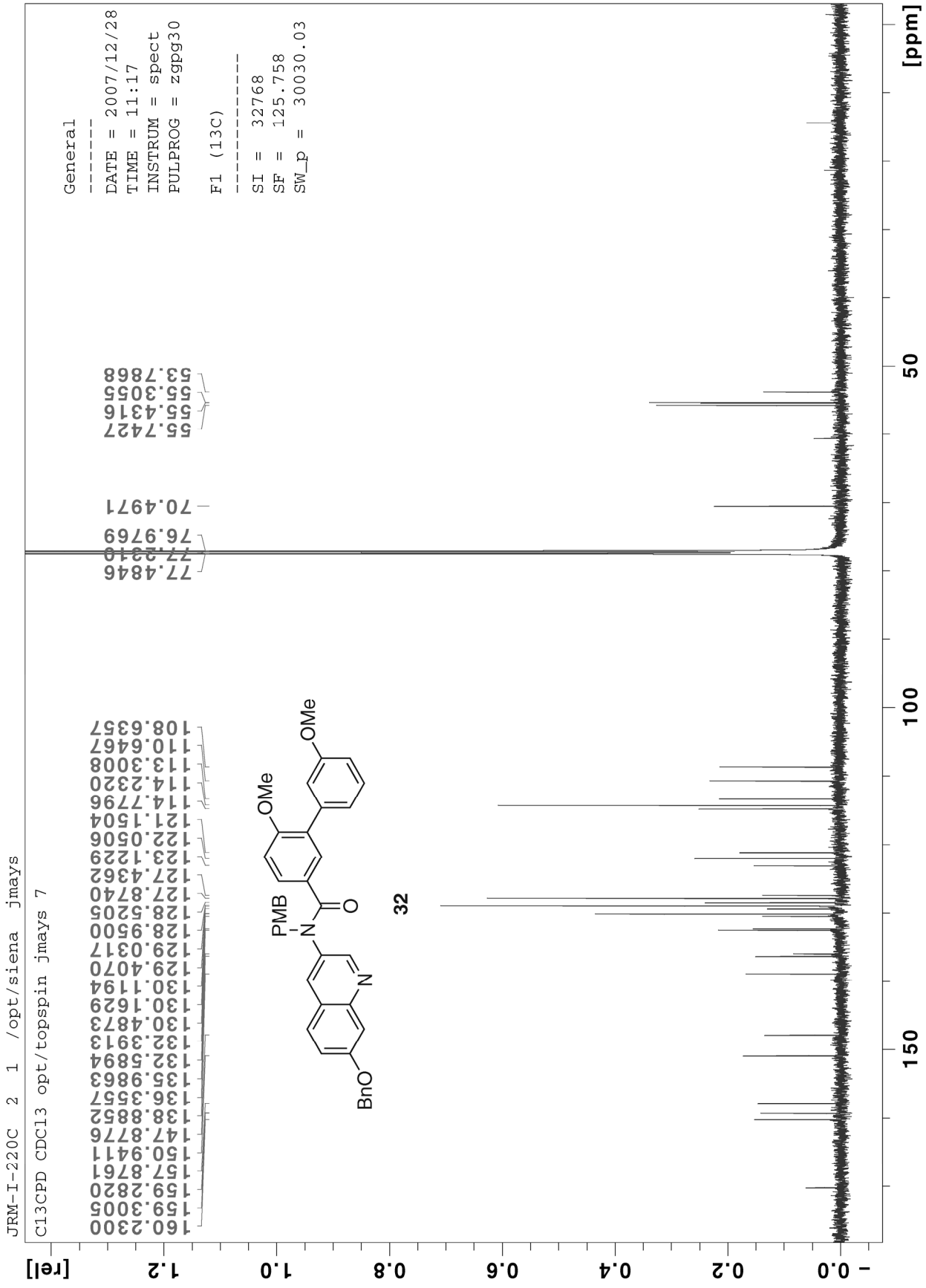

JRM-I-108B 1 1 /opt/siena jmays
PROTON CDC13 opt/topspin jmays 11
General
DATE = 2007/09/04
TIME = 18:00
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
8.9359
8.9308
8.9274
8.1803
8.1638
7.9061
7.9016
7.8518
7.8340
7.4441
7.4394
7.4264
7.4216
7.4168
7.4083
7.4002
7.3918
7.2701
1.6029
9.5944
2.0743
1.0704
1.0427
1.0000
BocO
N
28
[rel]
[ppm]

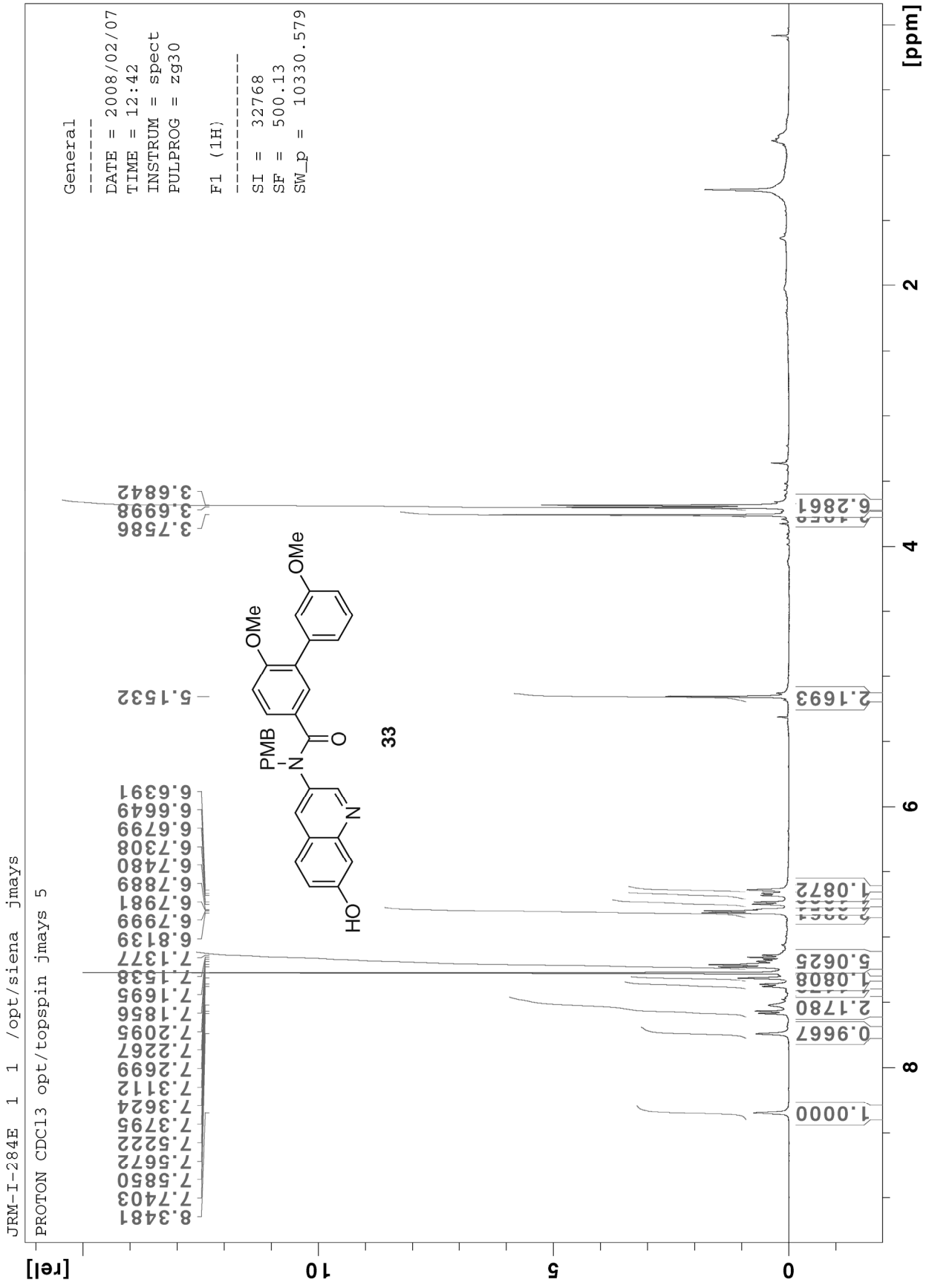

JRM-I-108B 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 11
General
DATE = 2007/09/04
TIME = 18:51
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
151.6795
151.6653
151.2267
148.8790
135.9146
128.9940
126.3359
121.9694
121.0148
120.1986
84.1786
77.3833
77.3362
76.8748
BocO
N
28
[rel]
[ppm]

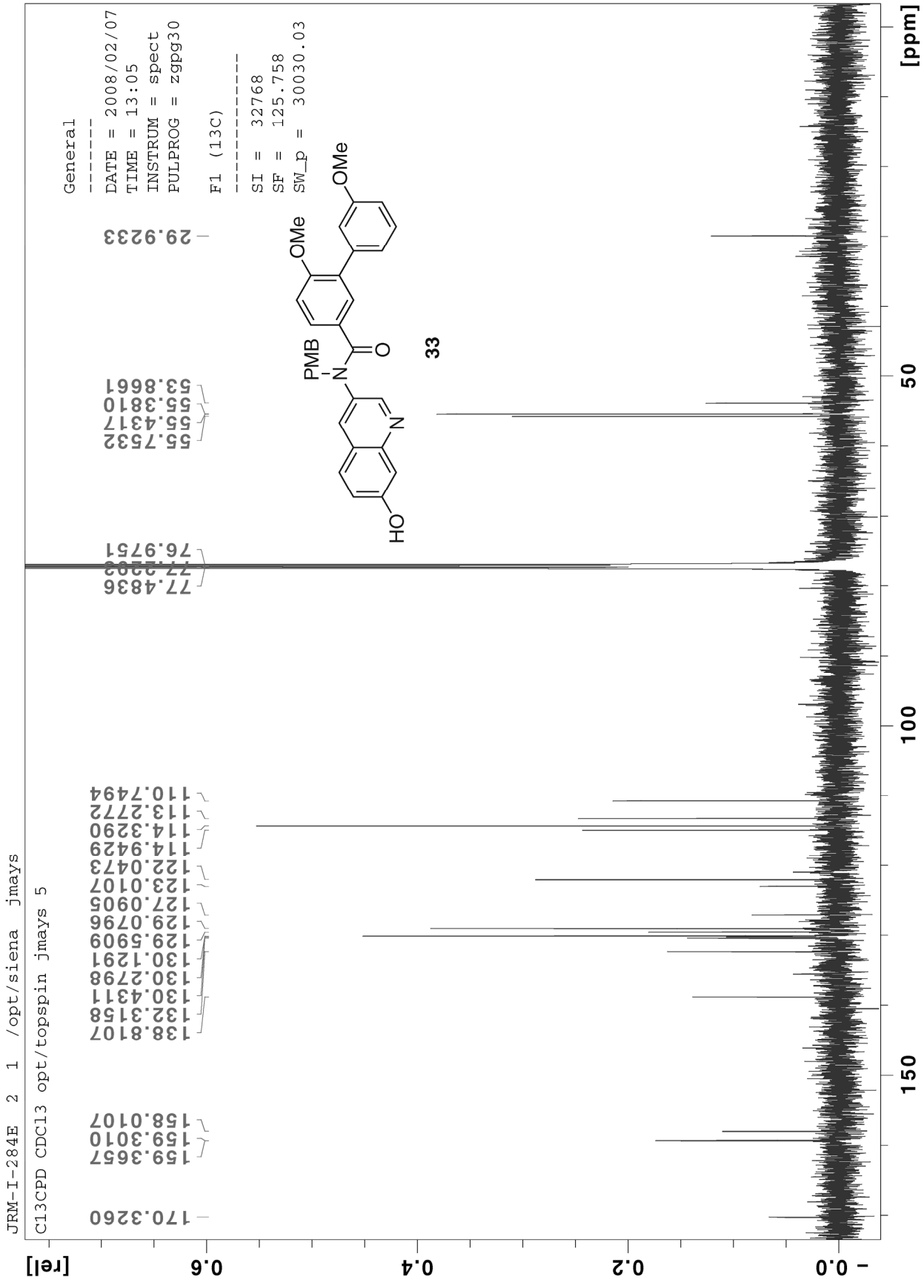

JRM-I-203A 1 1 /opt/siena jmays
PROTON CDCl3 opt/topspin jmays 5
General
DATE = 2007/12/13
TIME = 13:04
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
PMB
NH
N
BnO
31
[rel]
[ppm]
7.4132
7.4064
7.3933
7.3908
7.3553
7.3526
7.3451
7.3409
7.3362
7.3316
7.3279
7.2699
7.2121
7.2070
7.1943
7.1892
7.0653
7.0598
6.9221
6.9180
6.9089
6.9048
5.1731
4.3516
4.3420
4.1716
3.8231
1.0000
2.1171
3.1150
1.0046
2.1031
3.0908
1.0534
1.0563
2.0259

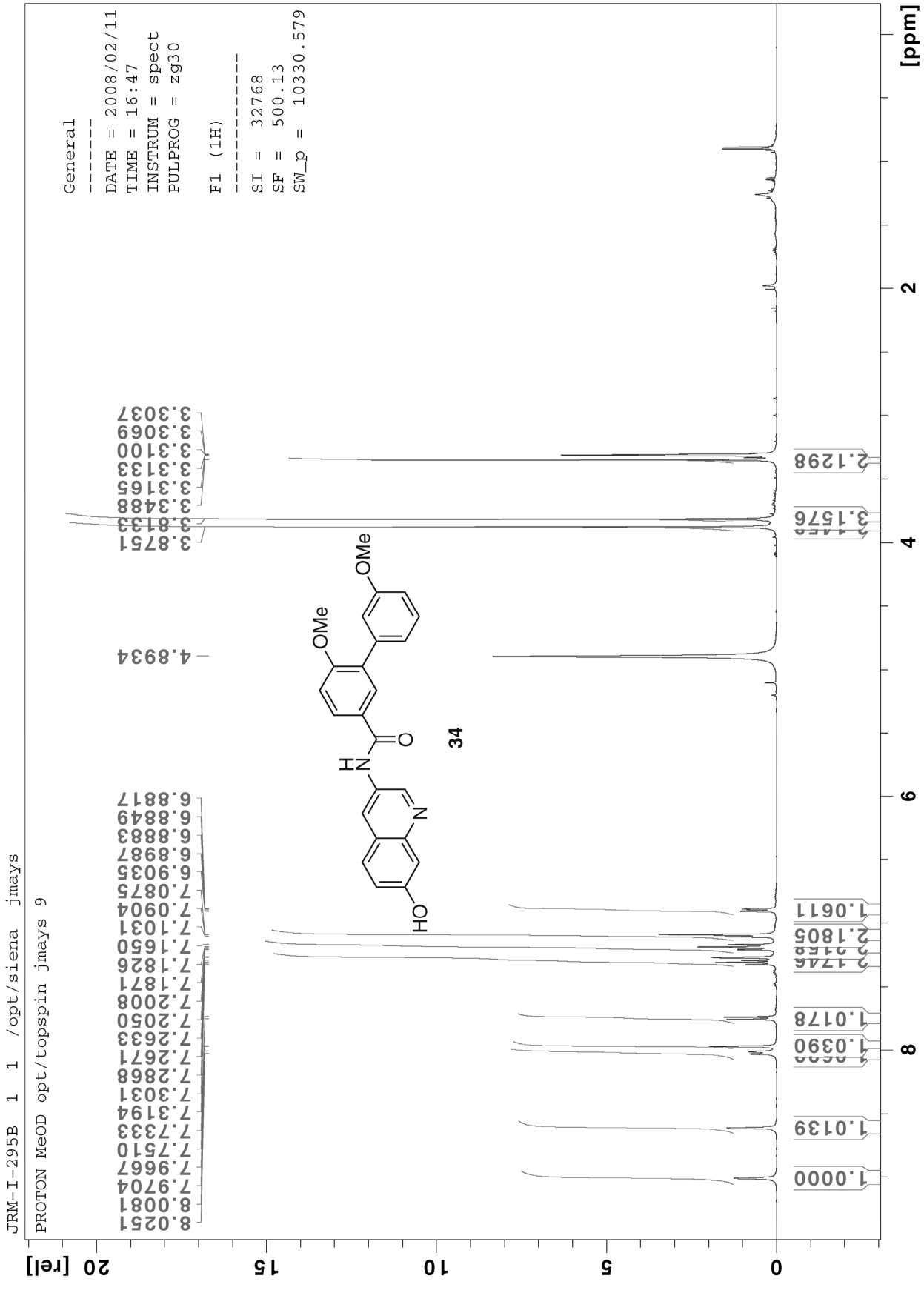

JRM-I-203A 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 5
General
DATE = 2007/12/13
TIME = 13:27
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
47.9523
55.5394
70.3263
76.9758
77.2296
77.4836
108.9593
111.9544
114.3864
120.3543
124.7125
127.2660
127.9100
128.2394
128.8215
129.0774
130.5631
137.0153
140.5309
143.2090
143.3913
159.2841
156.9301
PMB
NH
N
BnO
31
[rel]
[ppm]

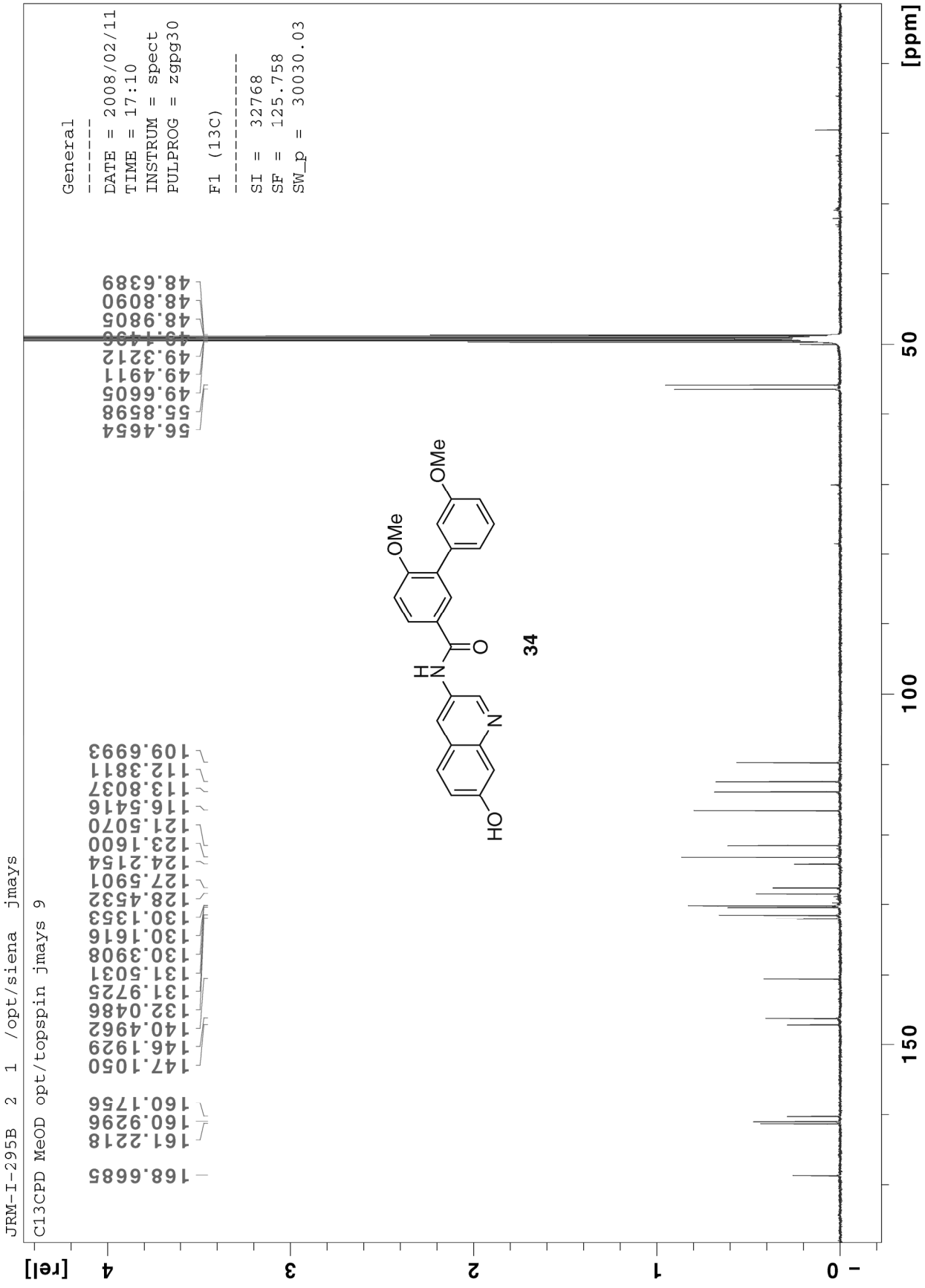

JRM-I-220C 1 1 /opt/siena jmays
PROTON CDCl3 opt/topspin jmays 7
General
DATE = 2007/12/28
TIME = 10:28
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
[rel]
[ppm]
PMB
OMe
OMe
BnO
32

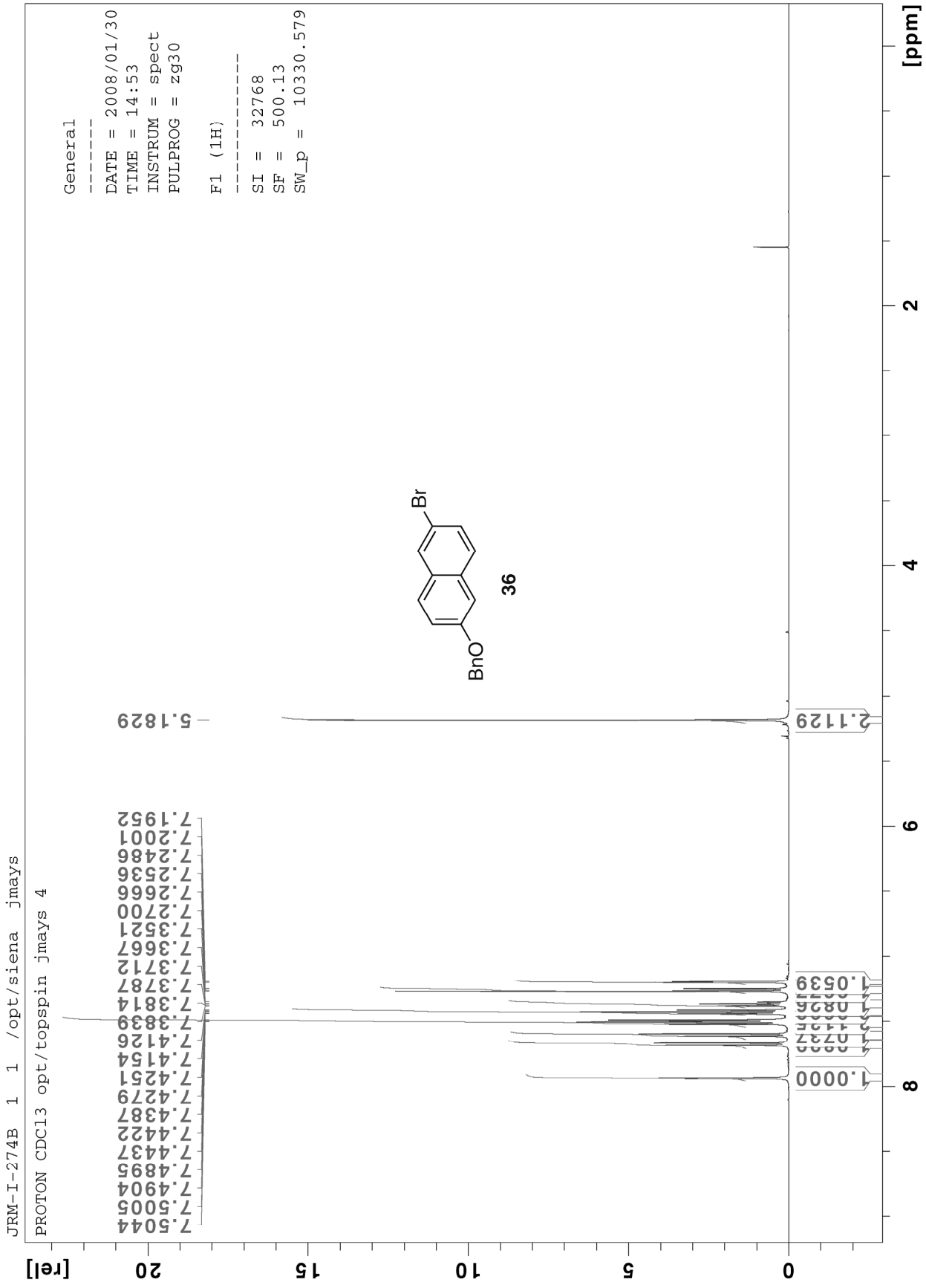

JRM-I-220C 2 1 /opt/siena jmays
C13CPD CDC13 opt/topspin jmays 7
General
DATE = 2007/12/28
TIME = 11:17
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
160.2300
159.3005
159.2820
157.8761
150.9411
147.8776
138.8852
136.3557
135.9863
132.5894
132.3913
130.4873
130.1629
130.1194
129.4070
129.0317
128.9500
128.5205
127.8740
127.4362
123.1229
122.0506
121.1504
114.7796
114.2320
113.3008
110.6467
108.6357
77.4846
77.2310
76.9769
70.4971
55.7427
55.4316
55.3055
53.7868
OMe
OMe
PMB
N
O
N
BnO
32
[rel]
1.2
1.0
0.8
0.6
0.4
0.2
0.0
150
100
50
[ppm]

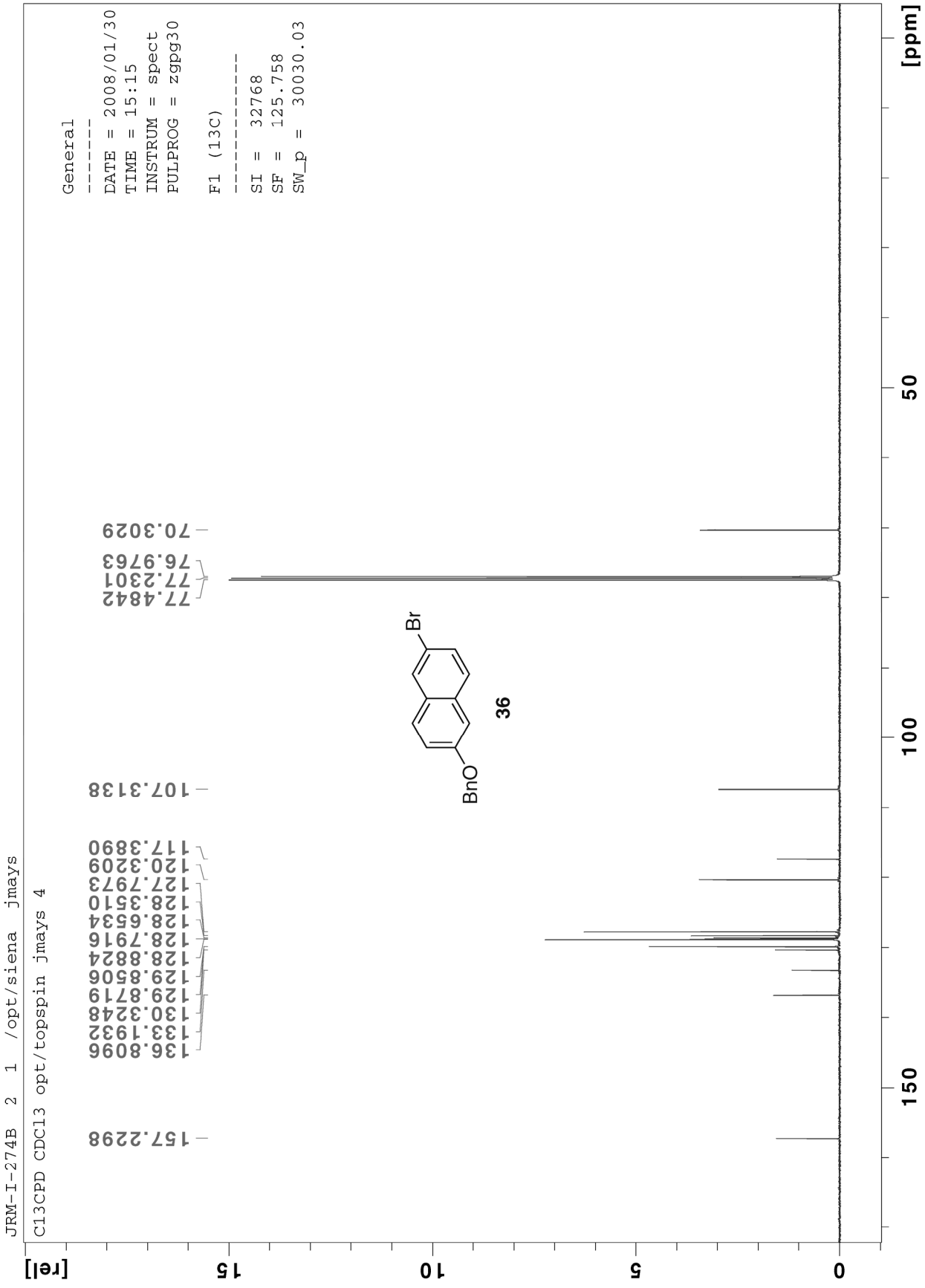

JRM-I-284E 1 1 /opt/siena jmays
PROTON CDCl3 opt/topspin jmays 5
General
DATE = 2008/02/07
TIME = 12:42
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
8.3481
7.7403
7.5850
7.5672
7.5222
7.3795
7.3624
7.3112
7.2699
7.2267
7.2095
7.1856
7.1695
7.1538
7.1377
6.8139
6.7999
6.7981
6.7889
6.7480
6.7308
6.7799
6.6649
6.6391
5.1532
3.7586
3.6998
3.6842
1.0000
0.9667
2.1780
1.0808
5.0625
1.0872
2.1693
6.2861
PMB
N
O
OMe
OMe
HO
N
33
[rel]
10
5
0
8
6
4
2
[ppm]

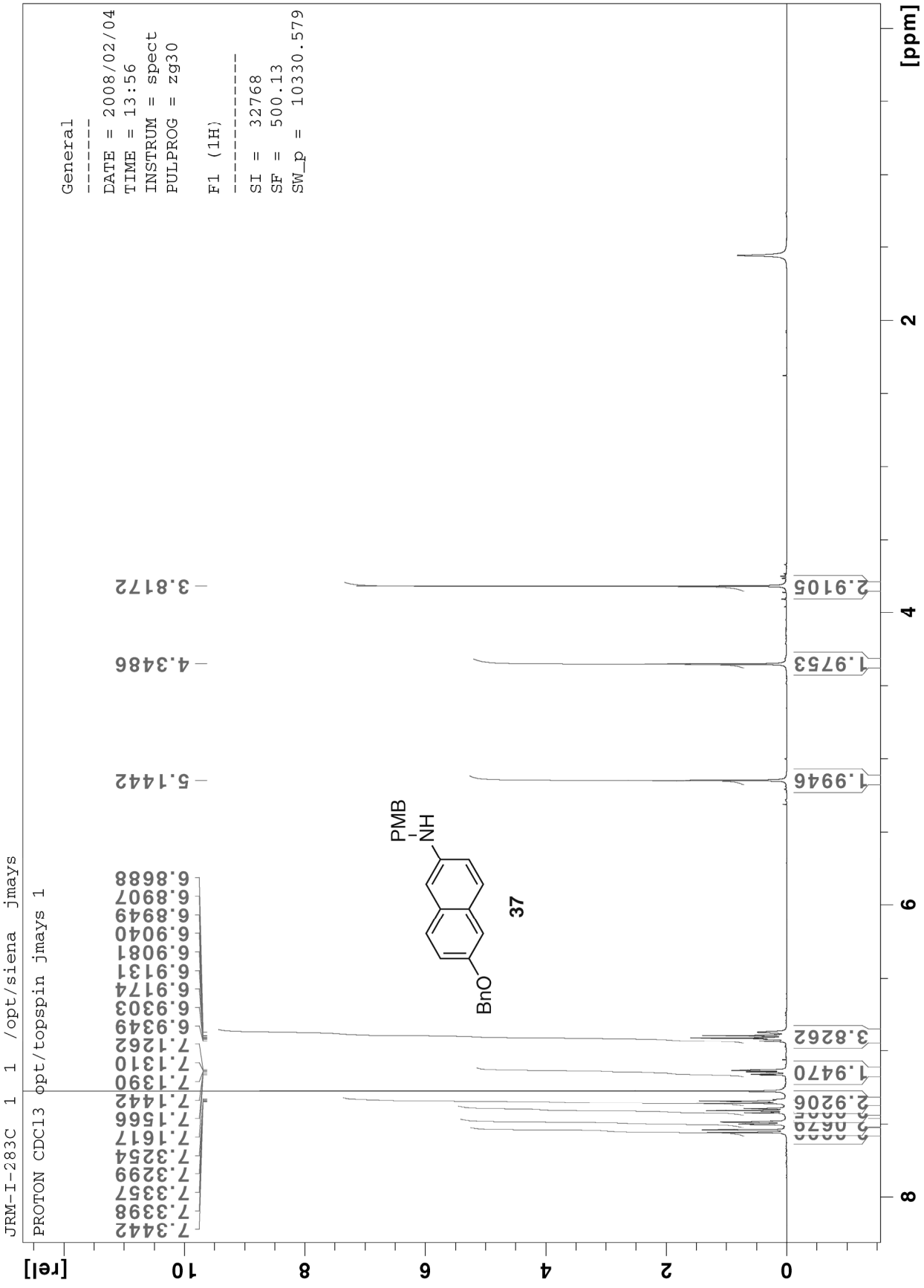

JRM-I-284E 2 1 /opt/siena jmays
C13CPD CDC13 opt/topspin jmays 5
General
DATE = 2008/02/07
TIME = 13:05
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
29.9233
53.8661
55.3810
55.4317
55.7532
76.9751
77.2302
77.4836
110.7494
113.2772
114.3290
114.9429
122.0473
123.0107
127.0905
129.0796
129.5909
130.1291
130.2798
130.4311
132.3158
138.8107
158.0107
159.3010
159.3657
170.3260
PMB
OMe
OMe
HO
33
[rel]
0.0
0.2
0.4
0.6
150
100
50
[ppm]

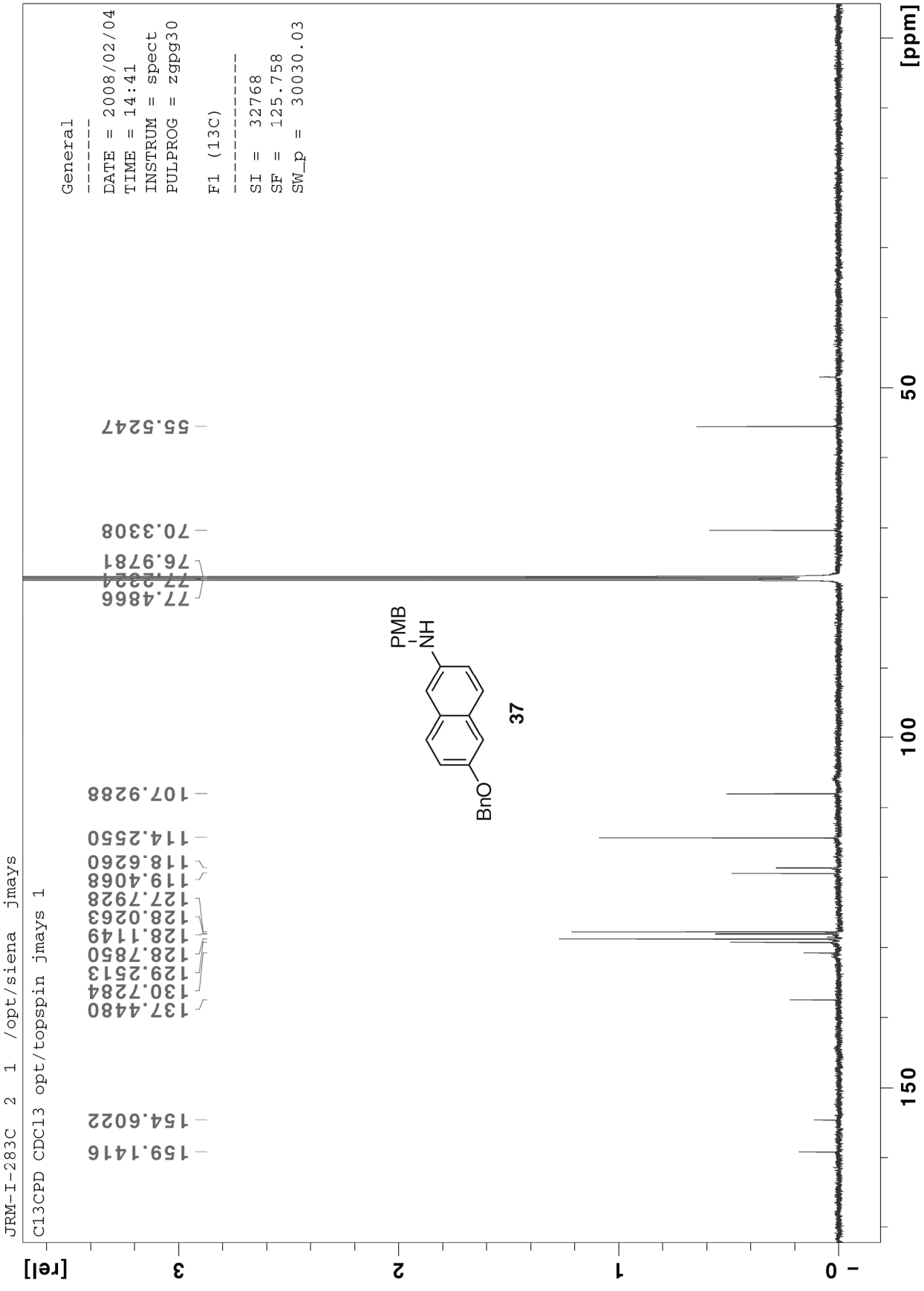

JRM-I-295B 1 1 /opt/siena jmays
PROTON MeOD opt/topspin jmays 9
General
DATE = 2008/02/11
TIME = 16:47
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
8.0251
8.0081
7.9704
7.9667
7.7510
7.7333
7.3194
7.3031
7.2868
7.2671
7.2633
7.2050
7.2008
7.1871
7.1826
7.1650
7.1031
7.0904
7.0875
6.9035
6.8987
6.8883
6.8849
6.8817
4.8934
3.8751
3.8133
3.3488
3.3165
3.3133
3.3100
3.3069
3.3037
1.0000
1.0139
1.0390
1.0178
2.1805
1.0611
2.1298
3.1576
OMe
OMe
HO
N
H
O
N
34
[rel]
20
15
10
5
0
8
6
4
2
[ppm]

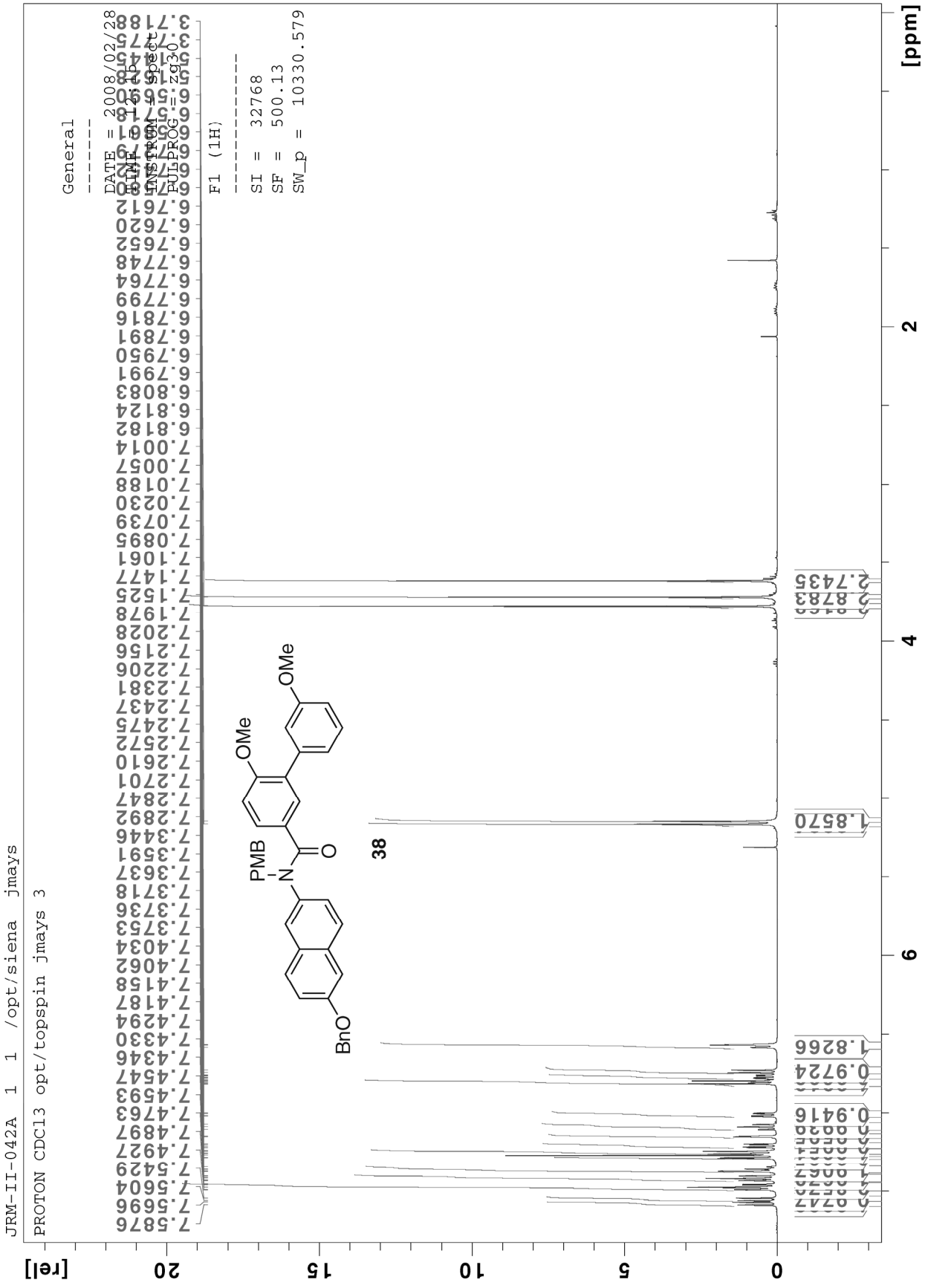

JRM-I-295B 2 1 /opt/siena jmays
C13CPD MeOD opt/topspin jmays 9
General
DATE = 2008/02/11
TIME = 17:10
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
168.6685
161.2218
160.9296
160.1756
147.1050
146.1929
140.4962
132.0486
131.9725
131.5031
130.3908
130.1616
130.1353
128.4532
127.5901
124.2154
123.1600
121.5070
116.5416
113.8037
112.3811
109.6993
56.4654
55.8598
49.6605
49.4911
49.3212
49.1436
48.9805
48.8090
48.6389
OMe
OMe
HO
N
H
N
O
34
[rel]
4
3
2
1
0
150
100
50
[ppm]

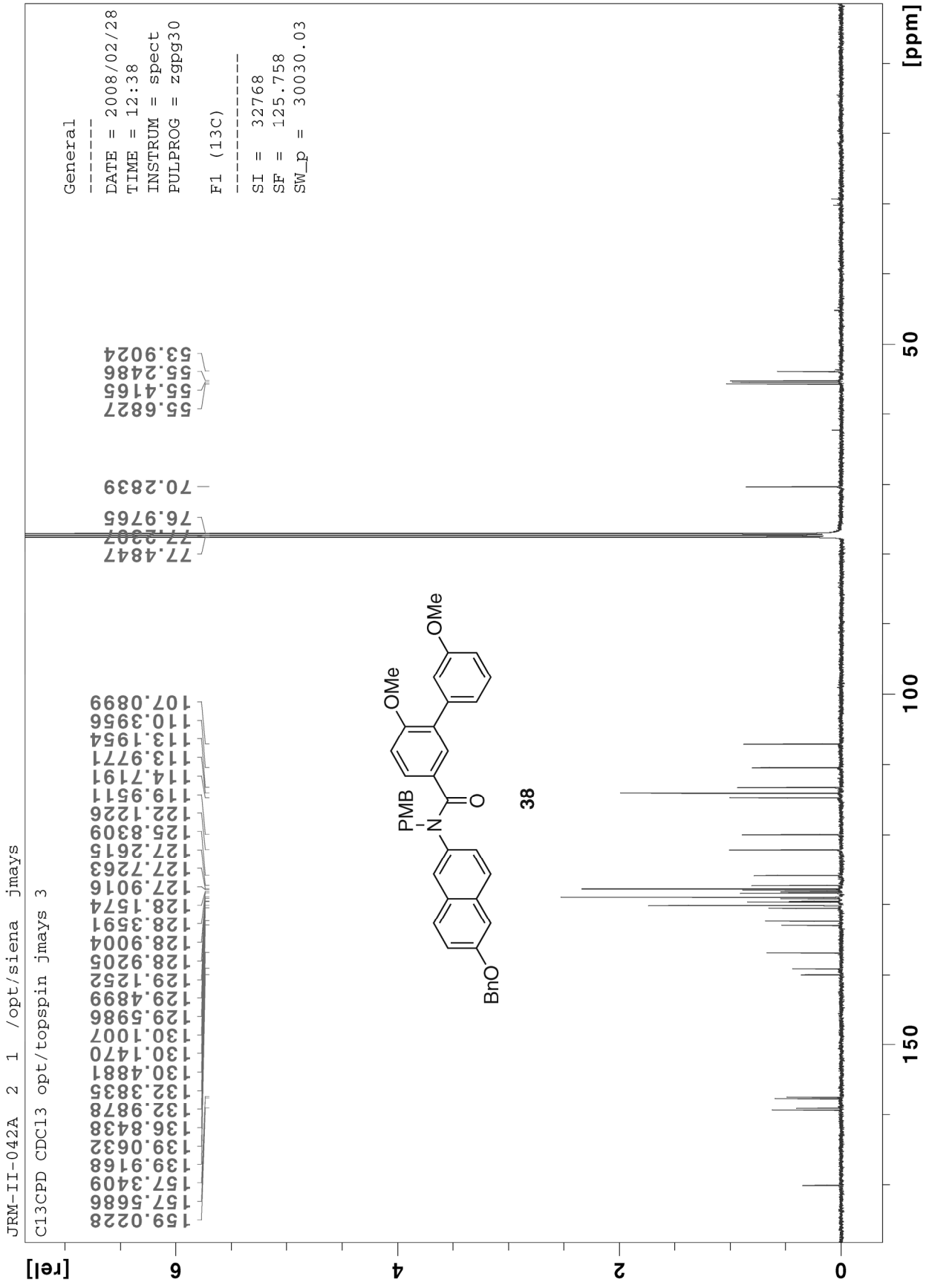

JRM-I-274B 1 1 /opt/siena jmays
PROTON CDCl3 opt/topspin jmays 4
General
DATE = 2008/01/30
TIME = 14:53
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
7.5044
7.5005
7.4904
7.4895
7.4437
7.4422
7.4387
7.4279
7.4251
7.4154
7.4126
7.3839
7.3814
7.3787
7.3712
7.3667
7.3521
7.2700
7.2666
7.2536
7.2486
7.2001
7.1952
5.1829
1.0000
1.0539
2.1129
Br
BnO
36
[rel]
20
15
10
5
0
8
6
4
2
[ppm]

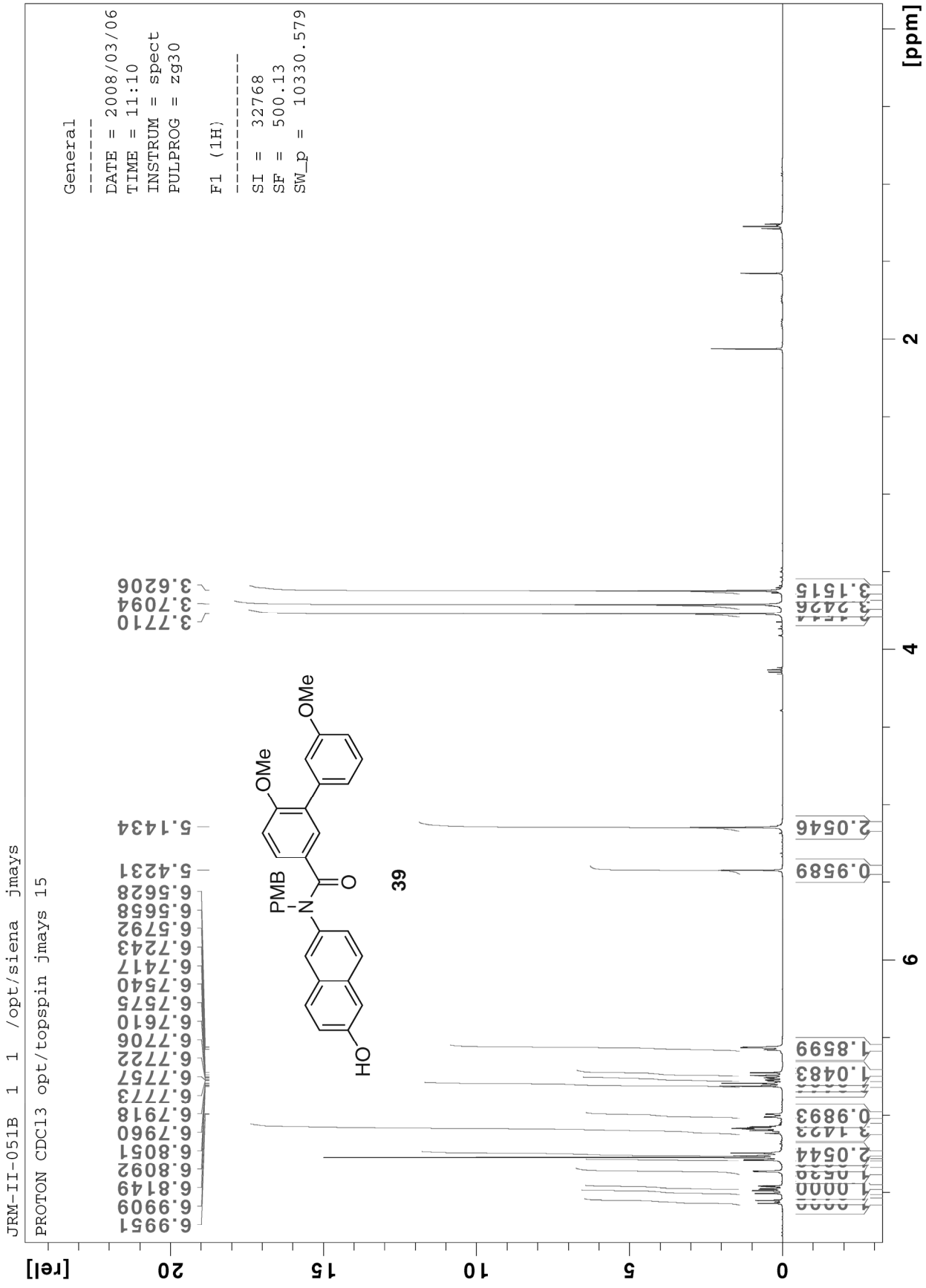

JRM-I-274B 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 4
General
DATE = 2008/01/30
TIME = 15:15
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
157.2298
136.8096
133.1932
130.3248
129.8719
129.8506
128.8824
128.7916
128.6534
128.3510
127.7973
120.3209
117.3890
107.3138
77.4842
77.2301
76.9763
70.3029
Br
BnO
36
[rel]
[ppm]

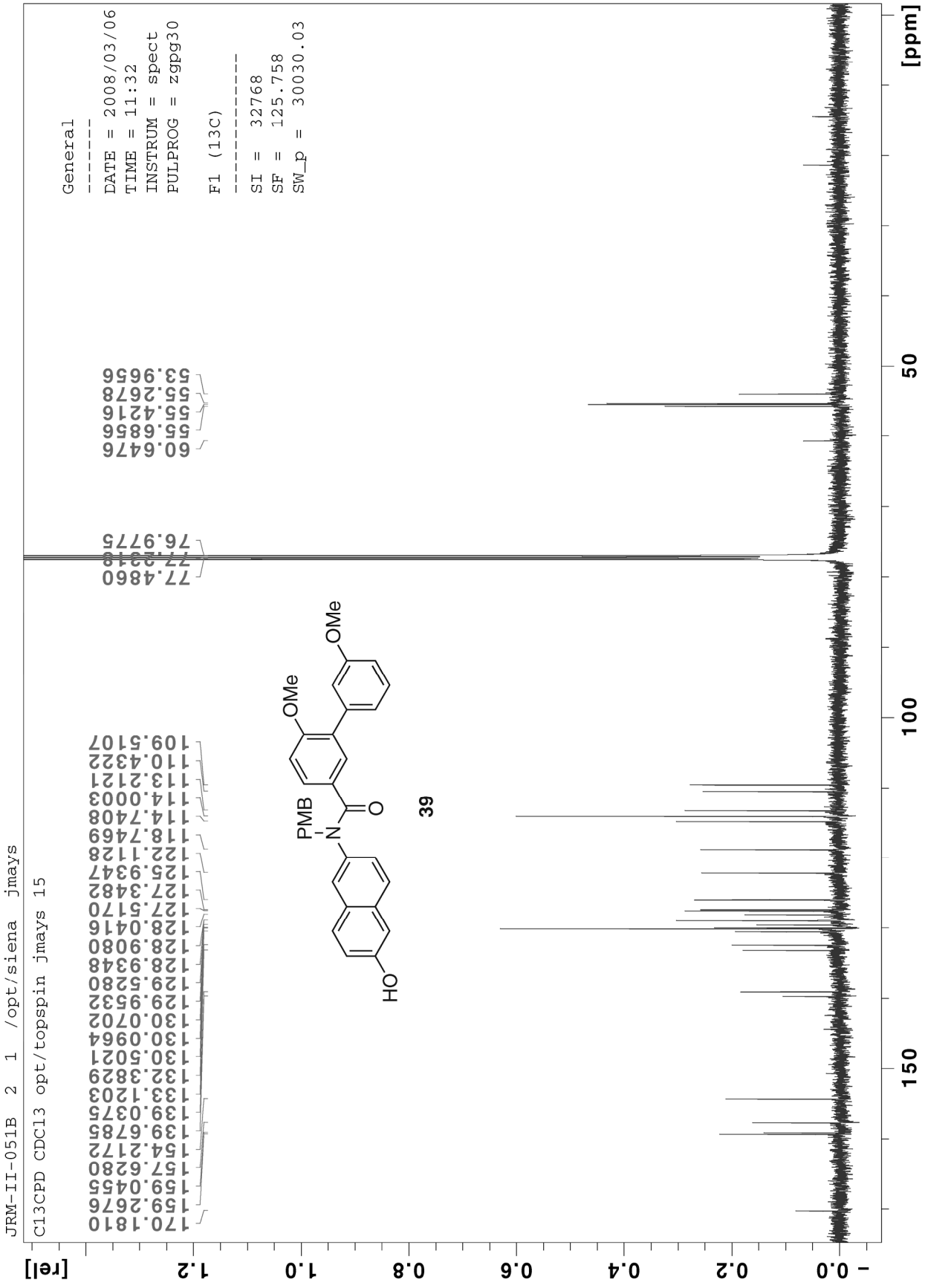

JRM-I-283C 1 1 /opt/siena jmays
PROTON CDCl3 opt/topspin jmays 1
General
DATE = 2008/02/04
TIME = 13:56
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
7.3442
7.3398
7.3357
7.3299
7.3254
7.1617
7.1566
7.1442
7.1390
7.1310
7.1262
6.9349
6.9303
6.9174
6.9131
6.9081
6.9040
6.8949
6.8907
6.8688
5.1442
4.3486
3.8172
2.9105
1.9753
1.9946
3.8262
1.9470
2.9206
PMB
NH
BnO
37
[rel]
[ppm]

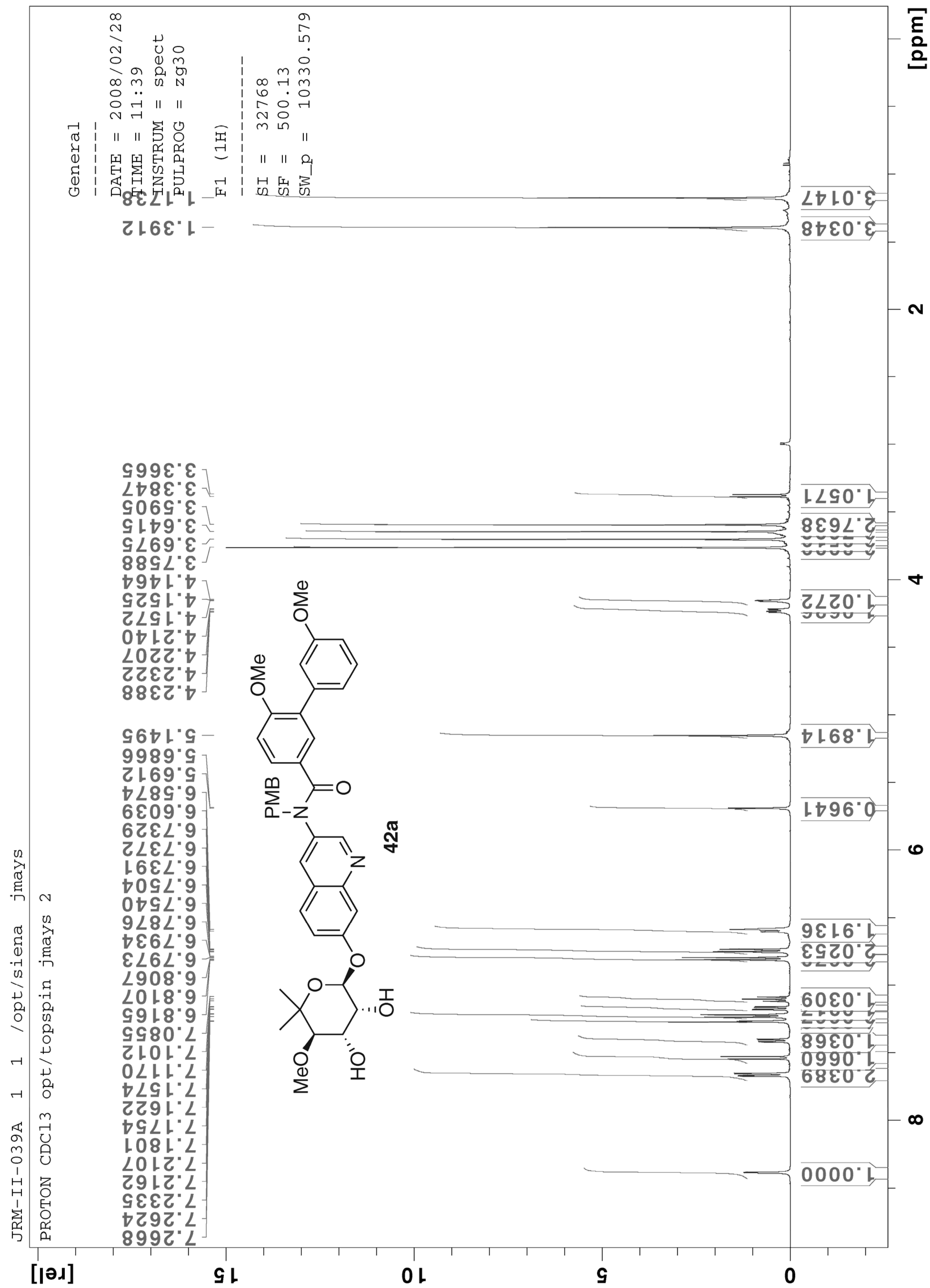

JRM-I-283C 2 1 /opt/siena jmays
C13CPD CDC13 opt/topspin jmays 1
General
DATE = 2008/02/04
TIME = 14:41
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
55.5247
70.3308
76.9781
77.2334
77.4866
107.9288
114.2550
118.6260
119.4068
127.7928
128.0263
128.1149
128.7850
129.2513
130.7284
137.4480
154.6022
159.1416
PMB
NH
BnO
37
[rel]
[ppm]


JRM-II-042A 1 1 /opt/siena jmays
PROTON CDC13 opt/topspin jmays 3
General
DATE = 2008/02/28
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
OMe
OMe
PMB
N
O
BnO
38
1.8570
1.8266
0.9724
0.9416
2.7435
[rel]
[ppm]

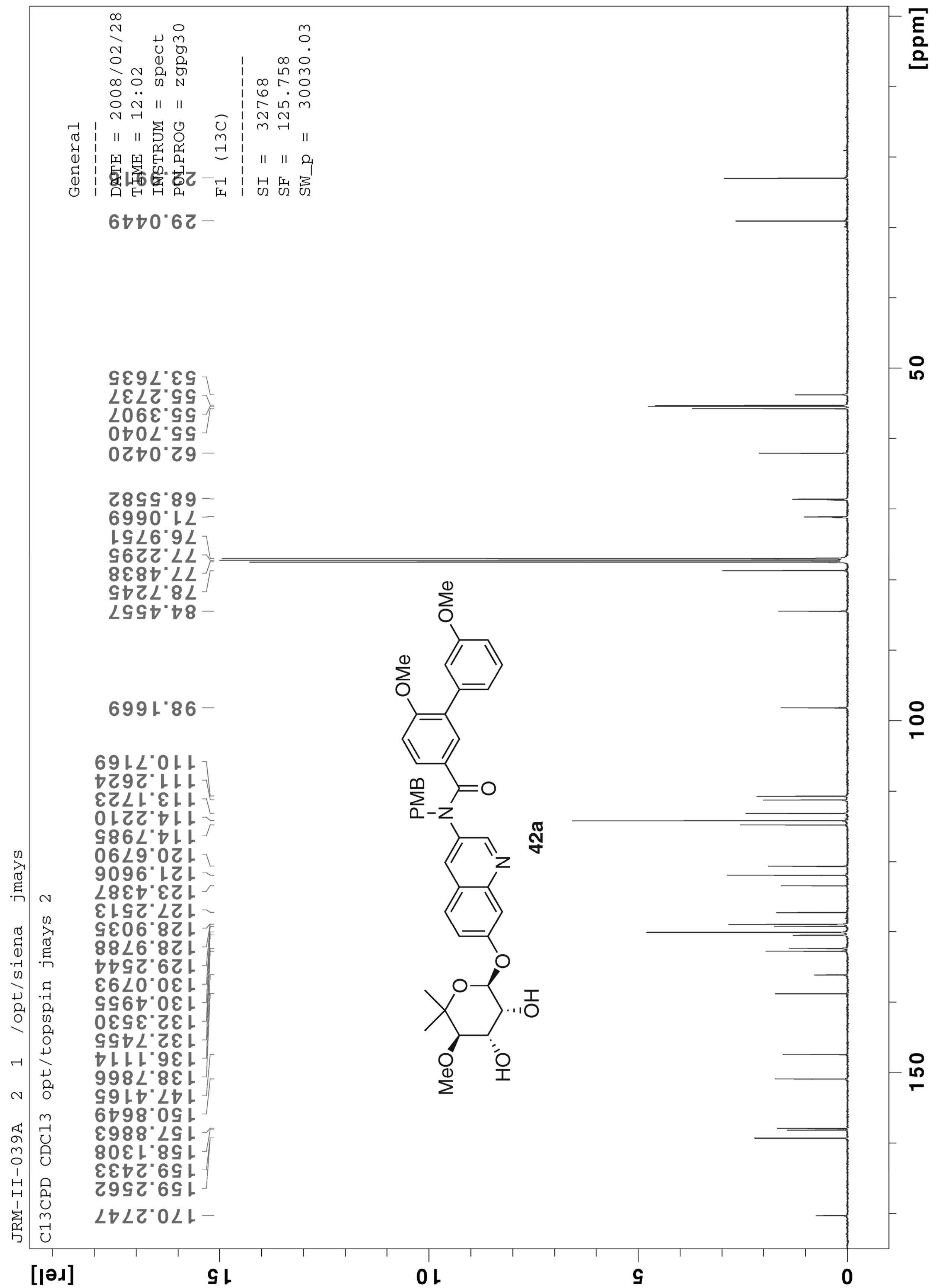

JRM-II-042A 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 3
General
DATE = 2008/02/28
TIME = 12:38
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
159.0228
157.5686
157.3409
139.9168
139.0632
136.8438
132.9878
132.3835
130.4881
130.1470
130.1007
129.5986
129.4899
129.1252
128.9205
128.9004
128.3591
128.1574
127.9016
127.7263
127.2615
125.8309
122.1226
119.9511
114.7191
113.9771
113.1954
110.3956
107.0899
77.4847
77.2307
76.9765
70.2839
55.6827
55.4165
55.2486
53.9024
OMe
OMe
PMB
N
O
BnO
38
[rel]
6
4
2
0
150
100
50
[ppm]

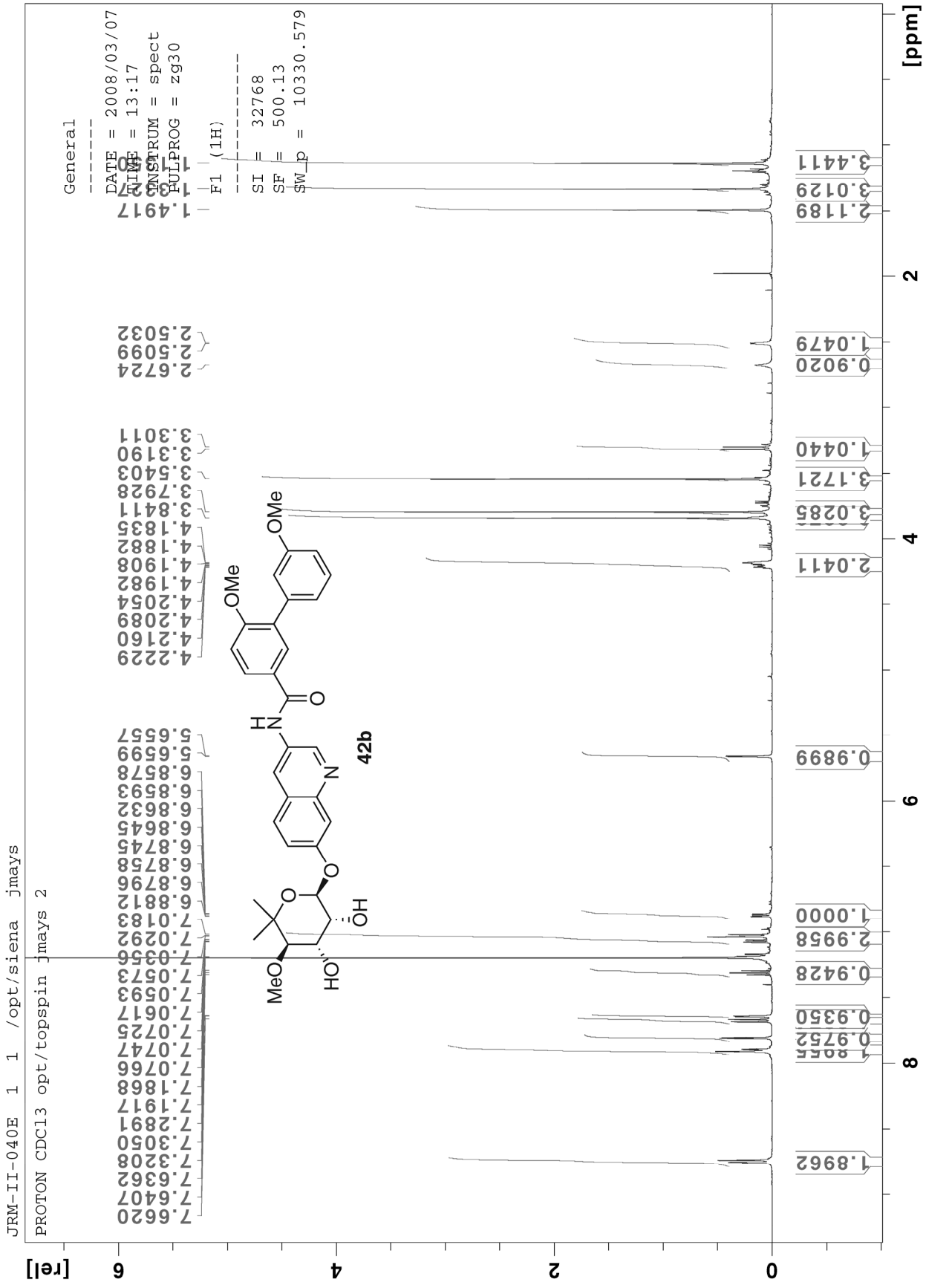

JRM-II-051B 1 1 /opt/siena jmays
PROTON CDCl3 opt/topspin jmays 15
General
DATE = 2008/03/06
TIME = 11:10
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
OMe
OMe
PMB
N
O
HO
39
[rel]
[ppm]

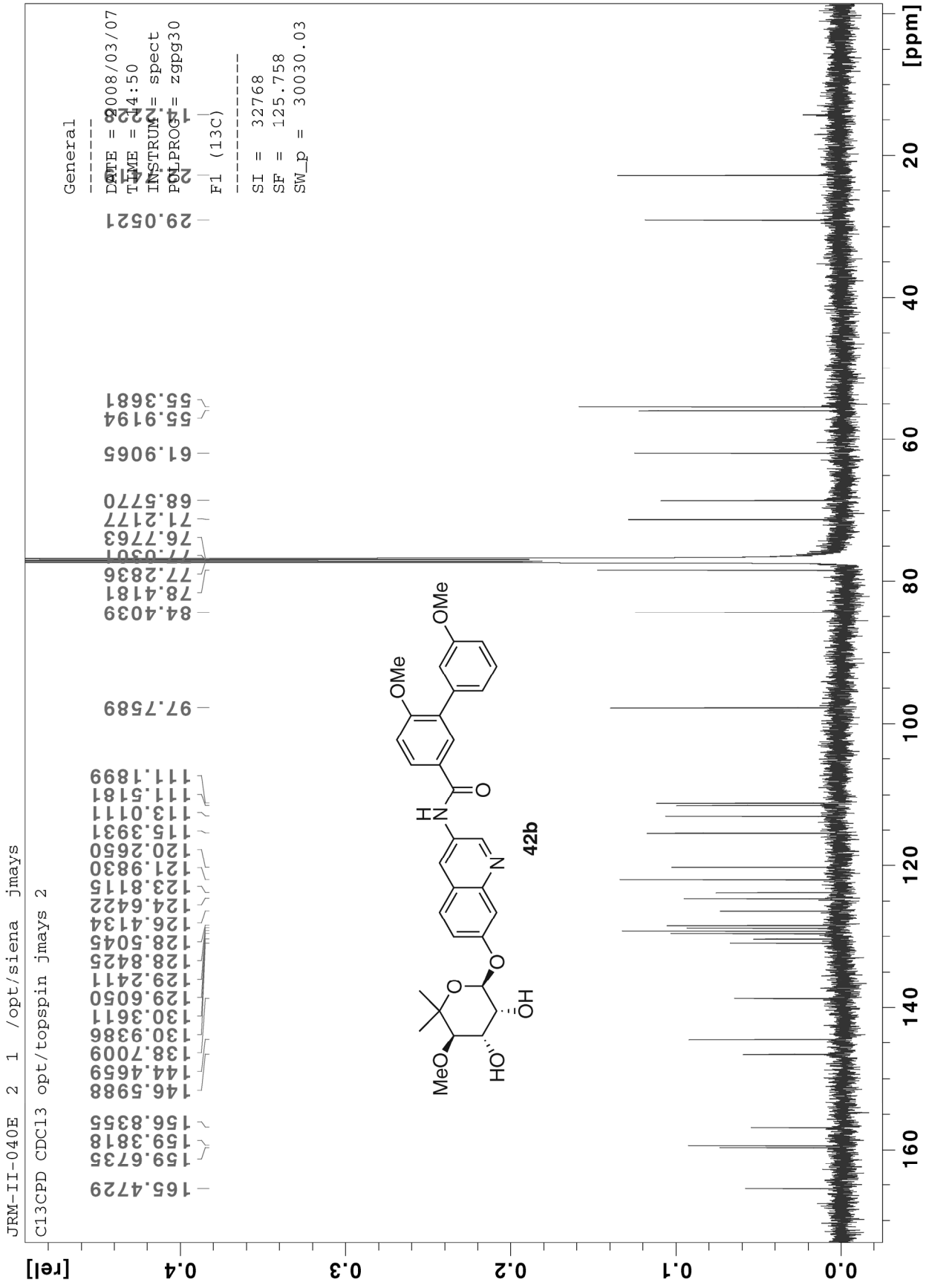

JRM-II-051B 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 15
General
DATE = 2008/03/06
TIME = 11:32
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
170.1810
159.2676
159.0455
157.6280
154.2172
139.6785
139.0375
133.1203
132.3829
130.5021
130.0964
130.0702
129.9532
129.5280
128.9348
128.9080
128.0416
127.5170
127.3482
125.9347
122.1128
118.7469
114.7408
114.0003
113.2121
110.4322
109.5107
77.4860
77.2318
76.9775
60.6476
55.6856
55.4216
55.2678
53.9656
OMe
OMe
PMB
N
O
HO
39
[rel]
[ppm]

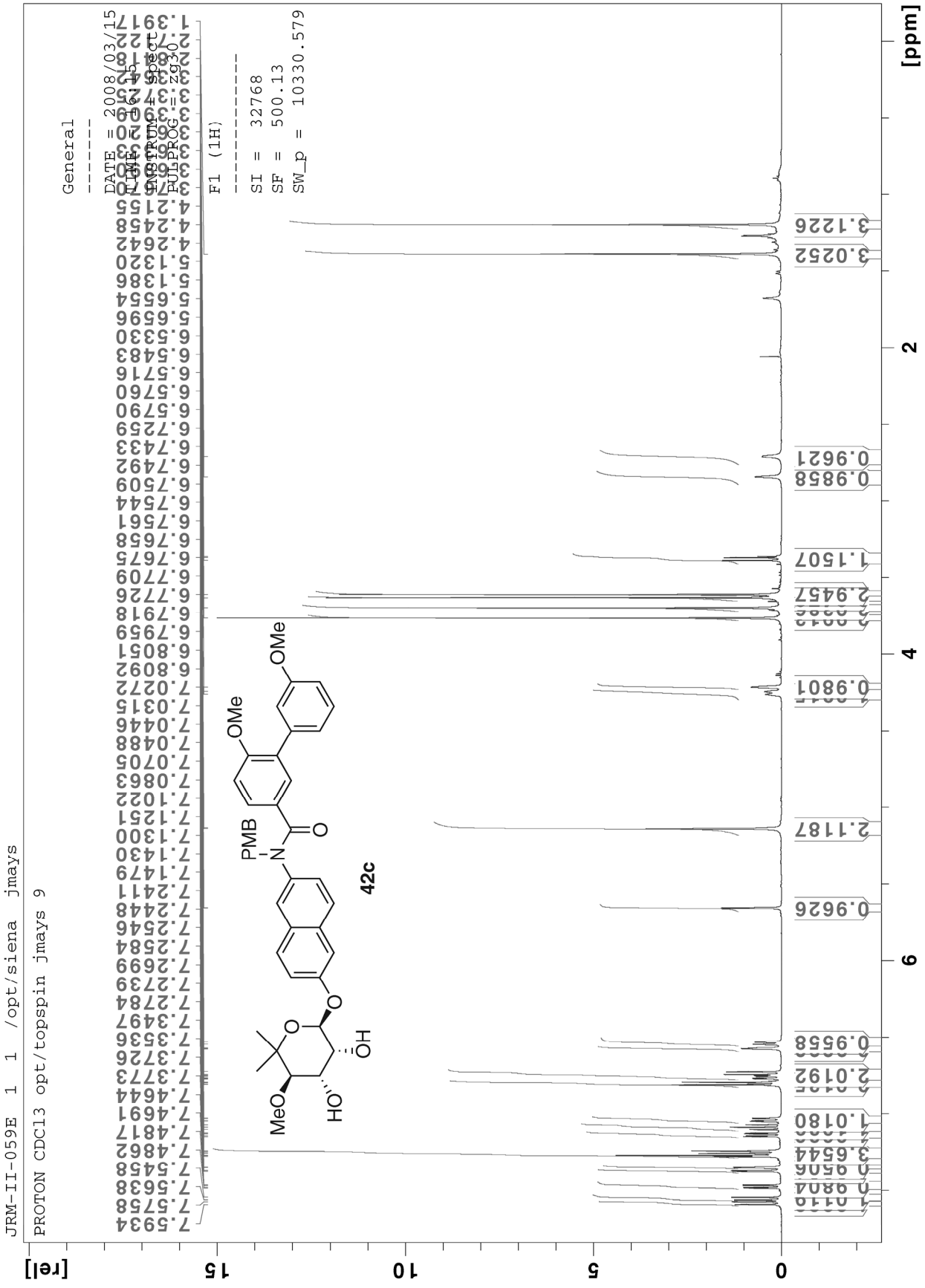


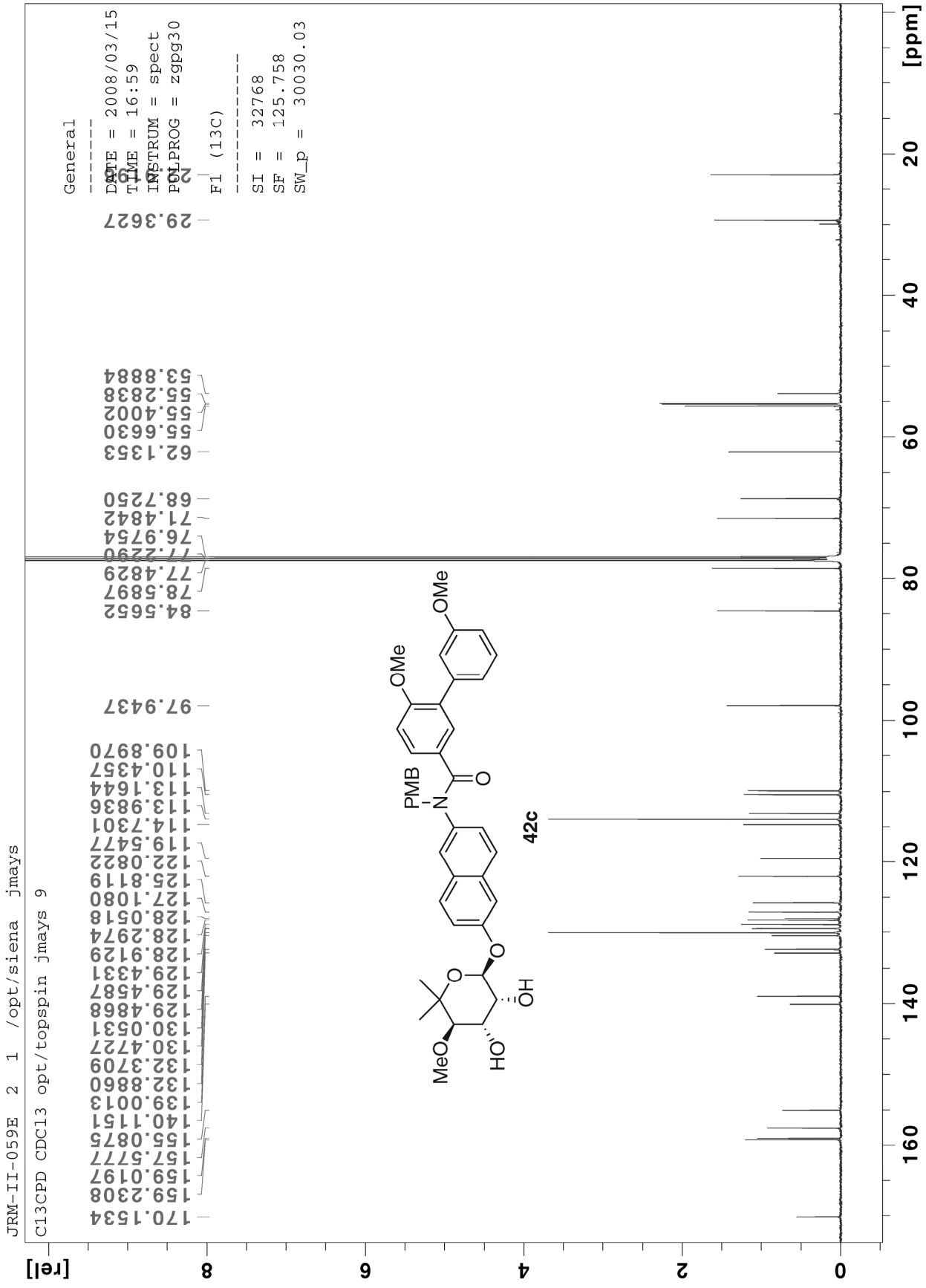
JRM-II-039A 1 1 /opt/siena jmays
PROTON CDCl3 opt/topspin jmays 2
General
DATE = 2008/02/28
TIME = 11:39
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
42a
PMB
OMe
MeO
HO
OH
N
O
[ppm]
[rel]

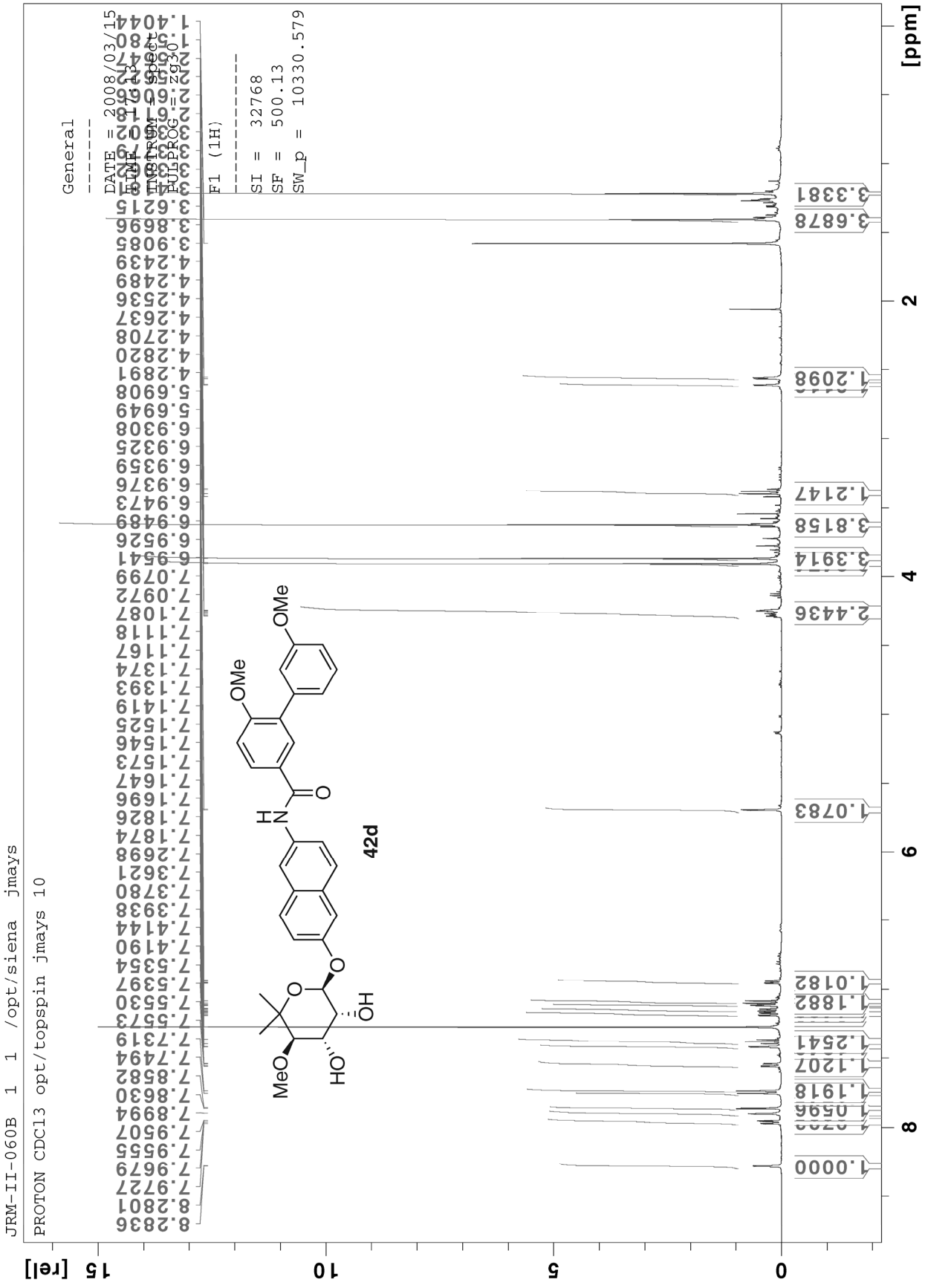

JRM-II-039A 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 2
General
DATE = 2008/02/28
TIME = 12:02
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
170.2747
159.2562
159.2433
158.1308
157.8863
150.8649
147.4165
138.7866
136.1114
132.7455
132.3530
130.4955
130.0793
129.2544
128.9788
128.9035
127.2513
123.4387
121.9606
120.6790
114.7985
114.2210
113.1723
111.2624
110.7169
98.1669
84.4557
78.7245
77.4838
77.2295
76.9751
71.0669
68.5582
62.0420
55.7040
55.3907
55.2737
53.7635
29.0449
42a
[rel]
[ppm]

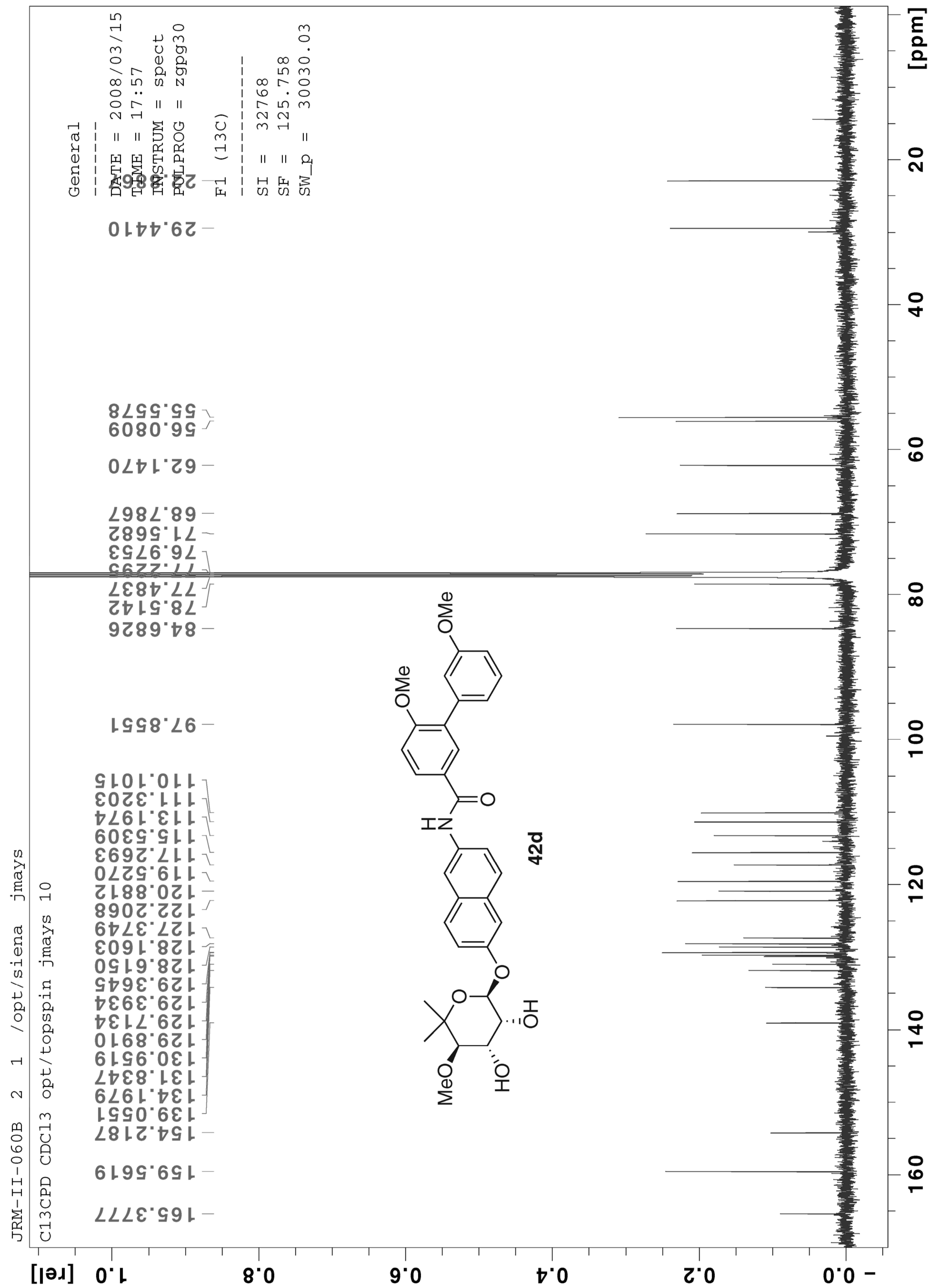

JRM-II-040E 1 1 /opt/siena jmays
PROTON CDC13 opt/topspin jmays 2
General
DATE = 2008/03/07
TIME = 13:17
INSTRUM = spect
PULPROG = zg30
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
42b
OMe
OMe
MeO
HO
OH
[rel]
[ppm]


JRM-II-040E 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 2
General
DATE = 2008/03/07
TIME = 14:50
INSTRUM = spect
PULPROG = zgpg30
F2
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
29.0521
55.3681
55.9194
61.9065
68.5770
71.2177
76.7763
77.0301
77.2836
78.4181
84.4039
97.7589
111.1899
111.5181
113.0111
115.3931
120.2650
121.9830
123.8115
124.6422
126.4134
128.5045
128.8425
129.2411
129.6050
130.3611
130.9386
138.7009
144.4659
146.5988
156.8355
159.3818
159.6735
165.4729
OMe
OMe
N
H
O
N
O
O
OH
HO
MeO
42b
[rel]
0.0
0.1
0.2
0.3
0.4
[ppm]
160
140
120
100
80
60
40
20


JRM-II-059E 1 1 /opt/siena jmays
PROTON CDC13 opt/topspin jmays 9
General
DATE = 2008/03/15
F1 (1H)
SI = 32768
SF = 500.13
SW_p = 10330.579
[rel]
[ppm]
PMB
OMe
OMe
MeO
HO
OH
42c
3.1226
3.0252
0.9858
0.9621
1.1507
2.9457
0.9801
2.1187
0.9626
2.0192
0.9558
3.6544
1.0180


JRM-II-059E 2 1 /opt/siena jmays
C13CPD CDC13 opt/topspin jmays 9
General
DATE = 2008/03/15
TIME = 16:59
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
170.1534
159.2308
159.0197
157.5777
155.0875
140.1151
139.0013
132.8860
132.3709
130.4727
130.0531
129.4868
129.4587
129.4331
128.9129
128.2974
128.0518
127.1080
125.8119
122.0822
119.5477
114.7301
113.9836
113.1644
110.4357
109.8970
97.9437
84.5652
78.5897
77.4829
77.2290
76.9754
71.4842
68.7250
62.1353
55.6630
55.4002
55.2838
53.8884
29.3627
PMB
OMe
OMe
MeO
HO
OH
42c
[rel]
[ppm]


JRM-II-060B 1 1 /opt/siena jmays
PROTON CDC13 opt/topspin jmays 10
General
DATE = 2008/03/15
SI = 32768
SF = 500.13
SW_p = 10330.579
F1 (1H)
42d
OMe
OMe
MeO
HO
OH
1.0000
1.0596
1.1918
1.1207
1.2541
1.1882
1.0182
1.0783
2.4436
3.3914
3.8158
1.2147
1.2098
3.6878
3.3381
[rel]
[ppm]


JRM-II-060B 2 1 /opt/siena jmays
C13CPD CDCl3 opt/topspin jmays 10
General
DATE = 2008/03/15
TIME = 17:57
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
165.3777
159.5619
154.2187
139.0551
134.1979
131.8347
130.9519
129.8910
129.7134
129.3934
129.3645
128.6150
128.1603
127.3749
122.2068
120.8812
119.5270
117.2693
115.5309
113.1974
111.3203
110.1015
97.8551
84.6826
78.5142
77.4837
77.2295
76.9753
71.5682
68.7867
62.1470
56.0809
55.5578
29.4410
MeO
HO
OH
O
H
N
OMe
42d
[ppm]
[rel]