Supporting Information

Synthesis of Hydrocarbazole Derivatives by Oxidative Dearomative Cyclization of Diarylamines using a Hypervalent Iodine Reagent

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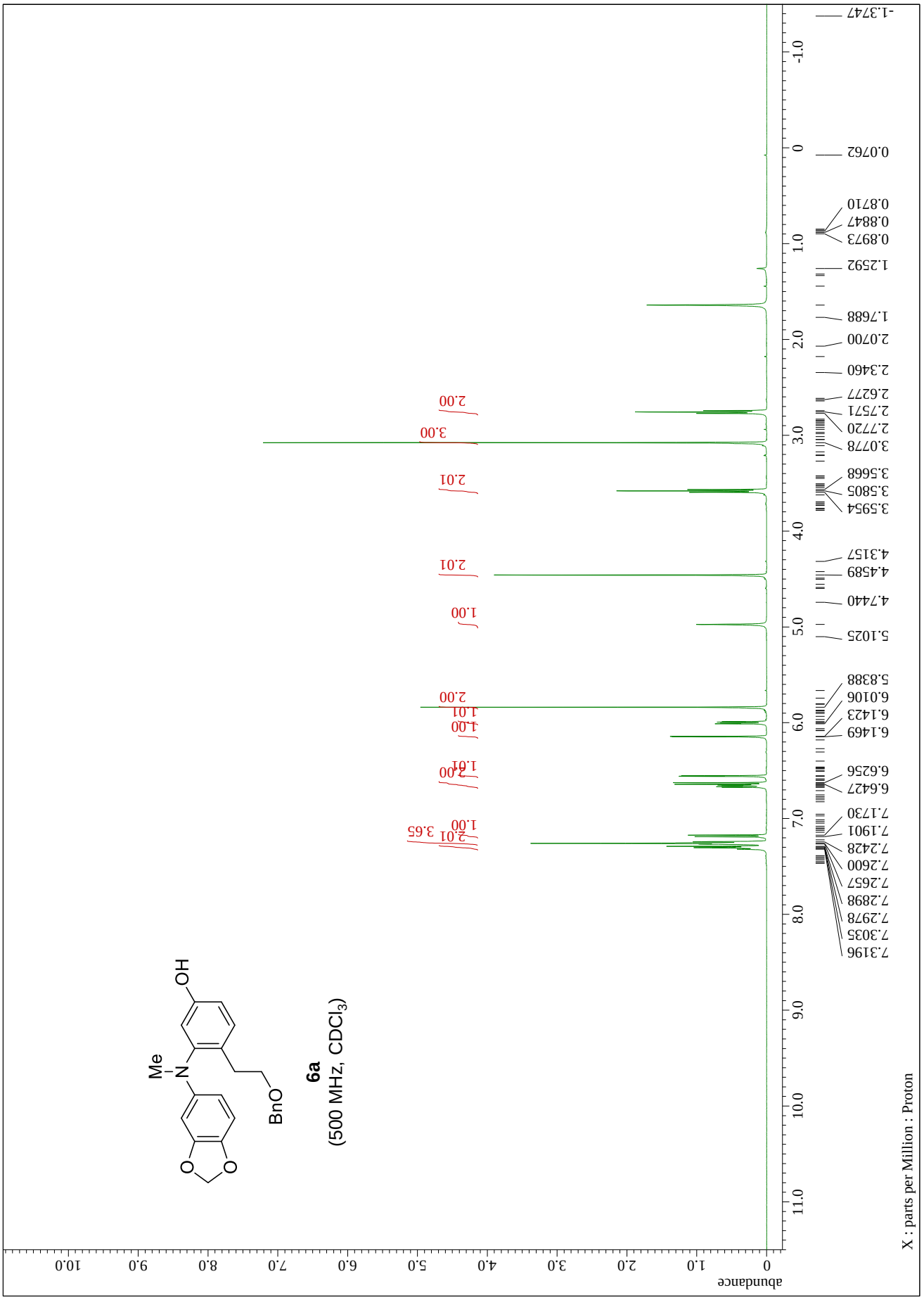
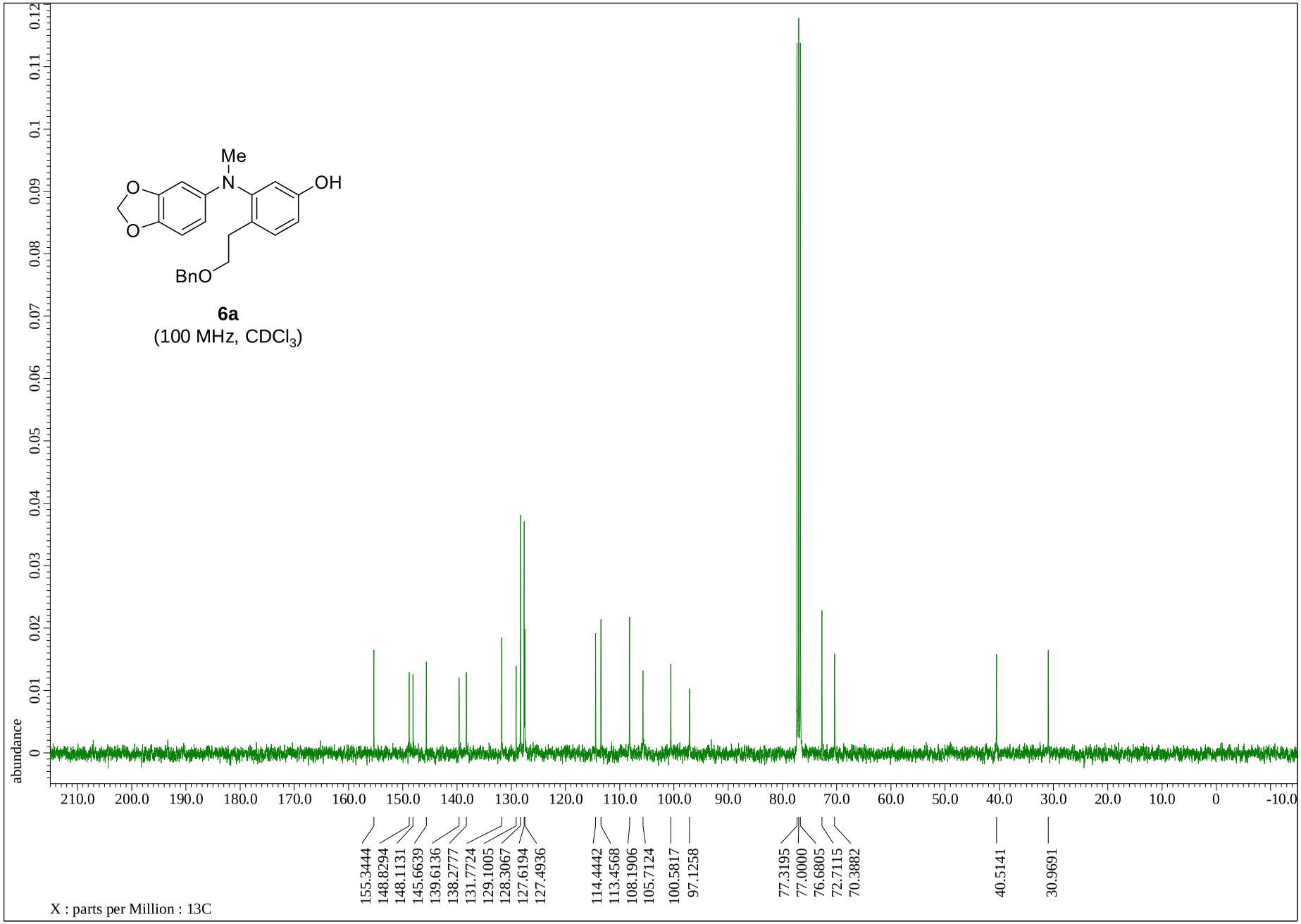
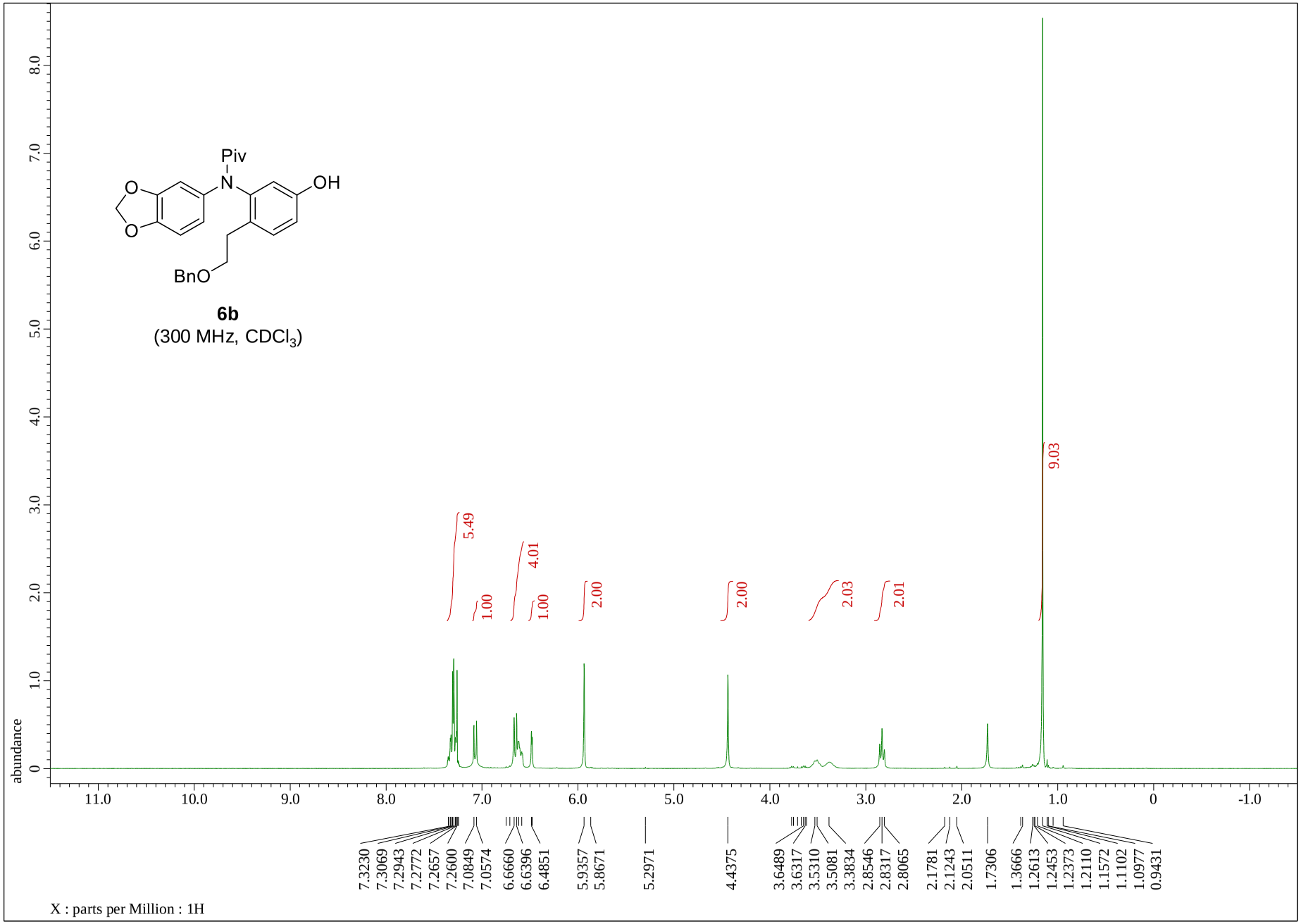
1. ^{1}H and ^{13}C NMR spectra of new compounds




Me
N
OH
O
O
BnO
6a
(100 MHz, CDCl3)
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
155.3444
148.8294
148.1131
145.6639
139.6136
138.2777
131.7724
129.1005
128.3067
127.6194
127.4936
114.4442
113.4568
108.1906
105.7124
100.5817
97.1258
77.3195
77.0000
76.6805
72.7115
70.3882
40.5141
30.9691
X : parts per Million : 13C


Piv
N
OH
O
O
BnO
6b
(300 MHz, CDCl3)
abundance
X : parts per Million : 1H
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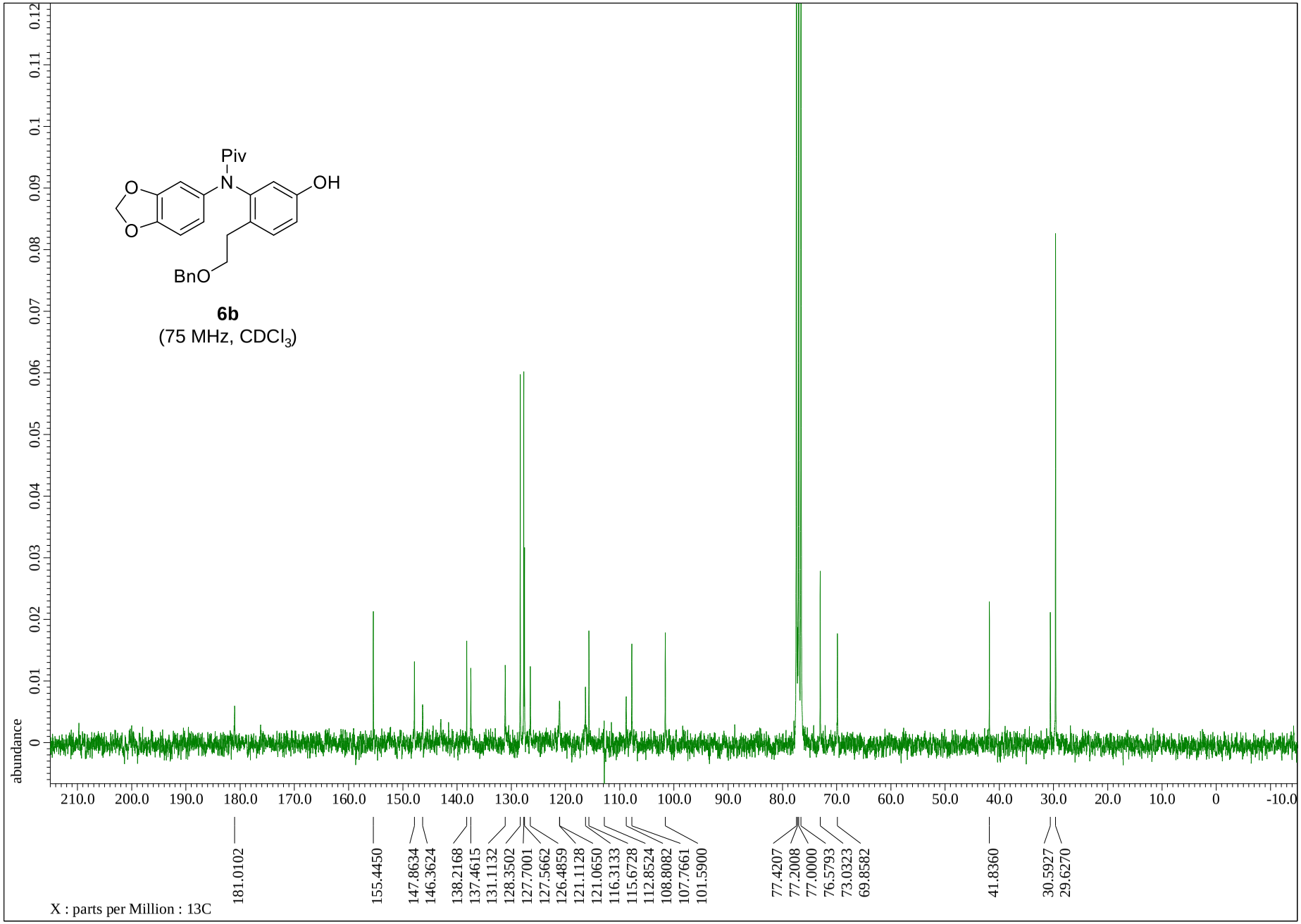
1.00
4.01
1.00
2.00
2.00
2.03
2.01
9.03
7.3230
7.3069
7.2943
7.2772
7.2657
7.2600
7.0849
7.0574
6.6660
6.6396
6.4851
5.9357
5.8671
5.2971
4.4375
3.6489
3.6317
3.5310
3.5081
3.3834
2.8546
2.8317
2.8065
2.1781
2.1243
2.0511
1.7306
1.3666
1.2613
1.2453
1.2373
1.2110
1.1572
1.1102
1.0977
0.9431


Piv
N
OH
O
O
BnO
6b
(75 MHz, CDCl3)
abundance
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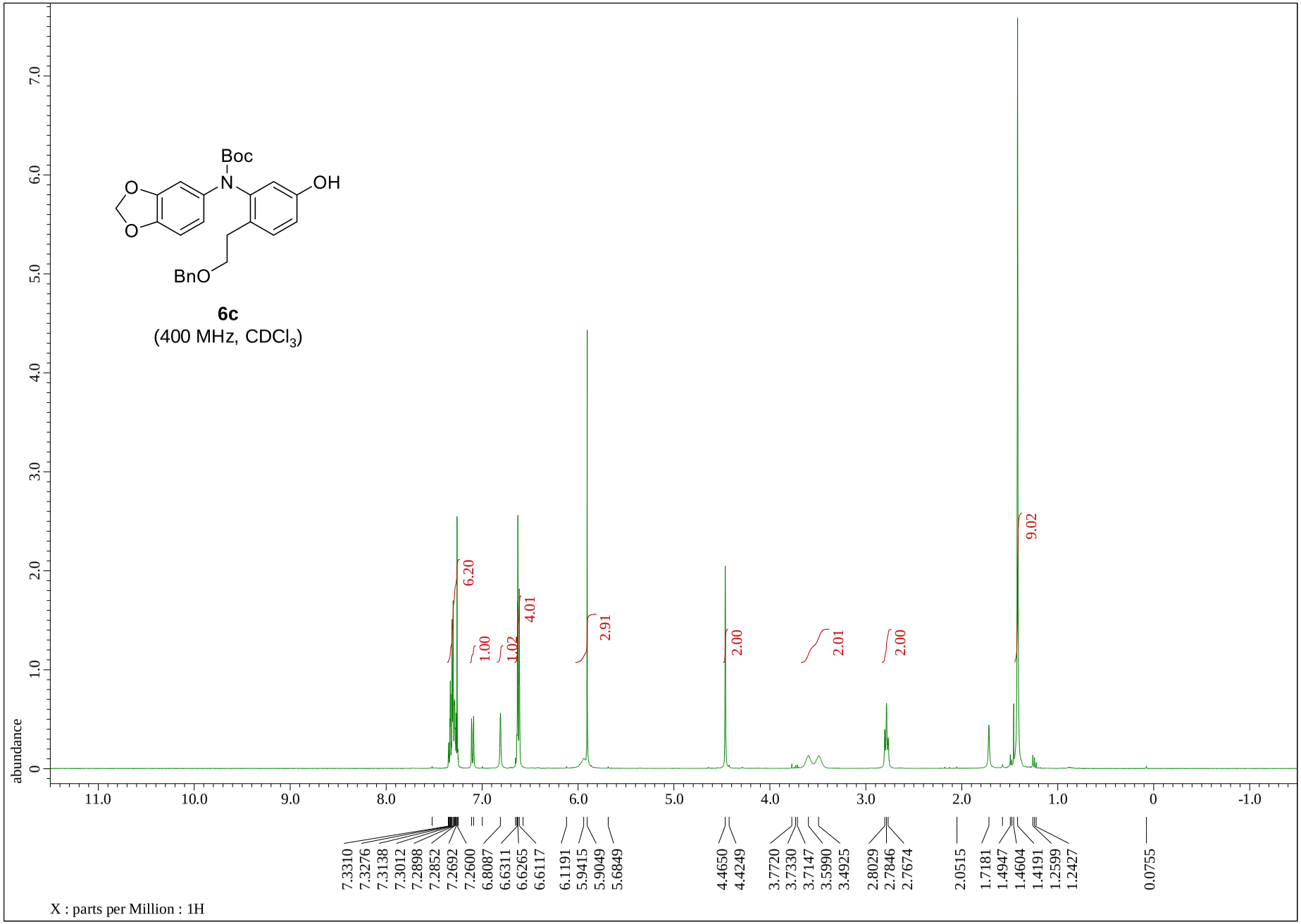
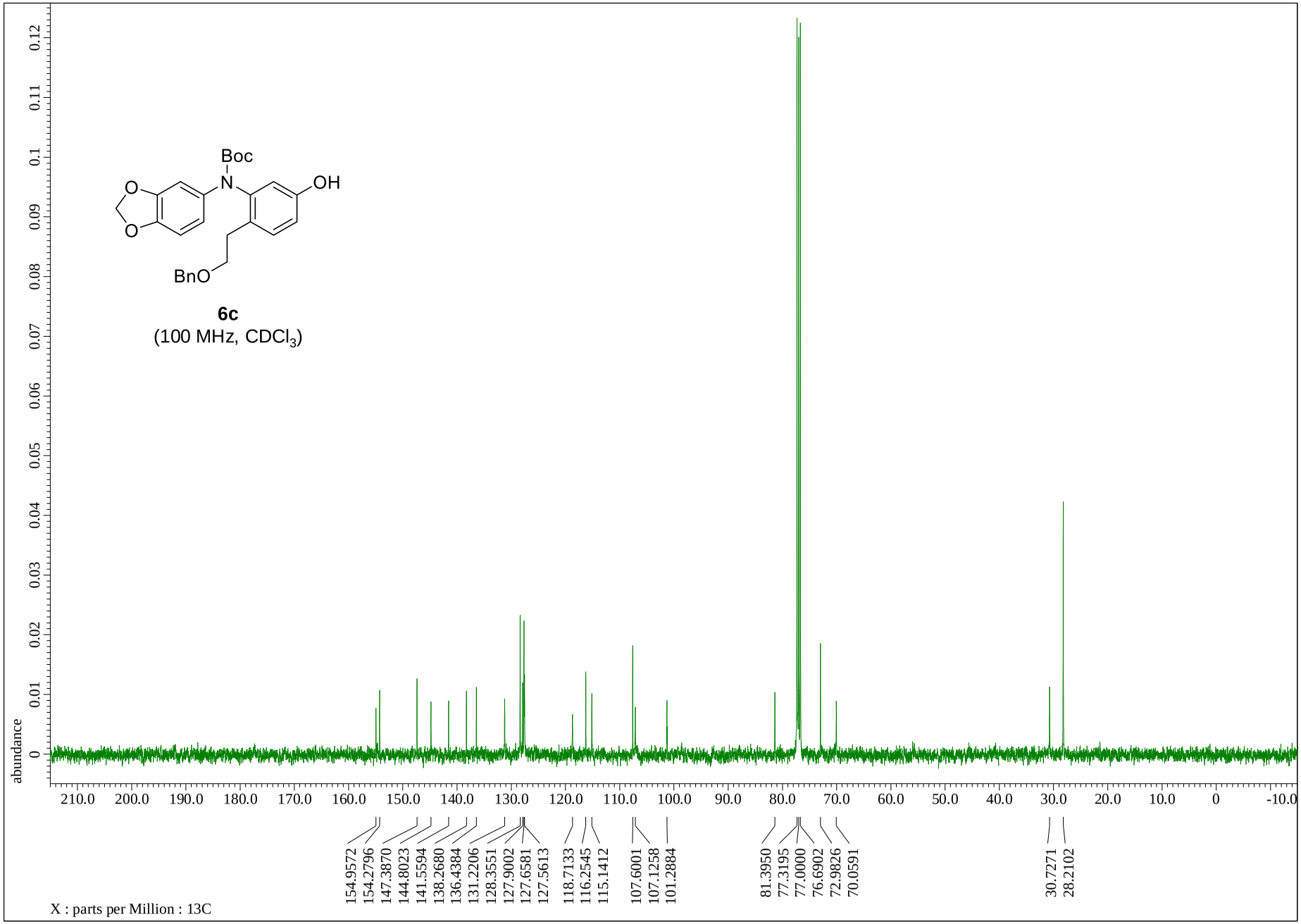
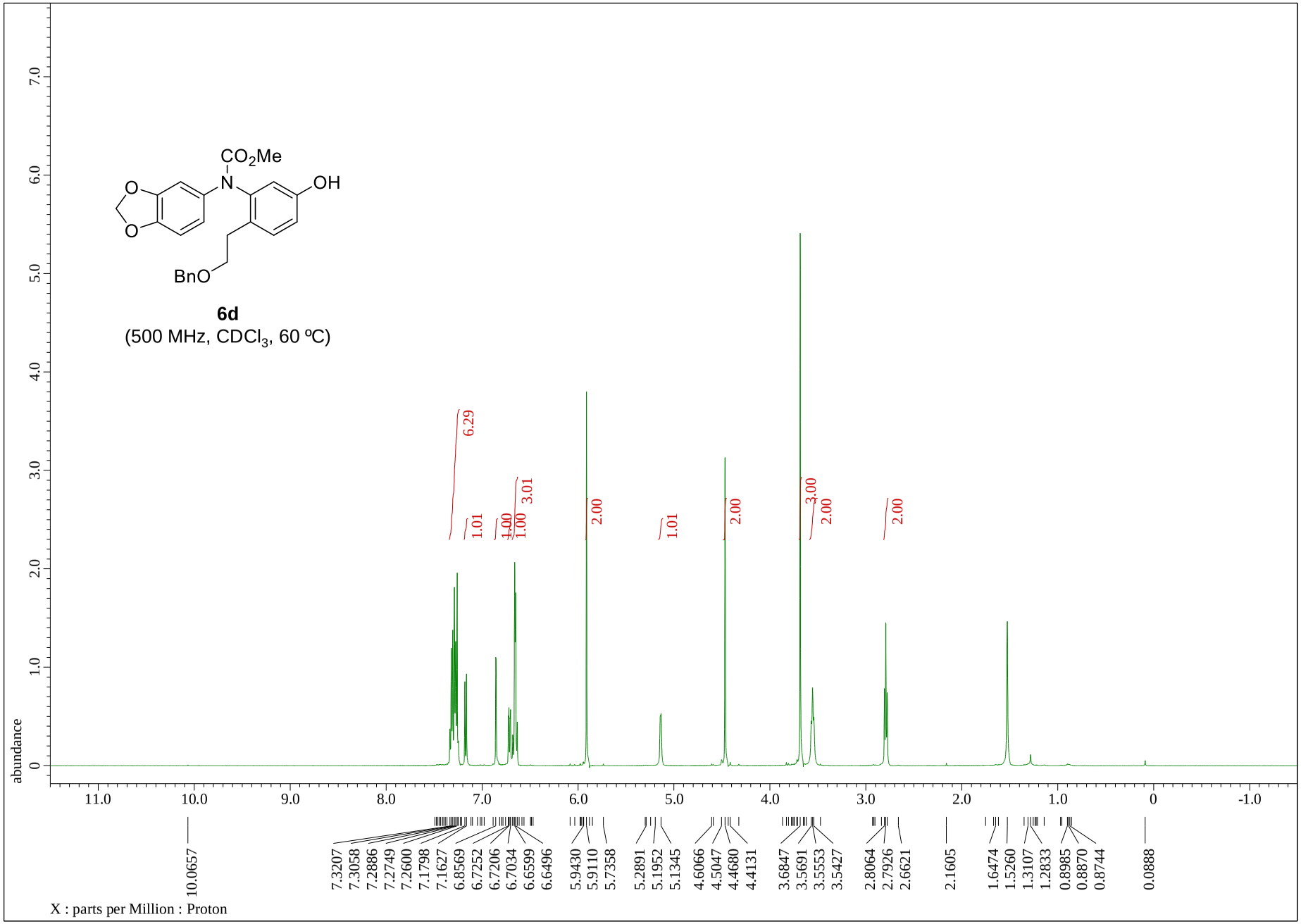
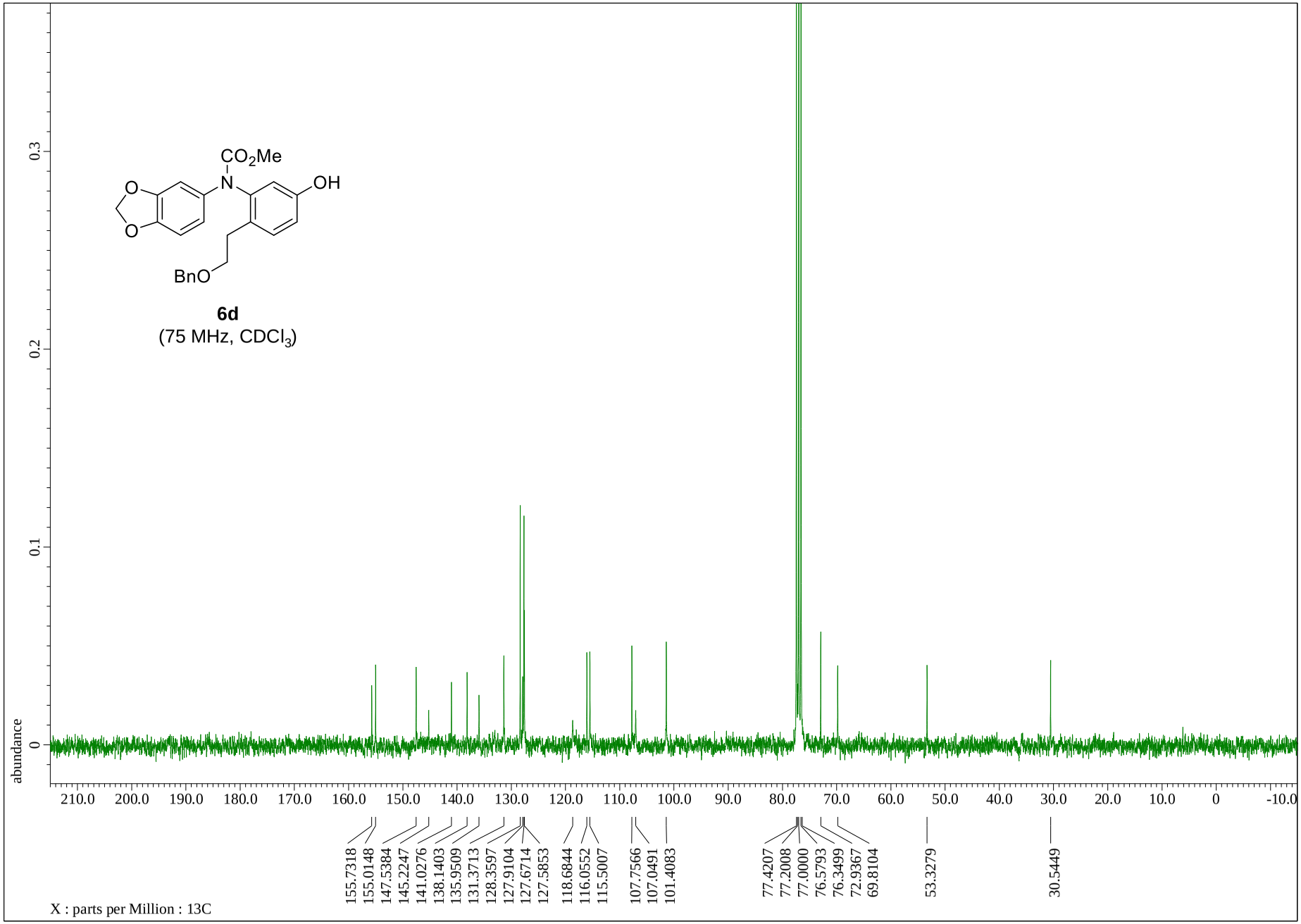
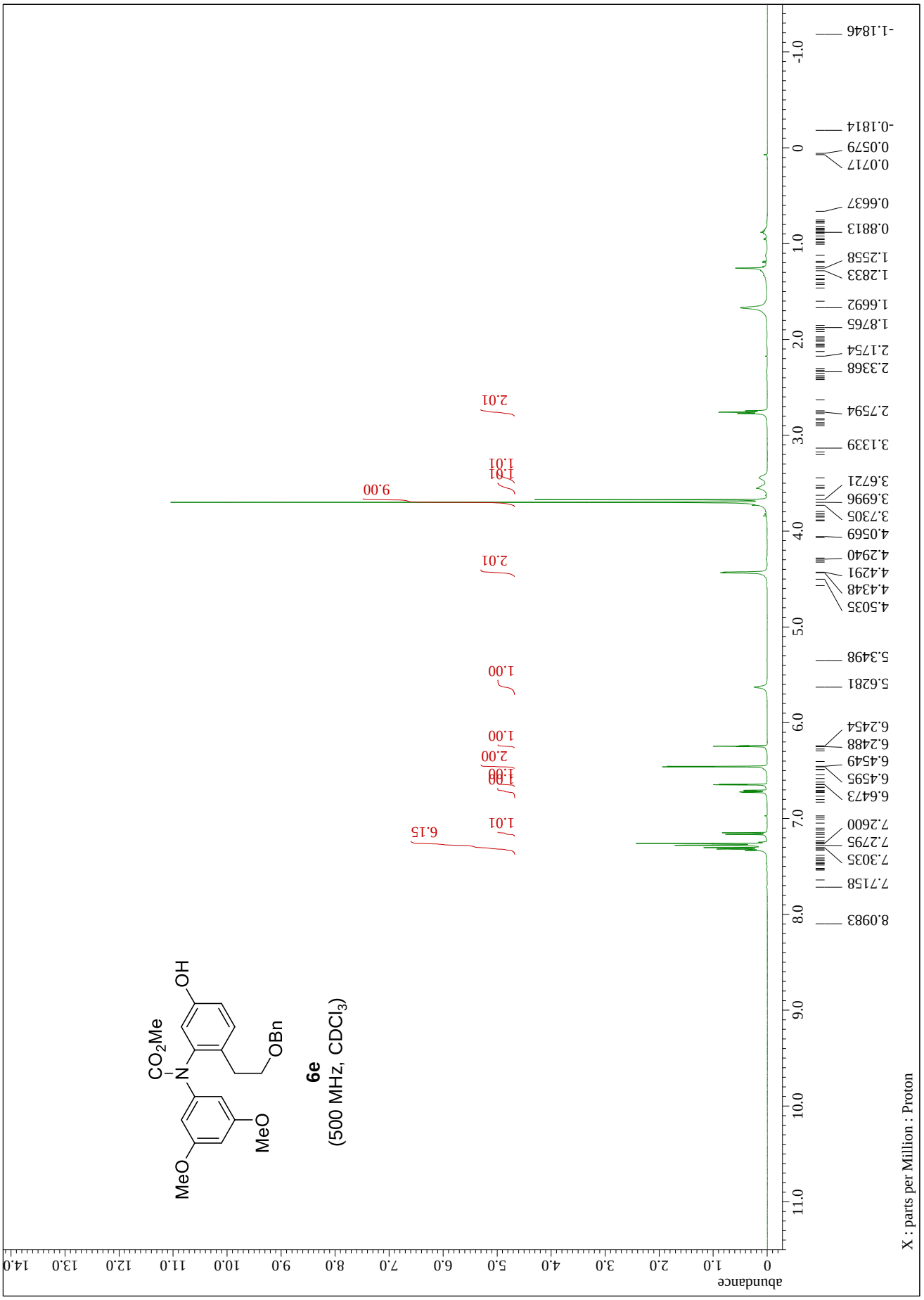
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
181.0102
155.4450
147.8634
146.3624
138.2168
137.4615
131.1132
128.3502
127.7001
127.5662
126.4859
121.1128
121.0650
116.3133
115.6728
112.8524
108.8082
107.7661
101.5900
77.4207
77.2008
77.0000
76.5793
73.0323
69.8582
41.8360
30.5927
29.6270
X : parts per Million : 13C


Boc
N
OH
O
O
BnO
6c
(400 MHz, CDCl3)
abundance
6.20
1.00
1.02
4.01
2.91
2.00
2.01
2.00
9.02
7.3310
7.3276
7.3138
7.3012
7.2898
7.2852
7.2692
7.2600
6.8087
6.6311
6.6265
6.6117
6.1191
5.9415
5.9049
5.6849
4.4650
4.4249
3.7720
3.7330
3.7147
3.5990
3.4925
2.8029
2.7846
2.7674
2.0515
1.7181
1.4947
1.4604
1.4191
1.2599
1.2427
0.0755
X : parts per Million : 1H


Boc
N
OH
O
O
BnO
6c
(100 MHz, CDCl3)
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
154.9572
154.2796
147.3870
144.8023
141.5594
138.2680
136.4384
131.2206
128.3551
127.9002
127.6581
127.5613
118.7133
116.2545
115.1412
107.6001
107.1258
101.2884
81.3950
77.3195
77.0000
76.6902
72.9826
70.0591
30.7271
28.2102
X : parts per Million : 13C


CO2Me
N
OH
O
O
BnO
6d
(500 MHz, CDCl3, 60 ºC)
abundance
6.29
1.01
1.00
1.00
3.01
2.00
1.01
2.00
3.00
2.00
2.00
10.0657
7.3207
7.3058
7.2886
7.2749
7.2600
7.1798
7.1627
6.8569
6.7252
6.7206
6.7034
6.6599
6.6496
5.9430
5.9110
5.7358
5.2891
5.1952
5.1345
4.6066
4.5047
4.4680
4.4131
3.6847
3.5691
3.5553
3.5427
2.8064
2.7926
2.6621
2.1605
1.6474
1.5260
1.3107
1.2833
0.8985
0.8870
0.8744
0.0888
X : parts per Million : Proton


CO2Me
N
OH
O
O
BnO
6d
(75 MHz, CDCl3)
abundance
0.3
0.2
0.1
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
155.7318
155.0148
147.5384
145.2247
141.0276
138.1403
135.9509
131.3713
128.3597
127.9104
127.6714
127.5853
118.6844
116.0552
115.5007
107.7566
107.0491
101.4083
77.4207
77.2008
77.0000
76.5793
76.3499
72.9367
69.8104
53.3279
30.5449
X : parts per Million : 13C


MeO
MeO
N
CO2Me
OH
OBn
6e
(500 MHz, CDCl3)
X : parts per Million : Proton
abundance
8.0983
7.7158
7.3035
7.2795
7.2600
6.6473
6.4595
6.4549
6.2488
6.2454
5.6281
5.3498
4.5035
4.4348
4.4291
4.2940
4.0569
3.7305
3.6996
3.6721
3.1339
2.7594
2.3368
2.1754
1.8765
1.6692
1.2833
1.2558
0.8813
0.6637
0.0717
0.0579
-0.1814
-1.1846
6.15
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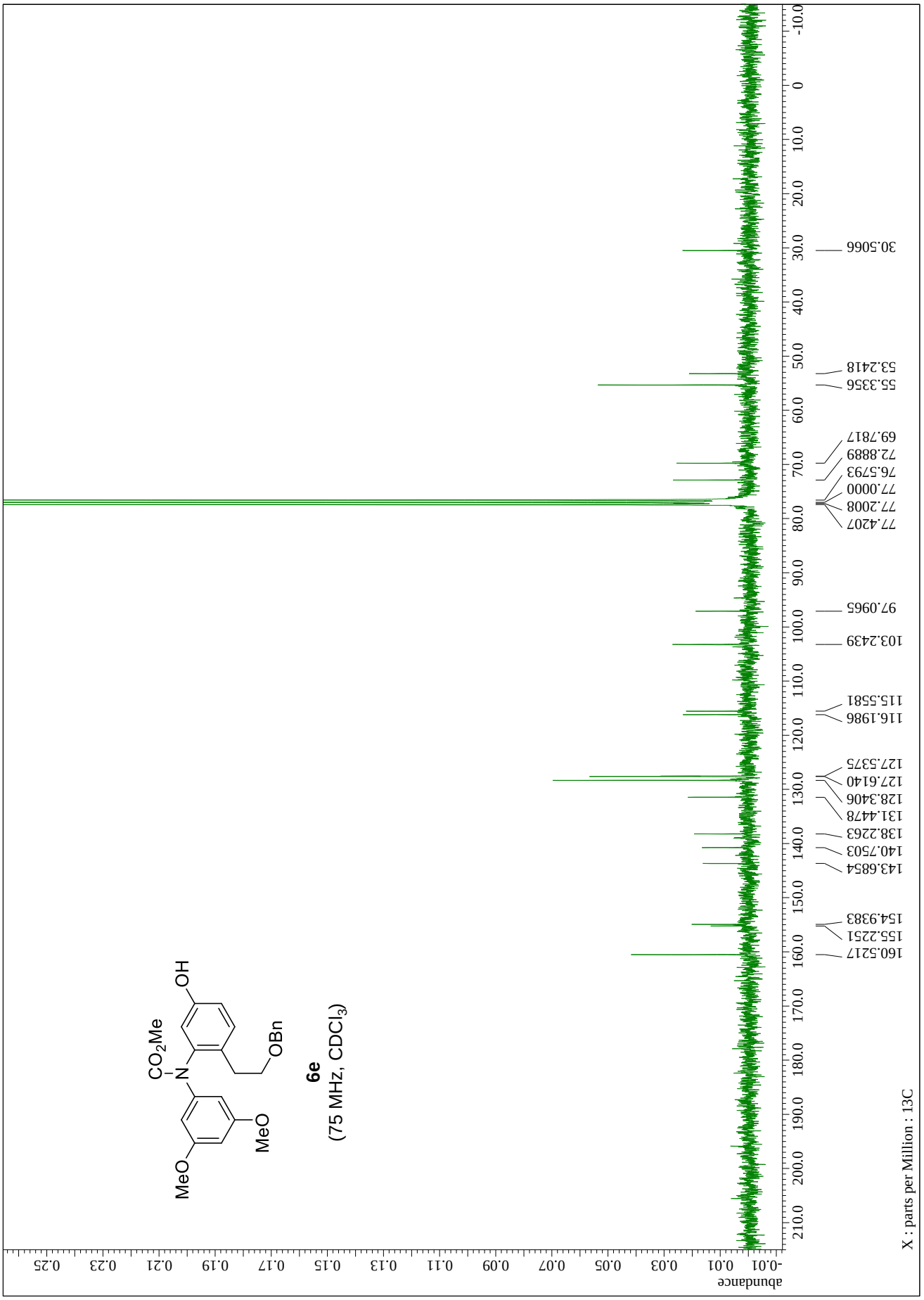
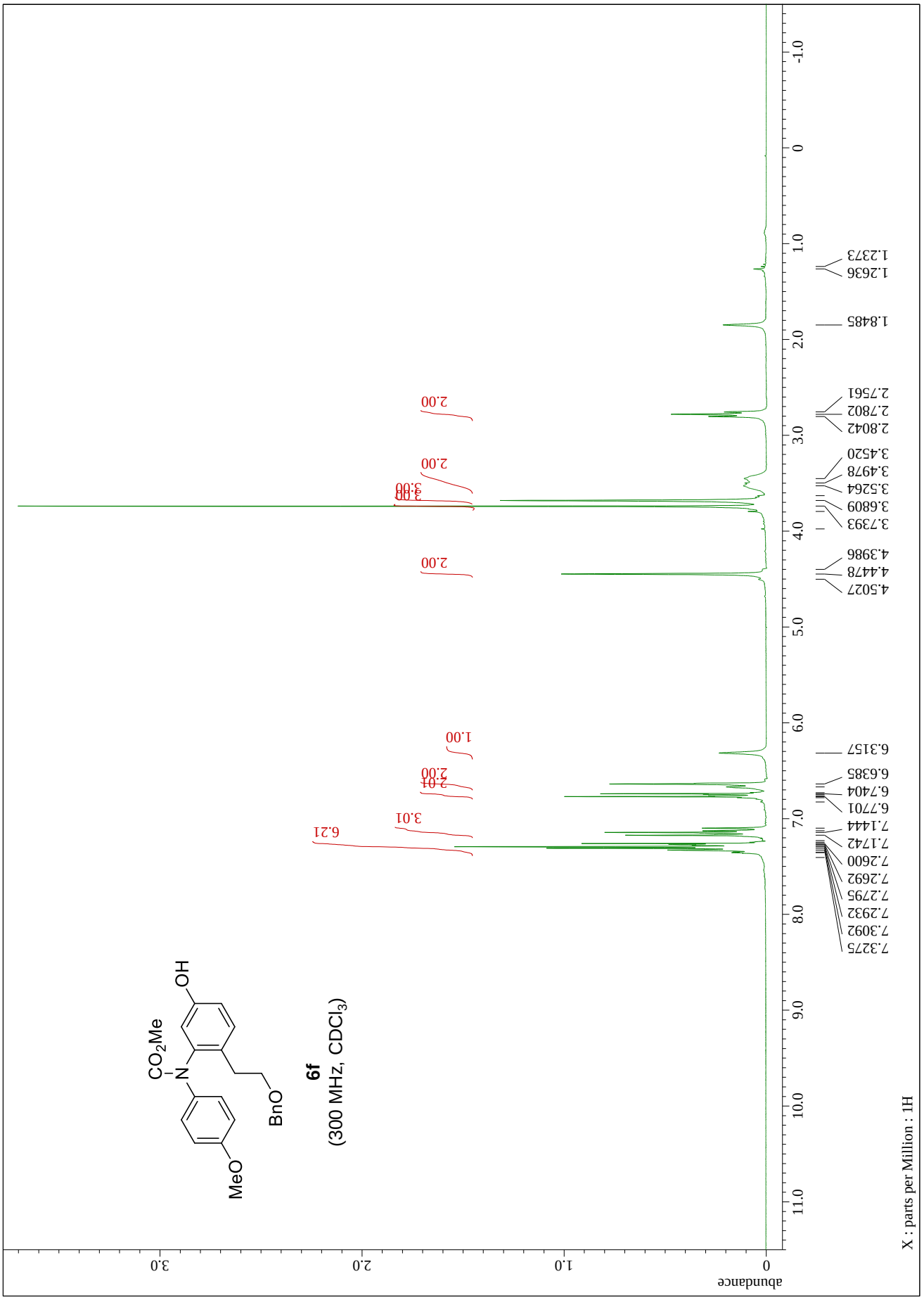
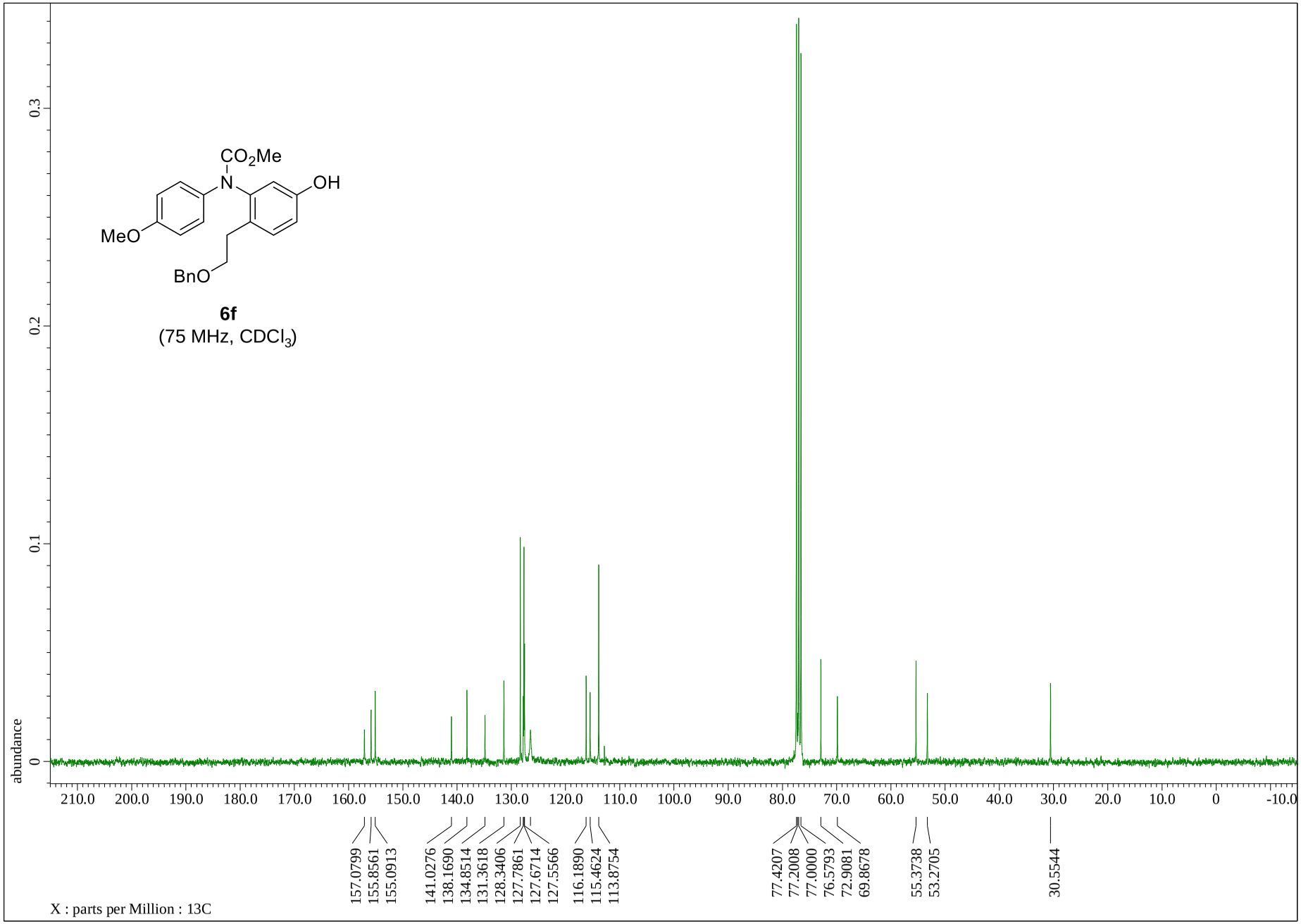
1.00
1.00
2.00
1.00
1.00
2.01
9.00
1.01
1.01
2.01


MeO
MeO
N
CO2Me
OH
OBn
6e
(75 MHz, CDCl3)
X : parts per Million : 13C
abundance
160.5217
155.2251
154.9383
143.6854
140.7503
138.2263
131.4478
128.3406
127.6140
127.5375
116.1986
115.5581
103.2439
97.0965
77.4207
77.2008
77.0000
76.5793
72.8889
69.7817
55.3356
53.2418
30.5066


MeO
BnO
N
CO2Me
OH
6f
(300 MHz, CDCl3)
X : parts per Million : 1H
abundance
7.3275
7.3092
7.2932
7.2795
7.2692
7.2600
7.1742
7.1444
6.7701
6.7404
6.6385
6.3157
4.5027
4.4478
4.3986
3.7393
3.6809
3.5264
3.4978
3.4520
2.8042
2.7802
2.7561
1.8485
1.2636
1.2373
6.21
3.01
2.01
2.00
1.00
2.00
2.00
3.00
3.00
2.00
2.00


CO2Me
N
OH
MeO
BnO
6f
(75 MHz, CDCl3)
abundance
0.3
0.2
0.1
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
157.0799
155.8561
155.0913
141.0276
138.1690
134.8514
131.3618
128.3406
127.7861
127.6714
127.5566
116.1890
115.4624
113.8754
77.4207
77.2008
77.0000
76.5793
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69.8678
55.3738
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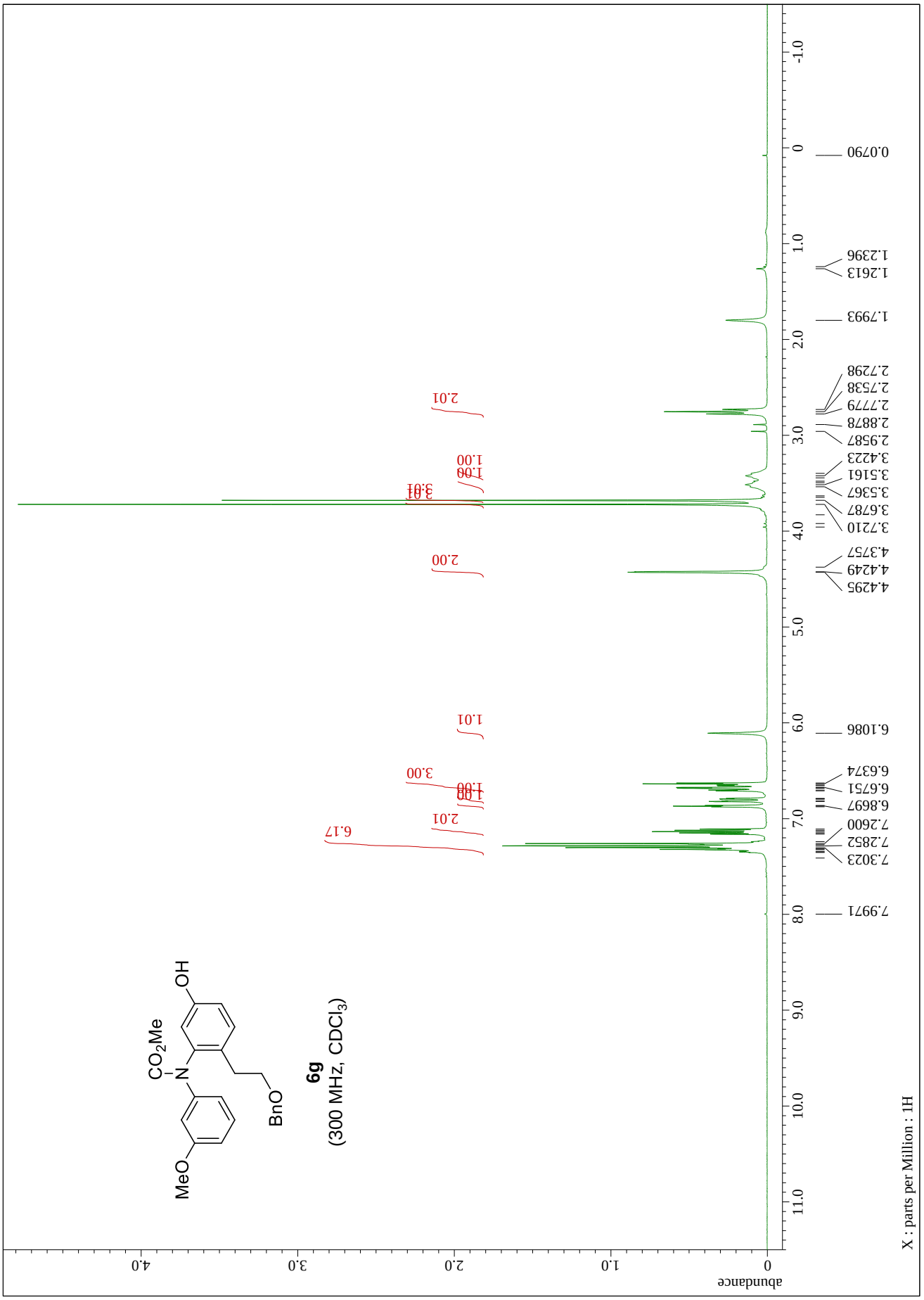
X : parts per Million : 13C


MeO
N
CO2Me
OH
BnO
6g
(300 MHz, CDCl3)
X : parts per Million : 1H
abundance
0.0790
1.2613
1.2396
1.7993
2.7298
2.7538
2.7779
2.8878
2.9587
3.4223
3.5161
3.5367
3.6787
3.7210
4.4295
4.4249
4.3757
6.1086
6.6374
6.6751
6.8697
7.2600
7.2852
7.3023
7.9971
6.17
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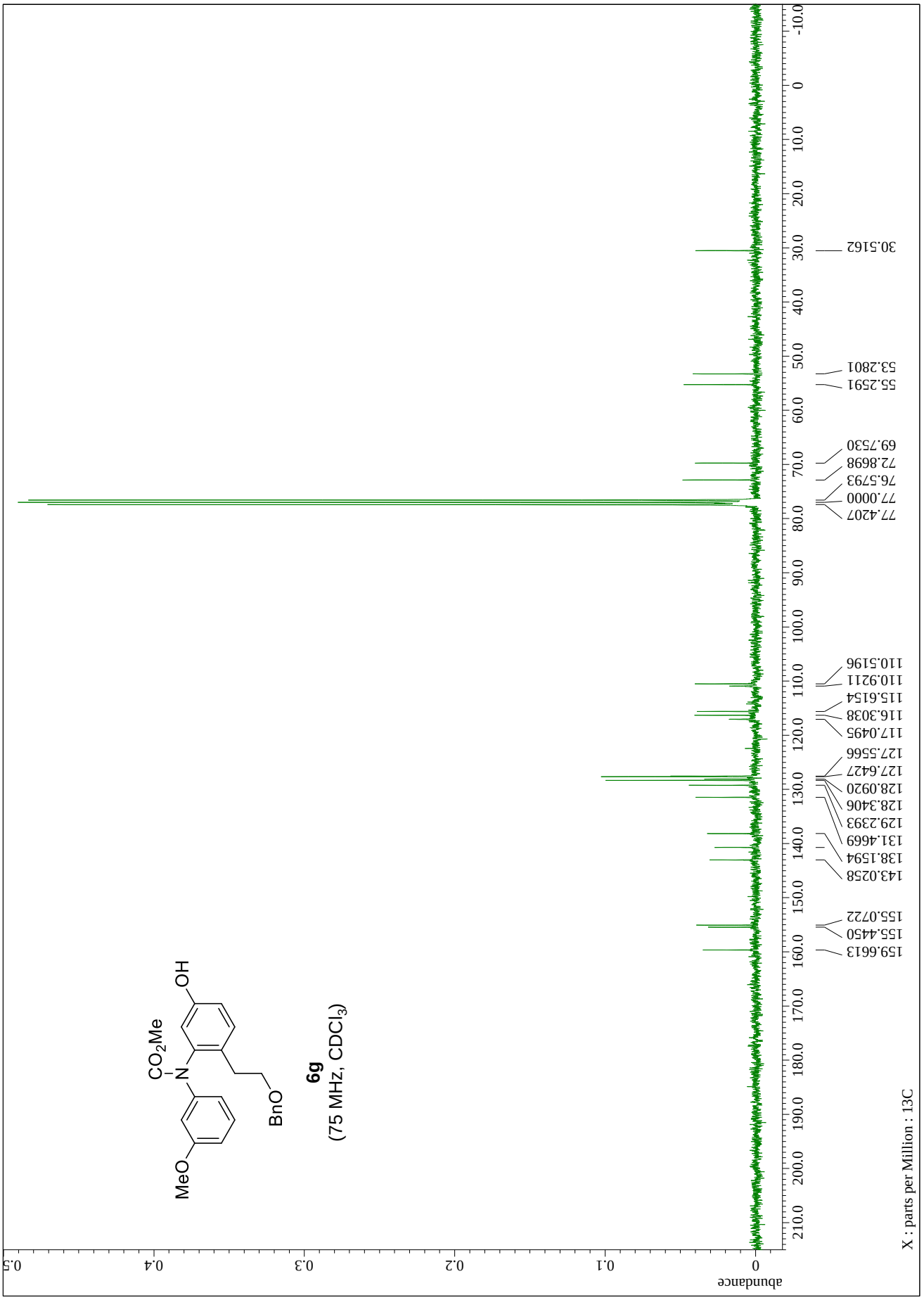
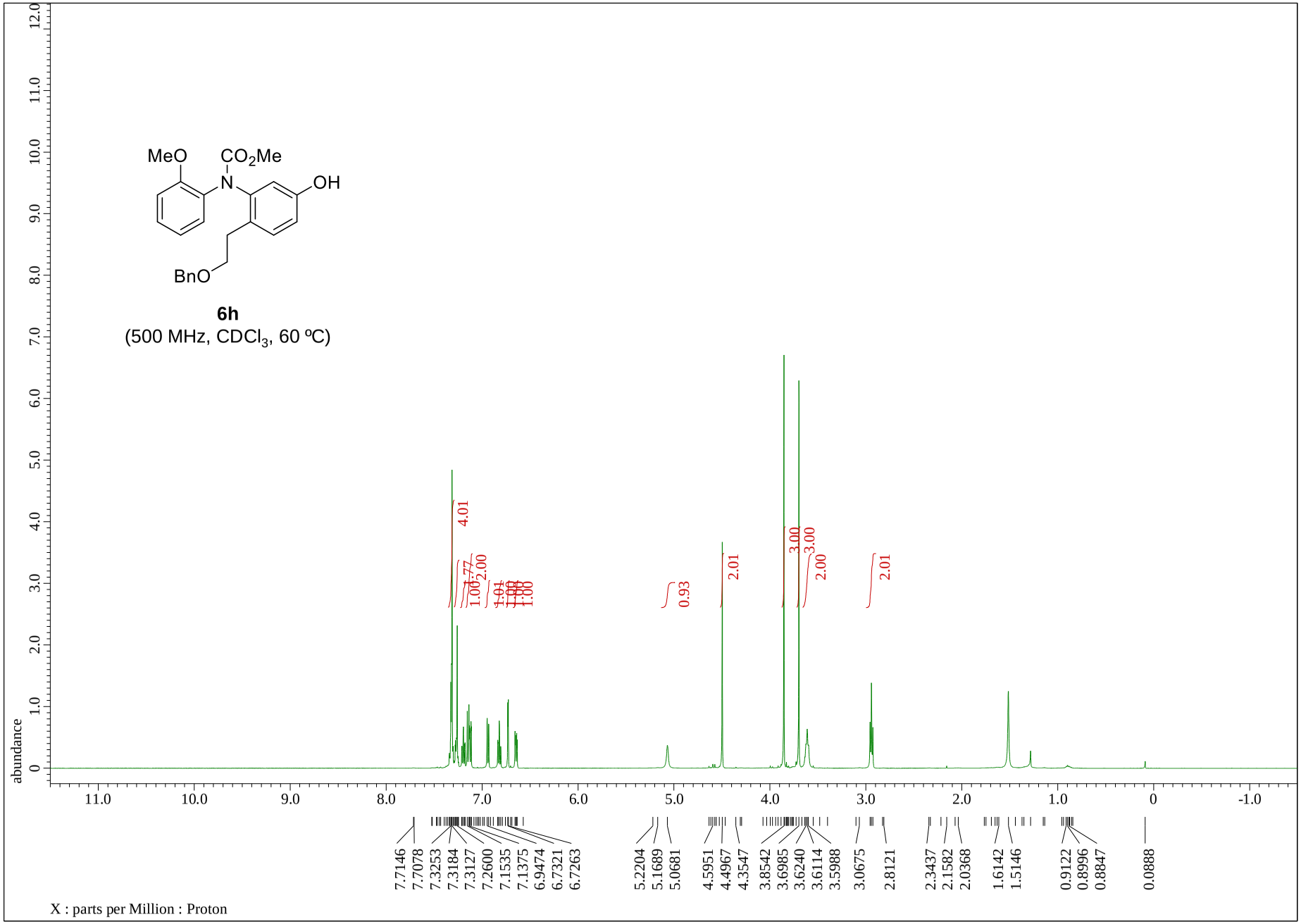
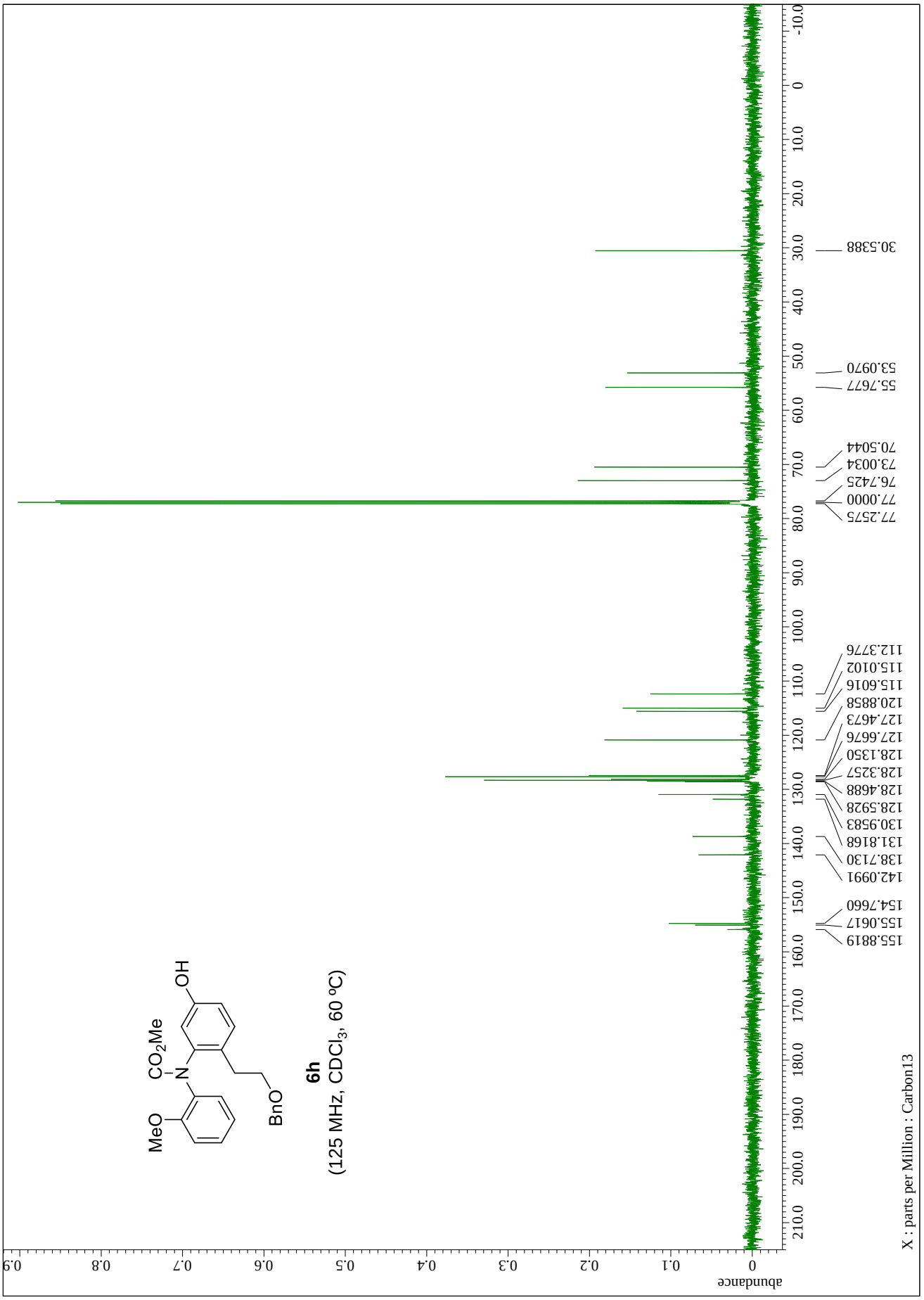
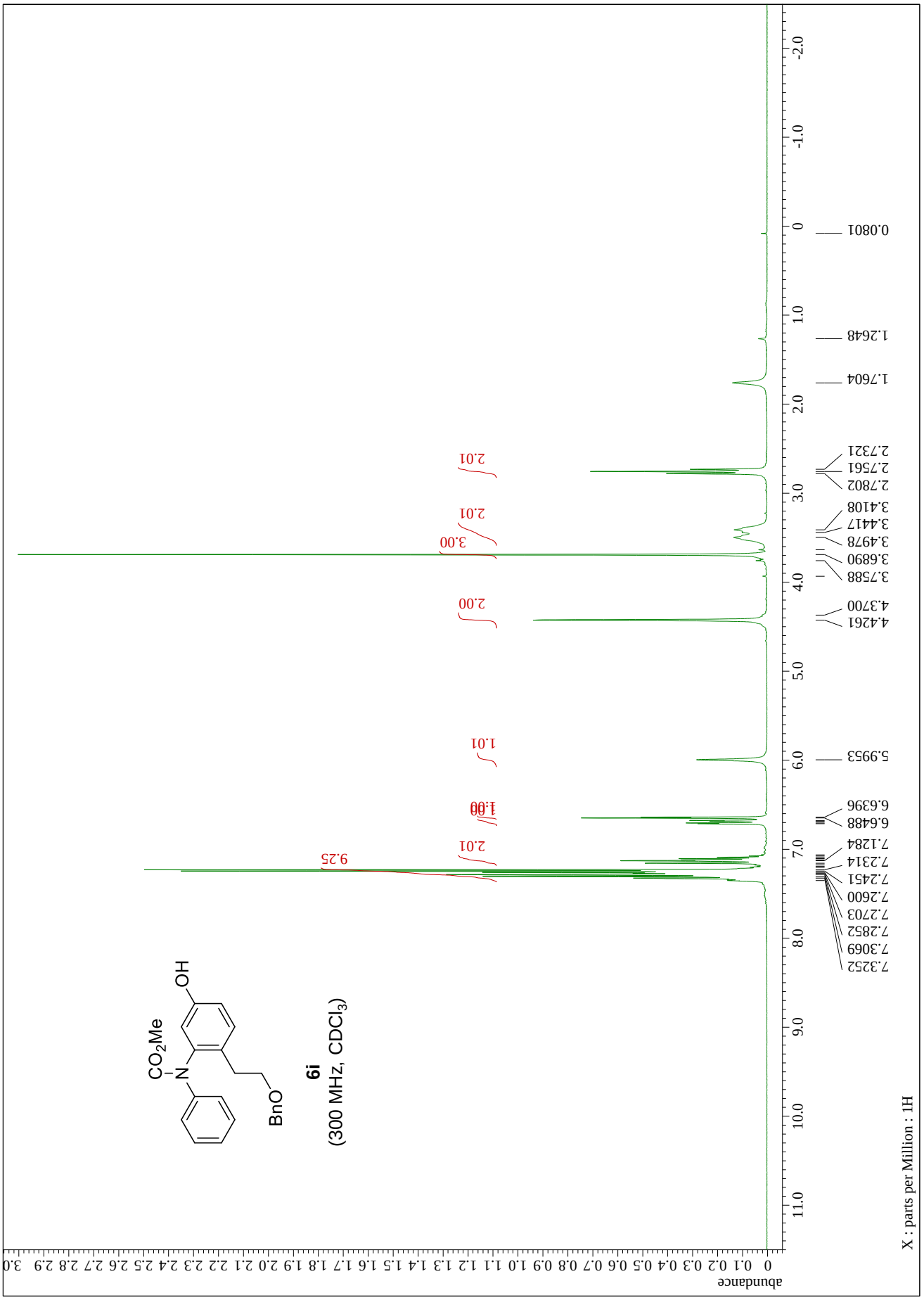
1.00
1.00
3.00
1.01
2.00
3.01
1.00
1.00
2.01


MeO
N
CO2Me
OH
BnO
6g
(75 MHz, CDCl3)
159.6613
155.4450
155.0722
143.0258
138.1594
131.4669
129.2393
128.3406
128.0920
127.6427
127.5566
117.0495
116.3038
115.6154
110.9211
110.5196
77.4207
77.0000
76.5793
72.8698
69.7530
55.2591
53.2801
30.5162
X : parts per Million : 13C
abundance


MeO
CO2Me
N
OH
BnO
6h
(500 MHz, CDCl3, 60 ºC)
abundance
4.01
2.00
1.77
1.00
0.93
2.01
3.00
3.00
2.00
2.01
7.7146
7.7078
7.3253
7.3184
7.3127
7.2600
7.1535
7.1375
6.9474
6.7321
6.7263
5.2204
5.1689
5.0681
4.5951
4.4967
4.3547
3.8542
3.6985
3.6240
3.6114
3.5988
3.0675
2.8121
2.3437
2.1582
2.0368
1.6142
1.5146
0.9122
0.8996
0.8847
0.0888
X : parts per Million : Proton


MeO
CO2Me
N
OH
BnO
6h
(125 MHz, CDCl3, 60 ºC)
155.8819
155.0617
154.7660
142.0991
138.7130
131.8168
130.9583
128.5928
128.4688
128.3257
128.1350
127.6676
127.4673
120.8858
115.6016
115.0102
112.3776
77.2575
77.0000
76.7425
73.0034
70.5044
55.7677
53.0970
30.5388
X : parts per Million : Carbon13
abundance


CO2Me
N
OH
BnO
6i
(300 MHz, CDCl3)
X : parts per Million : 1H
abundance
7.3252
7.3069
7.2852
7.2703
7.2600
7.2451
7.2314
7.1284
6.6488
6.6396
5.9953
4.4261
4.3700
3.7588
3.6890
3.4978
3.4417
3.4108
2.7802
2.7561
2.7321
1.7604
1.2648
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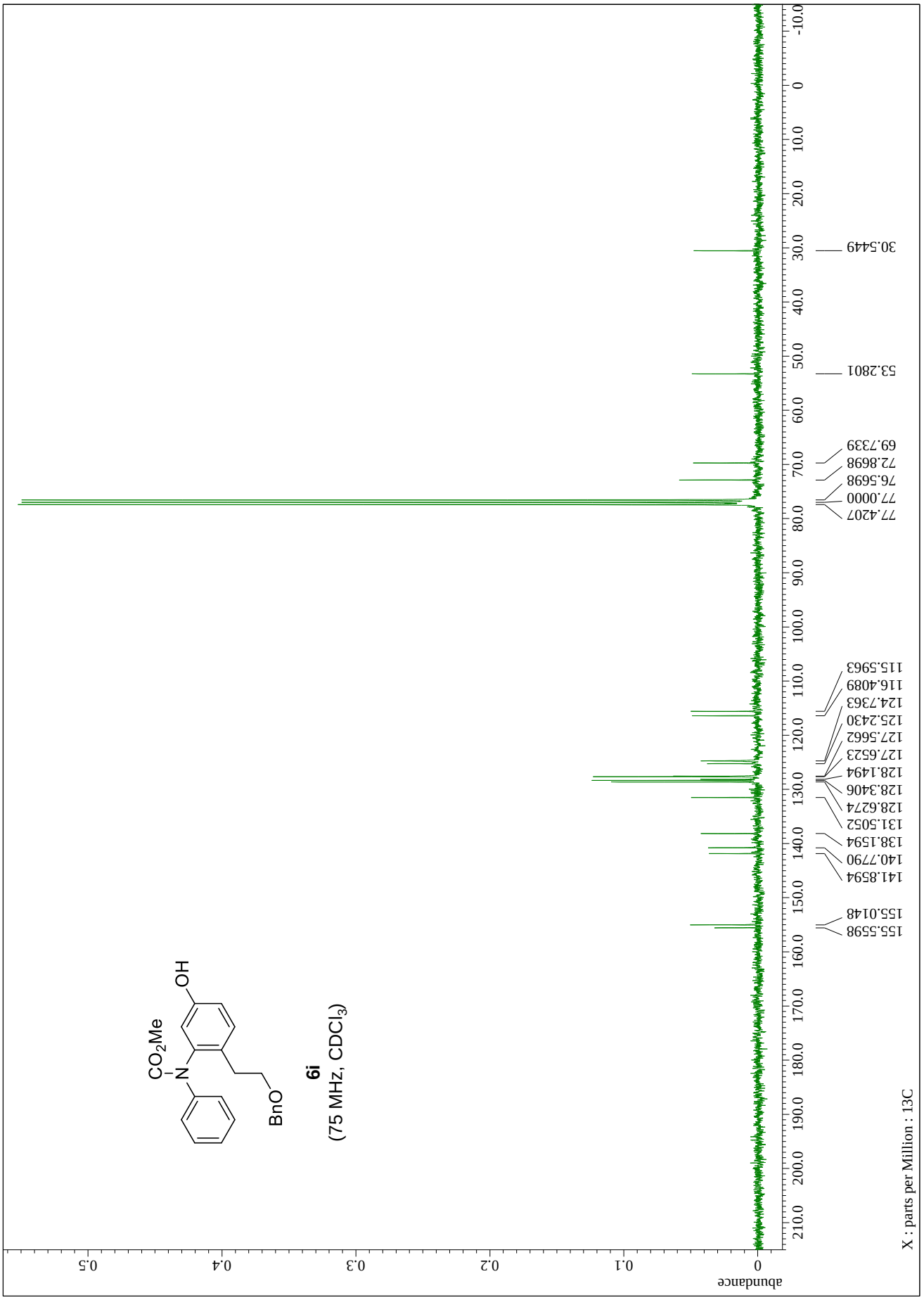
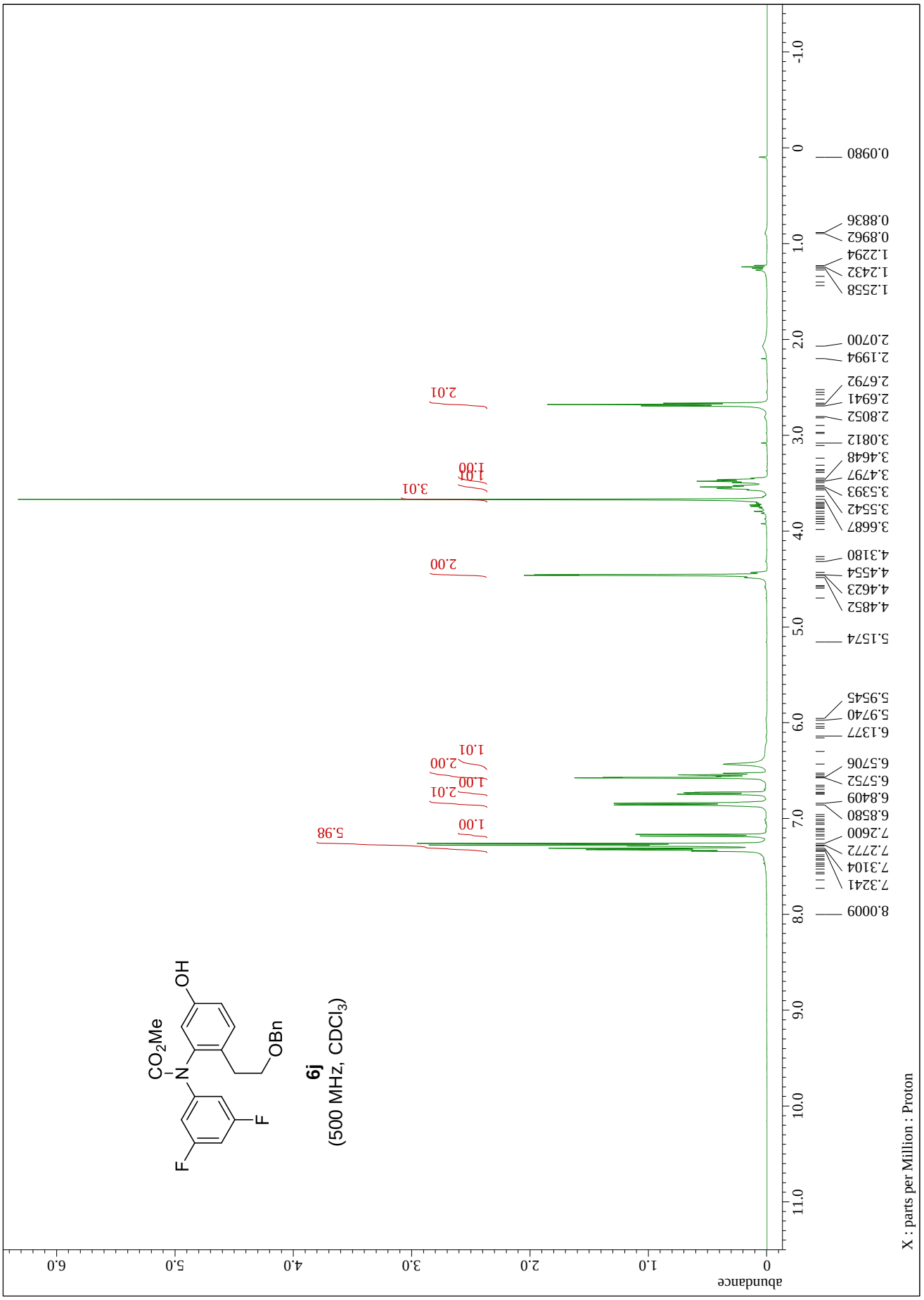
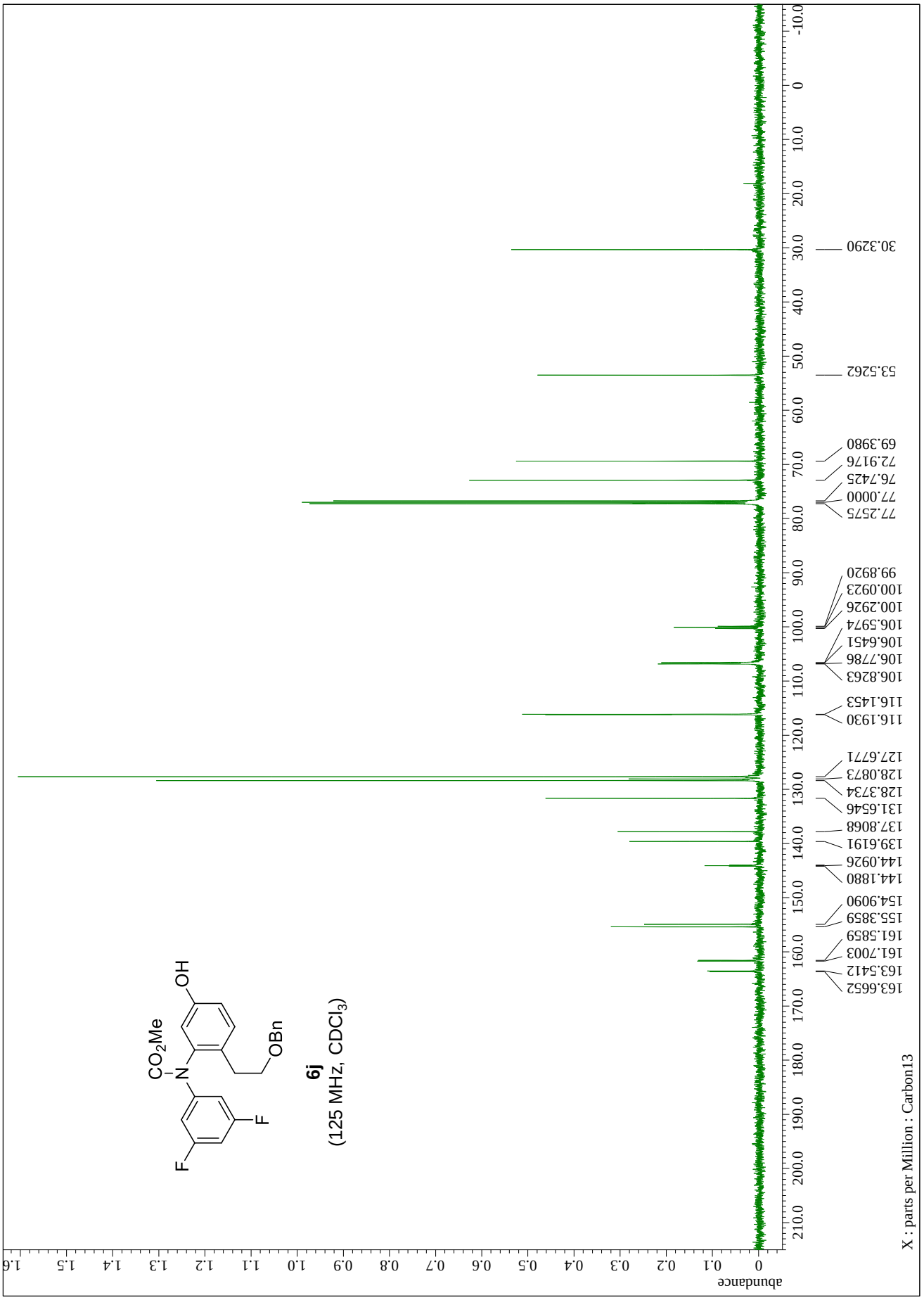
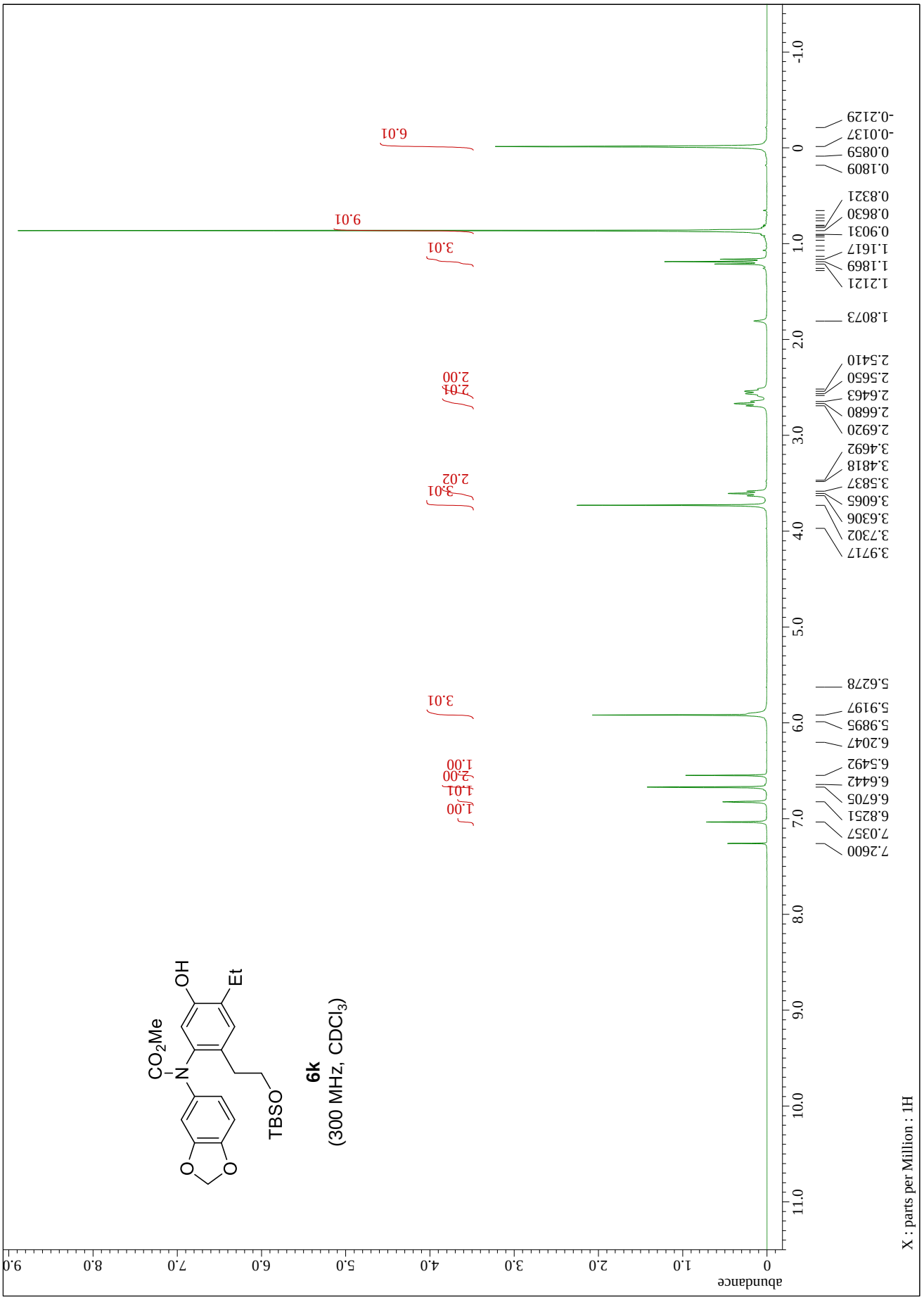
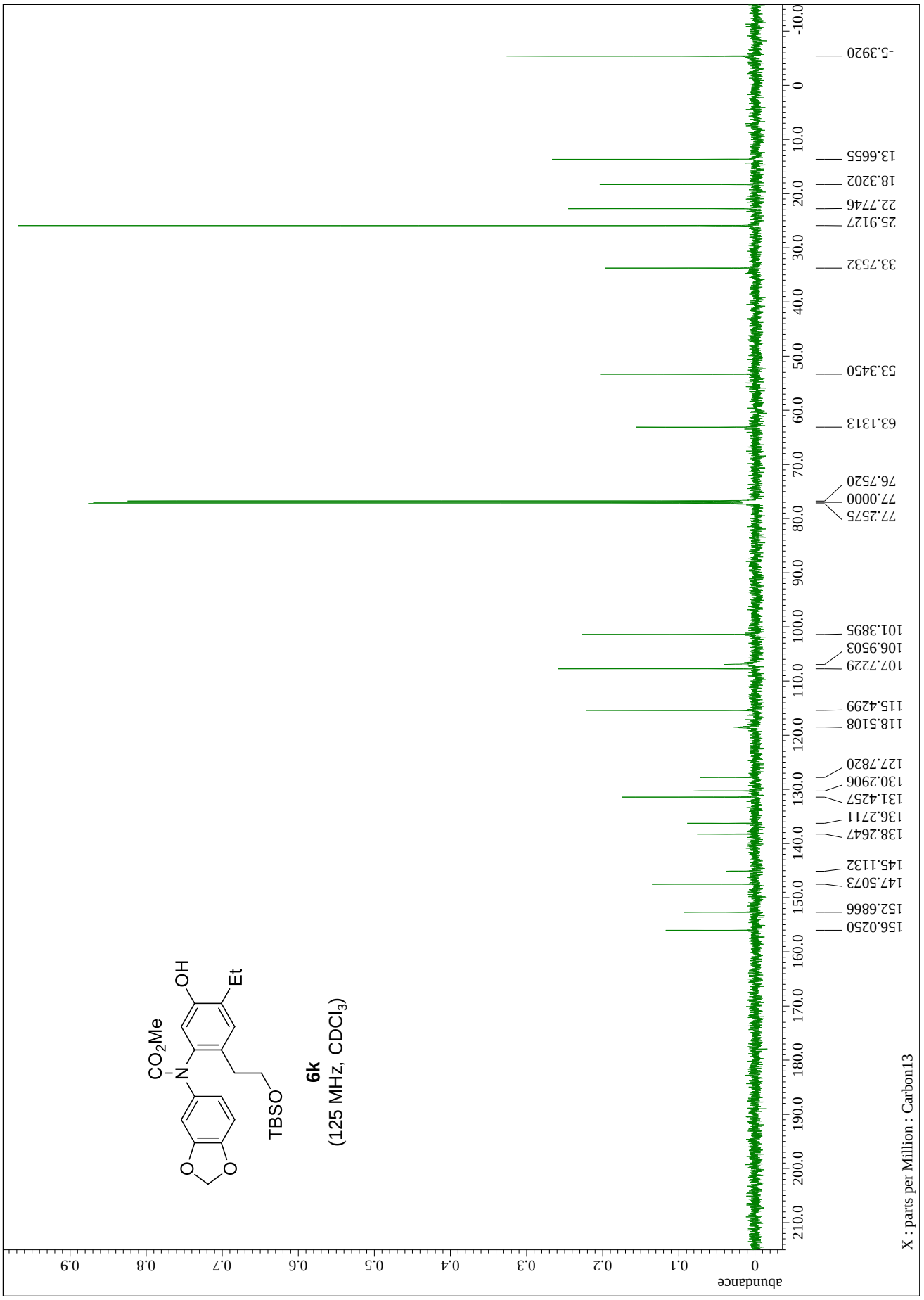
2.01
1.00
1.00
1.01
2.00
3.00
2.01
2.01

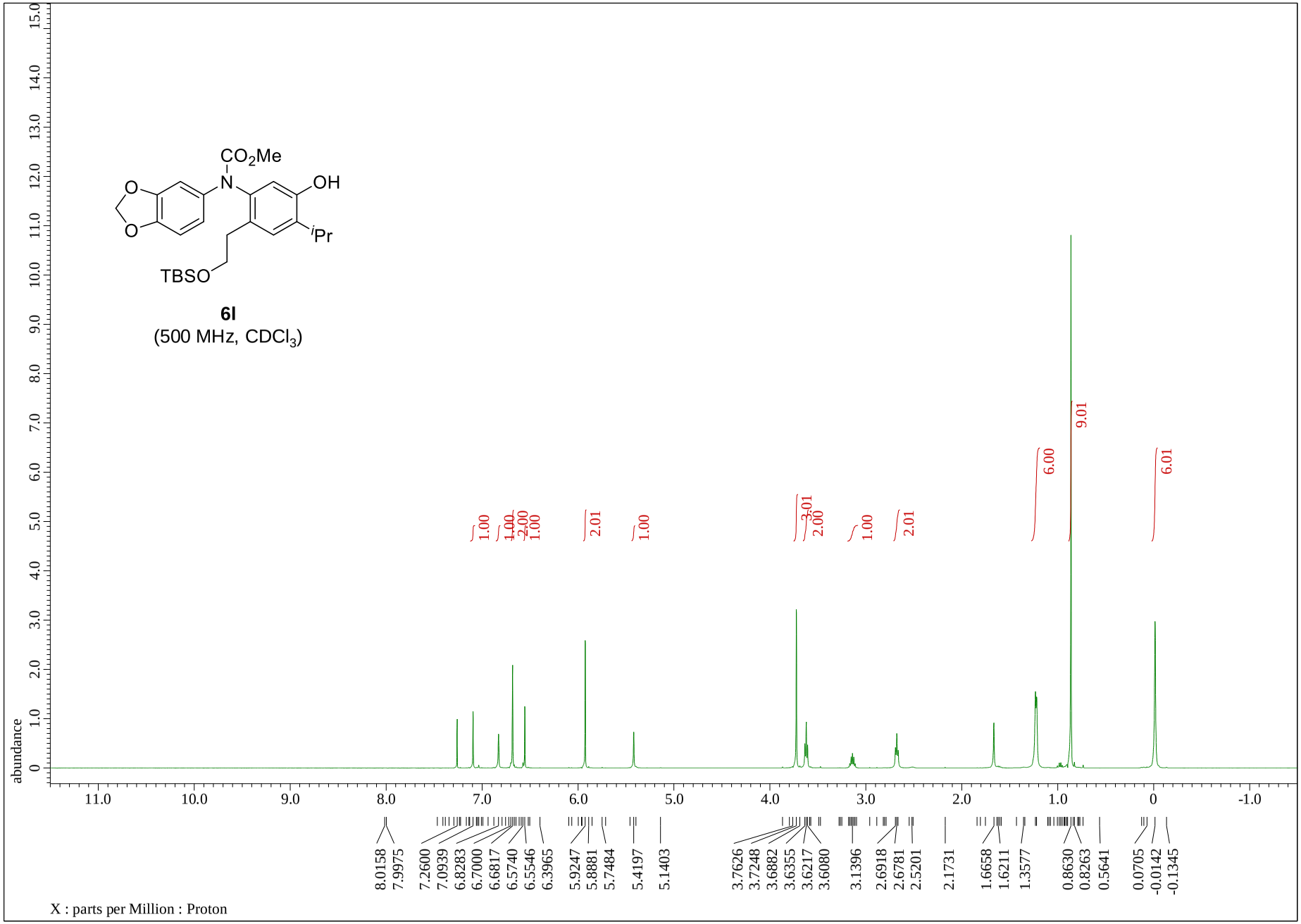

CO2Me
N
OH
BnO
6i
(75 MHz, CDCl3)
155.5598
155.0148
141.8594
140.7790
138.1594
131.5052
128.6274
128.3406
128.1494
127.6523
127.5662
125.2430
124.7363
116.4089
115.5963
77.4207
77.0000
76.5698
72.8698
69.7339
53.2801
30.5449
X : parts per Million : 13C
abundance

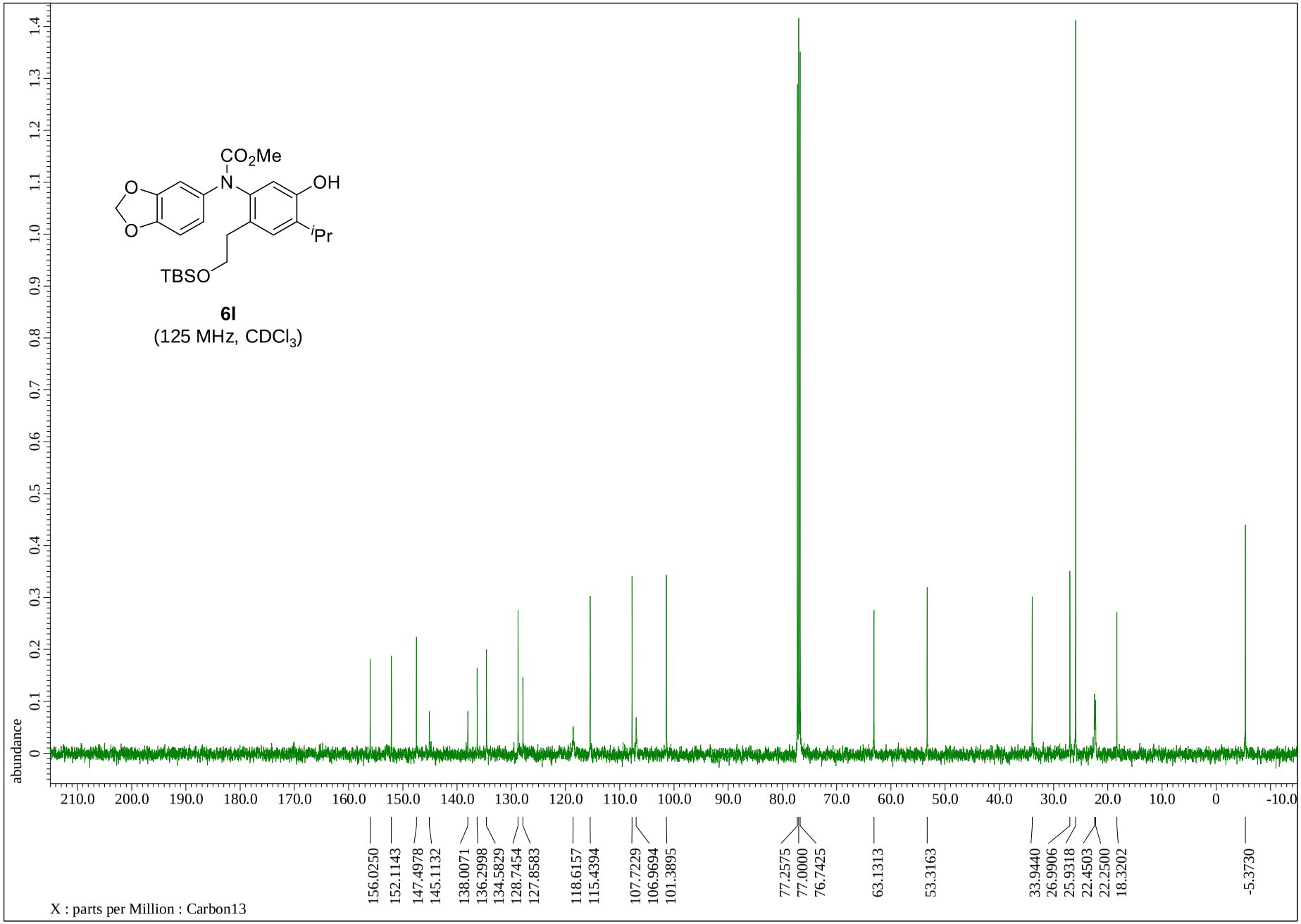

CO2Me
N
OH
OBn
F
F
6j
(500 MHz, CDCl3)
X : parts per Million : Proton
abundance
8.0009
7.3241
7.3104
7.2772
7.2600
6.8580
6.8409
6.5752
6.5706
6.1377
5.9740
5.9545
5.1574
4.4852
4.4623
4.4554
4.3180
3.6687
3.5542
3.5393
3.4797
3.4648
3.0812
2.8052
2.6941
2.6792
2.1994
2.0700
1.2558
1.2432
1.2294
0.8962
0.8836
0.0980
5.98
1.00
2.01
1.00
2.00
1.01
2.00
3.01
1.01
1.00
2.01

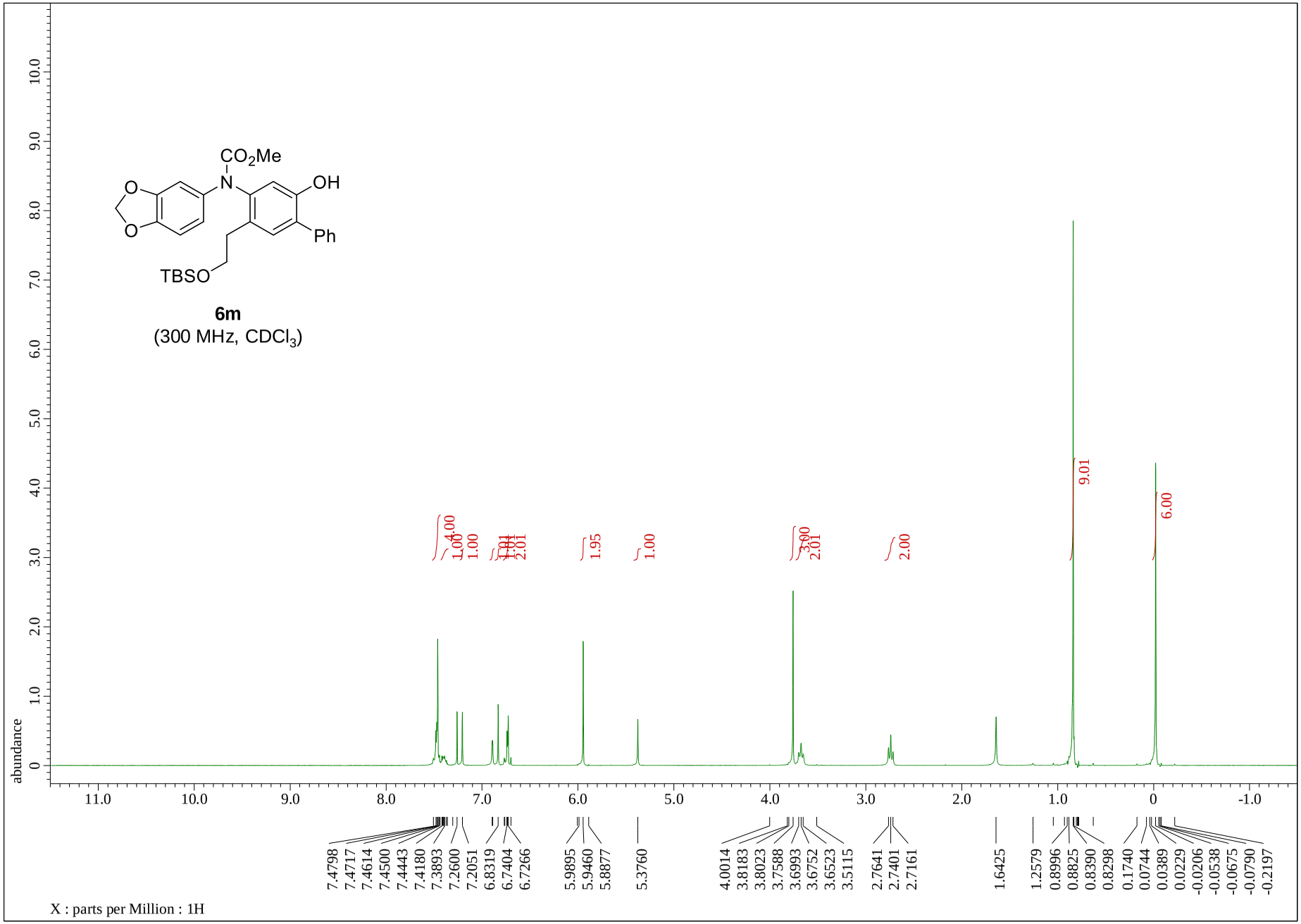

CO2Me
N
OH
OBn
F
F
6j
(125 MHz, CDCl3)
163.6652
163.5412
161.7003
161.5859
155.3859
154.9090
144.1880
144.0926
139.6191
137.8068
131.6546
128.3734
128.0873
127.6771
116.1930
116.1453
106.8263
106.7786
106.6451
106.5974
100.2926
100.0923
99.8920
77.2575
77.0000
76.7425
72.9176
69.3980
53.5262
30.3290
X : parts per Million : Carbon13
abundance

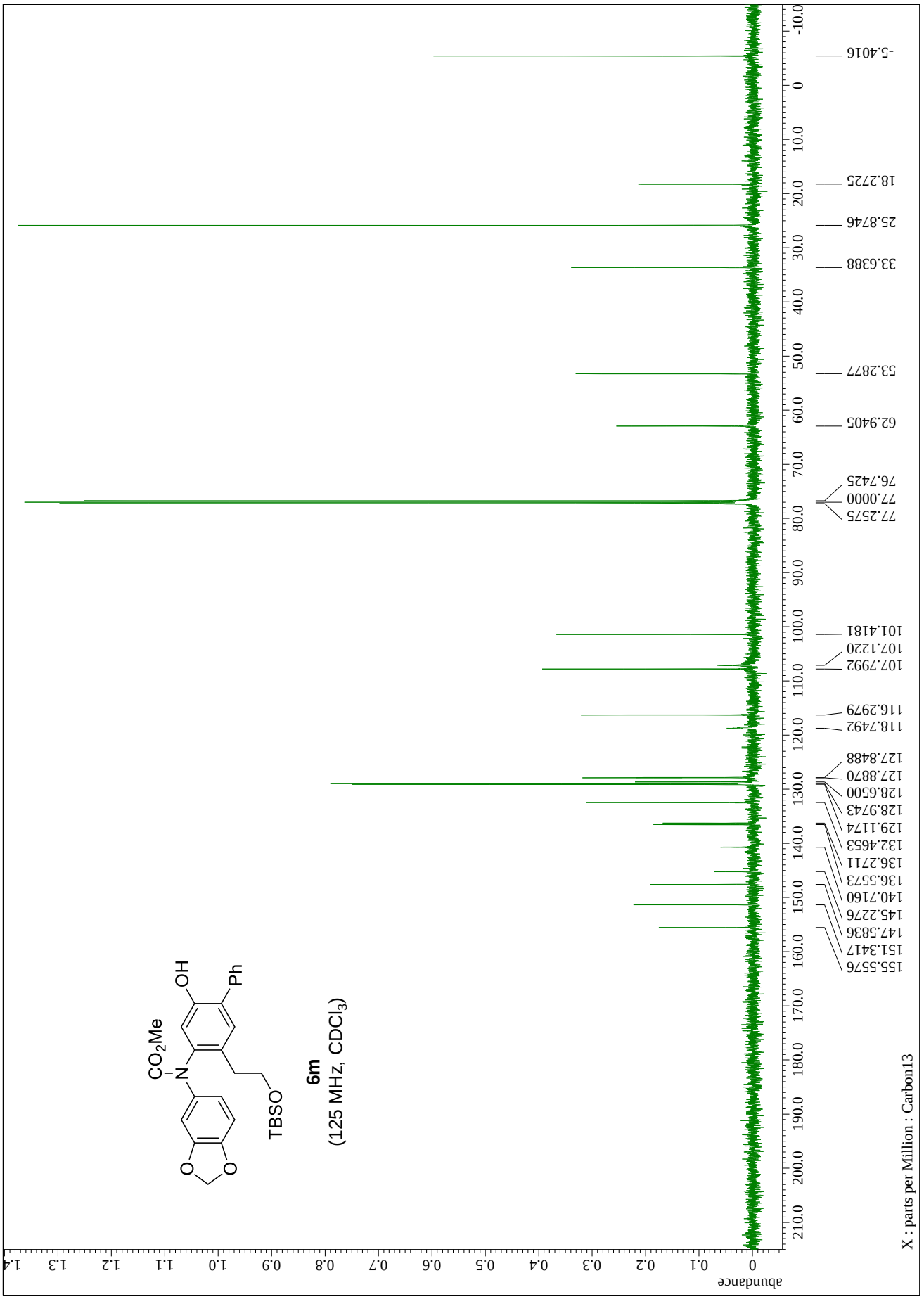

CO2Me
N
OH
Et
TBSO
O
O
6k
(300 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.2600
7.0357
6.8251
6.6705
6.6442
6.5492
6.2047
5.9895
5.9197
5.6278
3.9717
3.7302
3.6306
3.6065
3.5837
3.4818
3.4692
2.6920
2.6680
2.6463
2.5650
2.5410
1.8073
1.2121
1.1869
1.1617
0.9031
0.8630
0.8321
0.1809
0.0859
-0.0137
-0.2129
1.00
1.01
2.00
1.00
3.01
3.01
2.02
2.01
2.00
3.01
9.01
6.01

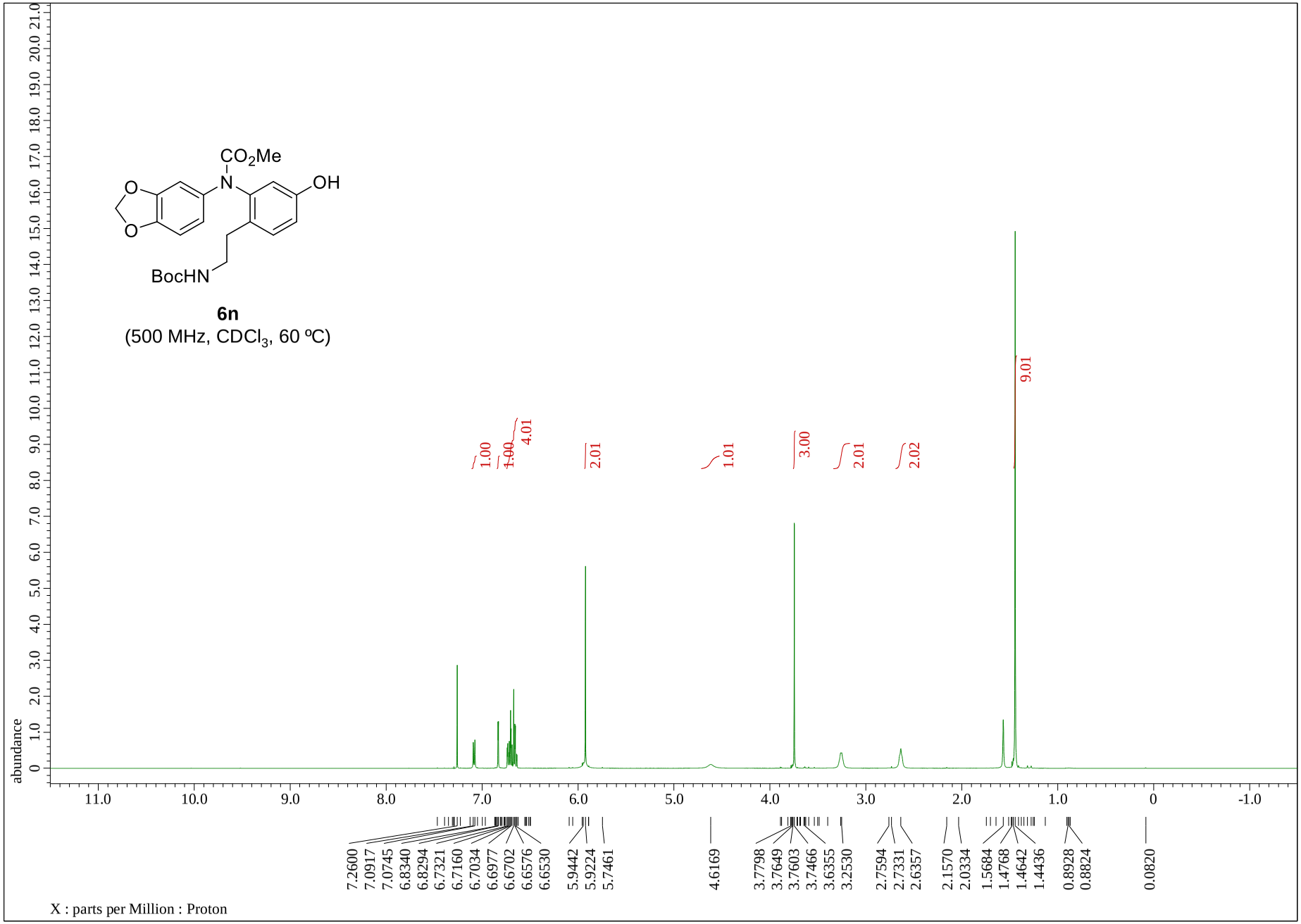

CO2Me
N
OH
Et
TBSO
O
O
6k
(125 MHz, CDCl3)
-5.3920
13.6655
18.3202
22.7746
25.9127
33.7532
53.3450
63.1313
76.7520
77.0000
77.2575
101.3895
106.9503
107.7229
115.4299
118.5108
127.7820
130.2906
131.4257
136.2711
138.2647
145.1132
147.5073
152.6866
156.0250
X : parts per Million : Carbon13
abundance

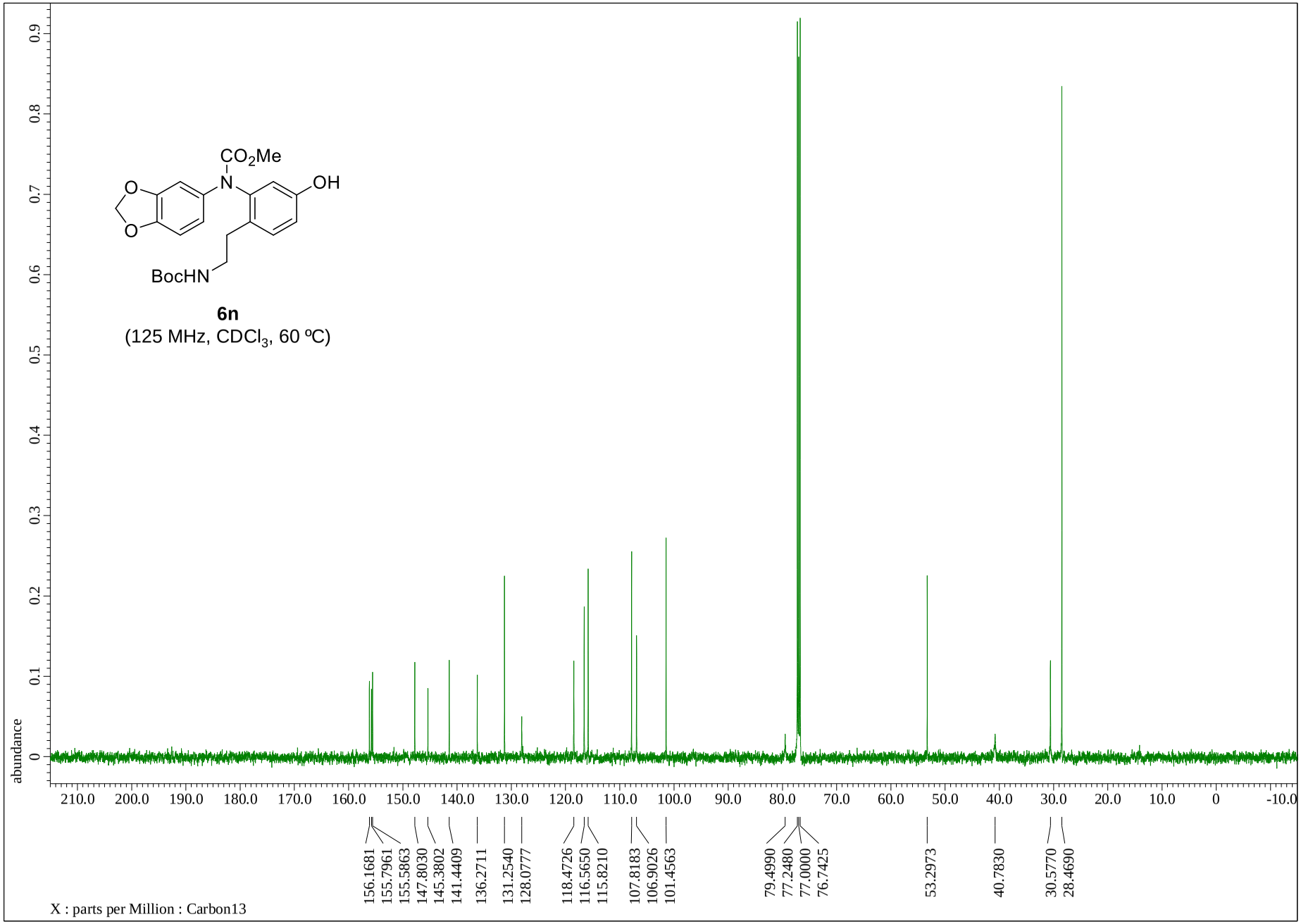

CO2Me
N
OH
O
O
iPr
TBSO
6l
(500 MHz, CDCl3)
abundance
X : parts per Million : Proton
8.0158
7.9975
7.2600
7.0939
6.8283
6.7000
6.6817
6.5740
6.5546
6.3965
5.9247
5.8881
5.7484
5.4197
5.1403
3.7626
3.7248
3.6882
3.6355
3.6217
3.6080
3.1396
2.6918
2.6781
2.5201
2.1731
1.6658
1.6211
1.3577
0.8630
0.8263
0.5641
0.0705
-0.0142
-0.1345
1.00
1.00
2.00
1.00
2.01
1.00
3.01
2.00
1.00
2.01
6.00
9.01
6.01

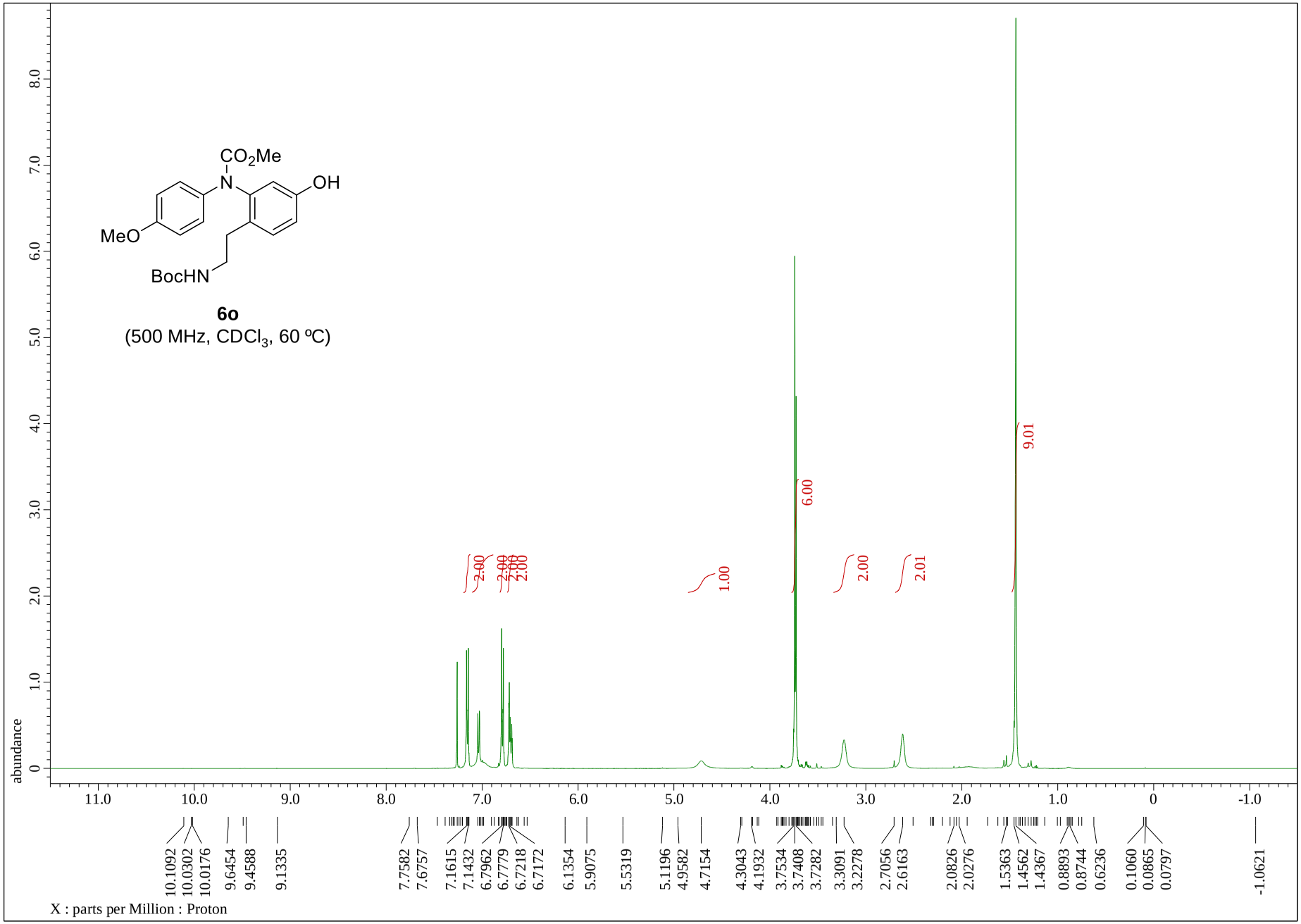

CO2Me
N
OH
O
O
iPr
TBSO
6l
(125 MHz, CDCl3)
abundance
156.0250
152.1143
147.4978
145.1132
138.0071
136.2998
134.5829
128.7454
127.8583
118.6157
115.4394
107.7229
106.9694
101.3895
77.2575
77.0000
76.7425
63.1313
53.3163
33.9440
26.9906
25.9318
22.4503
22.2500
18.3202
-5.3730
X : parts per Million : Carbon13

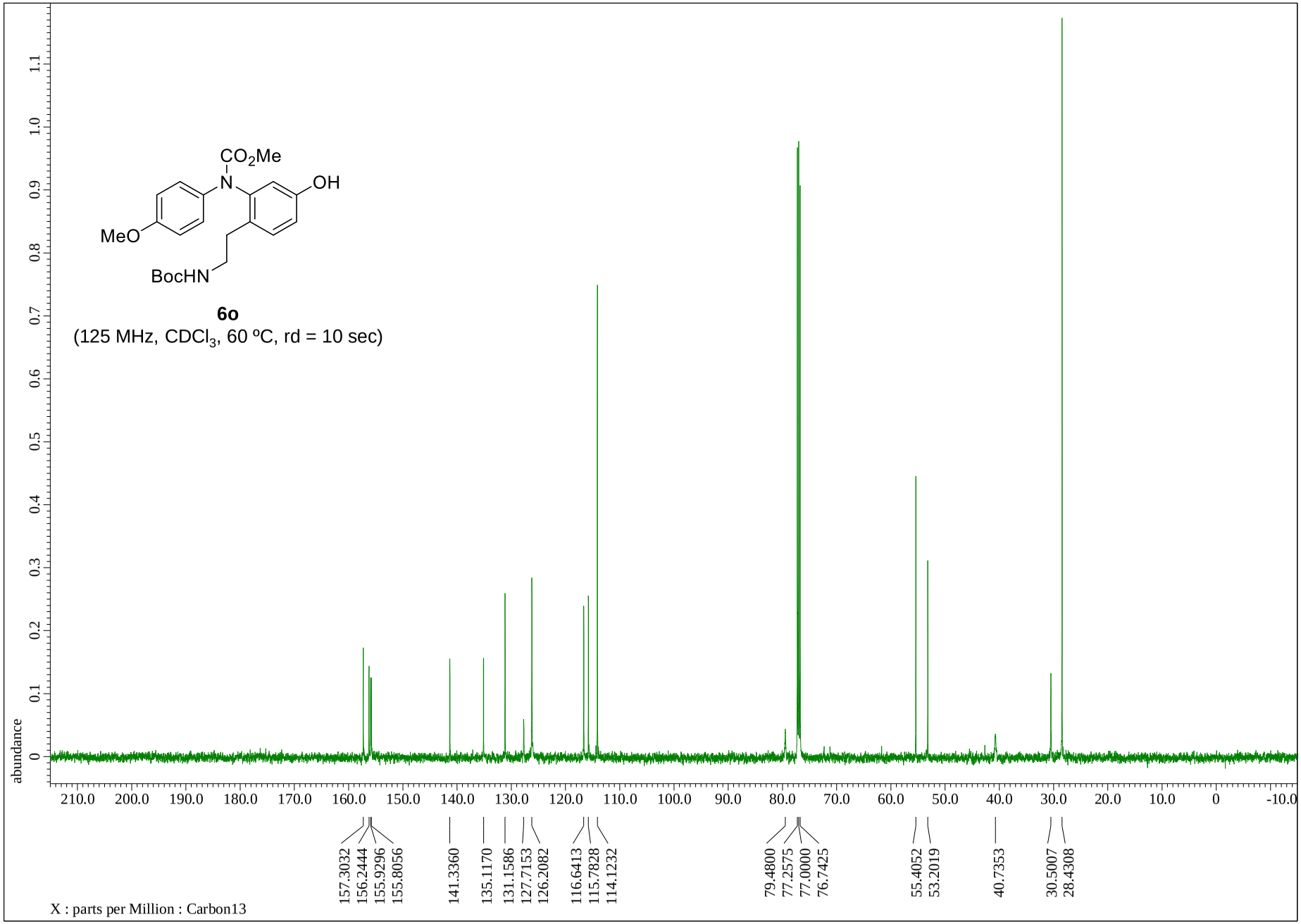

CO2Me
N
OH
O
O
Ph
TBSO
6m
(300 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.4798
7.4717
7.4614
7.4500
7.4443
7.4180
7.3893
7.2600
7.2051
6.8319
6.7404
6.7266
5.9895
5.9460
5.8877
5.3760
4.0014
3.8183
3.8023
3.7588
3.6993
3.6752
3.6523
3.5115
2.7641
2.7401
2.7161
1.6425
1.2579
0.8996
0.8825
0.8390
0.8298
0.1740
0.0744
0.0389
0.0229
-0.0206
-0.0538
-0.0675
-0.0790
-0.2197
4.00
1.00
1.00
2.01
1.95
1.00
3.00
2.01
2.00
9.01
6.00

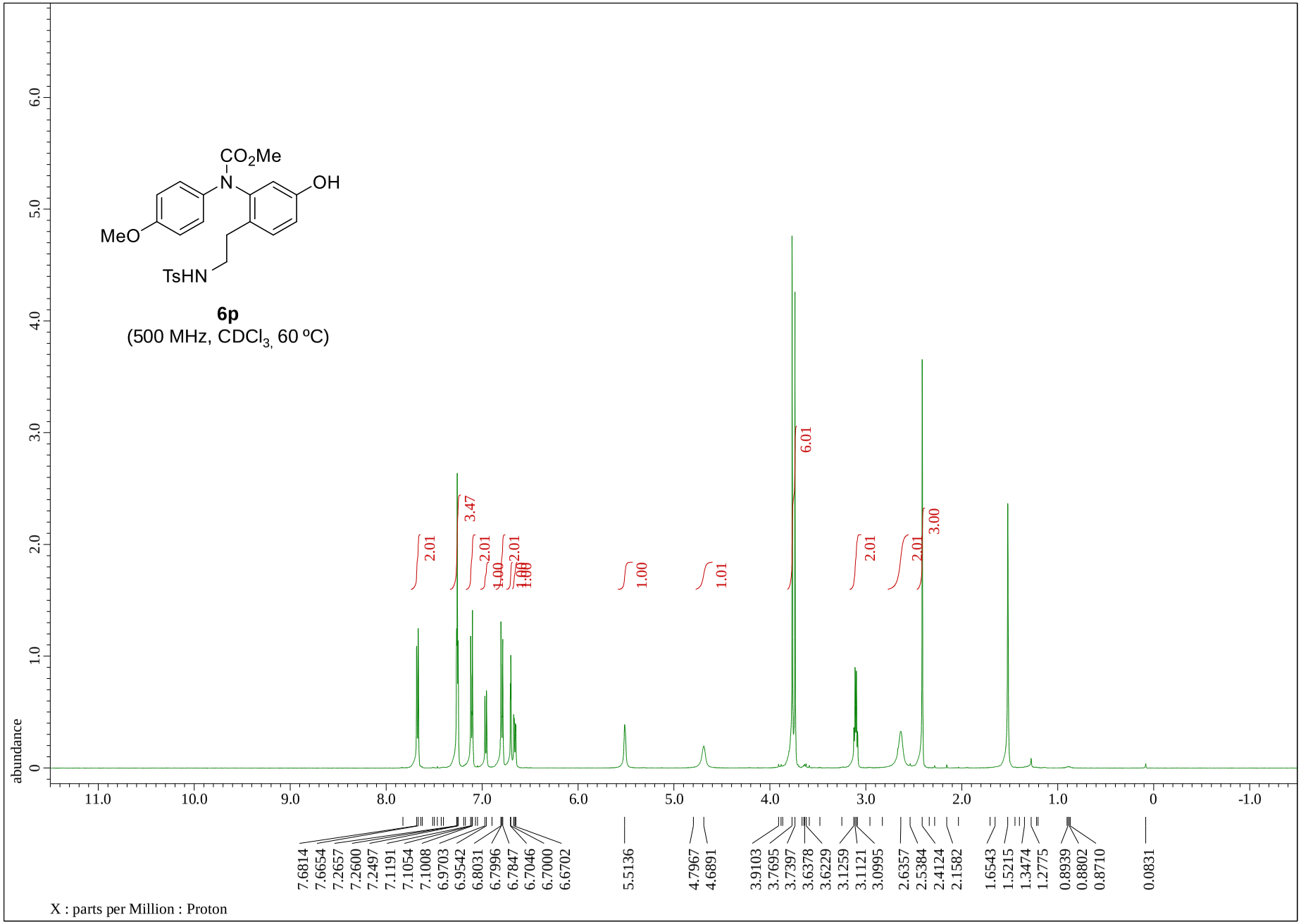

CO2Me
N
OH
Ph
TBSO
O
O
6m
(125 MHz, CDCl3)
-5.4016
18.2725
25.8746
33.6388
53.2877
62.9405
77.2575
77.0000
76.7425
101.4181
107.7992
107.1220
118.7492
116.2979
155.5576
151.3417
147.5836
145.2276
140.7160
136.5573
136.2711
132.4653
129.1174
128.9743
128.6500
127.8870
127.8488
X : parts per Million : Carbon13
abundance

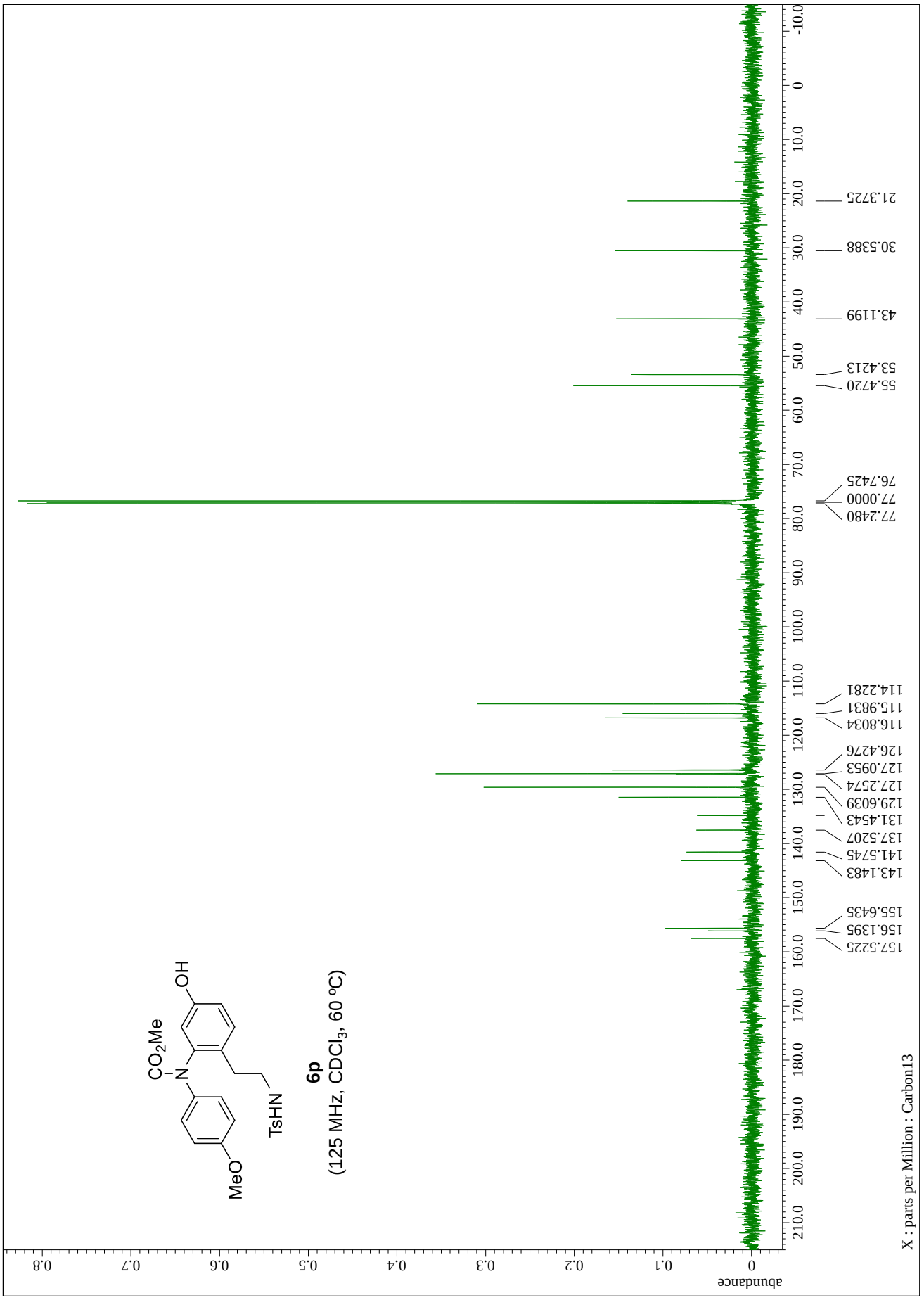

CO2Me
N
OH
O
O
BocHN
6n
(500 MHz, CDCl3, 60 ºC)
abundance
1.00
1.00
4.01
2.01
1.01
3.00
2.01
2.02
9.01
7.2600
7.0917
7.0745
6.8340
6.8294
6.7321
6.7160
6.7034
6.6977
6.6702
6.6576
6.6530
5.9442
5.9224
5.7461
4.6169
3.7798
3.7649
3.7603
3.7466
3.6355
3.2530
2.7594
2.7331
2.6357
2.1570
2.0334
1.5684
1.4768
1.4642
1.4436
0.8928
0.8824
0.0820
X : parts per Million : Proton

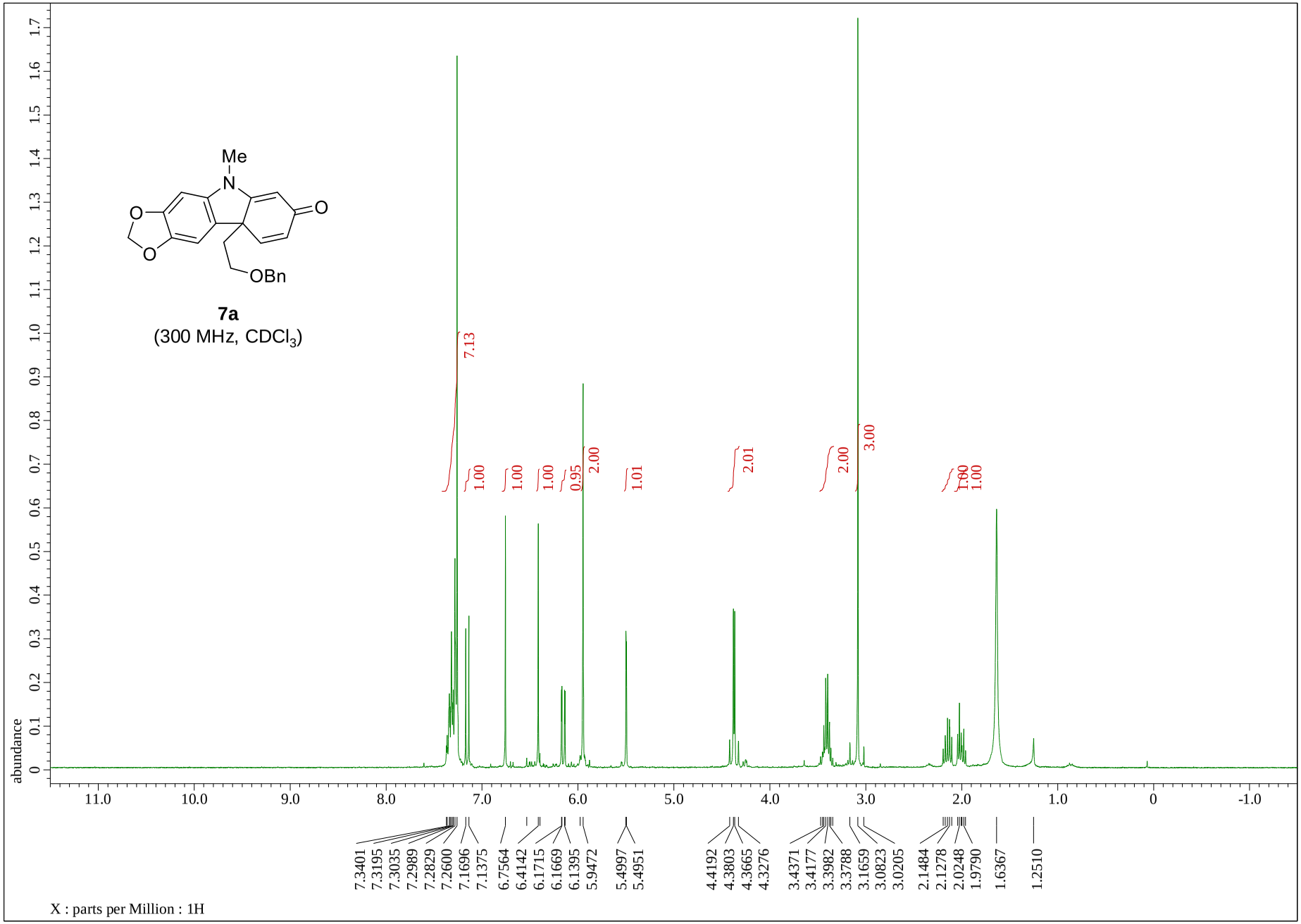

CO2Me
N
OH
O
O
BocHN
6n
(125 MHz, CDCl3, 60 ºC)
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
156.1681
155.7961
155.5863
147.8030
145.3802
141.4409
136.2711
131.2540
128.0777
118.4726
116.5650
115.8210
107.8183
106.9026
101.4563
79.4990
77.2480
77.0000
76.7425
53.2973
40.7830
30.5770
28.4690
X : parts per Million : Carbon13

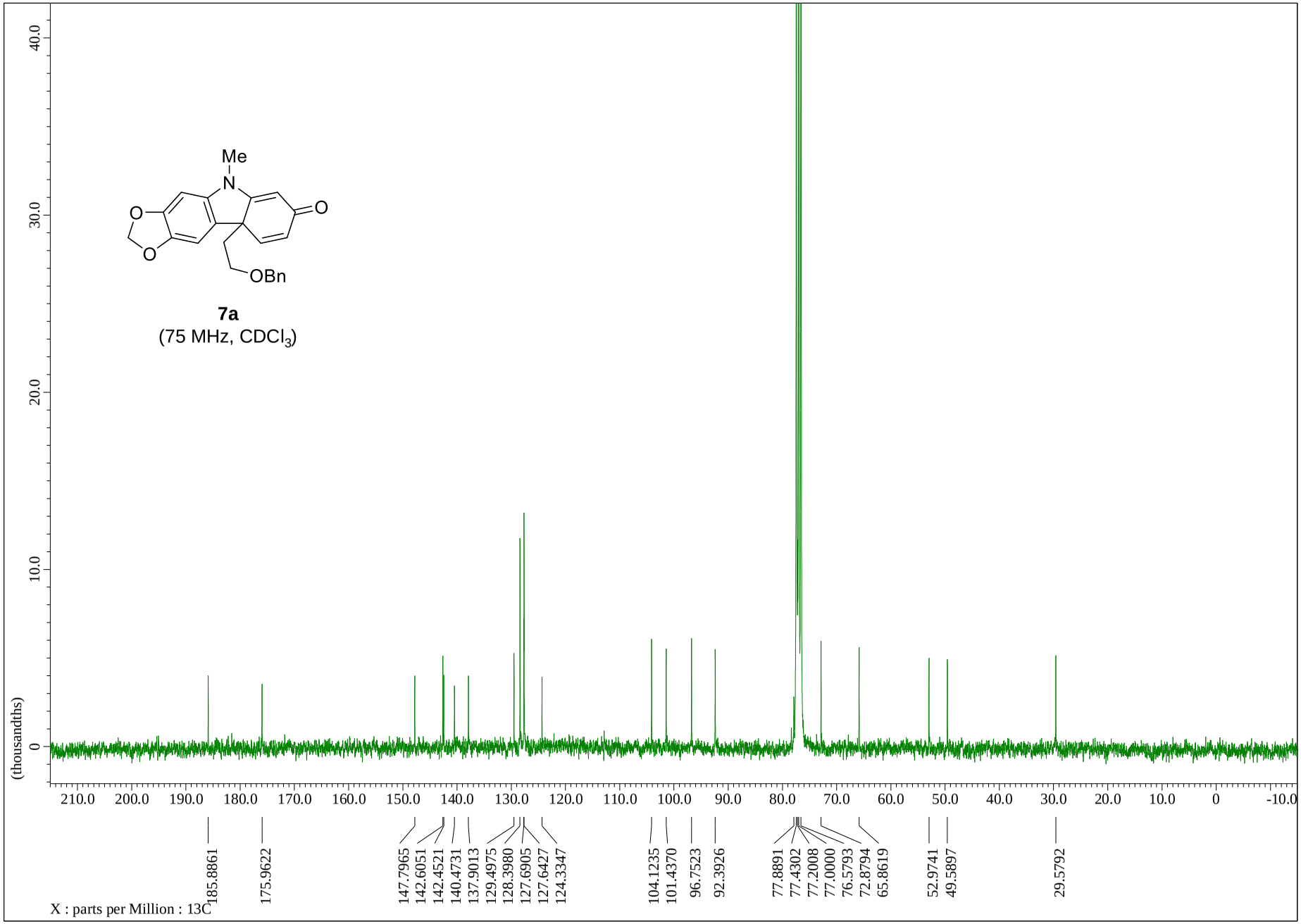

CO2Me
N
OH
MeO
BocHN
6o
(500 MHz, CDCl3, 60 ºC)
abundance
2.00
1.00
6.00
2.00
2.01
9.01
10.1092
10.0302
10.0176
9.6454
9.4588
9.1335
7.7582
7.6757
7.1615
7.1432
6.7962
6.7779
6.7218
6.7172
6.1354
5.9075
5.5319
5.1196
4.9582
4.7154
4.3043
4.1932
3.7534
3.7408
3.7282
3.3091
3.2278
2.7056
2.6163
2.0826
2.0276
1.5363
1.4562
1.4367
0.8893
0.8744
0.6236
0.1060
0.0865
0.0797
-1.0621
X : parts per Million : Proton

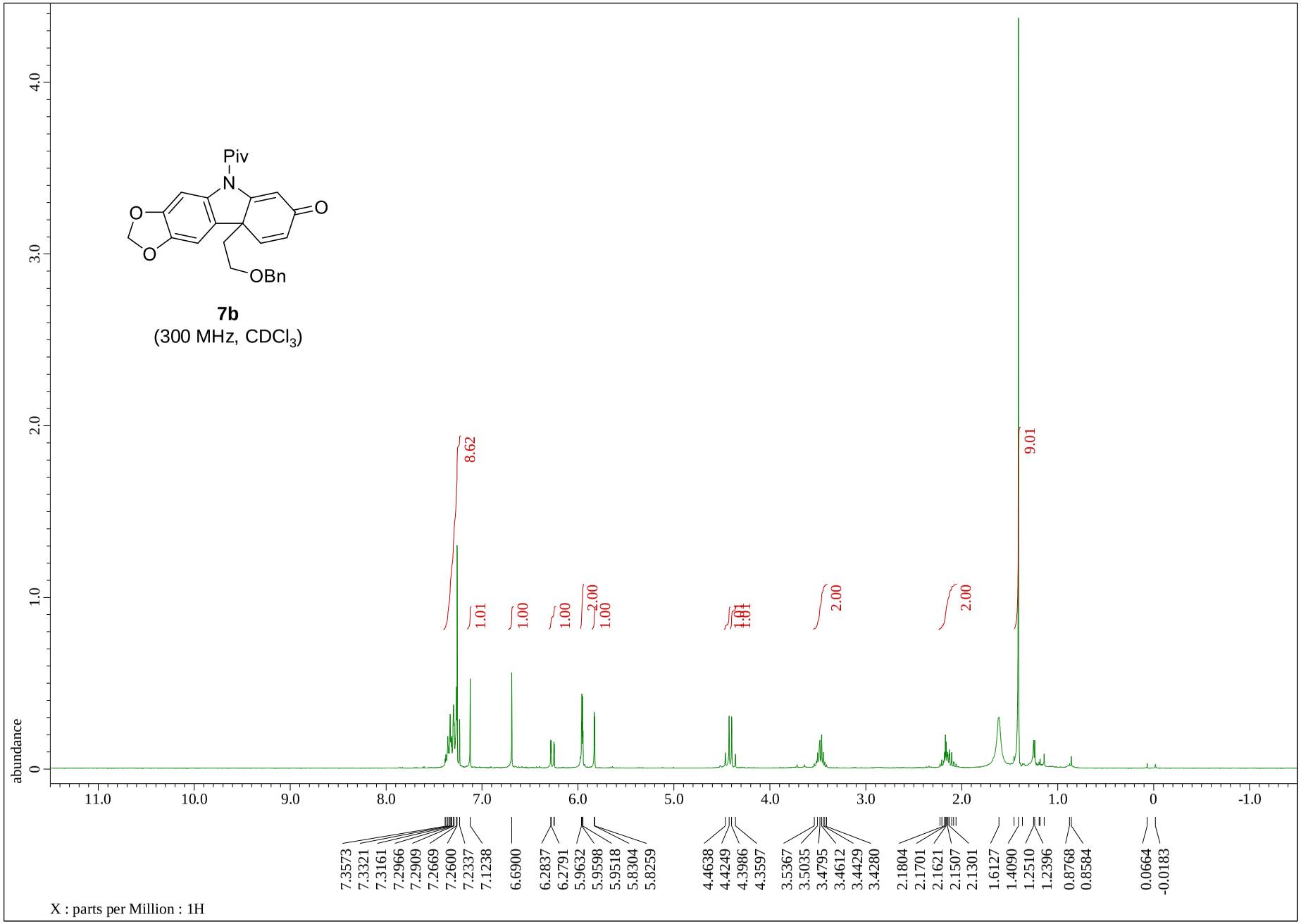

CO2Me
N
OH
MeO
BocHN
6o
(125 MHz, CDCl3, 60 ºC, rd = 10 sec)
abundance
157.3032
156.2444
155.9296
155.8056
141.3360
135.1170
131.1586
127.7153
126.2082
116.6413
115.7828
114.1232
79.4800
77.2575
77.0000
76.7425
55.4052
53.2019
40.7353
30.5007
28.4308
X : parts per Million : Carbon13

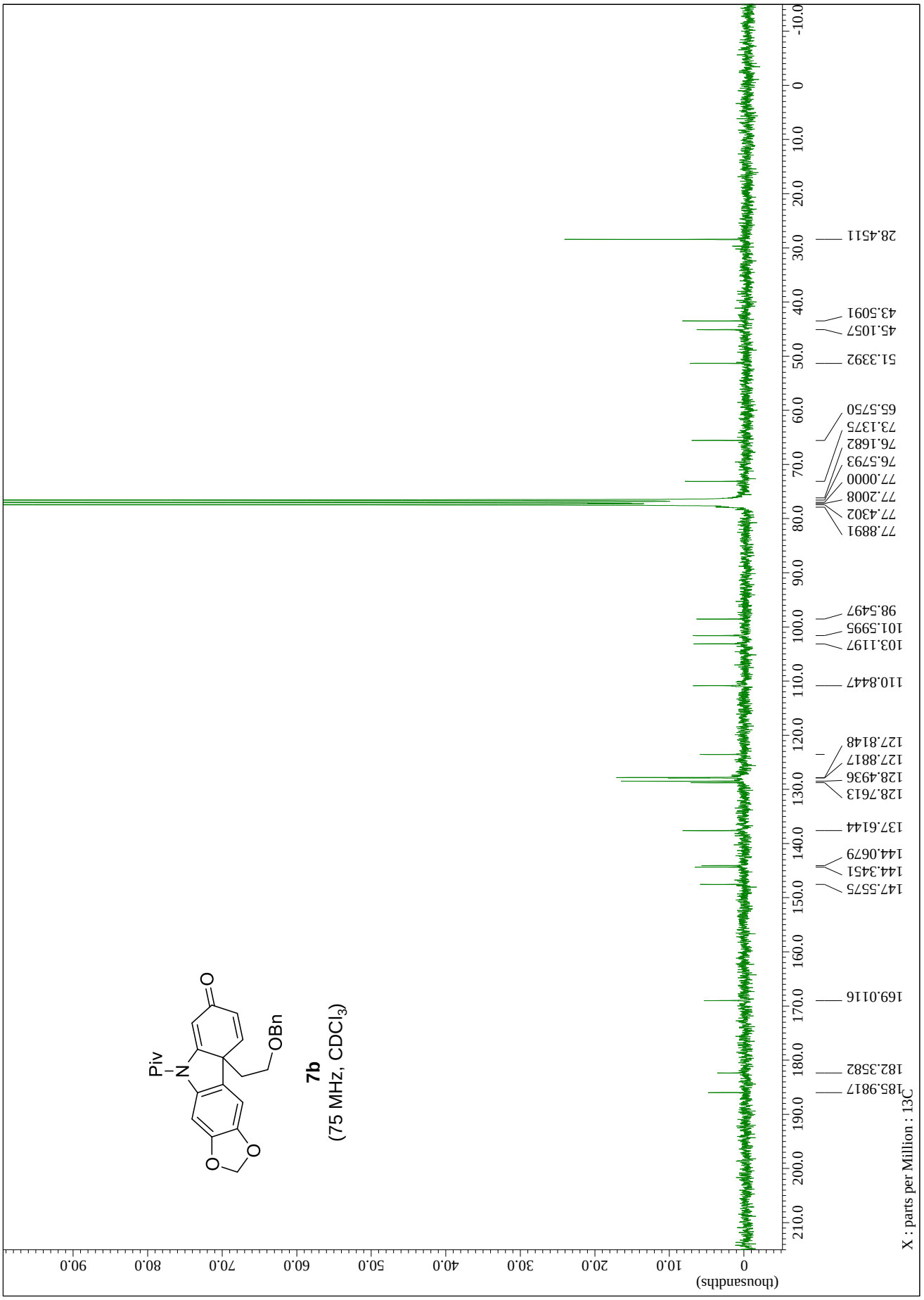

CO2Me
N
OH
MeO
TsHN
6p
(500 MHz, CDCl3, 60 ºC)
abundance
X : parts per Million : Proton
7.6814
7.6654
7.2657
7.2600
7.2497
7.1191
7.1054
7.1008
6.9703
6.9542
6.8031
6.7996
6.7847
6.7046
6.7000
6.6702
5.5136
4.7967
4.6891
3.9103
3.7695
3.7397
3.6378
3.6229
3.1259
3.1121
3.0995
2.6357
2.5384
2.4124
2.1582
1.6543
1.5215
1.3474
1.2775
0.8939
0.8802
0.8710
0.0831
2.01
3.47
2.01
1.00
2.01
1.00
1.01
6.01
2.01
2.01
3.00


MeO
CO2Me
N
OH
TsHN
6p
(125 MHz, CDCl3, 60 ºC)
157.5225
156.1395
155.6435
143.1483
141.5745
137.5207
131.4543
129.6039
127.2574
127.0953
126.4276
116.8034
115.9831
114.2281
77.2480
77.0000
76.7425
55.4720
53.4213
43.1199
30.5388
21.3725
X : parts per Million : Carbon13
abundance

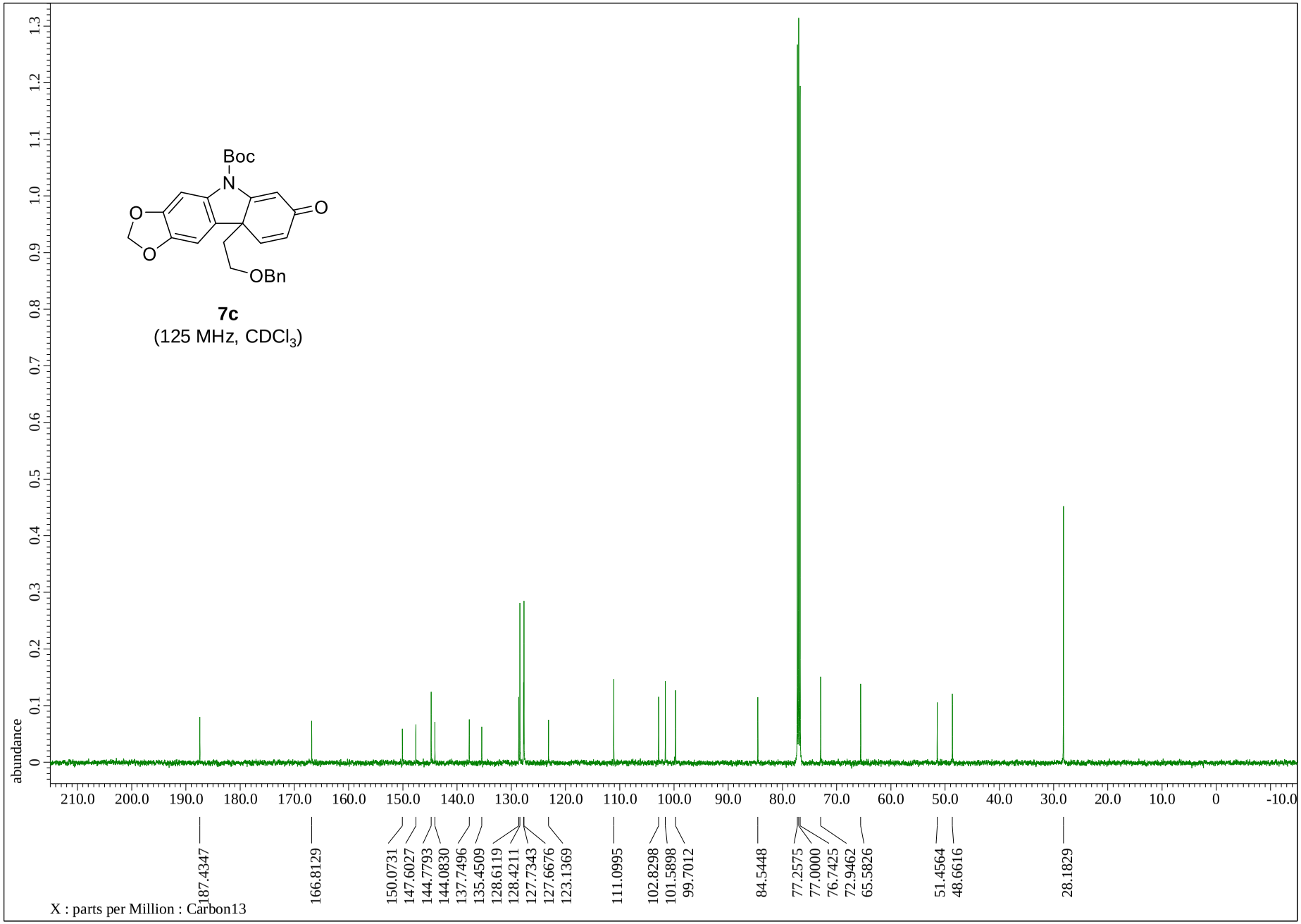

Me
N
O
O
O
OBn
7a
(300 MHz, CDCl3)
abundance
7.13
1.00
1.00
1.00
0.95
2.00
1.01
2.01
2.00
3.00
1.00
1.00
7.3401
7.3195
7.3035
7.2989
7.2829
7.2600
7.1696
7.1375
6.7564
6.4142
6.1715
6.1669
6.1395
5.9472
5.4997
5.4951
4.4192
4.3803
4.3665
4.3276
3.4371
3.4177
3.3982
3.3788
3.1659
3.0823
3.0205
2.1484
2.1278
2.0248
1.9790
1.6367
1.2510
X : parts per Million : 1H

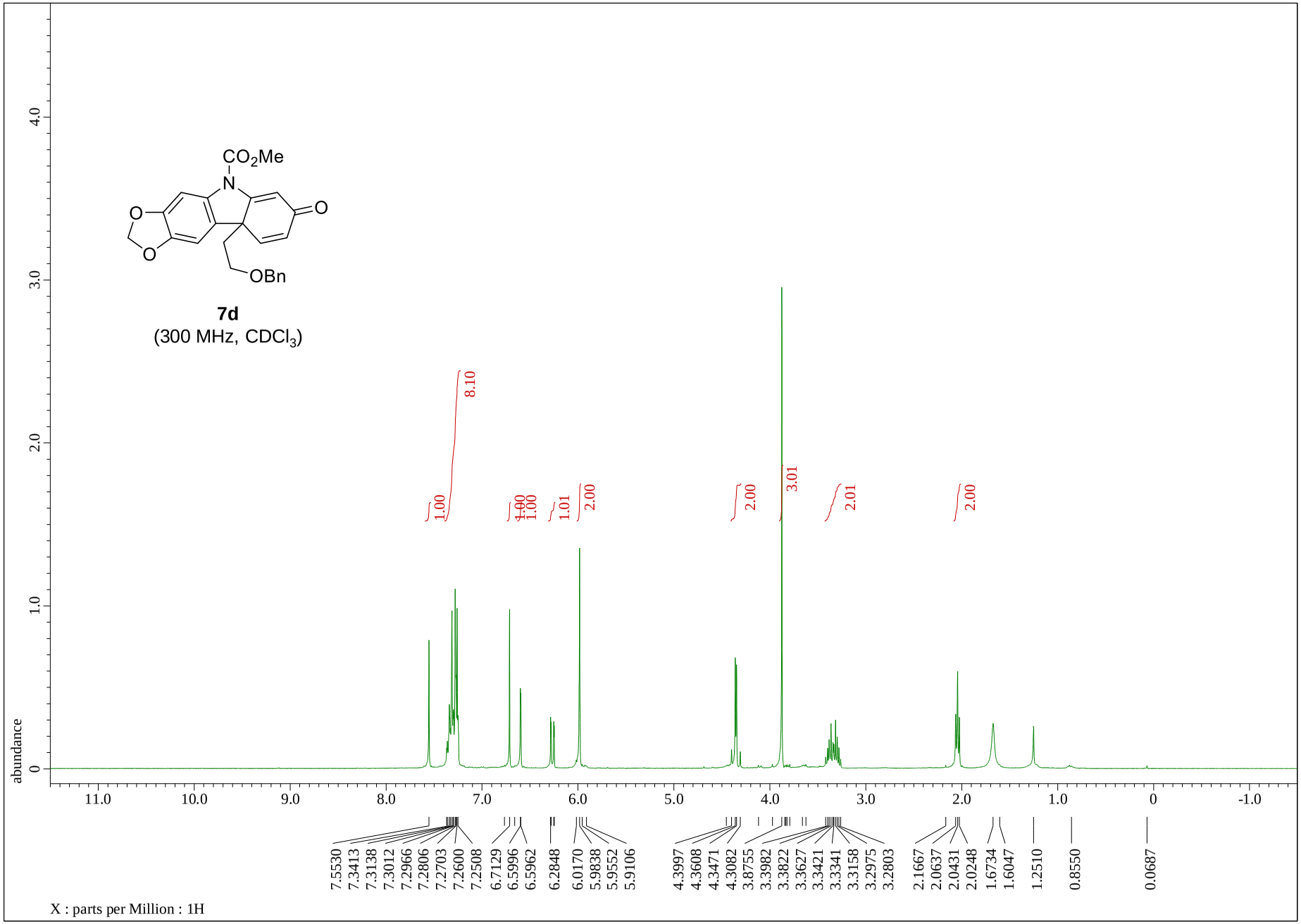

Me
N
O
O
O
OBn
7a
(75 MHz, CDCl3)
(thousandths)
40.0
30.0
20.0
10.0
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
185.8861
175.9622
147.7965
142.6051
142.4521
140.4731
137.9013
129.4975
128.3980
127.6905
127.6427
124.3347
104.1235
101.4370
96.7523
92.3926
77.8891
77.4302
77.2008
77.0000
76.5793
72.8794
65.8619
52.9741
49.5897
29.5792
X : parts per Million : 13C

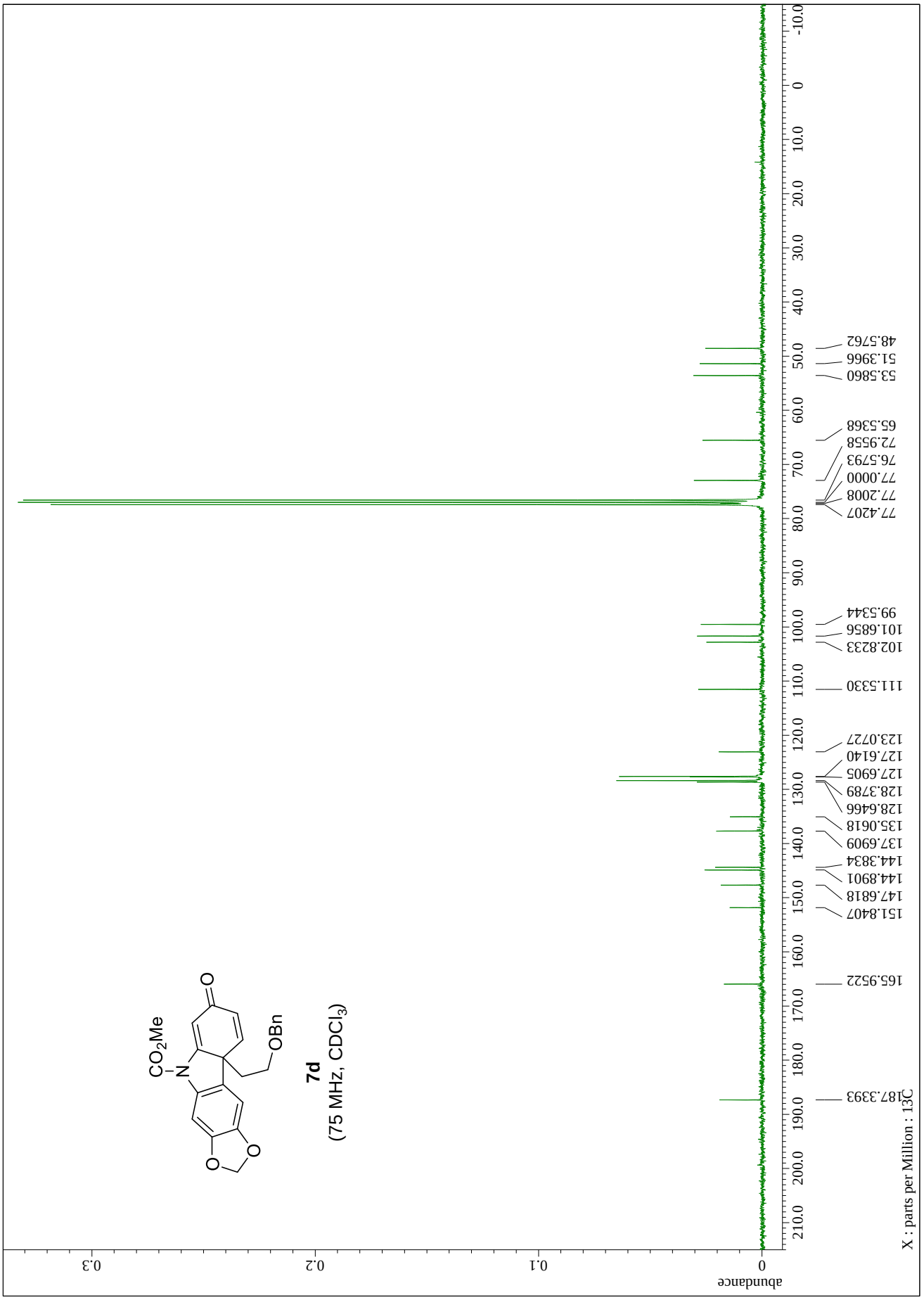

Piv
N
O
O
O
OBn
7b
(300 MHz, CDCl3)
abundance
8.62
1.01
1.00
1.00
2.00
1.00
2.00
2.00
9.01
7.3573
7.3321
7.3161
7.2966
7.2909
7.2669
7.2600
7.2337
7.1238
6.6900
6.2837
6.2791
5.9632
5.9598
5.9518
5.8304
5.8259
4.4638
4.4249
4.3986
4.3597
3.5367
3.5035
3.4795
3.4612
3.4429
3.4280
2.1804
2.1701
2.1621
2.1507
2.1301
1.6127
1.4090
1.2510
1.2396
0.8768
0.8584
0.0664
-0.0183
X : parts per Million : 1H

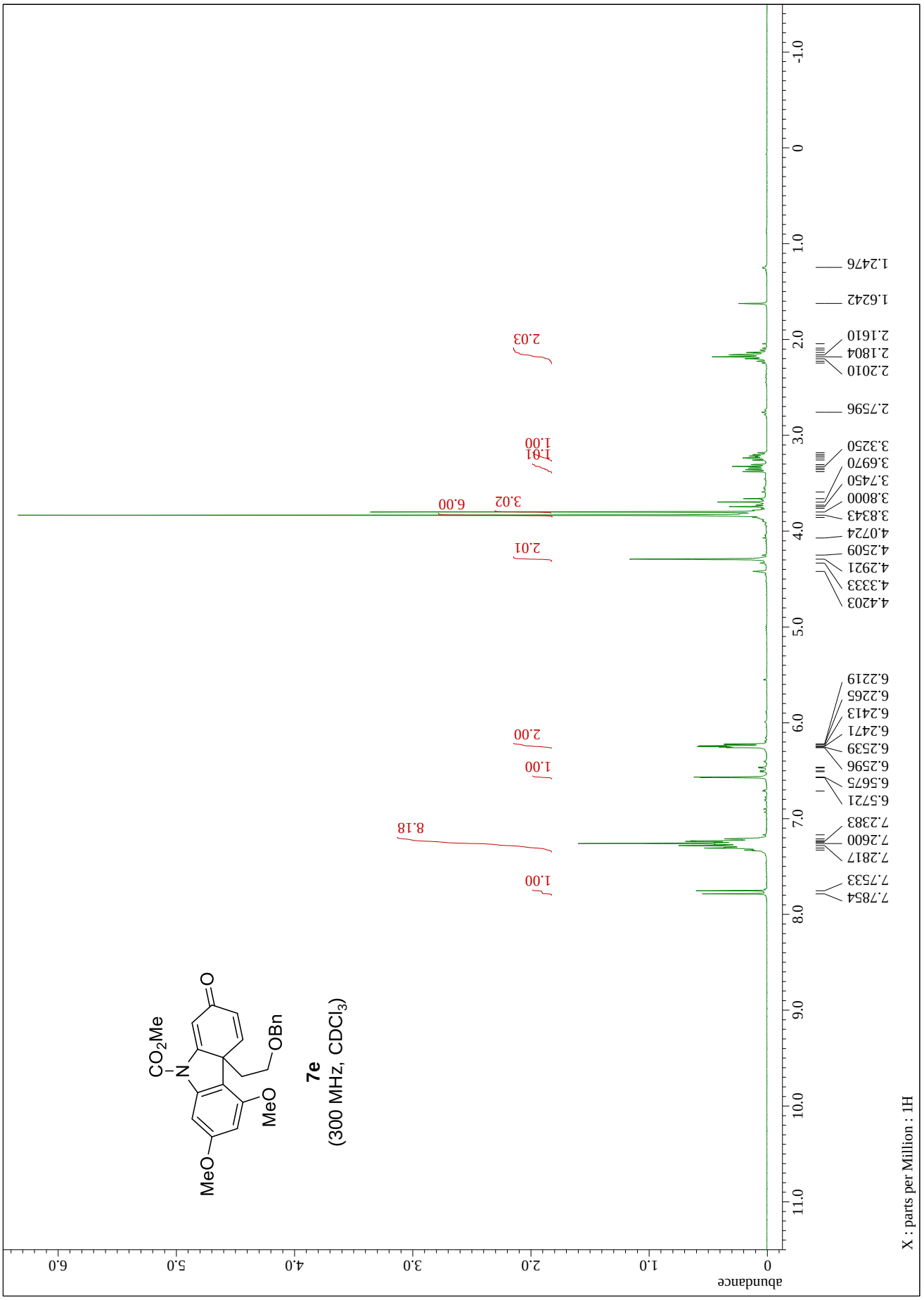

Piv
N
OBn
O
O
O
7b
(75 MHz, CDCl3)
28.4511
43.5091
45.1057
51.3392
65.5750
73.1375
76.1682
76.5793
77.0000
77.2008
77.4302
77.8891
98.5497
101.5995
103.1197
110.8447
127.8148
127.8817
128.4936
128.7613
137.6144
144.0679
144.3451
147.5575
169.0116
182.3582
185.9817
X : parts per Million : 13C
(thousandths)

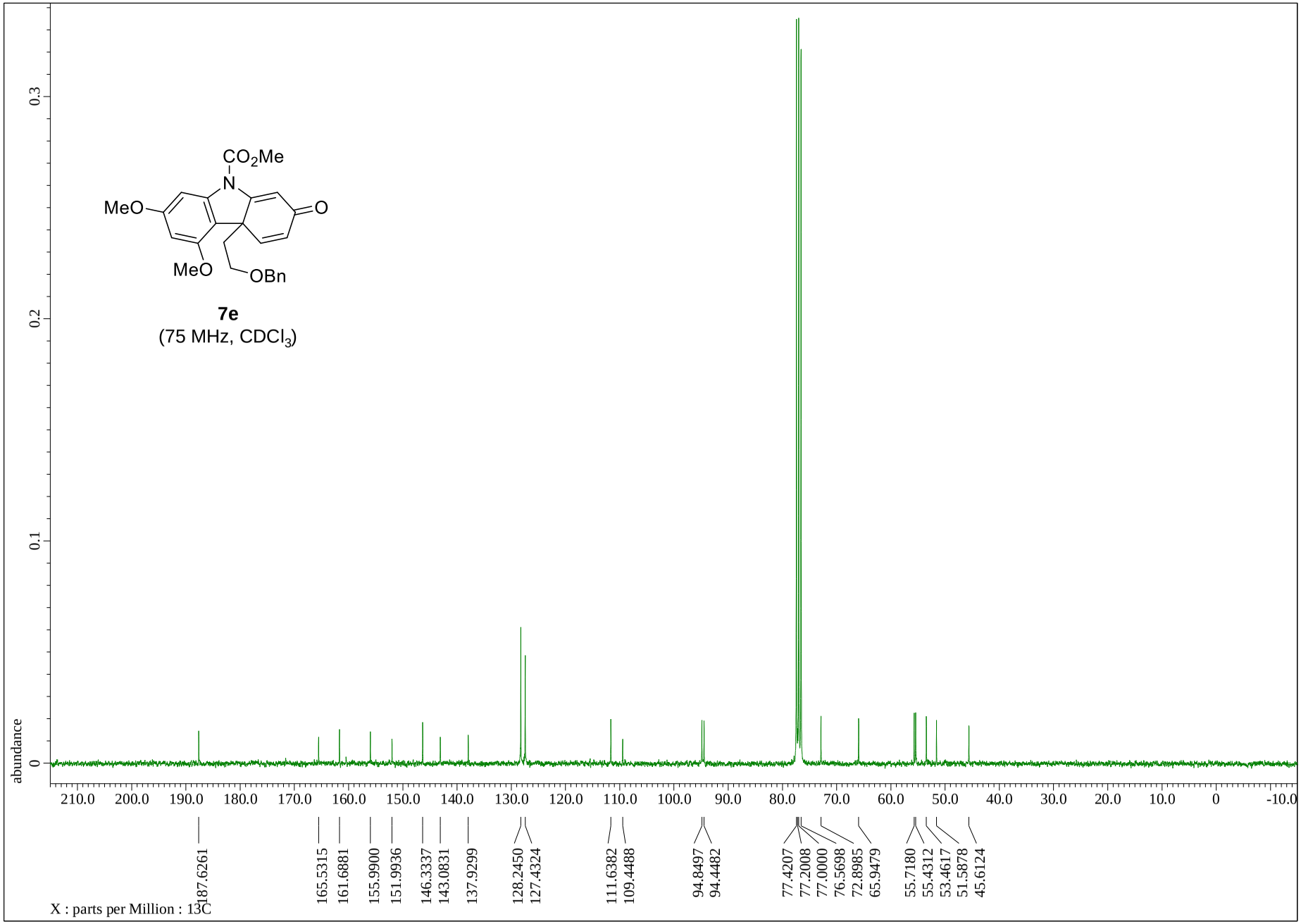
Boc
N
OBn
O
O
O
7c
(500 MHz, CDCl3)
X : parts per Million : Proton
abundance

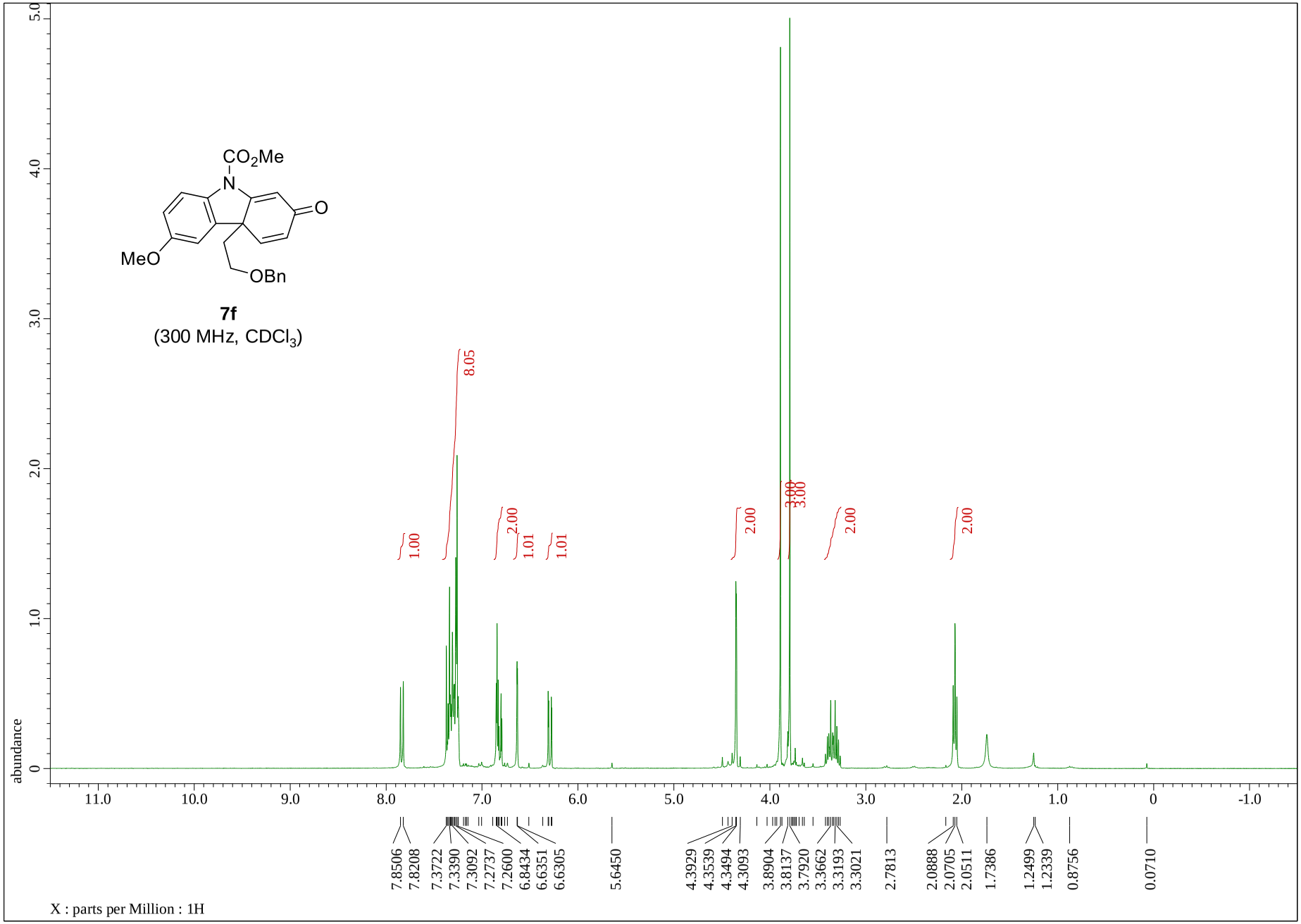

Boc
N
O
O
O
OBn
7c
(125 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
187.4347
166.8129
150.0731
147.6027
144.7793
144.0830
137.7496
135.4509
128.6119
128.4211
127.7343
127.6676
123.1369
111.0995
102.8298
101.5898
99.7012
84.5448
77.2575
77.0000
76.7425
72.9462
65.5826
51.4564
48.6616
28.1829

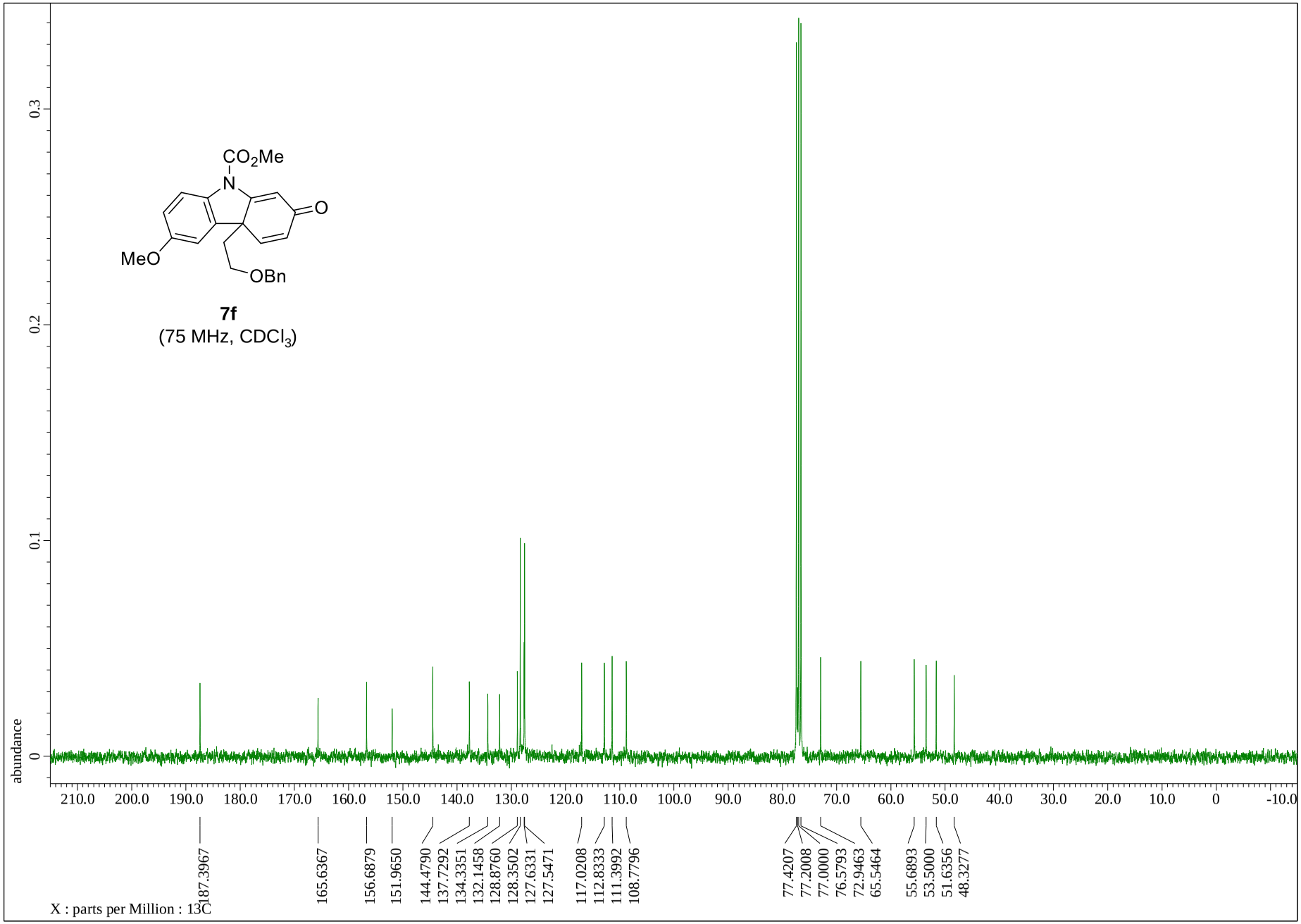

CO2Me
N
O
O
O
OBn
7d
(300 MHz, CDCl3)
abundance
X : parts per Million : 1H
1.00
8.10
1.00
1.00
1.01
2.00
2.00
3.01
2.01
2.00
7.5530
7.3413
7.3138
7.3012
7.2966
7.2806
7.2703
7.2600
7.2508
6.7129
6.5996
6.5962
6.2848
6.0170
5.9838
5.9552
5.9106
4.3997
4.3608
4.3471
4.3082
3.8755
3.3982
3.3822
3.3627
3.3421
3.3341
3.3158
3.2975
3.2803
2.1667
2.0637
2.0431
2.0248
1.6734
1.6047
1.2510
0.8550
0.0687

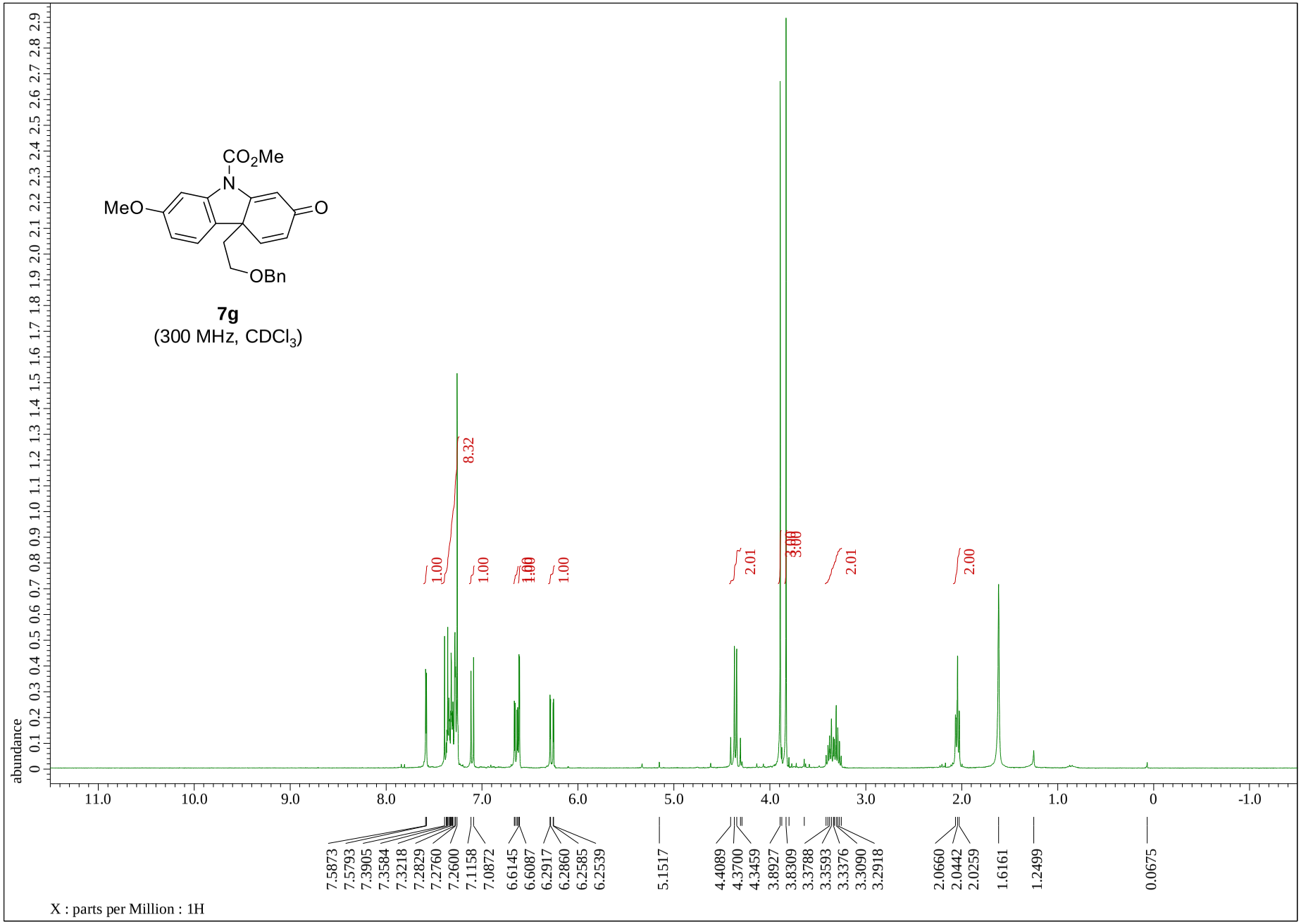

CO2Me
N
OBn
O
O
O
7d
(75 MHz, CDCl3)
187.3393
165.9522
151.8407
147.6818
144.8901
144.3834
137.6909
135.0618
128.6466
128.3789
127.6905
127.6140
123.0727
111.5330
102.8233
101.6856
99.5344
77.4207
77.2008
77.0000
76.5793
72.9558
65.5368
53.5860
51.3966
48.5762
abundance
X : parts per Million : 13C

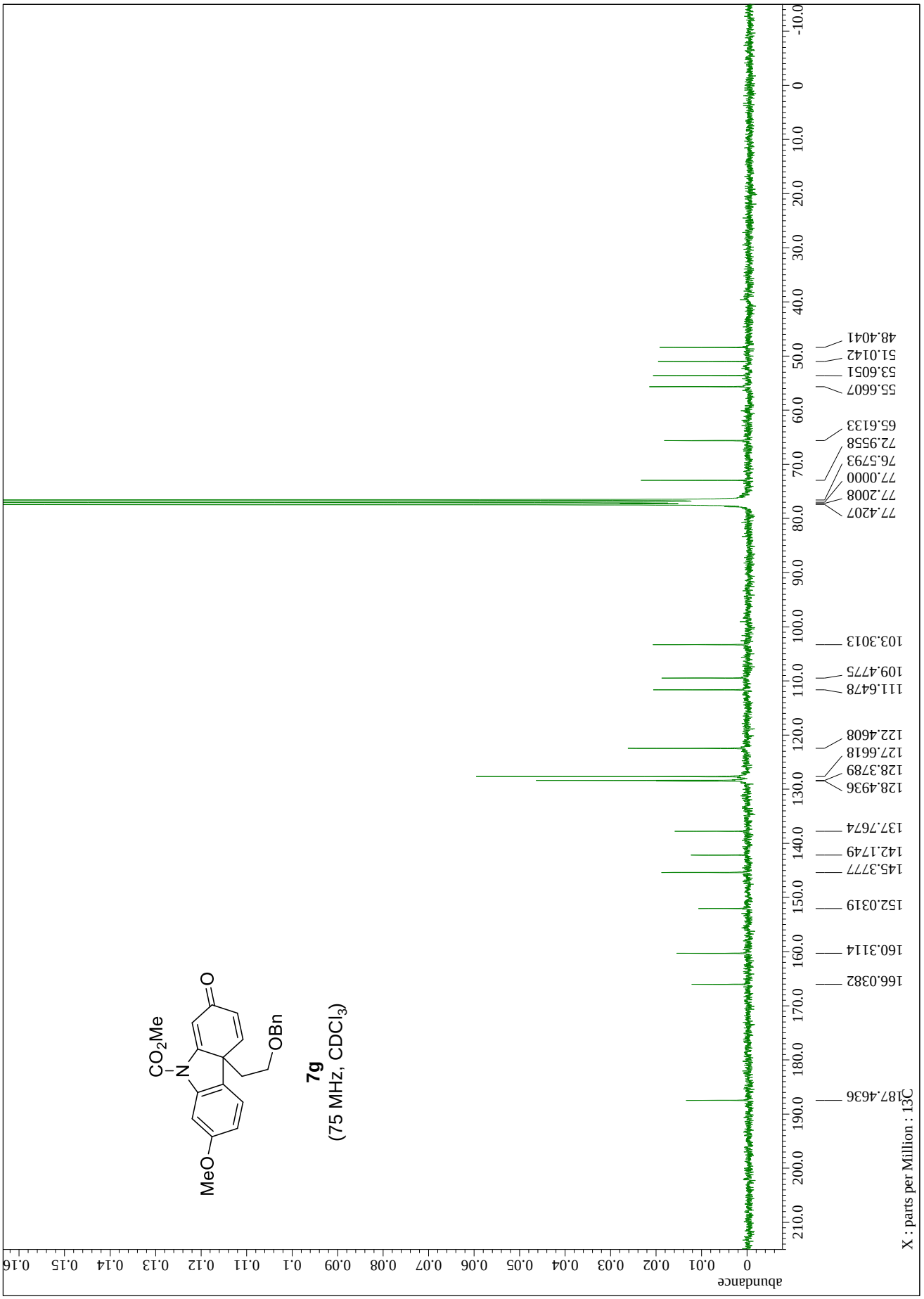

CO2Me
N
MeO
MeO
OBn
O
7e
(300 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.7854
7.7533
7.2817
7.2600
7.2383
6.5721
6.5675
6.2596
6.2539
6.2471
6.2413
6.2265
6.2219
4.4203
4.3333
4.2921
4.2509
4.0724
3.8343
3.8000
3.7450
3.6970
3.3250
2.7596
2.2010
2.1804
2.1610
1.6242
1.2476
1.00
8.18
1.00
2.00
2.01
6.00
3.02
1.01
1.00
2.03

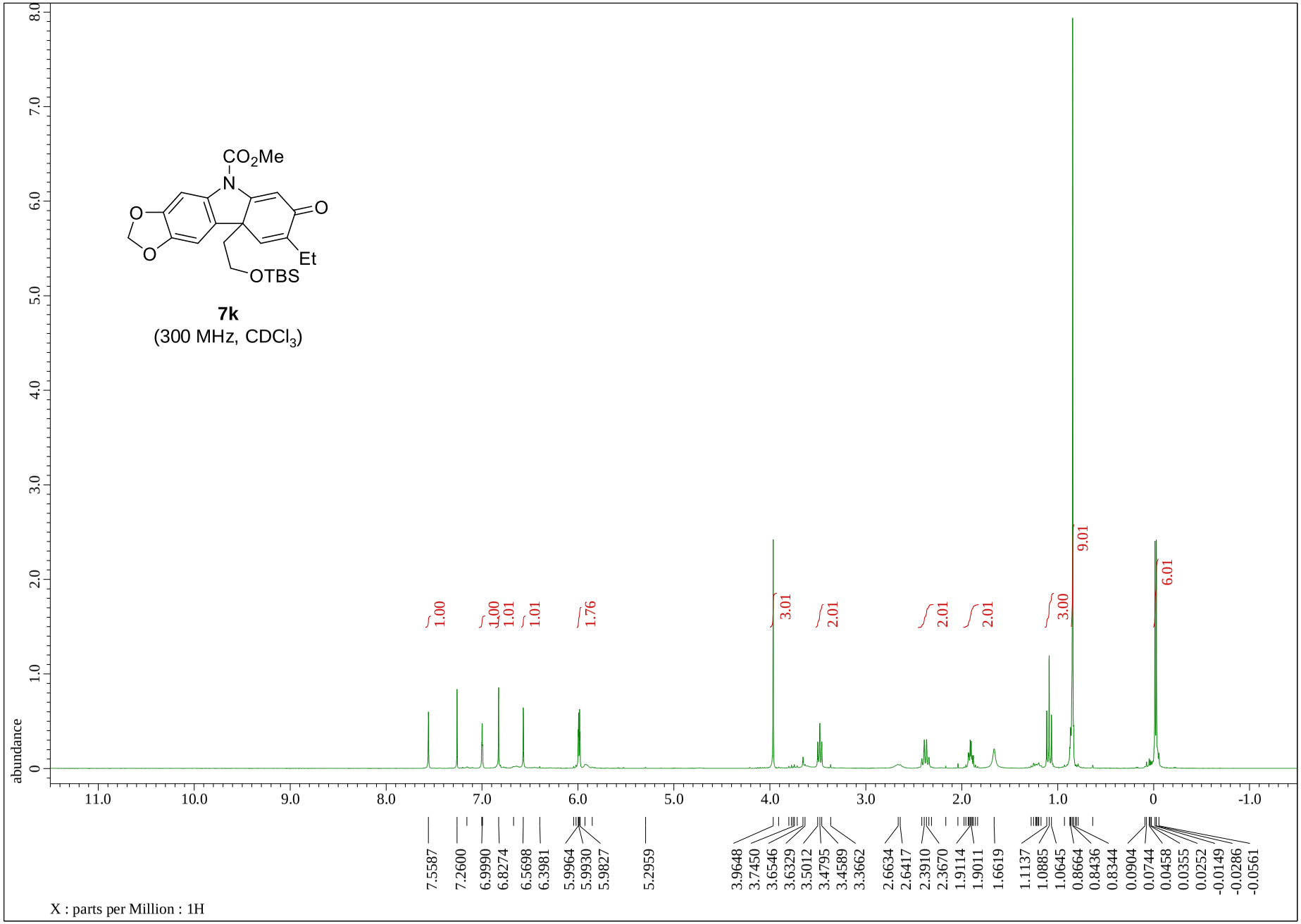

CO2Me
N
MeO
O
MeO
OBn
7e
(75 MHz, CDCl3)
abundance
0.3
0.2
0.1
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
187.6261
165.5315
161.6881
155.9900
151.9936
146.3337
143.0831
137.9299
128.2450
127.4324
111.6382
109.4488
94.8497
94.4482
77.4207
77.2008
77.0000
76.5698
72.8985
65.9479
55.7180
55.4312
53.4617
51.5878
45.6124
X : parts per Million : 13C

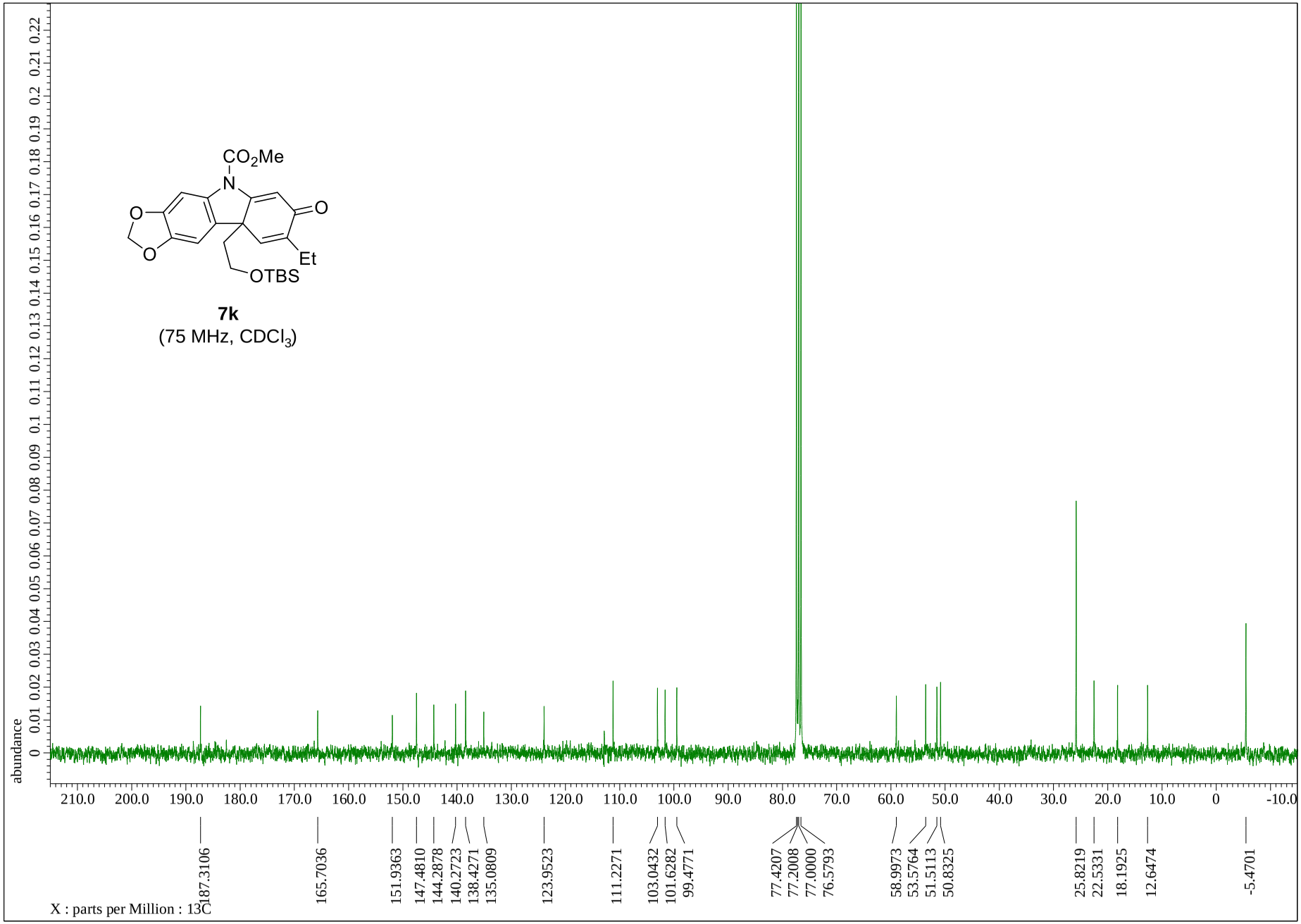

CO2Me
N
O
MeO
OBn
7f
(300 MHz, CDCl3)
abundance
1.00
8.05
2.00
1.01
1.01
2.00
3.00
3.00
2.00
2.00
7.8506
7.8208
7.3722
7.3390
7.3092
7.2737
7.2600
6.8434
6.6351
6.6305
5.6450
4.3929
4.3539
4.3494
4.3093
3.8904
3.8137
3.7920
3.3662
3.3193
3.3021
2.7813
2.0888
2.0705
2.0511
1.7386
1.2499
1.2339
0.8756
0.0710
X : parts per Million : 1H

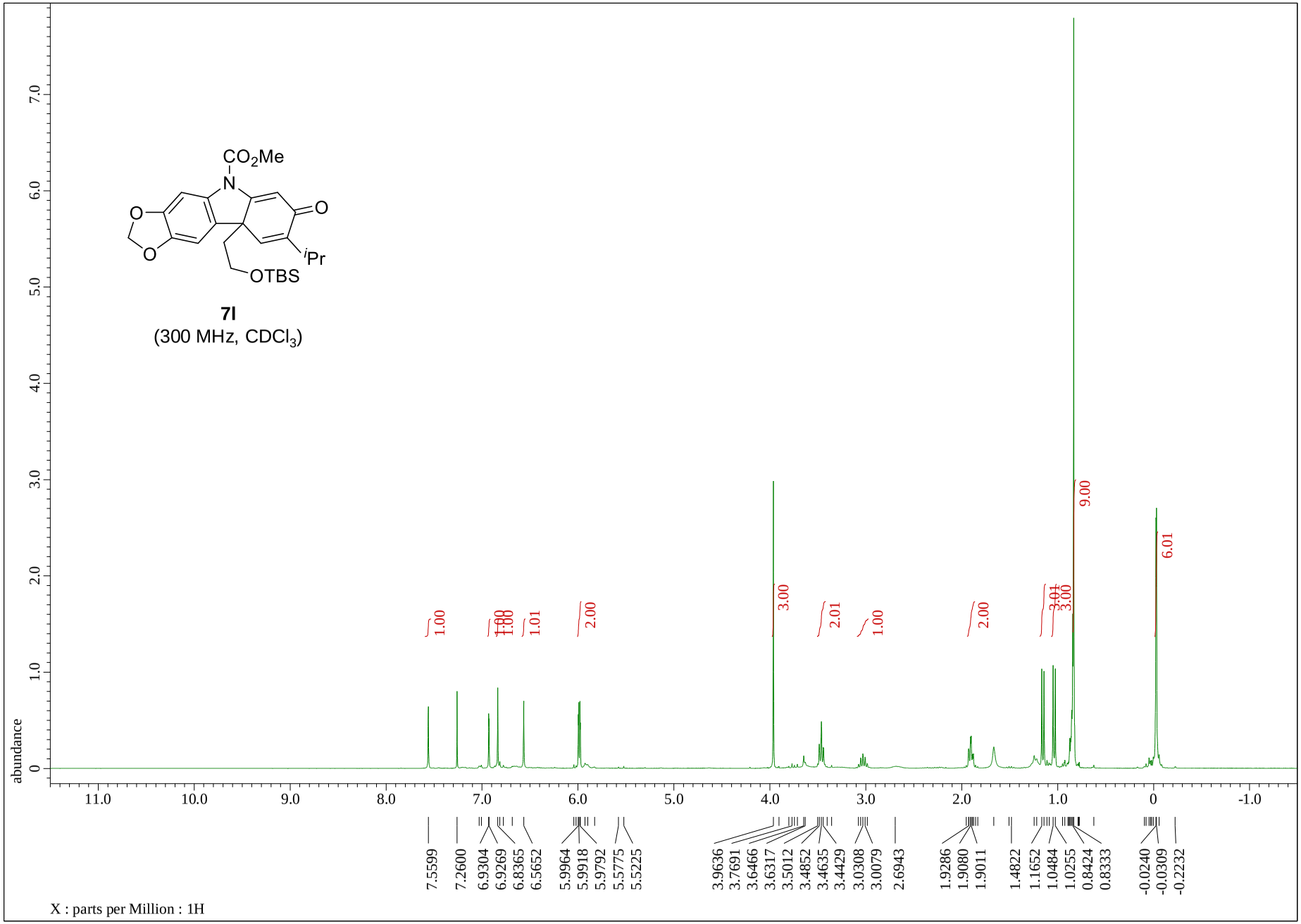

CO2Me
N
O
MeO
OBn
7f
(75 MHz, CDCl3)
abundance
0.3
0.2
0.1
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
187.3967
165.6367
156.6879
151.9650
144.4790
137.7292
134.3351
132.1458
128.8760
128.3502
127.6331
127.5471
117.0208
112.8333
111.3992
108.7796
77.4207
77.2008
77.0000
76.5793
72.9463
65.5464
55.6893
53.5000
51.6356
48.3277
X : parts per Million : 13C

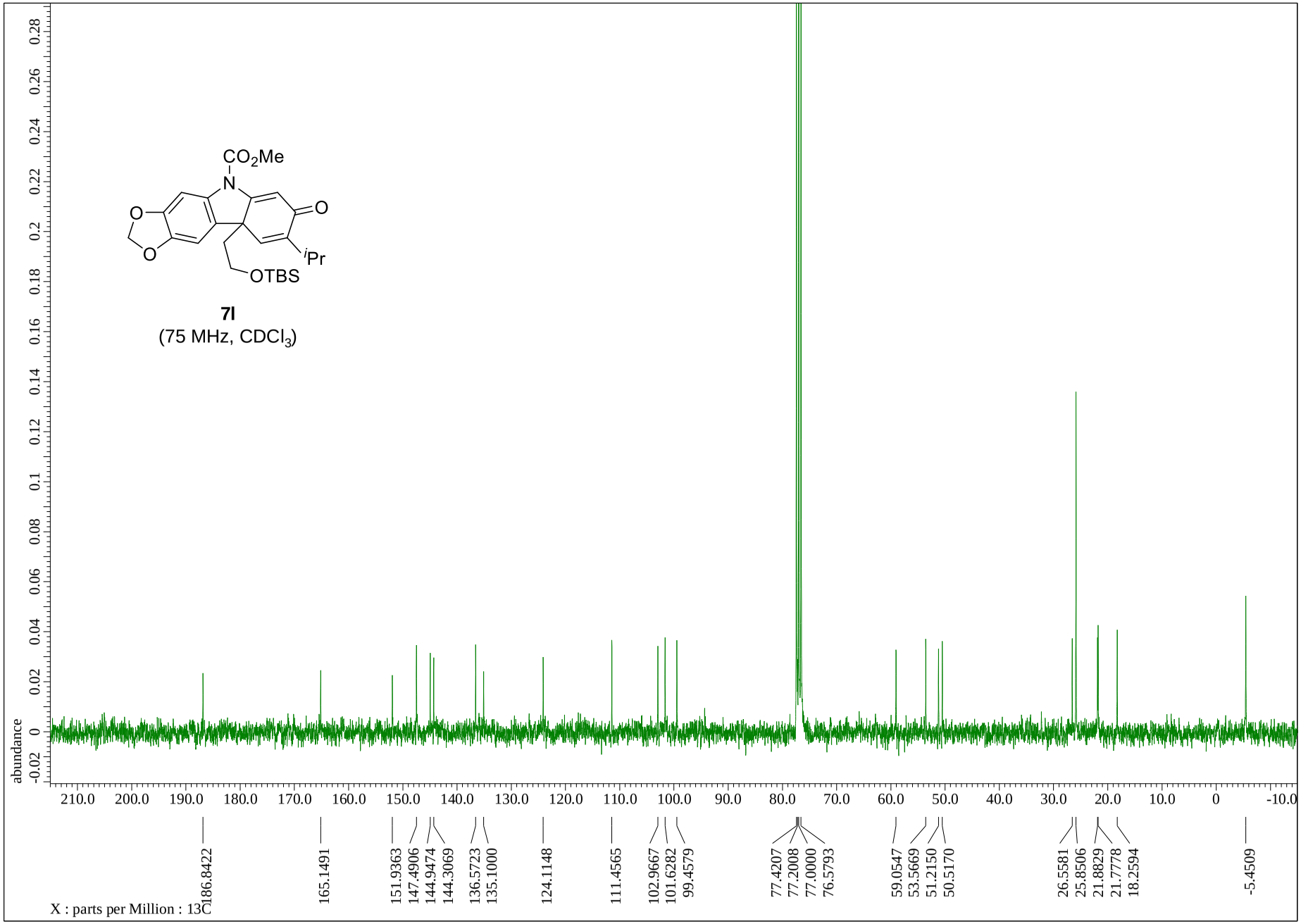

CO2Me
N
MeO
O
OBn
7g
(300 MHz, CDCl3)
abundance
8.32
1.00
1.00
1.00
1.00
2.01
3.00
2.01
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
7.5873
7.5793
7.3905
7.3584
7.3218
7.2829
7.2760
7.2600
7.1158
7.0872
6.6145
6.6087
6.2917
6.2860
6.2585
6.2539
5.1517
4.4089
4.3700
4.3459
3.8927
3.8309
3.3788
3.3593
3.3376
3.3090
3.2918
2.0660
2.0442
2.0259
1.6161
1.2499
0.0675
X : parts per Million : 1H

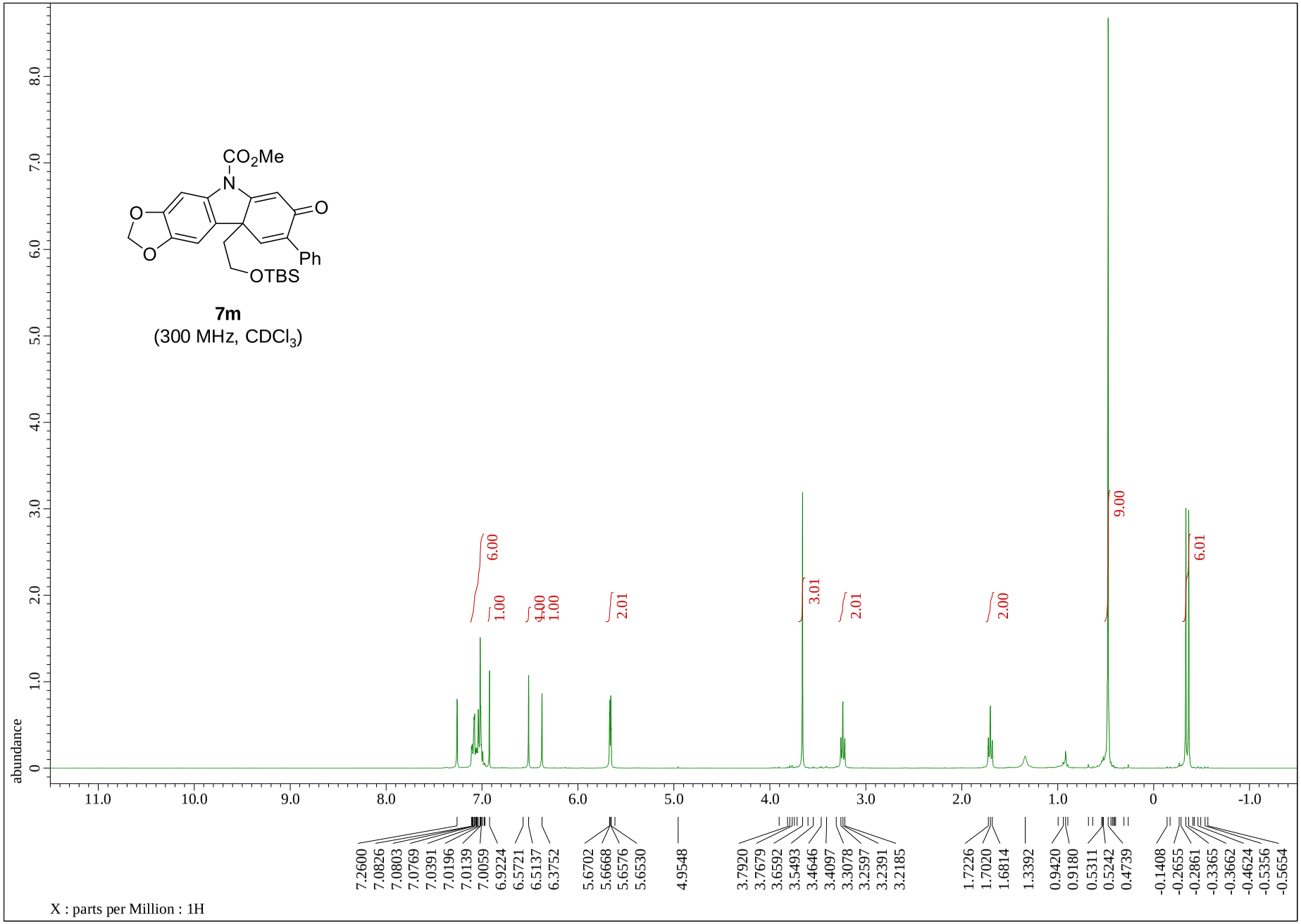

MeO
N
CO2Me
O
OBn
7g
(75 MHz, CDCl3)
X : parts per Million : 13C
abundance
187.4636
166.0382
160.3114
152.0319
145.3777
142.1749
137.7674
128.4936
128.3789
127.6618
122.4608
111.6478
109.4775
103.3013
77.4207
77.2008
77.0000
76.5793
72.9558
65.6133
55.6607
53.6051
51.0142
48.4041

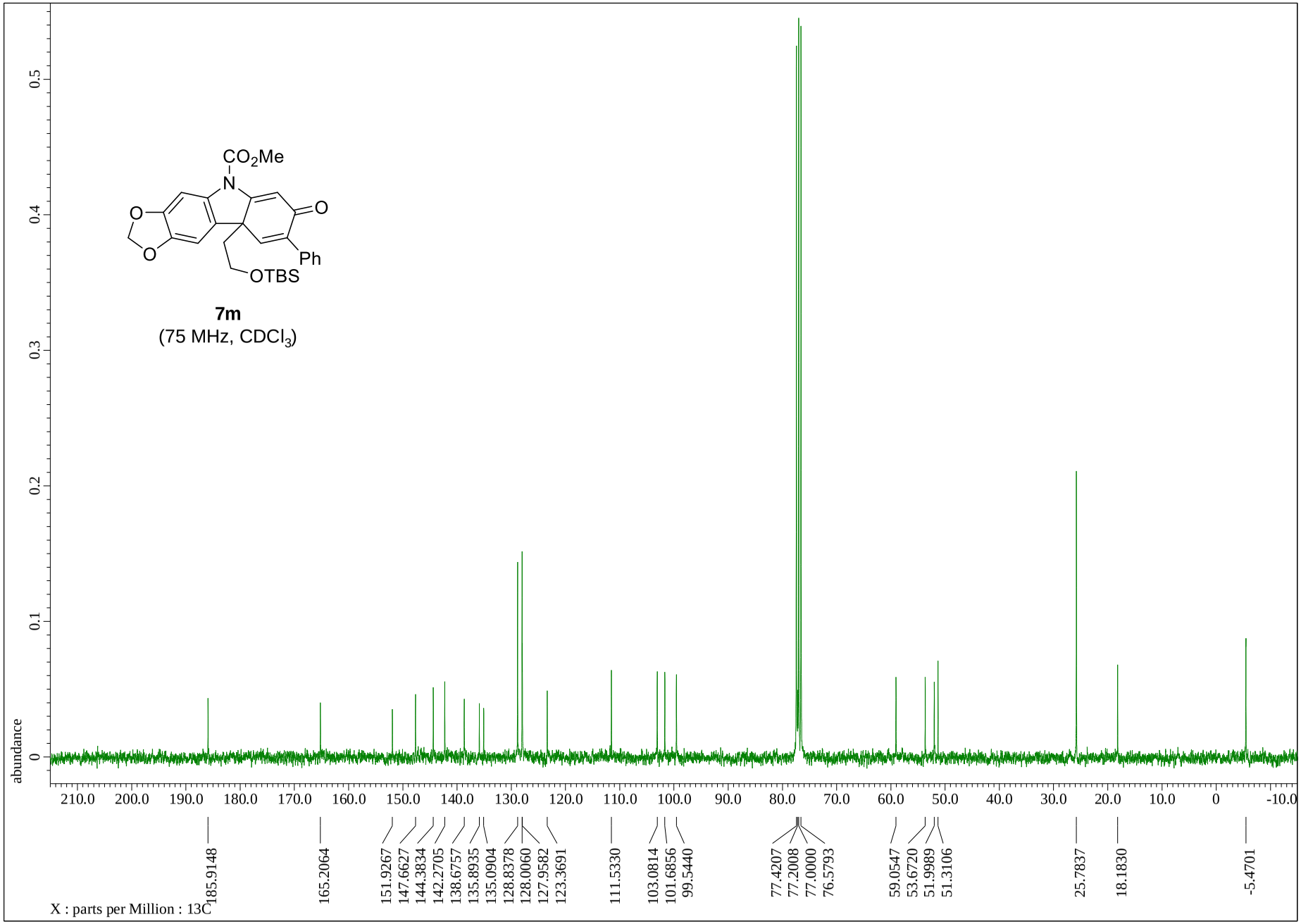

CO2Me
N
O
O
O
Et
OTBS
7k
(300 MHz, CDCl3)
abundance
1.00
1.00
1.01
1.01
1.76
3.01
2.01
2.01
2.01
3.00
9.01
6.01
7.5587
7.2600
6.9990
6.8274
6.5698
6.3981
5.9964
5.9930
5.9827
5.2959
3.9648
3.7450
3.6546
3.6329
3.5012
3.4795
3.4589
3.3662
2.6634
2.6417
2.3910
2.3670
1.9114
1.9011
1.6619
1.1137
1.0885
1.0645
0.8664
0.8436
0.8344
0.0904
0.0744
0.0458
0.0355
0.0252
-0.0149
-0.0286
-0.0561
X : parts per Million : 1H

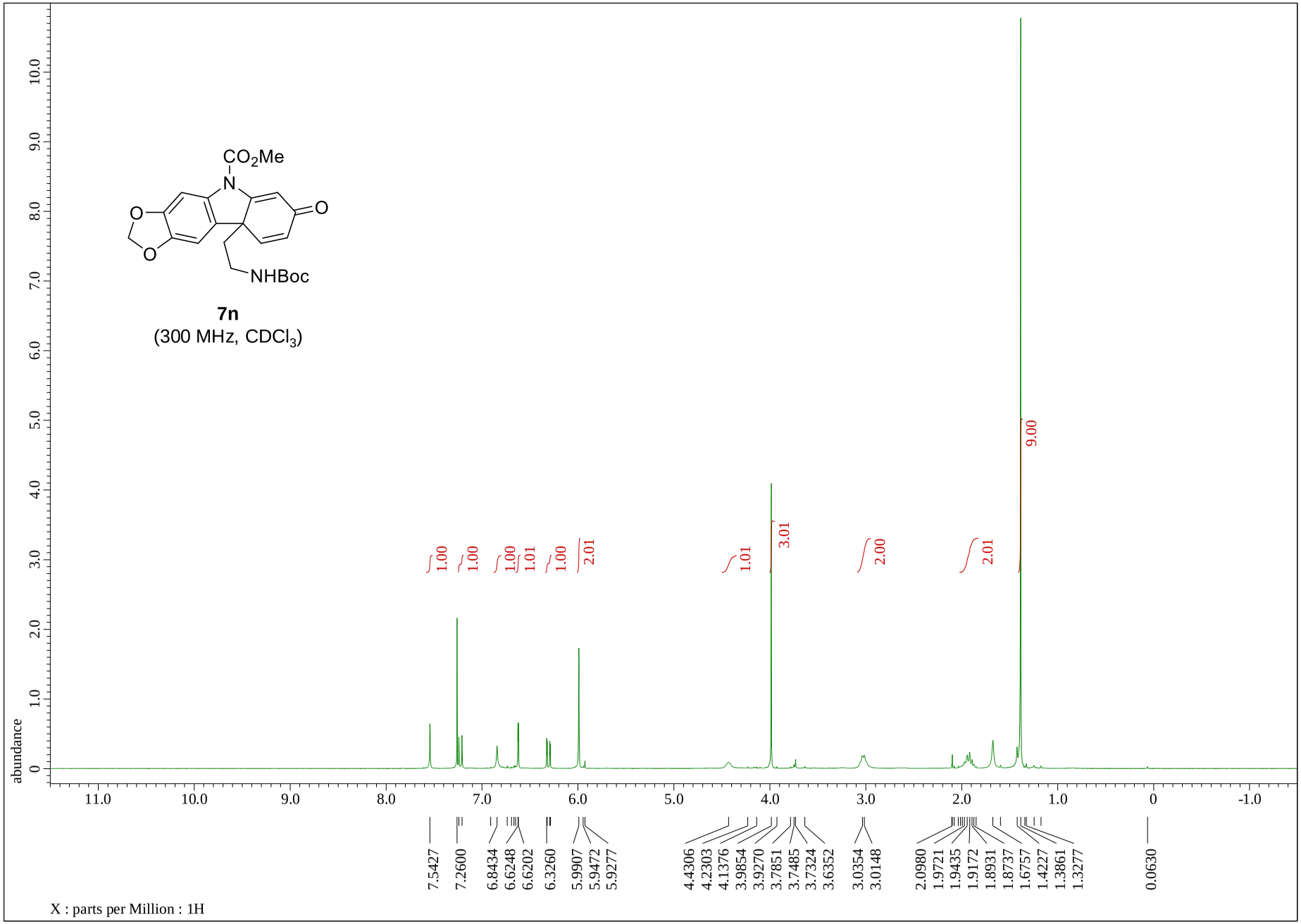

CO2Me
N
O
O
O
Et
OTBS
7k
(75 MHz, CDCl3)
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19 0.2 0.21 0.22
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
187.3106
165.7036
151.9363
147.4810
144.2878
140.2723
138.4271
135.0809
123.9523
111.2271
103.0432
101.6282
99.4771
77.4207
77.2008
77.0000
76.5793
58.9973
53.5764
51.5113
50.8325
25.8219
22.5331
18.1925
12.6474
-5.4701
X : parts per Million : 13C

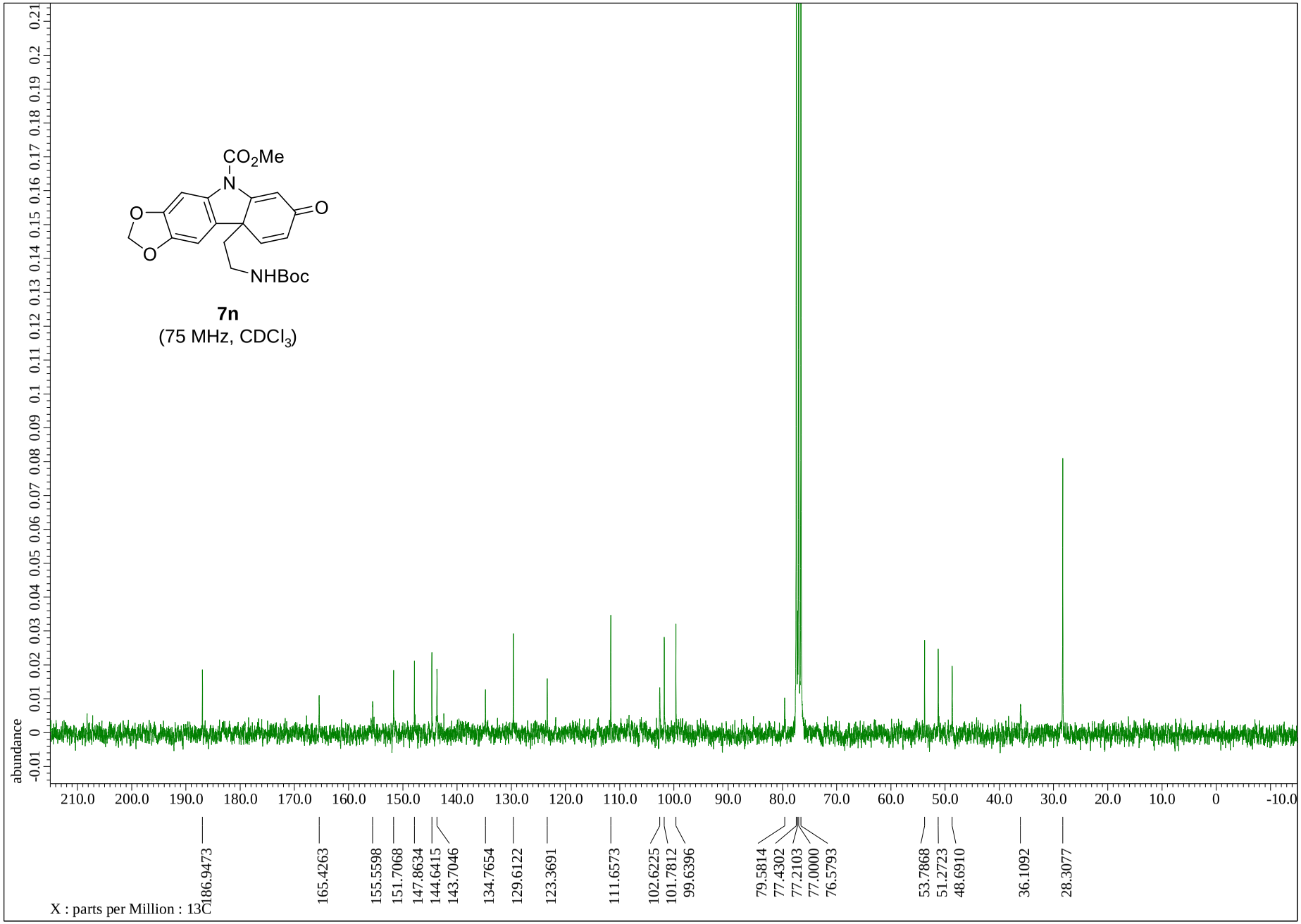

CO2Me
N
O
O
O
iPr
OTBS
7l
(300 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.5599
7.2600
6.9304
6.9269
6.8365
6.5652
5.9964
5.9918
5.9792
5.5775
5.5225
3.9636
3.7691
3.6466
3.6317
3.5012
3.4852
3.4635
3.4429
3.0308
3.0079
2.6943
1.9286
1.9080
1.9011
1.4822
1.1652
1.0484
1.0255
0.8424
0.8333
-0.0240
-0.0309
-0.2232
1.00
1.01
2.00
3.00
2.01
1.00
2.00
3.01
3.00
9.00
6.01

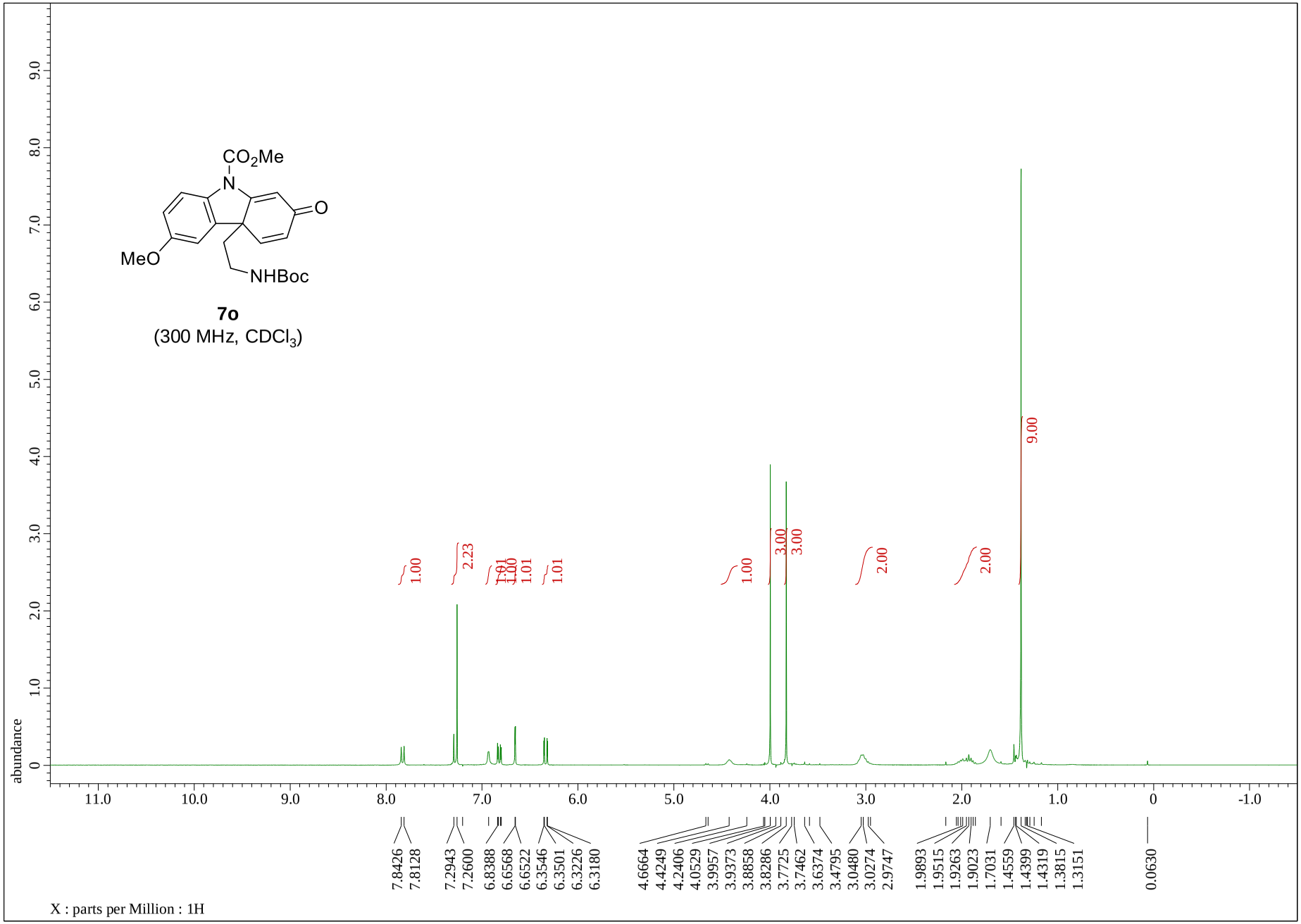

CO2Me
N
O
O
O
iPr
OTBS
7l
(75 MHz, CDCl3)
abundance
186.8422
165.1491
151.9363
147.4906
144.9474
144.3069
136.5723
135.1000
124.1148
111.4565
102.9667
101.6282
99.4579
77.4207
77.2008
77.0000
76.5793
59.0547
53.5669
51.2150
50.5170
26.5581
25.8506
21.8829
21.7778
18.2594
-5.4509
X : parts per Million : 13C

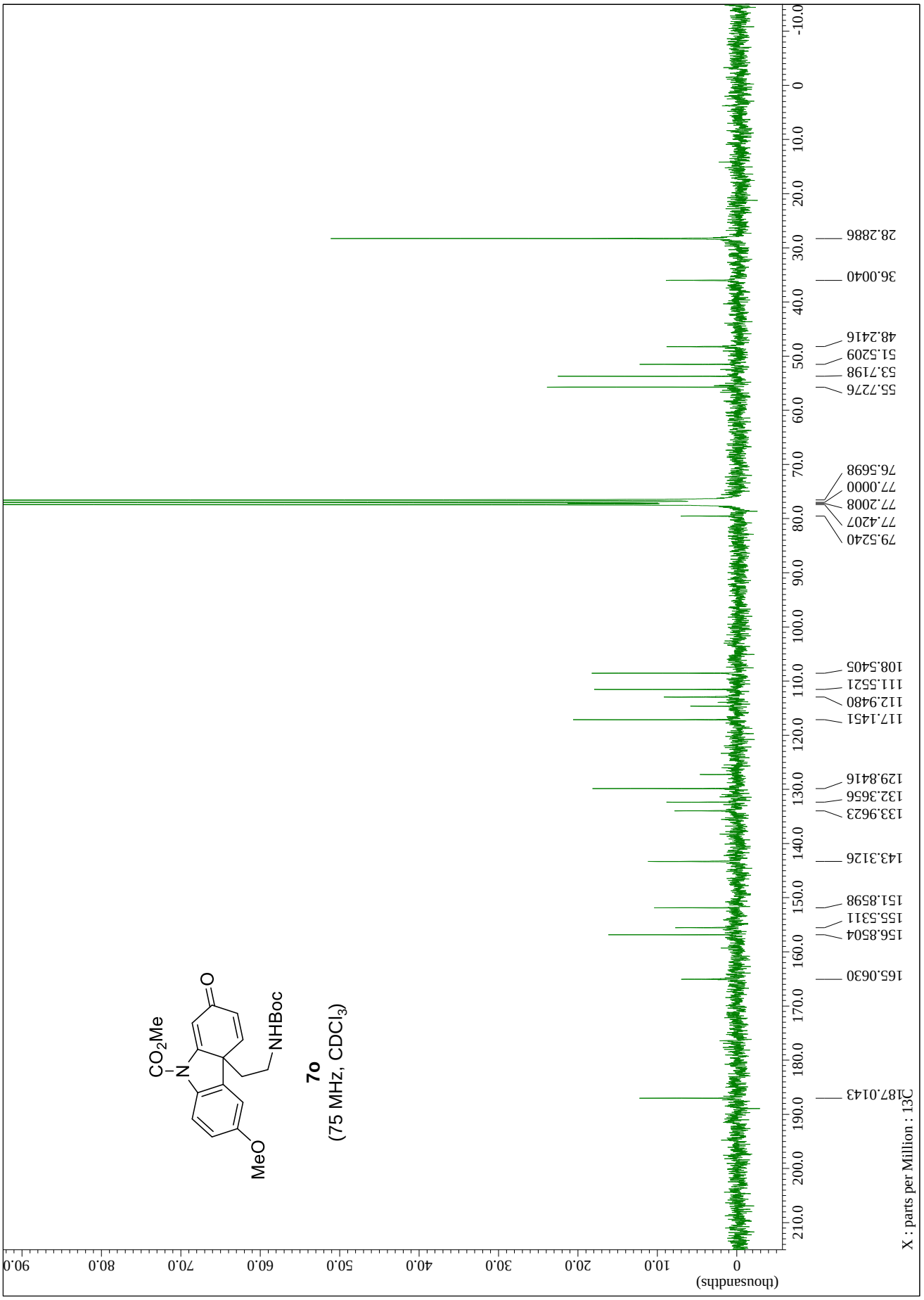

CO2Me
N
O
O
O
Ph
OTBS
7m
(300 MHz, CDCl3)
abundance
6.00
1.00
1.00
1.00
2.01
3.01
2.01
2.00
9.00
6.01
7.2600
7.0826
7.0803
7.0769
7.0391
7.0196
7.0139
7.0059
6.9224
6.5721
6.5137
6.3752
5.6702
5.6668
5.6576
5.6530
4.9548
3.7920
3.7679
3.6592
3.5493
3.4646
3.4097
3.3078
3.2597
3.2391
3.2185
1.7226
1.7020
1.6814
1.3392
0.9420
0.9180
0.5311
0.5242
0.4739
-0.1408
-0.2655
-0.2861
-0.3365
-0.3662
-0.4624
-0.5356
-0.5654
X : parts per Million : 1H

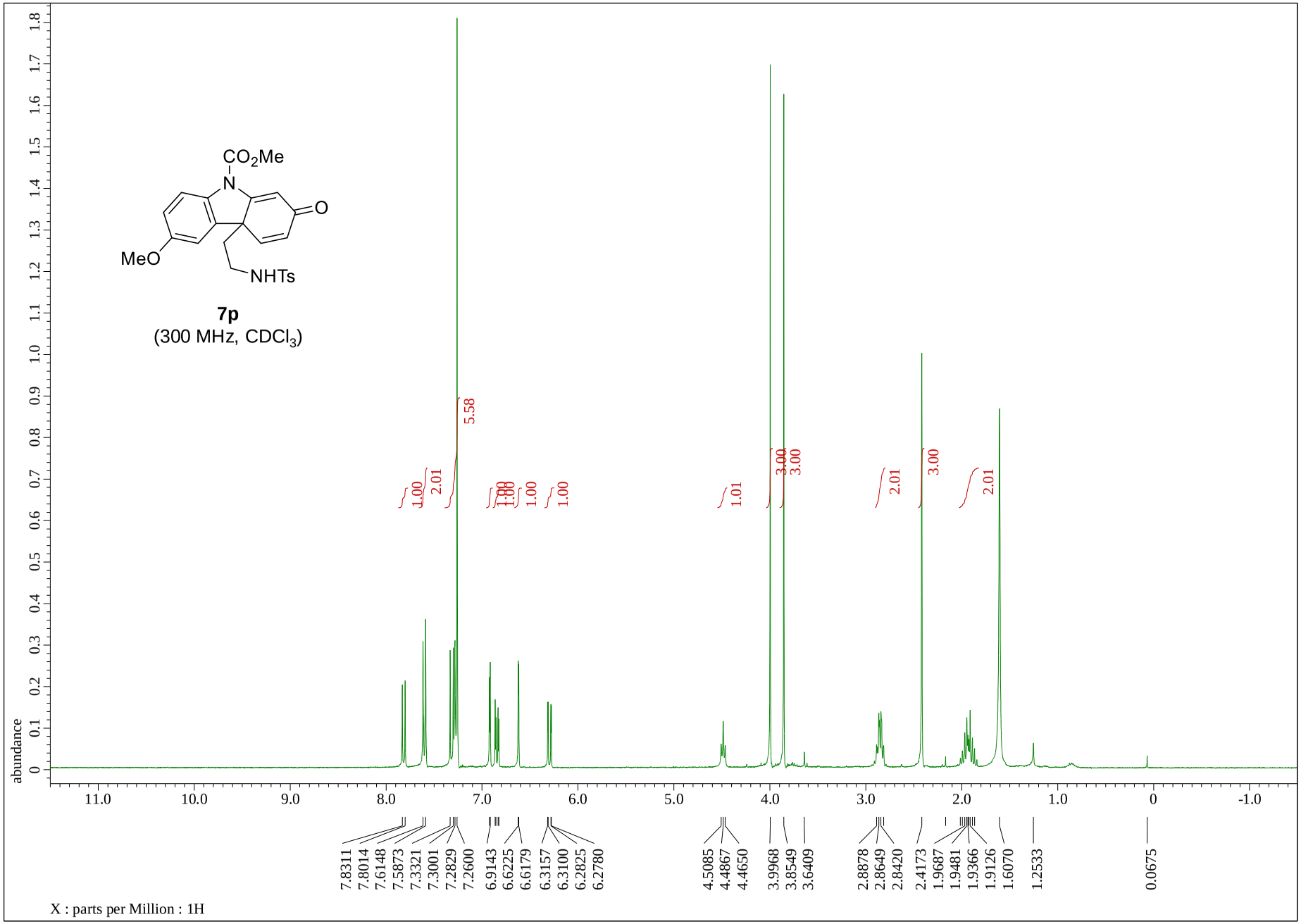

CO2Me
N
O
O
O
Ph
OTBS
7m
(75 MHz, CDCl3)
abundance
0
0.1
0.2
0.3
0.4
0.5
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
185.9148
165.2064
151.9267
147.6627
144.3834
142.2705
138.6757
135.8935
135.0904
128.8378
128.0060
127.9582
123.3691
111.5330
103.0814
101.6856
99.5440
77.4207
77.2008
77.0000
76.5793
59.0547
53.6720
51.9989
51.3106
25.7837
18.1830
-5.4701
X : parts per Million : 13C

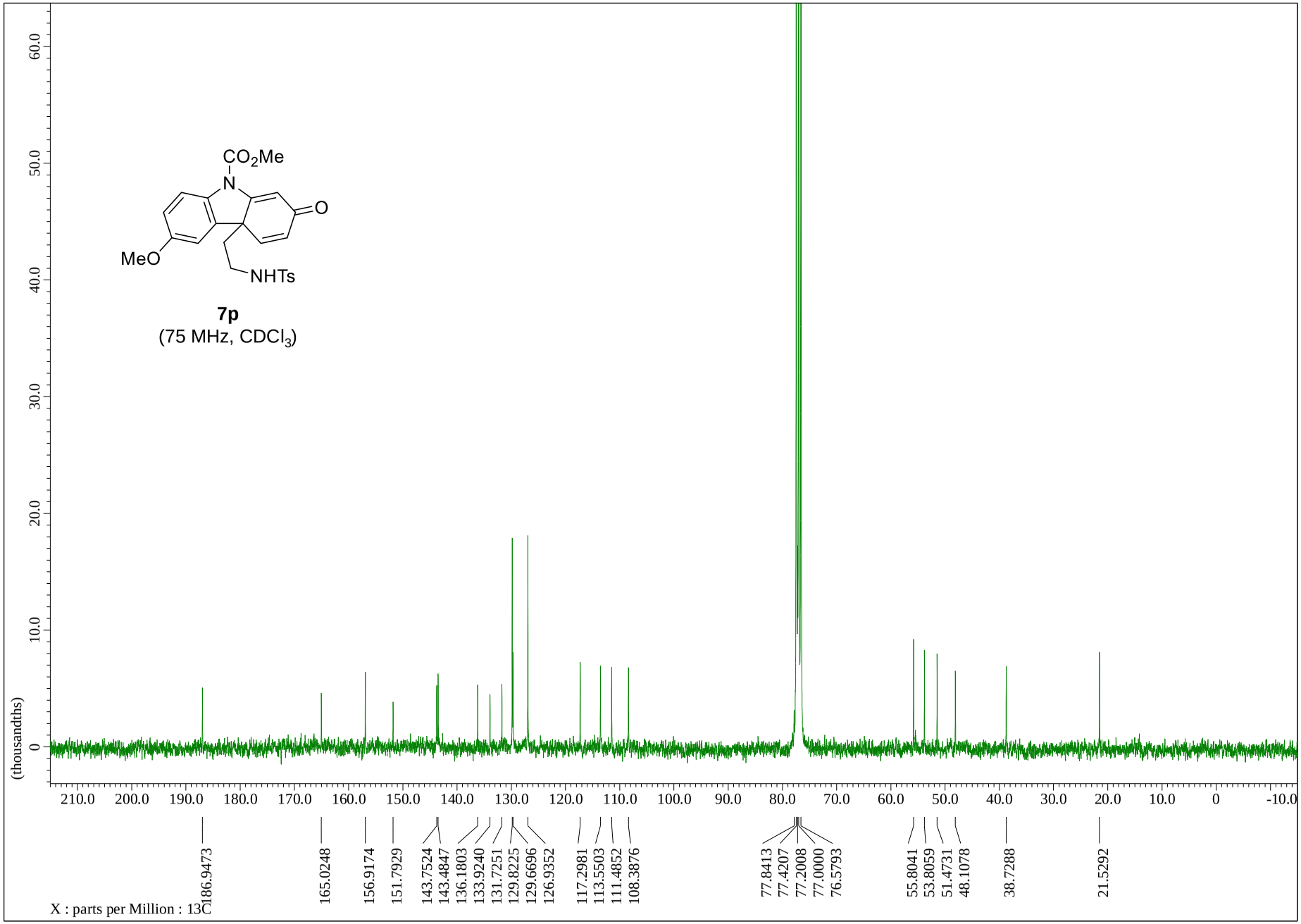

CO2Me
N
O
O
O
NHBoc
7n
(300 MHz, CDCl3)
abundance
1.00
1.00
1.00
1.01
1.00
2.01
1.01
3.01
2.00
2.01
9.00
7.5427
7.2600
6.8434
6.6248
6.6202
6.3260
5.9907
5.9472
5.9277
4.4306
4.2303
4.1376
3.9854
3.9270
3.7851
3.7485
3.7324
3.6352
3.0354
3.0148
2.0980
1.9721
1.9435
1.9172
1.8931
1.8737
1.6757
1.4227
1.3861
1.3277
0.0630
X : parts per Million : 1H

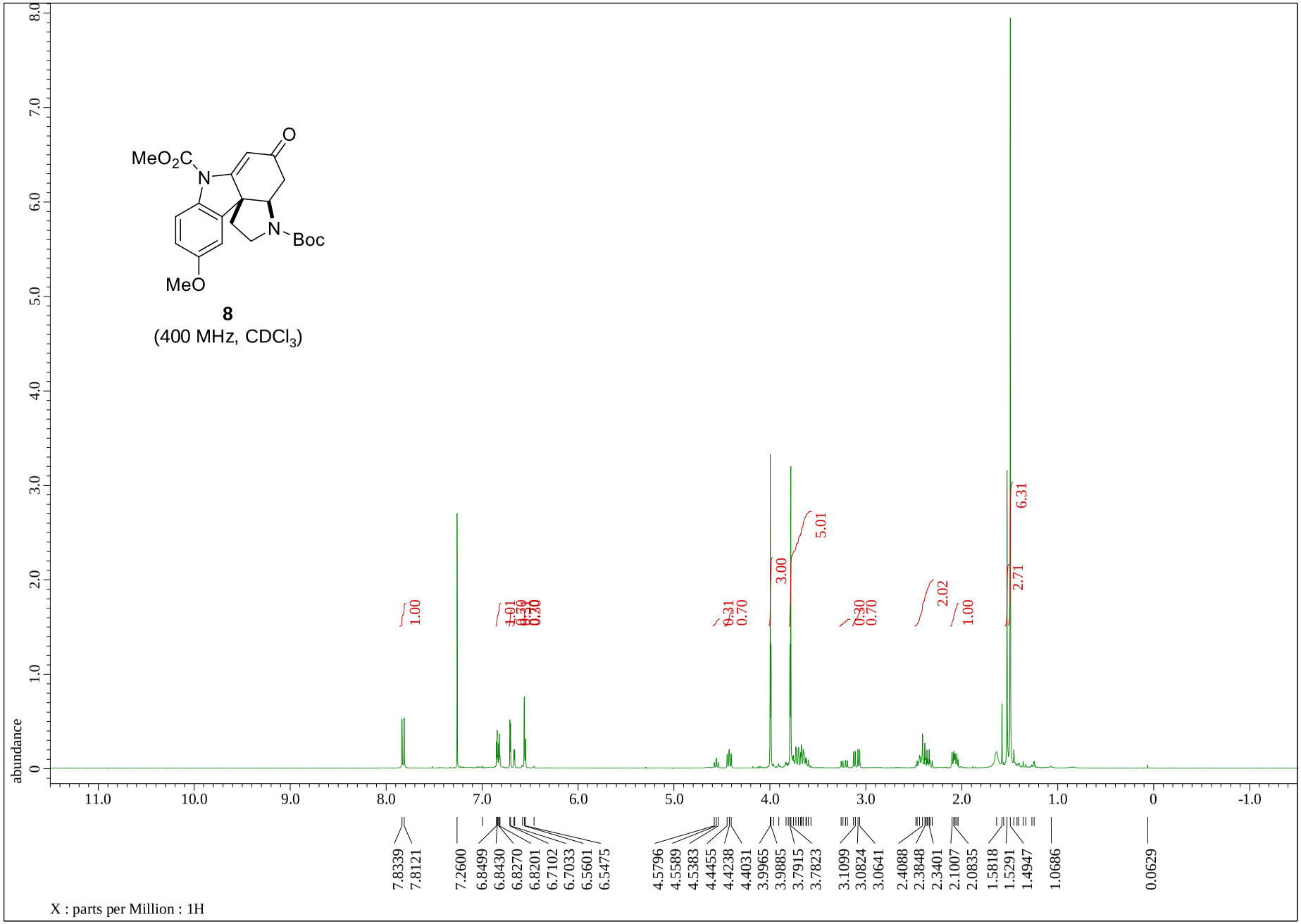

CO2Me
N
O
O
O
NHBoc
7n
(75 MHz, CDCl3)
abundance
186.9473
165.4263
155.5598
151.7068
147.8634
144.6415
143.7046
134.7654
129.6122
123.3691
111.6573
102.6225
101.7812
99.6396
79.5814
77.4302
77.2103
77.0000
76.5793
53.7868
51.2723
48.6910
36.1092
28.3077
X : parts per Million : 13C

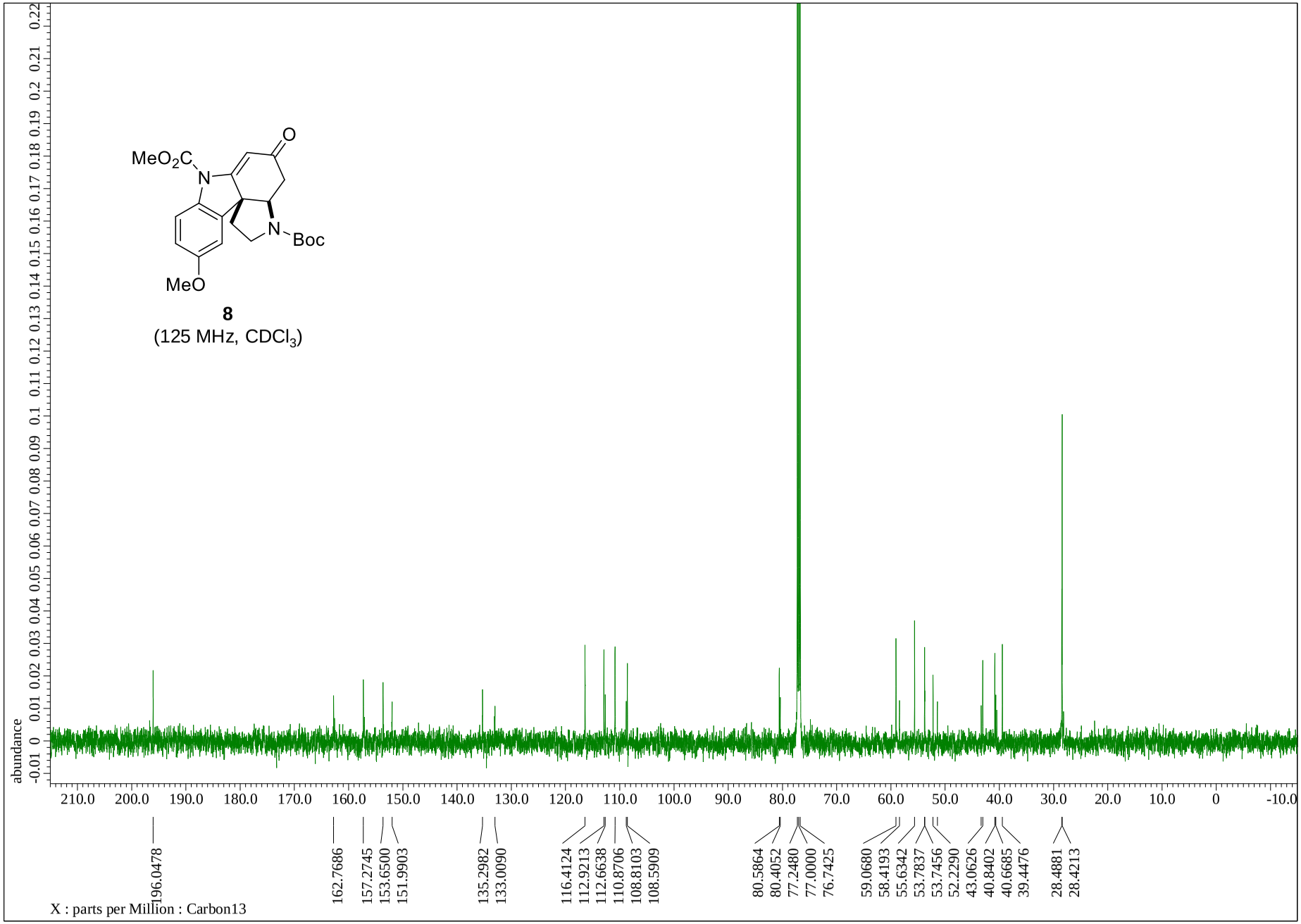

CO2Me
N
O
MeO
NHBoc
7o
(300 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.8426
7.8128
7.2943
7.2600
6.8388
6.6568
6.6522
6.3546
6.3501
6.3226
6.3180
4.6664
4.4249
4.2406
4.0529
3.9957
3.9373
3.8858
3.8286
3.7725
3.7462
3.6374
3.4795
3.0480
3.0274
2.9747
1.9893
1.9515
1.9263
1.9023
1.7031
1.4559
1.4399
1.4319
1.3815
1.3151
0.0630
1.00
2.23
1.01
1.01
1.00
3.00
3.00
2.00
2.00
9.00

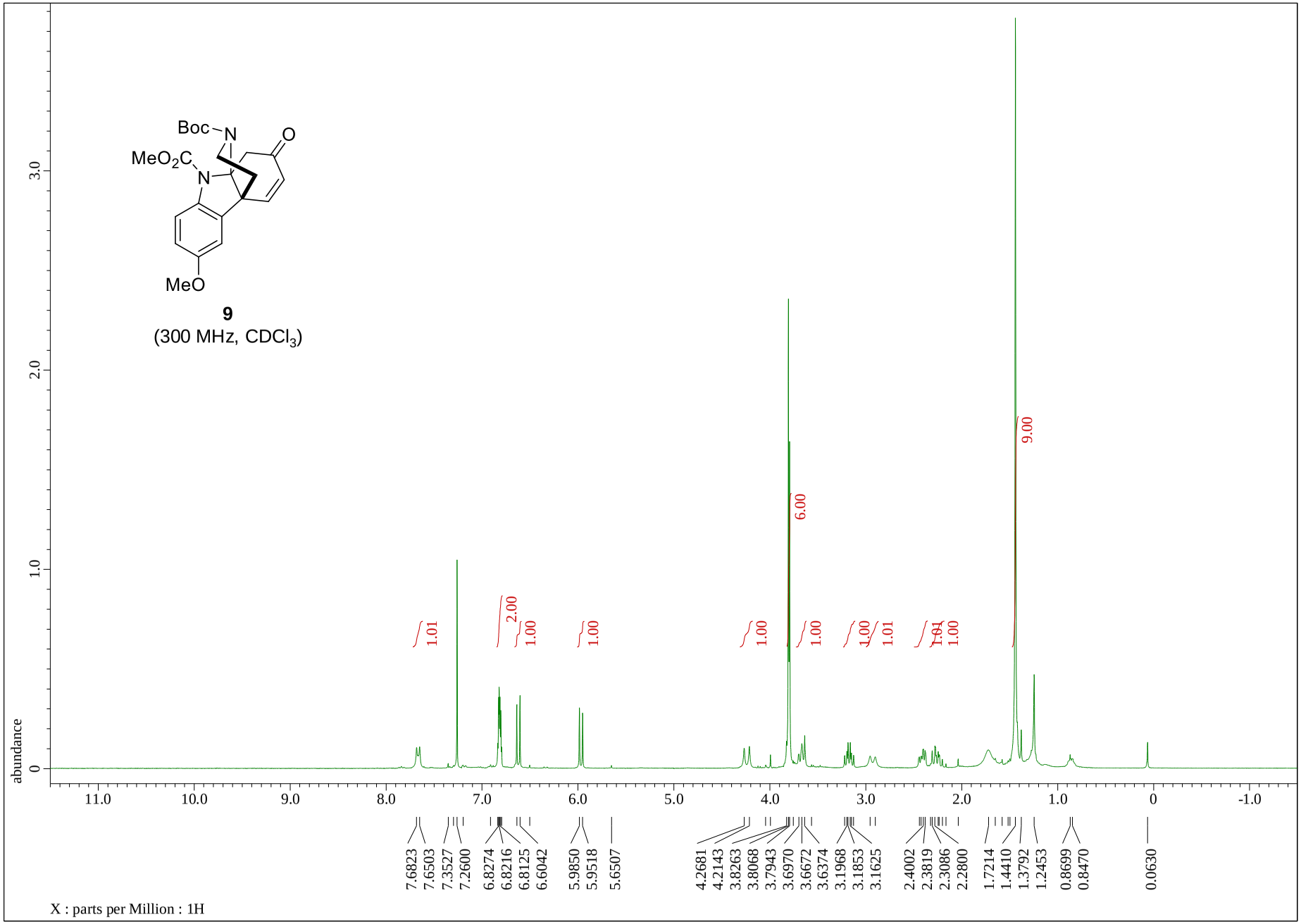

CO2Me
N
NHBoc
O
MeO
7o
(75 MHz, CDCl3)
(thousandths)
X : parts per Million : 13C
187.0143
165.0630
156.8504
155.5311
151.8598
143.3126
133.9623
132.3656
129.8416
117.1451
112.9480
111.5521
108.5405
79.5240
77.4207
77.2008
77.0000
76.5698
55.7276
53.7198
51.5209
48.2416
36.0040
28.2886

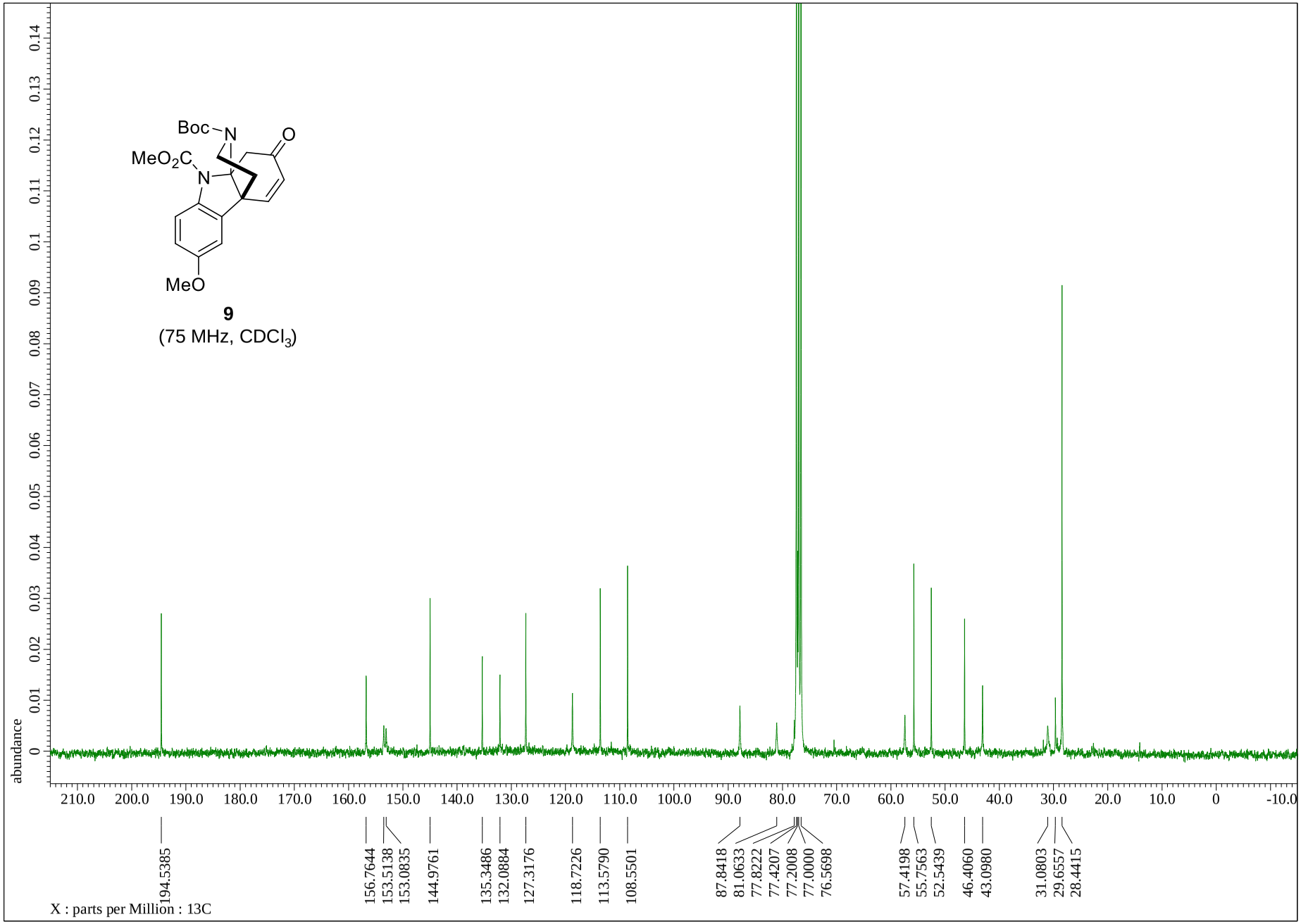

CO2Me
N
O
MeO
NHTs
7p
(300 MHz, CDCl3)
abundance
1.00
2.01
5.58
1.00
1.00
1.01
3.00
3.00
2.01
3.00
2.01
7.8311
7.8014
7.6148
7.5873
7.3321
7.3001
7.2829
7.2600
6.9143
6.6225
6.6179
6.3157
6.3100
6.2825
6.2780
4.5085
4.4867
4.4650
3.9968
3.8549
3.6409
2.8878
2.8649
2.8420
2.4173
1.9687
1.9481
1.9366
1.9126
1.6070
1.2533
0.0675
X : parts per Million : 1H


CO2Me
N
O
MeO
NHTs
7p
(75 MHz, CDCl3)
(thousandths)
186.9473
165.0248
156.9174
151.7929
143.7524
143.4847
136.1803
133.9240
131.7251
129.8225
129.6696
126.9352
117.2981
113.5503
111.4852
108.3876
77.8413
77.4207
77.2008
77.0000
76.5793
55.8041
53.8059
51.4731
48.1078
38.7288
21.5292
X : parts per Million : 13C


MeO2C
N
O
N
Boc
MeO
8
(400 MHz, CDCl3)
abundance
X : parts per Million : 1H
7.8339
7.8121
7.2600
6.8499
6.8430
6.8270
6.8201
6.7102
6.7033
6.5601
6.5475
4.5796
4.5589
4.5383
4.4455
4.4238
4.4031
3.9965
3.9885
3.7915
3.7823
3.1099
3.0824
3.0641
2.4088
2.3848
2.3401
2.1007
2.0835
1.5818
1.5291
1.4947
1.0686
0.0629
1.00
3.00
5.01
6.31
2.71
2.02
1.00


MeO2C
N
O
N
Boc
MeO
8
(125 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
196.0478
162.7686
157.2745
153.6500
151.9903
135.2982
133.0090
116.4124
112.9213
112.6638
110.8706
108.8103
108.5909
80.5864
80.4052
77.2480
77.0000
76.7425
59.0680
58.4193
55.6342
53.7837
53.7456
52.2290
43.0626
40.8402
40.6685
39.4476
28.4881
28.4213


Boc
N
O
MeO2C
N
MeO
9
(300 MHz, CDCl3)
abundance
3.0
2.0
1.0
0
1.01
2.00
1.00
1.00
1.00
6.00
1.00
1.00
1.01
1.01
1.00
9.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
7.6823
7.6503
7.3527
7.2600
6.8274
6.8216
6.8125
6.6042
5.9850
5.9518
5.6507
4.2681
4.2143
3.8263
3.8068
3.7943
3.6970
3.6672
3.6374
3.1968
3.1853
3.1625
2.4002
2.3819
2.3086
2.2800
1.7214
1.4410
1.3792
1.2453
0.8699
0.8470
0.0630
X : parts per Million : 1H


Boc
N
O
MeO2C
N
MeO
9
(75 MHz, CDCl3)
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
194.5385
156.7644
153.5138
153.0835
144.9761
135.3486
132.0884
127.3176
118.7226
113.5790
108.5501
87.8418
81.0633
77.8222
77.4207
77.2008
77.0000
76.5698
57.4198
55.7563
52.5439
46.4060
43.0980
31.0803
29.6557
28.4415
X : parts per Million : 13C