SUPPLEMENTARY MATERIAL

Synthesis and Hetero-Michael Addition Reactions of 2-Alkynyl Oxazoles and Oxazolines

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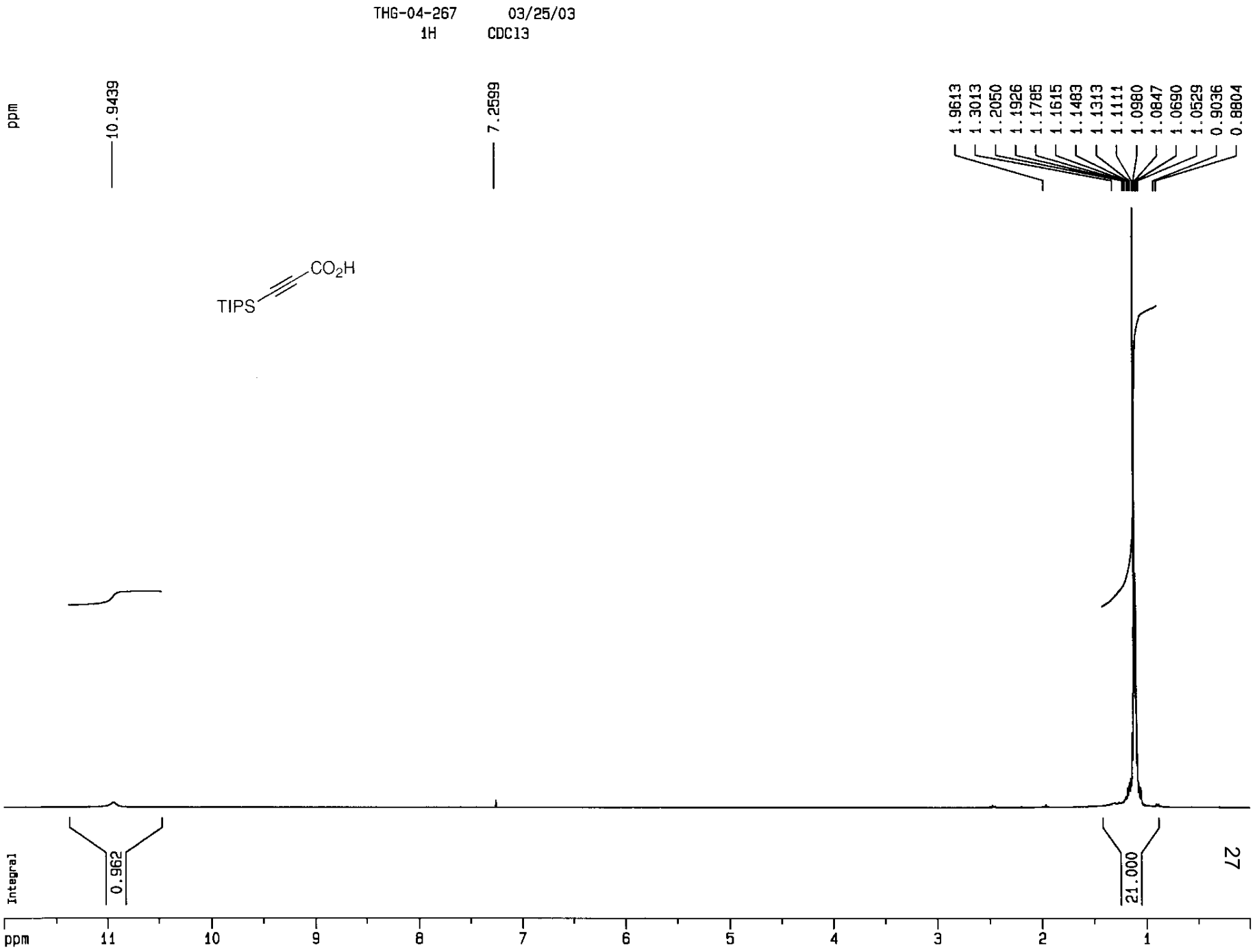
E-mail: pwipf@pitt.edu

Experimental procedures and spectral data for all new compounds, including copies of ^{1}H and ^{13}C NMR spectra.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1.0529
0.9036
0.8804
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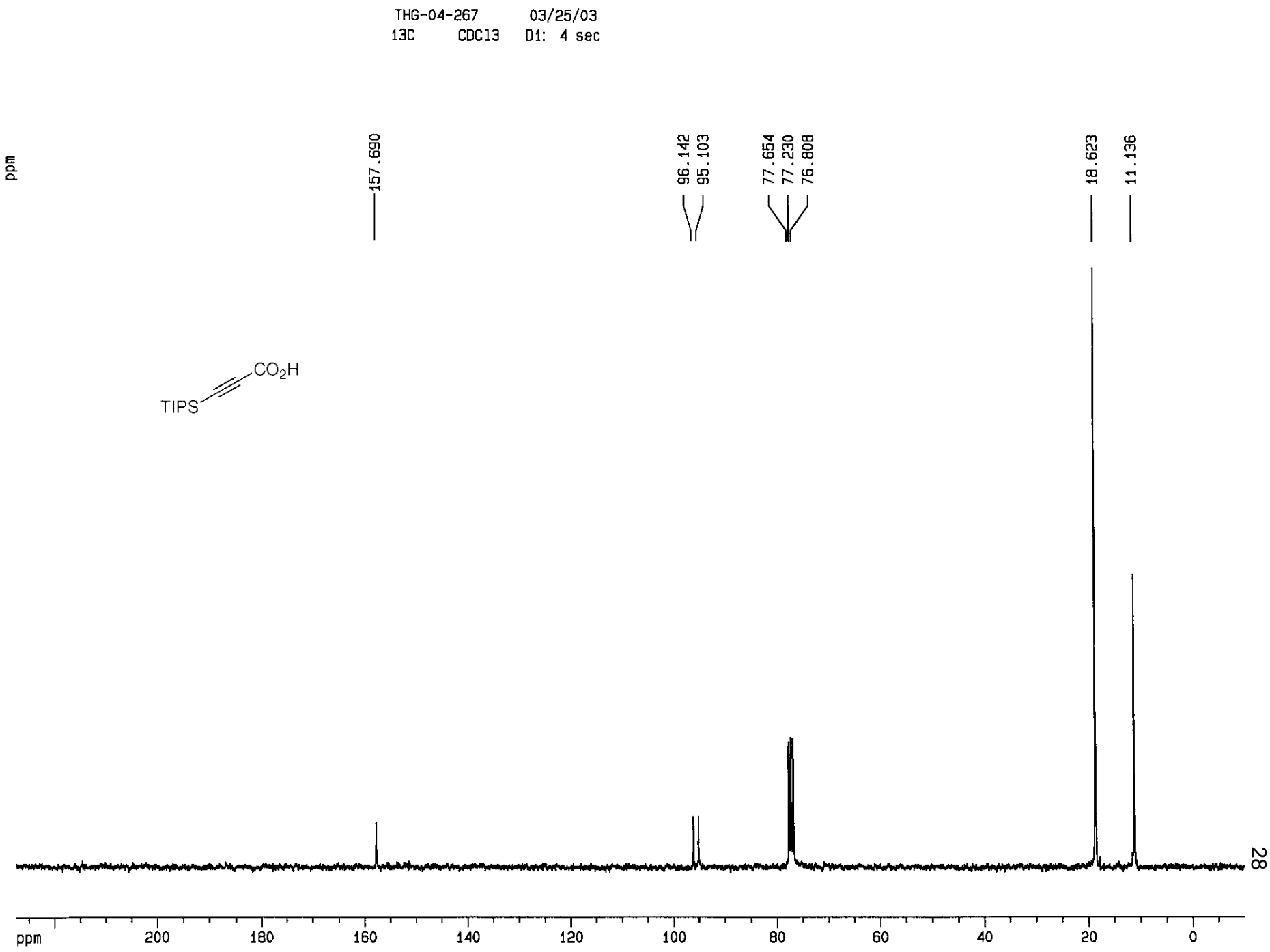
8
7
6
5
4
3
2
1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TIPS
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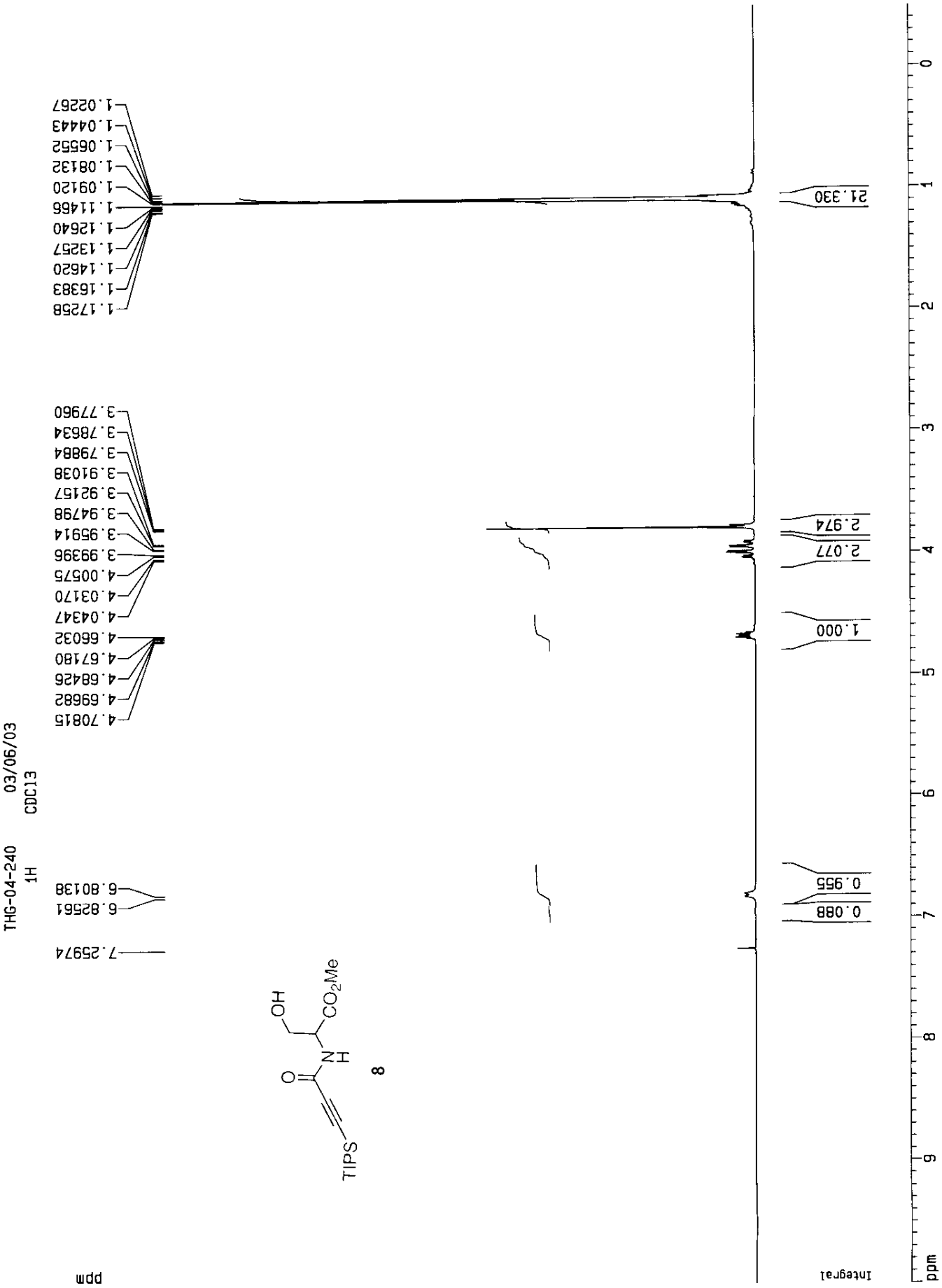
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3.91038
3.79884
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1.12640
1.11466
1.09120
1.08132
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1.04443
1.02267
21.330
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2.077
1.000
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Integral
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N
H
OH
CO2Me
8

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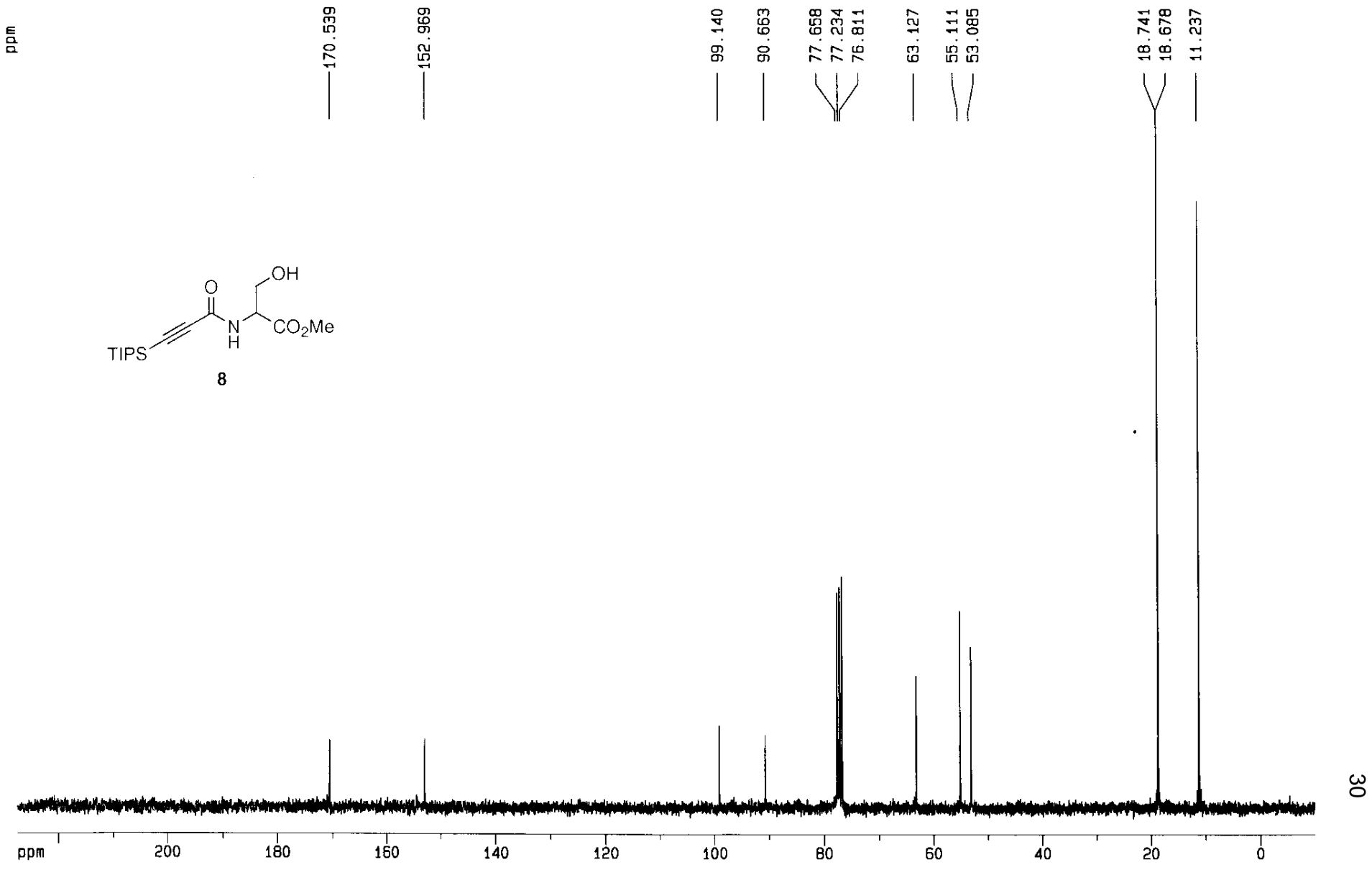

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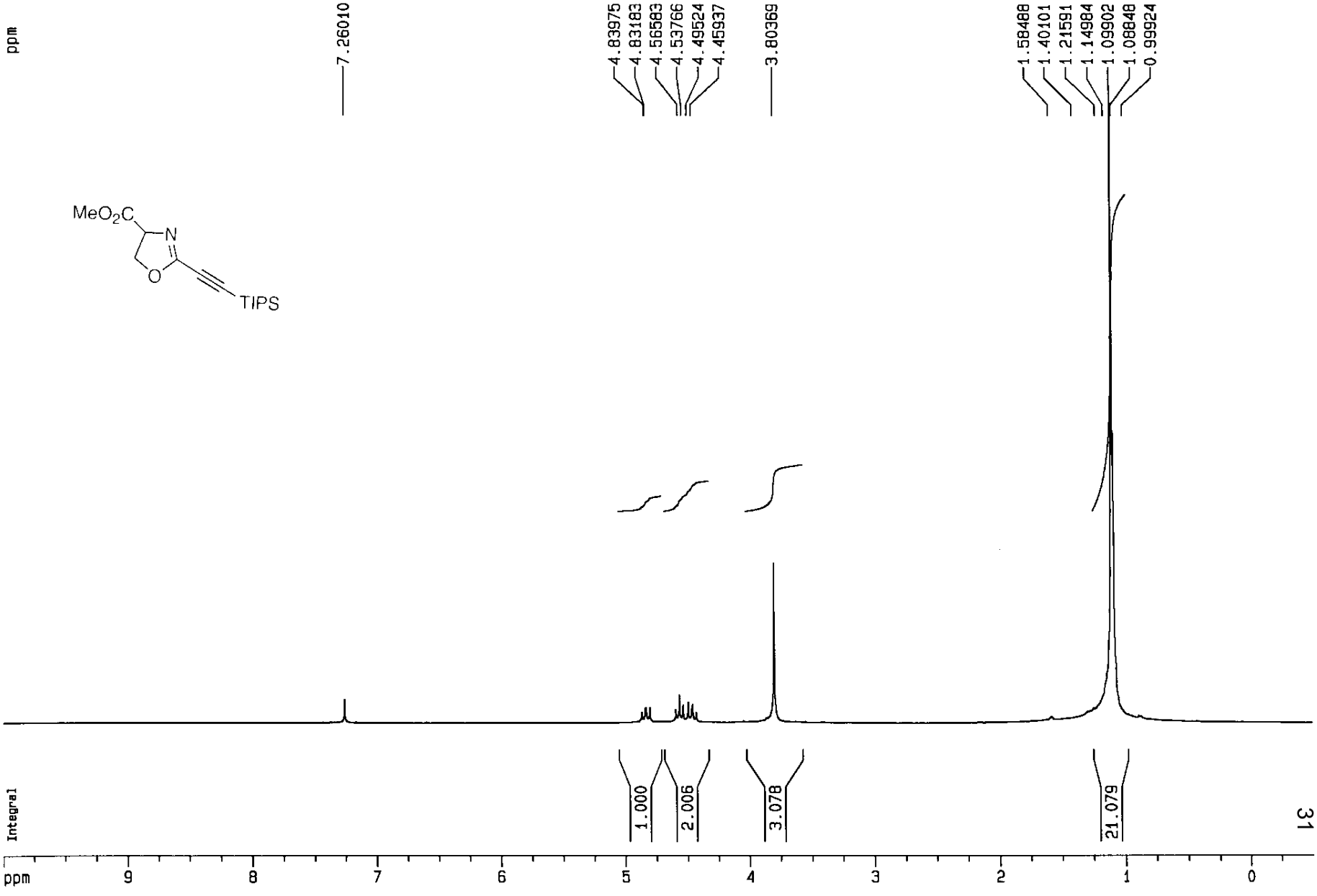
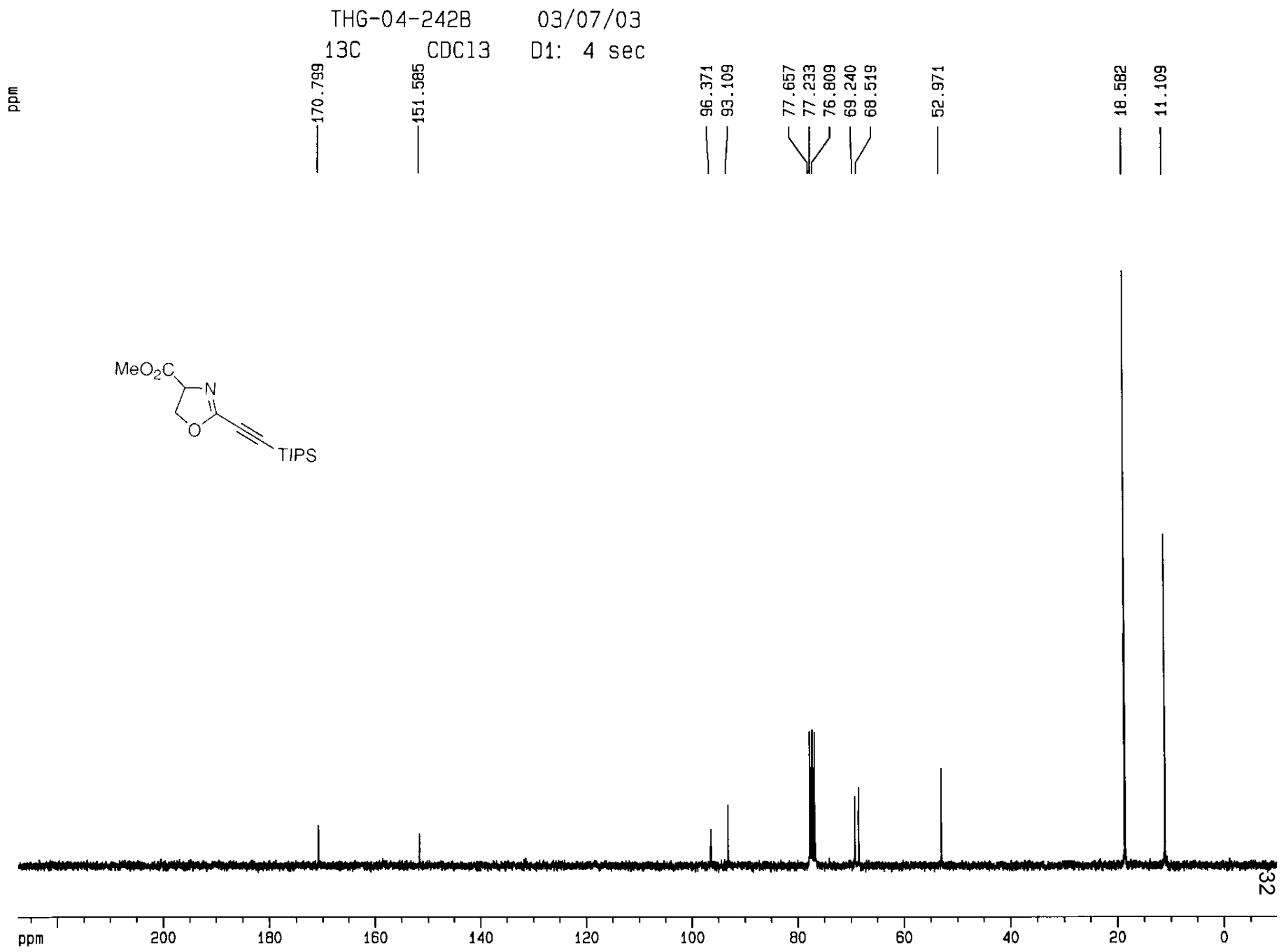
THG-04-252 03/14/03

1H CDC13

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76.809
69.240
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18.582
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MeO2C
N
O
TIPS
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ppm
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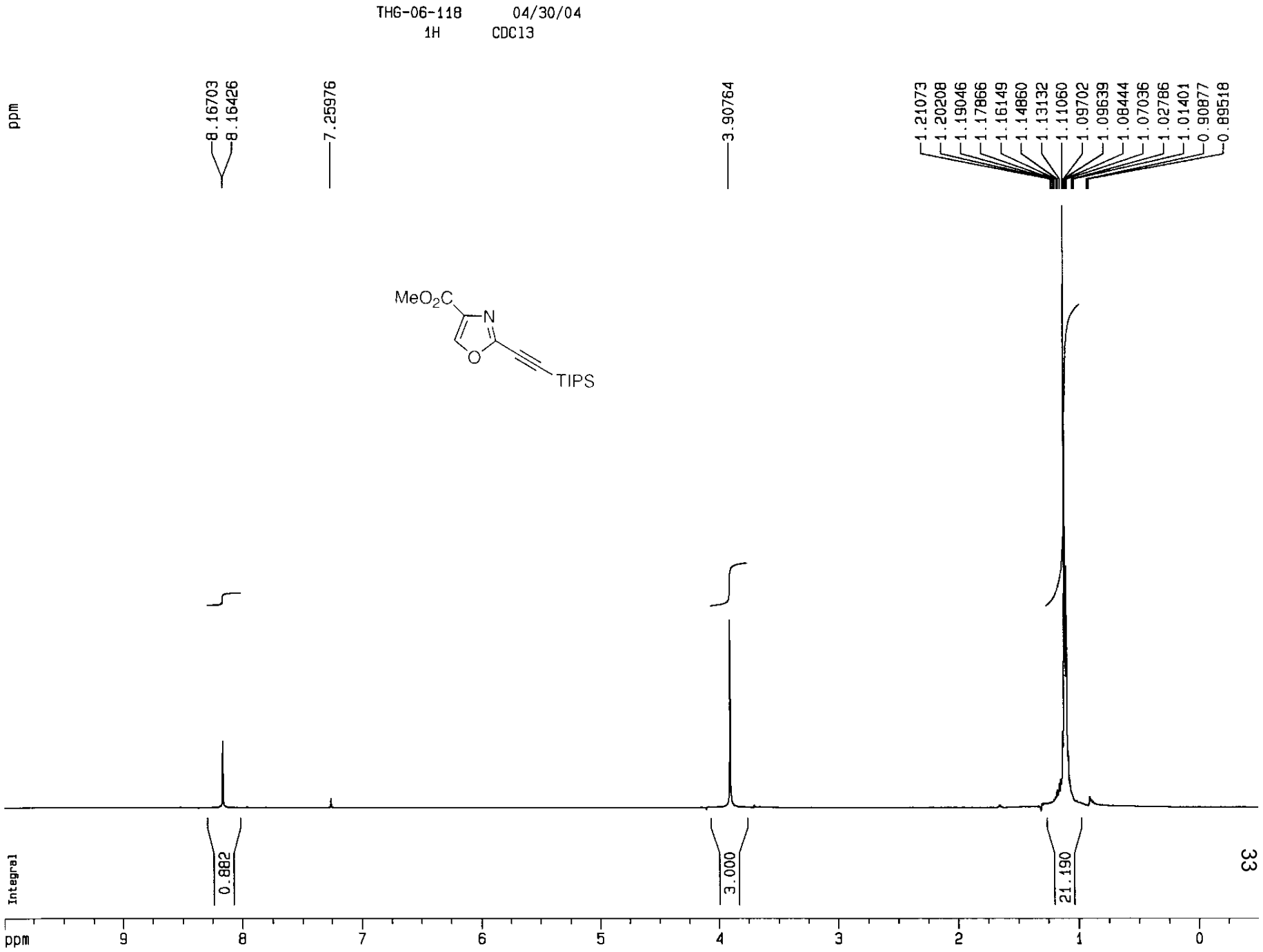
180
160
140
120
100
80
60
40
20
0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1.19046
1.17866
1.16149
1.14860
1.13132
1.11060
1.09702
1.09639
1.08444
1.07036
1.02786
1.01401
0.90877
0.89518
MeO2C
N
O
TIPS
Integral
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3.000
21.190
ppm
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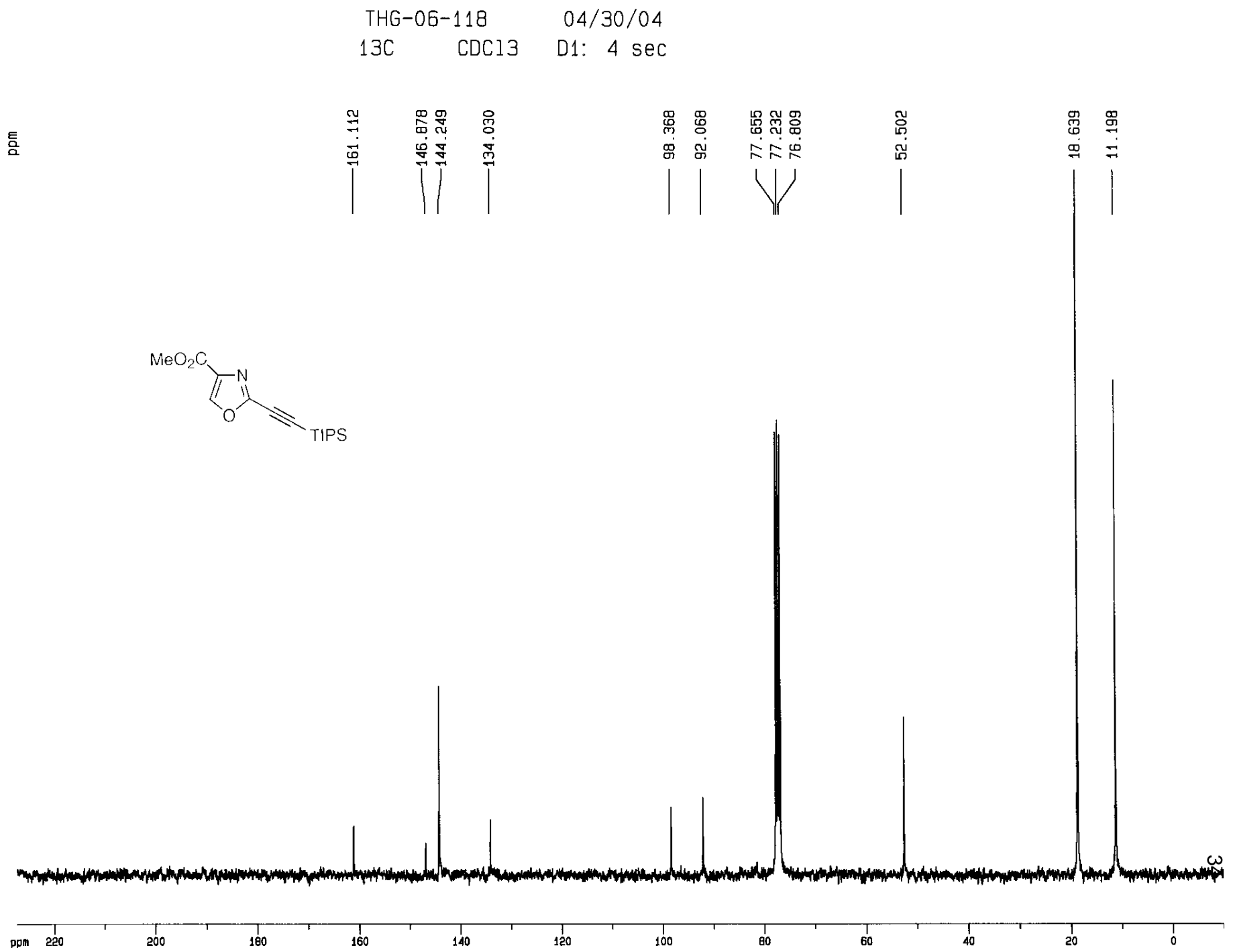
8
7
6
5
4
3
2
1
0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134.030
98.368
92.068
77.655
77.232
76.809
52.502
18.639
11.198
MeO2C
N
O
TIPS
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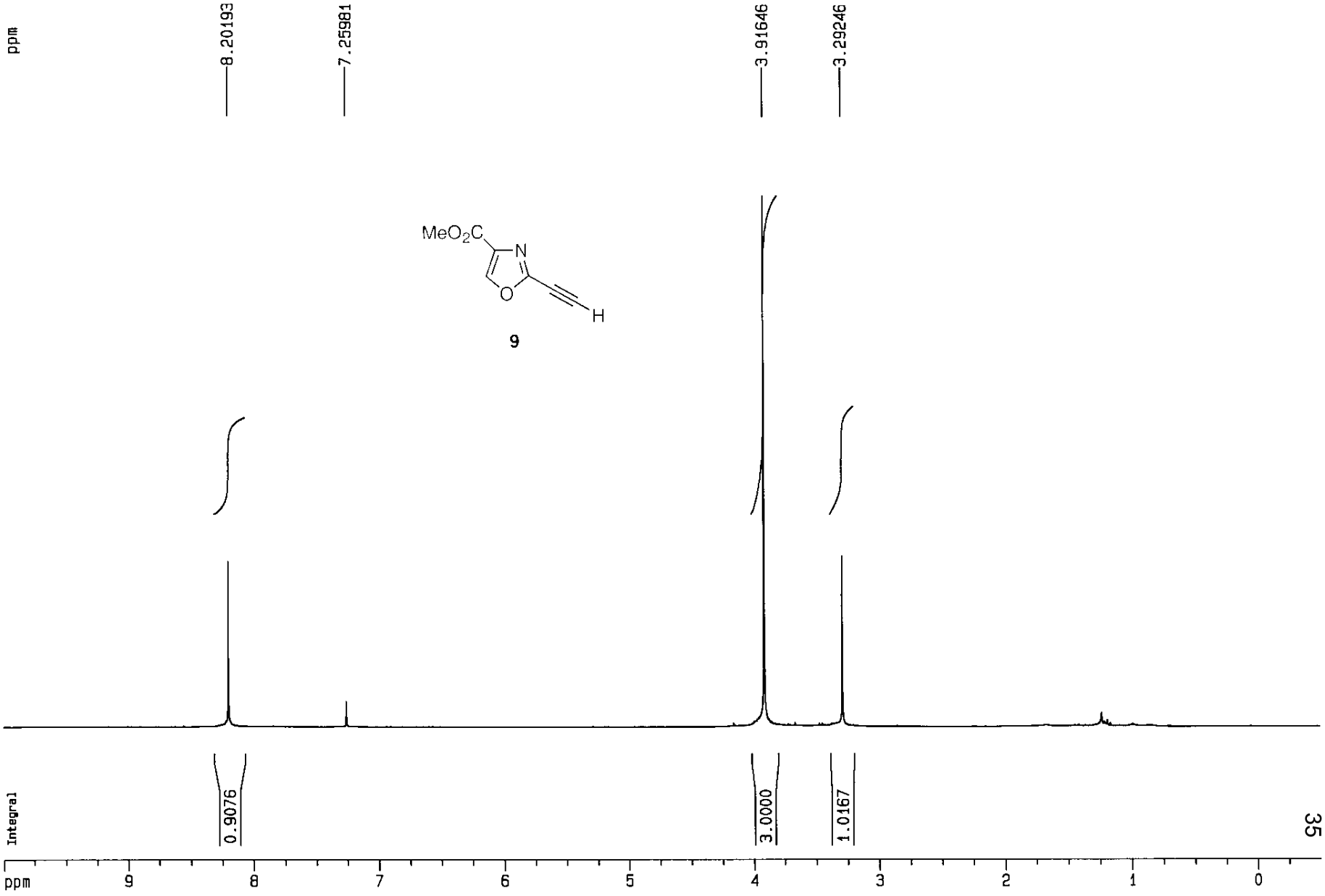
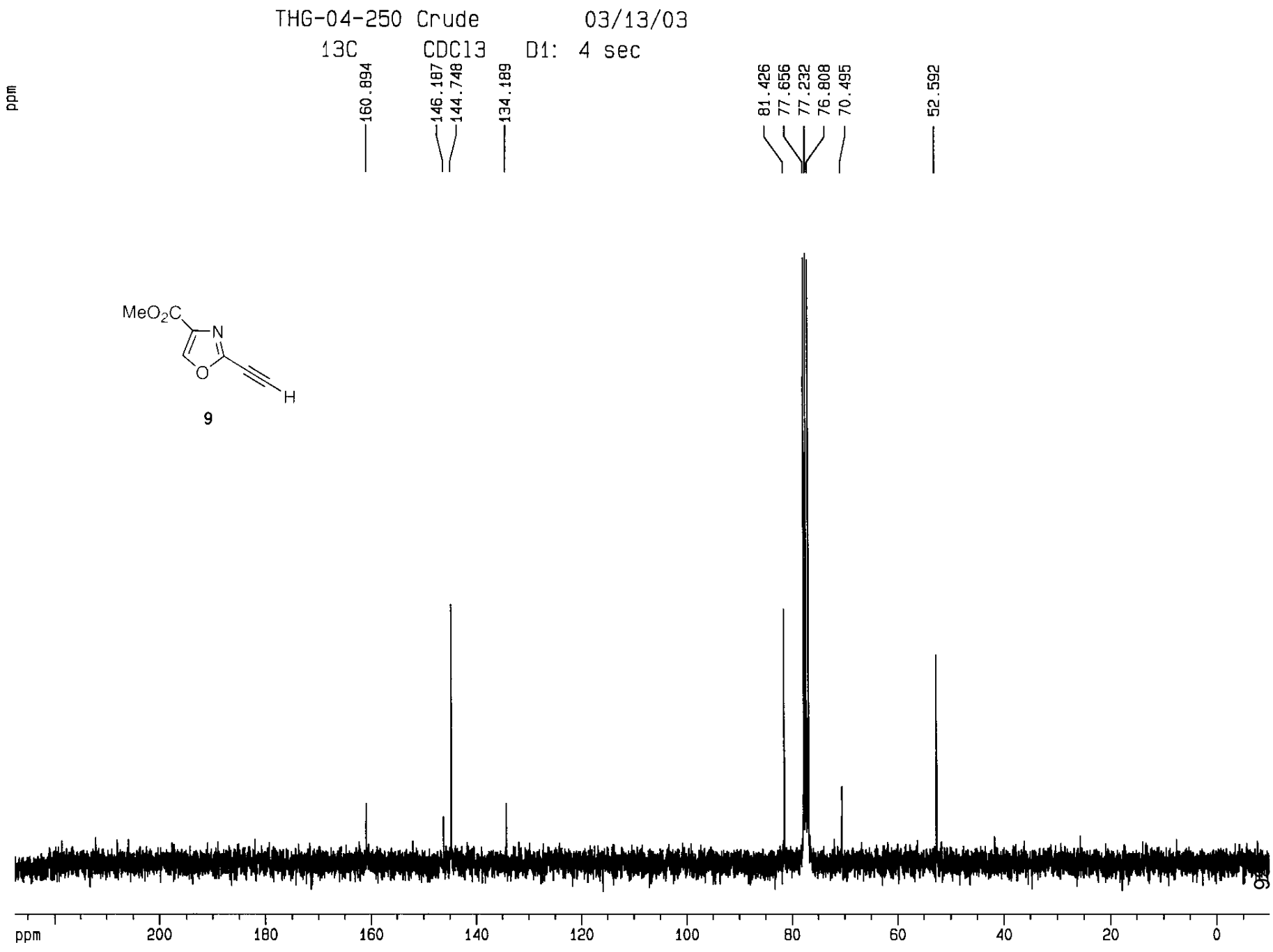
THG-04-250 Crude 03/13/03

1H CDCl3

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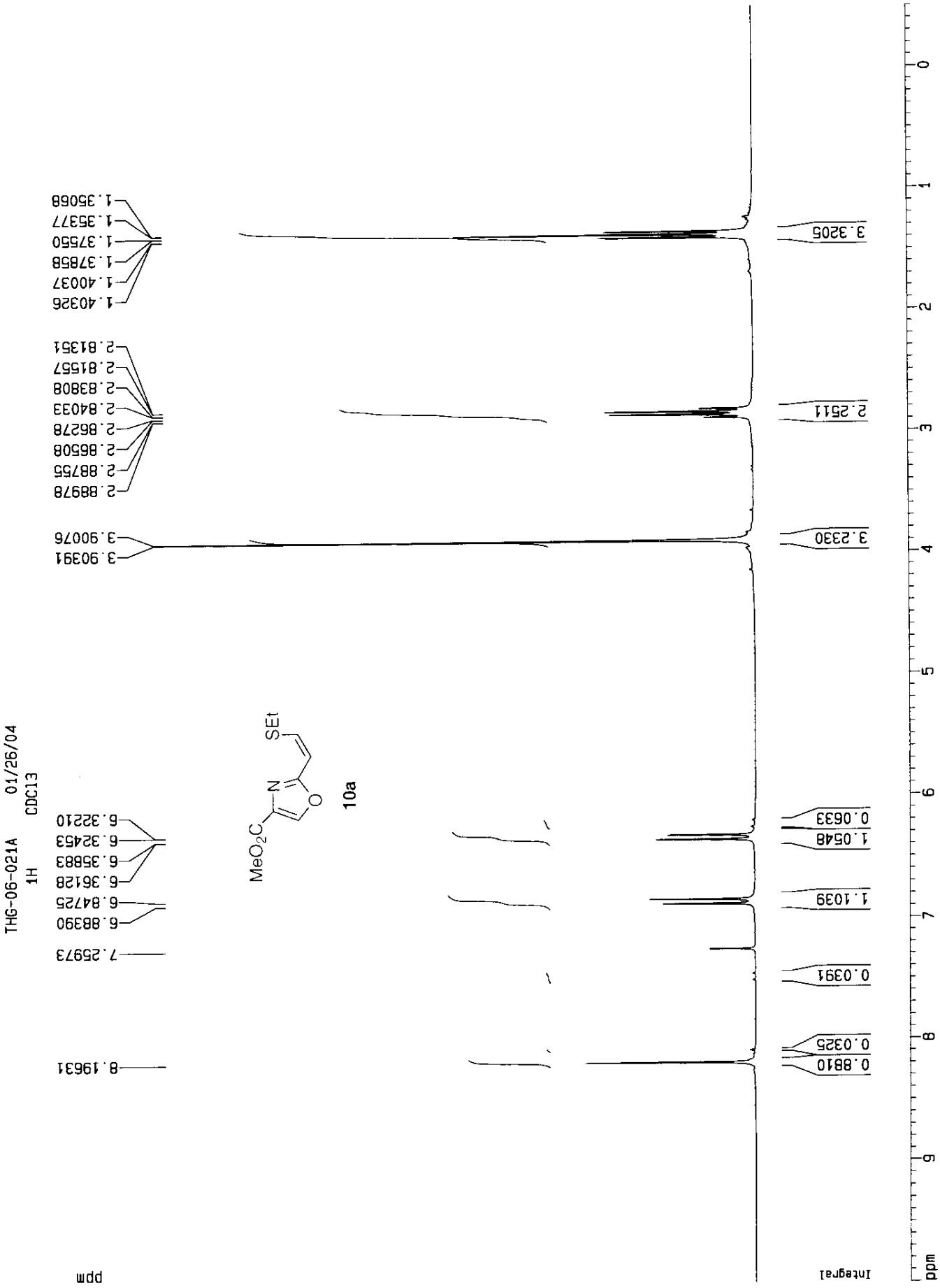
146.187
144.748
134.189
81.426
77.656
77.232
76.808
70.495
52.592
MeO2C
N
O
H
9
ppm
200
180
160
140
120
100
80
60
40
20
0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1H CDCl3
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7.25973
6.88390
6.84725
6.36128
6.35883
6.32453
6.32210
3.90391
3.90076
2.88978
2.88755
2.86508
2.86278
2.84033
2.83808
2.81557
2.81351
1.40326
1.40037
1.37858
1.37550
1.35377
1.35068
MeO2C
SEt
N
O
10a
0.8810
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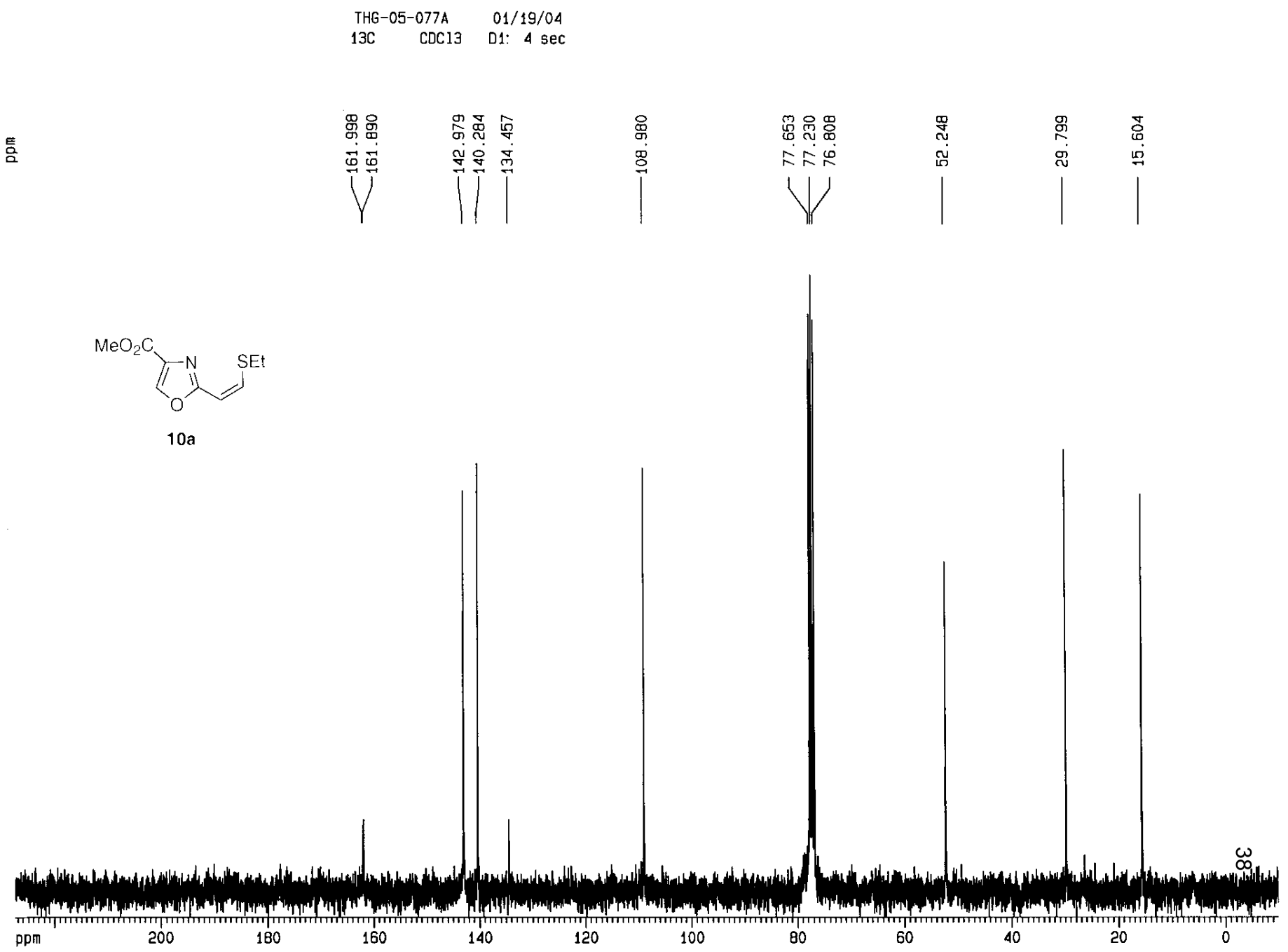
3.2330
2.2511
3.2205
Integral
ppm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77.653
77.230
76.808
52.248
29.799
15.604
MeO2C
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SEt
O
10a
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140
120
100
80
60
40
20
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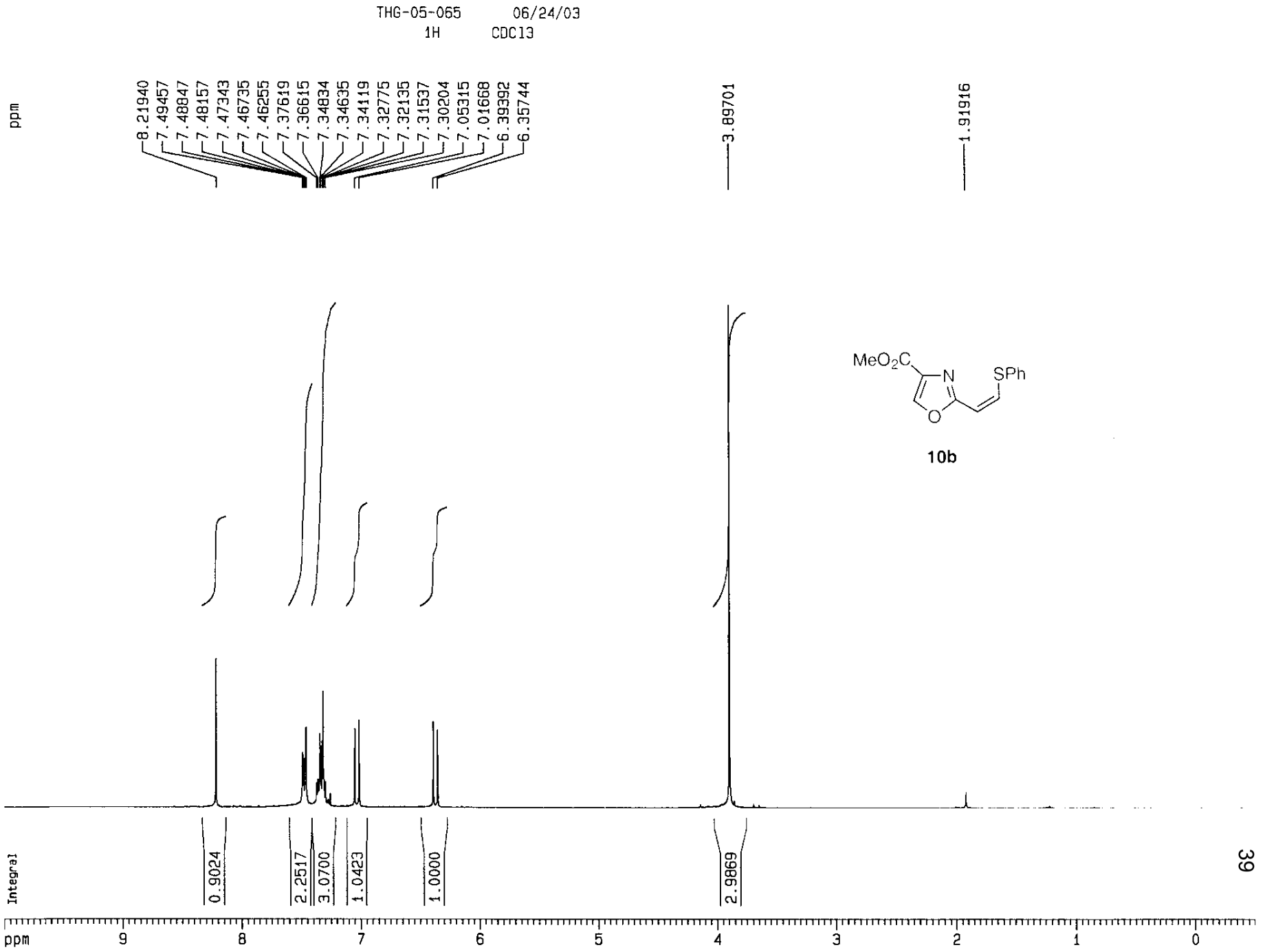
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7.46735
7.46255
7.37619
7.36615
7.34834
7.34635
7.34119
7.32775
7.32135
7.31537
7.30204
7.05315
7.01668
6.39392
6.35744
3.89701
1.91916
MeO2C
N
SPh
O
10b
Integral
0.9024
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3.0700
1.0423
1.0000
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8
7
6
5
4
3
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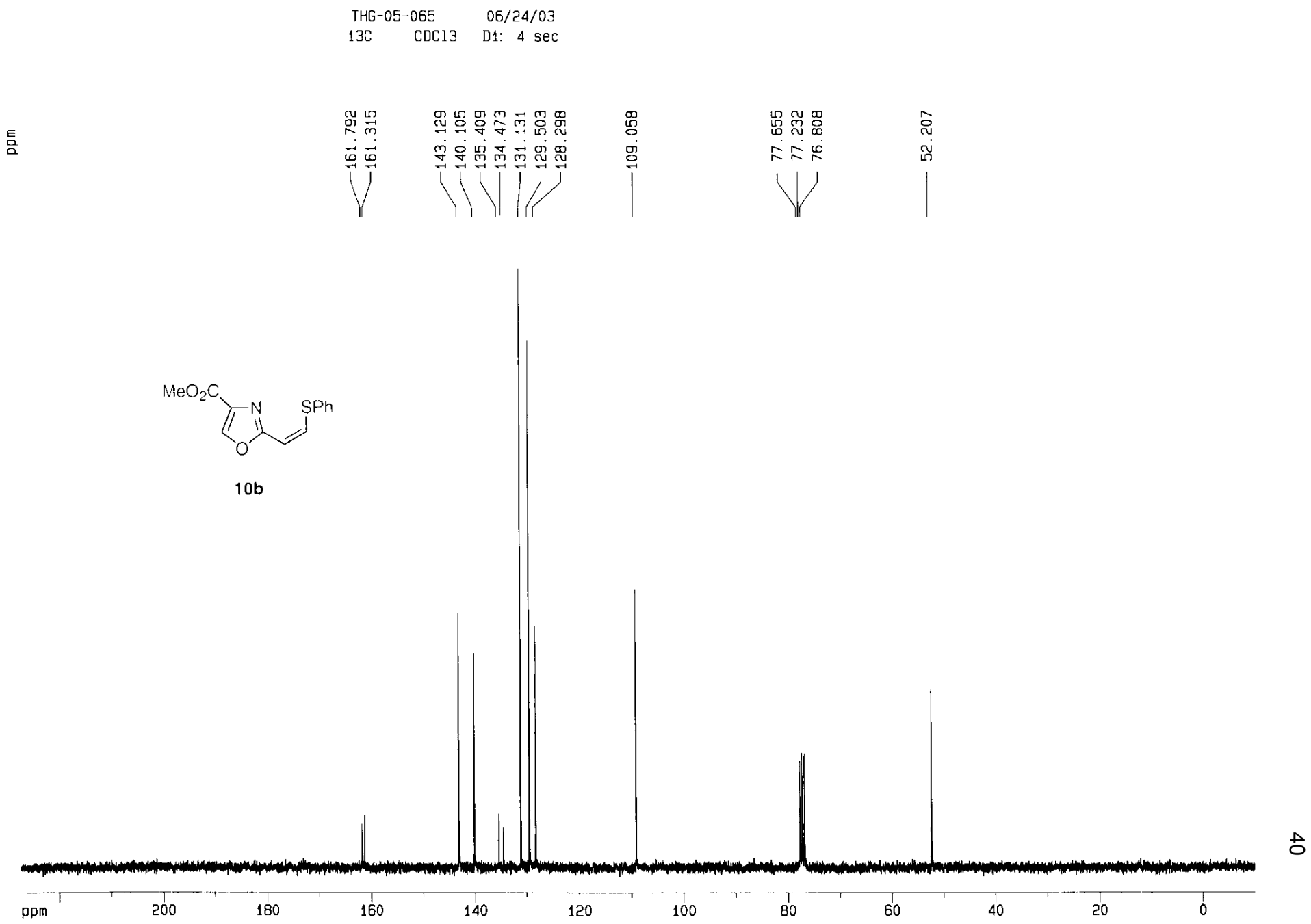
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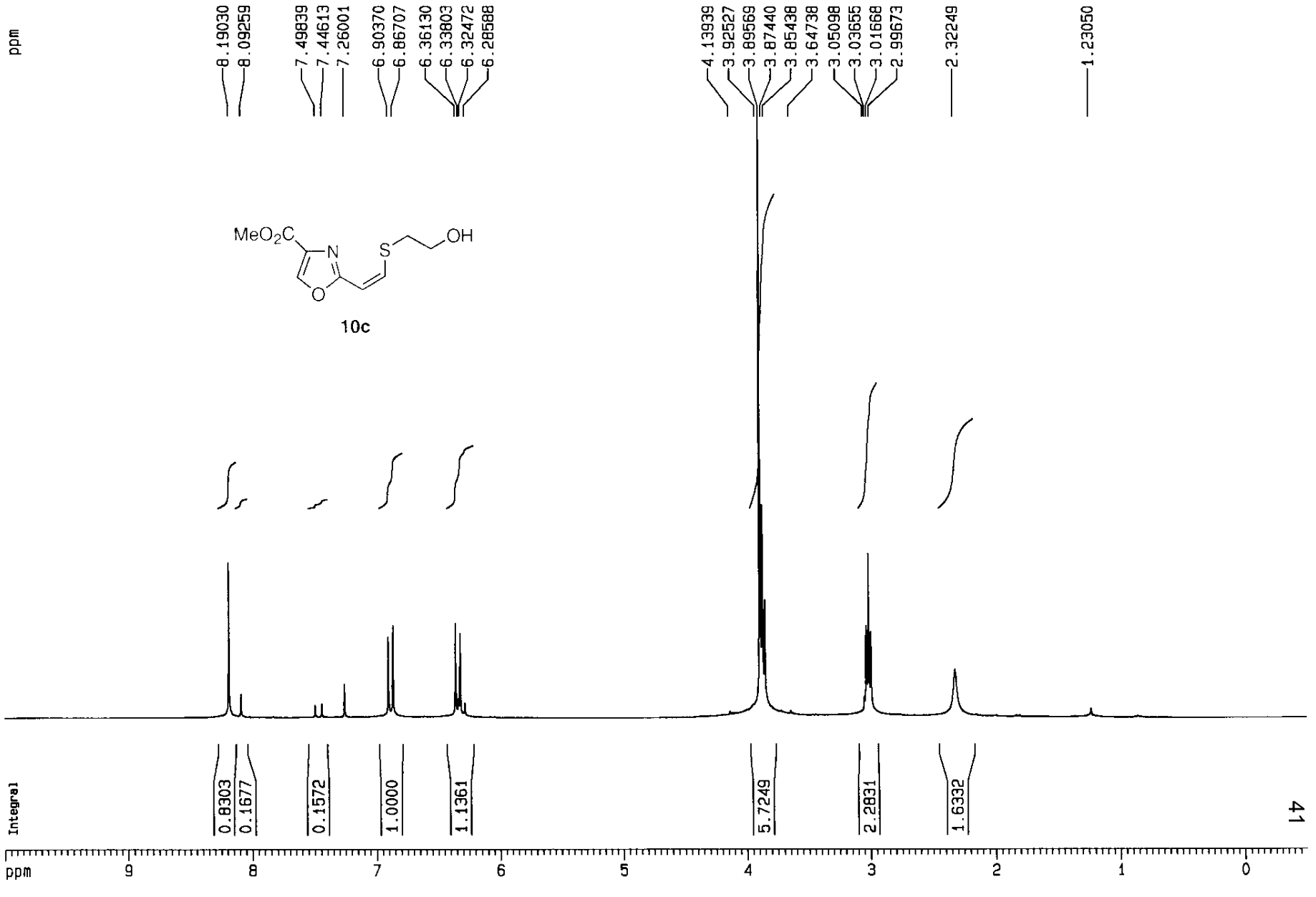
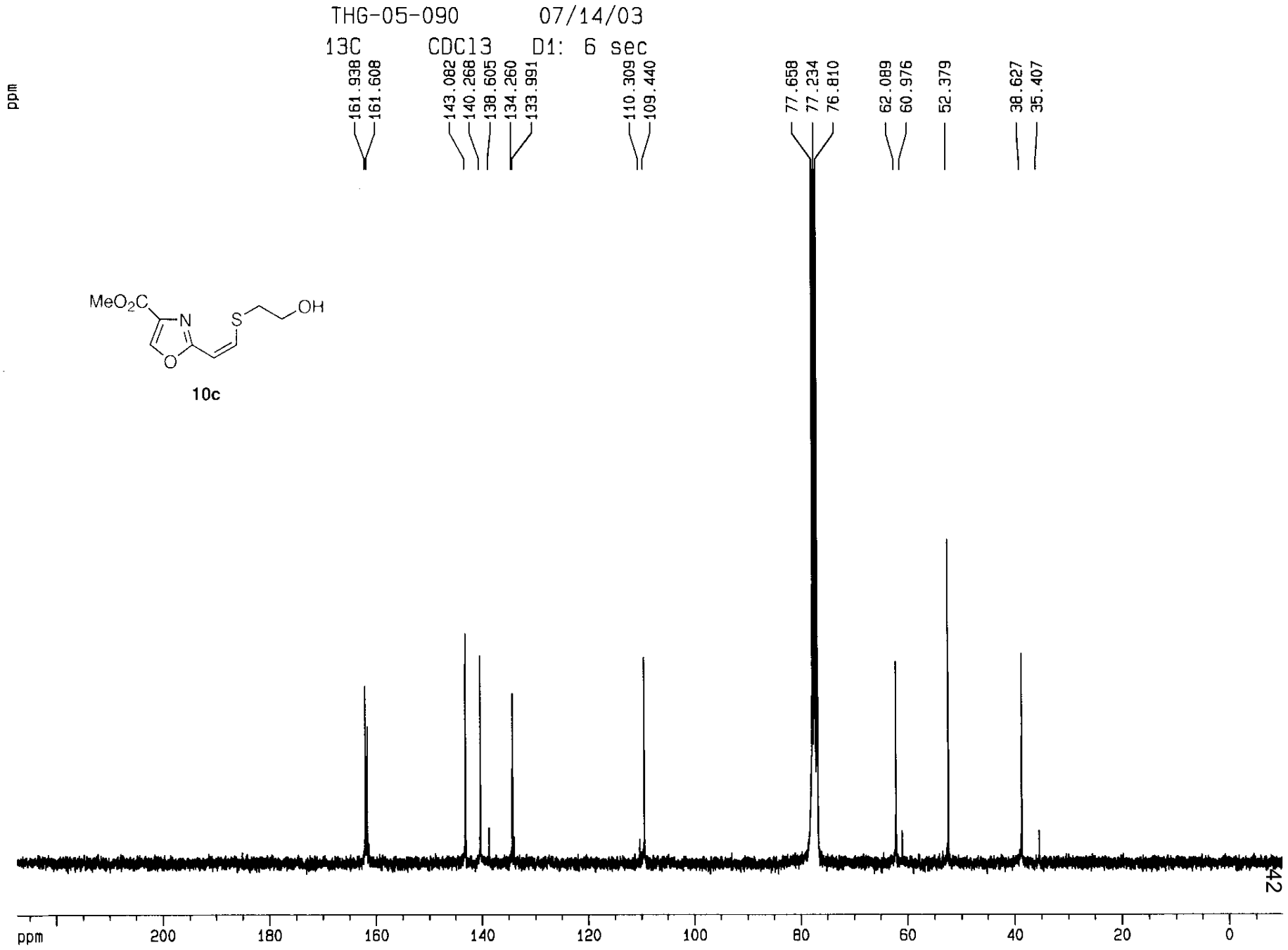
131.131
129.503
128.298
109.058
77.655
77.232
76.808
52.207
MeO2C
N
SPh
O
10b
ppm
200
180
160
140
120
100
80
60
40
20
0

THG-05-090 07/14/03

1H CDCl3

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143.082
140.268
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134.260
133.991
110.309
109.440
77.658
77.234
76.810
62.089
60.976
52.379
38.627
35.407
MeO2C
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S
OH
O
10c
42
ppm
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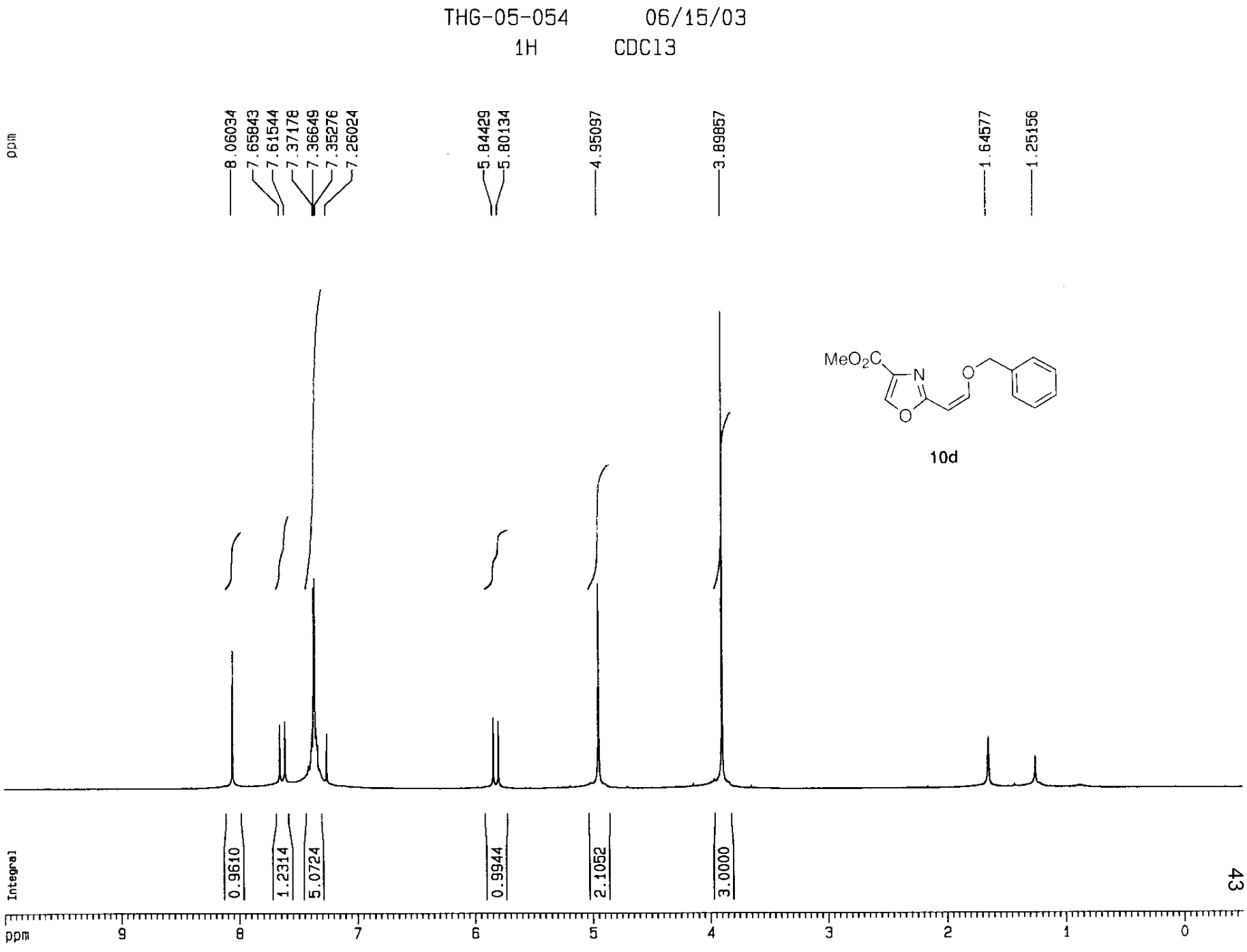
180
160
140
120
100
80
60
40
20
0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1H CDCl3
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7.36649
7.35276
7.26024
5.84429
5.80134
4.95097
3.89857
1.64577
1.25156
MeO2C
N
O
O
10d
Integral
0.9610
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7
6
5
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3
2
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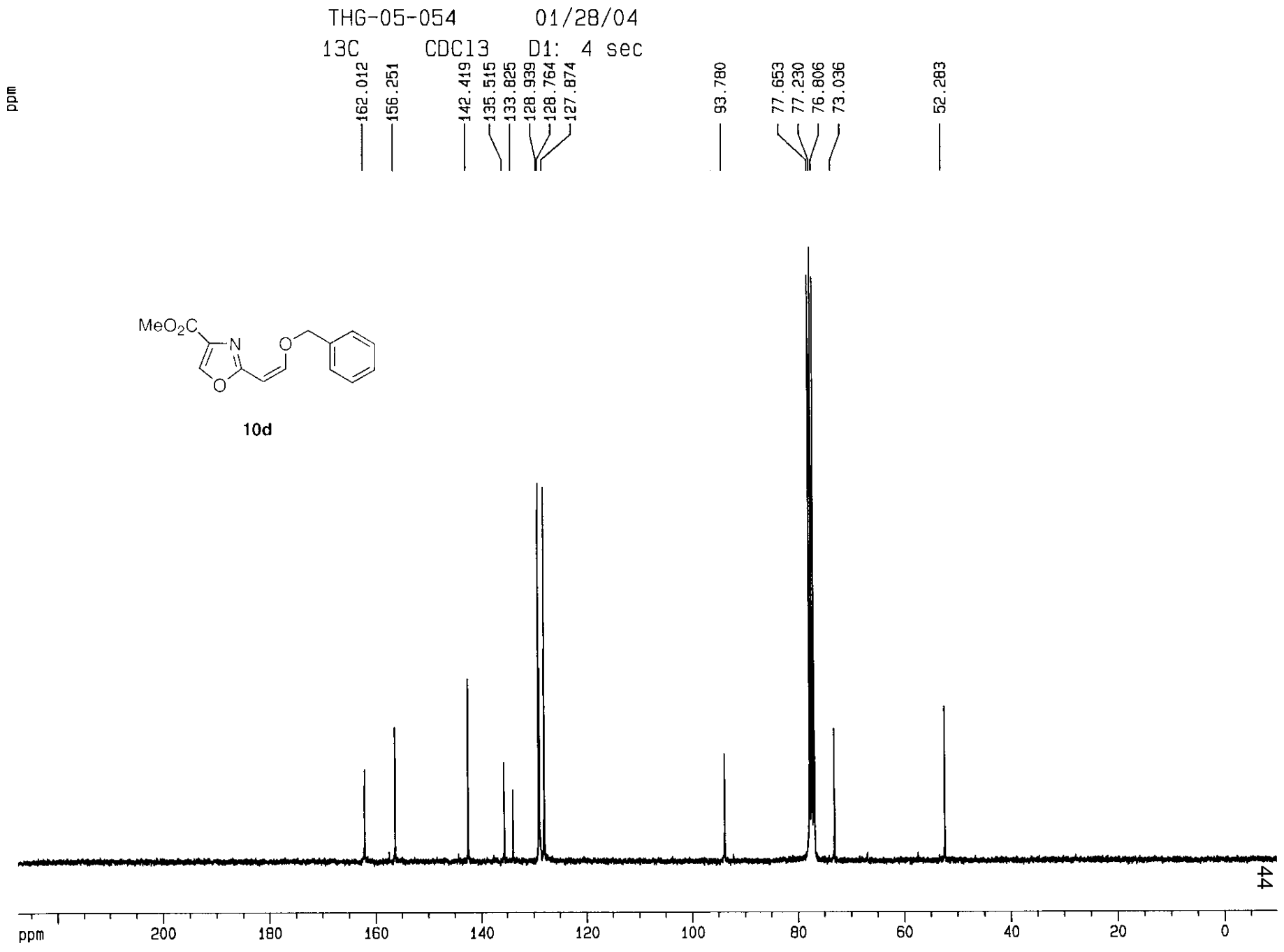
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128.764
127.874
93.780
77.653
77.230
76.806
73.036
52.283
MeO2C
N
O
O
10d
44
ppm
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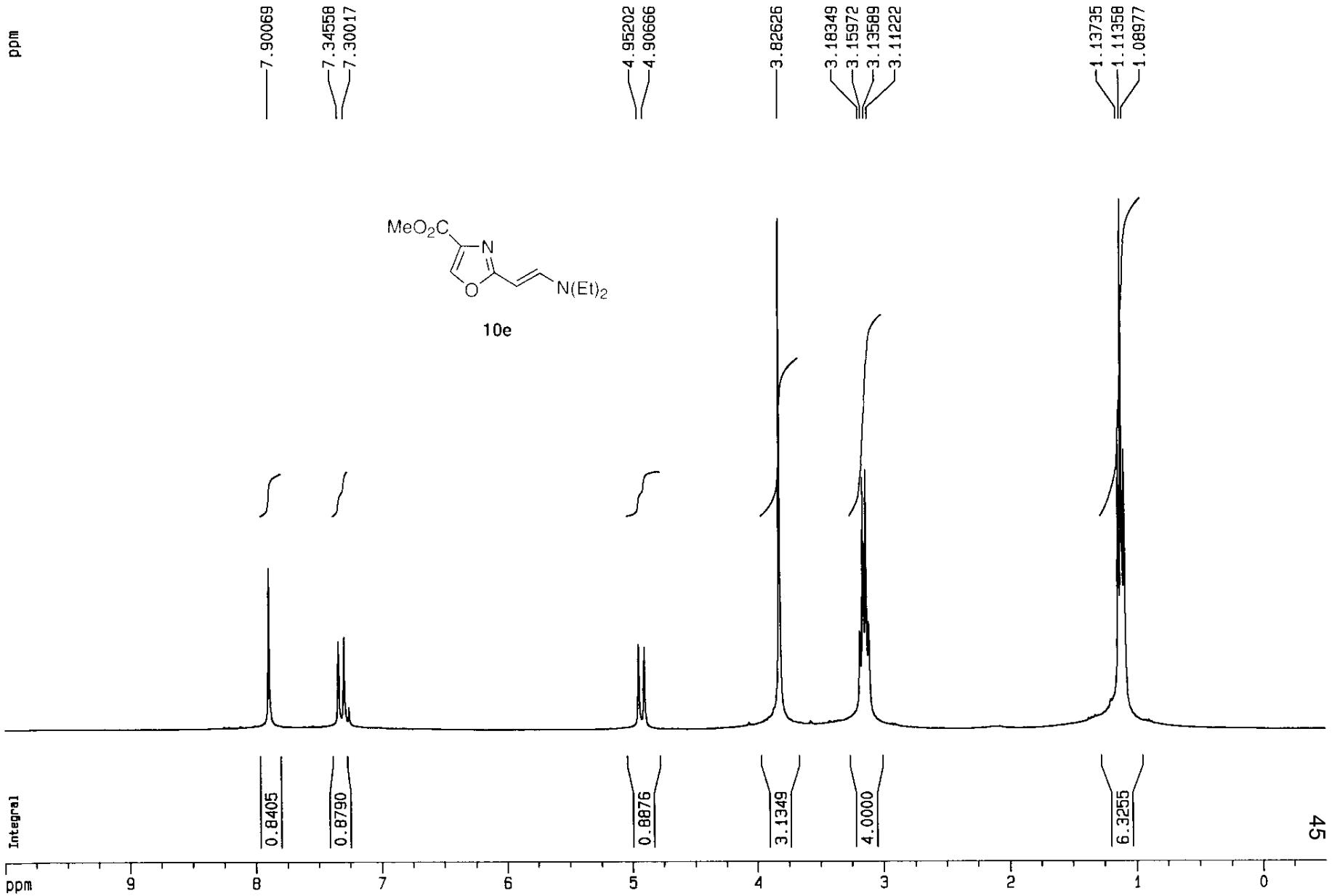
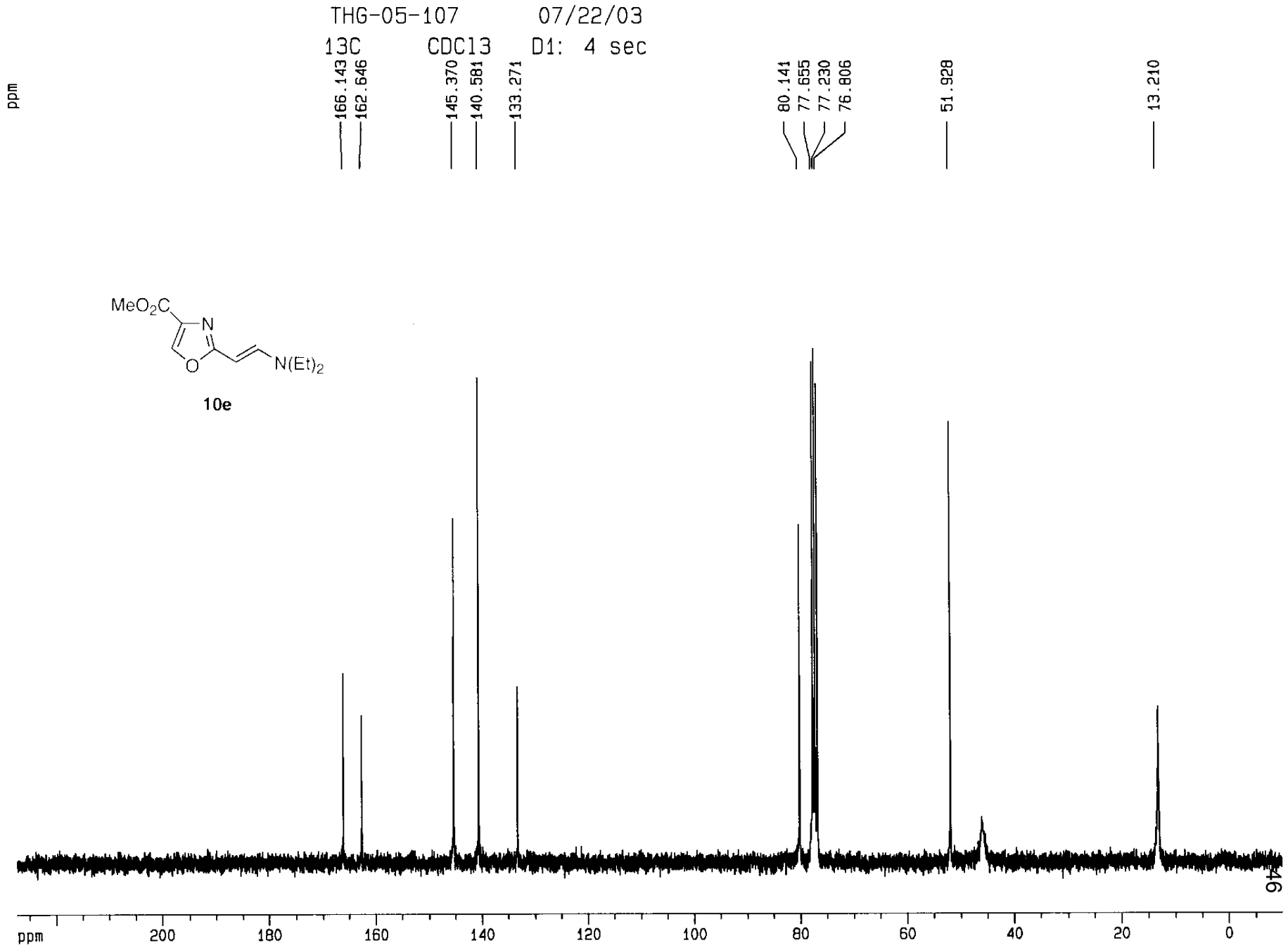
180
160
140
120
100
80
60
40
20
0

THG-05-107 07/22/03

1H CDC13

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77.230
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10e
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140
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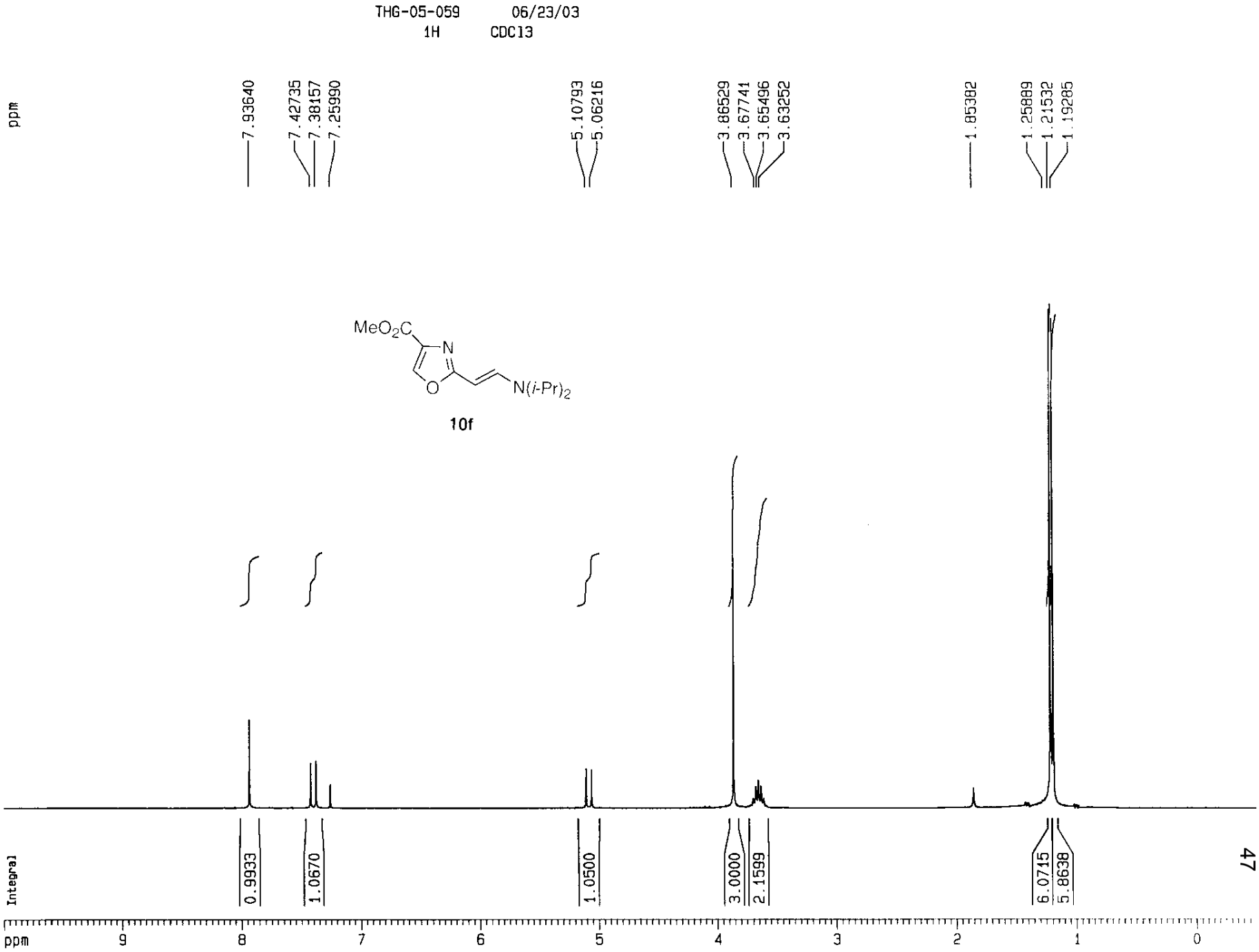
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3.86529
3.67741
3.65496
3.63252
1.85382
1.25889
1.21532
1.19285
MeO2C
N
O
N(i-Pr)2
10f
Integral
0.9933
1.0670
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6.0715
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8
7
6
5
4
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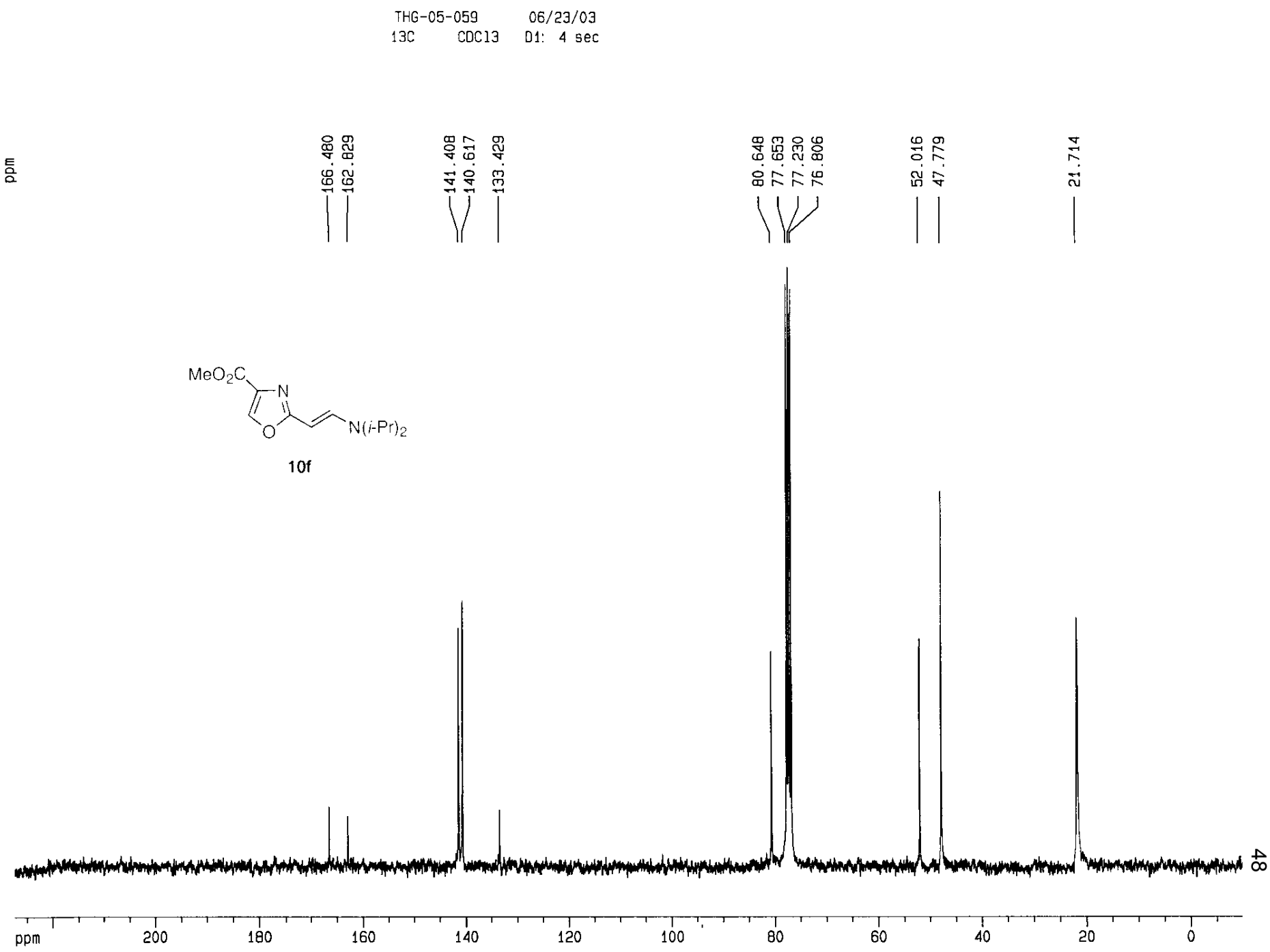
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166.480
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133.429
80.648
77.653
77.230
76.806
52.016
47.779
21.714
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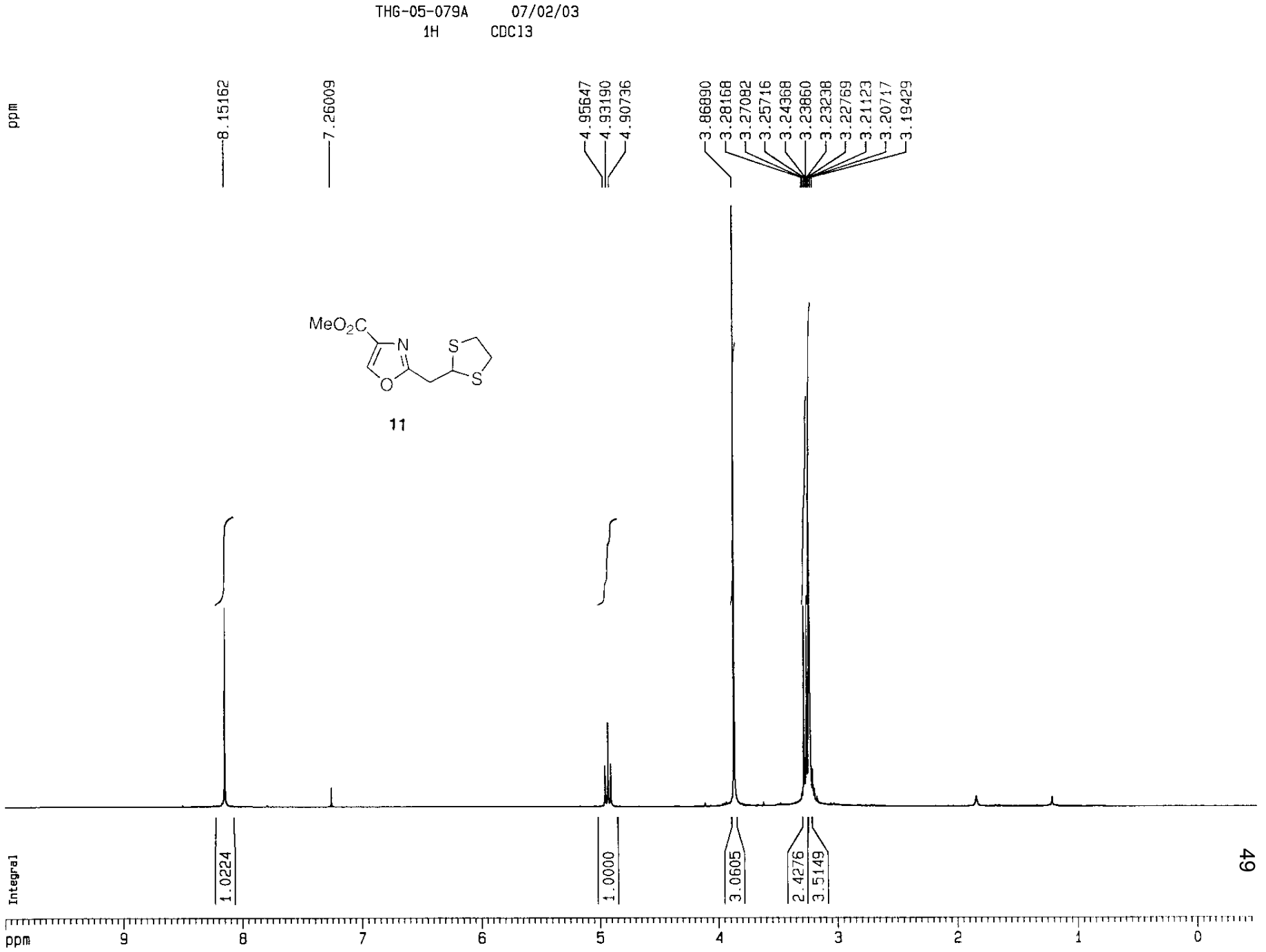
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4.90736
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3.28168
3.27082
3.25716
3.24368
3.23860
3.23238
3.22769
3.21123
3.20717
3.19429
MeO2C
N
S
S
O
11
Integral
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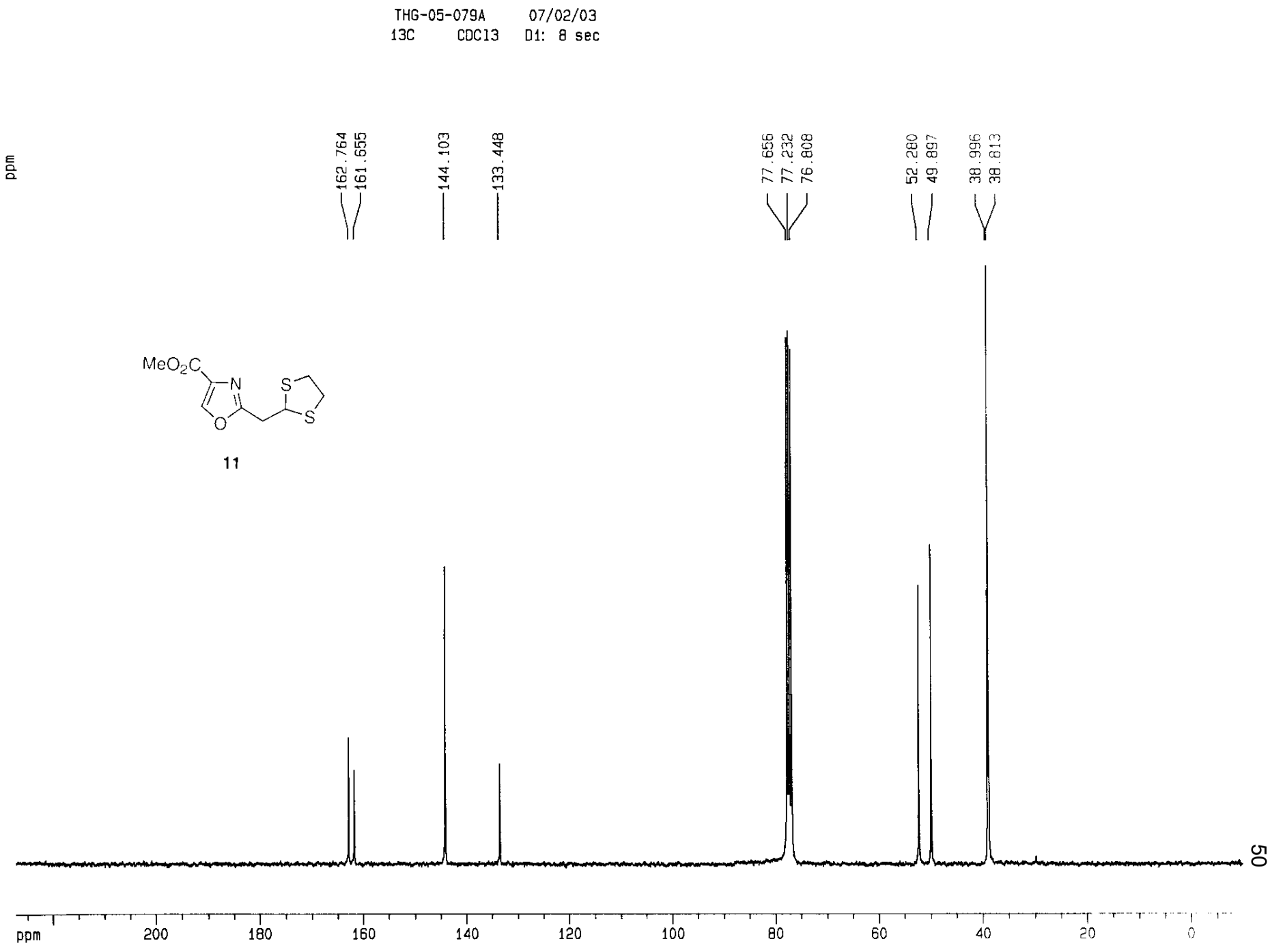
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77.232
76.808
52.280
49.897
38.996
38.813
MeO2C
N
S
S
O
11
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140
120
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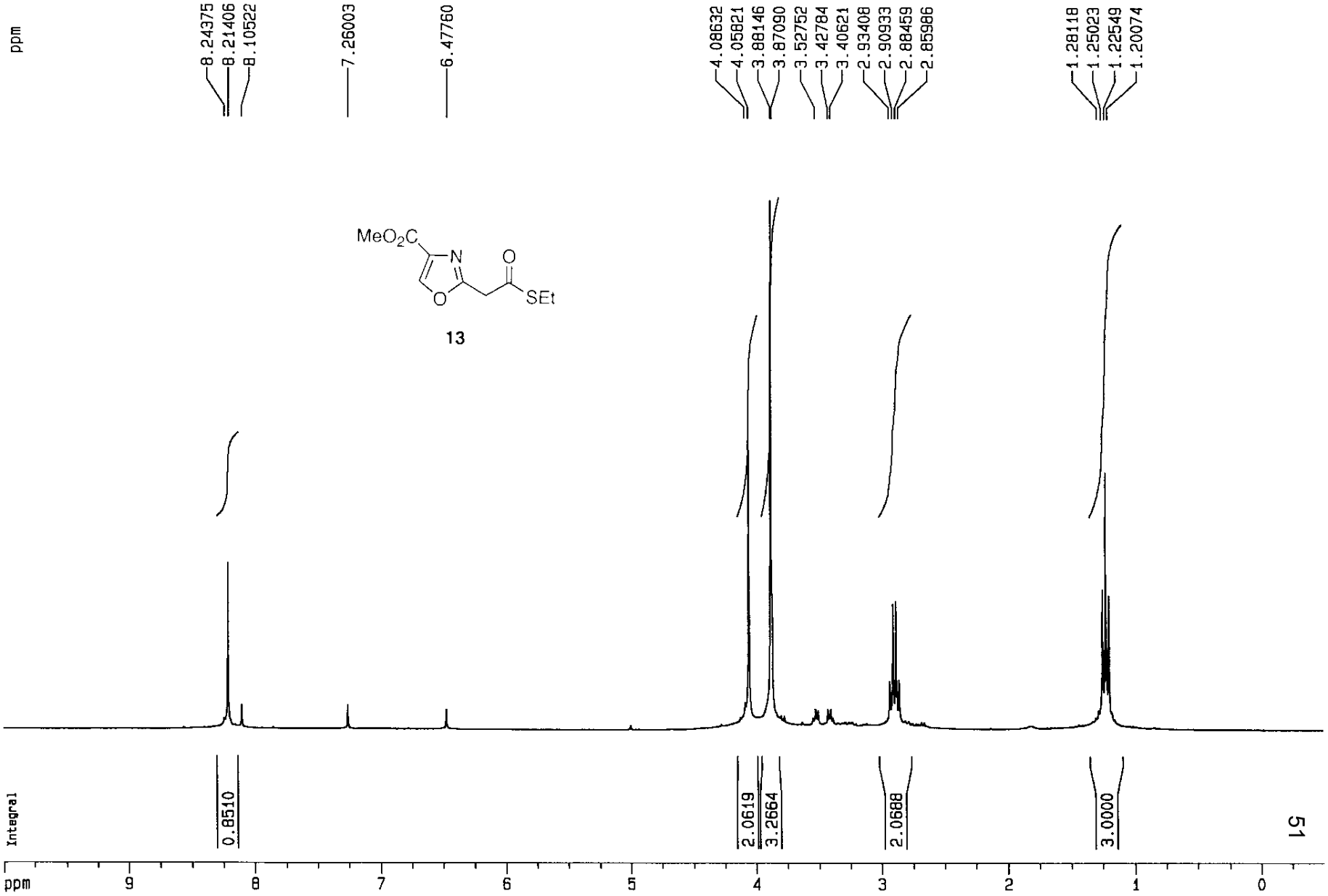
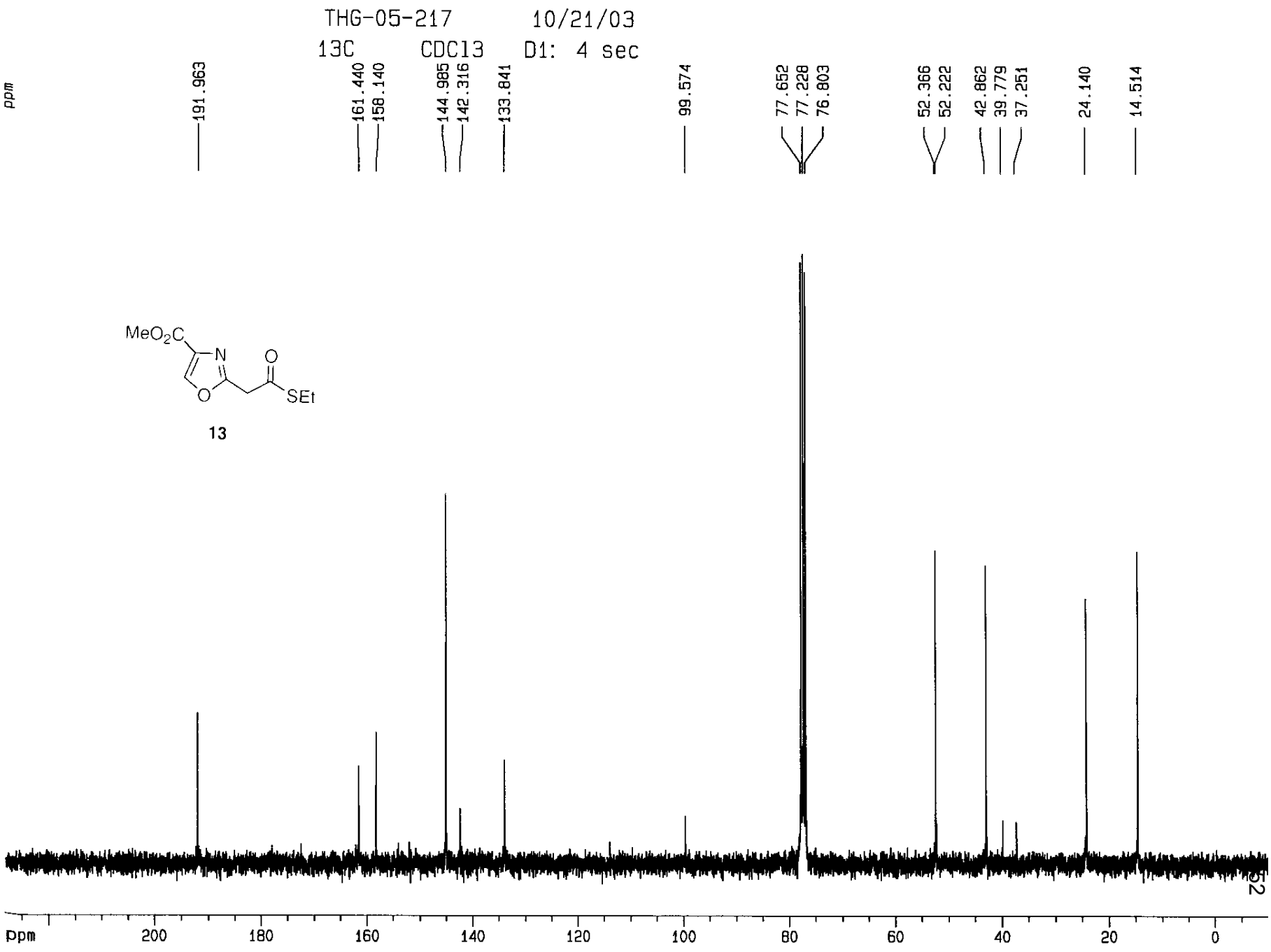
40
20
0

THG-05-217 10/21/03

1H CDCl3

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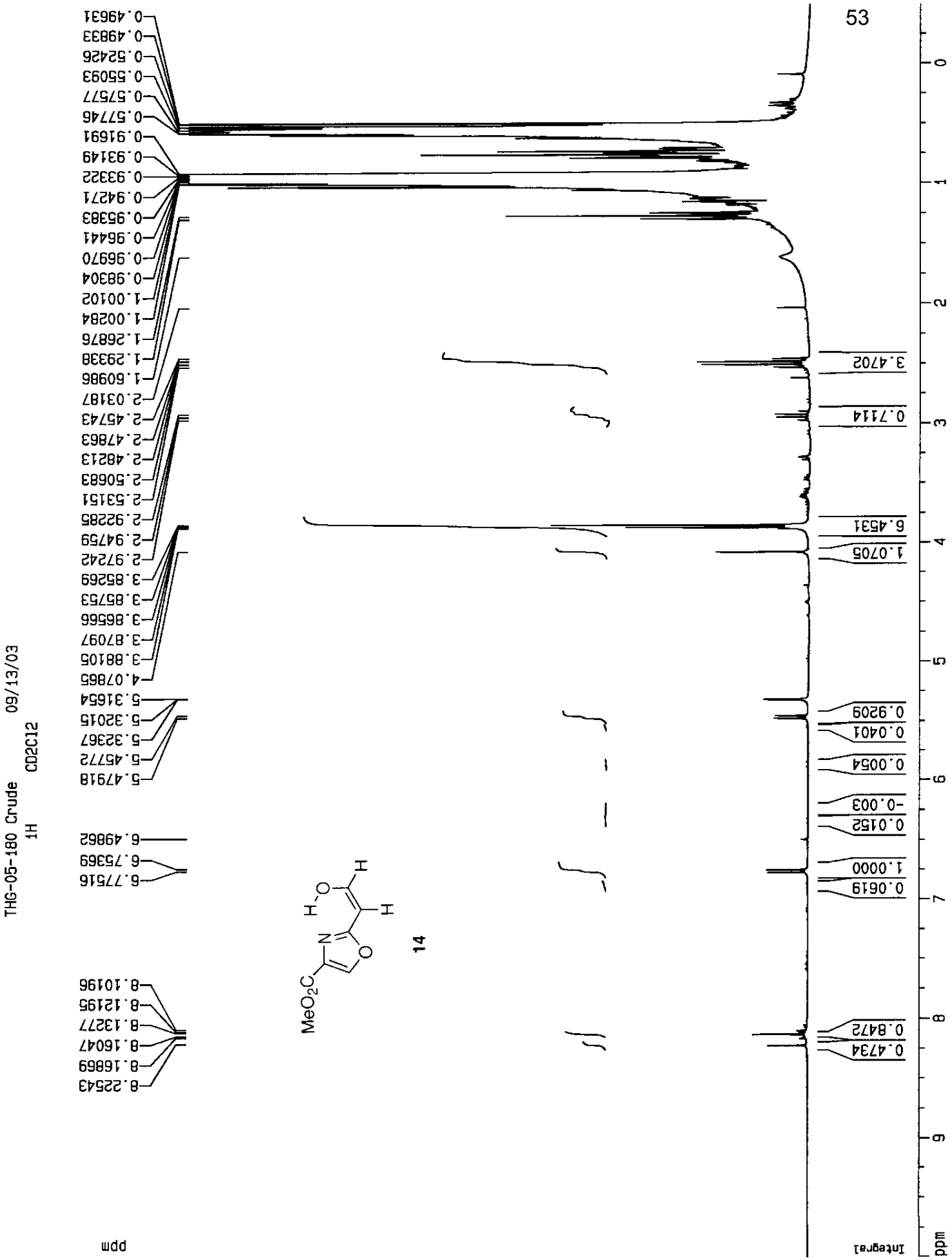
191.963
161.440
158.140
144.985
142.316
133.841
99.574
77.652
77.228
76.803
52.366
52.222
42.862
39.779
37.251
24.140
14.514
MeO2C
N
O
O
SEt
13
52
ppm
200
180
160
140
120
100
80
60
40
20
0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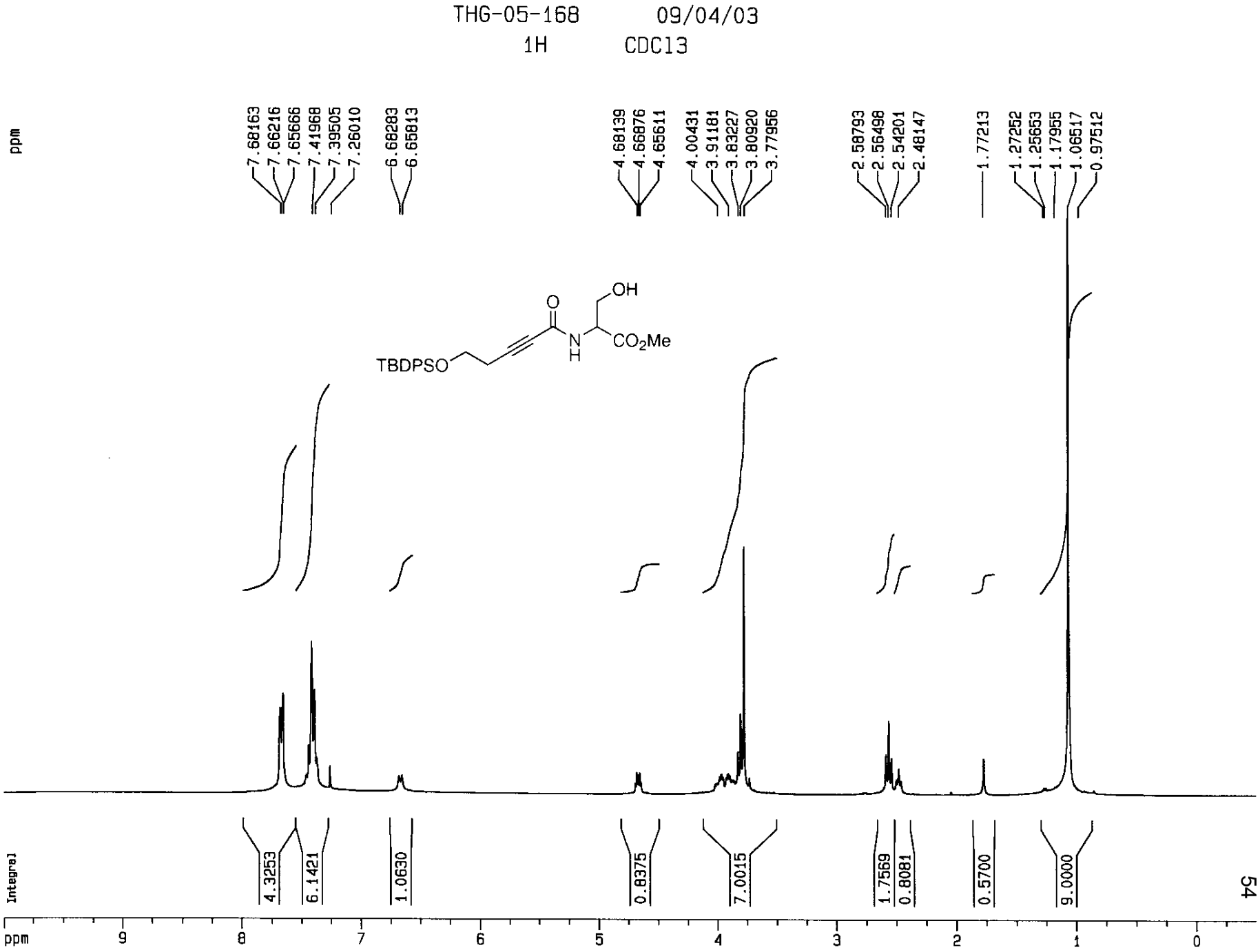
1H
CD2Cl2
09/13/03
14
MeO2C
ppm
Integral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7.68163
7.66216
7.65666
7.41968
7.39505
7.26010
6.68283
6.65813
4.68139
4.66876
4.65611
4.00431
3.91181
3.83227
3.80920
3.77956
2.58793
2.56498
2.54201
2.48147
1.77213
1.27252
1.25653
1.17955
1.06517
0.97512
OH
O
N
H
CO2Me
TBDPSO
Integral
4.3253
6.1421
1.0630
0.8375
7.0015
1.7569
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9
8
7
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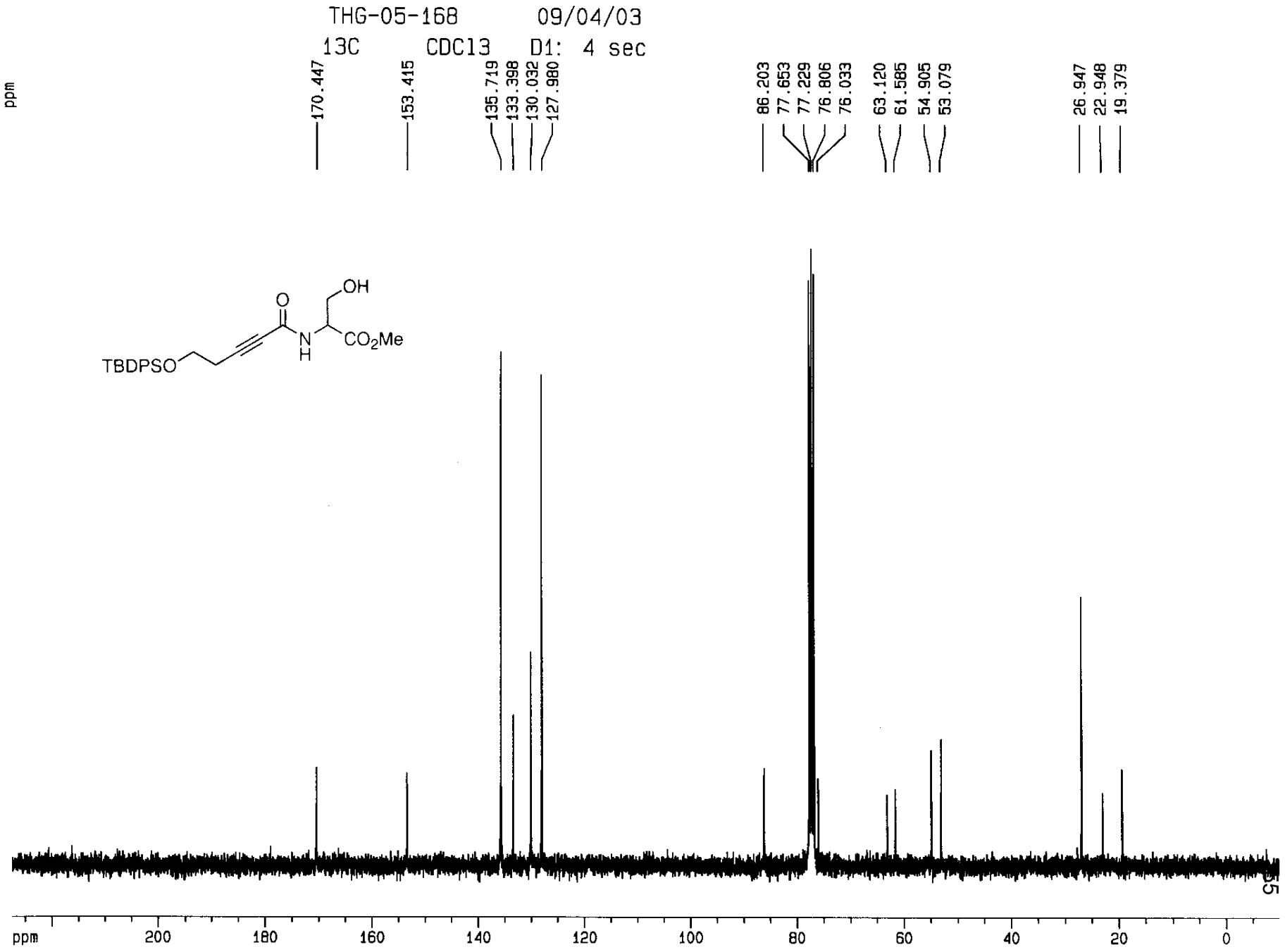
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13C CDCl3 D1: 4 sec
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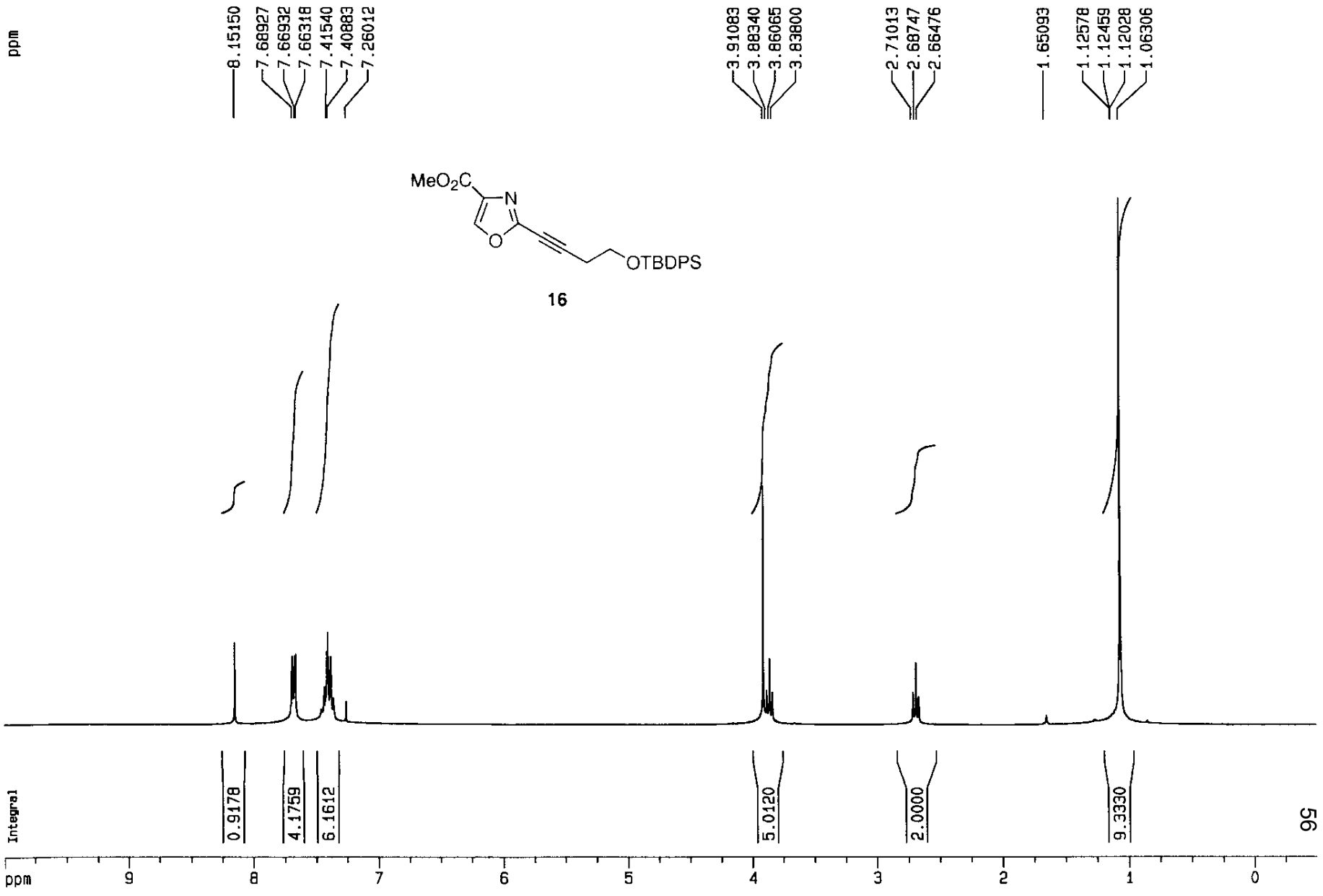
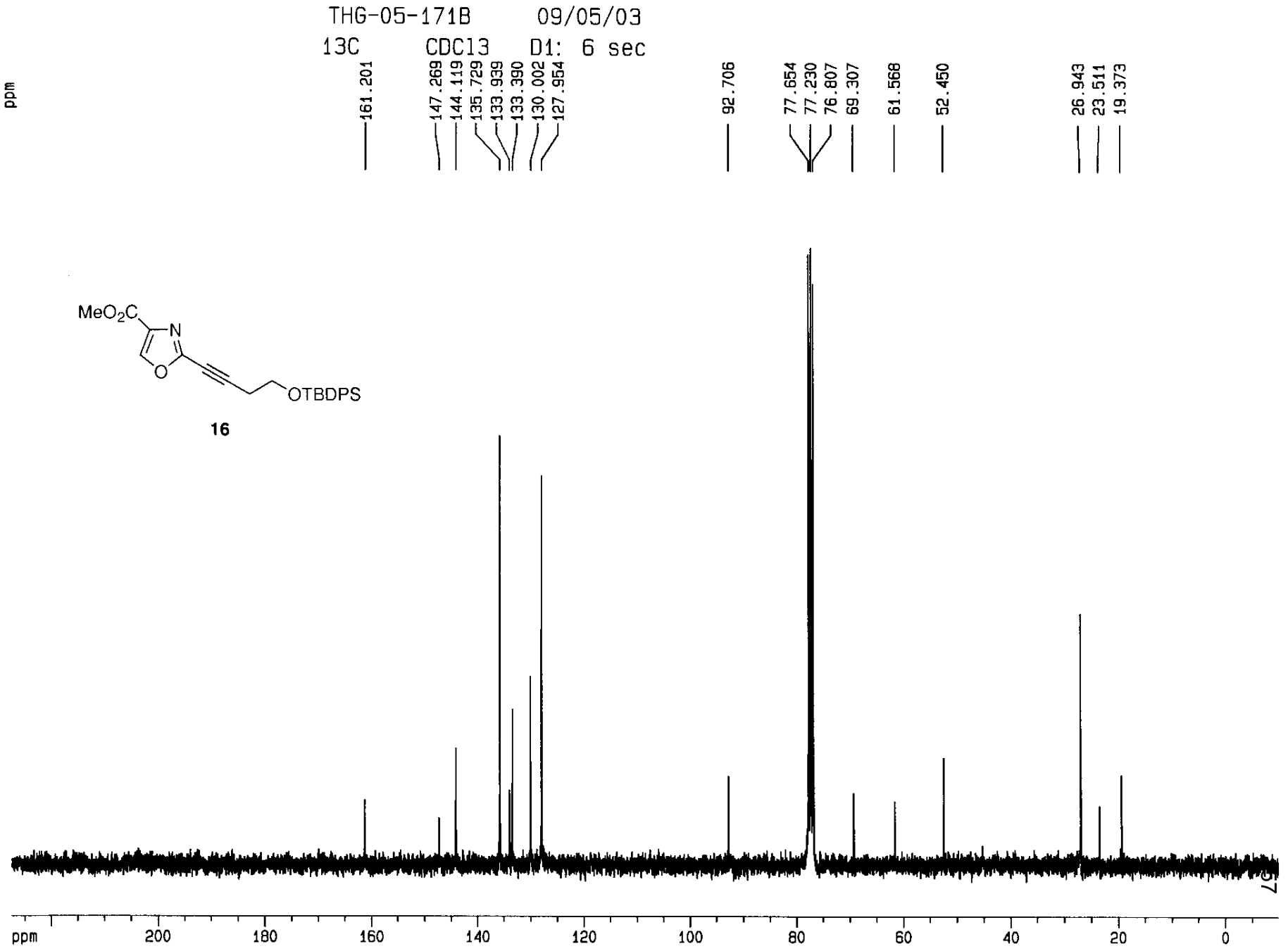
153.415
135.719
133.398
130.032
127.980
86.203
77.653
77.229
76.806
76.033
63.120
61.585
54.905
53.079
26.947
22.948
19.379
OH
O
N
H
CO2Me
TBDPSO
ppm
200
180
160
140
120
100
80
60
40
20
0

THG-05-171B 09/05/03

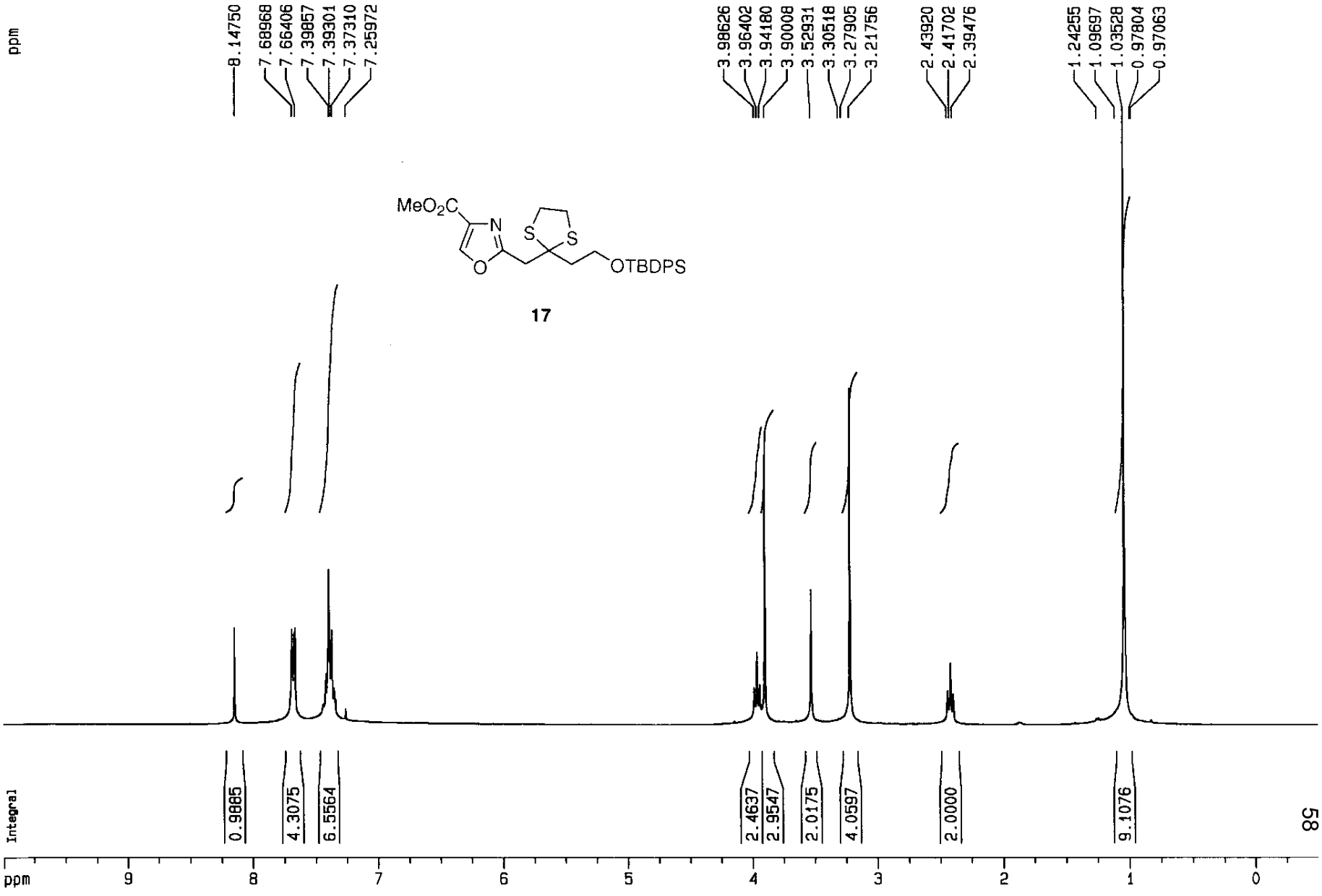
1H CDCl3



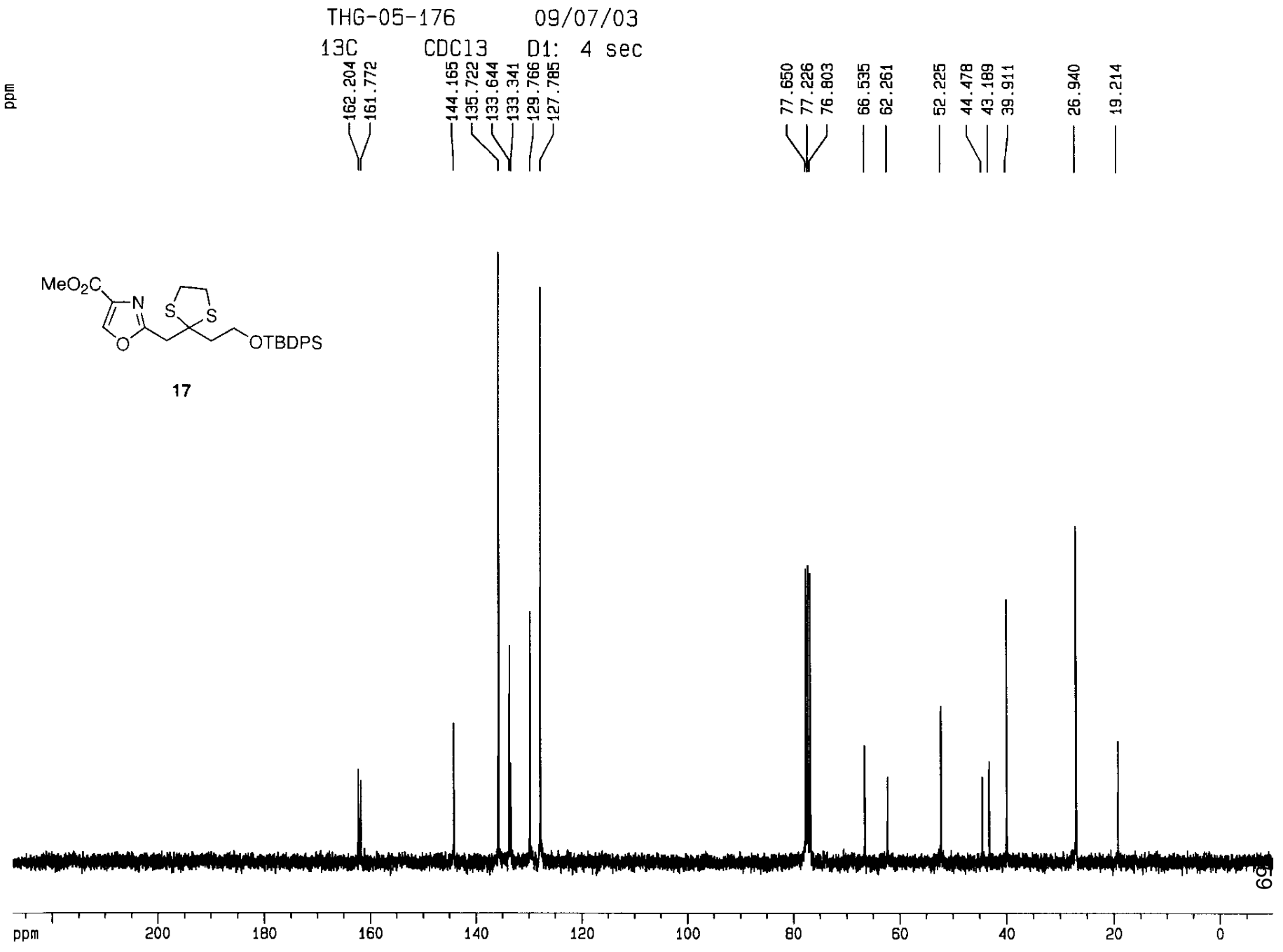

THG-05-171B 09/05/03
13C CDCl3 D1: 6 sec
ppm
161.201
147.269
144.119
135.729
133.939
133.390
130.002
127.954
92.706
77.654
77.230
76.807
69.307
61.568
52.450
26.943
23.511
19.373
MeO2C
N
O
OTBDPS
16
ppm
200
180
160
140
120
100
80
60
40
20
0

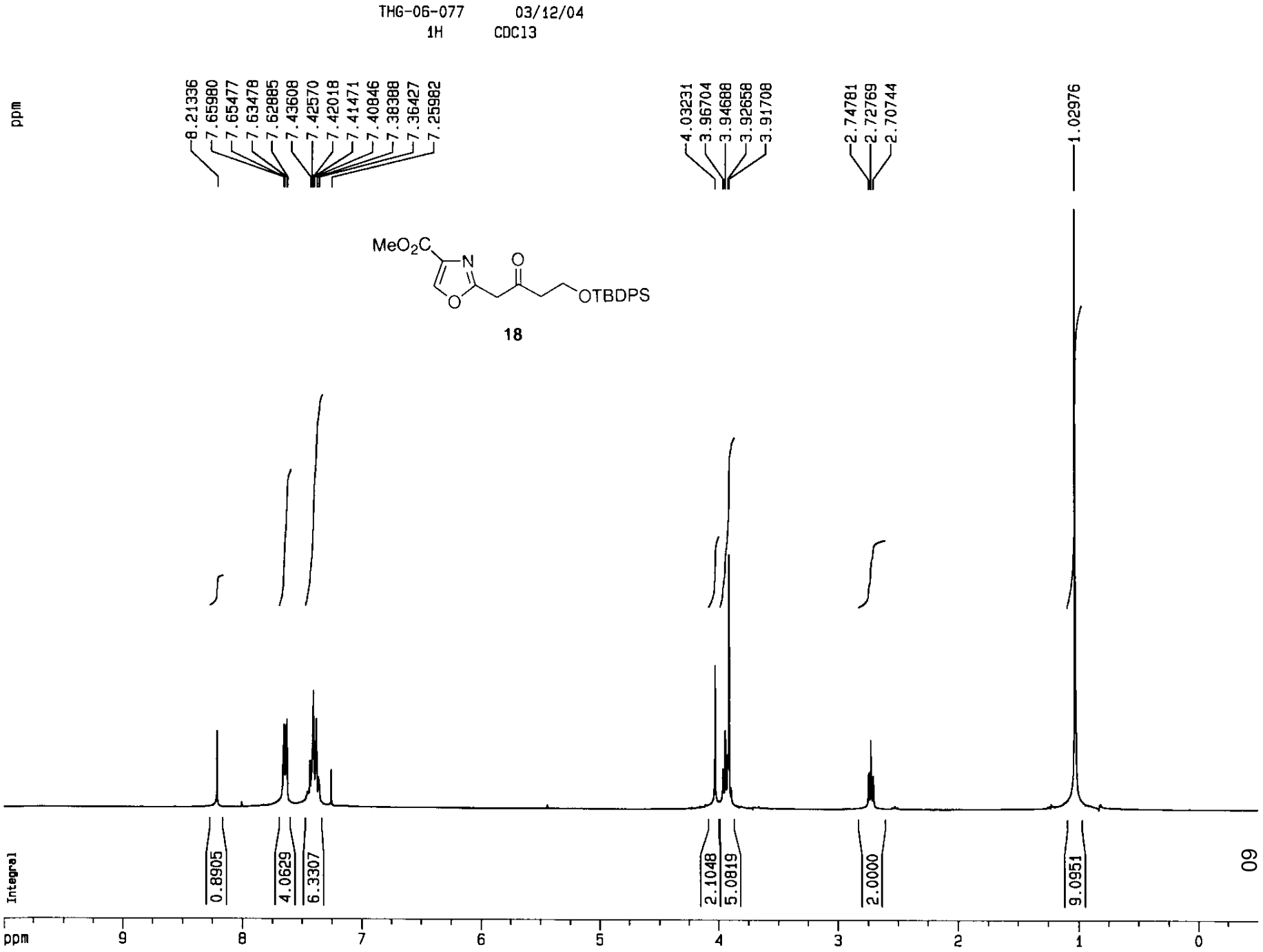
THG-05-176 09/07/03

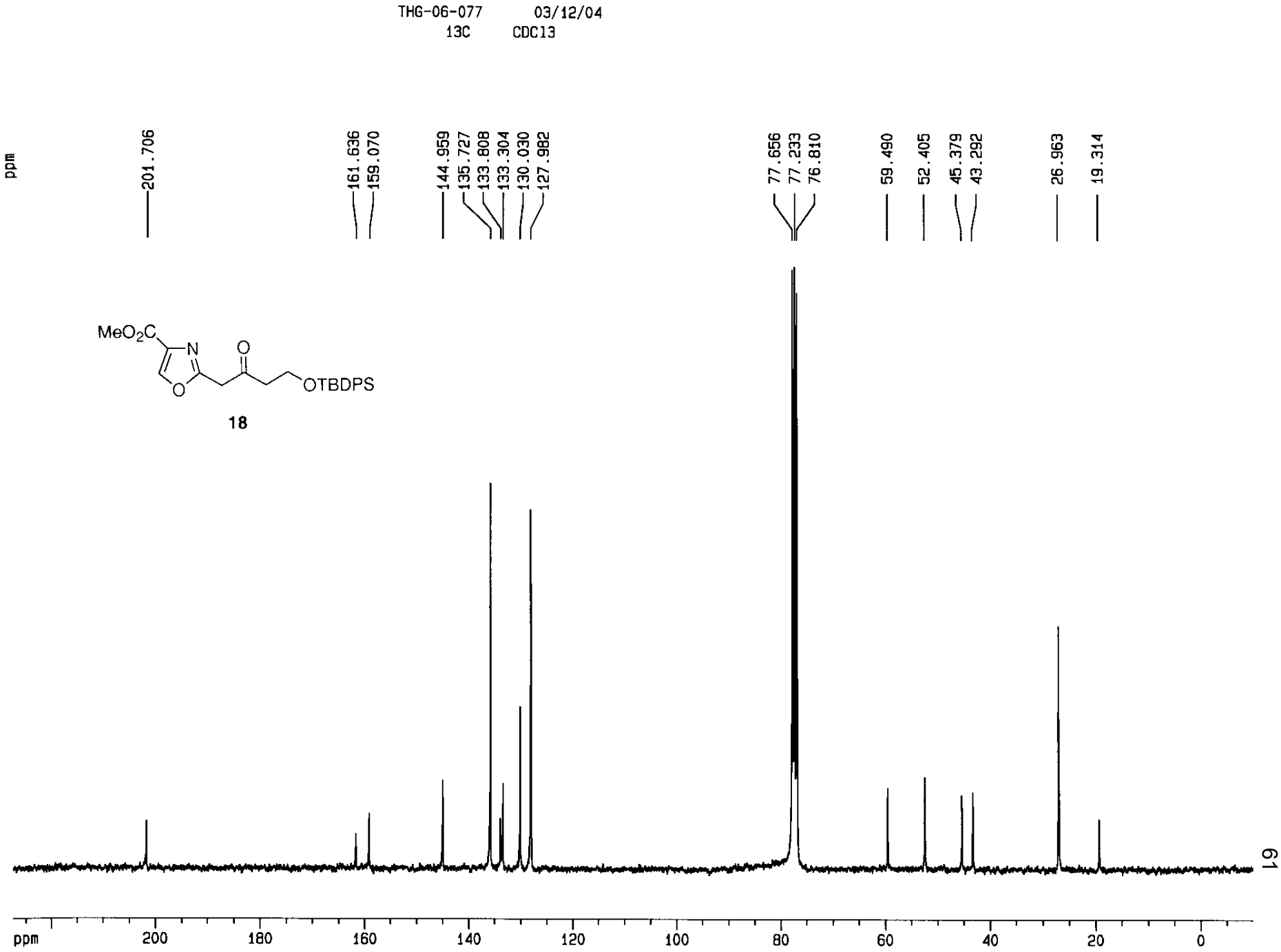
1H CDCl3



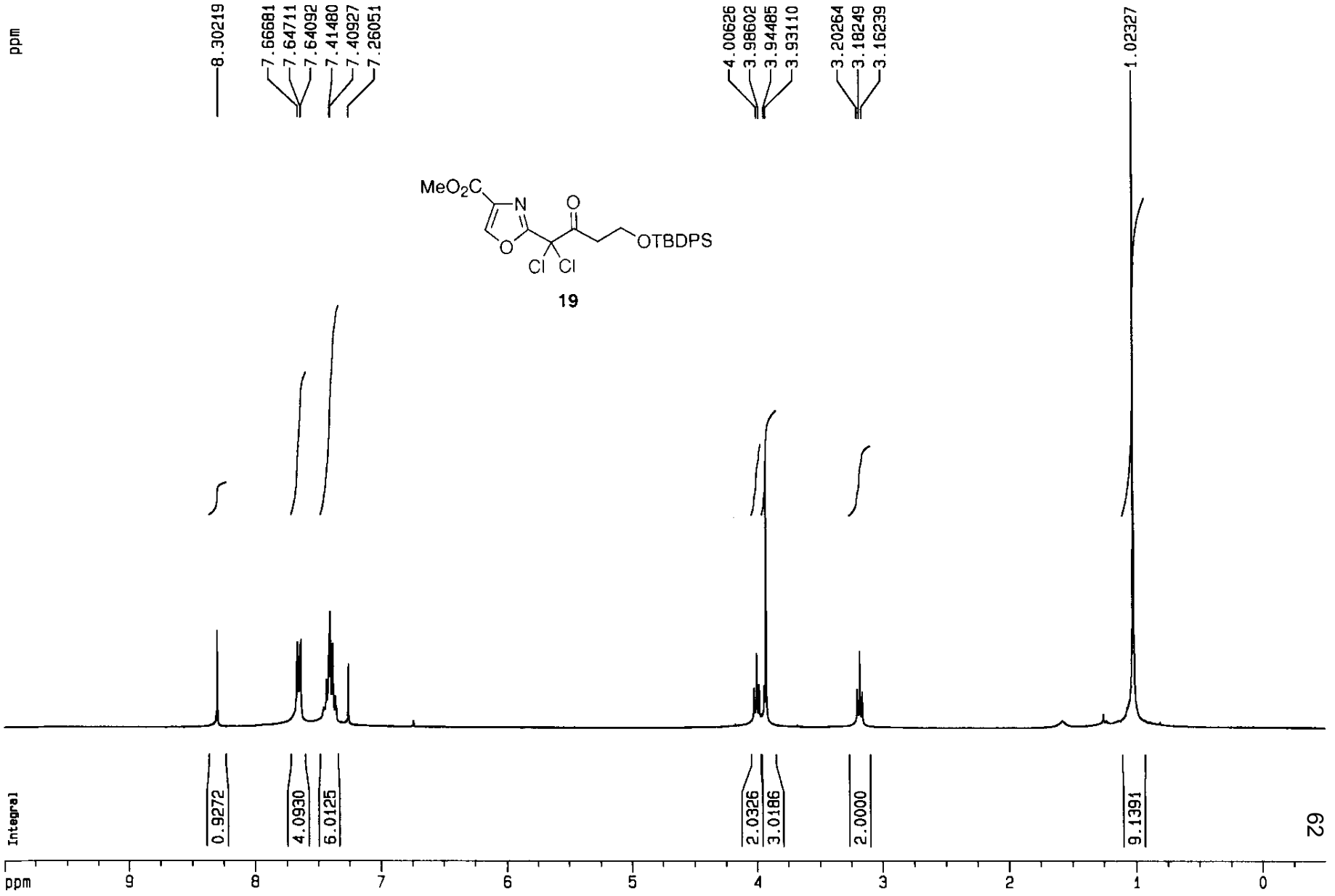
17

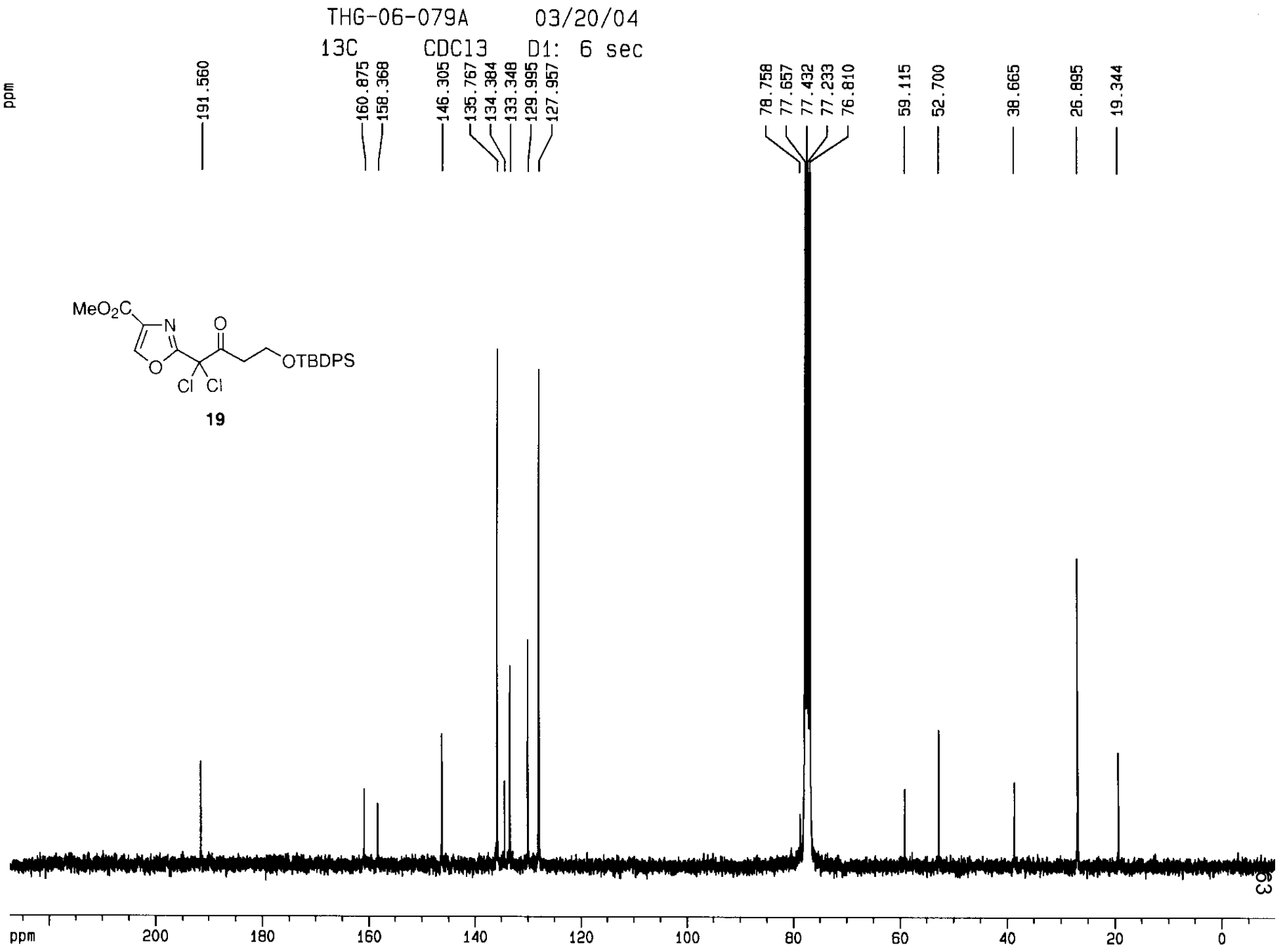

THG-05-176 09/07/03
13C CDCl3 D1: 4 sec
ppm
162.204
161.772
144.165
135.722
133.644
133.341
129.766
127.785
77.650
77.226
76.803
66.535
62.261
52.225
44.478
43.189
39.911
26.940
19.214
MeO2C
N
S
S
O
OTBDPS
17
69
ppm
200
180
160
140
120
100
80
60
40
20
0


THG-06-077 03/12/04
1H CDCl3
ppm
8.21336
7.65980
7.65477
7.63478
7.62885
7.43608
7.42570
7.42018
7.41471
7.40846
7.38388
7.36427
7.25982
4.03231
3.96704
3.94688
3.92658
3.91708
2.74781
2.72769
2.70744
1.02976
MeO2C
N
O
O
OTBDPS
18
Integral
0.8905
4.0629
6.3307
2.1048
5.0819
2.0000
9.0951
ppm
9
8
7
6
5
4
3
2
1
0
09


THG-06-077 03/12/04
13C CDCl3
ppm
201.706
161.636
159.070
144.959
135.727
133.808
133.304
130.030
127.982
77.656
77.233
76.810
59.490
52.405
45.379
43.292
26.963
19.314
MeO2C
N
O
O
OTBDPS
18
ppm
200
180
160
140
120
100
80
60
40
20
0

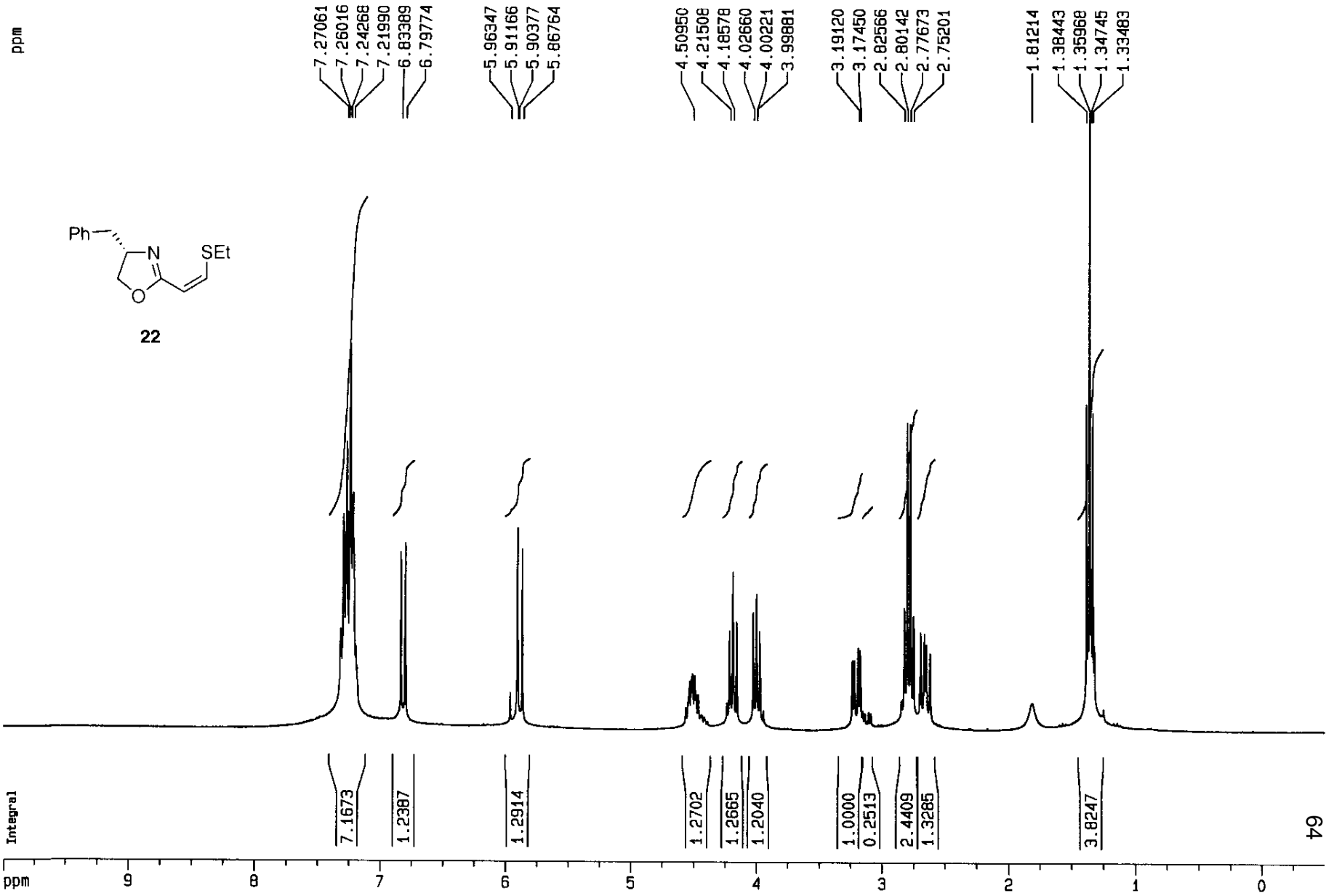
THG-06-079A 03/20/04
1H CDC13

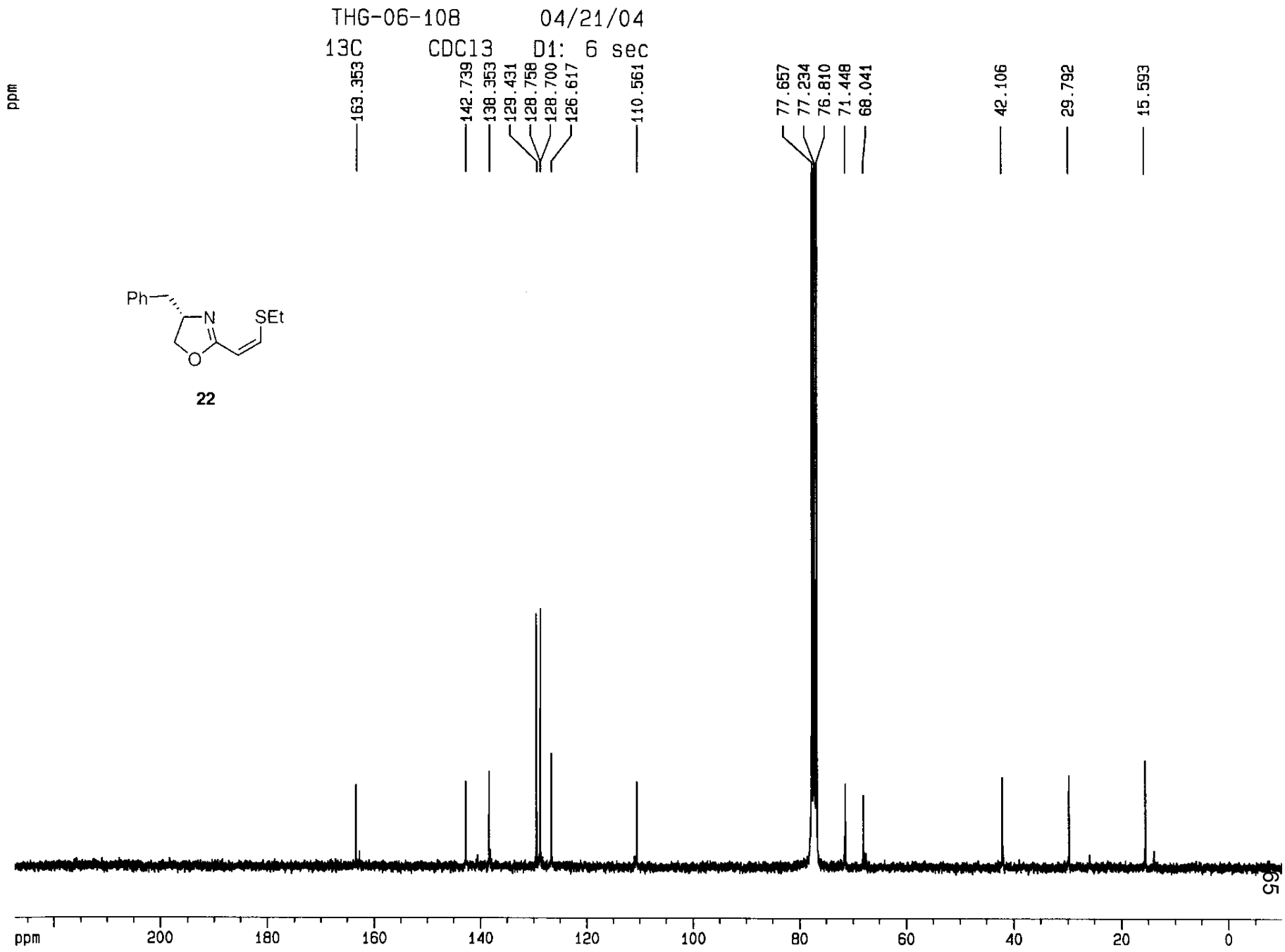



THG-06-079A 03/20/04
13C CDCl3 D1: 6 sec
ppm
191.560
160.875
158.368
146.305
135.767
134.384
133.348
129.995
127.957
78.758
77.657
77.432
77.233
76.810
59.115
52.700
38.665
26.895
19.344
MeO2C
N
O
O
OTBDPS
Cl Cl
19
ppm
200
180
160
140
120
100
80
60
40
20
0

THG-06-108 04/21/04

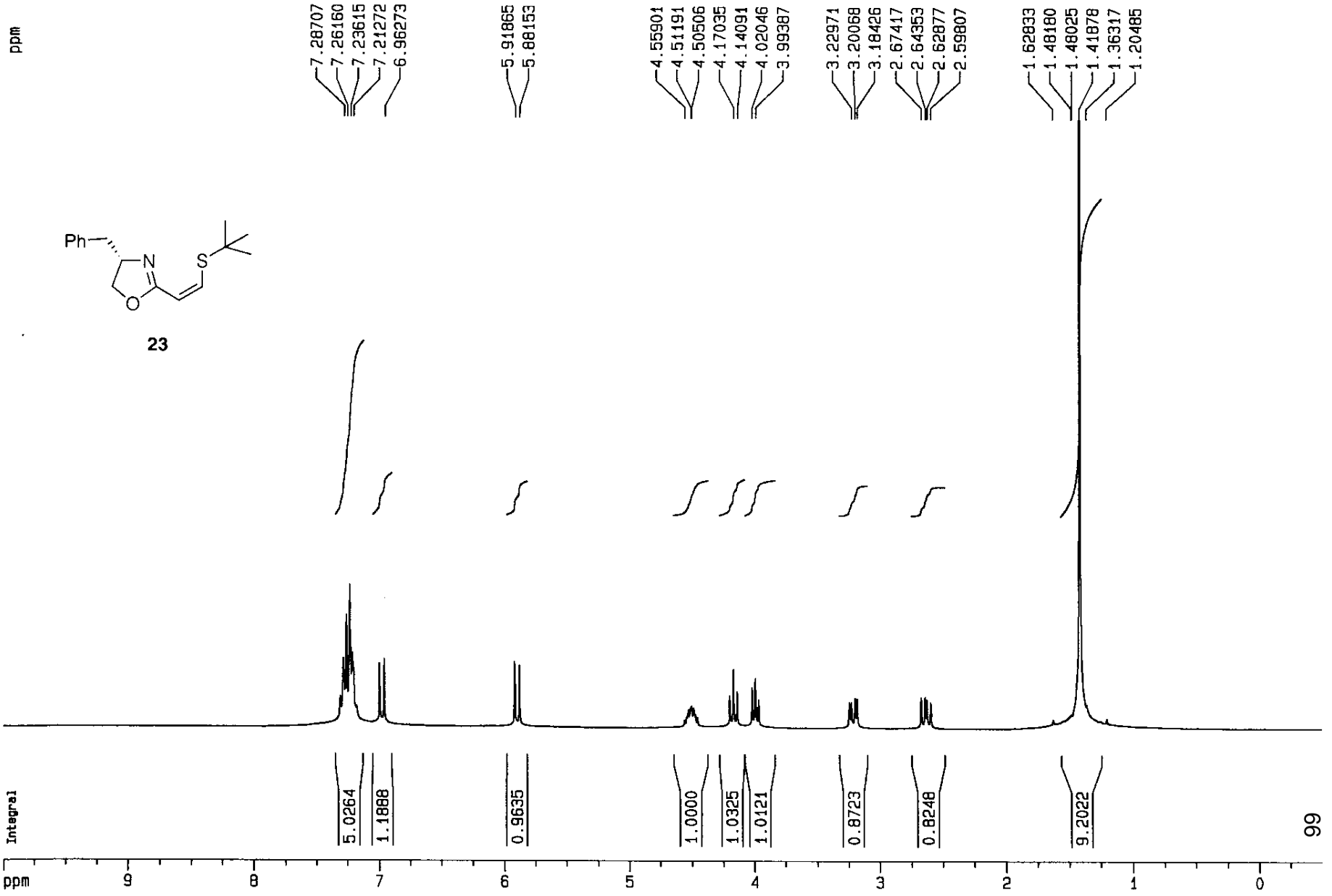
1H CDCl3

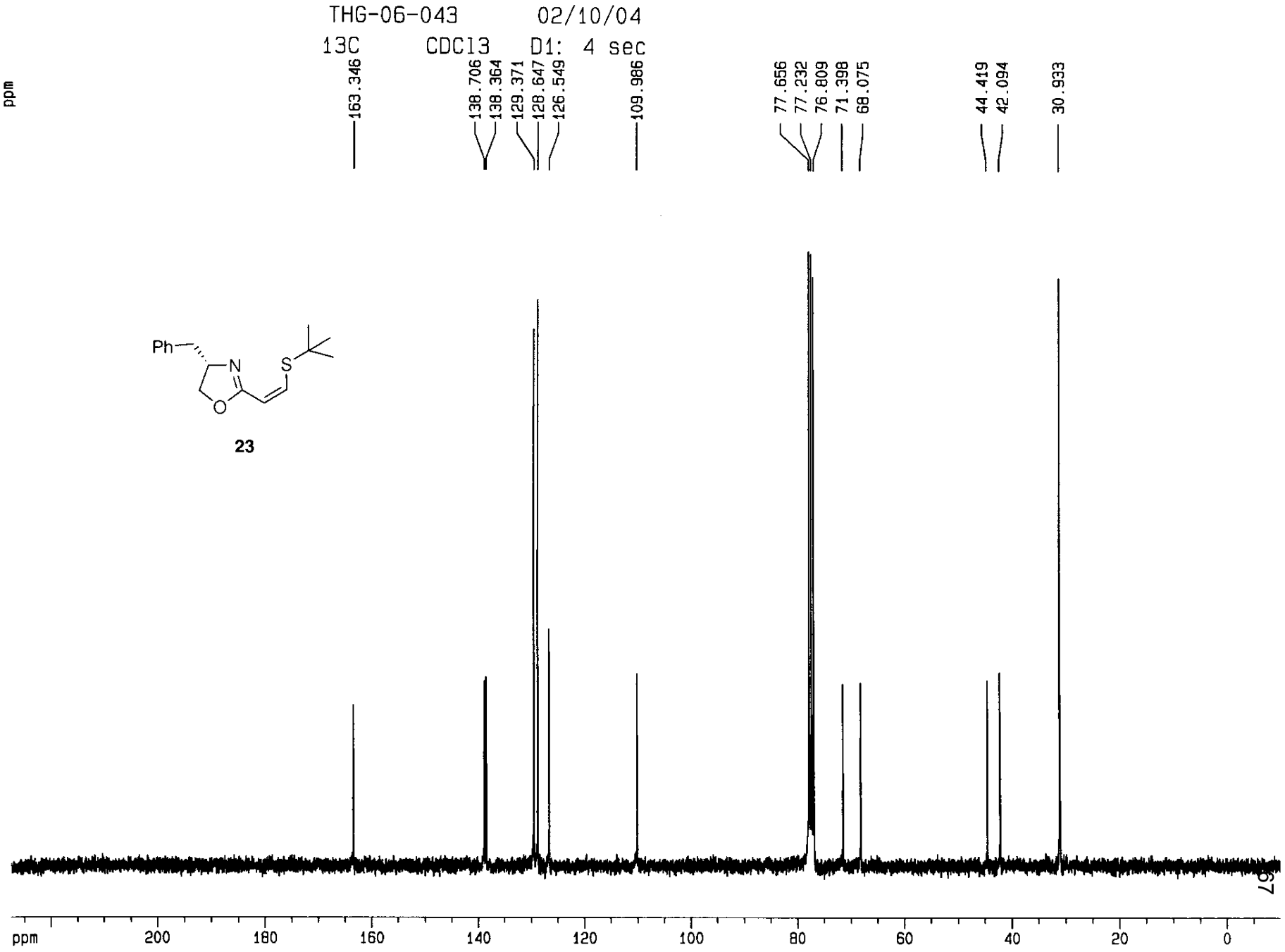


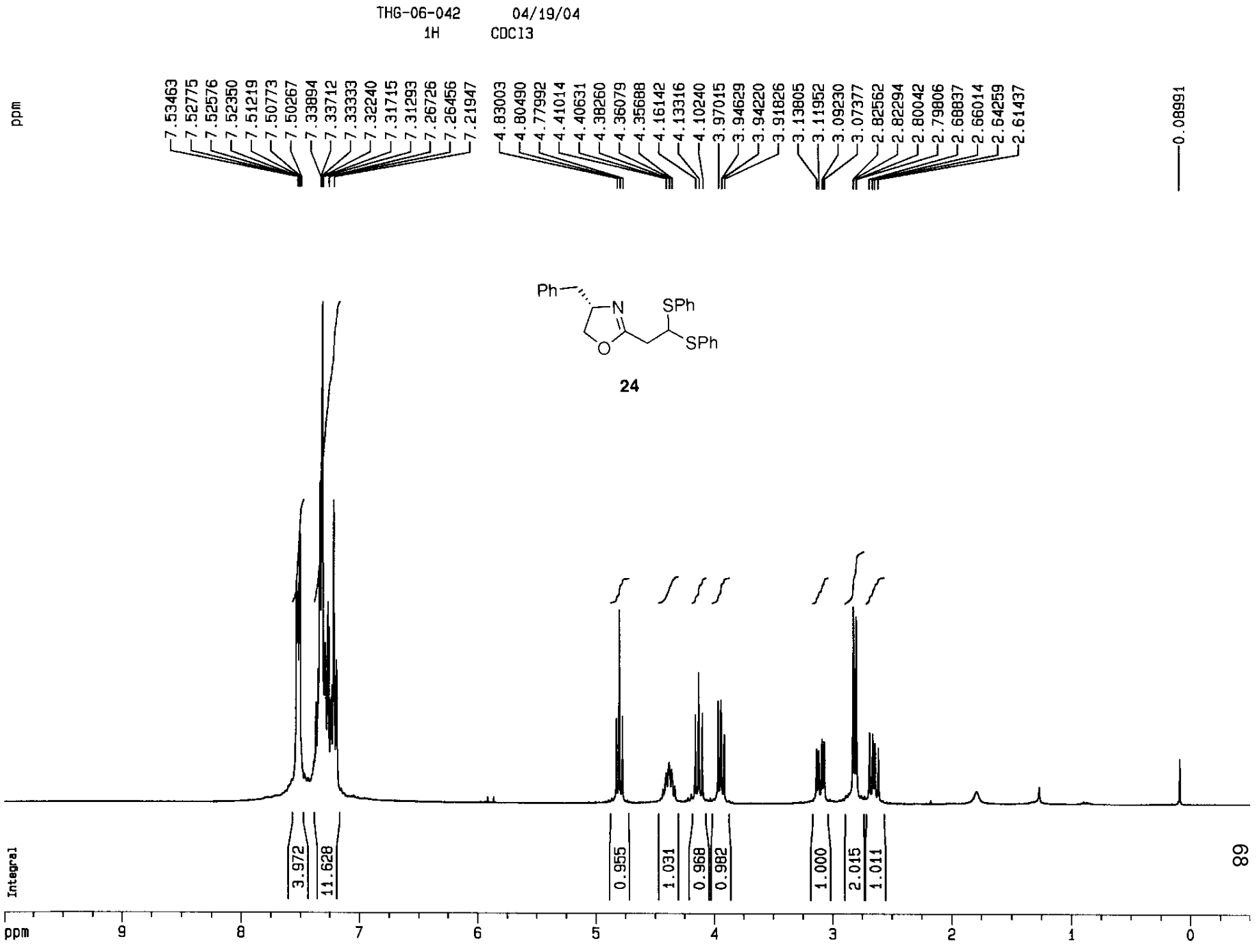

THG-06-108 04/21/04
13C CDCl3 D1: 6 sec
ppm
163.353
142.739
138.353
129.431
128.758
128.700
126.617
110.561
77.657
77.234
76.810
71.448
68.041
42.106
29.792
15.593
Ph
N
SEt
O
22
ppm
200
180
160
140
120
100
80
60
40
20
0

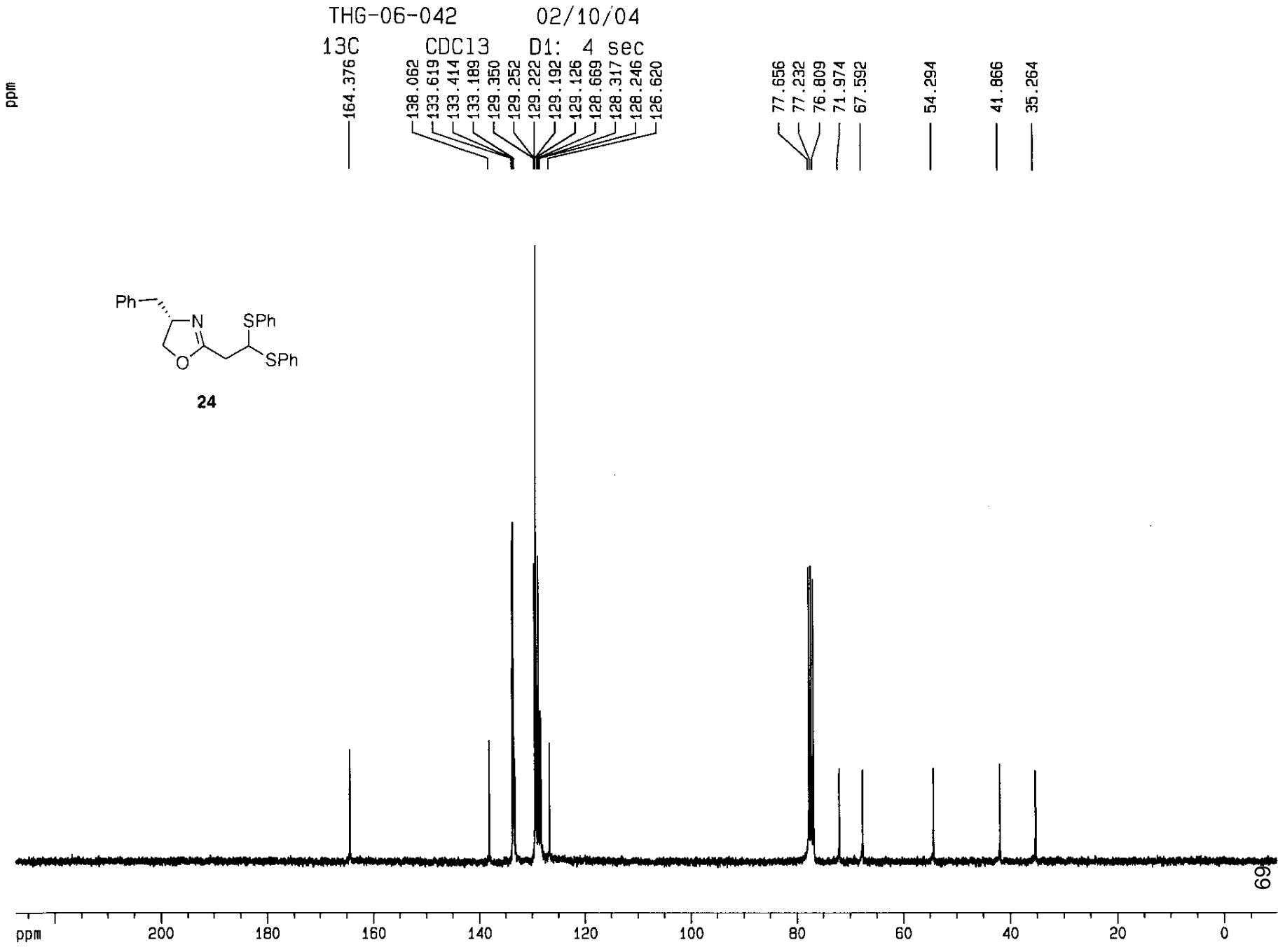
THG-06-043 02/10/04

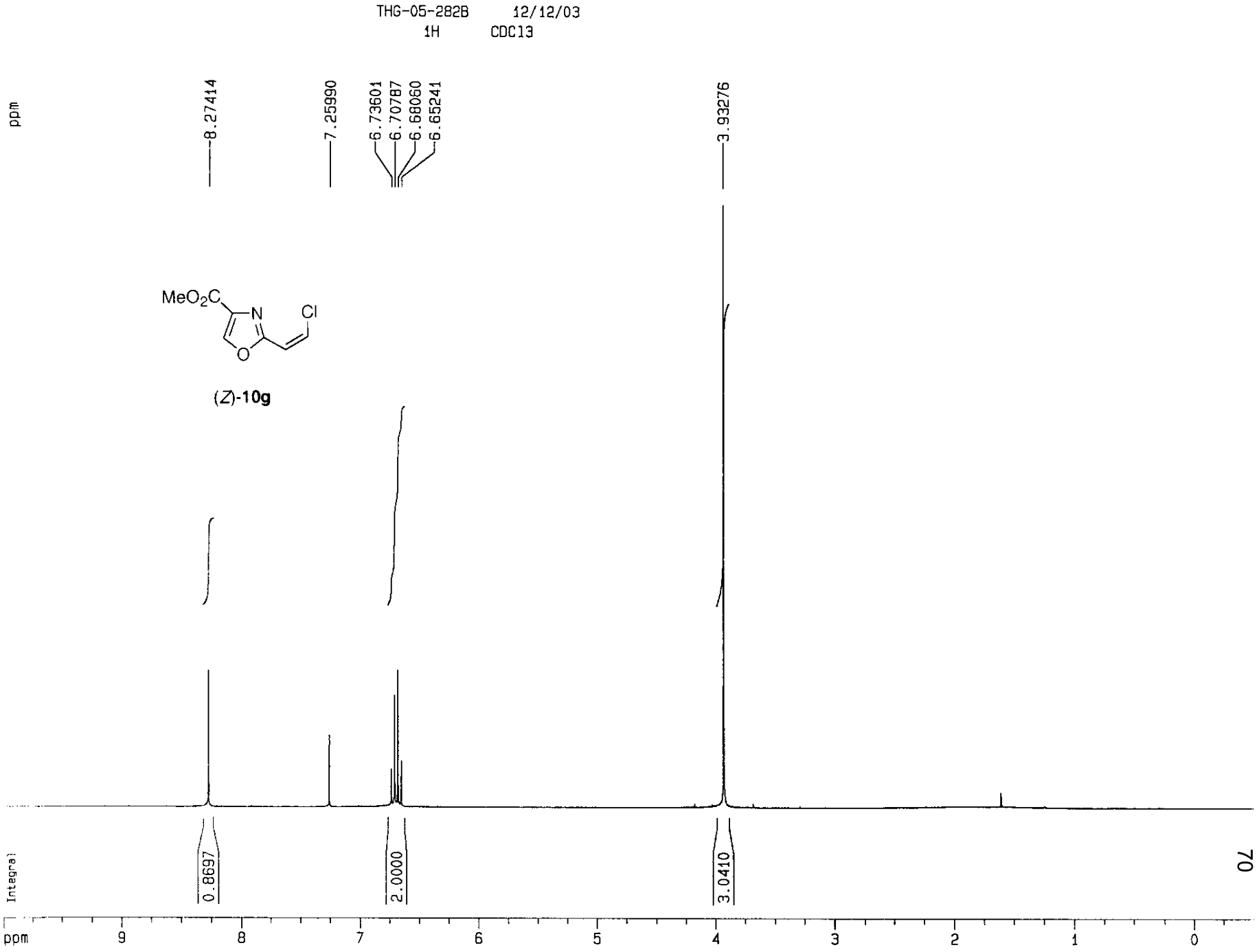
1H CDC13

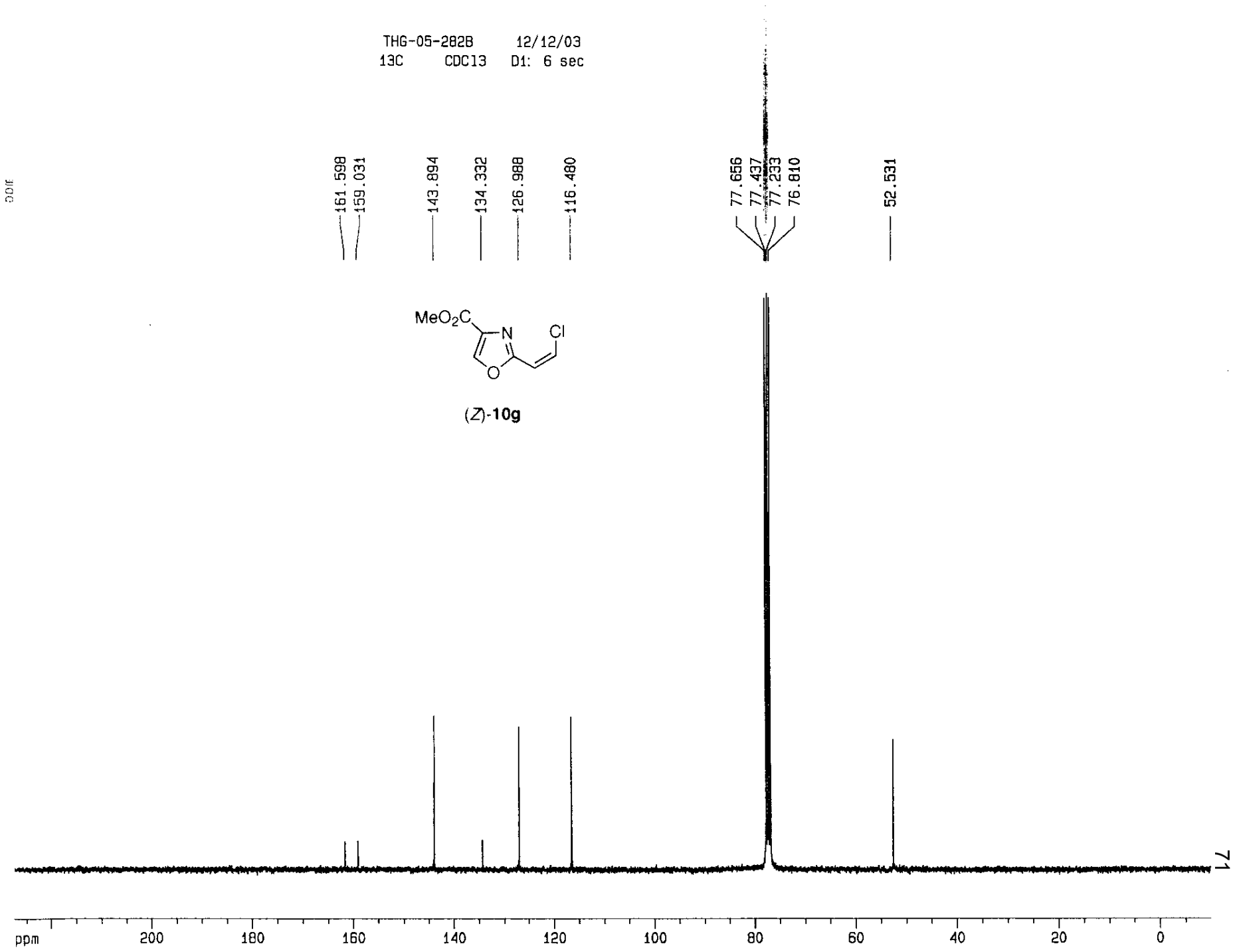


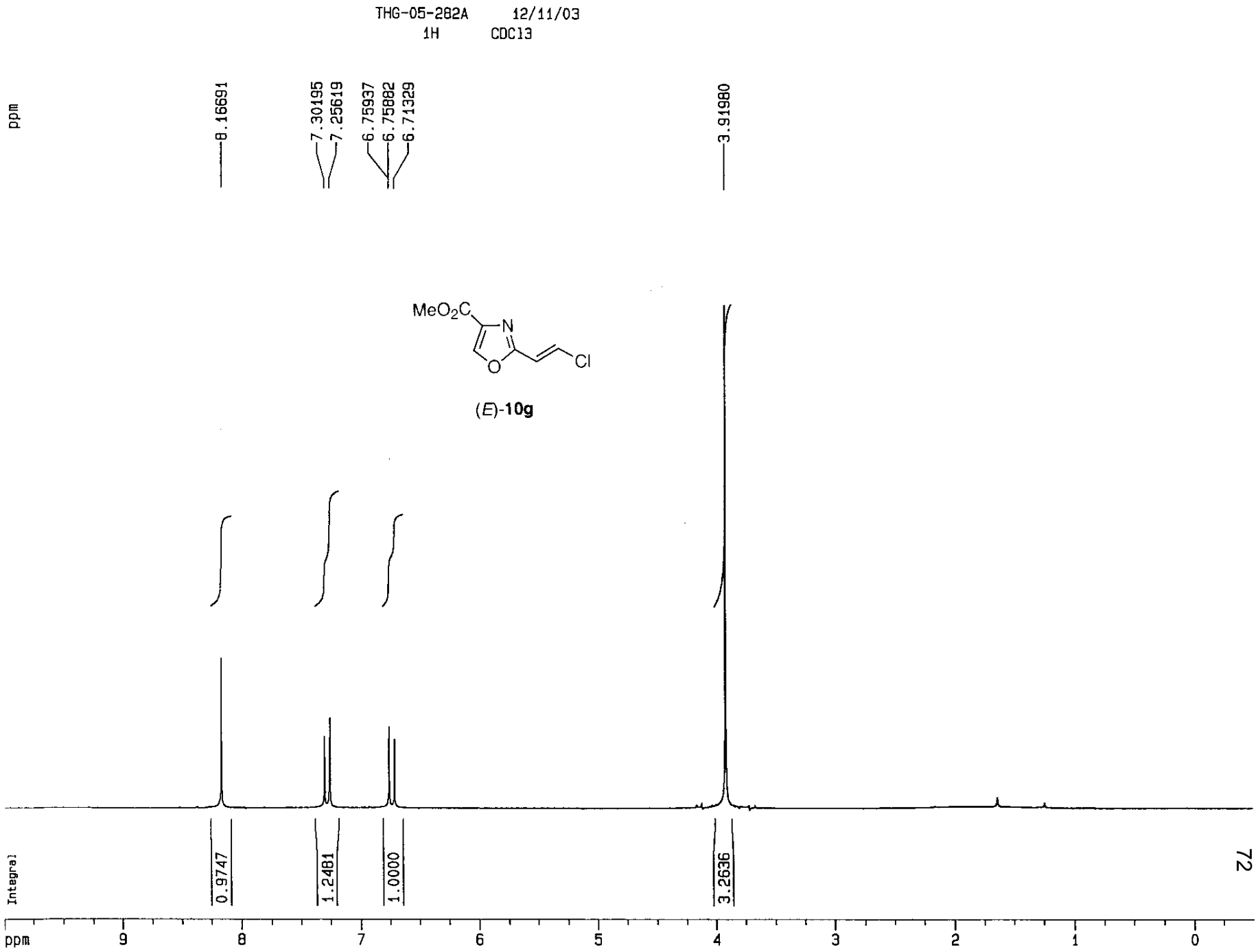

THG-06-043 02/10/04
13C CDCl3 D1: 4 sec
ppm
163.346
138.706
138.364
129.371
128.647
126.549
109.986
77.656
77.232
76.809
71.398
68.075
44.419
42.094
30.933
Ph
N
S
O
23
67
ppm
200
180
160
140
120
100
80
60
40
20
0

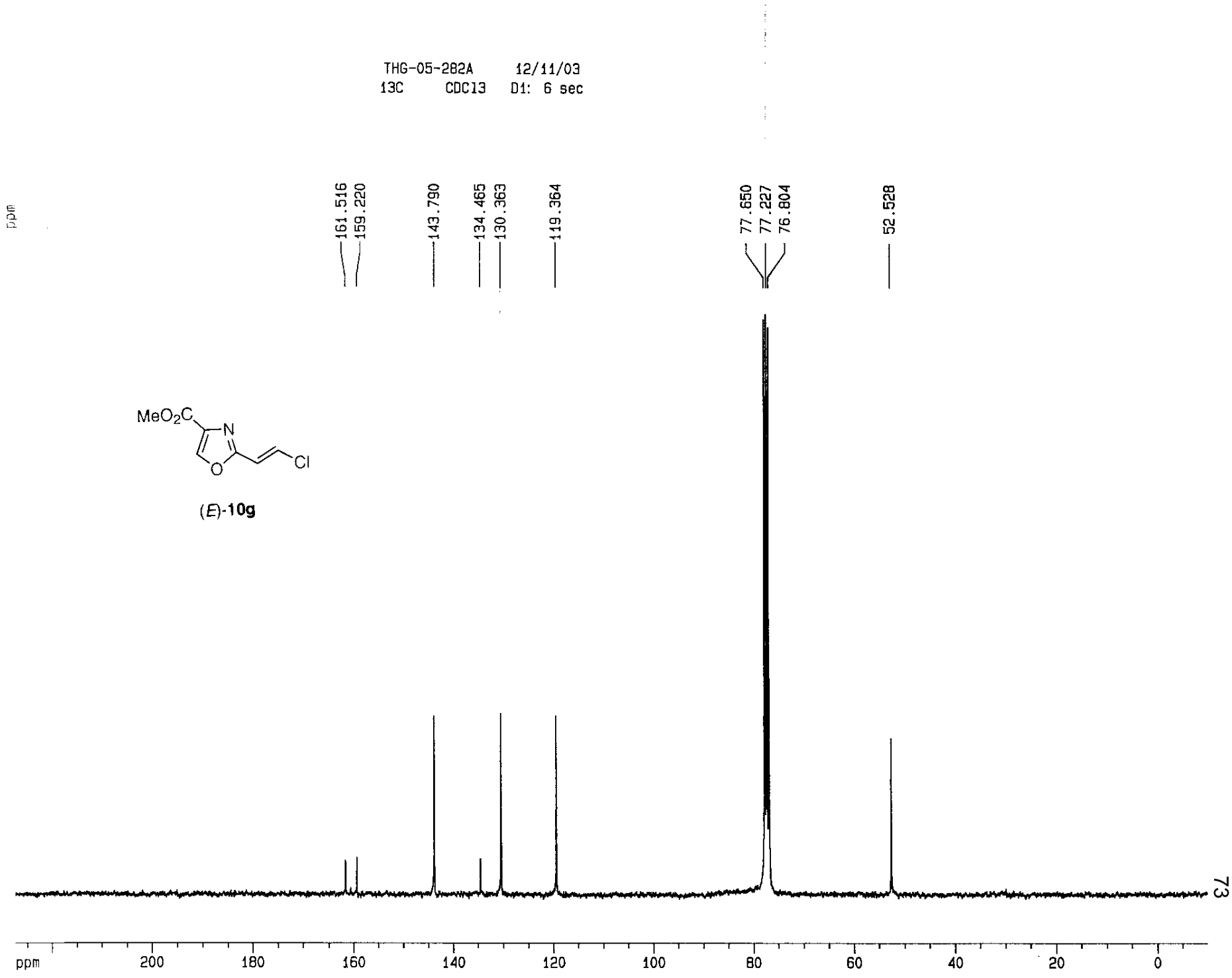

THG-06-042 04/19/04
1H CDCl3
ppm
7.53463
7.52775
7.52576
7.52350
7.51219
7.50773
7.50267
7.33894
7.33712
7.33333
7.32240
7.31715
7.31293
7.26726
7.26456
7.21947
4.83003
4.80490
4.77992
4.41014
4.40631
4.38260
4.36079
4.35688
4.16142
4.13316
4.10240
3.97015
3.94629
3.94220
3.91826
3.13805
3.11952
3.09230
3.07377
2.82562
2.82294
2.80042
2.79806
2.68837
2.66014
2.64259
2.61437
0.08991
Ph
N
SPh
SPh
O
24
Integral
3.972
11.628
0.955
1.031
0.968
0.982
1.000
2.015
1.011
ppm
9
8
7
6
5
4
3
2
1
0


THG-06-042 02/10/04
13C CDCl3 D1: 4 sec
ppm
164.376
138.062
133.619
133.414
133.189
129.350
129.252
129.222
129.192
129.126
128.669
128.317
128.246
126.620
77.656
77.232
76.809
71.974
67.592
54.294
41.866
35.264
Ph
N
SPh
SPh
O
24
69
ppm
200
180
160
140
120
100
80
60
40
20
0

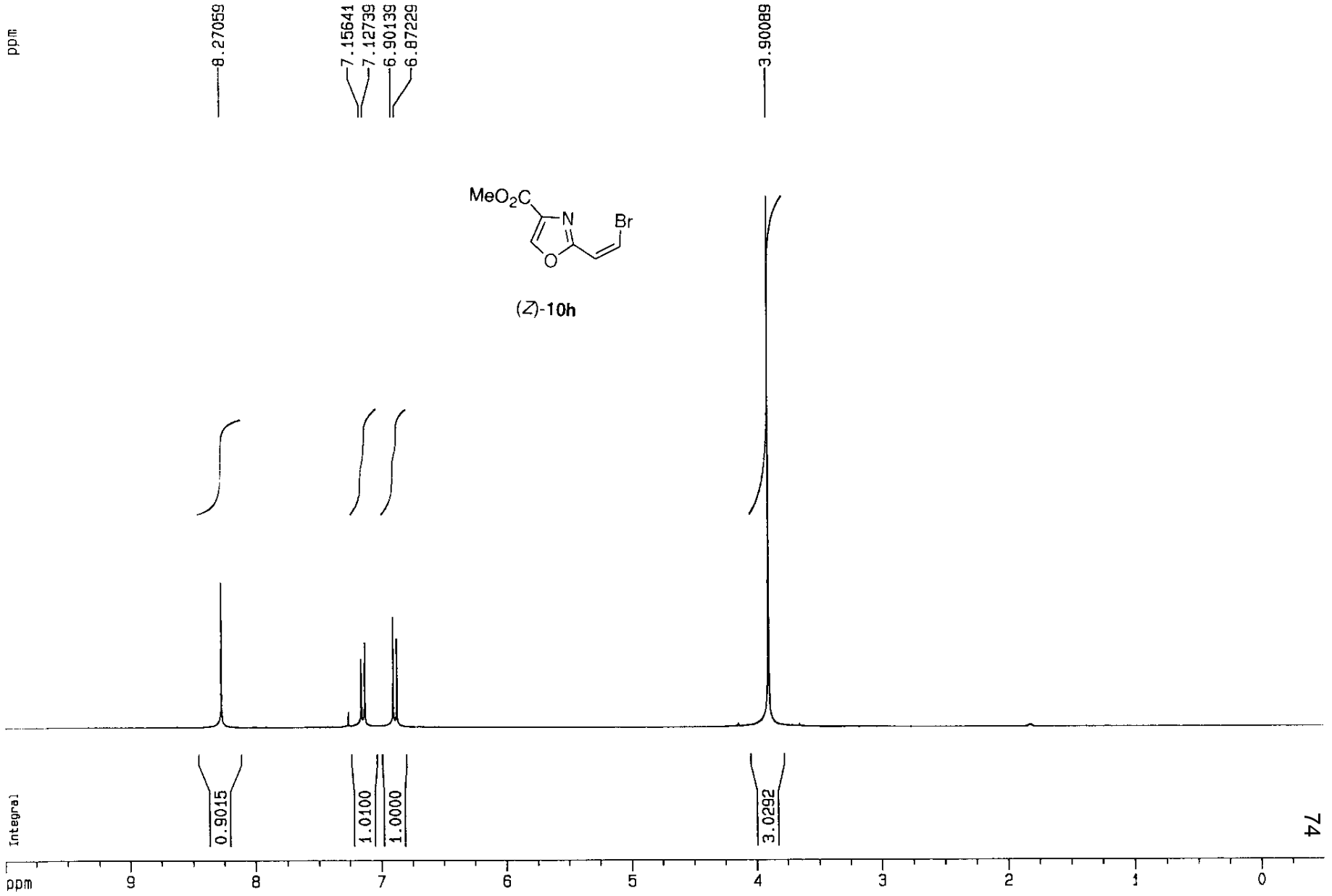

THG-05-282B 12/12/03
1H CDCl3
ppm
8.27414
7.25990
6.73601
6.70787
6.68060
6.65241
3.93276
MeO2C
N
Cl
O
(Z)-10g
Integral
0.8697
2.0000
3.0410
ppm
9
8
7
6
5
4
3
2
1
0
70

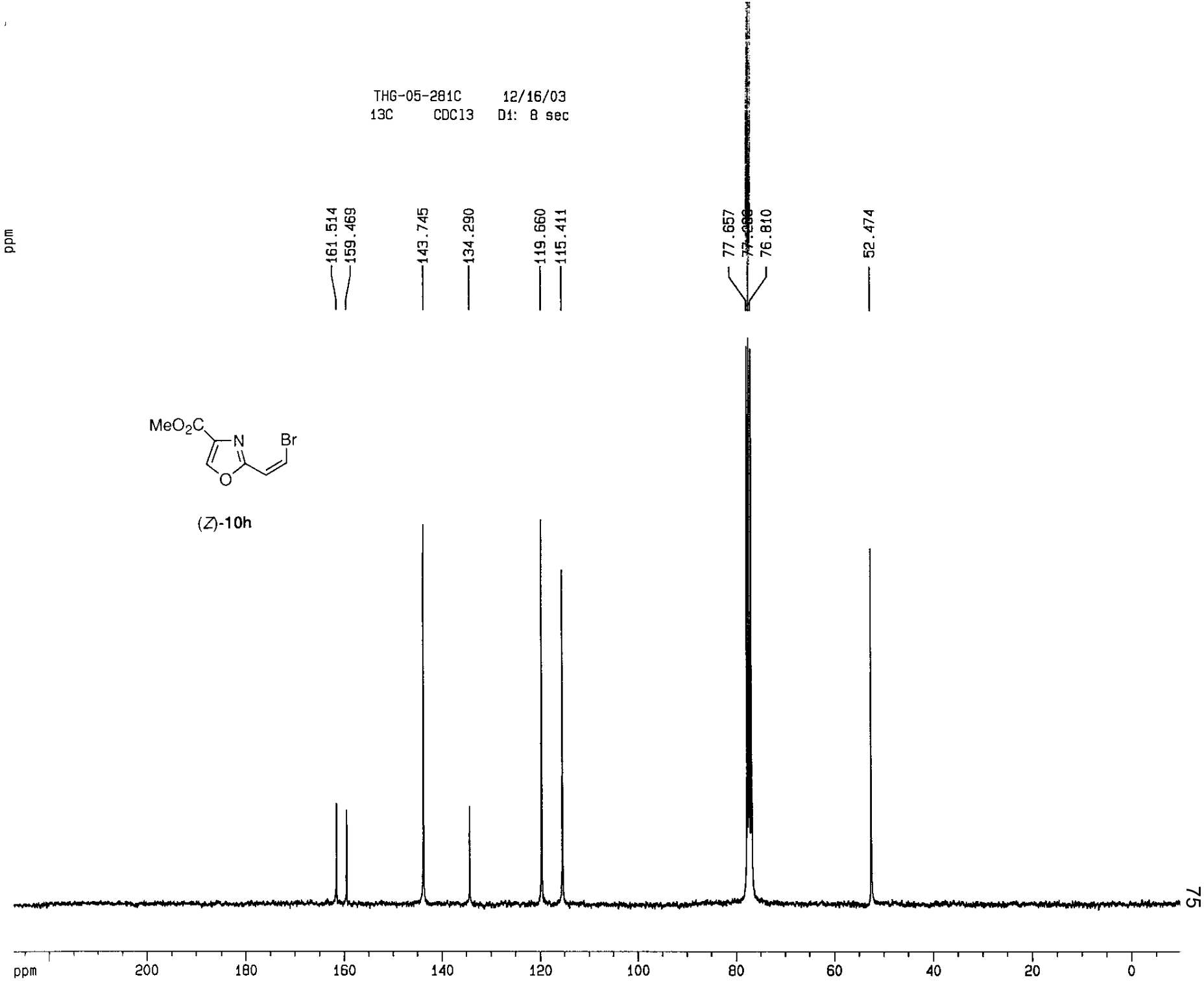

THG-05-282B 12/12/03
13C CDCl3 D1: 6 sec
161.598
159.031
143.894
134.332
126.988
116.480
77.656
77.437
77.233
76.810
52.531
MeO2C
N
Cl
O
(Z)-10g
ppm
200
180
160
140
120
100
80
60
40
20
0

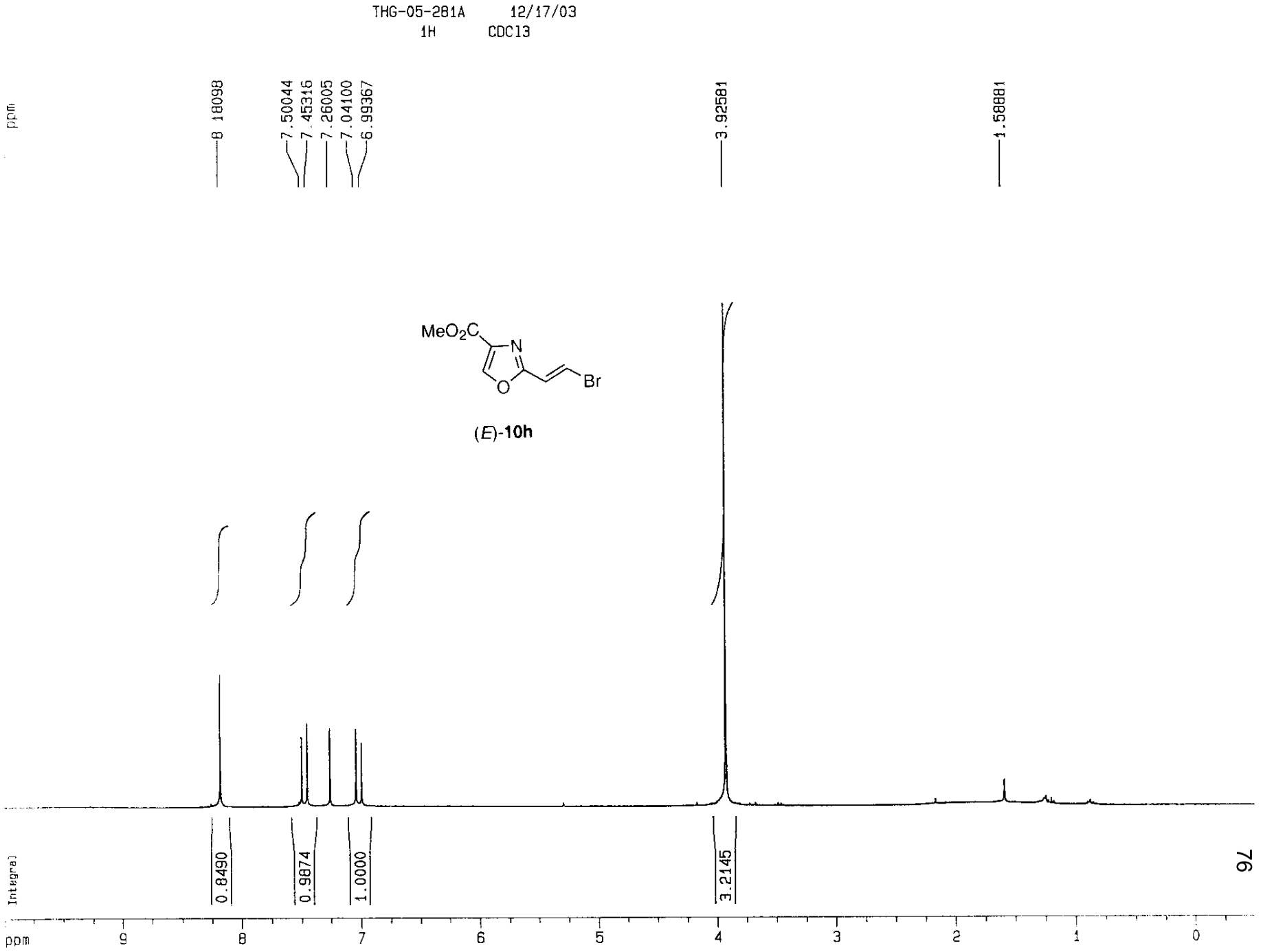

THG-05-282A 12/11/03
1H CDCl3
ppm
8.16691
7.30195
7.25619
6.75937
6.75882
6.71329
3.91980
MeO2C
N
O
Cl
(E)-10g
Integral
0.9747
1.2481
1.0000
3.2636
ppm
9
8
7
6
5
4
3
2
1
0

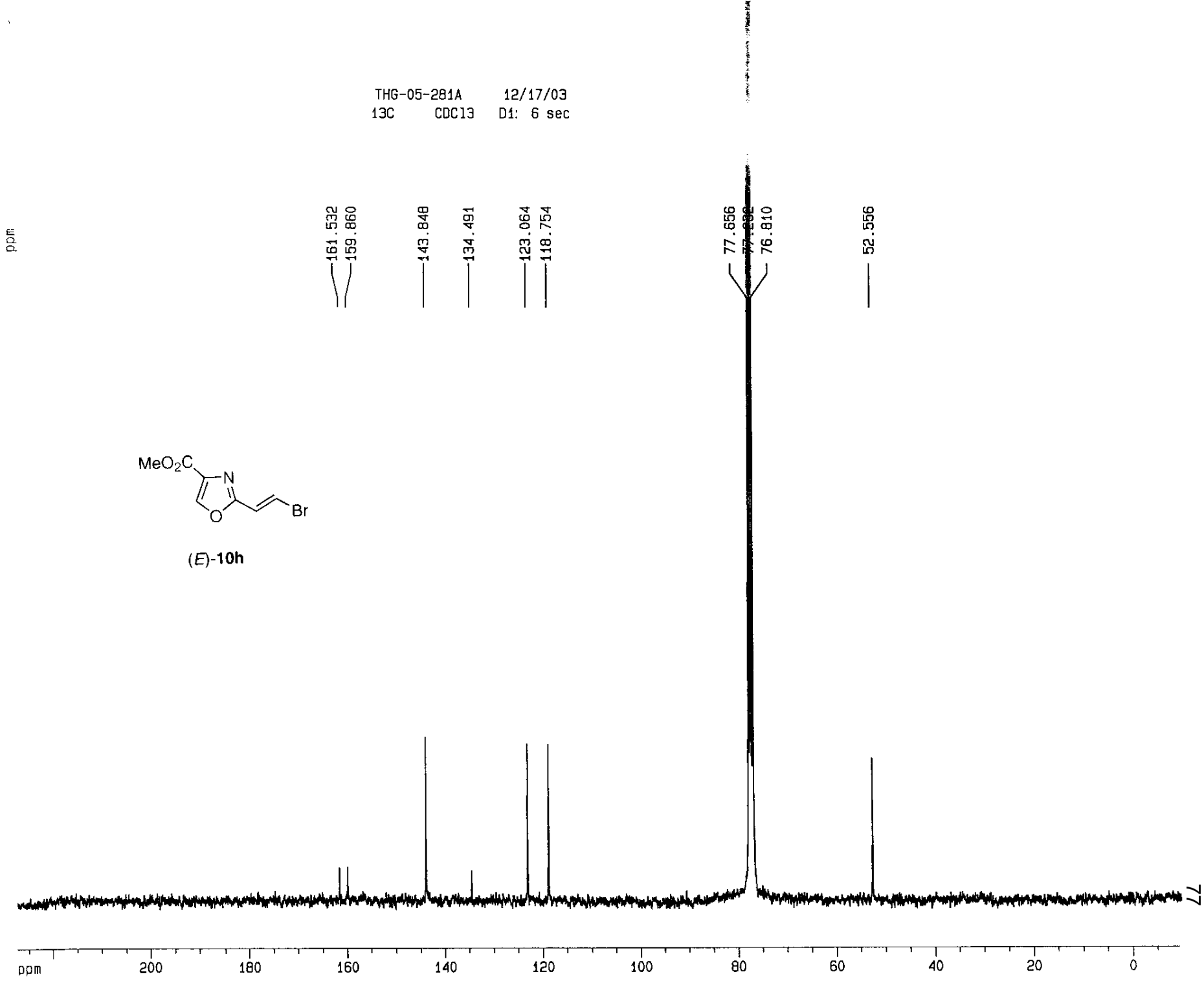

THG-05-282A 12/11/03
13C CDCl3 D1: 6 sec
ppm
161.516
159.220
143.790
134.465
130.363
119.364
77.650
77.227
76.804
52.528
MeO2C
N
O
Cl
(E)-10g
ppm
200
180
160
140
120
100
80
60
40
20
0

THG-05-281C 12/17/03
1H CDCl3



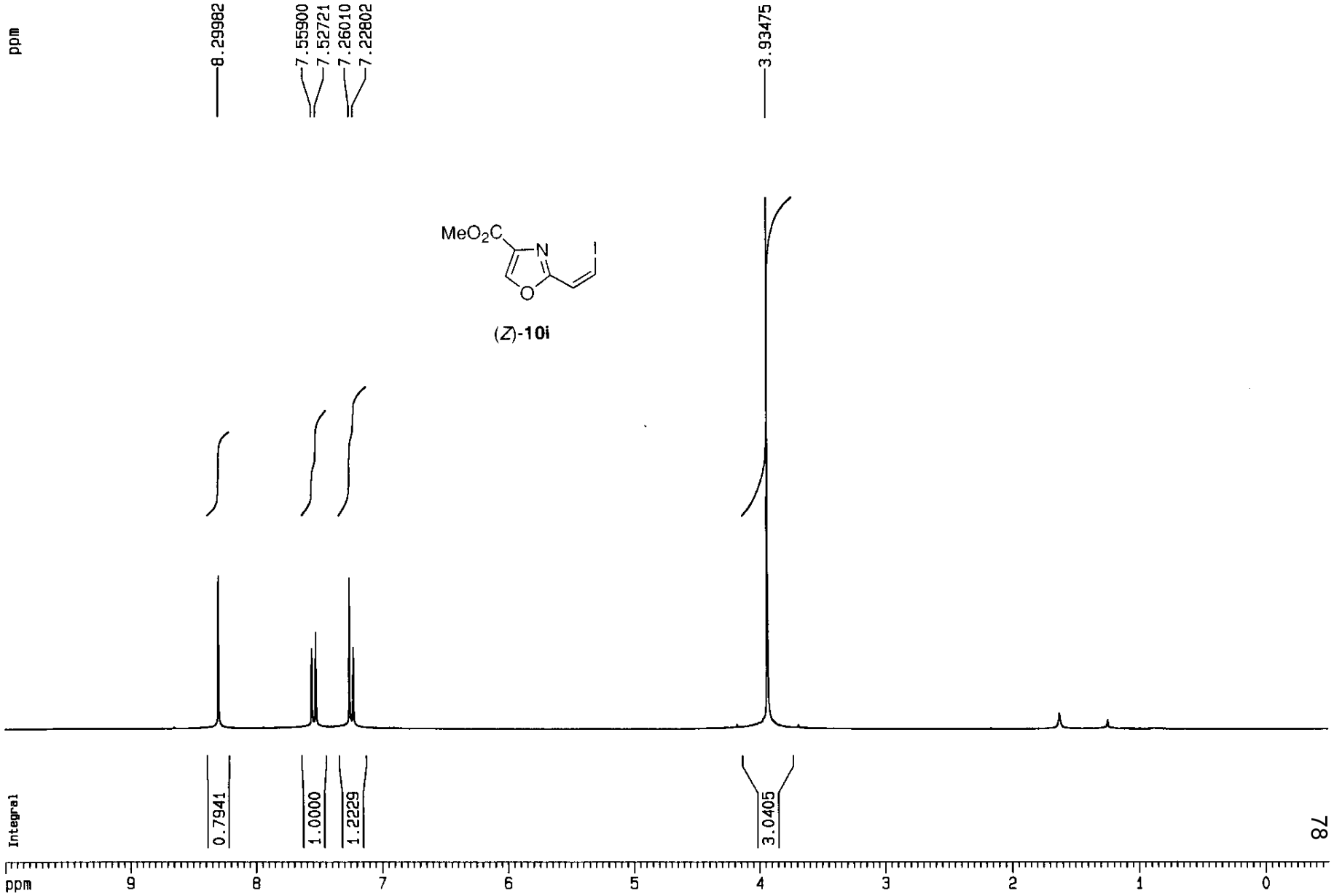

THG-05-281C 12/16/03
13C CDCl3 D1: 8 sec
ppm
161.514
159.469
143.745
134.290
119.660
115.411
77.657
76.810
52.474
MeO2C
N
Br
O
(Z)-10h
ppm
200
180
160
140
120
100
80
60
40
20
0

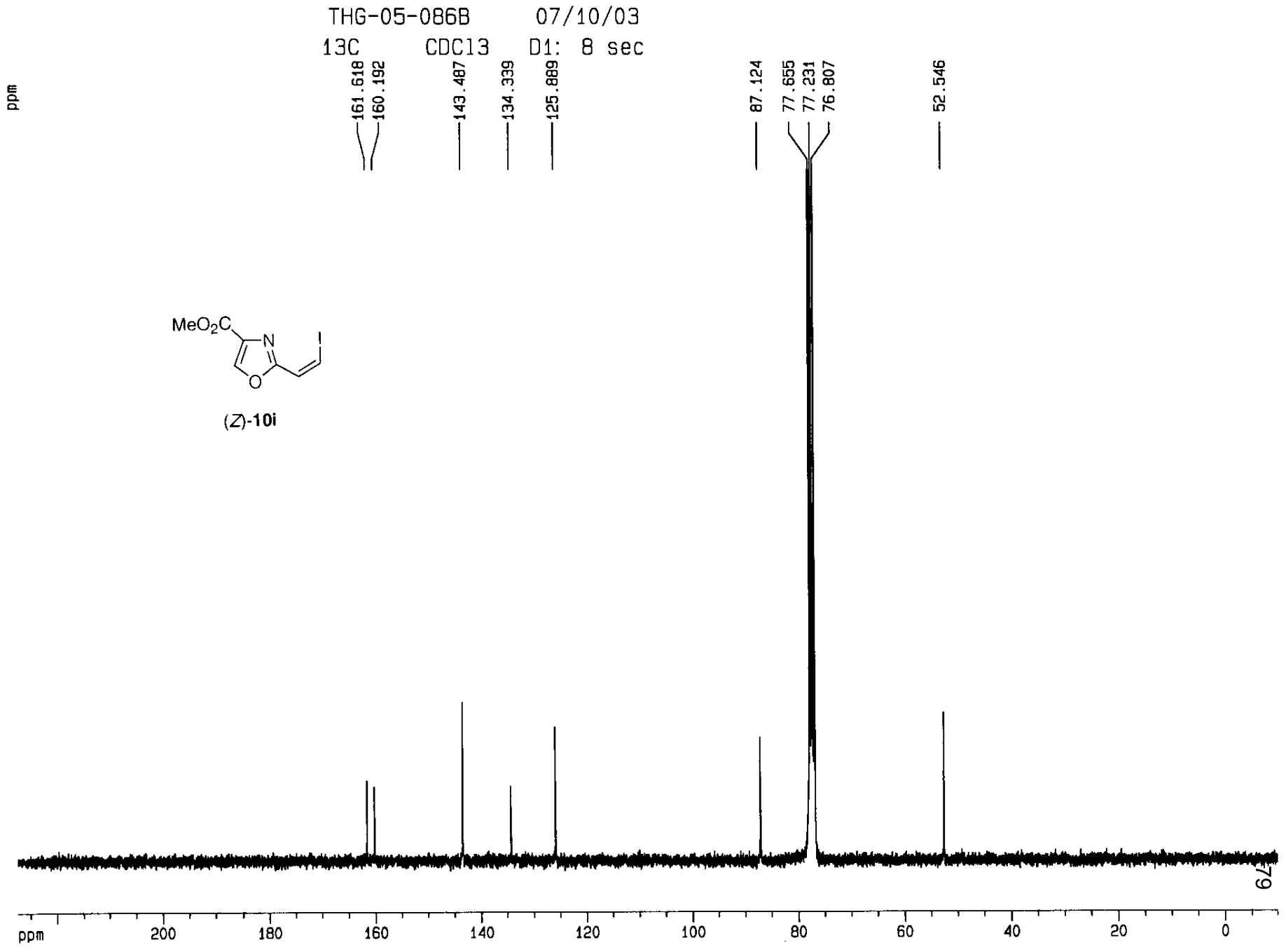

THG-05-281A 12/17/03
1H CDCl3
ppm
8.18098
7.50044
7.45316
7.26005
7.04100
6.99367
3.92581
1.58881
MeO2C
N
O
Br
(E)-10h
Integral
0.8490
0.9874
1.0000
3.2145
ppm
9
8
7
6
5
4
3
2
1
0


THG-05-281A 12/17/03
13C CDCl3 D1: 6 sec
ppm
161.532
159.860
143.848
134.491
123.064
118.754
77.656
76.810
52.556
MeO2C
N
O
Br
(E)-10h
77
ppm
200
180
160
140
120
100
80
60
40
20
0

THG-05-086B 07/10/03

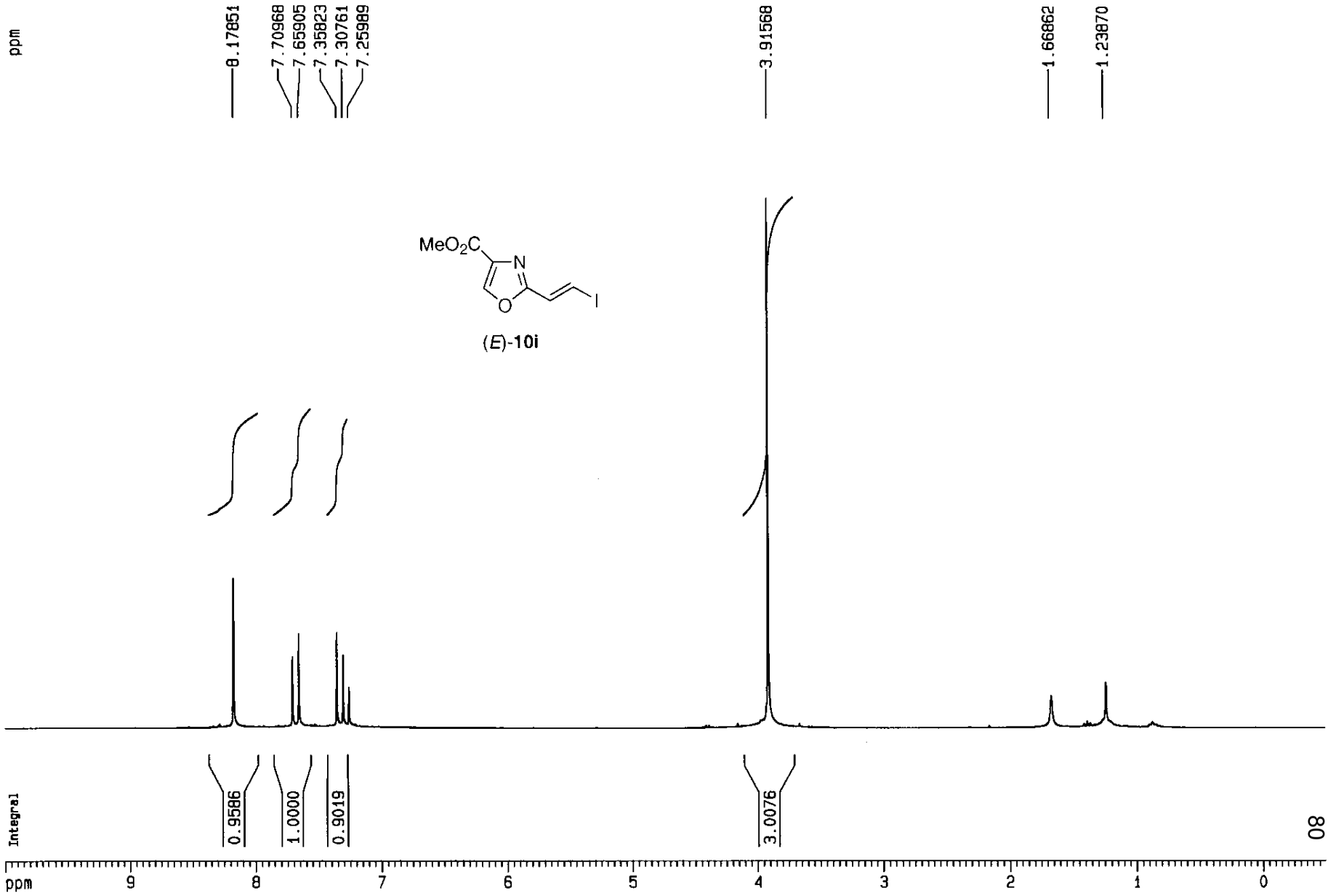
1H CDCl3

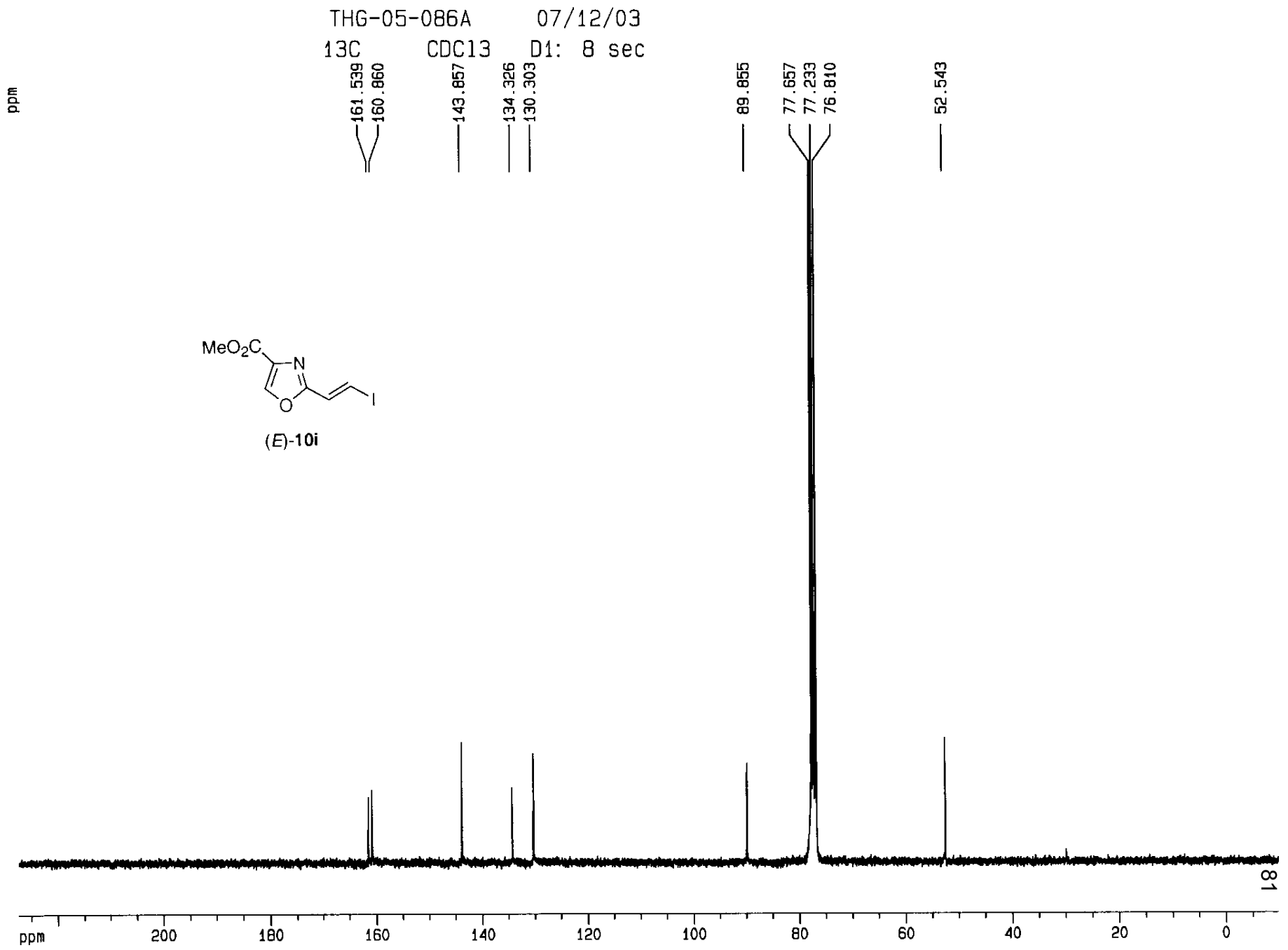



THG-05-086B 07/10/03
13C CDCl3 D1: 8 sec
ppm
161.618
160.192
143.487
134.339
125.889
87.124
77.655
77.231
76.807
52.546
MeO2C
N
O
I
(Z)-10i
79
ppm
200
180
160
140
120
100
80
60
40
20
0

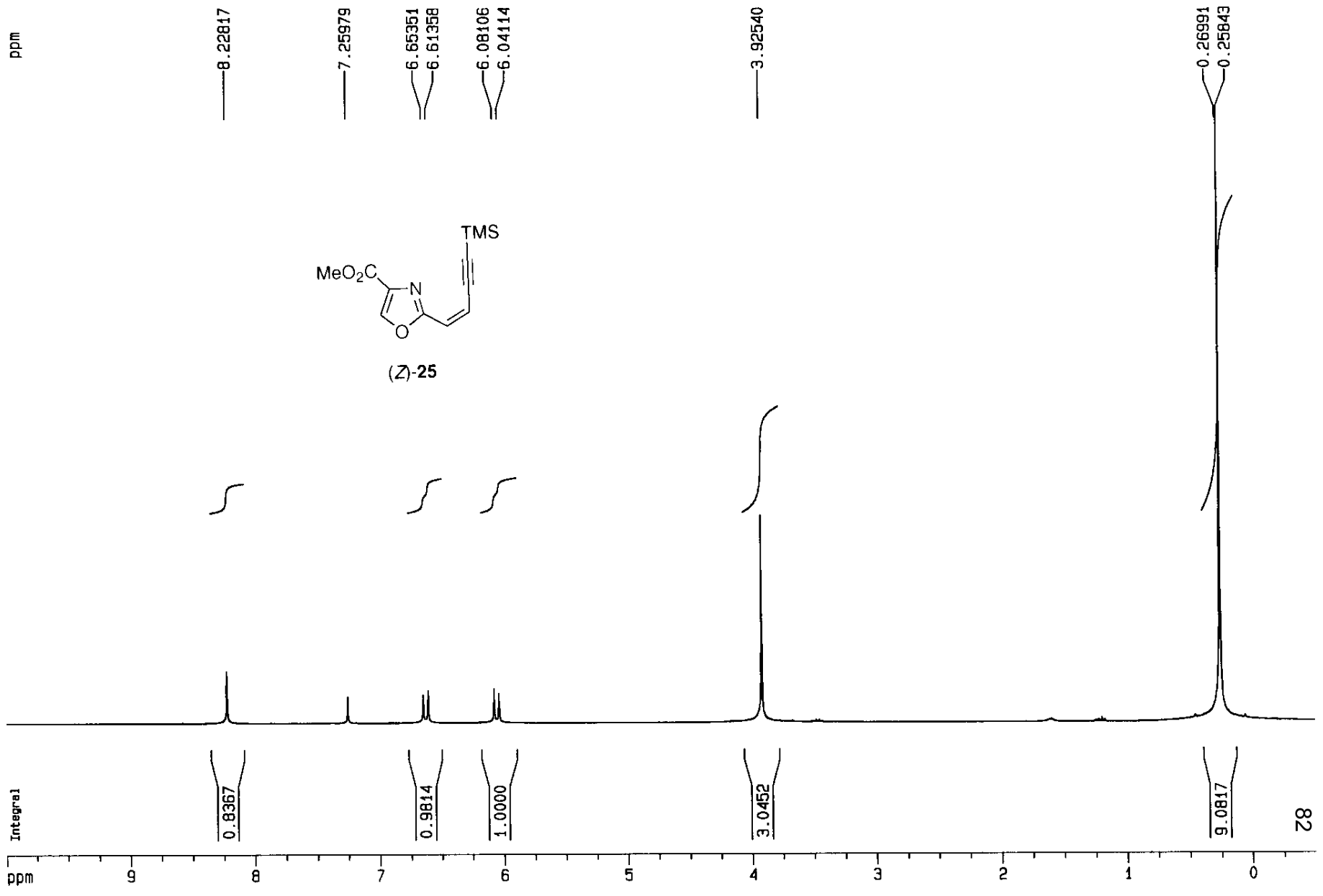
THG-05-086A 07/12/03

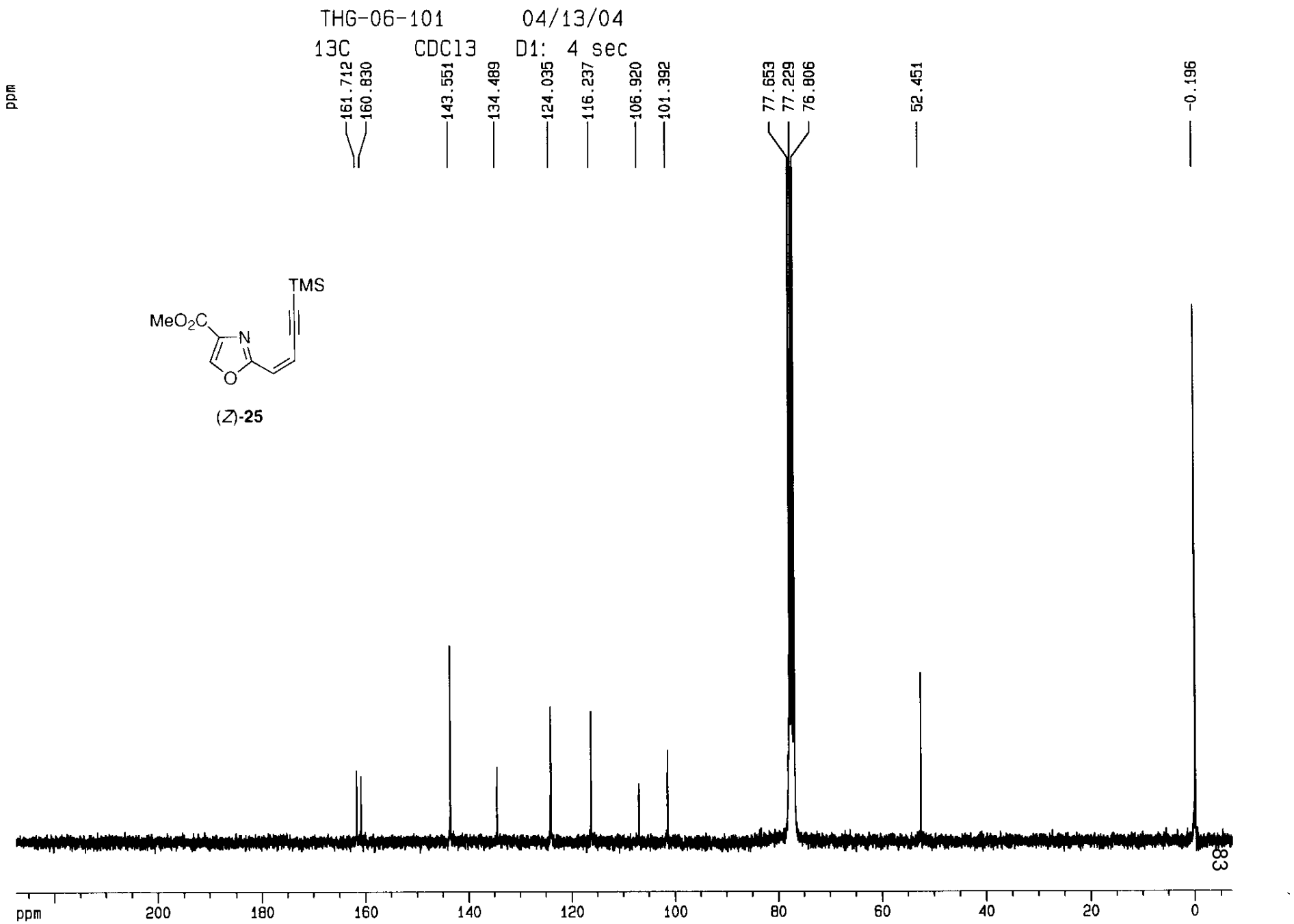
1H CDCl3

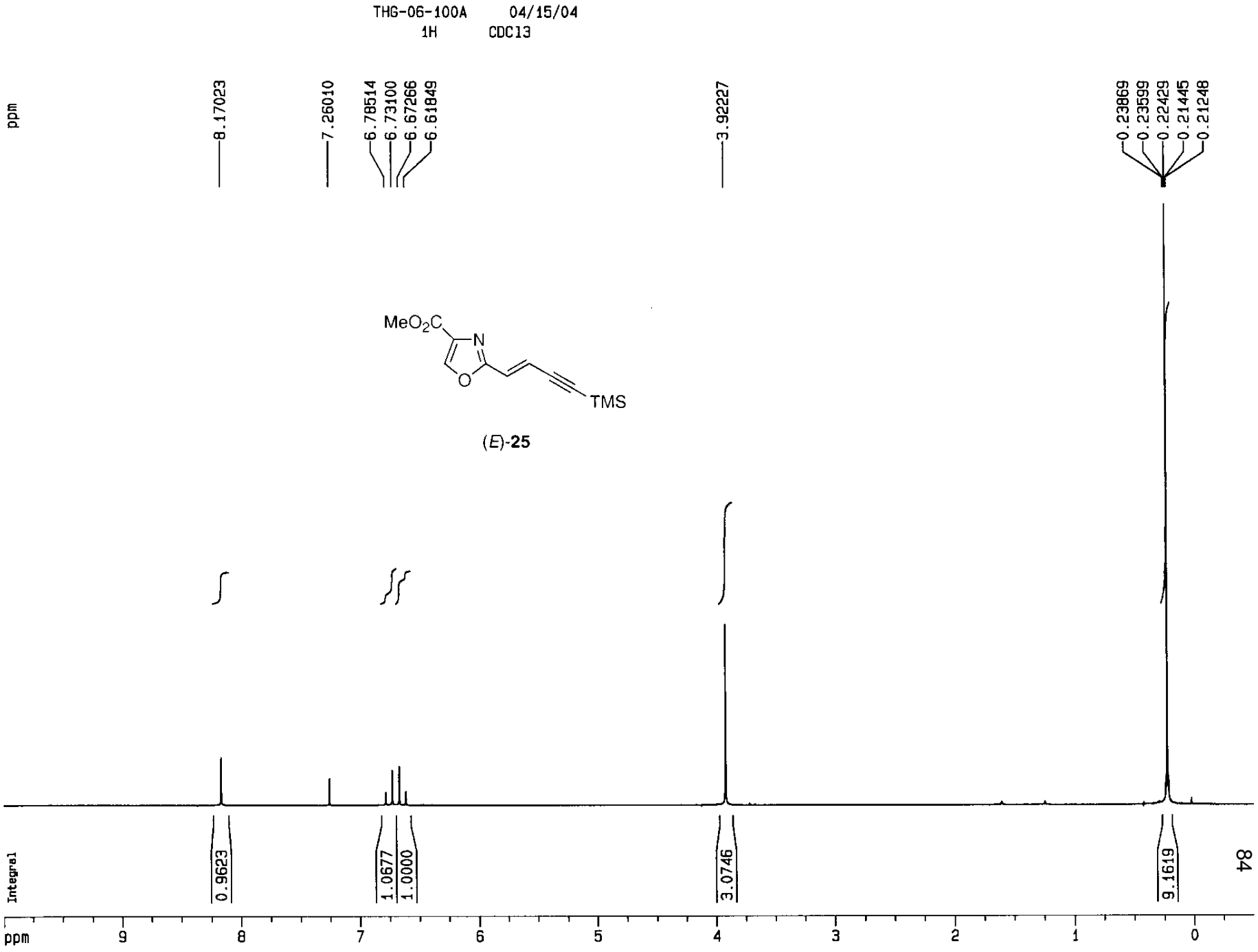


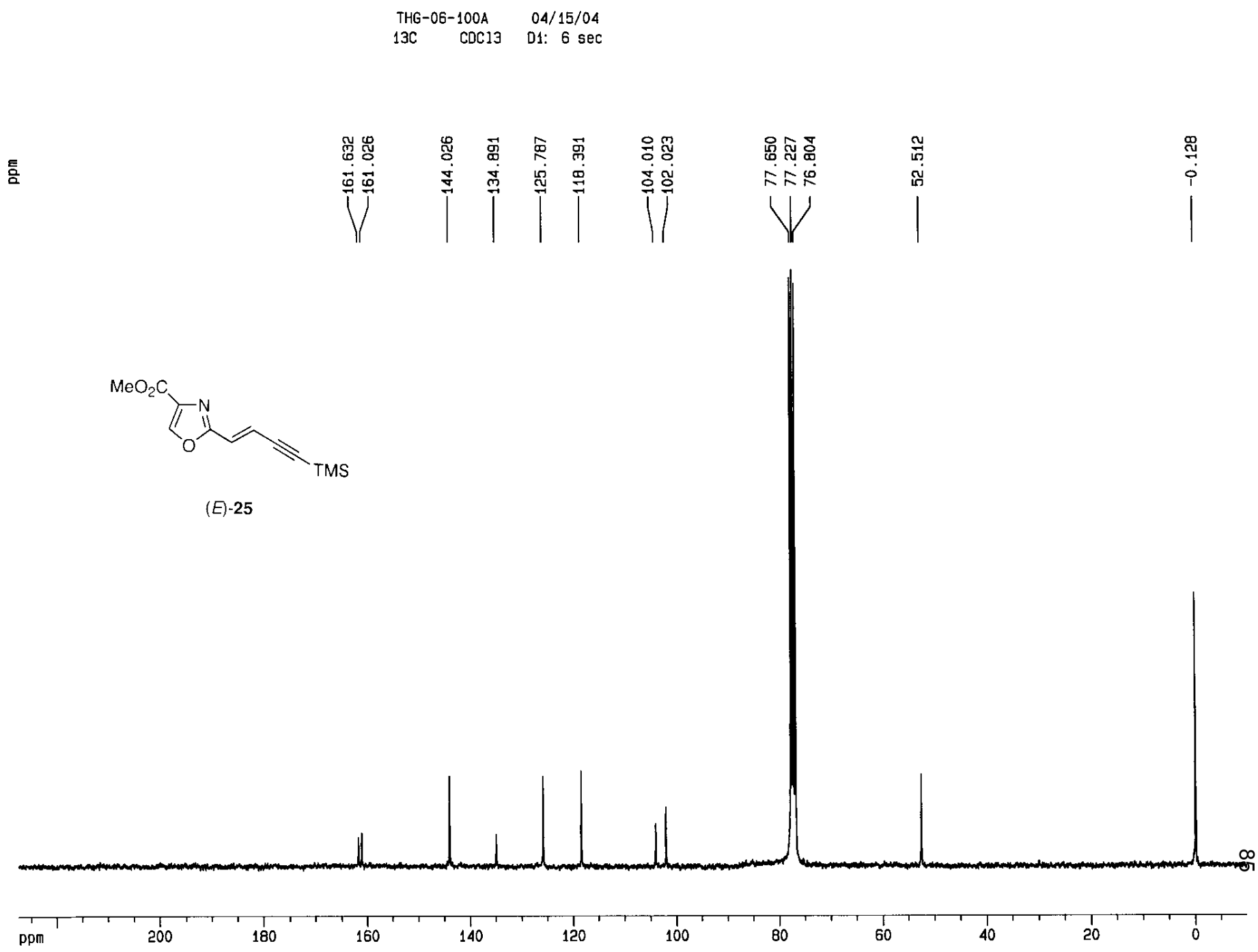

THG-05-086A 07/12/03
13C CDCl3 D1: 8 sec
ppm
161.539
160.860
143.857
134.326
130.303
89.855
77.657
77.233
76.810
52.543
MeO2C
N
O
I
(E)-10i
181
ppm
200
180
160
140
120
100
80
60
40
20
0

THG-06-101 04/13/04
1H CDC13




THG-06-101 04/13/04
13C CDCl3 D1: 4 sec
ppm
161.712
160.830
143.551
134.489
124.035
116.237
106.920
101.392
77.653
77.229
76.806
52.451
-0.196
TMS
MeO2C
N
O
(Z)-25
ppm
200
180
160
140
120
100
80
60
40
20
0


THG-06-100A 04/15/04
1H CDCl3
ppm
8.17023
7.26010
6.78514
6.73100
6.67266
6.61849
3.92227
0.23869
0.23599
0.22429
0.21445
0.21248
MeO2C
N
O
TMS
(E)-25
Integral
0.9623
1.0677
1.0000
3.0746
9.1619
ppm
9
8
7
6
5
4
3
2
1
0


THG-06-100A 04/15/04
13C CDCl3 D1: 6 sec
ppm
161.632
161.026
144.026
134.891
125.787
118.391
104.010
102.023
77.650
77.227
76.804
52.512
-0.128
MeO2C
N
O
TMS
(E)-25
ppm
200
180
160
140
120
100
80
60
40
20
0