Catalytic enantioselective construction of quaternary stereocenter by direct vinylogous Michael addition of deconjugated butenolides to nitroolefins

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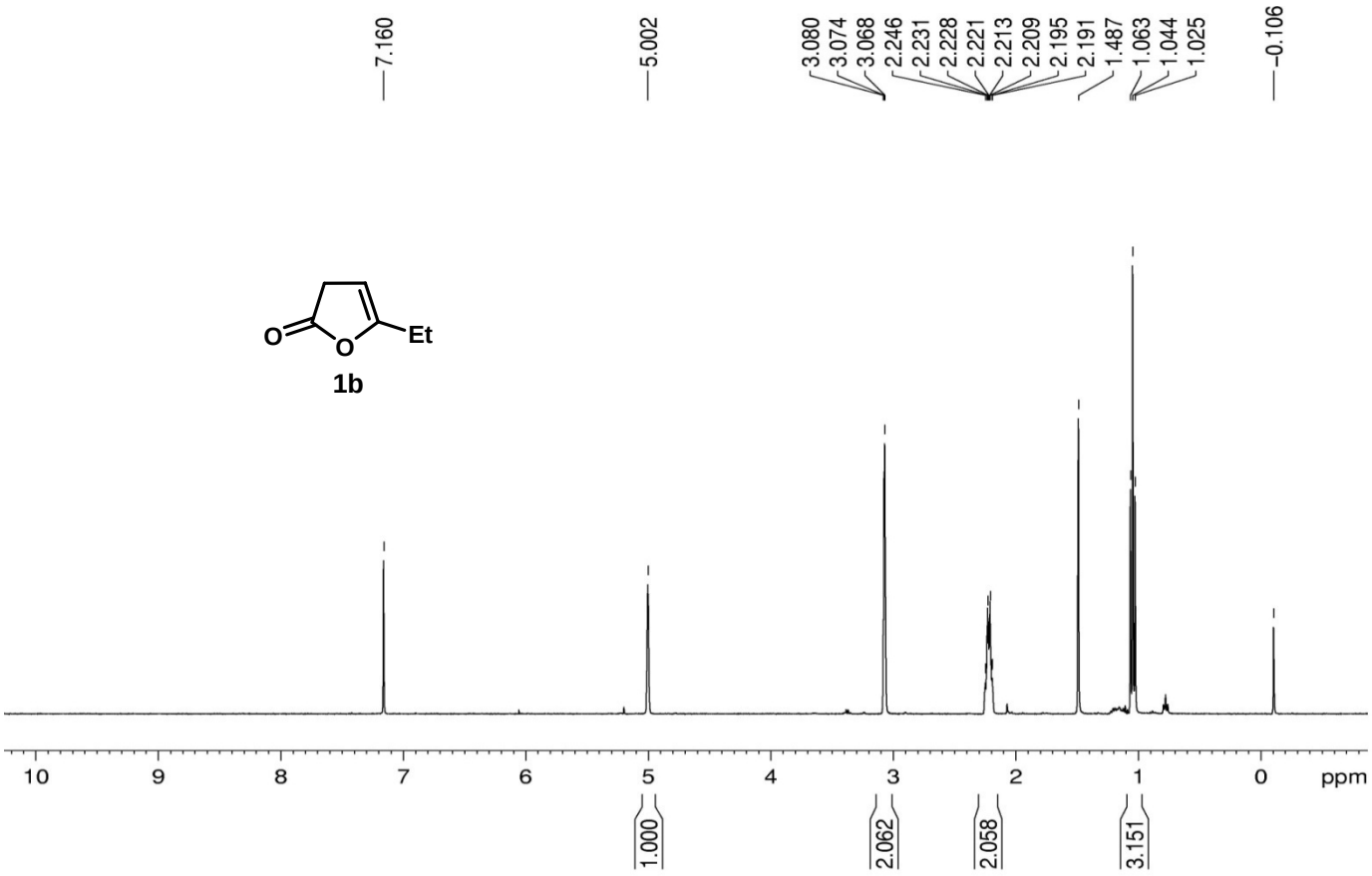
sm@orgchem.iisc.ernet.in

SUPPORTING INFORMATION: PART B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O
O
Et
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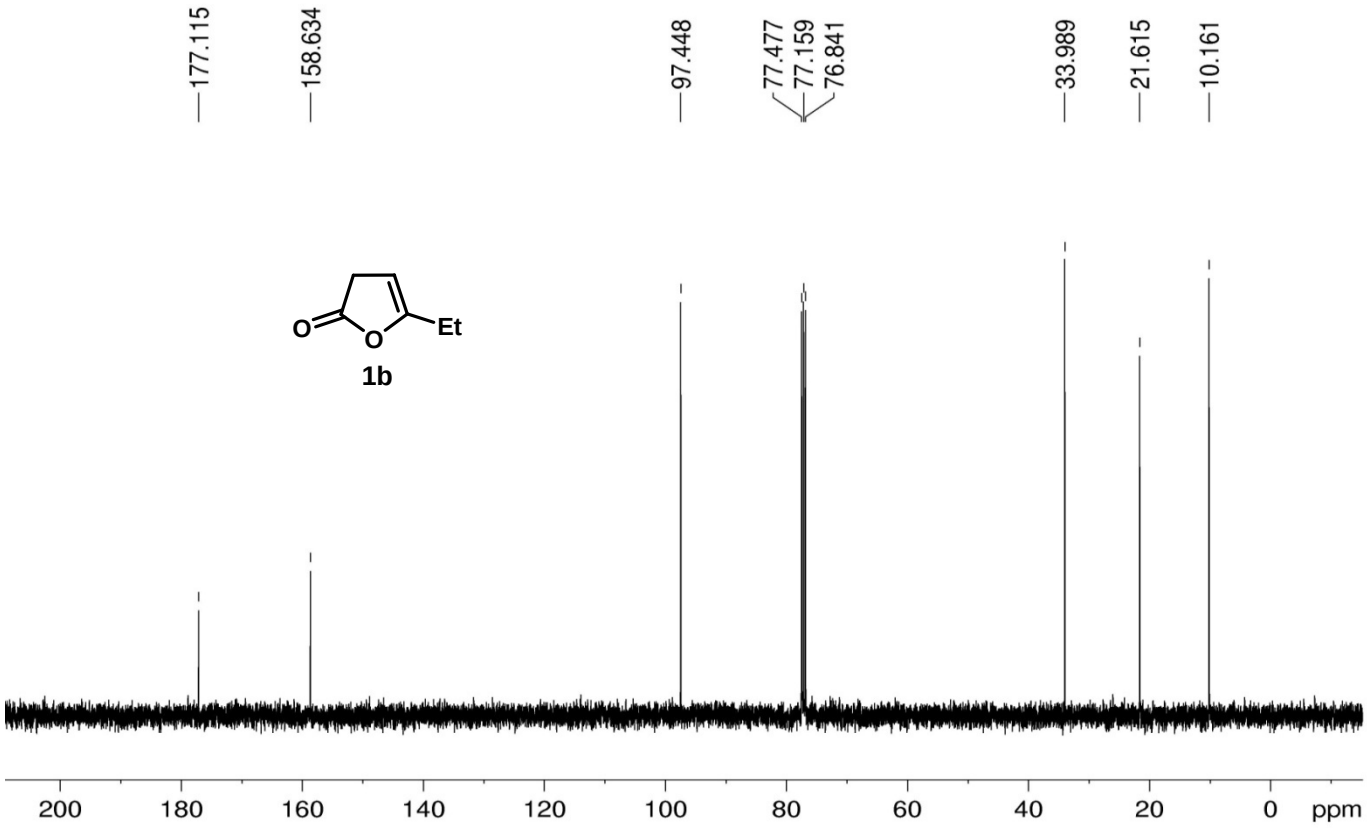
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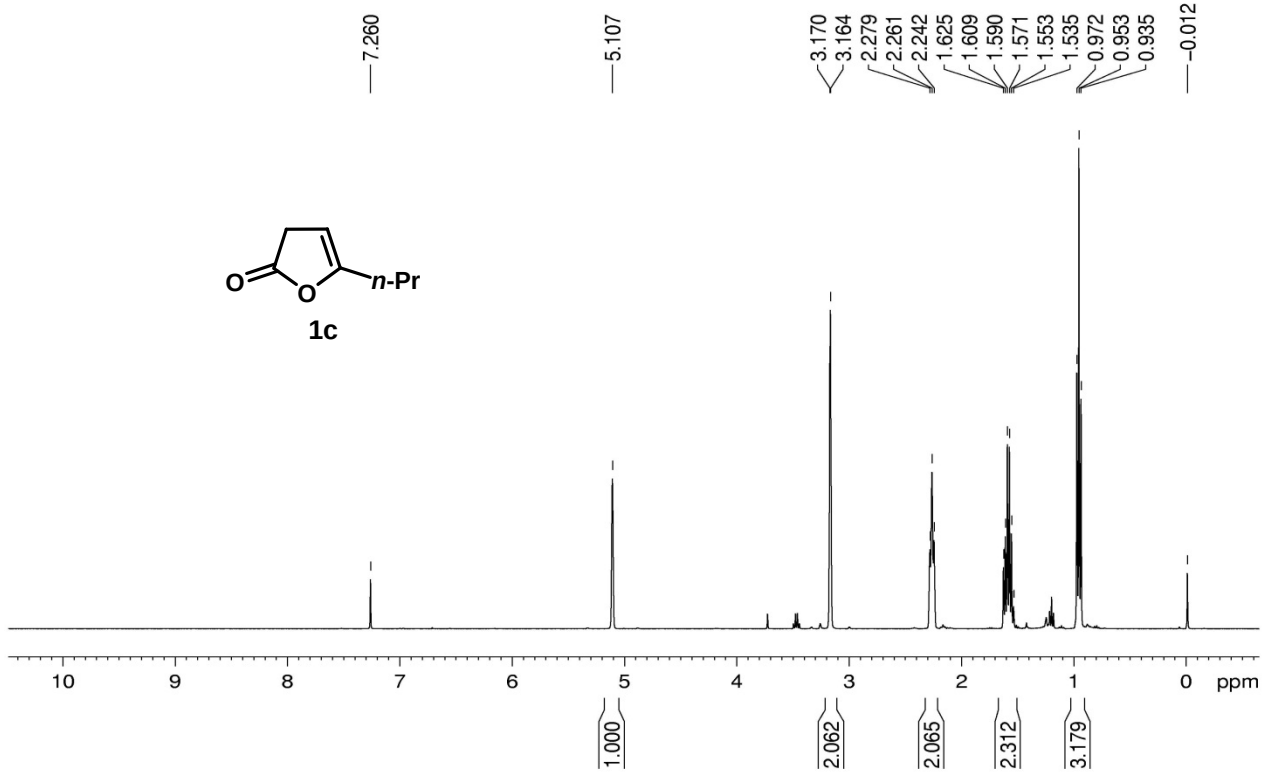
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O
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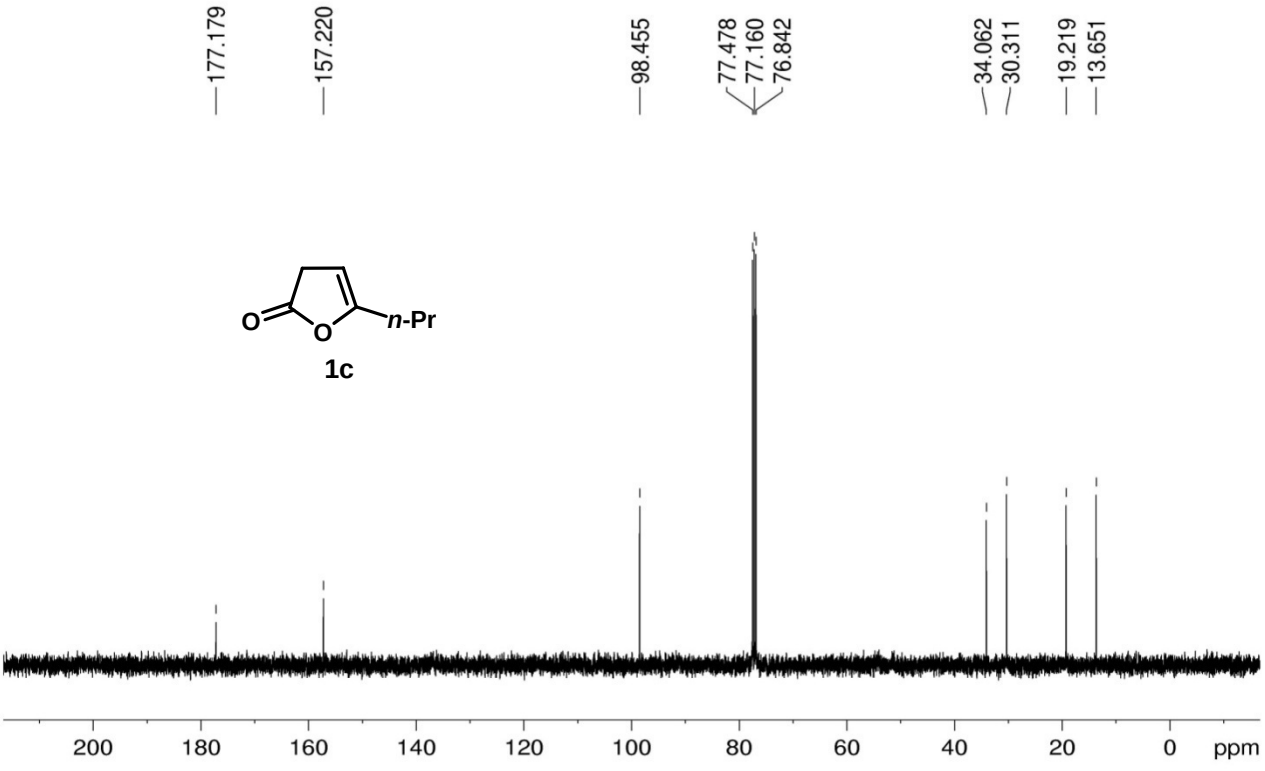
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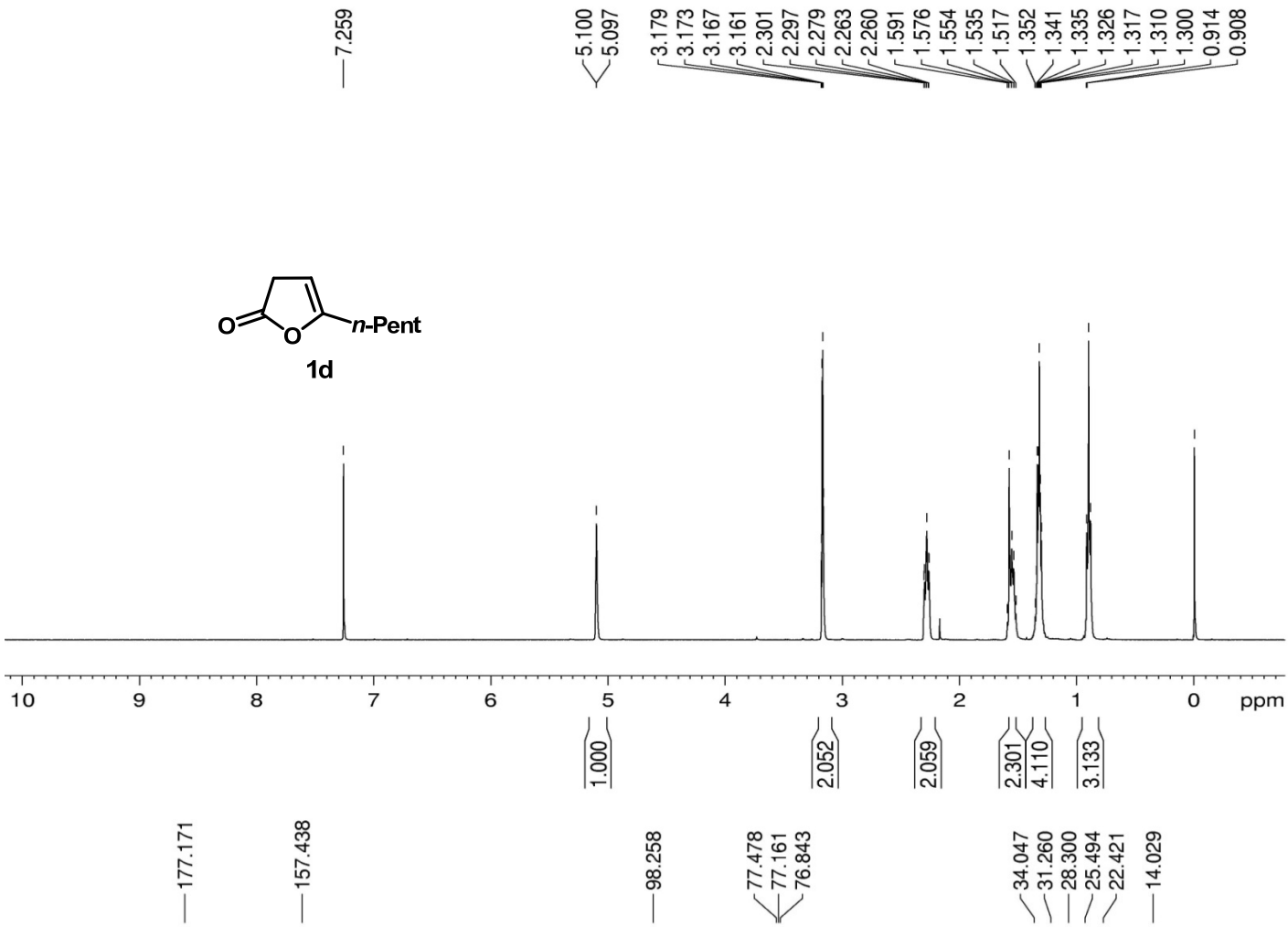
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1.576
1.554
1.535
1.517
1.352
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1.326
1.317
1.310
1.300
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0.908
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O
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1d
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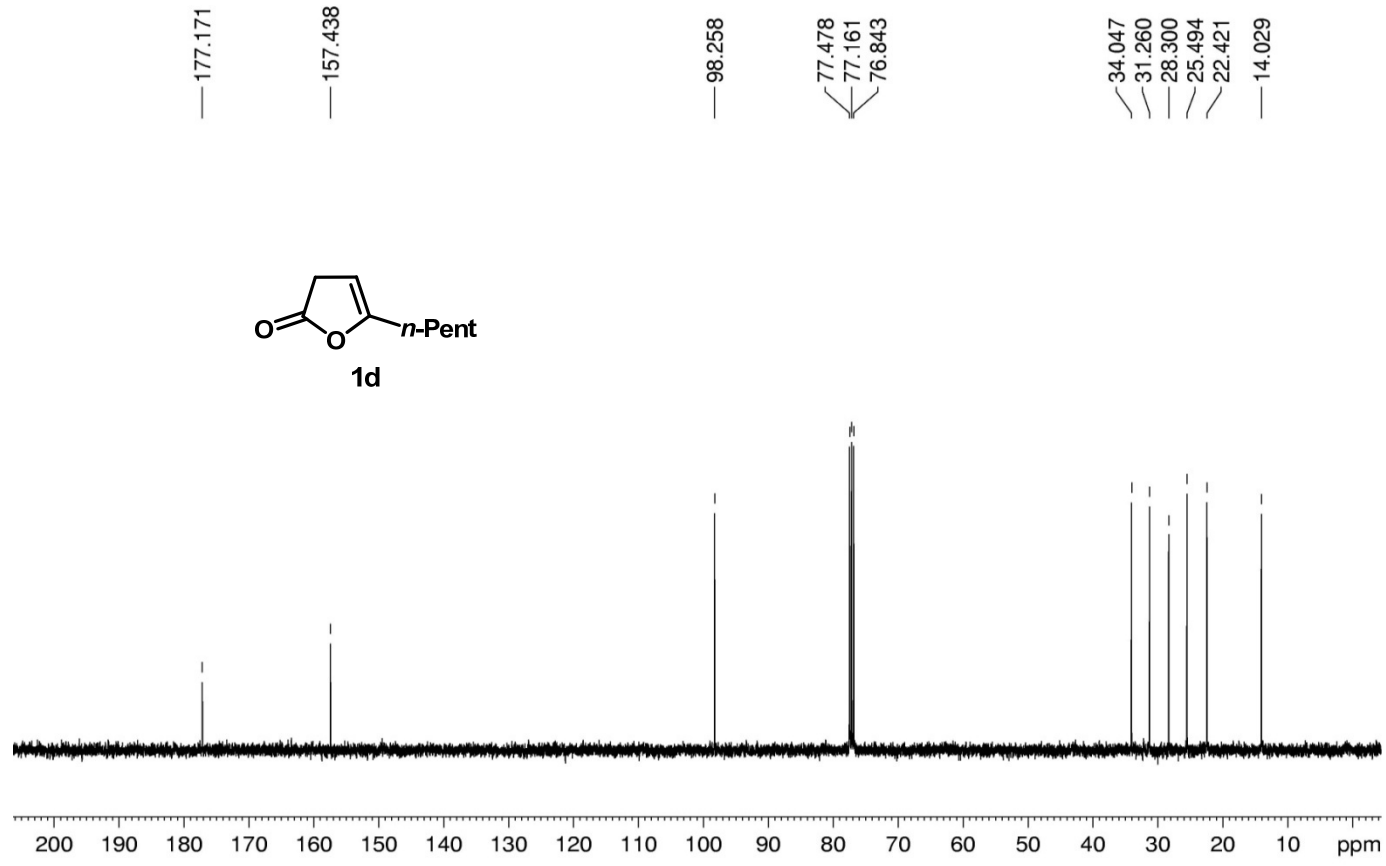
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O
n-Pent
1d
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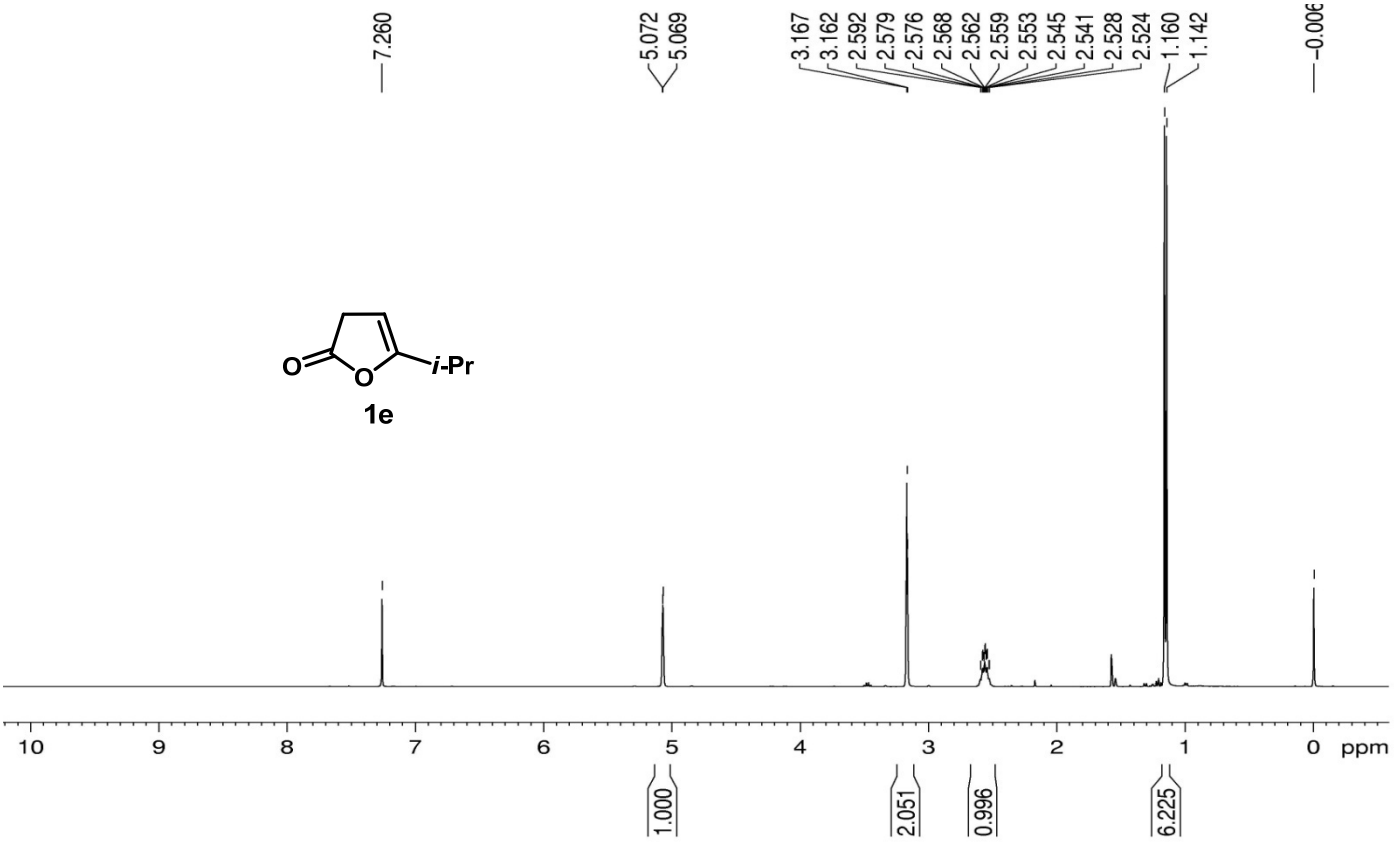
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2.541
2.528
2.524
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-0.006
i-Pr
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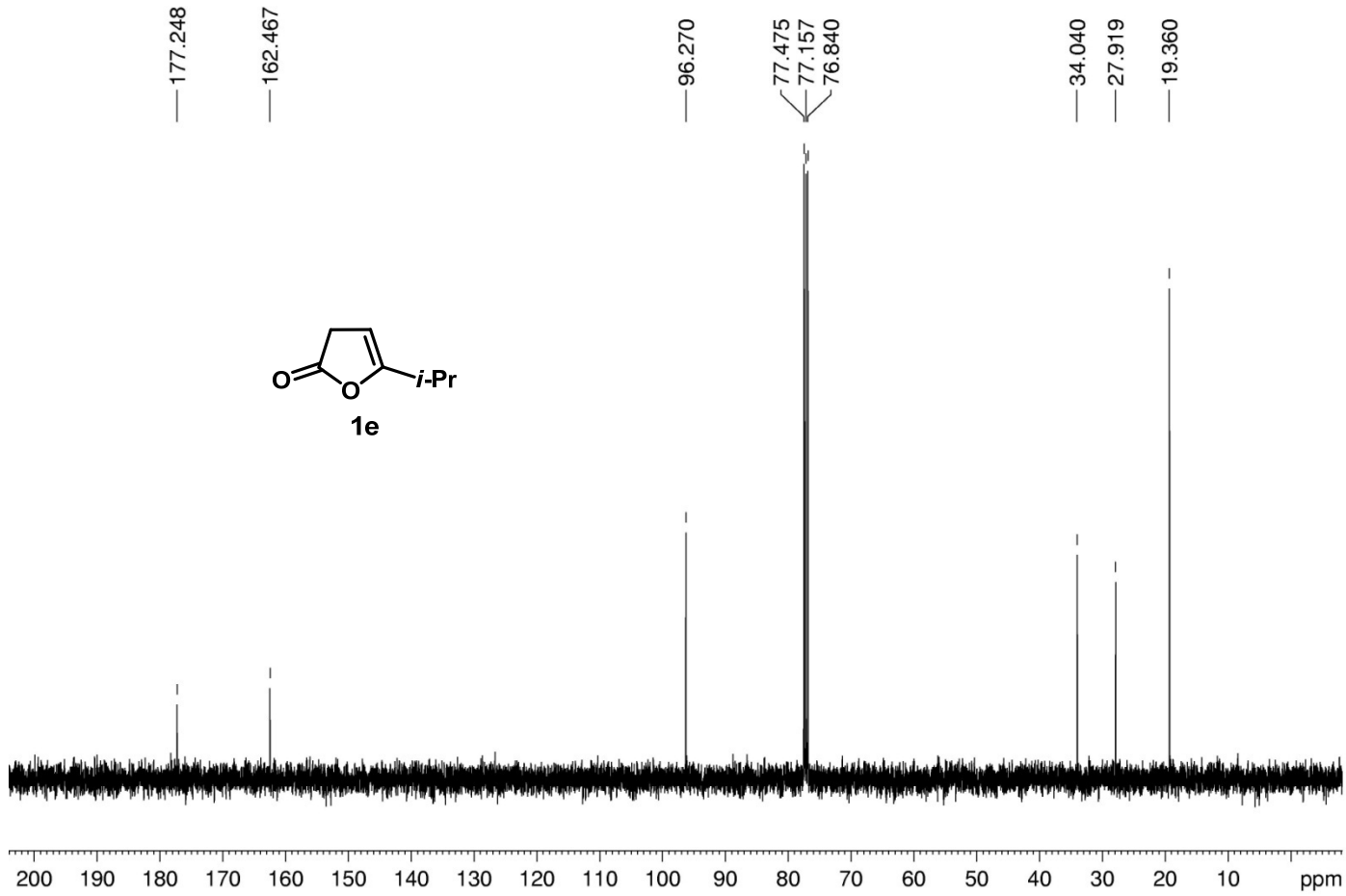
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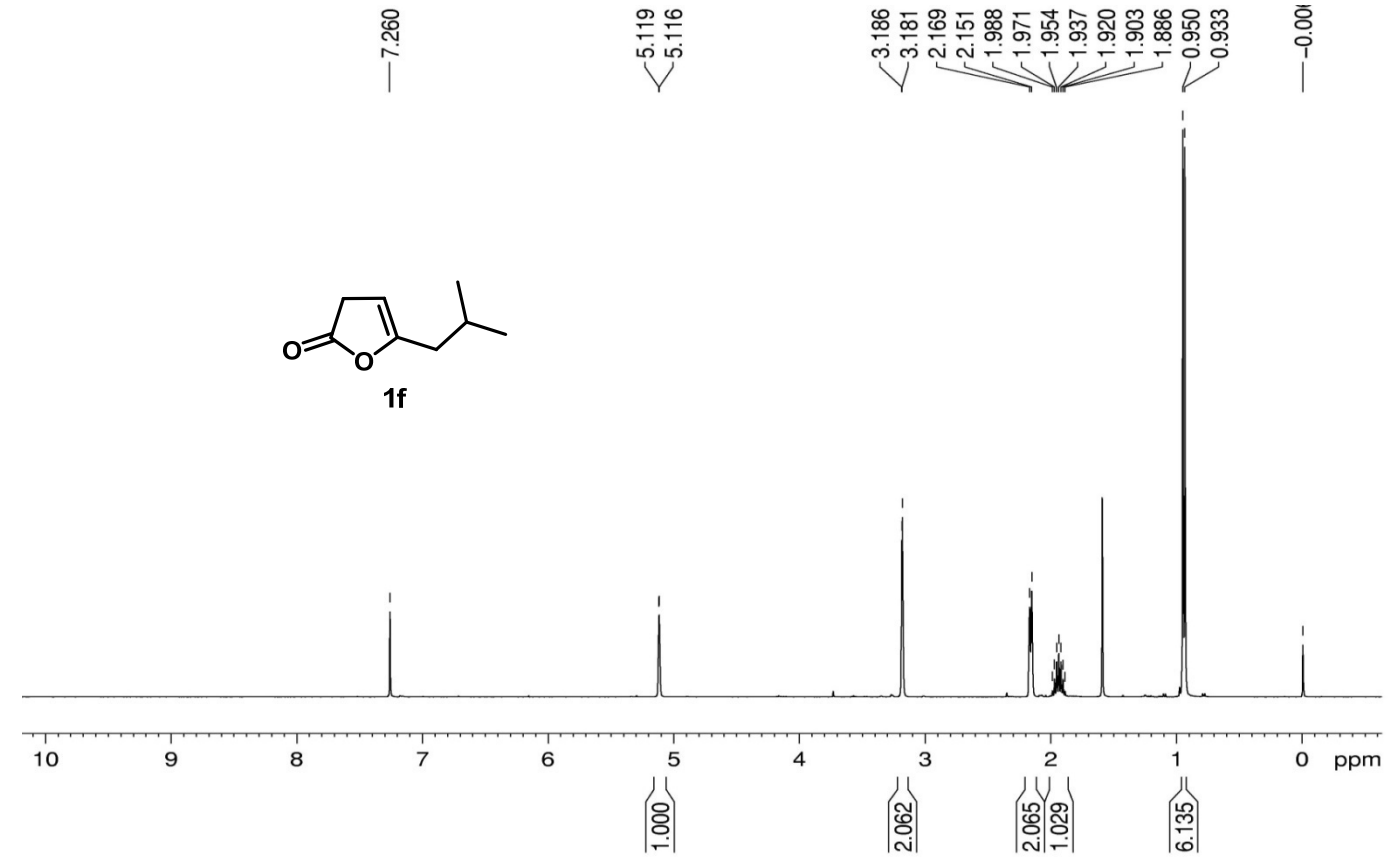
20
10
ppm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0.950
0.933
1f
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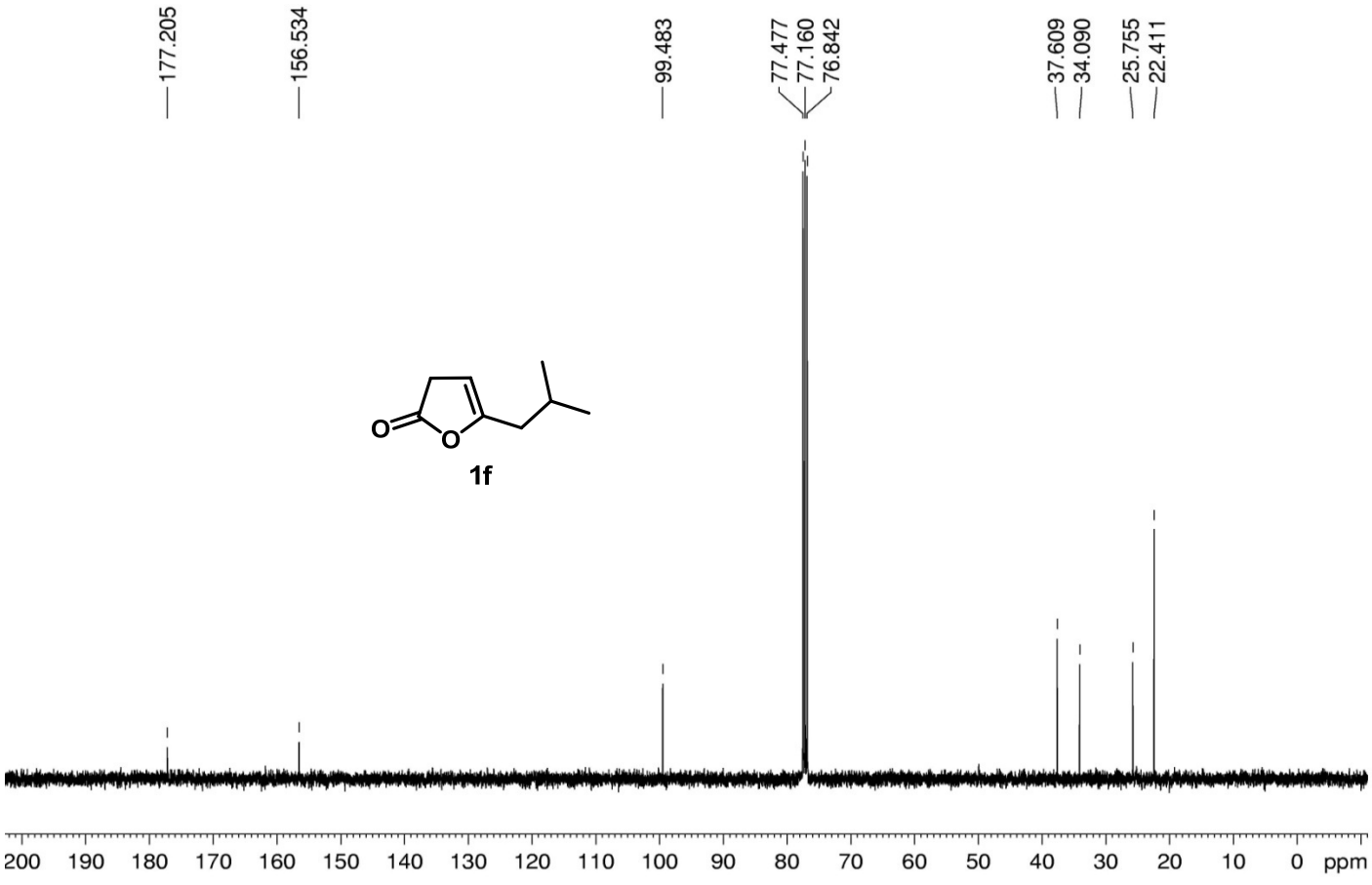
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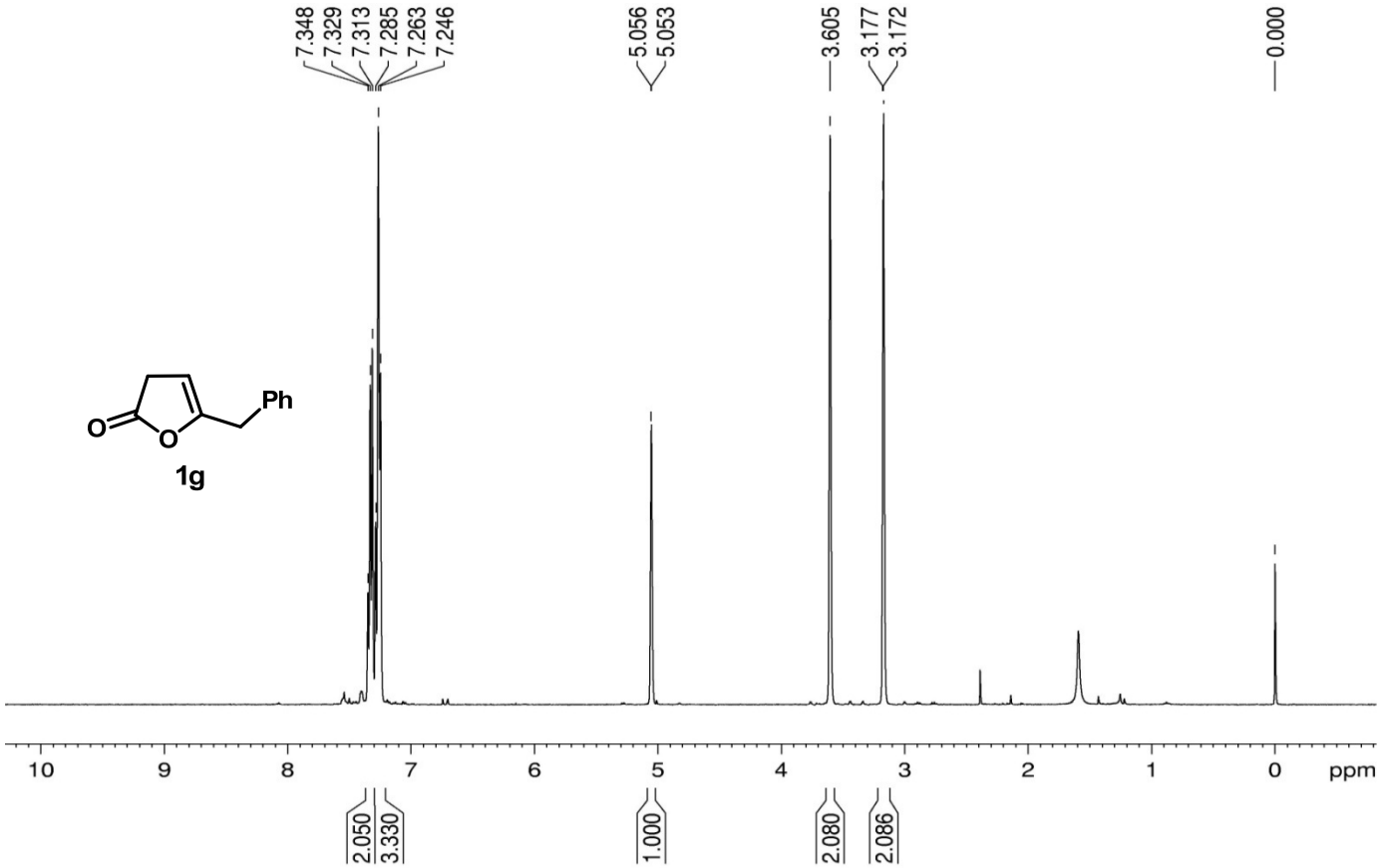
ppm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O
1g
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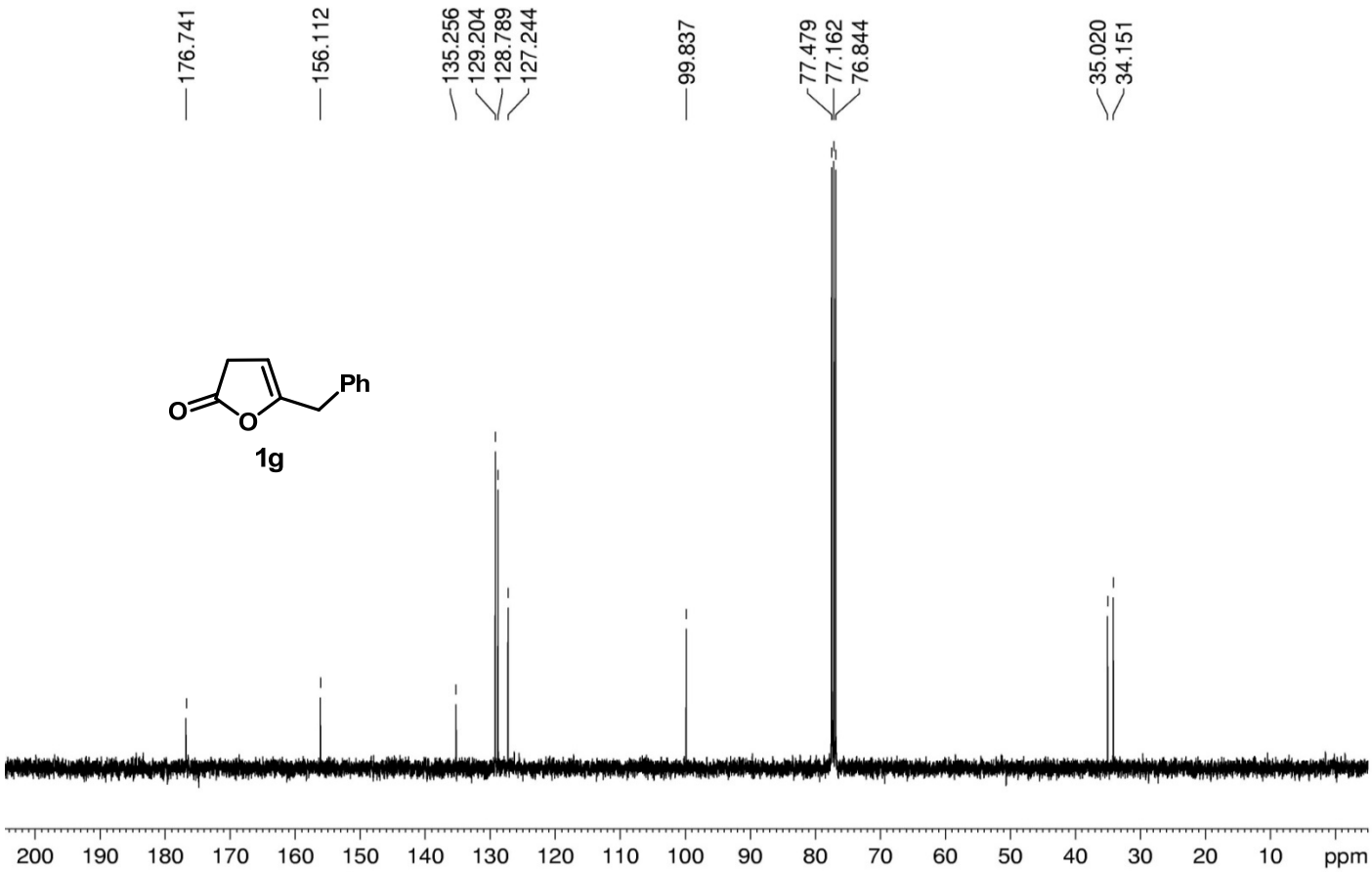
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Ph
O
O
1g
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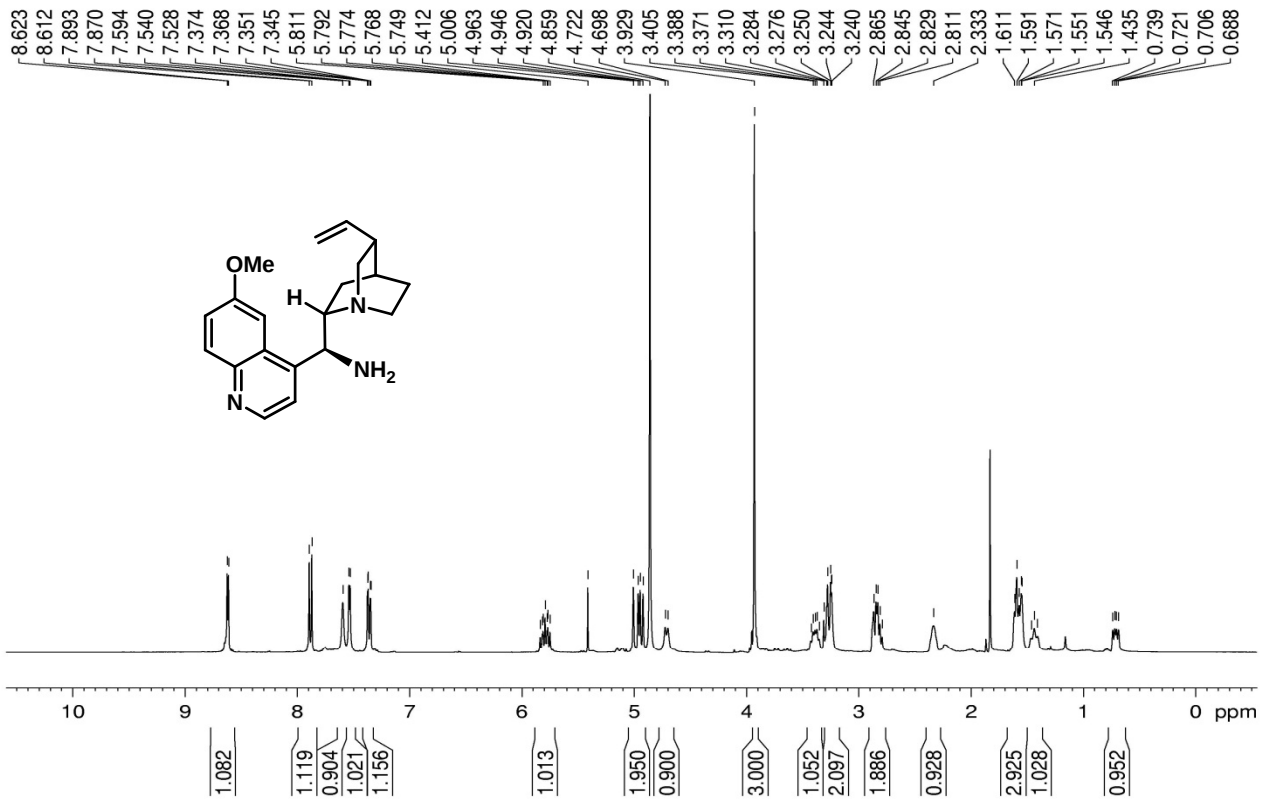
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4.722
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1.546
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0.688
OMe
H
N
NH2
N
10
9
8
7
6
5
4
3
2
1
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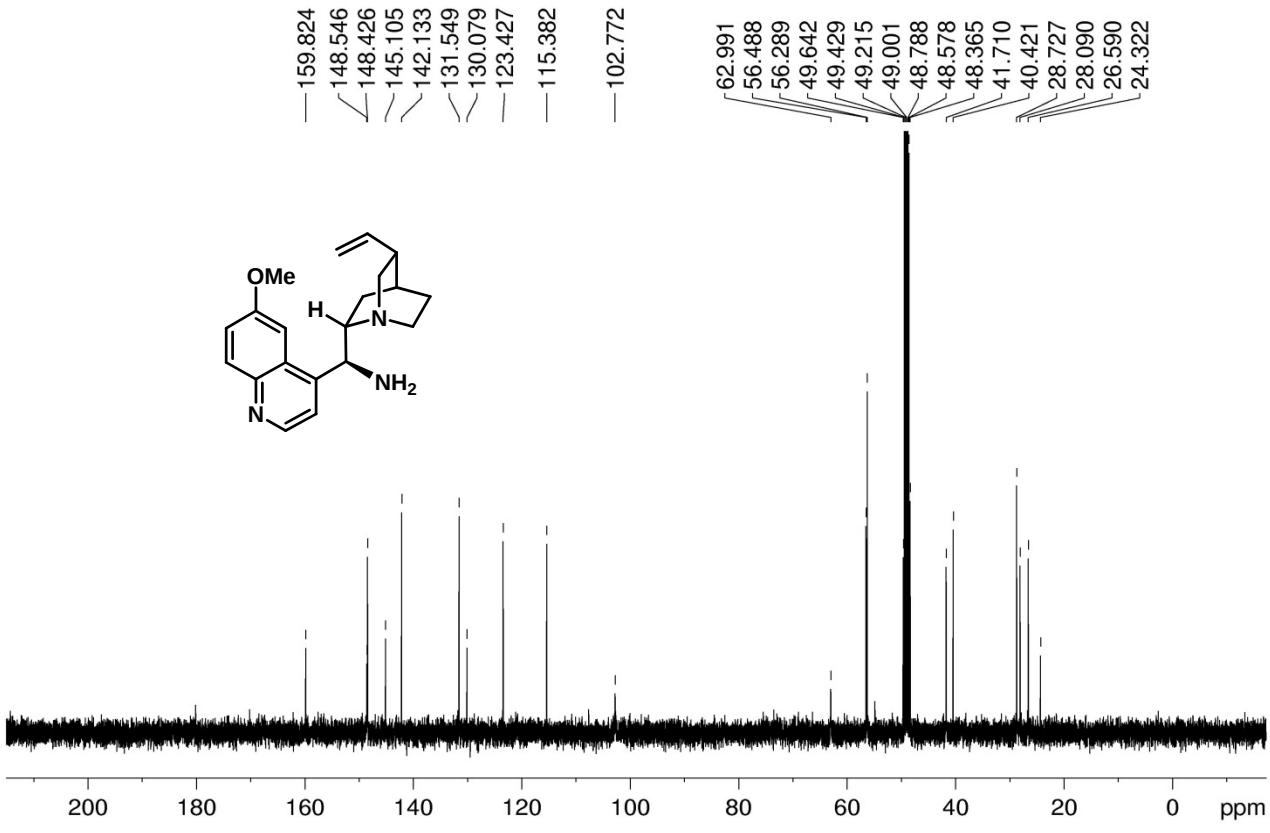
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28.090
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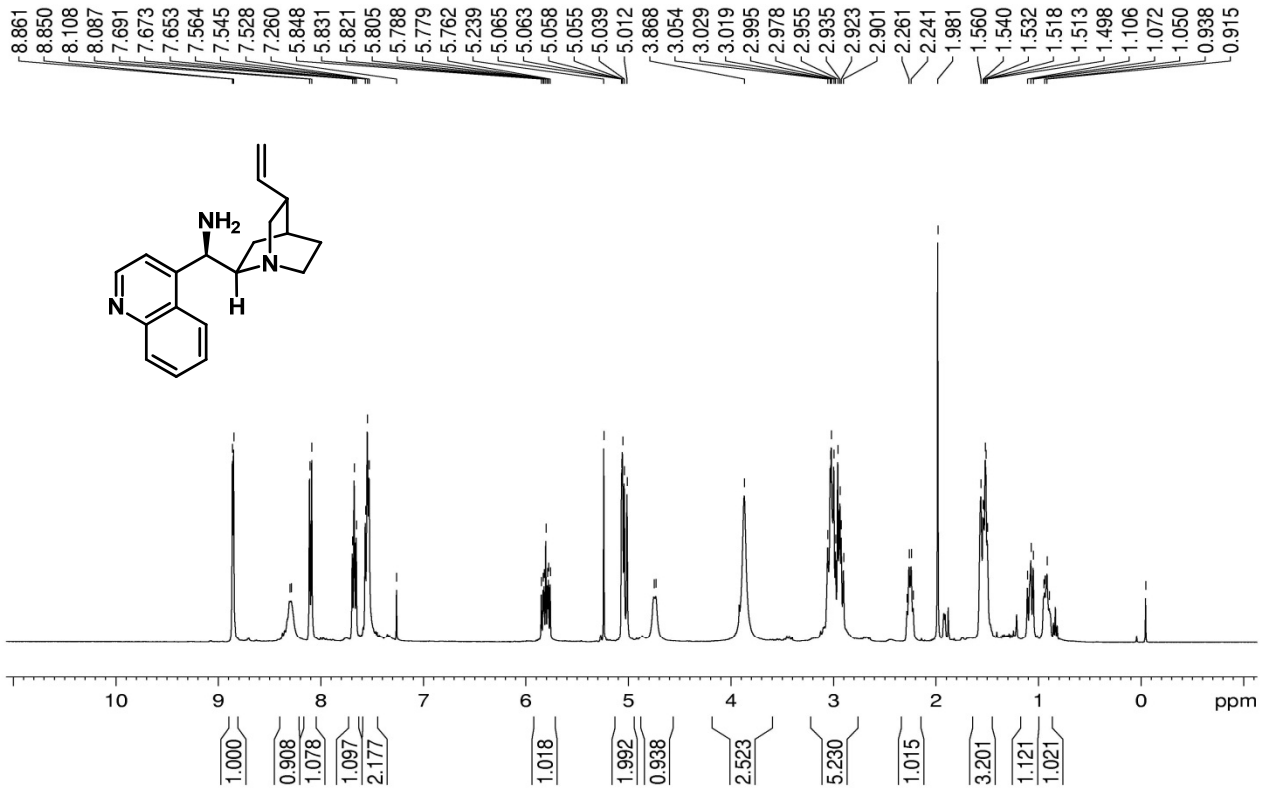
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5.055
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2.978
2.955
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N
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H
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9
8
7
6
5
4
3
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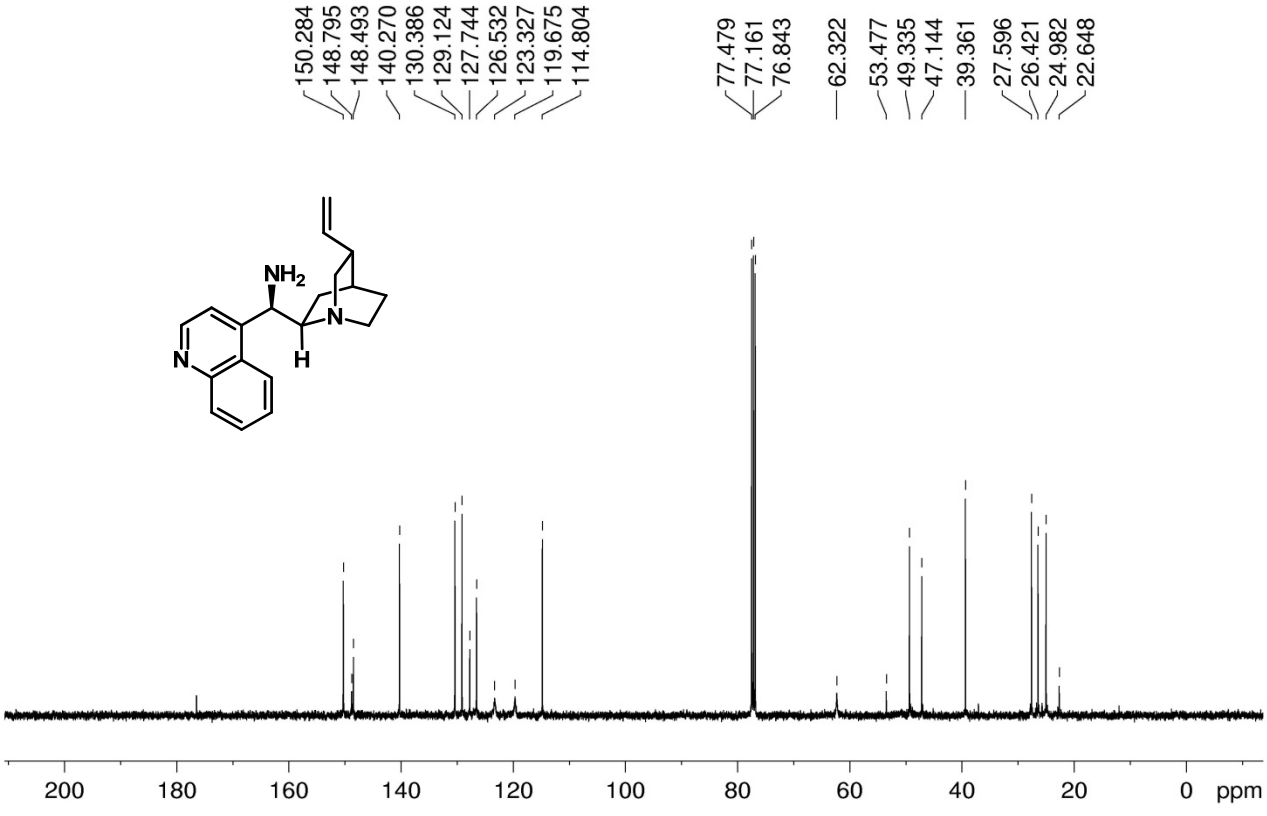
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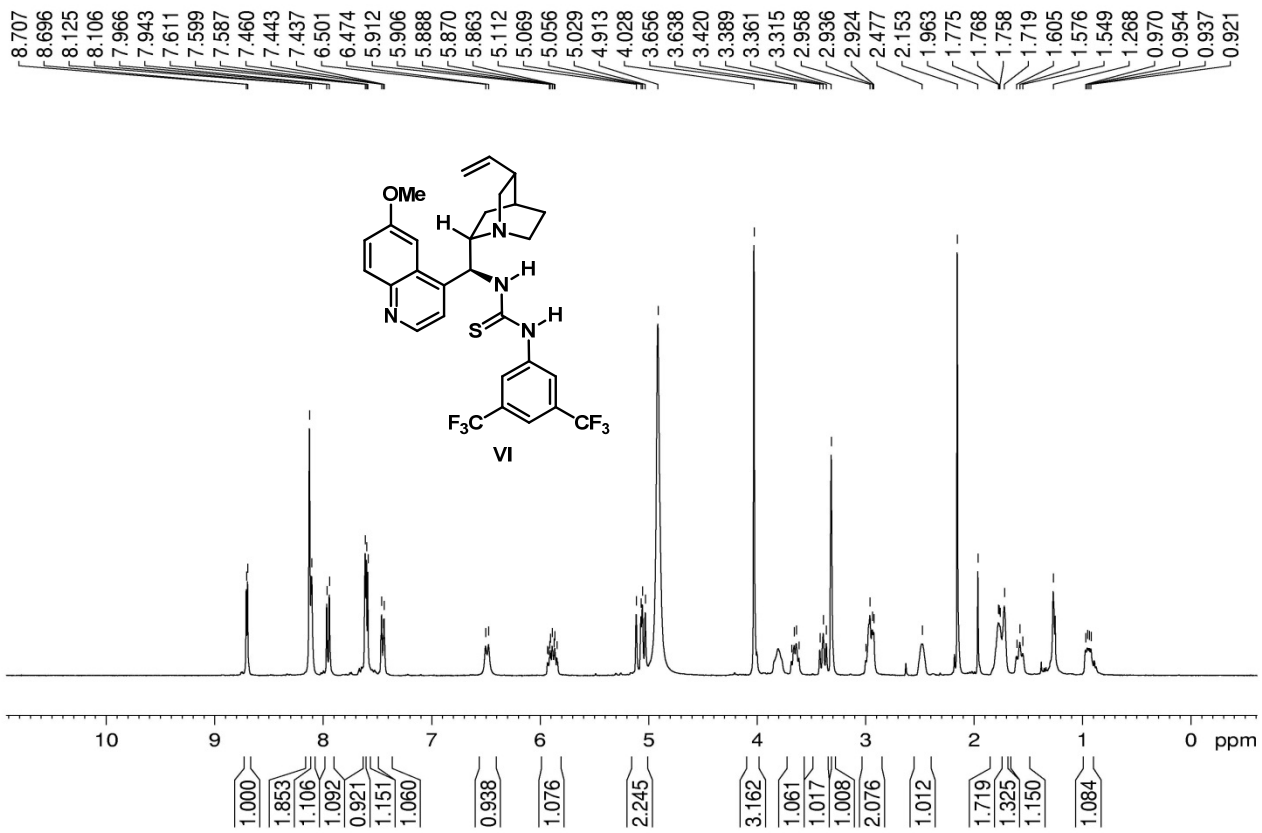
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F3C
CF3
VI
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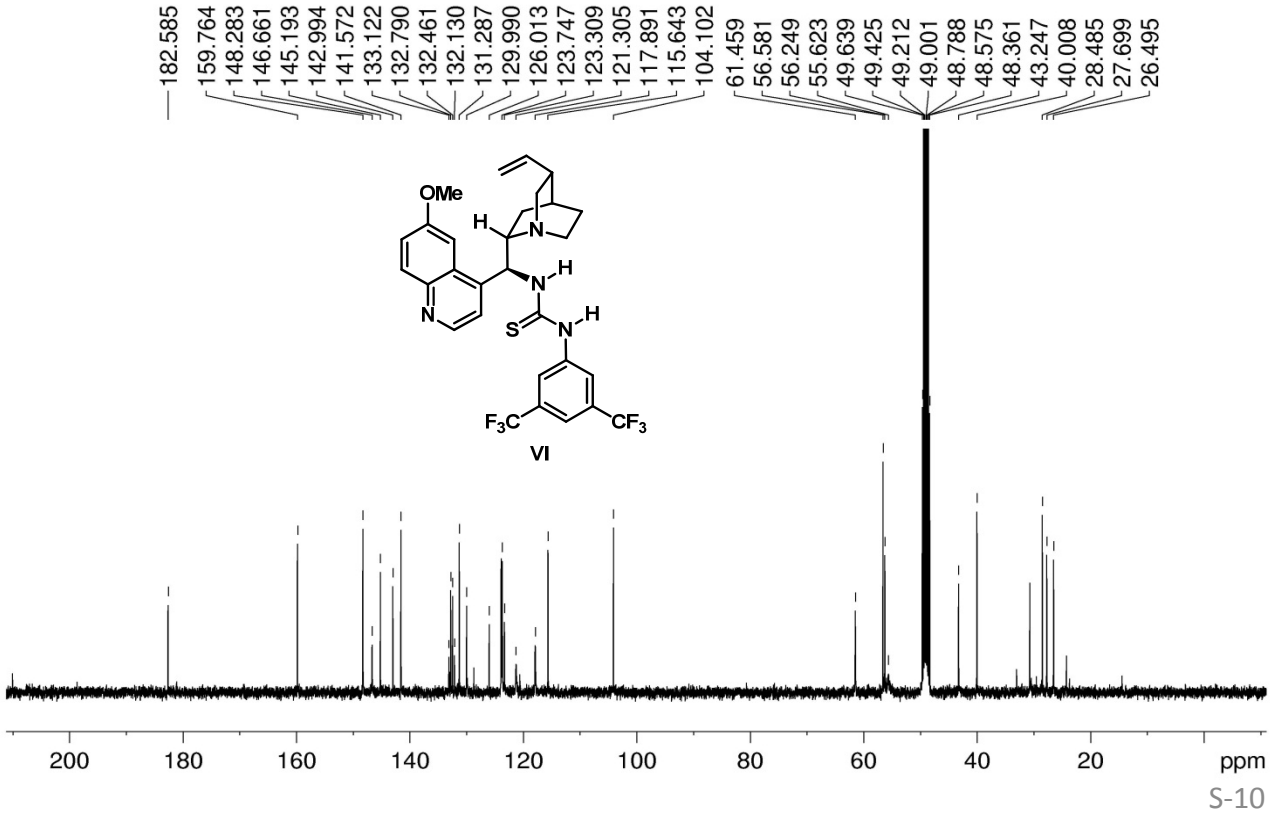
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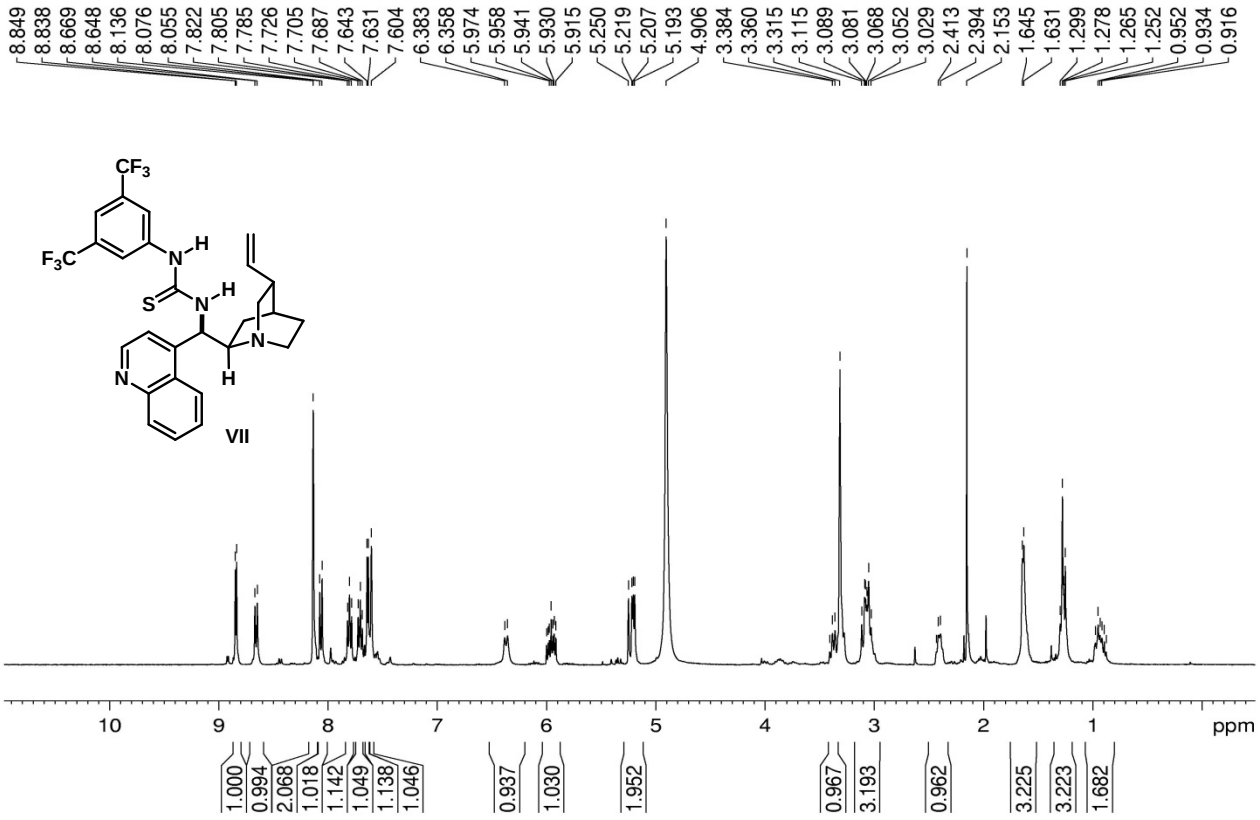
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F3C
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H
S
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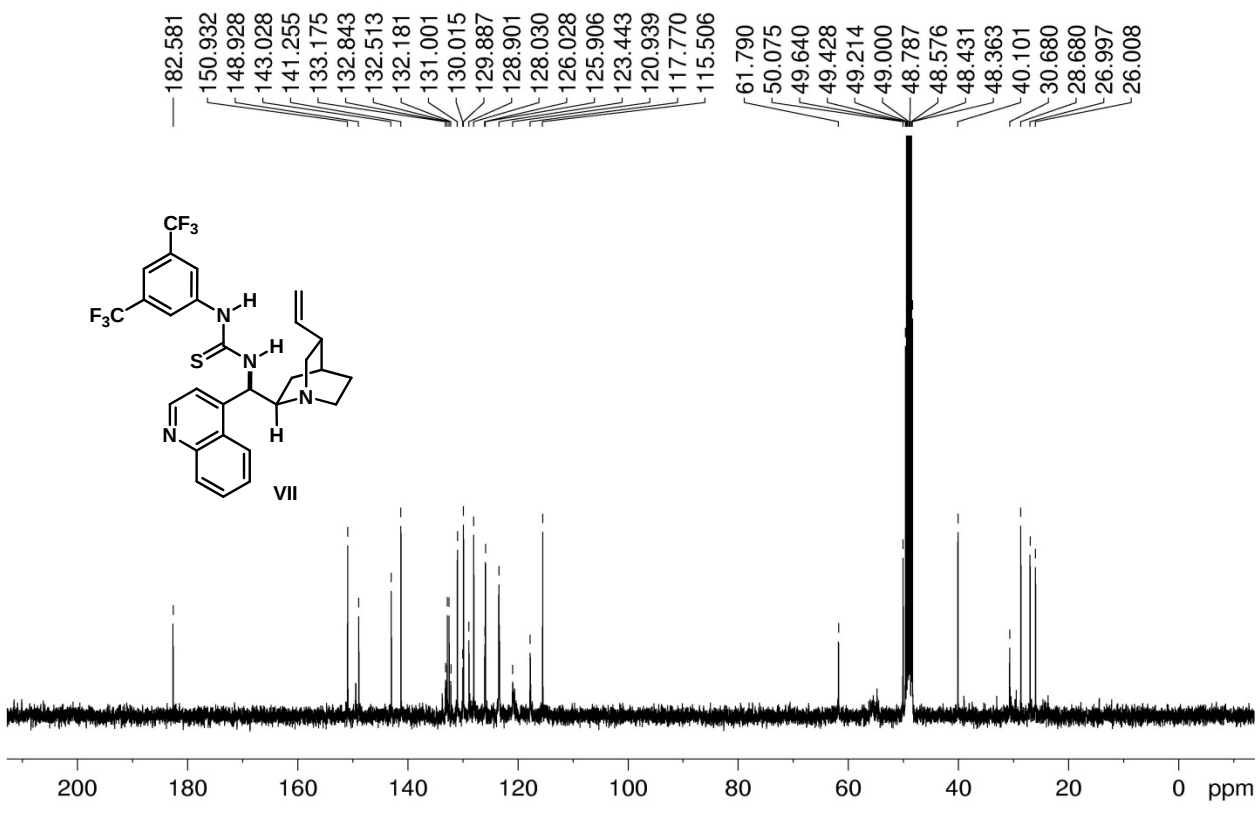
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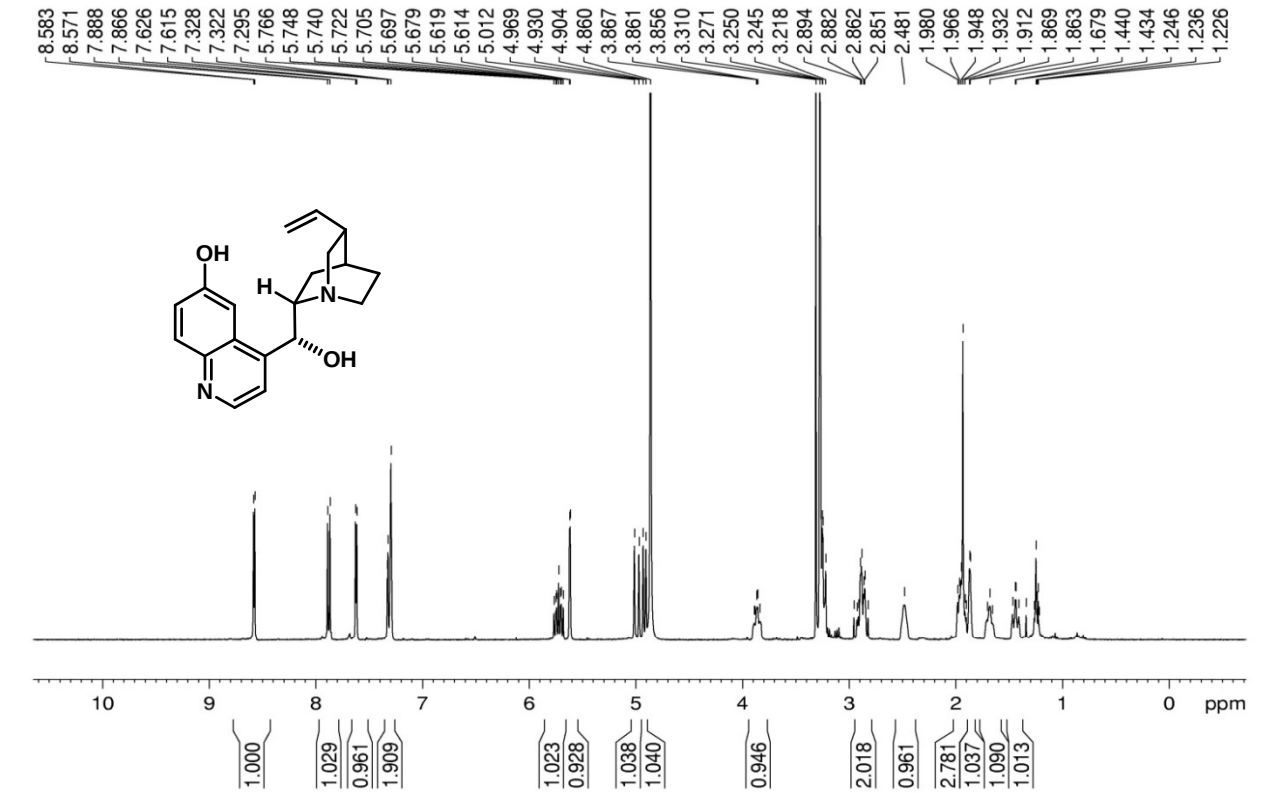
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OH
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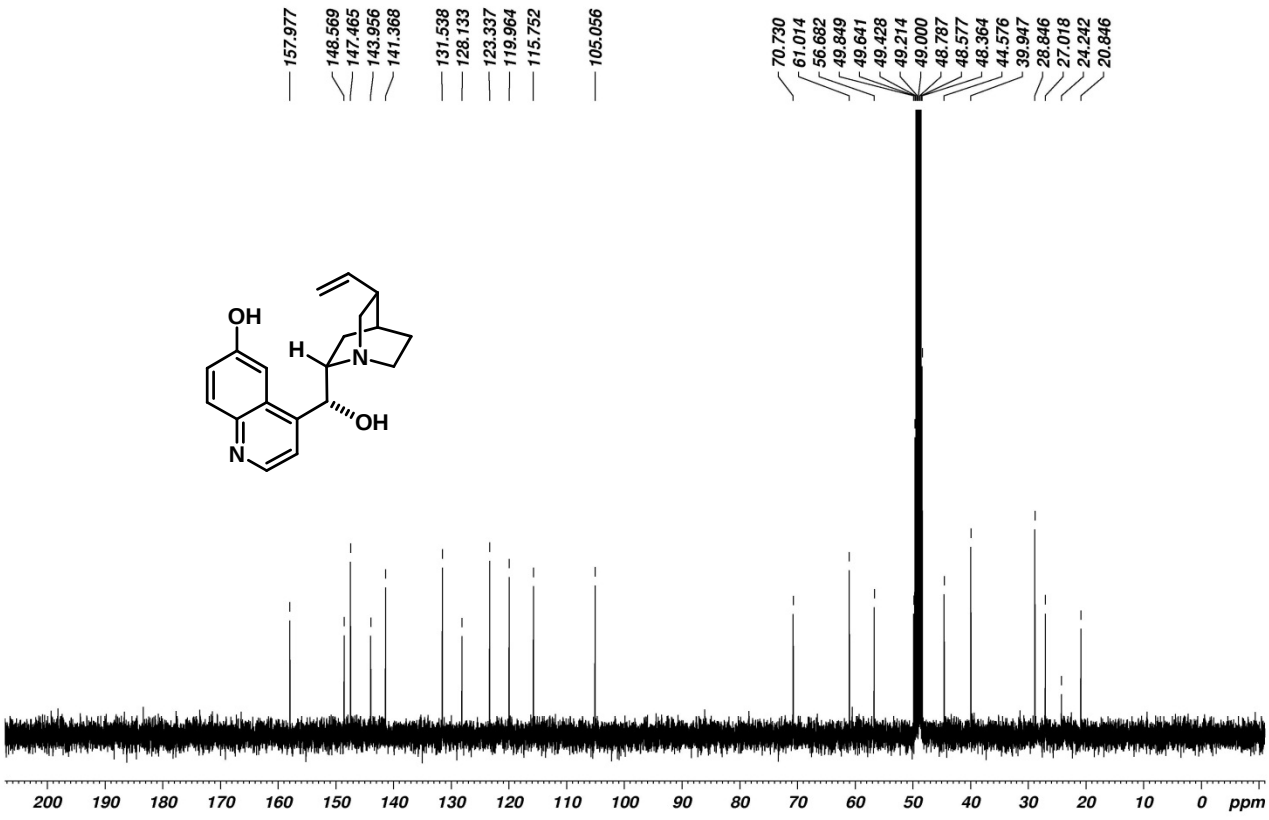
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48.364
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20.846
OH
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OH
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200
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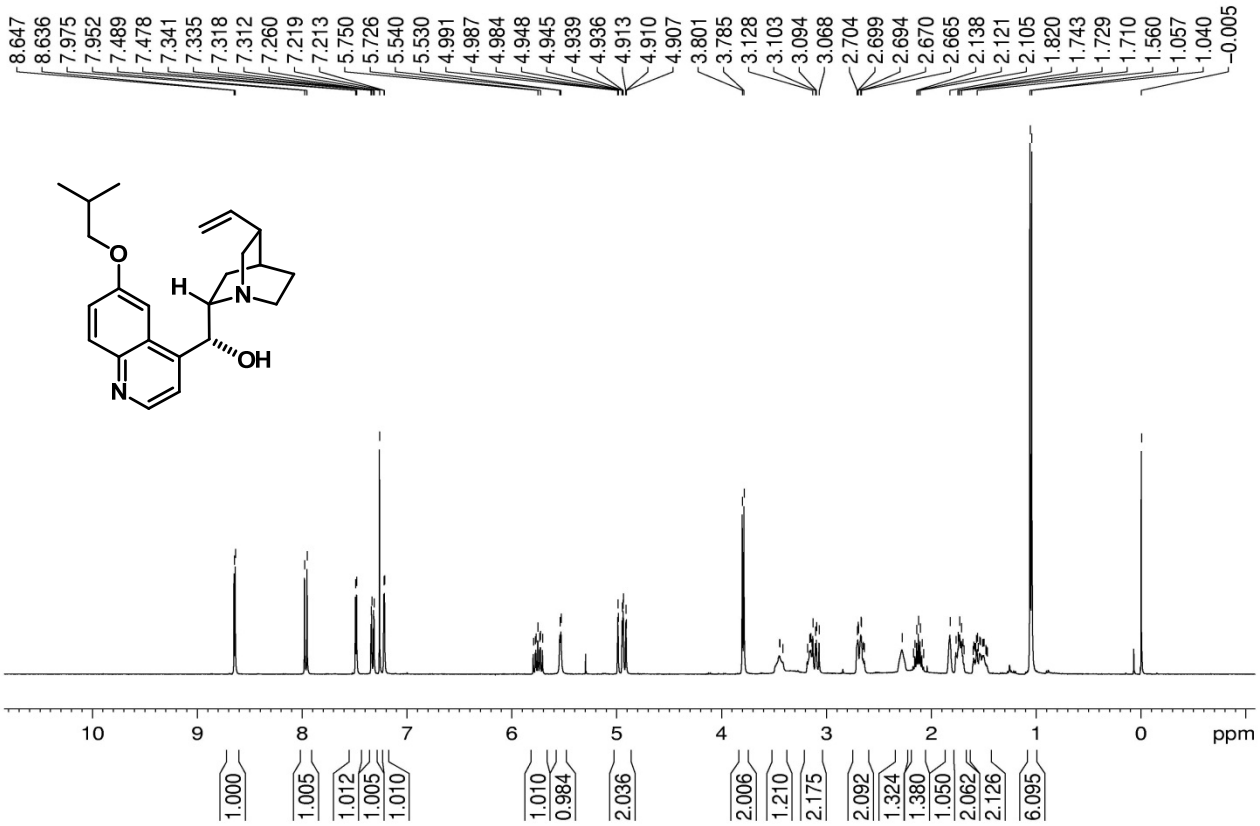
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4.945
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4.936
4.913
4.910
4.907
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3.128
3.103
3.094
3.068
2.704
2.699
2.694
2.670
2.665
2.138
2.121
2.105
1.820
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1.729
1.710
1.560
1.057
1.040
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H
N
OH
N
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6
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4
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1.010
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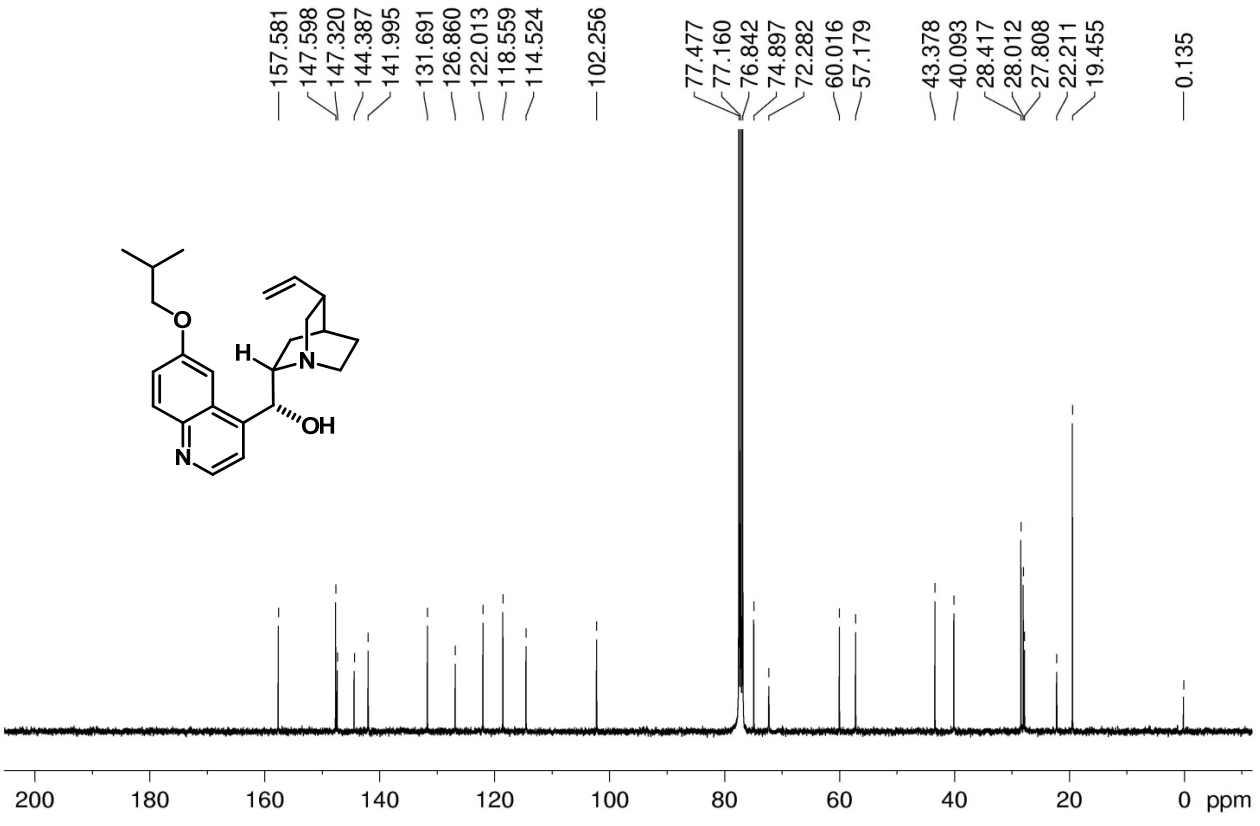
6.095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72.282
60.016
57.179
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27.808
22.211
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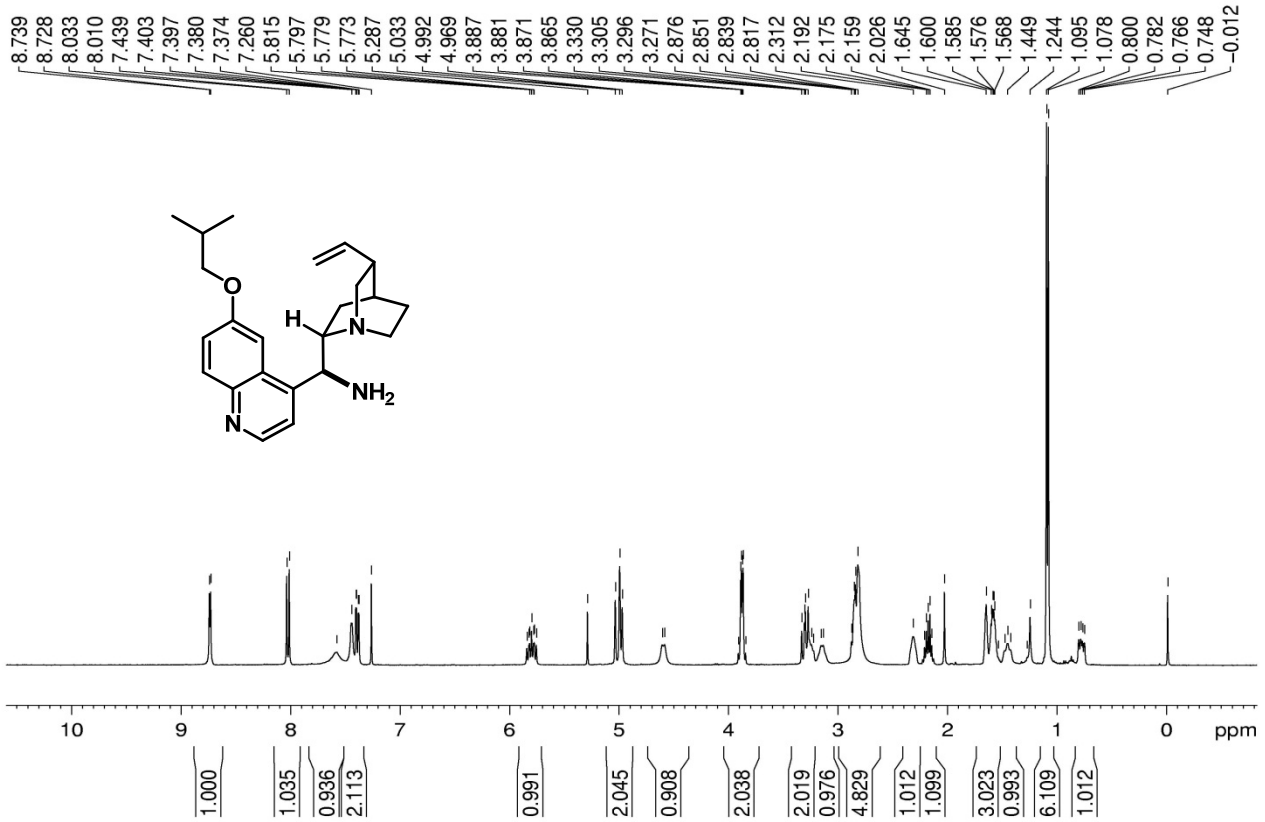
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5.779
5.773
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5.033
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4.969
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3.881
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3.305
3.296
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2.312
2.192
2.175
2.159
2.026
1.645
1.600
1.585
1.576
1.568
1.449
1.244
1.095
1.078
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0.782
0.766
0.748
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O
H
N
NH2
N
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9
8
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6
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4
3
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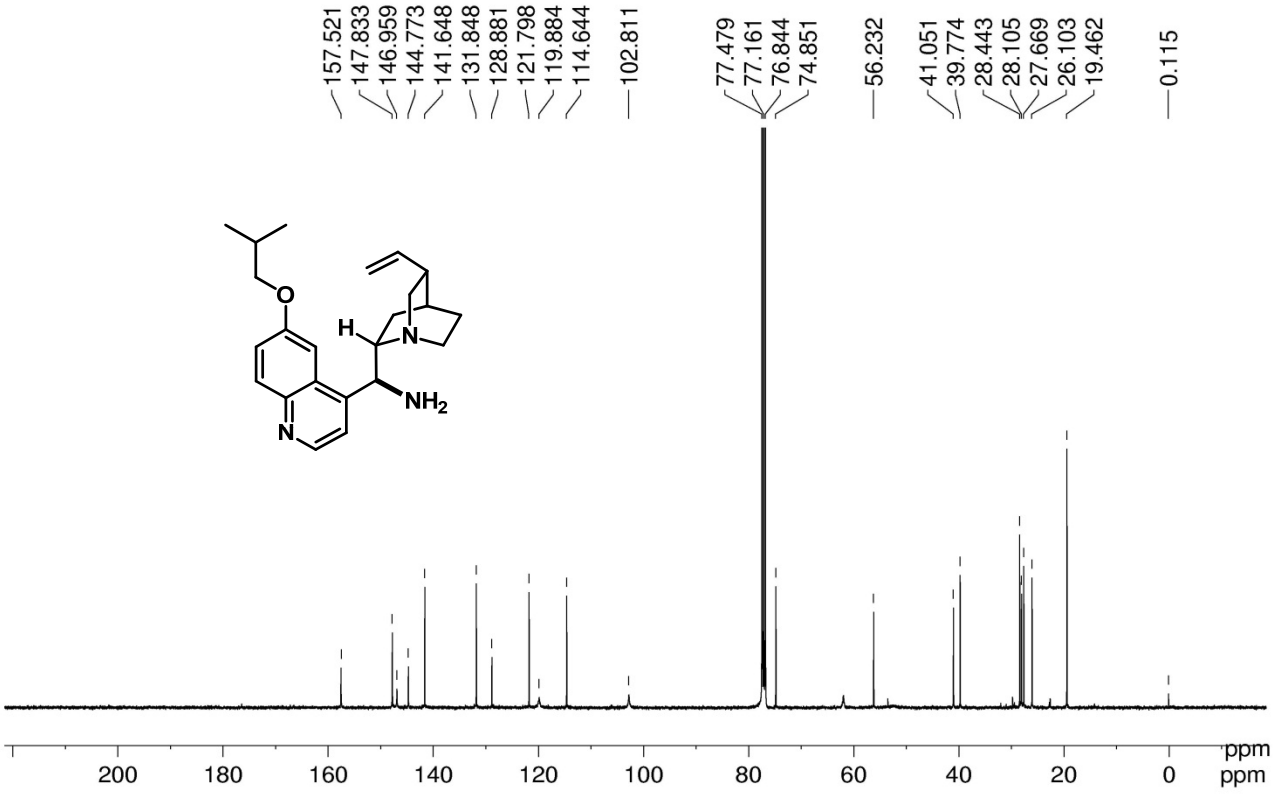
1.012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77.161
76.844
74.851
56.232
41.051
39.774
28.443
28.105
27.669
26.103
19.462
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NH2
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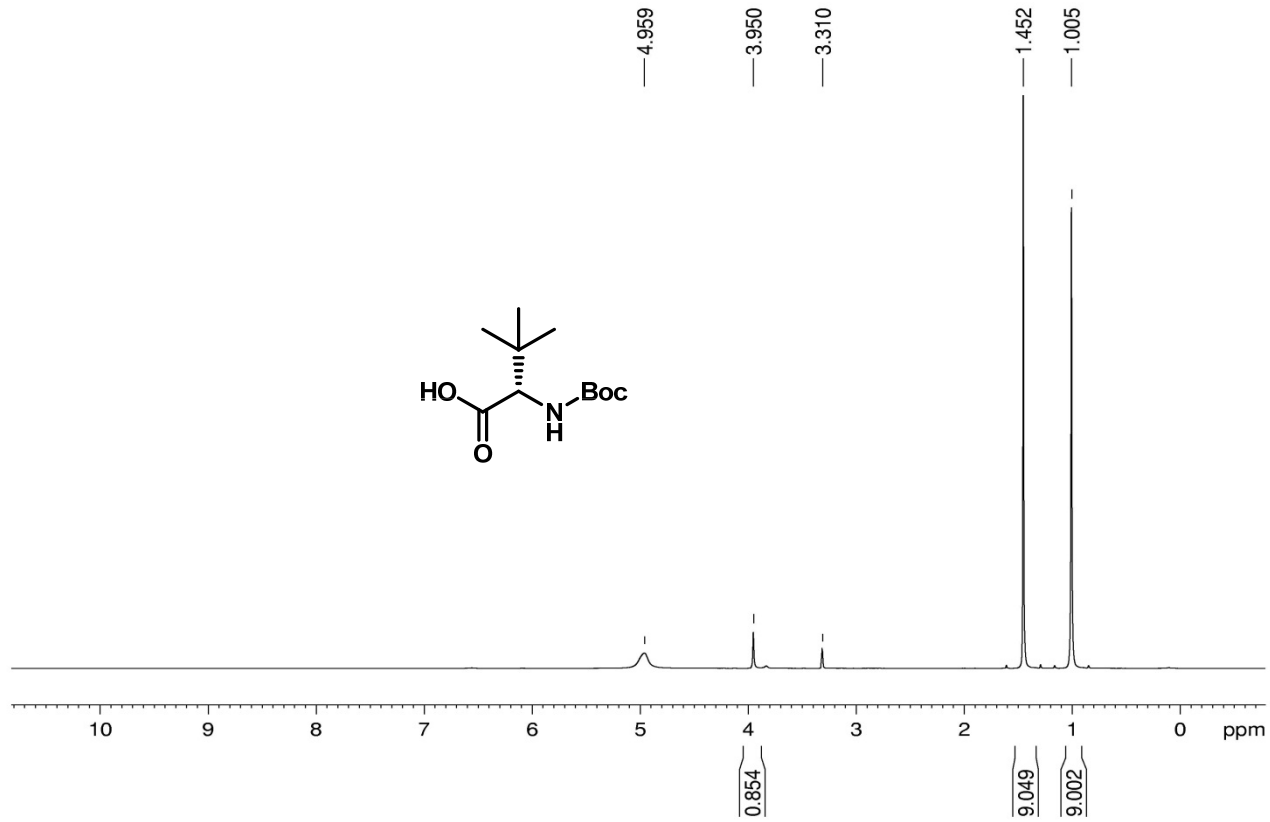
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Boc
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H
O
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9
8
7
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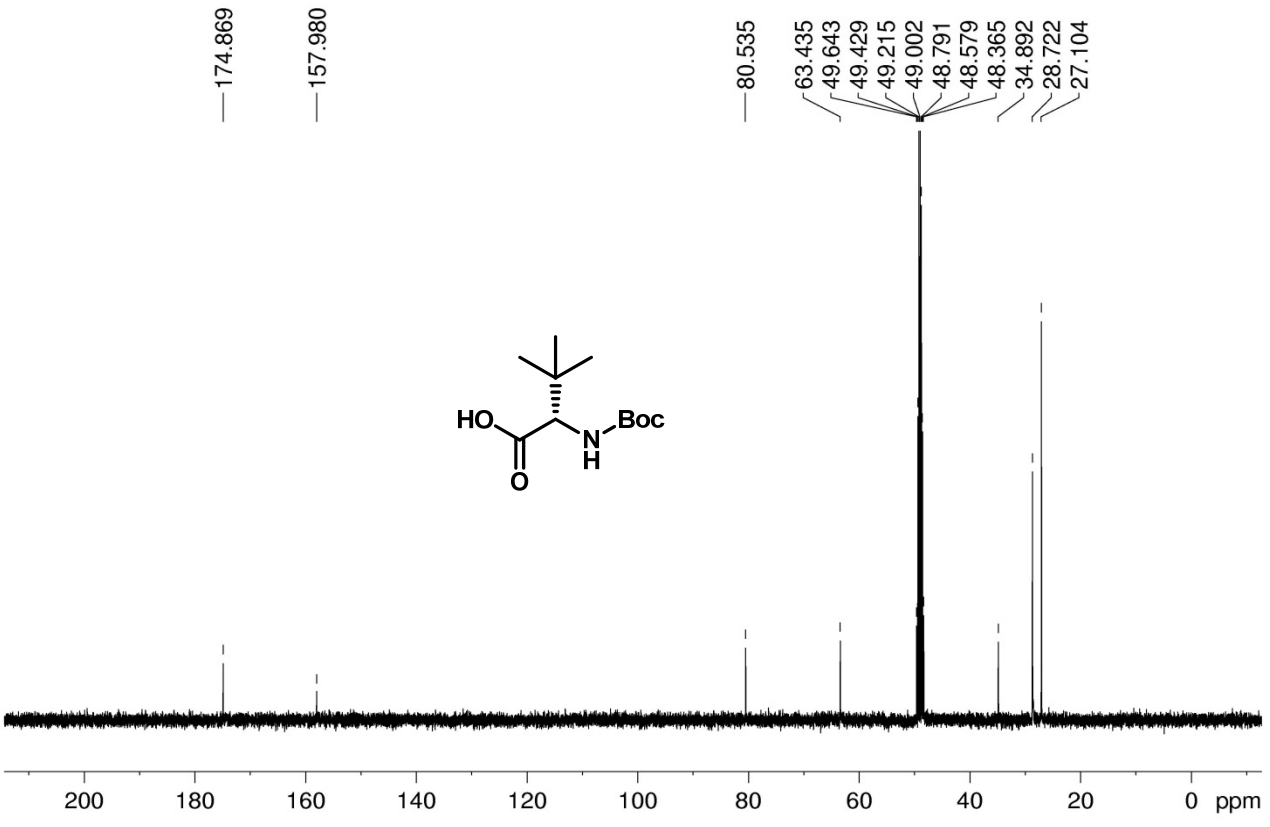
9.002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80.535
63.435
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49.429
49.215
49.002
48.791
48.579
48.365
34.892
28.722
27.104
HO
Boc
N
H
O
200
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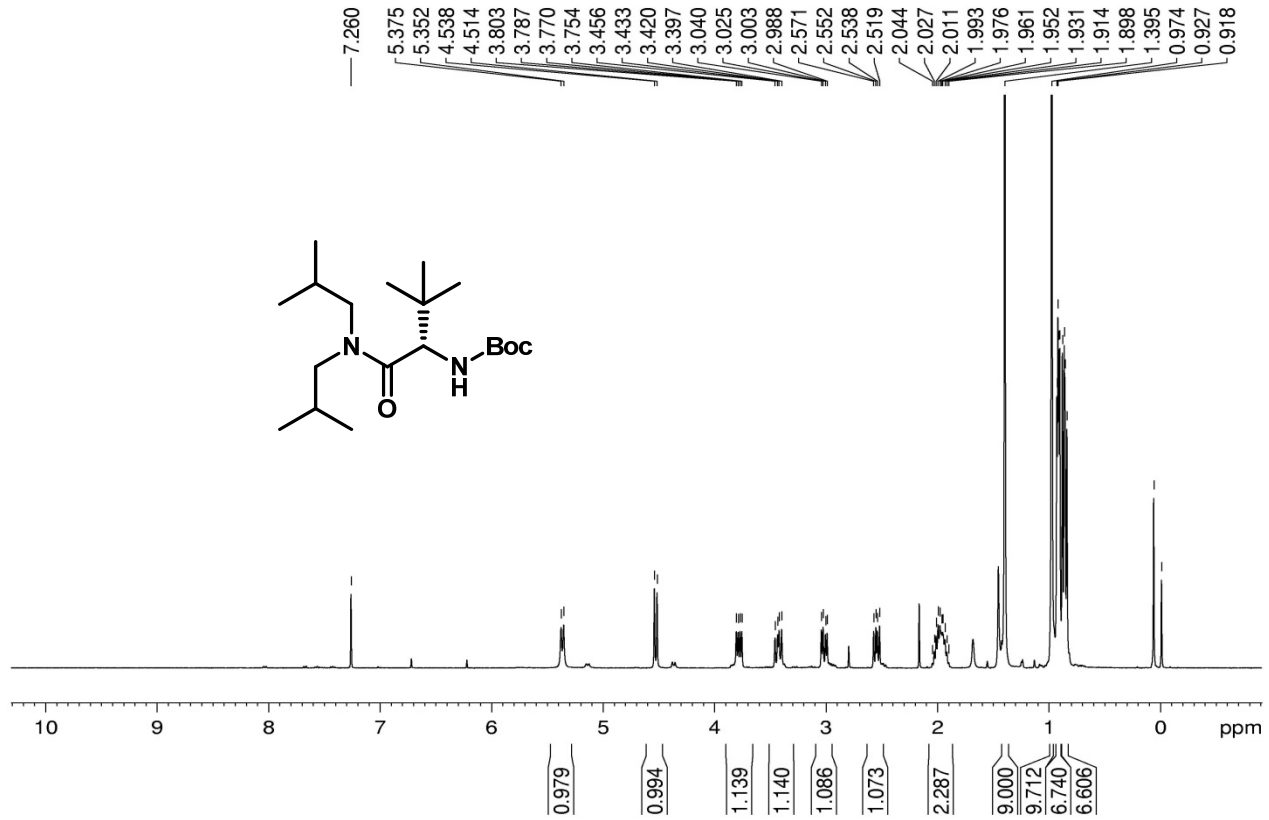
160
140
120
100
80
60
40
20
0
ppm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5.352
4.538
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3.787
3.770
3.754
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3.420
3.397
3.040
3.025
3.003
2.988
2.571
2.552
2.538
2.519
2.044
2.027
2.011
1.993
1.976
1.961
1.952
1.931
1.914
1.898
1.395
0.974
0.927
0.918
N
Boc
N
H
O
10
9
8
7
6
5
4
3
2
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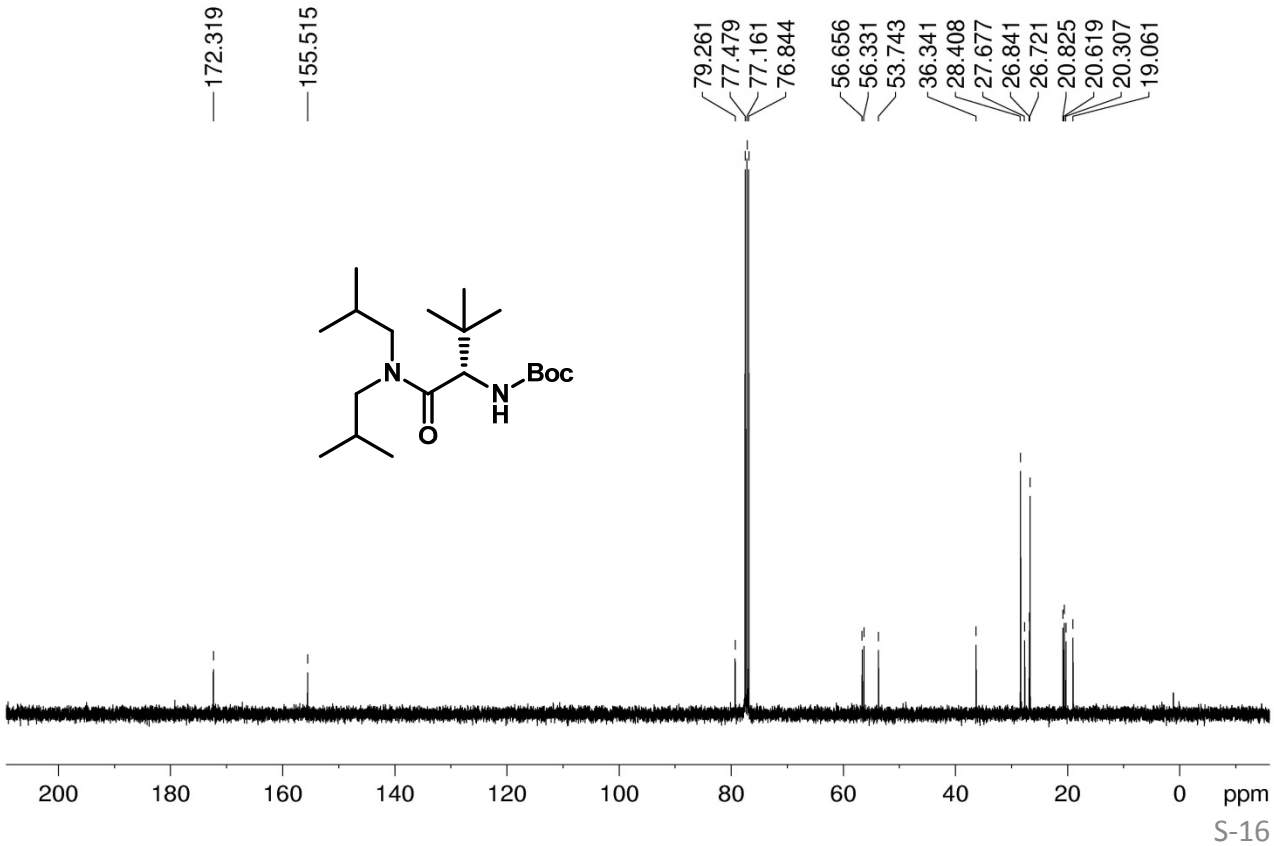
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77.161
76.844
56.656
56.331
53.743
36.341
28.408
27.677
26.841
26.721
20.825
20.619
20.307
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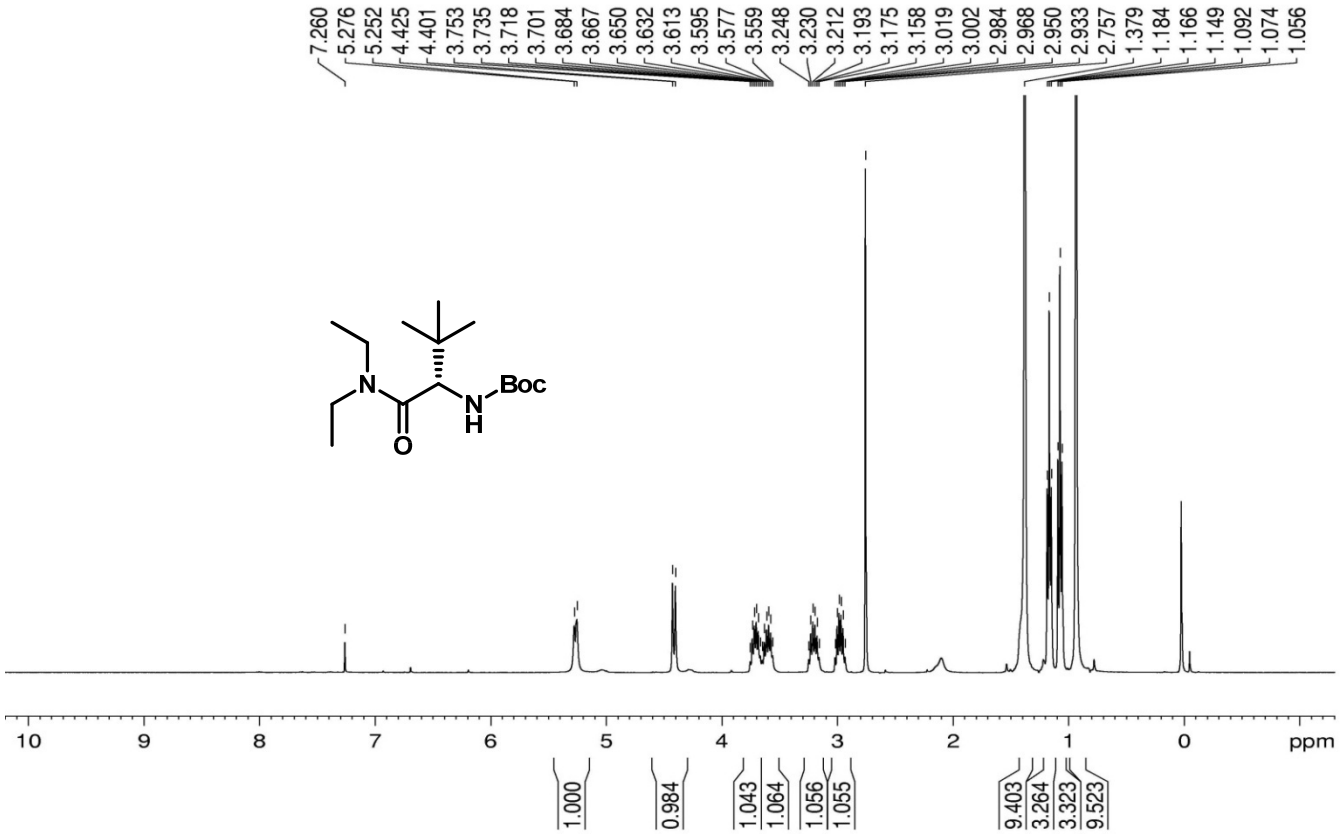
Boc
N
H
O
200
180
160
140
120
100
80
60
40
20
0
ppm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5.252
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4.401
3.753
3.735
3.718
3.701
3.684
3.667
3.650
3.632
3.613
3.595
3.577
3.559
3.248
3.230
3.212
3.193
3.175
3.158
3.019
3.002
2.984
2.968
2.950
2.933
2.757
1.379
1.184
1.166
1.149
1.092
1.074
1.056
N
Boc
N
H
O
10
9
8
7
6
5
4
3
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1.055
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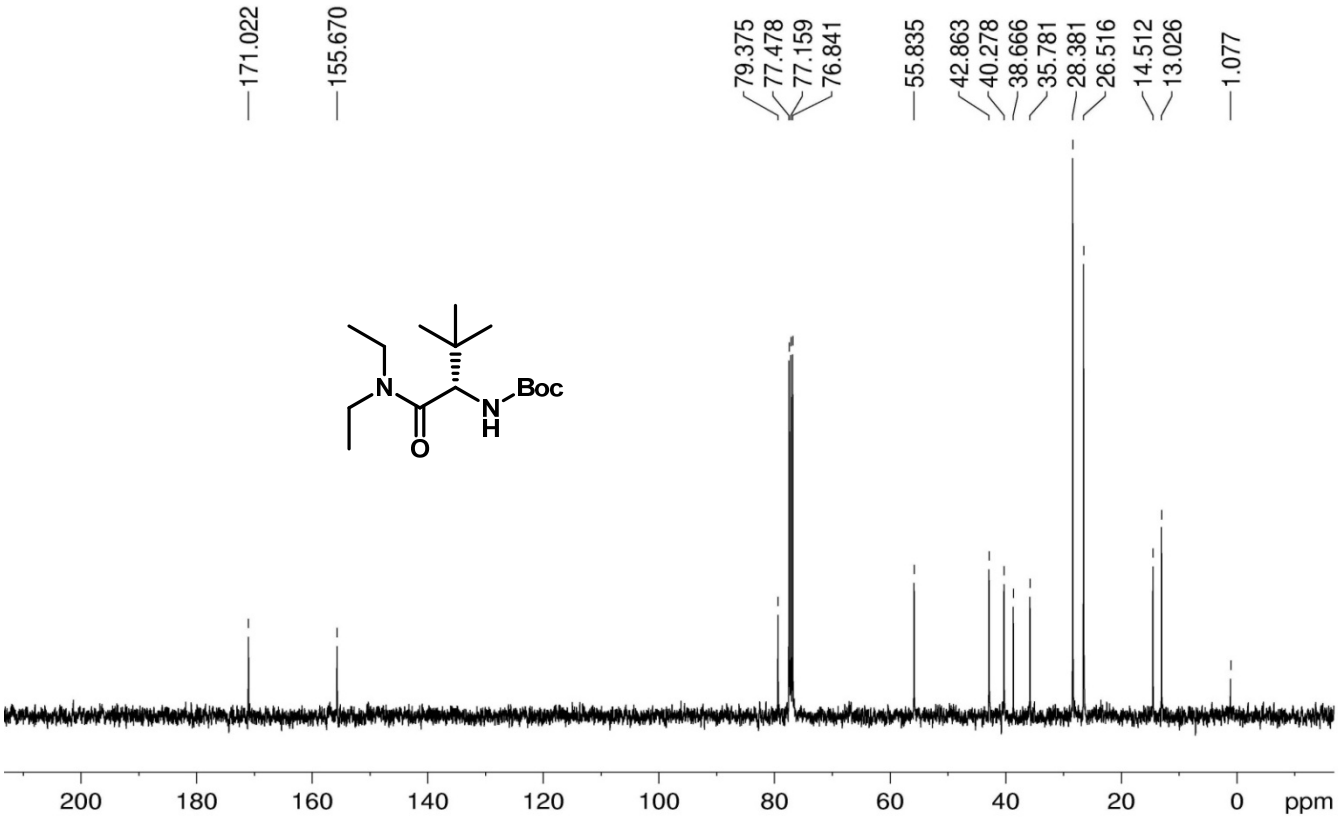
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76.841
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42.863
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38.666
35.781
28.381
26.516
14.512
13.026
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Boc
N
H
O
200
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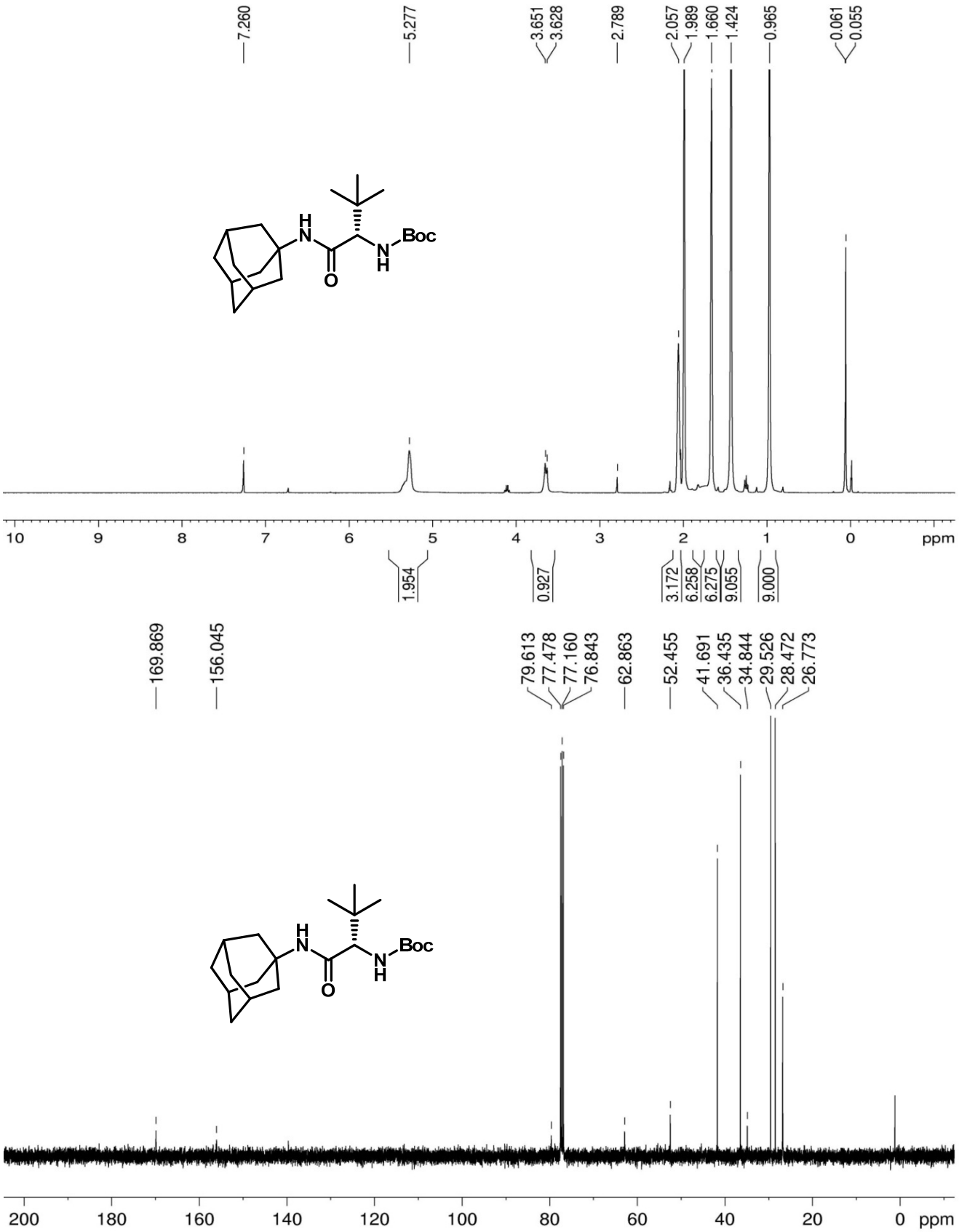
160
140
120
100
80
60
40
20
0
ppm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3.628
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1.660
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0.965
0.061
0.055
Boc
ppm
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0.927
3.172
6.258
6.275
9.055
9.000
169.869
156.045
79.613
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62.863
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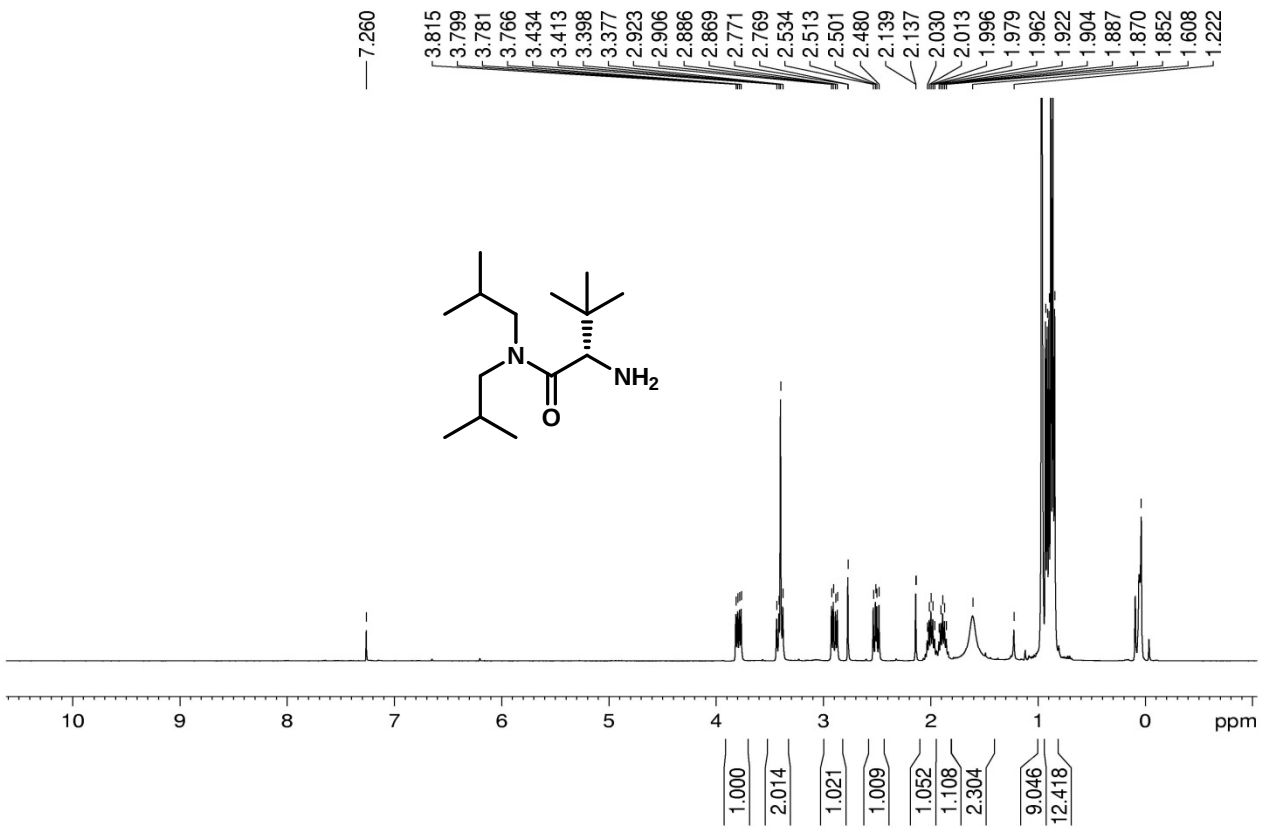
26.773
Boc
ppm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3.398
3.377
2.923
2.906
2.886
2.869
2.771
2.769
2.534
2.513
2.501
2.480
2.139
2.137
2.030
2.013
1.996
1.979
1.962
1.922
1.904
1.887
1.870
1.852
1.608
1.222
N
NH2
O
10
9
8
7
6
5
4
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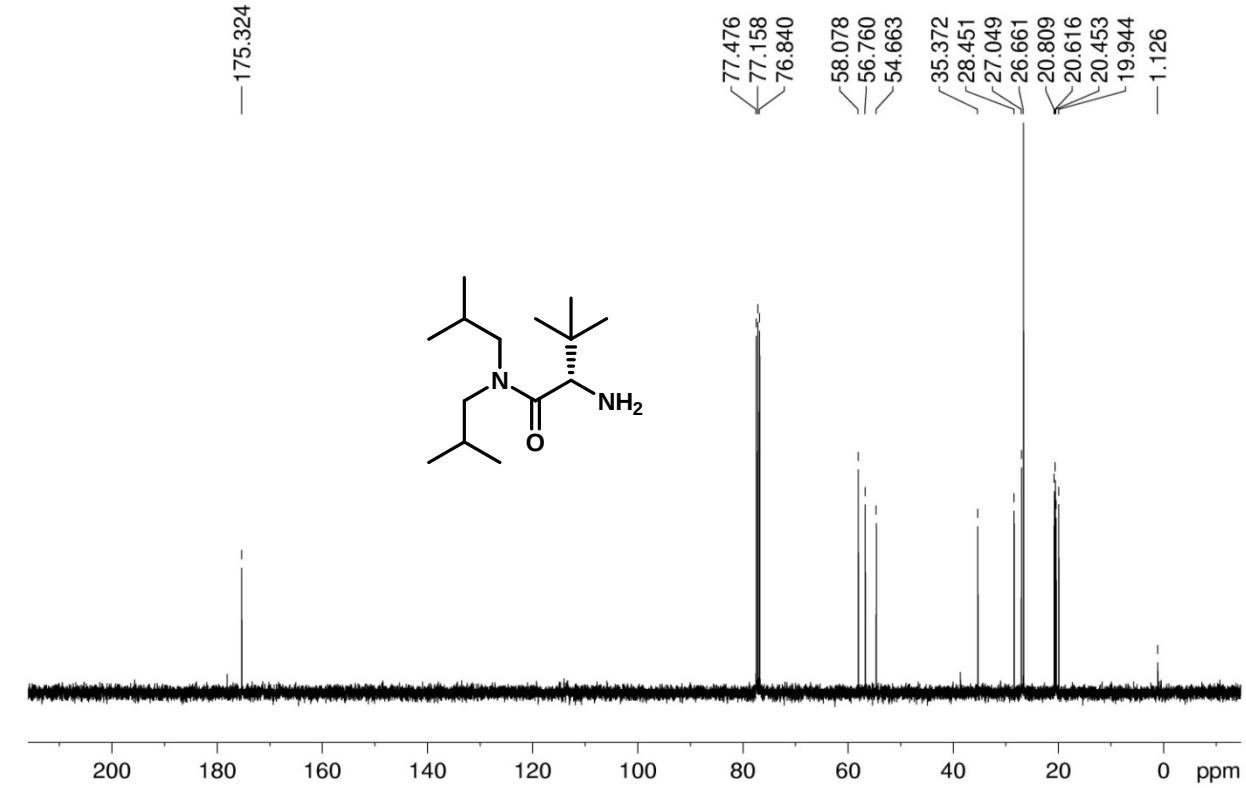
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54.663
35.372
28.451
27.049
26.661
20.809
20.616
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NH2
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120
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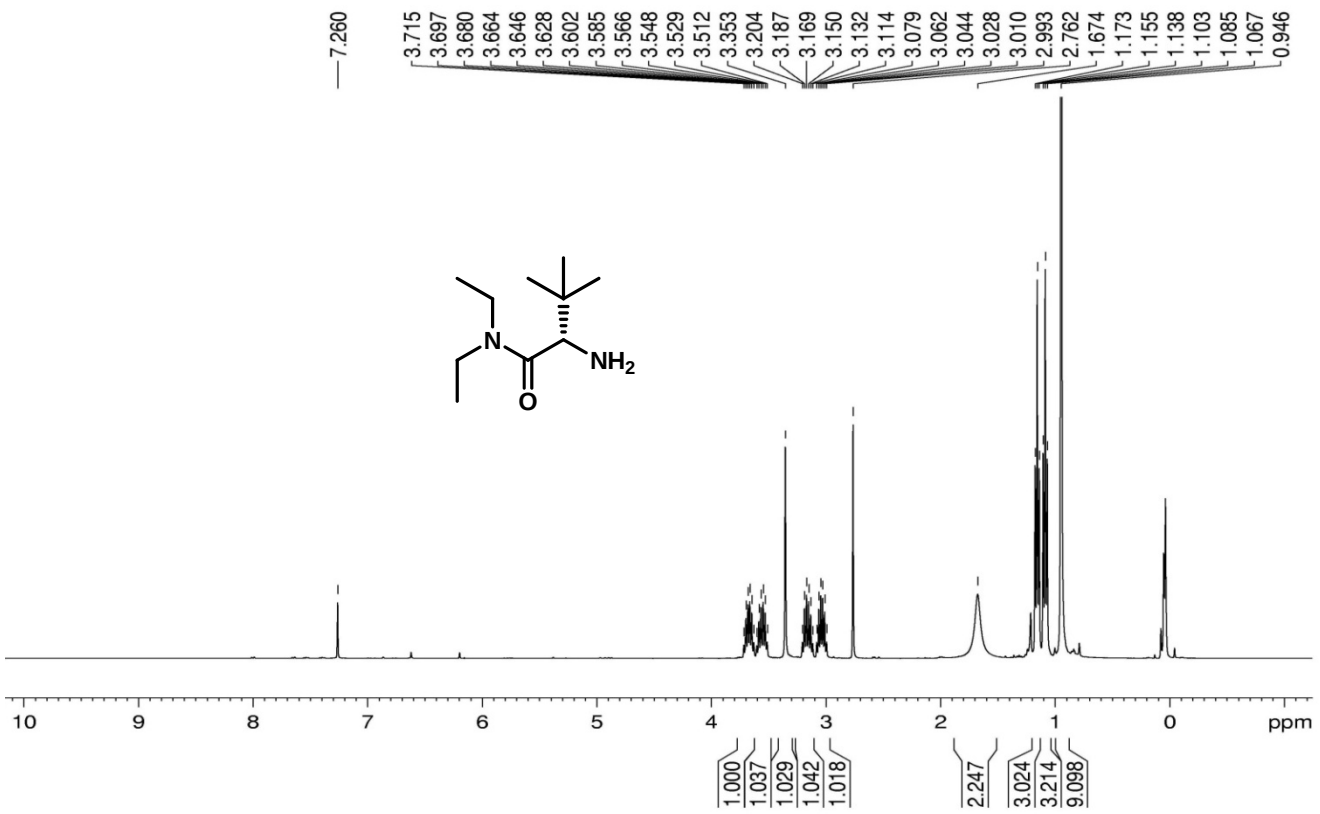
20
0
ppm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3.646
3.628
3.602
3.585
3.566
3.548
3.529
3.512
3.353
3.204
3.187
3.169
3.150
3.132
3.114
3.079
3.062
3.044
3.028
3.010
2.993
2.762
1.674
1.173
1.155
1.138
1.103
1.085
1.067
0.946
N
NH2
O
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9
8
7
6
5
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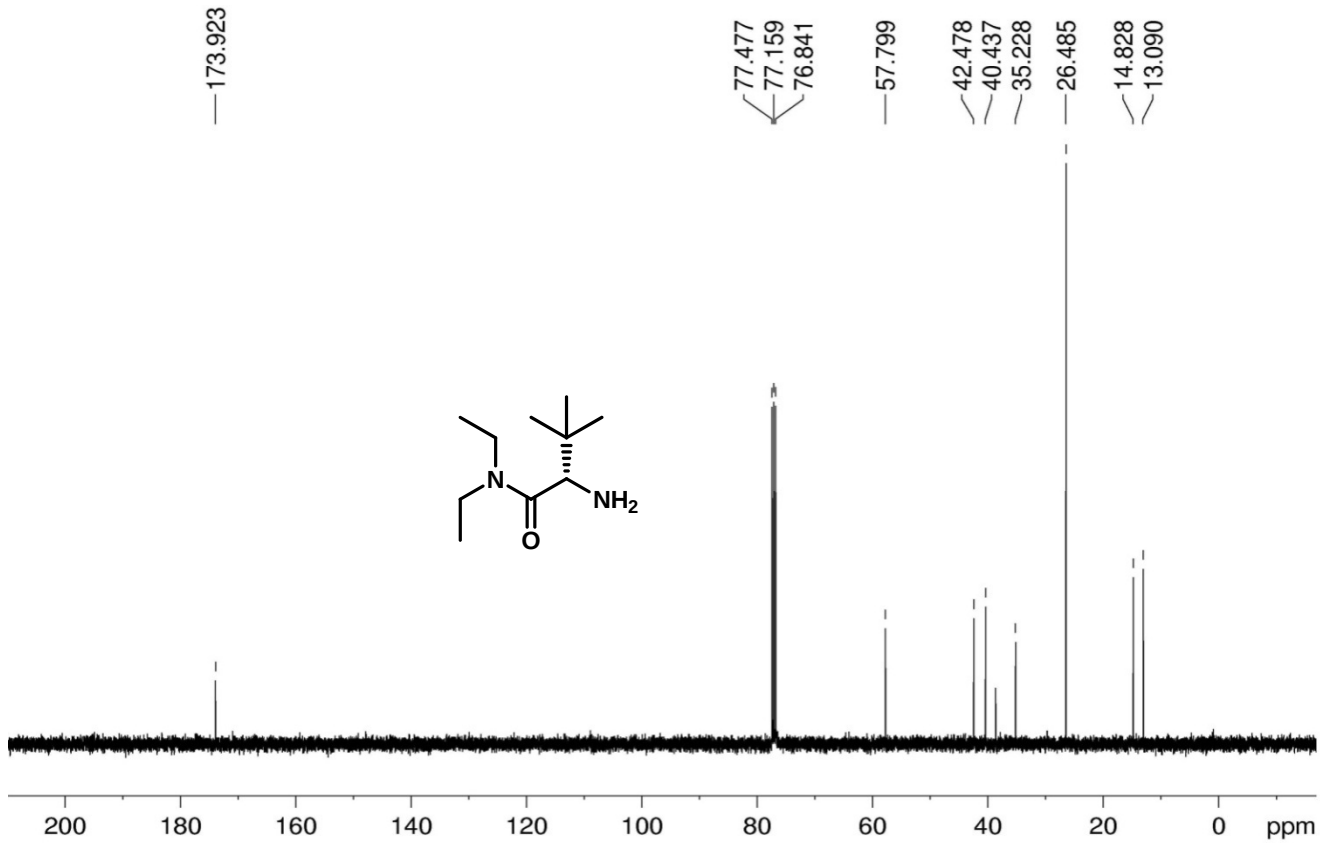
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140
120
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60
40
20
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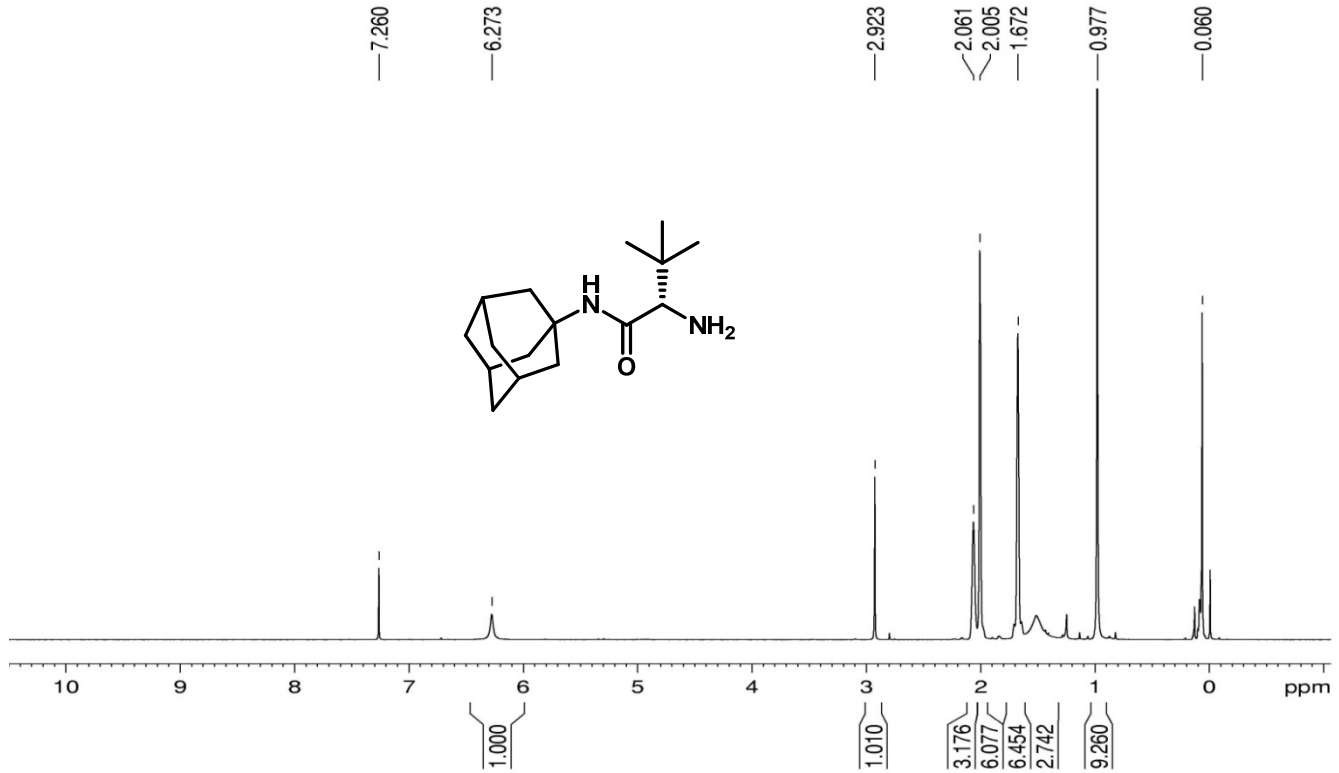
ppm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0.060
H
N
O
NH2
10
9
8
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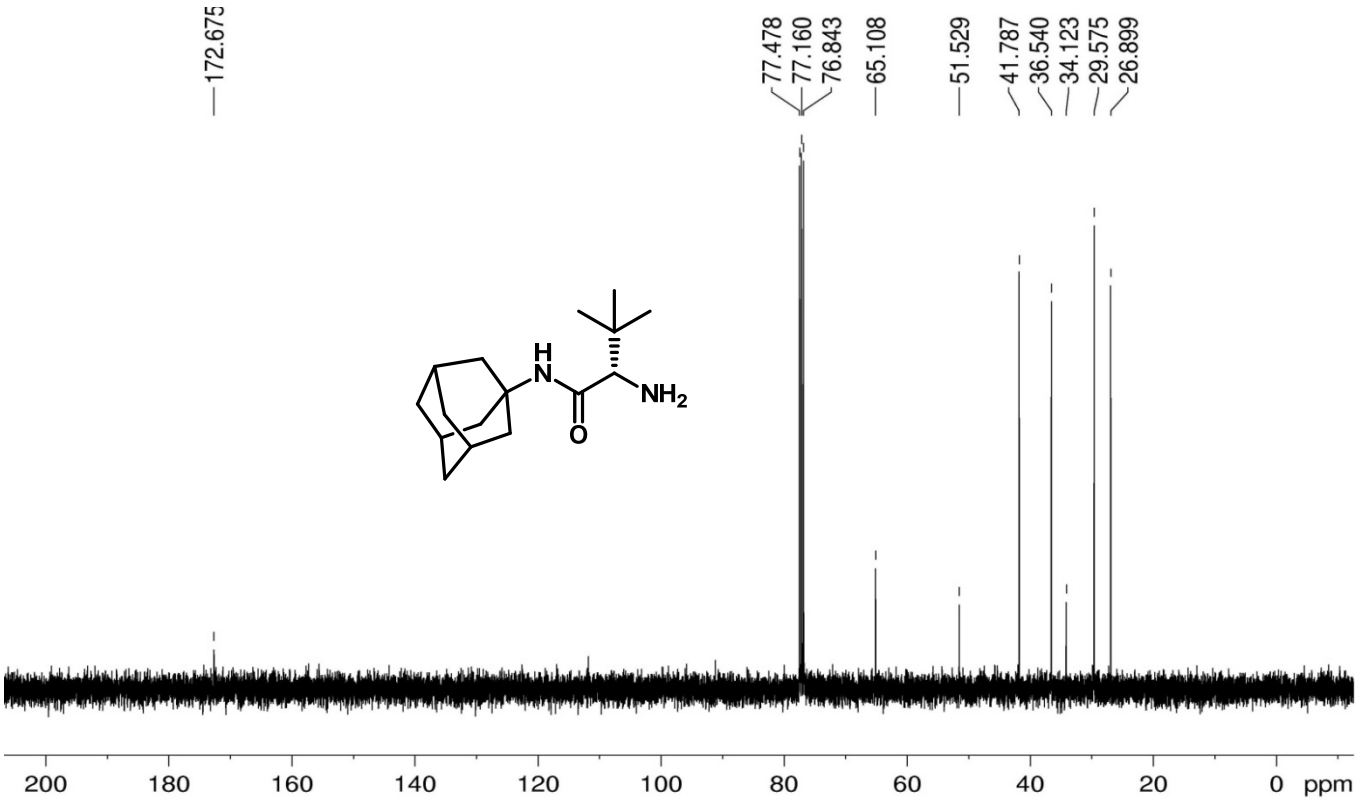
9.260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O
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120
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0
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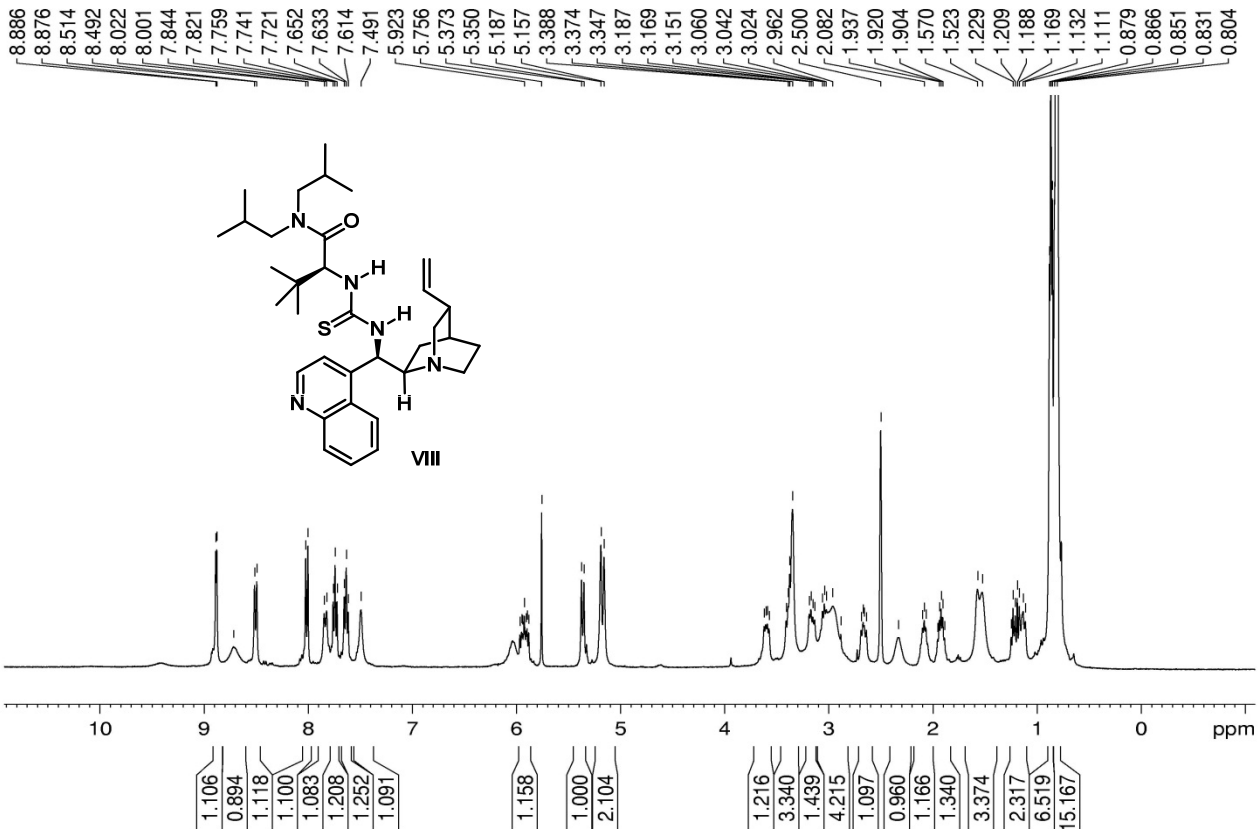
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7.614
7.491
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5.157
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3.347
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3.151
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3.024
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1.920
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1.570
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1.229
1.209
1.188
1.169
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0.866
0.851
0.831
0.804
VIII
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.100
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1.208
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1.158
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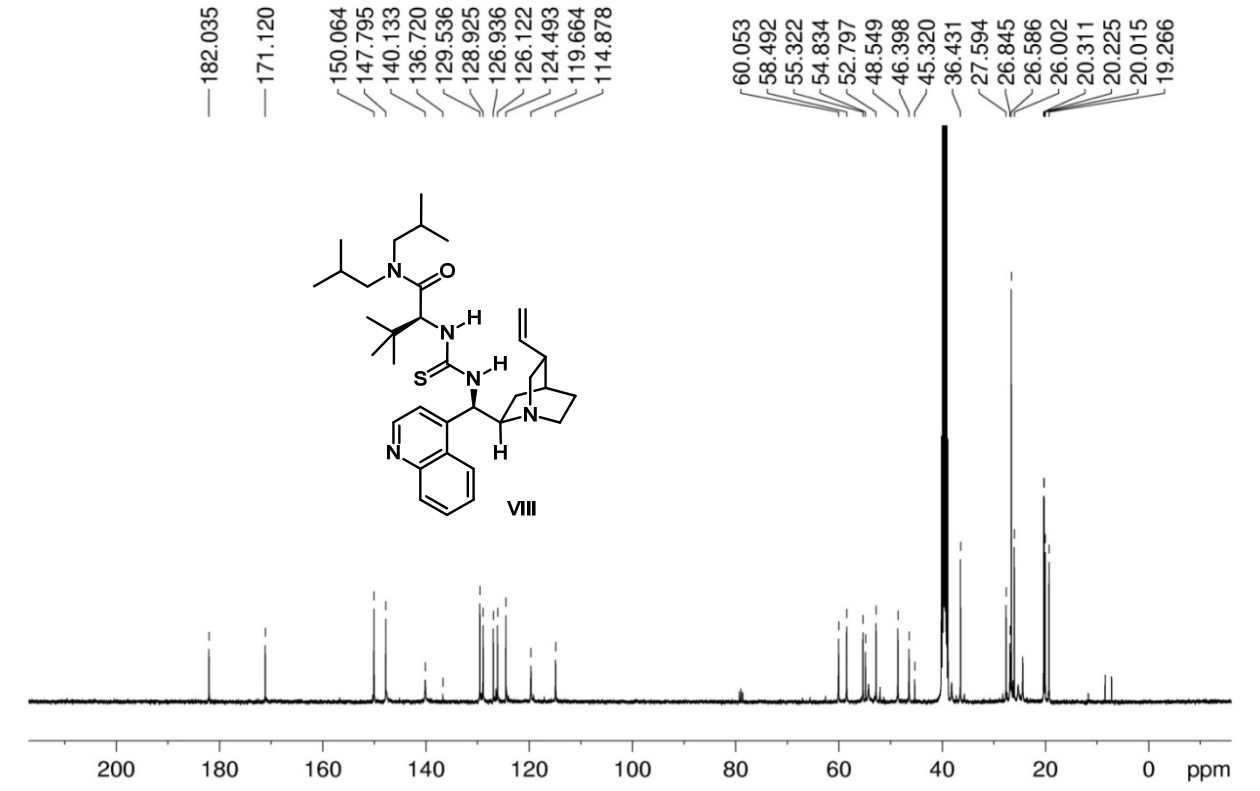
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114.878
60.053
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52.797
48.549
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45.320
36.431
27.594
26.845
26.586
26.002
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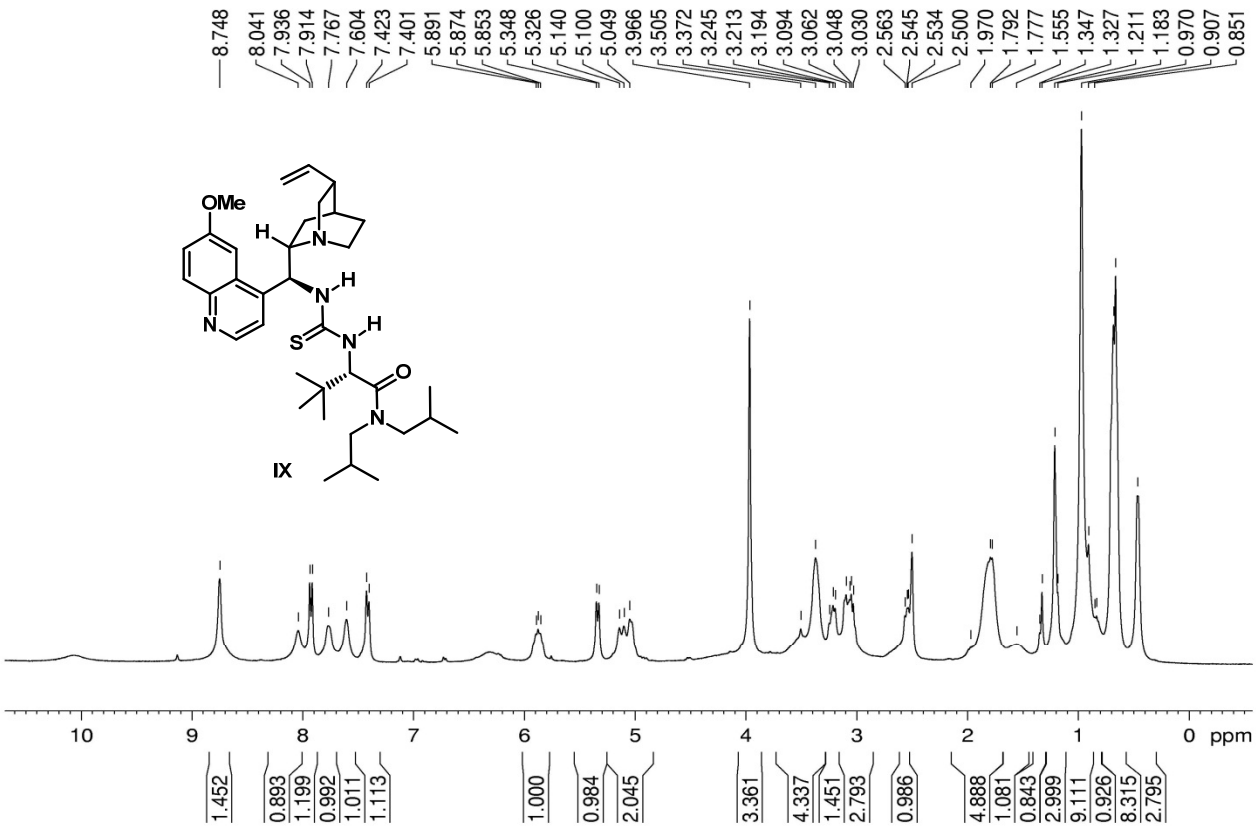
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5.326
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5.100
5.049
3.966
3.505
3.372
3.245
3.213
3.194
3.094
3.062
3.048
3.030
2.563
2.545
2.534
2.500
1.970
1.792
1.777
1.555
1.347
1.327
1.211
1.183
0.970
0.907
0.851
OMe
H
N
N
H
N
H
S
N
O
N
IX
10
9
8
7
6
5
4
3
2
1
0 ppm
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0.893
1.199
0.992
1.011
1.113
1.000
0.984
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3.361
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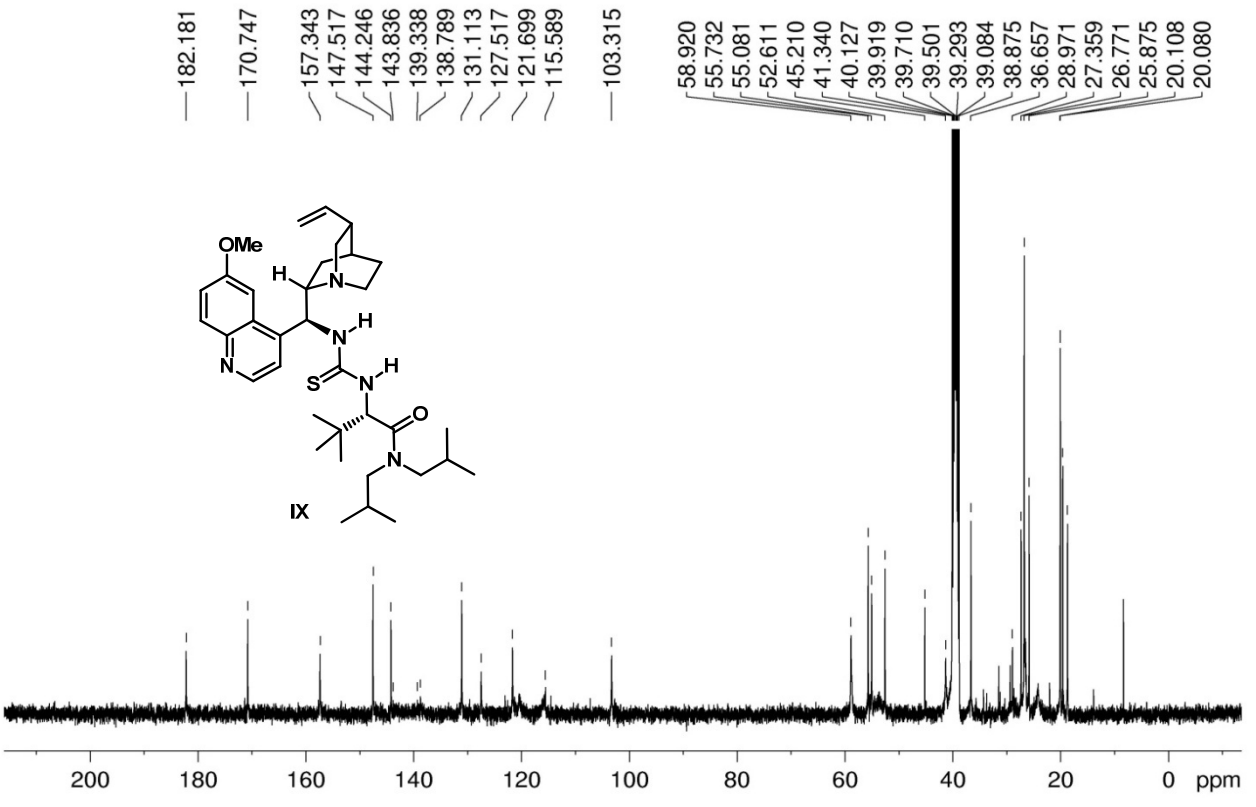
2.795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103.315
58.920
55.732
55.081
52.611
45.210
41.340
40.127
39.919
39.710
39.501
39.293
39.084
38.875
36.657
28.971
27.359
26.771
25.875
20.108
20.080
OMe
H
N
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O
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IX
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140
120
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20
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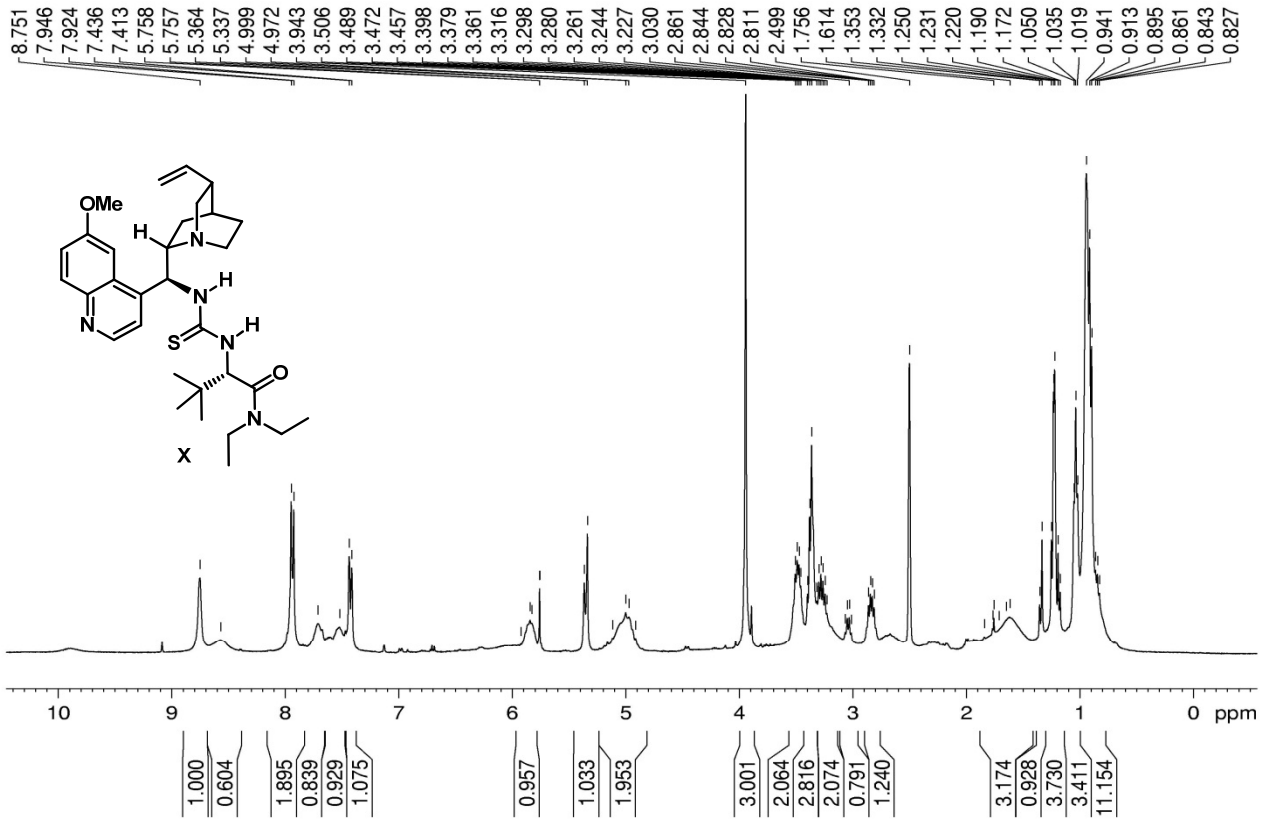
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3.457
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OMe
H
N
N
H
N
H
S
N
O
N
X
10
9
8
7
6
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2
1
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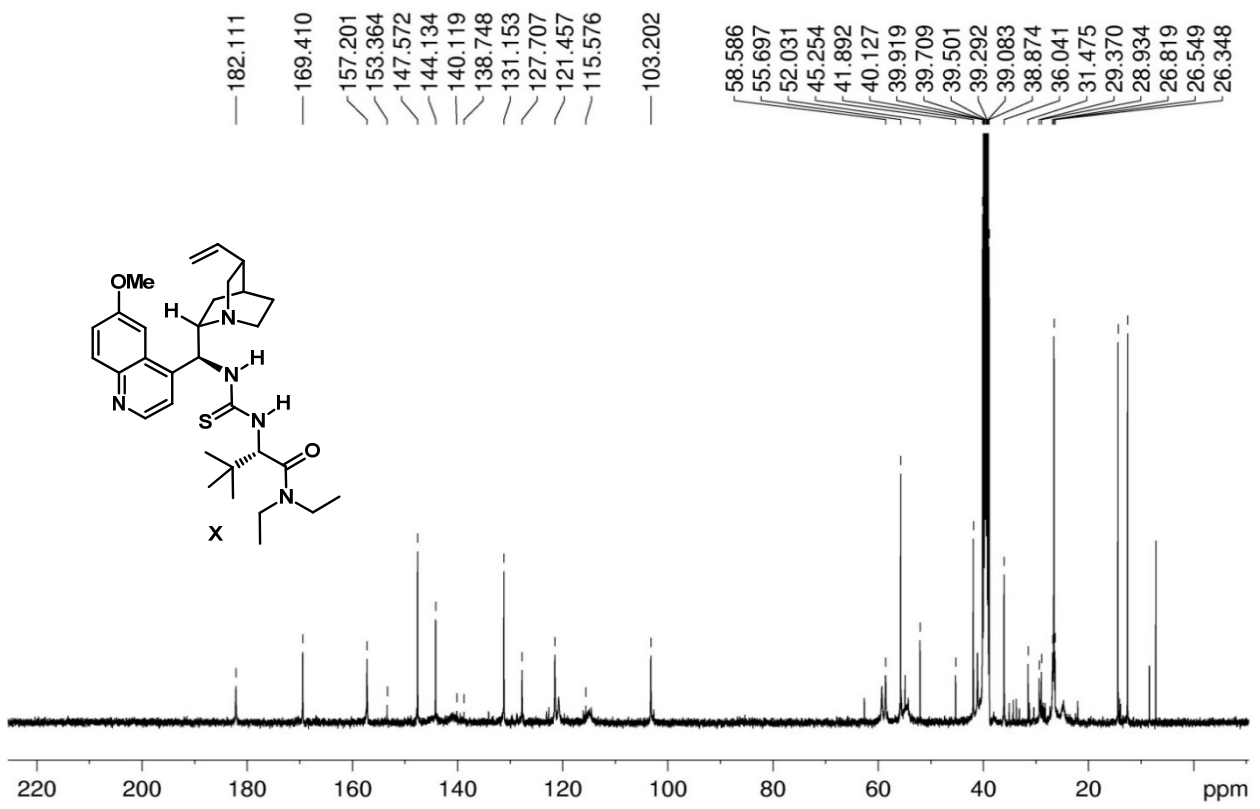
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45.254
41.892
40.127
39.919
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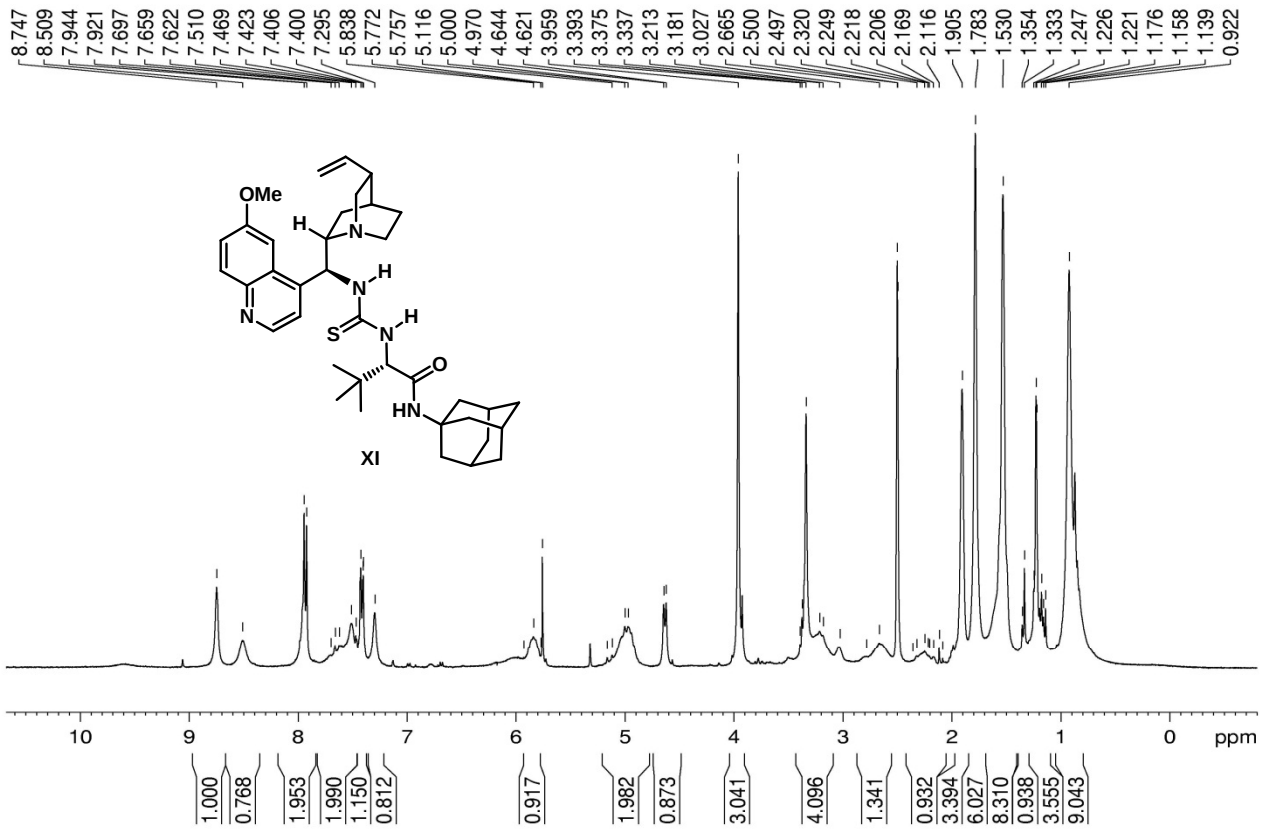
39.501
39.292
39.083
38.874
36.041
31.475
29.370
28.934
26.819
26.549
26.348
OMe
H
N
N
H
N
H
S
N
O
N
X
220
200
180
160
140
120
100
80
60
40
20
ppm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7.944
7.921
7.697
7.659
7.622
7.510
7.469
7.423
7.406
7.400
7.295
5.838
5.772
5.757
5.116
5.000
4.970
4.644
4.621
3.959
3.393
3.375
3.337
3.213
3.181
3.027
2.665
2.500
2.497
2.320
2.249
2.218
2.206
2.169
2.116
1.905
1.783
1.530
1.354
1.333
1.247
1.226
1.221
1.176
1.158
1.139
0.922
OMe
H
N
H
N
N
H
S
N
H
O
HN
XI
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
0.768
1.953
1.990
1.150
0.812
0.917
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4.096
1.341
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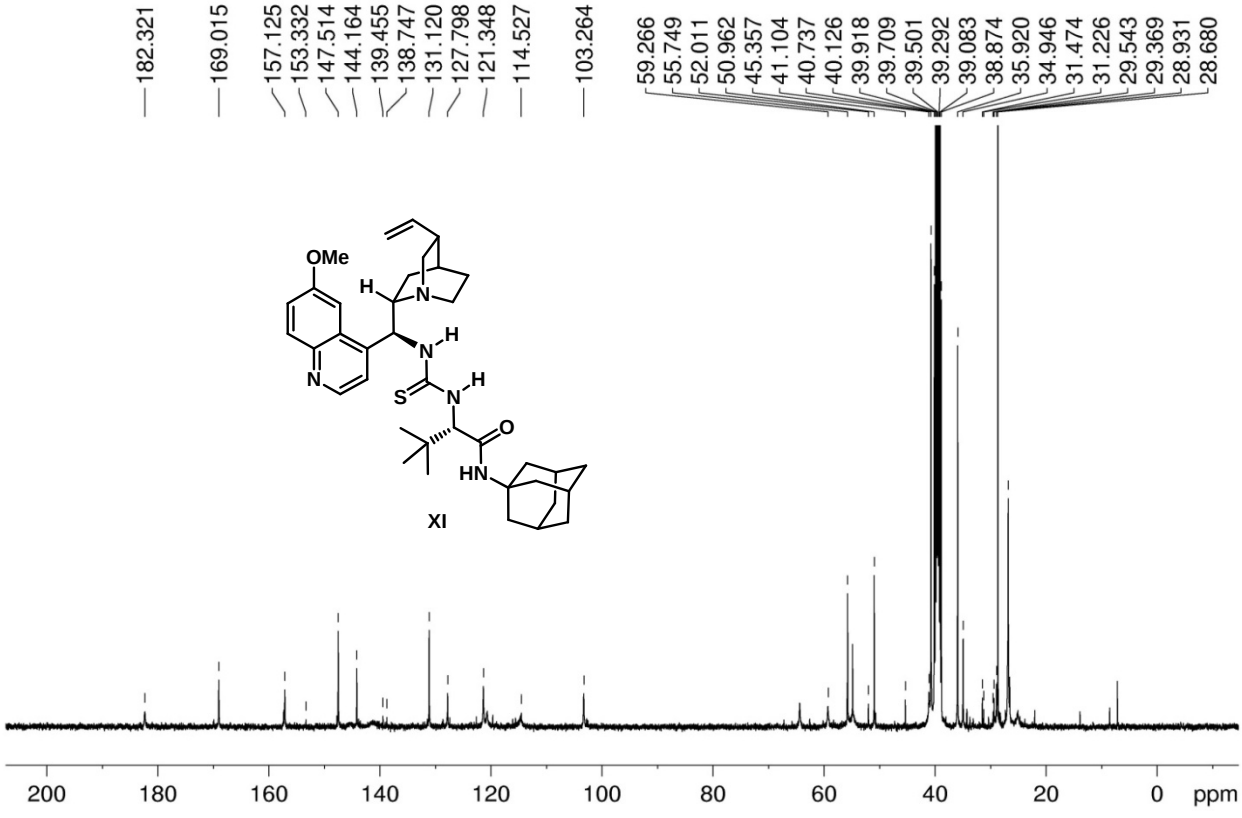
9.043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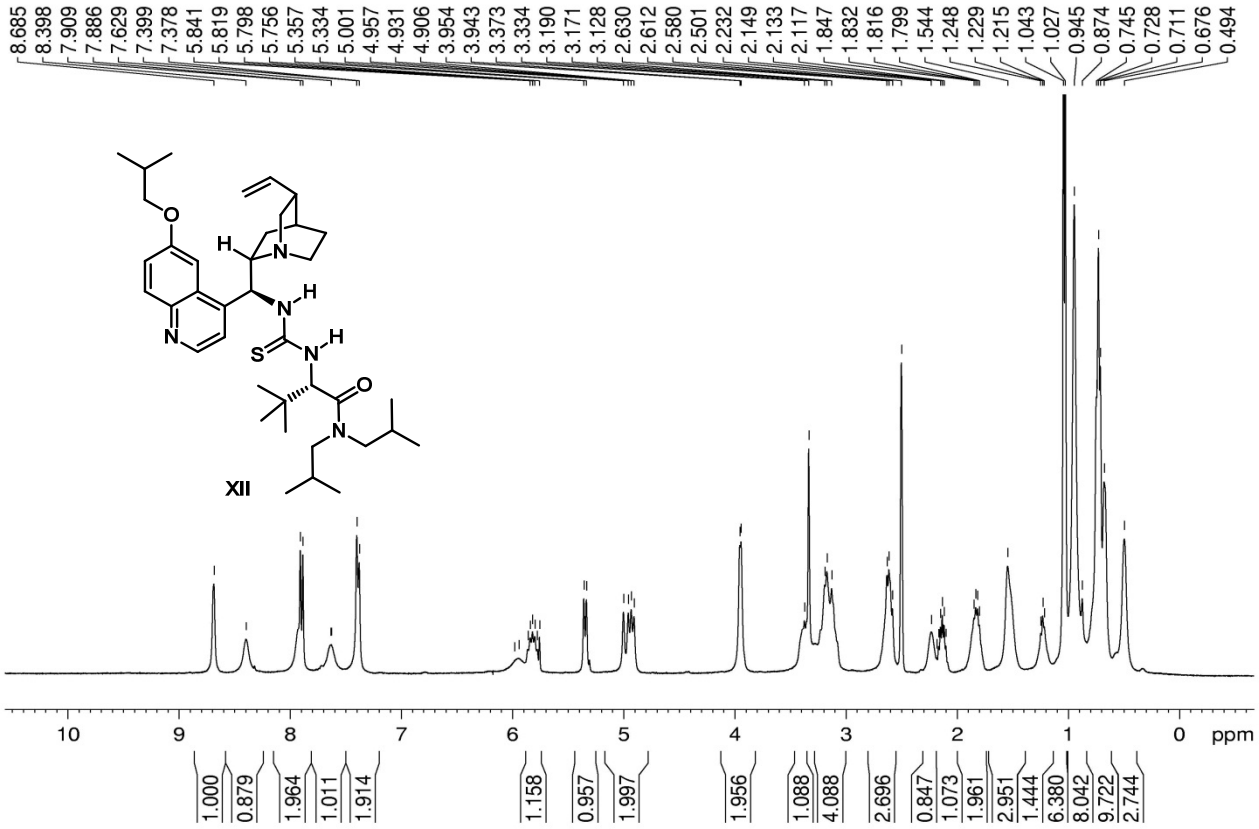
157.125
153.332
147.514
144.164
139.455
138.747
131.120
127.798
121.348
114.527
103.264
59.266
55.749
52.011
50.962
45.357
41.104
40.737
40.126
39.918
39.709
39.501
39.292
39.083
38.874
35.920
34.946
31.474
31.226
29.543
29.369
28.931
28.680
OMe
H
N
H
N
N
H
S
N
H
O
HN
XI
200
180
160
140
120
100
80
60
40
20
0
ppm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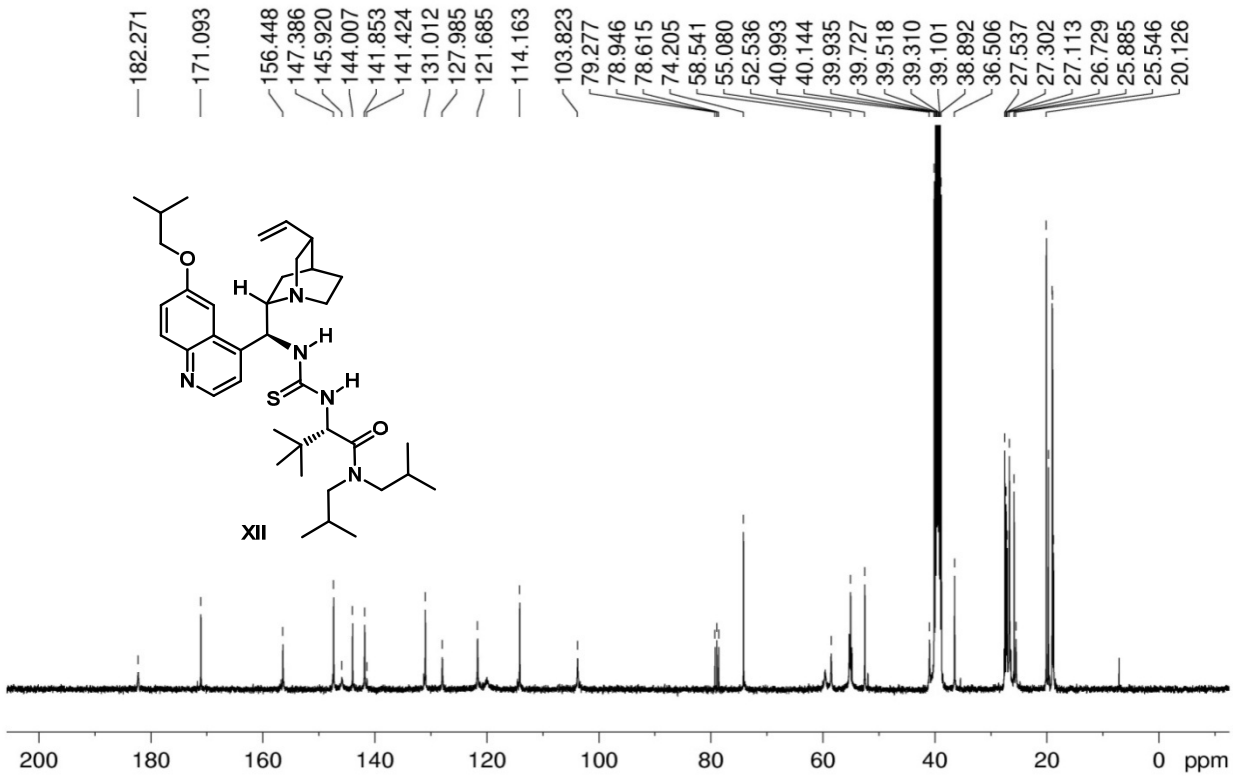
7.909
7.886
7.629
7.399
7.378
5.841
5.819
5.798
5.756
5.357
5.334
5.001
4.957
4.931
4.906
3.954
3.943
3.373
3.334
3.190
3.171
3.128
2.630
2.612
2.580
2.501
2.232
2.149
2.133
2.117
1.847
1.832
1.816
1.799
1.544
1.248
1.229
1.215
1.043
1.027
0.945
0.874
0.745
0.728
0.711
0.676
0.494
XII
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
0.879
1.964
1.011
1.914
1.158
0.957
1.997
1.956
1.088
4.088
2.696
0.847
1.073
1.961
2.951
1.444
6.380
8.042
9.722
2.744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156.448
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145.920
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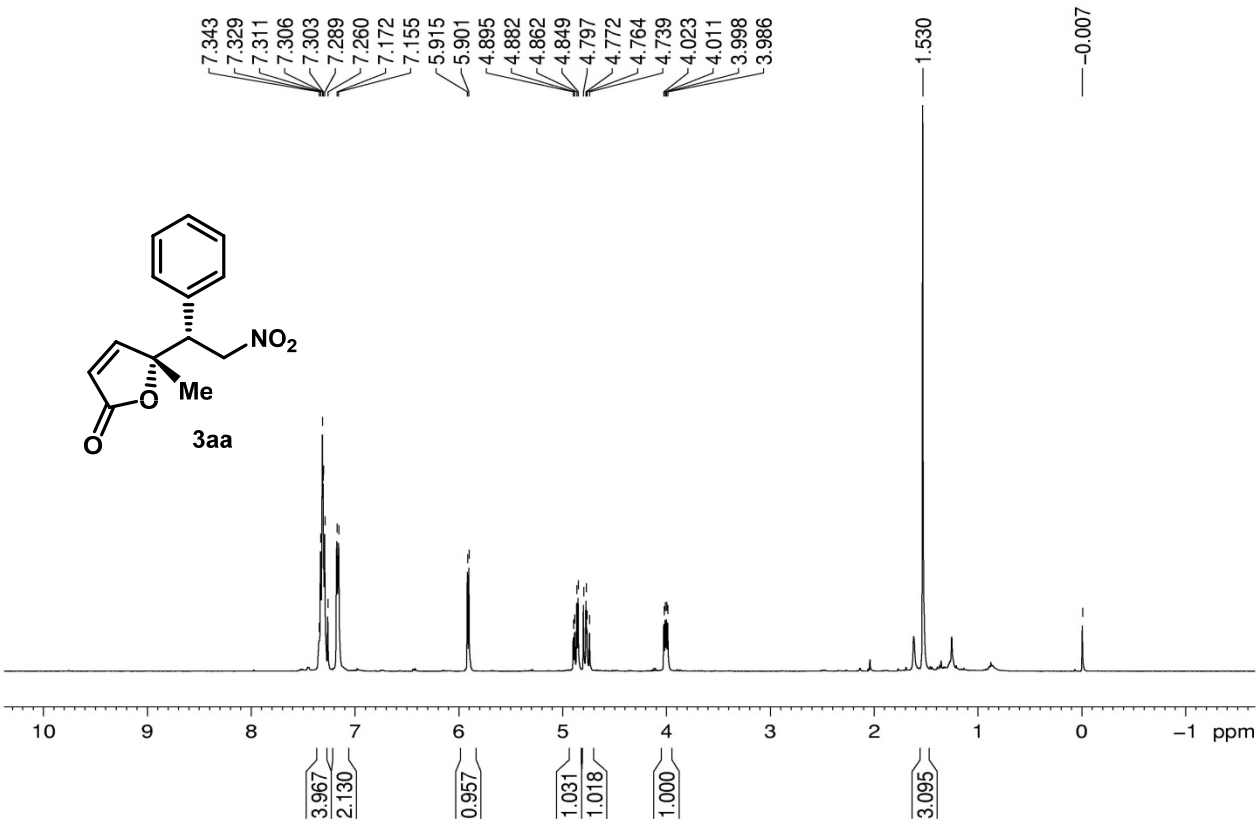
141.853
141.424
131.012
127.985
121.685
114.163
103.823
79.277
78.946
78.615
74.205
58.541
55.080
52.536
40.993
40.144
39.935
39.727
39.518
39.310
39.101
38.892
36.506
27.537
27.302
27.113
26.729
25.885
25.546
20.126
XII
200
180
160
140
120
100
80
60
40
20
0
ppm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7.329
7.311
7.306
7.303
7.289
7.260
7.172
7.155
5.915
5.901
4.895
4.882
4.862
4.849
4.797
4.772
4.764
4.739
4.023
4.011
3.998
3.986
1.530
0.007
NO2
Me
O
O
3aa
10
9
8
7
6
5
4
3
2
1
0
−1 ppm
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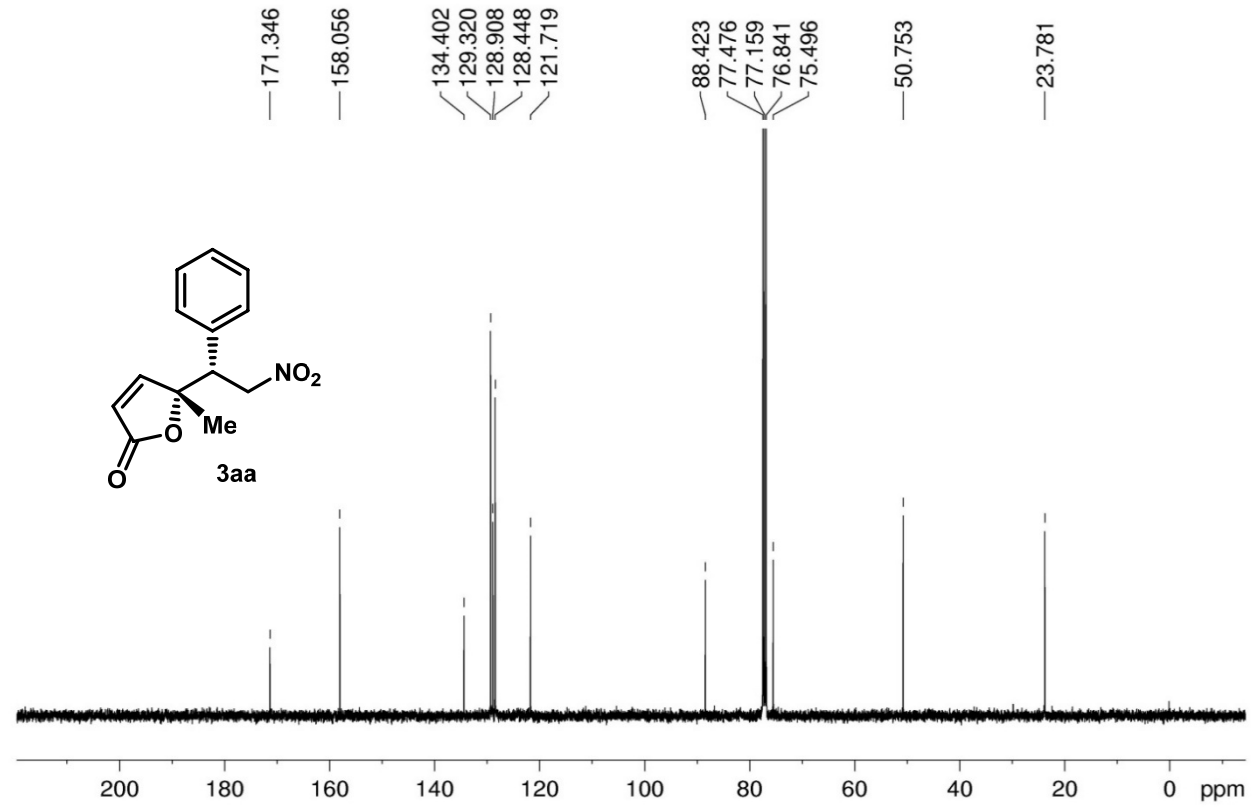
2.130
0.957
1.031
1.018
1.000
3.095


171.346
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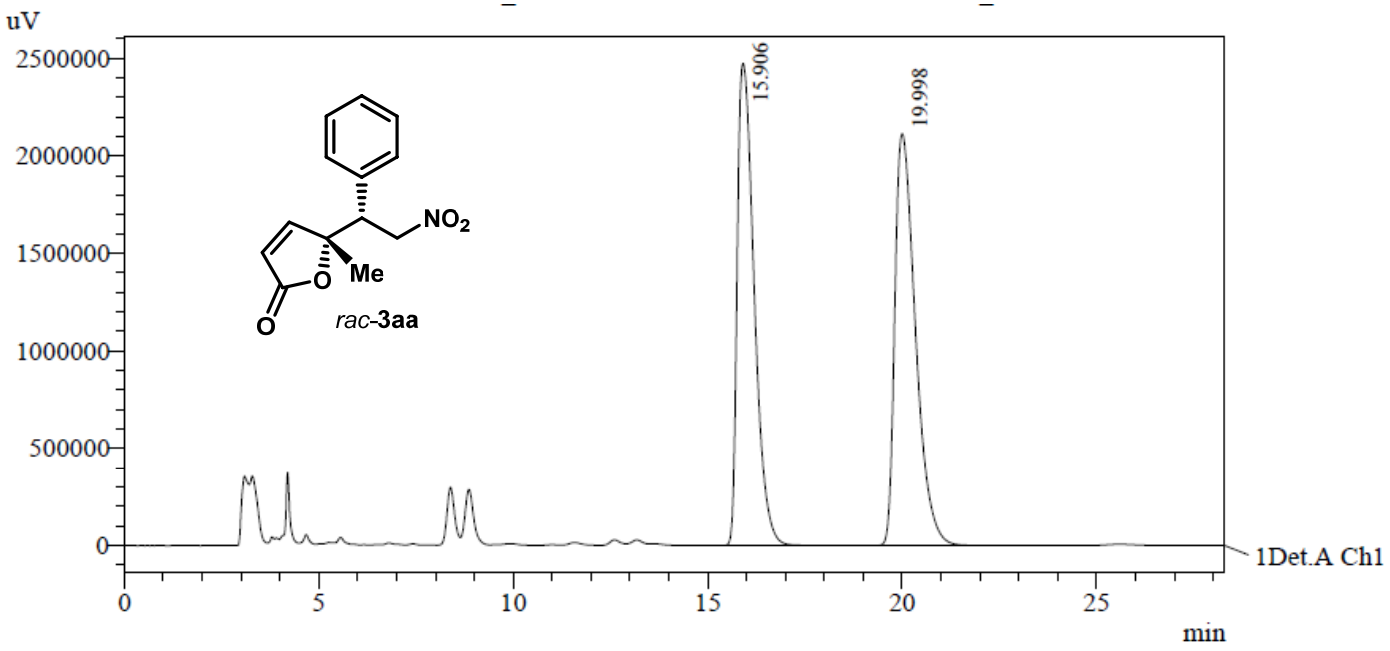
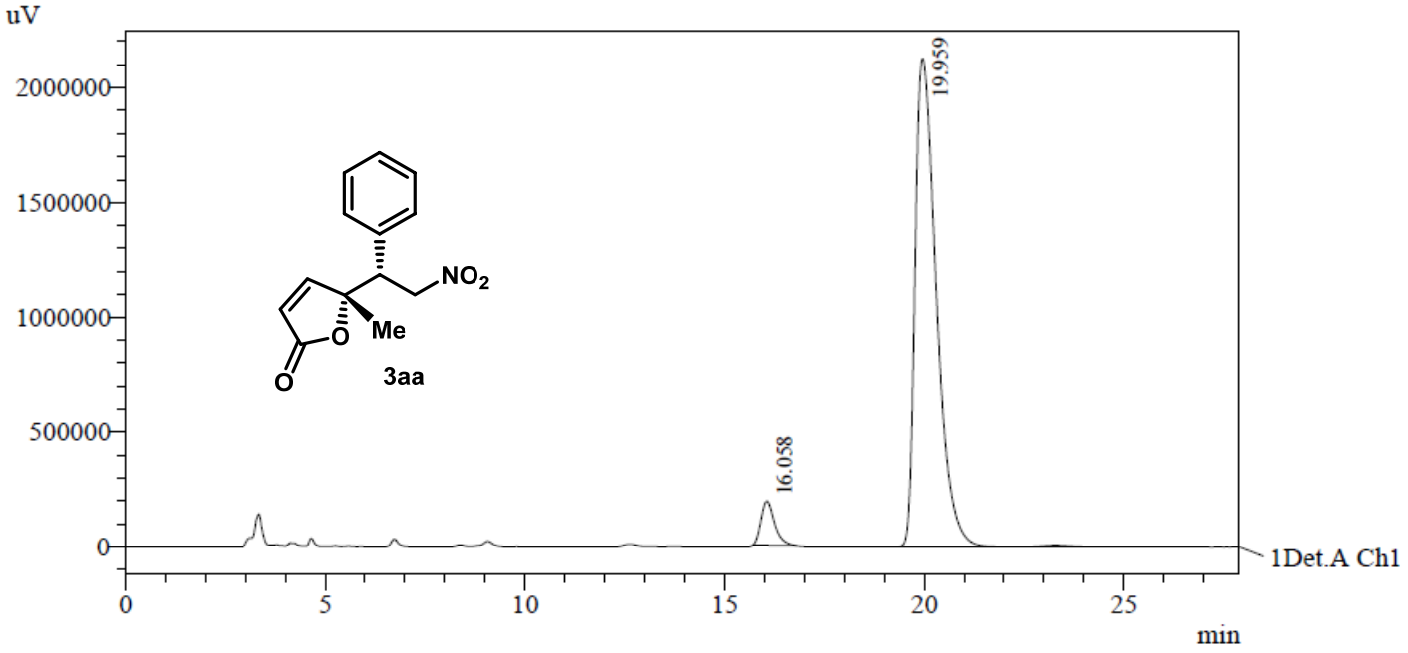
134.402
129.320
128.908
128.448
121.719
88.423
77.476
77.159
76.841
75.496
50.753
23.781
NO2
Me
O
O
3aa
200
180
160
140
120
100
80
60
40
20
0 ppm



PeakTable

Detector A Ch1 210nm

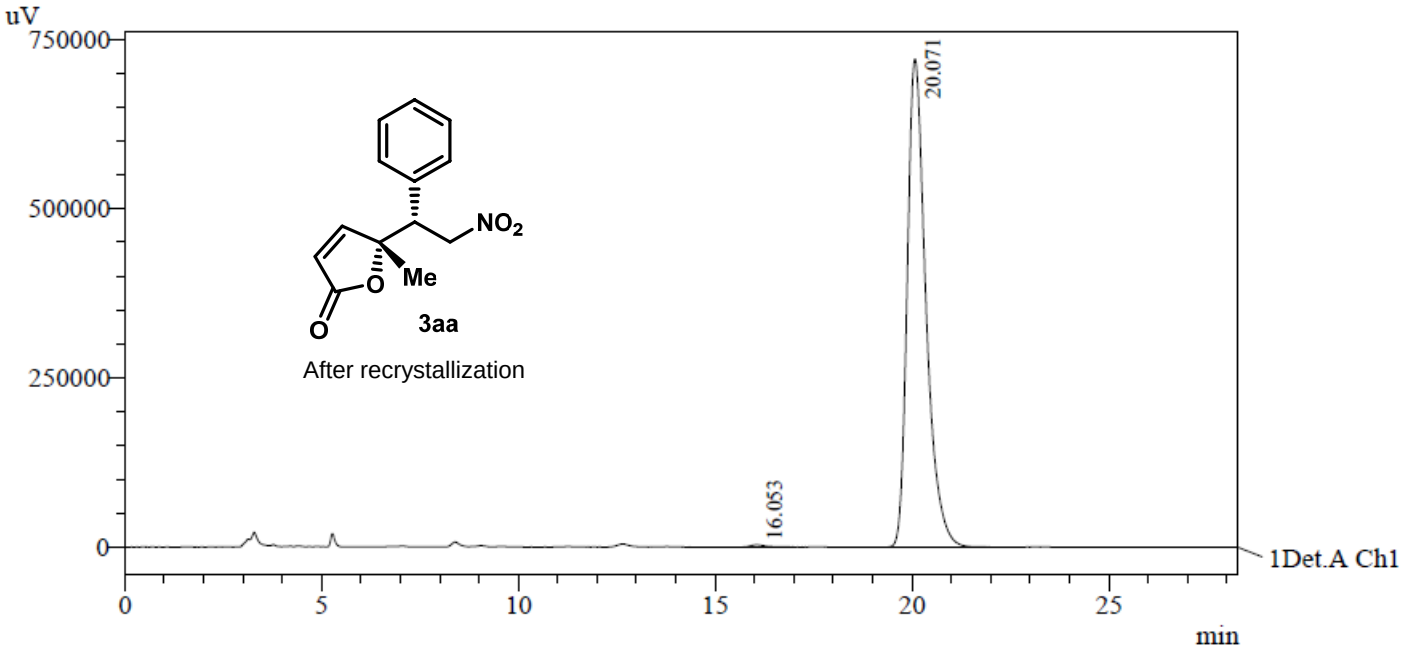
Peak#	Ret. Time	Area	Area %
1	15.906	74738100	48.991
2	19.998	77816421	51.009
Total		152554520	100.000



PeakTable

Detector A Ch1 210nm

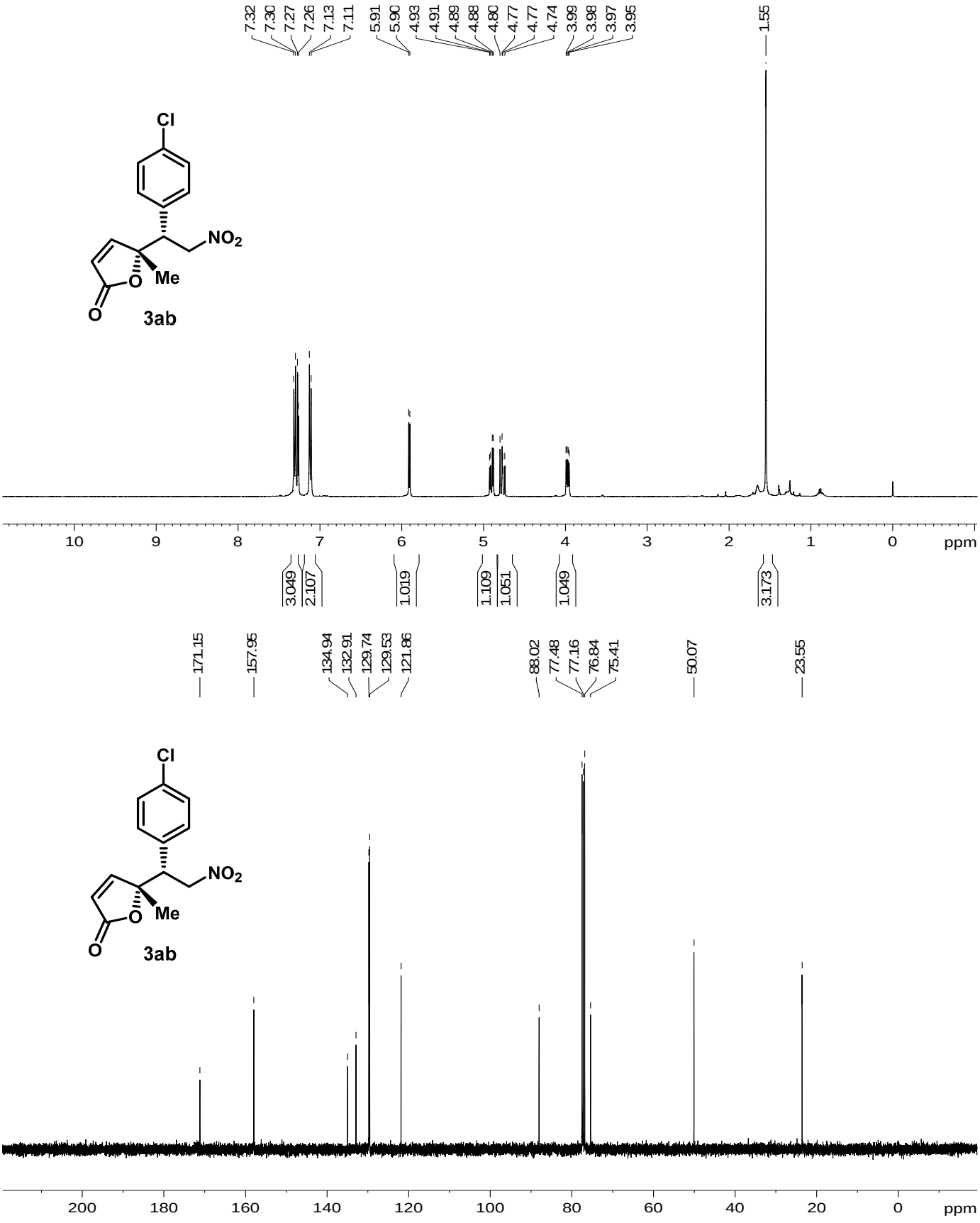
Peak#	Ret. Time	Area	Area %
1	16.058	4604234	5.502
2	19.959	79071492	94.498
Total		83675726	100.000



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	16.053	85559	0.359
2	20.071	23776017	99.641
Total		23861575	100.000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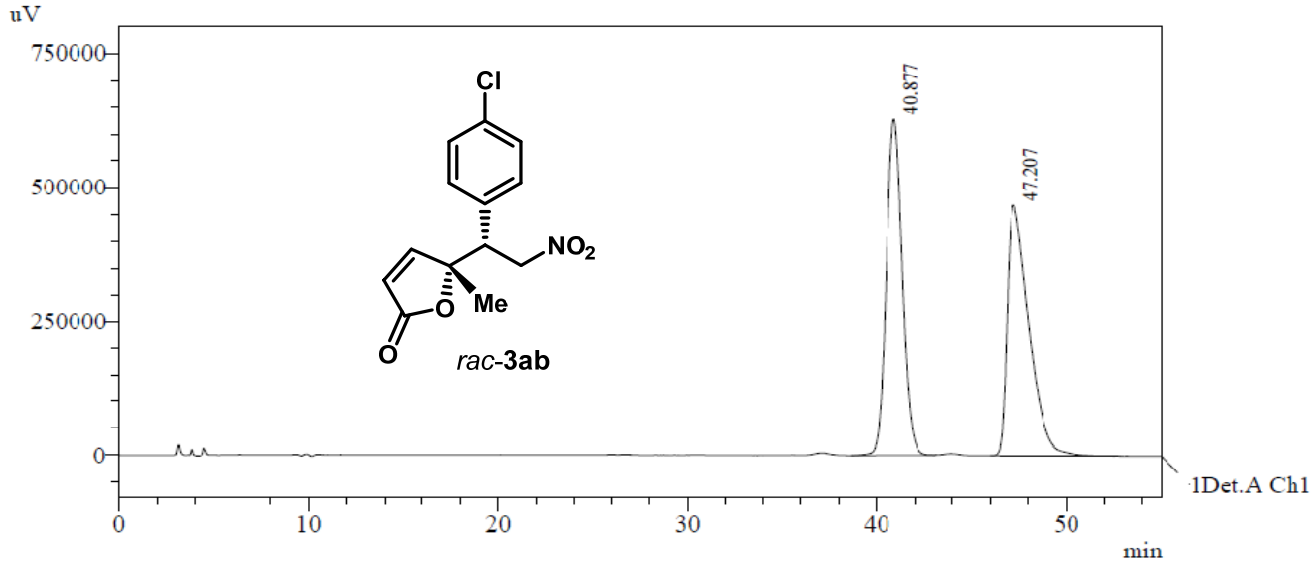
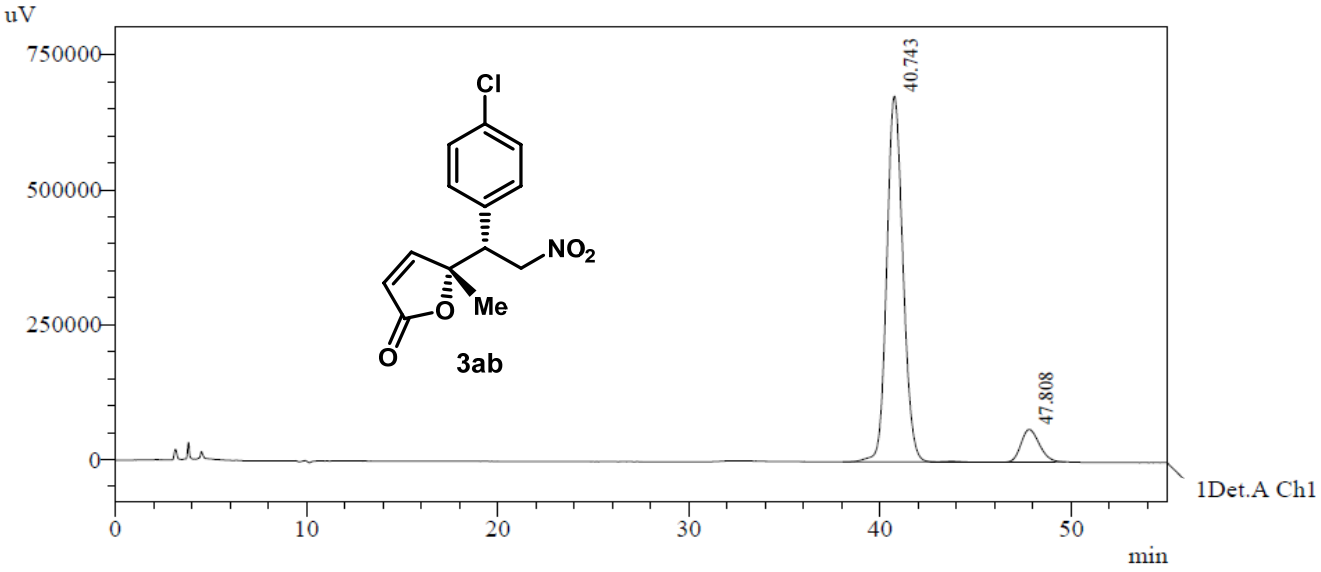
7.27
7.26
7.13
7.11
5.91
5.90
4.93
4.91
4.89
4.88
4.80
4.77
4.77
4.74
3.99
3.98
3.97
3.95
1.55
Cl
NO2
Me
O
O
3ab
10
9
8
7
6
5
4
3
2
1
0
ppm
3.049
2.107
1.019
1.109
1.051
1.049
3.173
171.15
157.95
134.94
132.91
129.74
129.53
121.86
88.02
77.48
77.16
76.84
75.41
50.07
23.55
Cl
NO2
Me
O
O
3ab
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

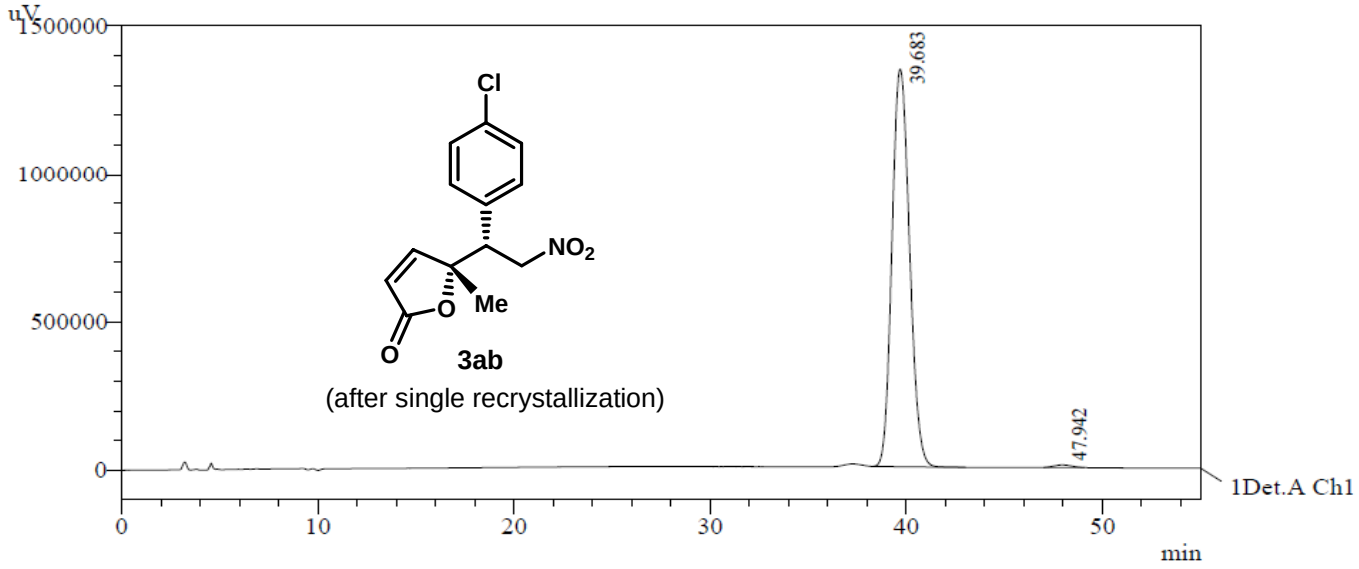
Peak#	Ret. Time	Area	Area %
1	40.877	36534265	49.720
2	47.207	36945932	50.280
Total		73480197	100.000



PeakTable

Detector A Ch1 210nm

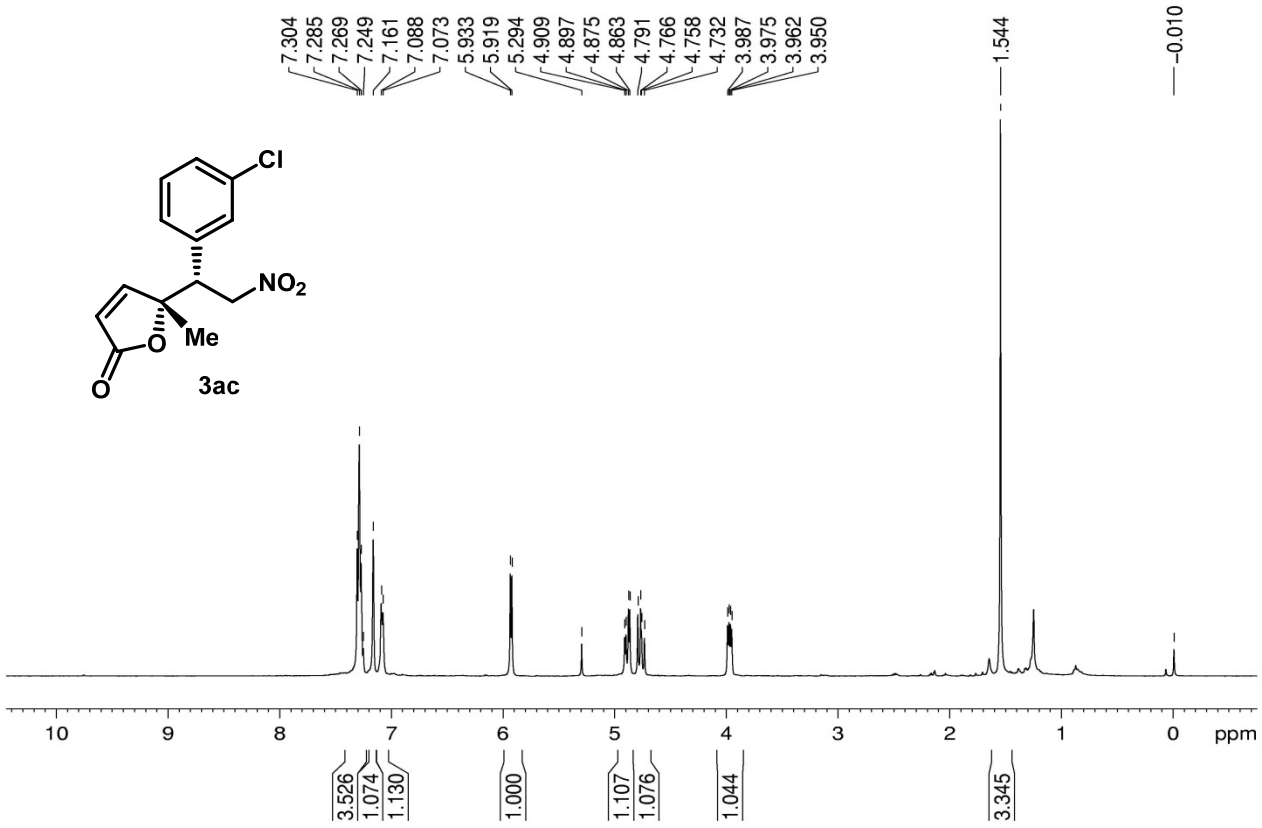
Peak#	Ret. Time	Area	Area %
1	40.743	40011675	90.836
2	47.808	4036399	9.164
Total		44048074	100.000

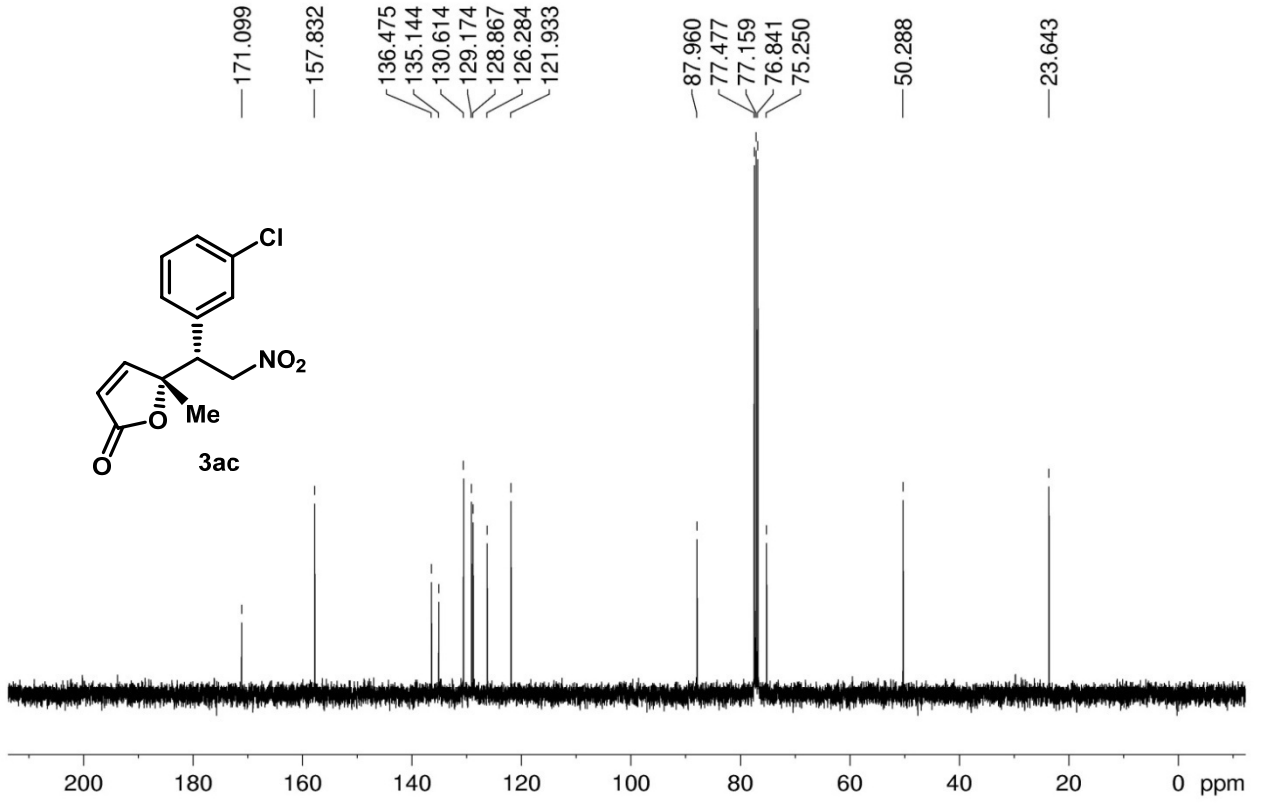


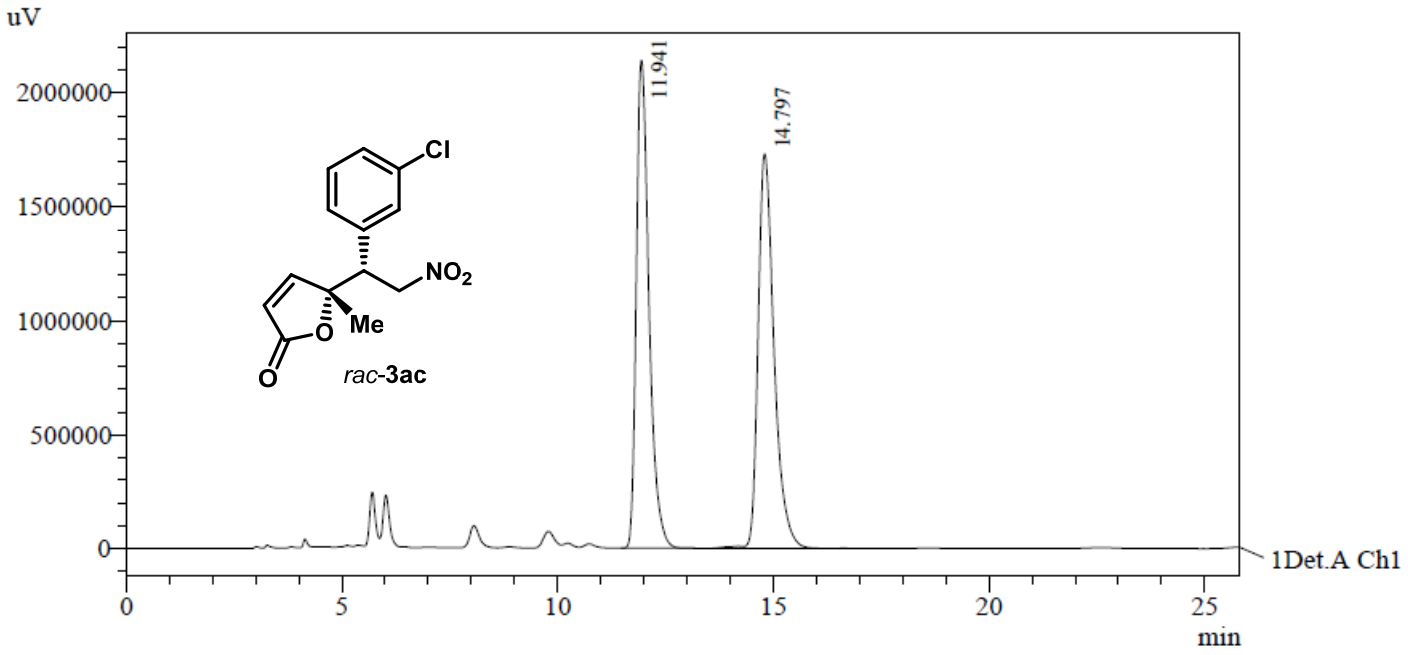
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	39.683	83643108	99.382
2	47.942	520248	0.618
Total		84163355	100.000


7.304
7.285
7.269
7.249
7.161
7.088
7.073
5.933
5.919
5.294
4.909
4.897
4.875
4.863
4.791
4.766
4.758
4.732
3.987
3.975
3.962
3.950
1.544
-0.010
Cl
NO2
Me
O
O
3ac
10
9
8
7
6
5
4
3
2
1
0
ppm
3.526
1.074
1.130
1.000
1.107
1.076
1.044
3.345

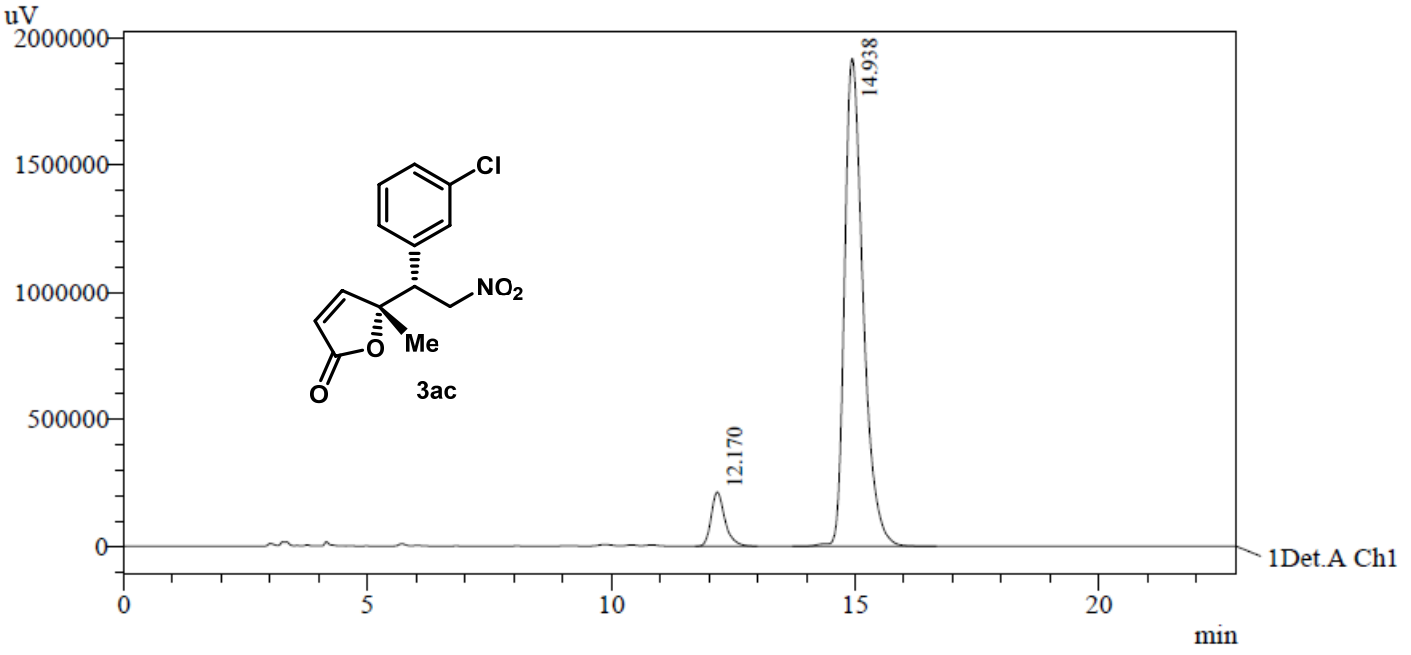

171.099
157.832
136.475
135.144
130.614
129.174
128.867
126.284
121.933
87.960
77.477
77.159
76.841
75.250
50.288
23.643
Cl
NO2
Me
O
O
3ac
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

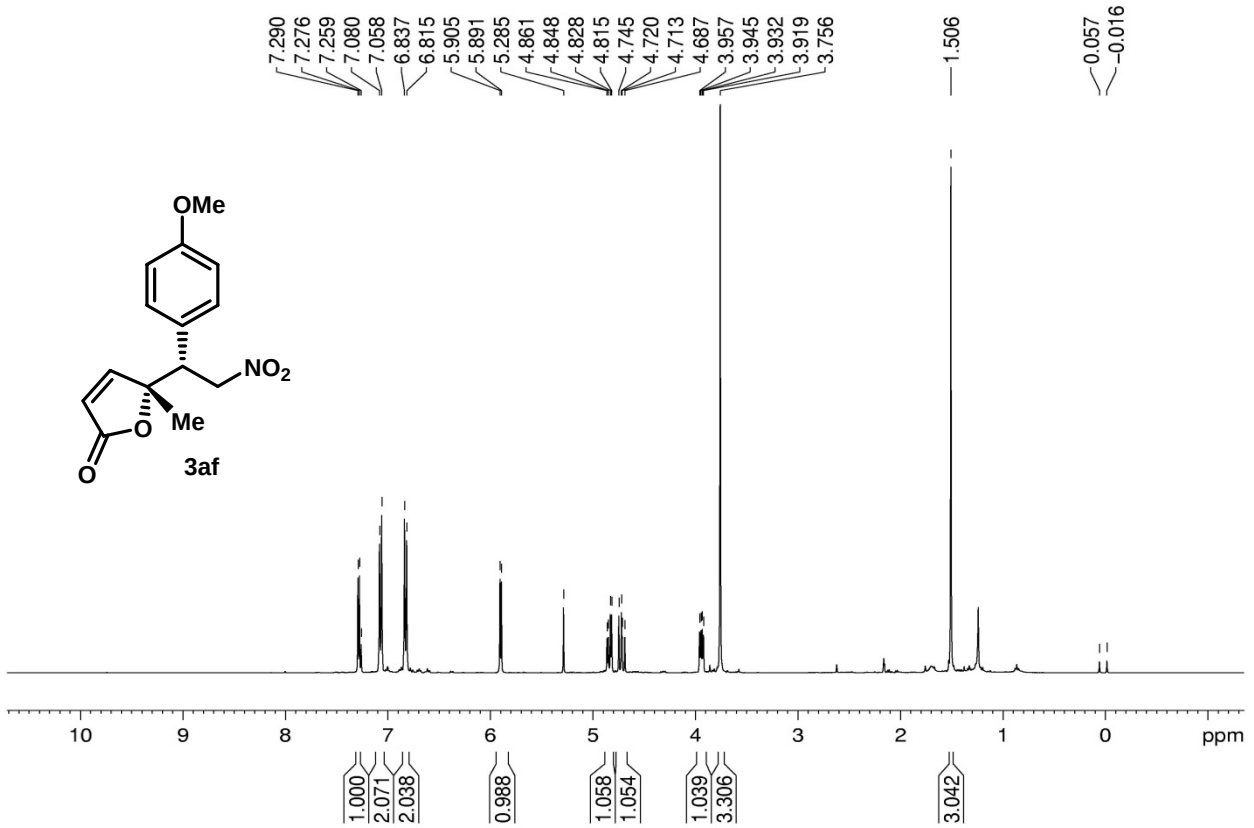
Peak#	Ret. Time	Area	Area %
1	11.941	43960741	49.744
2	14.797	44413168	50.256
Total		88373908	100.000



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	12.170	4257631	7.716
2	14.938	50924123	92.284
Total		55181754	100.000


7.290
7.276
7.259
7.080
7.058
6.837
6.815
5.905
5.891
5.285
4.861
4.848
4.828
4.815
4.745
4.720
4.713
4.687
3.957
3.945
3.932
3.919
3.756
1.506
0.057
-0.016
OMe
NO2
Me
O
O
3af
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.071
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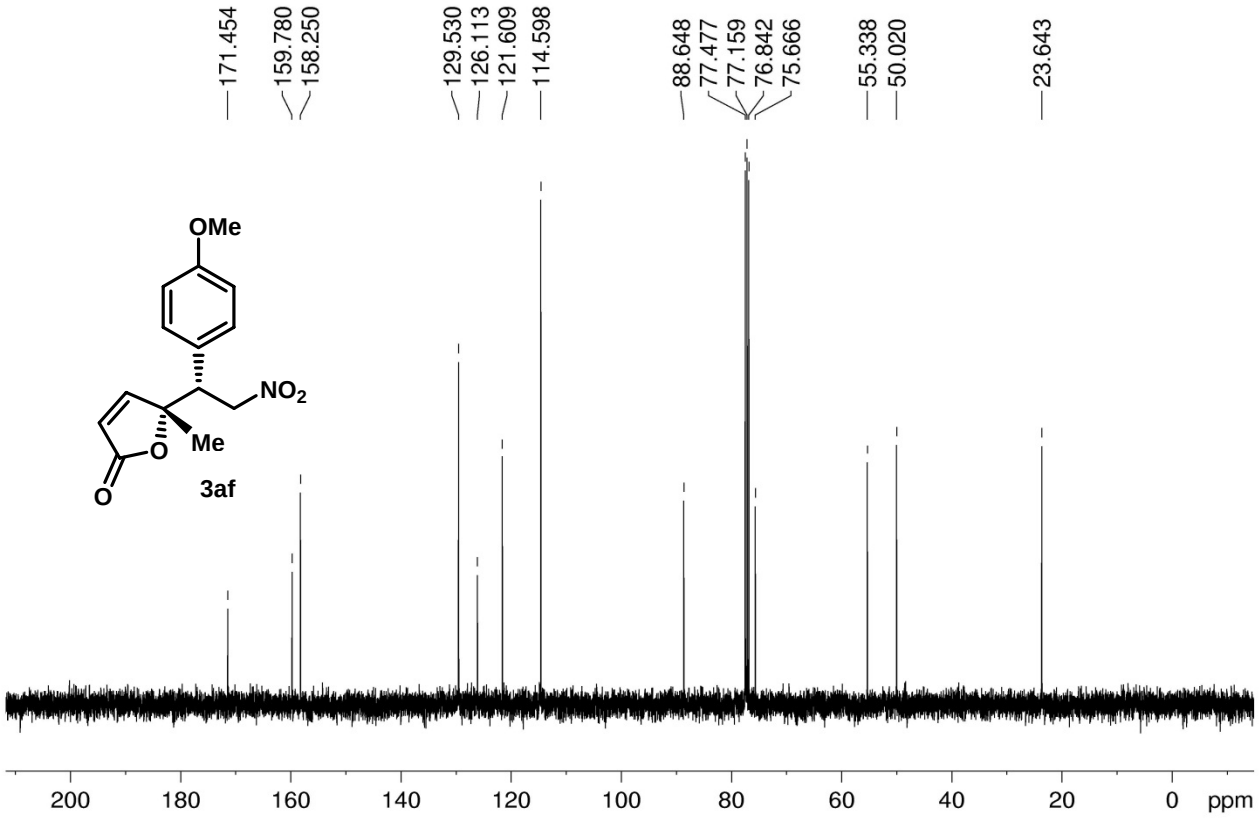
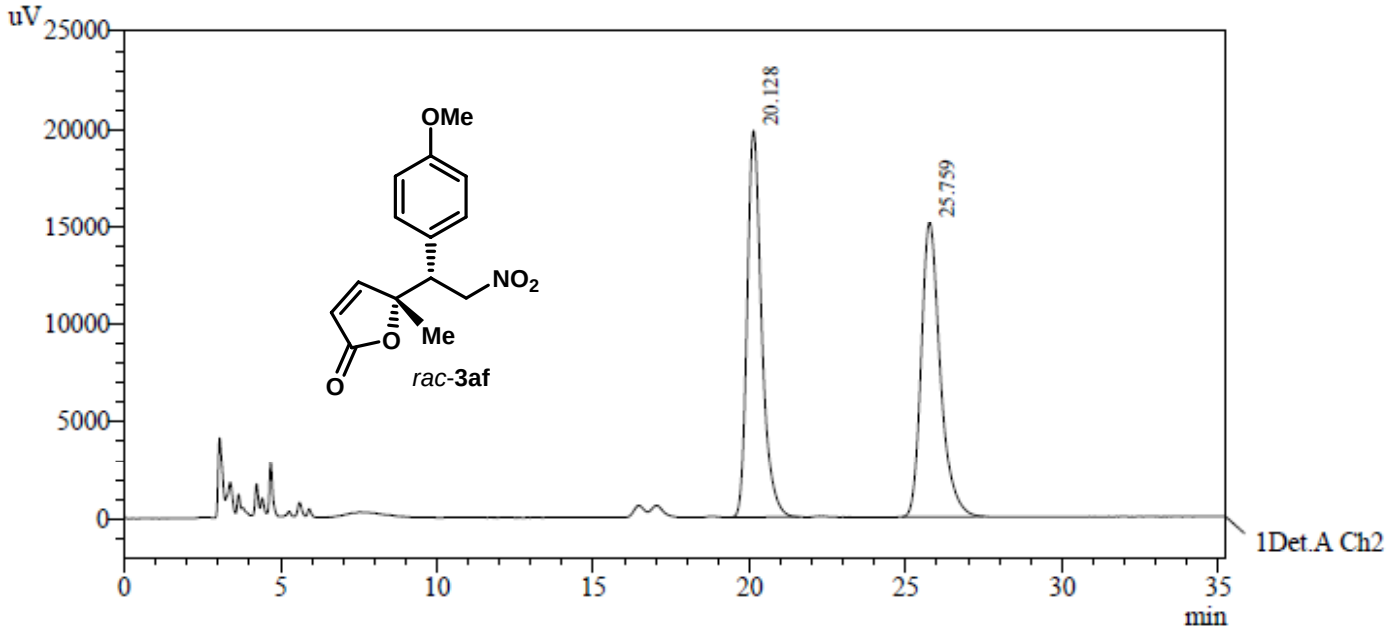
1.058
1.054
1.039
3.306
3.042

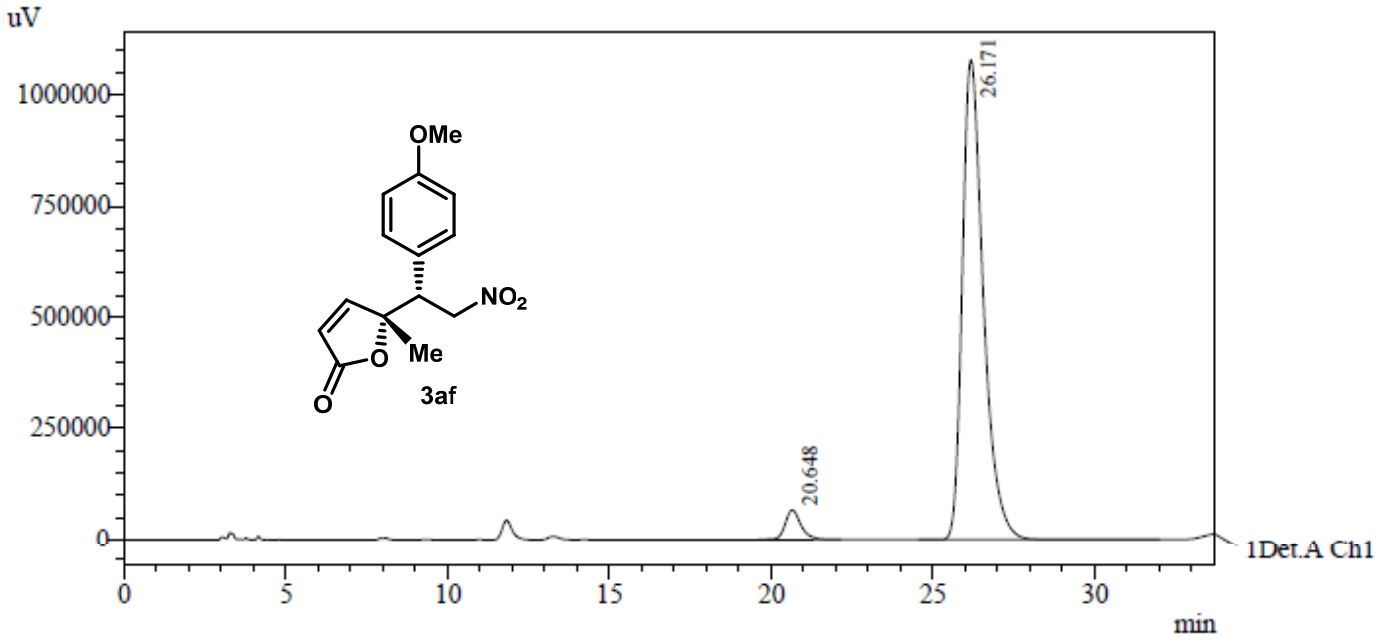

171.454
159.780
158.250
129.530
126.113
121.609
114.598
88.648
77.477
77.159
76.842
75.666
55.338
50.020
23.643
OMe
NO2
Me
O
O
3af
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch2 254nm

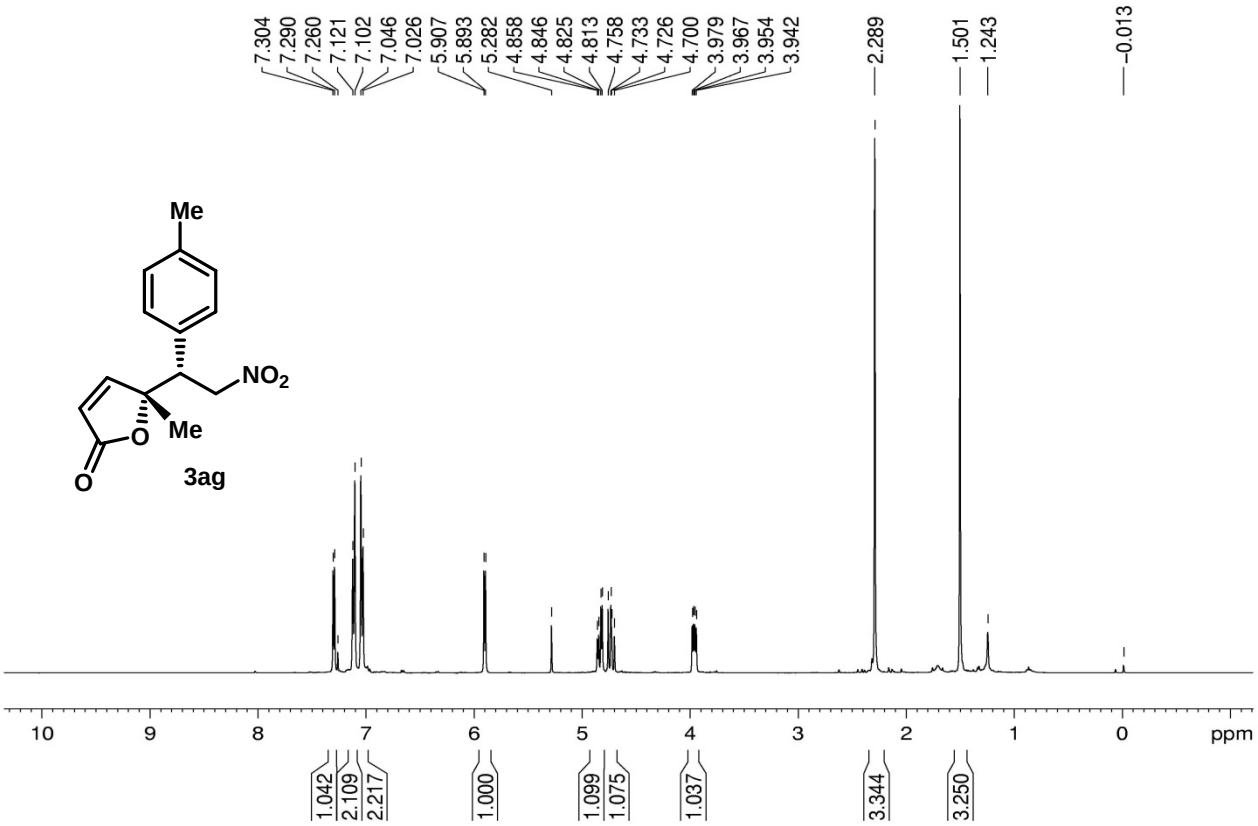
Peak#	Ret. Time	Area	Area %	Resolution
1	20.128	642052	50.036	0.000
2	25.759	641120	49.964	5.948
Total		1283172	100.000	

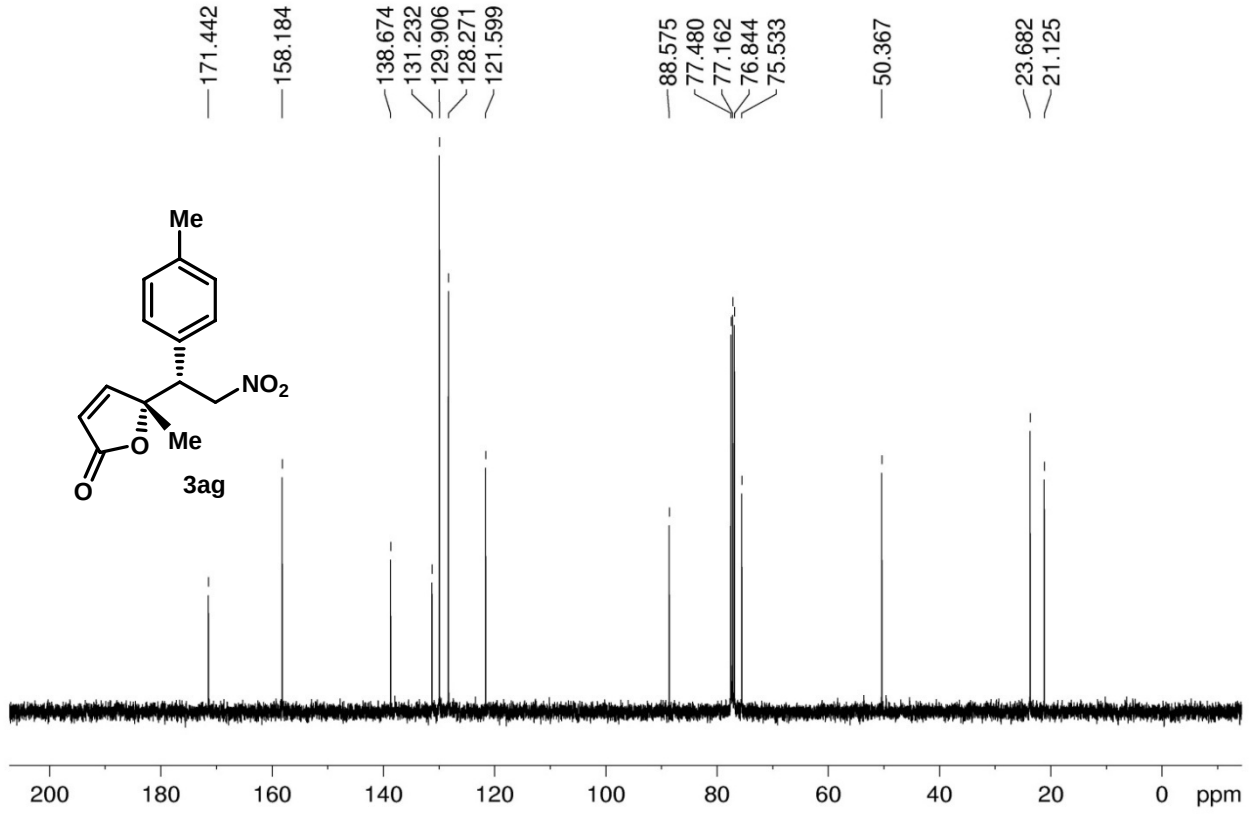


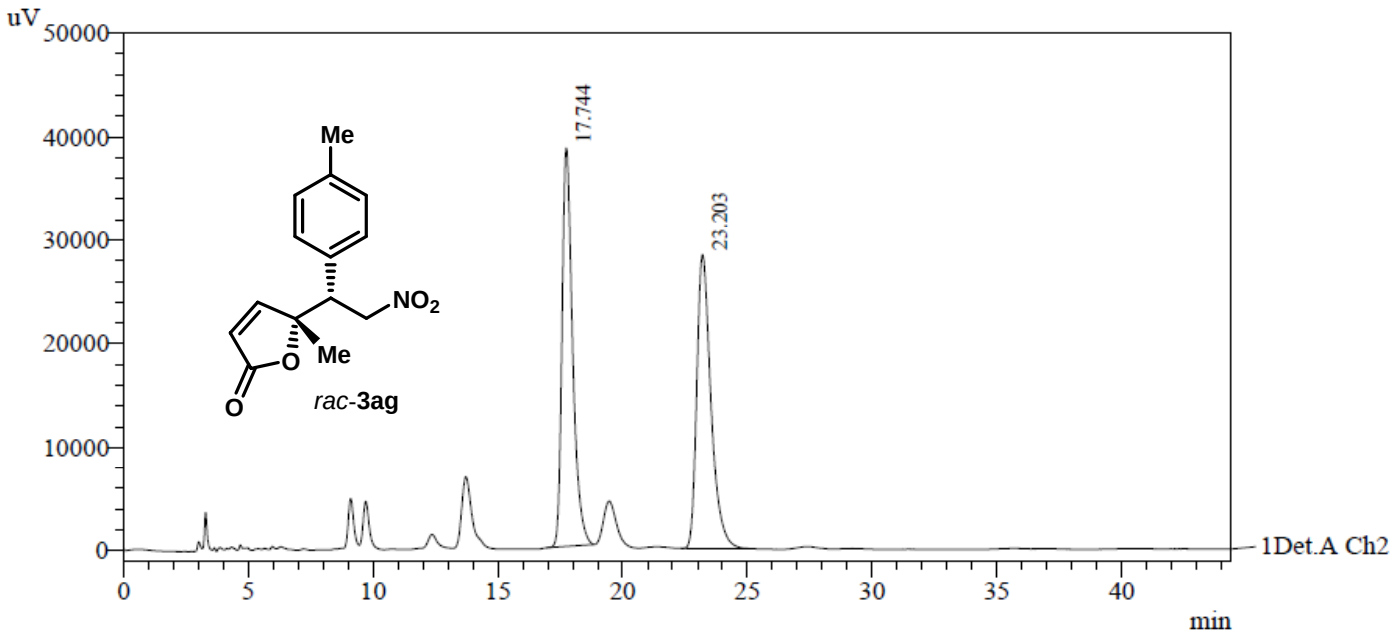
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	20.648	2296603	4.498
2	26.171	48759494	95.502
Total		51056097	100.000


7.304
7.290
7.260
7.121
7.102
7.046
7.026
5.907
5.893
5.282
4.858
4.846
4.825
4.813
4.758
4.733
4.726
4.700
3.979
3.967
3.954
3.942
2.289
1.501
1.243
0.013
Me
NO2
Me
O
O
3ag
10
9
8
7
6
5
4
3
2
1
0
ppm
1.042
2.109
2.217
1.000
1.099
1.075
1.037
3.344
3.250

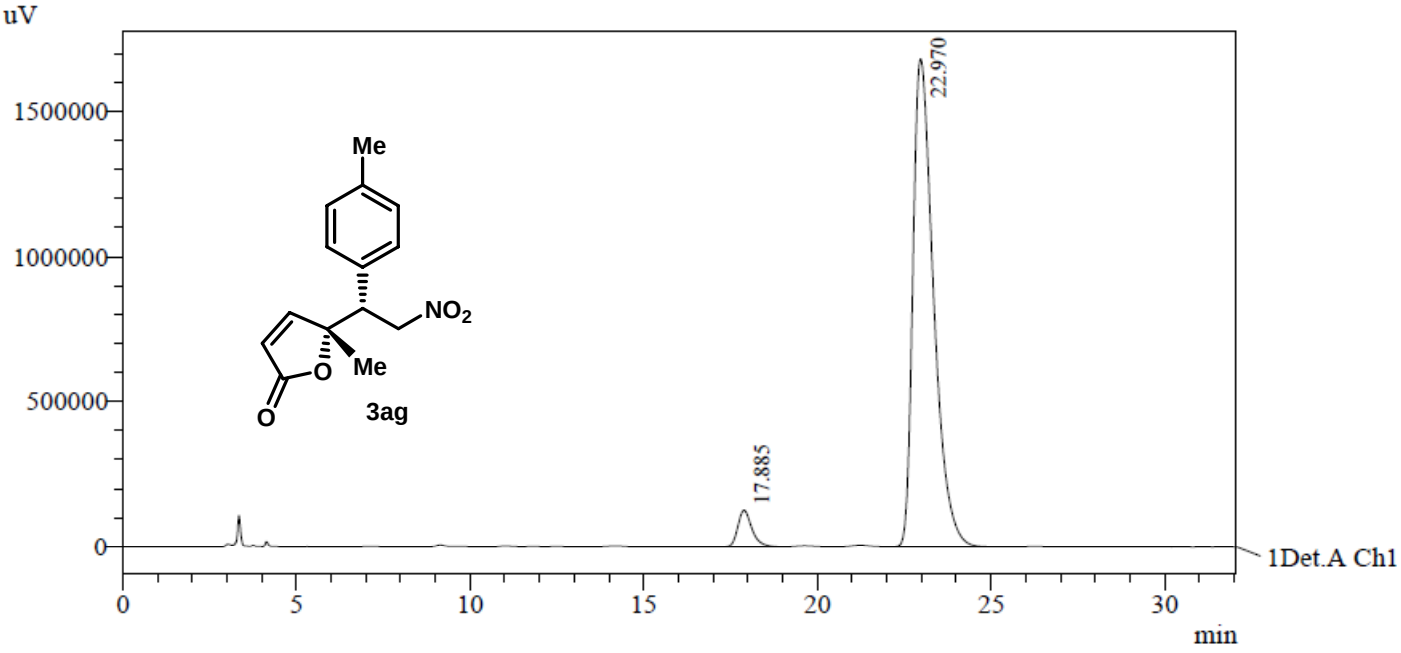

171.442
158.184
138.674
131.232
129.906
128.271
121.599
88.575
77.480
77.162
76.844
75.533
50.367
23.682
21.125
Me
NO2
Me
O
O
3ag
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch2 254nm

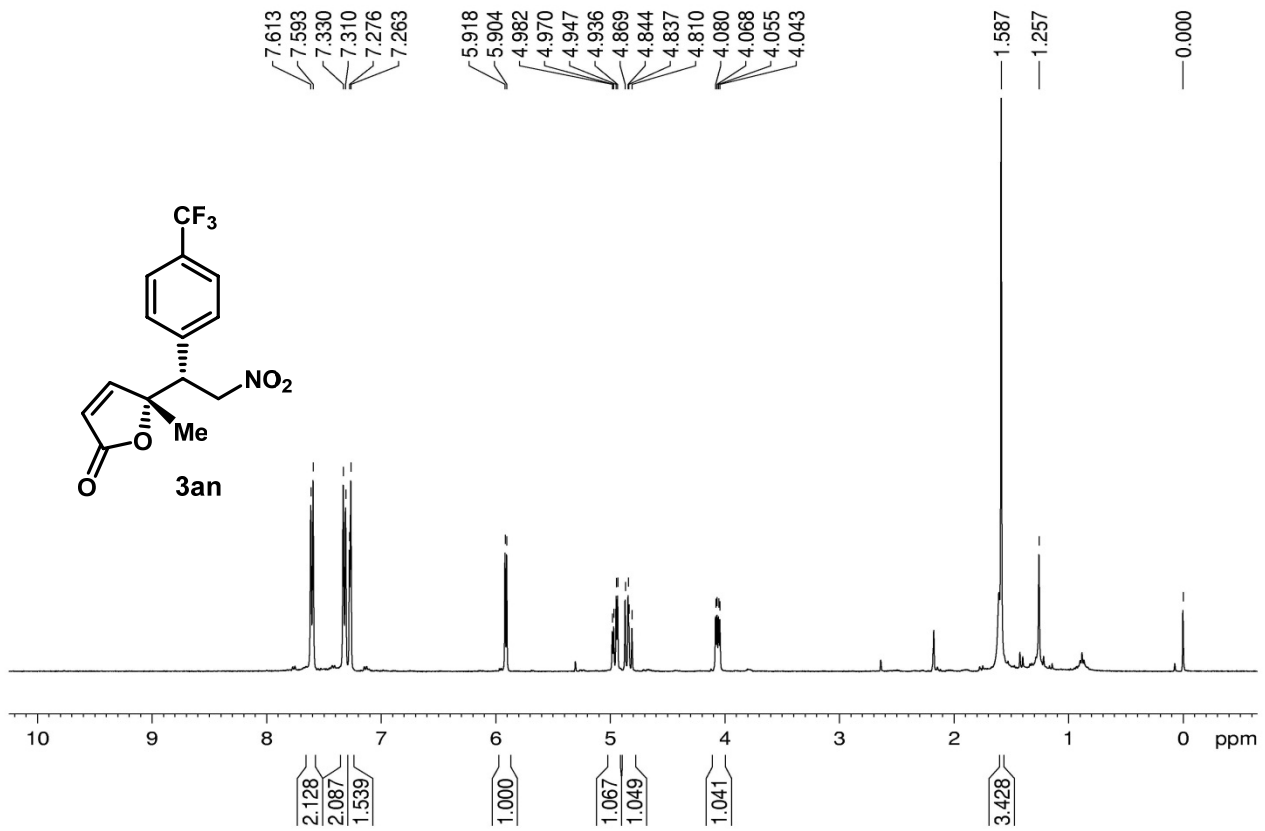
Peak#	Ret. Time	Area	Area %	Resolution
1	17.744	1134434	50.290	0.000
2	23.203	1121345	49.710	6.220
Total		2255780	100.000	

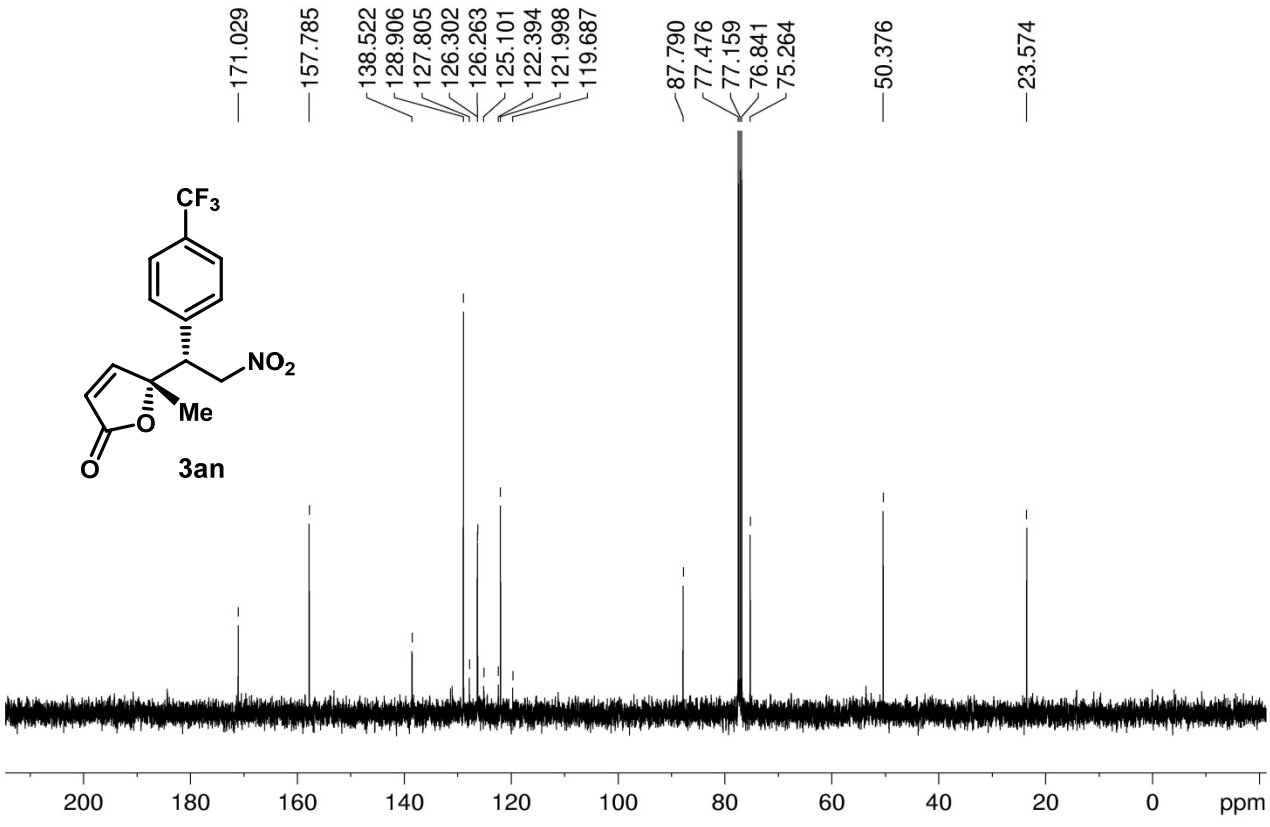


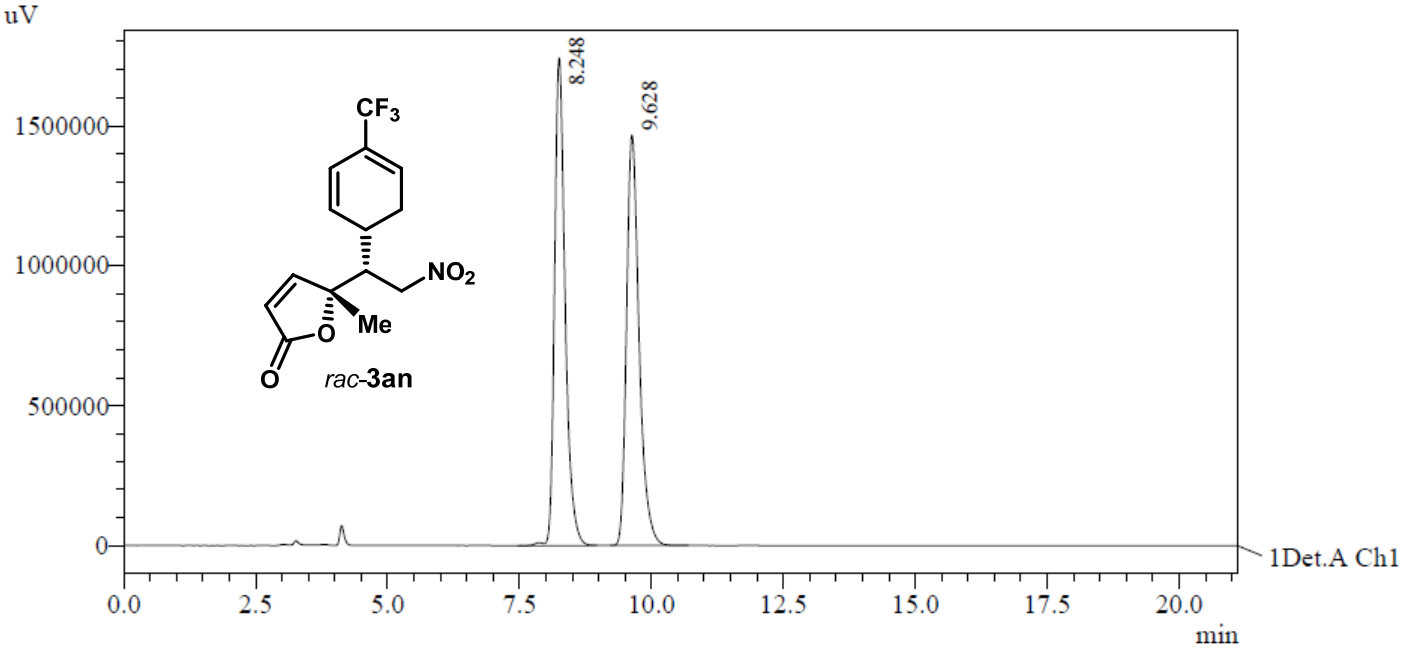
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	17.885	3614947	4.946
2	22.970	69470195	95.054
Total		73085143	100.000


7.613
7.593
7.330
7.310
7.276
7.263
5.918
5.904
4.982
4.970
4.947
4.936
4.869
4.844
4.837
4.810
4.080
4.068
4.055
4.043
1.587
1.257
0.000
CF3
NO2
Me
O
O
3an
10
9
8
7
6
5
4
3
2
1
0
ppm
2.128
2.087
1.539
1.000
1.067
1.049
1.041
3.428

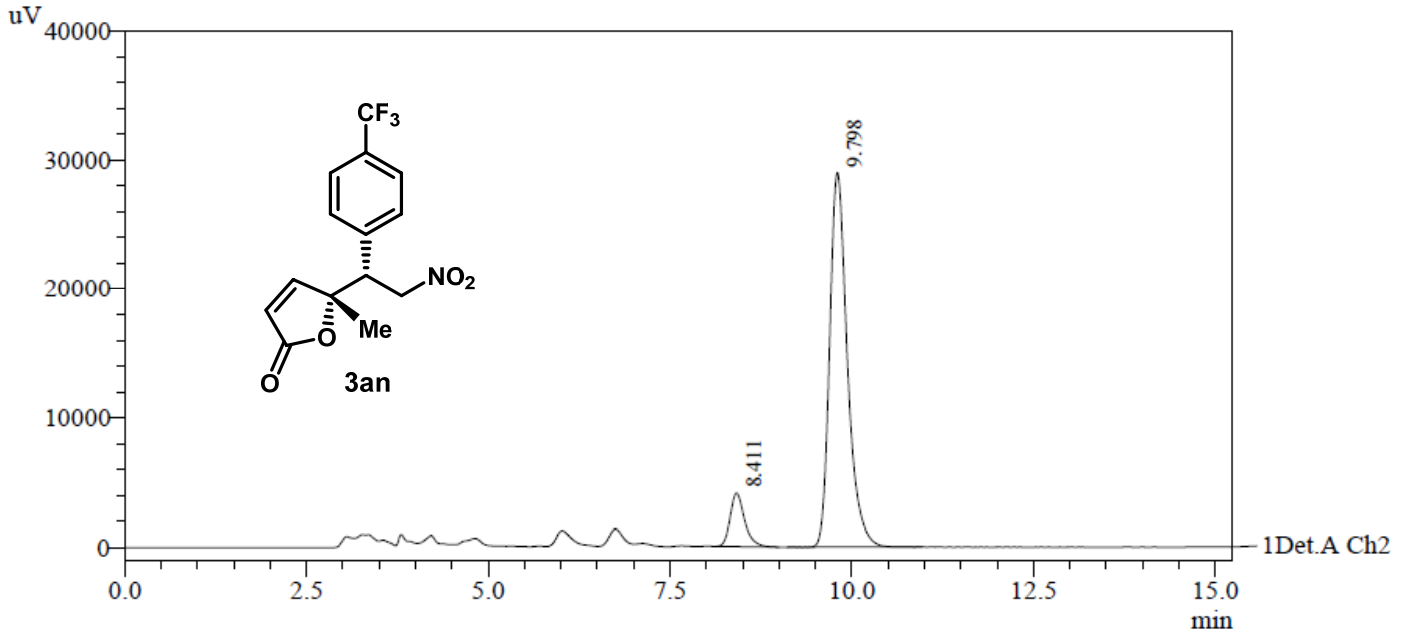

171.029
157.785
138.522
128.906
127.805
126.302
126.263
125.101
122.394
121.998
119.687
87.790
77.476
77.159
76.841
75.264
50.376
23.574
CF3
NO2
Me
O
O
3an
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

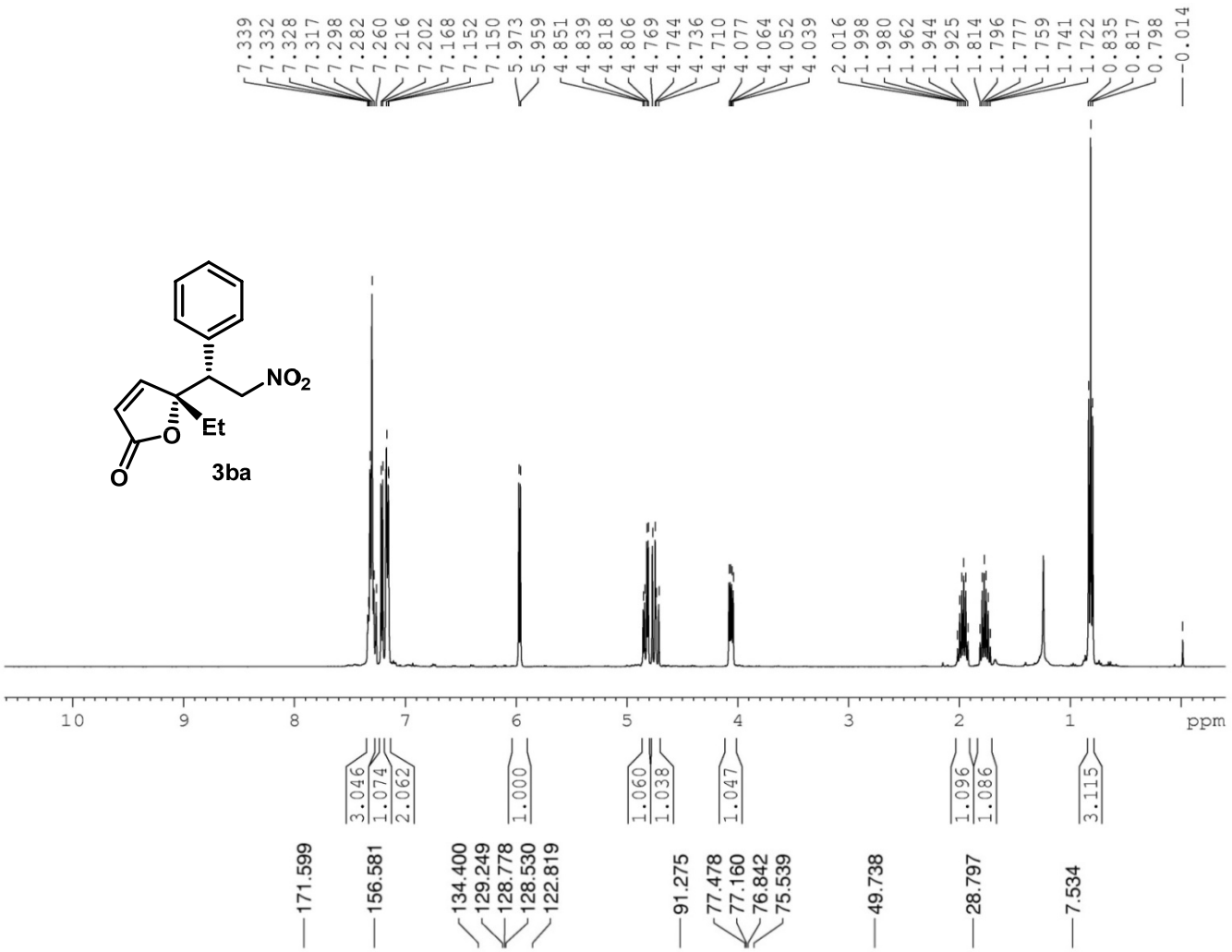
Peak#	Ret. Time	Area	Area %
1	8.248	24364501	50.067
2	9.628	24299158	49.933
Total		48663659	100.000

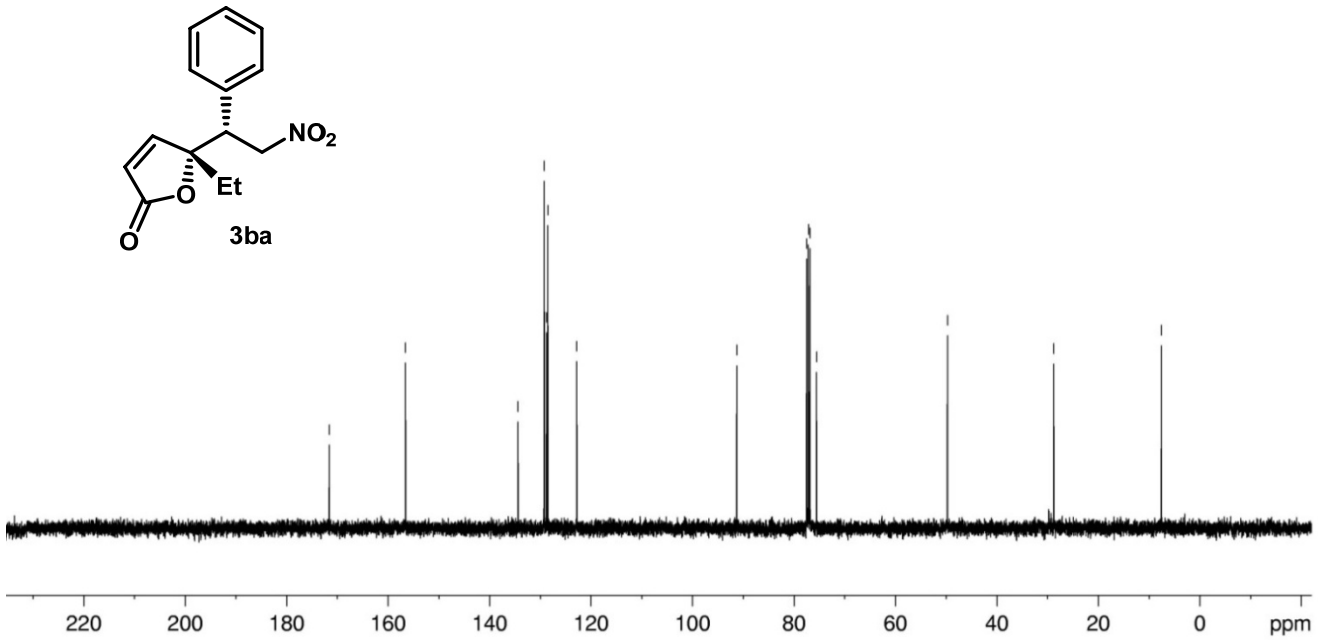


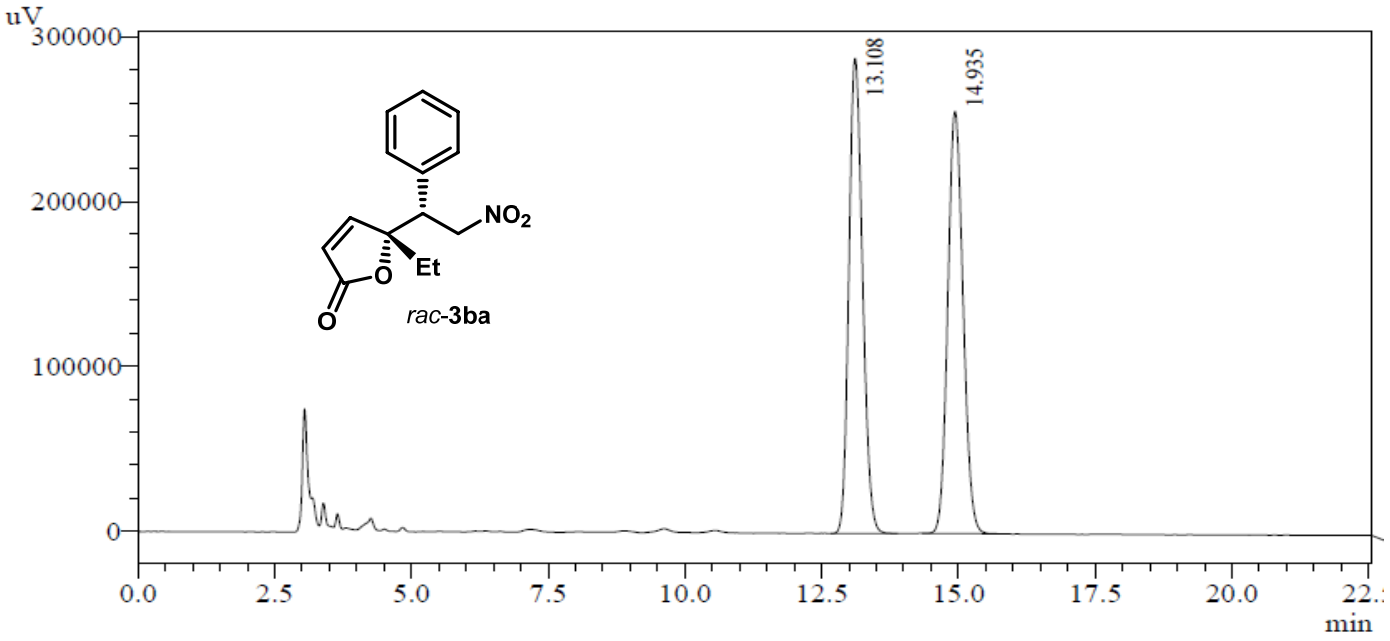
PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %	Resolution
1	8.411	56647	10.379	0.000
2	9.798	489118	89.621	3.491
Total		545765	100.000	


7.339
7.332
7.328
7.317
7.298
7.282
7.260
7.216
7.202
7.168
7.152
7.150
5.973
5.959
4.851
4.839
4.818
4.806
4.769
4.744
4.736
4.710
4.077
4.064
4.052
4.039
2.016
1.998
1.980
1.962
1.944
1.925
1.814
1.796
1.777
1.759
1.741
1.722
0.835
0.817
0.798
-0.014
NO2
Et
O
O
3ba
10
9
8
7
6
5
4
3
2
1
ppm
3.046
1.074
2.062
1.000
1.060
1.038
1.047
1.096
1.086
3.115

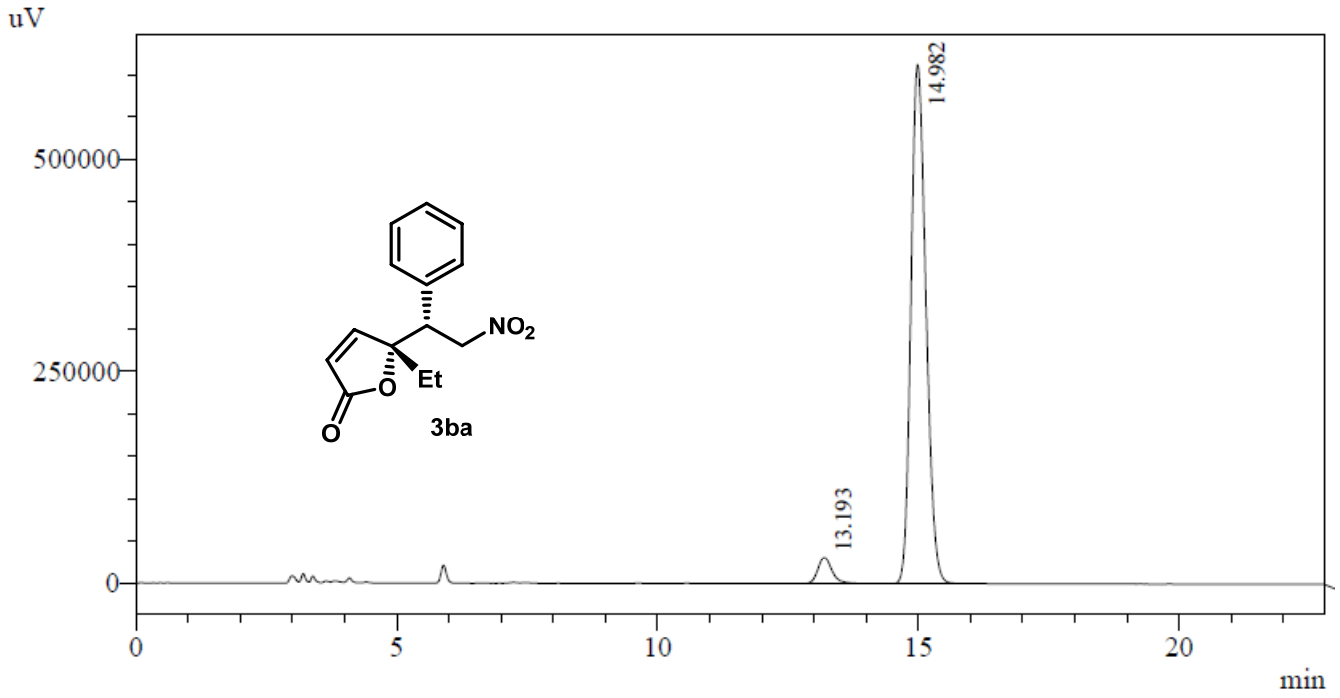

171.599
156.581
134.400
129.249
128.778
128.530
122.819
91.275
77.478
77.160
76.842
75.539
49.738
28.797
7.534
NO2
Et
O
O
3ba
220
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

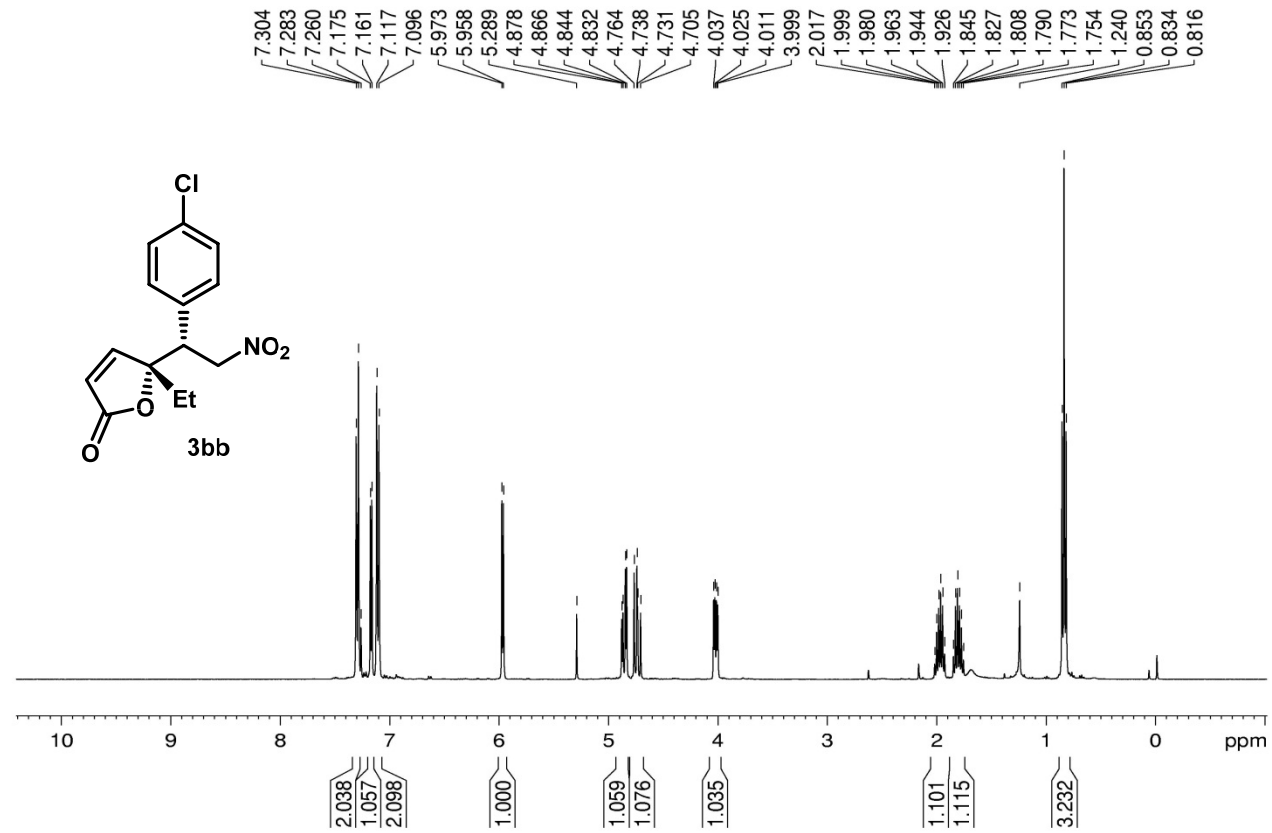
Peak#	Ret. Time	Area	Area %
1	13.108	4993852	50.044
2	14.935	4985067	49.956
Total		9978919	100.000

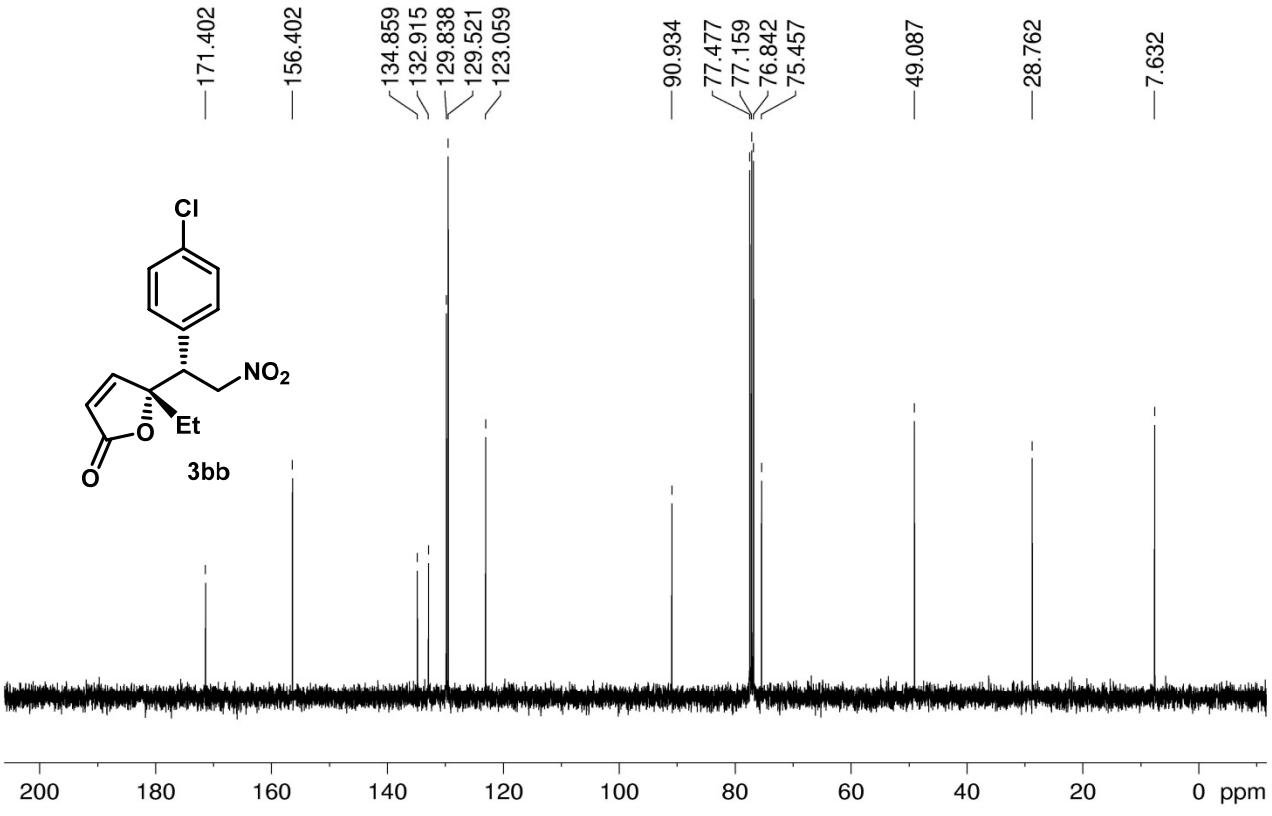


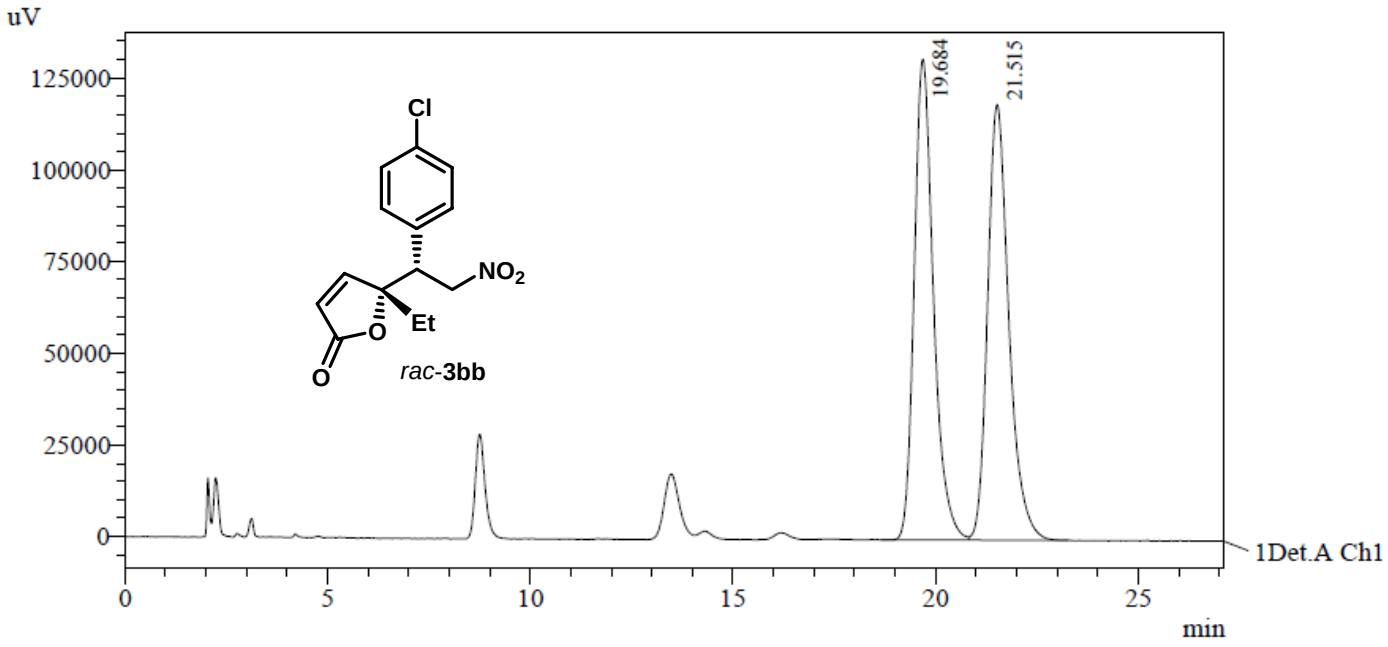
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	13.193	574487	4.485
2	14.982	12234171	95.515
Total		12808658	100.000


7.304
7.283
7.260
7.175
7.161
7.117
7.096
5.973
5.958
5.289
4.878
4.866
4.844
4.832
4.764
4.738
4.731
4.705
4.037
4.025
4.011
3.999
2.017
1.999
1.980
1.963
1.944
1.926
1.845
1.827
1.808
1.790
1.773
1.754
1.240
0.853
0.834
0.816
Cl
NO2
Et
O
O
3bb
10
9
8
7
6
5
4
3
2
1
0
ppm
2.038
1.057
2.098
1.000
1.059
1.076
1.035
1.101
1.115
3.232

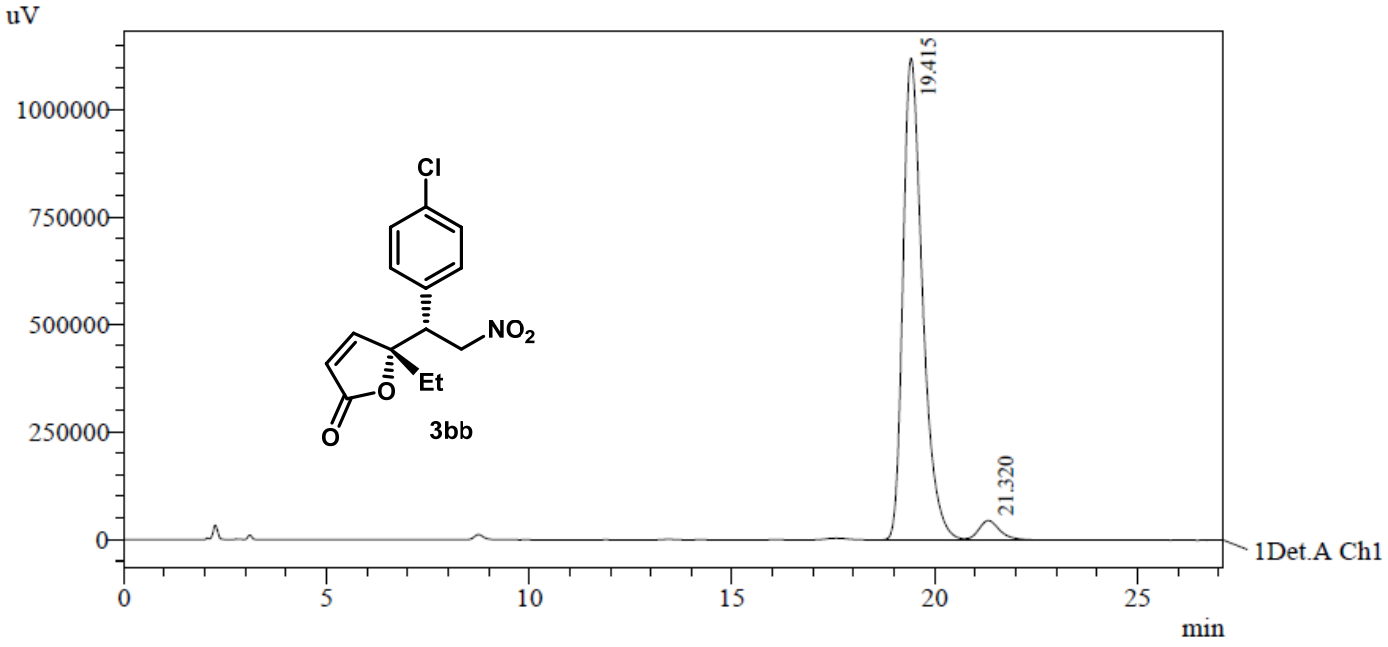

171.402
156.402
134.859
132.915
129.838
129.521
123.059
90.934
77.477
77.159
76.842
75.457
49.087
28.762
7.632
Cl
NO2
Et
O
O
3bb
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

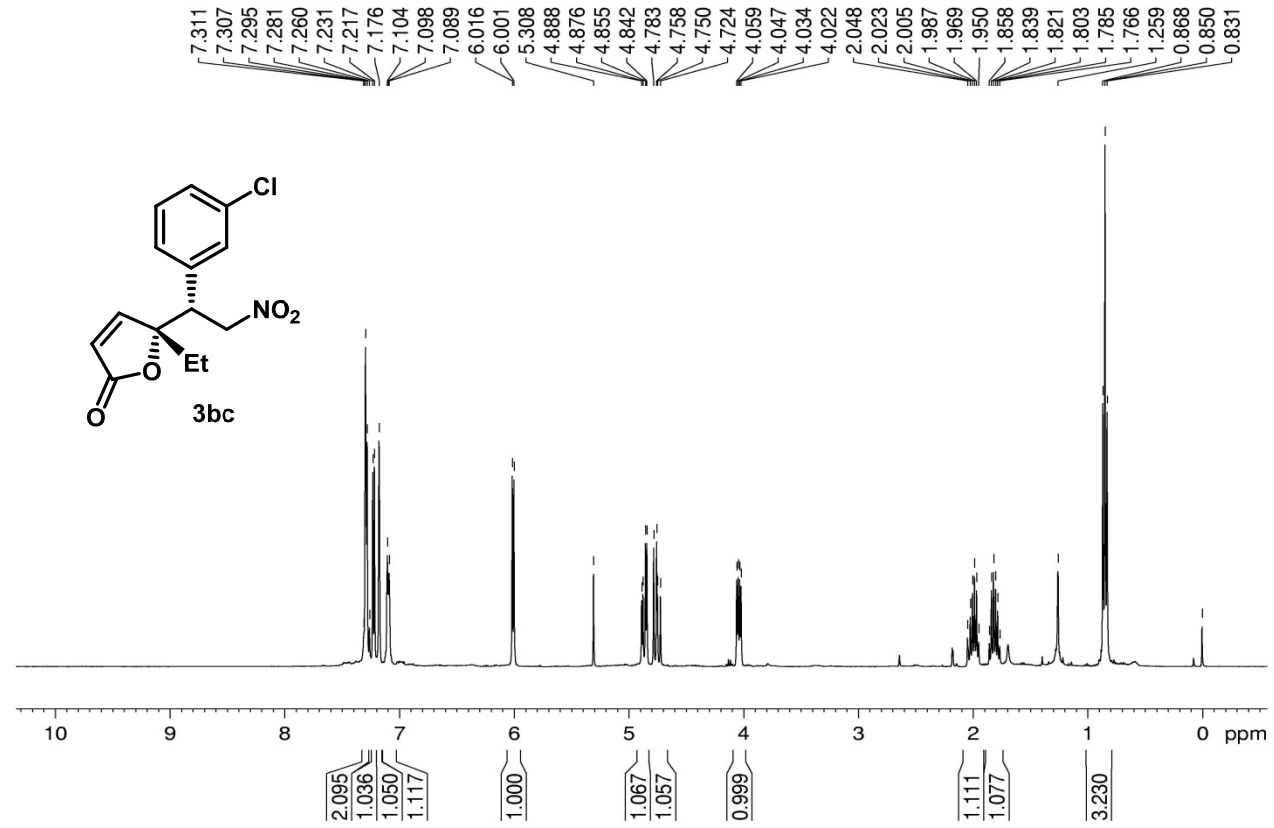
Peak#	Ret. Time	Area	Area %
1	19.684	4332915	49.956
2	21.515	4340460	50.044
Total		8673375	100.000

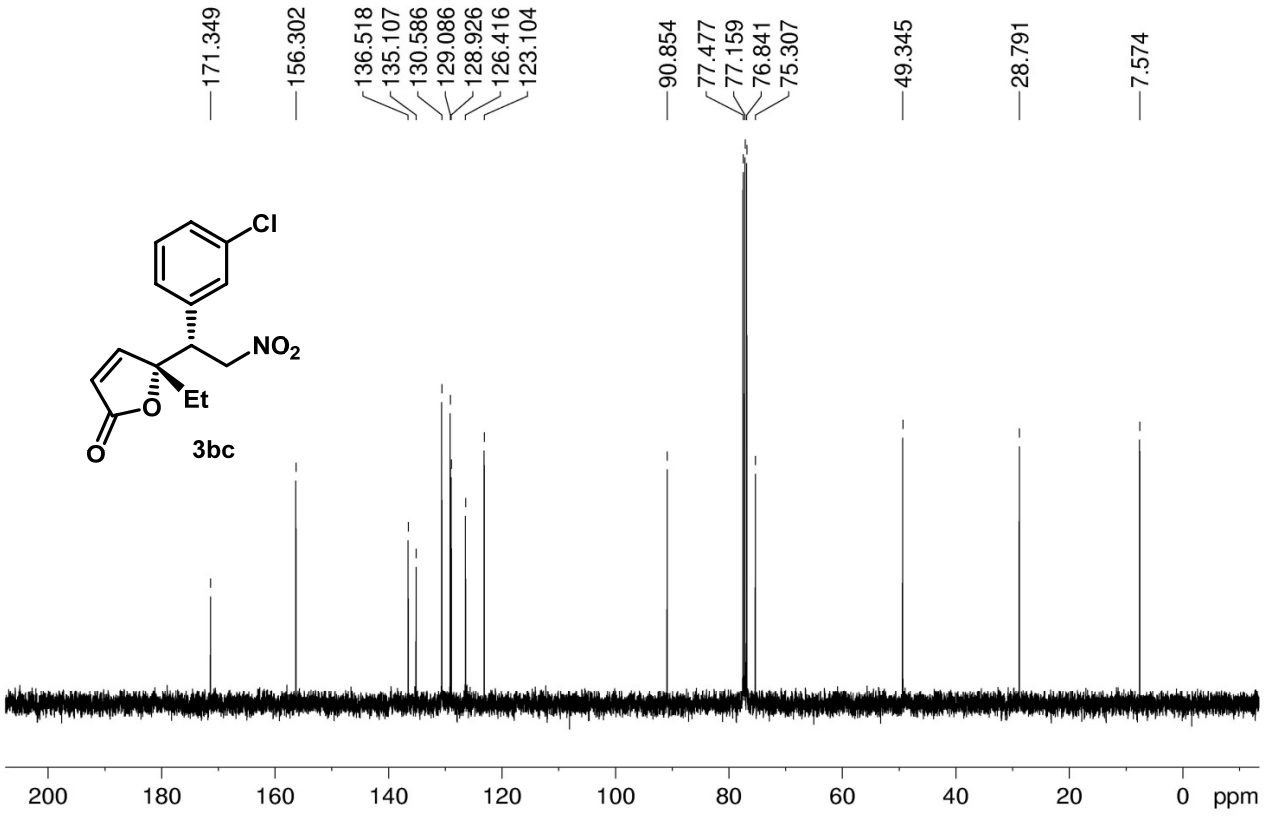


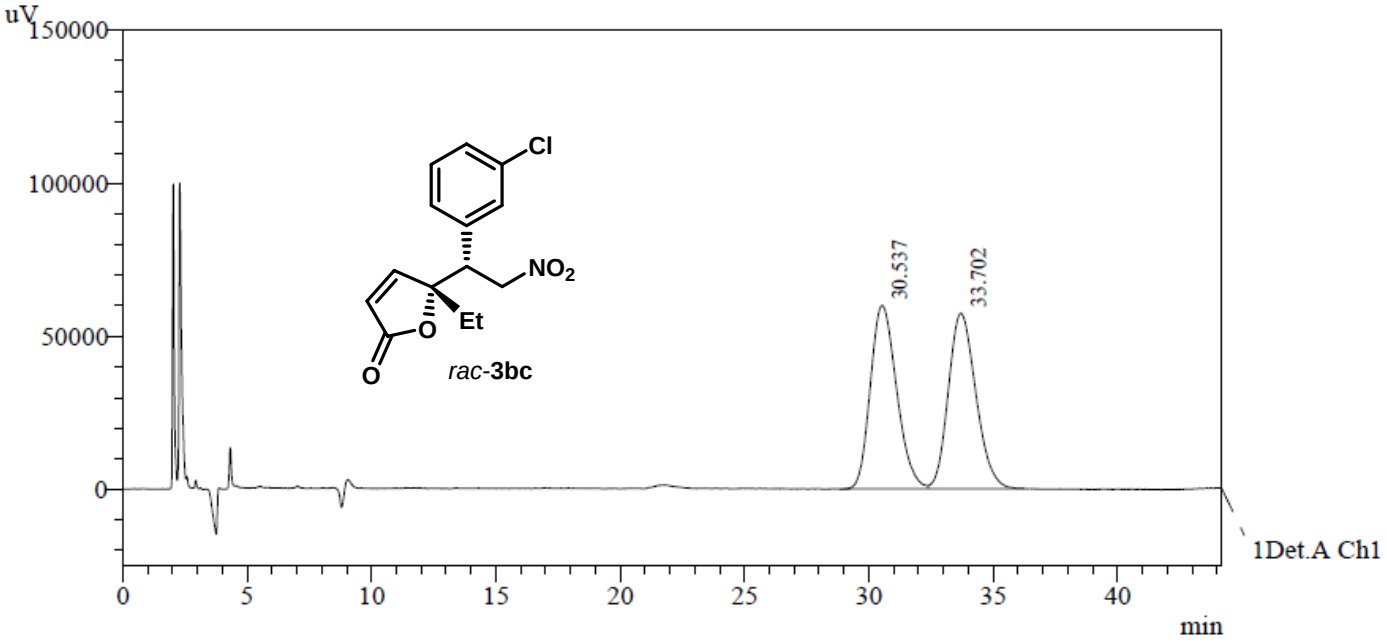
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	19.415	37692542	95.920
2	21.320	1603100	4.080
Total		39295641	100.000


7.311
7.307
7.295
7.281
7.260
7.231
7.217
7.176
7.104
7.098
7.089
6.016
6.001
5.308
4.888
4.876
4.855
4.842
4.783
4.758
4.750
4.724
4.059
4.047
4.034
4.022
2.048
2.023
2.005
1.987
1.969
1.950
1.858
1.839
1.821
1.803
1.785
1.766
1.259
0.868
0.850
0.831
Cl
NO2
Et
O
O
3bc
10
9
8
7
6
5
4
3
2
1
0 ppm
2.095
1.036
1.050
1.117
1.000
1.067
1.057
0.999
1.111
1.077
3.230

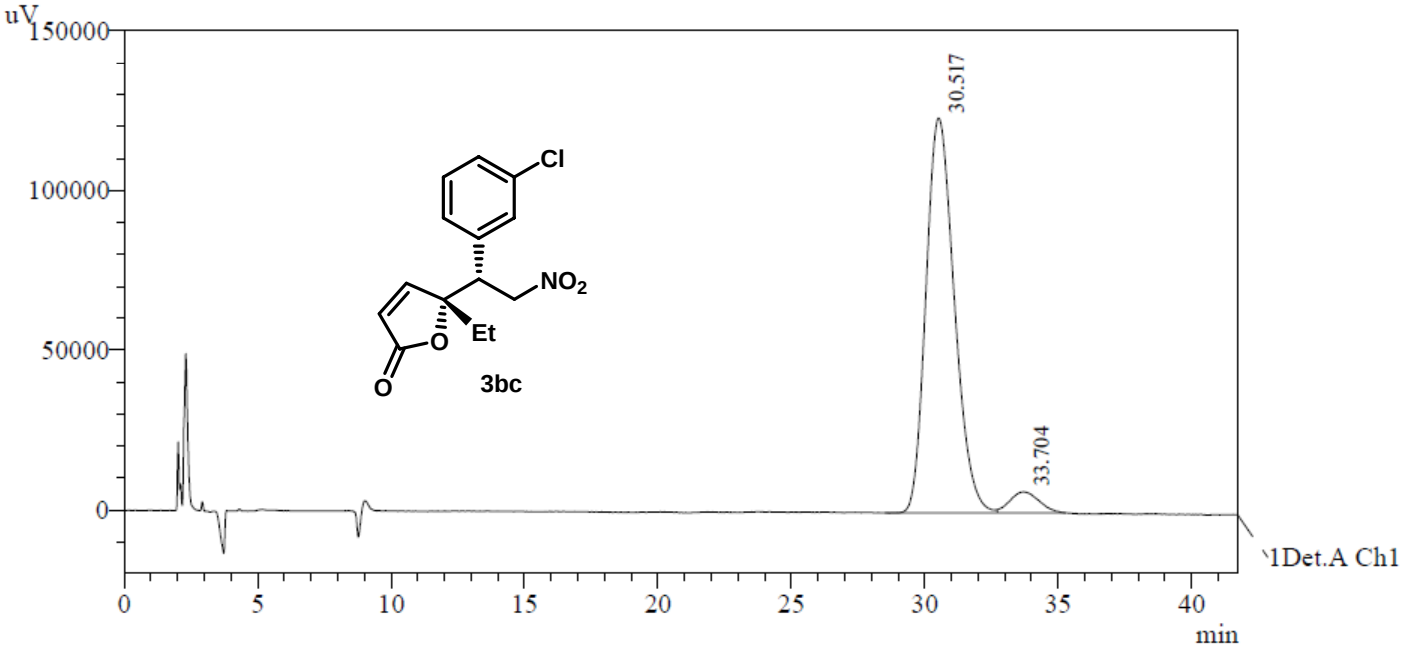

171.349
156.302
136.518
135.107
130.586
129.086
128.926
126.416
123.104
90.854
77.477
77.159
76.841
75.307
49.345
28.791
7.574
Cl
NO2
Et
O
O
3bc
200
180
160
140
120
100
80
60
40
20
0 ppm



PeakTable

Detector A Ch1 210nm

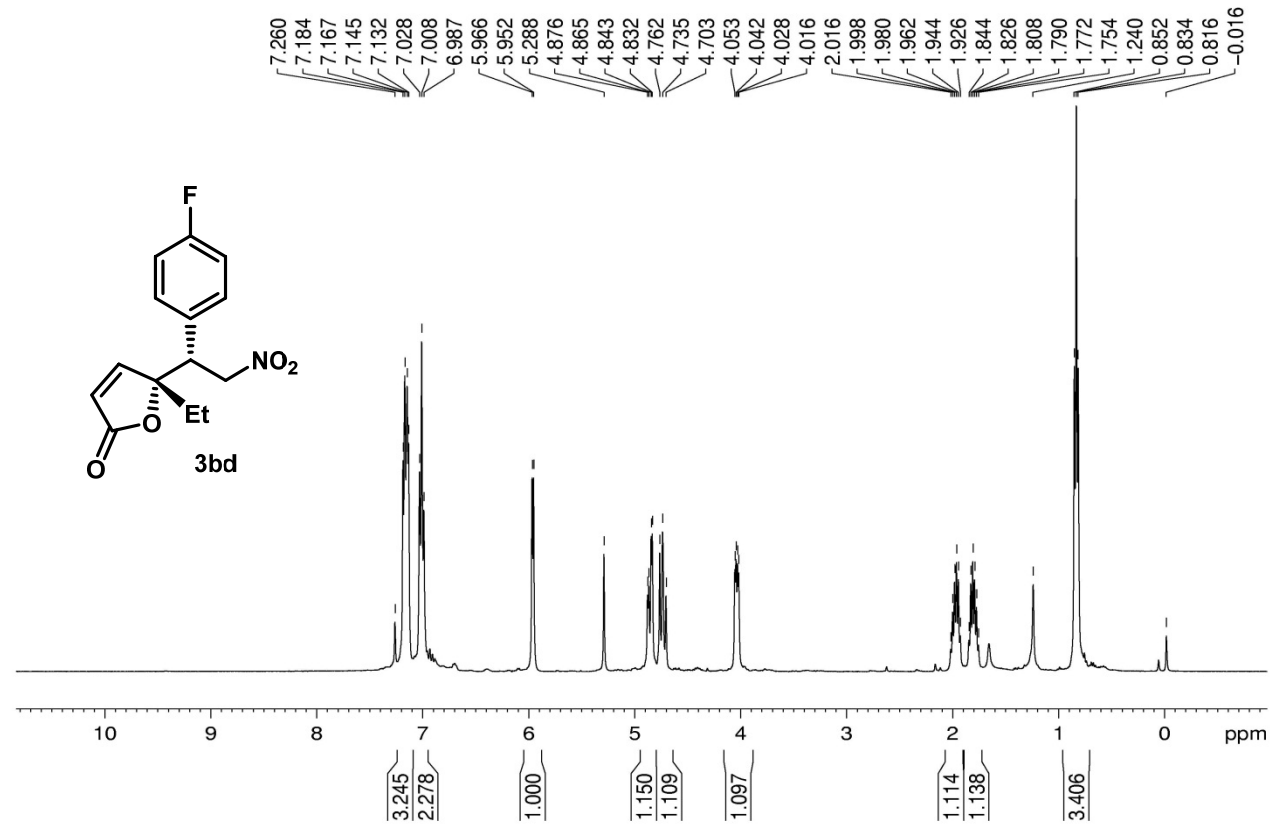
Peak#	Ret. Time	Area	Area %
1	30.537	4428476	49.979
2	33.702	4432269	50.021
Total		8860744	100.000

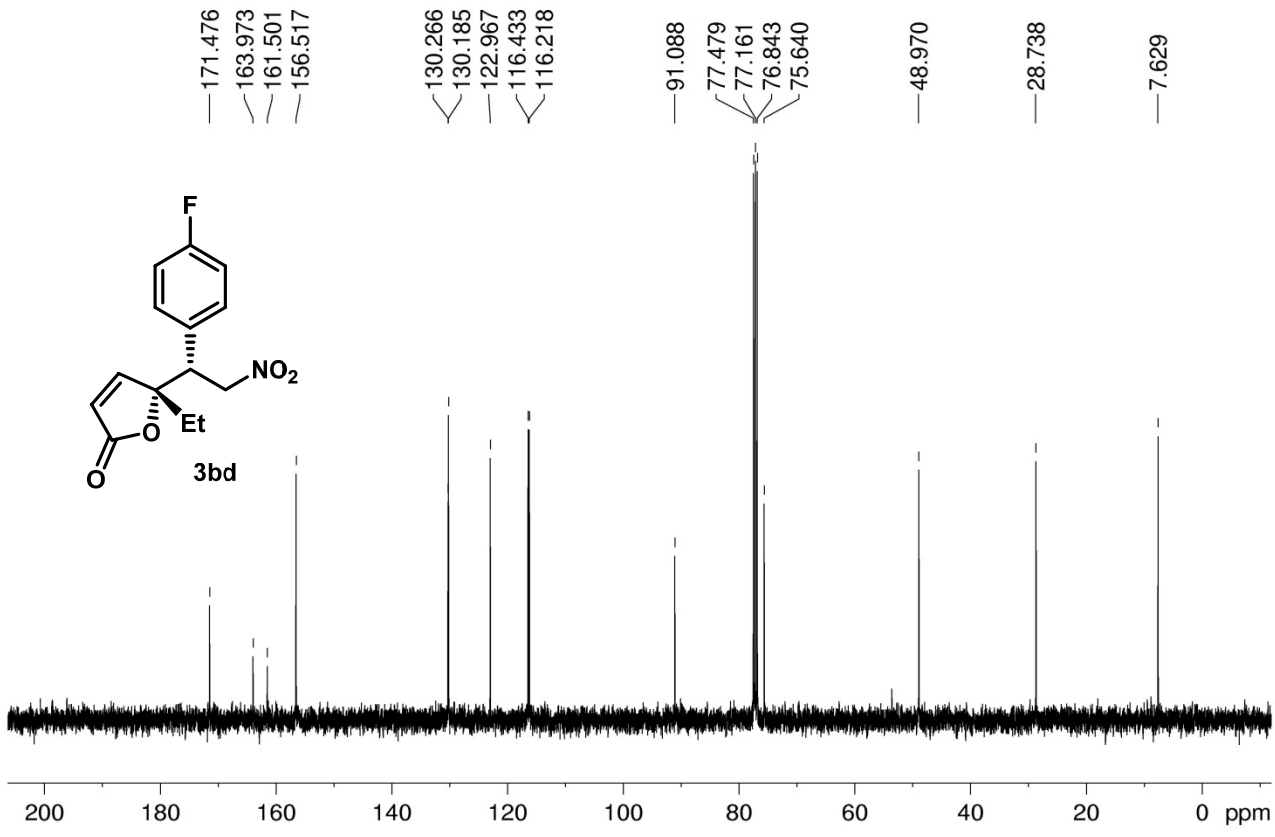


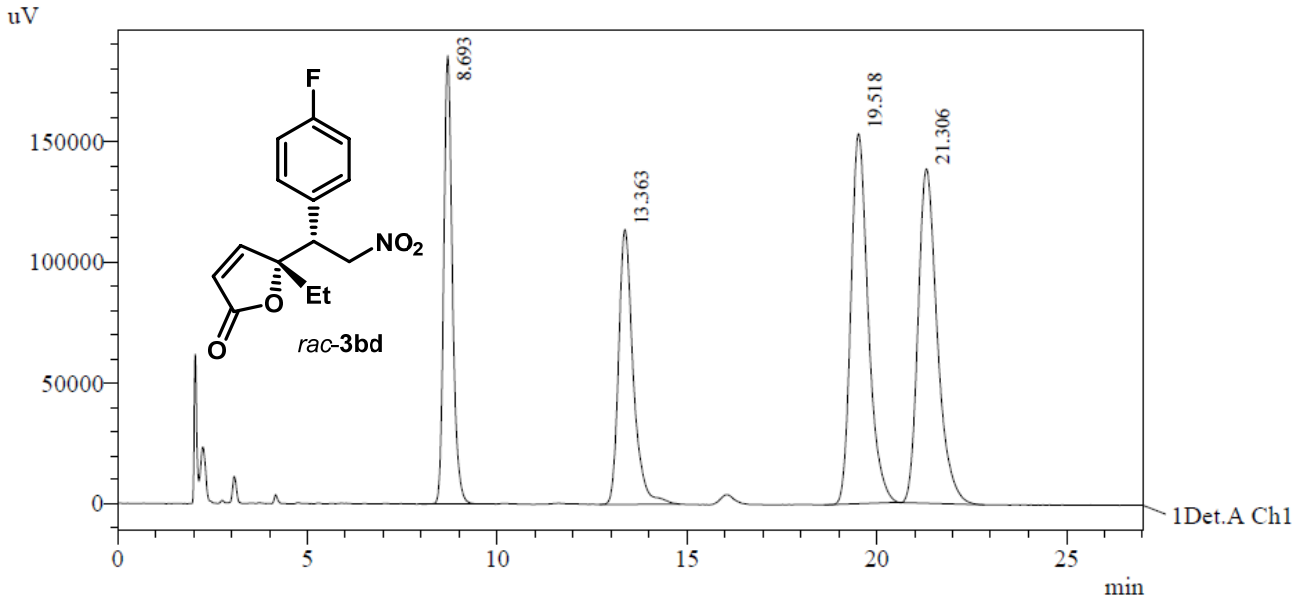
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	30.517	9127889	94.743
2	33.704	506458	5.257
Total		9634348	100.000


7.260
7.184
7.167
7.145
7.132
7.028
7.008
6.987
5.966
5.952
5.288
4.876
4.865
4.843
4.832
4.762
4.735
4.703
4.053
4.042
4.028
4.016
2.016
1.998
1.980
1.962
1.944
1.926
1.844
1.826
1.808
1.790
1.772
1.754
1.240
0.852
0.834
0.816
-0.016
F
NO2
Et
O
O
3bd
10
9
8
7
6
5
4
3
2
1
0
ppm
3.245
2.278
1.000
1.150
1.109
1.097
1.114
1.138
3.406

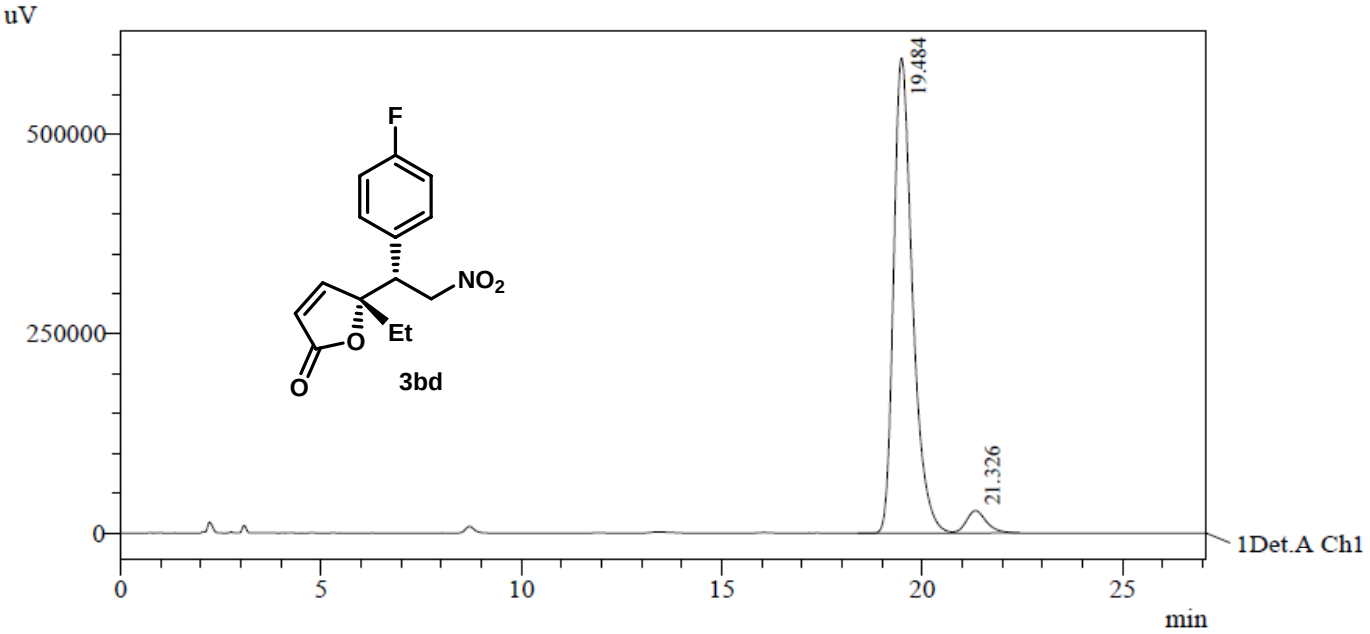

171.476
163.973
161.501
156.517
130.266
130.185
122.967
116.433
116.218
91.088
77.479
77.161
76.843
75.640
48.970
28.738
7.629
F
NO2
Et
O
O
3bd
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

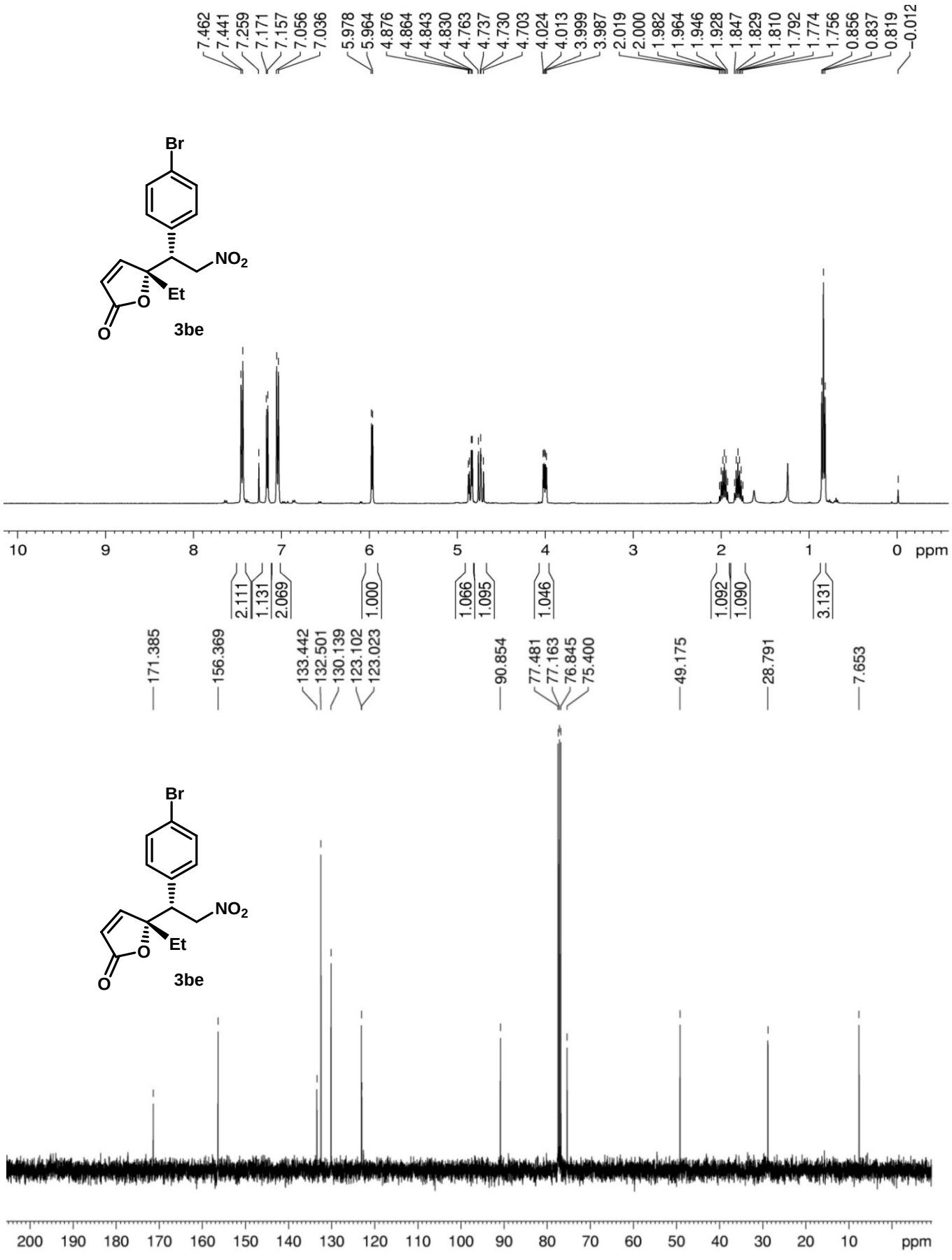
Peak#	Ret. Time	Area	Area %
1	8.693	2946077	18.691
2	13.363	3050442	19.353
3	19.518	4876050	30.936
4	21.306	4889324	31.020
Total		15761893	100.000

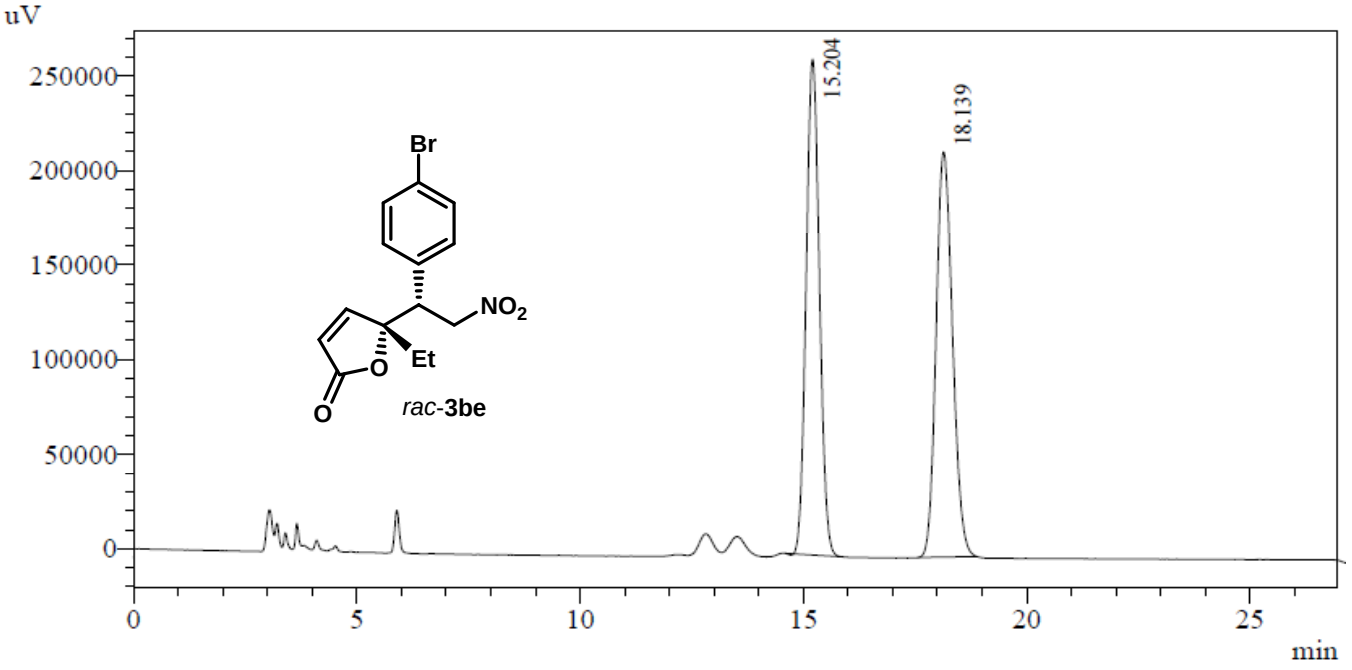


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	19.484	19543704	95.242
2	21.326	976247	4.758
Total		20519951	100.000

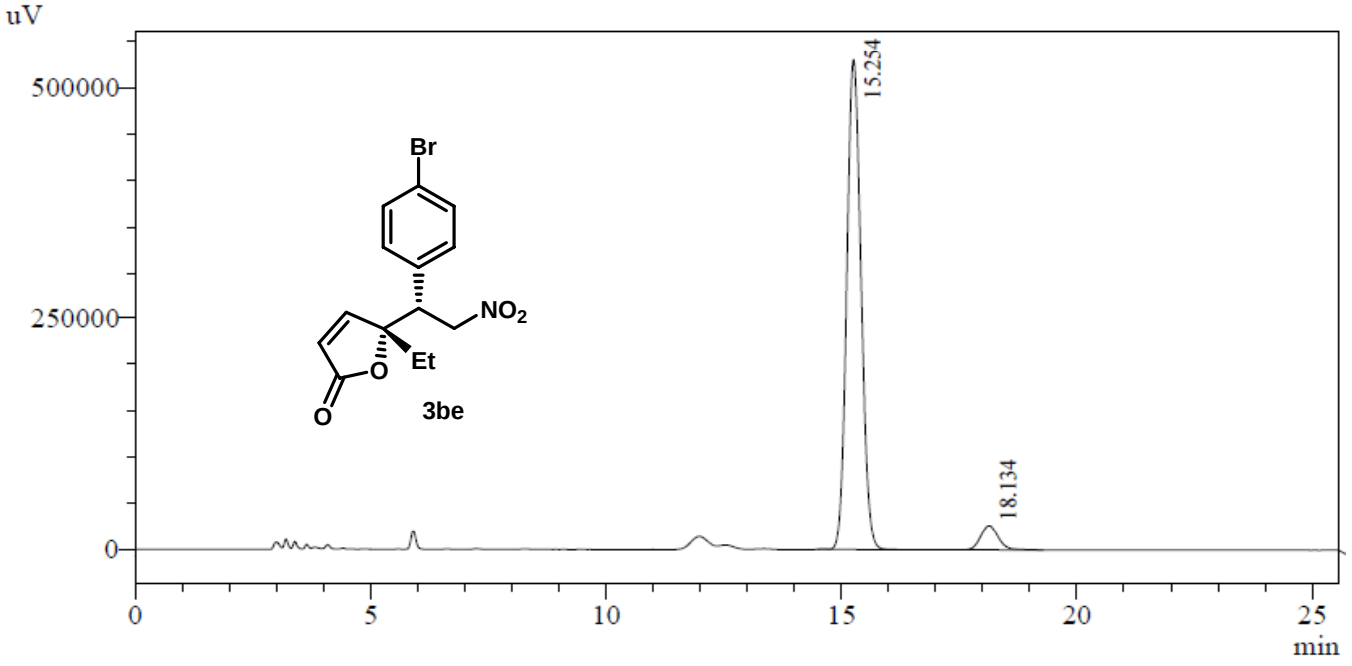

7.462
7.441
7.259
7.171
7.157
7.056
7.036
5.978
5.964
4.876
4.864
4.843
4.830
4.763
4.737
4.730
4.703
4.024
4.013
3.999
3.987
2.019
2.000
1.982
1.964
1.946
1.928
1.847
1.829
1.810
1.792
1.774
1.756
0.856
0.837
0.819
-0.012
Br
NO2
Et
O
O
3be
10 9 8 7 6 5 4 3 2 1 0 ppm
2.111
1.131
2.069
1.000
1.066
1.095
1.046
1.092
1.090
3.131
171.385
156.369
133.442
132.501
130.139
123.102
123.023
90.854
77.481
77.163
76.845
75.400
49.175
28.791
7.653
Br
NO2
Et
O
O
3be
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



PeakTable

Detector A Ch1 210nm

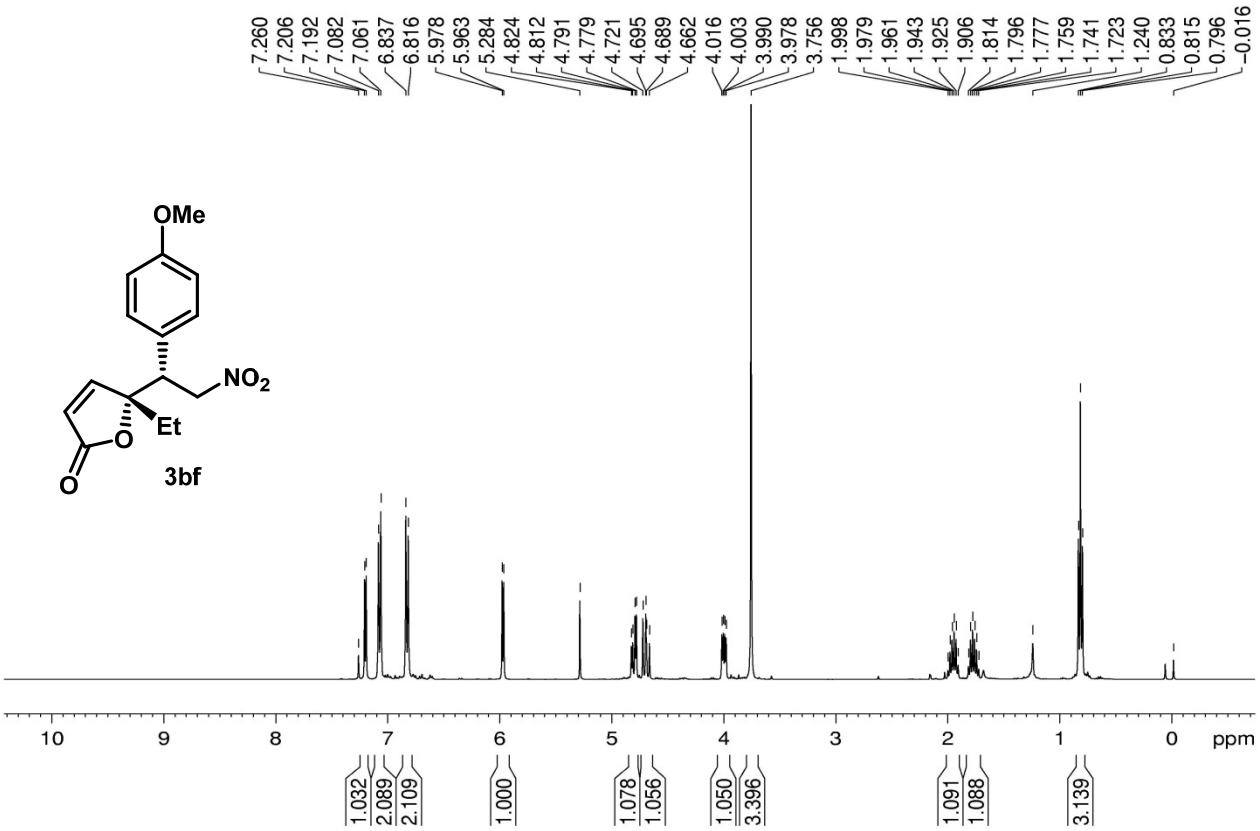
Peak#	Ret. Time	Area	Area %
1	15.204	5423316	49.659
2	18.139	5497726	50.341
Total		10921041	100.000

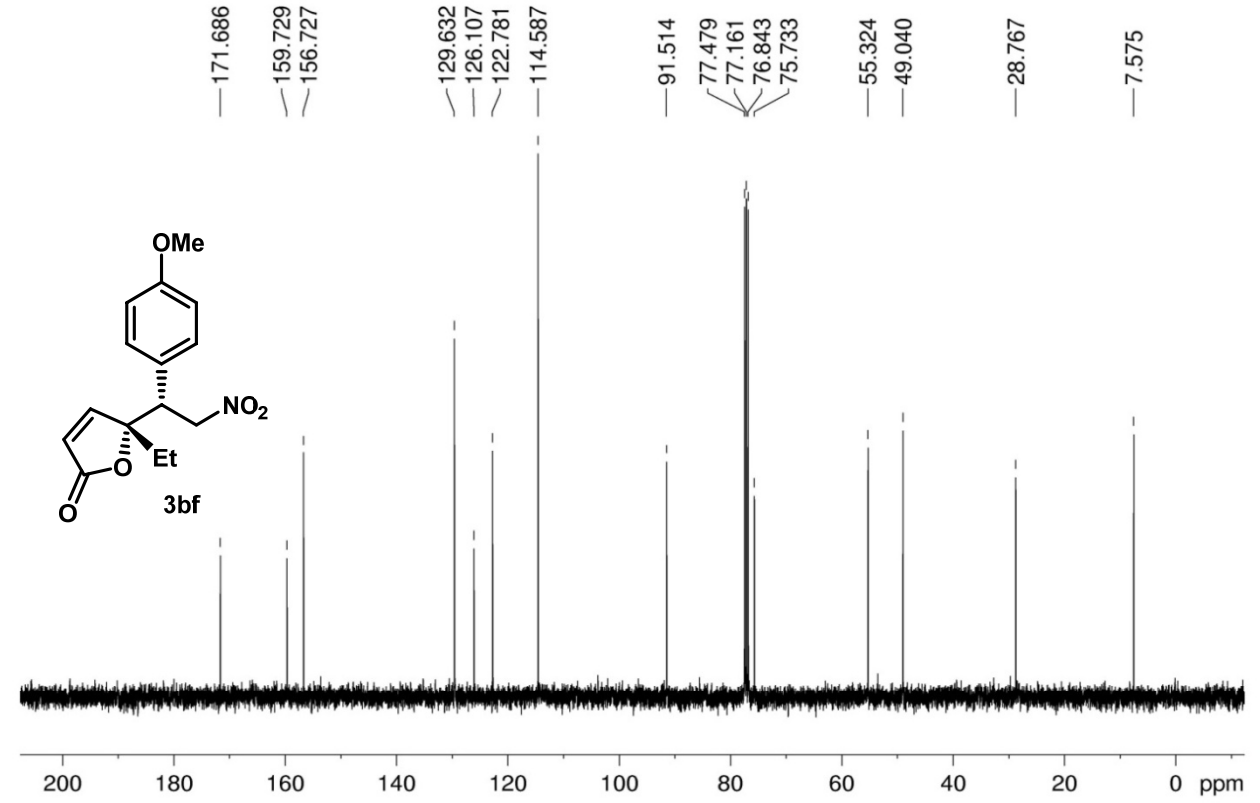


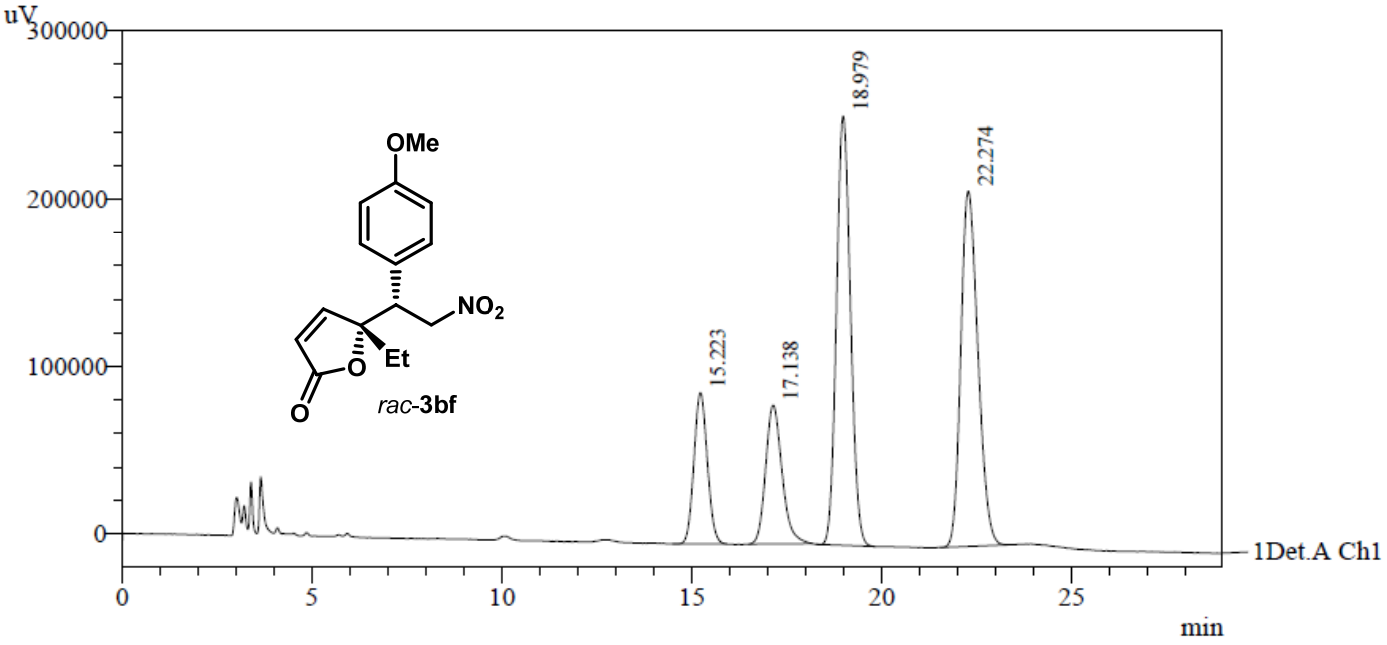
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	15.254	11192758	94.144
2	18.134	696265	5.856
Total		11889023	100.000


7.260
7.206
7.192
7.082
7.061
6.837
6.816
5.978
5.963
5.284
4.824
4.812
4.791
4.779
4.721
4.695
4.689
4.662
4.016
4.003
3.990
3.978
3.756
1.998
1.979
1.961
1.943
1.925
1.906
1.814
1.796
1.777
1.759
1.741
1.723
1.240
0.833
0.815
0.796
-0.016
OMe
NO2
Et
O
O
3bf
10
9
8
7
6
5
4
3
2
1
0
ppm
1.032
2.089
2.109
1.000
1.078
1.056
1.050
3.396
1.091
1.088
3.139

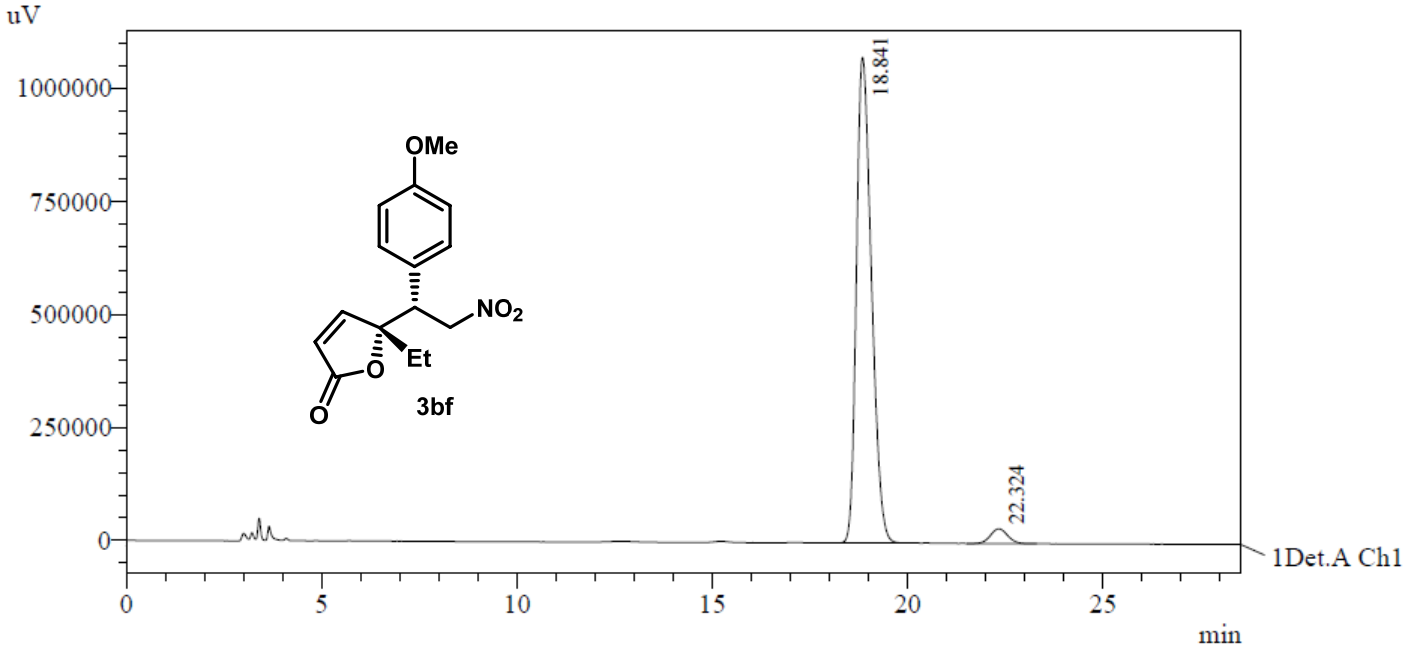

171.686
159.729
156.727
129.632
126.107
122.781
114.587
91.514
77.479
77.161
76.843
75.733
55.324
49.040
28.767
7.575
OMe
NO2
Et
O
O
3bf
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

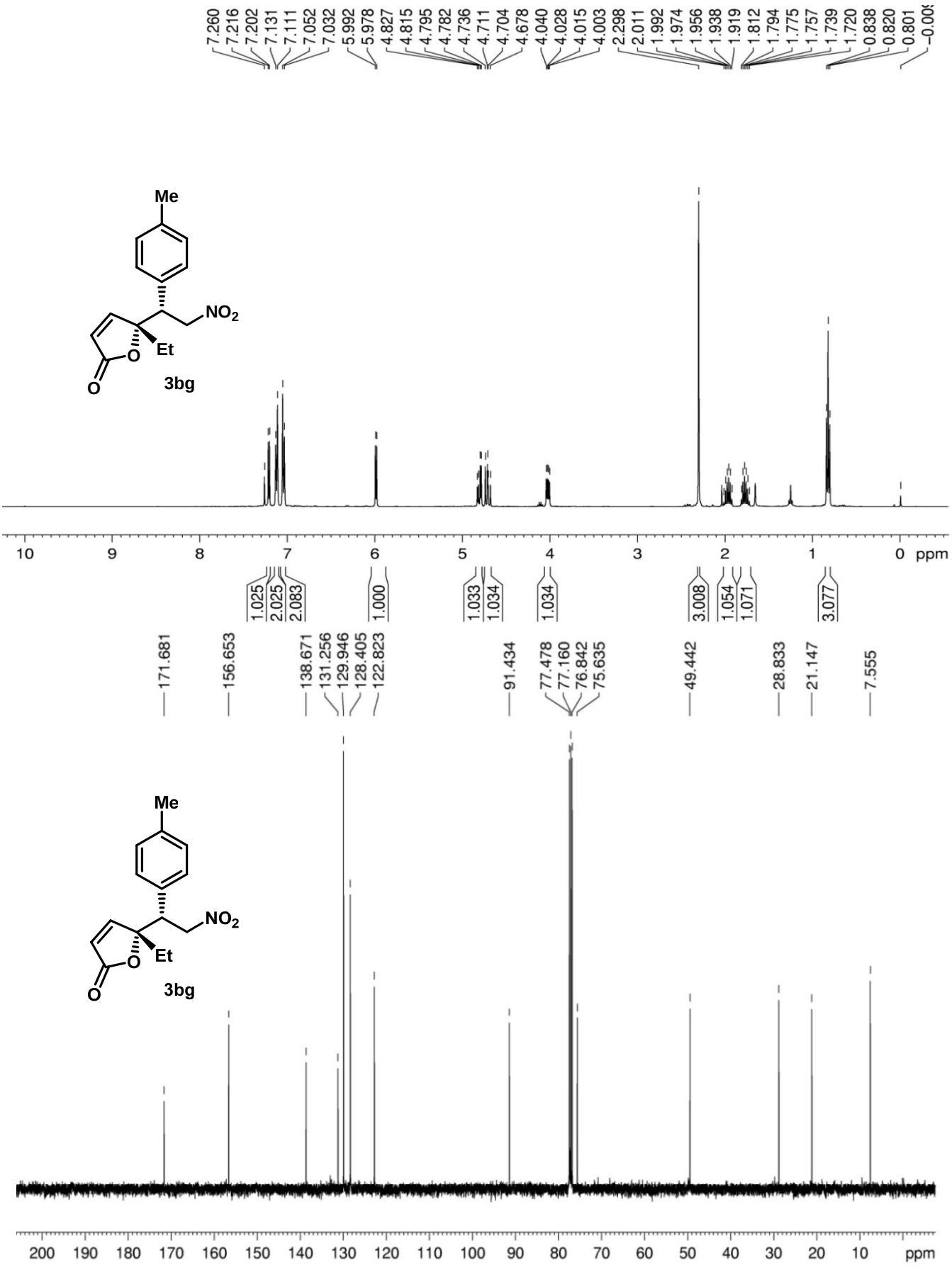
Peak#	Ret. Time	Area	Area %
1	15.223	2223525	12.359
2	17.138	2500017	13.896
3	18.979	6605960	36.718
4	22.274	6661442	37.027
Total		17990943	100.000

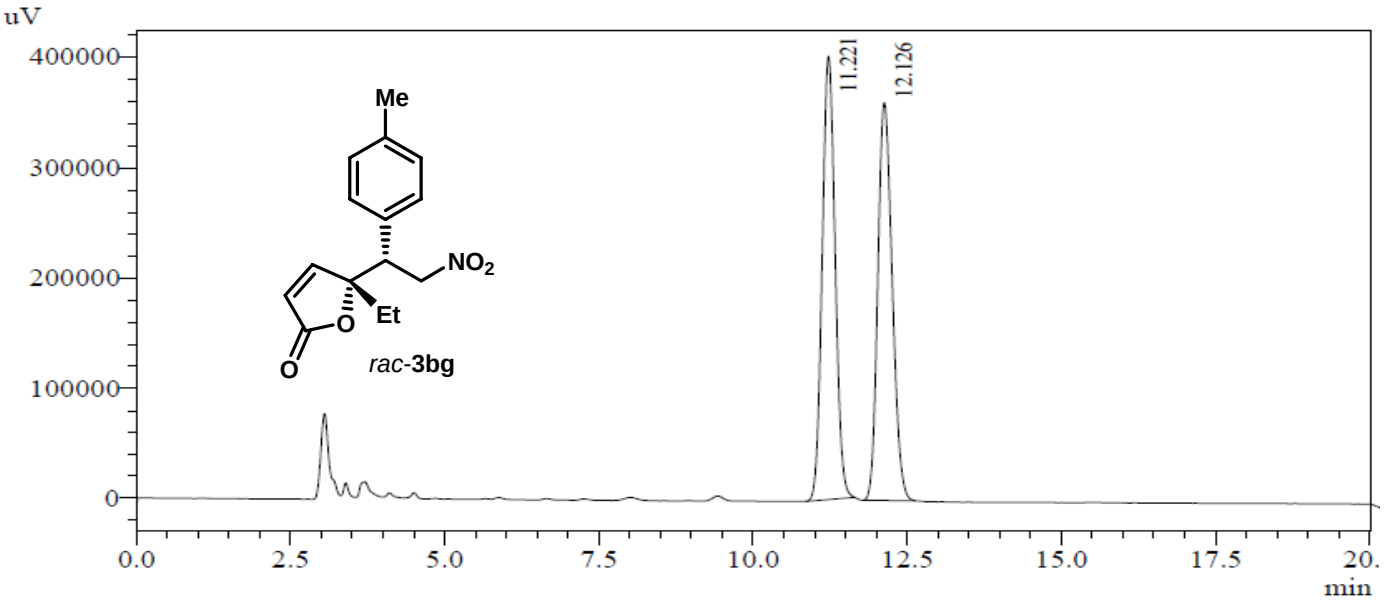


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	18.841	28814217	96.692
2	22.324	985778	3.308
Total		29799994	100.000

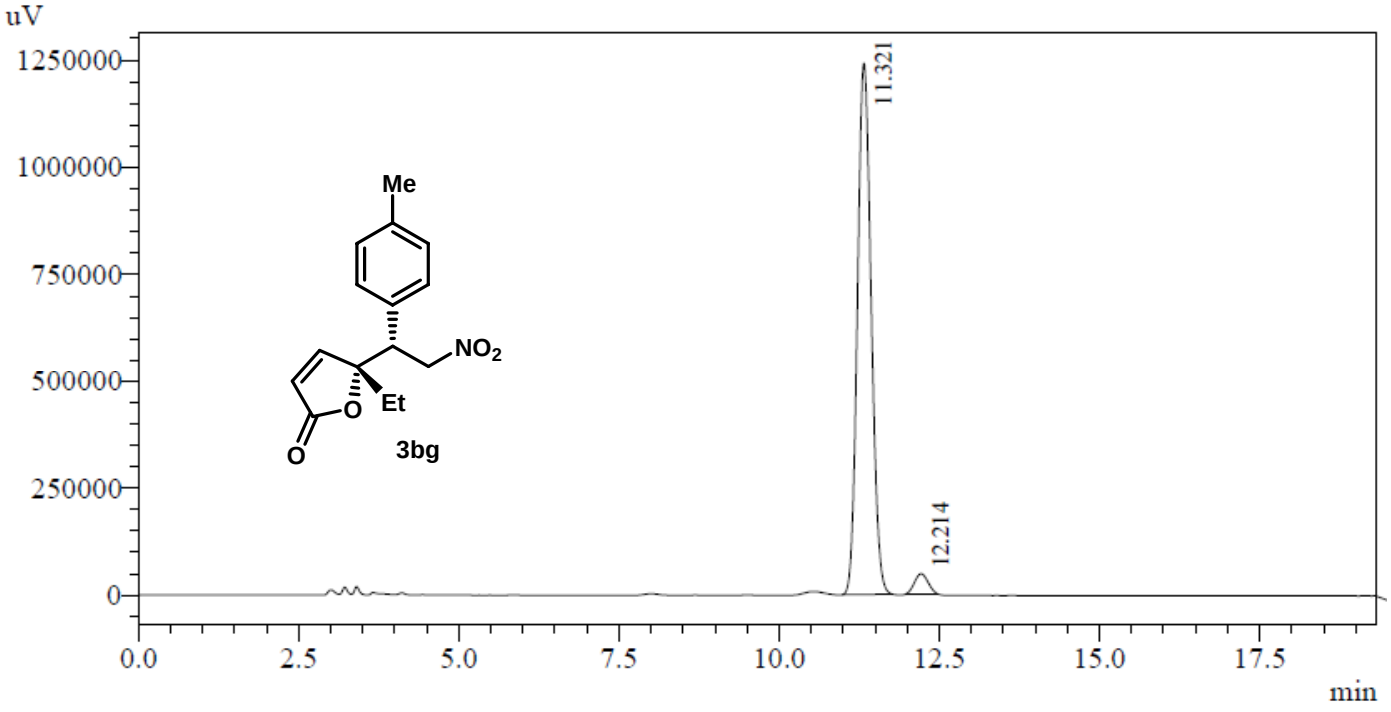

7.260
7.216
7.202
7.131
7.111
7.052
7.032
5.992
5.978
4.827
4.815
4.795
4.782
4.736
4.711
4.704
4.678
4.040
4.028
4.015
4.003
2.298
2.011
1.992
1.974
1.956
1.938
1.919
1.812
1.794
1.775
1.757
1.739
1.720
0.838
0.820
0.801
Me
NO2
Et
O
O
3bg
10 9 8 7 6 5 4 3 2 1 0 ppm
1.025
2.025
2.083
1.000
1.033
1.034
1.034
3.008
1.054
1.071
3.077
171.681
156.653
138.671
131.256
129.946
128.405
122.823
91.434
77.478
77.160
76.842
75.635
49.442
28.833
21.147
7.555
Me
NO2
Et
O
O
3bg
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



PeakTable

Detector A Ch1 210nm

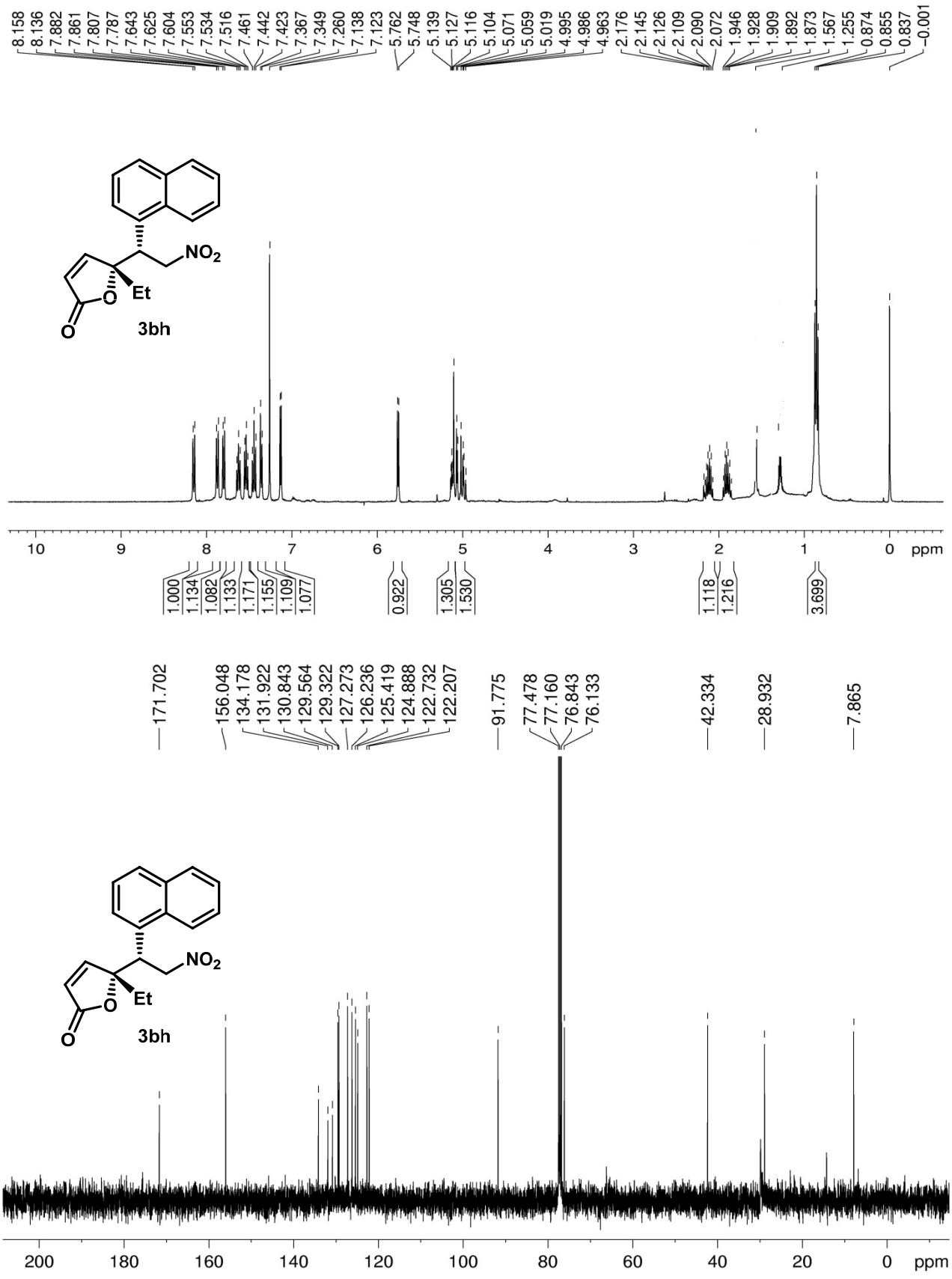
Peak#	Ret. Time	Area	Area %
1	11.221	5858816	49.948
2	12.126	5871083	50.052
Total		11729899	100.000

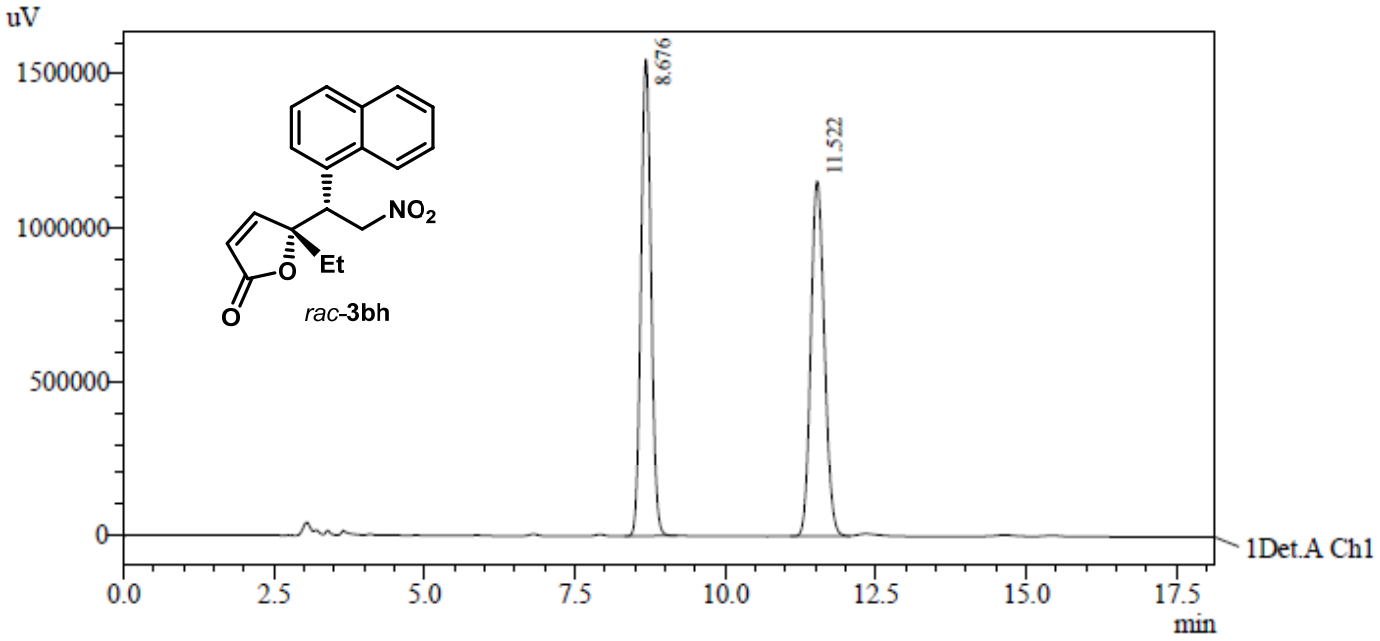


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	11.321	18492120	96.309
2	12.214	708750	3.691
Total		19200870	100.000

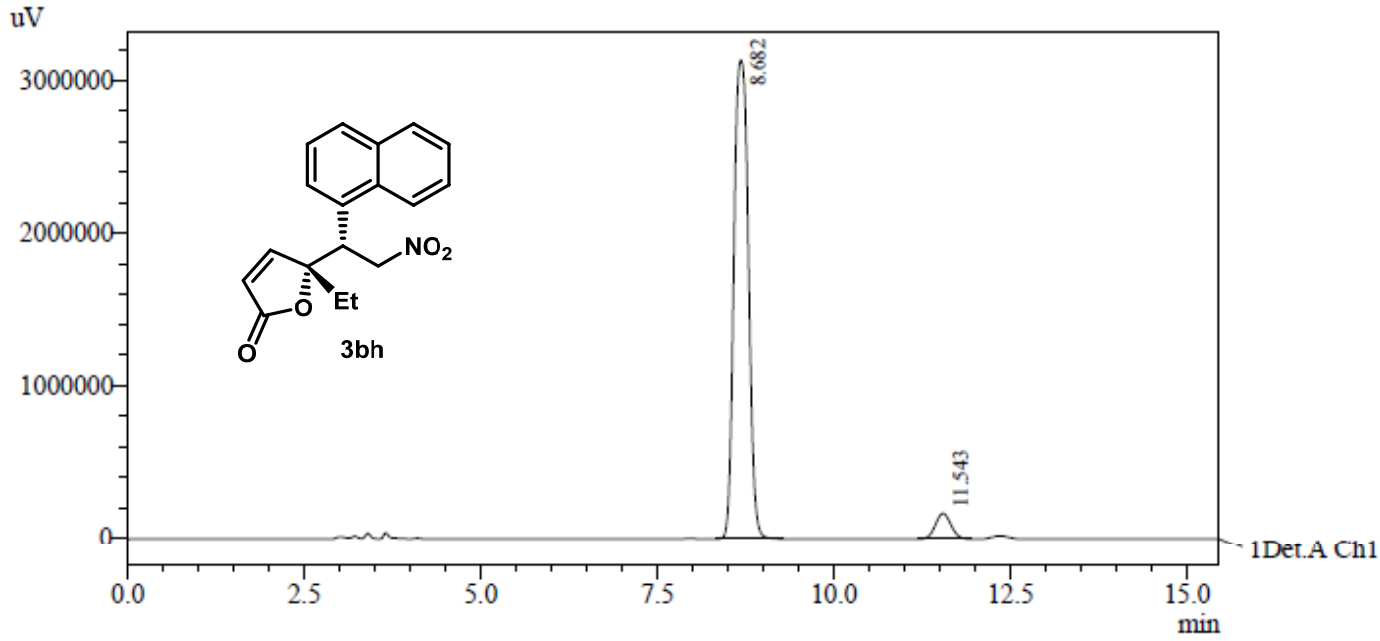

8.158
8.136
7.882
7.861
7.807
7.787
7.643
7.625
7.604
7.553
7.534
7.516
7.461
7.442
7.423
7.367
7.349
7.260
7.138
7.123
5.762
5.748
5.139
5.127
5.116
5.104
5.071
5.059
5.019
4.995
4.986
4.963
2.176
2.145
2.126
2.109
2.090
2.072
1.946
1.928
1.909
1.892
1.873
1.567
1.255
0.874
0.855
0.837
-0.001
NO2
Et
O
O
3bh
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.134
1.082
1.133
1.171
1.155
1.109
1.077
0.922
1.305
1.530
1.118
1.216
3.699
171.702
156.048
134.178
131.922
130.843
129.564
129.322
127.273
126.236
125.419
124.888
122.732
122.207
91.775
77.478
77.160
76.843
76.133
42.334
28.932
7.865
NO2
Et
O
O
3bh
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

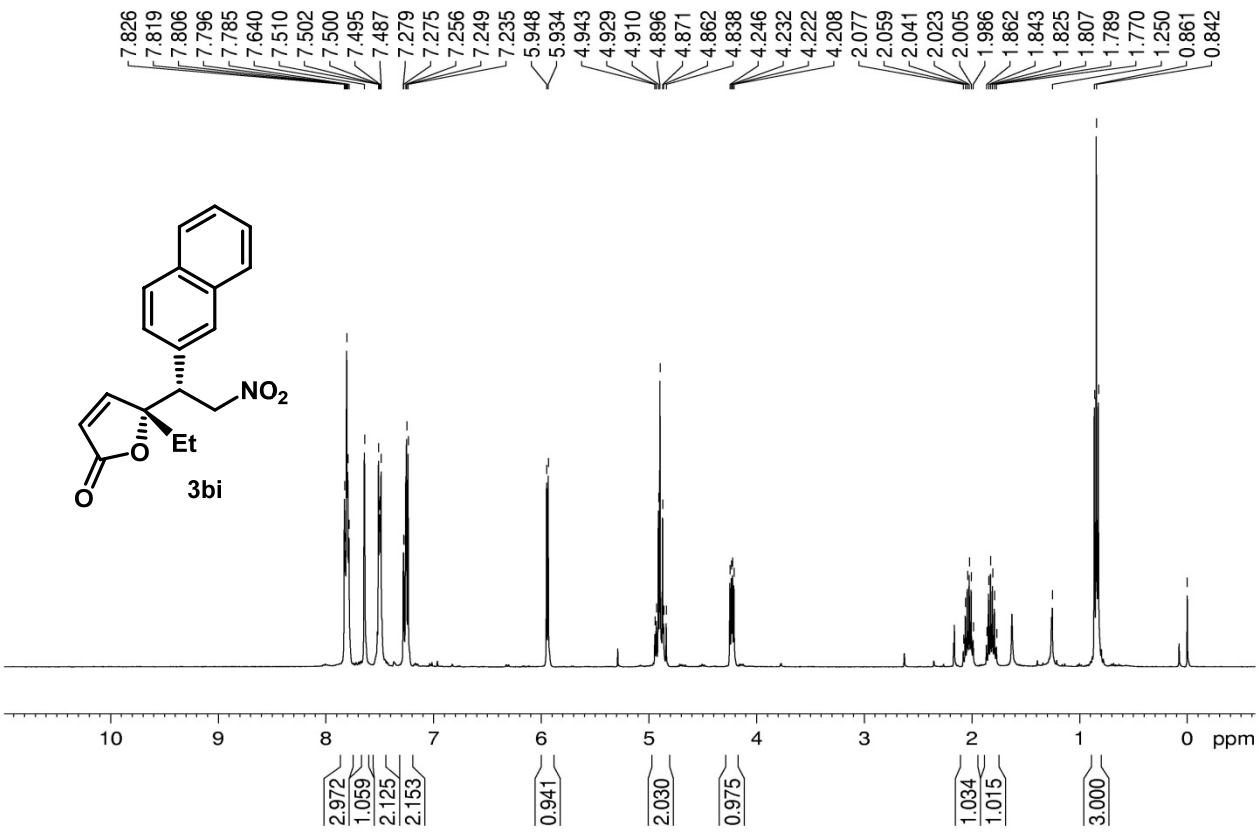
Peak#	Ret. Time	Area	Area %
1	8.676	18088111	49.841
2	11.522	18203188	50.159
Total		36291300	100.000

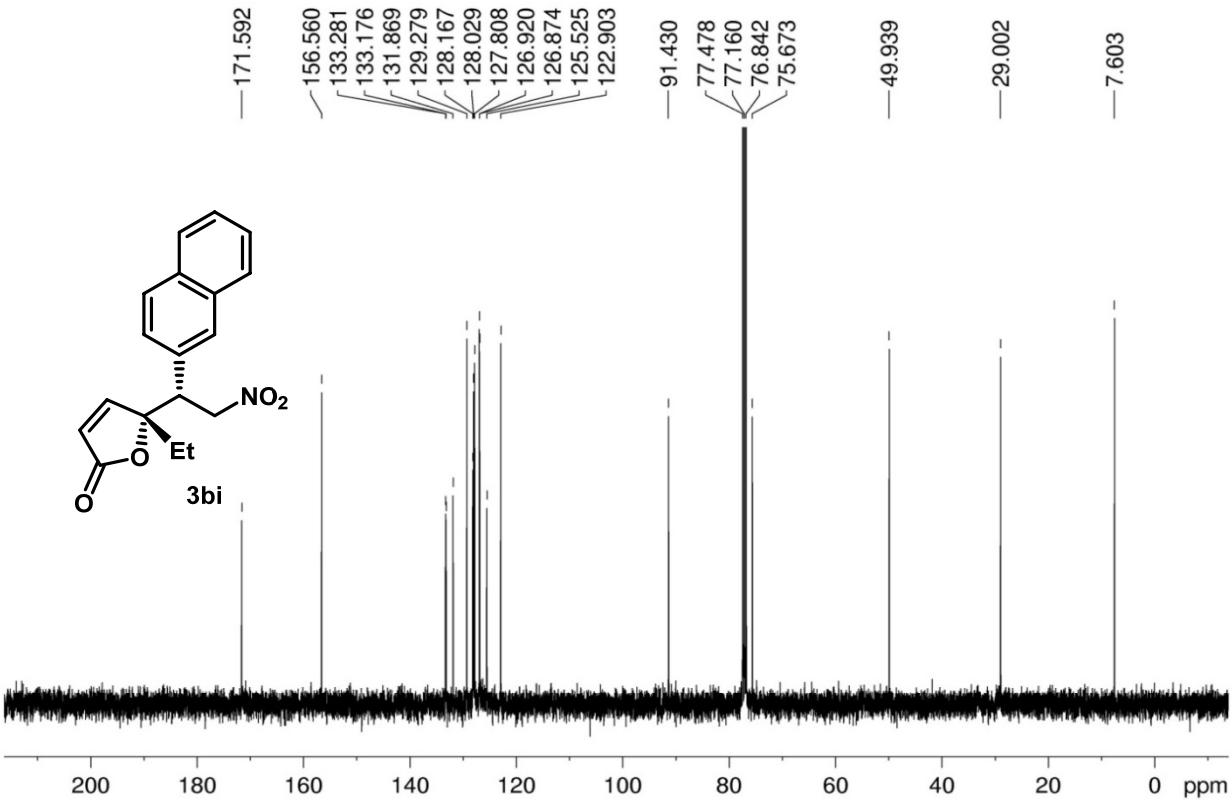


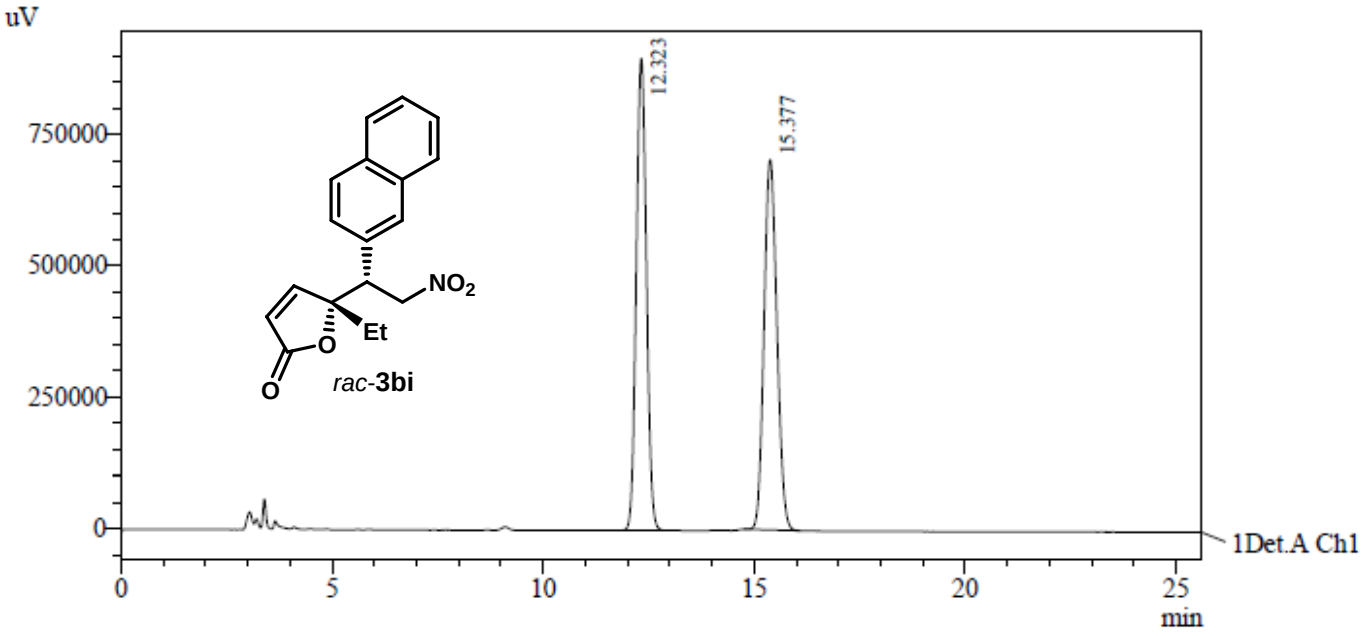
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	8.682	44554458	94.550
2	11.543	2568332	5.450
Total		47122790	100.000


7.826
7.819
7.806
7.796
7.785
7.640
7.510
7.502
7.500
7.495
7.487
7.279
7.275
7.256
7.249
7.235
5.948
5.934
4.943
4.929
4.910
4.896
4.871
4.862
4.838
4.246
4.232
4.222
4.208
2.077
2.059
2.041
2.023
2.005
1.986
1.862
1.843
1.825
1.807
1.789
1.770
1.250
0.861
0.842
NO2
Et
O
O
3bi
10
9
8
7
6
5
4
3
2
1
0
ppm
2.972
1.059
2.125
2.153
0.941
2.030
0.975
1.034
1.015
3.000

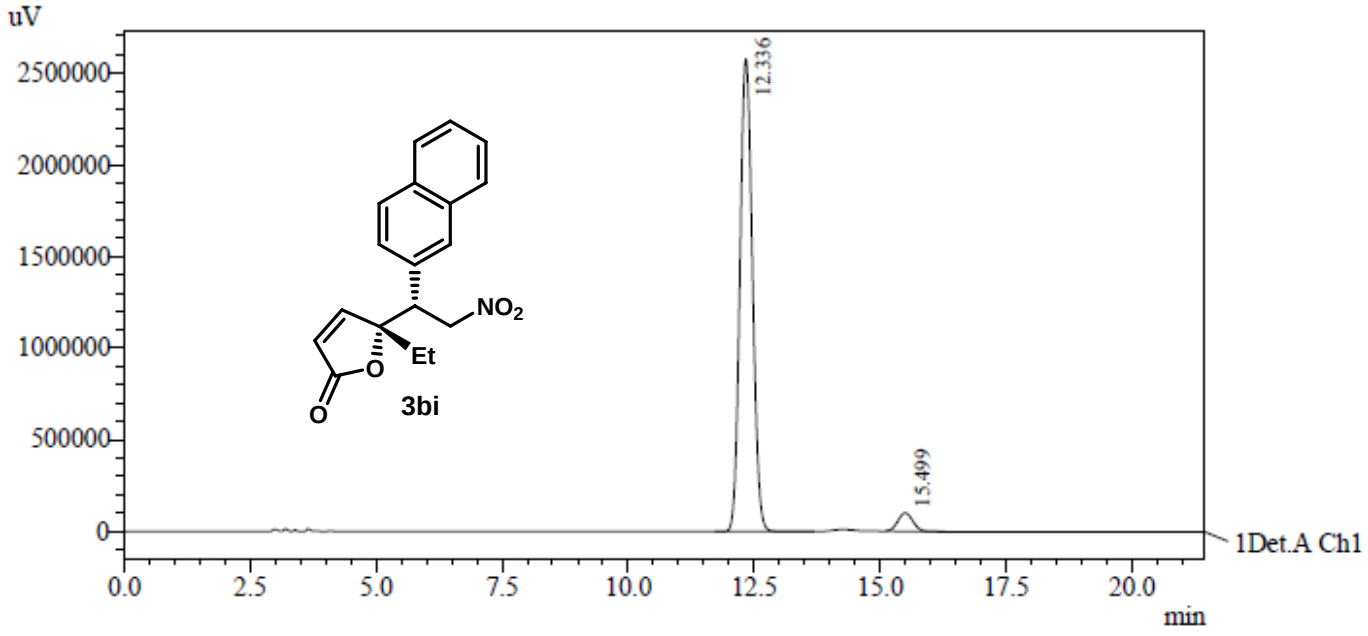

171.592
156.560
133.281
133.176
131.869
129.279
128.167
128.029
127.808
126.920
126.874
125.525
122.903
91.430
77.478
77.160
76.842
75.673
49.939
29.002
7.603
NO2
Et
O
O
3bi
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

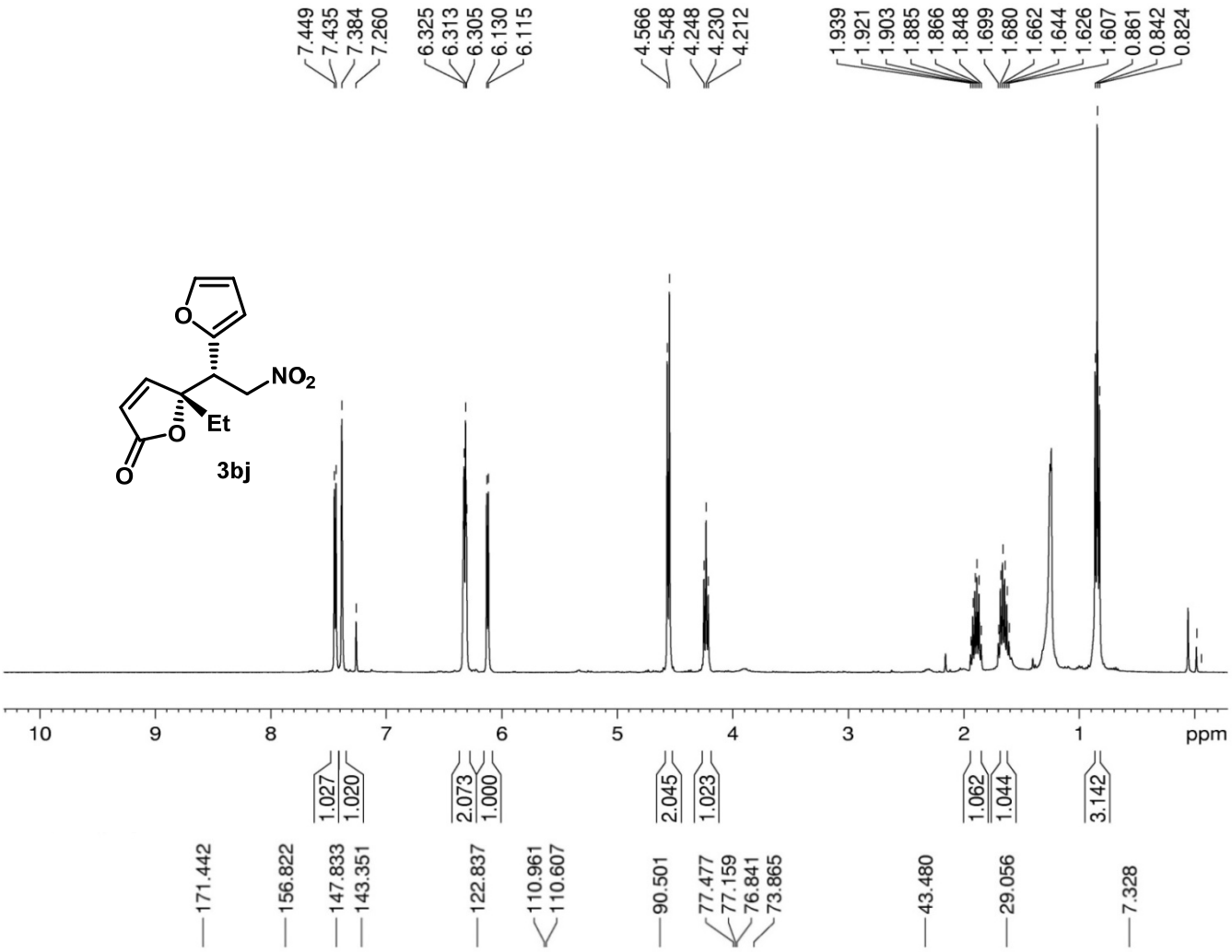
Peak#	Ret. Time	Area	Area %
1	12.323	14961419	50.083
2	15.377	14911663	49.917
Total		29873082	100.000

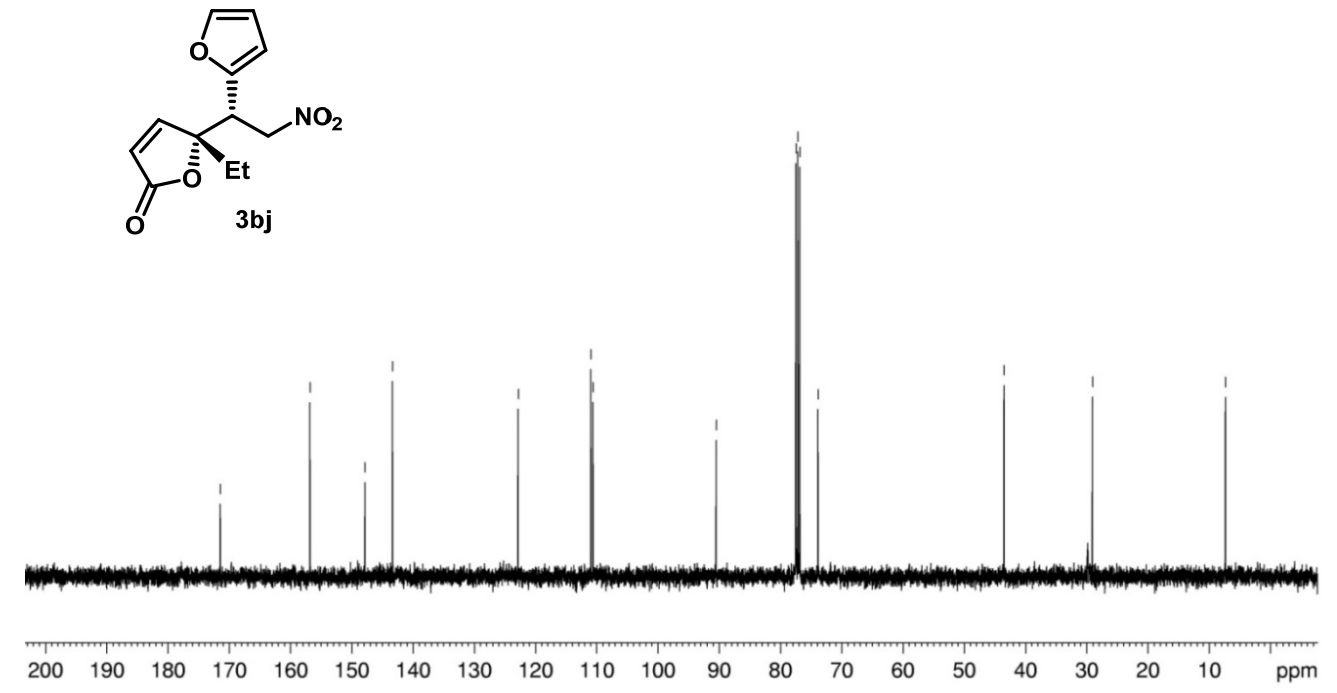


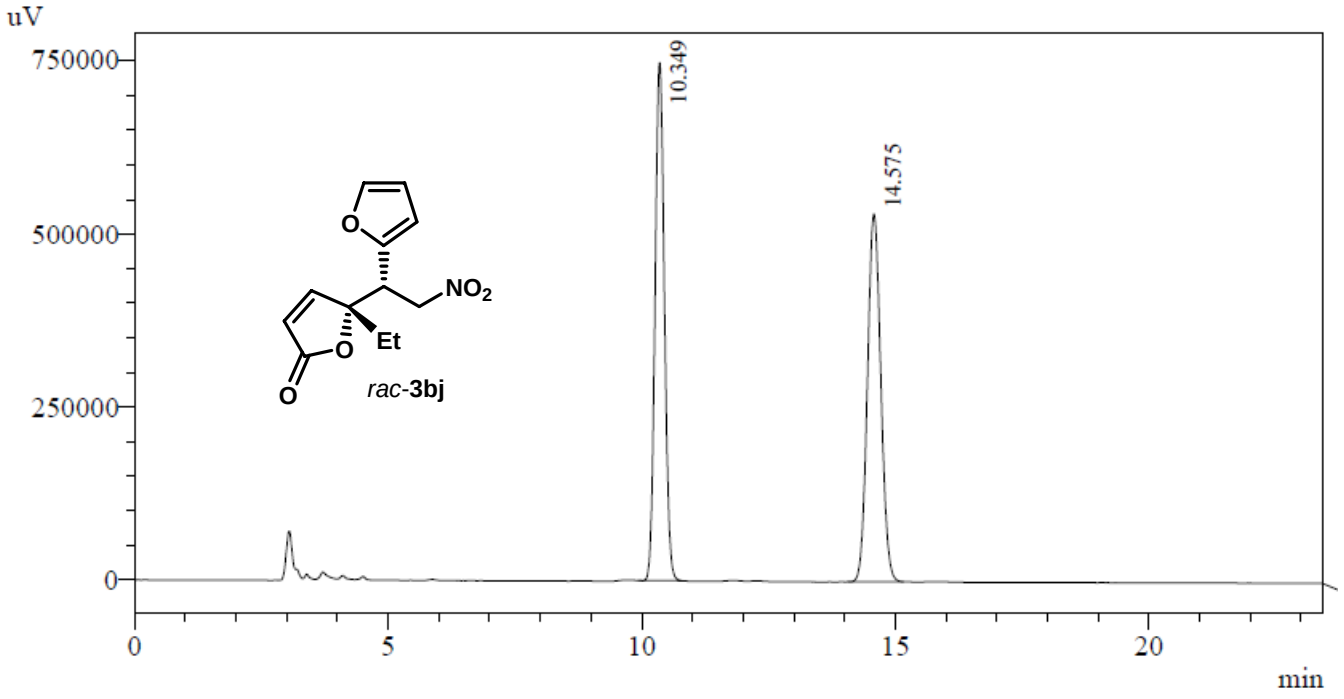
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	12.336	44453895	95.569
2	15.499	2061160	4.431
Total		46515056	100.000


7.449
7.435
7.384
7.260
6.325
6.313
6.305
6.130
6.115
4.566
4.548
4.248
4.230
4.212
1.939
1.921
1.903
1.885
1.866
1.848
1.699
1.680
1.662
1.644
1.626
1.607
0.861
0.842
0.824
NO2
Et
O
O
O
3bj
10
9
8
7
6
5
4
3
2
1
ppm
1.027
1.020
2.073
1.000
2.045
1.023
1.062
1.044
3.142

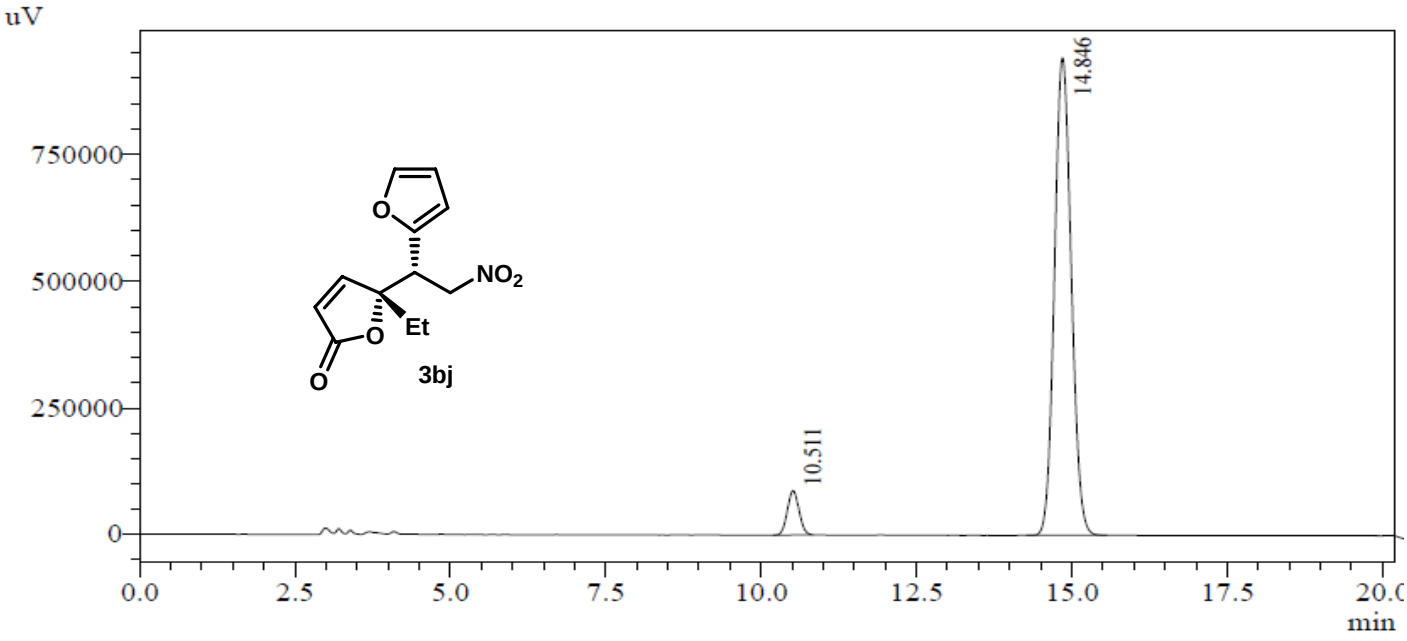

171.442
156.822
147.833
143.351
122.837
110.961
110.607
90.501
77.477
77.159
76.841
73.865
43.480
29.056
7.328
NO2
Et
O
O
O
3bj
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

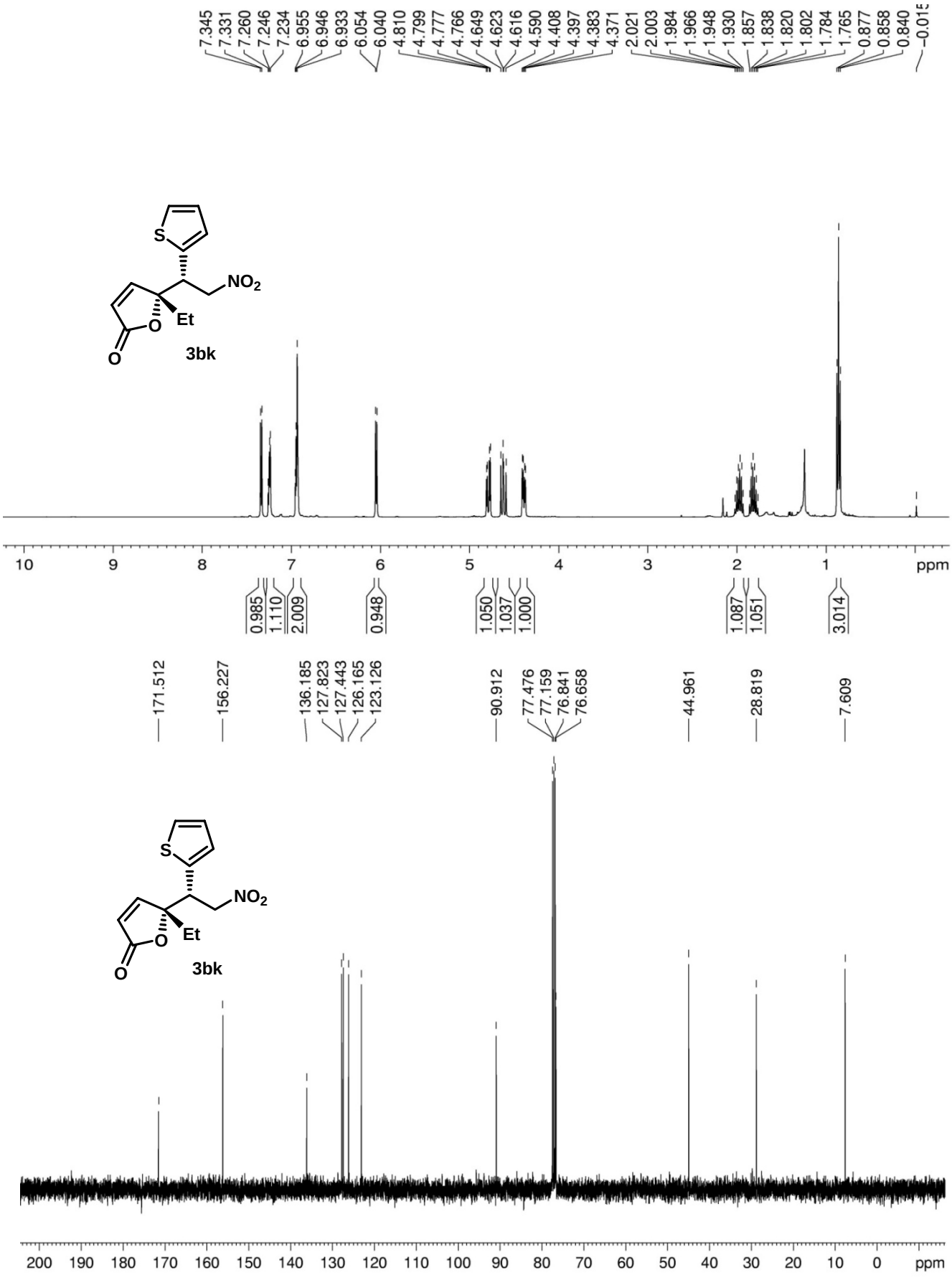
Peak#	Ret. Time	Area	Area %
1	10.349	9573668	49.546
2	14.575	9749175	50.454
Total		19322842	100.000

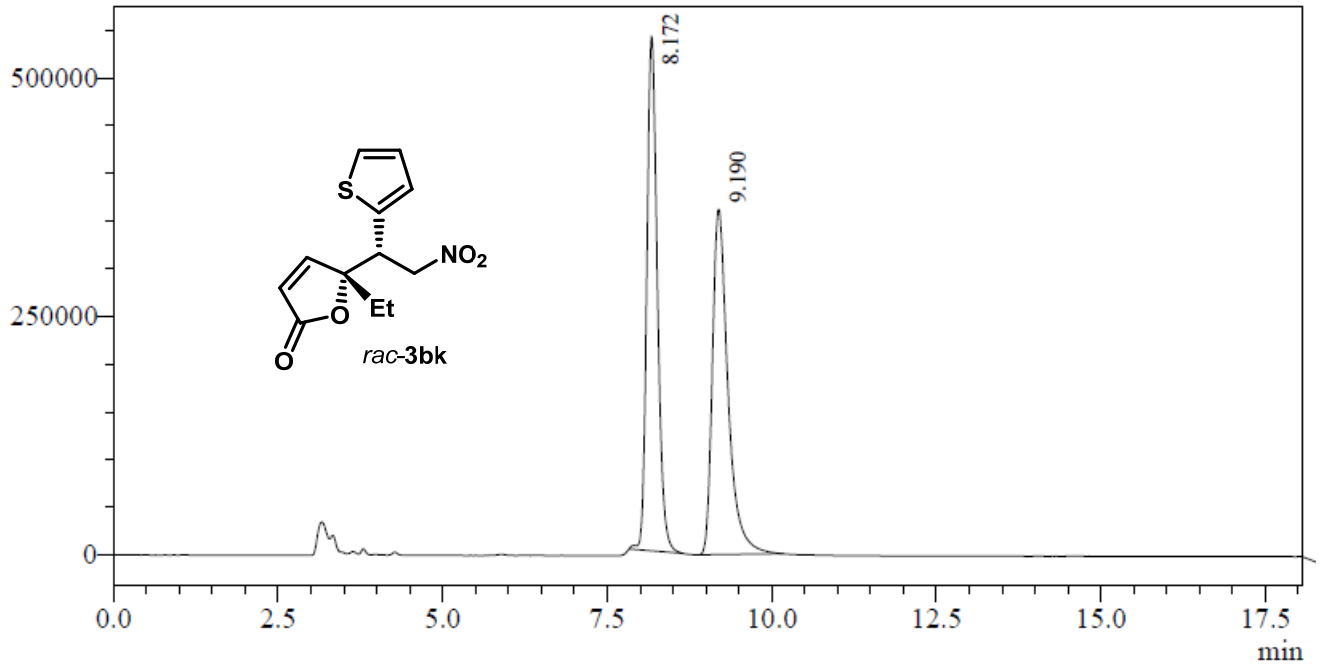


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	10.511	1156579	6.091
2	14.846	17831957	93.909
Total		18988536	100.000

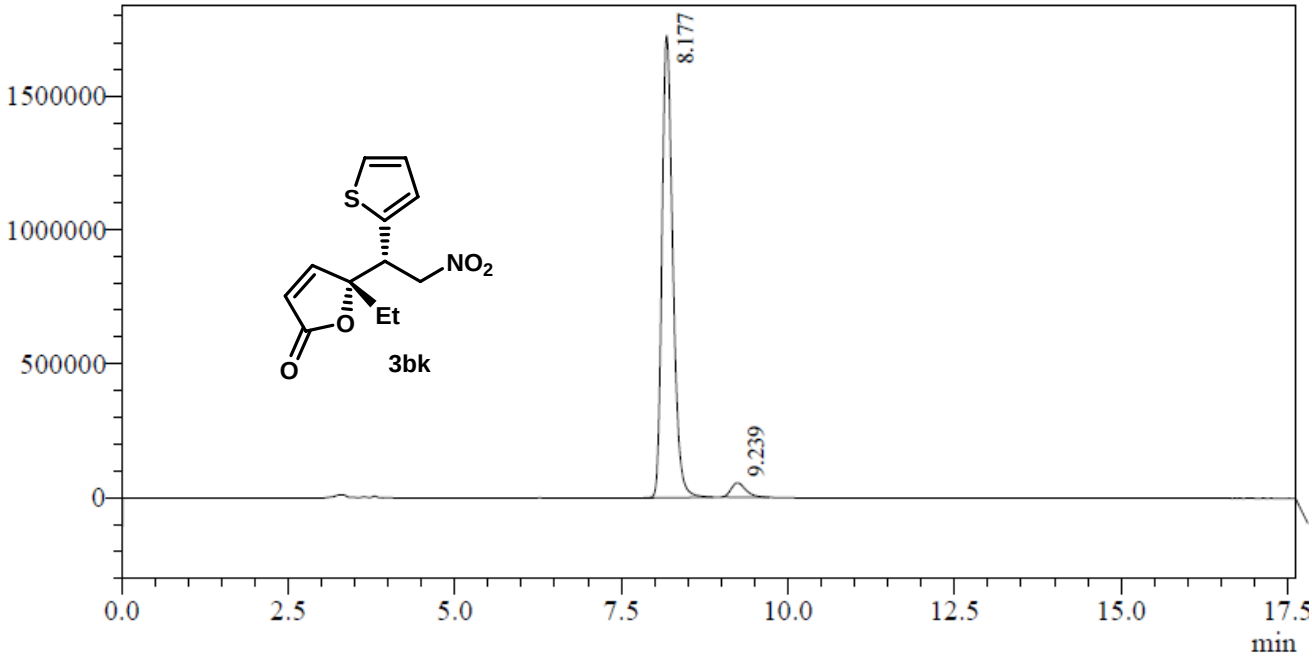

7.345
7.331
7.260
7.246
7.234
6.955
6.946
6.933
6.054
6.040
4.810
4.799
4.777
4.766
4.649
4.623
4.616
4.590
4.408
4.397
4.383
4.371
2.021
2.003
1.984
1.966
1.948
1.930
1.857
1.838
1.820
1.802
1.784
1.765
0.877
0.858
0.840
S
NO2
Et
O
O
3bk
10
9
8
7
6
5
4
3
2
1
ppm
0.985
1.110
2.009
0.948
1.050
1.037
1.000
1.087
1.051
3.014
171.512
156.227
136.185
127.823
127.443
126.165
123.126
90.912
77.476
77.159
76.841
76.658
44.961
28.819
7.609
S
NO2
Et
O
O
3bk
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



PeakTable

Detector A Ch1 210nm

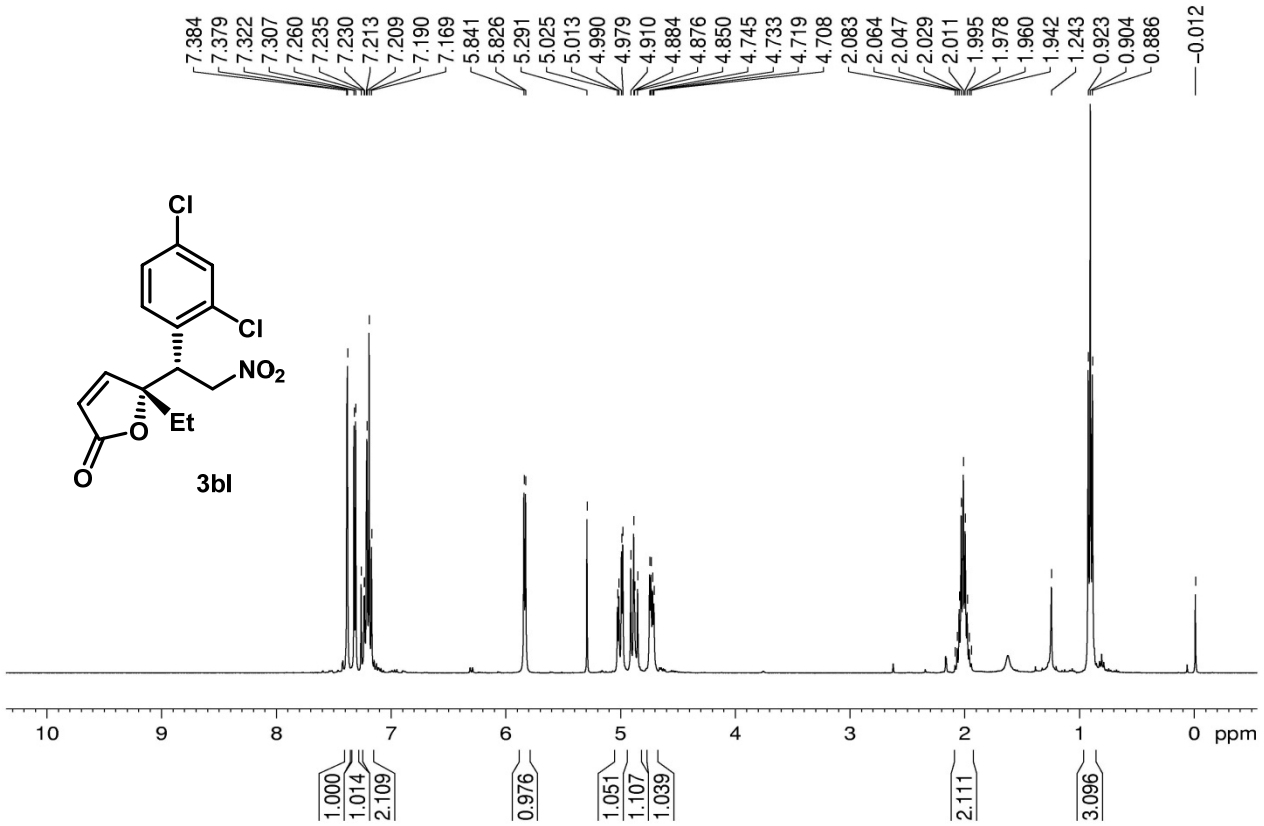
Peak#	Ret. Time	Area	Area %
1	8.172	5988697	50.148
2	9.190	5953437	49.852
Total		11942134	100.000

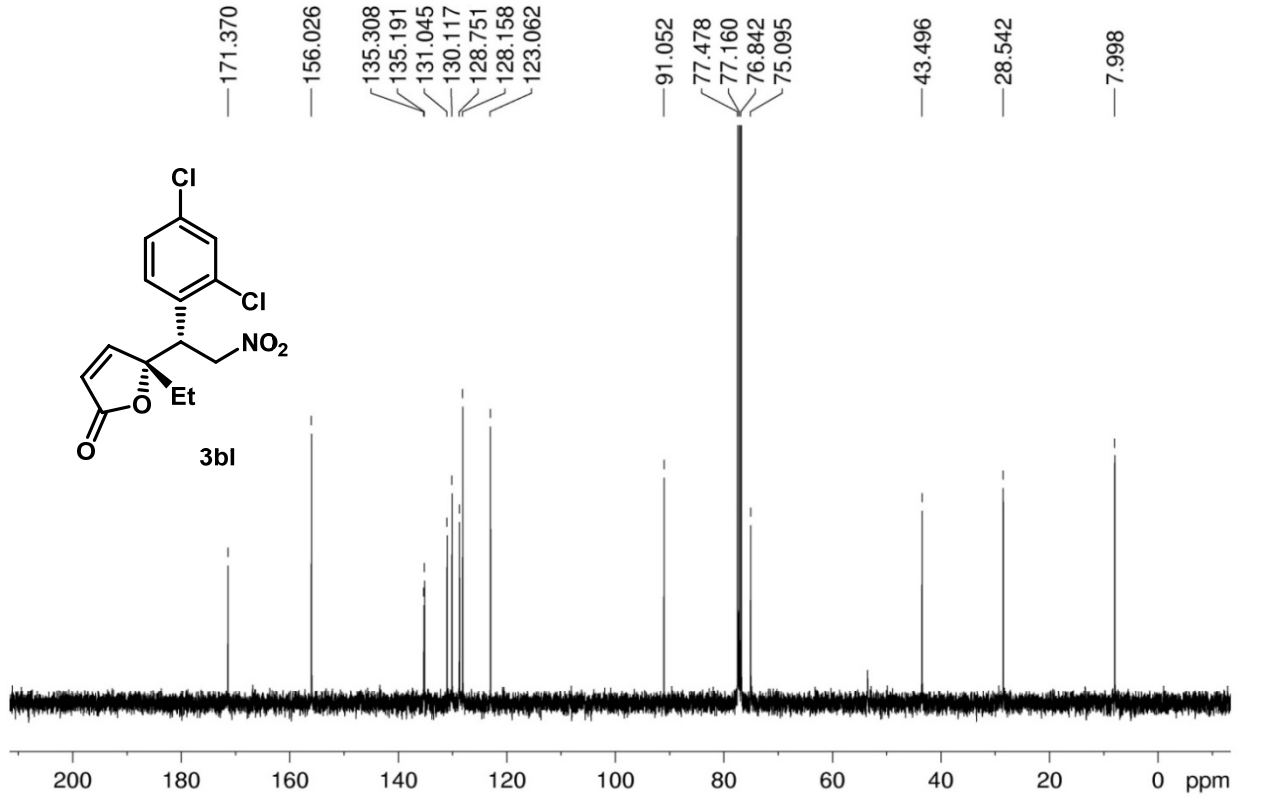


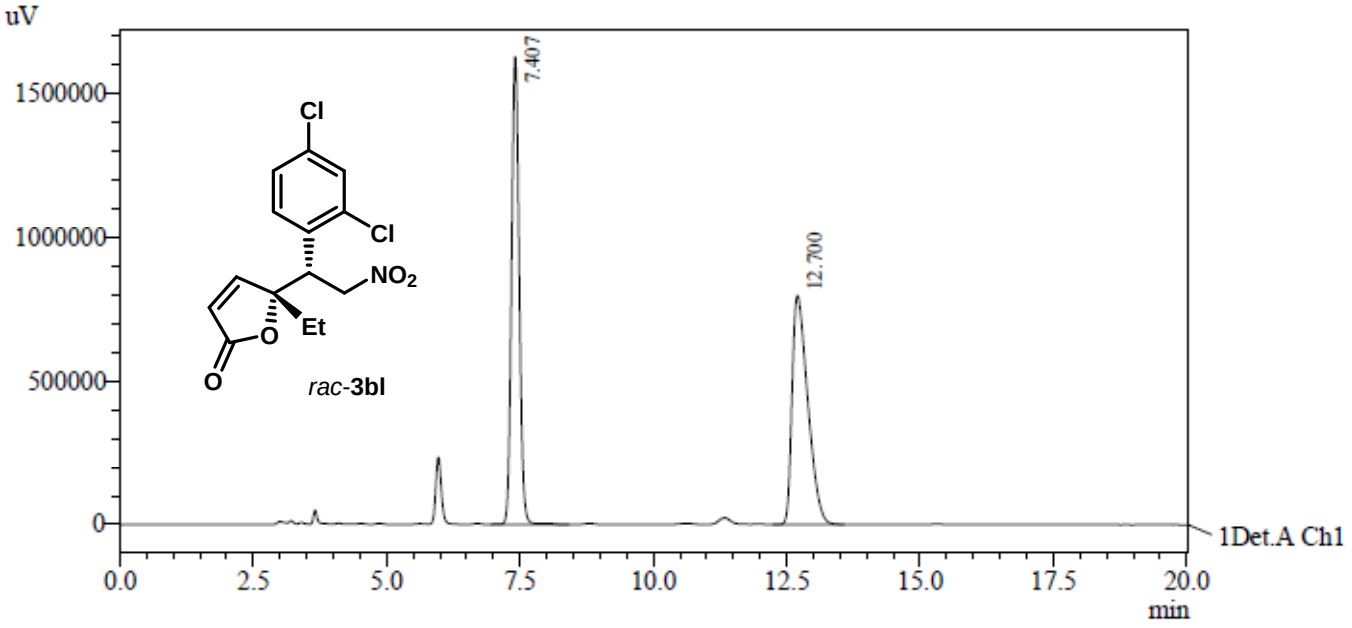
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	8.177	19565396	95.993
2	9.239	816768	4.007
Total		20382164	100.000


7.384
7.379
7.322
7.307
7.260
7.235
7.230
7.213
7.209
7.190
7.169
5.841
5.826
5.291
5.025
5.013
4.990
4.979
4.910
4.884
4.876
4.850
4.745
4.733
4.719
4.708
2.083
2.064
2.047
2.029
2.011
1.995
1.978
1.960
1.942
1.243
0.923
0.904
0.886
-0.012
Cl
Cl
NO2
Et
O
O
3bl
10
9
8
7
6
5
4
3
2
1
0 ppm
1.000
1.014
2.109
0.976
1.051
1.107
1.039
2.111
3.096

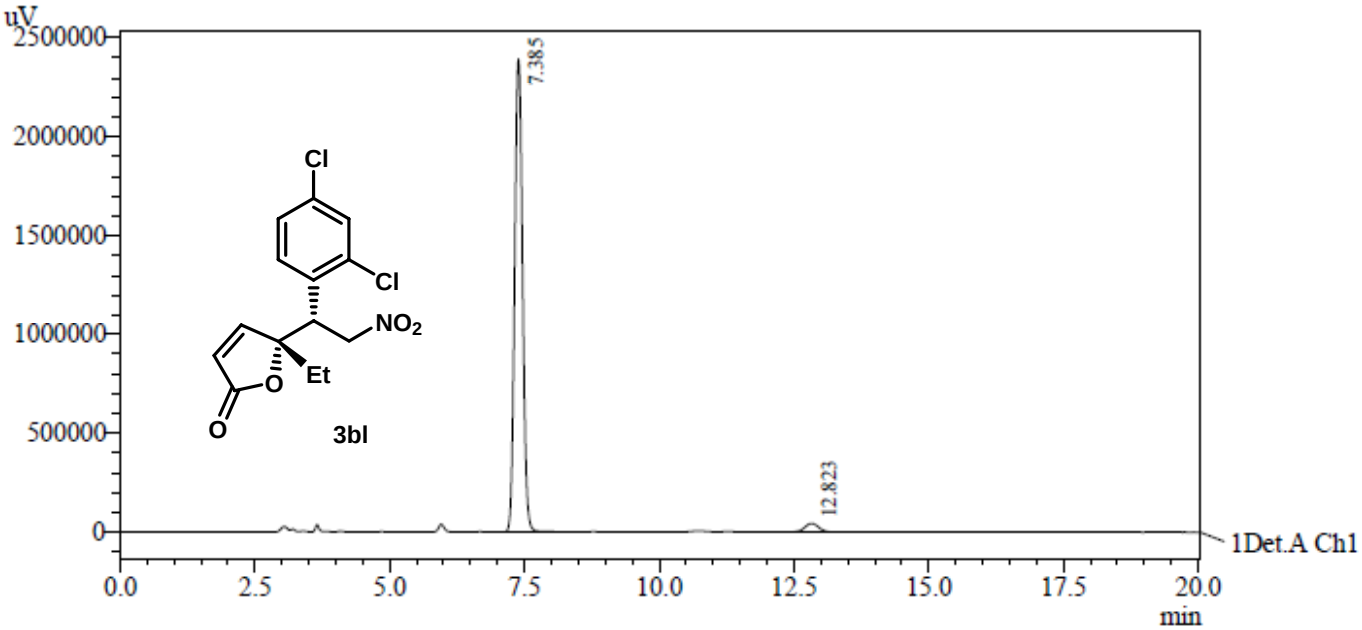

171.370
156.026
135.308
135.191
131.045
130.117
128.751
128.158
123.062
91.052
77.478
77.160
76.842
75.095
43.496
28.542
7.998
Cl
Cl
NO2
Et
O
O
3bl
200
180
160
140
120
100
80
60
40
20
0 ppm



PeakTable

Detector A Ch1 210nm

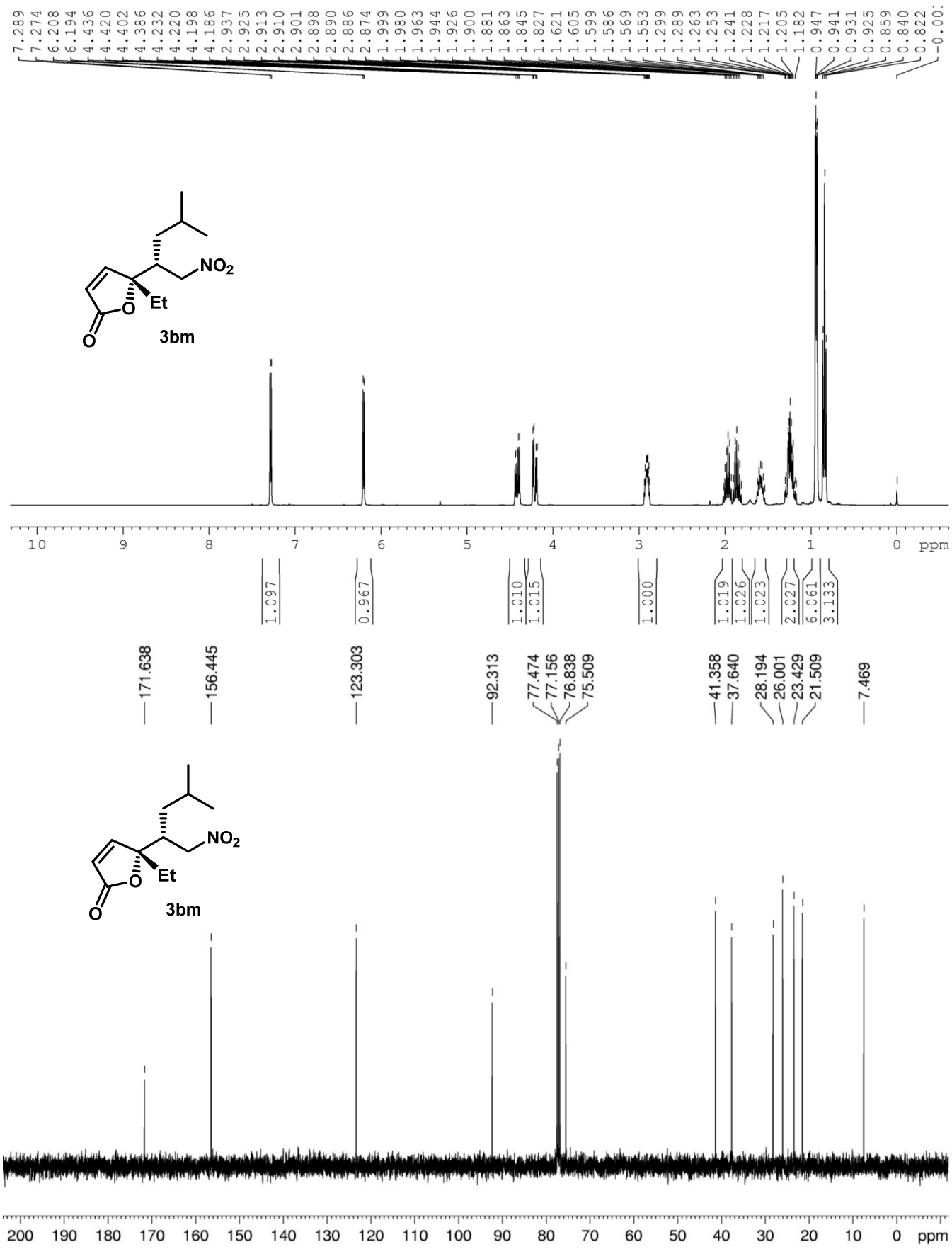
Peak#	Ret. Time	Area	Area %
1	7.407	16310897	49.953
2	12.700	16341518	50.047
Total		32652415	100.000

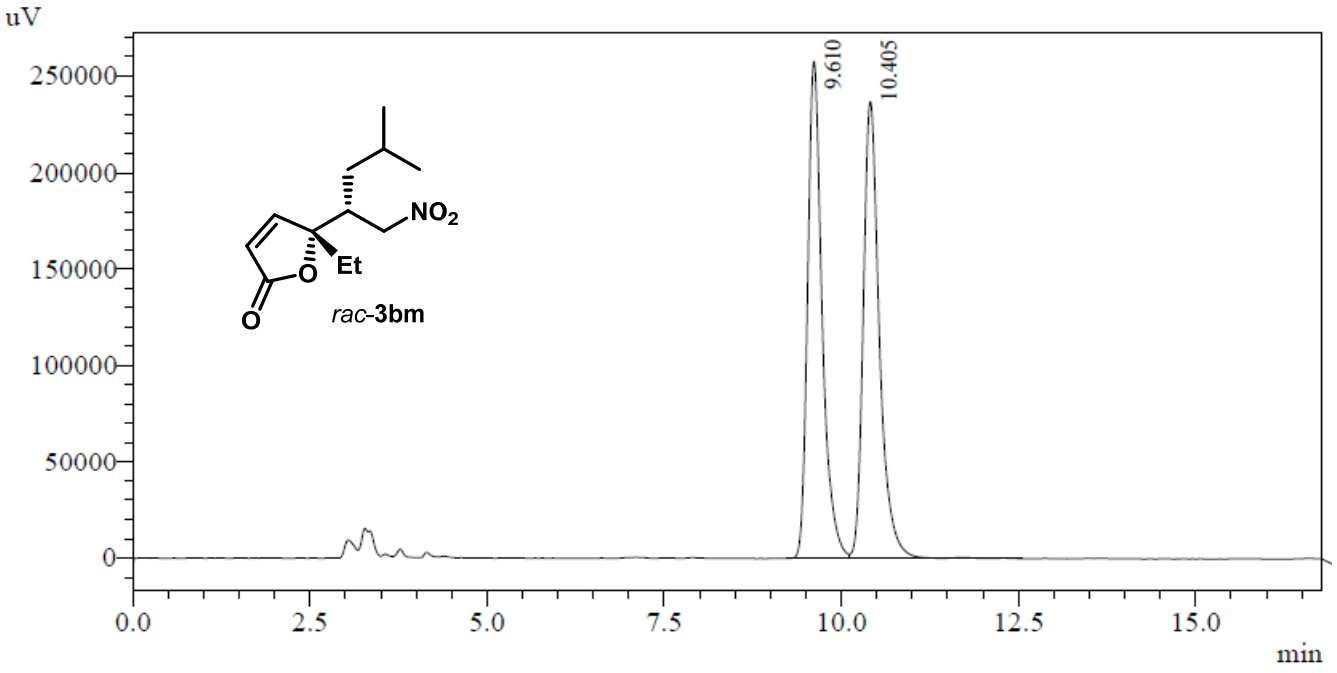


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	7.385	24397407	96.810
2	12.823	804035	3.190
Total		25201443	100.000

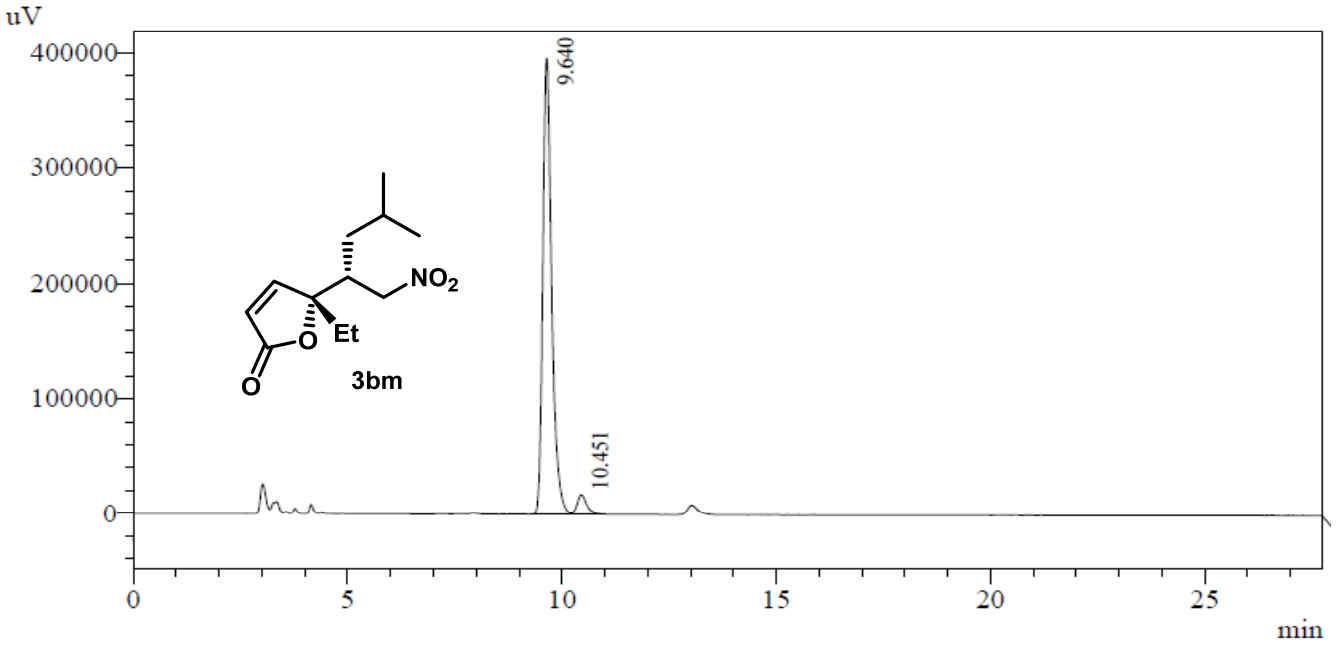

7.289
7.274
6.208
6.194
4.436
4.420
4.402
4.386
4.232
4.220
4.198
4.186
2.937
2.925
2.913
2.910
2.901
2.898
2.890
2.886
2.874
1.999
1.980
1.963
1.944
1.926
1.900
1.881
1.863
1.845
1.827
1.621
1.605
1.599
1.586
1.569
1.553
1.299
1.289
1.263
1.253
1.241
1.228
1.217
1.205
1.182
0.947
0.941
0.931
0.925
0.859
0.840
0.822
NO2
Et
O
O
3bm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.097
0.967
1.010
1.015
1.000
1.019
1.026
1.023
2.027
6.061
3.133
171.638
156.445
123.303
92.313
77.474
77.156
76.838
75.509
41.358
37.640
28.194
26.001
23.429
21.509
7.469
NO2
Et
O
O
3bm
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



PeakTable

Detector A Ch1 210nm

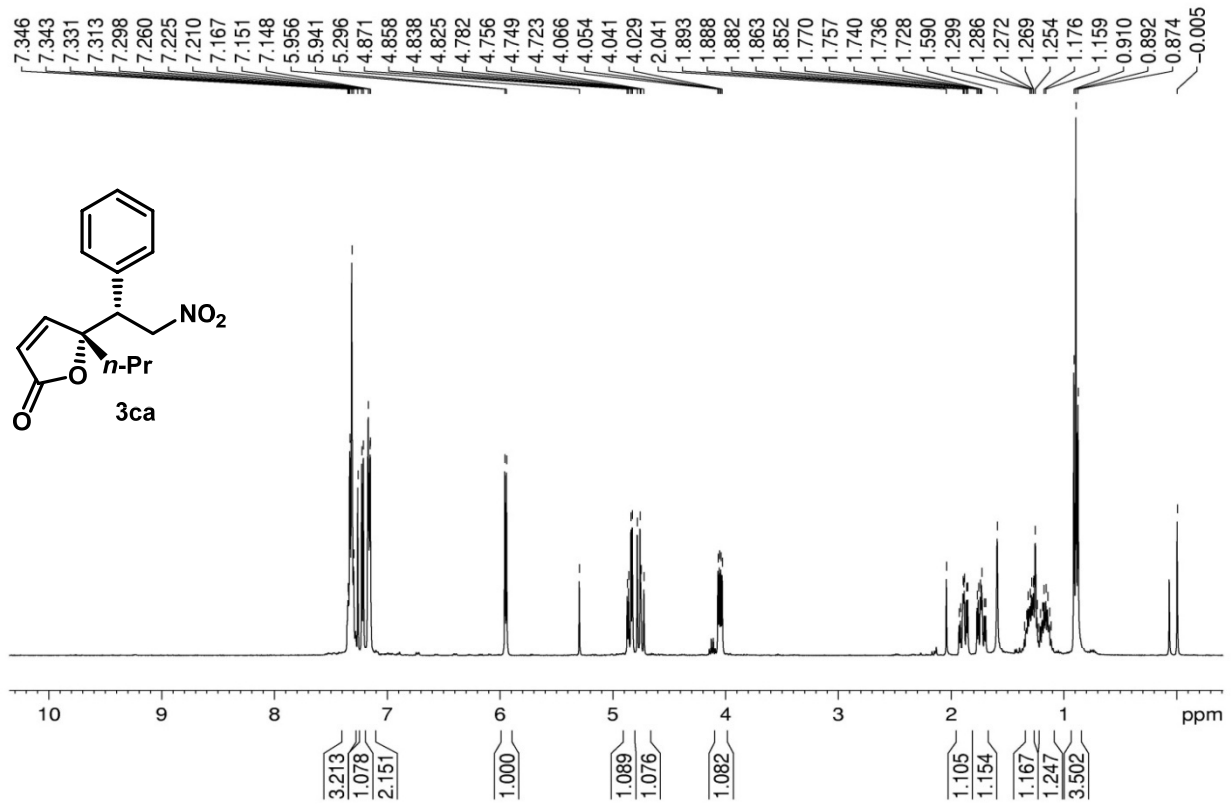
Peak#	Ret. Time	Area	Area %
1	9.610	3691389	49.694
2	10.405	3736792	50.306
Total		7428181	100.000

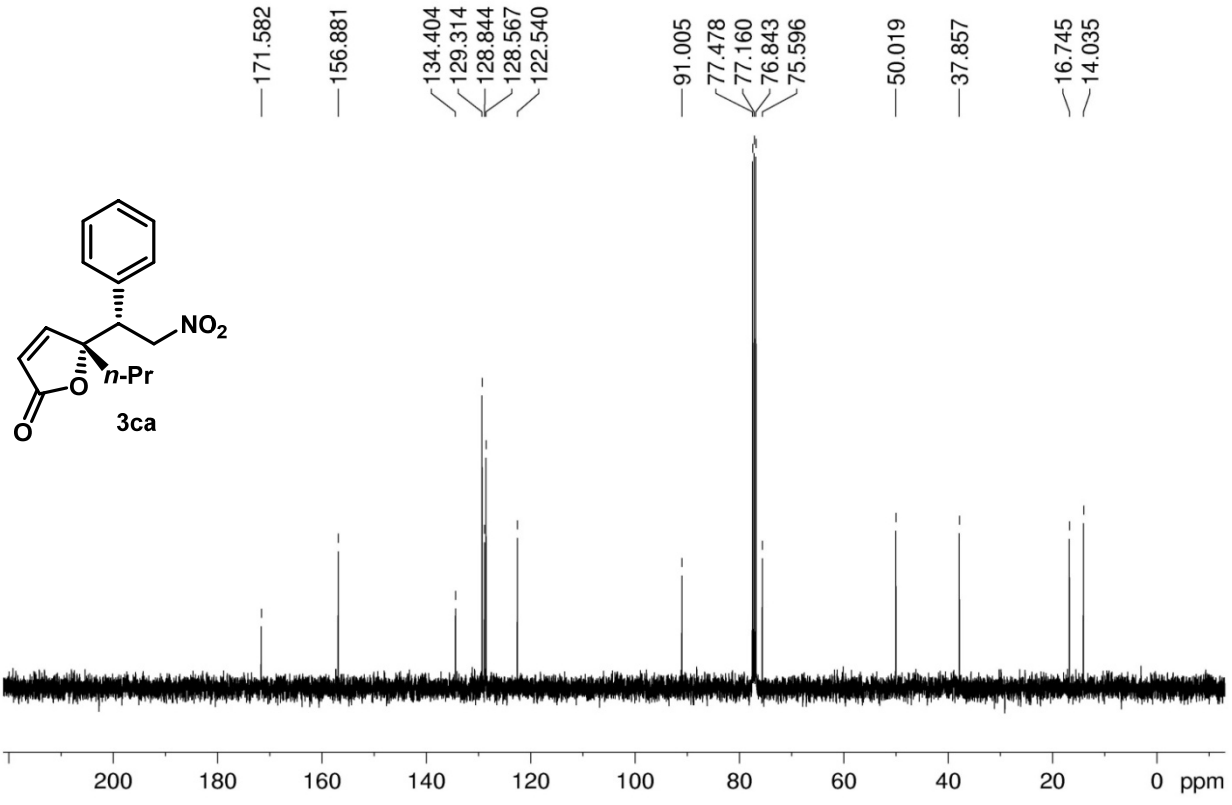


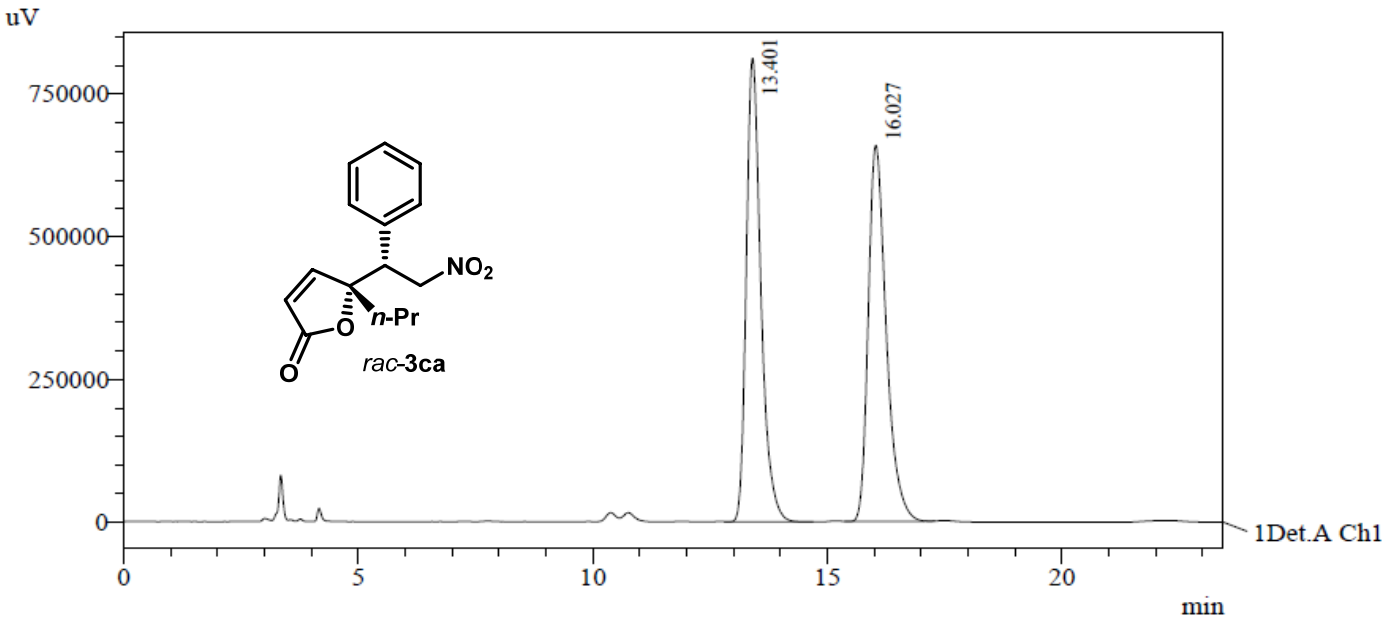
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	9.640	5706384	95.543
2	10.451	266214	4.457
Total		5972598	100.000


7.346
7.343
7.331
7.313
7.298
7.260
7.225
7.210
7.167
7.151
7.148
5.956
5.941
5.296
4.871
4.858
4.838
4.825
4.782
4.756
4.749
4.723
4.066
4.054
4.041
4.029
2.041
1.893
1.888
1.882
1.863
1.852
1.770
1.757
1.740
1.736
1.728
1.590
1.299
1.286
1.272
1.269
1.254
1.176
1.159
0.910
0.892
0.874
-0.005
NO2
n-Pr
O
O
3ca
10
9
8
7
6
5
4
3
2
1
ppm
3.213
1.078
2.151
1.000
1.089
1.076
1.082
1.105
1.154
1.167
1.247
3.502

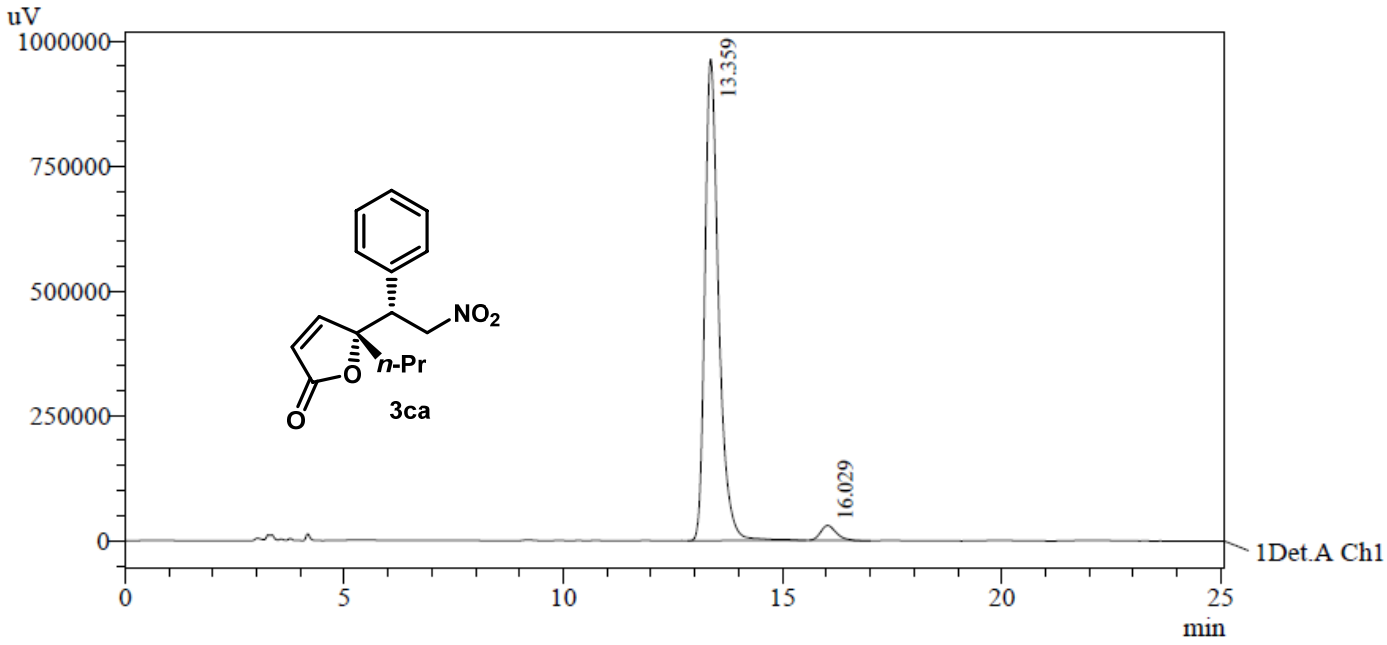

171.582
156.881
134.404
129.314
128.844
128.567
122.540
91.005
77.478
77.160
76.843
75.596
50.019
37.857
16.745
14.035
NO2
n-Pr
O
O
3ca
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

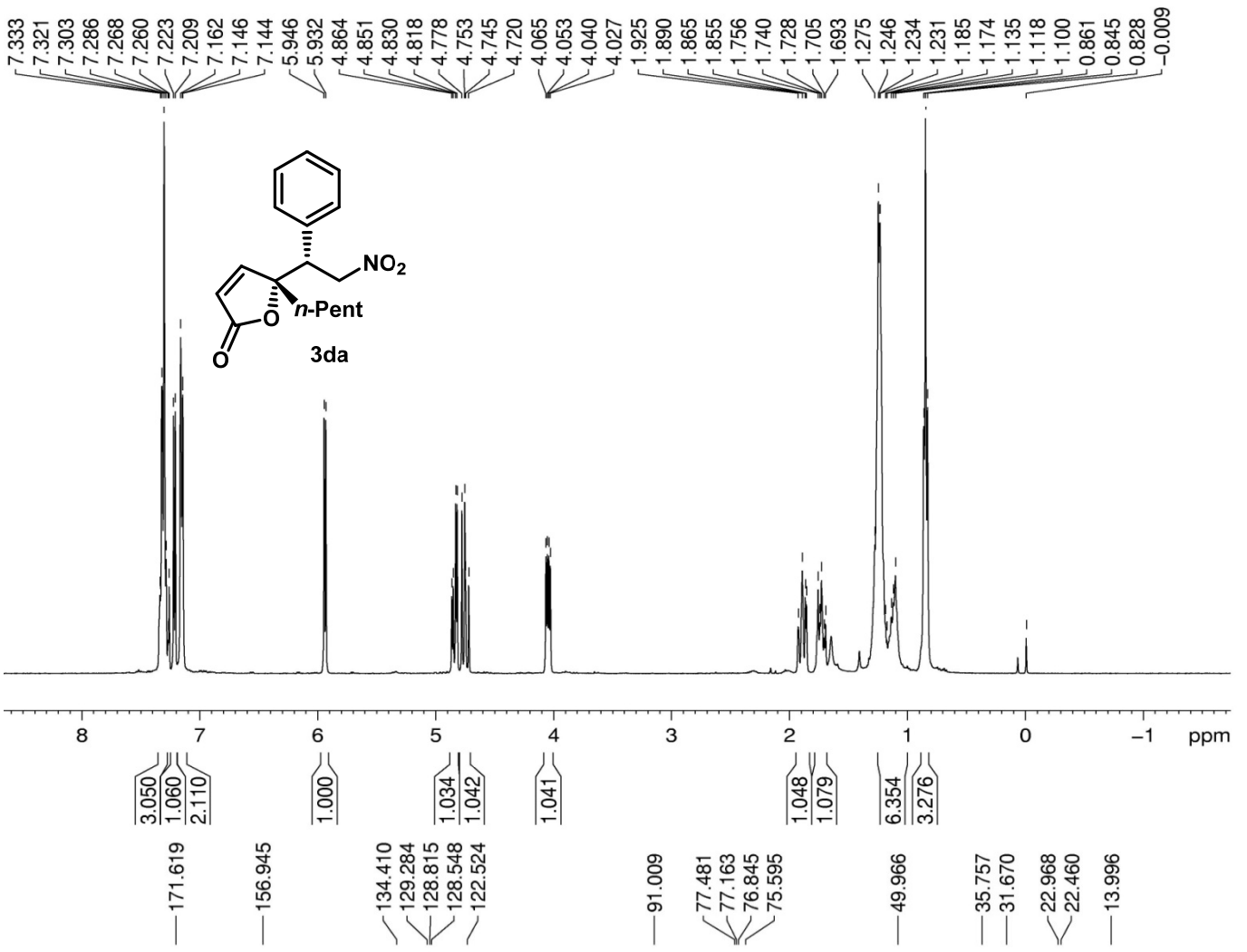
Peak#	Ret. Time	Area	Area %
1	13.401	17620843	50.036
2	16.027	17595667	49.964
Total		35216511	100.000

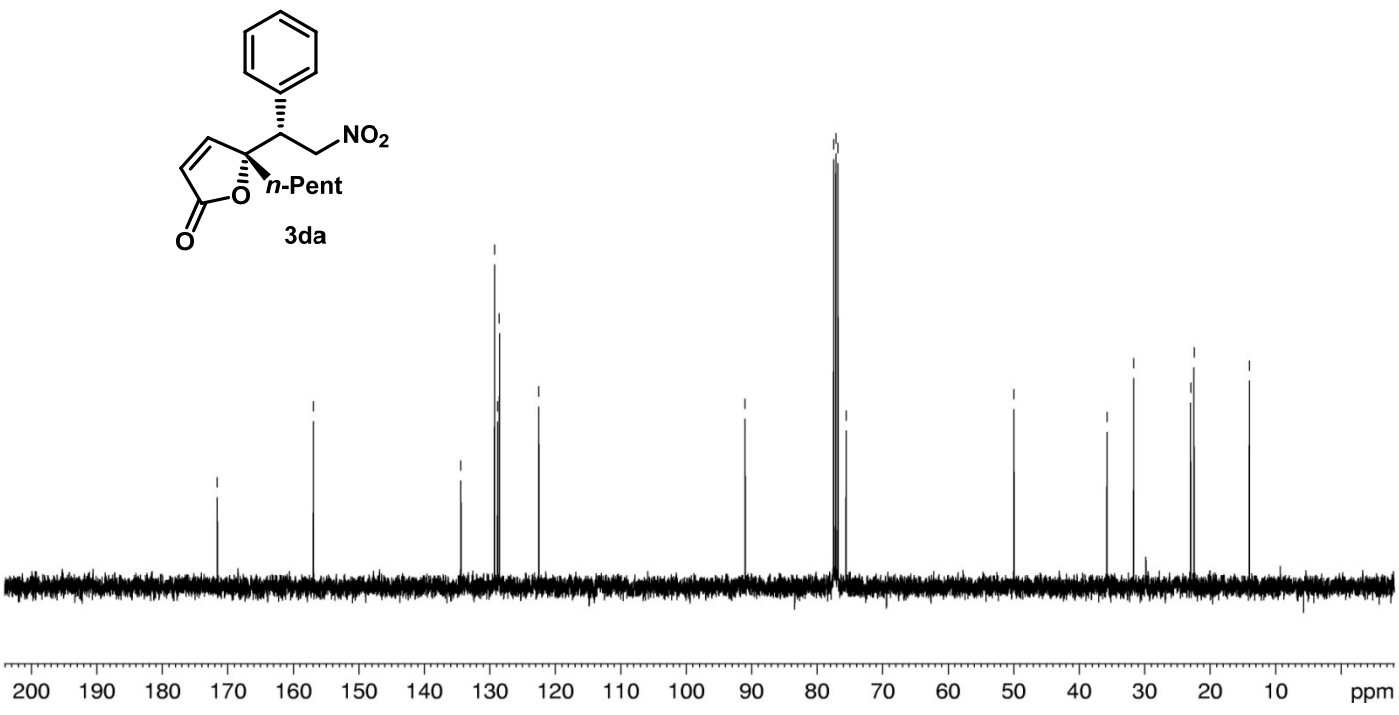


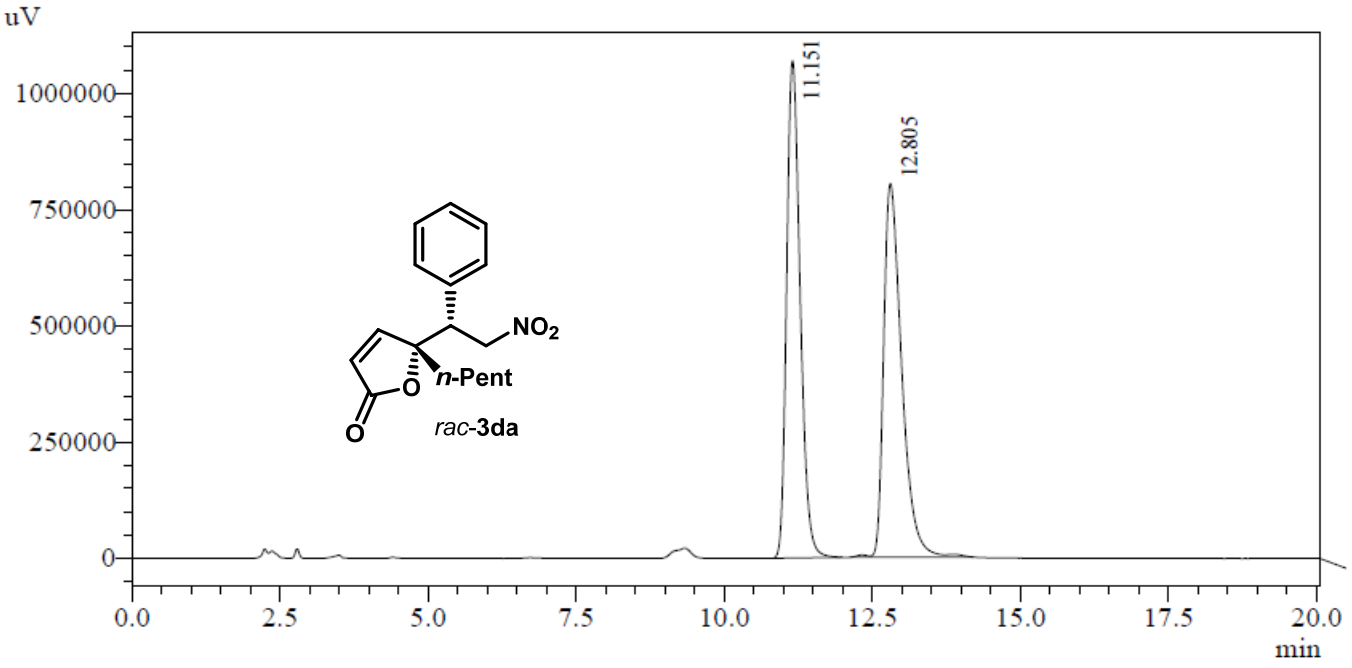
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	13.359	21185237	96.617
2	16.029	741714	3.383
Total		21926951	100.000


7.333
7.321
7.303
7.286
7.268
7.260
7.223
7.209
7.162
7.146
7.144
5.946
5.932
4.864
4.851
4.830
4.818
4.778
4.753
4.745
4.720
4.065
4.053
4.040
4.027
1.925
1.890
1.865
1.855
1.756
1.740
1.728
1.705
1.693
1.275
1.246
1.234
1.231
1.185
1.174
1.135
1.118
1.100
0.861
0.845
0.828
−0.009
NO2
n-Pent
O
O
3da
8
7
6
5
4
3
2
1
0
−1
ppm
3.050
1.060
2.110
1.000
1.034
1.042
1.041
1.048
1.079
6.354
3.276

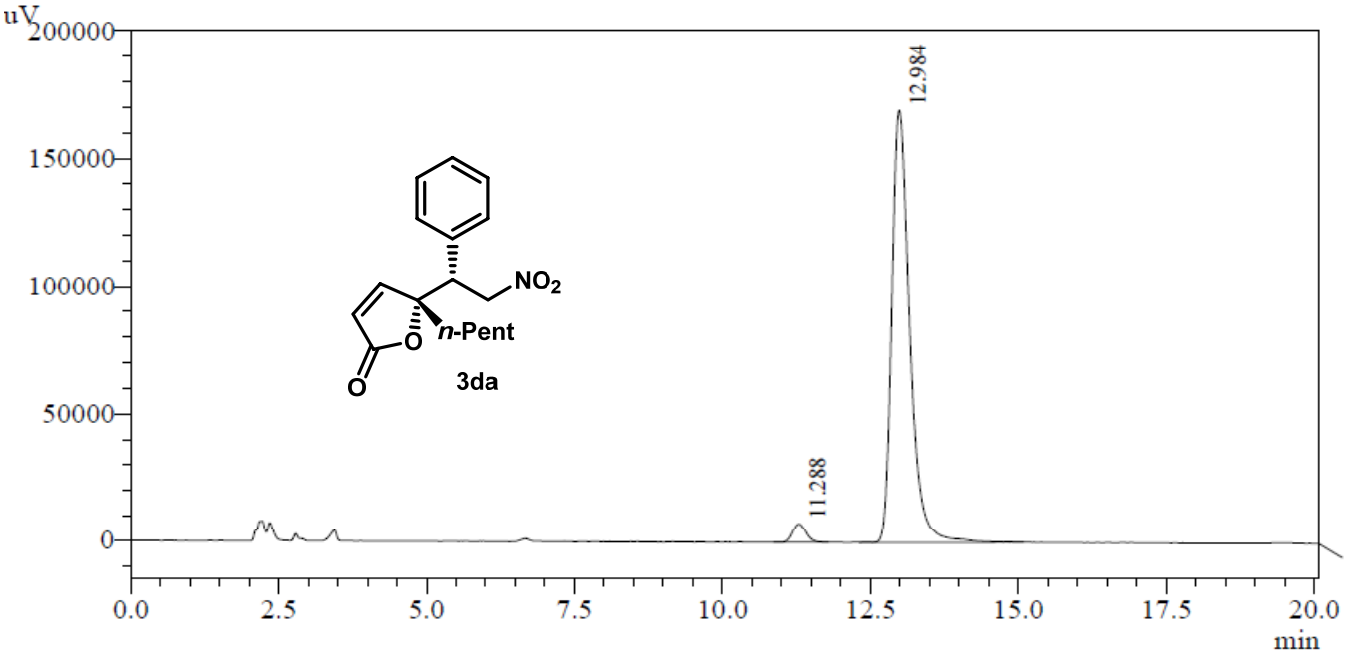

171.619
156.945
134.410
129.284
128.815
128.548
122.524
91.009
77.481
77.163
76.845
75.595
49.966
35.757
31.670
22.968
22.460
13.996
NO2
n-Pent
O
O
3da
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

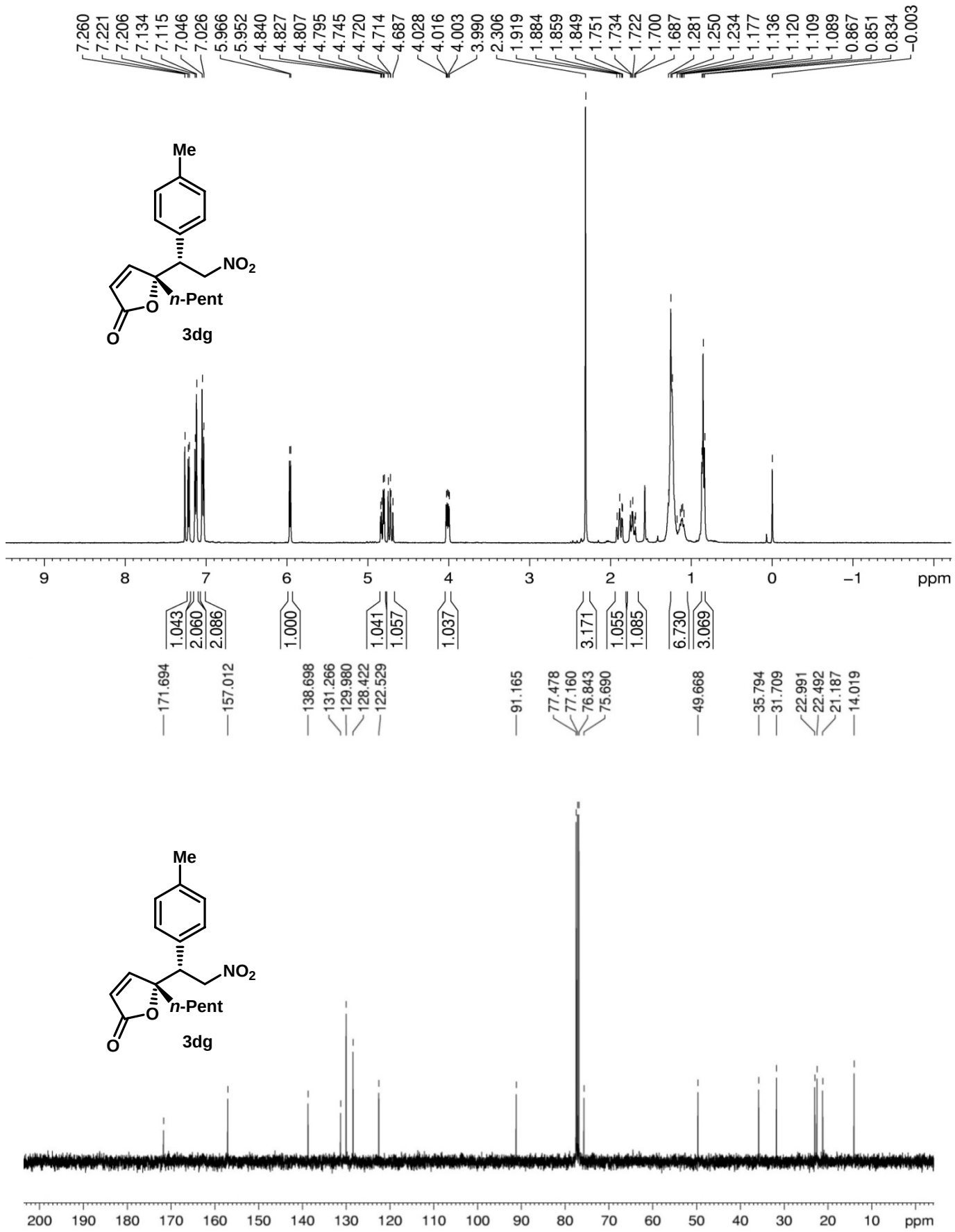
Peak#	Ret. Time	Area	Area %
1	11.151	16979737	49.797
2	12.805	17117919	50.203
Total		34097656	100.000

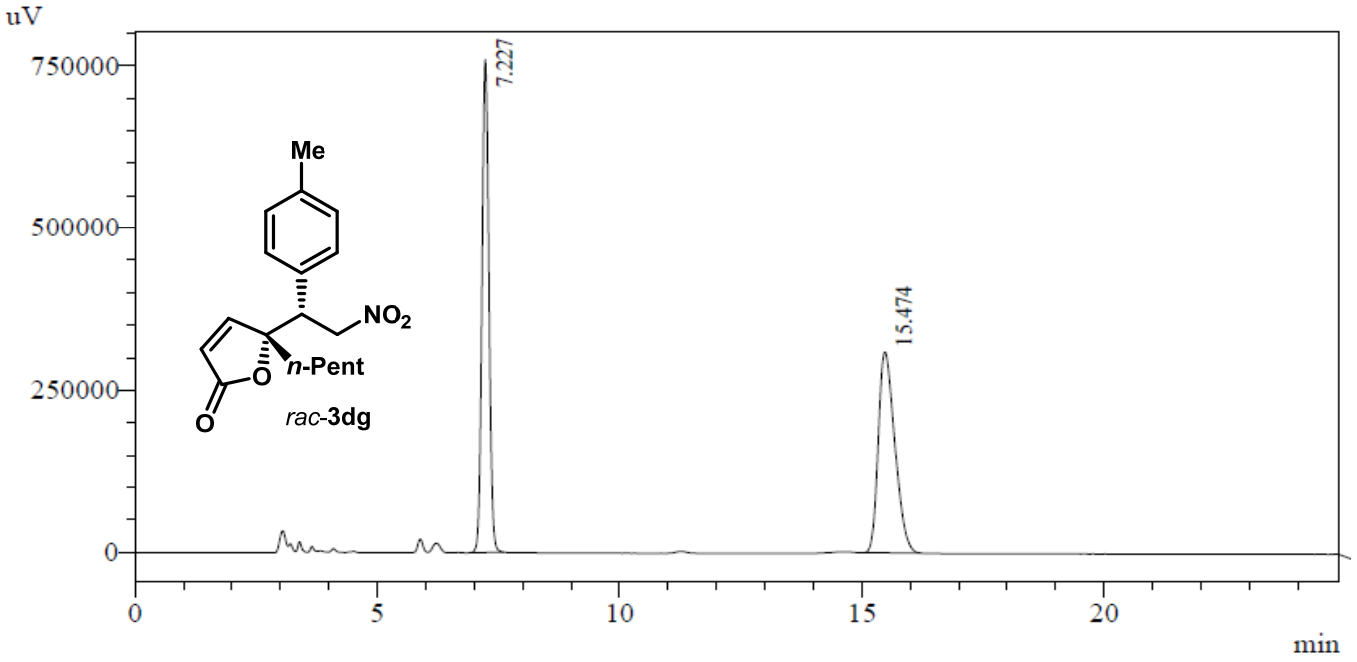


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	11.288	120076	3.223
2	12.984	3605196	96.777
Total		3725272	100.000

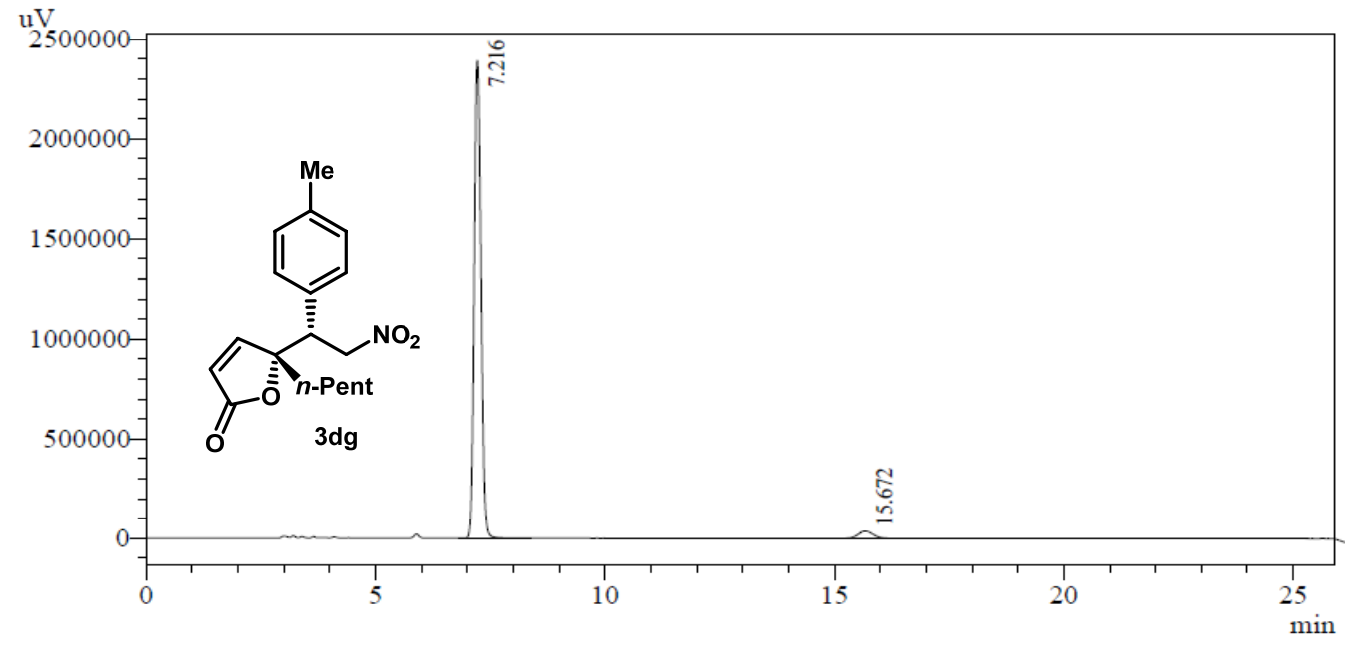

7.260
7.221
7.206
7.134
7.115
7.046
7.026
5.966
5.952
4.840
4.827
4.807
4.795
4.745
4.720
4.714
4.687
4.028
4.016
4.003
3.990
2.306
1.919
1.884
1.859
1.849
1.751
1.734
1.722
1.700
1.687
1.281
1.250
1.234
1.177
1.136
1.120
1.109
1.089
0.867
0.851
0.834
−0.003
Me
NO2
n-Pent
O
O
3dg
9
8
7
6
5
4
3
2
1
0
−1
ppm
1.043
2.060
2.086
1.000
1.041
1.057
1.037
3.171
1.055
1.085
6.730
3.069
171.694
157.012
138.698
131.266
129.980
128.422
122.529
91.165
77.478
77.160
76.843
75.690
49.668
35.794
31.709
22.991
22.492
21.187
14.019
Me
NO2
n-Pent
O
O
3dg
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

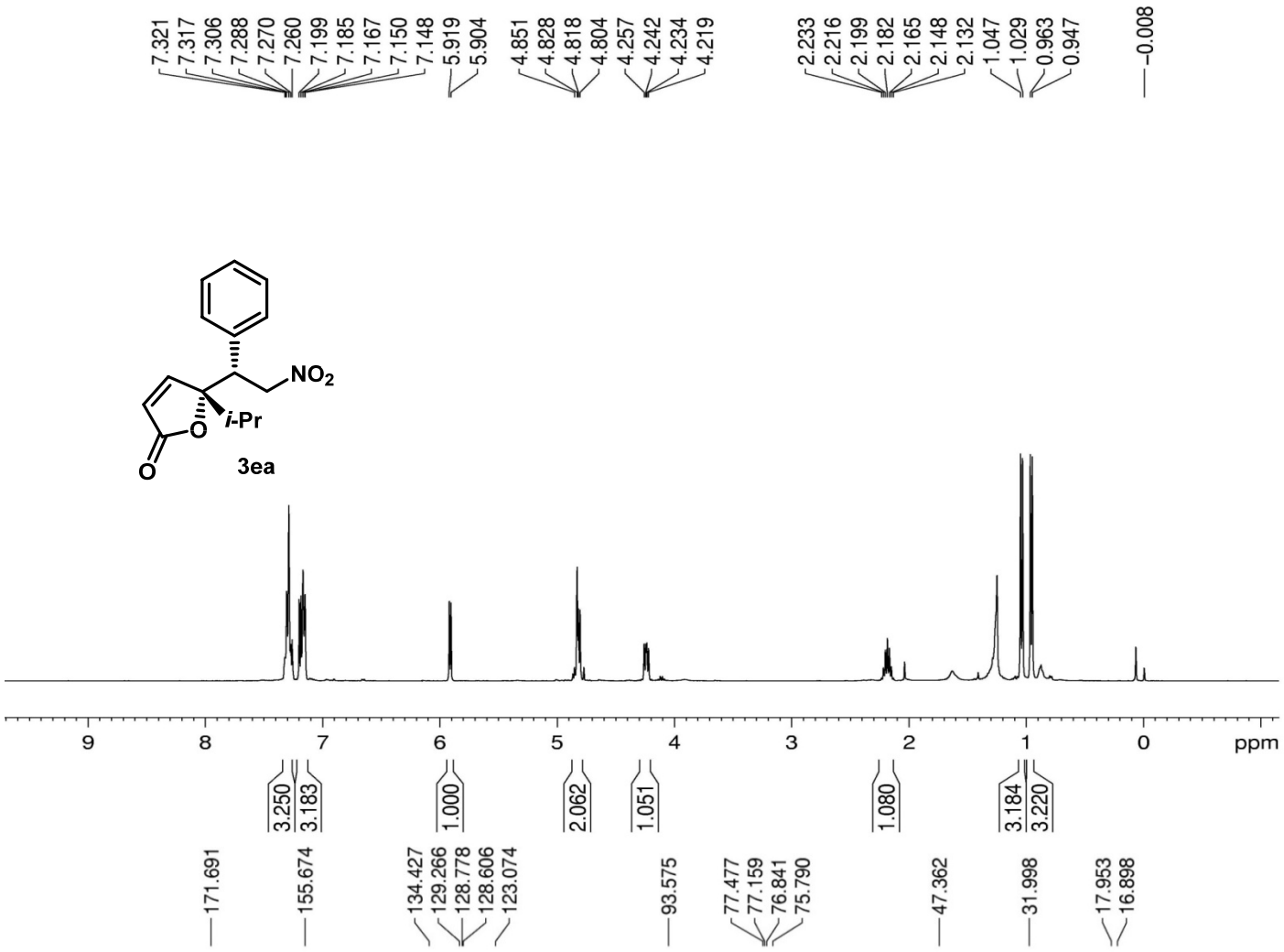
Peak#	Ret. Time	Area	Area %
1	7.227	7512496	50.495
2	15.474	7365090	49.505
Total		14877587	100.000

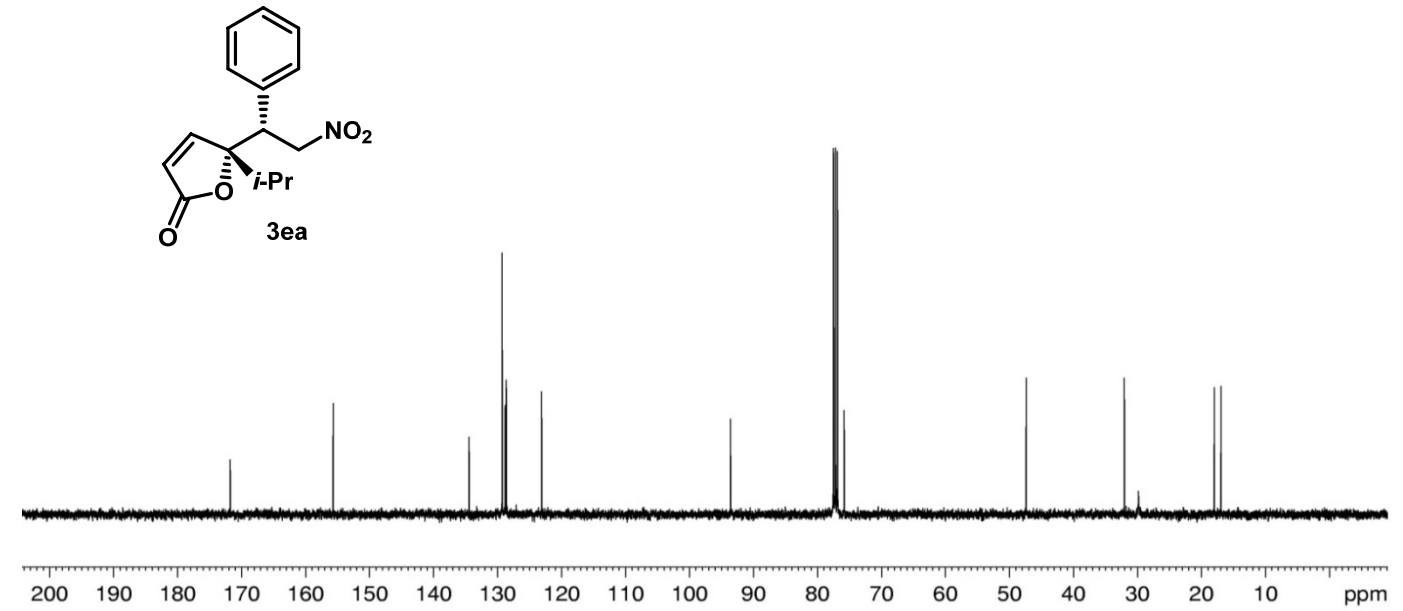


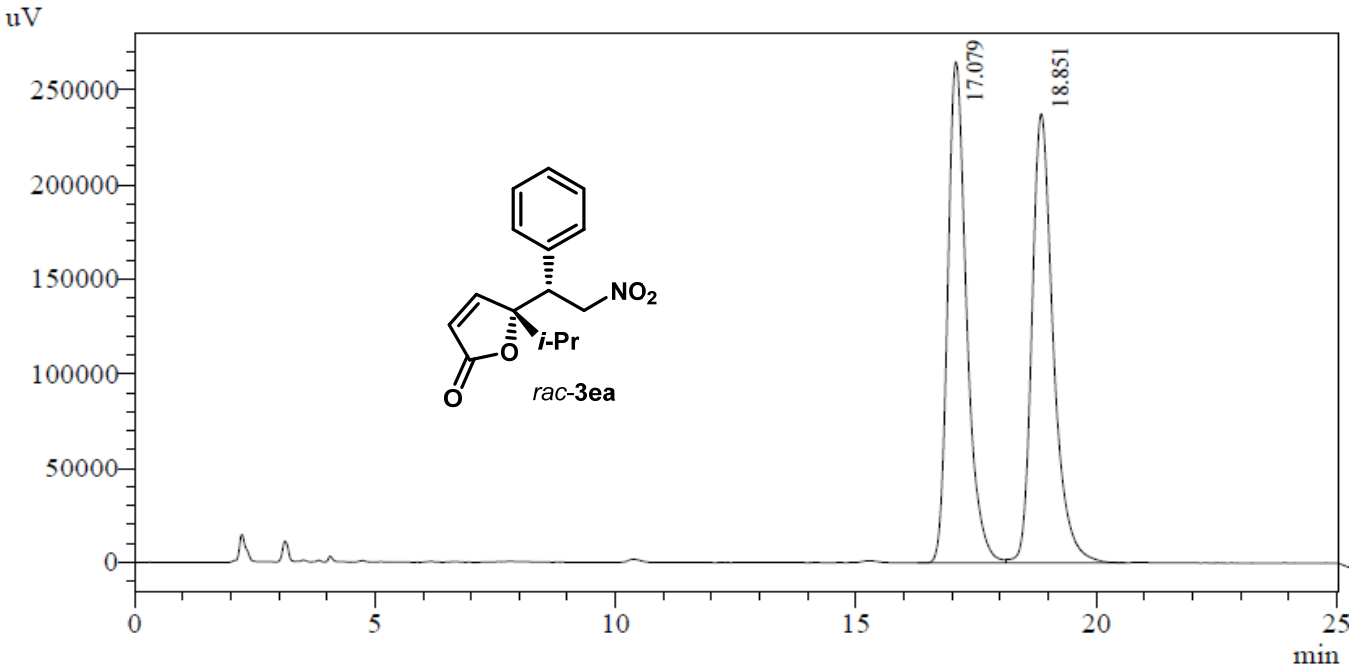
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	7.216	24814386	96.682
2	15.672	851670	3.318
Total		25666056	100.000


7.321
7.317
7.306
7.288
7.270
7.260
7.199
7.185
7.167
7.150
7.148
5.919
5.904
4.851
4.828
4.818
4.804
4.257
4.242
4.234
4.219
2.233
2.216
2.199
2.182
2.165
2.148
2.132
1.047
1.029
0.963
0.947
-0.008
NO2
i-Pr
O
O
3ea
9
8
7
6
5
4
3
2
1
0
ppm
3.250
3.183
1.000
2.062
1.051
1.080
3.184
3.220
171.691
155.674
134.427
129.266
128.778
128.606
123.074
93.575
77.477
77.159
76.841
75.790
47.362
31.998
17.953
16.898

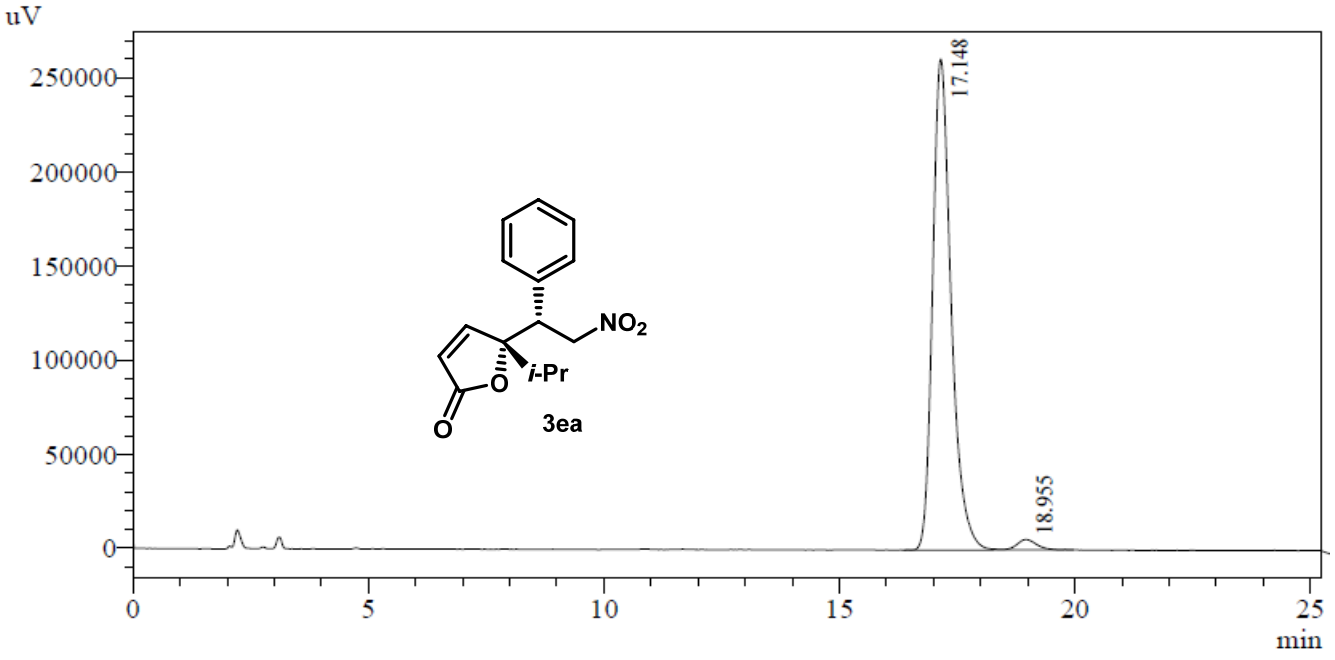

NO2
i-Pr
O
O
3ea
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

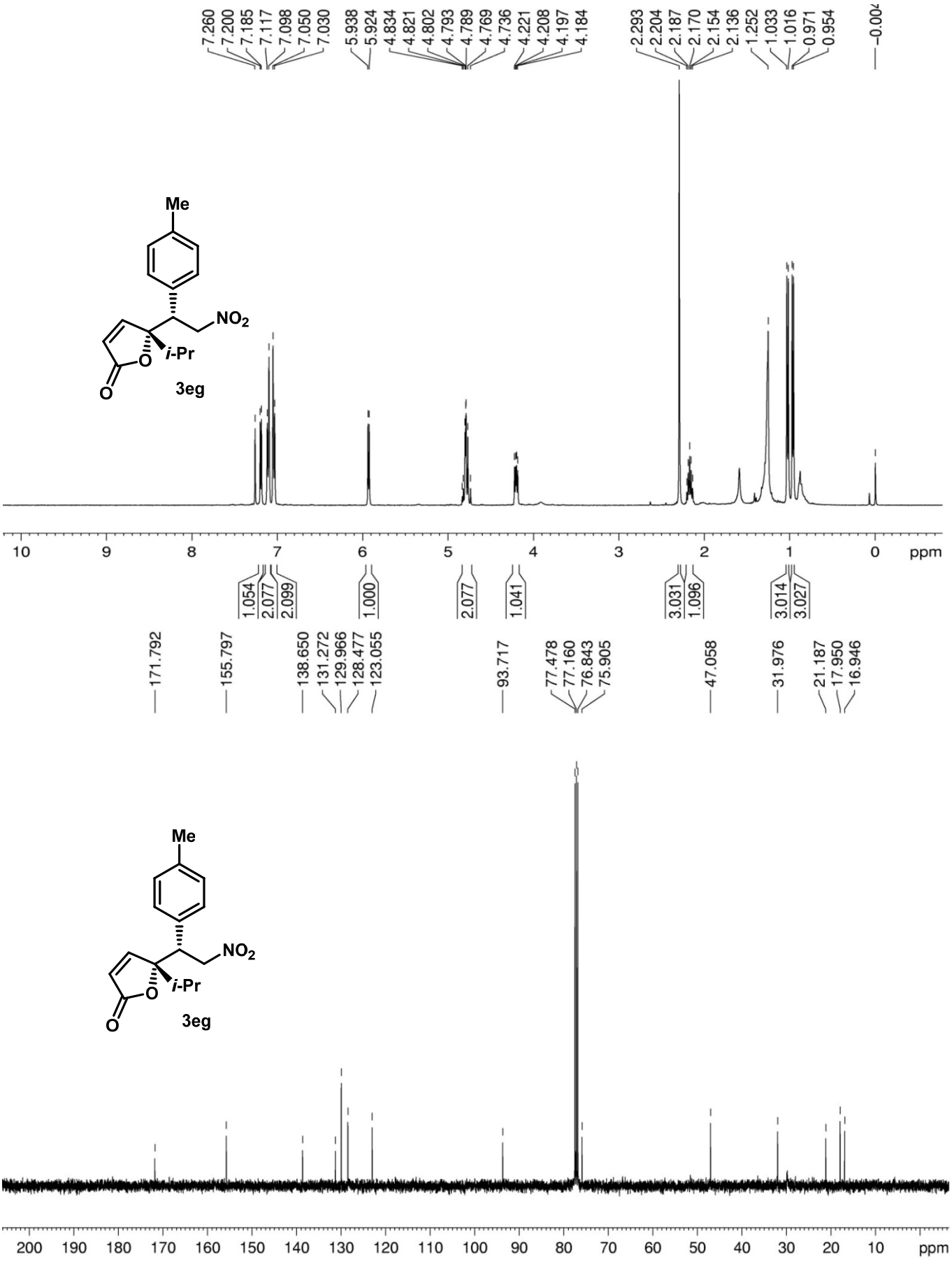
Peak#	Ret. Time	Area	Area %
1	17.079	7232318	49.640
2	18.851	7337111	50.360
Total		14569429	100.000

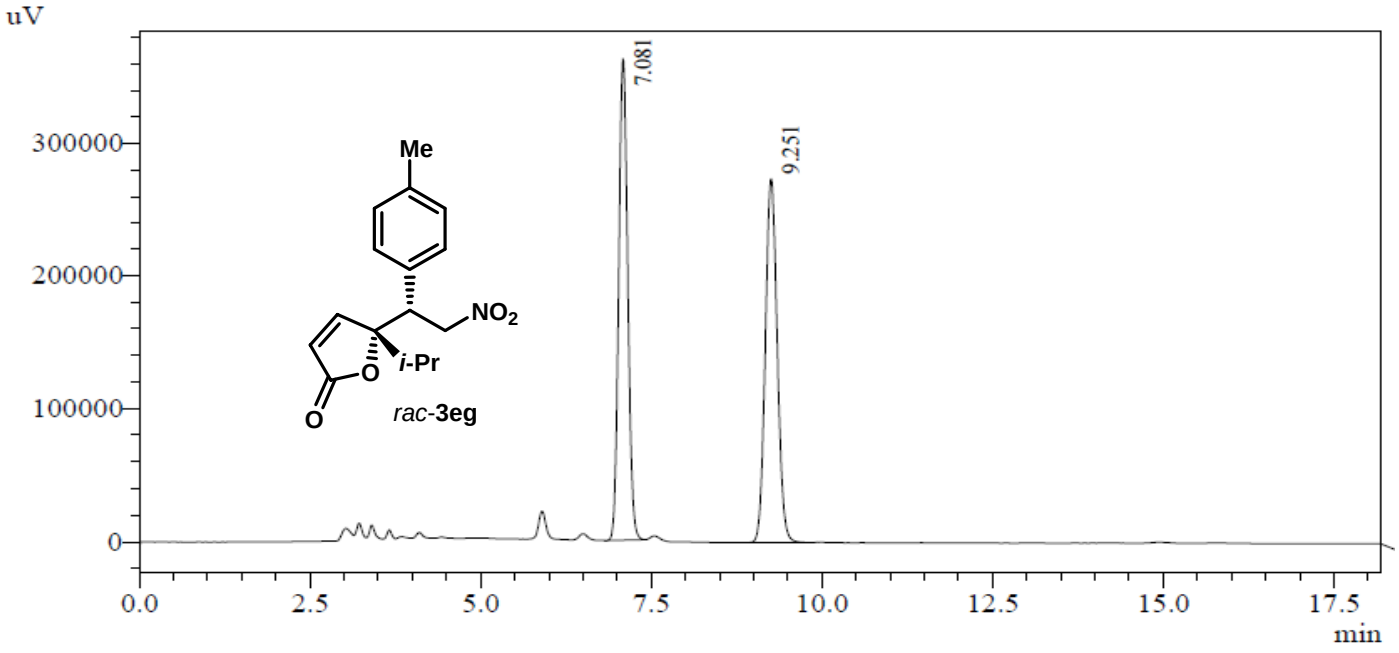


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	17.148	7174208	97.819
2	18.955	159932	2.181
Total		7334140	100.000

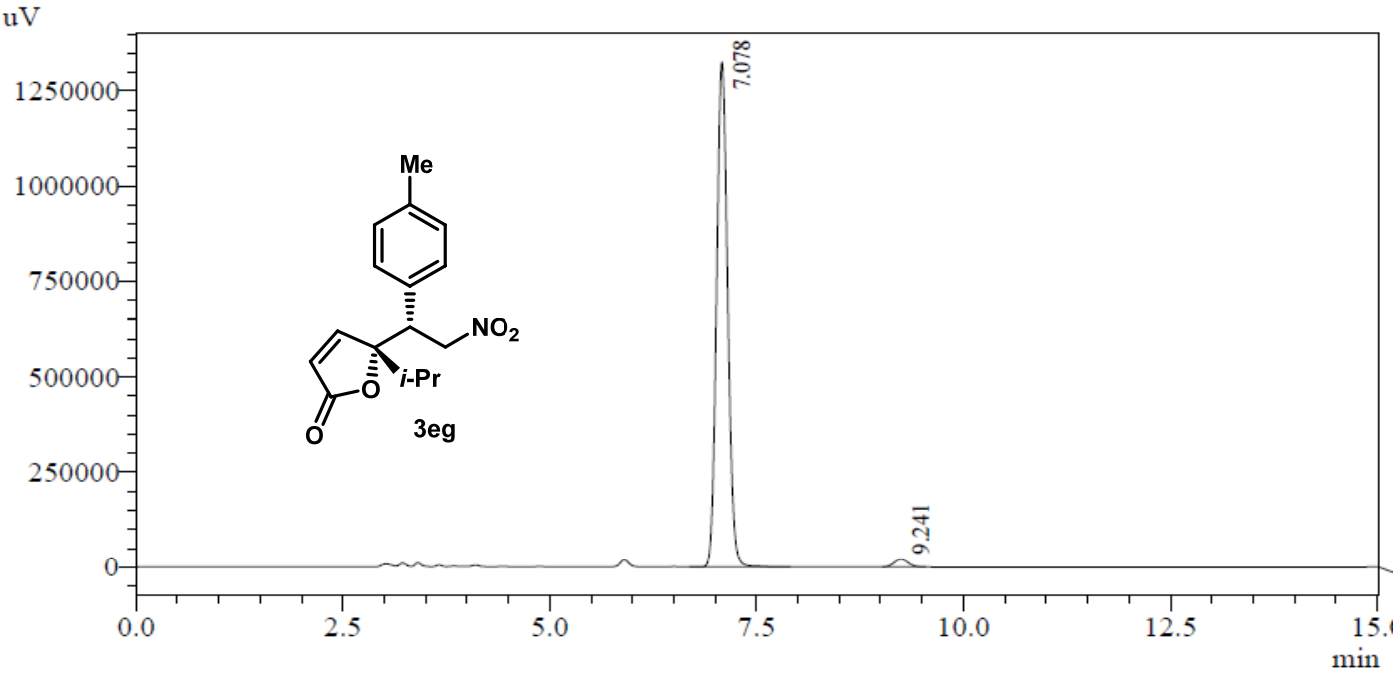

7.260
7.200
7.185
7.117
7.098
7.050
7.030
5.938
5.924
4.834
4.821
4.802
4.793
4.789
4.769
4.736
4.221
4.208
4.197
4.184
2.293
2.204
2.187
2.170
2.154
2.136
1.252
1.033
1.016
0.971
0.954
Me
NO2
i-Pr
O
O
3eg
10
9
8
7
6
5
4
3
2
1
0
ppm
1.054
2.077
2.099
1.000
2.077
1.041
3.031
1.096
3.014
3.027
171.792
155.797
138.650
131.272
129.966
128.477
123.055
93.717
77.478
77.160
76.843
75.905
47.058
31.976
21.187
17.950
16.946
Me
NO2
i-Pr
O
O
3eg
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

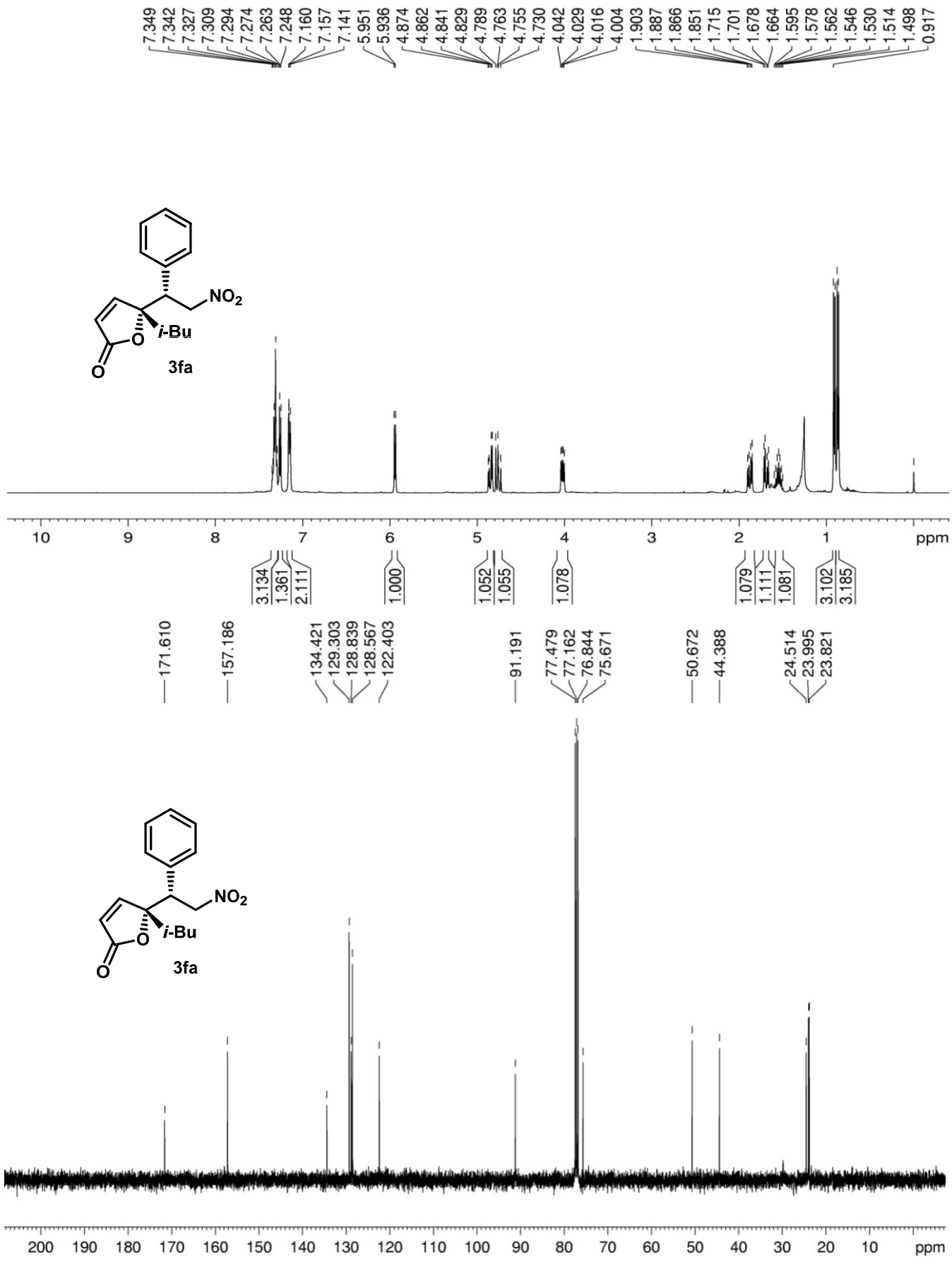
Peak#	Ret. Time	Area	Area %
1	7.081	3322008	50.039
2	9.251	3316804	49.961
Total		6638812	100.000

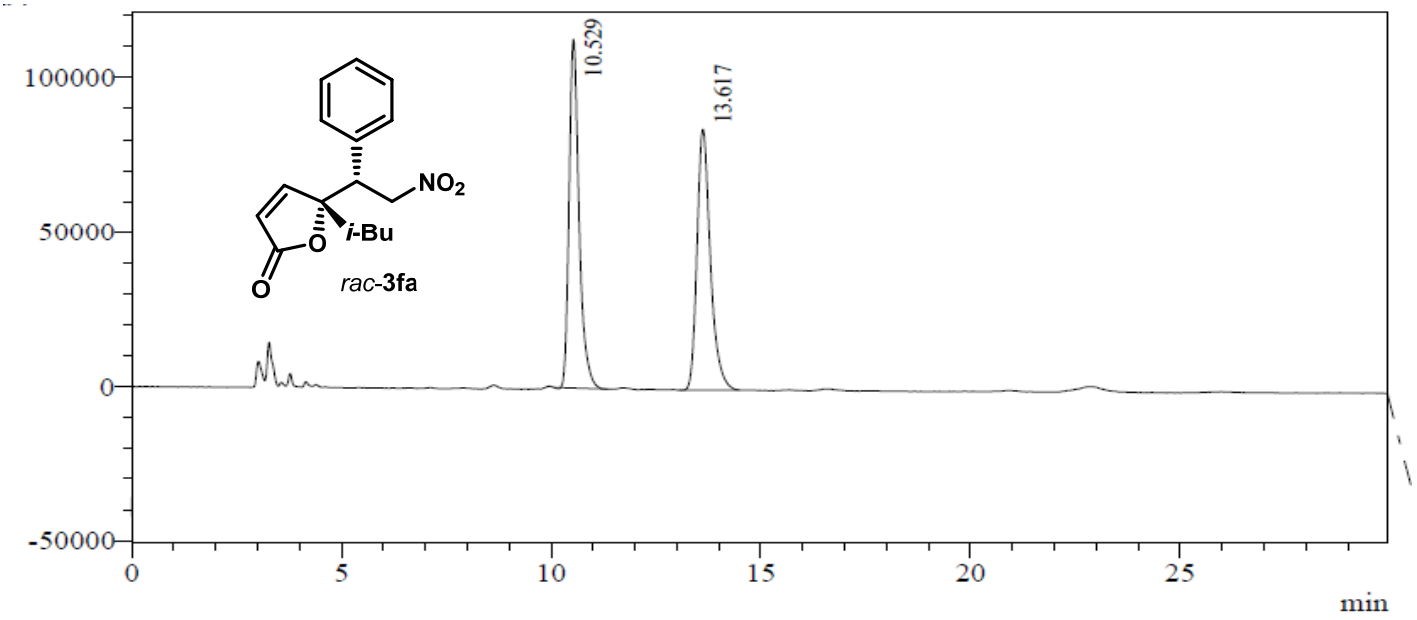


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	7.078	12352408	98.022
2	9.241	249263	1.978
Total		12601671	100.000

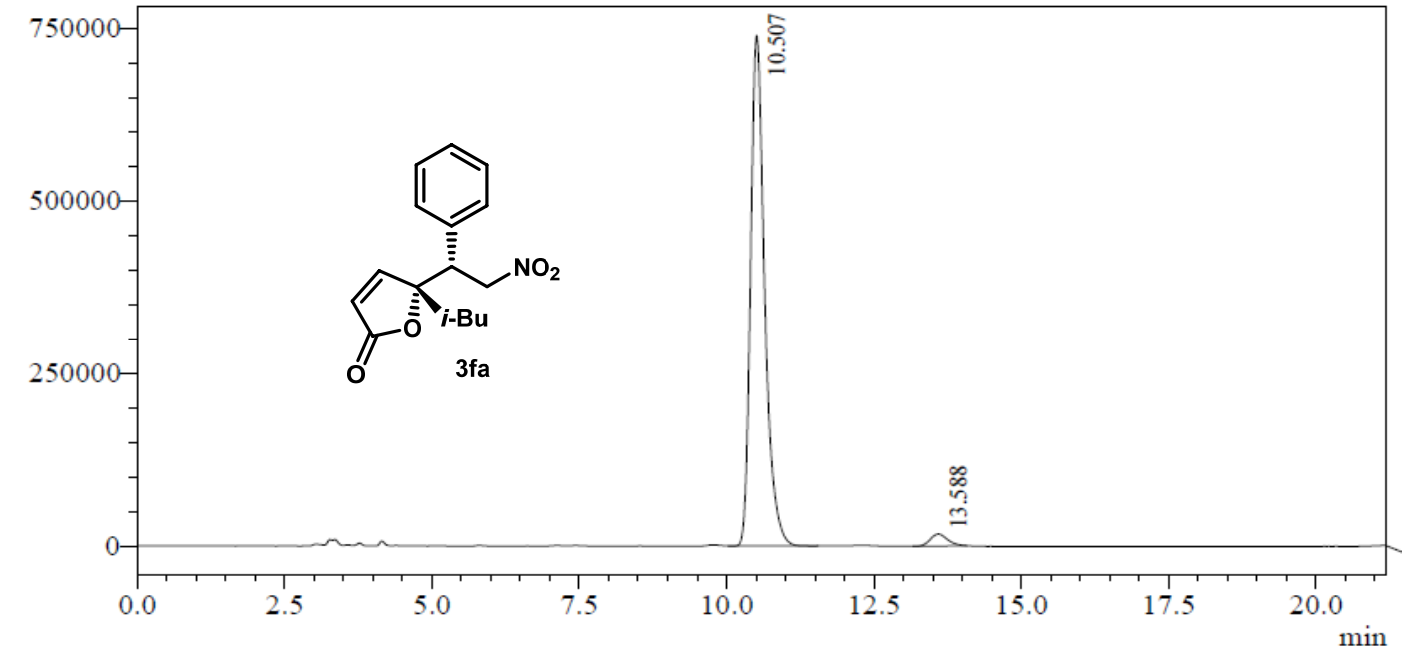

7.349
7.342
7.327
7.309
7.294
7.274
7.263
7.248
7.160
7.157
7.141
5.951
5.936
4.874
4.862
4.841
4.829
4.789
4.763
4.755
4.730
4.042
4.029
4.016
4.004
1.903
1.887
1.866
1.851
1.715
1.701
1.678
1.664
1.595
1.578
1.562
1.546
1.530
1.514
1.498
0.917
NO2
i-Bu
O
O
3fa
10
9
8
7
6
5
4
3
2
1
ppm
3.134
1.361
2.111
1.000
1.052
1.055
1.078
1.079
1.111
1.081
3.102
3.185
171.610
157.186
134.421
129.303
128.839
128.567
122.403
91.191
77.479
77.162
76.844
75.671
50.672
44.388
24.514
23.995
23.821
NO2
i-Bu
O
O
3fa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

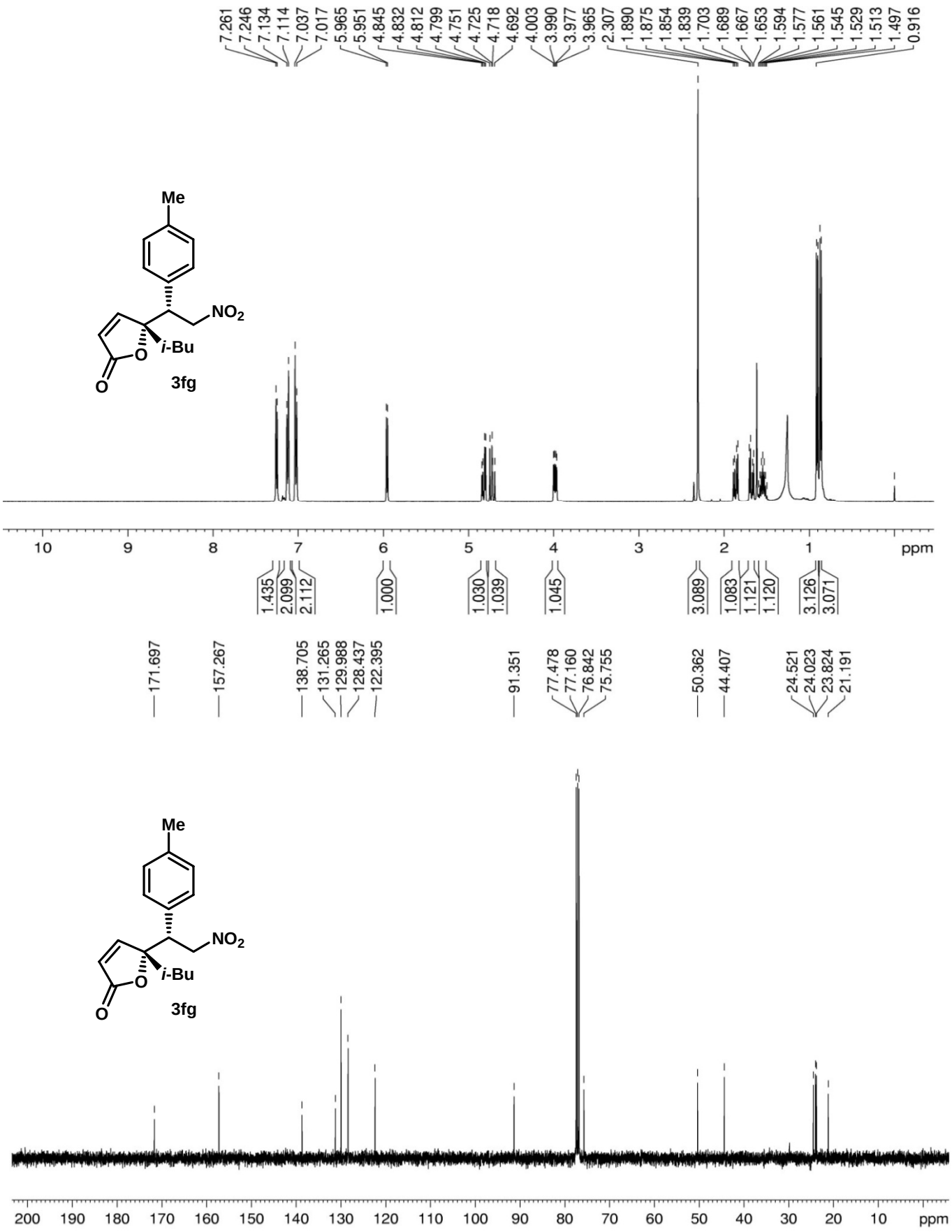
Peak#	Ret. Time	Area	Area %
1	10.529	1866644	50.000
2	13.617	1866670	50.000
Total		3733313	100.000

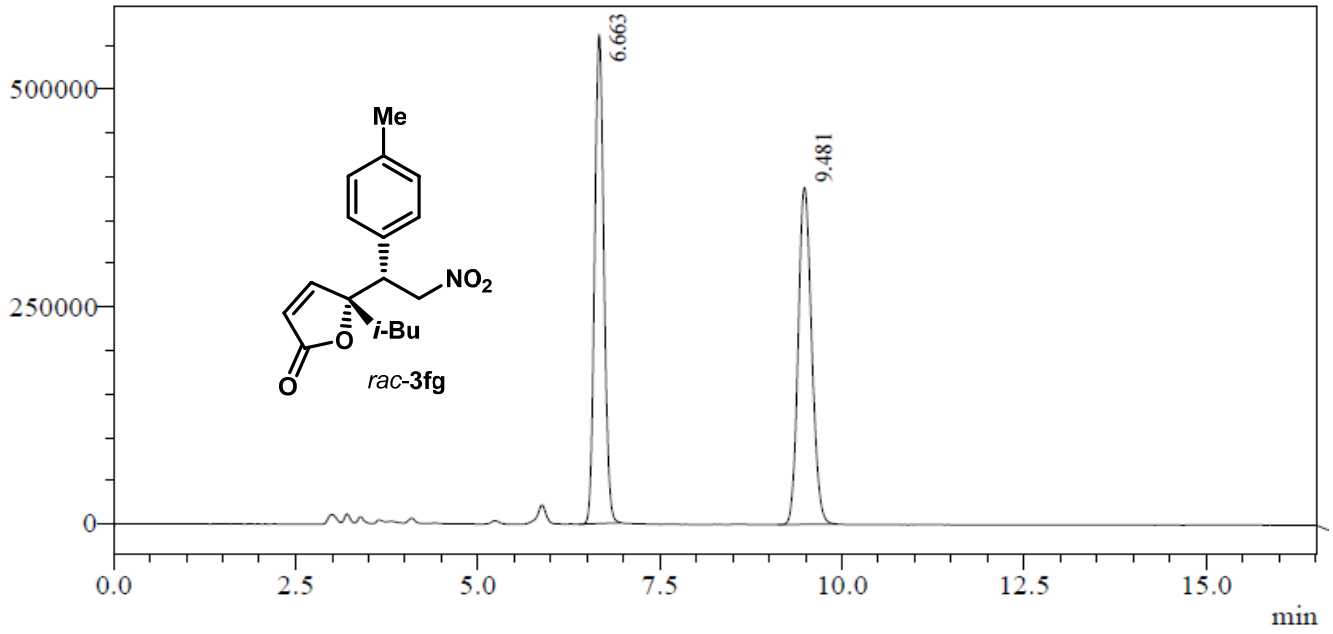


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	10.507	12282651	97.168
2	13.588	357953	2.832
Total		12640604	100.000

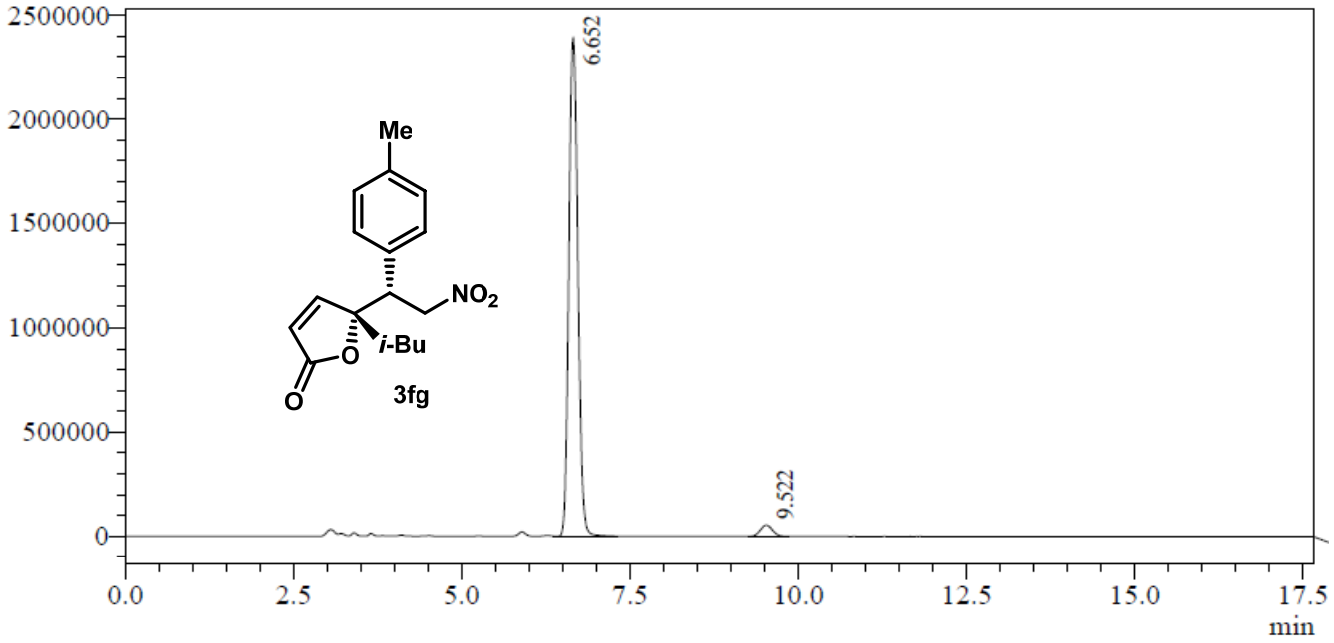

7.261
7.246
7.134
7.114
7.037
7.017
5.965
5.951
4.845
4.832
4.812
4.799
4.751
4.725
4.718
4.692
4.003
3.990
3.977
3.965
2.307
1.890
1.875
1.854
1.839
1.703
1.689
1.667
1.653
1.594
1.577
1.561
1.545
1.529
1.513
1.497
0.916
Me
NO2
i-Bu
O
O
3fg
10
9
8
7
6
5
4
3
2
1
ppm
1.435
2.099
2.112
1.000
1.030
1.039
1.045
3.089
1.083
1.121
1.120
3.126
3.071
171.697
157.267
138.705
131.265
129.988
128.437
122.395
91.351
77.478
77.160
76.842
75.755
50.362
44.407
24.521
24.023
23.824
21.191
Me
NO2
i-Bu
O
O
3fg
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

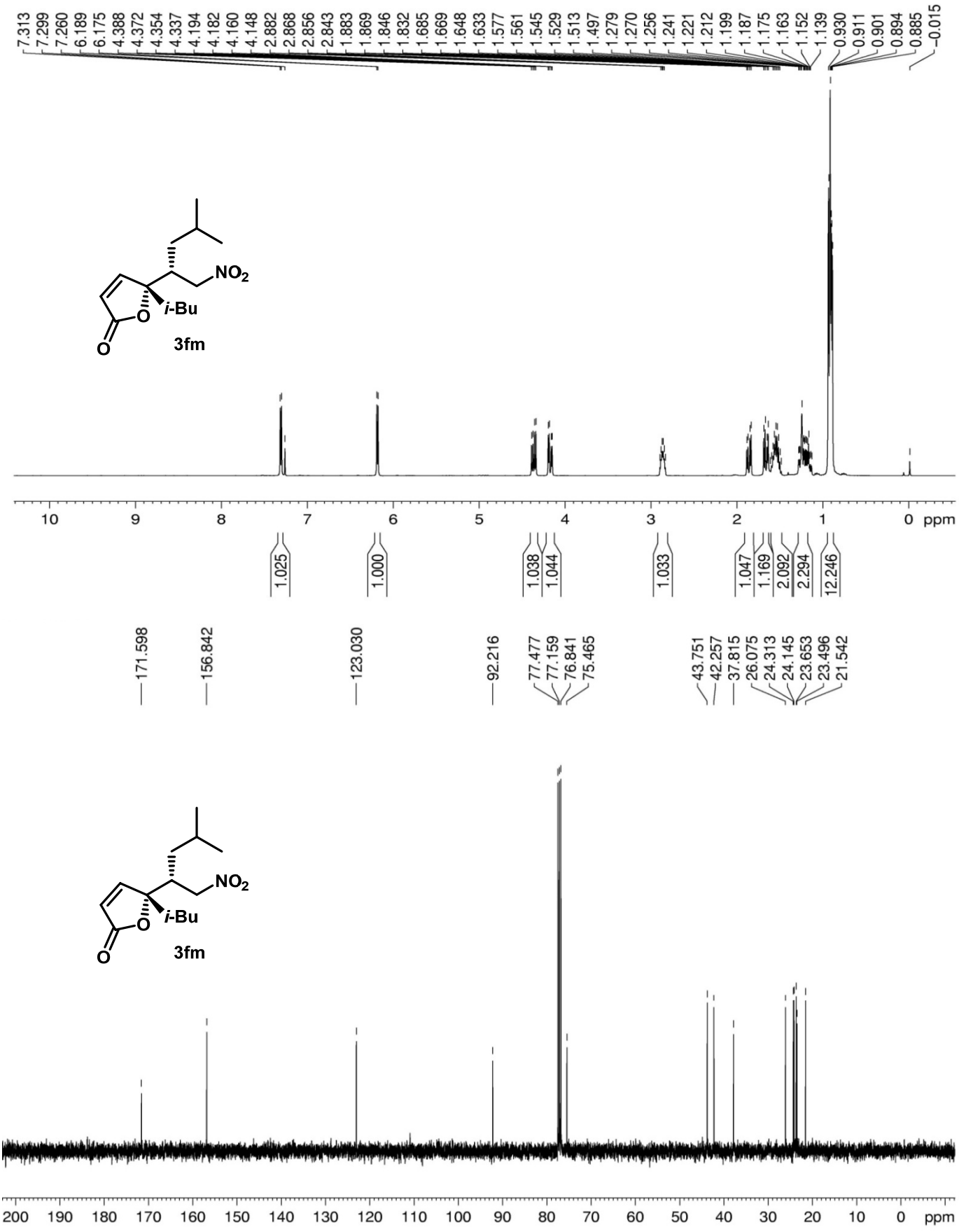
Peak#	Ret. Time	Area	Area %
1	6.663	4971897	49.844
2	9.481	5002944	50.156
Total		9974841	100.000

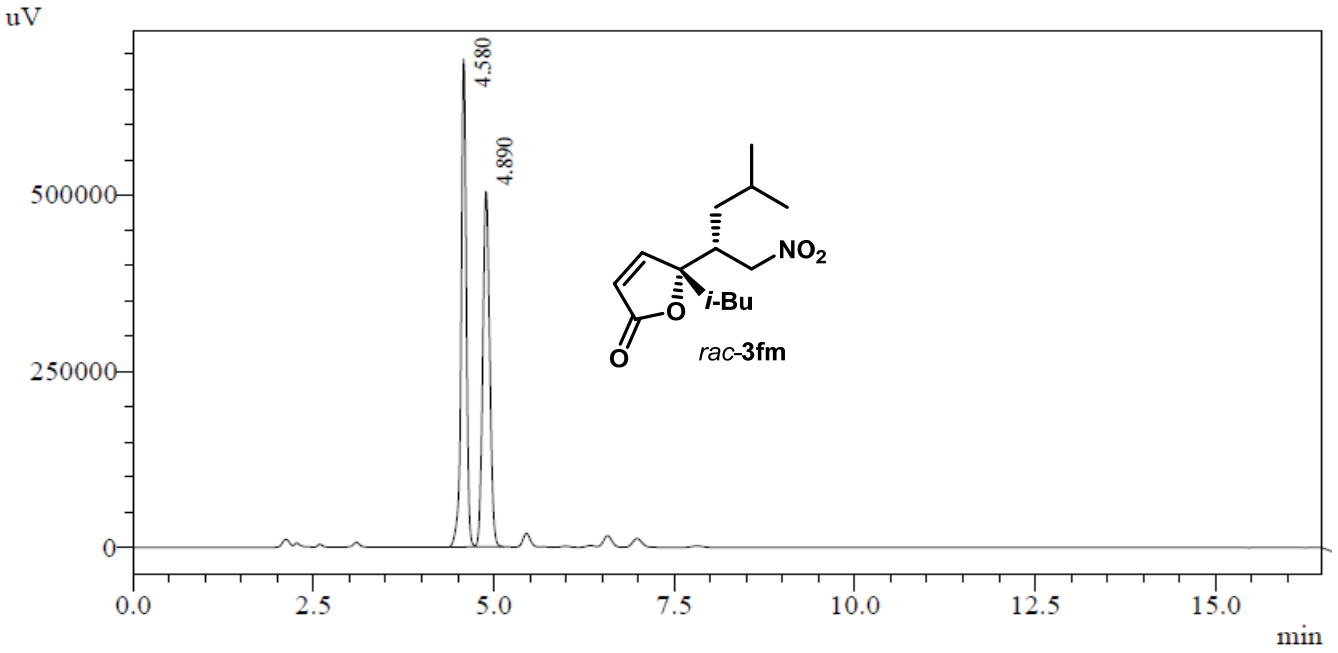


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	6.652	22326543	97.013
2	9.522	687324	2.987
Total		23013868	100.000

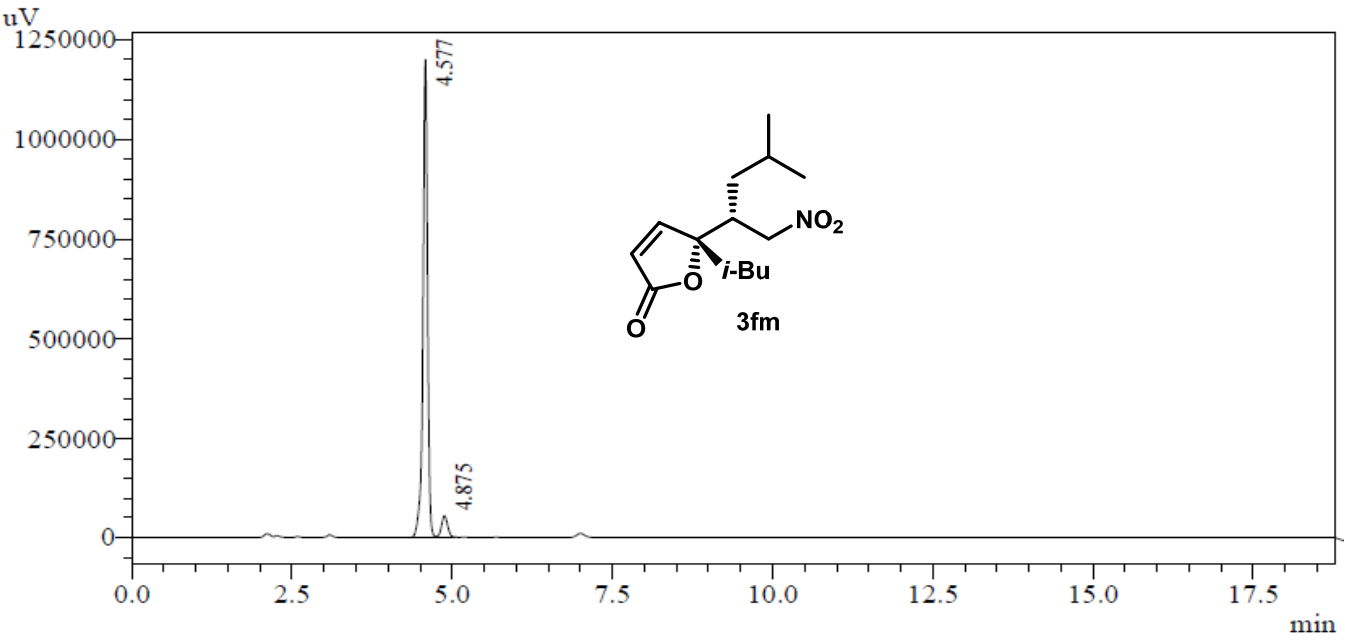

7.313
7.299
7.260
6.189
6.175
4.388
4.372
4.354
4.337
4.194
4.182
4.160
4.148
2.882
2.868
2.856
2.843
1.883
1.869
1.846
1.832
1.685
1.669
1.648
1.633
1.577
1.561
1.545
1.529
1.513
1.497
1.279
1.270
1.256
1.241
1.221
1.212
1.199
1.187
1.175
1.163
1.152
1.139
0.930
0.911
0.901
0.894
0.885
-0.015
NO2
i-Bu
O
O
3fm
10
9
8
7
6
5
4
3
2
1
0 ppm
1.025
1.000
1.038
1.044
1.033
1.047
1.169
2.092
2.294
12.246
171.598
156.842
123.030
92.216
77.477
77.159
76.841
75.465
43.751
42.257
37.815
26.075
24.313
24.145
23.653
23.496
21.542
NO2
i-Bu
O
O
3fm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm



PeakTable

Detector A Ch1 210nm

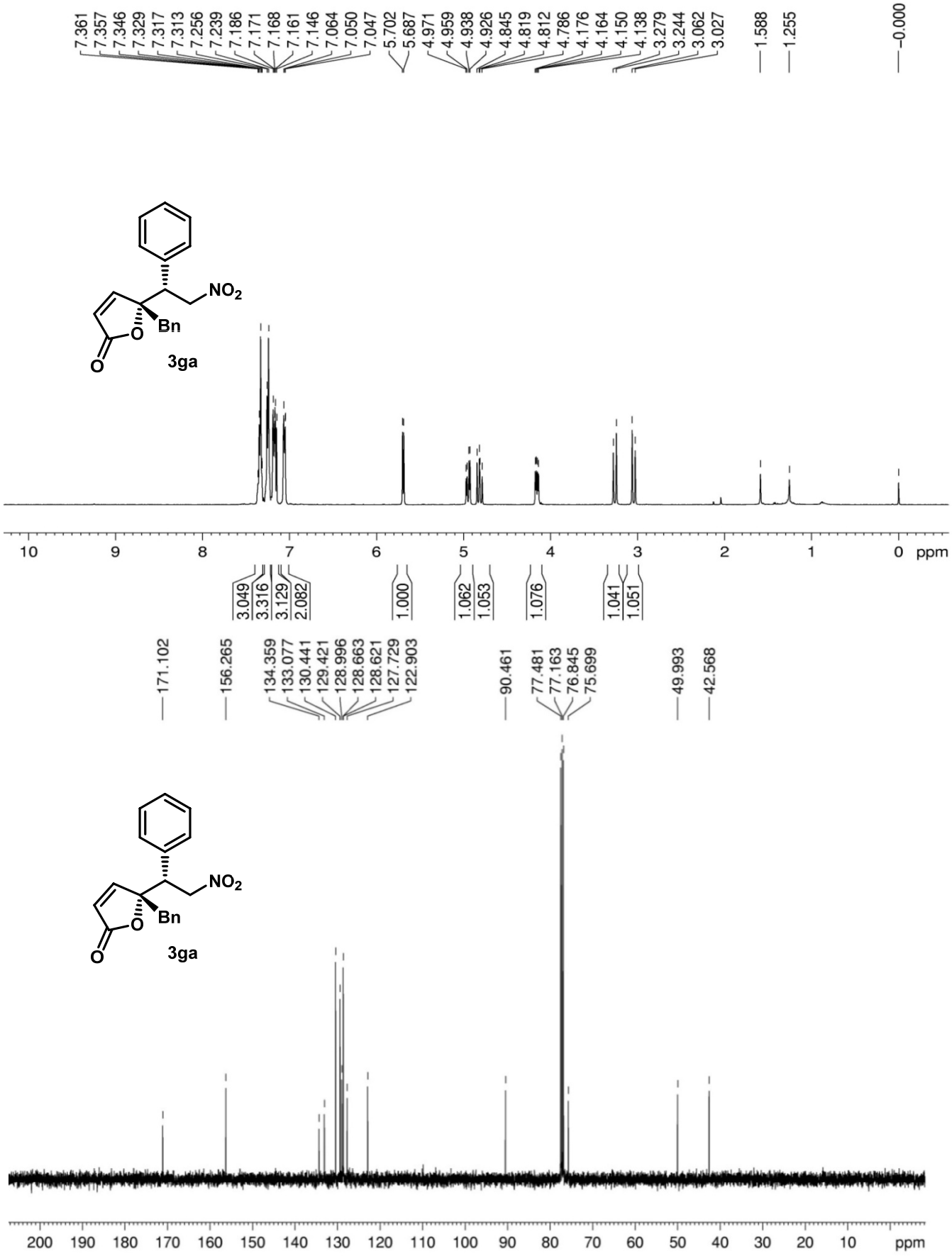
Peak#	Ret. Time	Area	Area %
1	4.580	3365054	49.947
2	4.890	3372221	50.053
Total		6737275	100.000

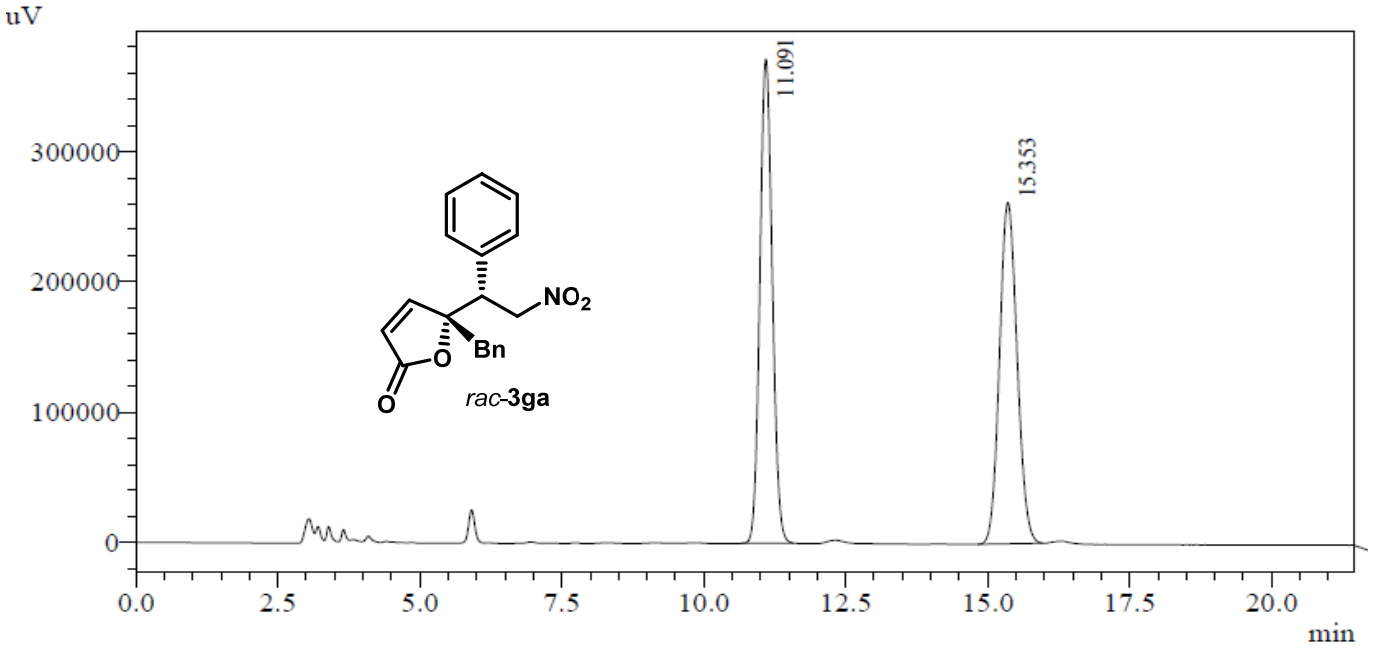


PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	4.577	5937933	94.266
2	4.875	361193	5.734
Total		6299126	100.000

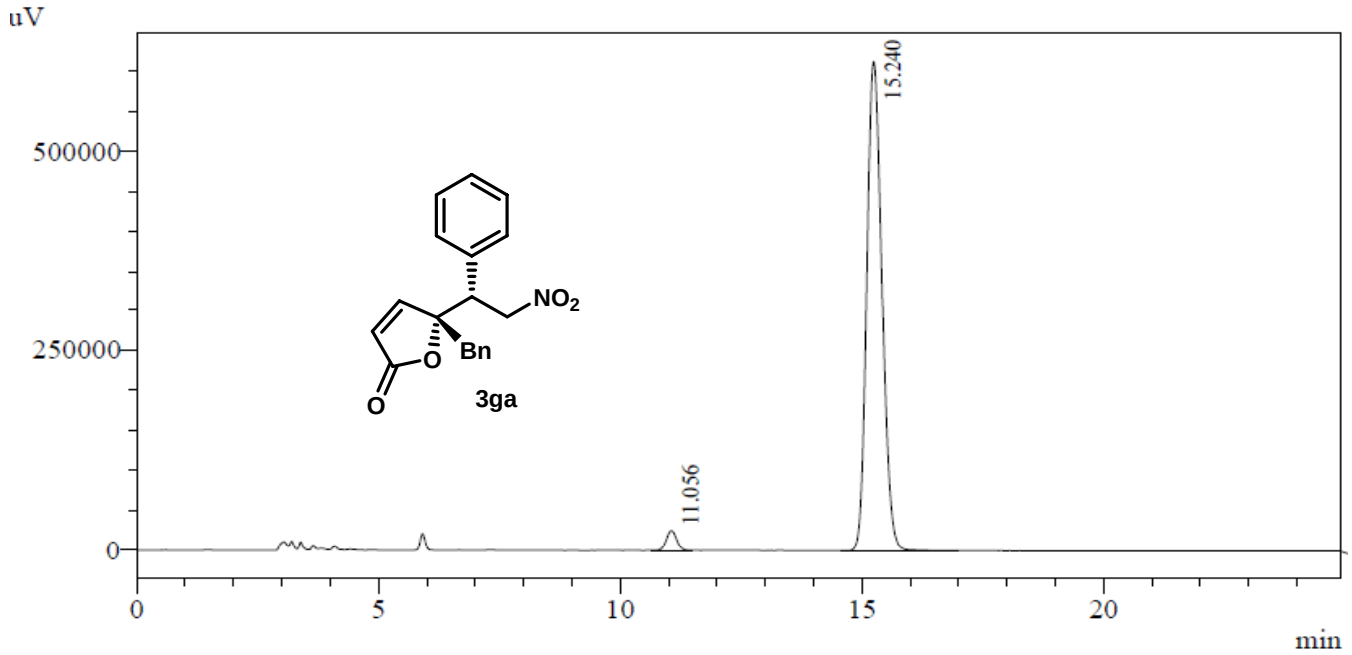

7.361
7.357
7.346
7.329
7.317
7.313
7.256
7.239
7.186
7.171
7.168
7.161
7.146
7.064
7.050
7.047
5.702
5.687
4.971
4.959
4.938
4.926
4.845
4.819
4.812
4.786
4.176
4.164
4.150
4.138
3.279
3.244
3.062
3.027
1.588
1.255
0.000
NO2
Bn
O
O
3ga
10
9
8
7
6
5
4
3
2
1
0 ppm
3.049
3.316
3.129
2.082
1.000
1.062
1.053
1.076
1.041
1.051
171.102
156.265
134.359
133.077
130.441
129.421
128.996
128.663
128.621
127.729
122.903
90.461
77.481
77.163
76.845
75.699
49.993
42.568
NO2
Bn
O
O
3ga
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



PeakTable

Detector A Ch1 210nm

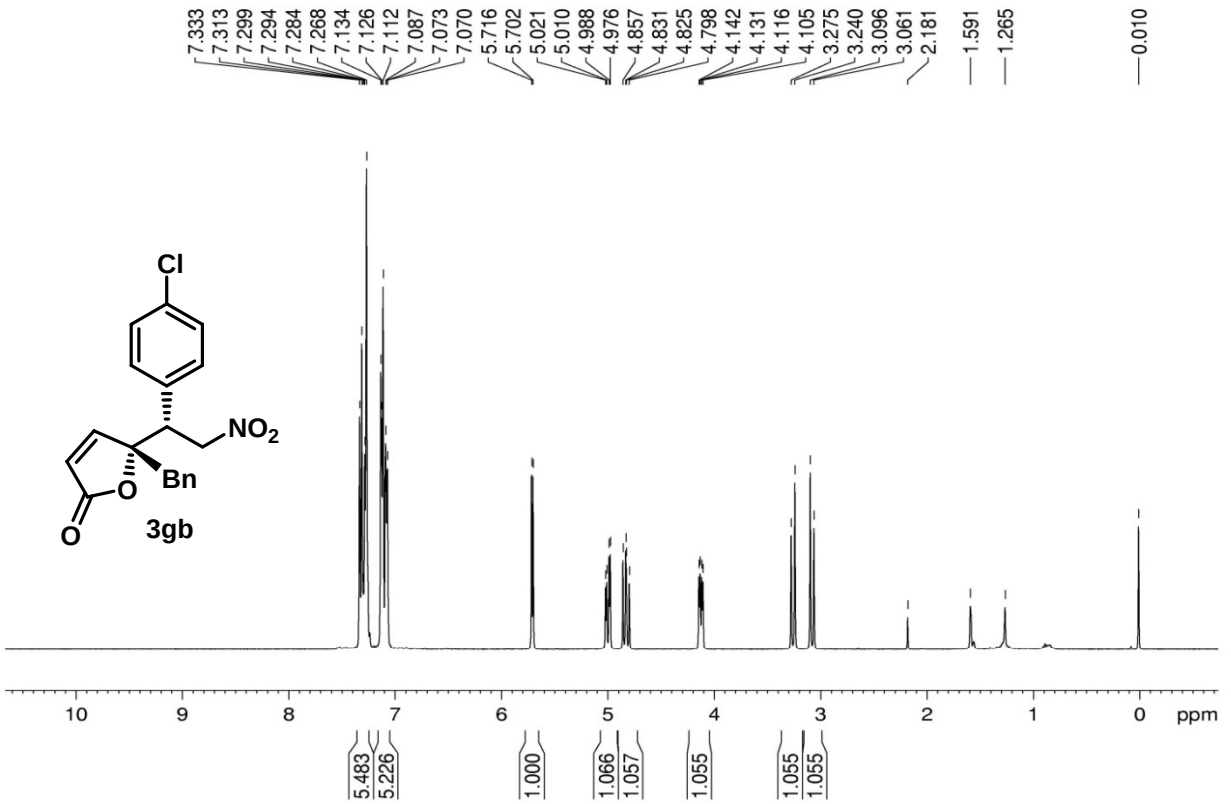
Peak#	Ret. Time	Area	Area %
1	11.091	5652608	49.980
2	15.353	5657043	50.020
Total		11309651	100.000



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	11.056	378656	2.746
2	15.240	13409862	97.254
Total		13788519	100.000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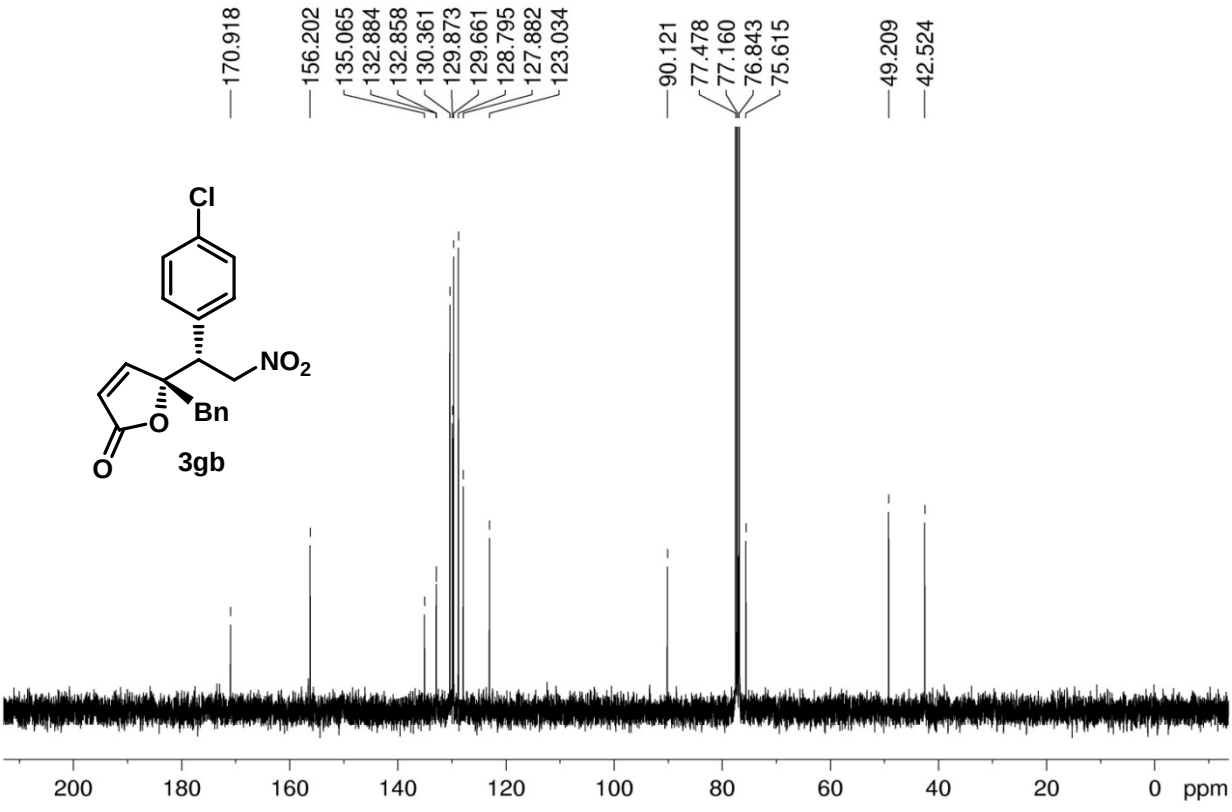
7.313
7.299
7.294
7.284
7.268
7.134
7.126
7.112
7.087
7.073
7.070
5.716
5.702
5.021
5.010
4.988
4.976
4.857
4.831
4.825
4.798
4.142
4.131
4.116
4.105
3.275
3.240
3.096
3.061
2.181
1.591
1.265
0.010
Cl
NO2
Bn
O
O
3gb
10
9
8
7
6
5
4
3
2
1
0
ppm
5.483
5.226
1.000
1.066
1.057
1.055
1.055
1.055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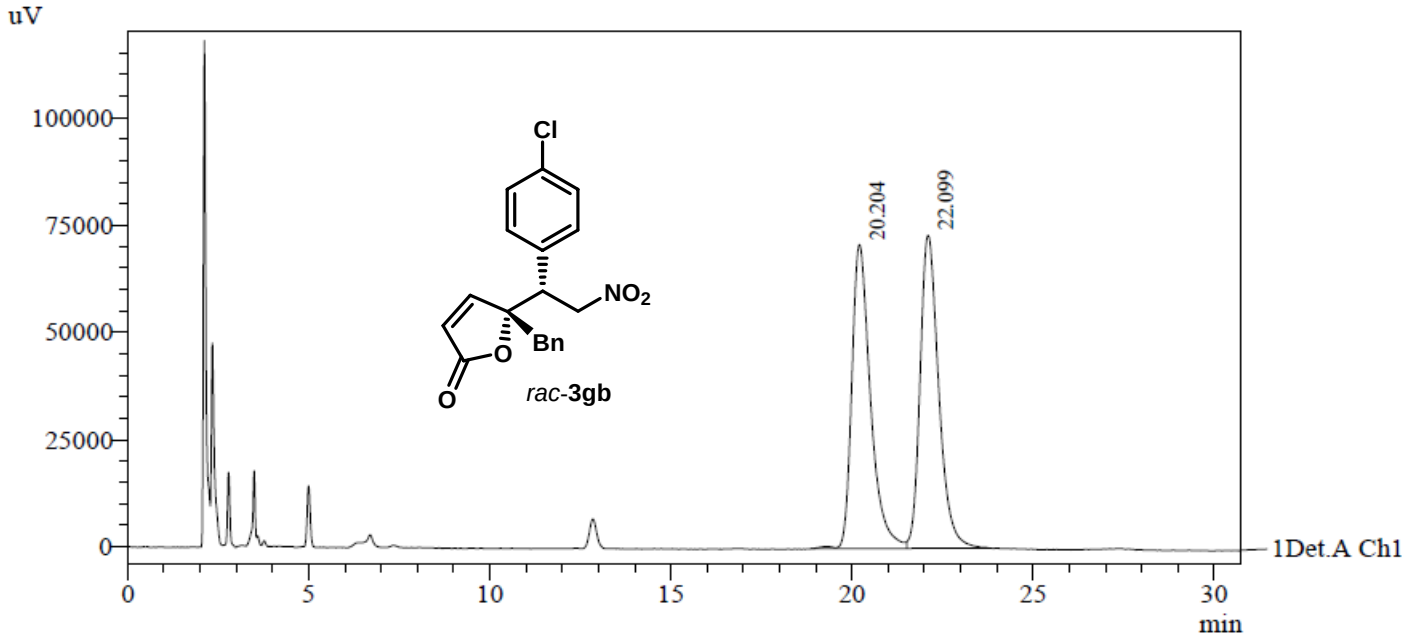
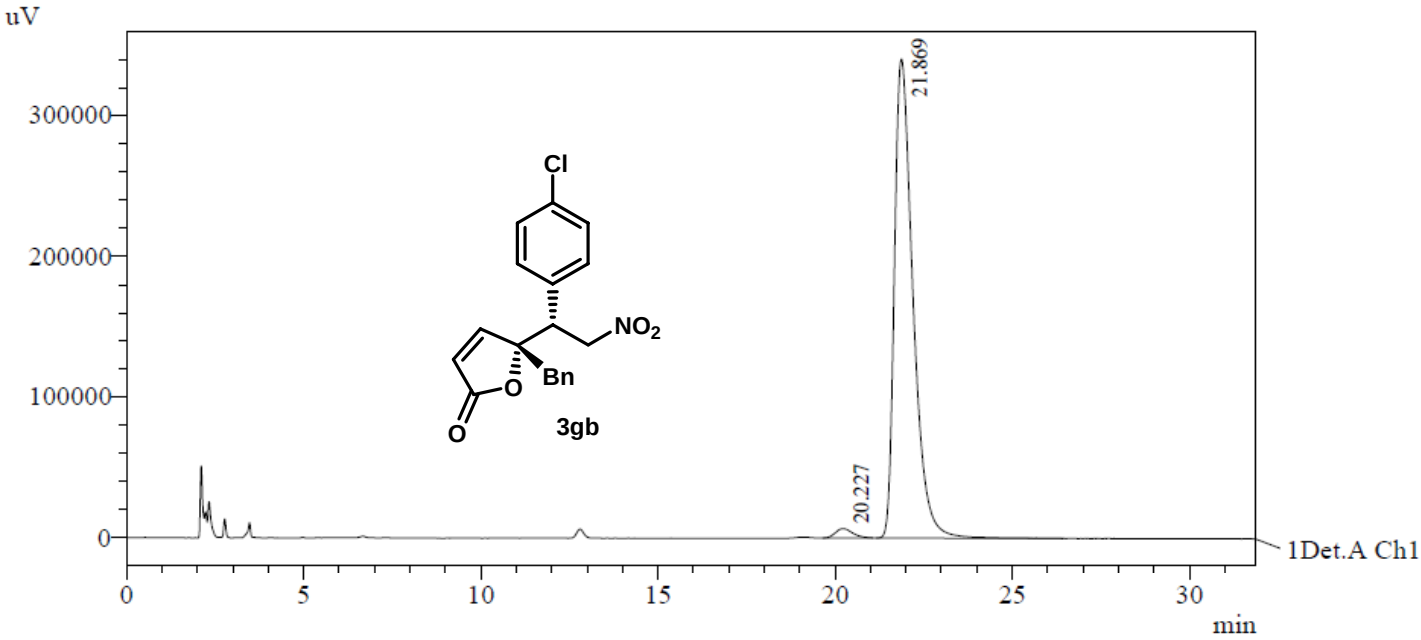
156.202
135.065
132.884
132.858
130.361
129.873
129.661
128.795
127.882
123.034
90.121
77.478
77.160
76.843
75.615
49.209
42.524
Cl
NO2
Bn
O
O
3gb
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

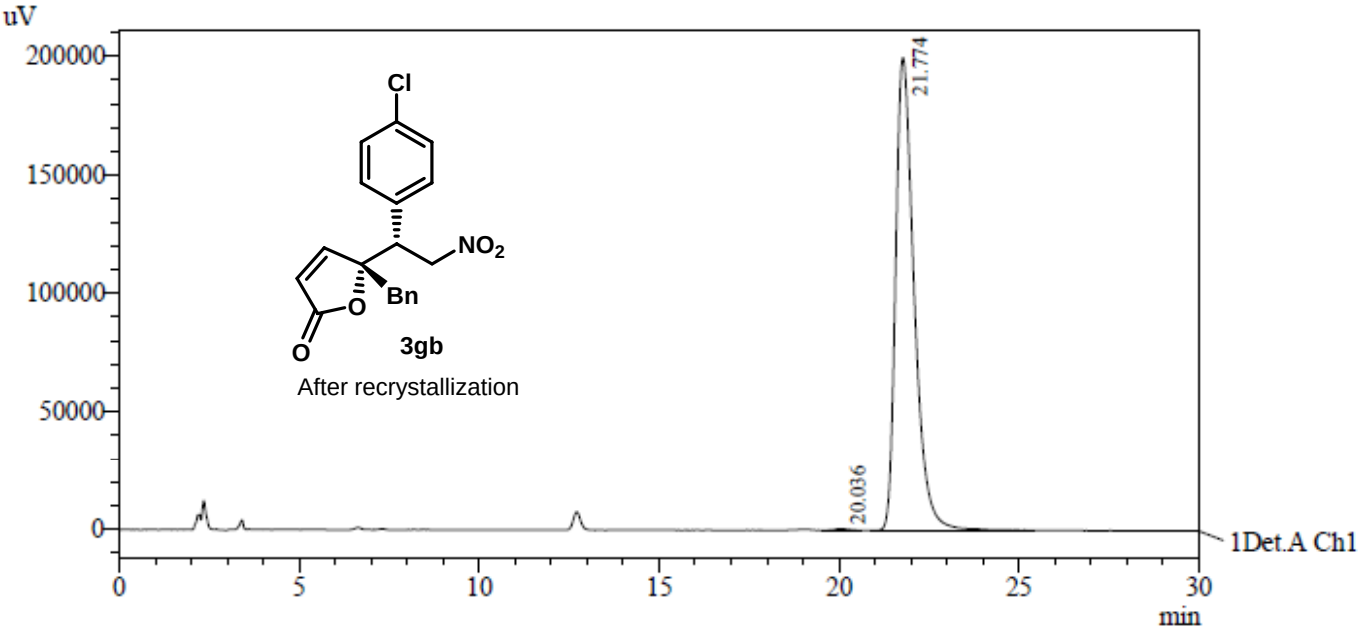
Peak#	Ret. Time	Area	Area %
1	20.204	2550699	49.466
2	22.099	2605787	50.534
Total		5156486	100.000



PeakTable

Detector A Ch1 210nm

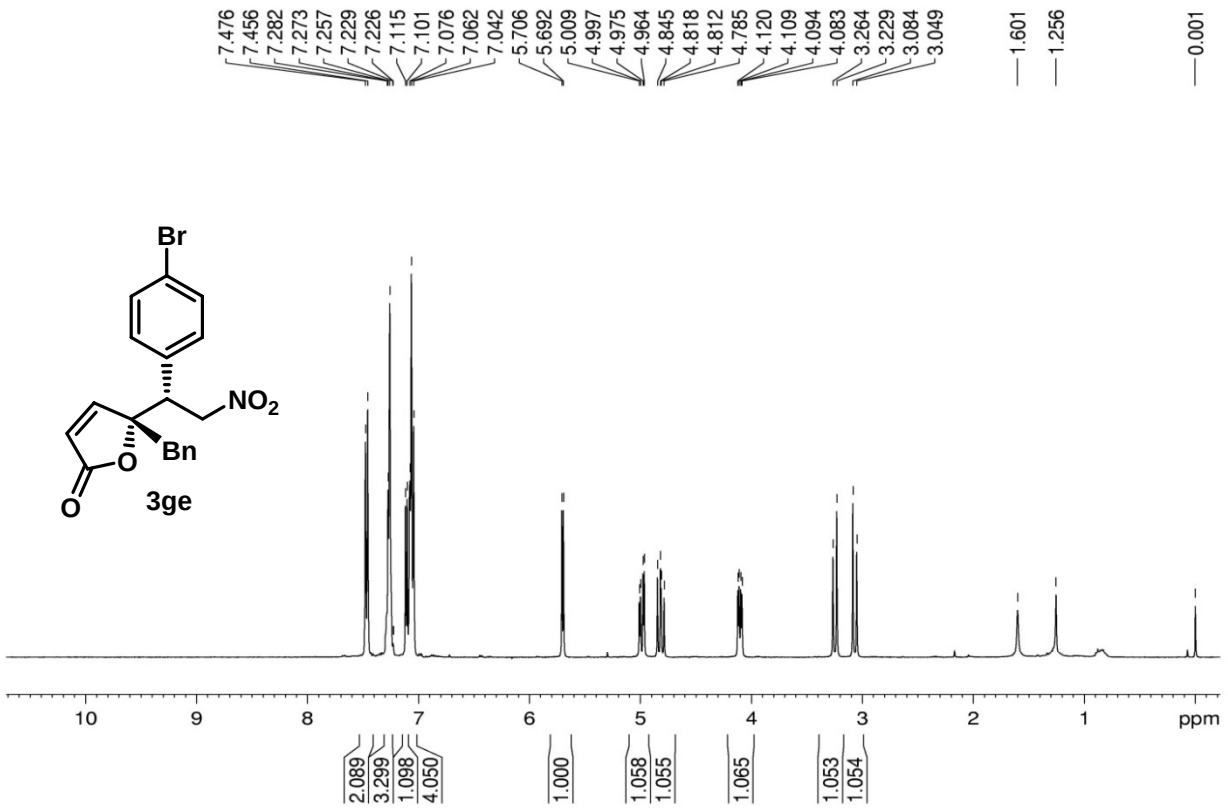
Peak#	Ret. Time	Area	Area %
1	20.227	227313	1.800
2	21.869	12399509	98.200
Total		12626822	100.000

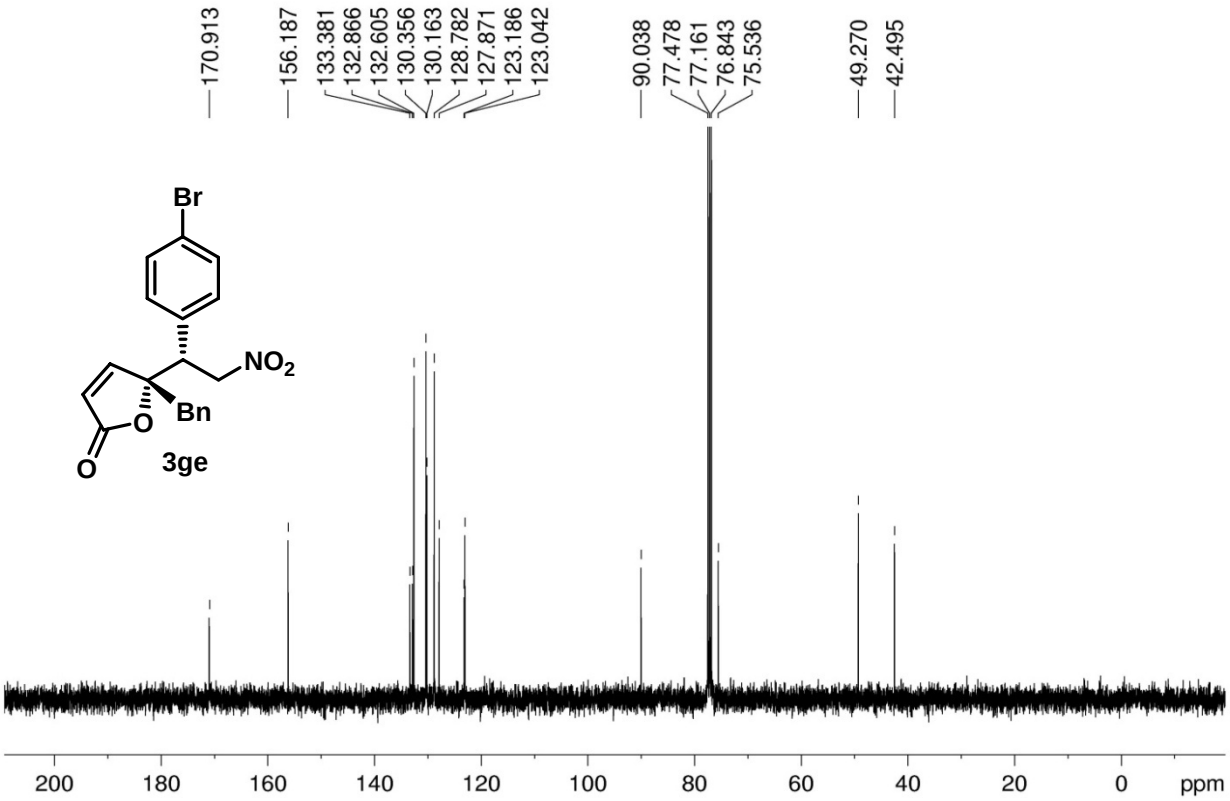


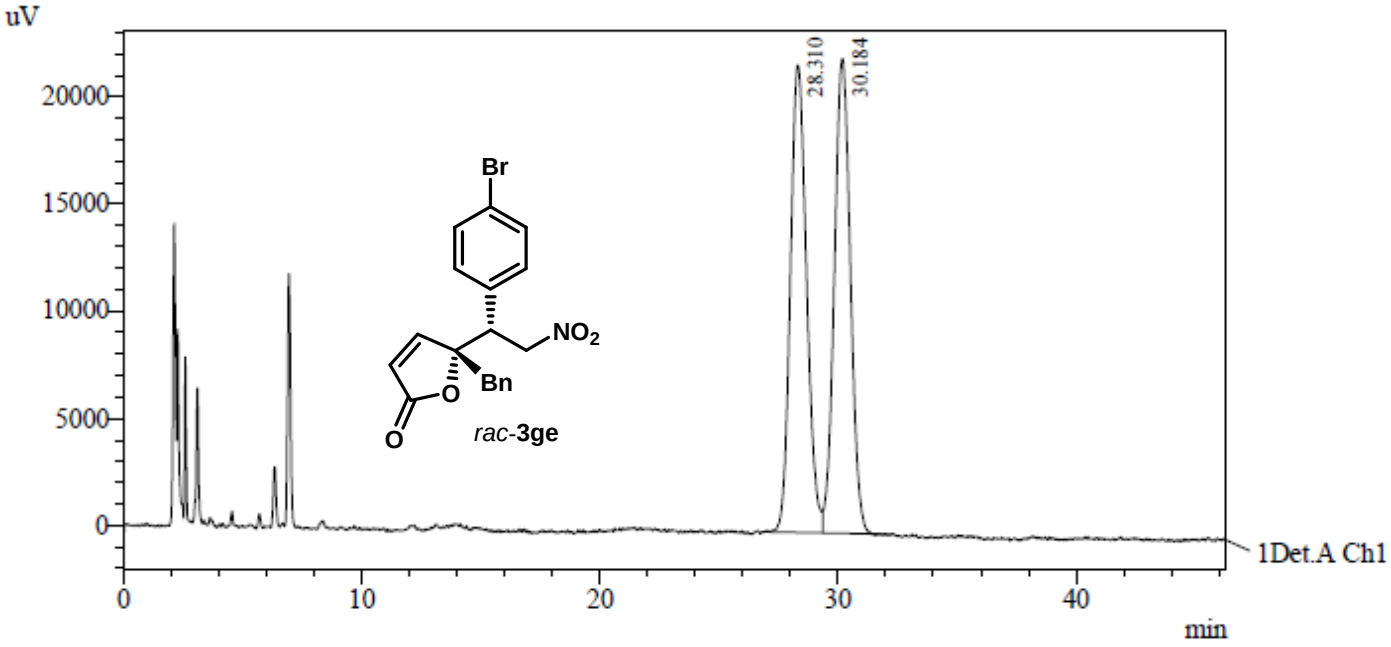
PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	20.036	14488	0.202
2	21.774	7171712	99.798
Total		7186200	100.000


7.476
7.456
7.282
7.273
7.257
7.229
7.226
7.115
7.101
7.076
7.062
7.042
5.706
5.692
5.009
4.997
4.975
4.964
4.845
4.818
4.812
4.785
4.120
4.109
4.094
4.083
3.264
3.229
3.084
3.049
1.601
1.256
0.001
Br
NO2
Bn
O
O
3ge
10
9
8
7
6
5
4
3
2
1
ppm
2.089
3.299
1.098
4.050
1.000
1.058
1.055
1.065
1.053
1.054

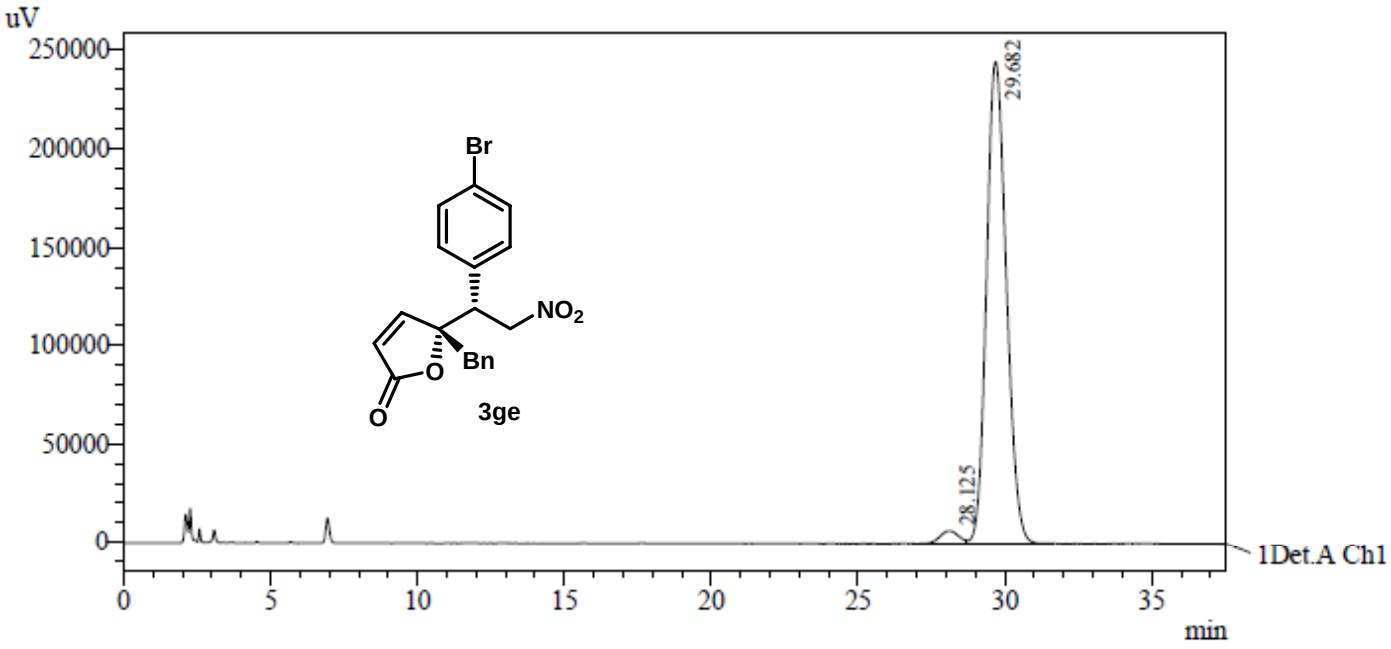

170.913
156.187
133.381
132.866
132.605
130.356
130.163
128.782
127.871
123.186
123.042
90.038
77.478
77.161
76.843
75.536
49.270
42.495
Br
NO2
Bn
O
O
3ge
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

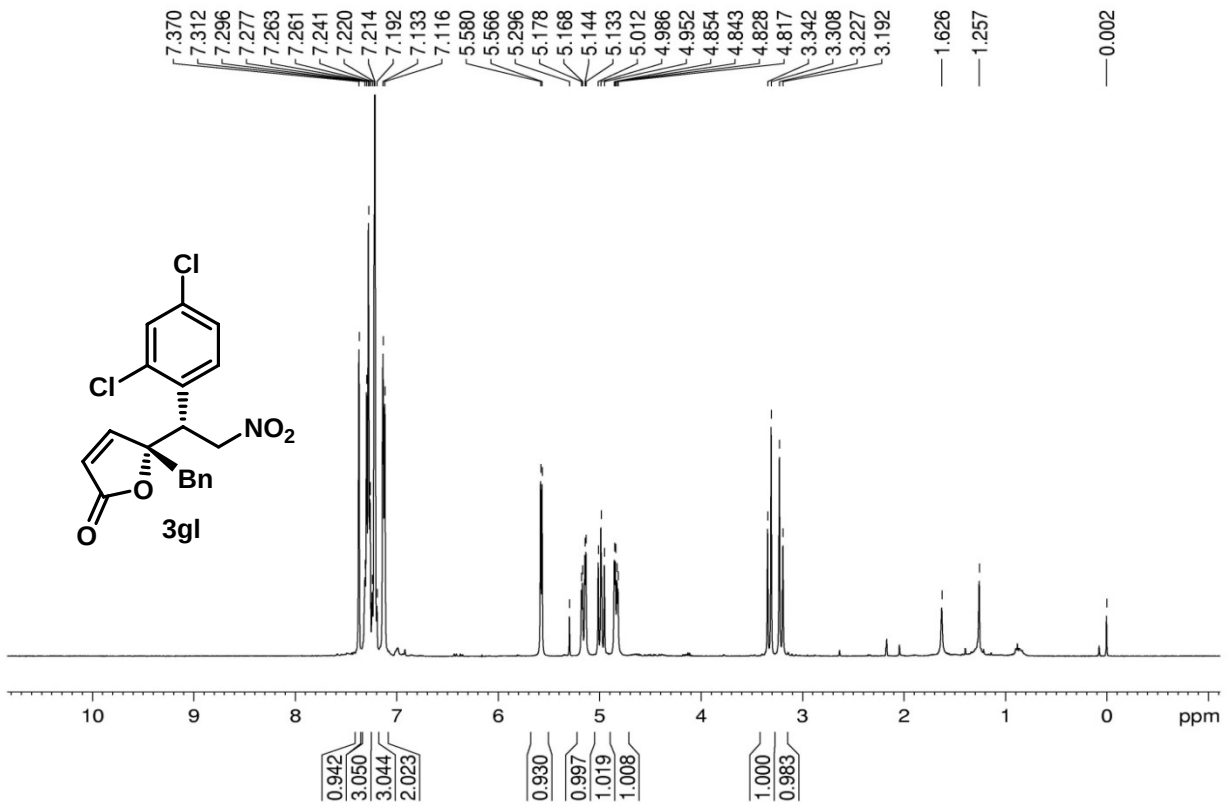
Peak#	Ret. Time	Area	Area %
1	28.310	1031911	49.915
2	30.184	1035440	50.085
Total		2067351	100.000



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	28.125	286326	2.435
2	29.682	11474118	97.565
Total		11760444	100.000


7.370
7.312
7.296
7.277
7.263
7.261
7.241
7.220
7.214
7.192
7.133
7.116
5.580
5.566
5.296
5.178
5.168
5.144
5.133
5.012
4.986
4.952
4.854
4.843
4.828
4.817
3.342
3.308
3.227
3.192
1.626
1.257
0.002
Cl
Cl
NO2
Bn
O
O
3gl
10
9
8
7
6
5
4
3
2
1
0
ppm
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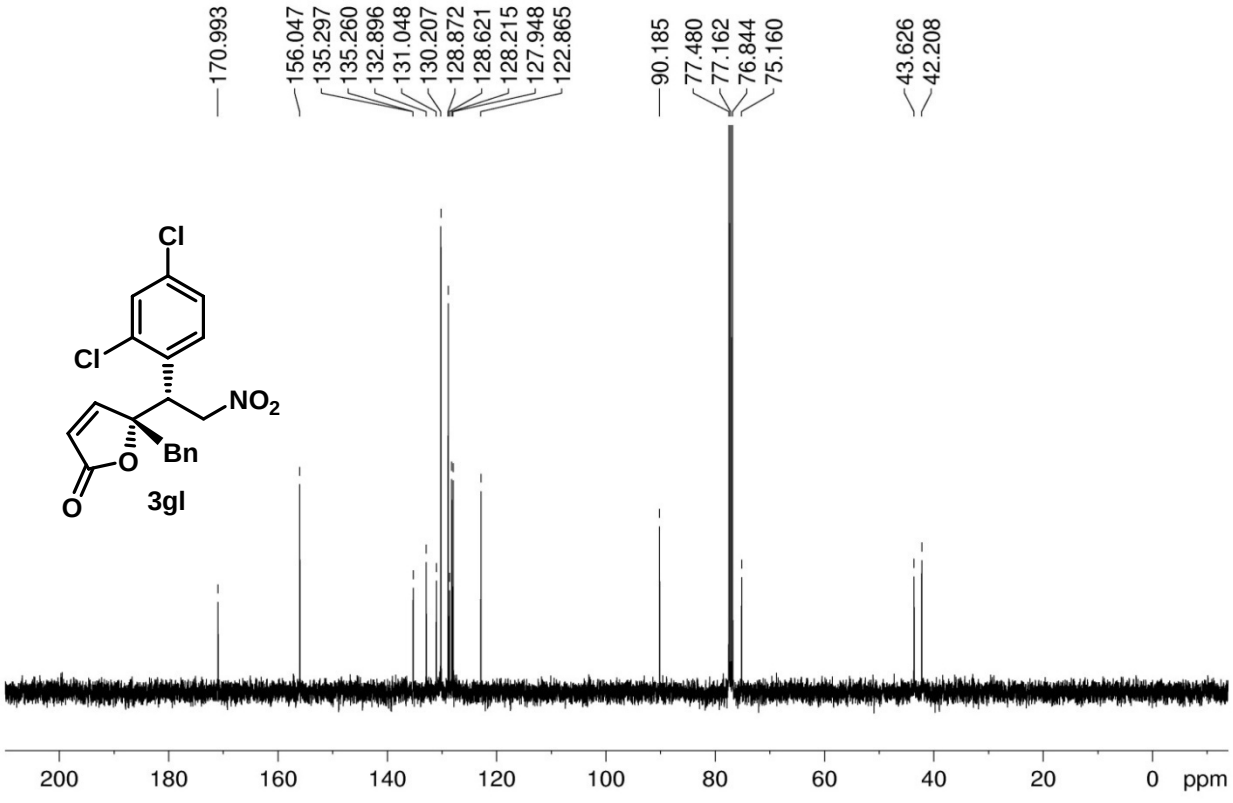
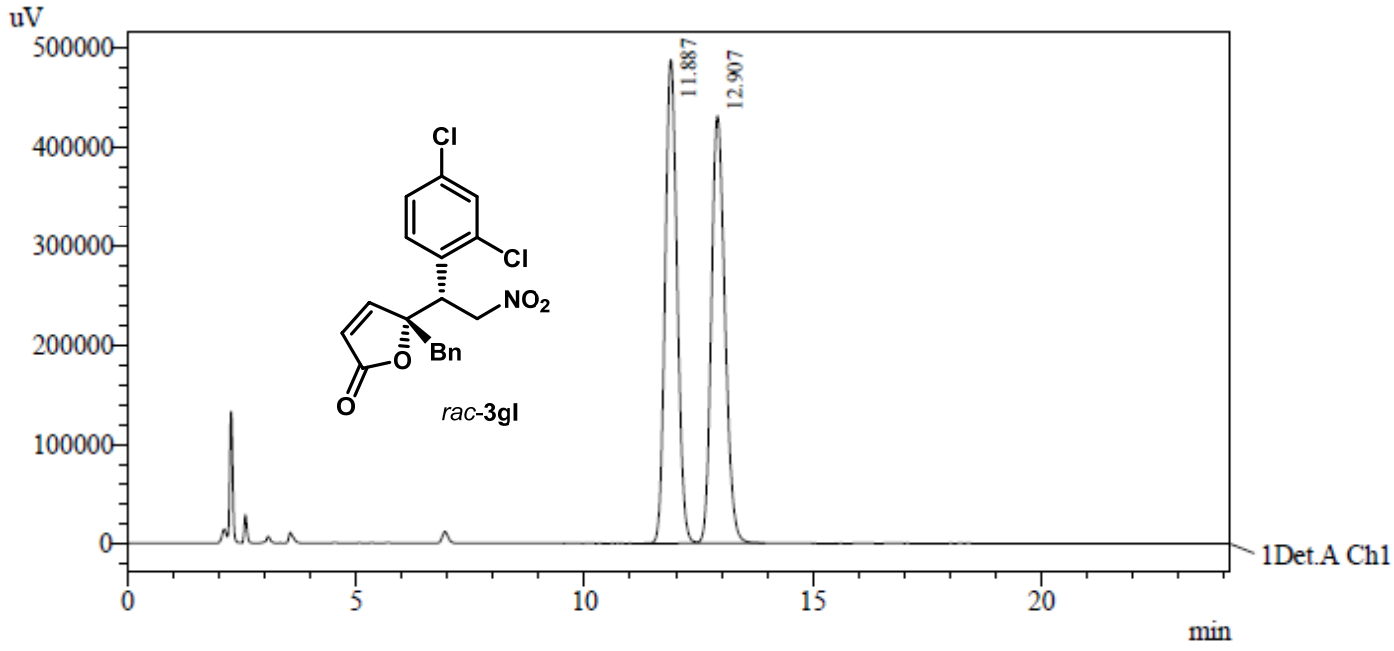
3.050
3.044
2.023
0.930
0.997
1.019
1.008
1.000
0.983

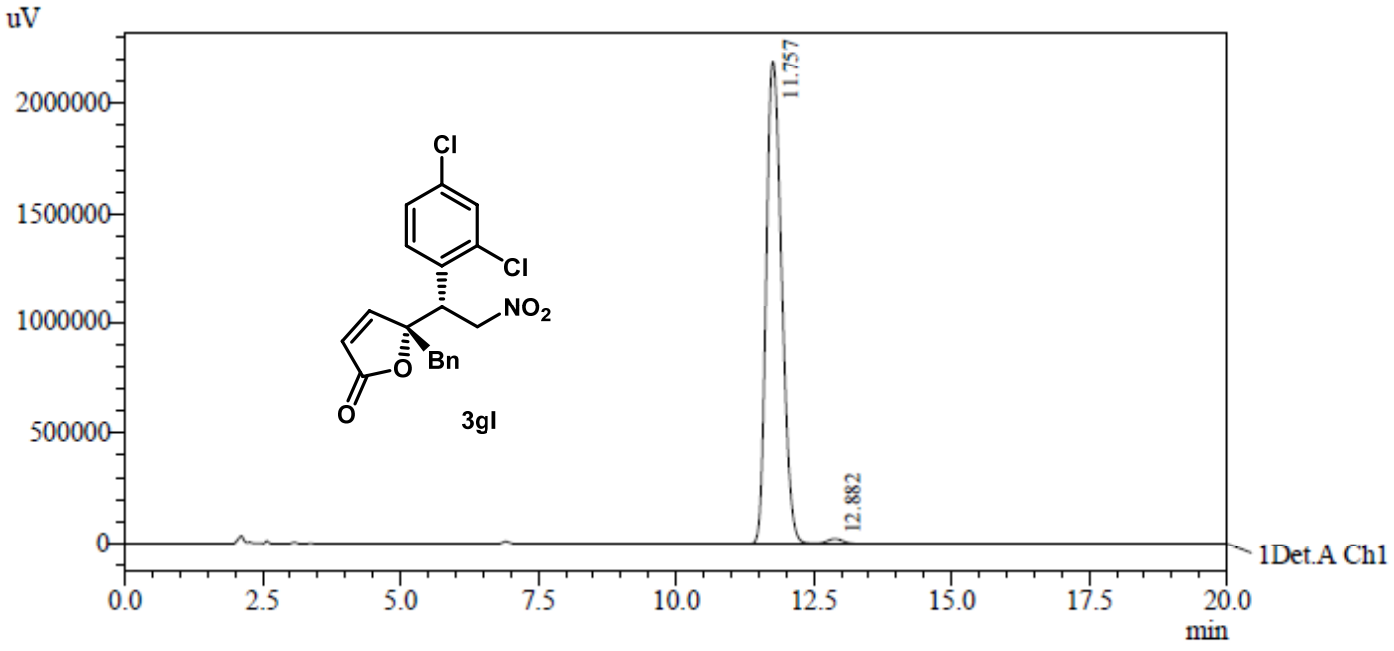

170.993
156.047
135.297
135.260
132.896
131.048
130.207
128.872
128.621
128.215
127.948
122.865
90.185
77.480
77.162
76.844
75.160
43.626
42.208
Cl
Cl
NO2
Bn
O
O
3gl
200
180
160
140
120
100
80
60
40
20
0
ppm



PeakTable

Detector A Ch1 210nm

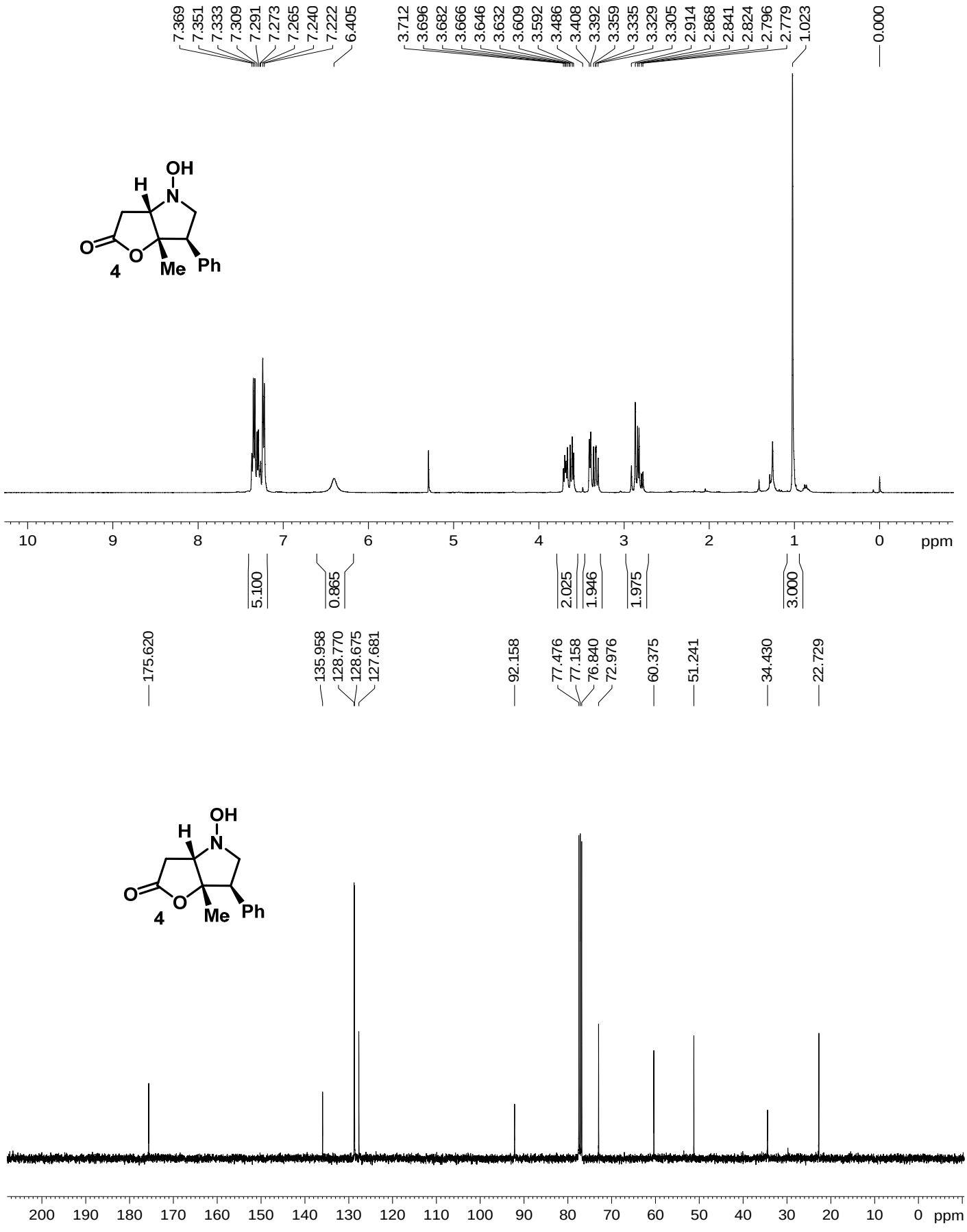
Peak#	Ret. Time	Area	Area %
1	11.887	8901660	49.970
2	12.907	8912346	50.030
Total		17814006	100.000



PeakTable

Detector A Ch1 210nm

Peak#	Ret. Time	Area	Area %
1	11.757	42819947	98.832
2	12.882	505838	1.168
Total		43325785	100.000


7.369
7.351
7.333
7.309
7.291
7.273
7.265
7.240
7.222
6.405
3.712
3.696
3.682
3.666
3.646
3.632
3.609
3.592
3.486
3.408
3.392
3.359
3.335
3.329
3.305
2.914
2.868
2.841
2.824
2.796
2.779
1.023
0.000
OH
H
N
O
O
4
Me
Ph
10
9
8
7
6
5
4
3
2
1
0
ppm
5.100
0.865
2.025
1.946
1.975
3.000
175.620
135.958
128.770
128.675
127.681
92.158
77.476
77.158
76.840
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H
N
O
O
4
Me
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm