Supporting Information

Total syntheses of several iridolactones and the putative structure of noriridoid scholarein A: An intramolecular Pauson-Khand reaction based one-stop synthetic solution

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Table of Contents

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Table 1: Comparison of ^{1}H NMR data of natural scholarein A with the synthetic one.

No. of H	^{1}H data for natural scholarein A reported in isolation paper[1]	^{1}H data reported for synthetic scholarein A by others[2]	^{1}H data for the presently synthesized scholarein A
CH2(1) or H-C(1)	3.39–3.42 (m)	3.85 – 3.80 (m, 1H), 3.68 (dd, J_1 = 12 Hz, J_2 = 3 Hz, 1H)	3.85 – 3.80 (m, 1H), 3.68 (dd, J_1 = 12 Hz, J_2 = 4 Hz, 1H)
CH2(3)	3.43–3.46(m), 3.30–3.33 (m)	3.85 – 3.80 (m, 1H), 3.33 (ddd, J = 11.6, 11.6, 2.4 Hz, 1H)	3.85 – 3.80 (m, 1H), 3.33 (td, J_1 = 11 Hz, J_2 = 2 Hz, 1H)
CH2(4)	1.66–1.69(m), 1.12–1.15 (m)	1.64-1.49 (m, 1H) 1.43-1.32 (m, 1H)	1.56 – 1.49 (m, 1H), 1.43 – 1.32 (m, 1H)
H-C(5)	2.16–2.19 (m)	2.26-2.17 (m, 1H)	2.26-2.17 (m, 1H)
CH2(6)	1.58–1.61 (m), 1.32–1.35 (m)	1.85 (ddd, J = 14.4, 6.4, 3.2 Hz, 1H), 1.77 (ddd, J = 14.8 Hz, 7.6, 3.2 Hz, 1H)	1.85 (ddd, J_1 = 14 Hz, J_2 = 6 Hz, J_3 = 3 Hz, 1H), 1.77 (ddd, J_1 = 14 Hz, J_2 = 8 Hz, J_3 = 3.0 Hz, 1H)
H-C(7)	3.86–3.88 (m)	4.29-4.25 (1H, m)	4.29-4.25 (1H, m)
H-C(8)	1.45–1.47 (m)	2.10 (ddq, J = 10.8, 6.8, 6.8 Hz, 1H)	2.15 – 2.04 (m, 1H)
H-C(9)	1.69–1.72 (m)	1.64-1.49 (m, 1H))	1.65 – 1.59 (m, 1H)
Me(10)	0.83 (d, J = 7)	1.01 (3H, d, J = 6.8 Hz)	1.01 (3H, d, J = 7 Hz)

Table 2: Comparison of ^{13}C NMR data of natural scholarein A with the synthetic one.

No. of C	^{13}C data for natural scholarein A reported in isolation paper[1]	^{13}C data reported for synthetic scholarein A by others[2]	^{13}C data for the presently synthesized scholarein A
CH2(1) or H-C(1)	62.2	67.0	66.9
CH2(3)	61.7	67.4	67.3
CH2(4)	33.2	30.3	30.2
H-C(5)	34.4	34.0	33.8
CH2(6)	40.9	41.7	41.6
H-C(7)	74.7	74.8	74.7
H-C(8)	41.3	37.8	37.6

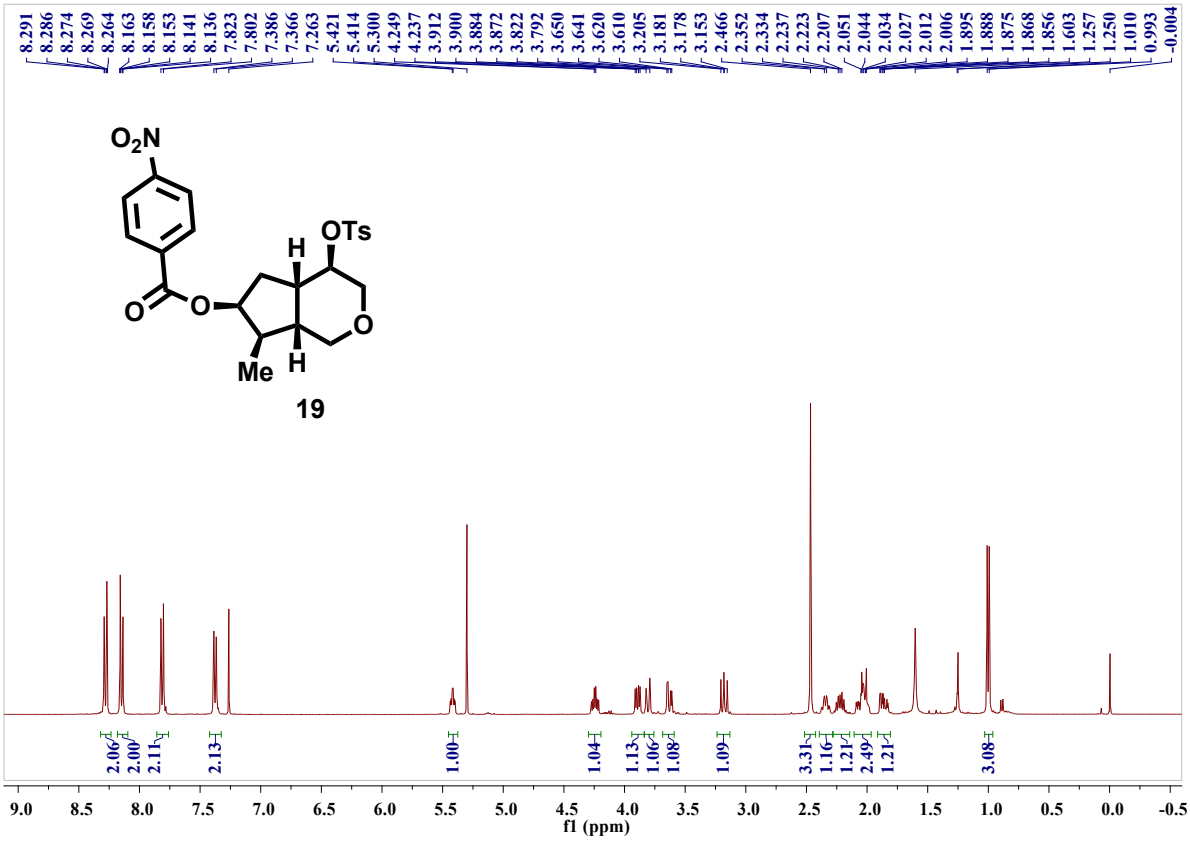
H-C(9)	48.4	43.3	43.2
Me(10)	13.5	11.9	11.7

CRYSTAL INFORMATION OF COMPOUND **32**

Compound (**32**) was crystallized from DCM solvent through slow-evaporation at room temperature. Single crystal X-ray diffraction data were collected on Bruker single-crystal X-ray diffractometer (D8 VENTURE) equipped with a PHOTON 100 CMOS detector. In this case data collection was smooth without any complication and crystal was stable throughout the data collection period. The structure were determined using intrinsic phasing method followed by full-matrix least-squares refinement against F^2 using SHELXTL-13. The data of colourless needle-like crystal collected at 110 K using graphite monochromated radiation (λ = 0.71073 Å) : $C_{16}H_{19}NO_5$, triclinic, P-1, a = 16.691(2), b = 7.895(3), c = 15.590(6) Å, α= 85.482(15), β = 85.127(10) °, γ =68.851(13), V = 764.3(4) $Å^3$, Z = 2, T = 110(2) K, μ = 0.099 mm^{-1} , 3863 reflection collected, 2724 independent (R (int) = 0.0837), 3863 observed [$I \geq 2\sigma(I)$], 200 parameters, R indices $R_1[I \geq 2\sigma(I)]$ = 0.0581 and wR_2 = 0.1493, final R (all data) = [$I \geq 2\sigma(I)$] R_1 = 0.0838 and wR_2 = 0.1723, GOF on F^2 = 1.034, max/min residual electron density = 0.26/-0.23 $e.A^{-3}$ .CCDC 1898028 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif.

Ref:

1) T. Feng, X.-H. Cai, Z.-Z. Du, X.-D. Luo, *Helv. Chim. Acta,* **2008**, *91*, 2247.
2) Y. Kawai, S. Megumi, T. Masahiro, *Heterocycles*, **2012**, *86*, 1093.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Me
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1.06
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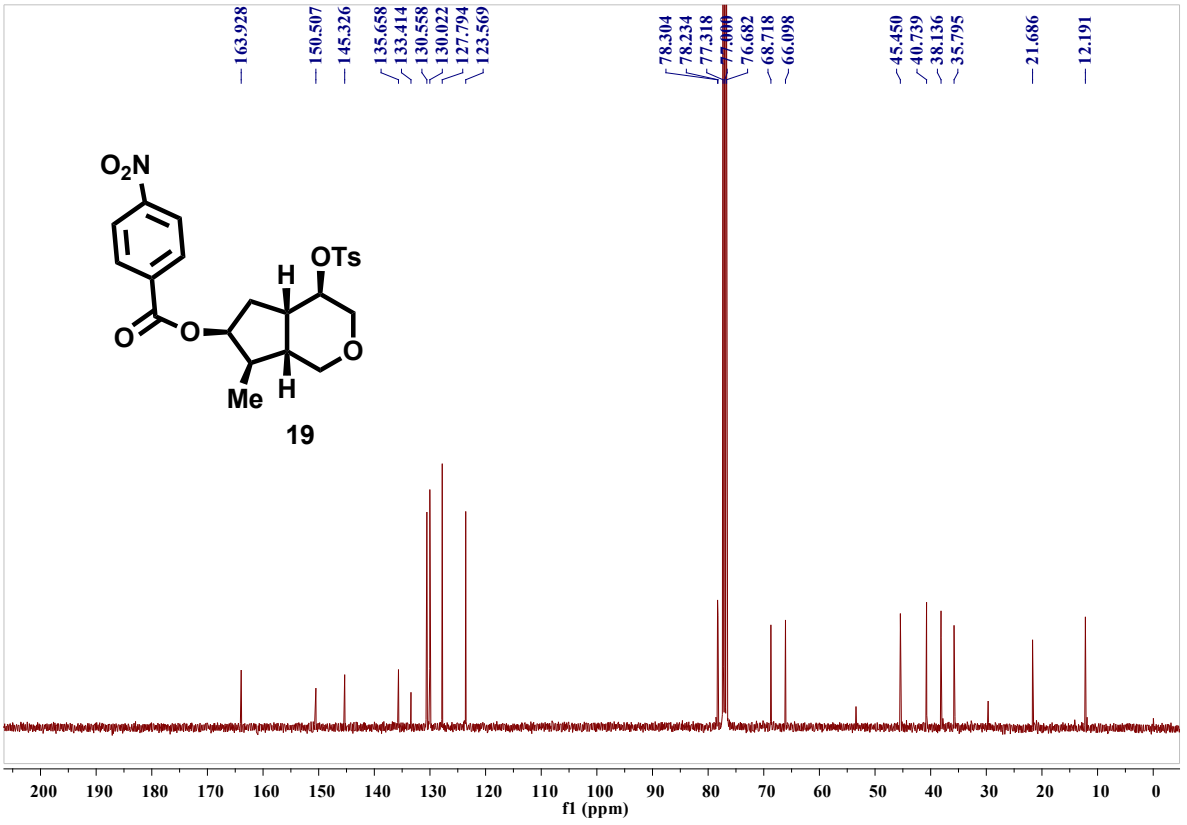
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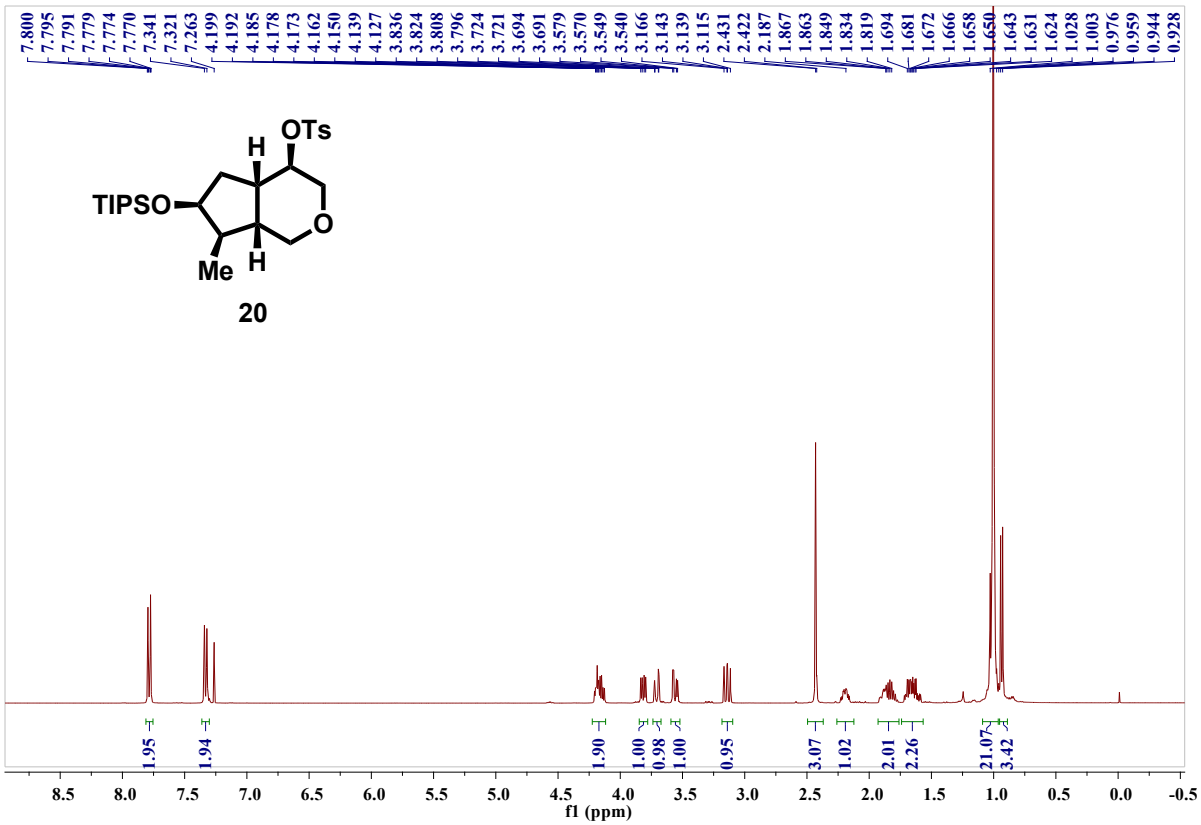
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TIPSO
O
Me
H
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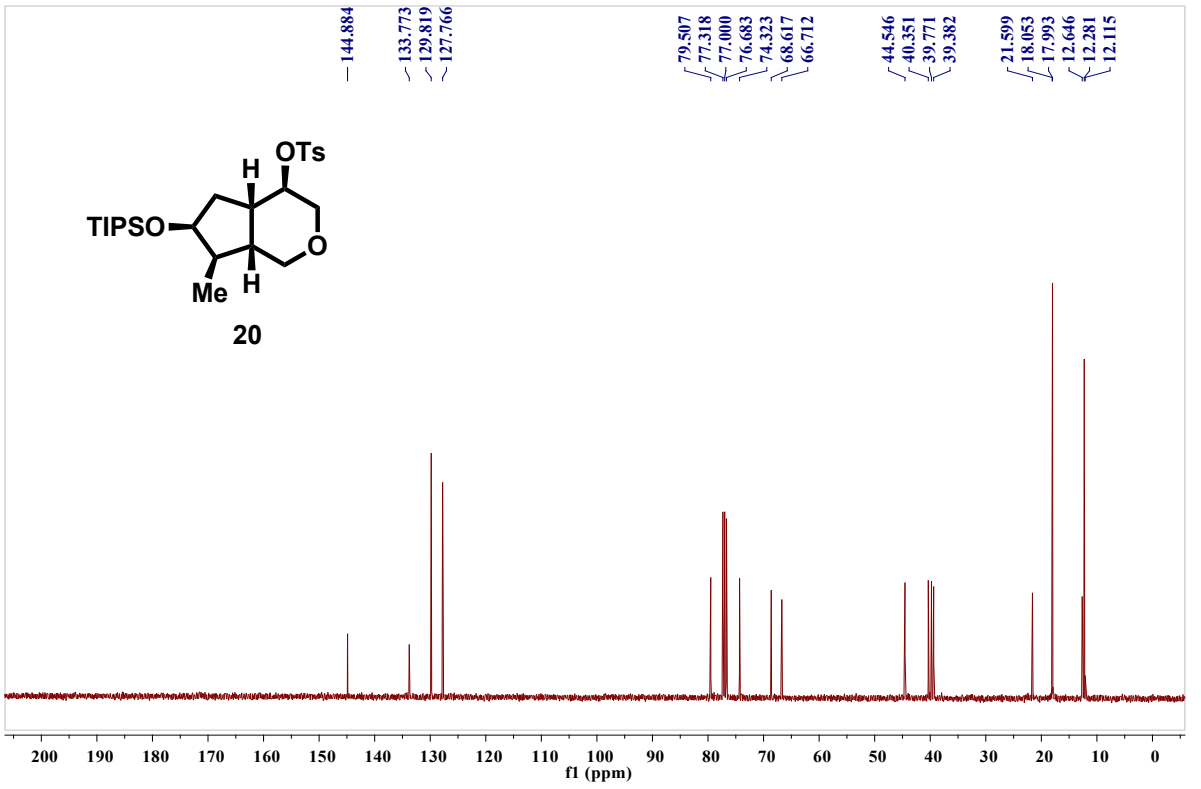
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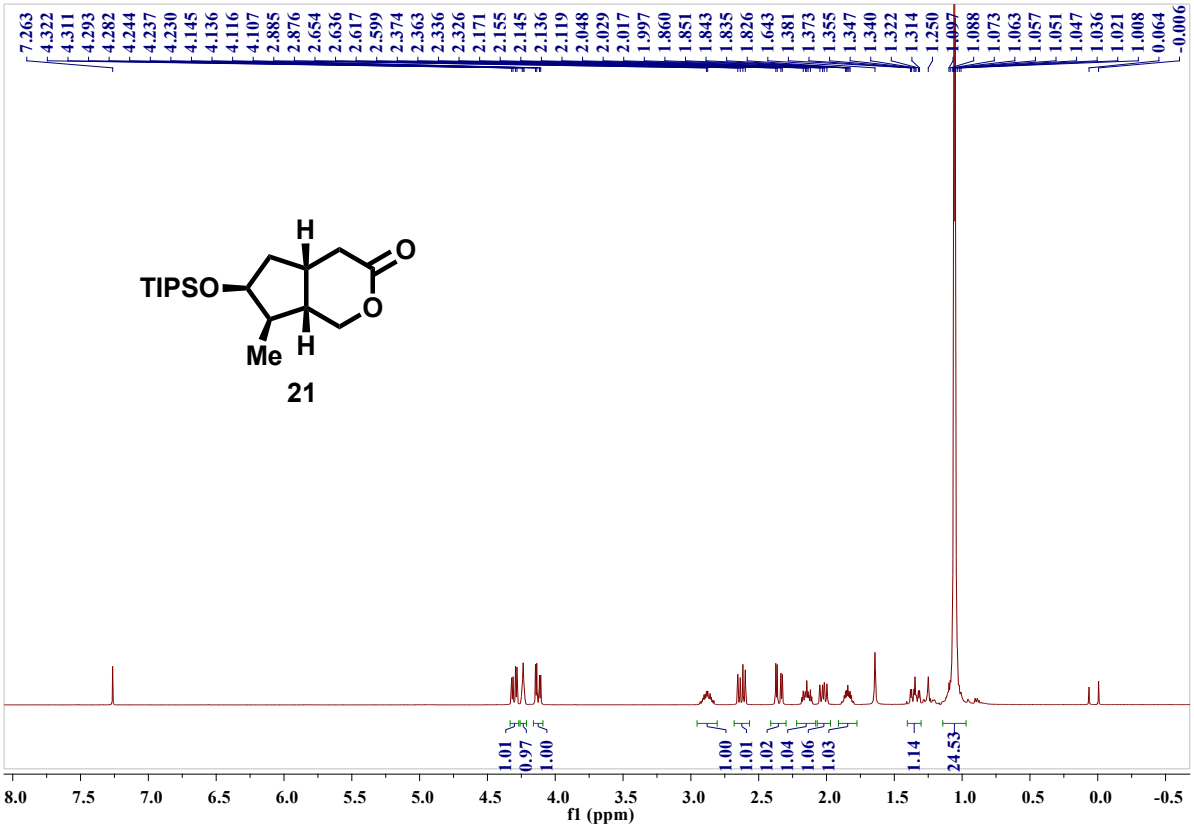
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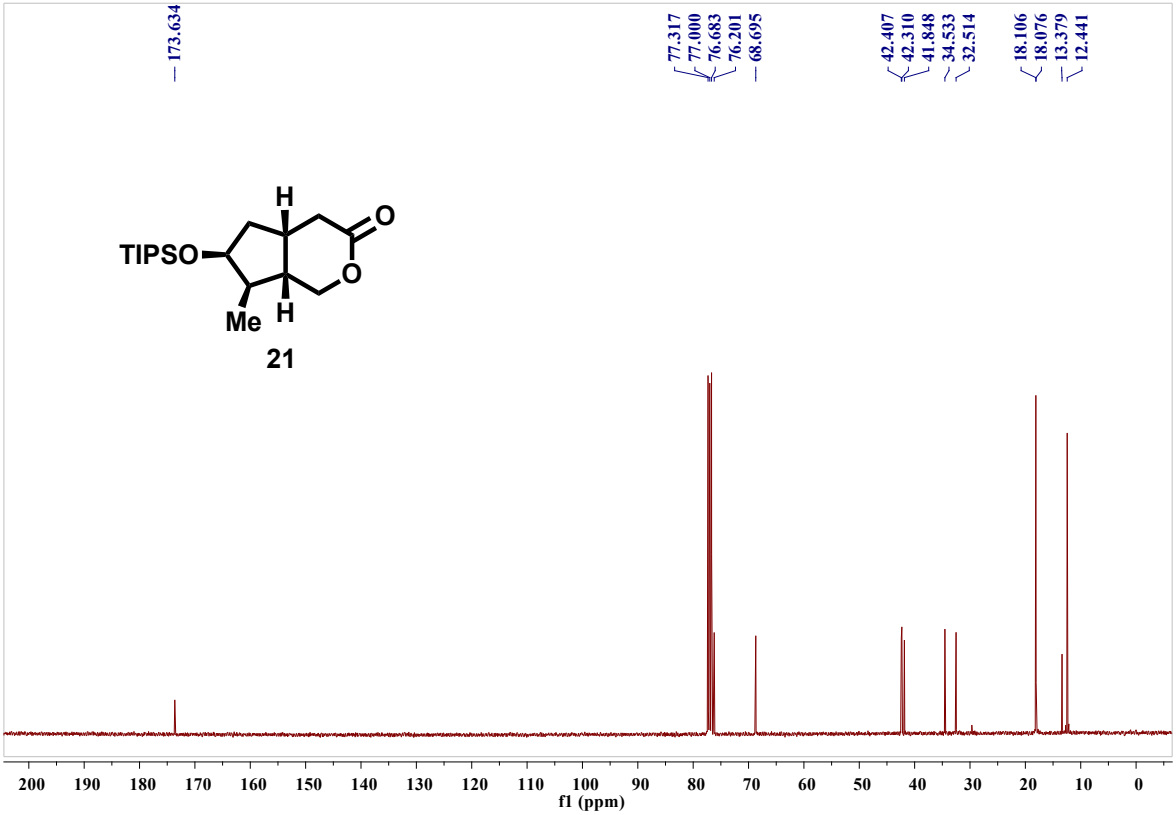
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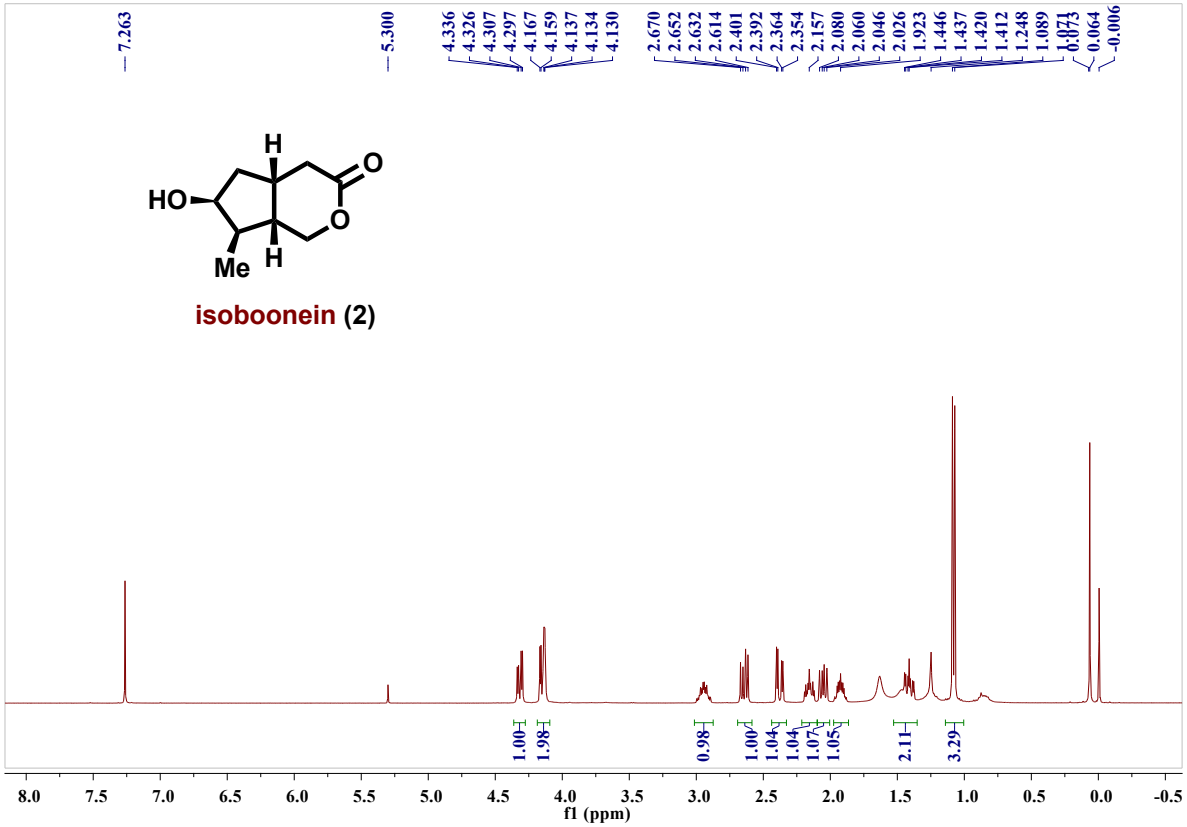
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H
O
O
H
Me
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1.00
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1.04
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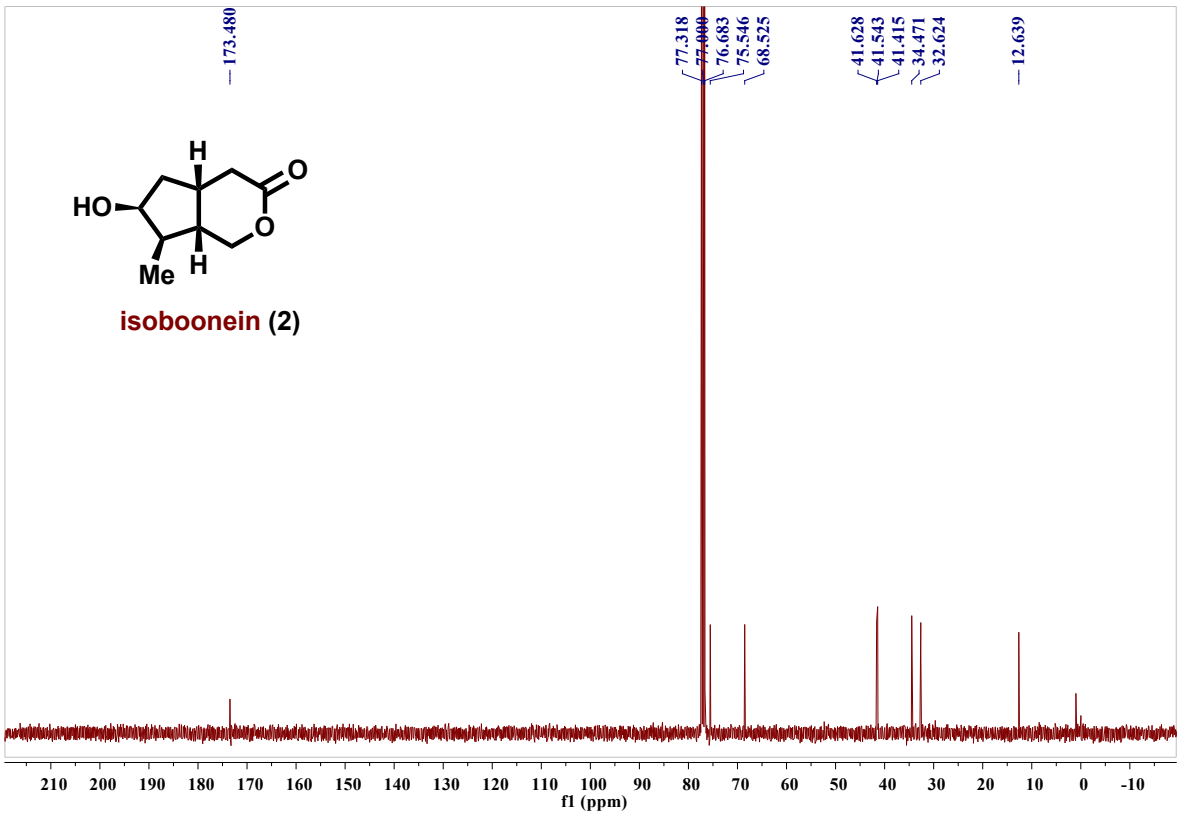
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Me
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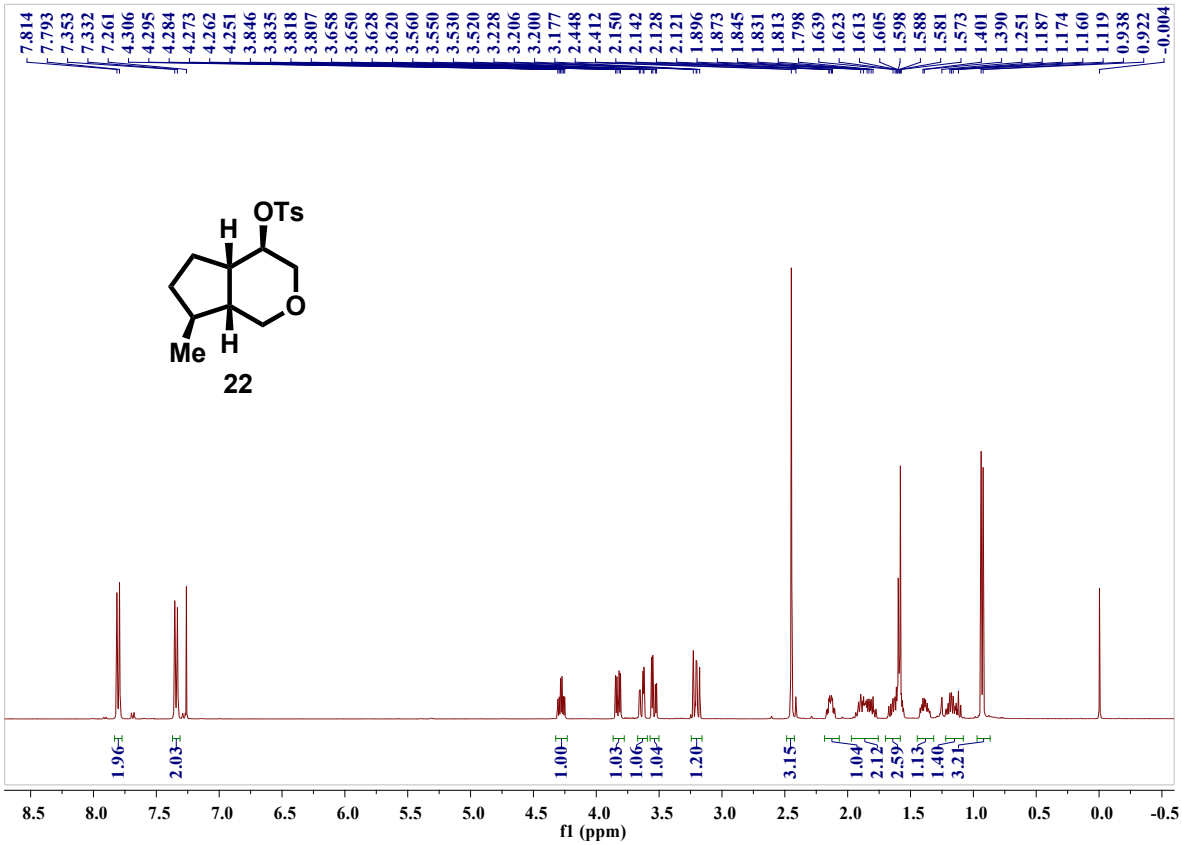
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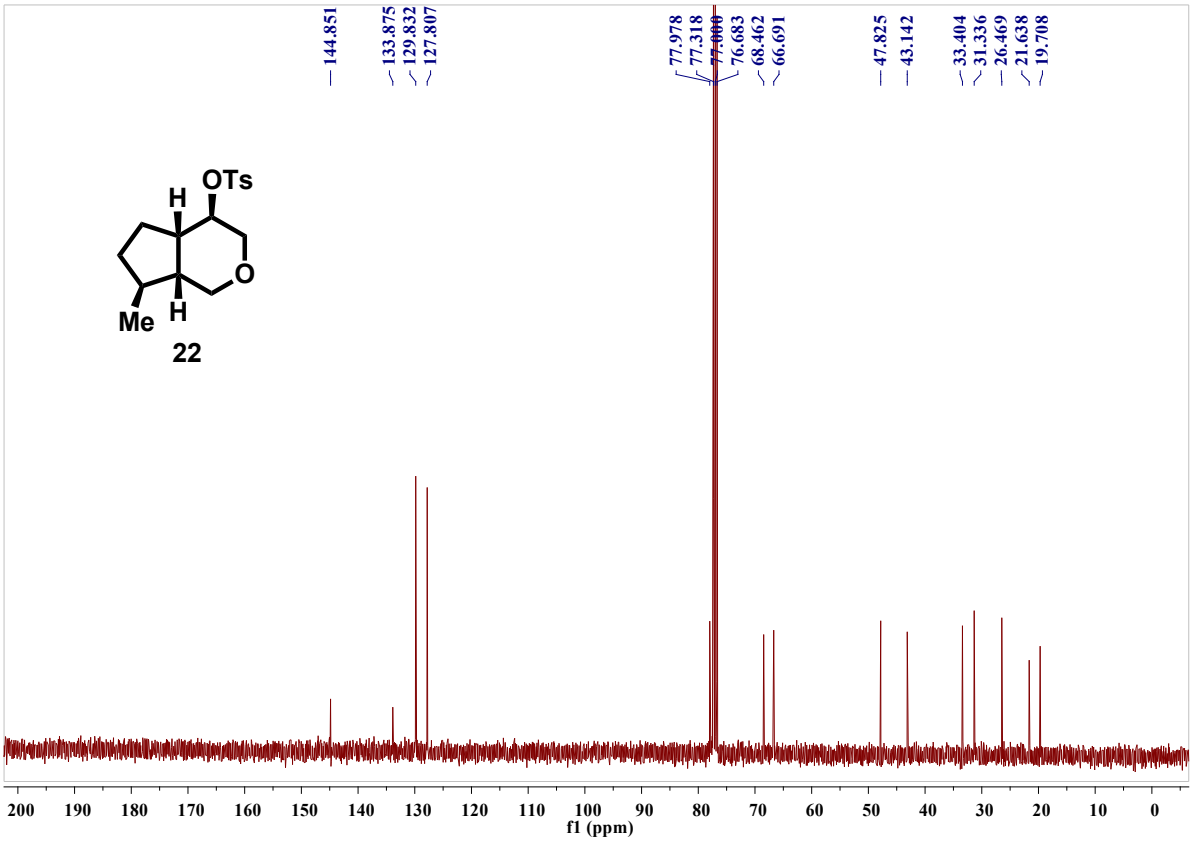
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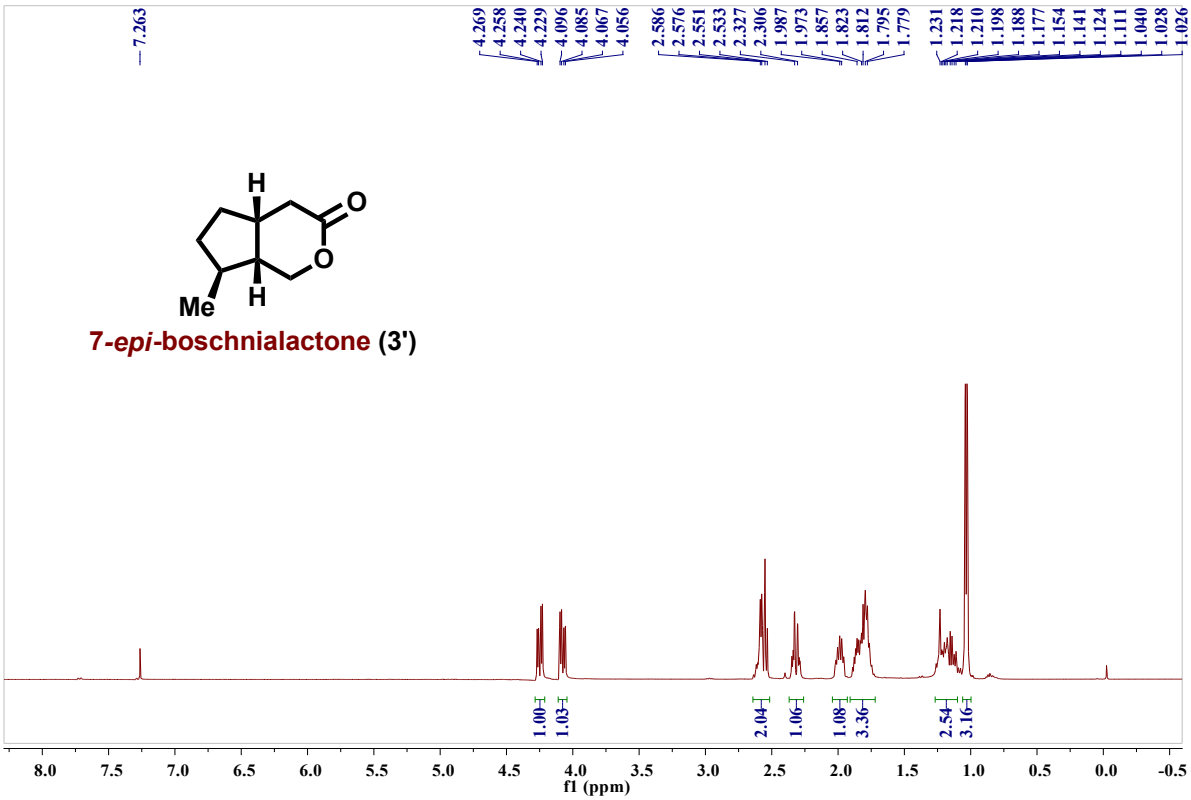

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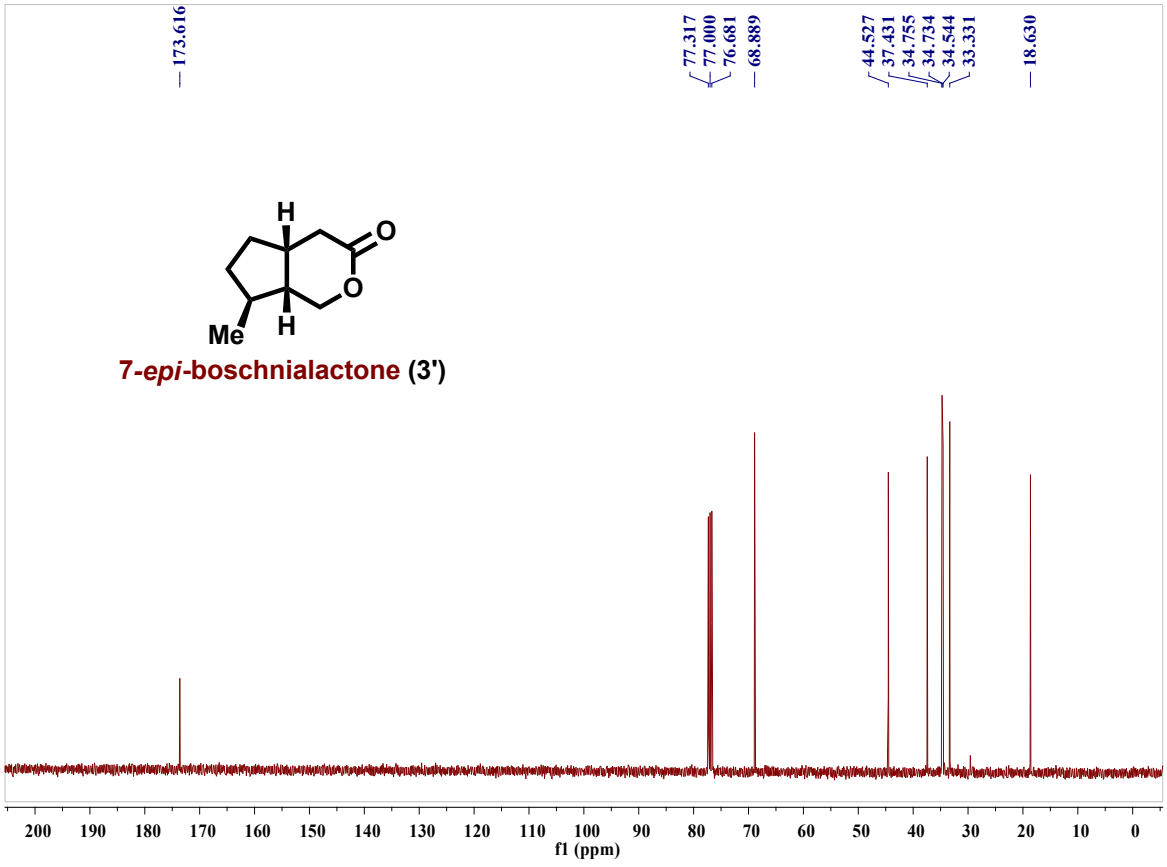

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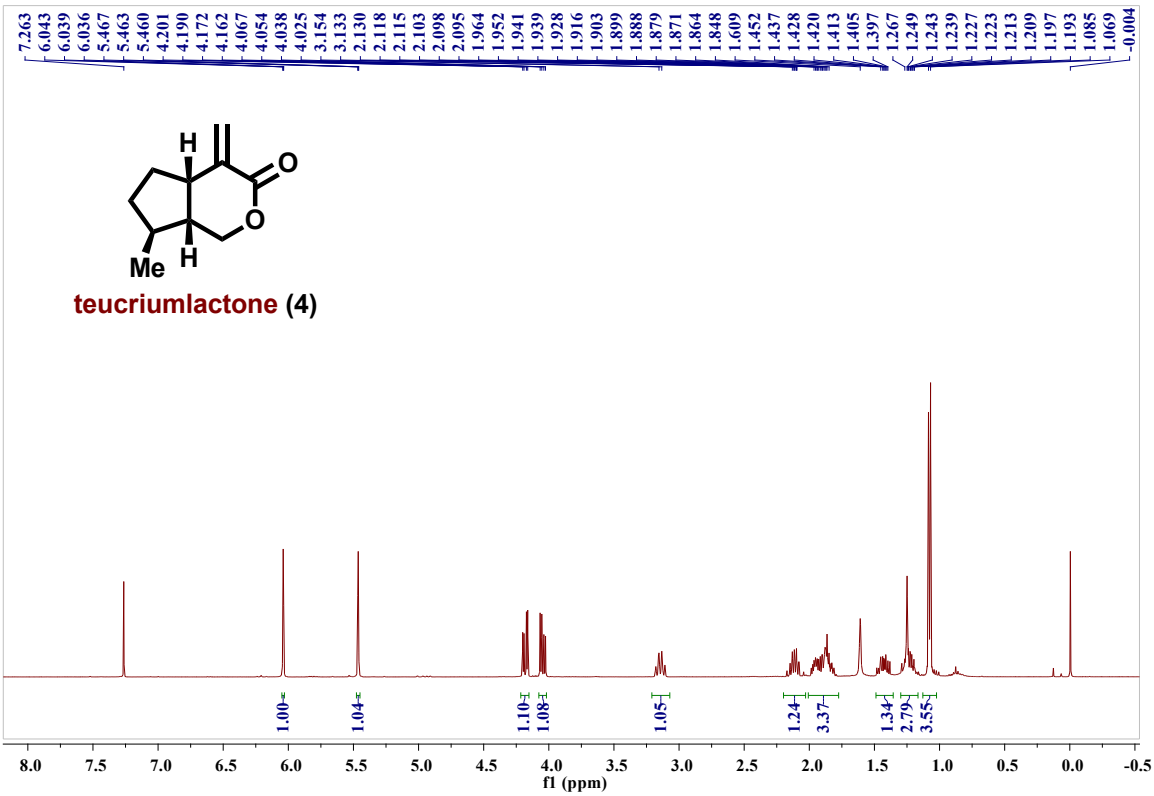

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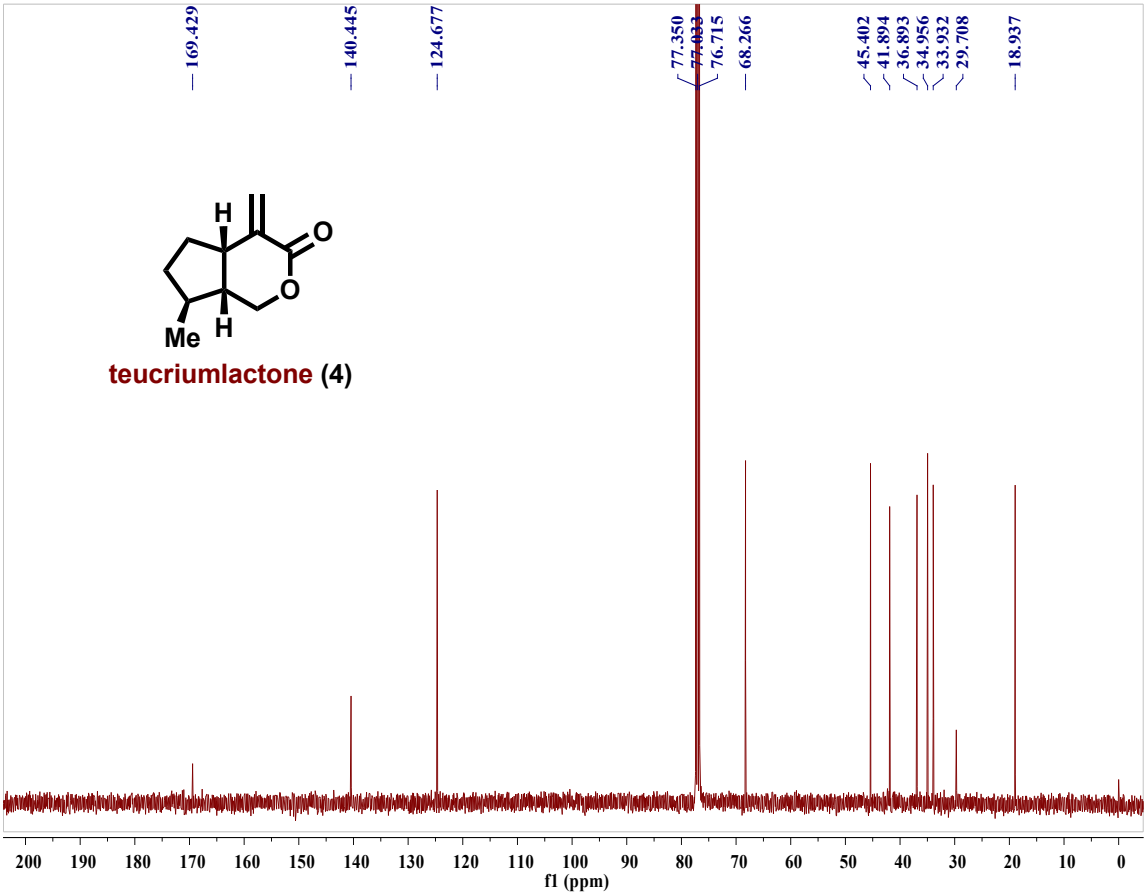

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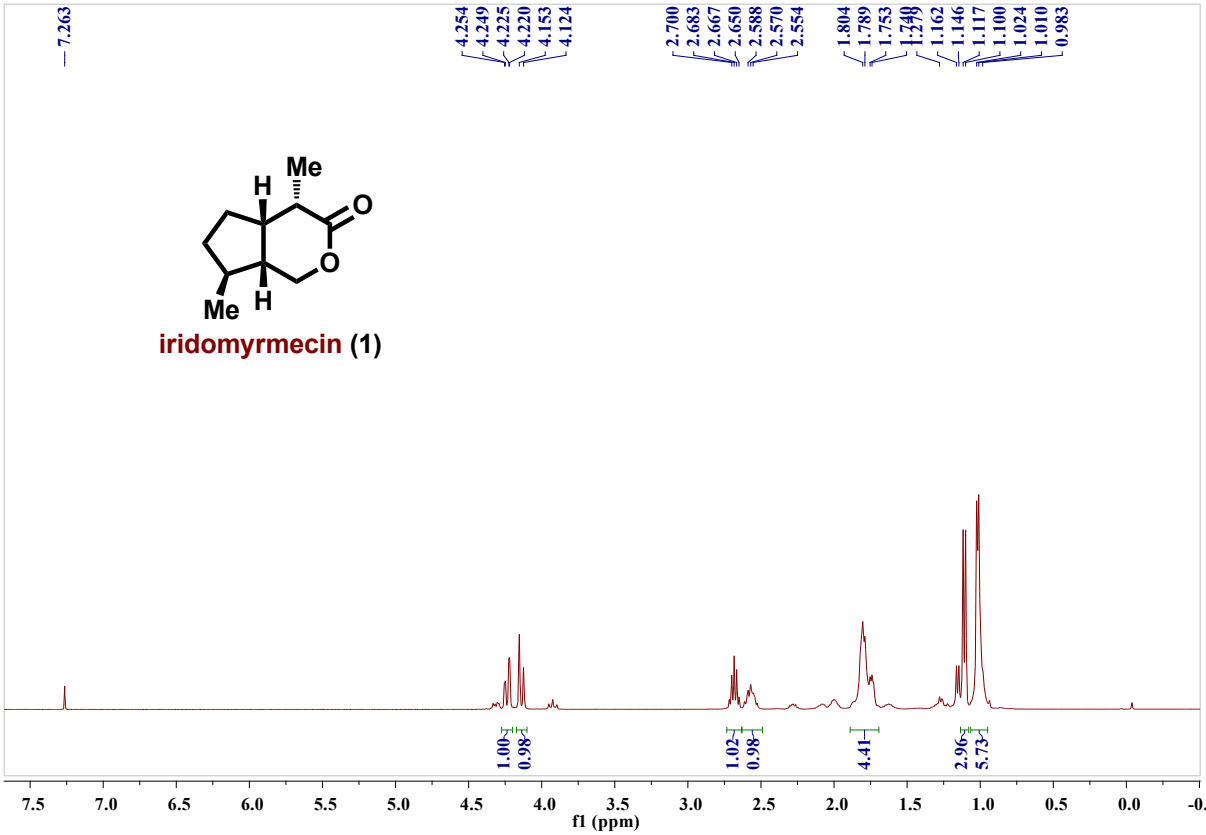

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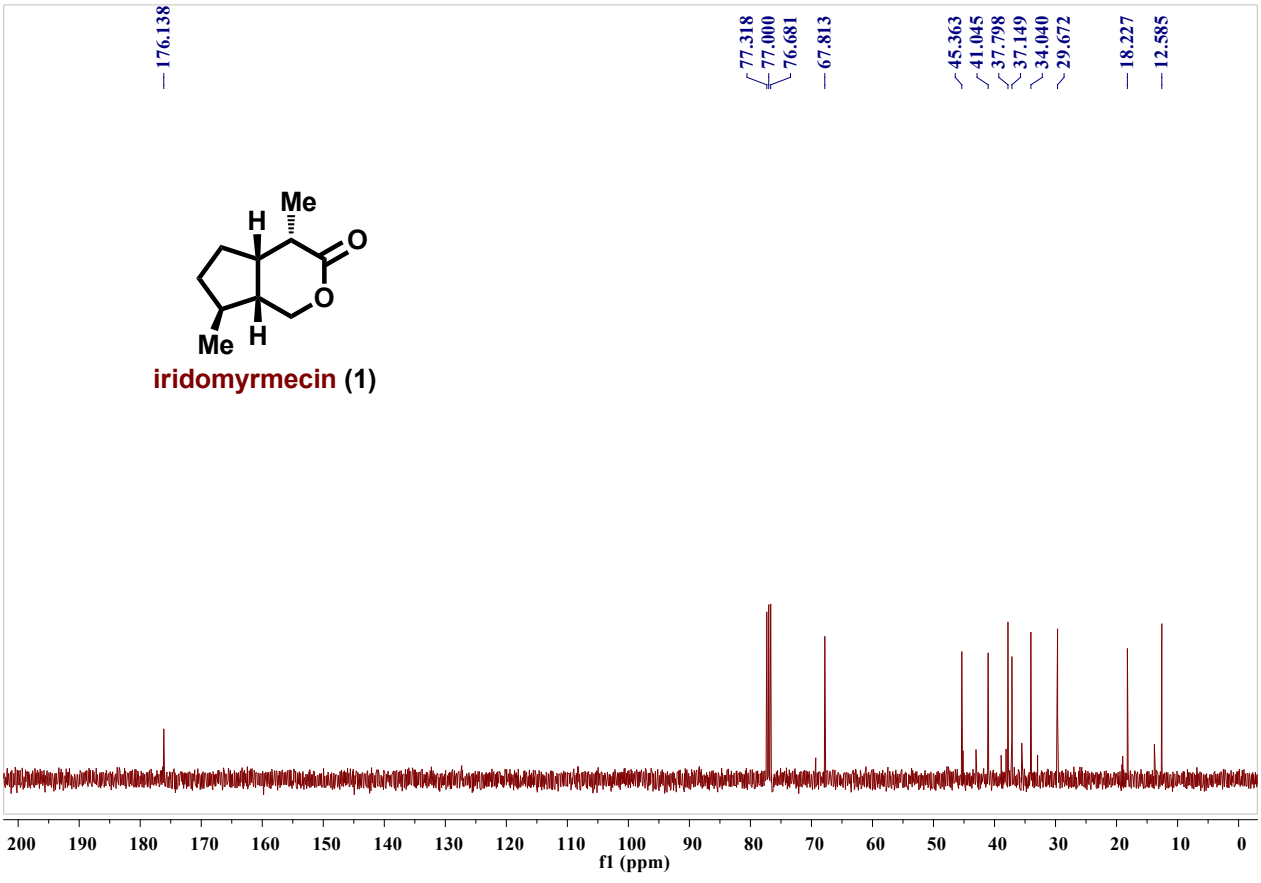

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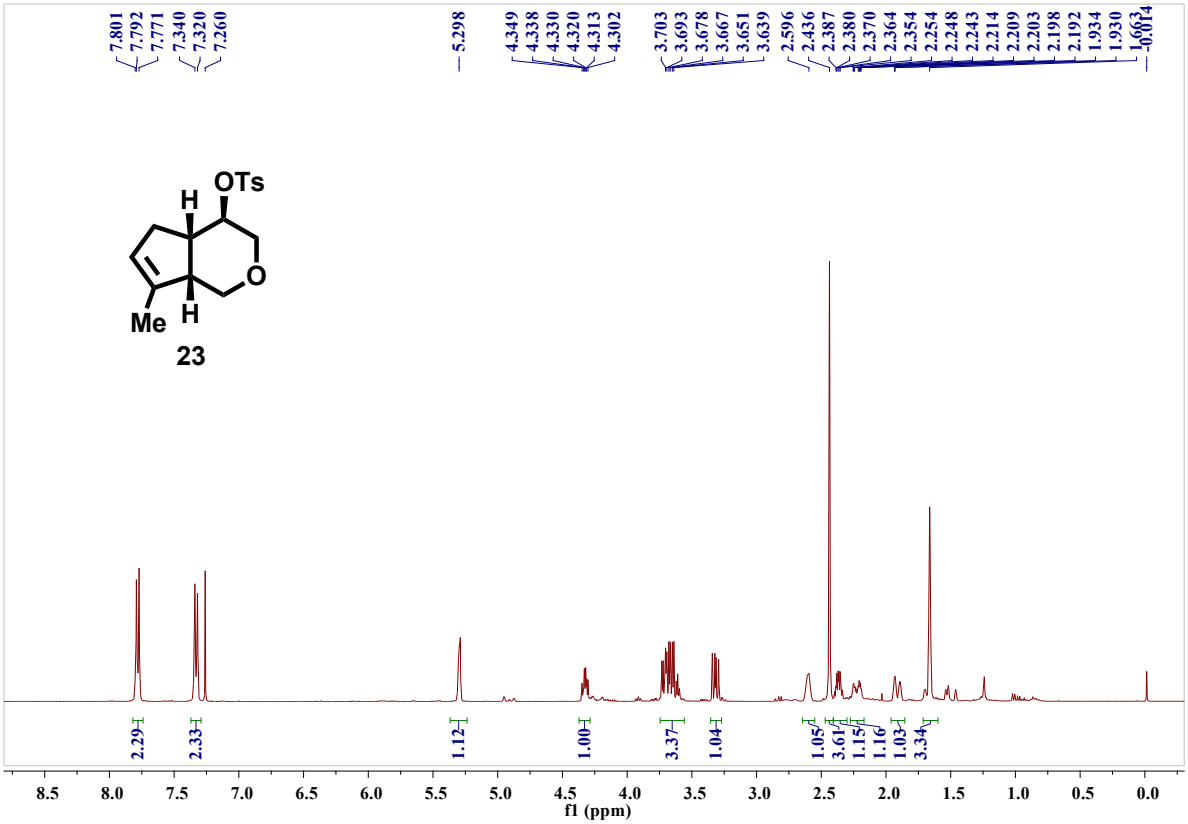
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OTs
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O
Me
H
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1.15
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1.03
3.34
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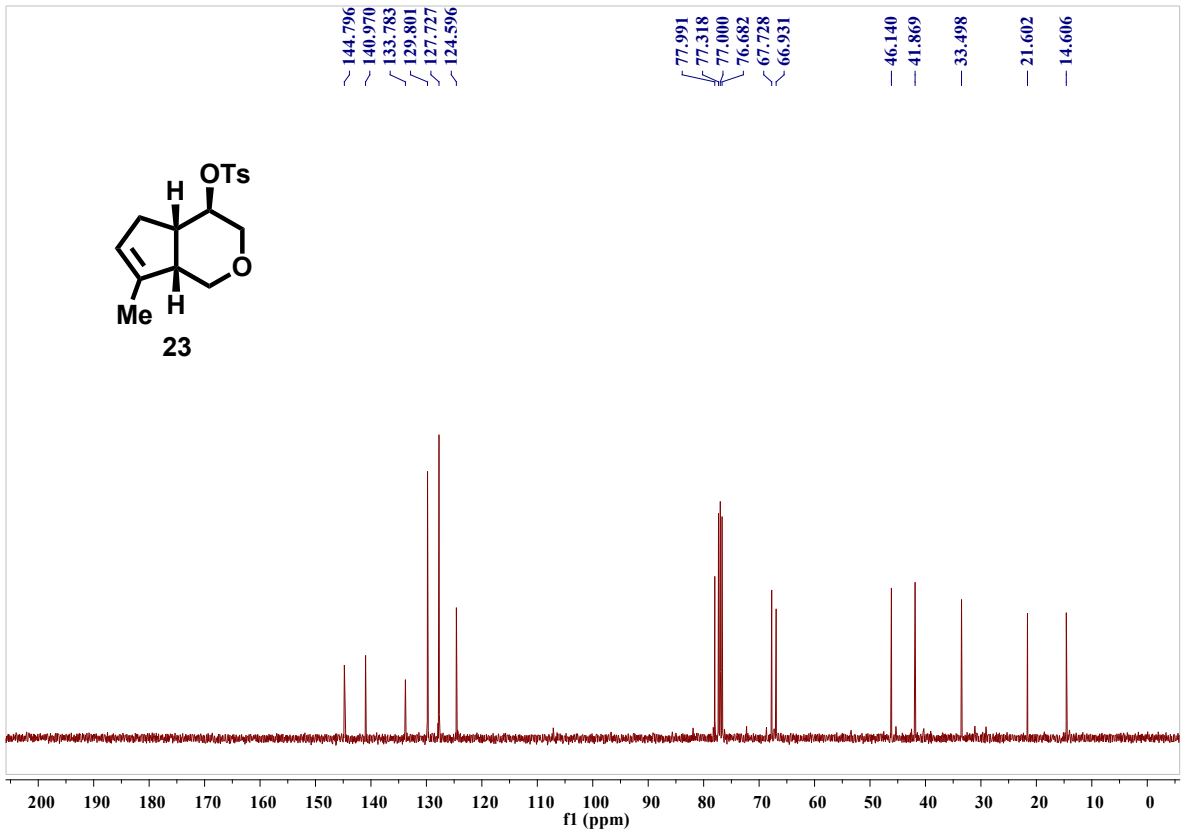
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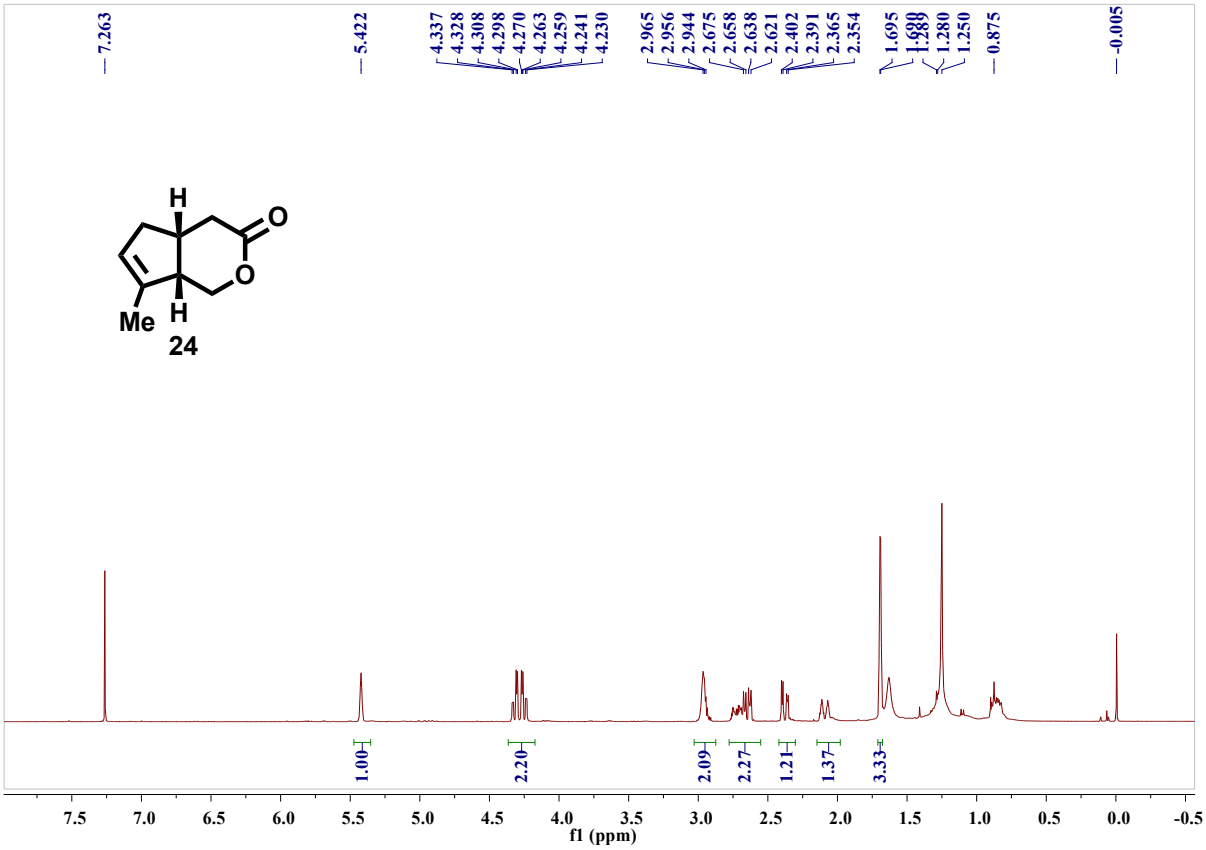
f1 (ppm)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Me
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1.37
3.33
7.5
7.0
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6.0
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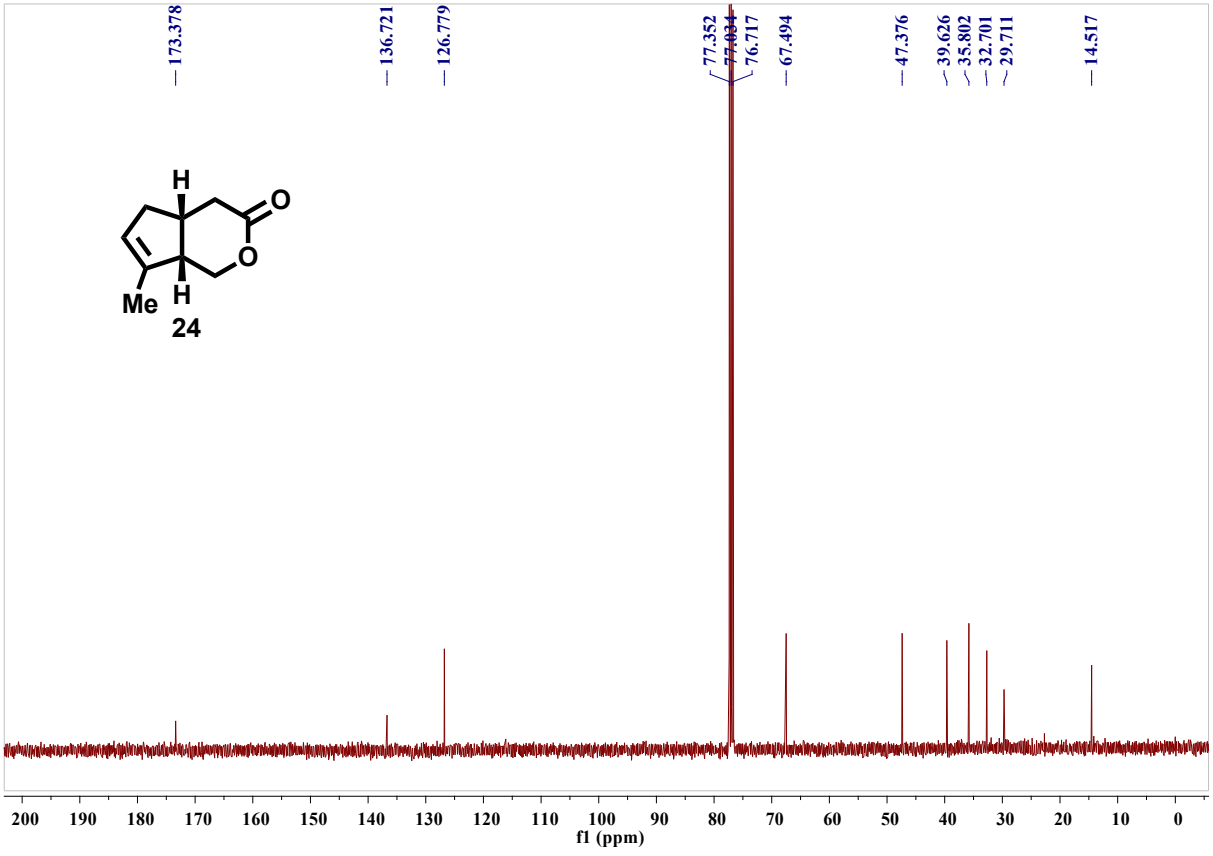
f1 (ppm)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H
O
O
Me
H
24
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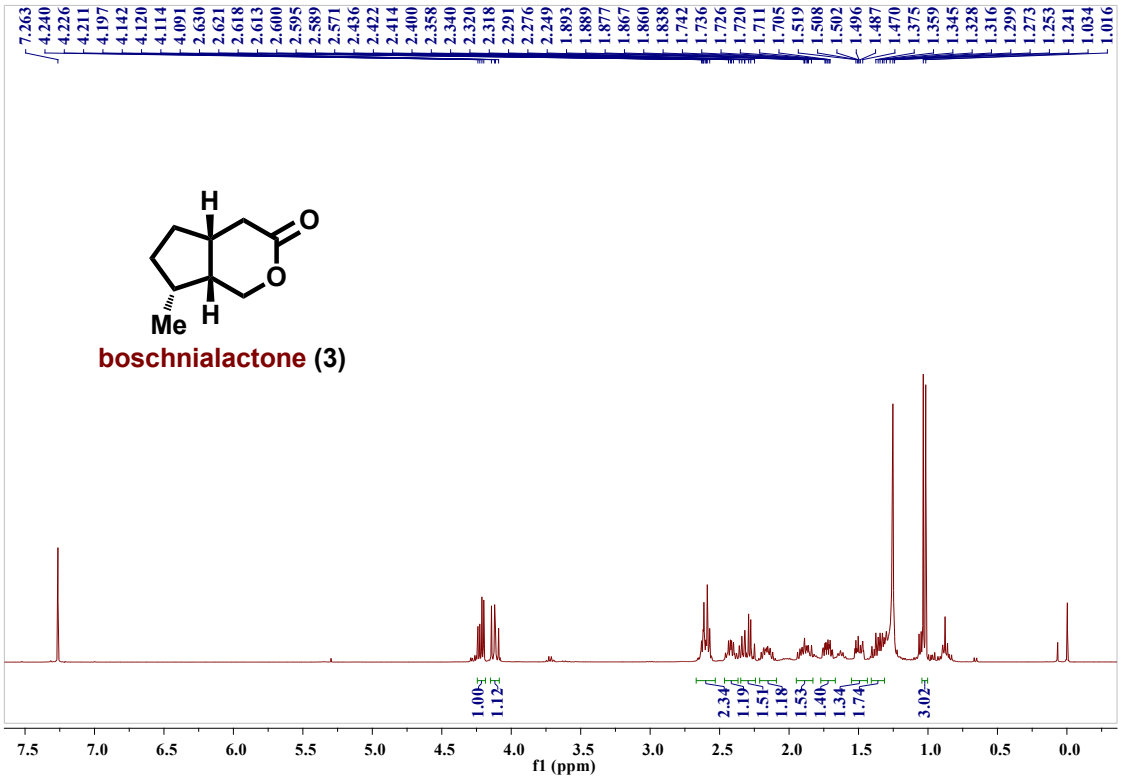
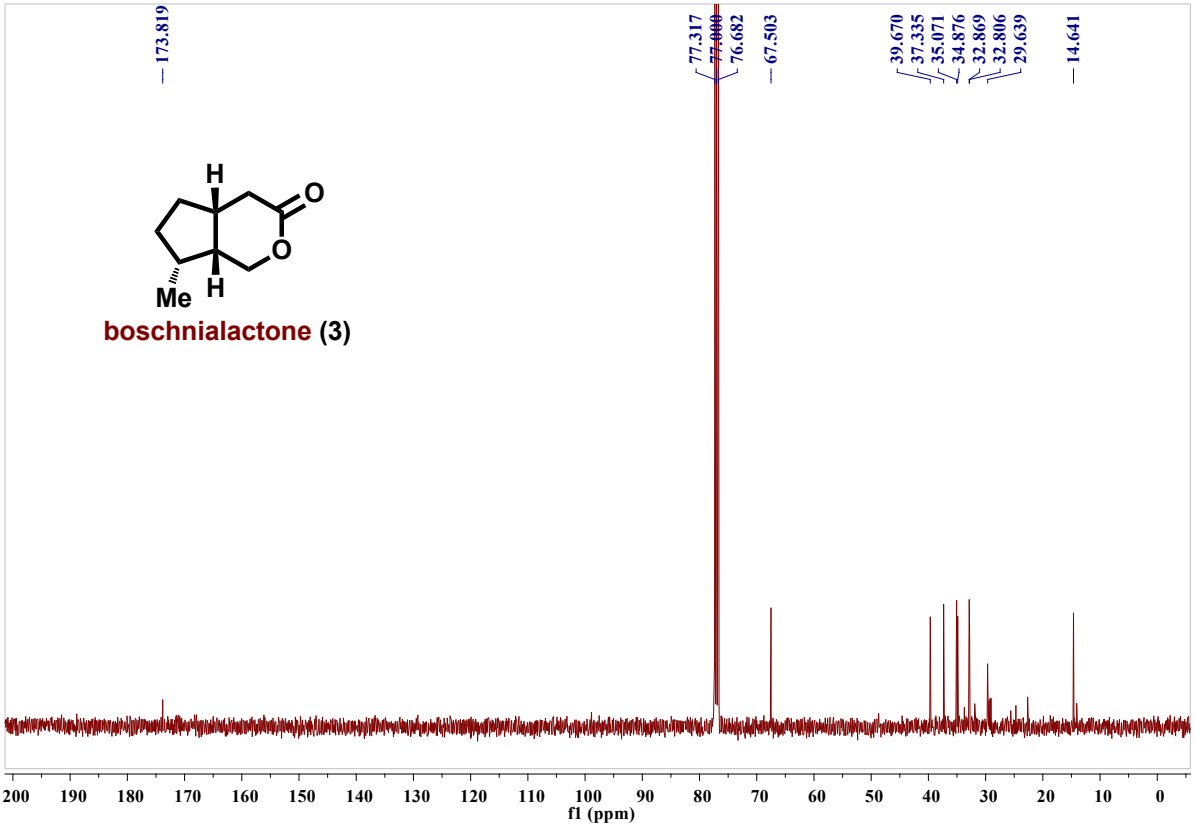
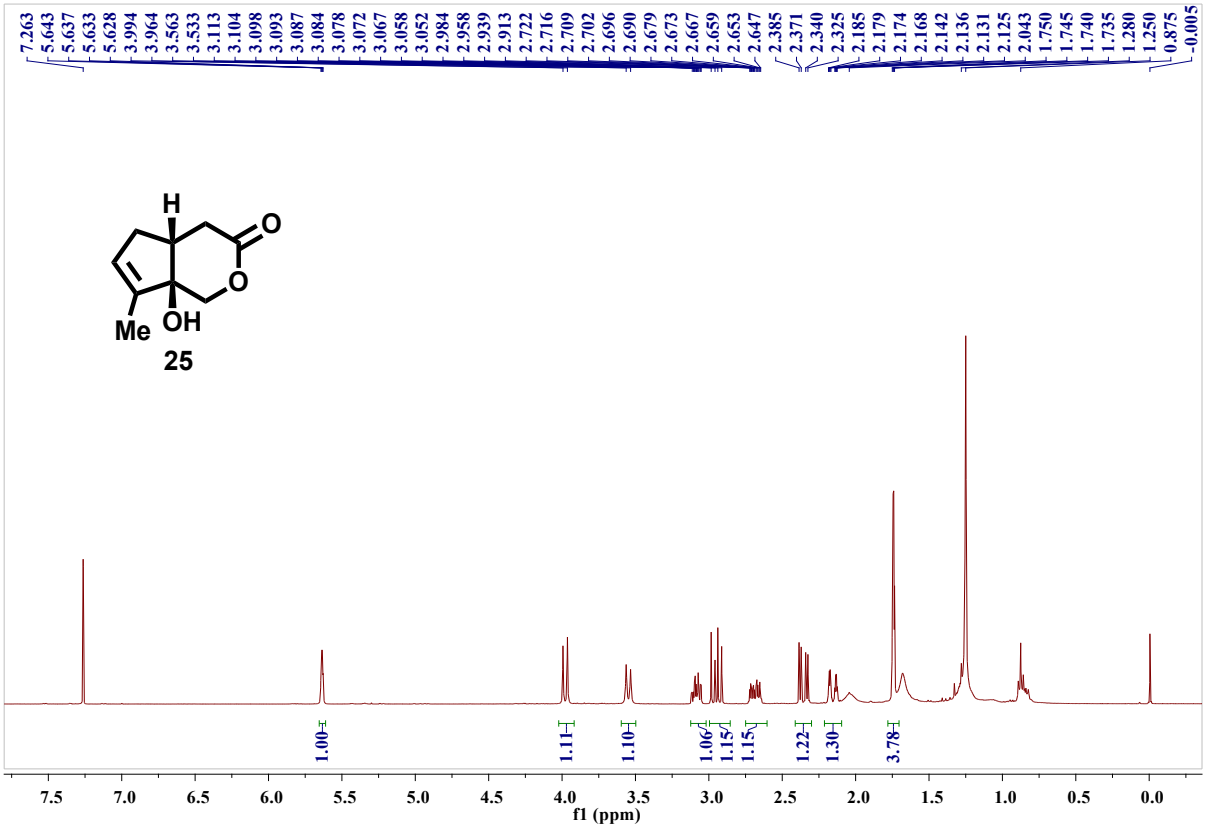
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

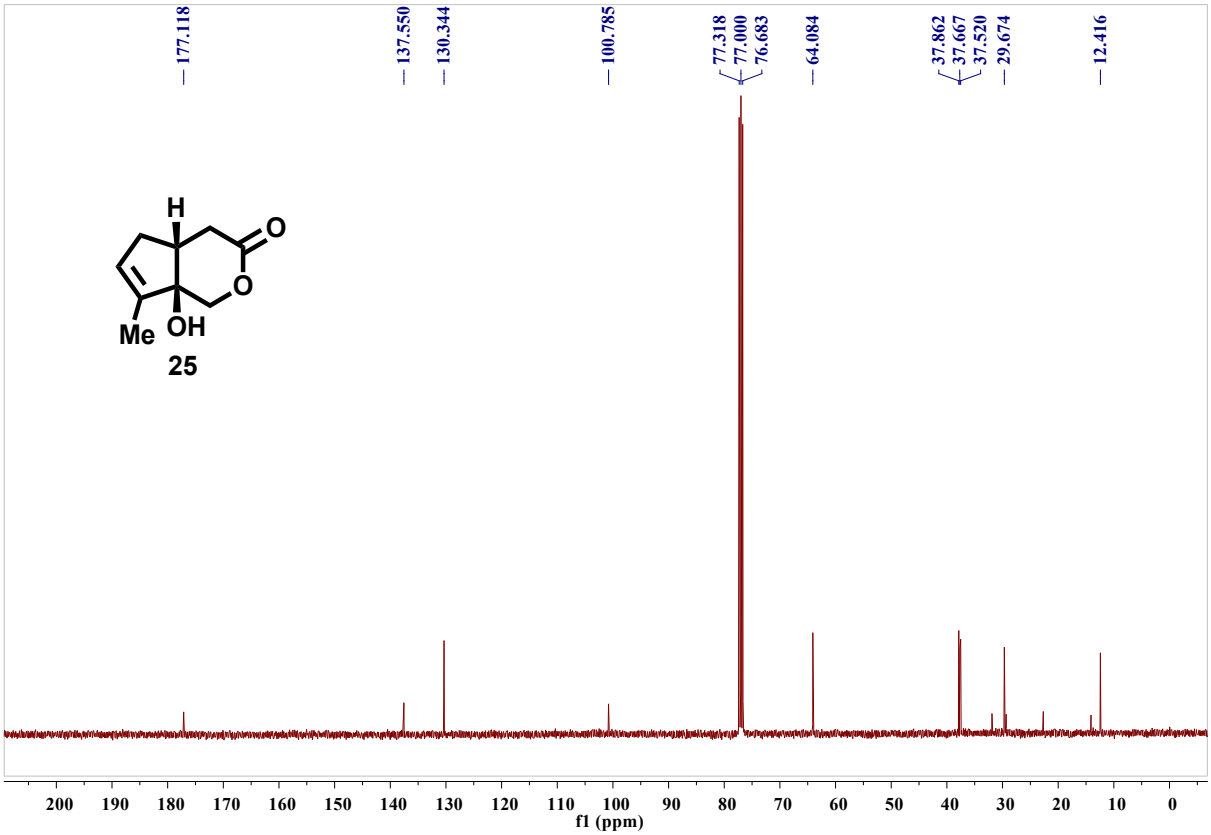


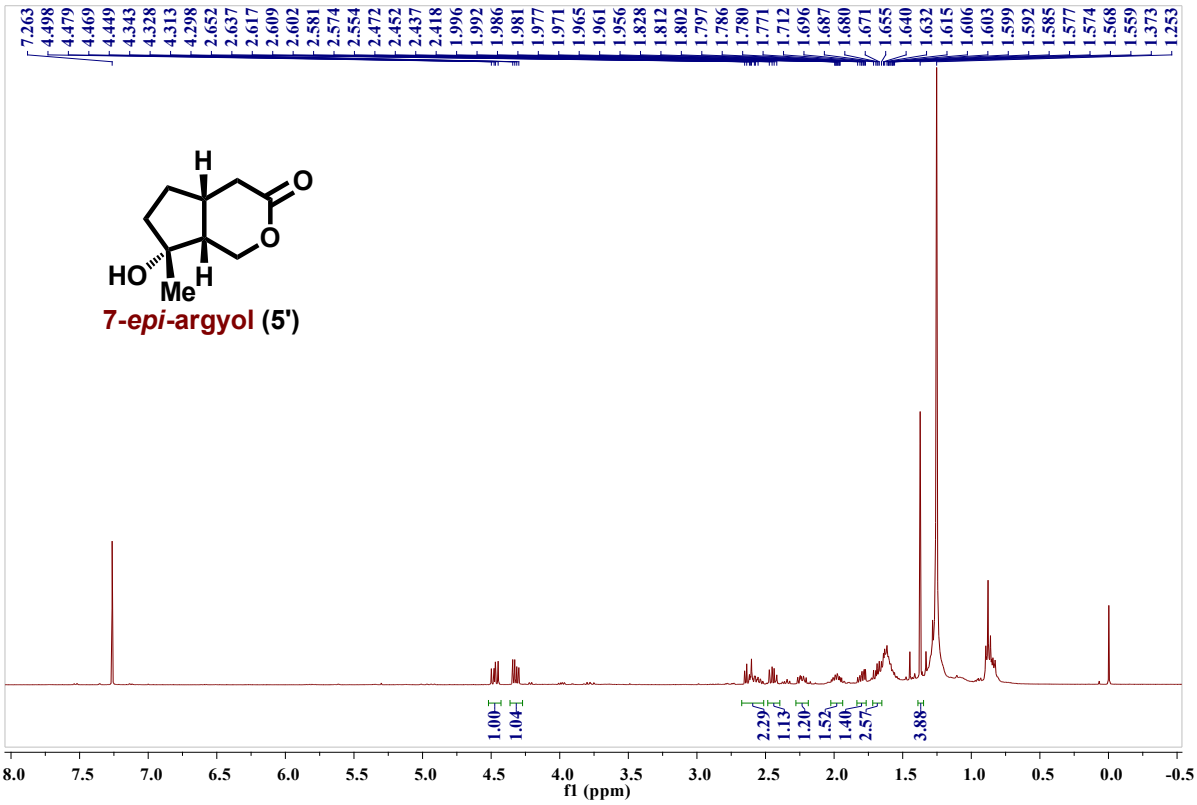
boschnialactone (3)

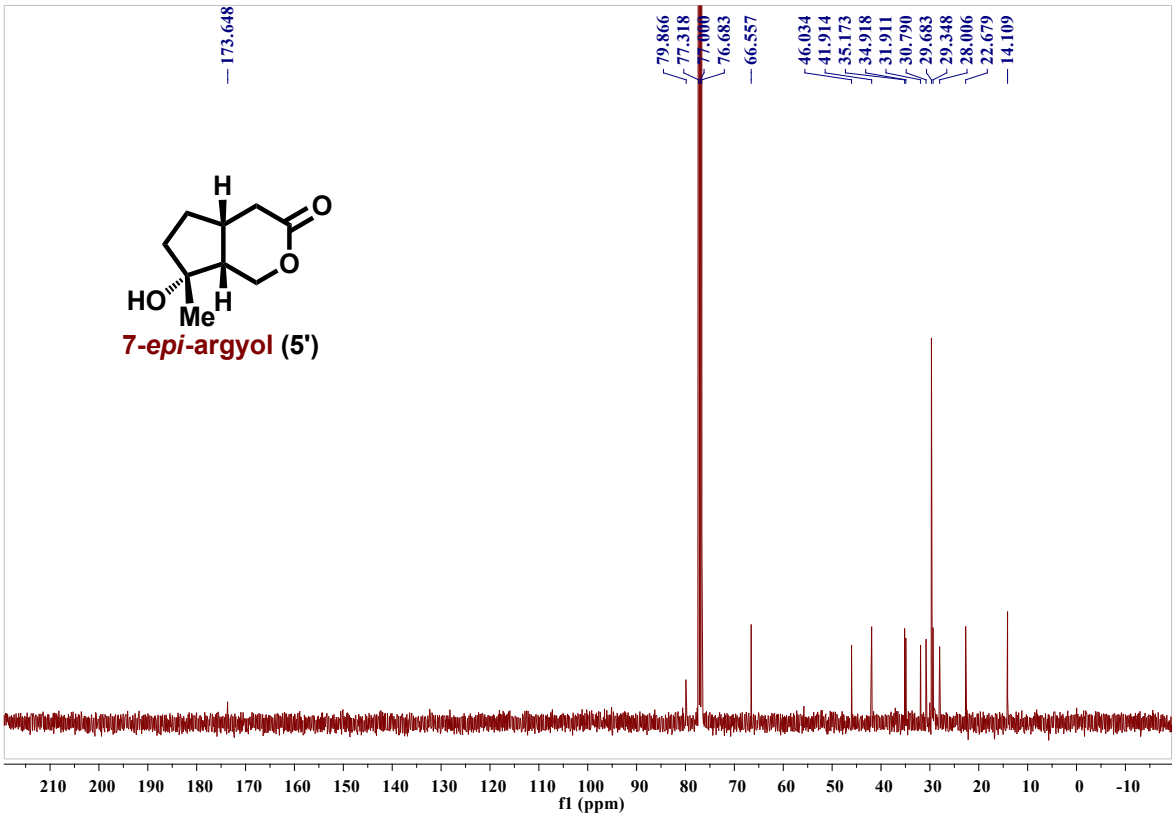


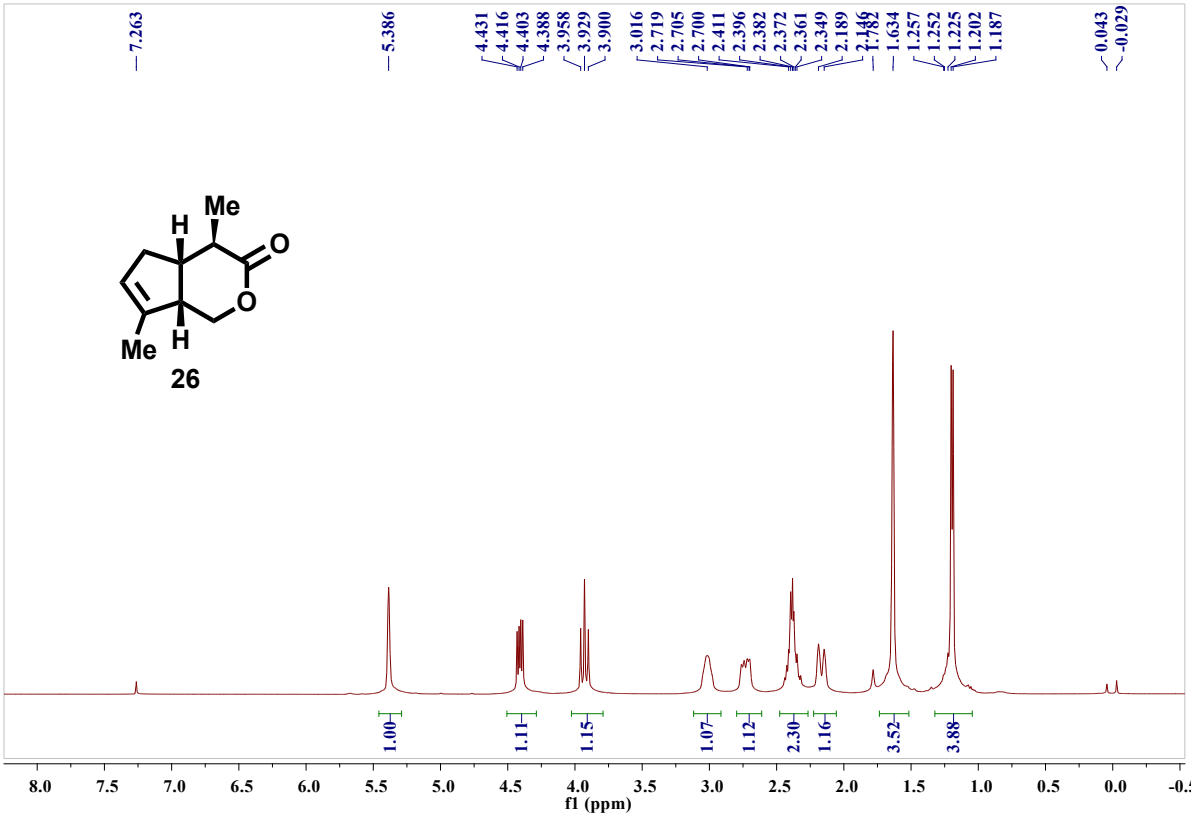
boschnialactone (3)

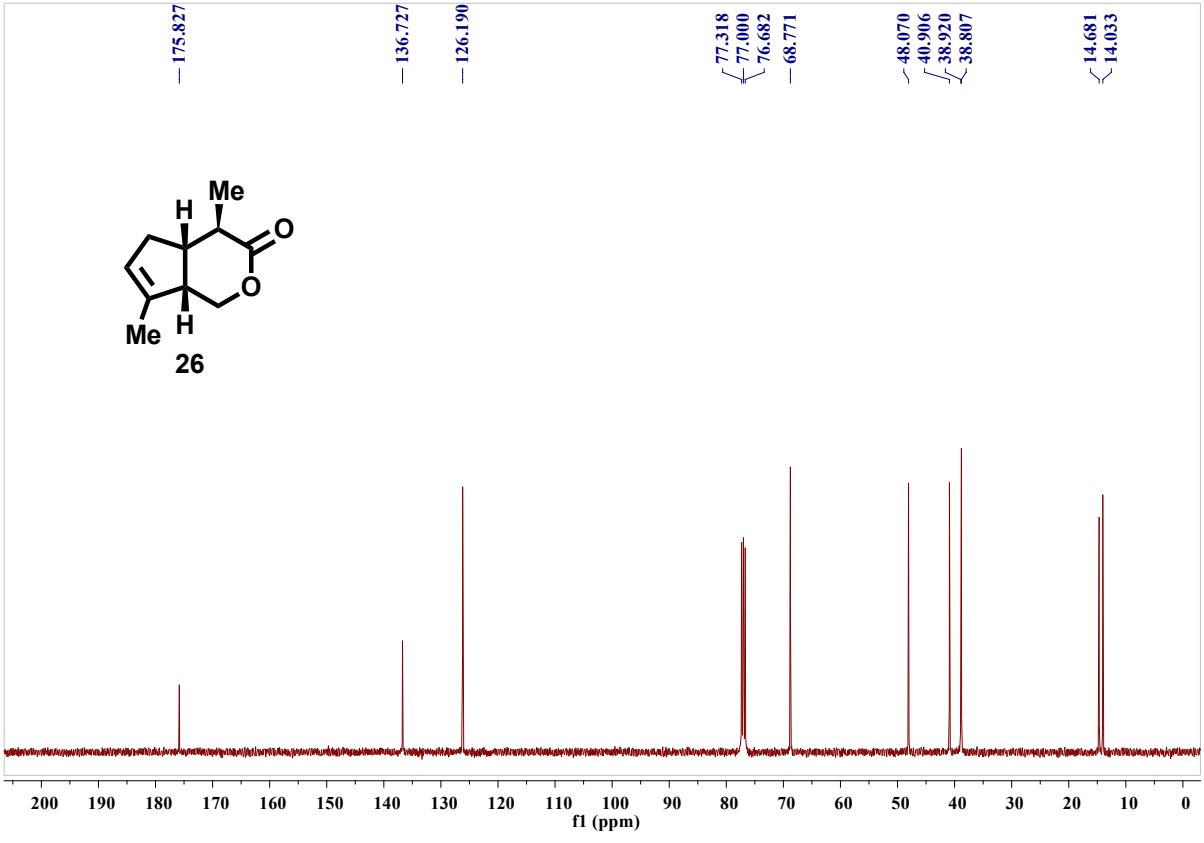

7.263
5.643
5.637
5.633
5.628
3.994
3.964
3.563
3.533
3.113
3.104
3.098
3.093
3.087
3.084
3.078
3.072
3.067
3.058
3.052
2.984
2.958
2.939
2.913
2.722
2.716
2.709
2.702
2.696
2.690
2.679
2.673
2.667
2.659
2.653
2.647
2.385
2.371
2.340
2.325
2.185
2.179
2.174
2.168
2.142
2.136
2.131
2.125
2.043
1.750
1.745
1.740
1.735
1.280
1.250
0.875
-0.005
H
O
O
Me
OH
25
1.00
1.11
1.10
1.06
1.15
1.15
1.22
1.30
3.78
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

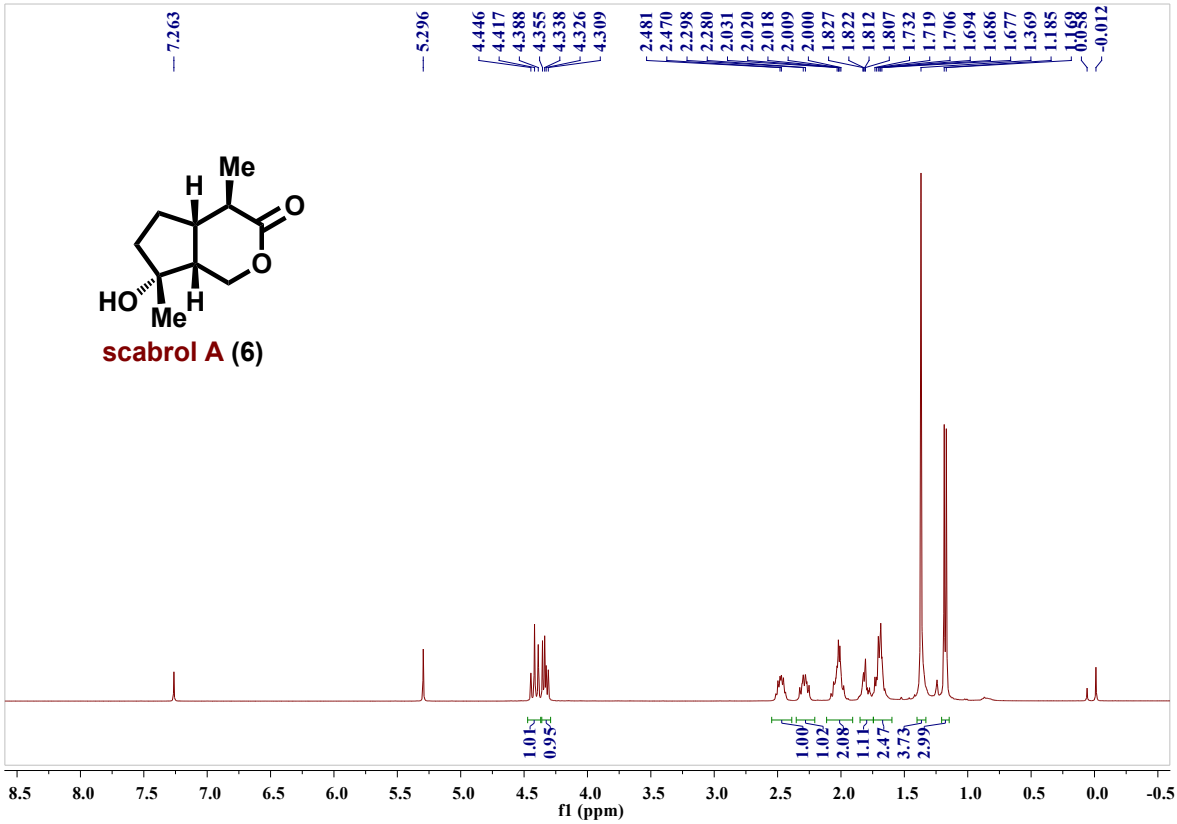

177.118
137.550
130.344
100.785
77.318
77.000
76.683
64.084
37.862
37.667
37.520
29.674
12.416
H
O
O
Me
OH
25
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

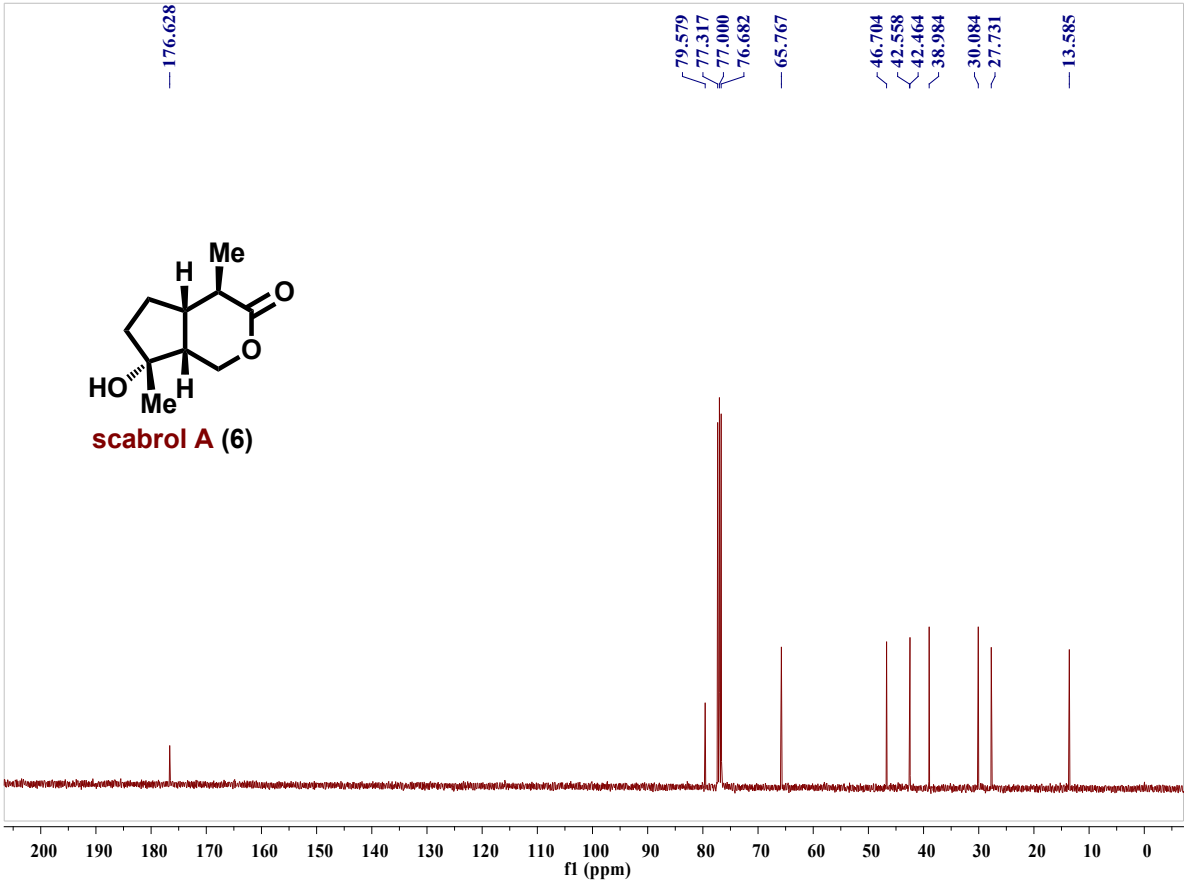

7.263
4.498
4.479
4.469
4.449
4.343
4.328
4.313
4.298
2.652
2.637
2.617
2.609
2.602
2.581
2.574
2.554
2.472
2.452
2.437
2.418
1.996
1.992
1.986
1.981
1.977
1.971
1.965
1.961
1.956
1.828
1.812
1.802
1.797
1.786
1.780
1.771
1.712
1.696
1.687
1.680
1.671
1.655
1.640
1.632
1.615
1.606
1.603
1.599
1.592
1.585
1.577
1.574
1.568
1.559
1.373
1.253
H
O
O
HO
Me
H
7-epi-argyol (5')
1.00
1.04
2.29
1.13
1.20
1.52
1.40
2.57
3.88
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

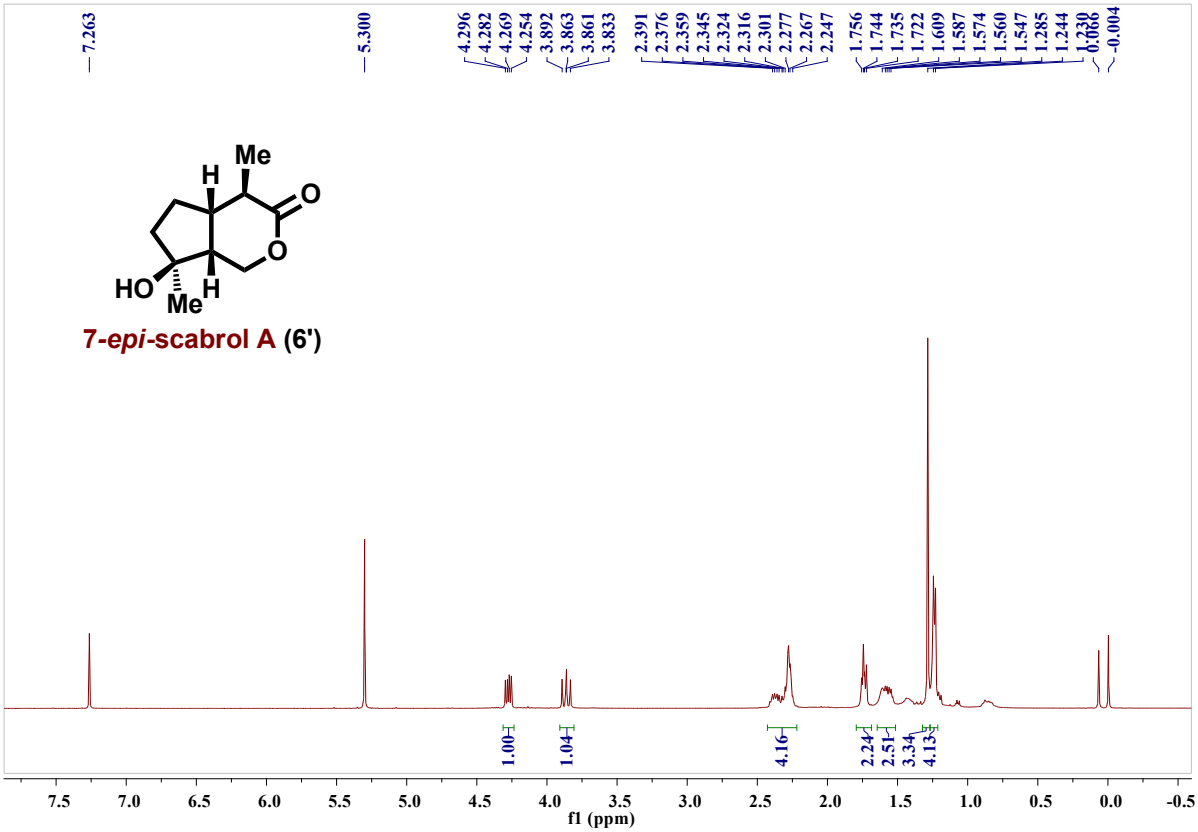

173.648
79.866
77.318
77.000
76.683
66.557
46.034
41.914
35.173
34.918
31.911
30.790
29.683
29.348
28.006
22.679
14.109
H
O
O
HO
Me
H
7-epi-argyol (5')
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

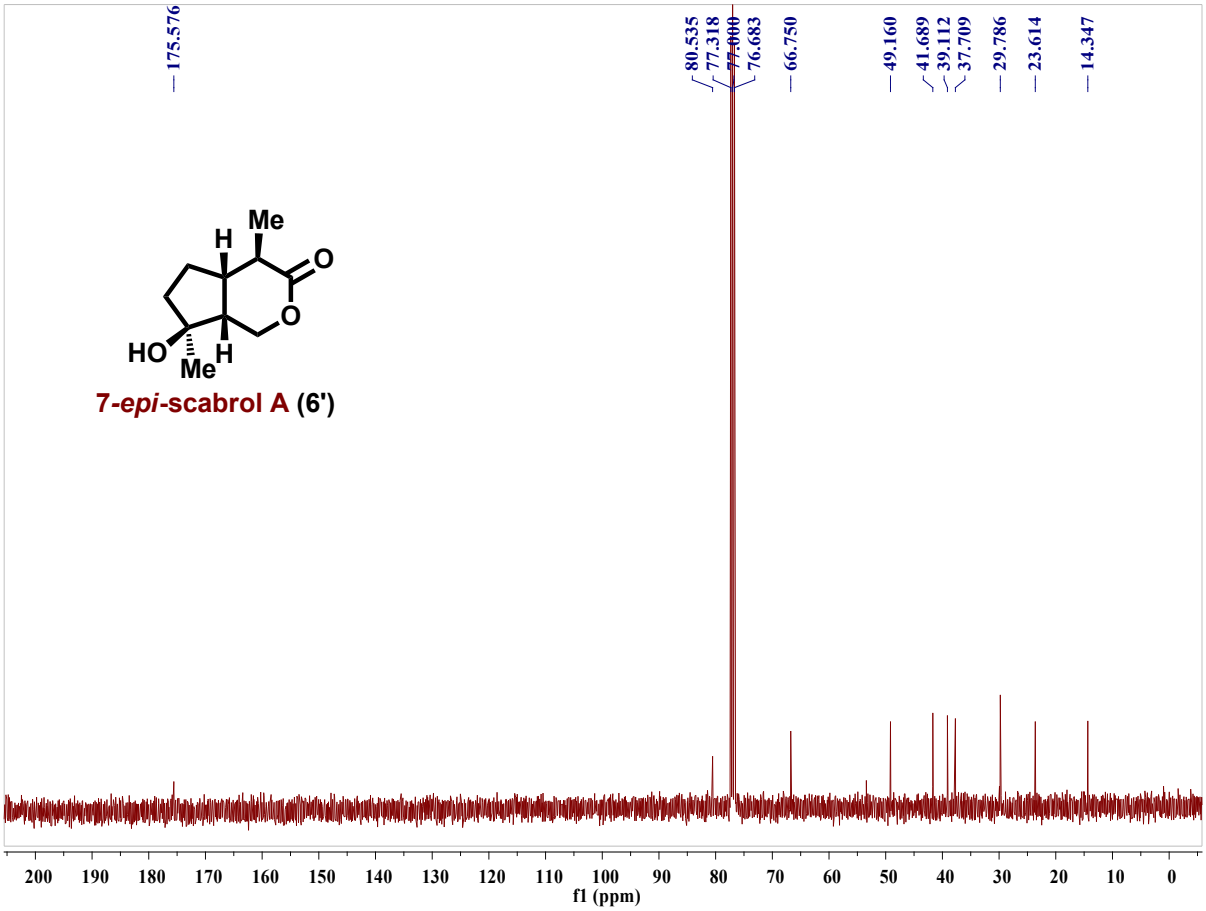

7.263
5.386
4.431
4.416
4.403
4.388
3.958
3.929
3.900
3.016
2.719
2.705
2.700
2.411
2.396
2.382
2.372
2.361
2.349
2.189
2.146
1.782
1.634
1.257
1.252
1.225
1.202
1.187
0.043
-0.029
Me
H
O
O
Me
H
26
1.00
1.11
1.15
1.07
1.12
2.30
1.16
3.52
3.88
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

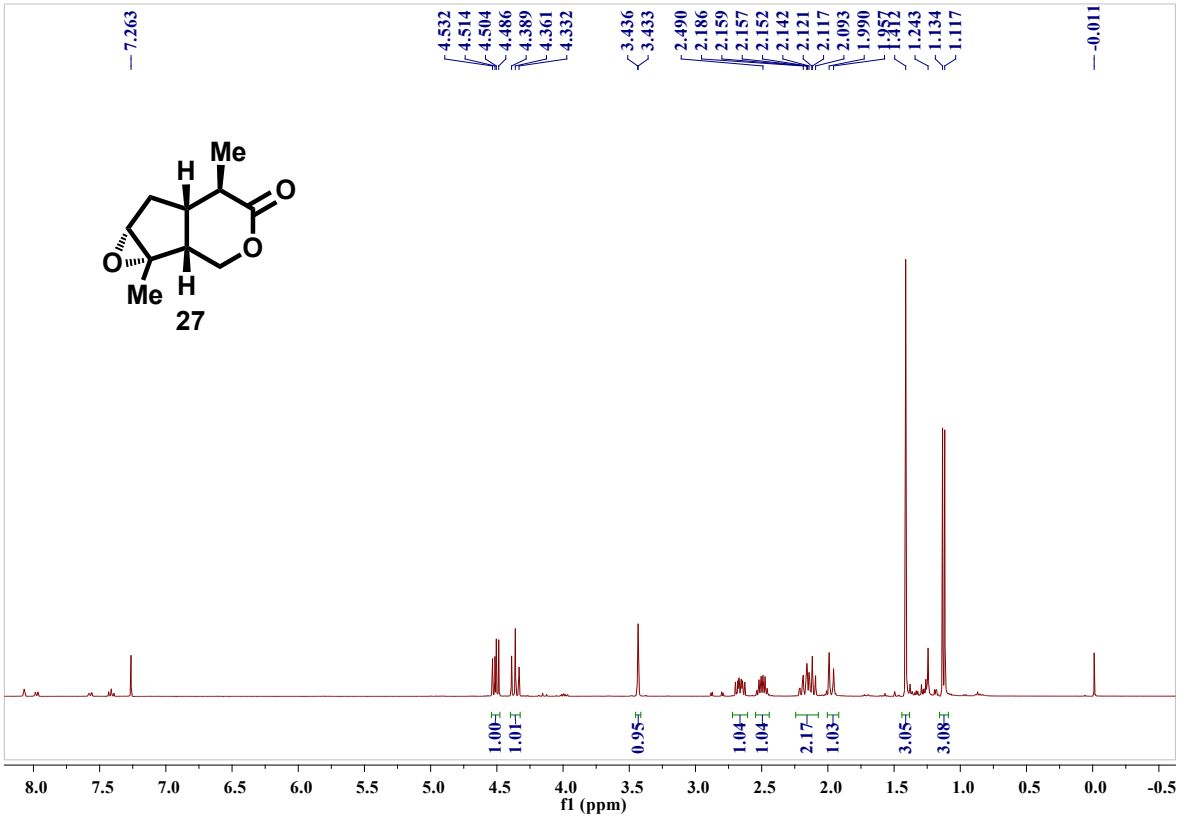

175.827
136.727
126.190
77.318
77.000
76.682
68.771
48.070
40.906
38.920
38.807
14.681
14.033
Me
H
O
O
Me
H
26
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

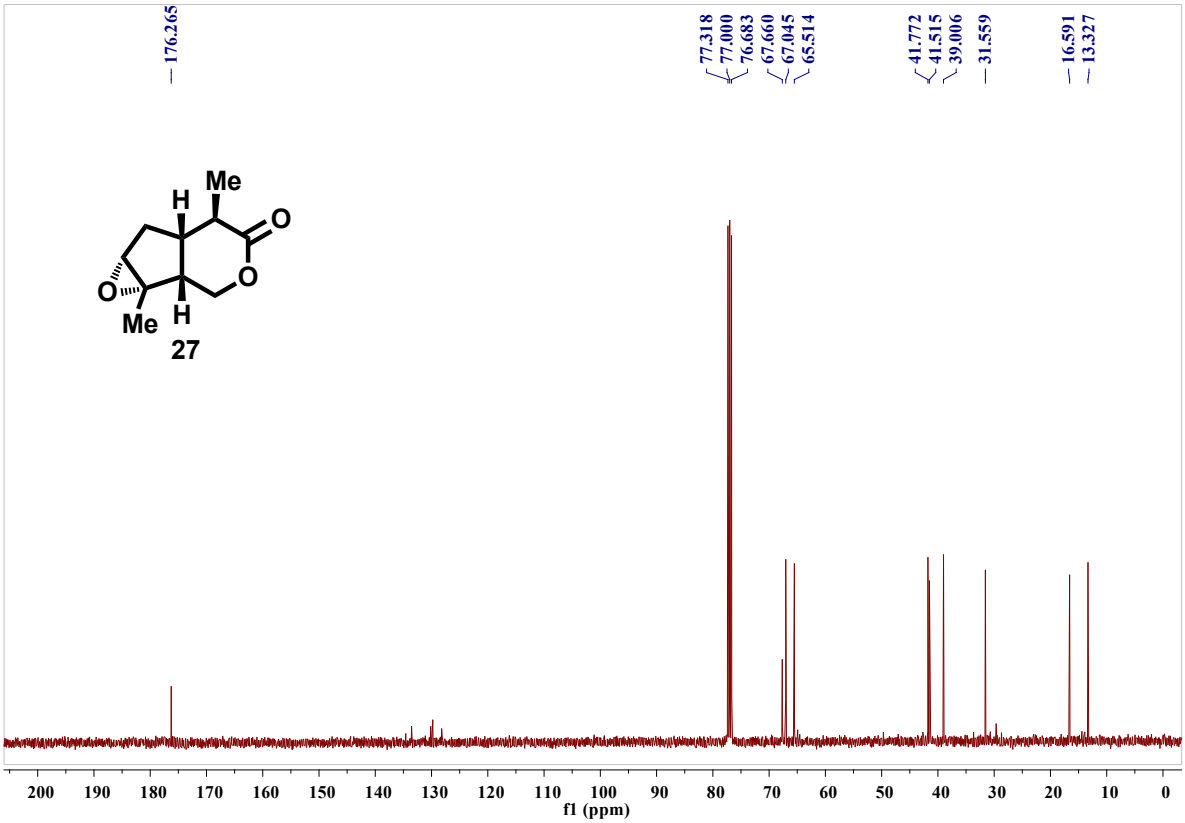

7.263
5.296
4.446
4.417
4.388
4.355
4.338
4.326
4.309
2.481
2.470
2.298
2.280
2.031
2.020
2.018
2.009
2.000
1.827
1.822
1.812
1.807
1.732
1.719
1.706
1.694
1.686
1.677
1.369
1.185
0.058
-0.012
Me
H
O
O
HO
Me
H
scabrol A (6)
1.01
0.95
1.00
1.02
2.08
1.11
2.47
3.73
2.99
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

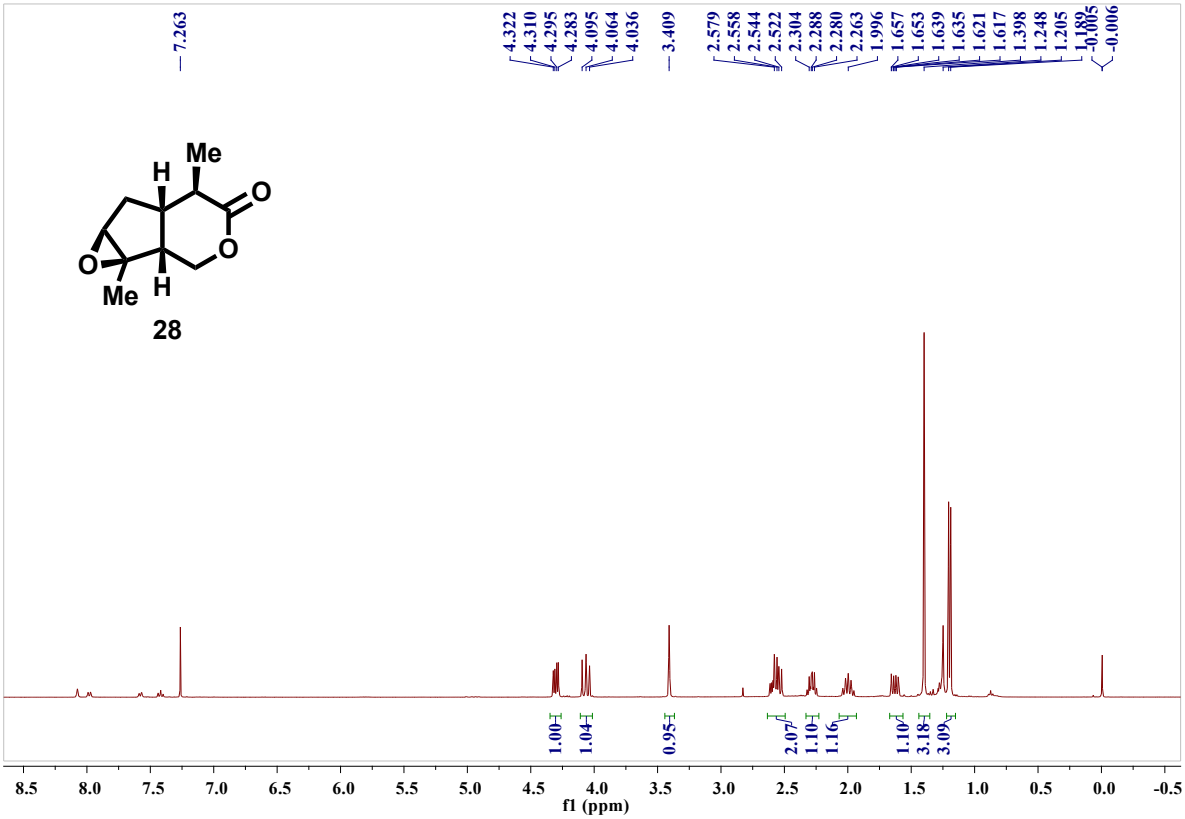

176.628
79.579
77.317
77.000
76.682
65.767
46.704
42.558
42.464
38.984
30.084
27.731
13.585
Me
H
O
O
HO
Me
H
scabrol A (6)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

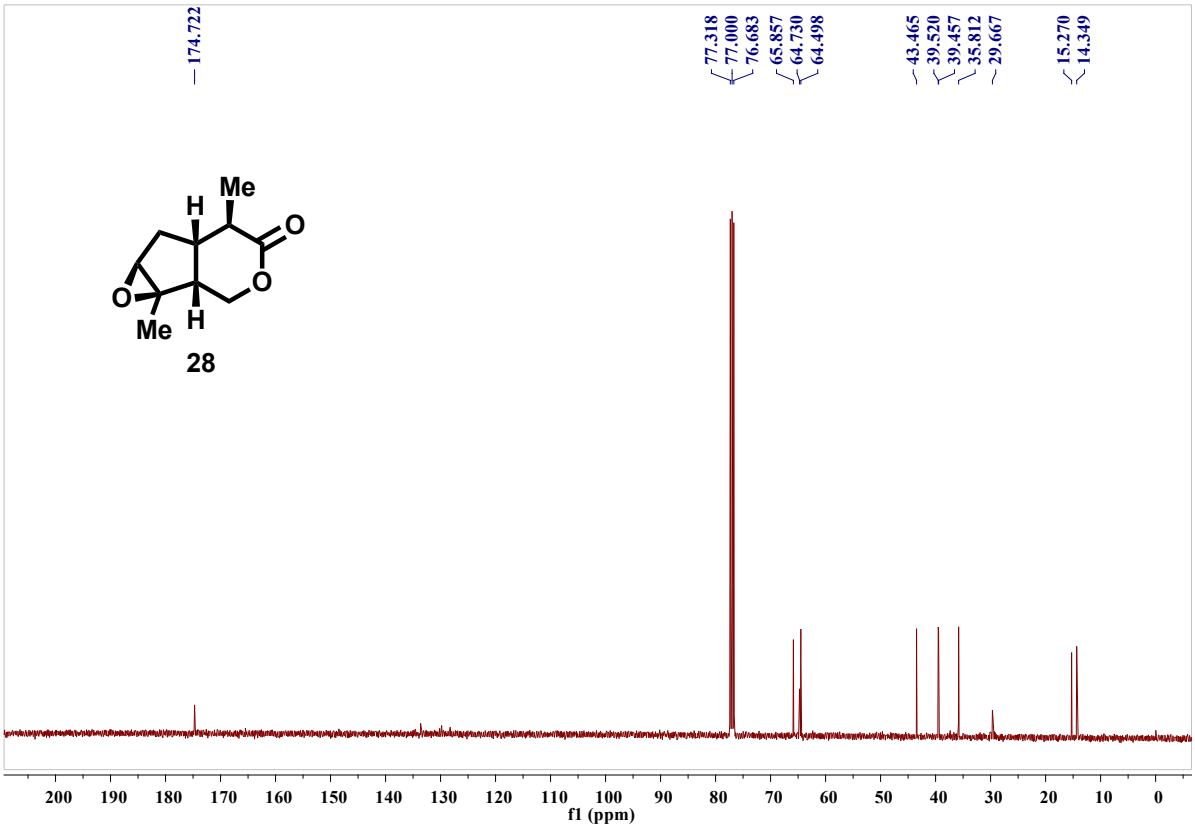

7.263
5.300
4.296
4.282
4.269
4.254
3.892
3.863
3.861
3.833
2.391
2.376
2.359
2.345
2.324
2.316
2.301
2.277
2.267
2.247
1.756
1.744
1.735
1.722
1.609
1.587
1.574
1.560
1.547
1.285
1.244
1.230
0.066
-0.004
Me
H
O
O
HO
H
Me
7-epi-scabrol A (6')
1.00
1.04
4.16
2.24
2.51
3.34
4.13
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

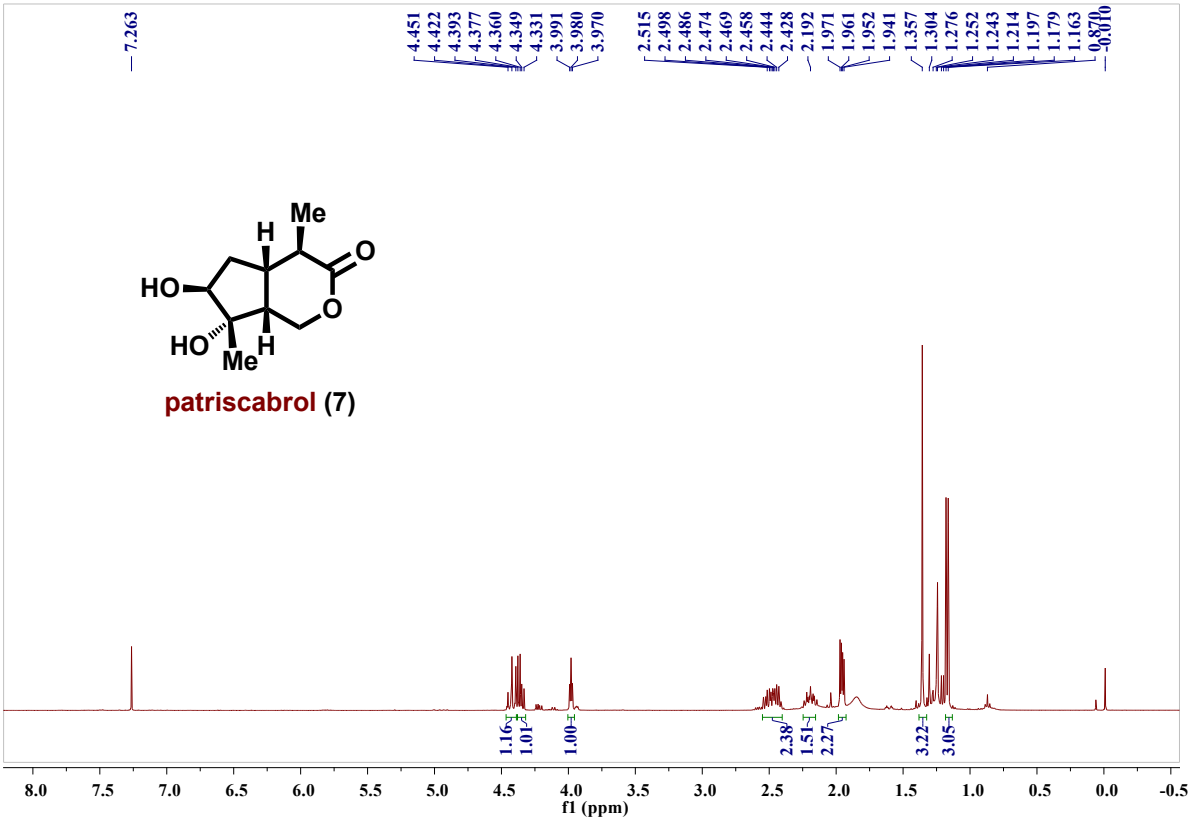

175.576
80.535
77.318
77.000
76.683
66.750
49.160
41.689
39.112
37.709
29.786
23.614
14.347
Me
H
O
O
HO
Me
H
7-epi-scabrol A (6')
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

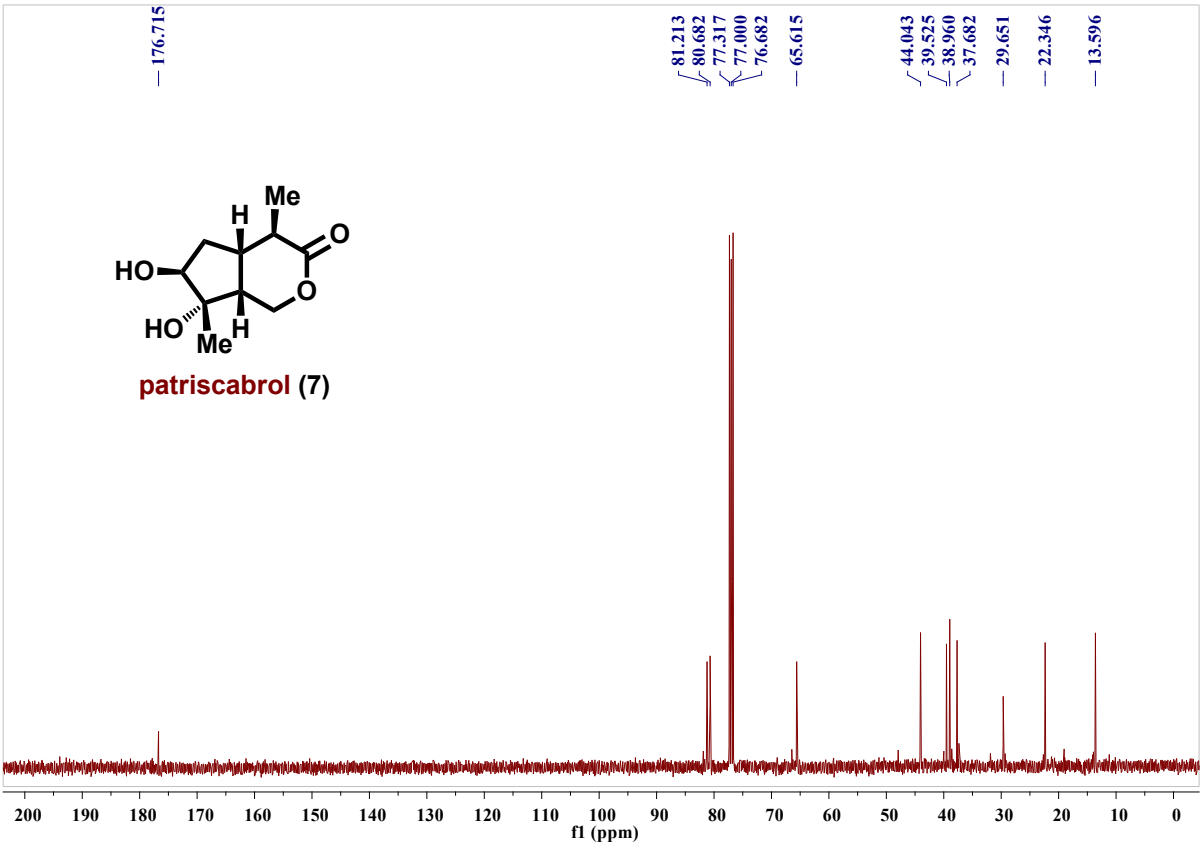

7.263
4.532
4.514
4.504
4.486
4.389
4.361
4.332
3.436
3.433
2.490
2.186
2.159
2.157
2.152
2.142
2.121
2.117
2.093
1.990
1.957
1.412
1.243
1.134
1.117
-0.011
Me
H
O
O
O
Me
H
27
1.00
1.01
0.95
1.04
1.04
2.17
1.03
3.05
3.08
f1 (ppm)

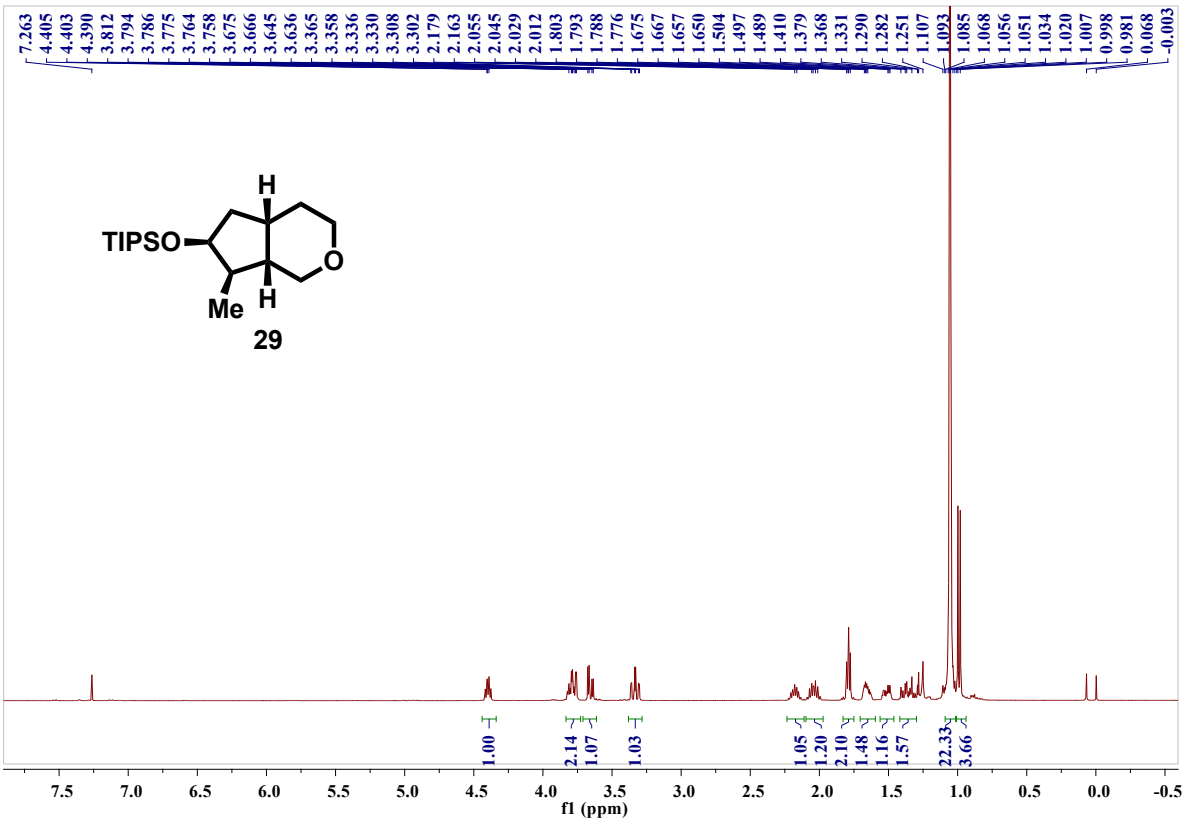

176.265
77.318
77.000
76.683
67.660
67.045
65.514
41.772
41.515
39.006
31.559
16.591
13.327
Me
H
O
O
O
Me
H
27
f1 (ppm)

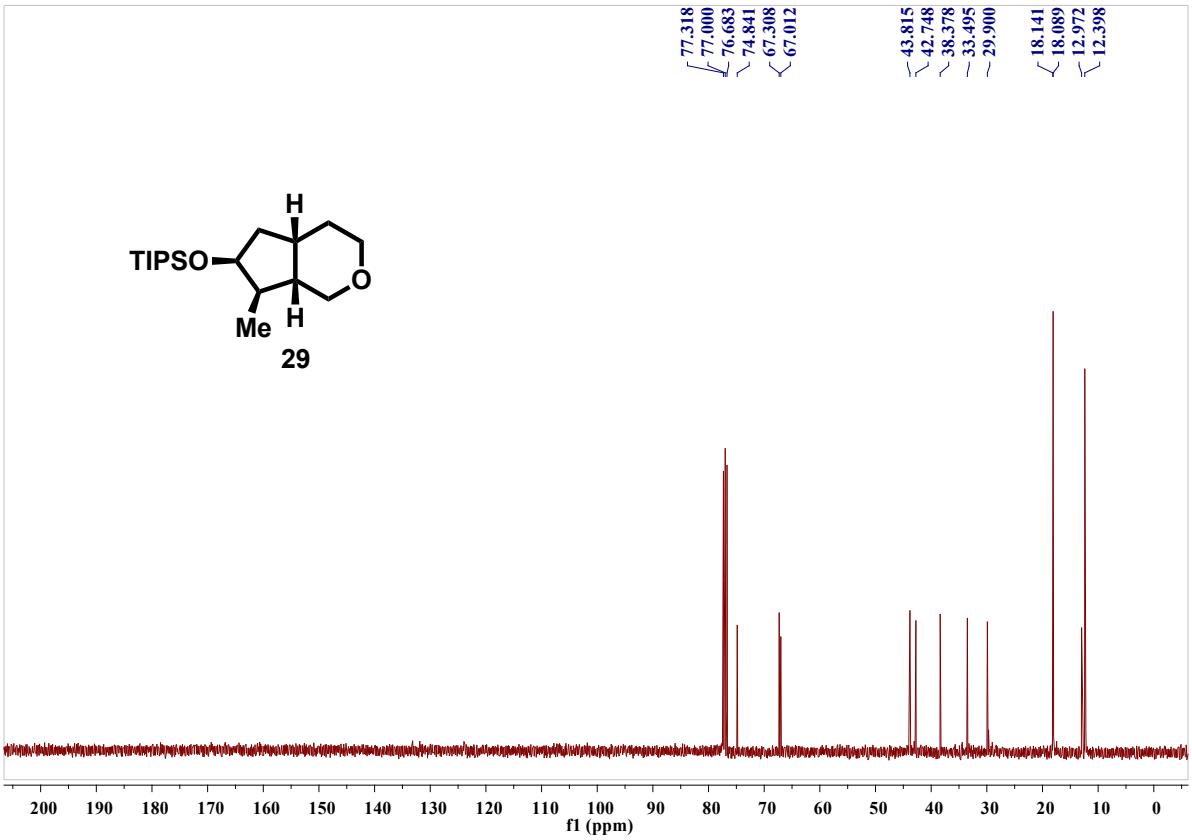

7.263
4.322
4.310
4.295
4.283
4.095
4.064
4.036
3.409
2.579
2.558
2.544
2.522
2.304
2.288
2.280
2.263
1.996
1.657
1.653
1.639
1.635
1.621
1.617
1.398
1.248
1.205
1.189
0.005
-0.006
Me
H
O
O
Me
H
28
1.00
1.04
0.95
2.07
1.10
1.16
1.10
3.18
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


174.722
77.318
77.000
76.683
65.857
64.730
64.498
43.465
39.520
39.457
35.812
29.667
15.270
14.349
Me
H
O
O
Me
H
28
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.263
4.451
4.422
4.393
4.377
4.360
4.349
4.331
3.991
3.980
3.970
2.515
2.498
2.486
2.474
2.469
2.458
2.444
2.428
2.192
1.971
1.961
1.952
1.941
1.357
1.304
1.276
1.252
1.243
1.214
1.197
1.179
1.163
0.870
0.010
Me
H
O
HO
O
HO
Me
H
patriscabrol (7)
1.16
1.01
1.00
2.38
1.51
2.27
3.22
3.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


176.715
81.213
80.682
77.317
77.000
76.682
65.615
44.043
39.525
38.960
37.682
29.651
22.346
13.596
Me
H
O
HO
O
HO
Me
H
patriscabrol (7)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.263
4.405
4.403
4.390
3.812
3.794
3.786
3.775
3.764
3.758
3.675
3.666
3.645
3.636
3.365
3.358
3.336
3.330
3.308
3.302
2.179
2.163
2.055
2.045
2.029
2.012
1.803
1.793
1.788
1.776
1.675
1.667
1.657
1.650
1.504
1.497
1.489
1.410
1.379
1.368
1.331
1.290
1.282
1.251
1.107
1.093
1.085
1.068
1.056
1.051
1.034
1.020
1.007
0.998
0.981
0.068
-0.003
TIPSO
H
O
Me
H
29
1.00
2.14
1.07
1.03
1.05
1.20
2.10
1.48
1.16
1.57
22.33
3.66
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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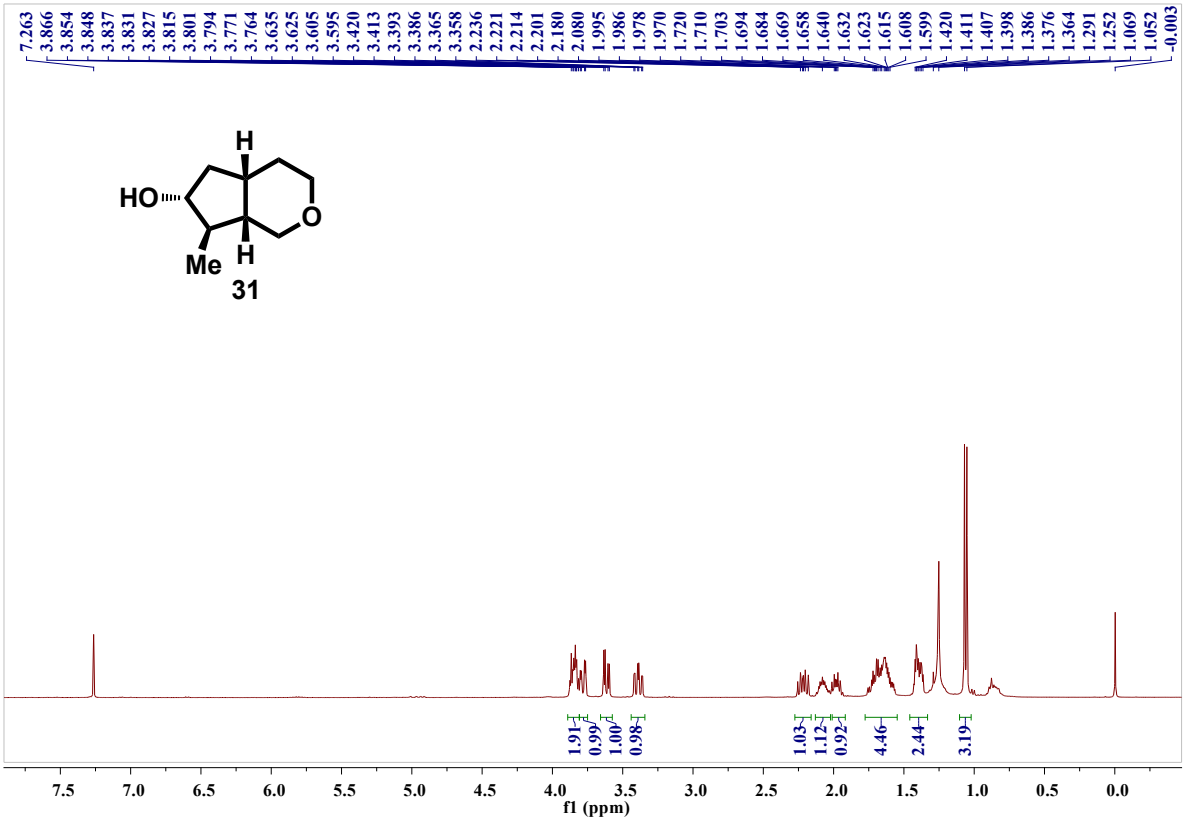
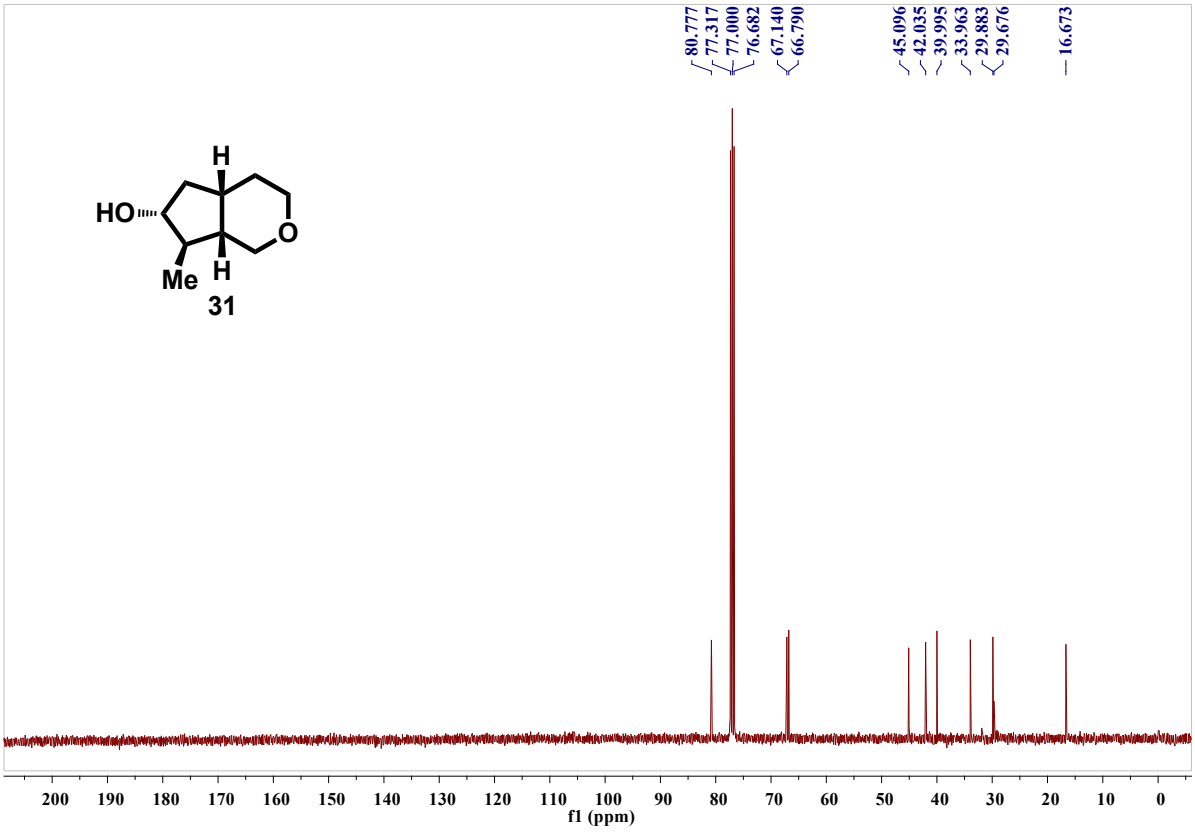
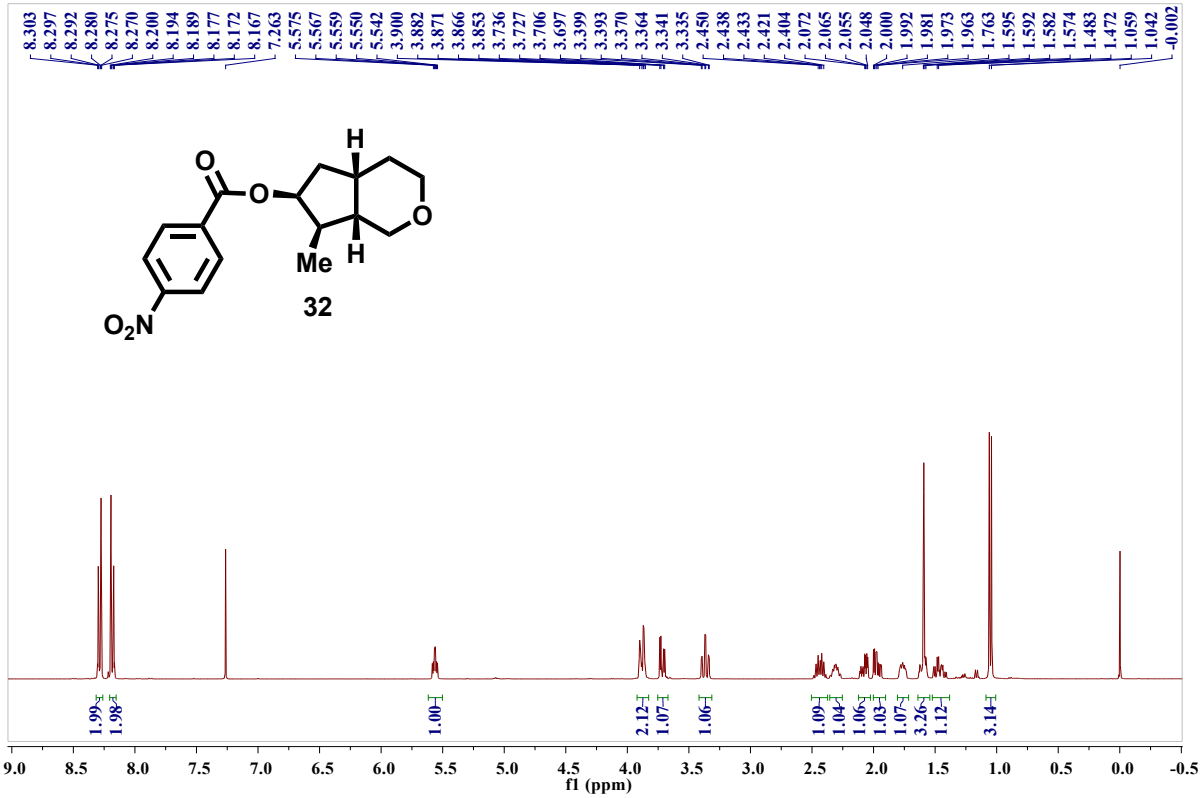
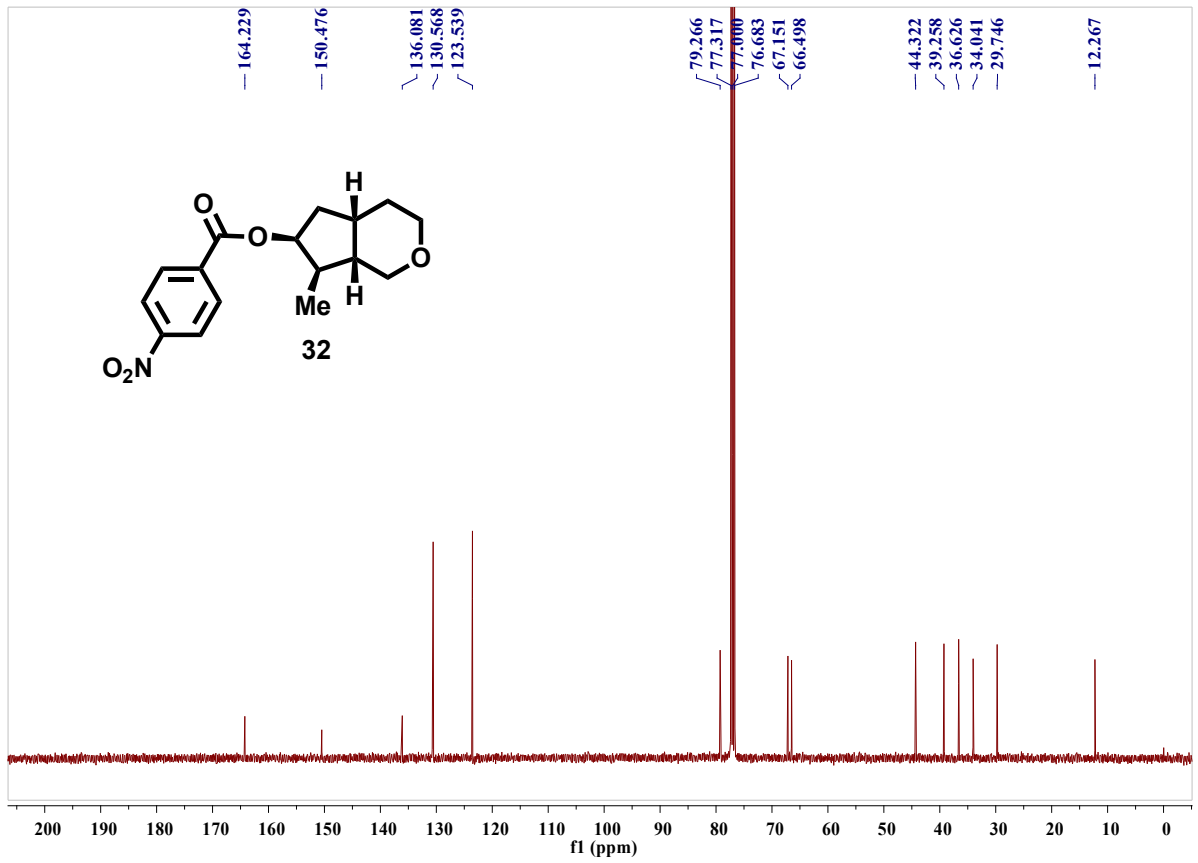
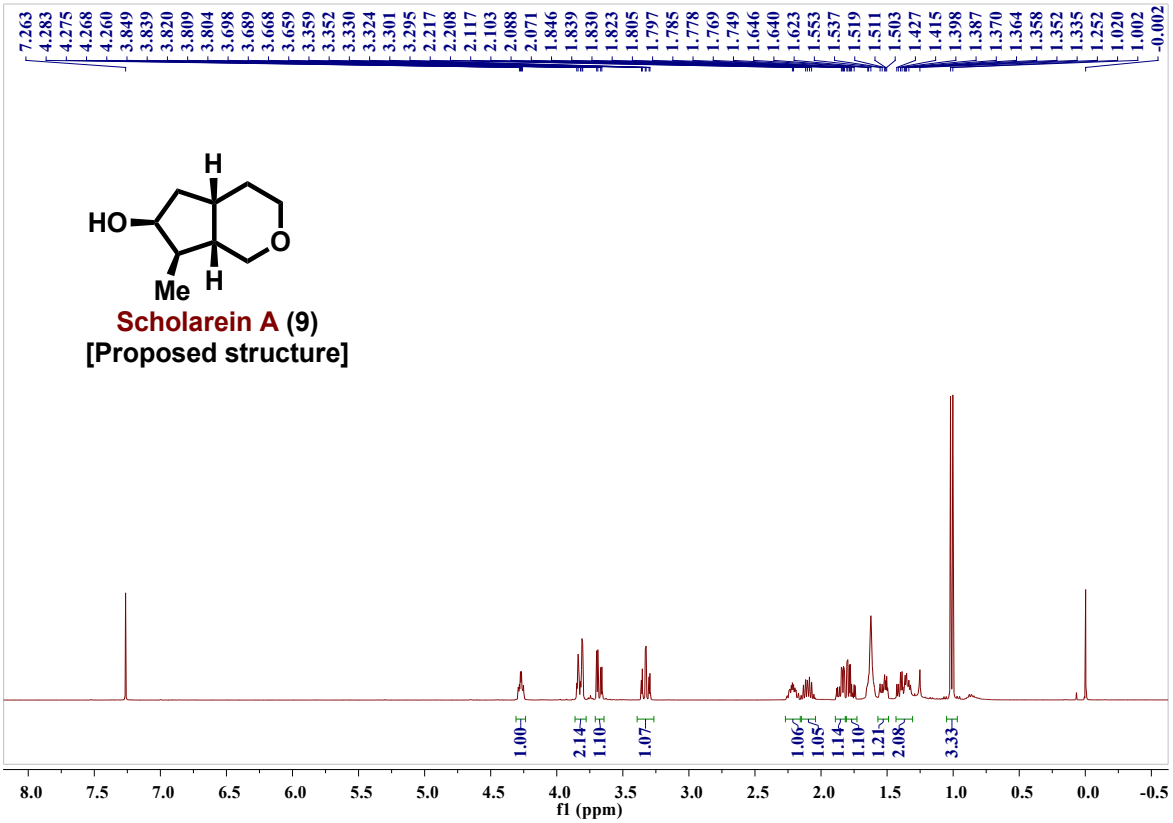
77.000
76.683
74.841
67.308
67.012
43.815
42.748
38.378
33.495
29.900
18.141
18.089
12.972
12.398
TIPSO
H
O
Me
H
29
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

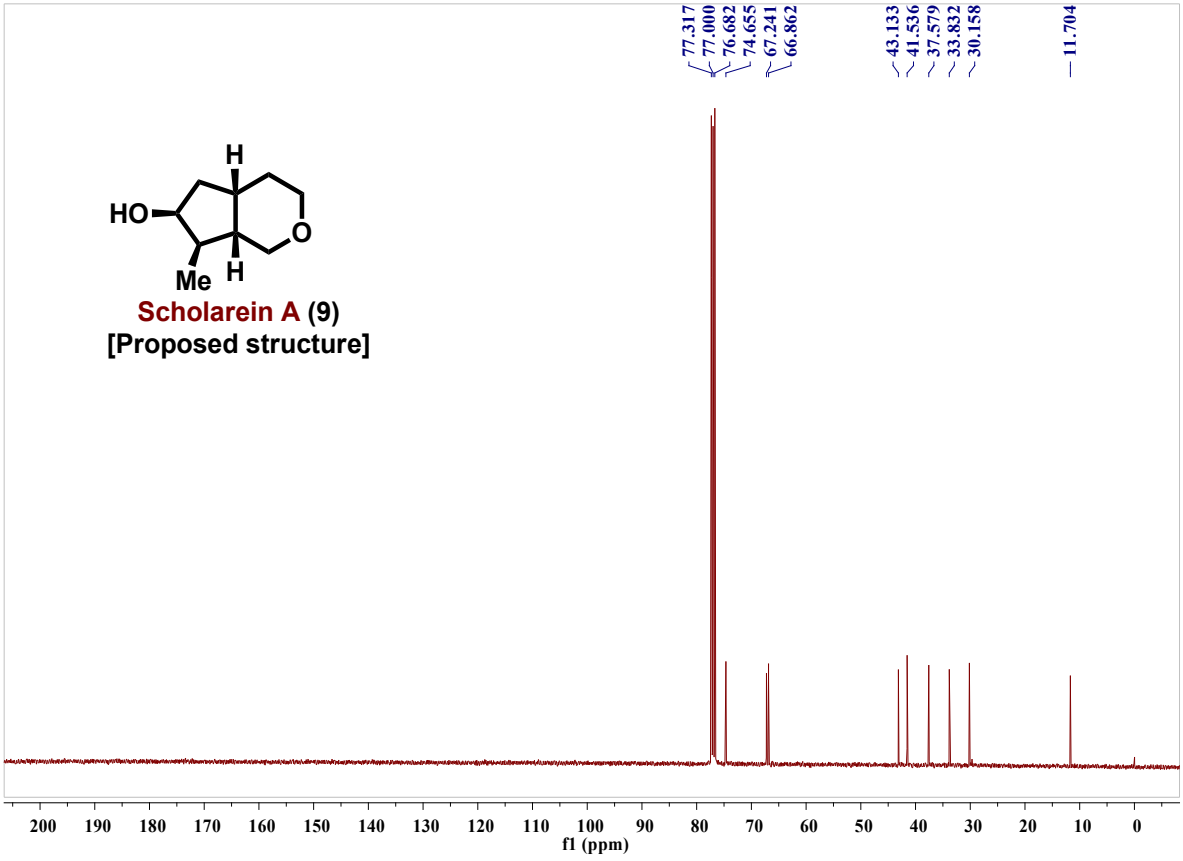

7.263
3.866
3.854
3.848
3.837
3.831
3.827
3.815
3.801
3.794
3.771
3.764
3.635
3.625
3.605
3.595
3.420
3.413
3.393
3.386
3.365
3.358
2.236
2.221
2.214
2.201
2.180
2.080
1.995
1.986
1.978
1.970
1.720
1.710
1.703
1.694
1.684
1.669
1.658
1.640
1.632
1.623
1.615
1.608
1.599
1.420
1.411
1.407
1.398
1.386
1.376
1.364
1.291
1.252
1.069
1.052
-0.003
HO
H
O
Me
H
31
1.91
0.99
1.00
0.98
1.03
1.12
0.92
4.46
2.44
3.19
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


80.777
77.317
77.000
76.682
67.140
66.790
45.096
42.035
39.995
33.963
29.883
29.676
16.673
HO
H
O
Me
H
31
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.303
8.297
8.292
8.280
8.275
8.270
8.200
8.194
8.189
8.177
8.172
8.167
7.263
5.575
5.567
5.559
5.550
5.542
3.900
3.882
3.871
3.866
3.853
3.736
3.727
3.706
3.697
3.399
3.393
3.370
3.364
3.341
3.335
2.450
2.438
2.433
2.421
2.404
2.072
2.065
2.055
2.048
2.000
1.992
1.981
1.973
1.963
1.763
1.595
1.592
1.582
1.574
1.483
1.472
1.059
1.042
-0.002
O
O
H
O
Me
H
O2N
32
1.99
1.98
1.00
2.12
1.07
1.06
1.09
1.04
1.06
1.03
1.07
3.26
1.12
3.14
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


164.229
150.476
136.081
130.568
123.539
79.266
77.317
77.000
76.683
67.151
66.498
44.322
39.258
36.626
34.041
29.746
12.267
O
O
H
O
Me
H
O2N
32
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.263
4.283
4.275
4.268
4.260
3.849
3.839
3.820
3.809
3.804
3.698
3.689
3.668
3.659
3.359
3.352
3.330
3.324
3.301
3.295
2.217
2.208
2.117
2.103
2.088
2.071
1.846
1.839
1.830
1.823
1.805
1.797
1.785
1.778
1.769
1.749
1.646
1.640
1.623
1.553
1.537
1.519
1.511
1.503
1.427
1.415
1.398
1.387
1.370
1.364
1.358
1.352
1.335
1.252
1.020
1.002
-0.002
H
HO
O
Me
H
Scholarein A (9)
[Proposed structure]
1.00
2.14
1.10
1.07
1.06
1.05
1.14
1.10
1.21
2.08
3.33
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


77.317
77.000
76.682
74.655
67.241
66.862
43.133
41.536
37.579
33.832
30.158
11.704
H
HO
O
Me
H
Scholarein A (9)
[Proposed structure]
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)