

Supporting Information-II

NMR Spectral Data

Direct Catalytic Asymmetric Synthesis of Highly Functionalized Tetronic acids/Tetrahydro-isobenzofuran-1, 5-diones via Combination of Cascade Three-Component Reductive Alkylations and Michael-Aldol Reactions

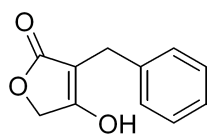
Dhevalapally B. Ramachary* and Mamillapalli Kishor

School of Chemistry, University of Hyderabad, Central University (P.O.),

Hyderabad 500 046, India

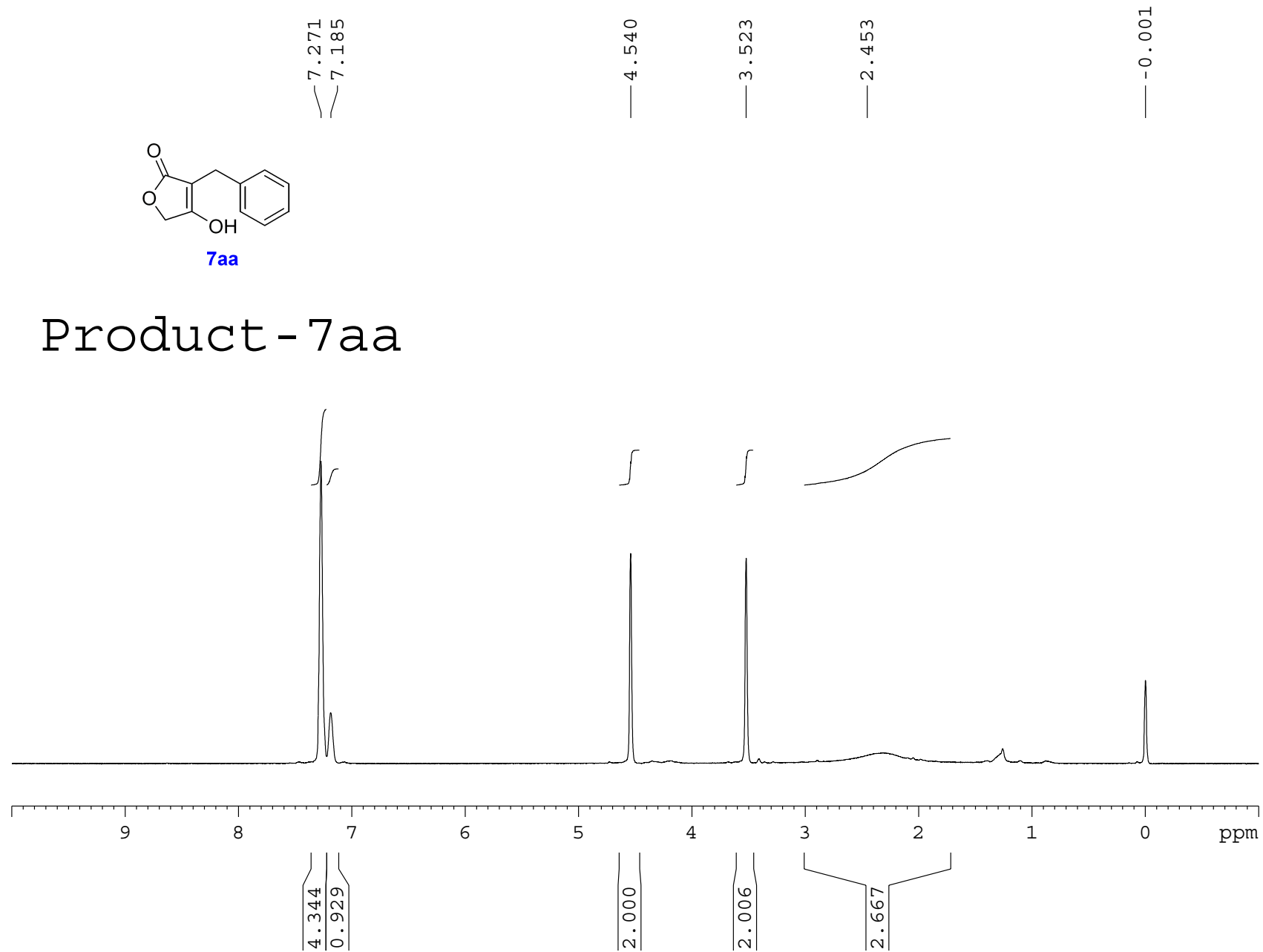
ramsc@uohyd.ernet.in

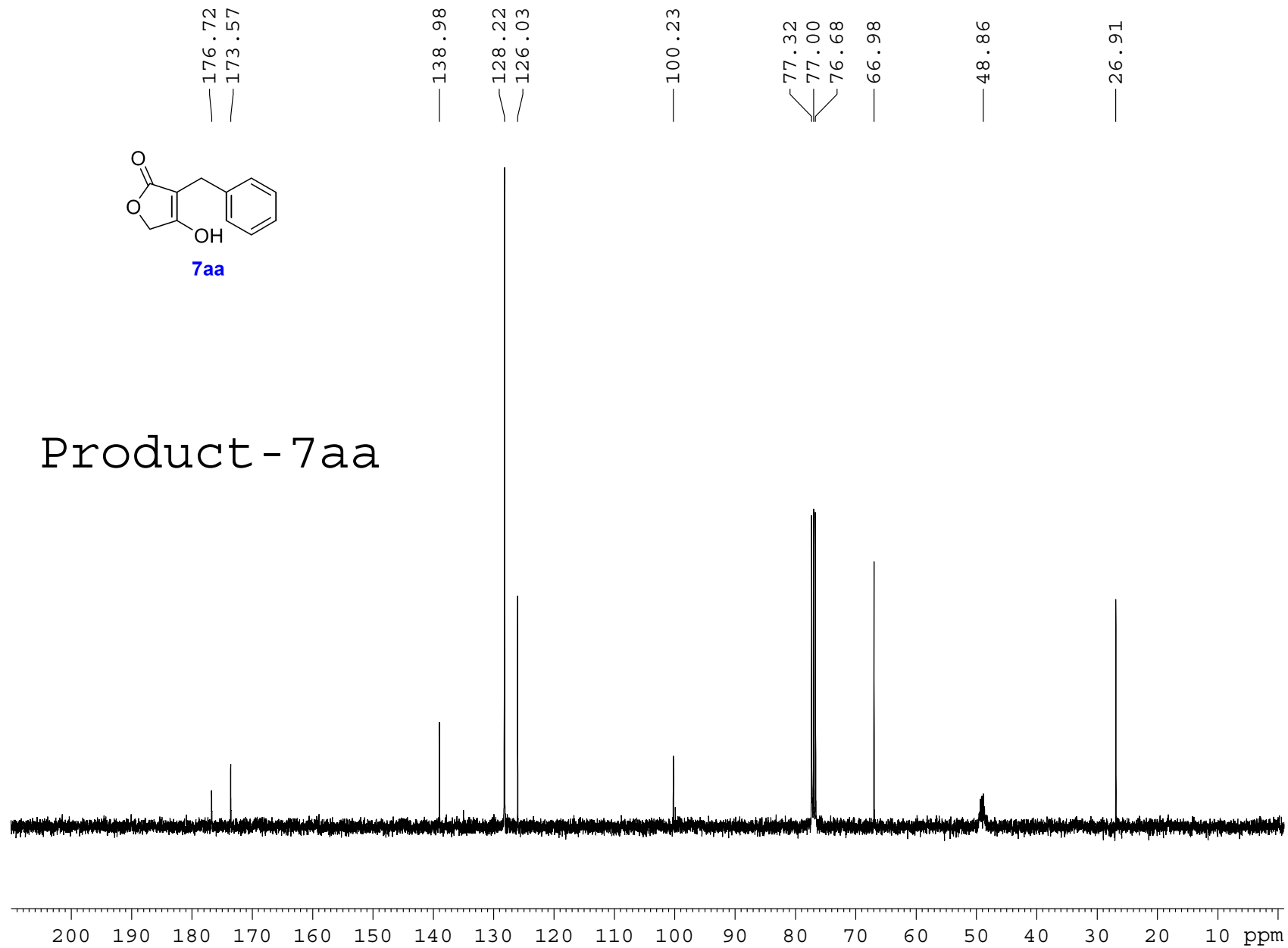
- *Because of solubility problem of cascade TCRA products 7aa-fm in CDCl₃, we have used three drops of CD₃OD for NMR analysis.*



7aa

Product - 7aa



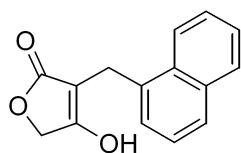


8.208
8.189
7.821
7.803
7.700
7.683
7.509
7.494
7.474
7.461
7.442
7.425
7.378
7.361

— 4.533

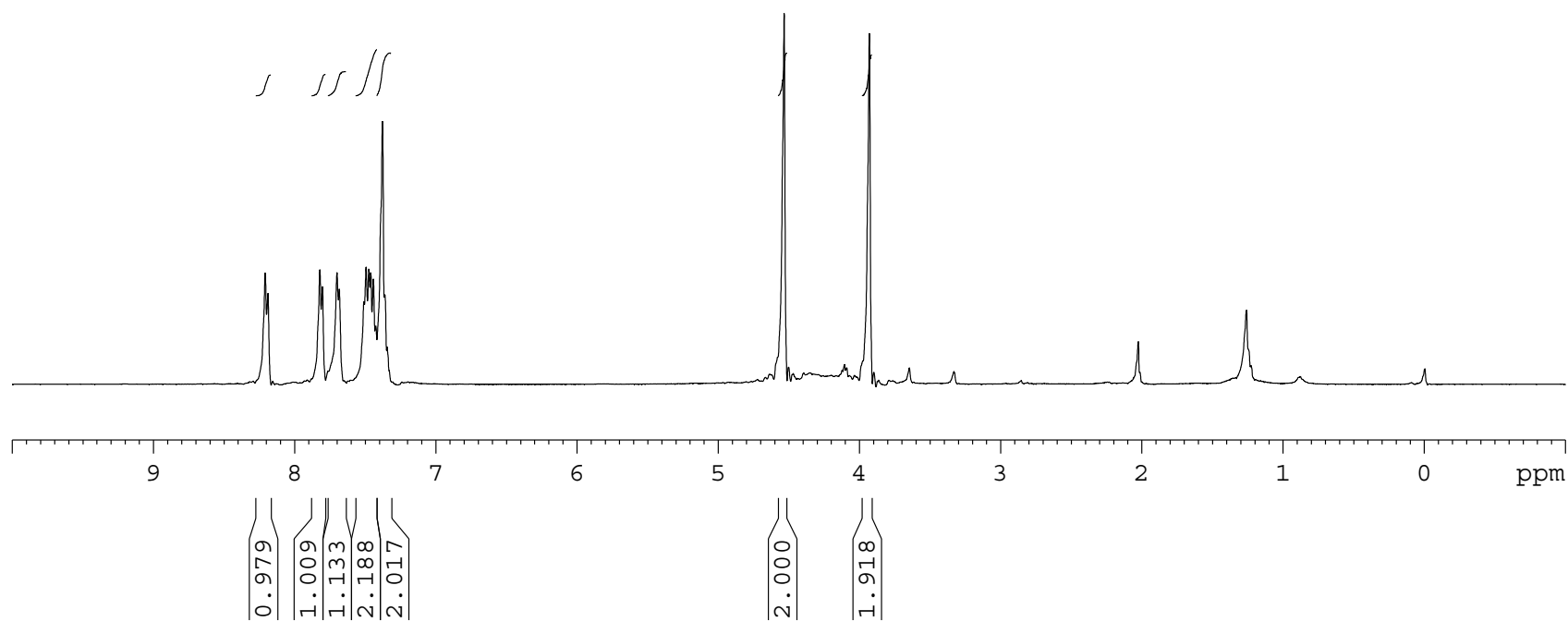
— 3.929

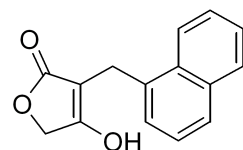
— -0.004



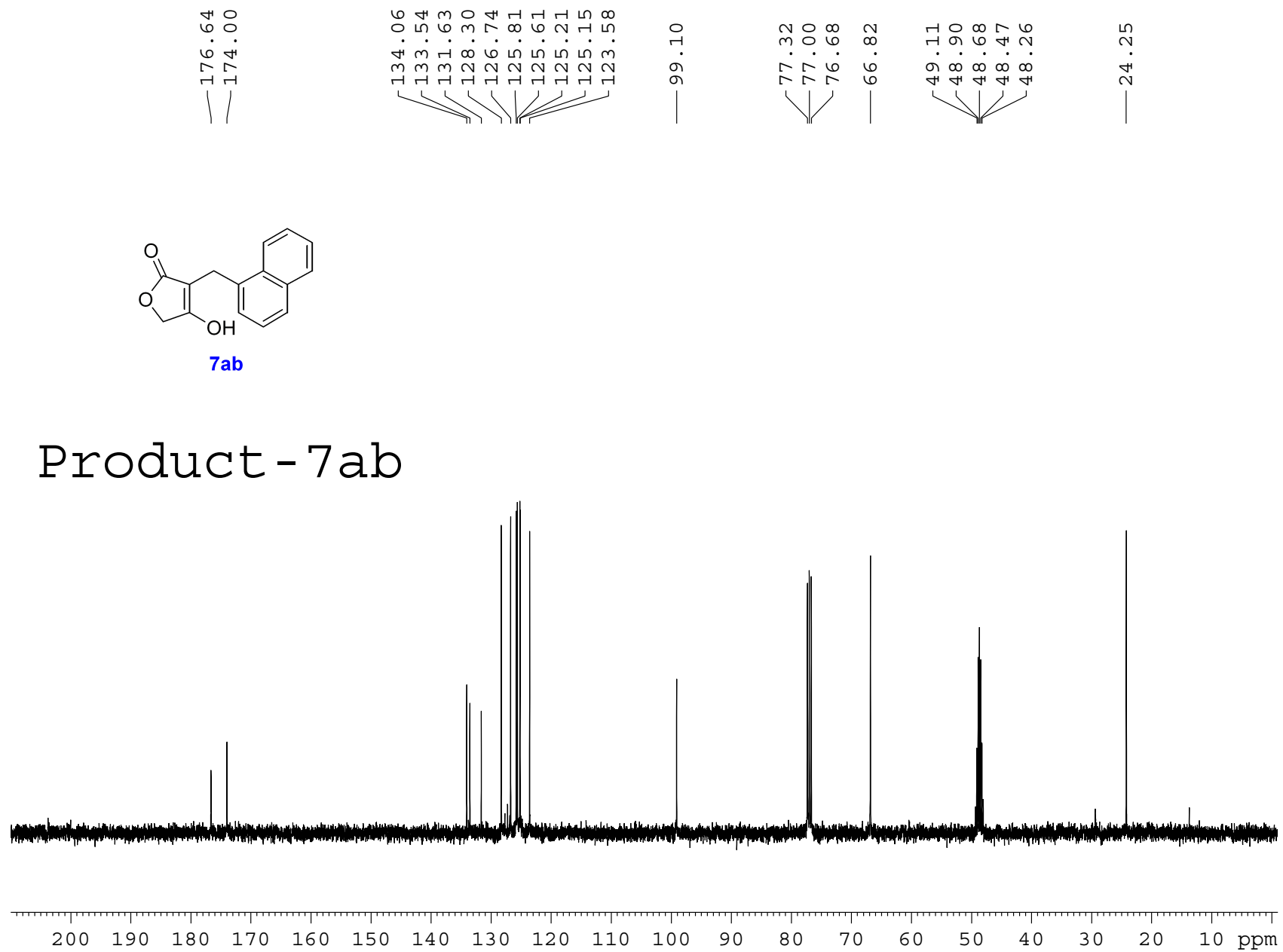
7ab

Product - 7ab





7ab

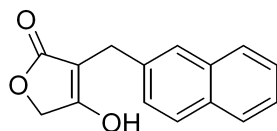


7.758
7.753
7.749
7.743
7.734
7.712
7.679
7.420
7.415
7.403
7.398
7.385
7.380
7.367
7.320

4.559

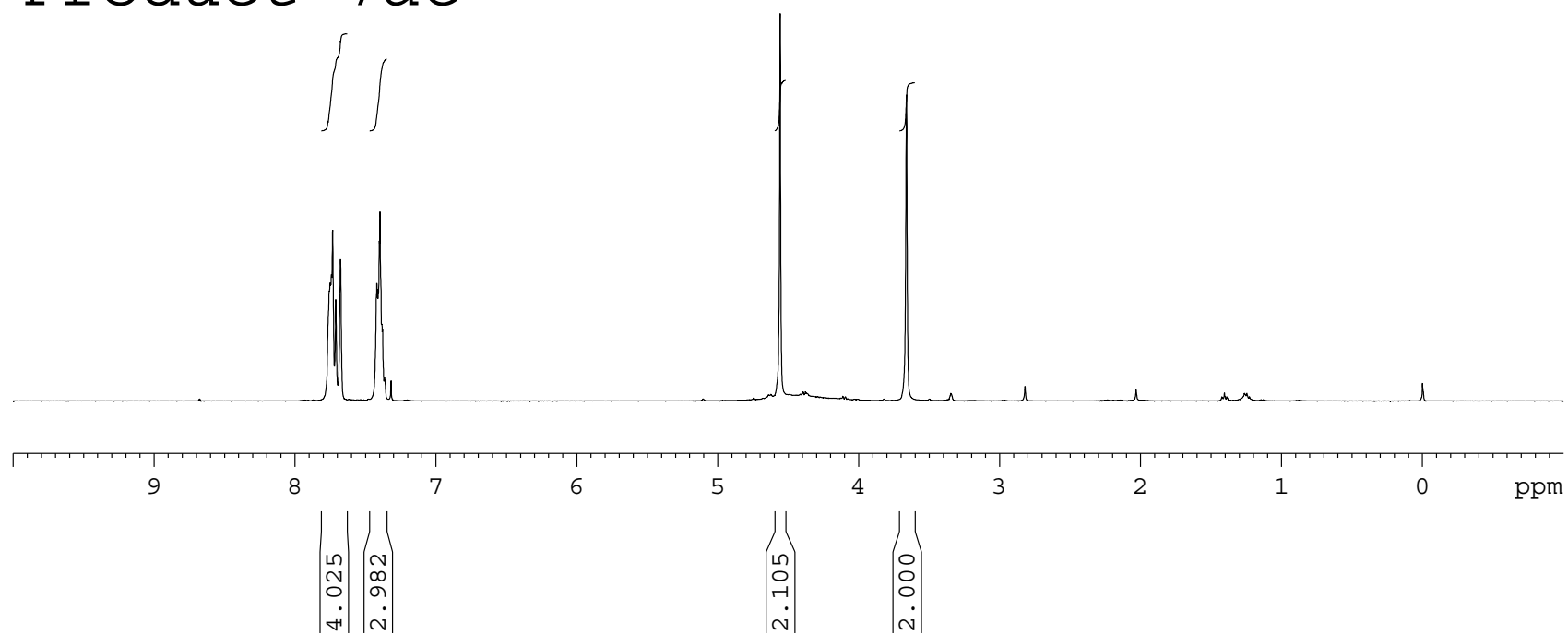
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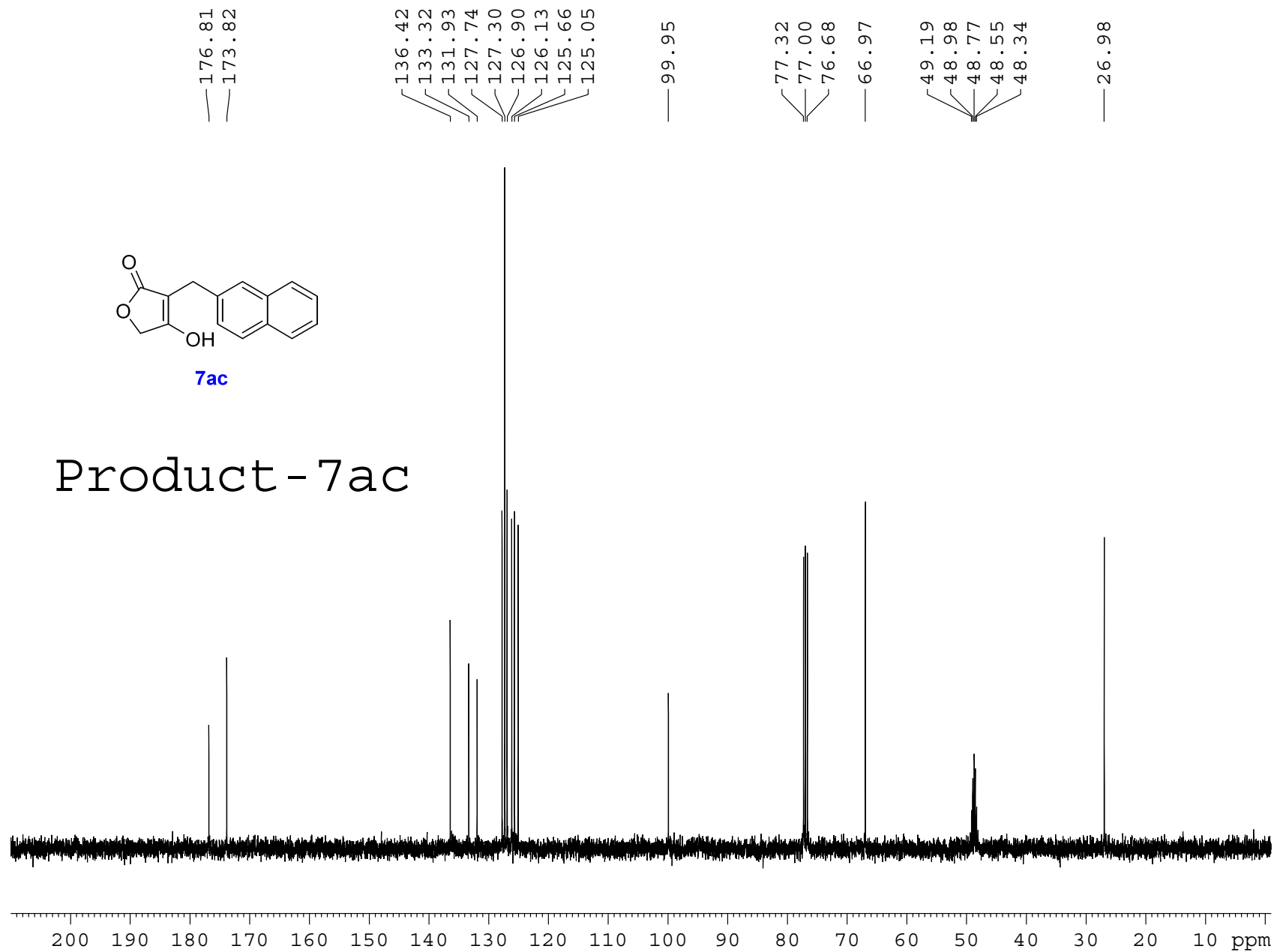
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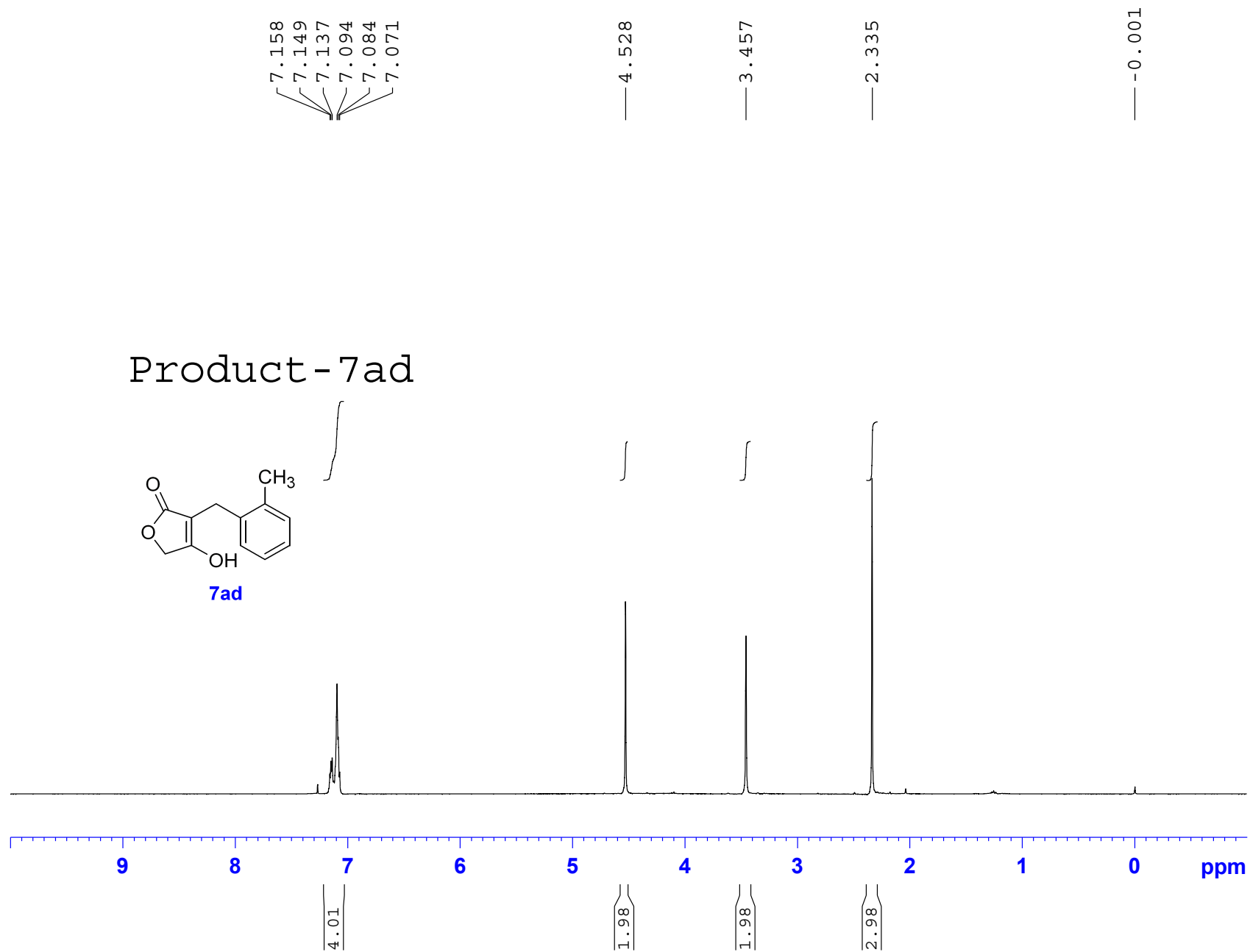
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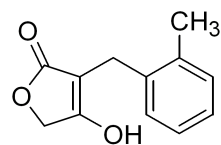
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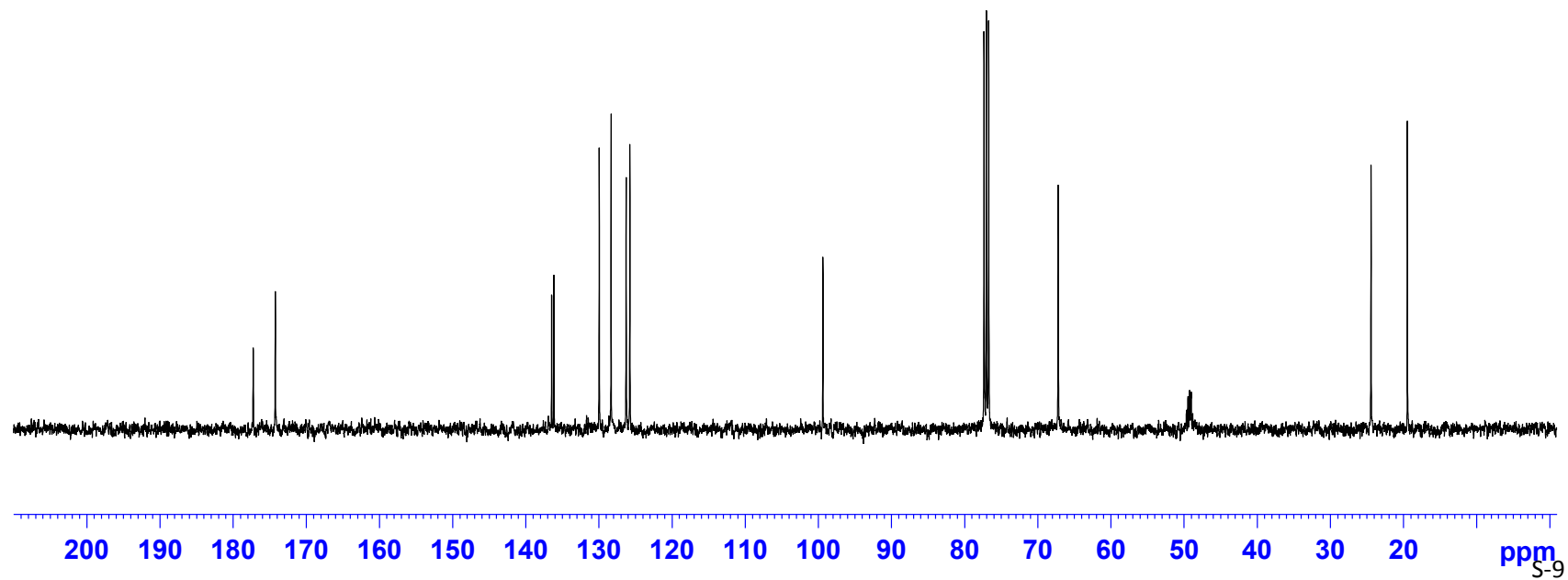
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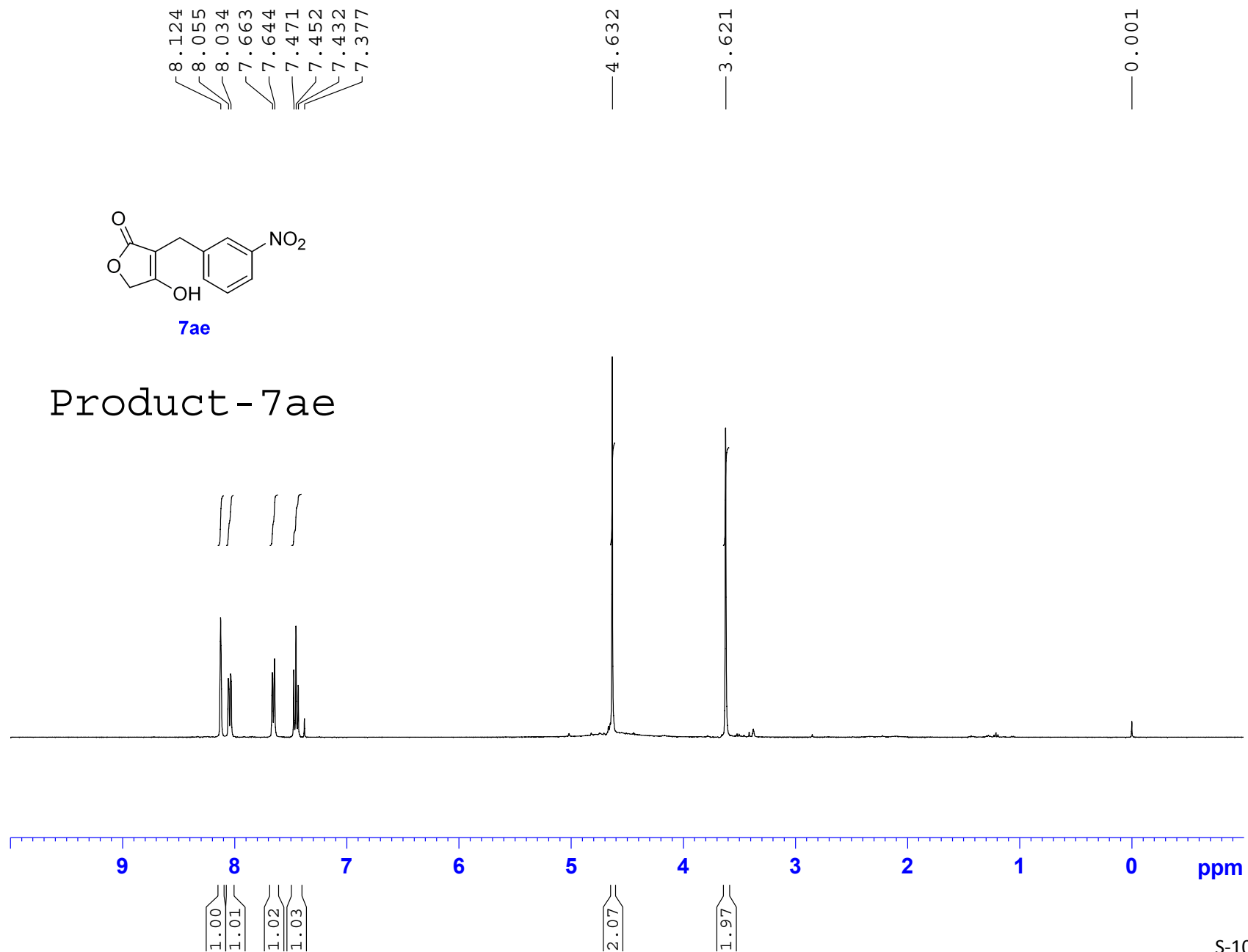


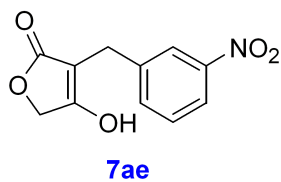


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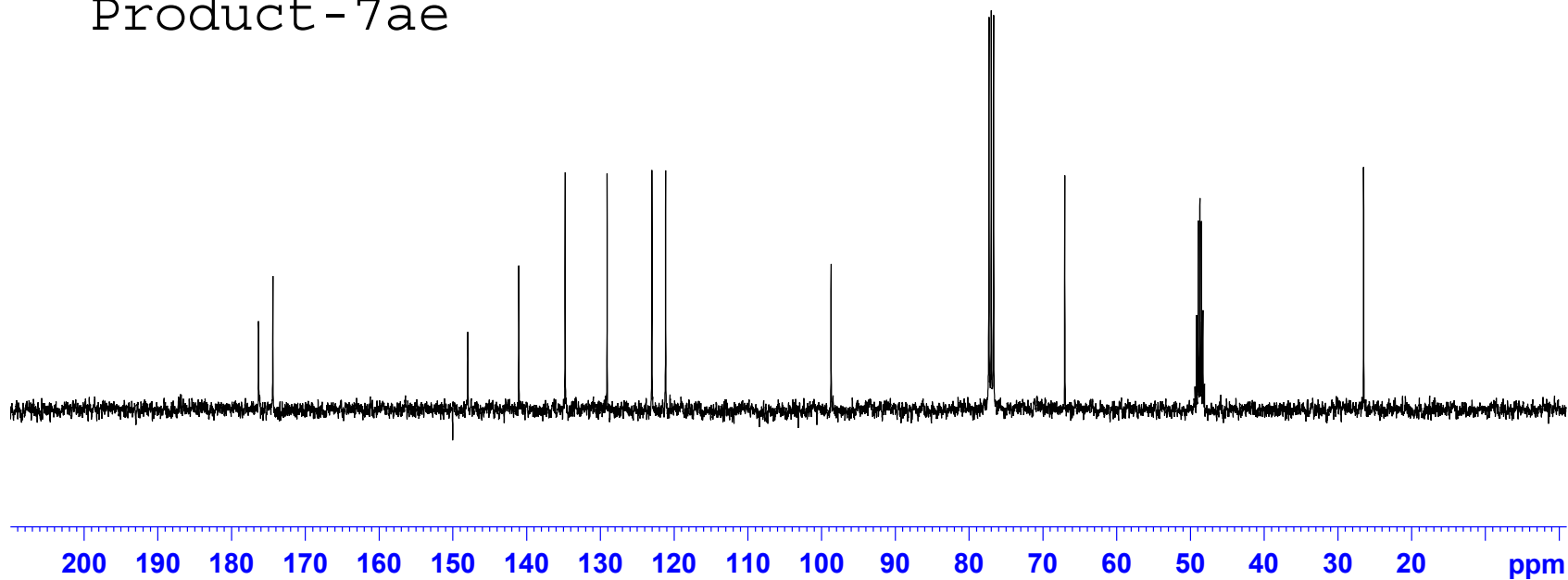
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Product - 7ae

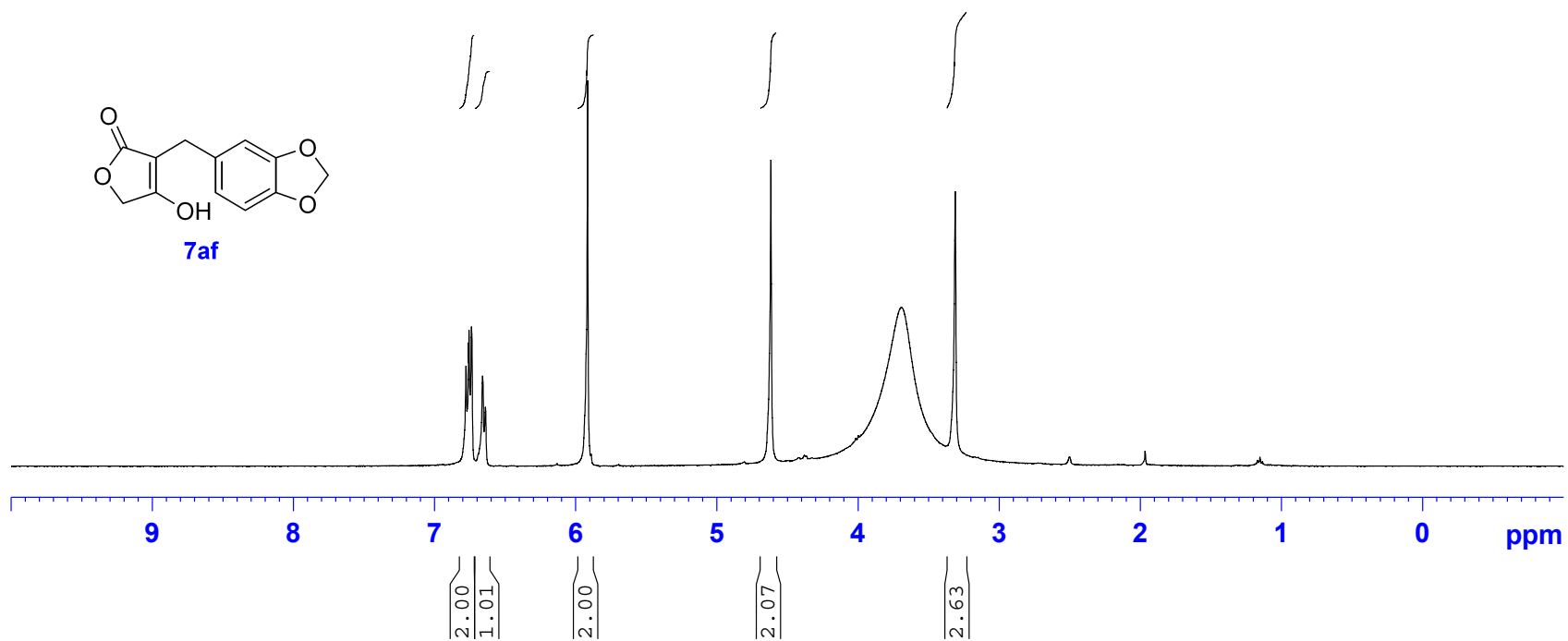


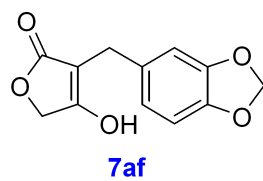
6.777
6.757
6.739
6.661
6.642
— 5.917

— 4.618

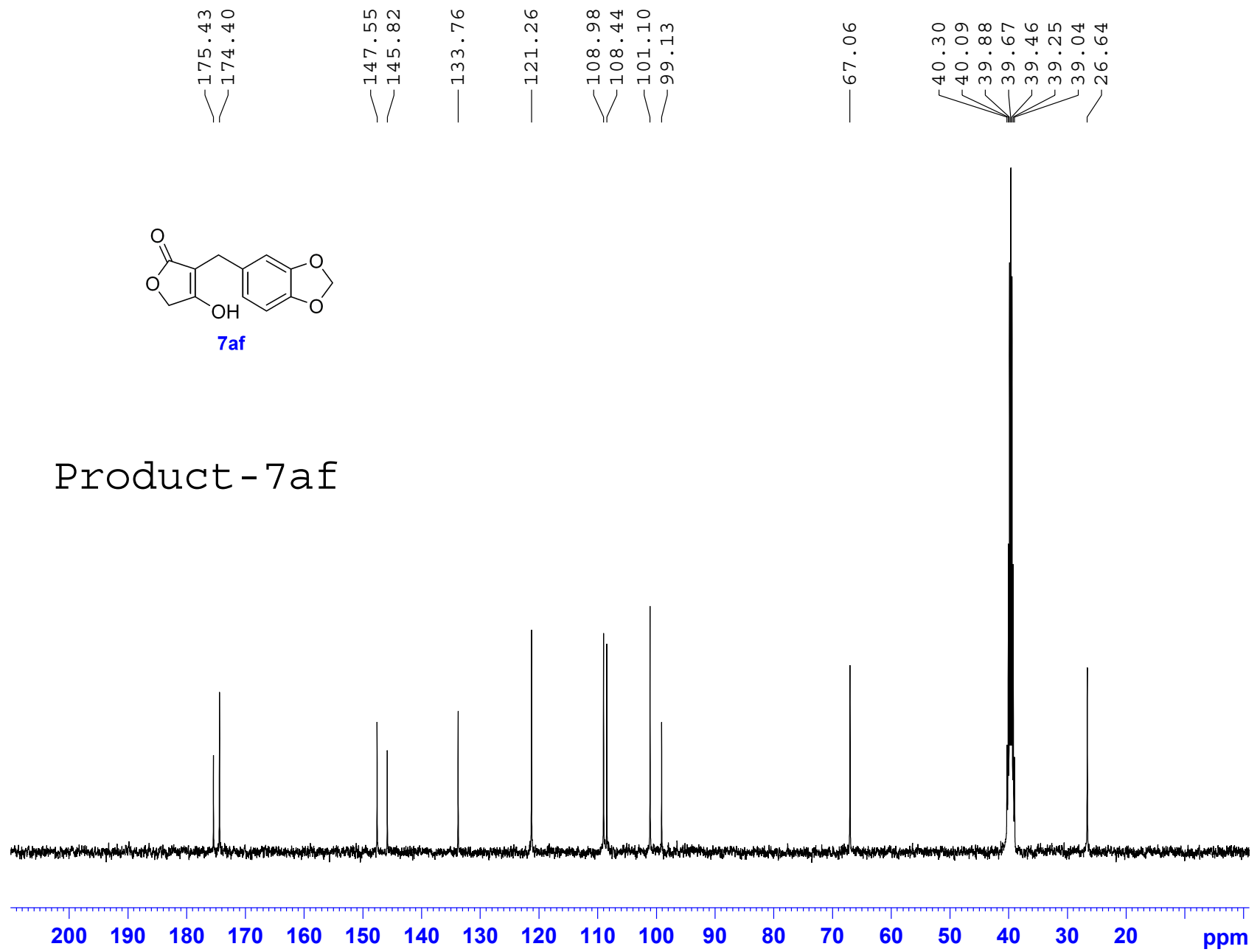
— 3.693
— 3.312

Product - 7af





Product - 7af

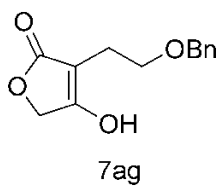


7.290
7.276
7.257
7.239
7.227
7.222
7.204
7.194

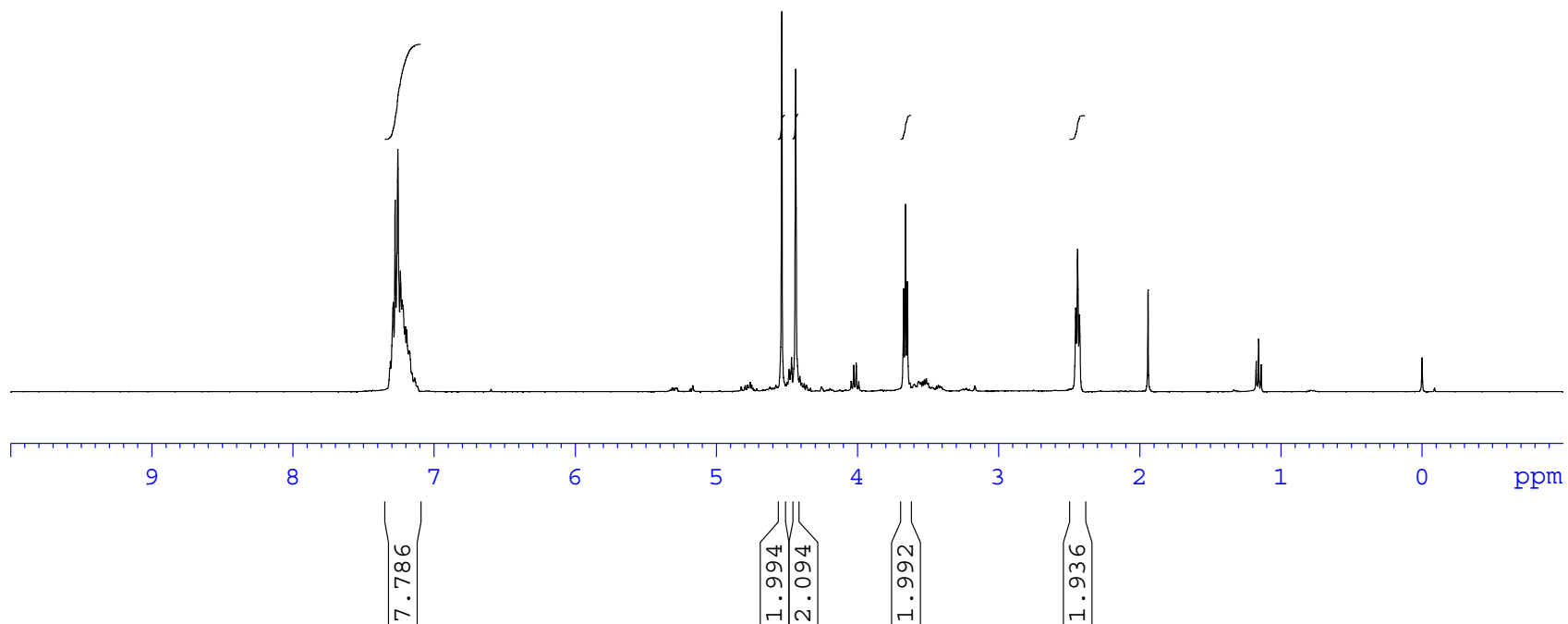
4.537
4.438

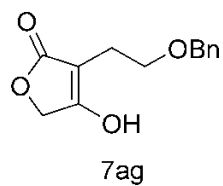
3.674
3.660
3.646

2.454
2.440
2.427

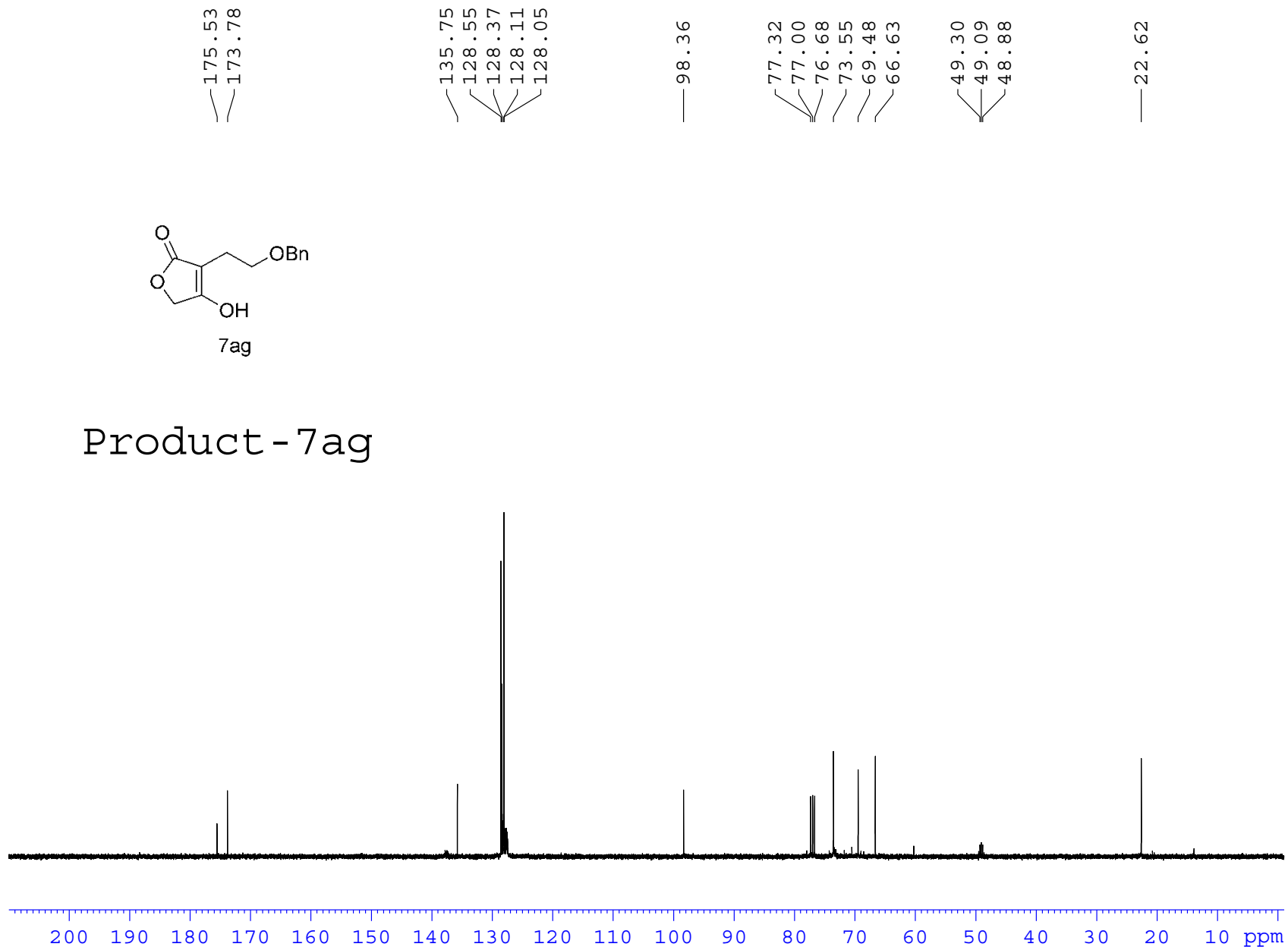


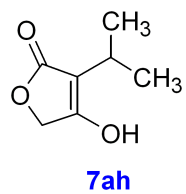
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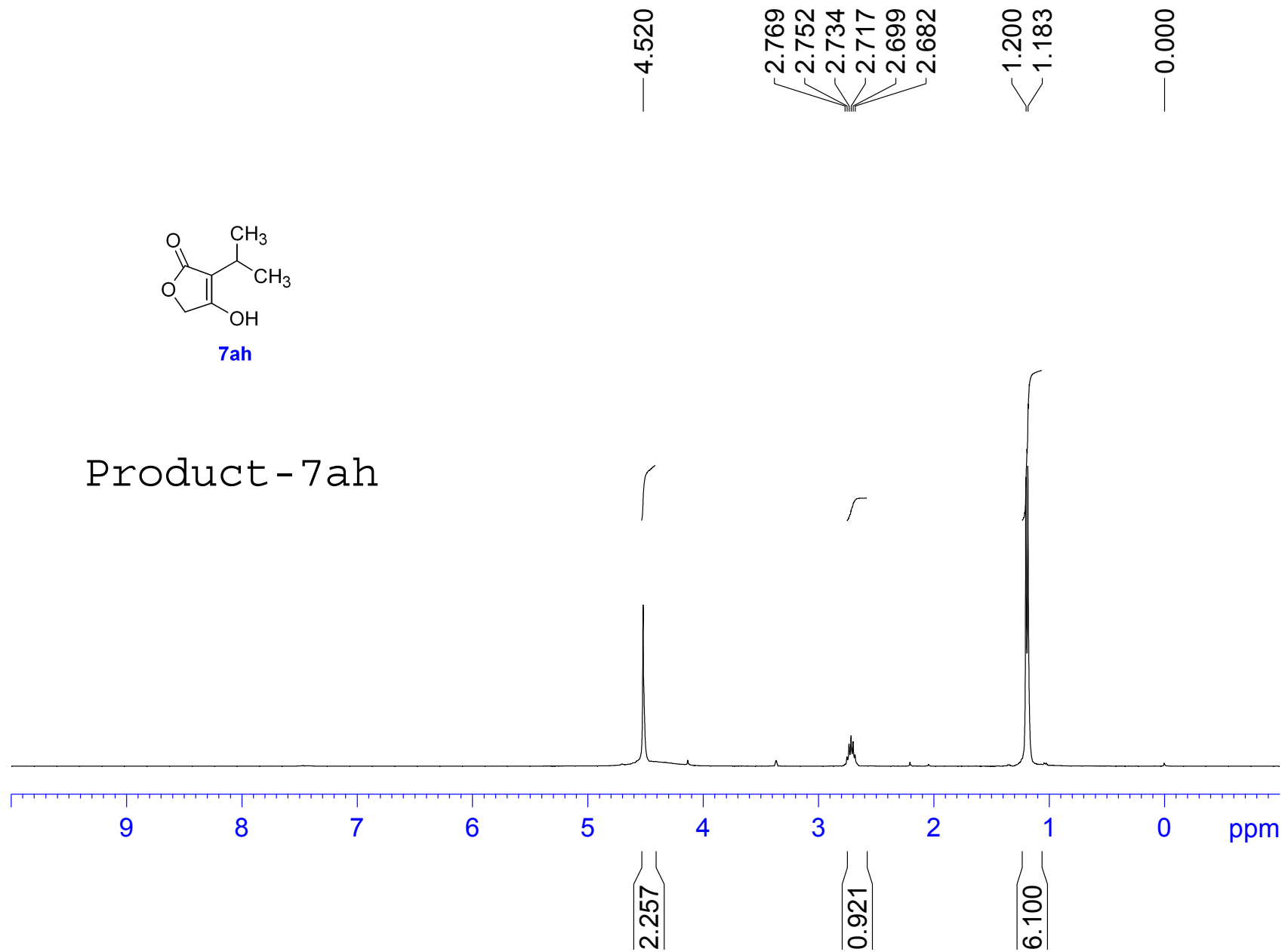


Product - 7ag





Product - 7ah



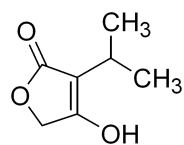
176.44
172.09

105.32

77.30
77.00
76.67
66.28

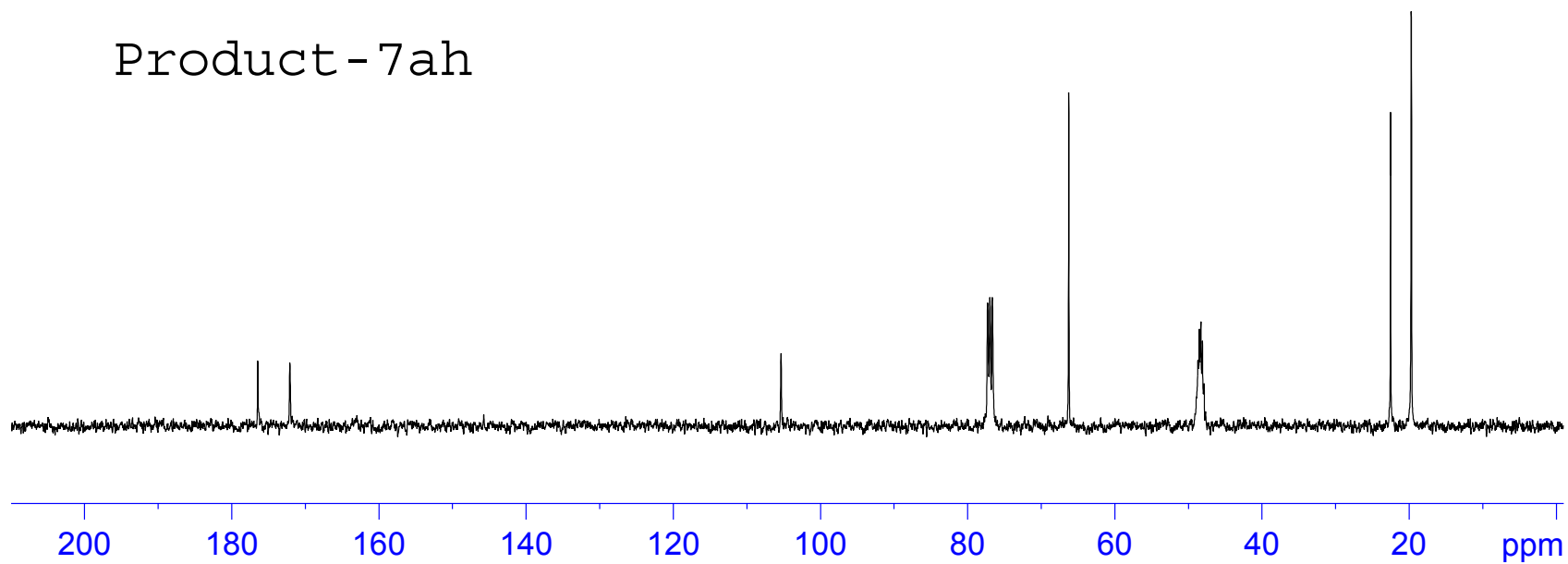
48.52
48.31
48.10

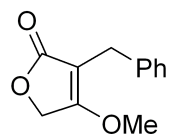
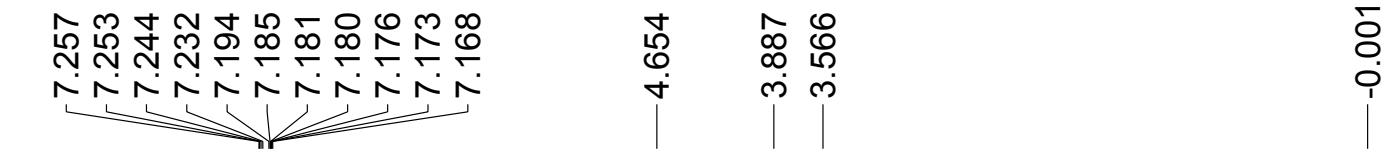
22.54
19.73



7ah

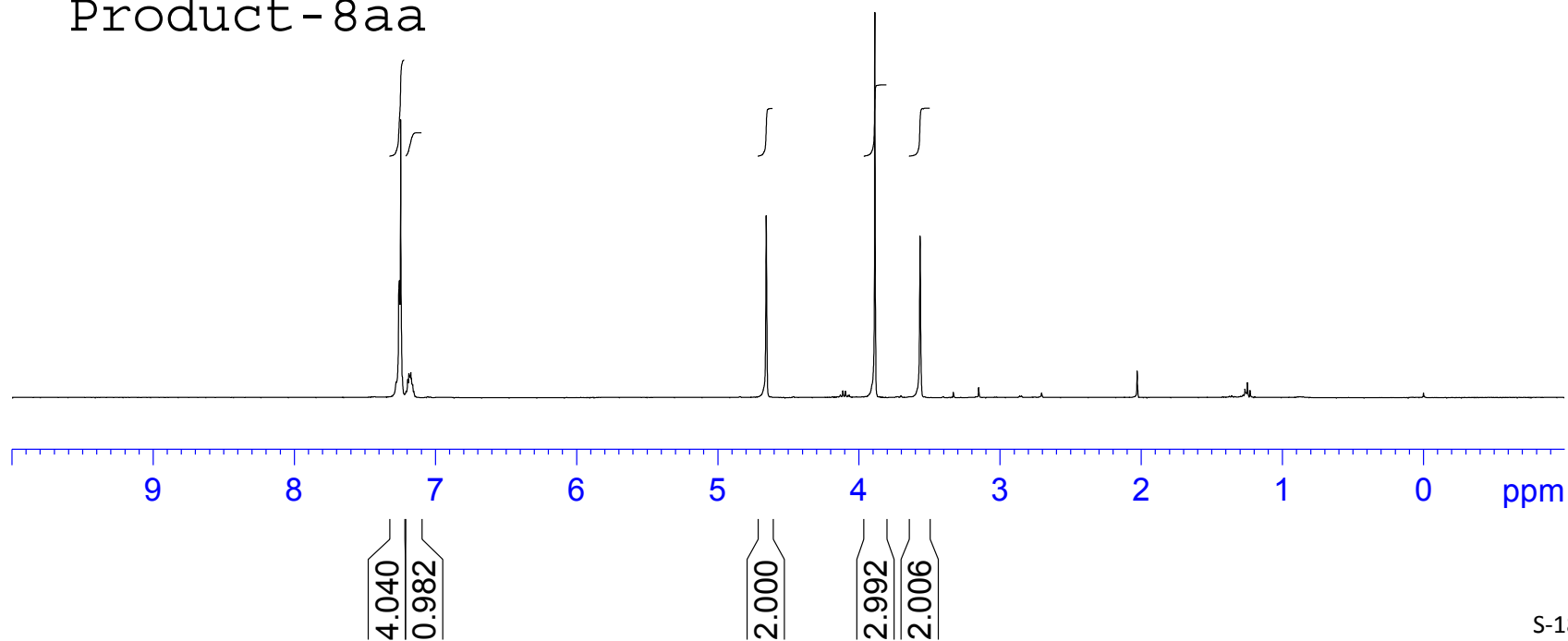
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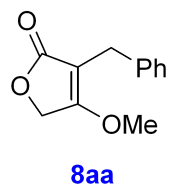
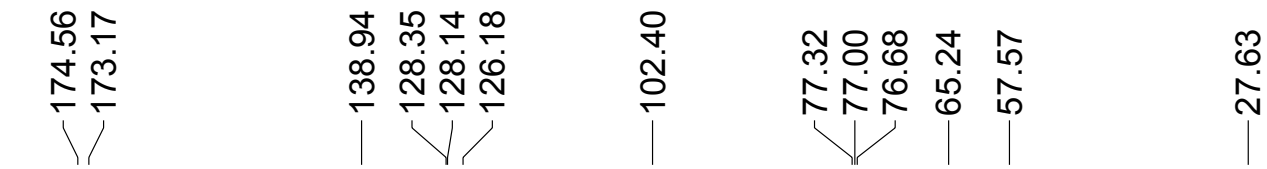




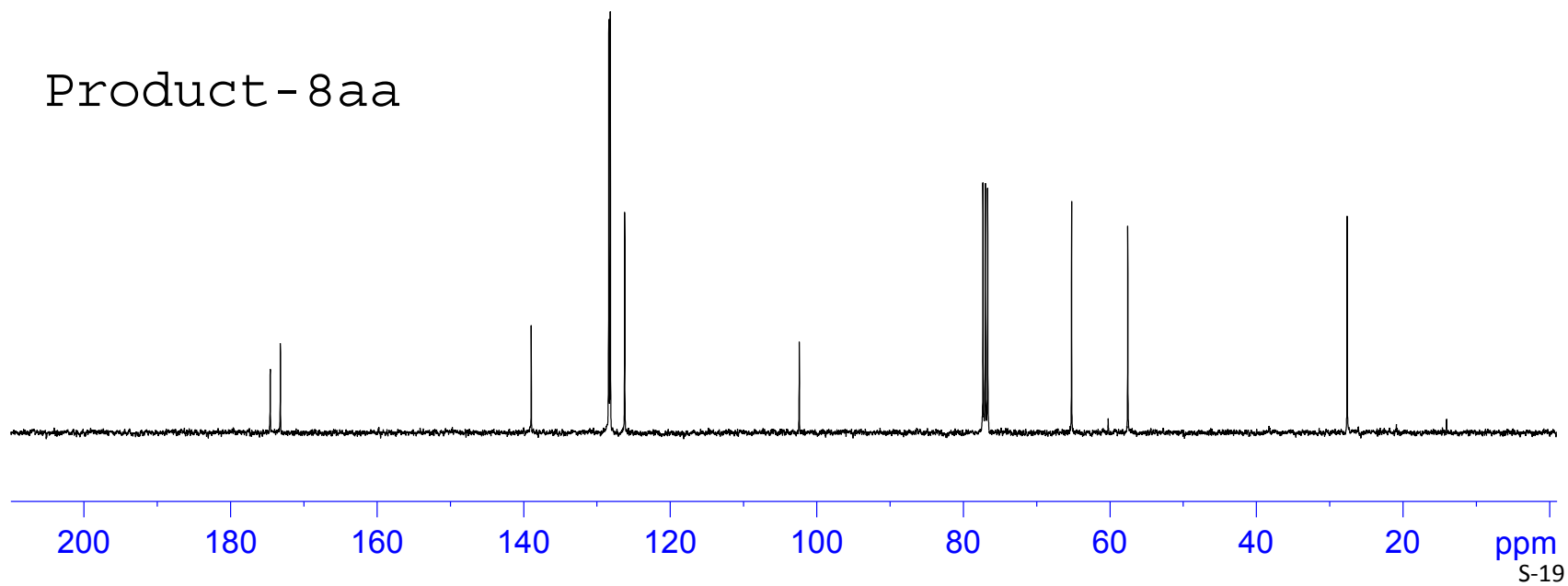
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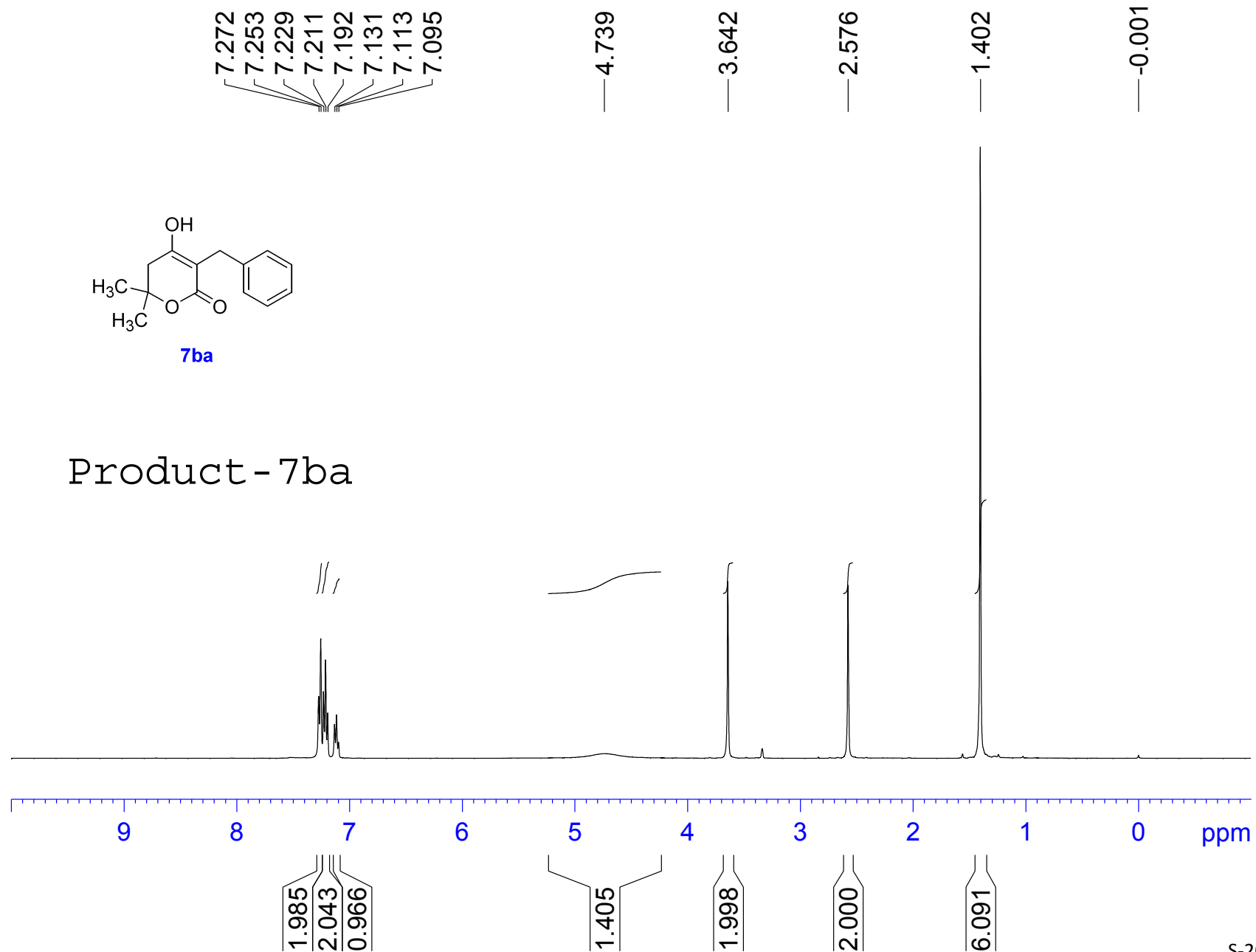
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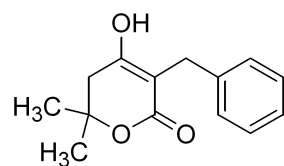




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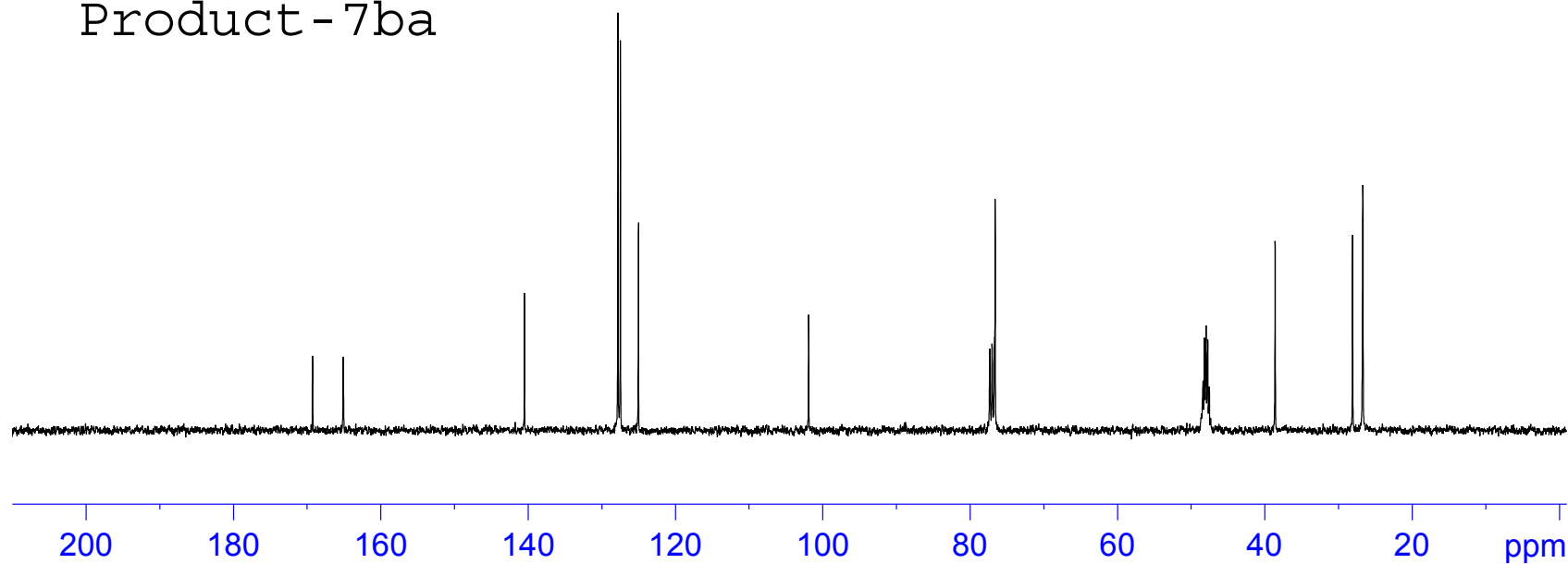


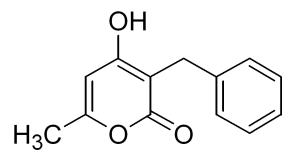




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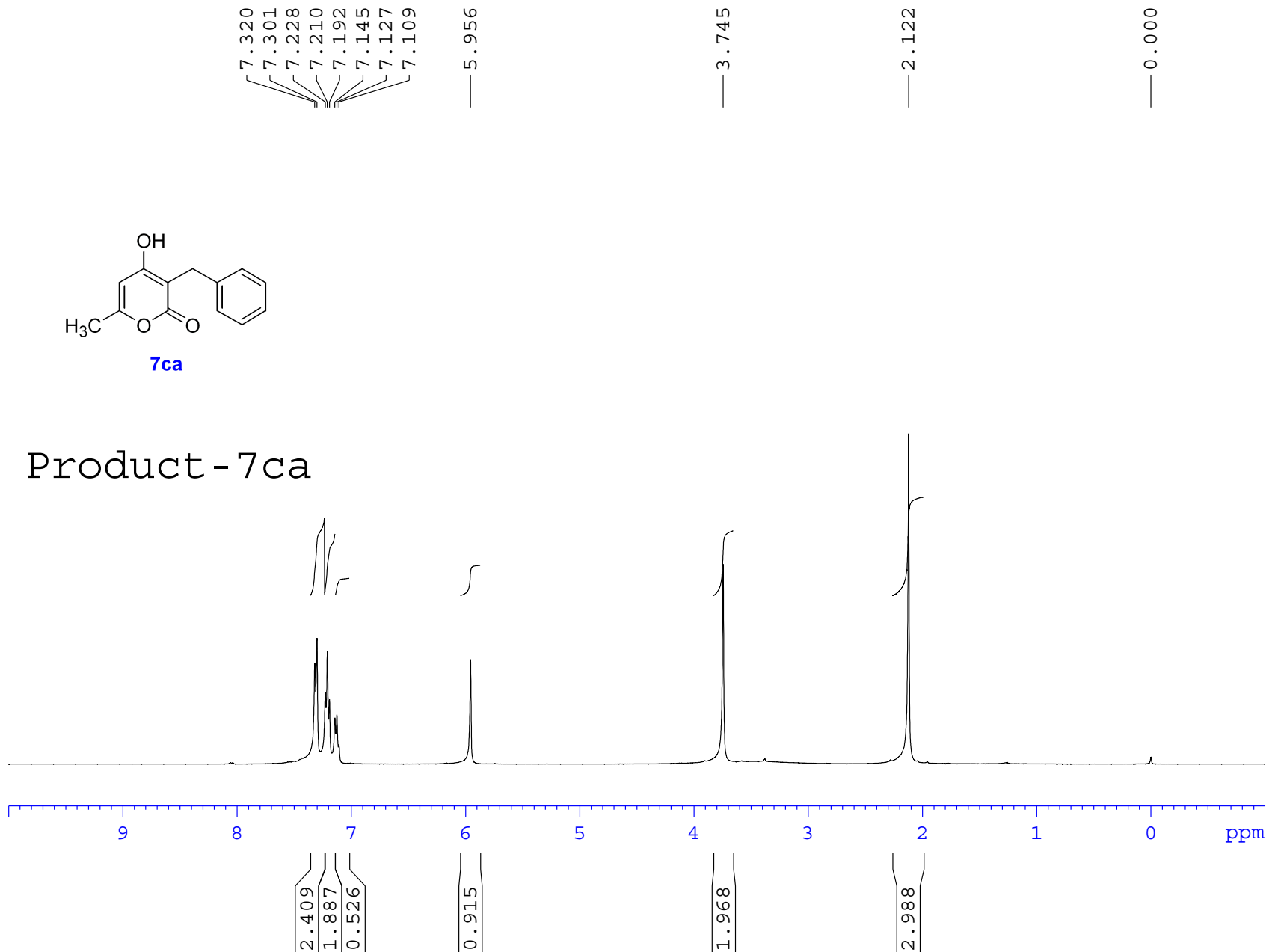
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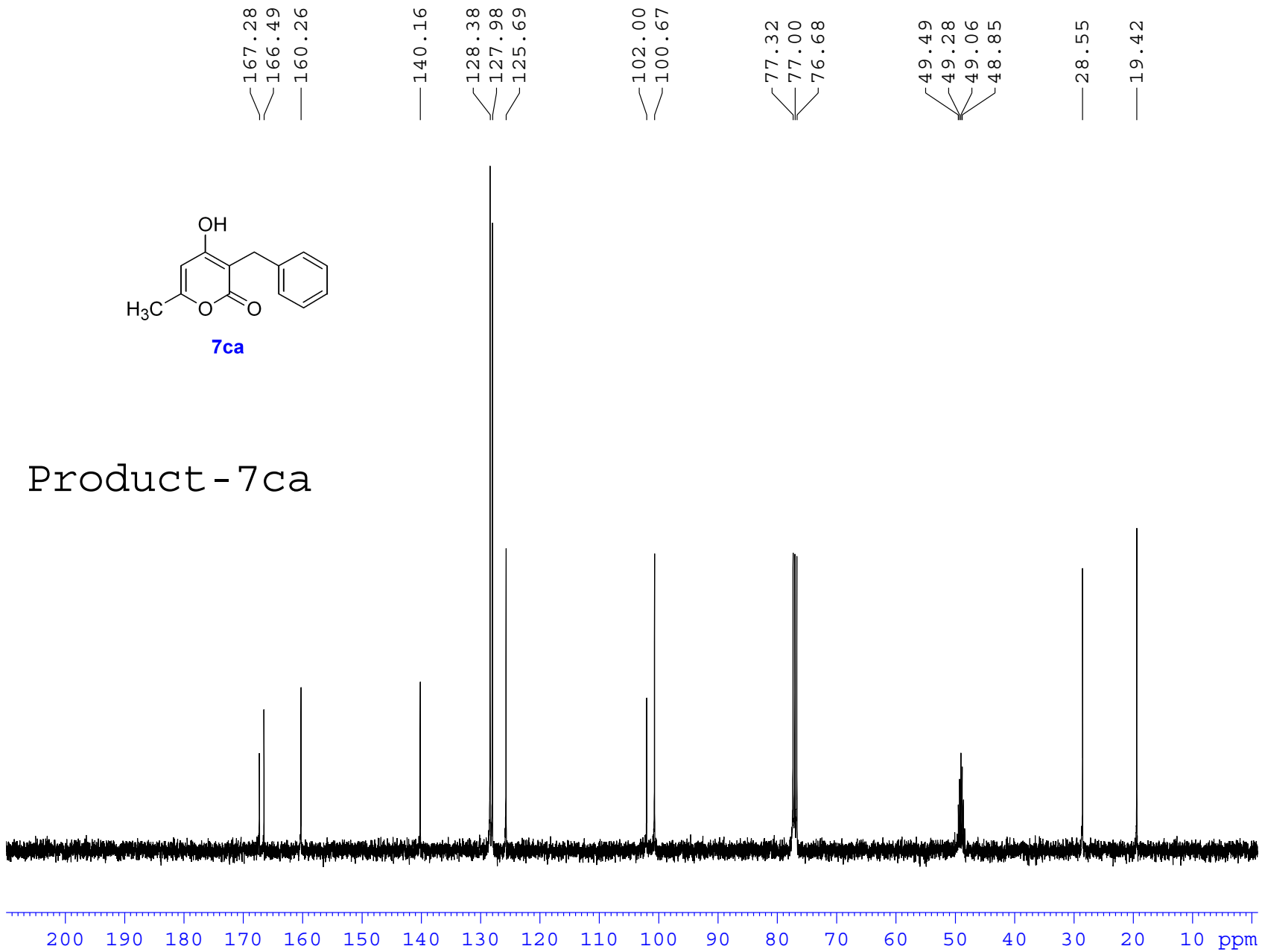
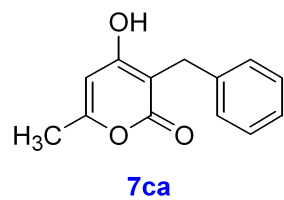


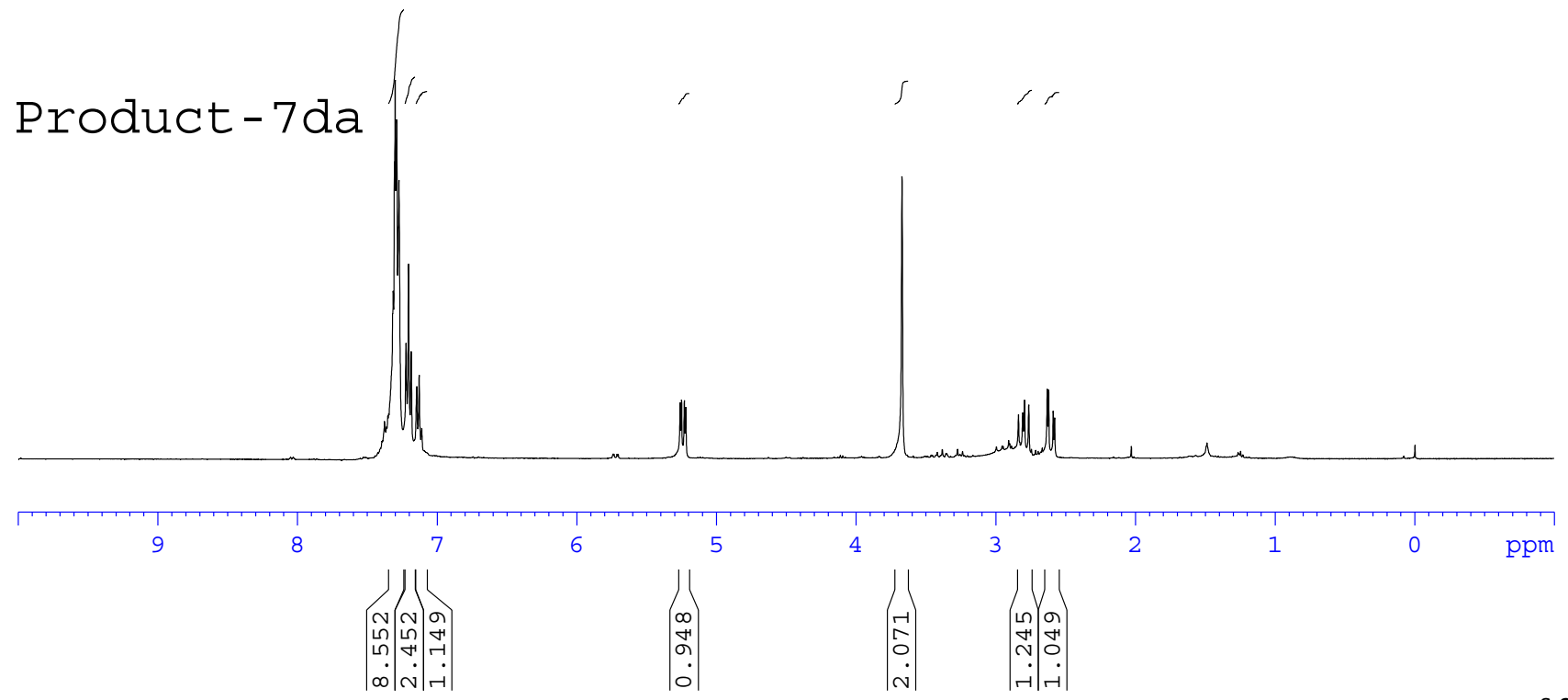
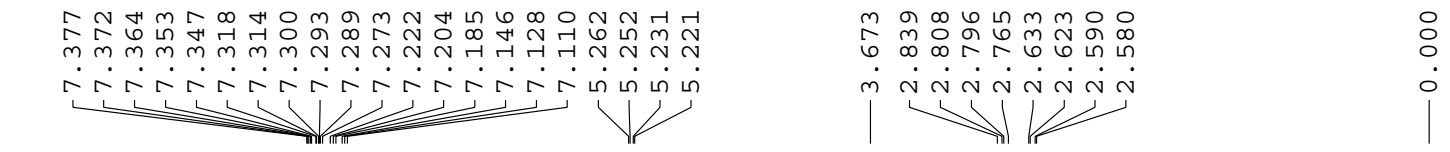


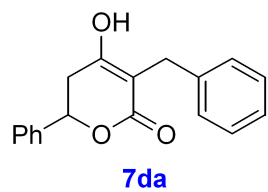
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Product - 7ca

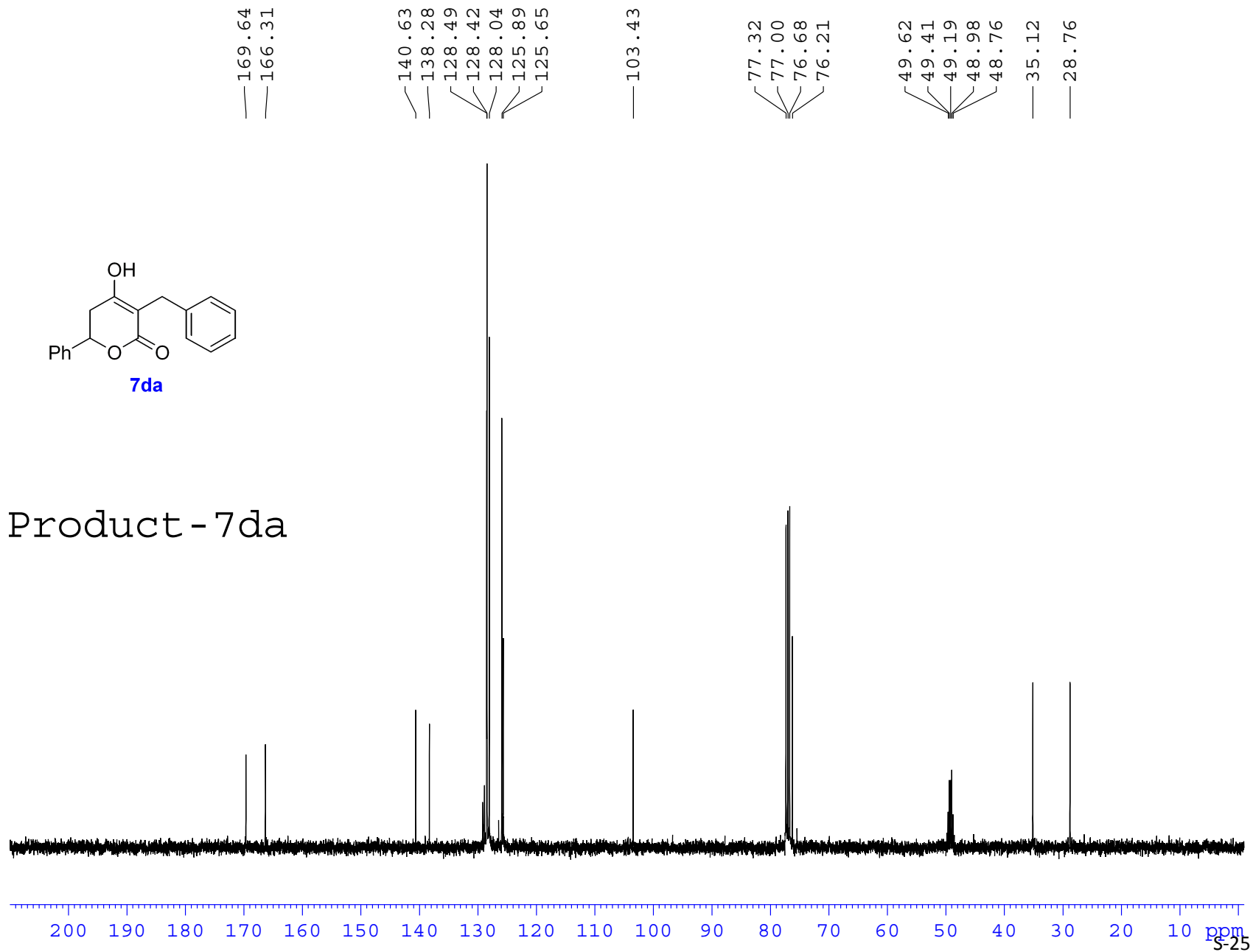






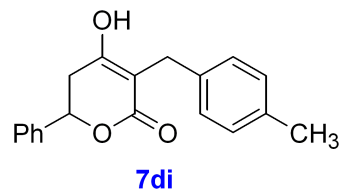


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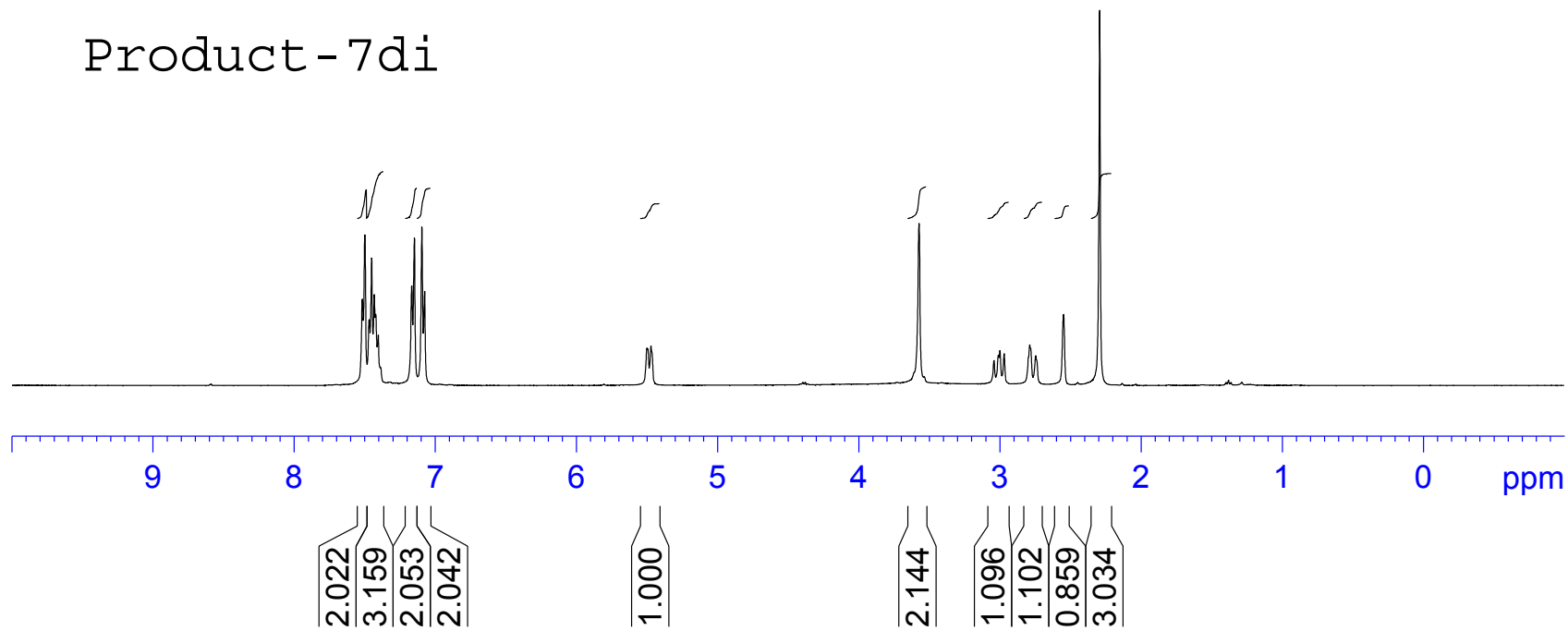


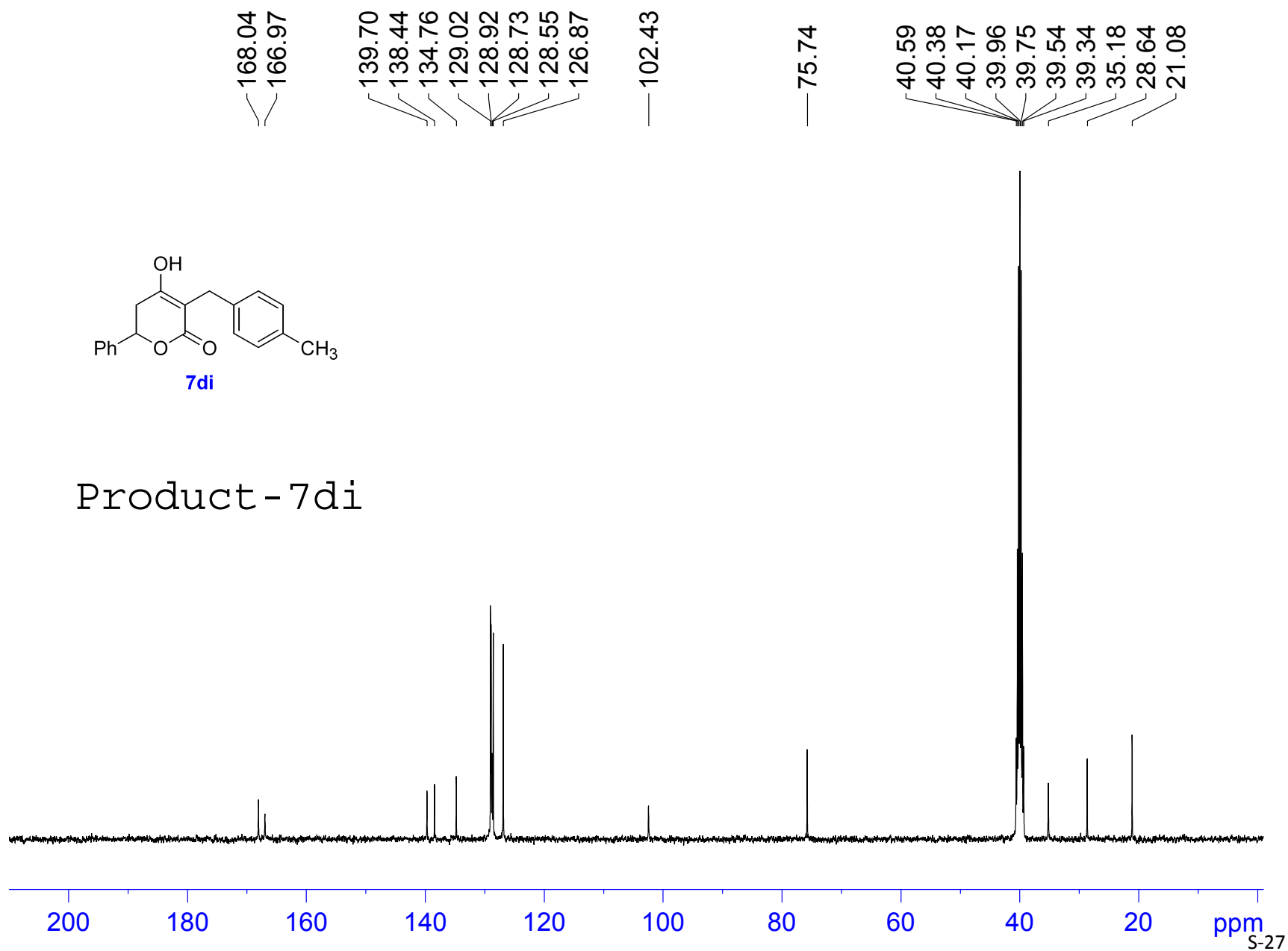
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7.467
7.450
7.431
7.422
7.402
7.387
7.166
7.147
7.094
7.075
5.500
5.493
5.471

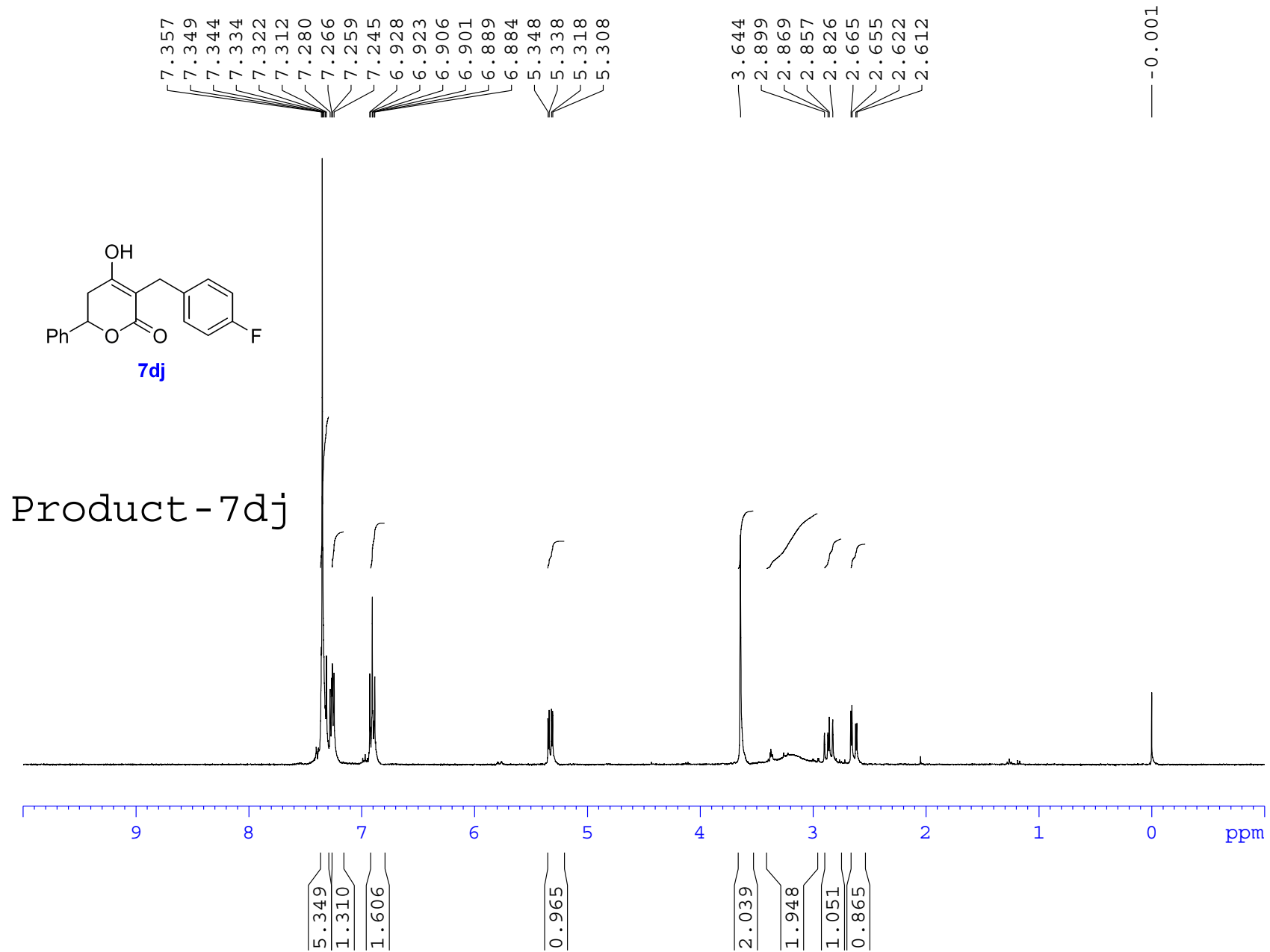
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3.043
3.012
3.000
2.970
2.790
2.747
2.550
2.293

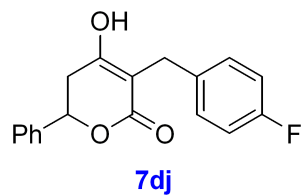
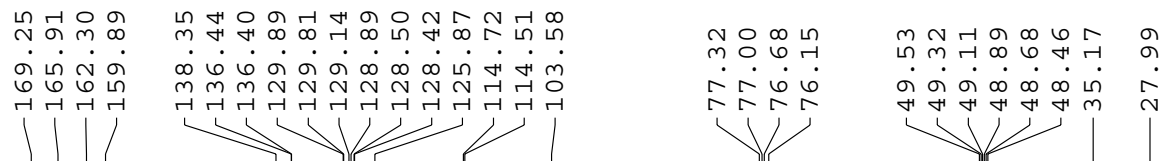


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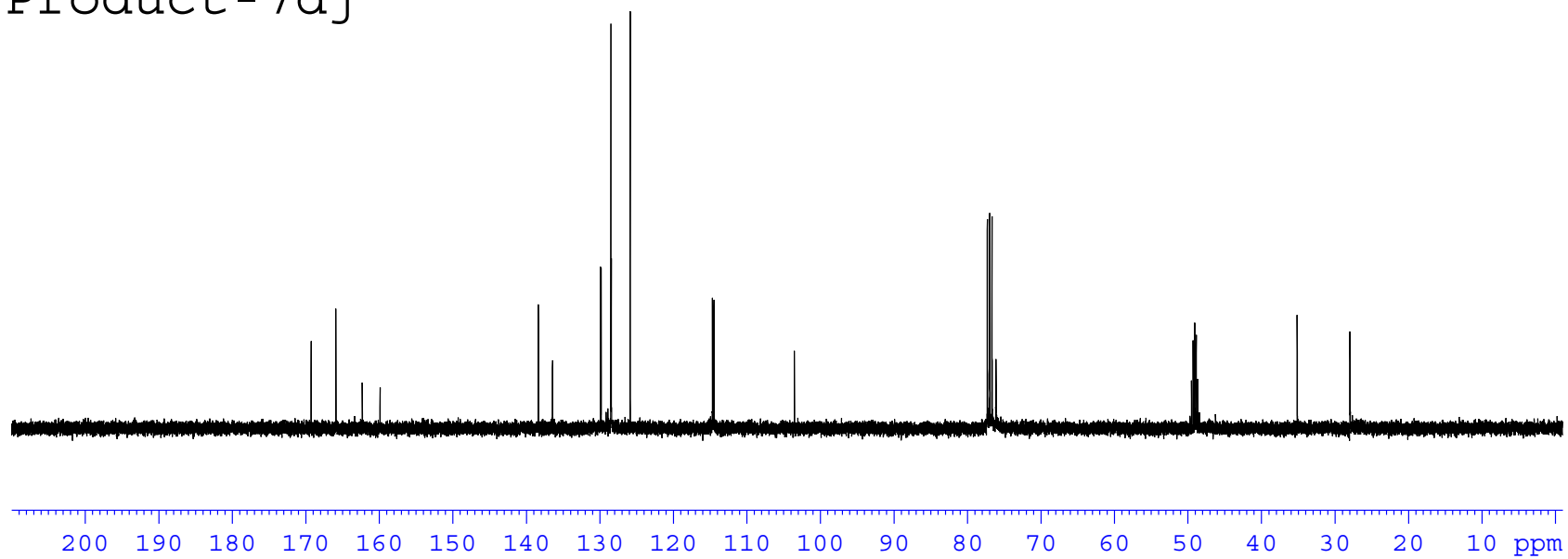


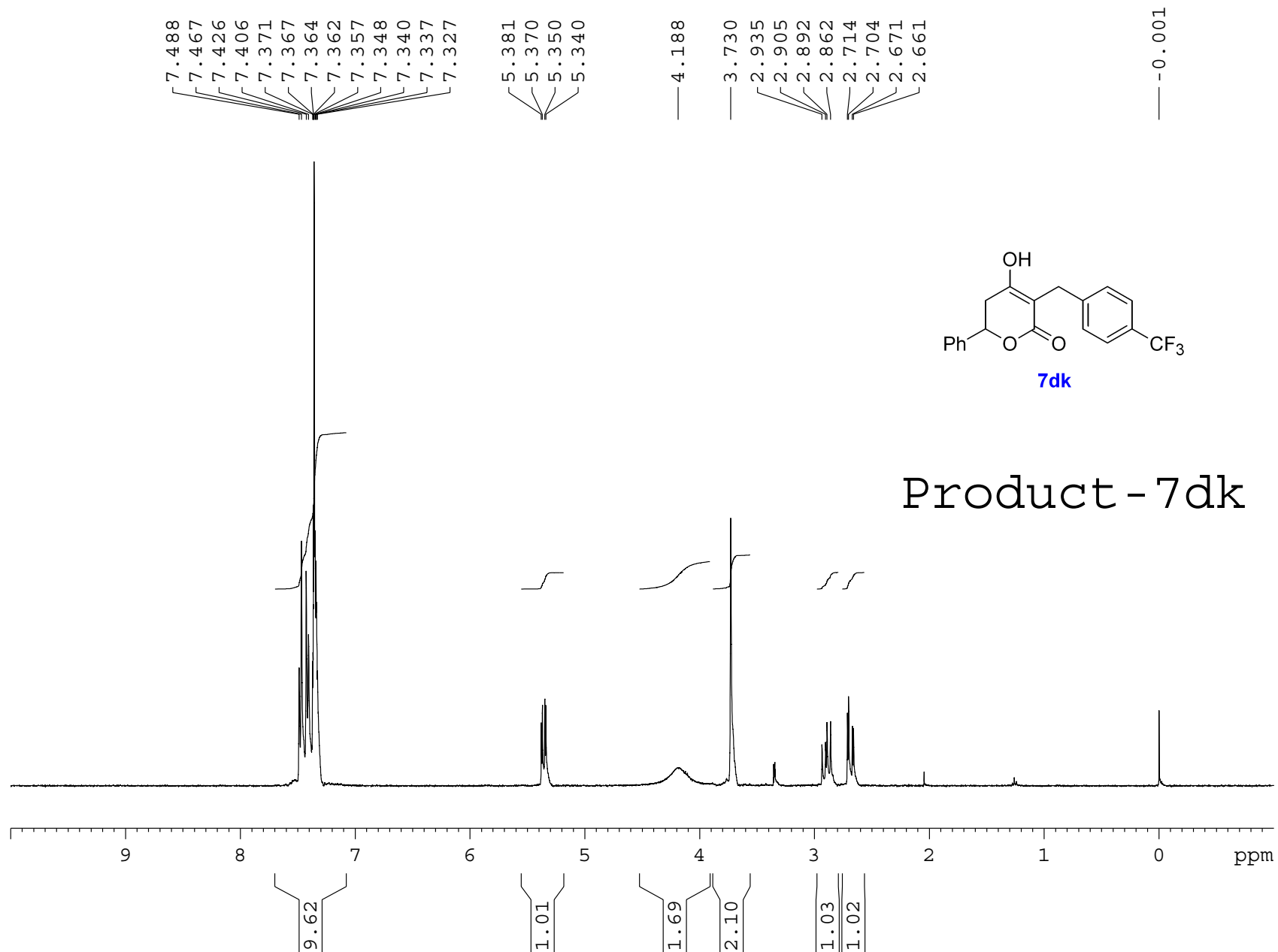


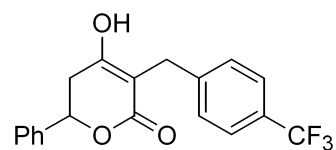




Product - 7dj

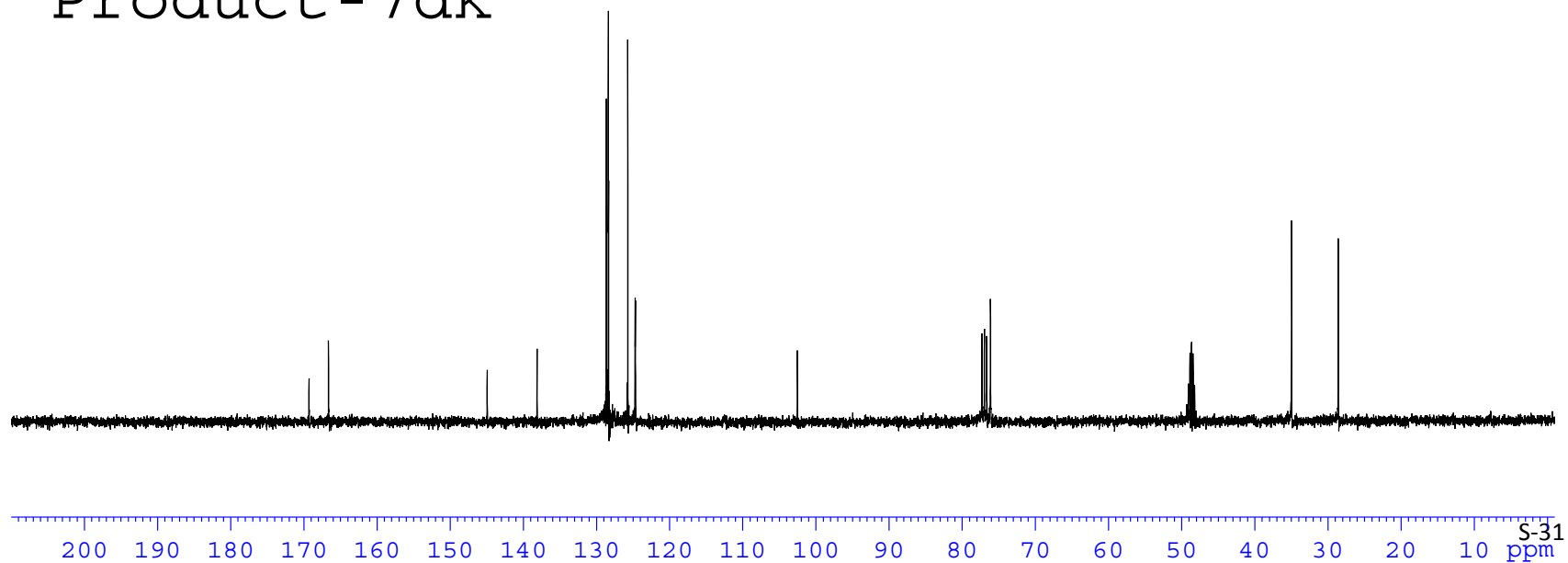






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Product - 7dk



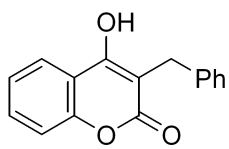
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7.497
7.331
7.316
7.288
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7.255
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7.185
7.167

3.981

2.278
2.252
2.177
2.048

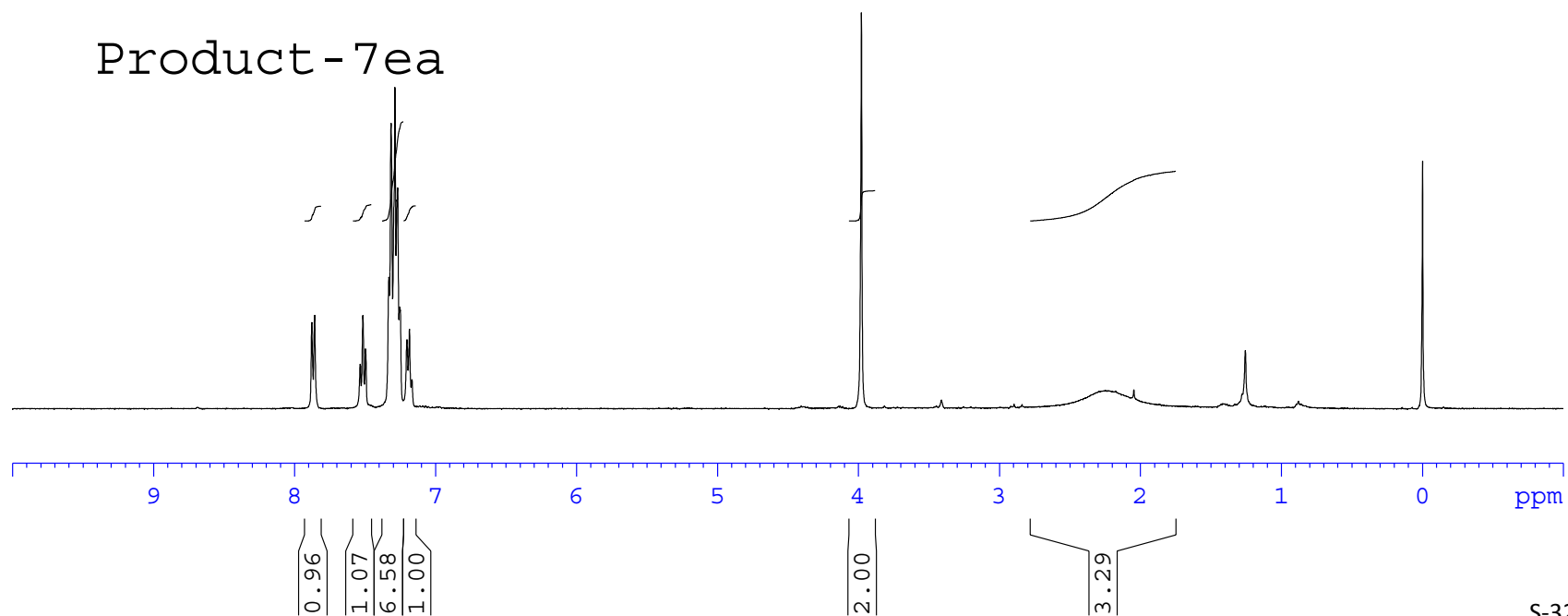
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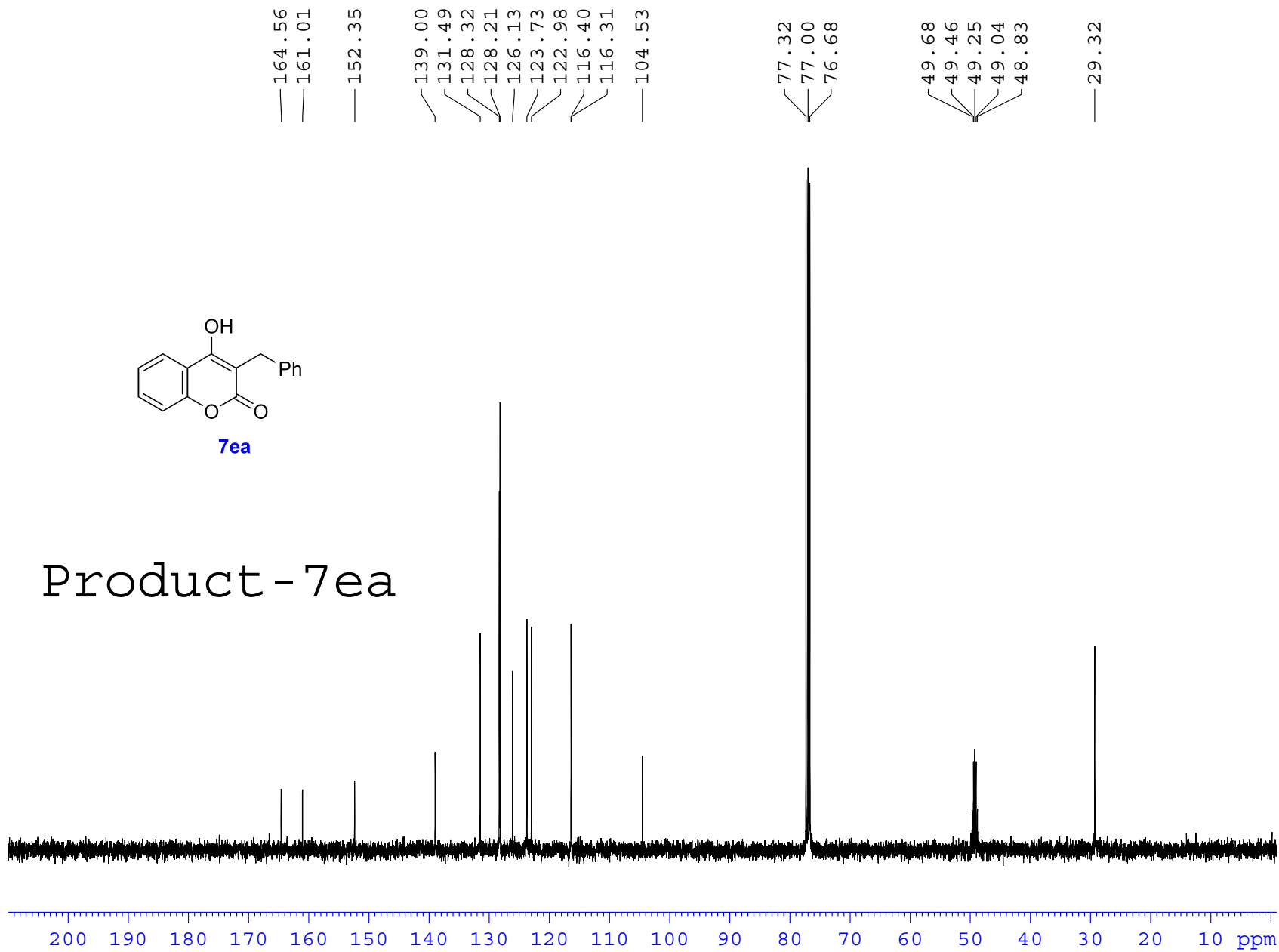
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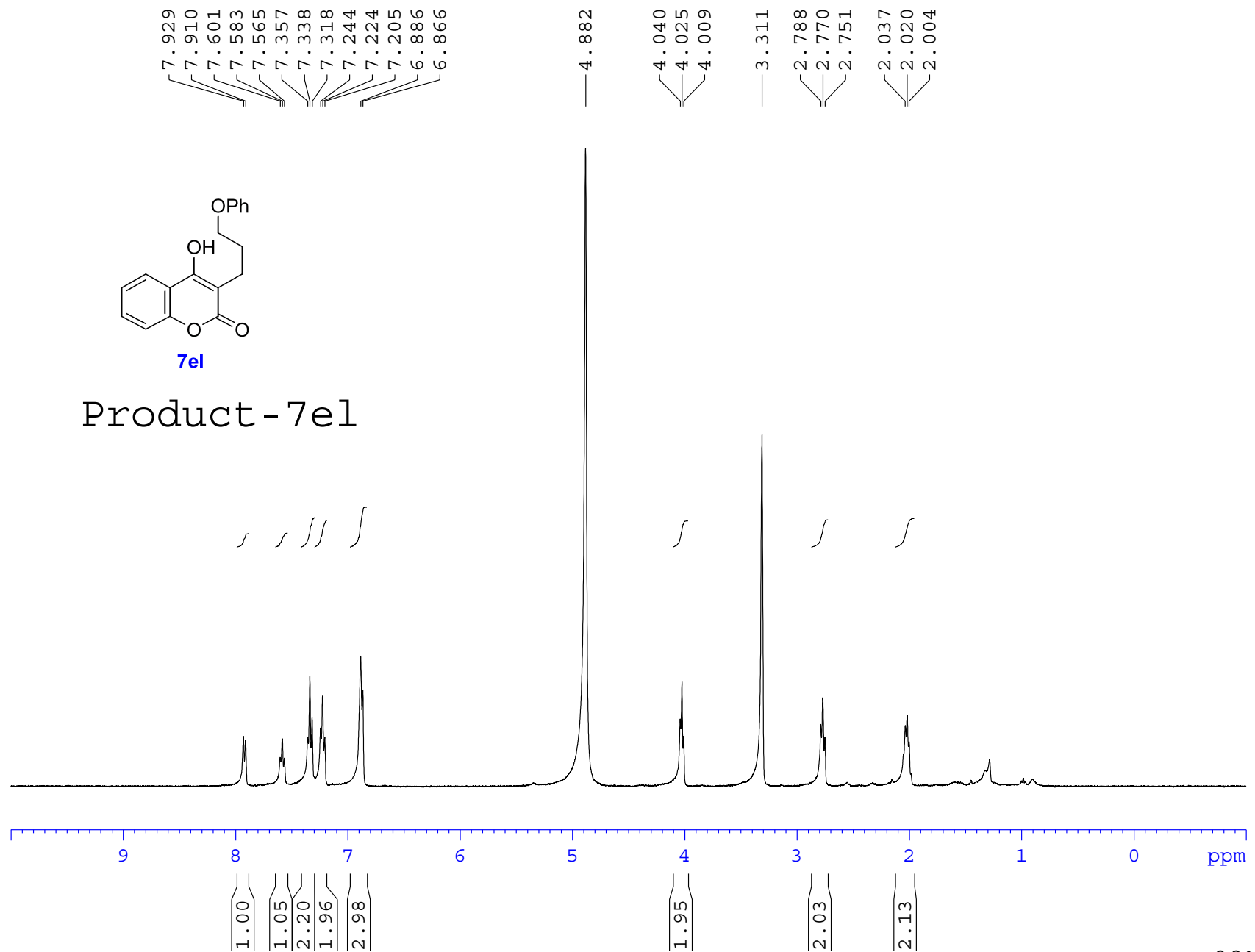


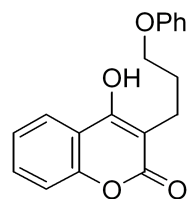
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Product - 7ea



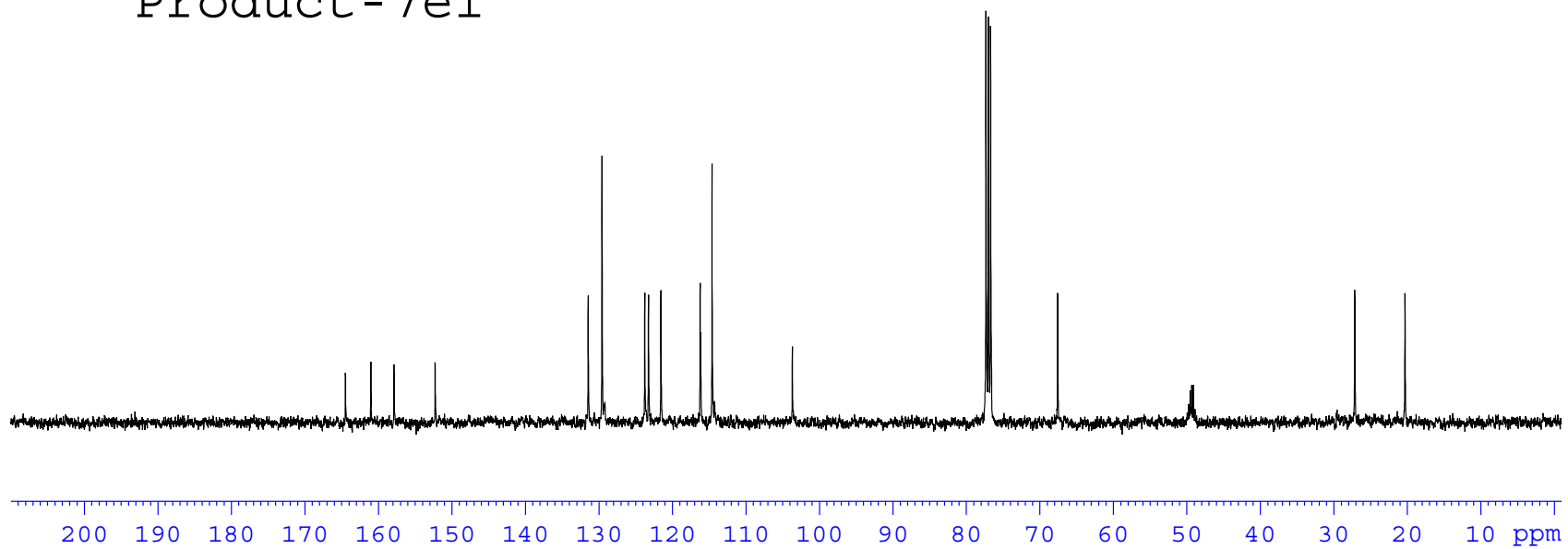


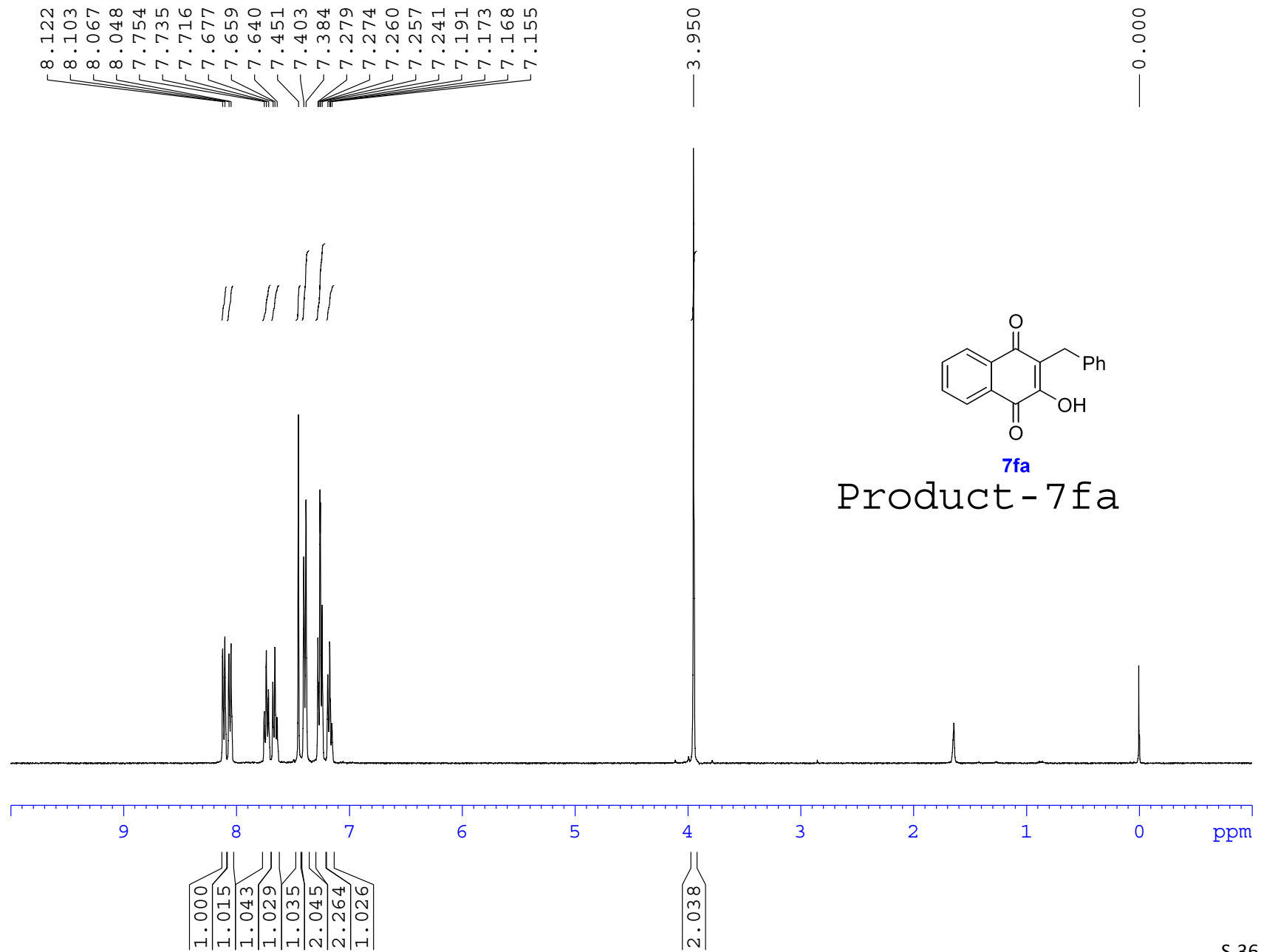




7el

Product - 7el



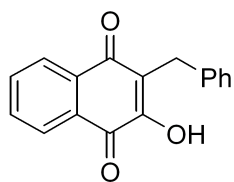


184.34
181.63

153.00
138.87
134.97
132.94
132.75
129.34
129.17
128.41
126.88
126.29
126.10
123.02

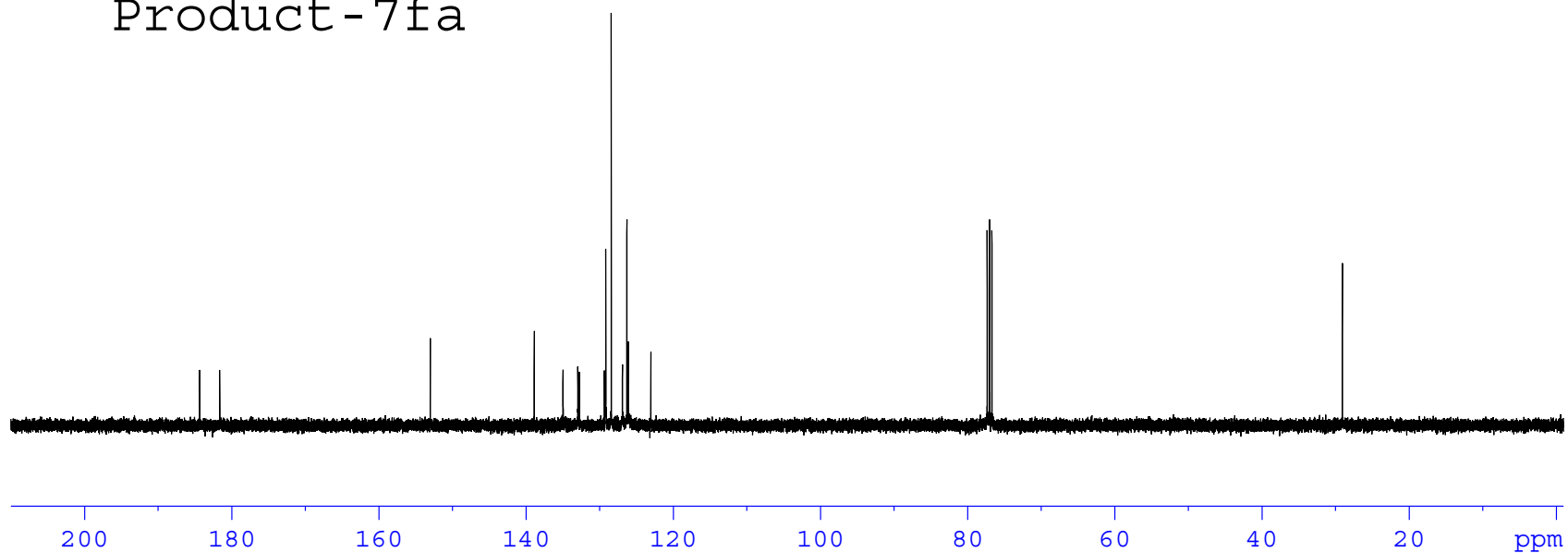
77.32
77.00
76.68

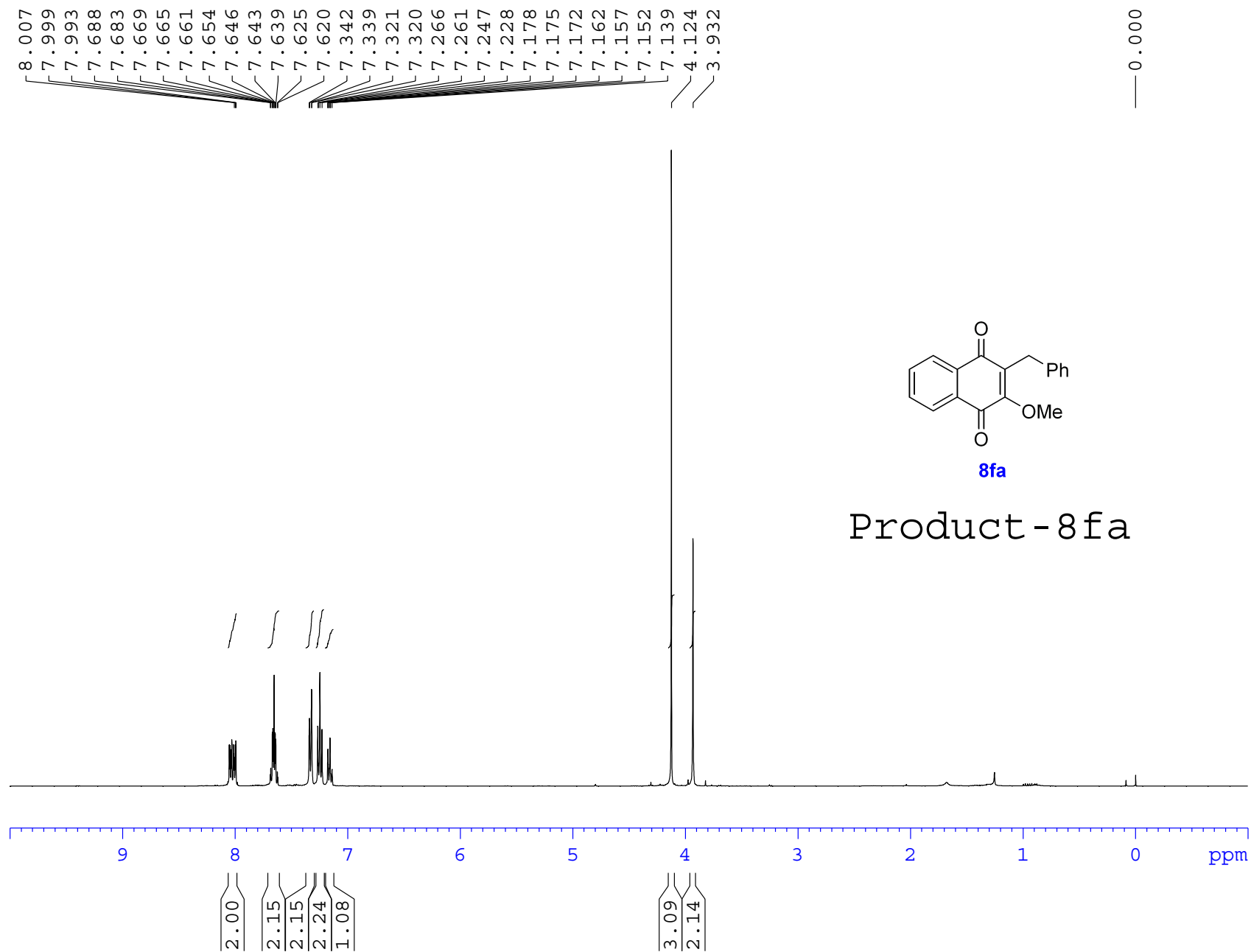
29.07

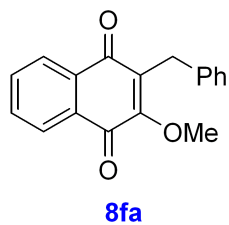
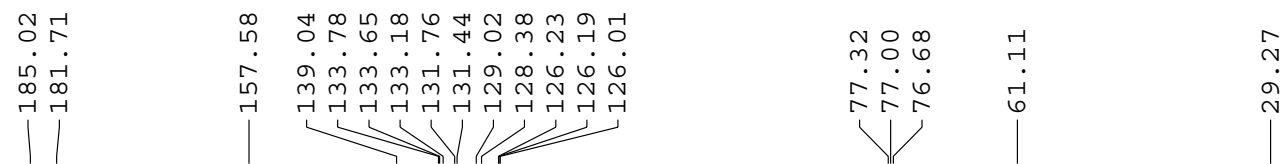


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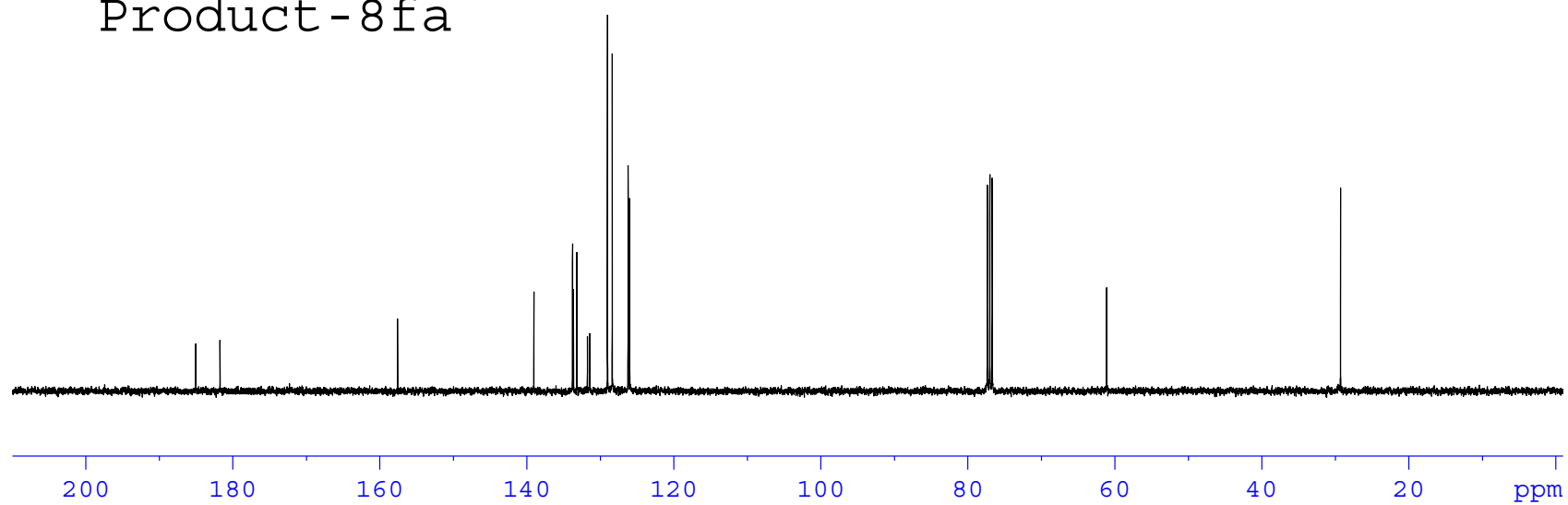
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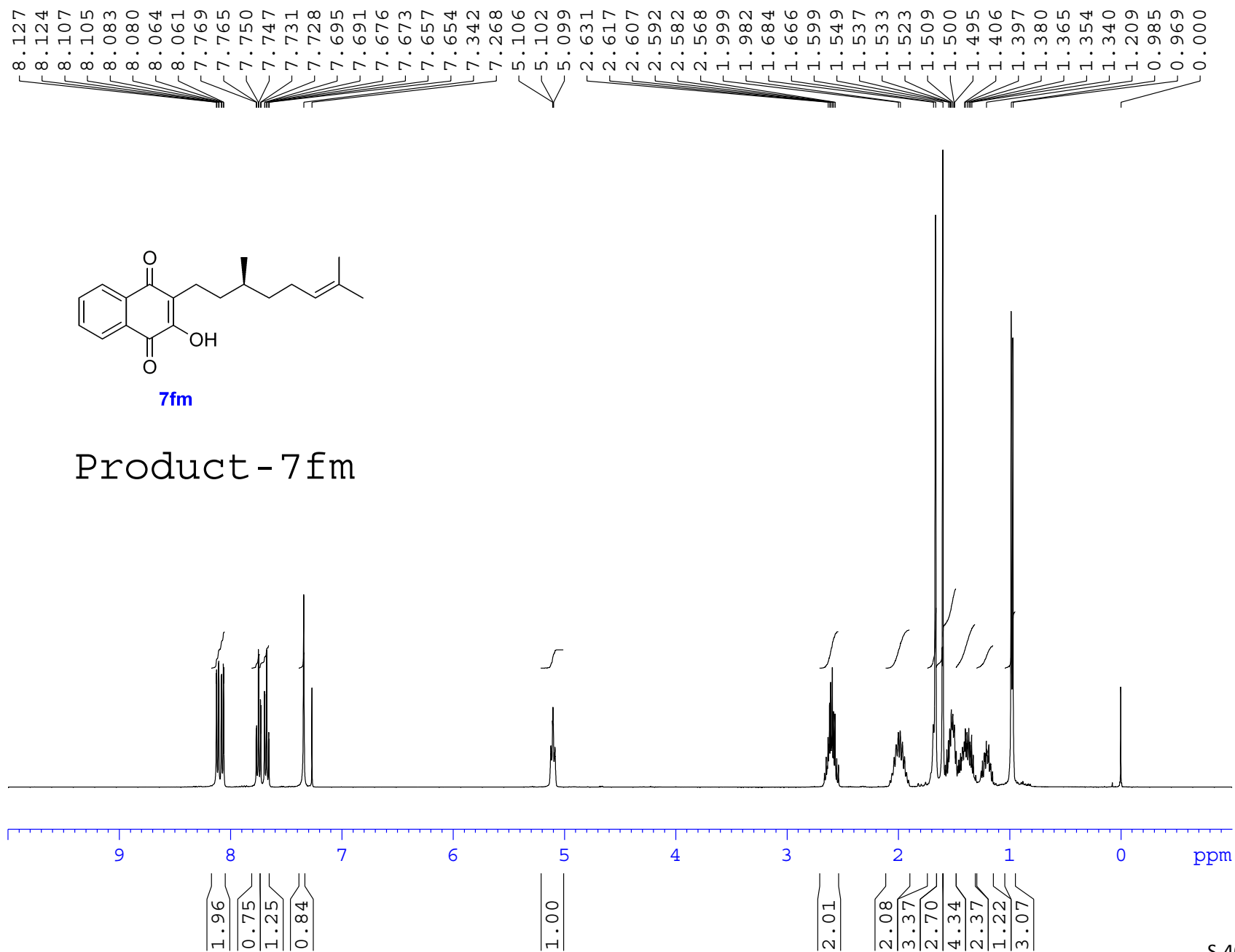






Product - 8fa



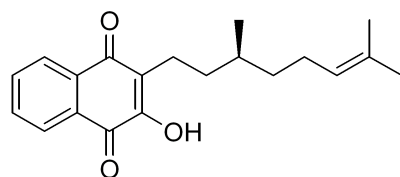


184.630
181.431

152.892
134.773
132.962
132.799
131.048
129.447
126.720
126.012
125.149
124.897

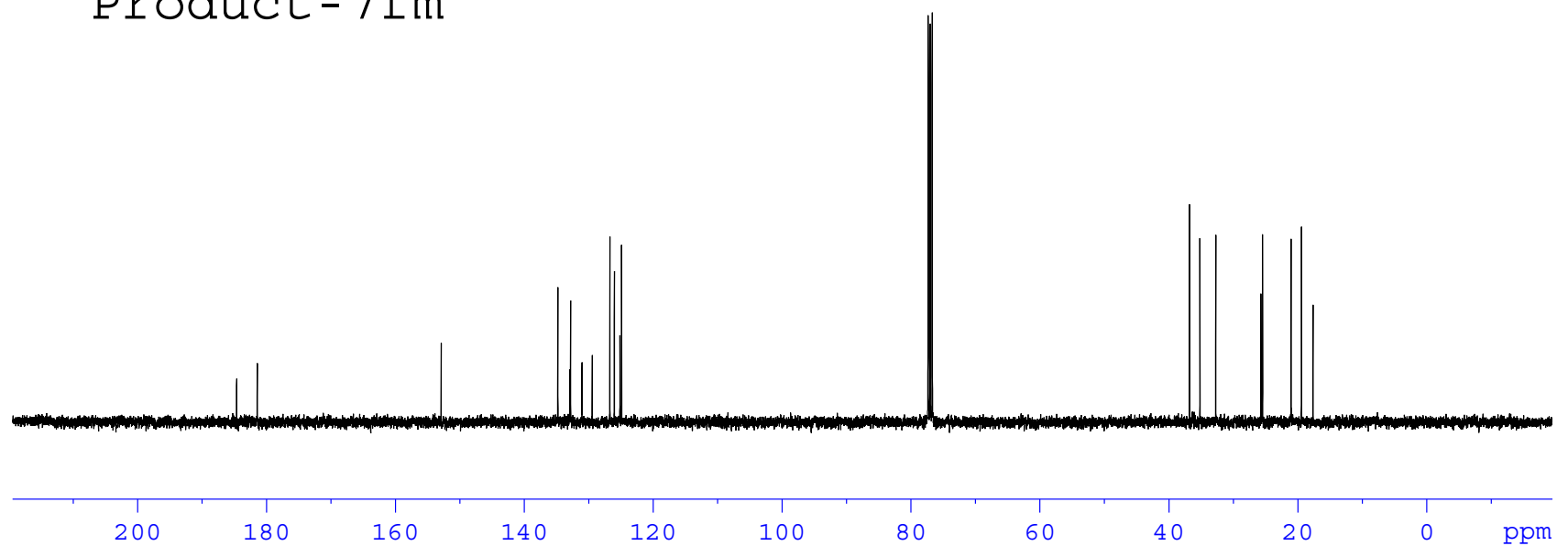
77.316
76.998
76.681

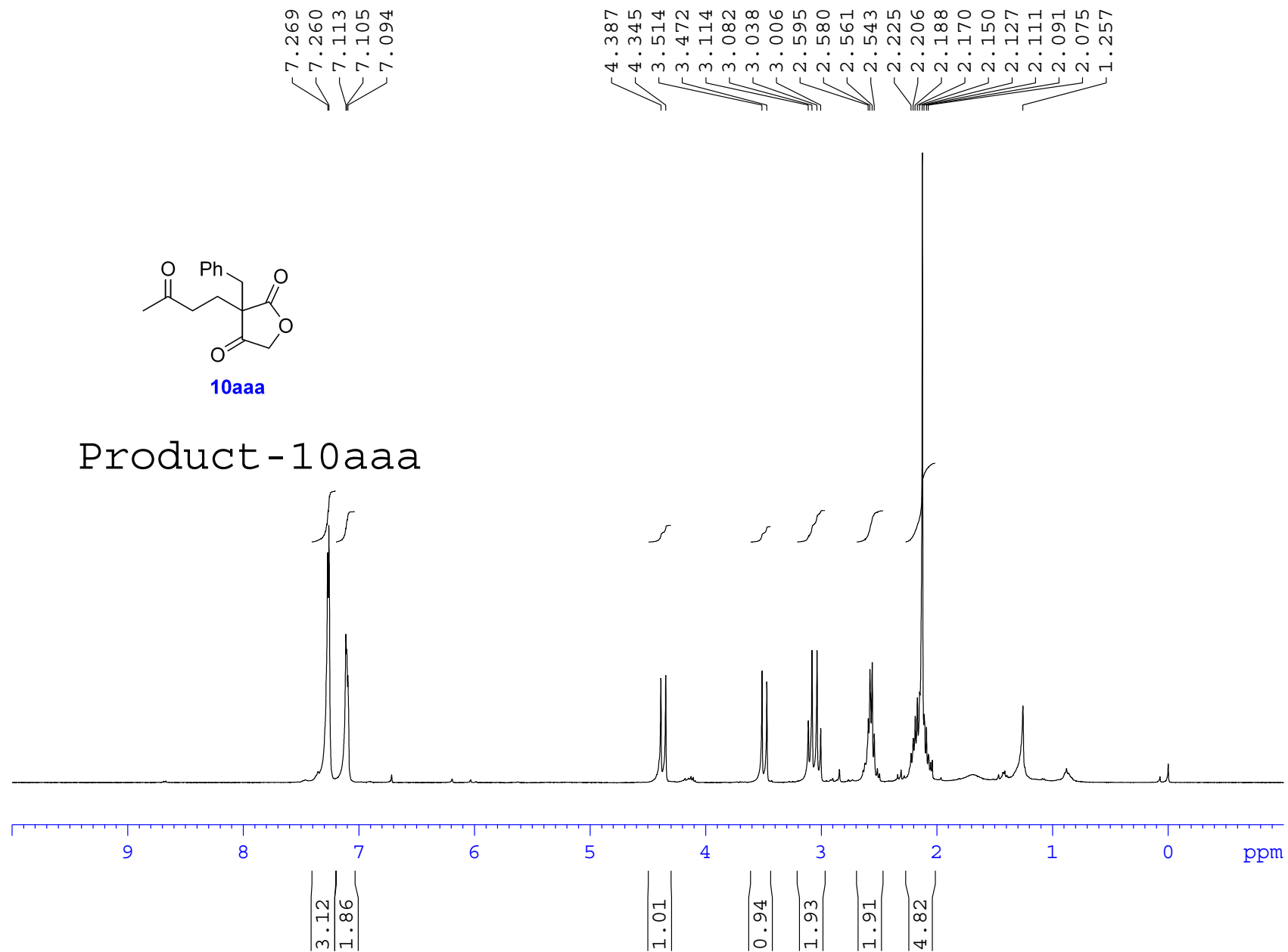
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35.141
32.684
25.678
25.440
21.004
19.385
17.593

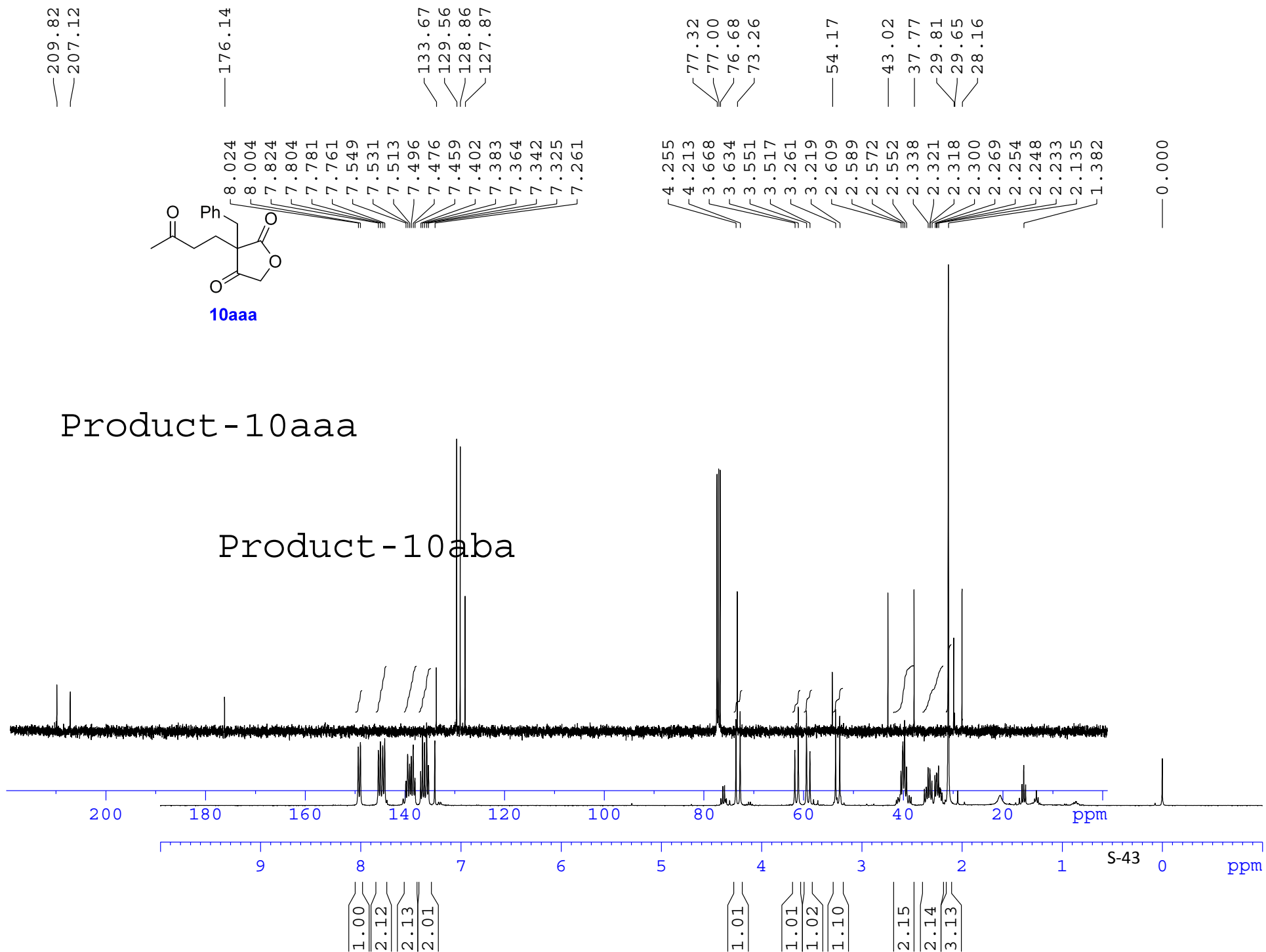


7fm

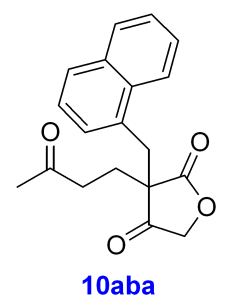
Product - 7fm







209.60
207.14



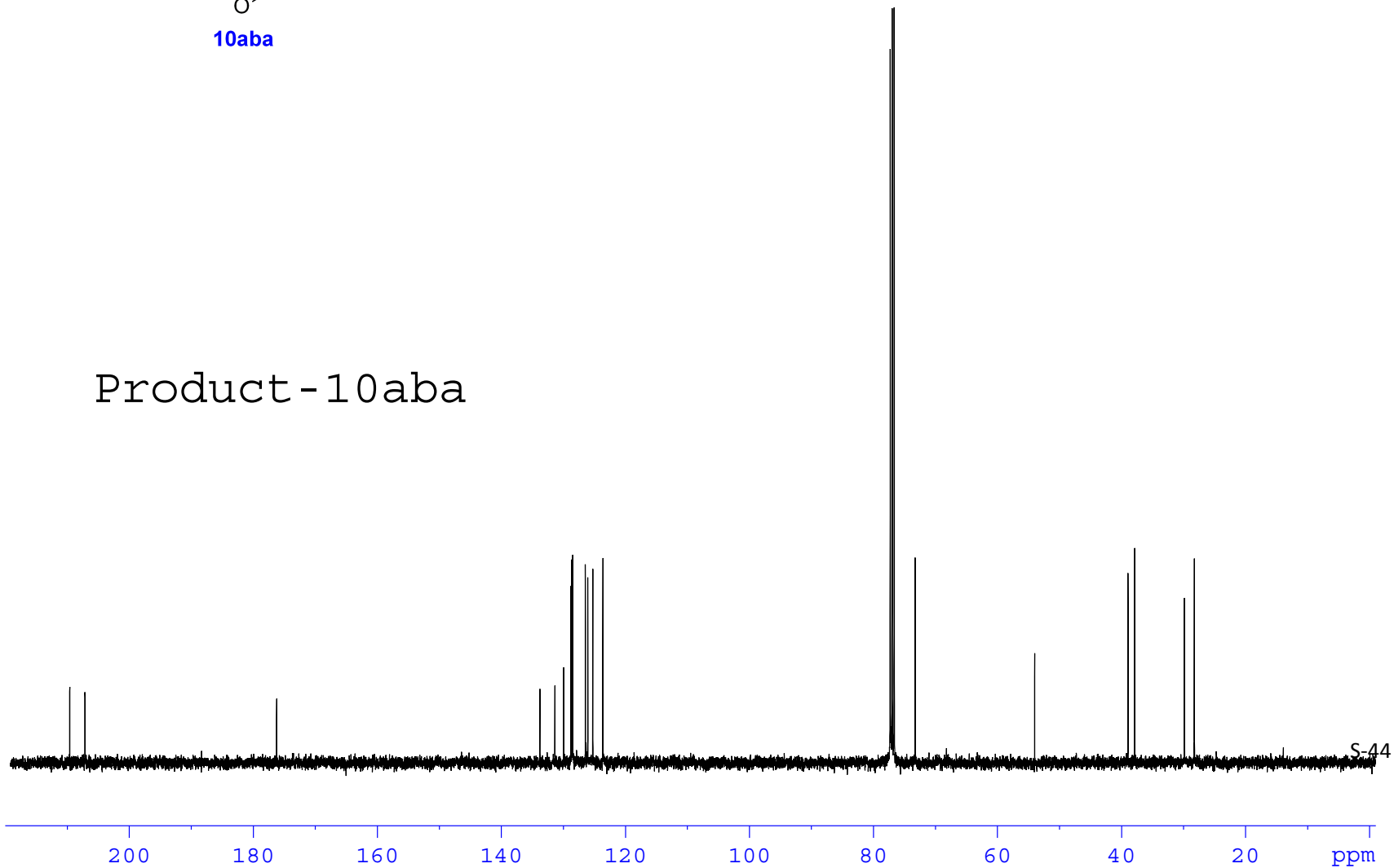
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131.39
129.99
128.82
128.67
128.53
126.48
126.10
125.29
123.66

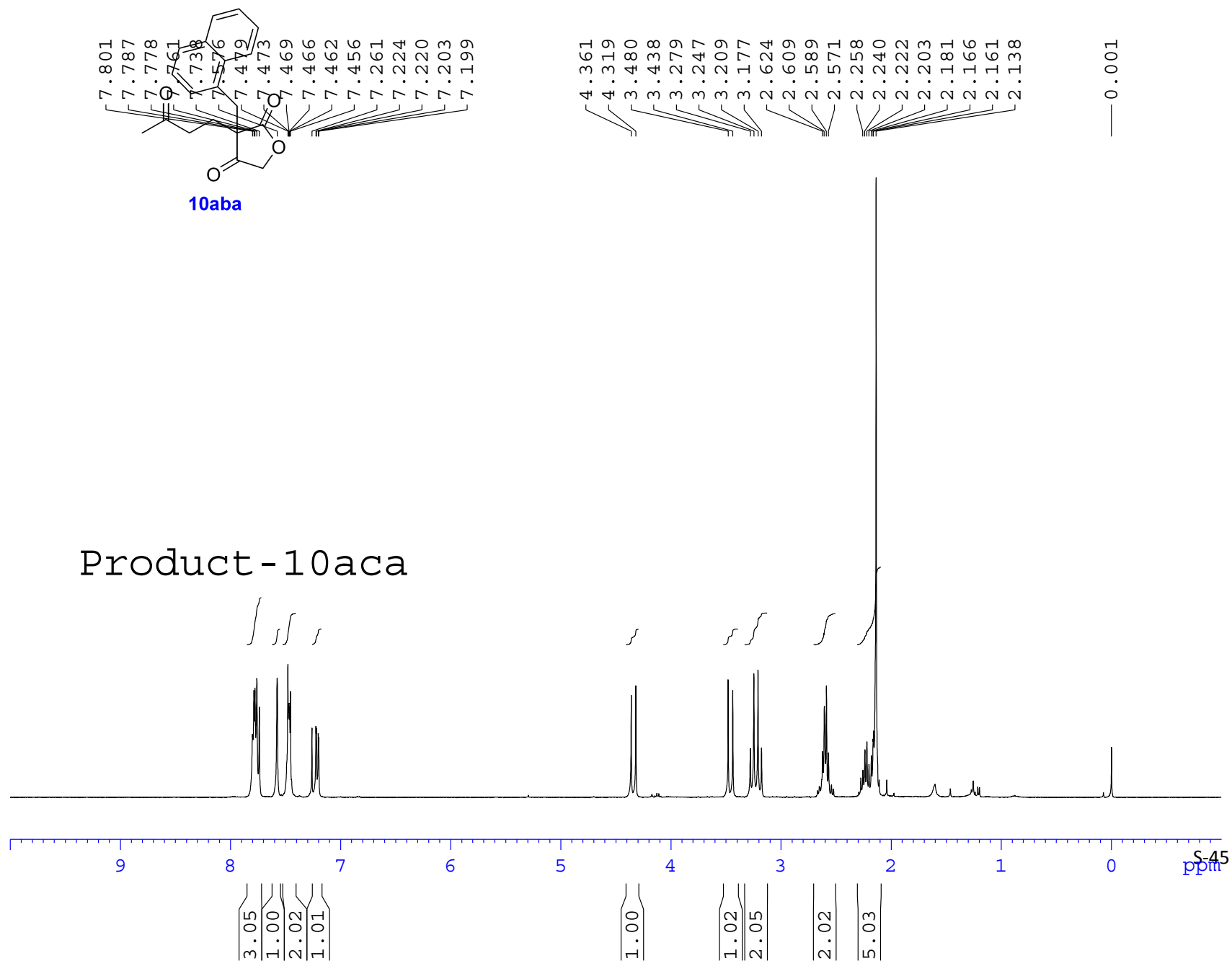
77.32
77.00
76.68
73.29

54.03

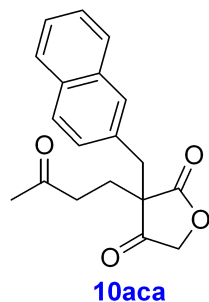
38.98
37.91
29.88
28.28

Product - 10aba





— 209.84
— 207.11



133.22
132.62
131.18
128.68
128.64
127.89
127.60
127.24
126.41
126.29

77.32
77.00
76.68
73.34

— 54.25

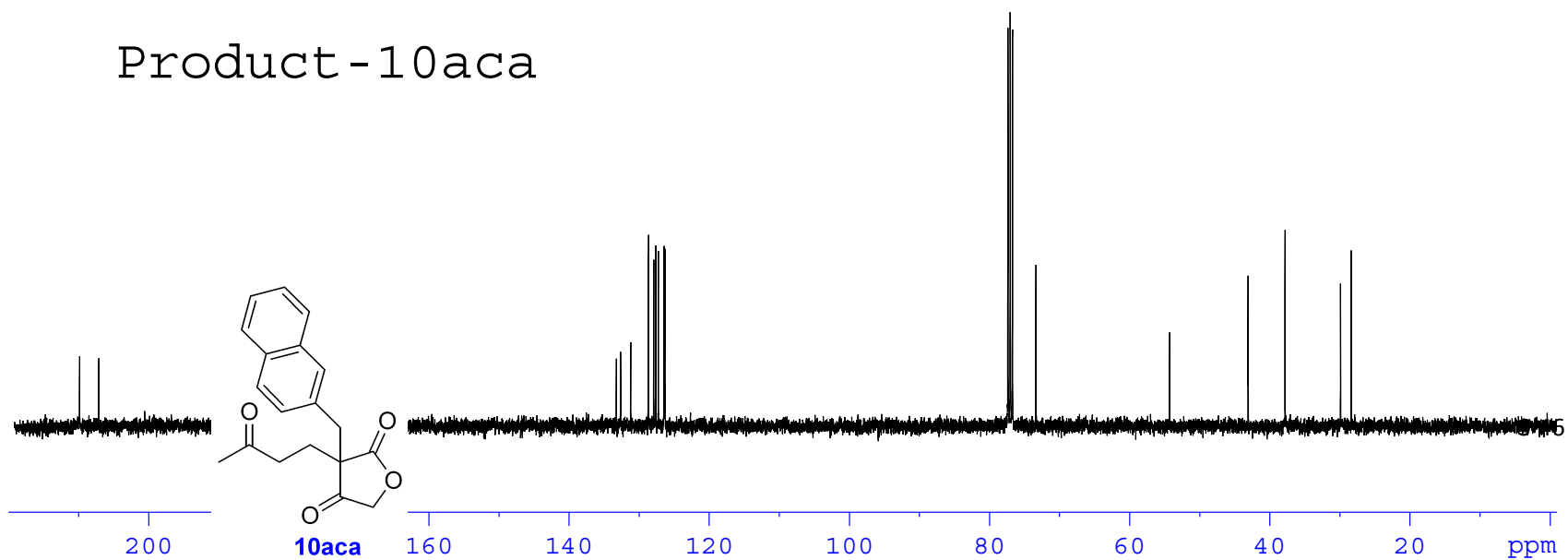
— 43.05

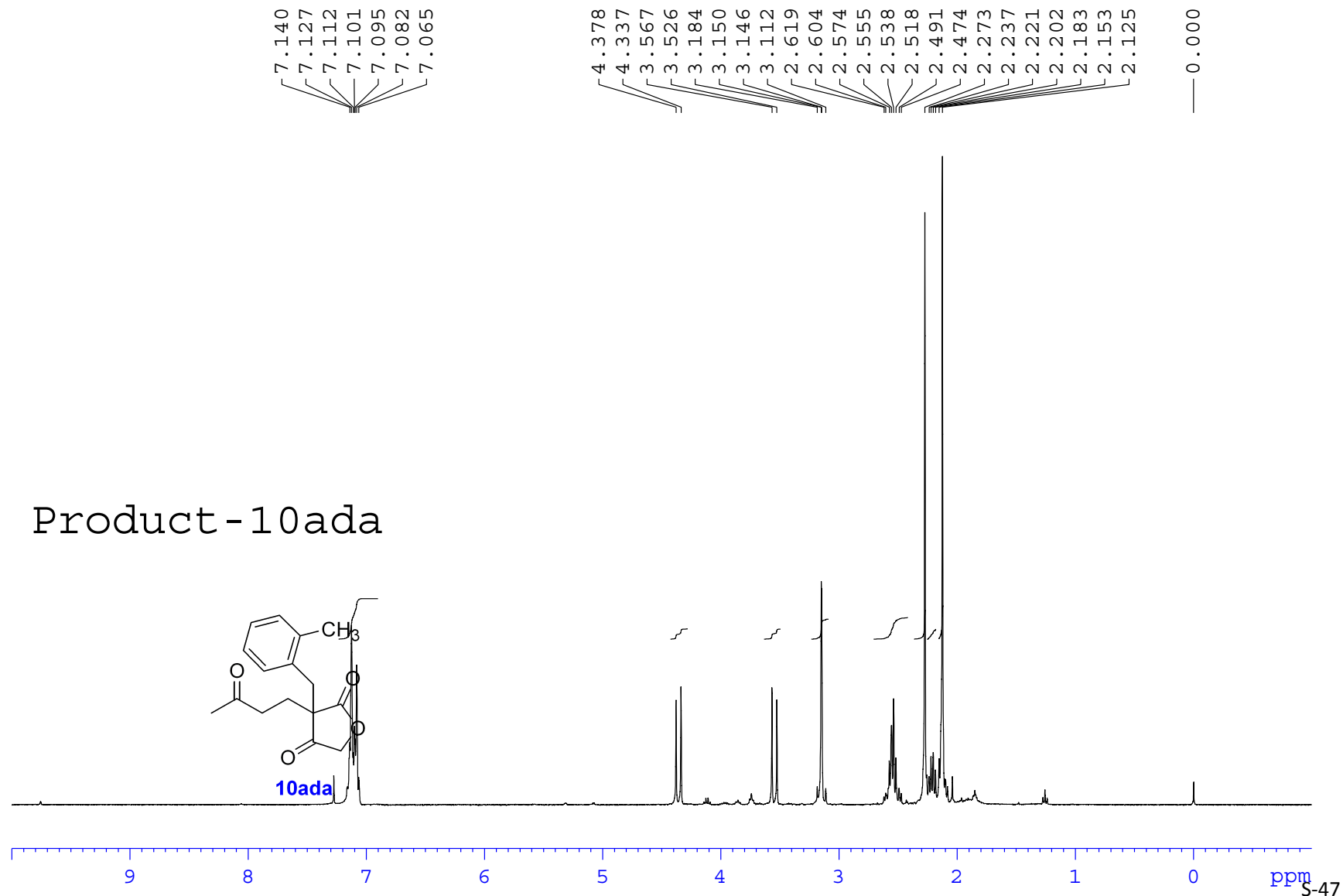
— 37.78

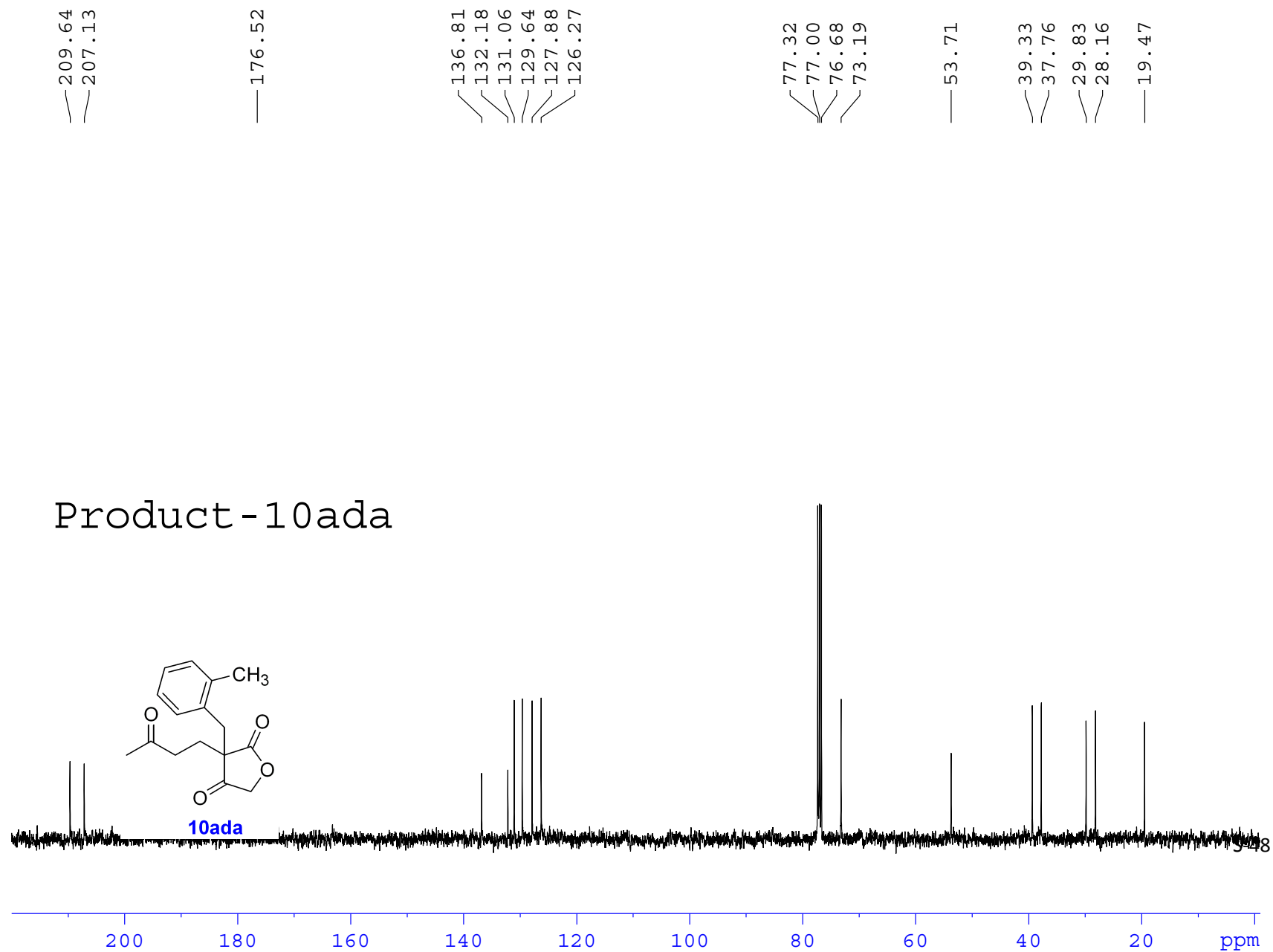
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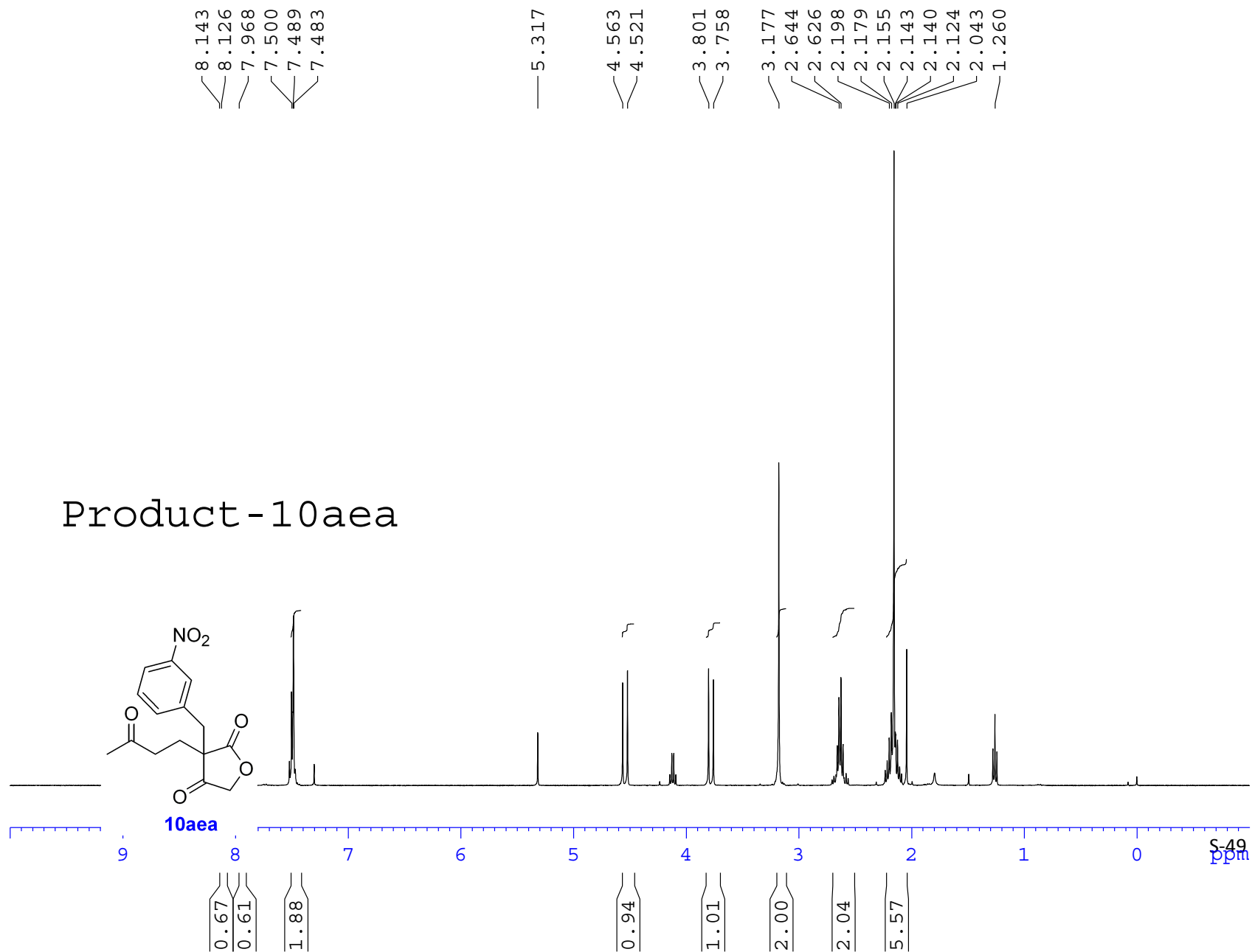
— 28.32

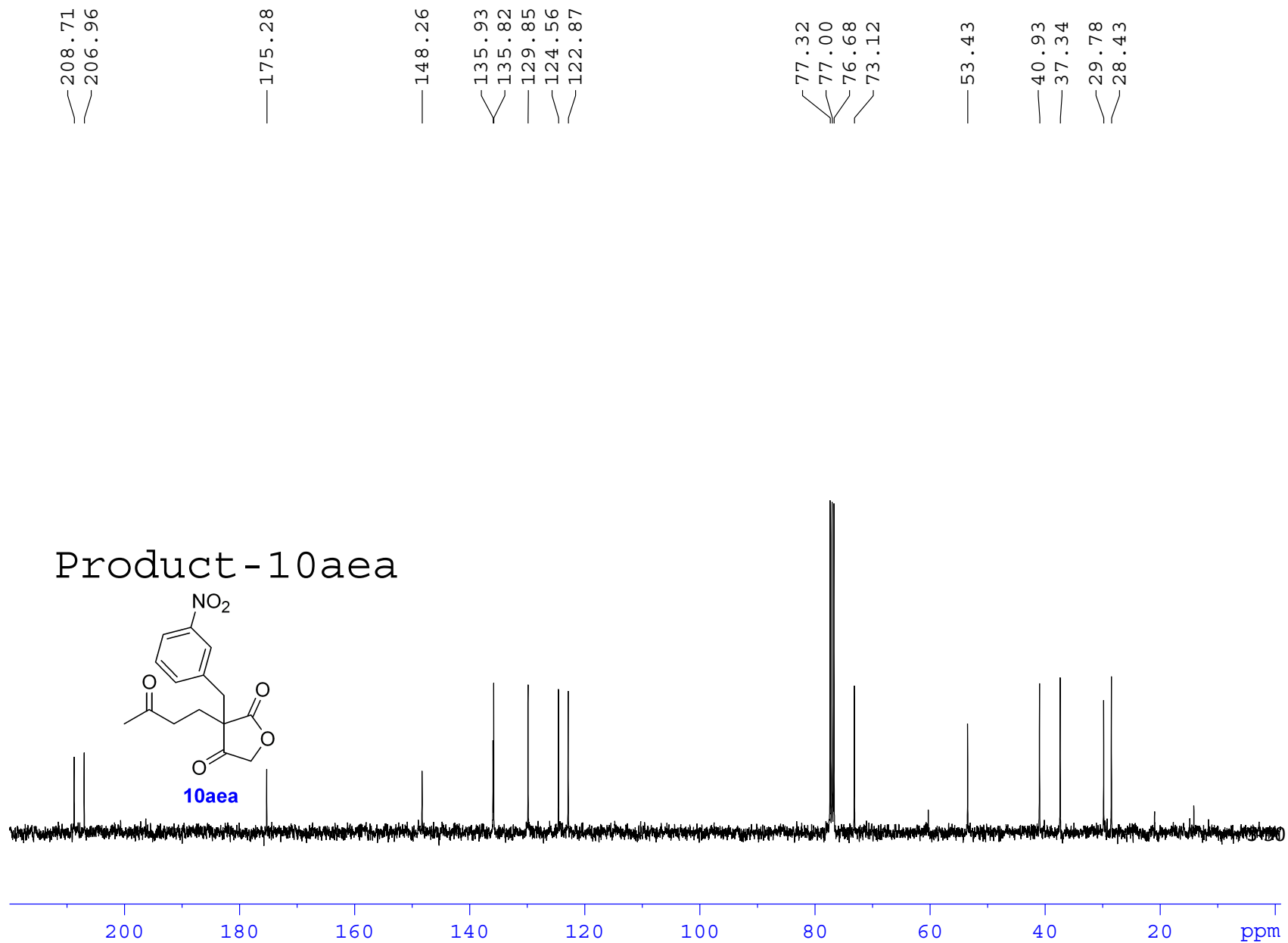
Product -10aca

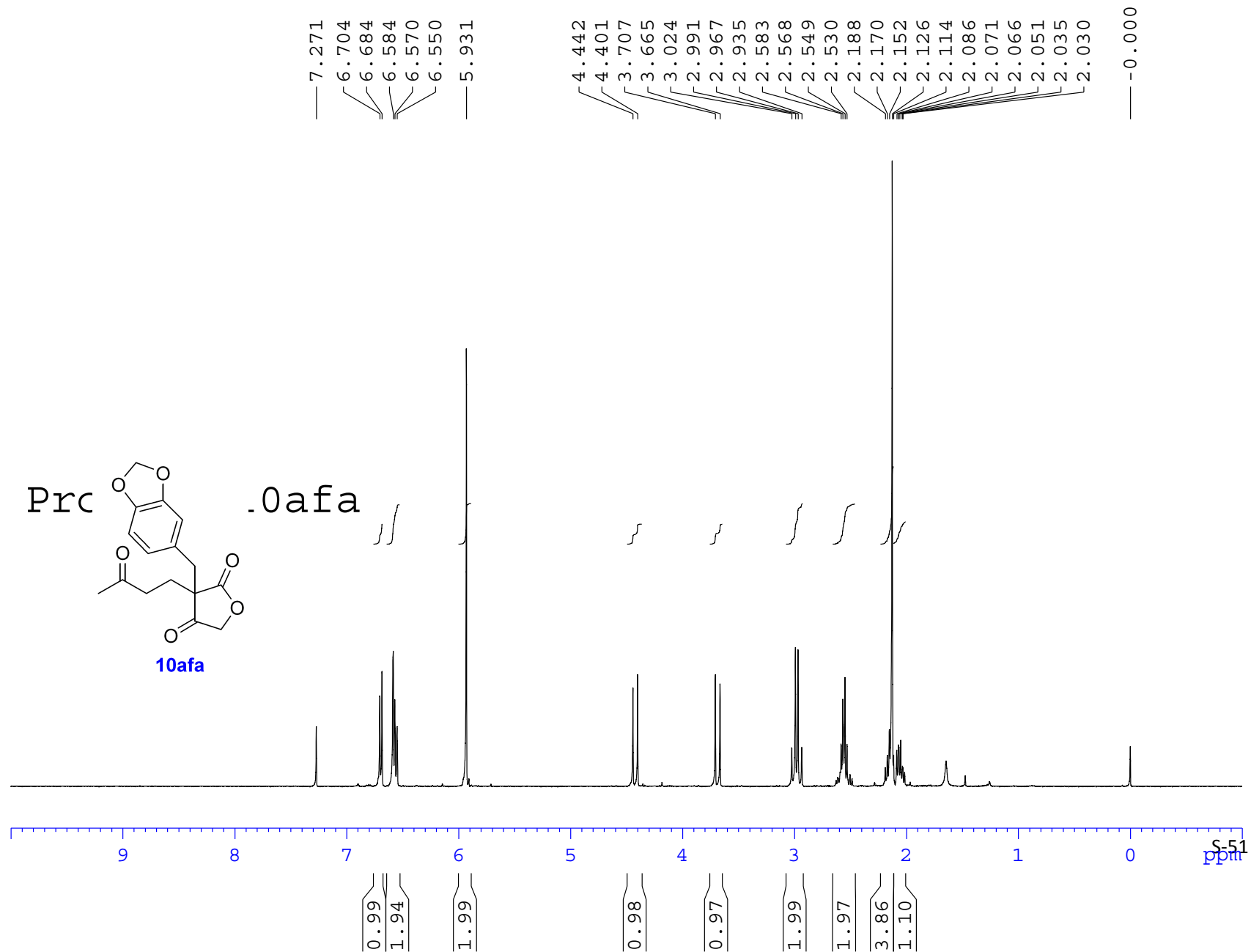


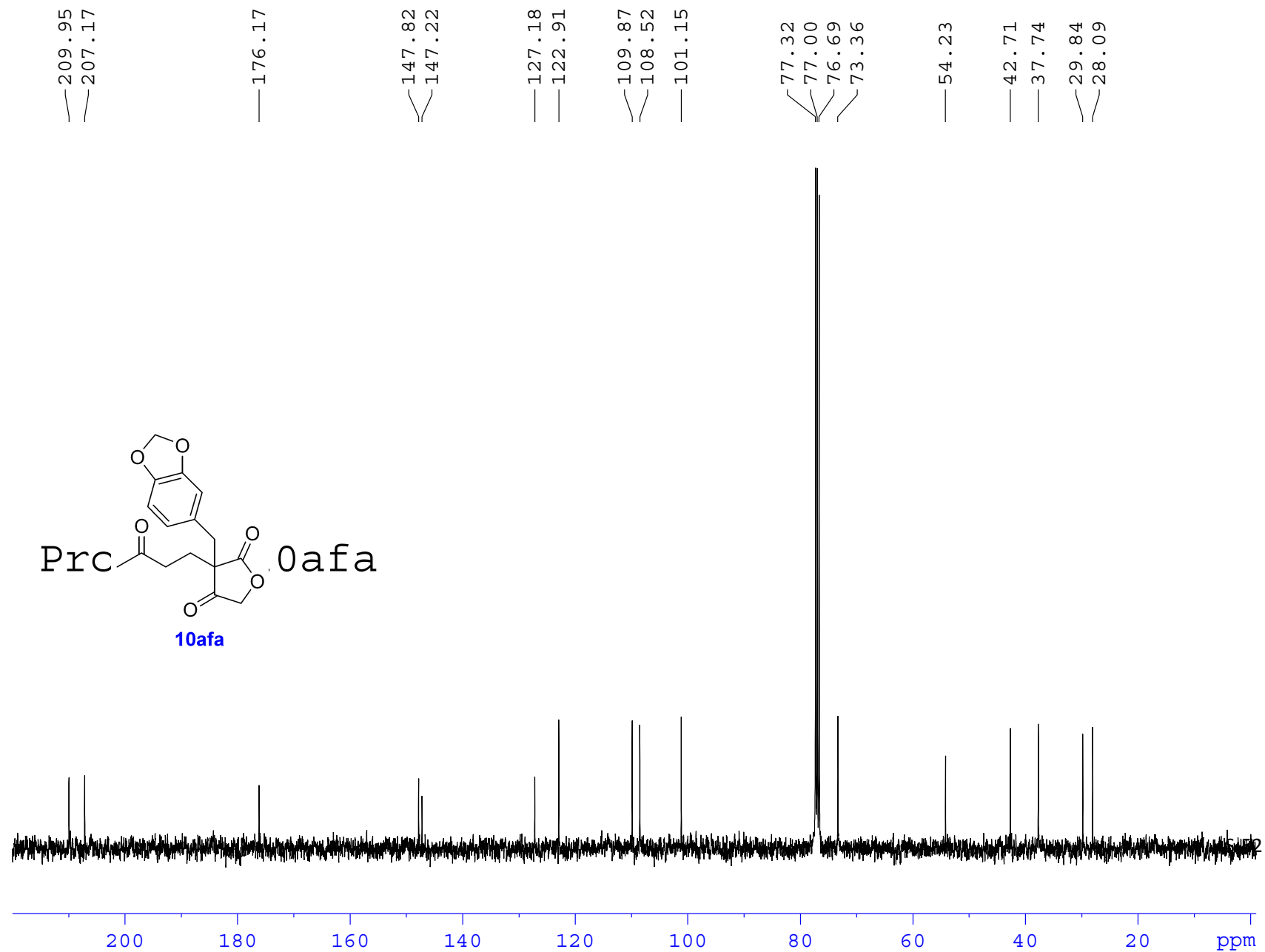


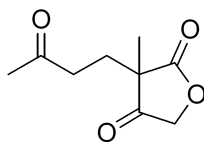






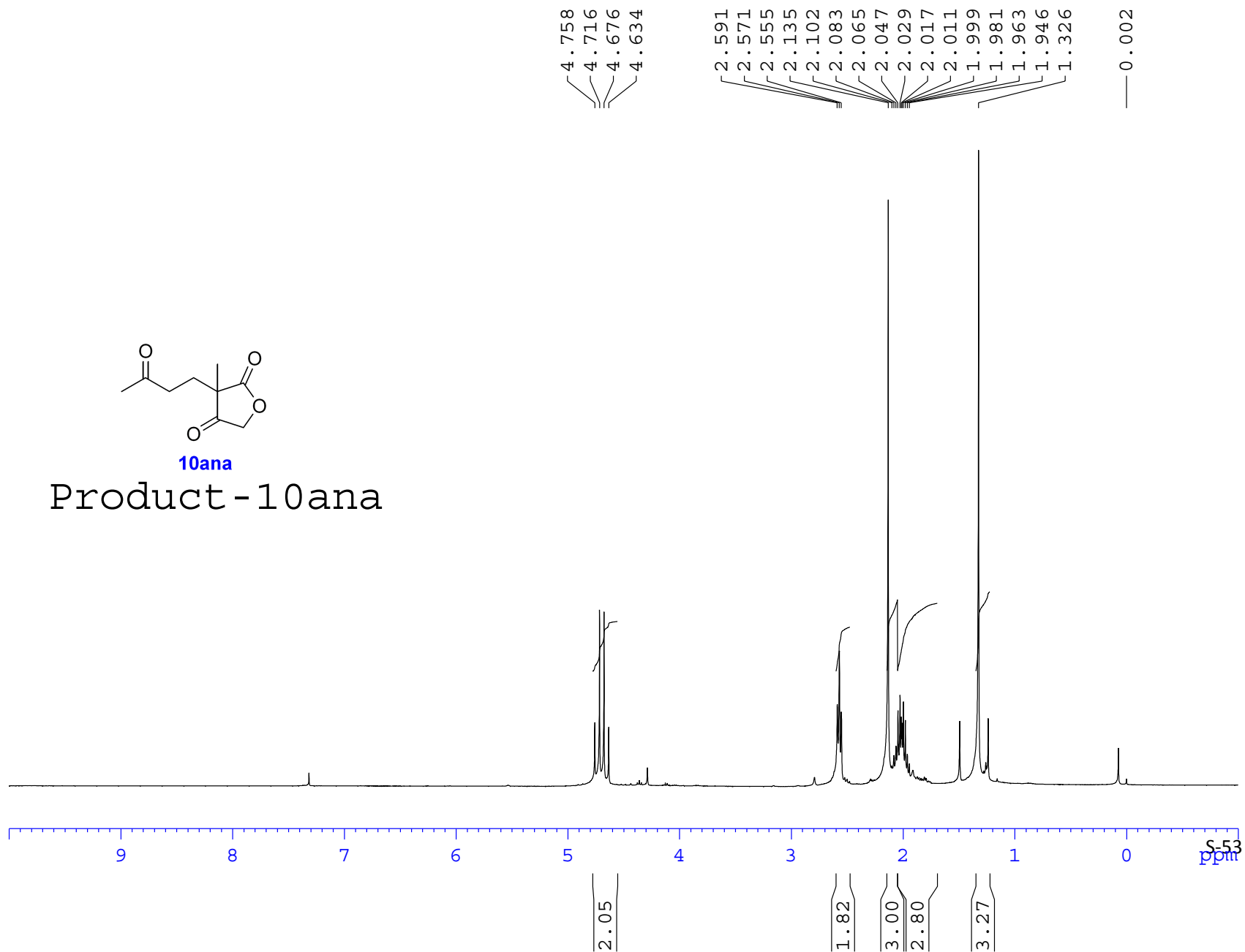






10ana

Product-10ana



209.046
207.350

176.754

77.319
77.000
76.681
72.167

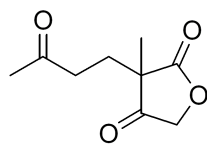
46.420

37.247

29.804

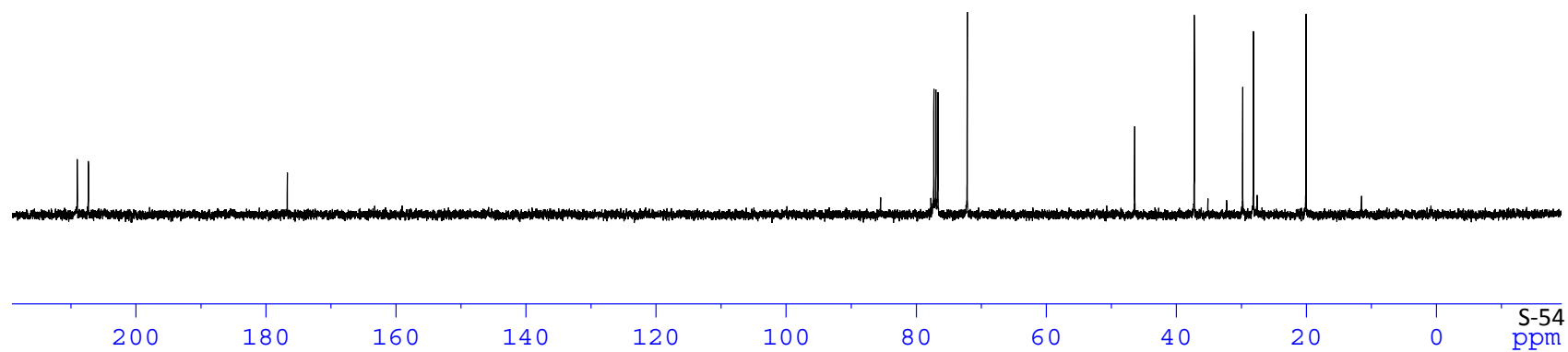
28.142

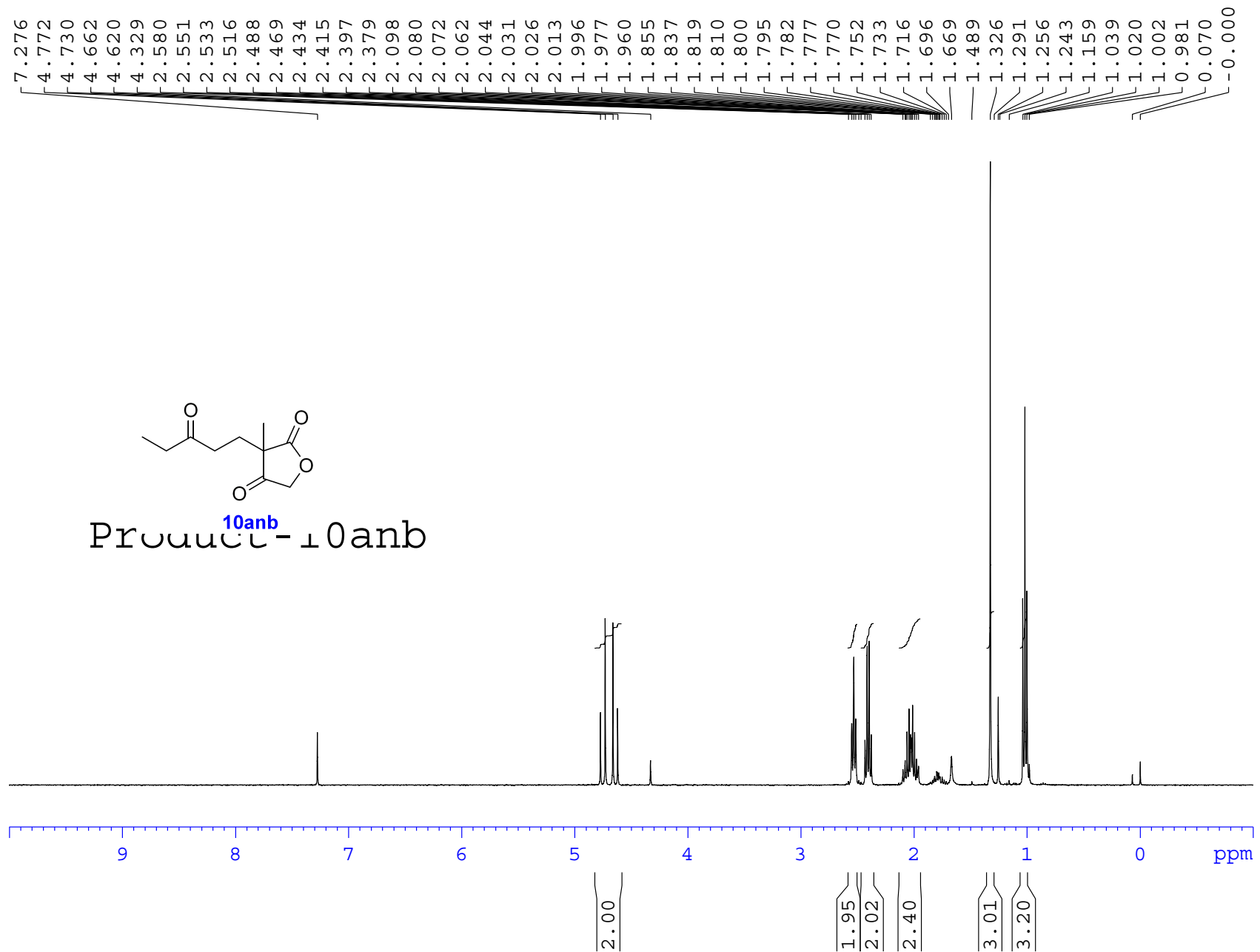
20.052



10ana

Product-10ana





210.28
209.05

176.85

77.32
77.00
76.68
72.26

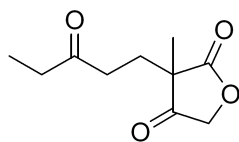
46.61

36.03
35.94

28.32

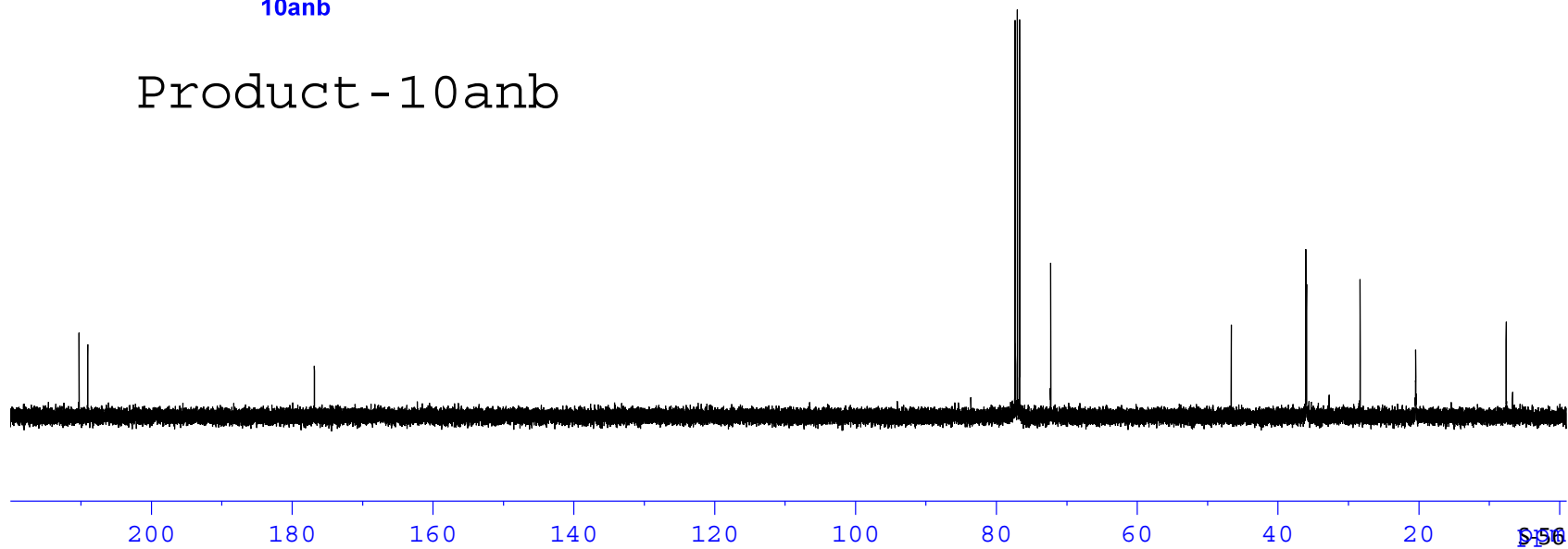
20.43

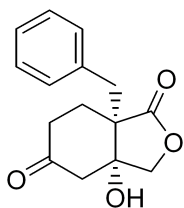
7.57



10anb

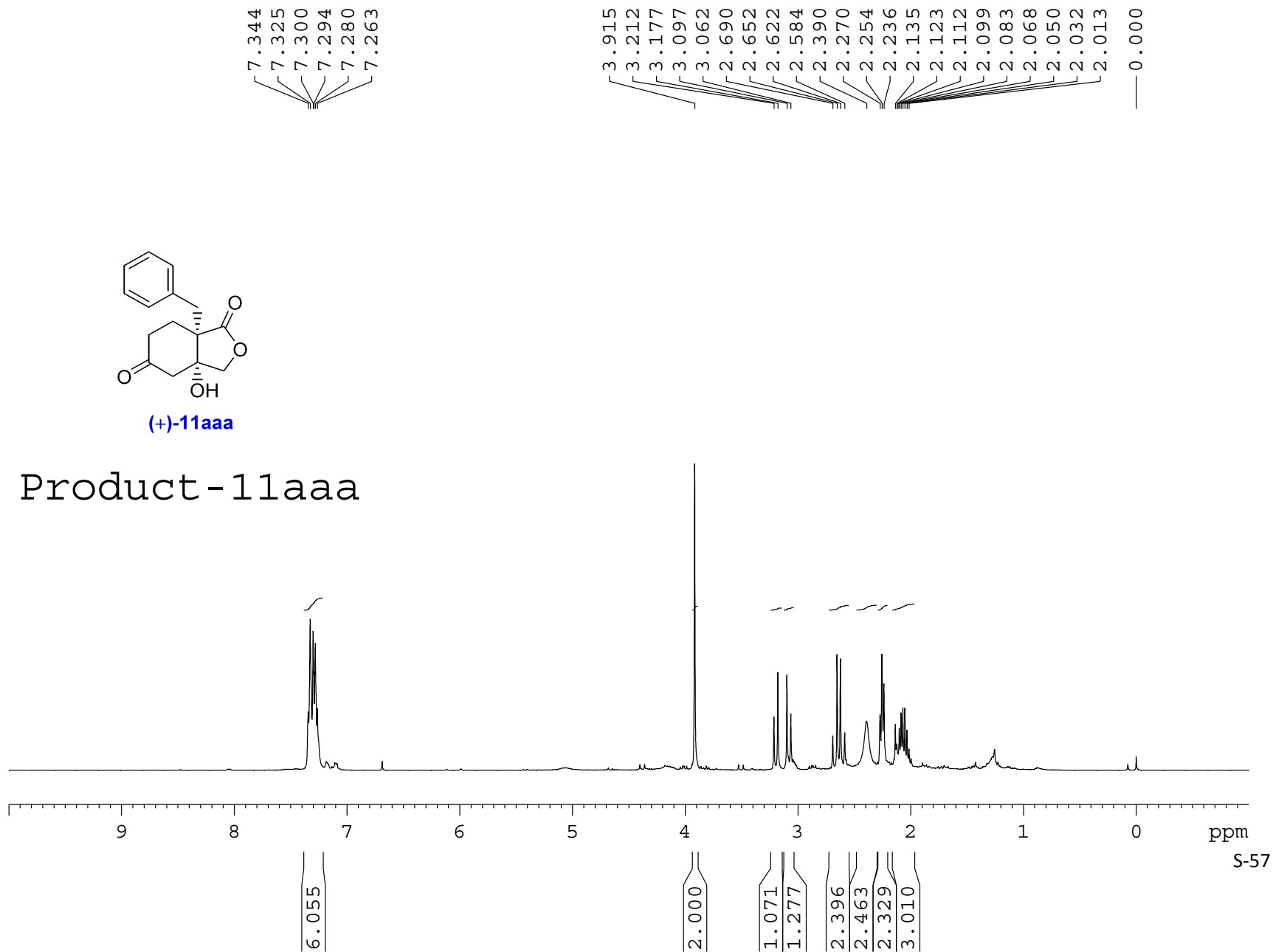
Product - 10anb





(+)-11aaa

Product - 11aaa



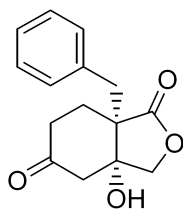
— 209.06

— 178.57

135.75
130.66
129.48
128.82
128.26
128.01
127.18

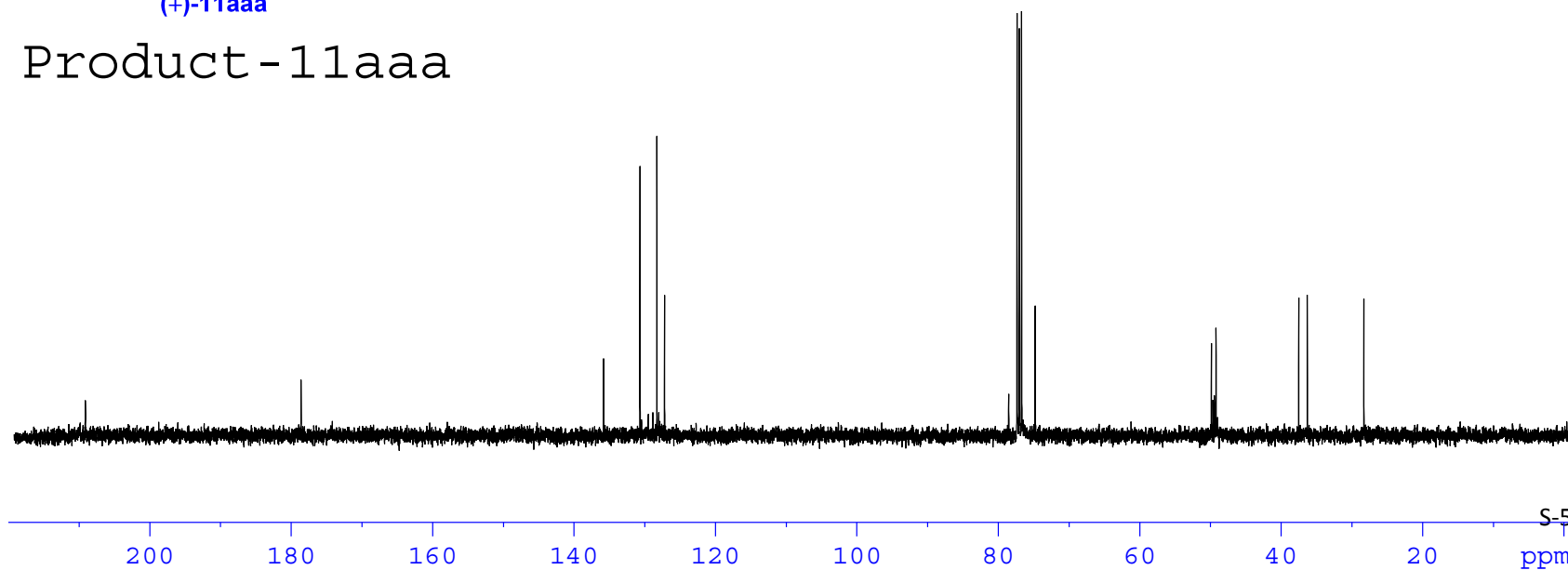
78.50
77.32
77.00
76.68
74.76

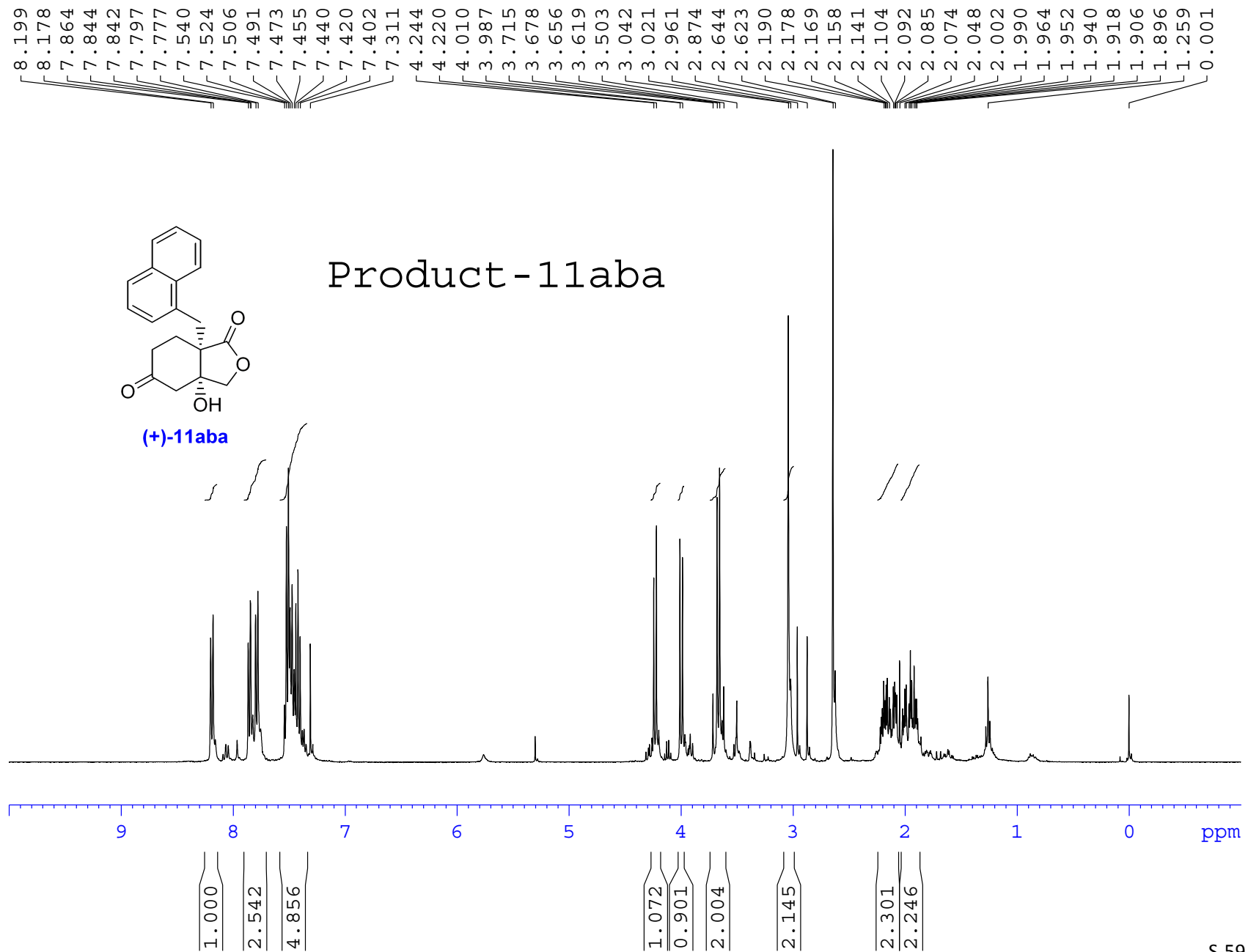
49.83
49.62
49.41
49.17
37.49
36.28
— 28.26



(+)-11aaa

Product-11aaa



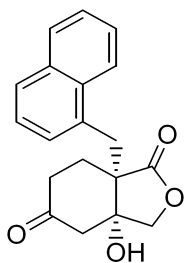


—209.12

—178.51

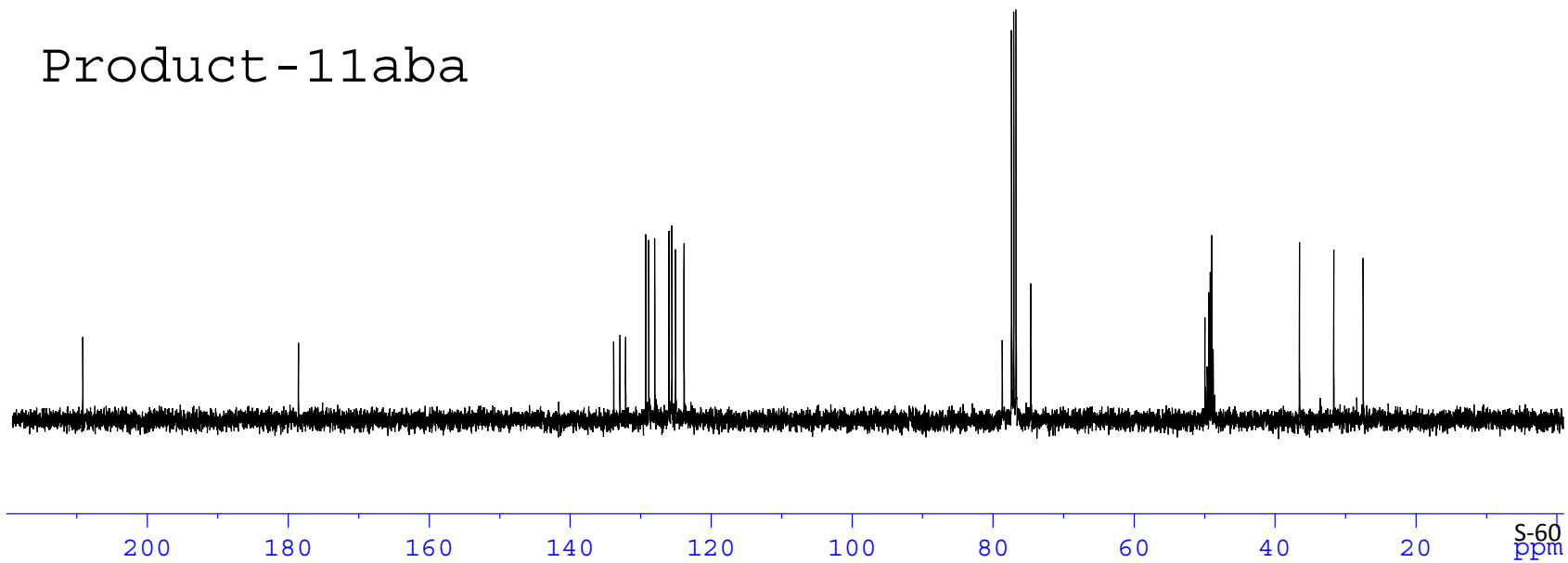
133.78
132.89
132.10
129.24
128.80
127.96
125.96
125.52
125.01
123.80

78.63
77.32
77.00
76.68
74.60
49.89
49.77
49.56
49.34
49.13
48.92
48.70
36.50
31.63
27.46



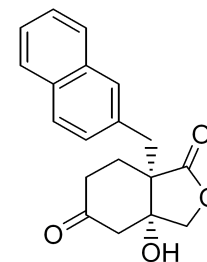
(+)-11aba

Product - 11aba



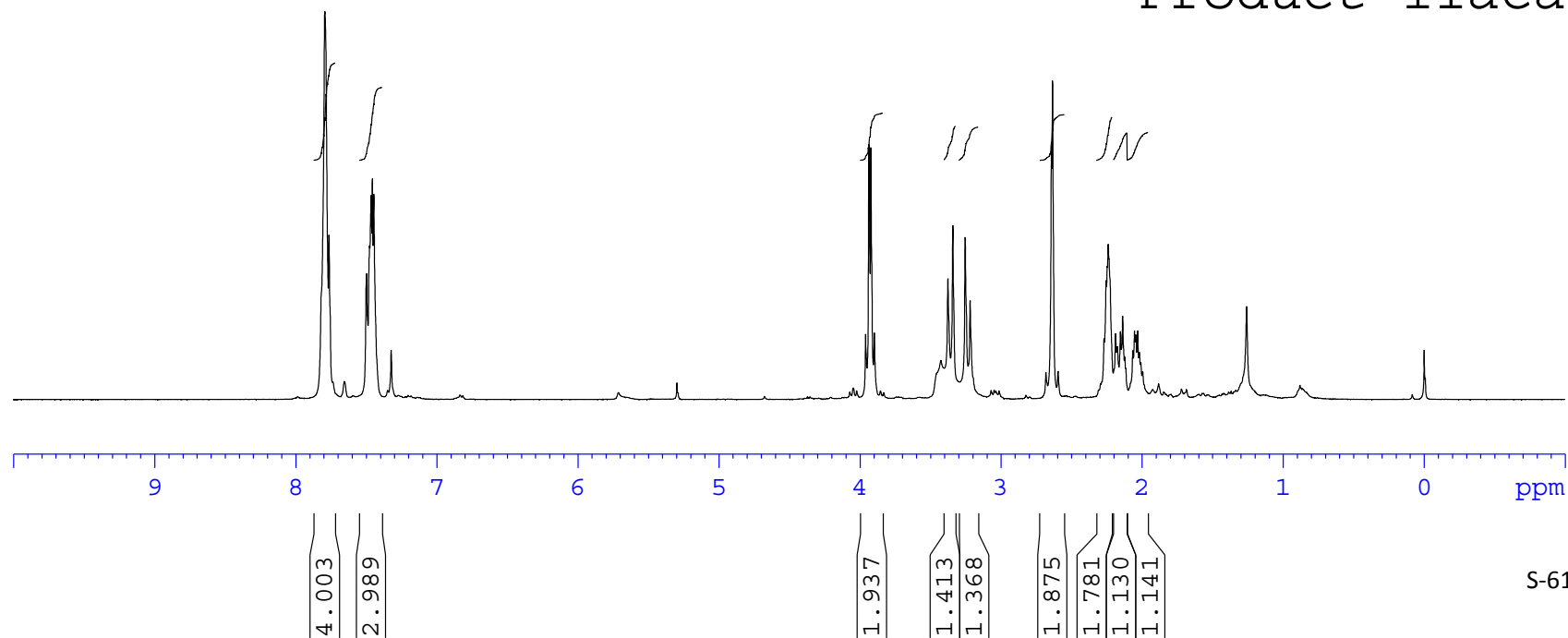
7.791
7.762
7.496
7.474
7.463
7.454
7.445
7.321

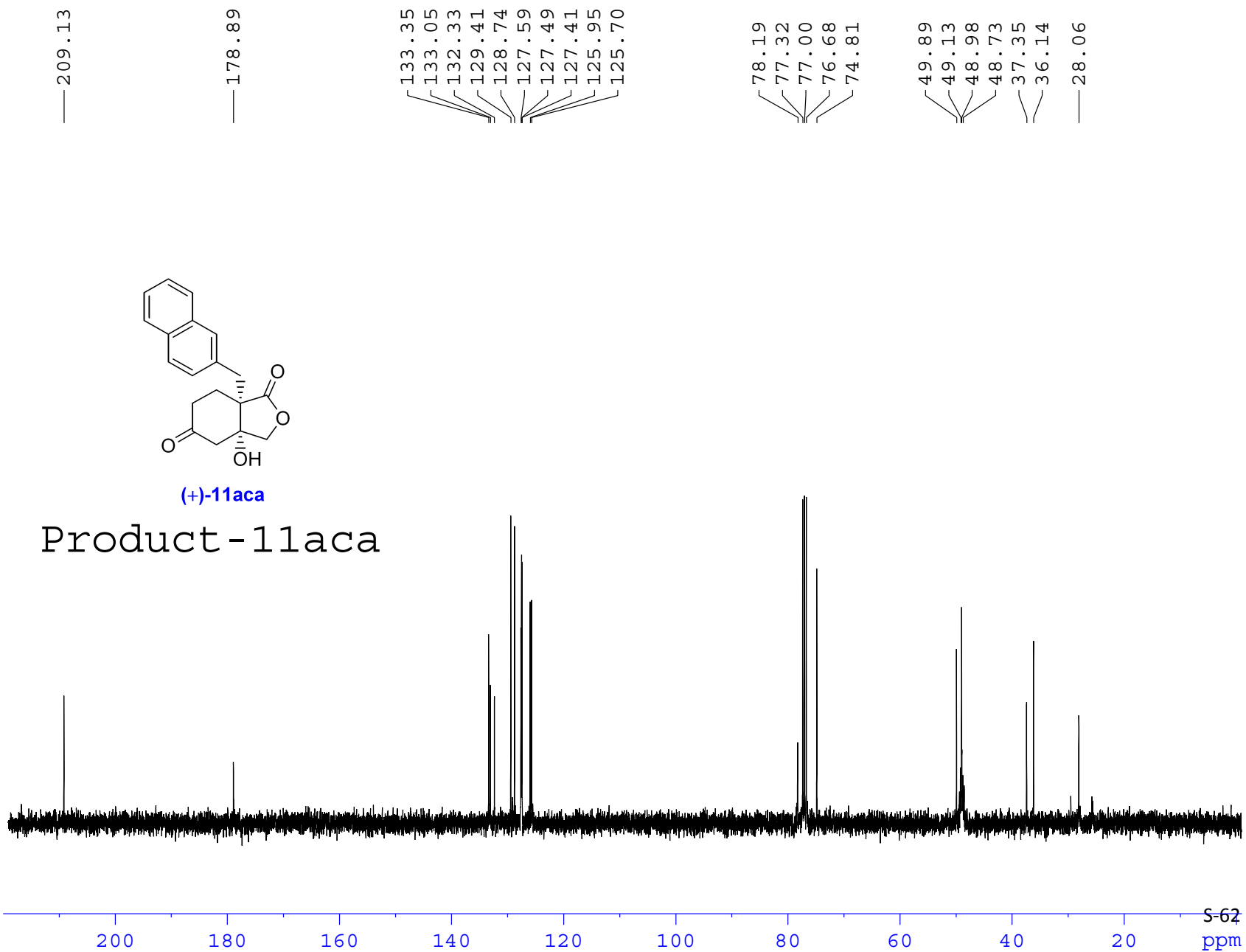
3.960
3.936
3.922
3.899
3.377
3.342
3.253
3.219
2.681
2.642
2.635
2.596

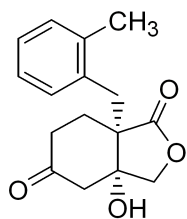


(+)-11aca

Product-11aca

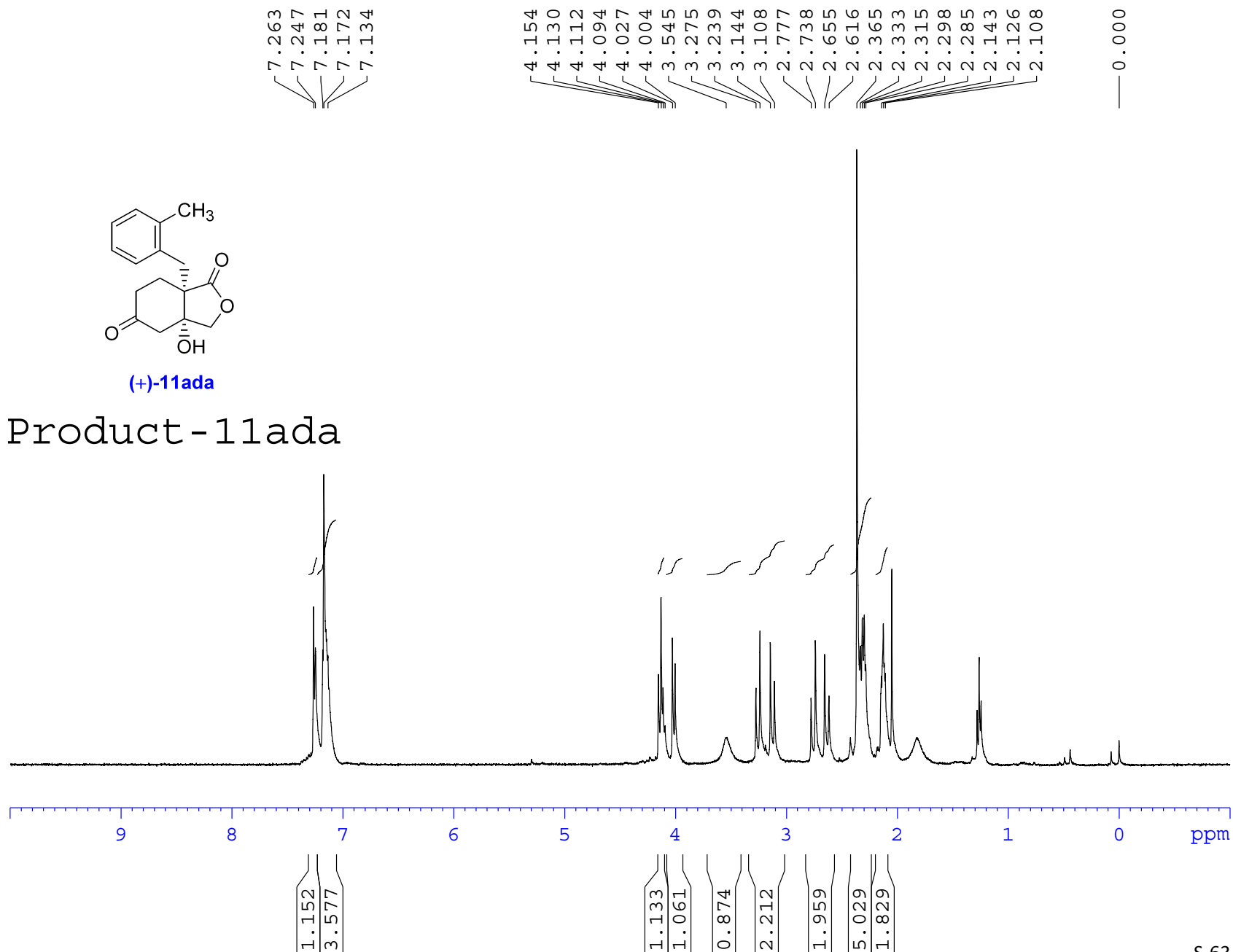


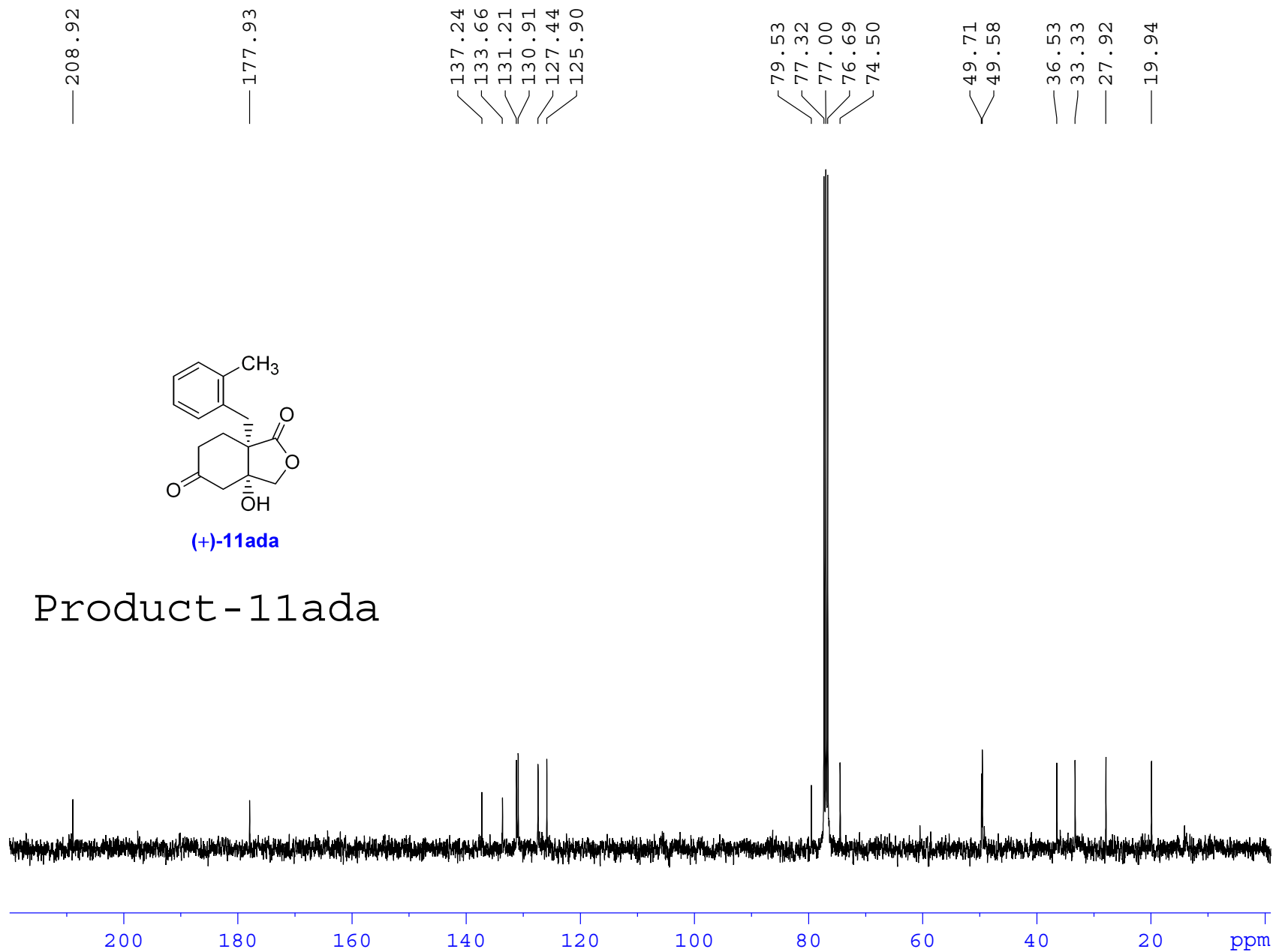


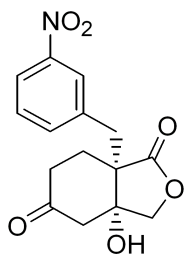


(+)-11ada

Product -11ada

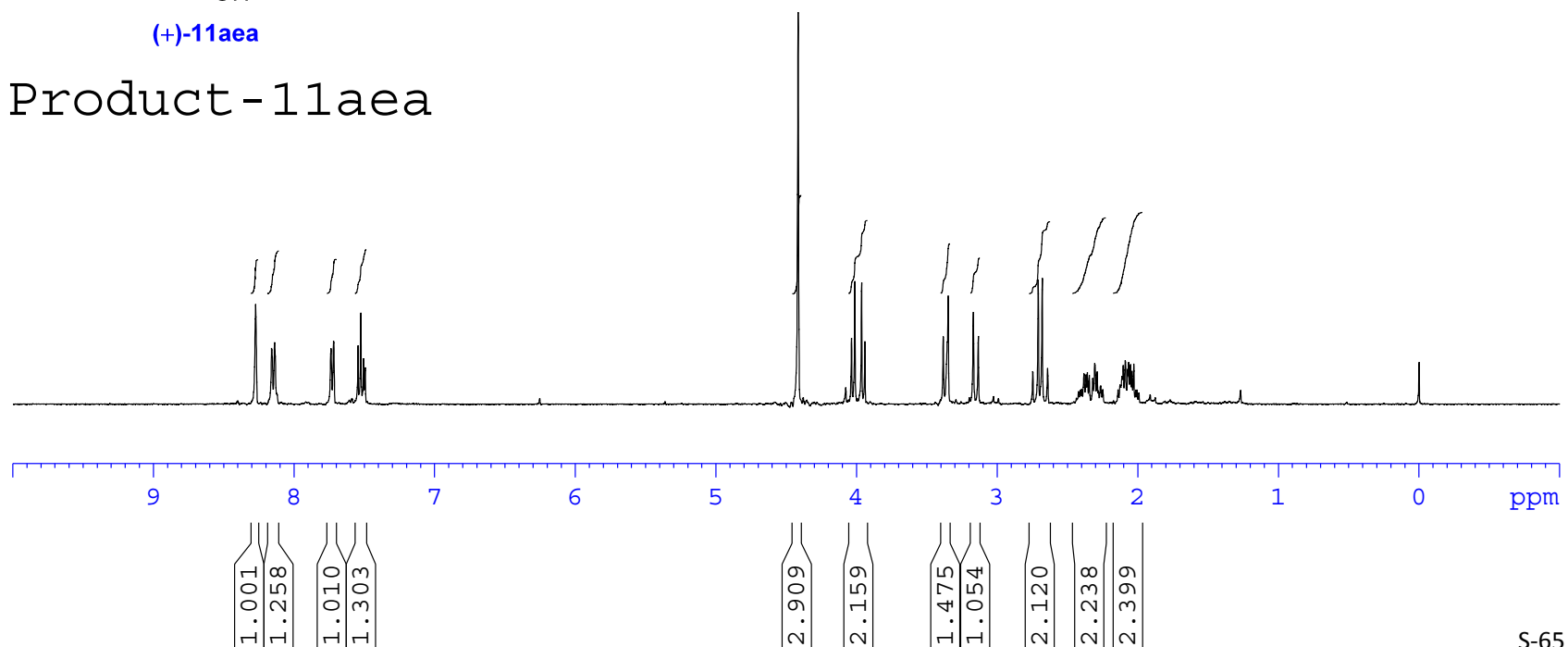


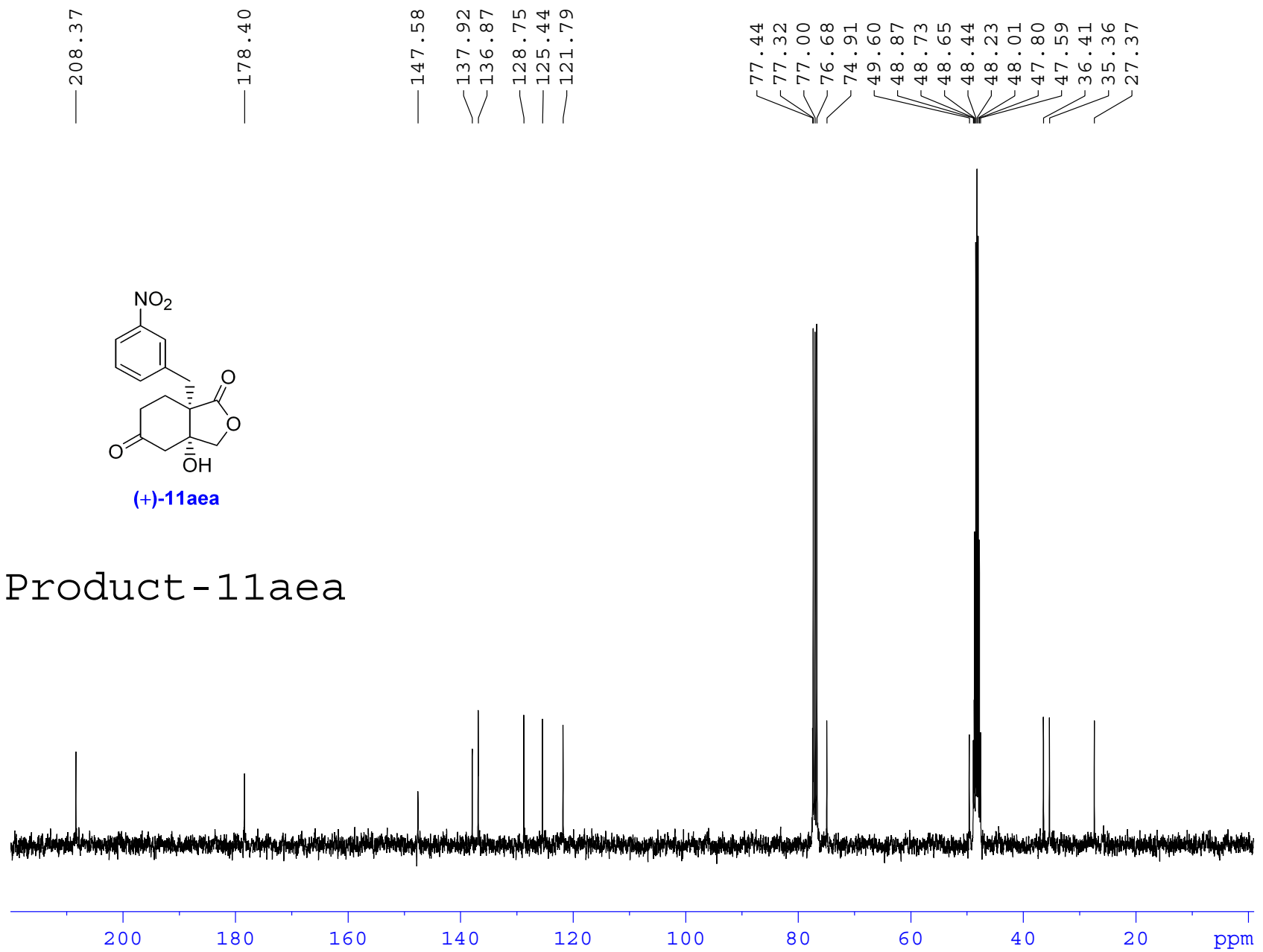


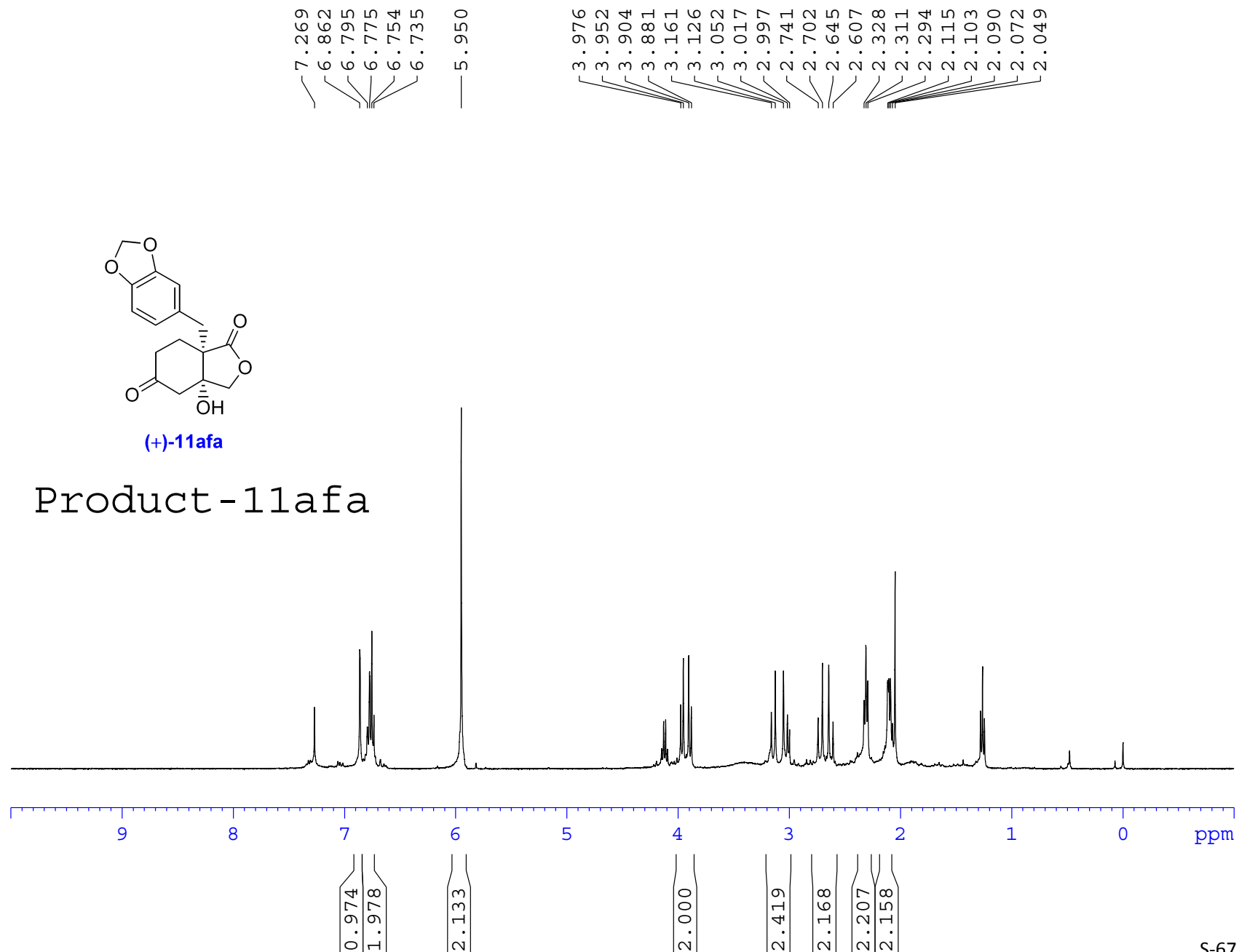


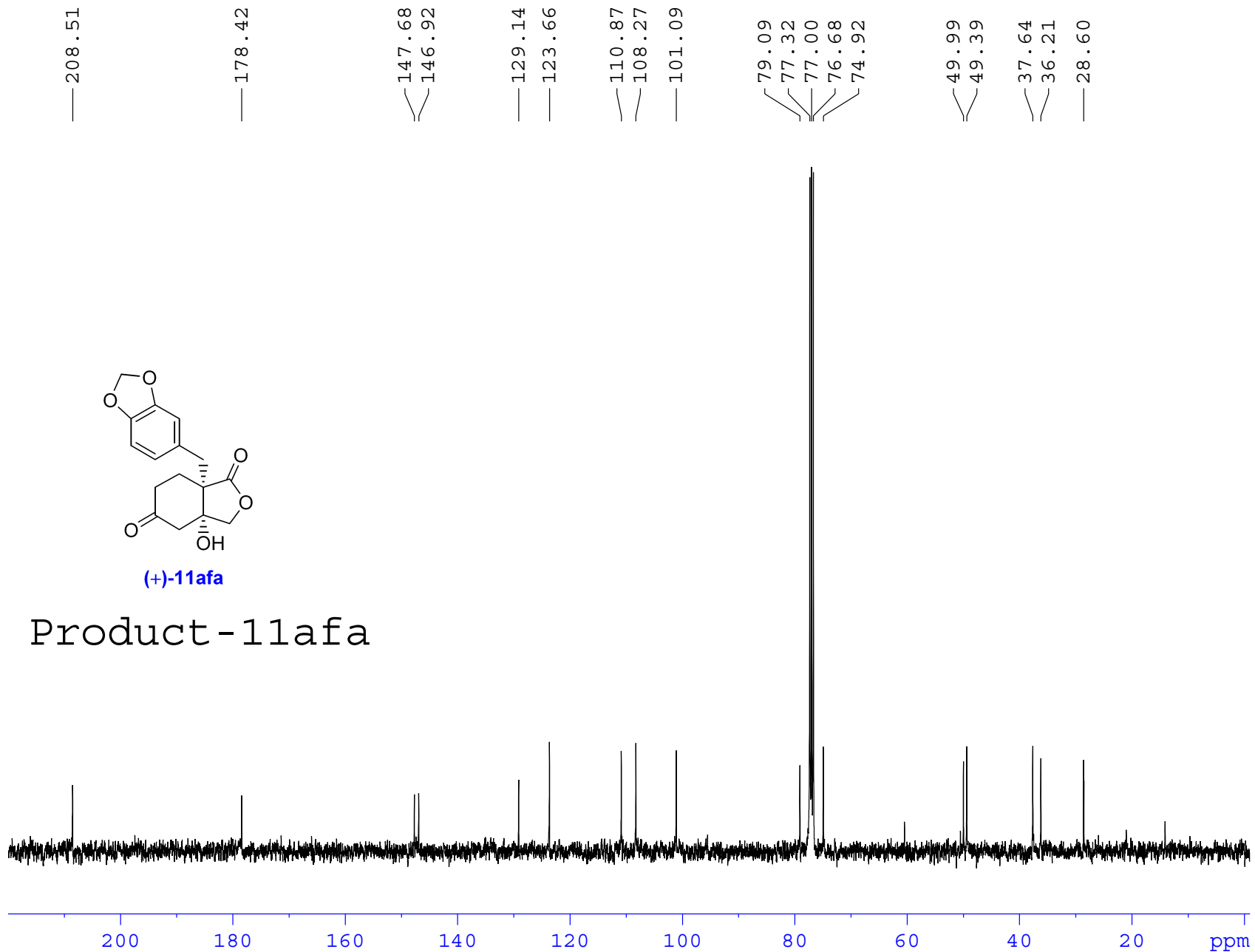
(+)-11aea

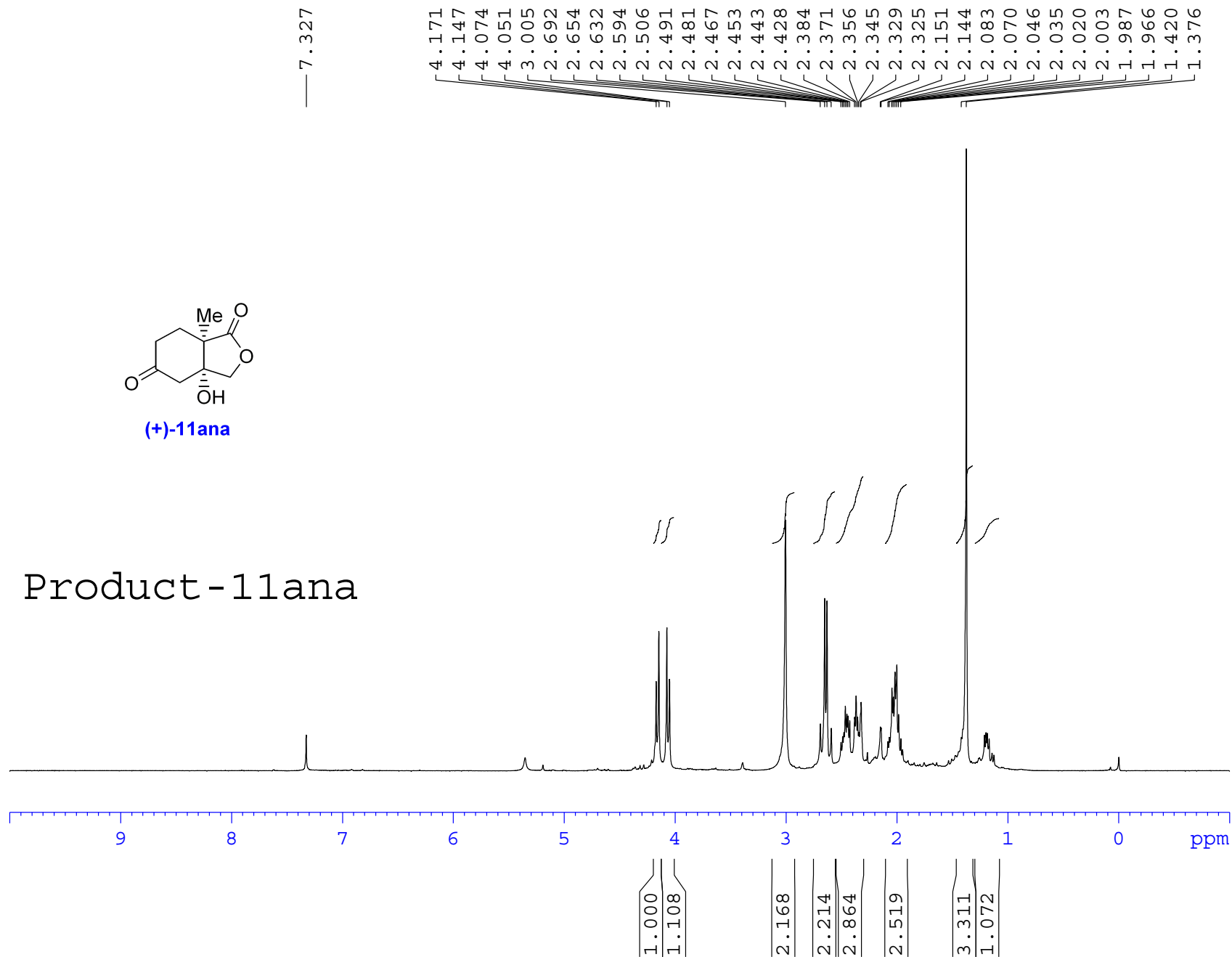
Product - 11aea







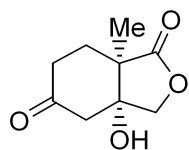




— 208.348

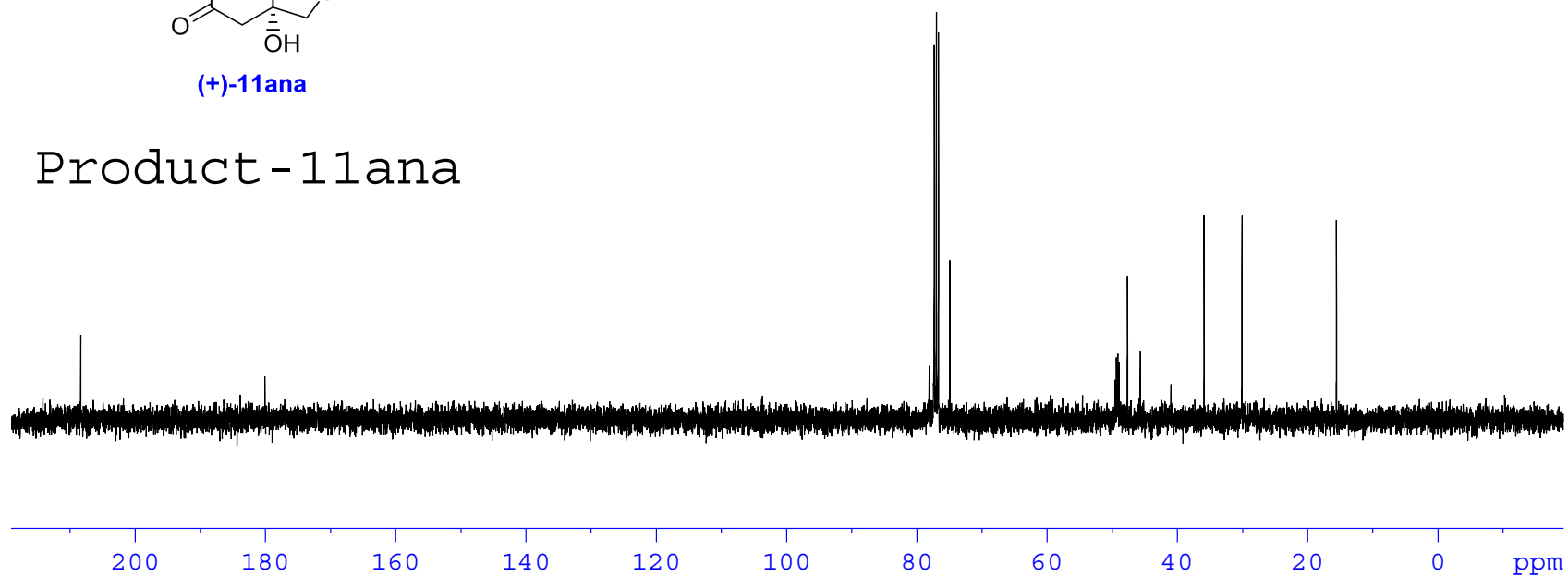
— 180.093

78.095
77.322
77.003
76.684
74.923
49.583
49.372
49.156
48.943
47.676
45.689
40.986
35.899
30.082
— 15.586

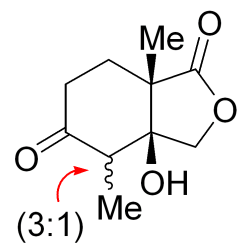


(+)-11ana

Product-11ana

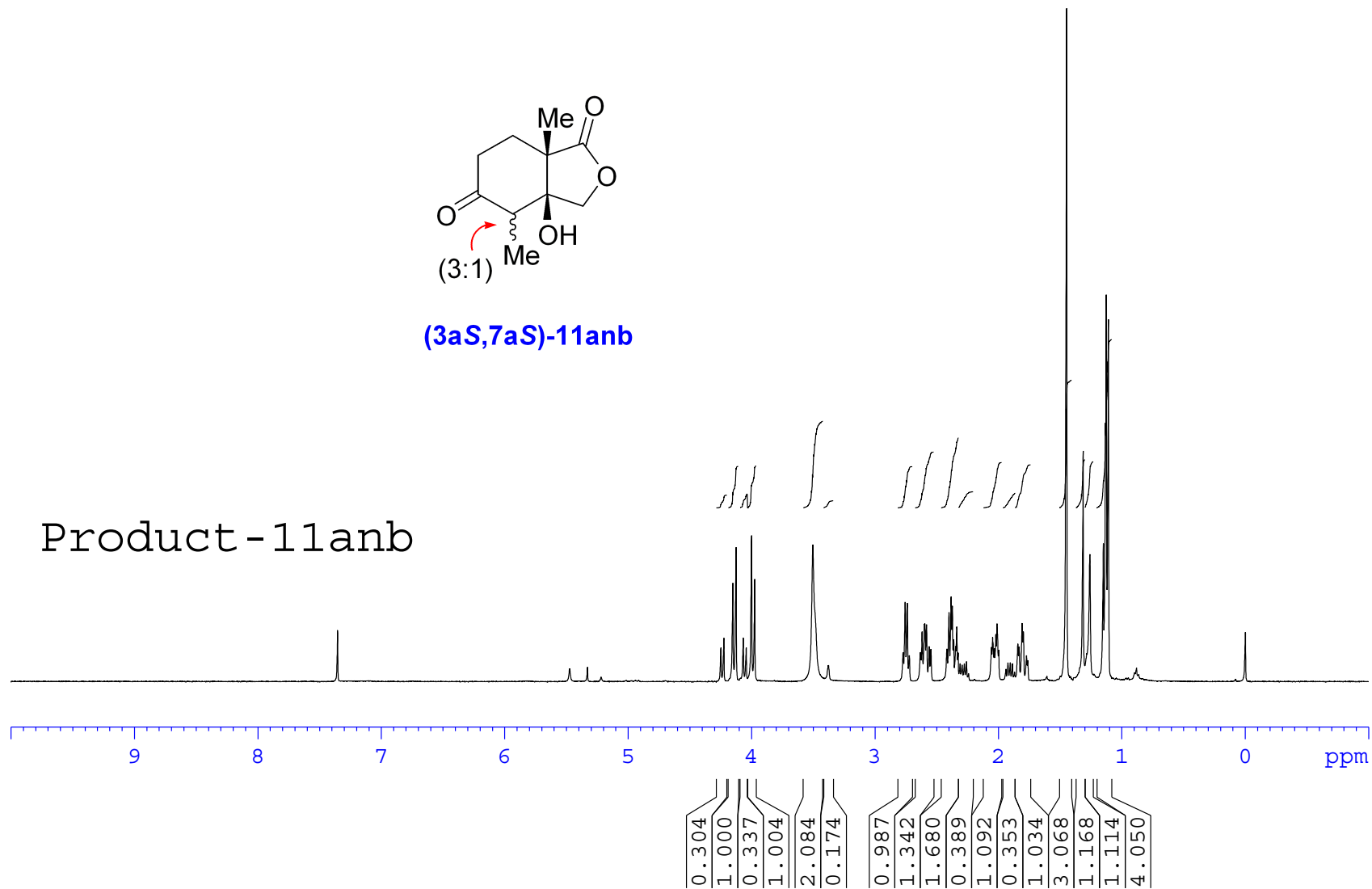


4.248
4.224
4.151
4.069
4.045
4.002
3.505
2.774
2.757
2.740
2.723
2.633
2.619
2.601
2.598
2.584
2.563
2.548
2.419
2.402
2.385
2.374
2.364
2.348
2.338
2.328
2.312
2.277
2.259
2.058
2.048
2.034
2.022
2.012
1.999
1.924
1.905
1.888
1.844
1.834
1.809
1.799
1.774
1.764
1.449
1.315
1.260
1.152
1.134
1.127
1.111
0.000



(3aS,7aS)-11anb

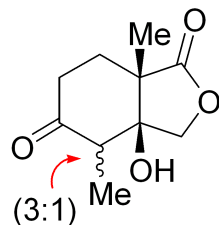
Product - 11anb



210.79
208.80

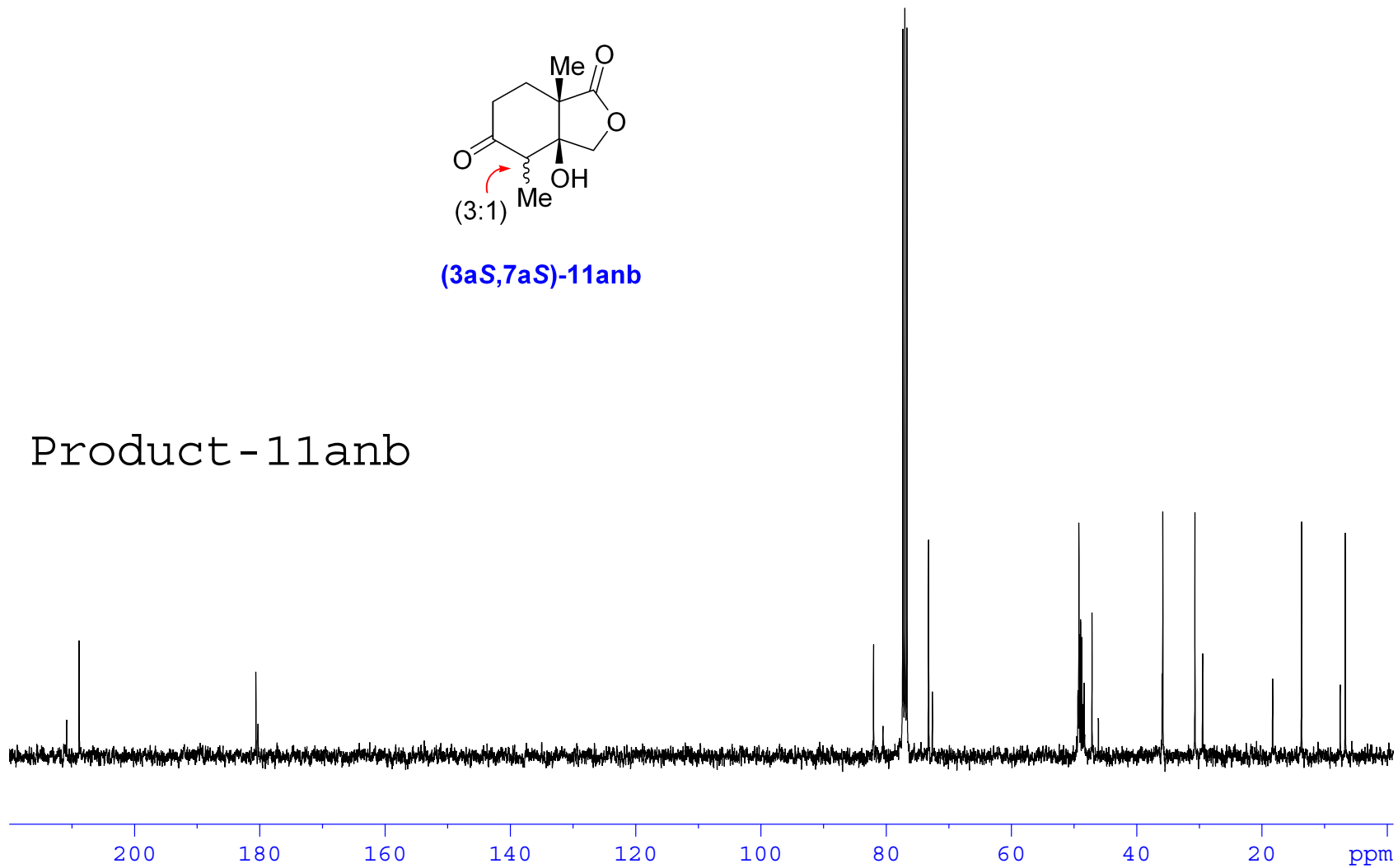
180.57
180.22

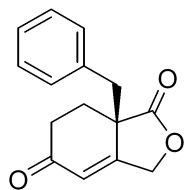
82.00
80.48
73.21
72.60
49.36
49.21
49.14
48.93
48.71
48.50
48.37
47.12
46.08
35.88
35.81
30.68
29.45
18.28
13.66
7.50
6.68



(3aS,7aS)-11anb

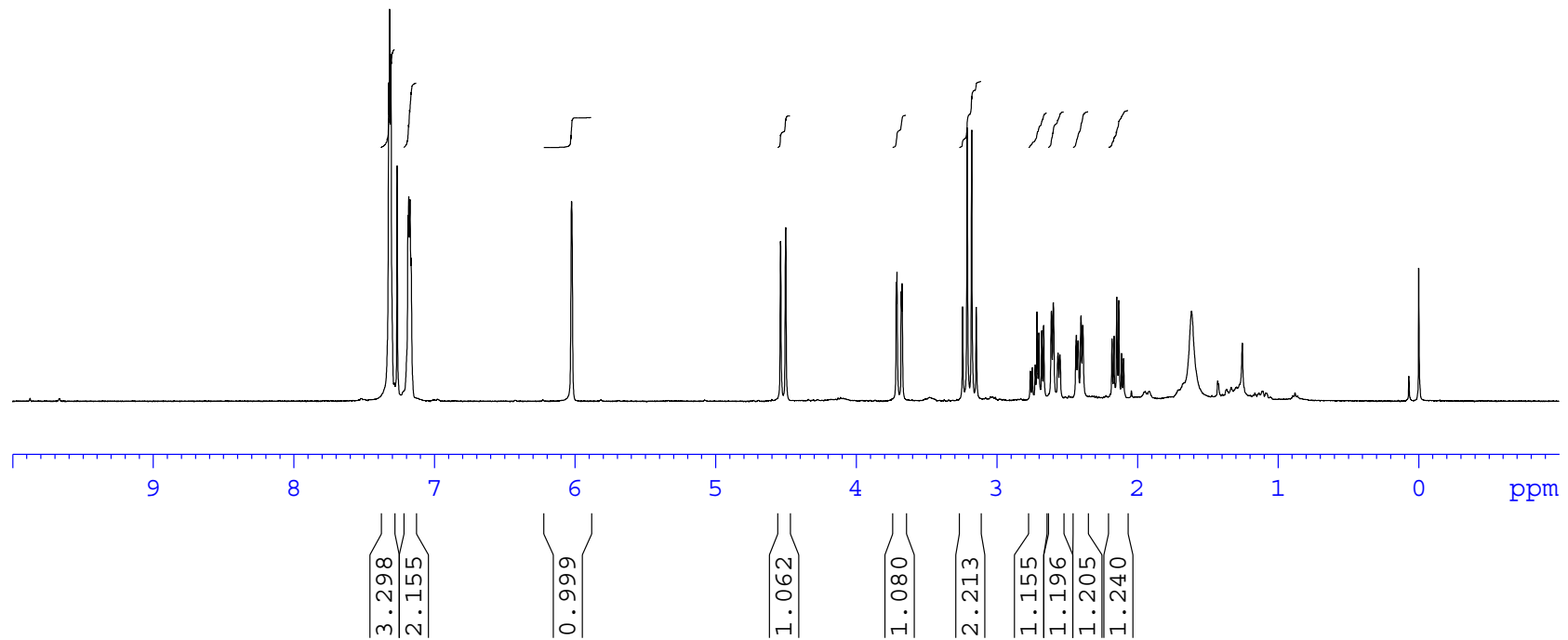
Product - 11anb

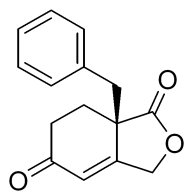




12aaa

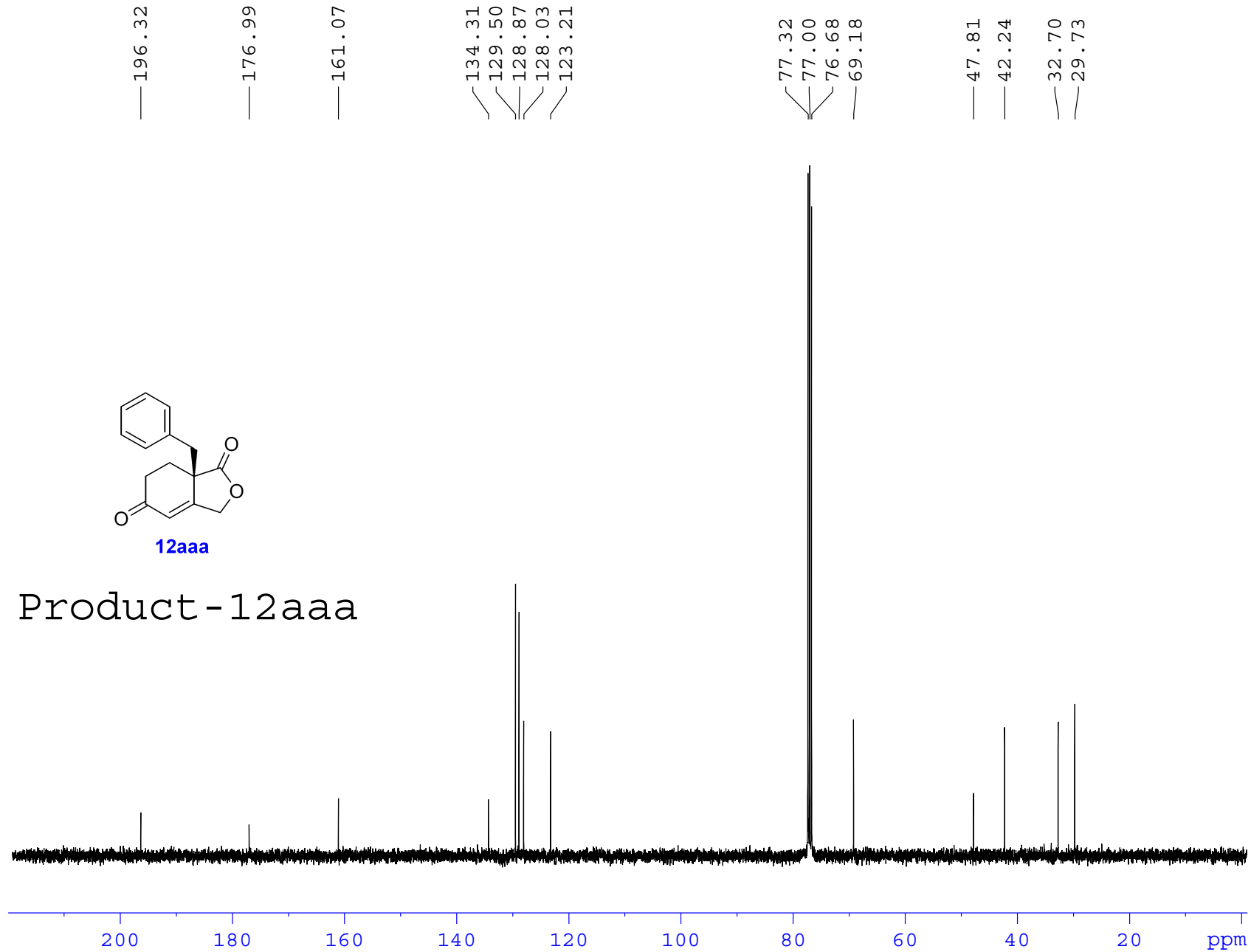
Product -- 12aaa

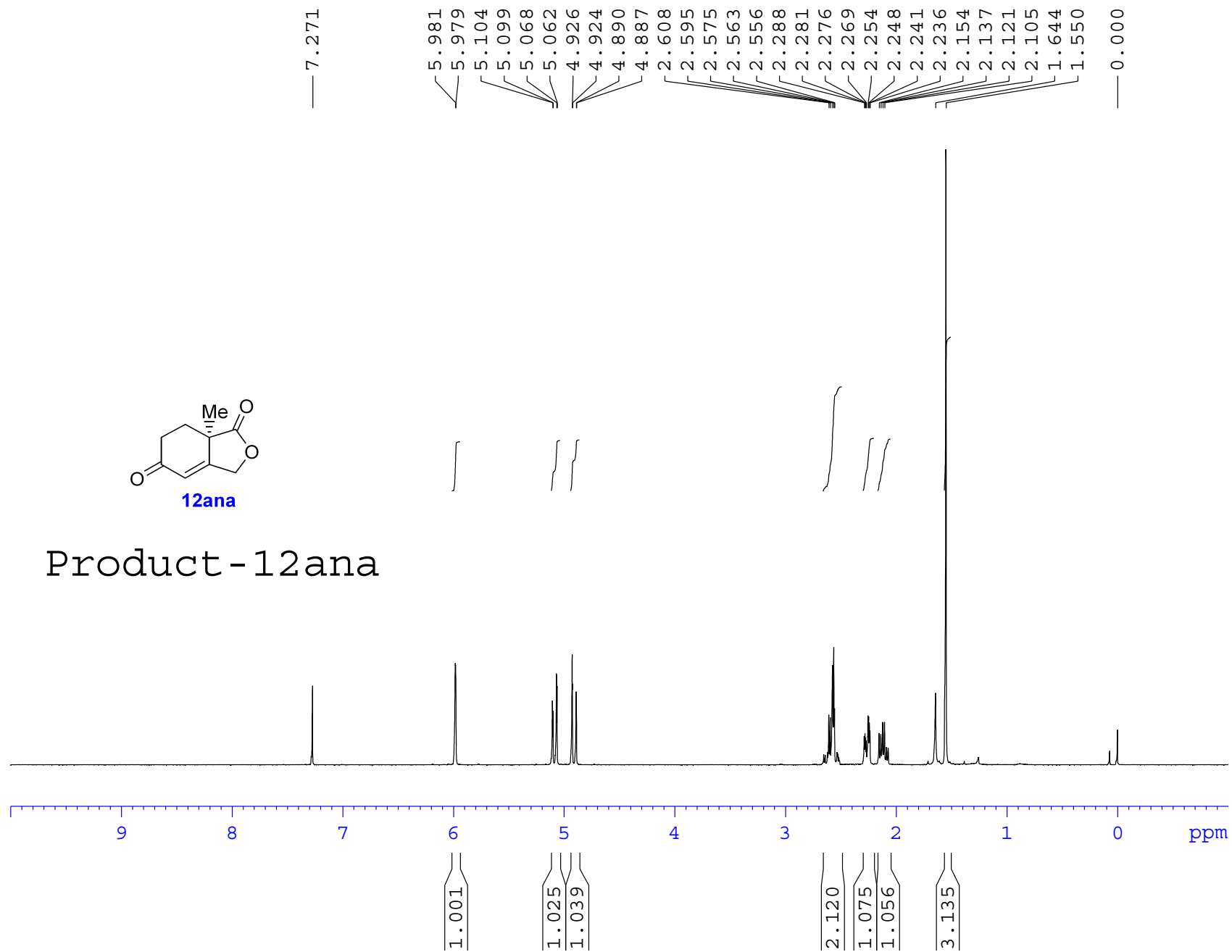




12aaa

Product-12aaa

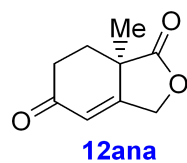




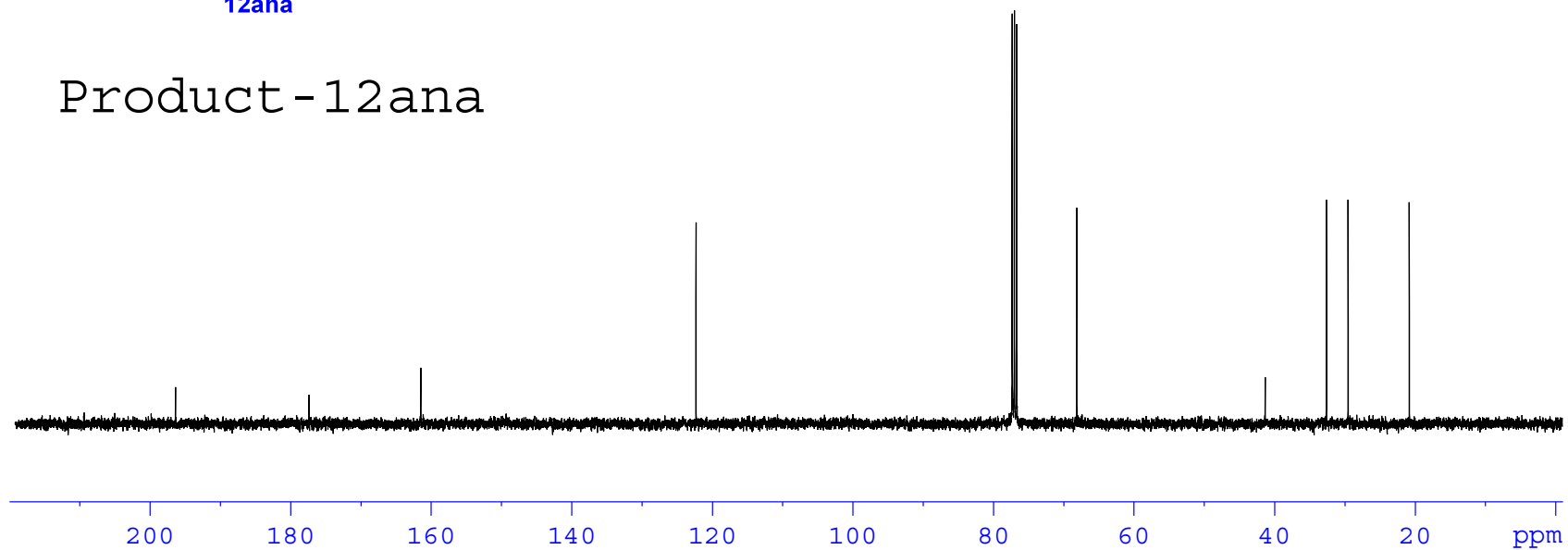
—196.34 —177.36 —161.45 —122.30

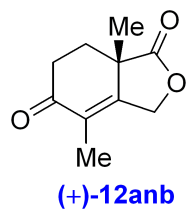
77.32
77.00
76.68
68.14

—41.31 —32.60 —29.50 —20.80

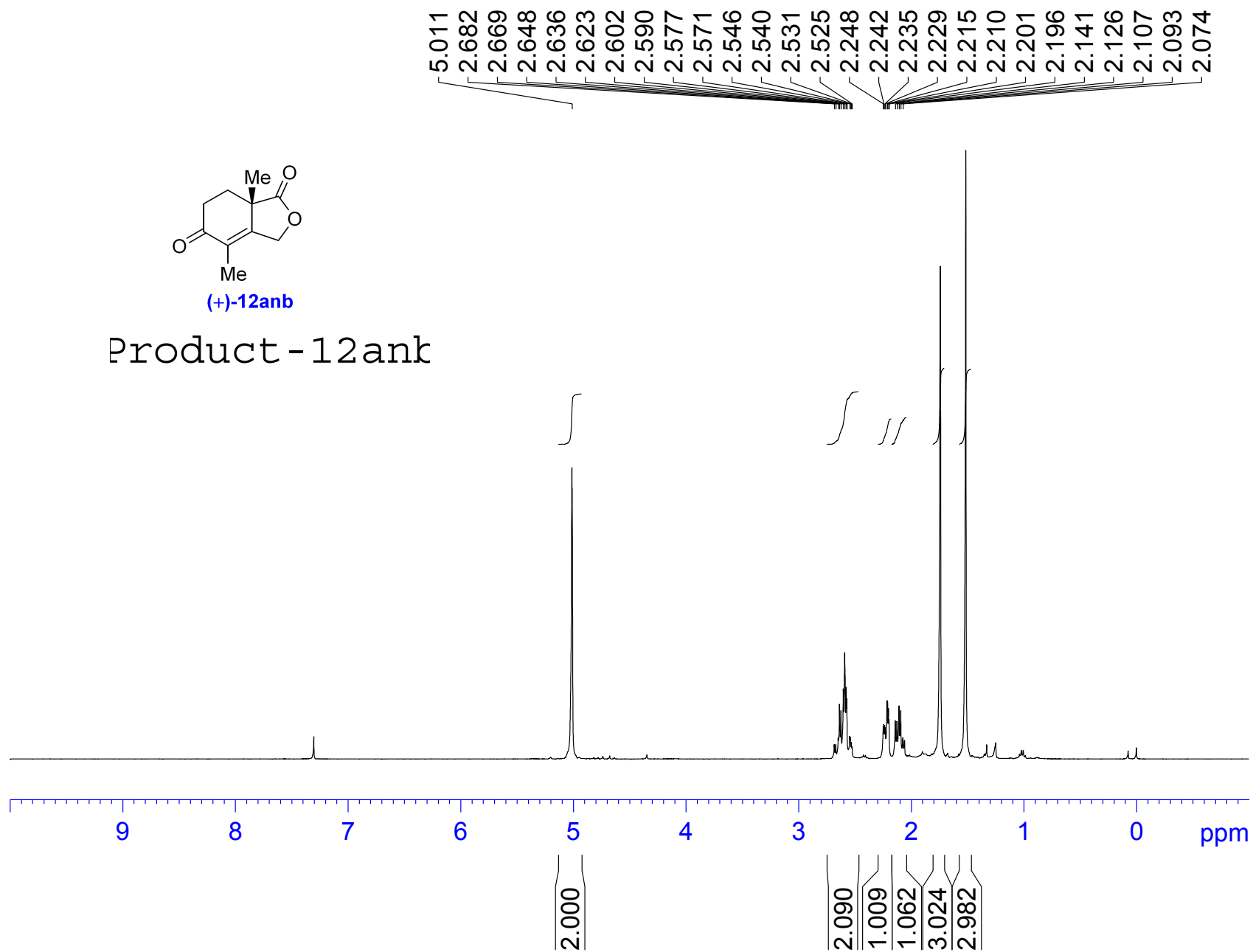


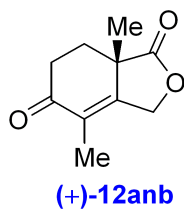
Product - 12ana



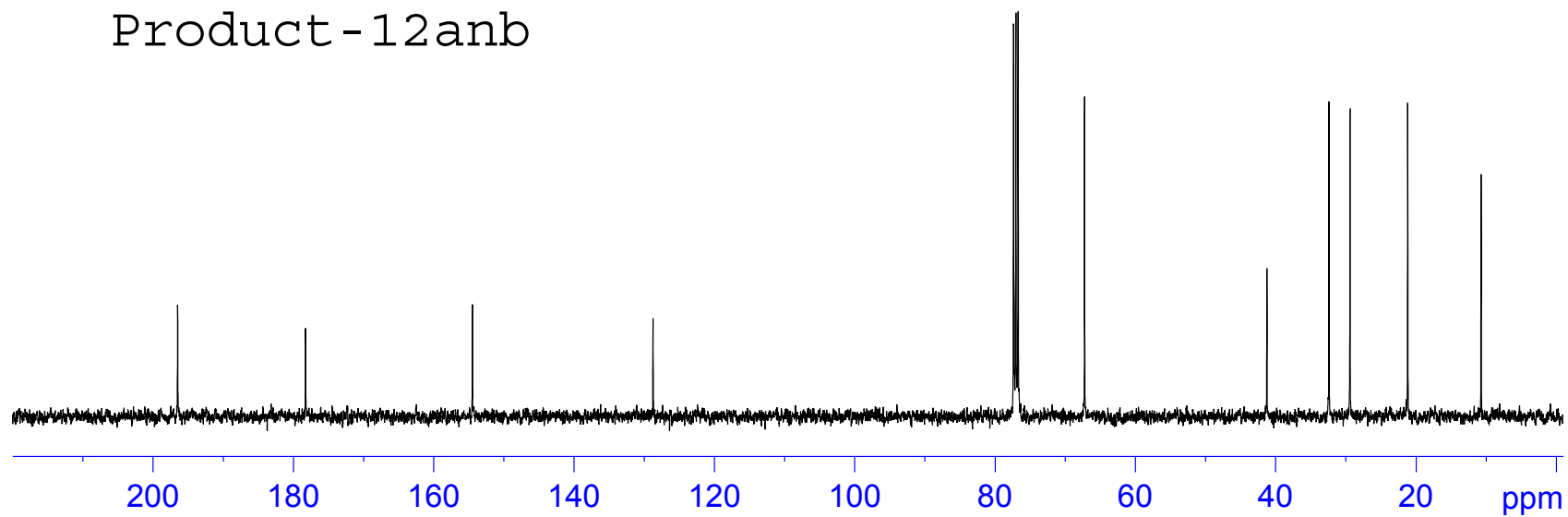


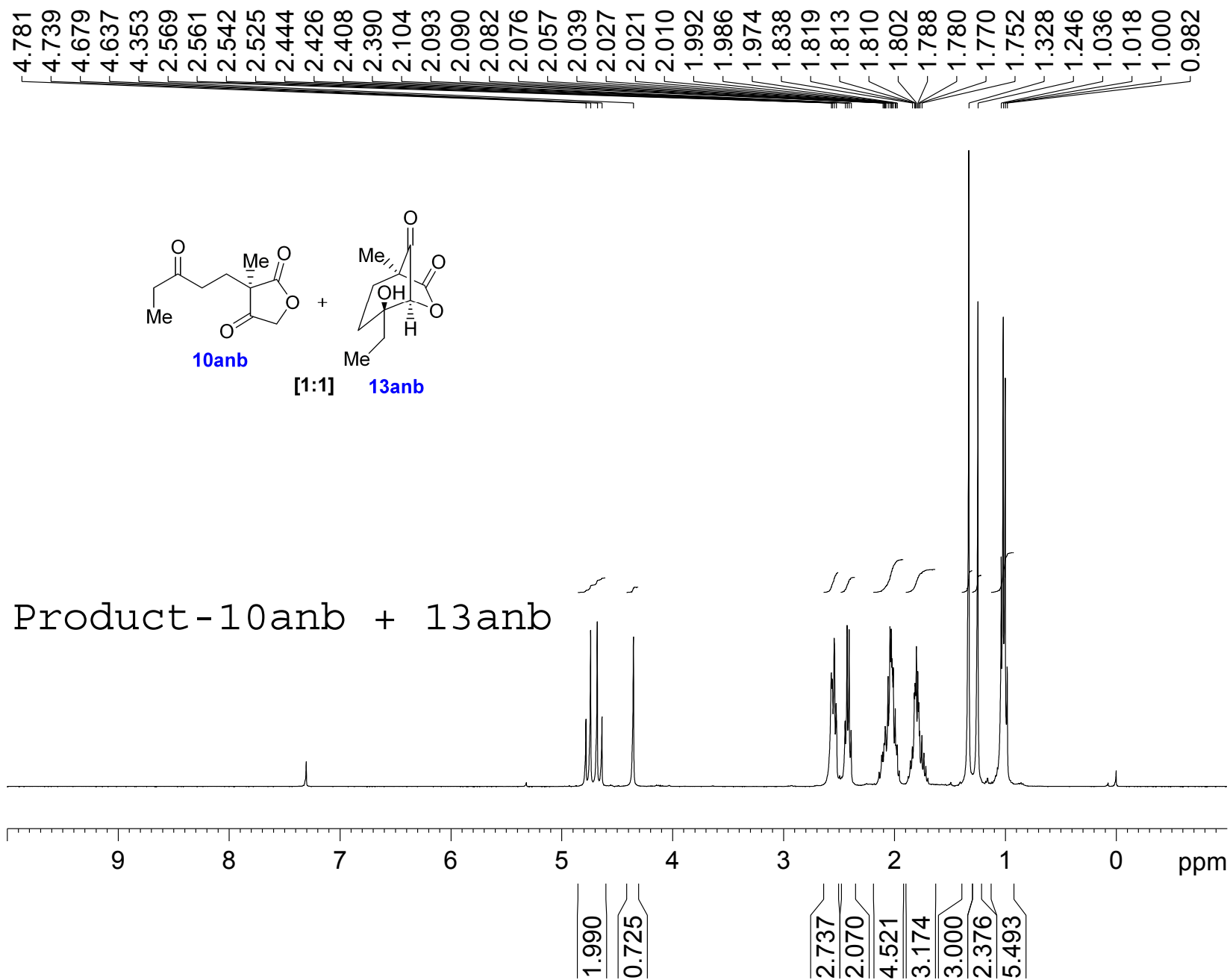
Product - 12ank





Product - 12anb

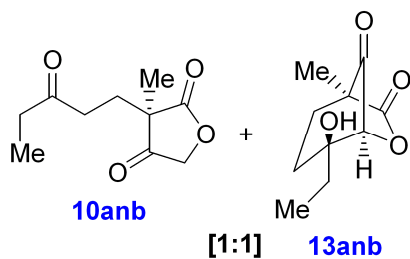




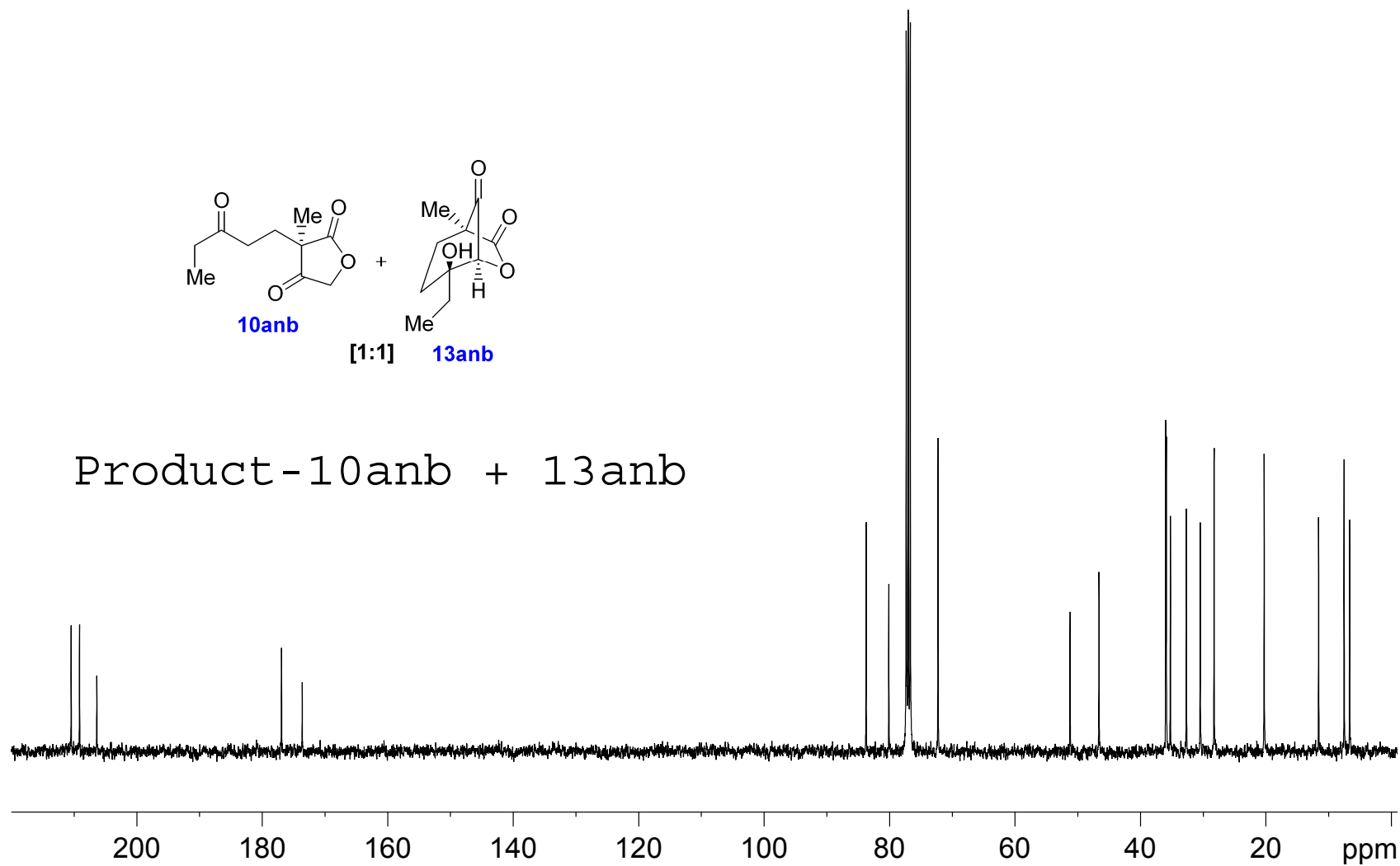
210.43
209.09
206.33

176.93
173.62

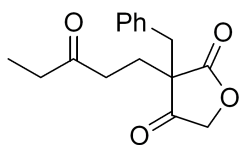
83.71
80.09
77.32
77.00
76.68
72.24
51.21
46.58
35.95
35.86
35.21
32.66
30.44
28.24
20.26
11.57
7.50



Product-10anb + 13anb

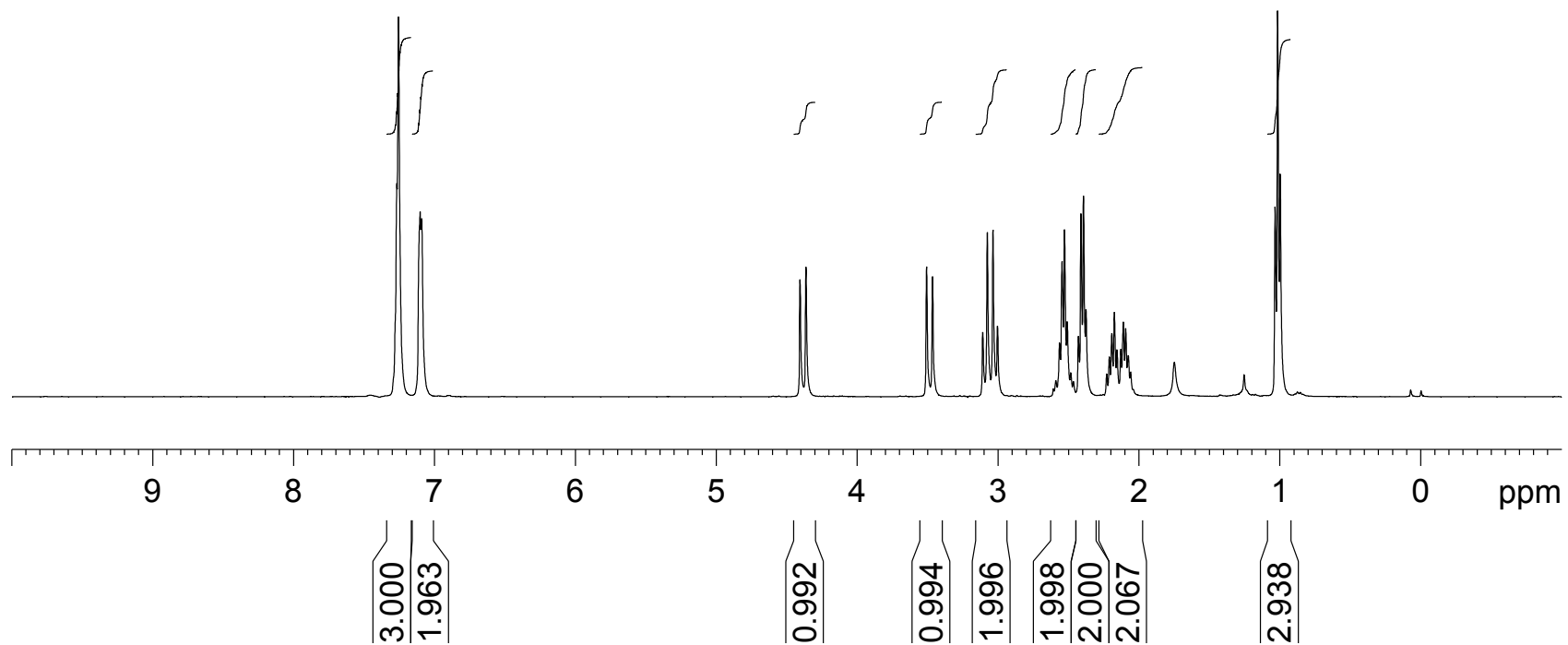


7.267
7.255
7.102
7.091
4.406
4.364
3.508
3.466
3.109
3.077
3.037
3.005
2.590
2.564
2.546
2.528
2.510
2.484
2.430
2.412
2.394
2.376
2.230
2.210
2.193
2.175
2.156
2.130
2.112
2.095
2.076
2.060



10aab

Product-10aab



209.99
209.79

176.16

133.65
129.53
128.81
127.82

77.32
77.00
76.68
73.26

54.24

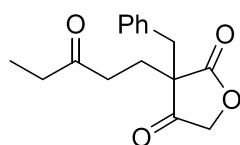
43.07

36.39

35.80

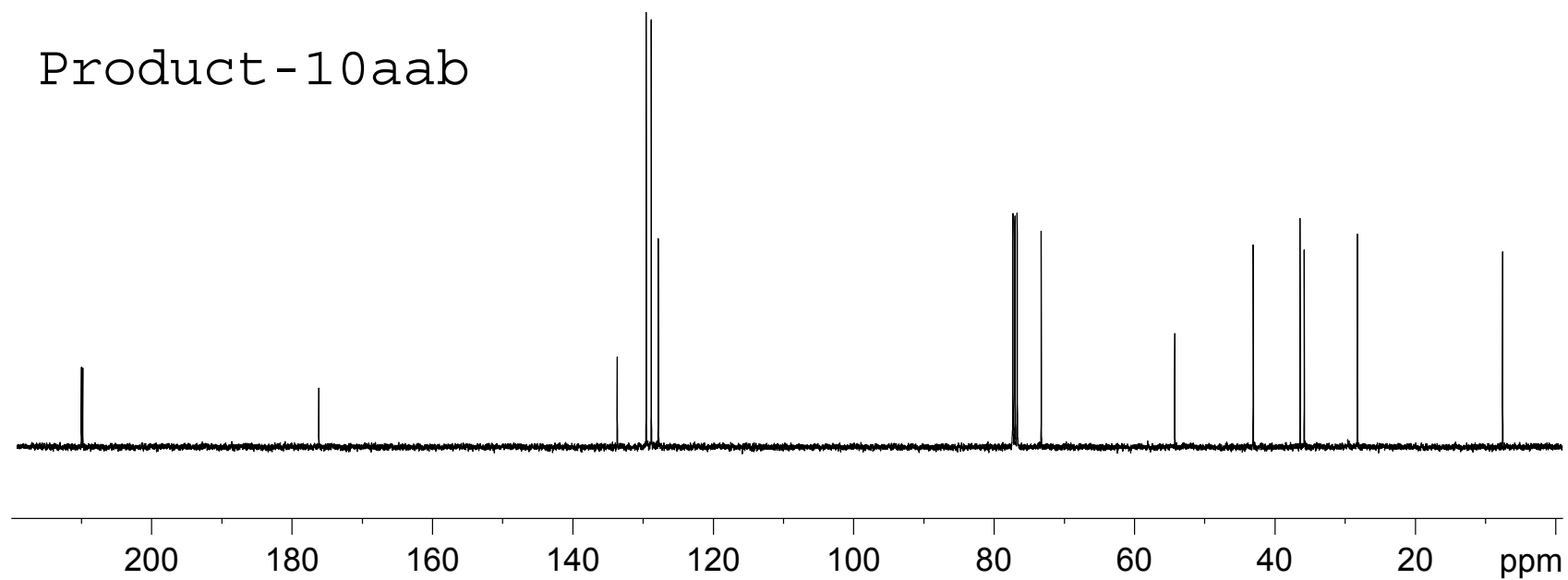
28.22

7.54

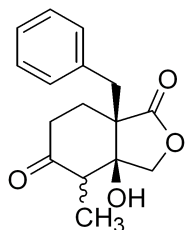


10aab

Product-10aab

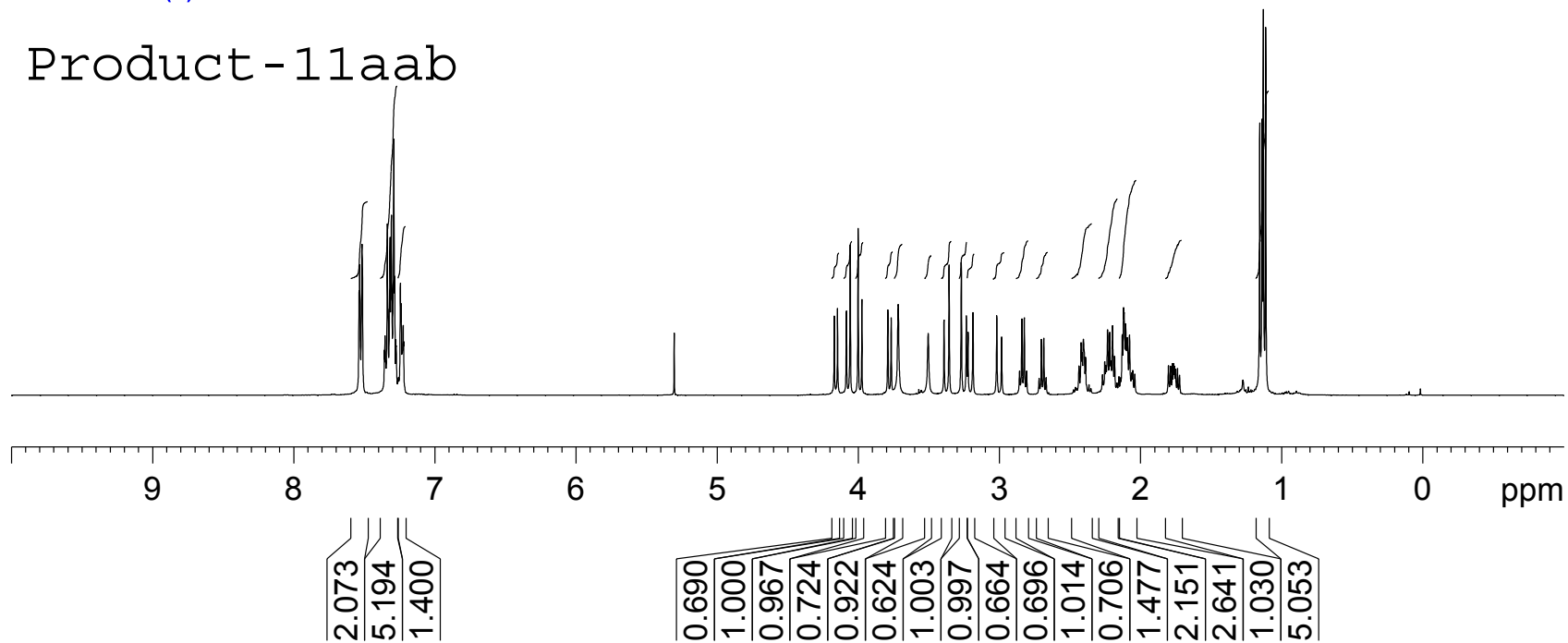


7.535
7.531
7.515
7.337
7.318
7.309
7.291
7.285
7.245
7.239
7.225
5.304
4.170
4.147
4.084
4.058
4.001
3.975
3.791
3.767
3.717
3.505
3.392
3.357
3.270
3.234
3.223
3.188
3.019
2.841
2.824
2.233
2.219
2.198
2.120
2.116
2.105
1.156
1.140
1.130
1.113



(-)-11aab

Product - 11aab



210.81
208.86

179.70
178.12

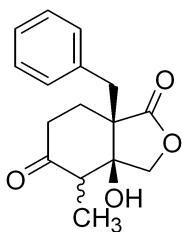
136.34
135.20
130.79
130.36
128.50
128.33
127.32
127.23

82.83
82.10
77.32
77.00
76.68
73.37
72.06

51.02
50.27
49.58
48.71

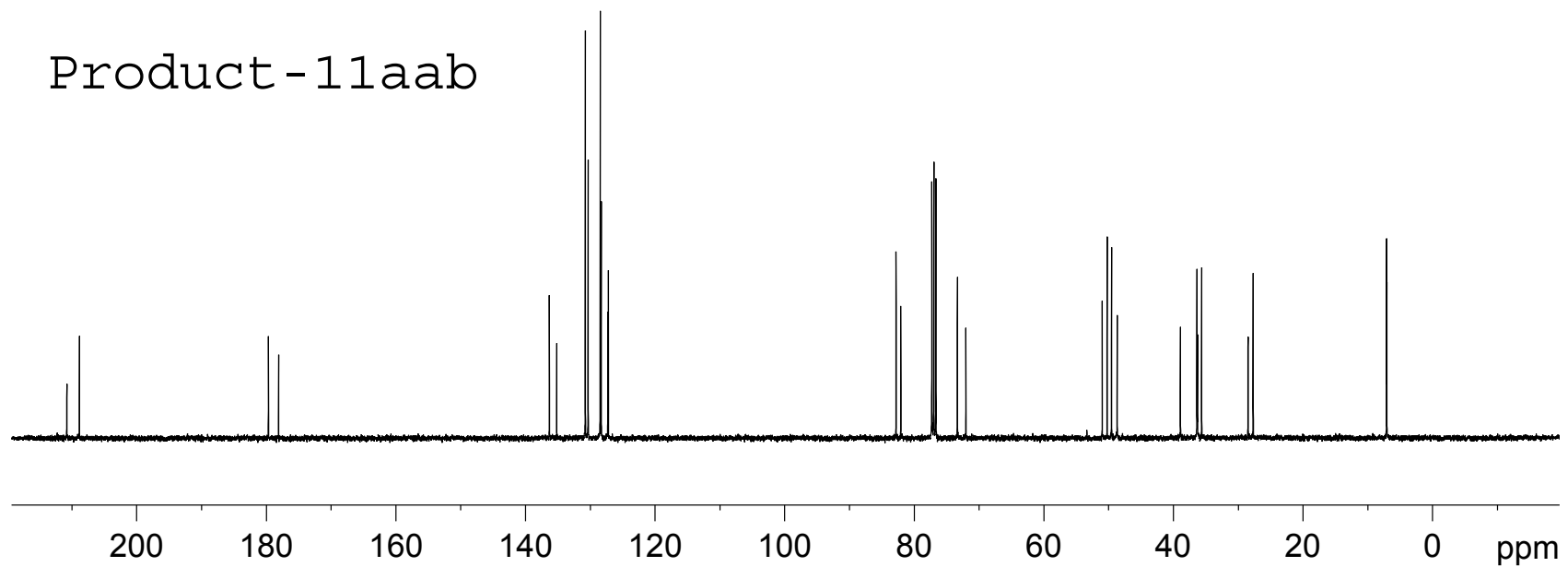
38.95
36.40
36.30
35.66
28.51
27.72

7.12
7.08

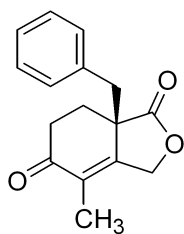


(-)-11aab

Product-11aab

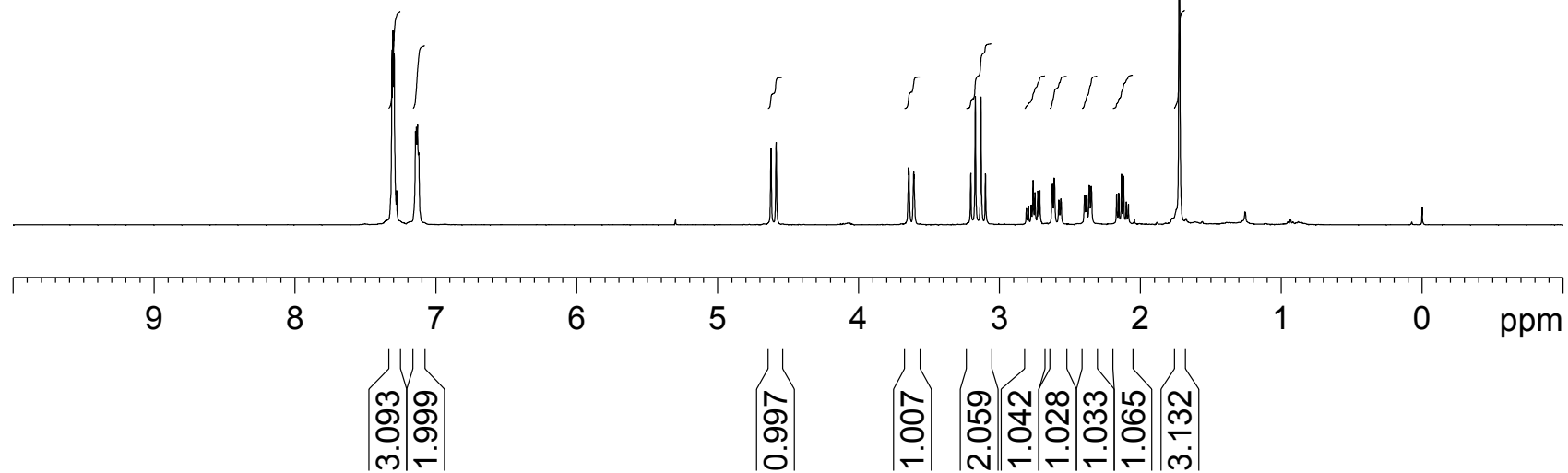


7.310
7.303
7.295
7.277
7.143
7.138
7.132
7.129
7.121
4.623
4.586
3.647
3.643
3.611
3.607
3.205
3.172
3.133
3.100
2.762
2.748
2.728
2.714
2.627
2.624
2.613
2.610
2.580
2.577
2.566
2.398
2.395
2.384
2.364
2.361
2.350
2.169
2.154
2.135
2.120
1.725



(+)-12aab

Product - 12aab



— 196.40

— 177.74

— 154.06

134.63

129.72

129.44

128.69

127.77

77.32

77.00

76.68

68.17

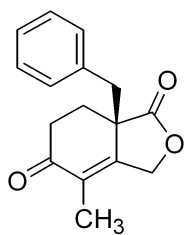
— 47.63

— 42.46

— 32.44

— 29.38

— 10.81



(+)-12aab

Product-12aab

