

Supporting Information-II

NMR Spectral Data

Sequential Combination of Michael and Acetalization Reactions: Direct Catalytic Asymmetric Synthesis of Functionalized 4-Nitromethylchromans as Drug Intermediates

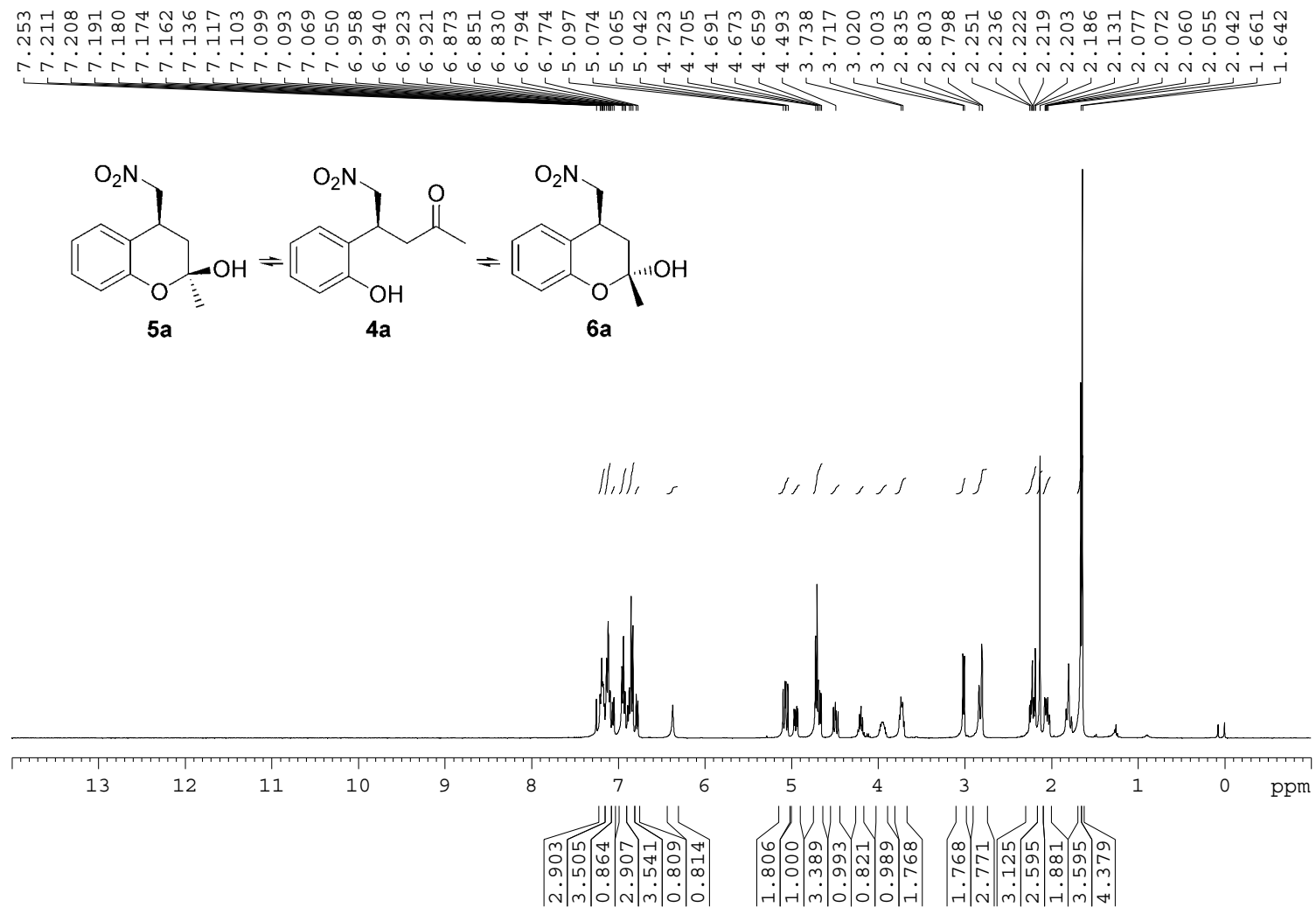
Dhevalapally B. Ramachary* and Rajasekar Sakthidevi

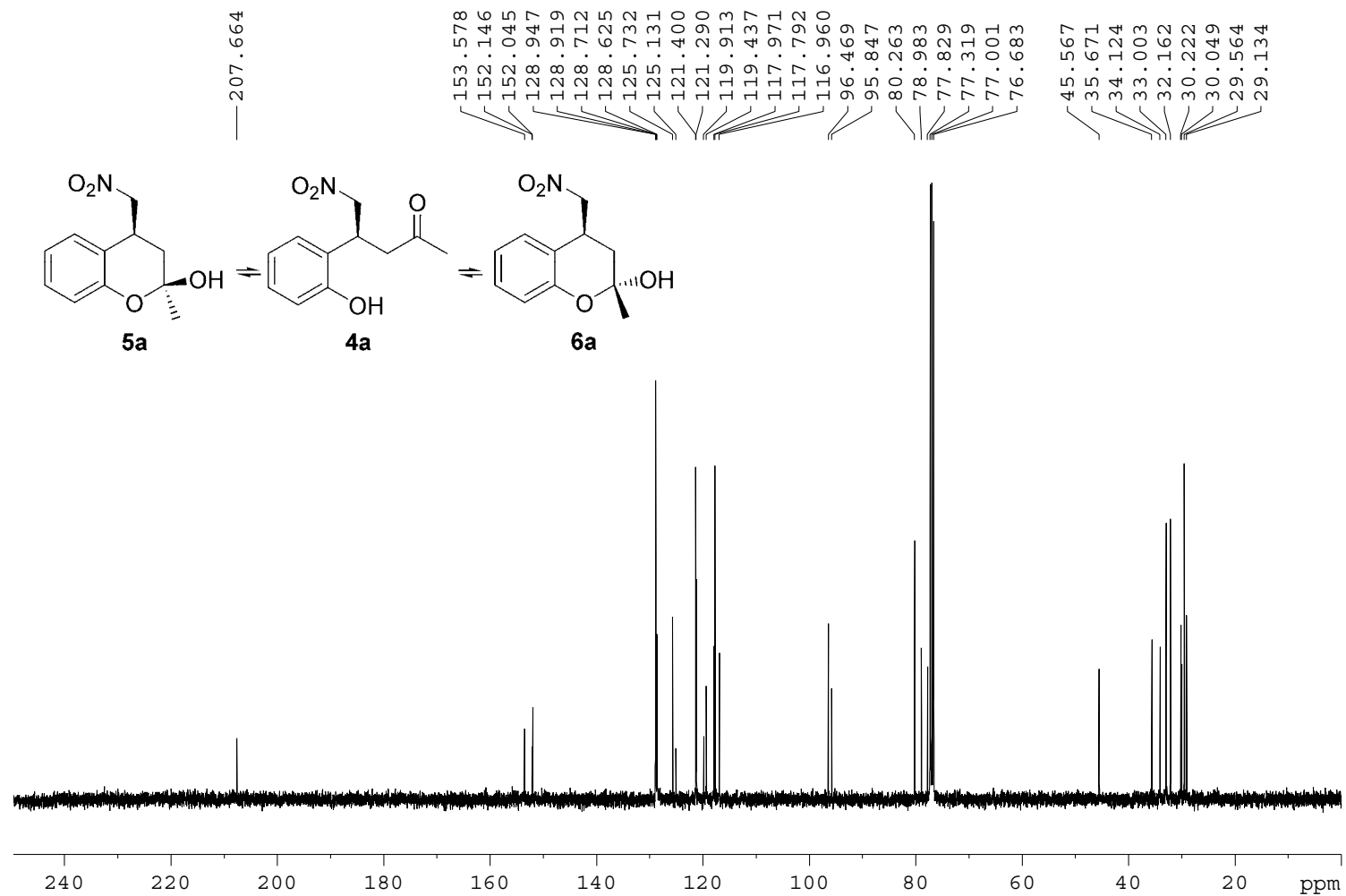
School of Chemistry, University of Hyderabad, Central University (P.O.),

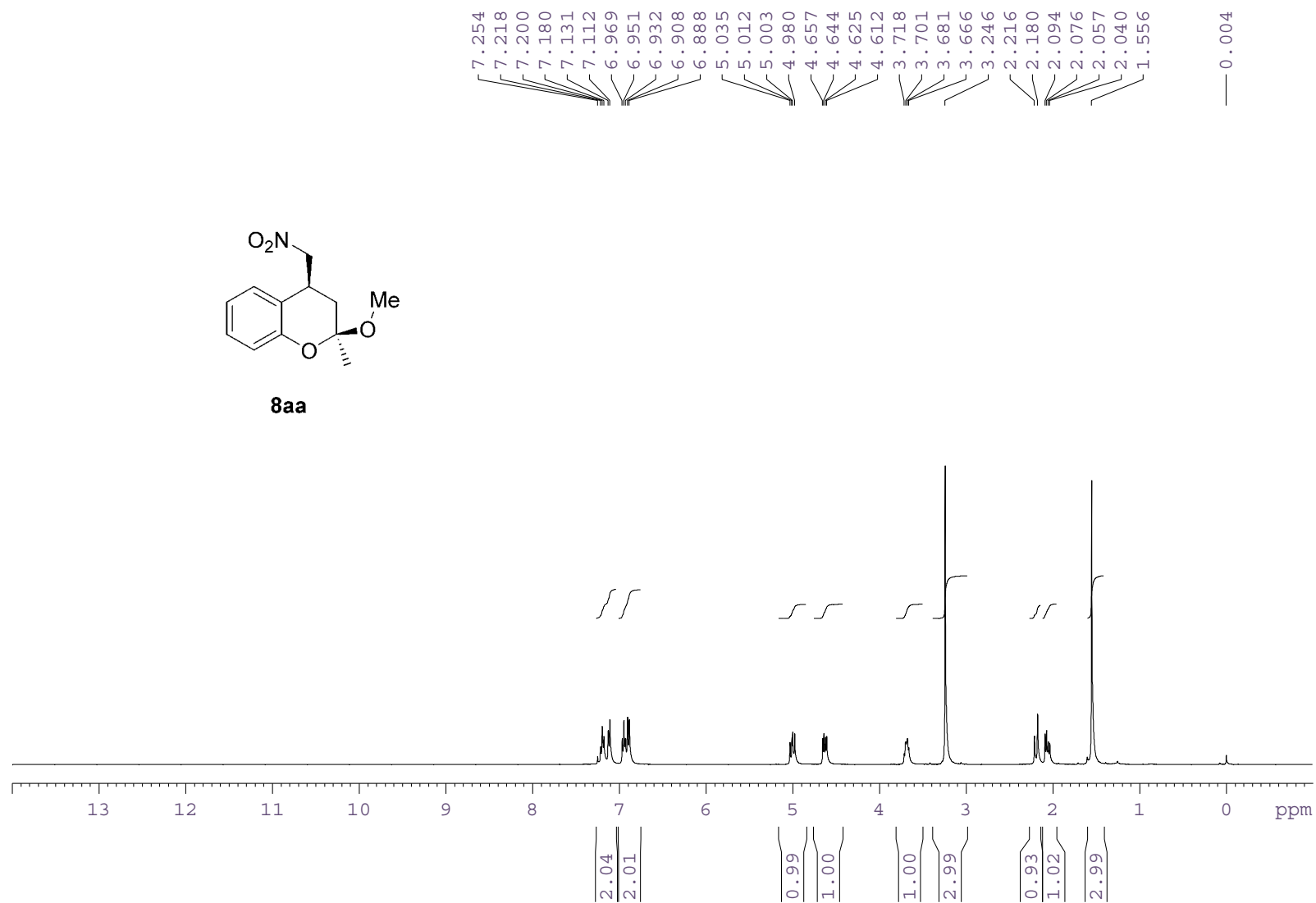
Hyderabad 500 046, India

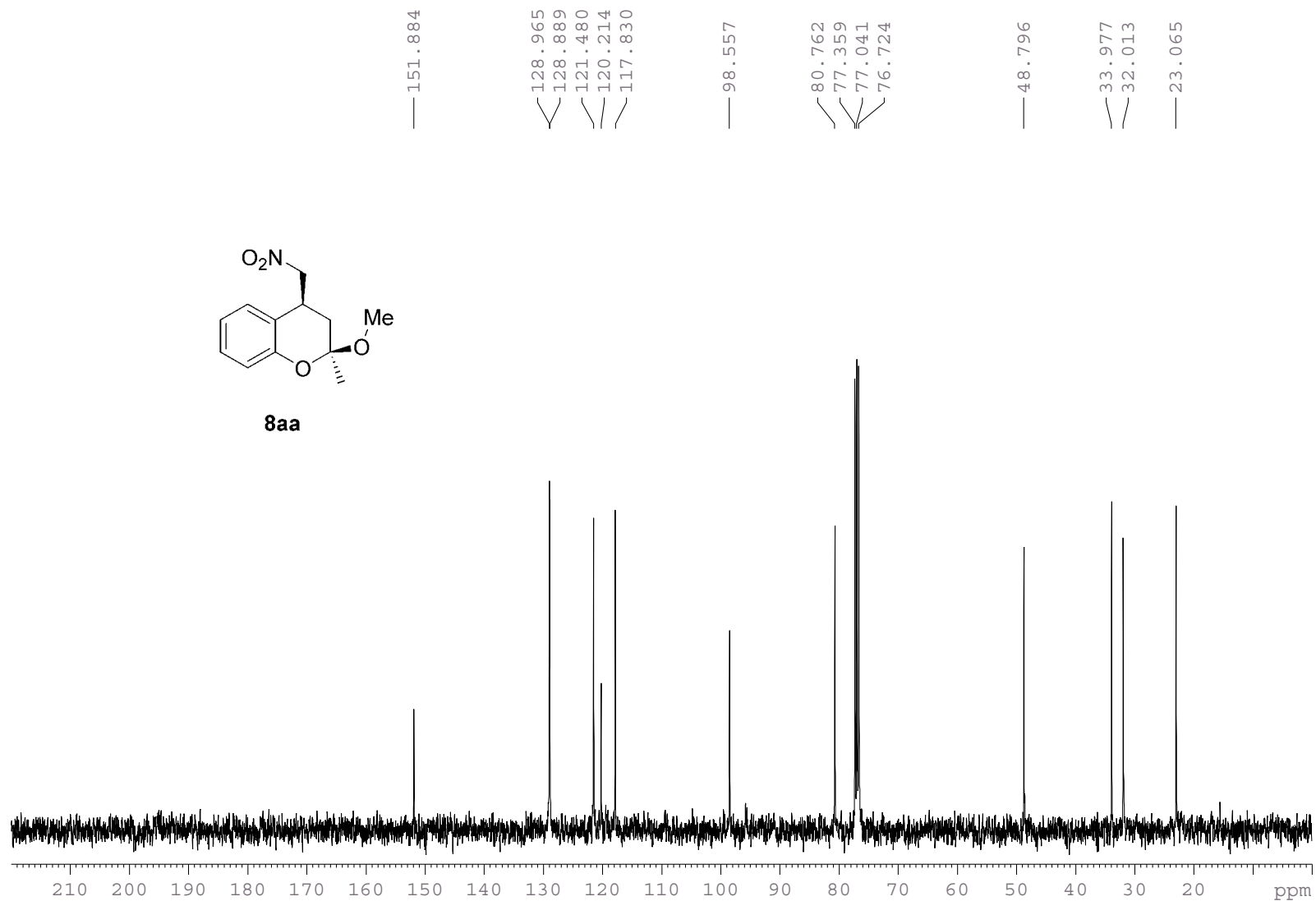
ramsc@uohyd.ernet.in

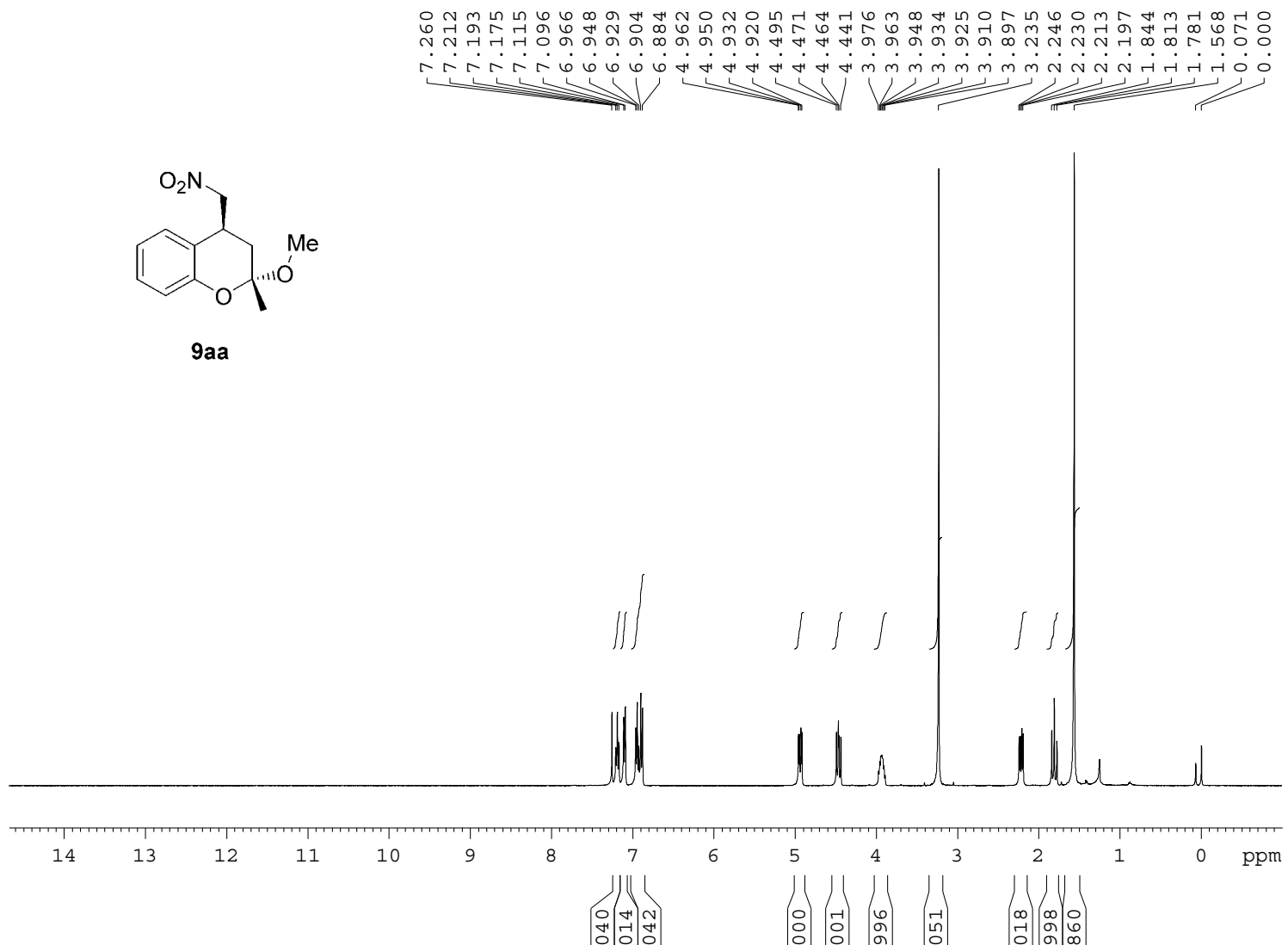
Key Note about the NMR plots: *Due to the Michael \leftrightarrow lactol isomerism in the SMA compounds 4/5/6, ^1H and ^{13}C NMR representing the signals of three compounds. The SMA products were found to exist in rapid equilibrium with 1:1:1 ratio of Michael \leftrightarrow cis-lactol \leftrightarrow trans-lactol products in solution (CDCl_3). The equilibrium is very rapid and therefore no pseudo-diastereomers are observed during HPLC analysis.*

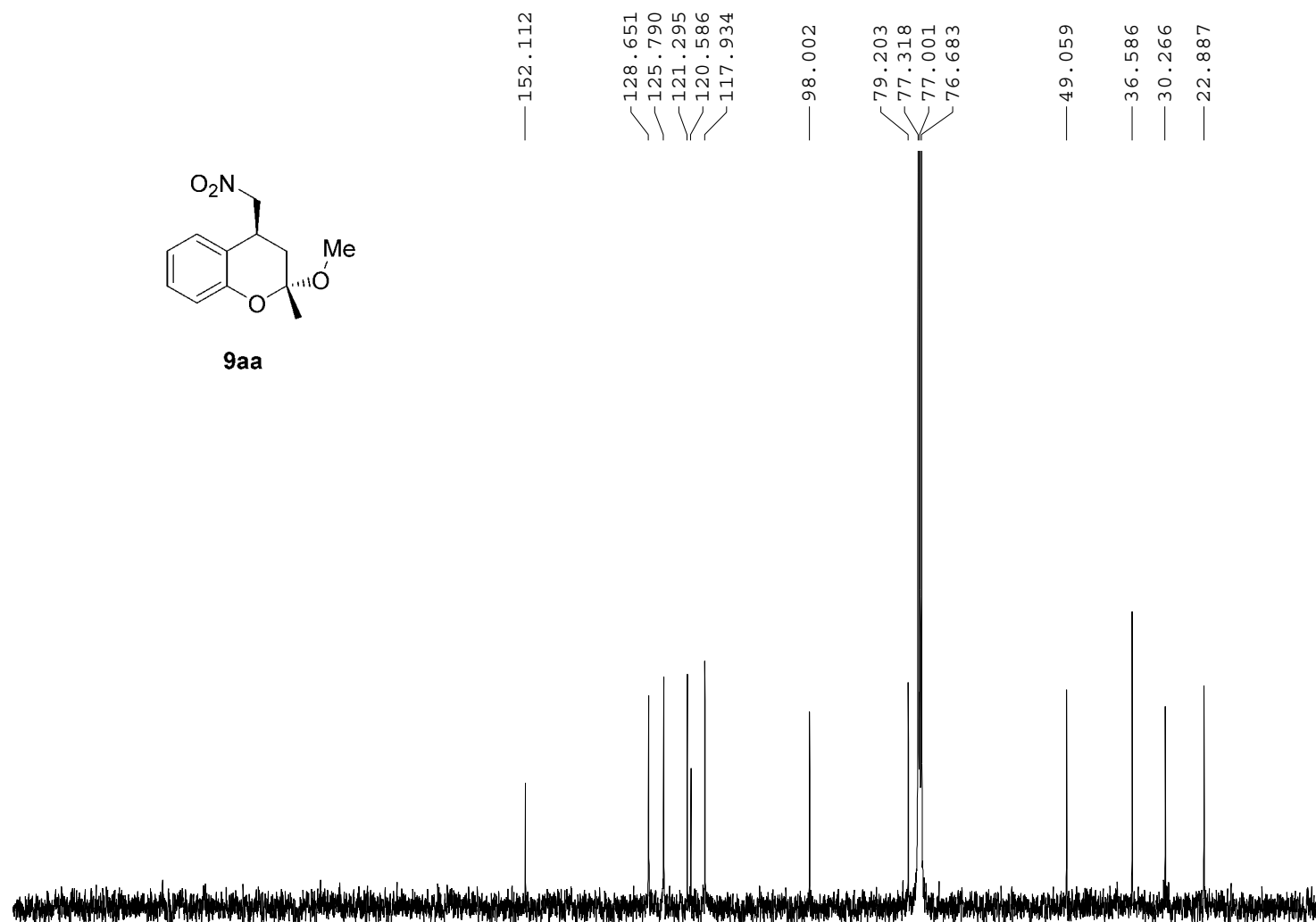
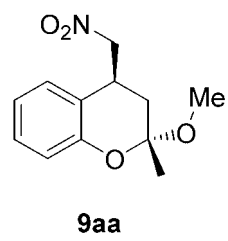


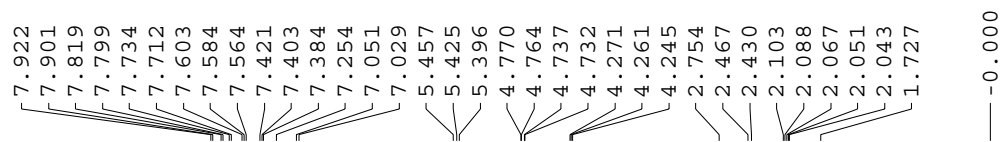
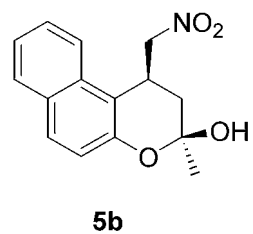


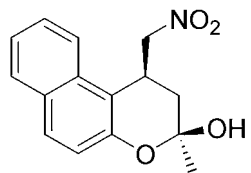




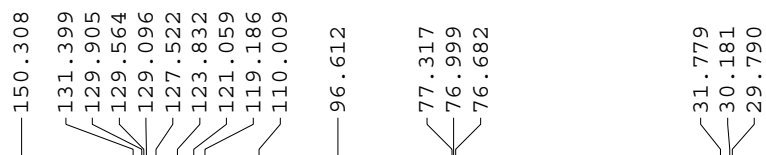


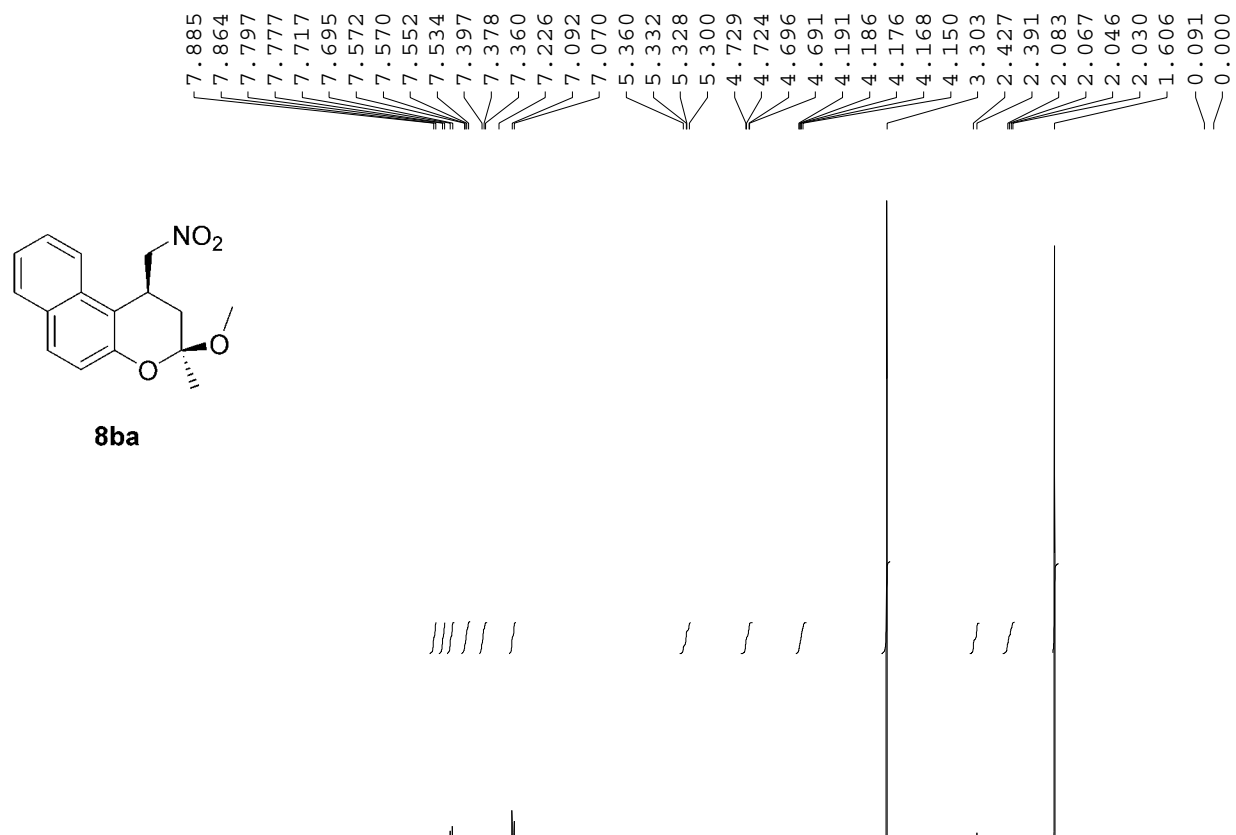


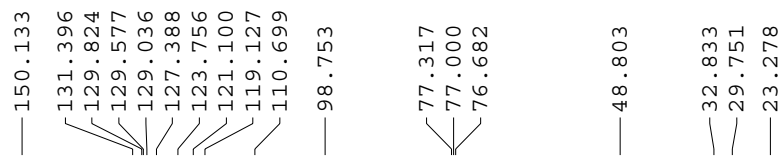
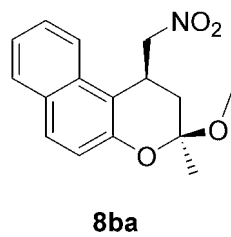


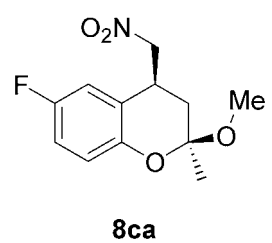


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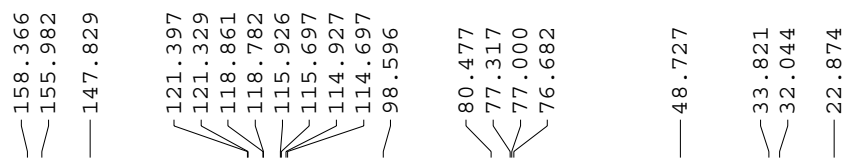
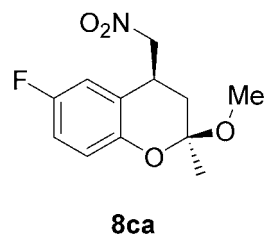


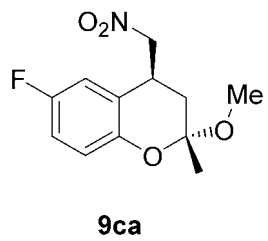




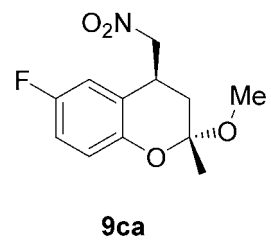


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2.057
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2.020
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0.000





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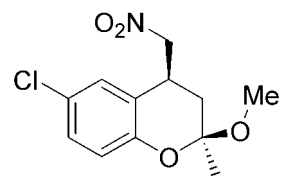
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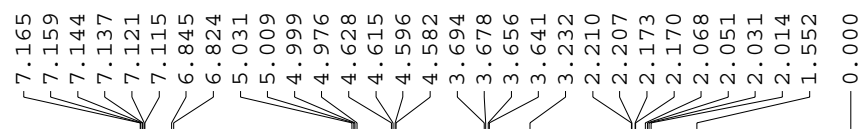
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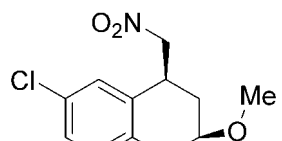
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8da





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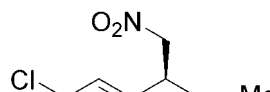
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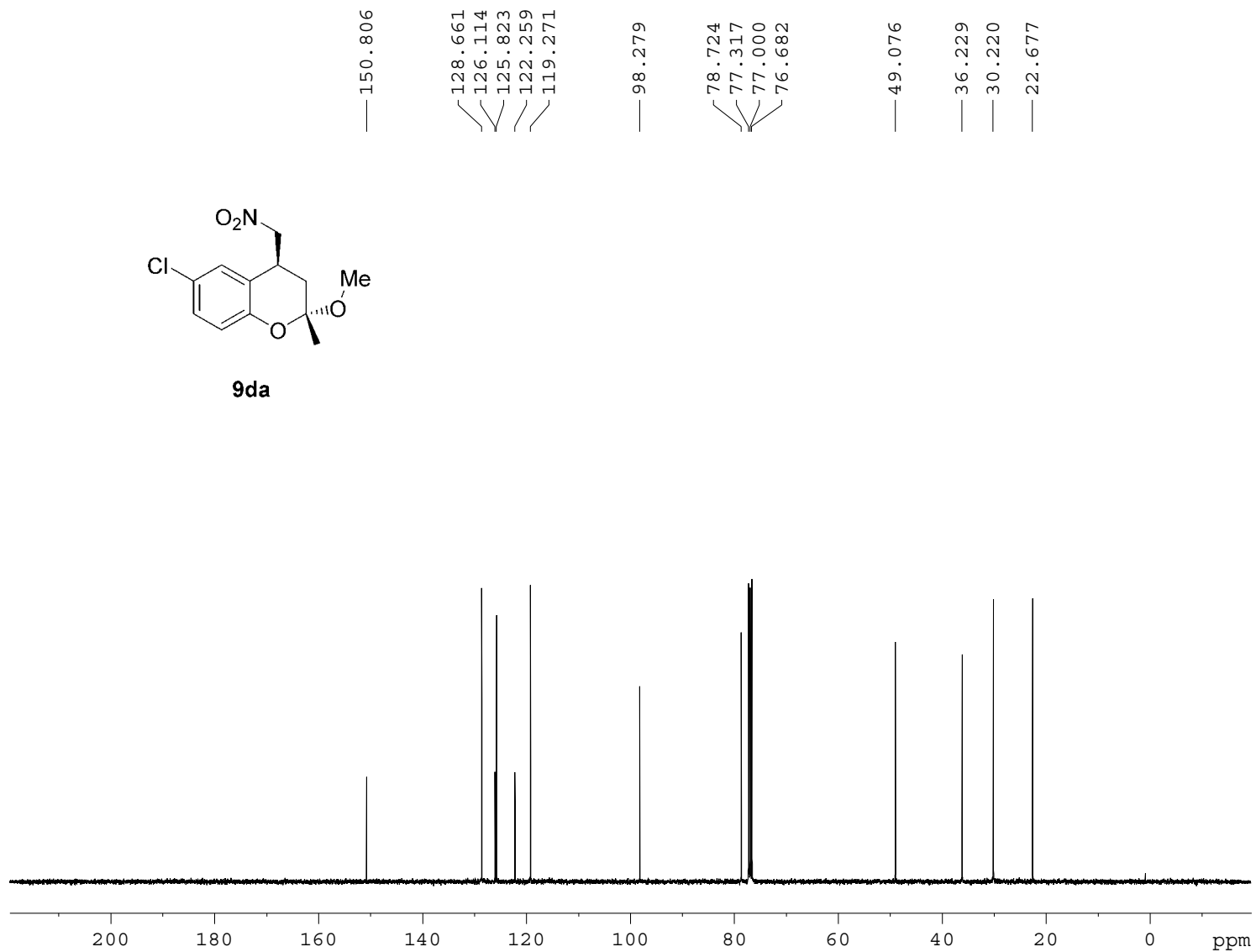
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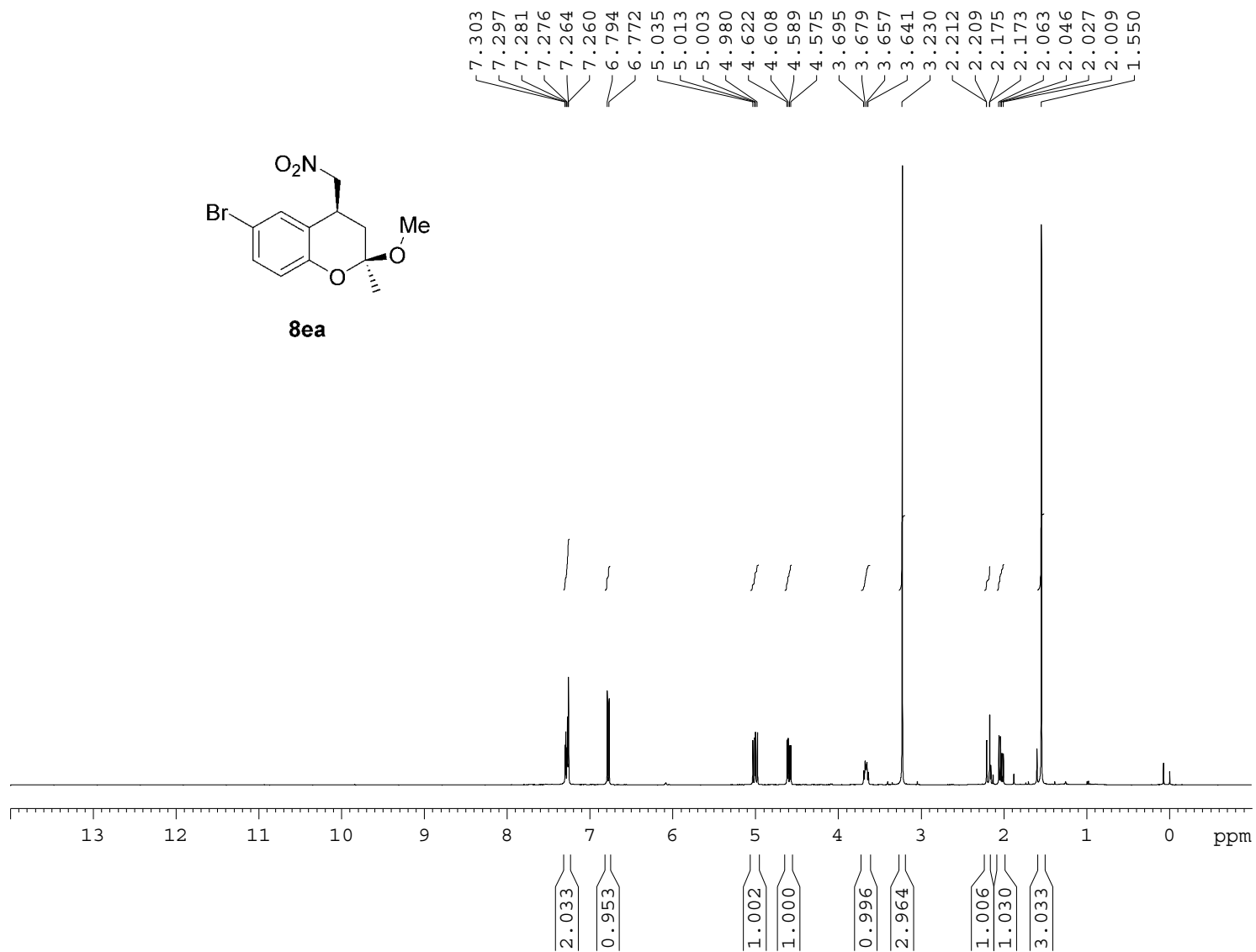


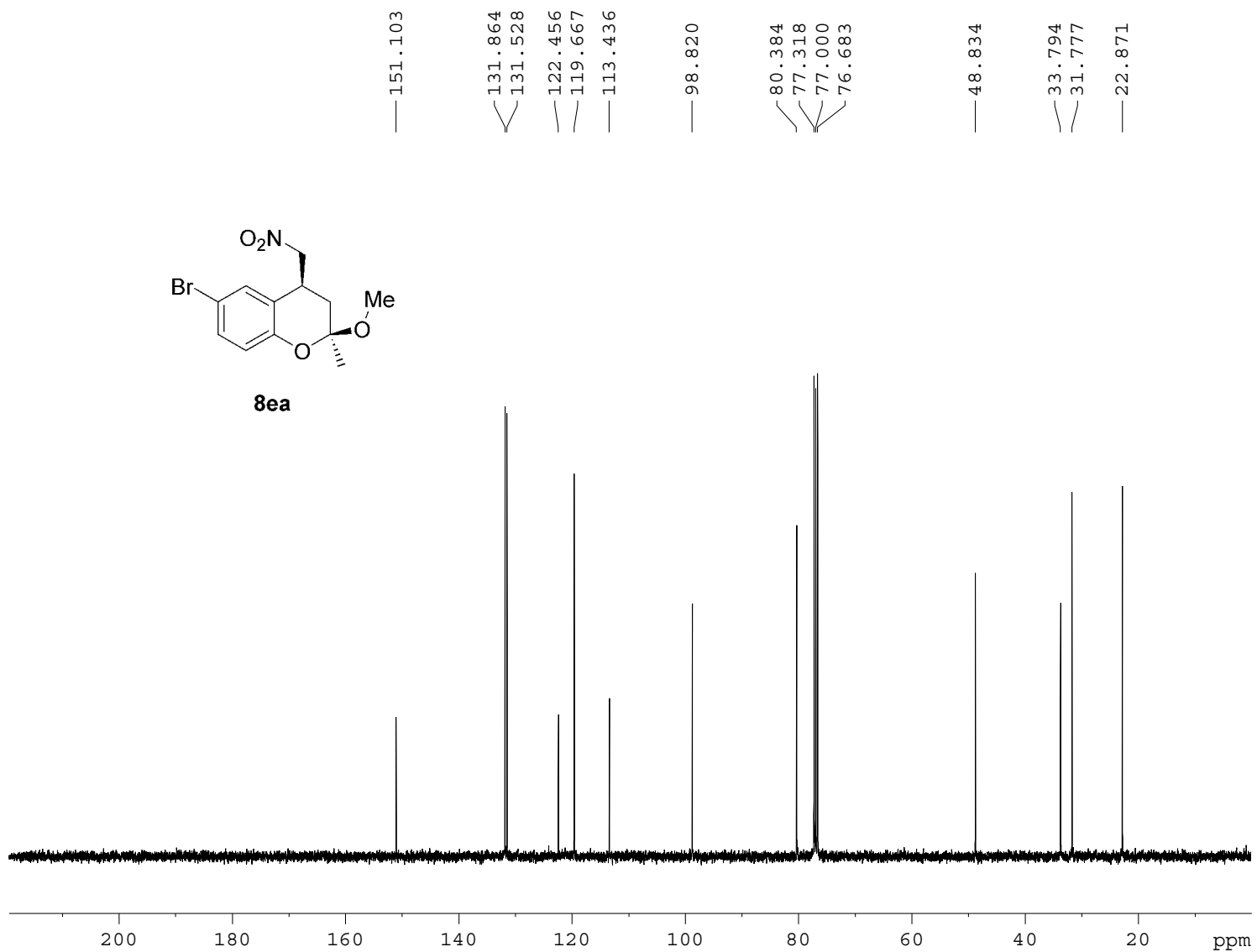
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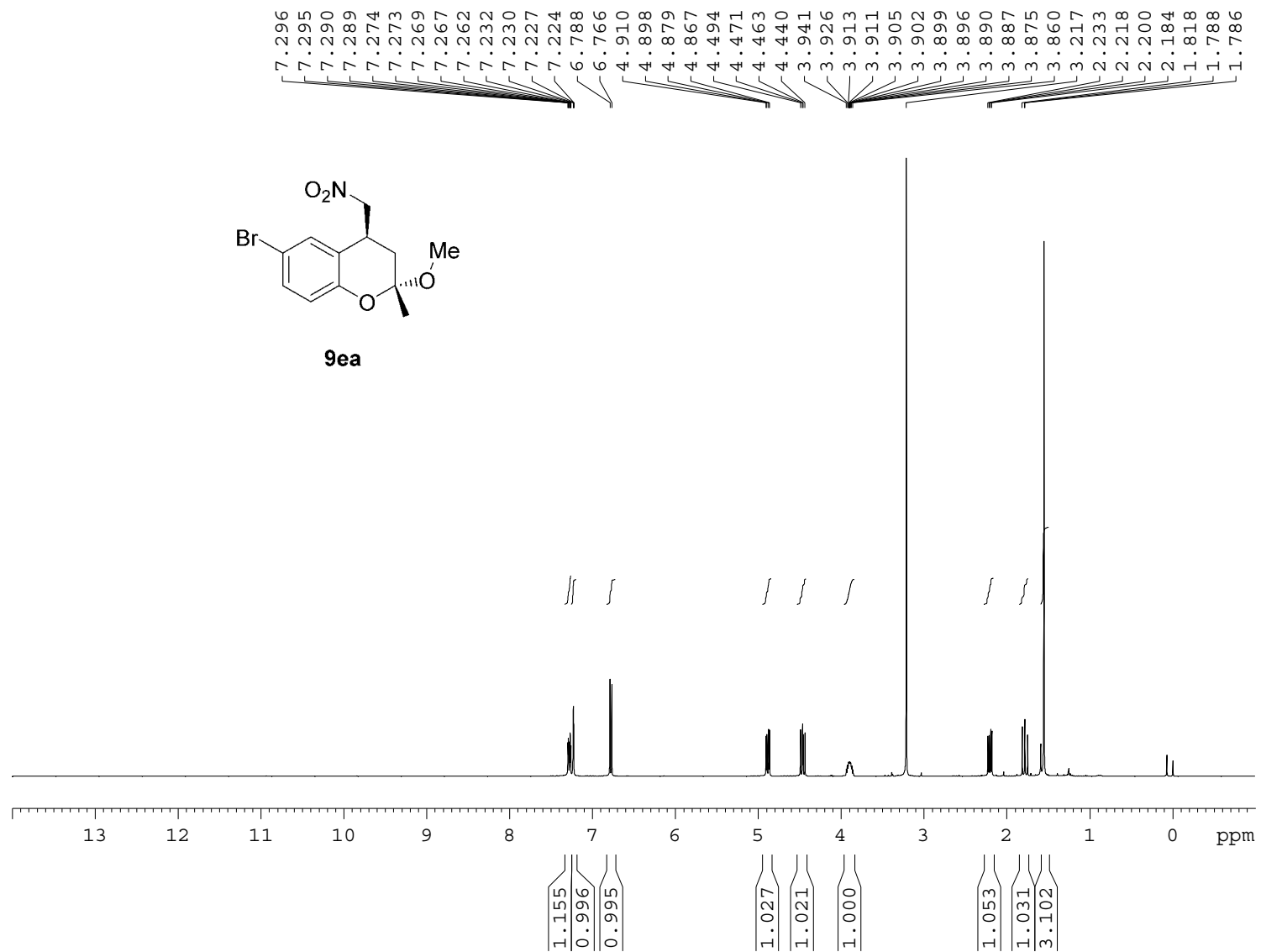
Supplementary Material (ESI) for Organic & Biomolecular Chemistry

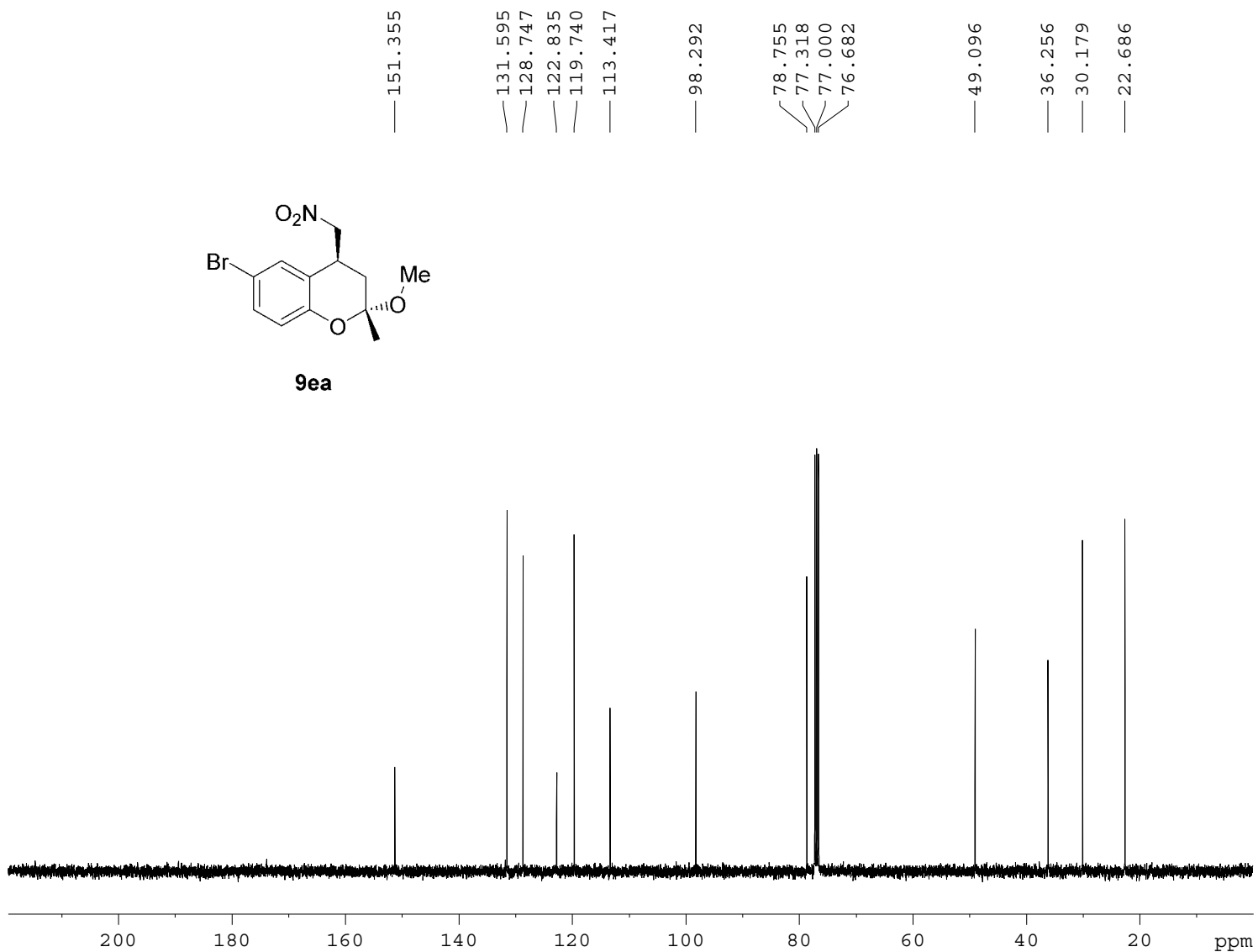
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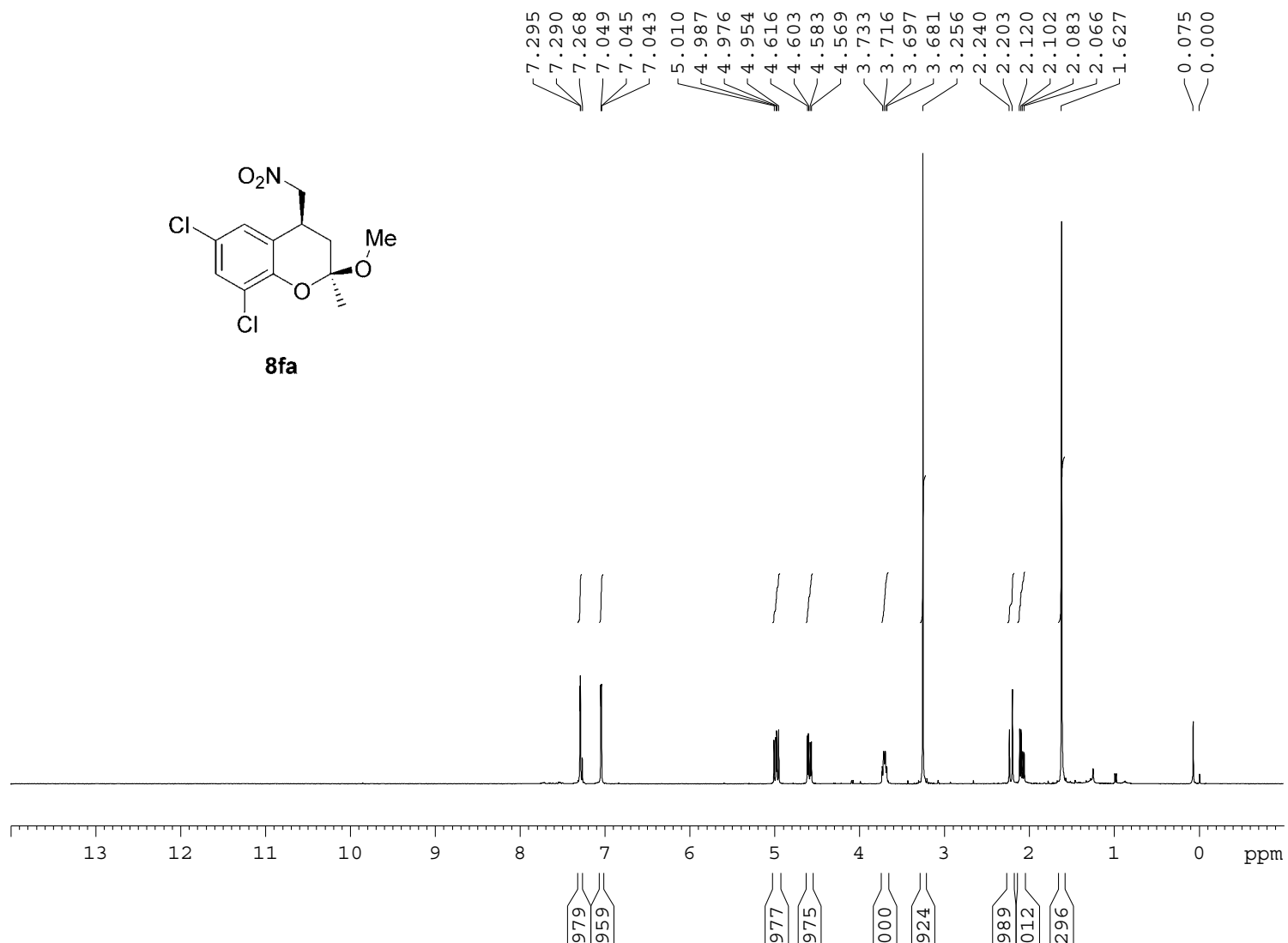


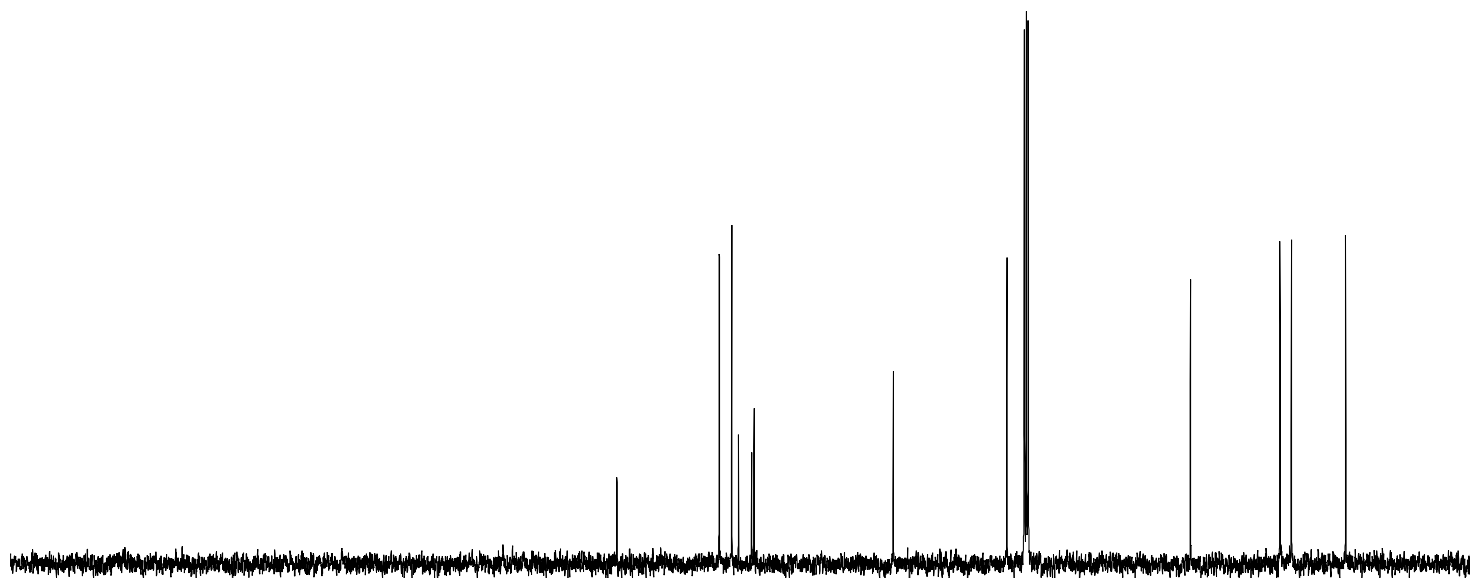
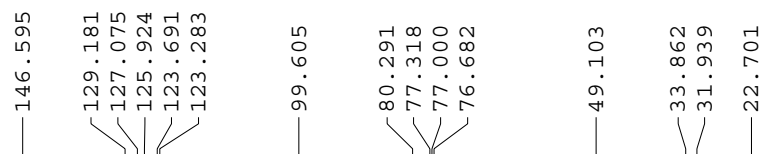
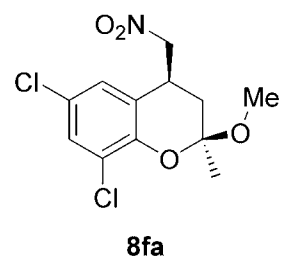


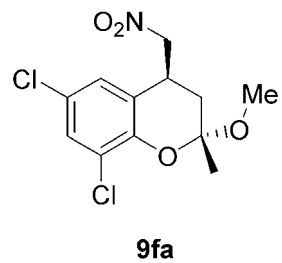




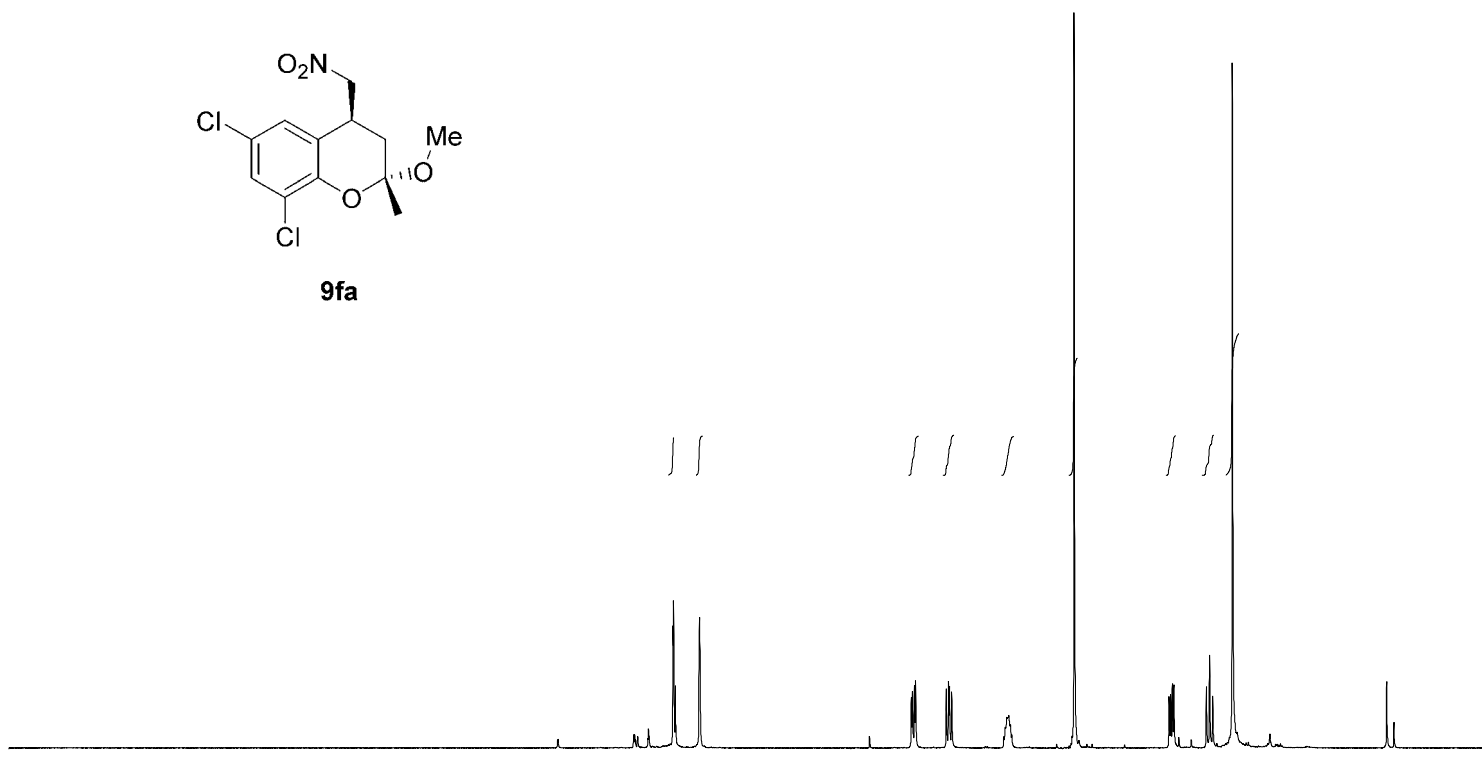


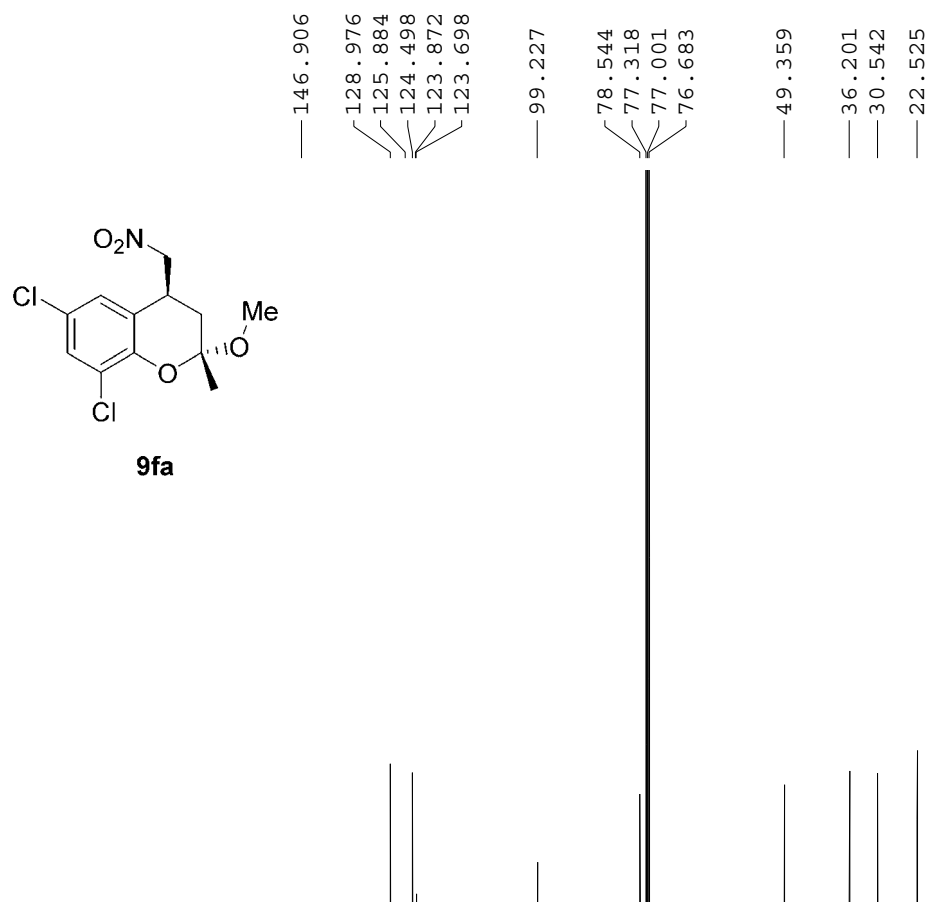


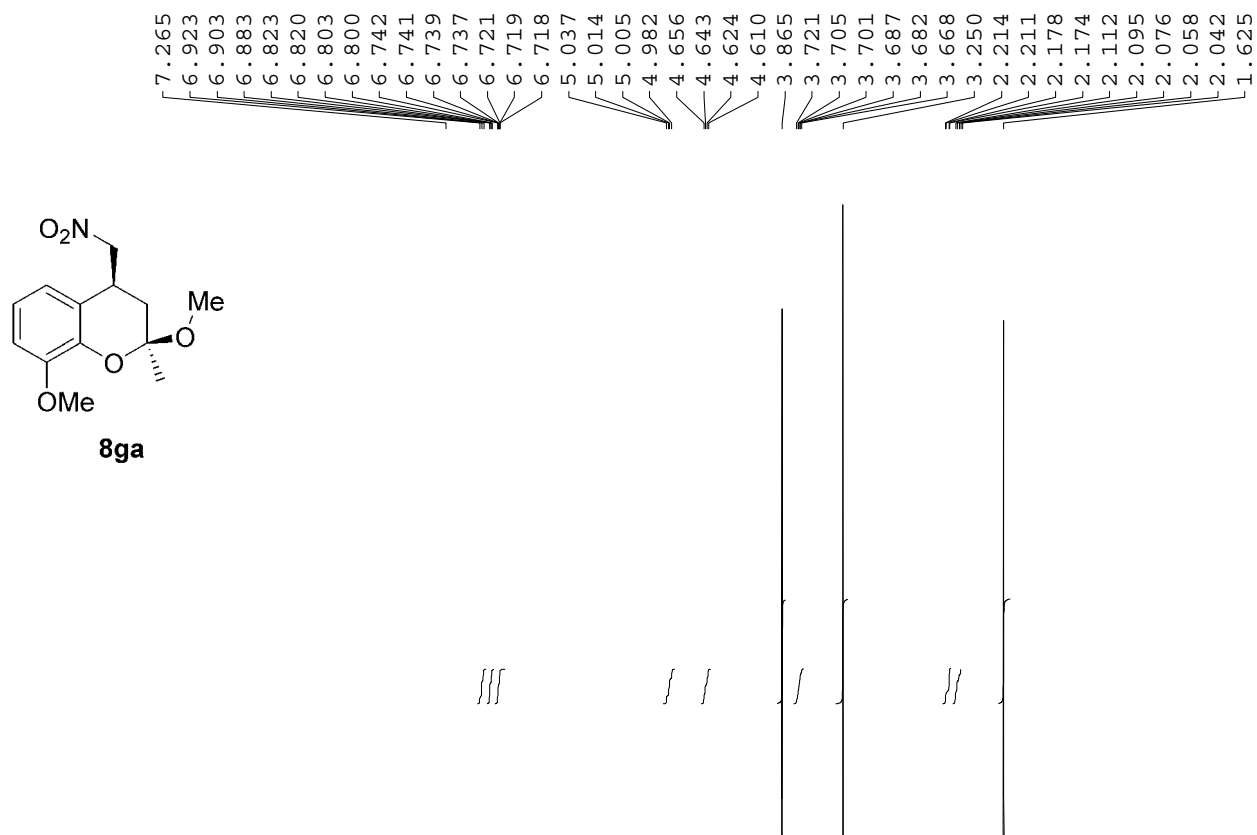


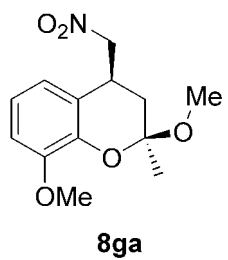


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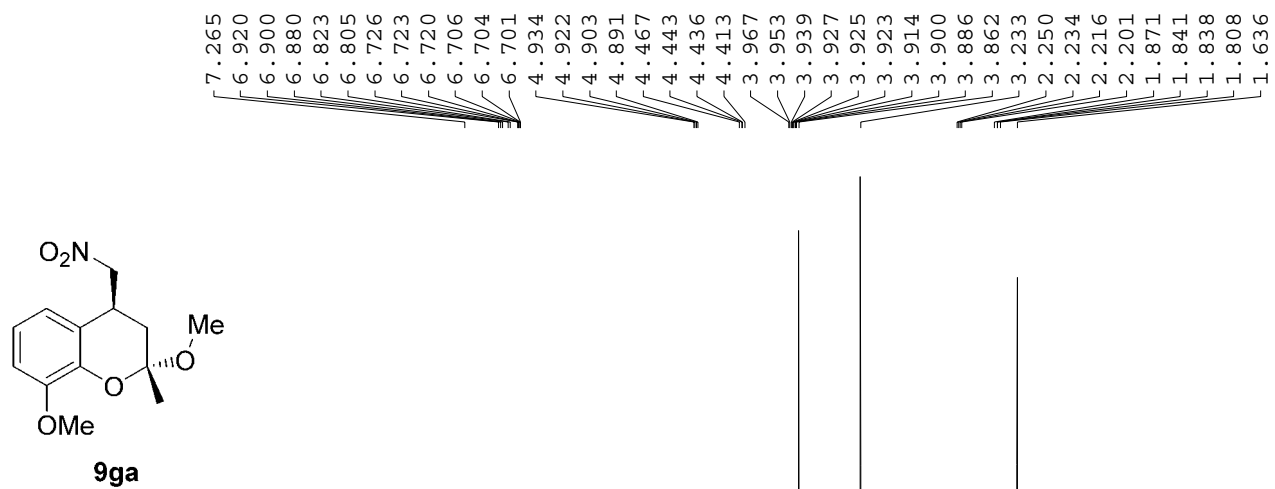
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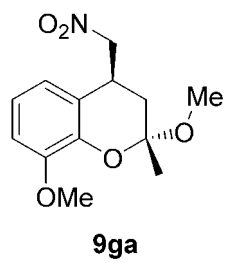
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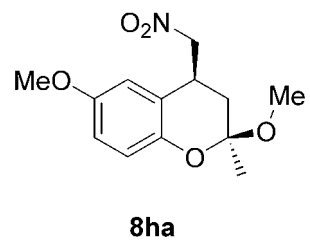
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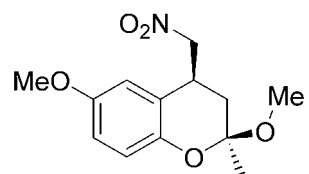
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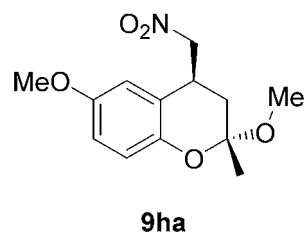
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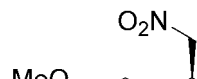
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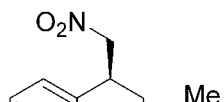
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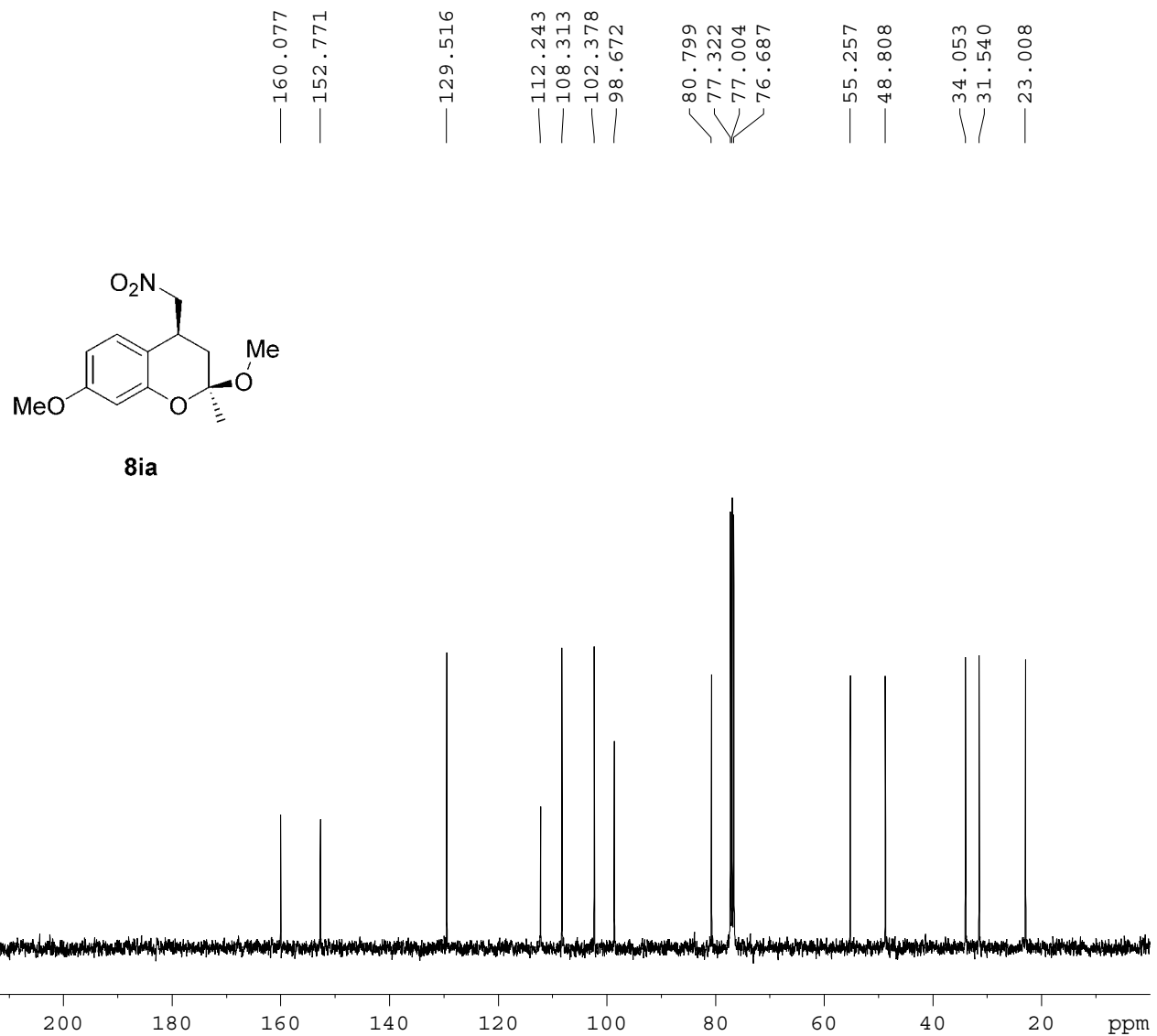


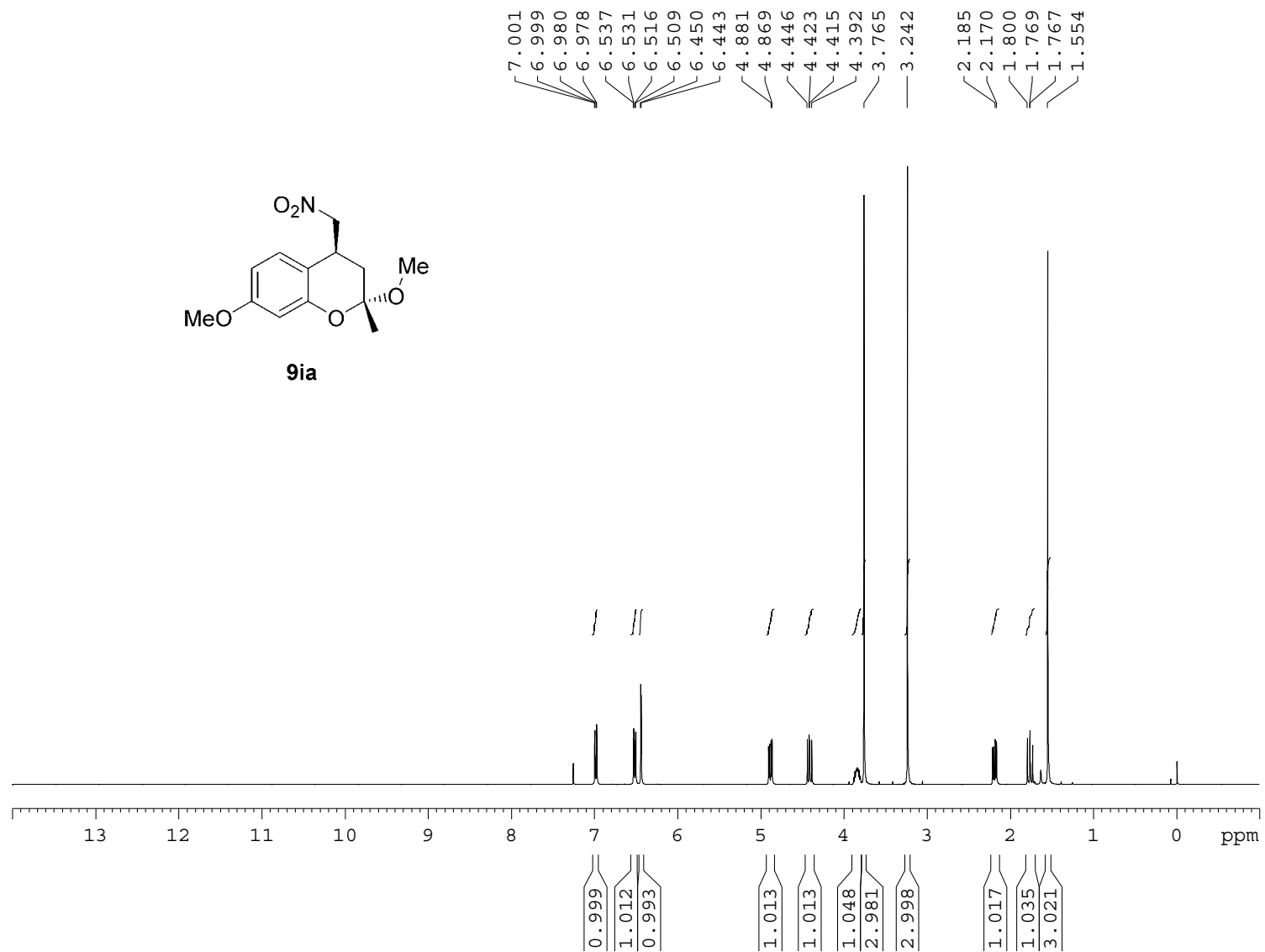


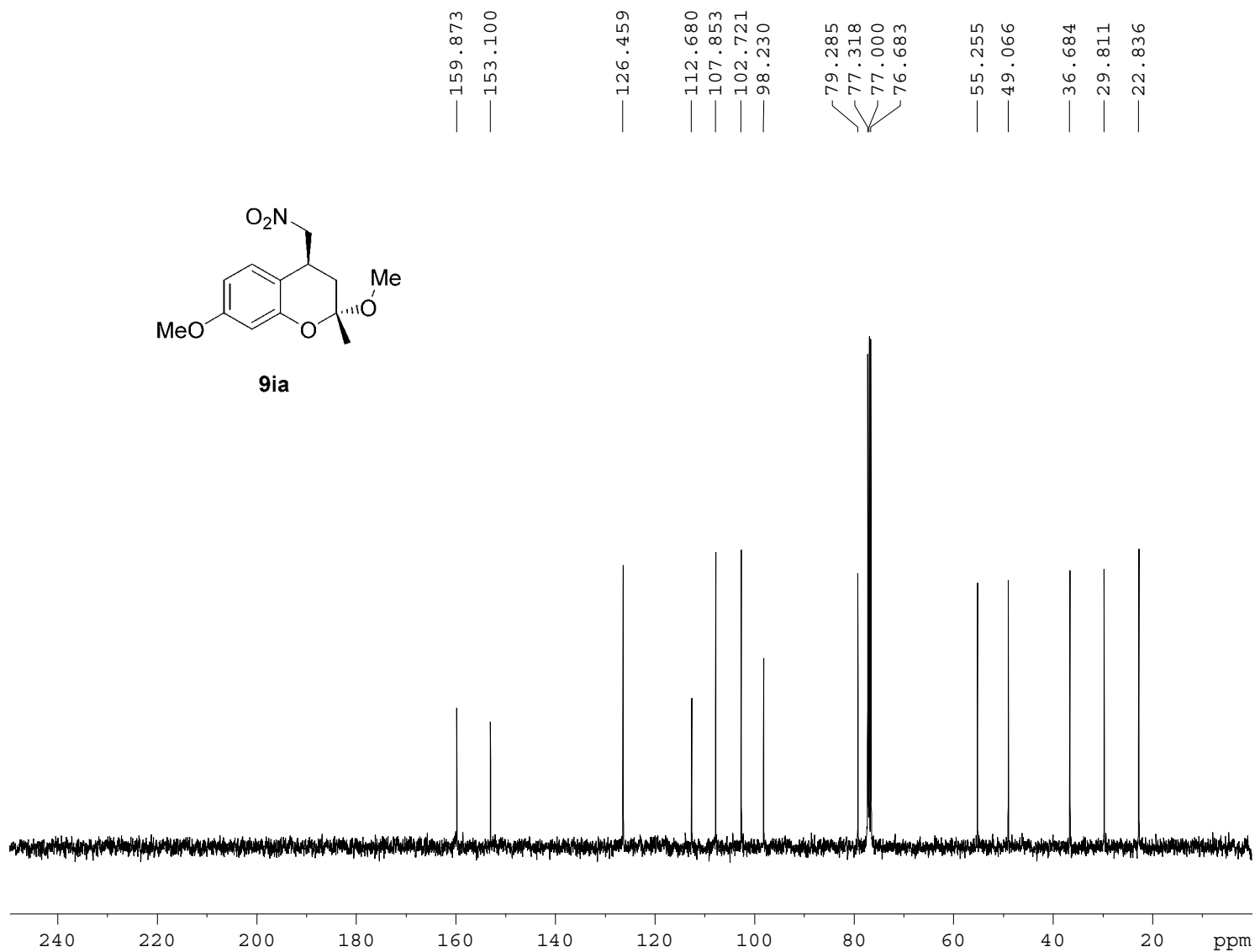
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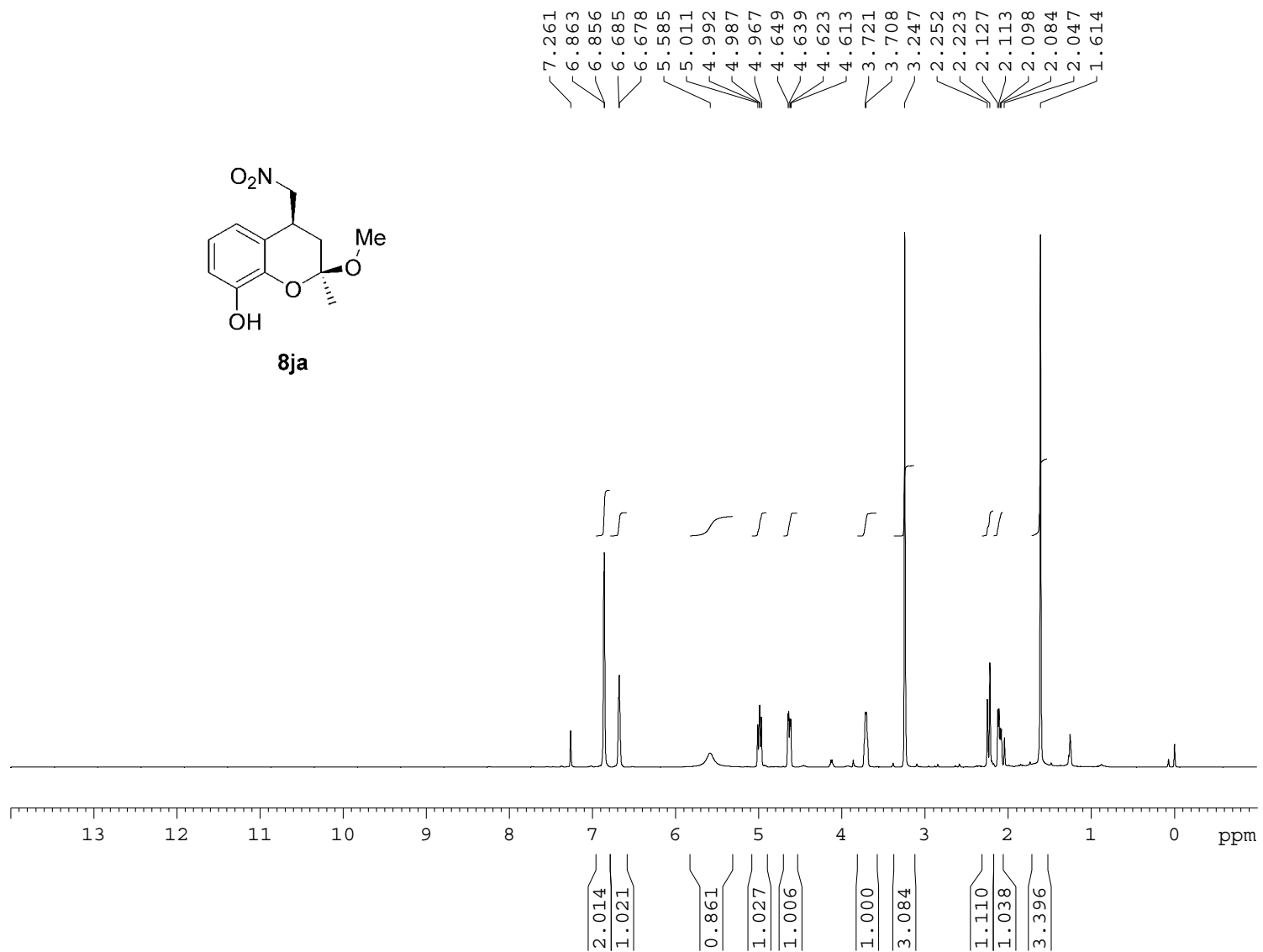
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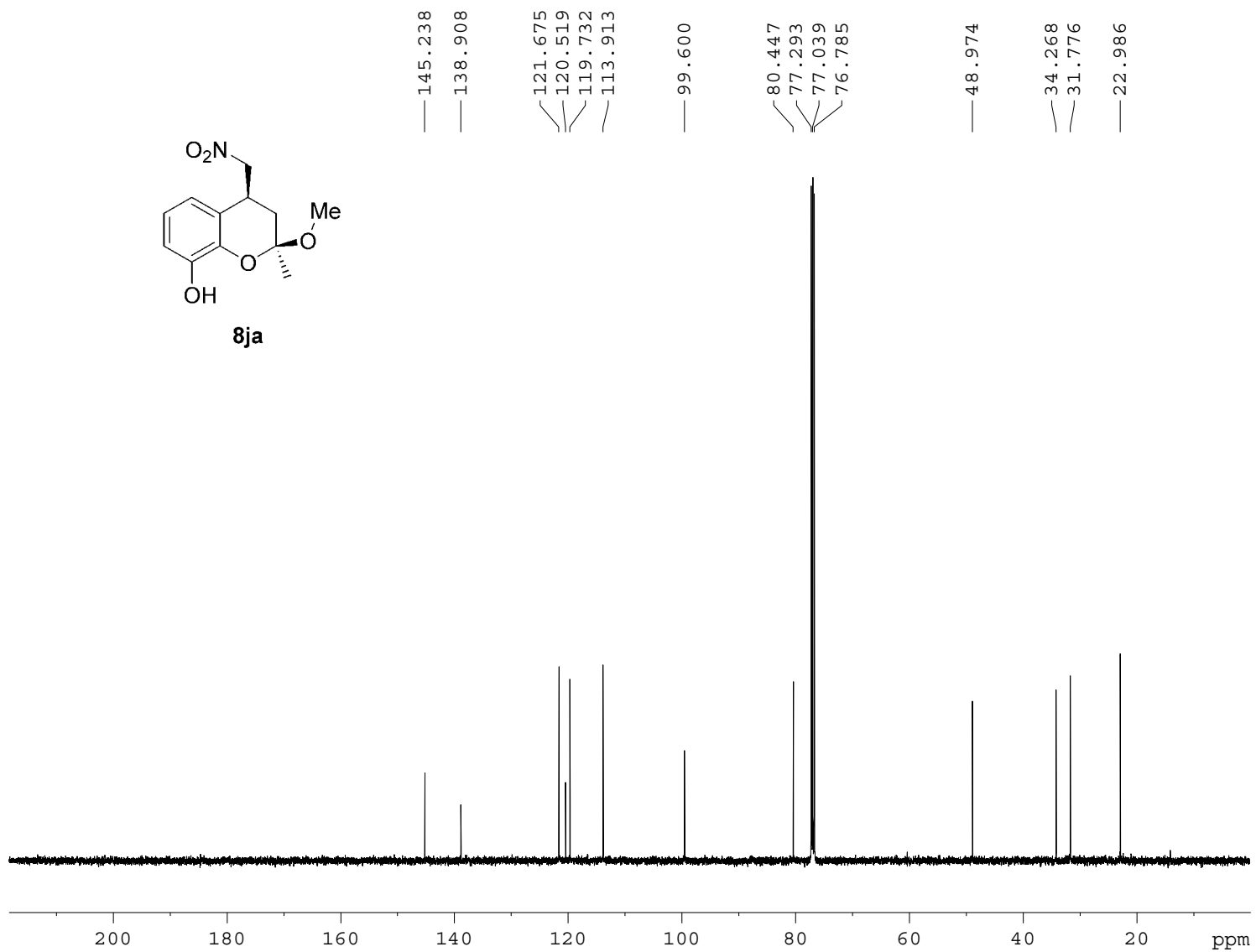
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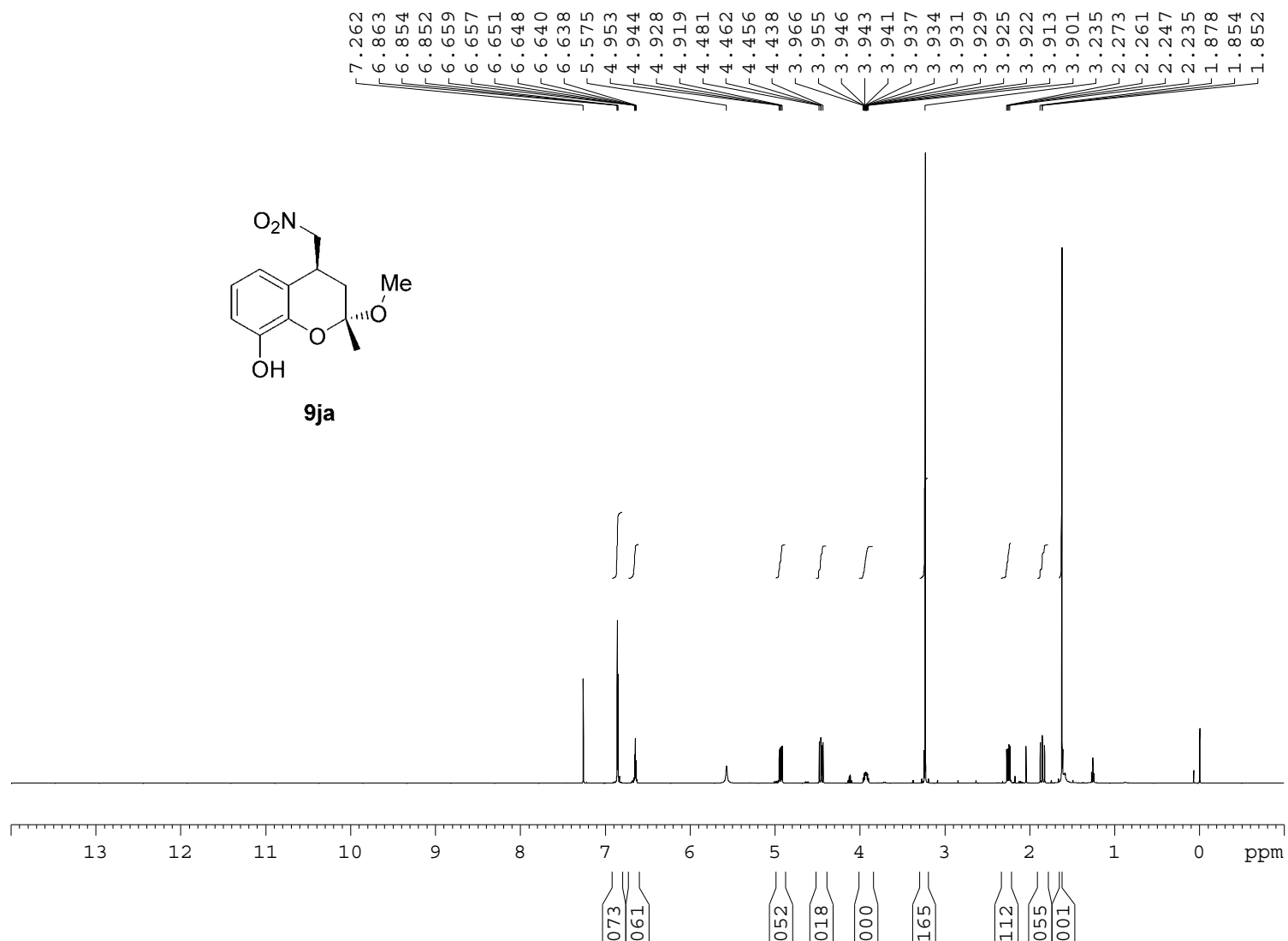


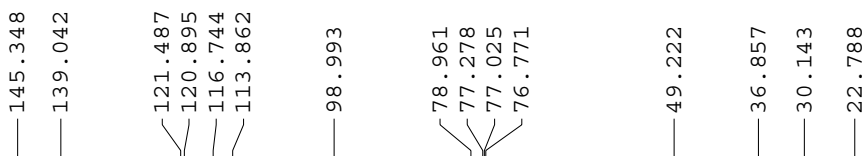
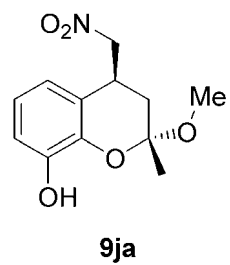


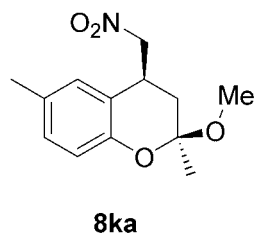




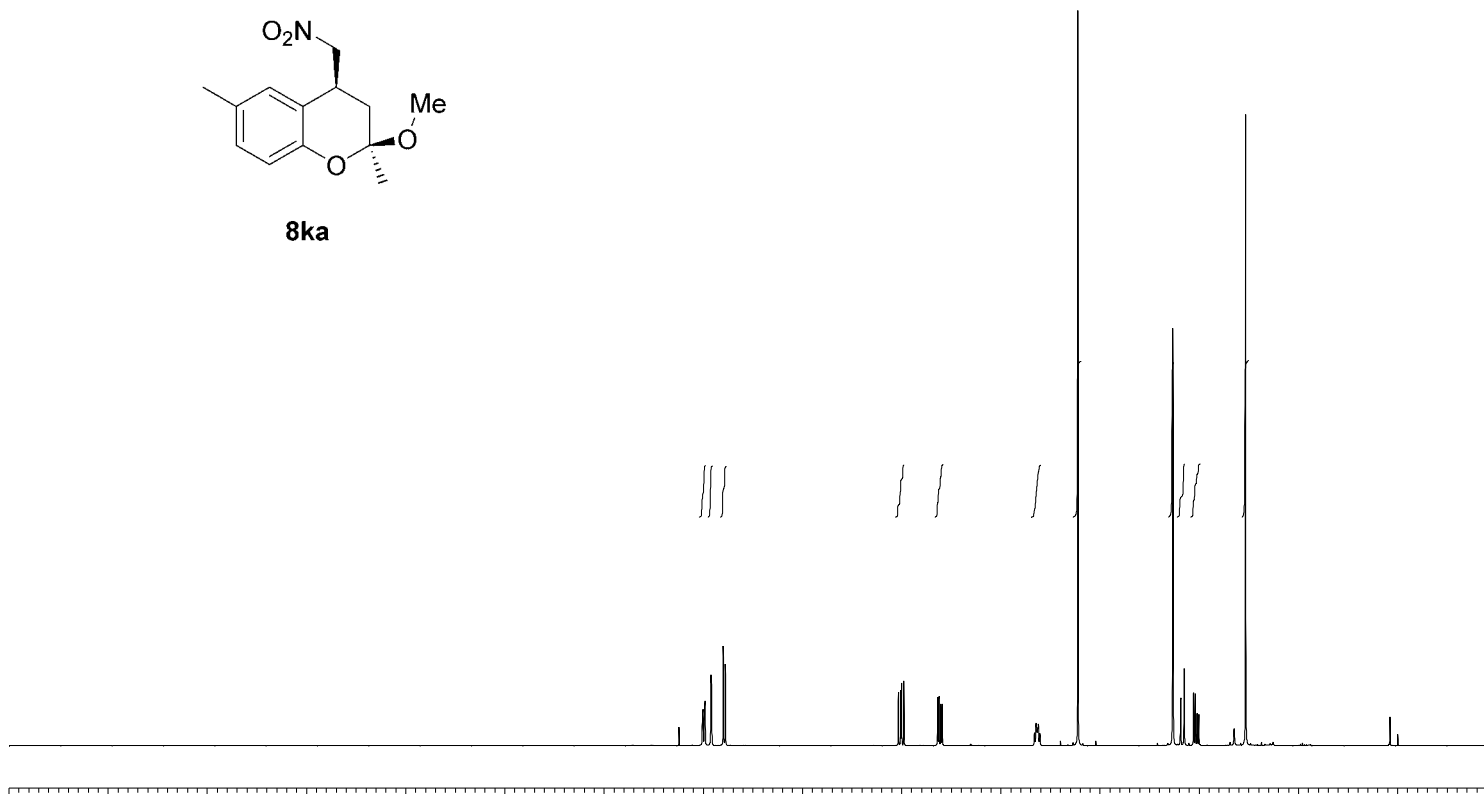


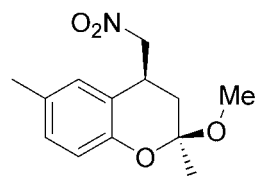






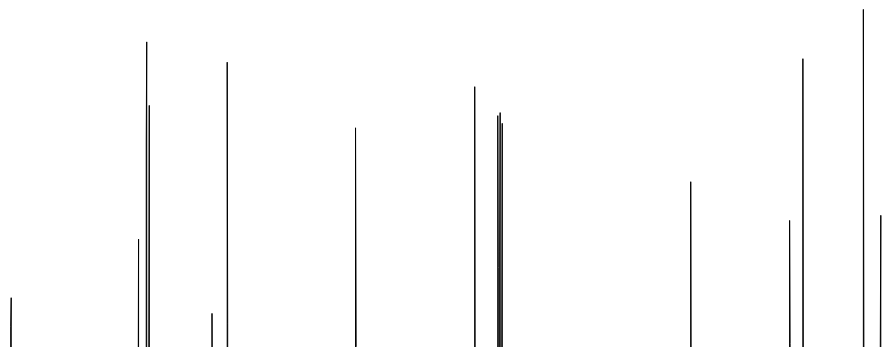
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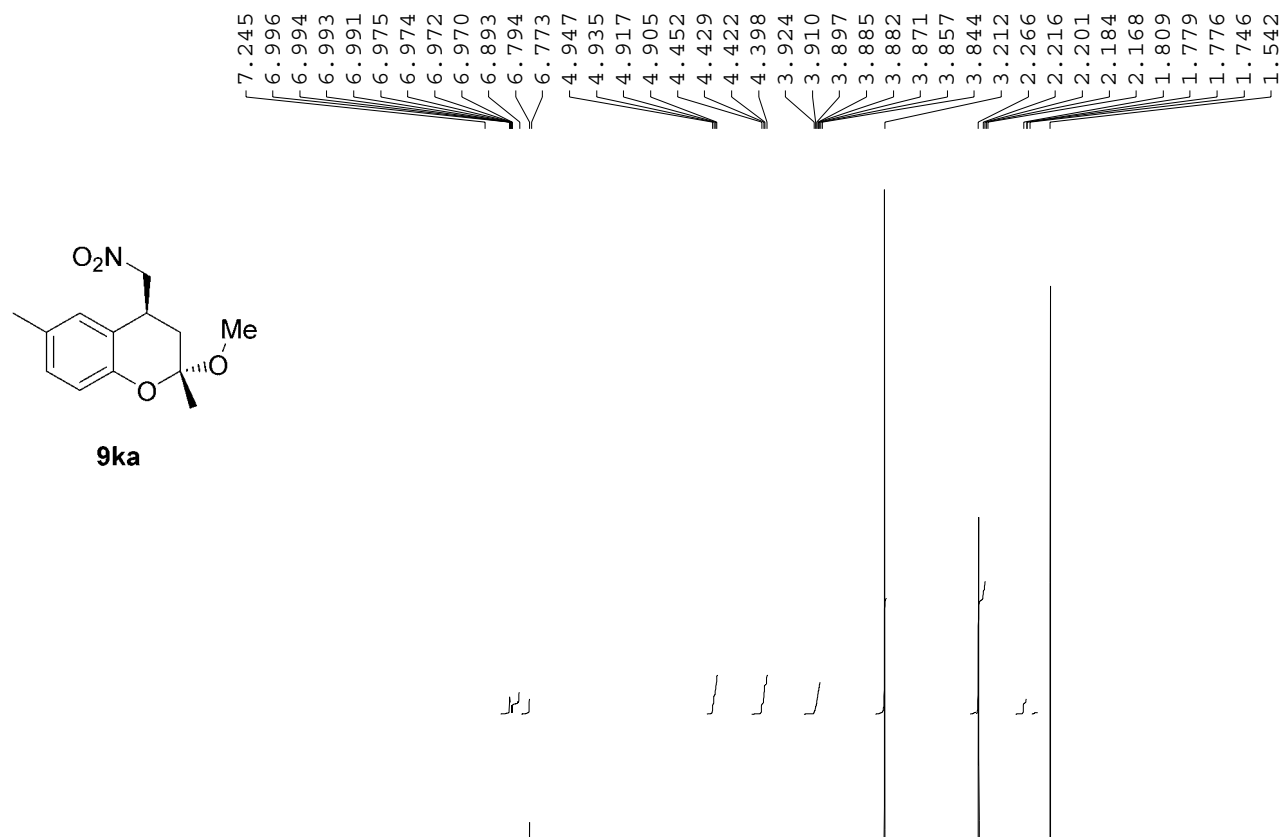


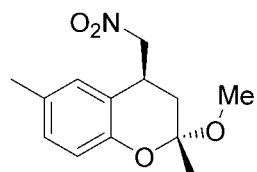


8ka

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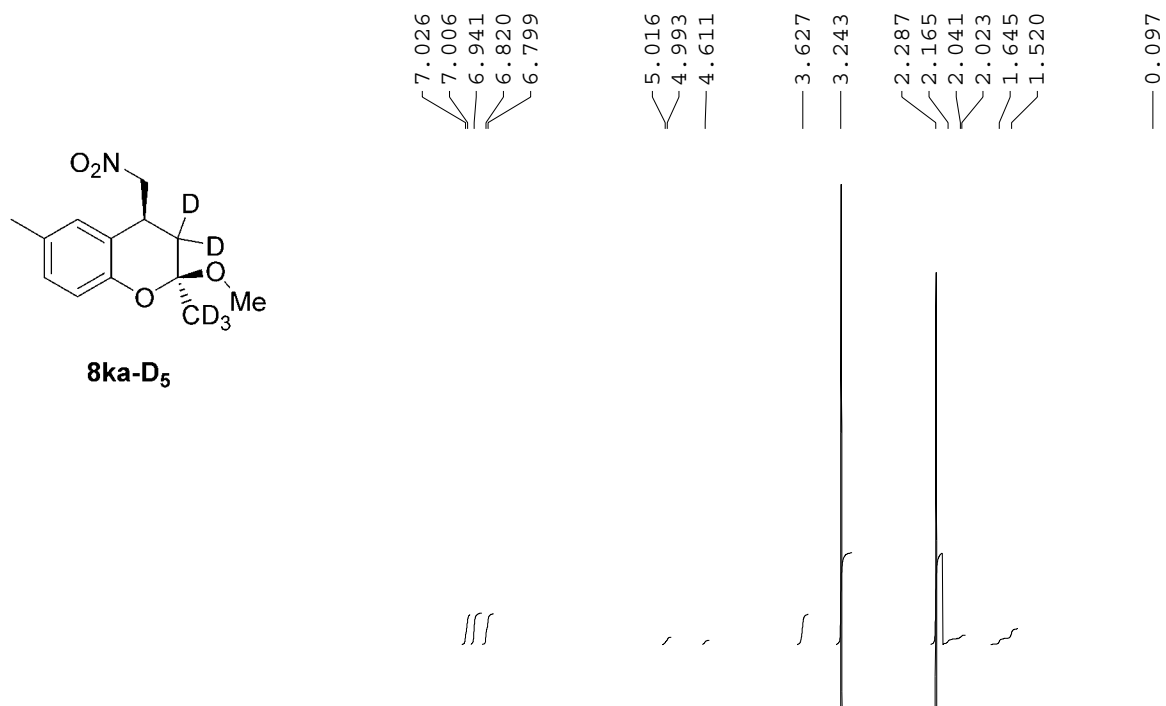


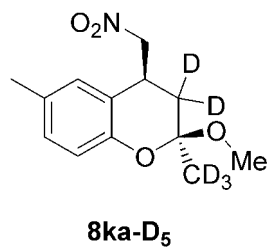




9ka

—	149.797
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—	77.318
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—	22.833
—	20.632





— 149.592

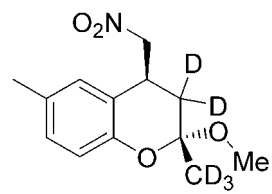
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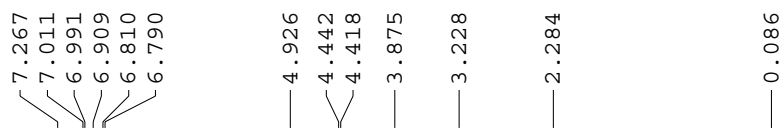
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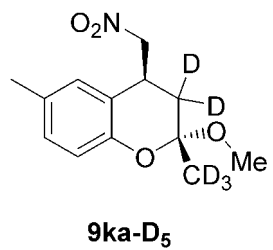
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9ka-D₅





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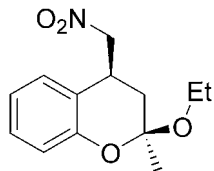
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117.709

—97.767

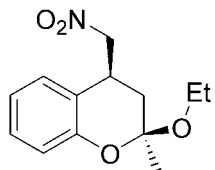
79.033
77.369
77.051
76.734

—49.013

30.040
29.967
22.081
20.721



7.256
7.207
7.189
7.172
7.169
7.125
7.107
6.957
6.939
6.920
6.880
6.859
5.090
5.067
5.057
5.035
4.672
4.658
4.640
4.626
3.720
3.704
3.683
3.667
3.615
3.598
3.580
3.564
2.224
2.188
2.068
2.051
2.032
2.015
1.561
1.046
1.029
1.011



— 151.996

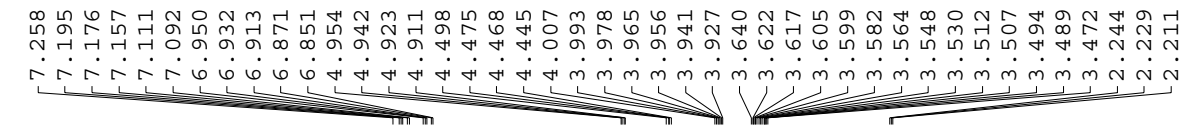
128.906
128.812
121.328
120.211
117.751

— 98.388

80.907
77.319
77.001
76.684

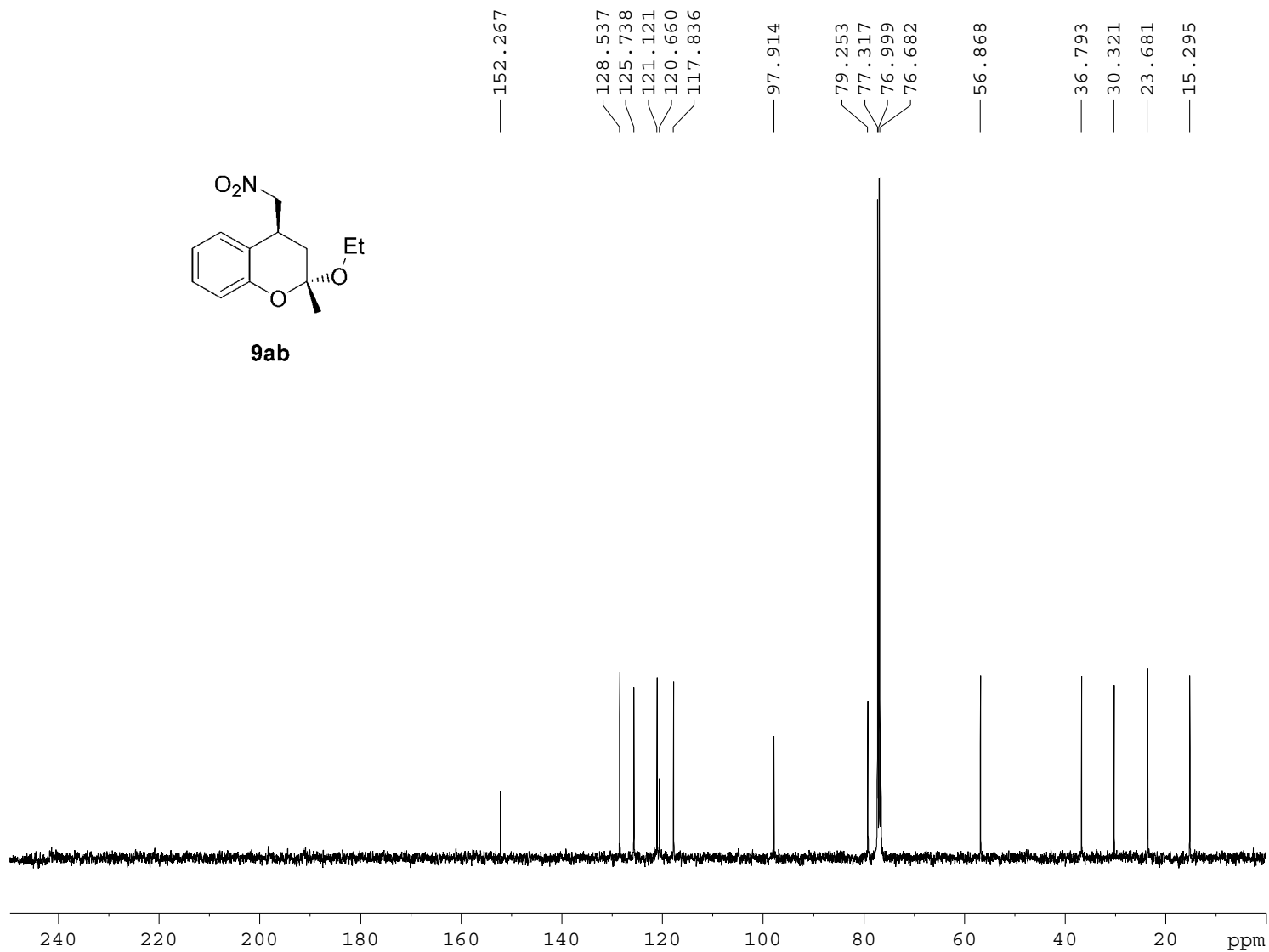
— 56.862

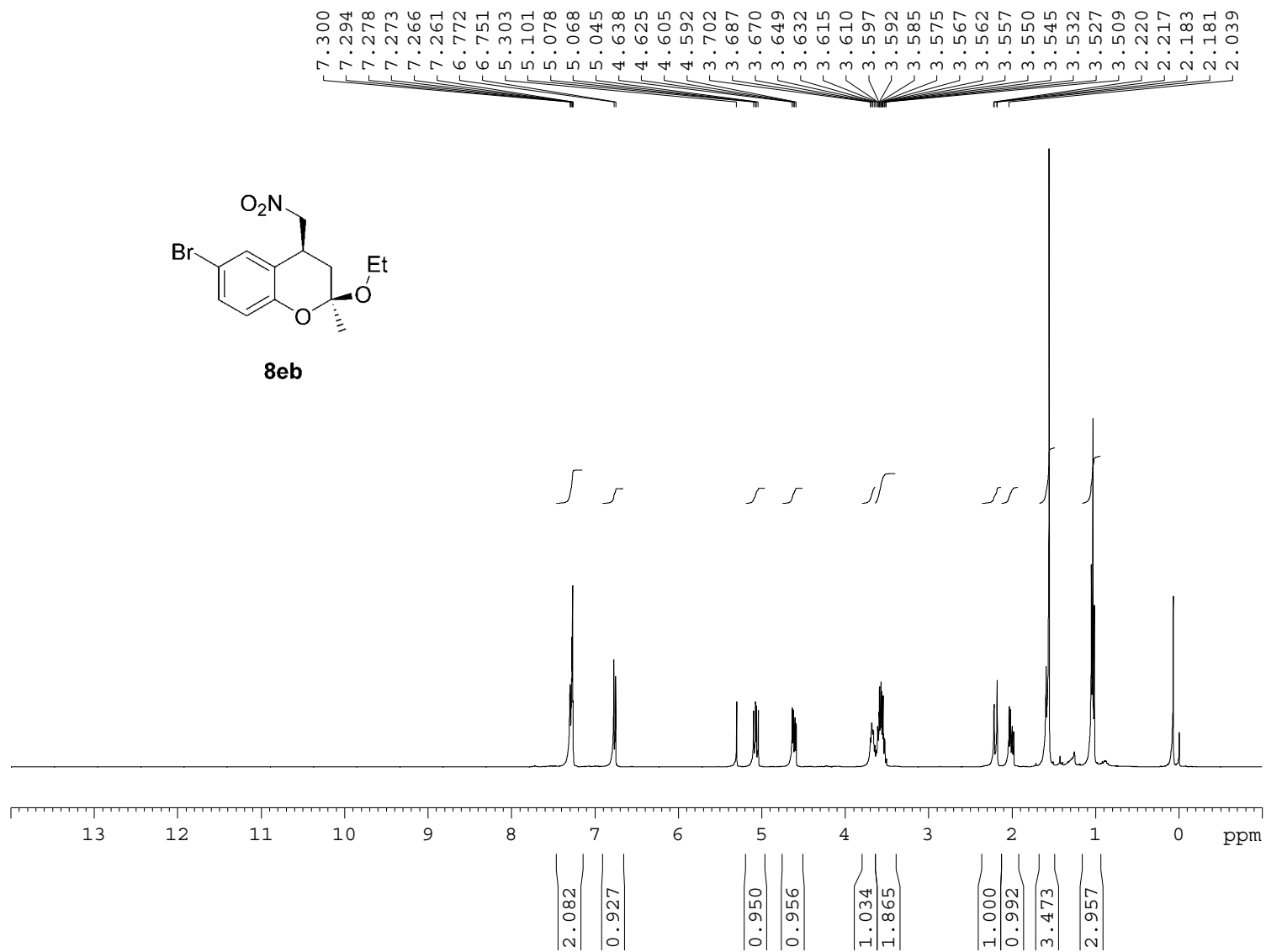
34.230
32.096
— 23.755
— 15.395

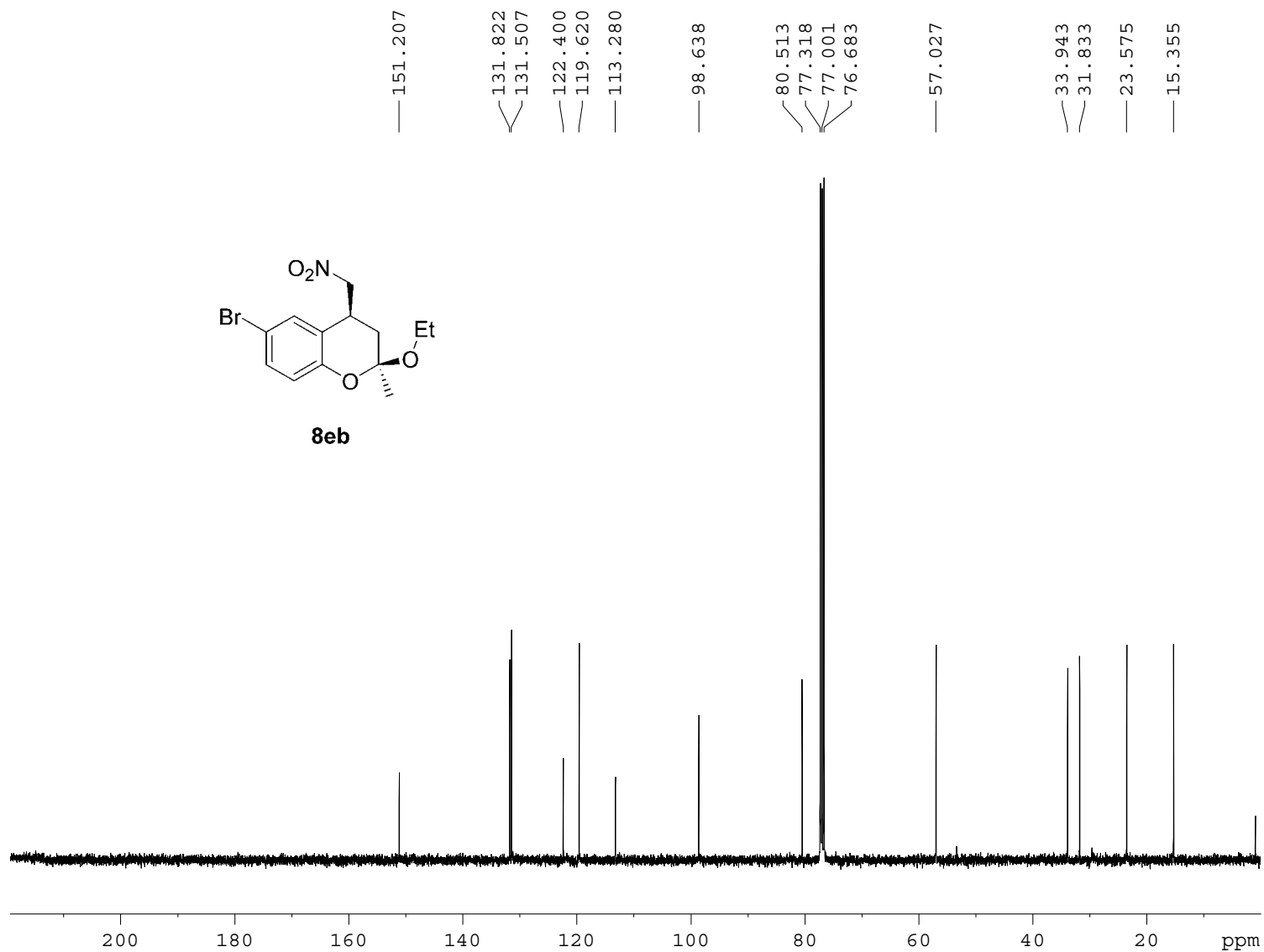


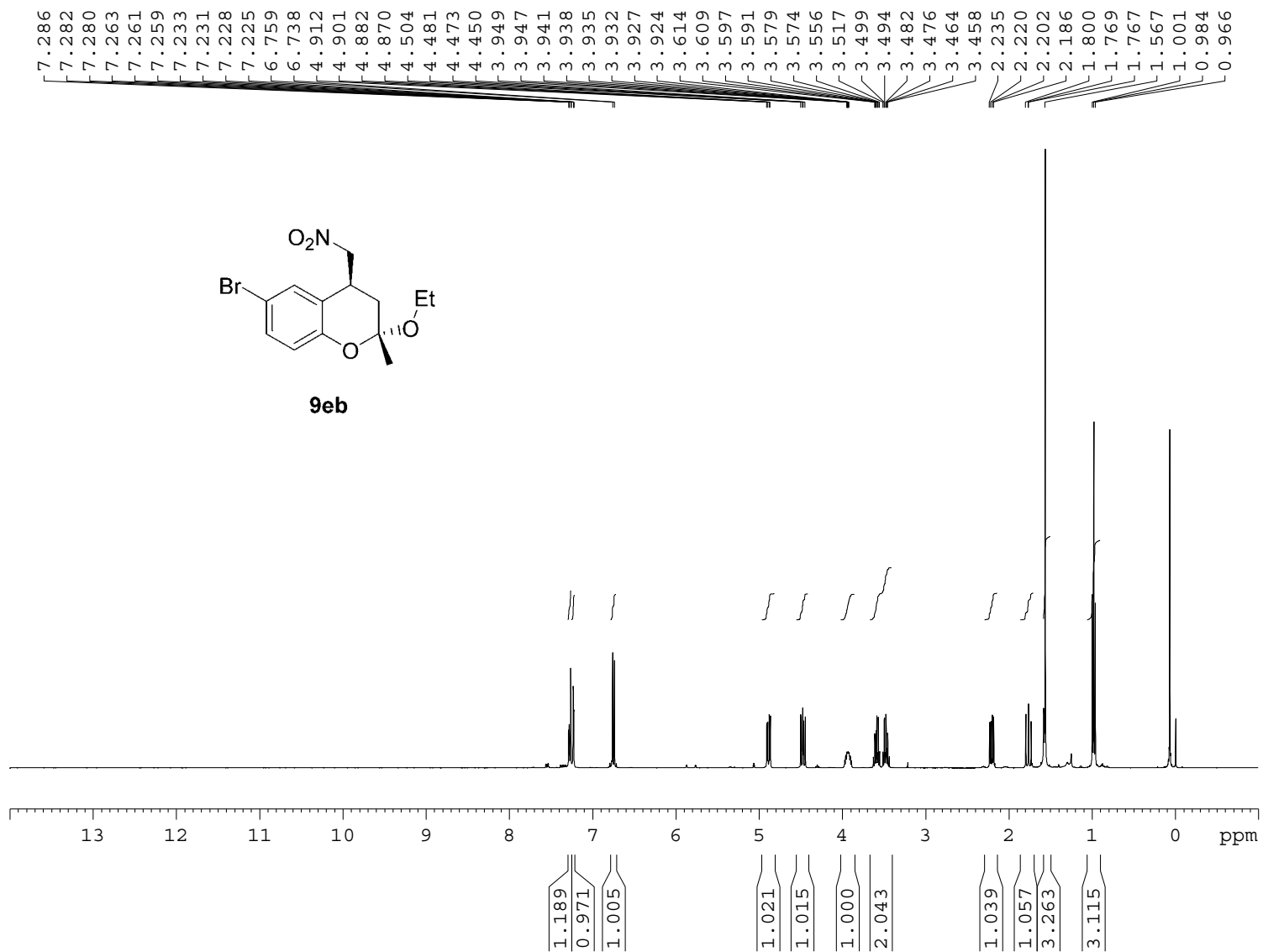
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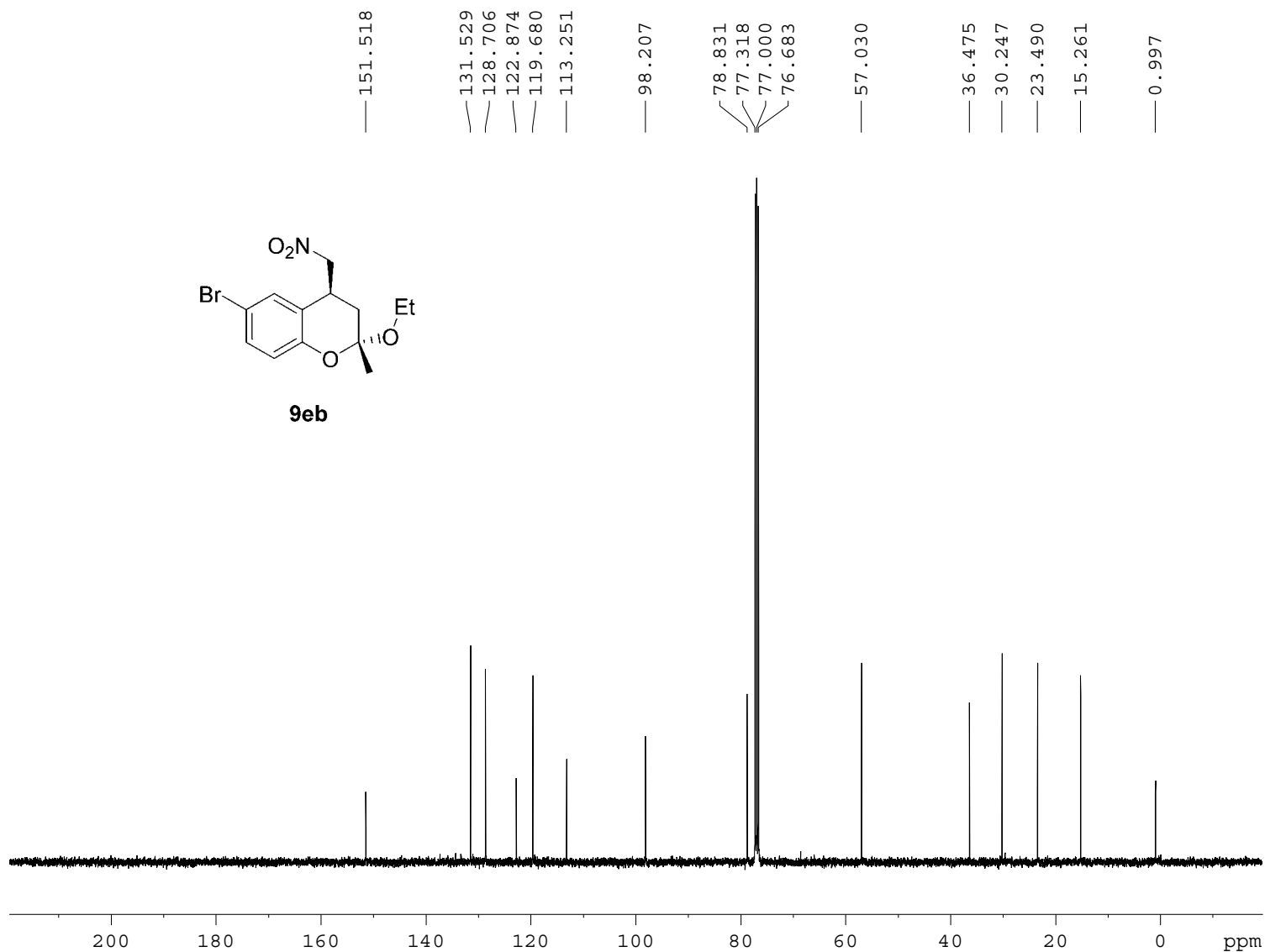
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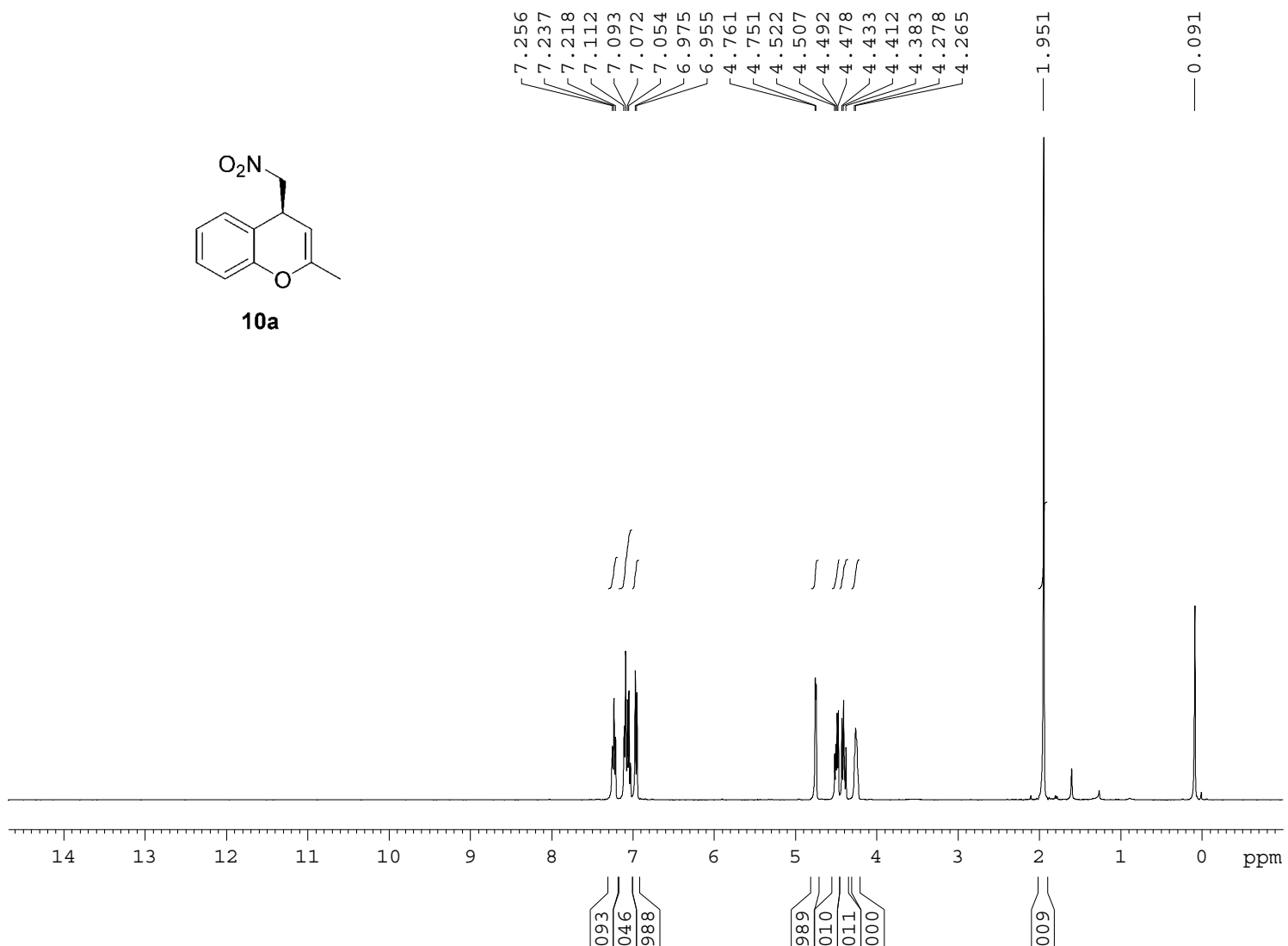


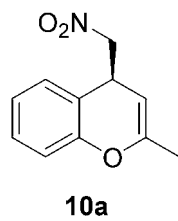












151.649
150.726

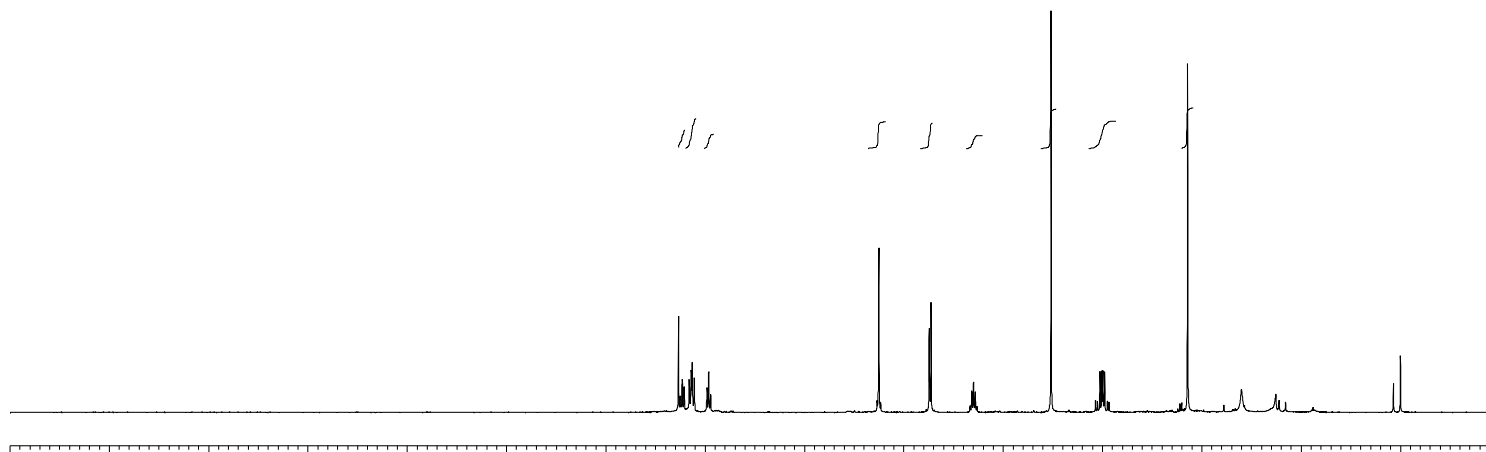
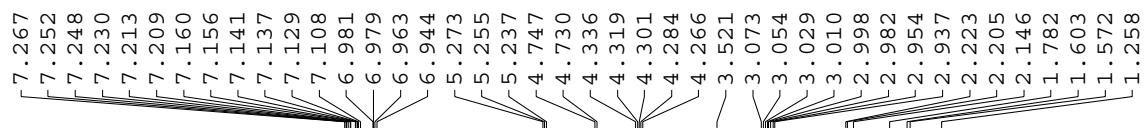
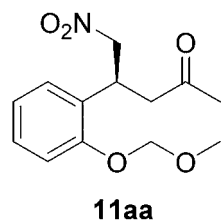
128.797
128.065
123.737
118.222
116.886

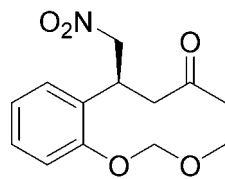
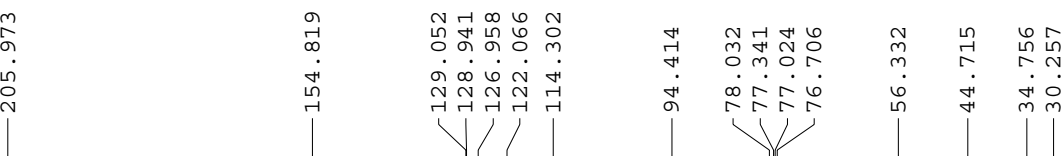
94.548

81.981
77.318
77.000
76.682

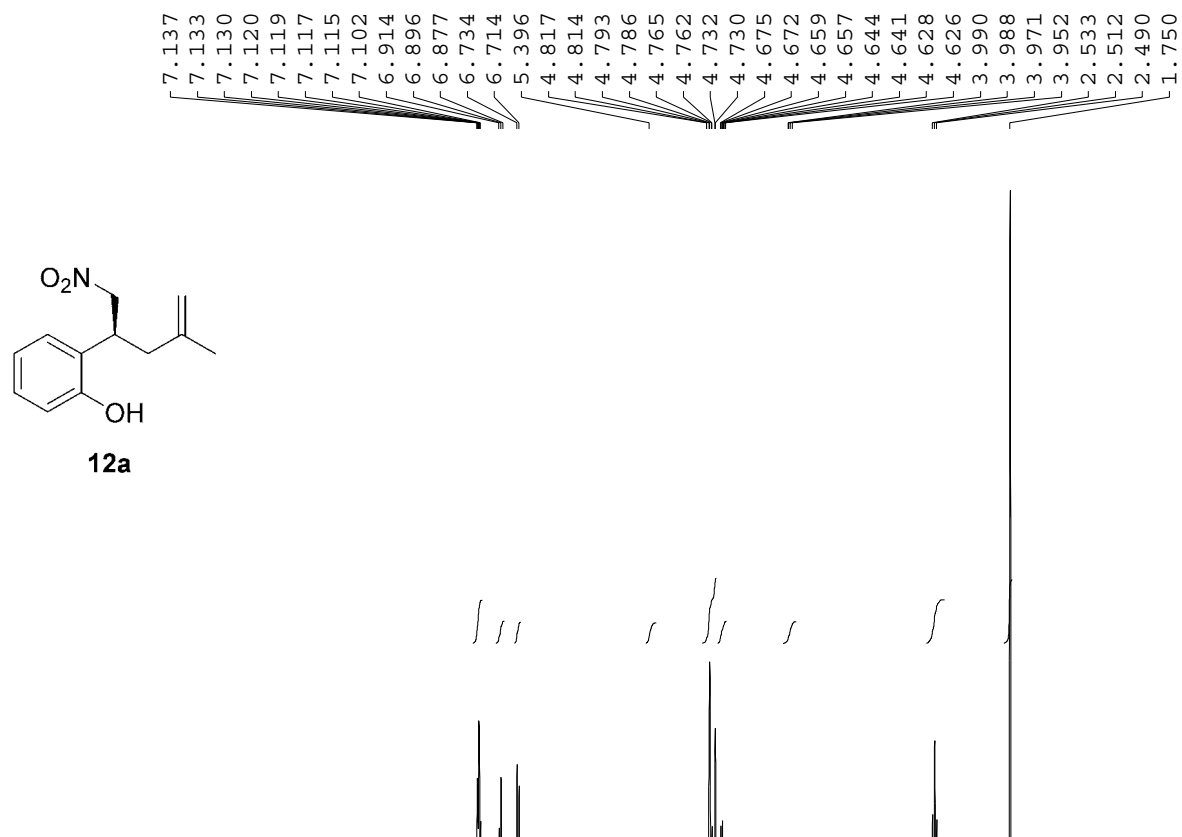
33.894

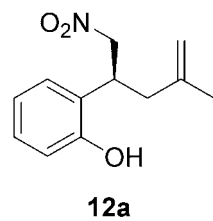
19.333





11aa





— 153.496

— 142.159

— 129.175

— 128.572

— 125.577

— 121.135

— 116.020

— 113.519

— 78.597

— 77.392

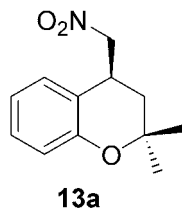
— 77.075

— 76.757

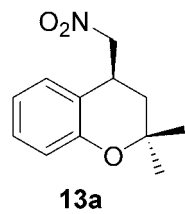
— 39.907

— 37.665

— 22.055



7.256
7.188
7.169
7.150
7.097
7.078
6.906
6.888
6.868
6.850
6.829
4.974
4.962
4.944
4.932
4.423
4.398
4.368
3.784
3.770
3.758
3.745
3.732
3.720
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1.770
1.741
1.708
1.598
1.444
1.269
0.075

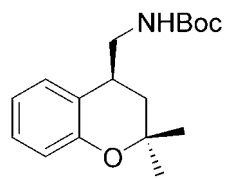


— 153.816

— 128.851
— 126.319
— 120.421
— 118.765
— 118.380

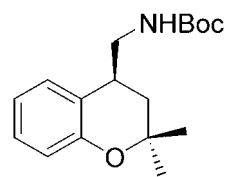
— 80.082
— 77.317
— 77.000
— 76.682
— 73.946

— 37.564
— 31.189
— 29.565
— 24.142



14a

7.264
7.240
7.144
7.126
7.106
6.899
6.881
6.862
6.812
6.794
6.792
4.502
3.820
3.794
3.786
3.774
3.399
3.387
3.364
3.095
3.082
1.907
1.892
1.873
1.858
1.717
1.685
1.653
1.437
1.428
1.235
0.071
0.000



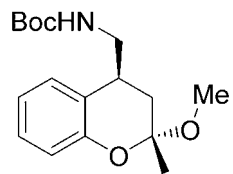
14a

156.179
154.419

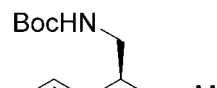
127.918
126.729
121.607
120.204
117.814

79.402
77.323
77.006
76.689
74.213

43.601
37.366
31.955
30.003
28.363
24.162



7.265
7.241
7.174
7.154
7.136
6.965
6.946
6.930
6.928
6.876
6.874
6.856
6.853
4.441
3.798
3.791
3.778
3.765
3.756
3.744
3.736
3.515
3.501
3.490
3.481
3.466
3.455
3.288
3.275
3.267
3.261
3.238
3.226
2.176
2.160
2.145
2.126
2.111
1.782
1.750



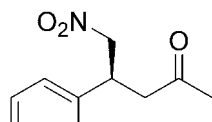
— 156.173
— 152.816

— 127.783
— 126.208
— 123.041
— 121.172
— 117.469

— 98.437

— 79.335
— 77.318
— 77.203
— 77.000
— 76.683

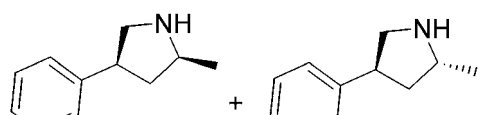
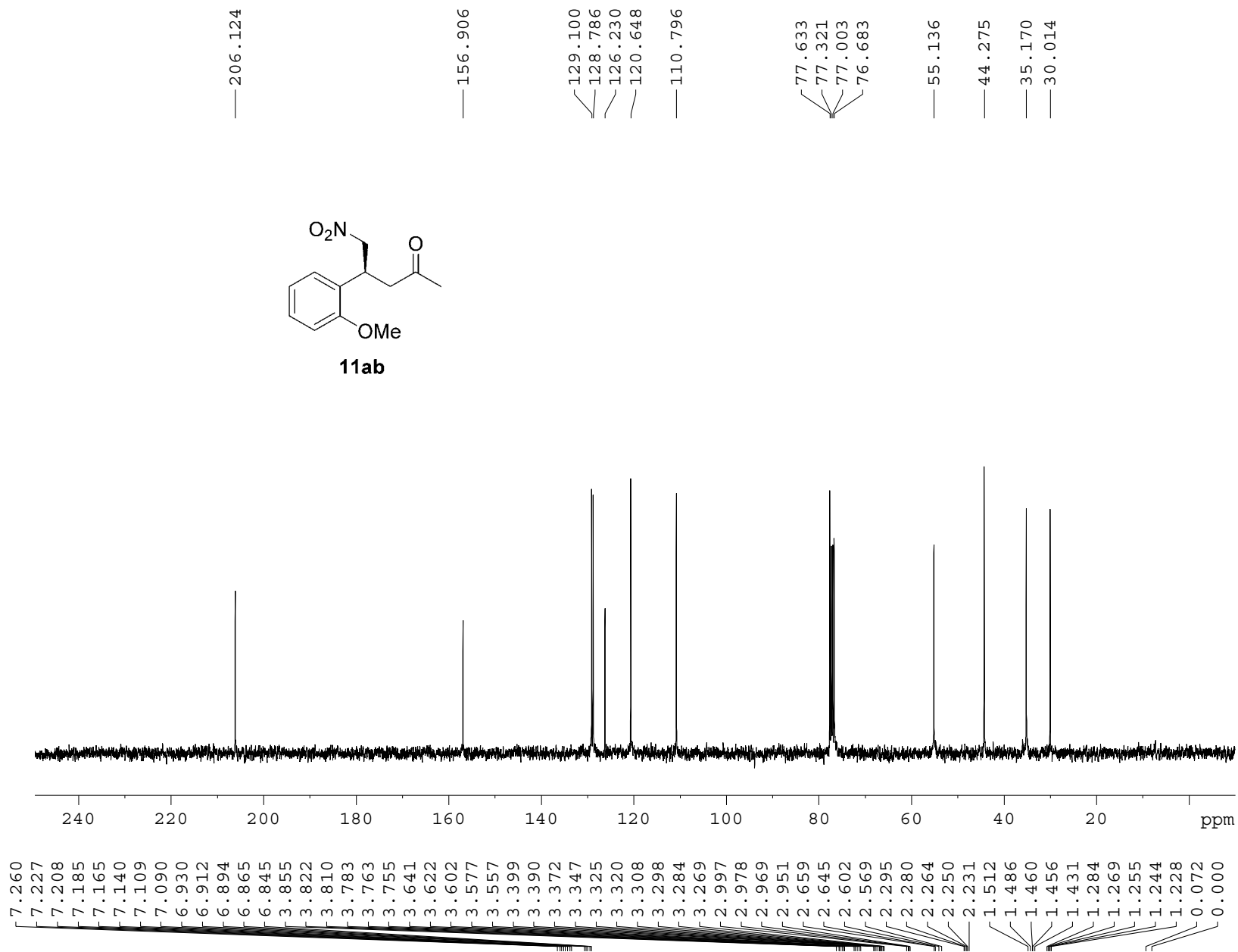
— 48.995
— 42.468
— 36.179
— 30.992
— 28.344
— 23.140



7.251
7.231
7.212
7.133
7.114
6.898
6.882
6.862
4.757
4.726
4.709
4.695
4.682
4.664
4.220
4.203
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3.837
3.038
3.019
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2.910
2.100

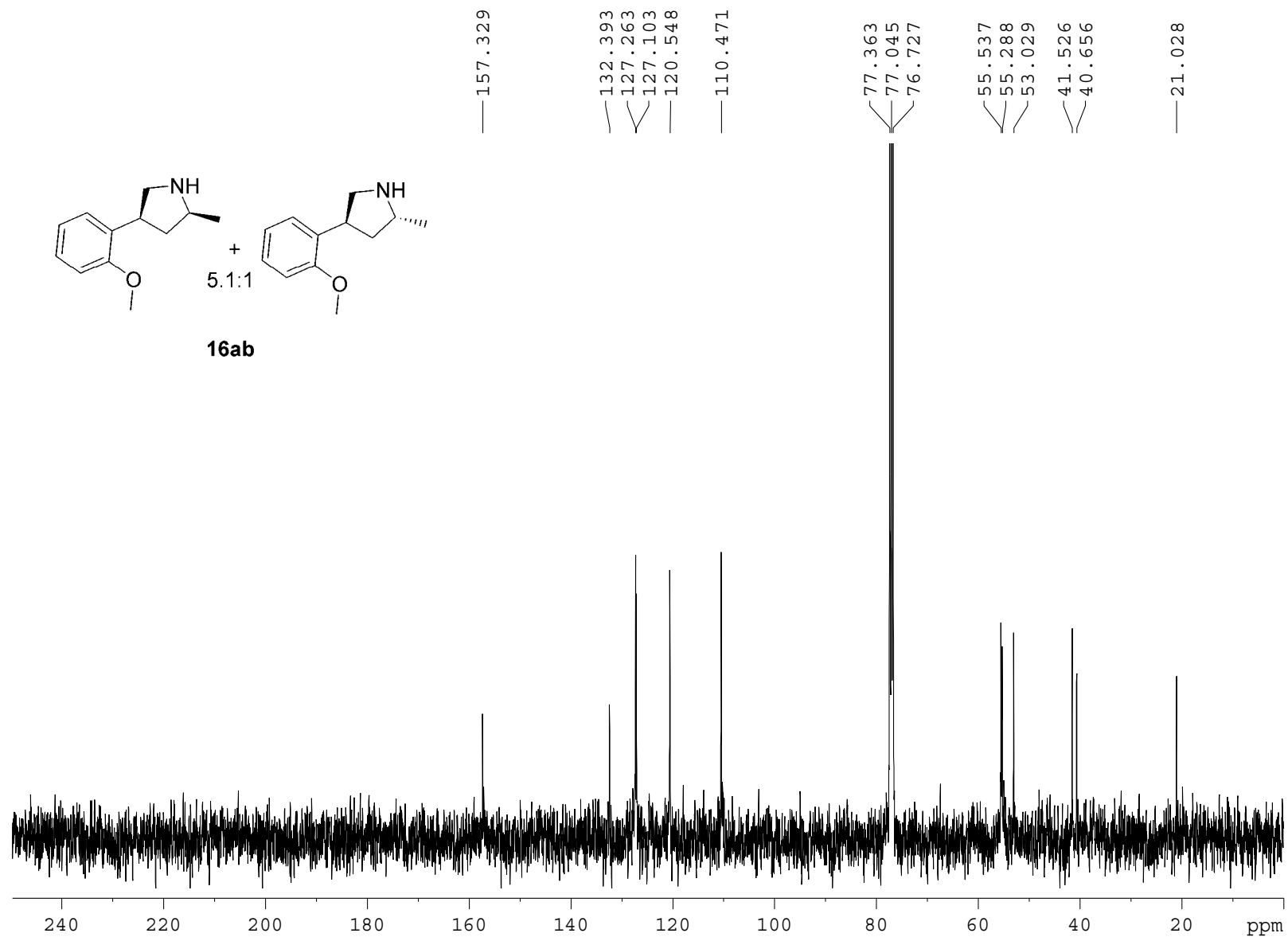
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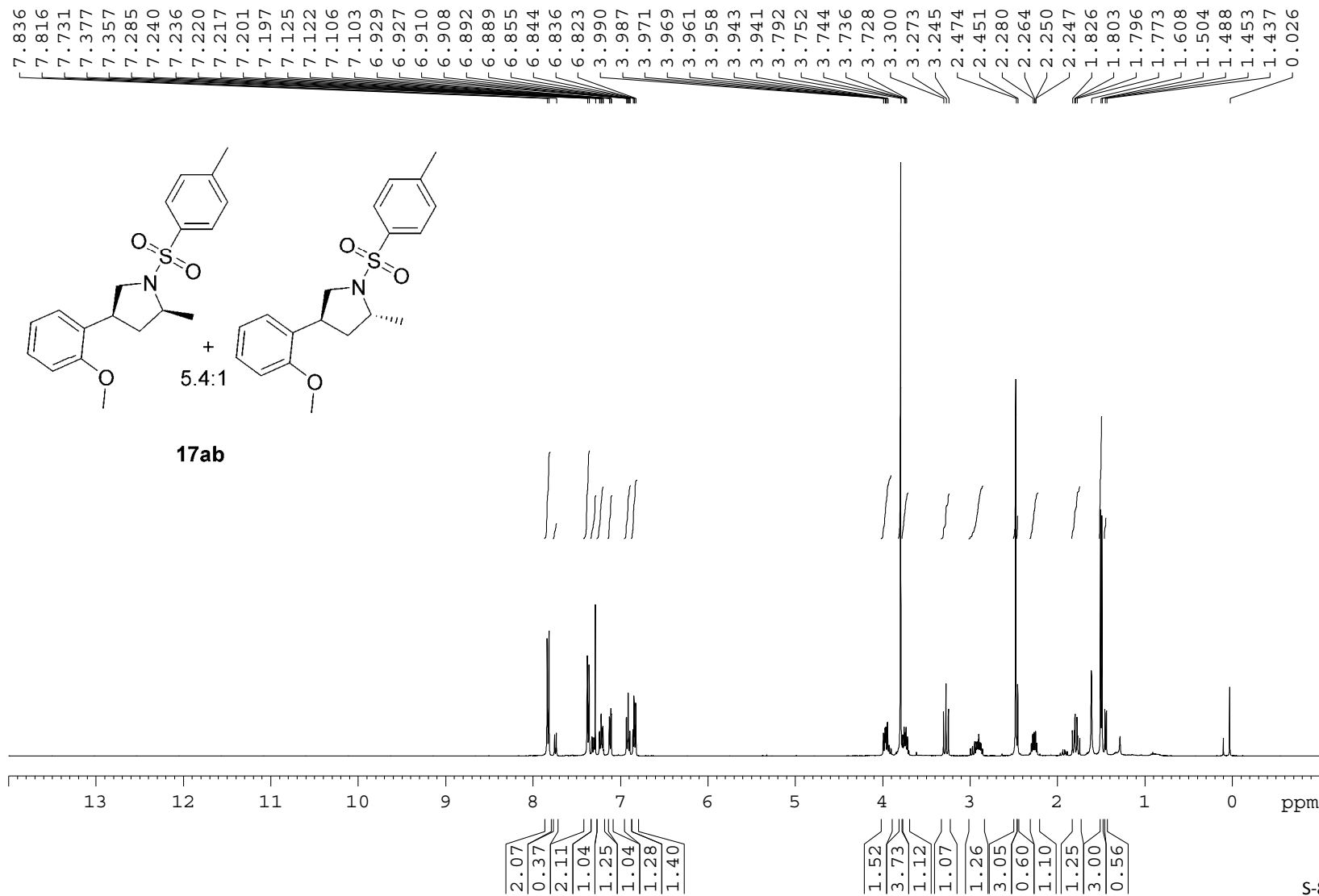
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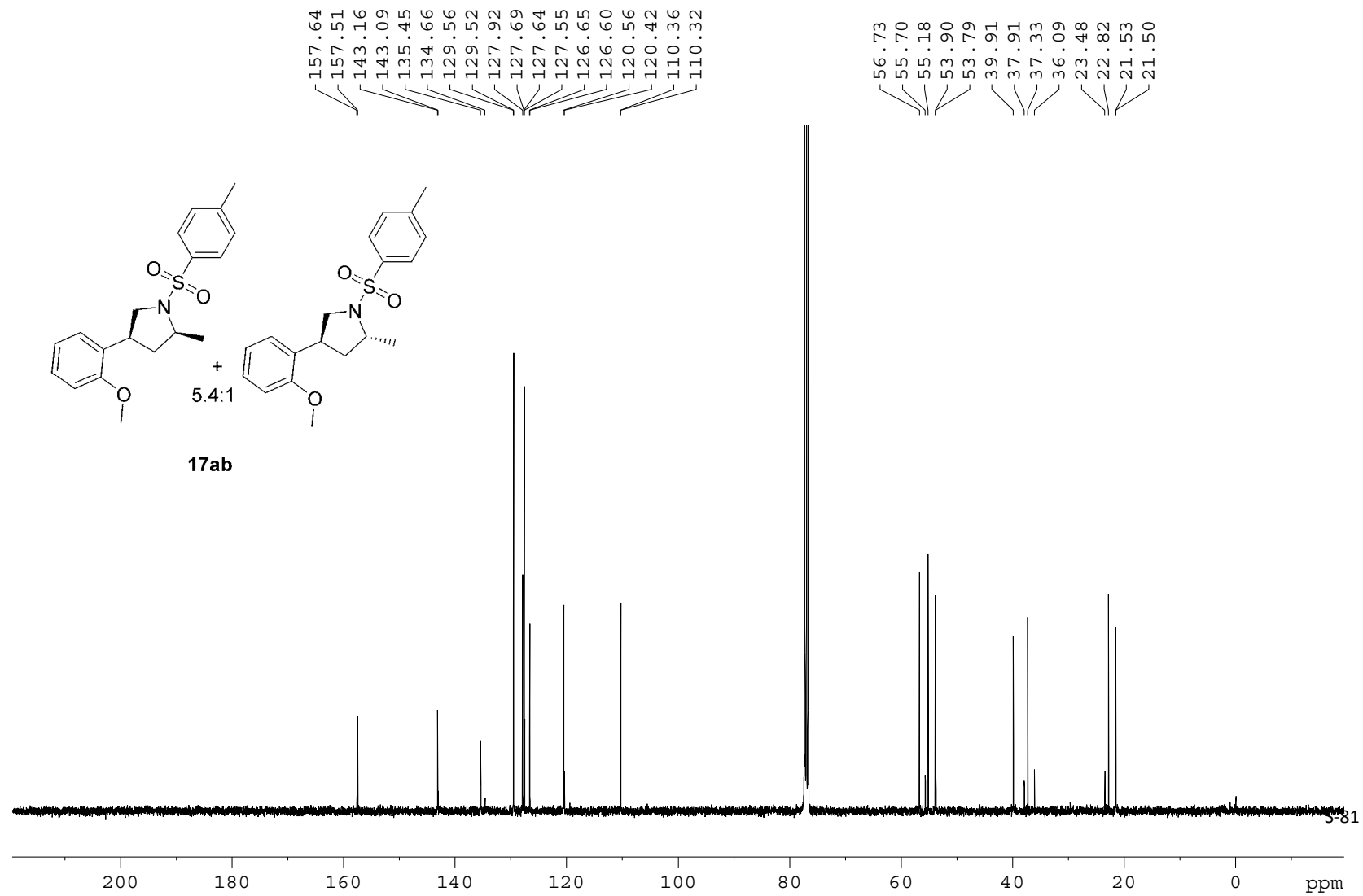


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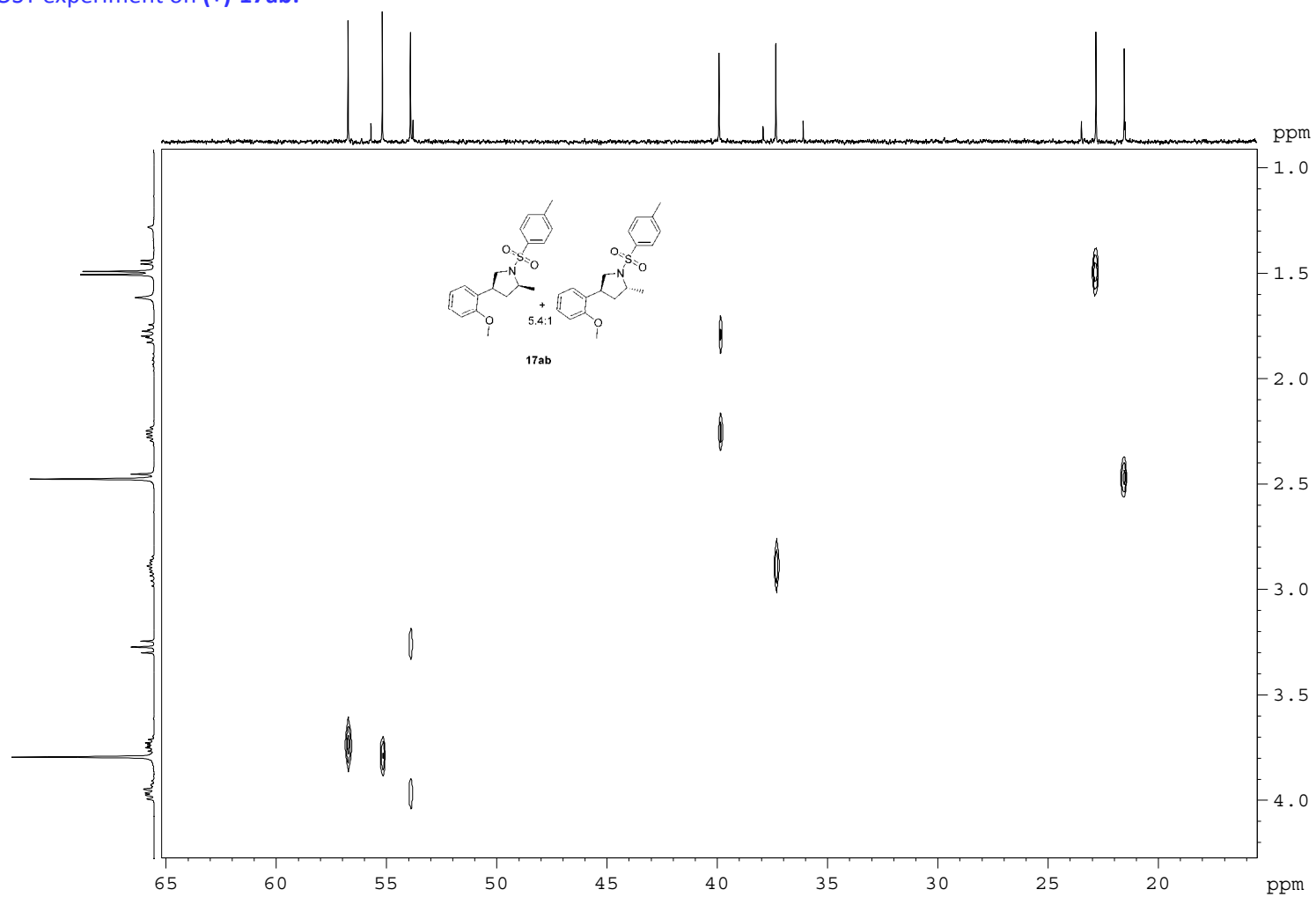
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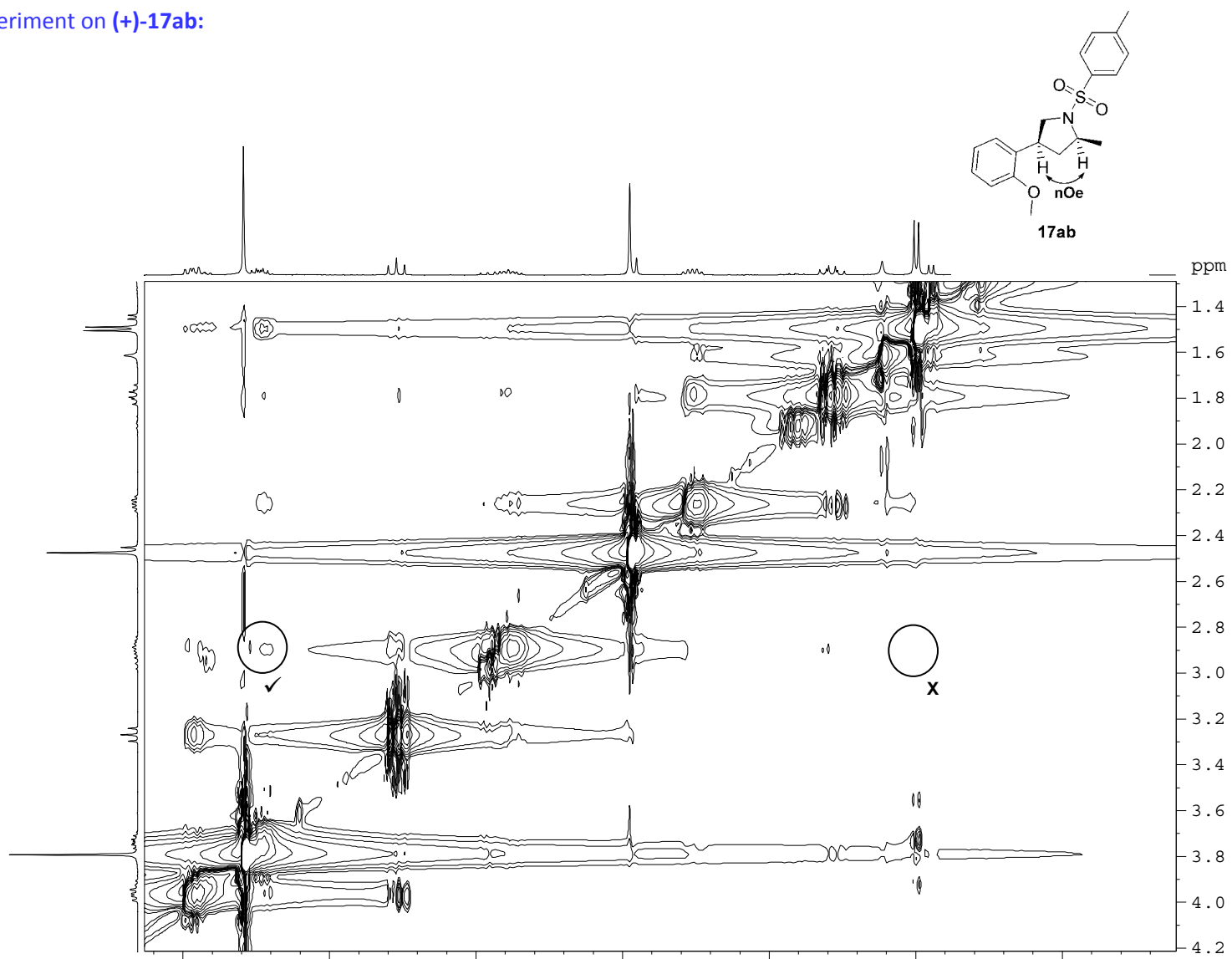




Hetero-COSY experiment on (+)-17ab:



NOSEY Experiment on (+)-17ab:



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