

Supporting Information

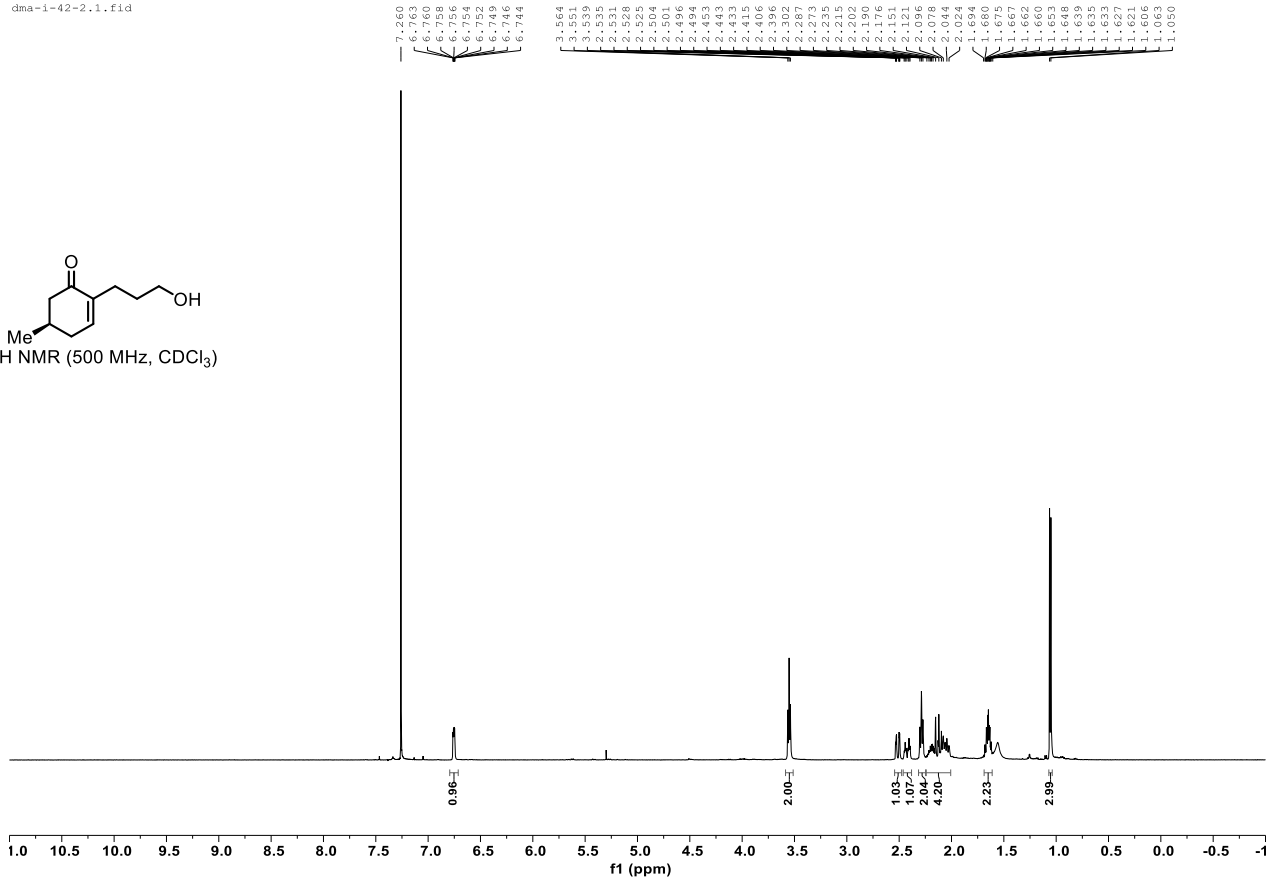
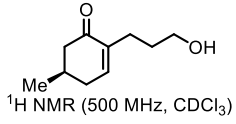
Concise Total Synthesis of Complanadine A Enabled by Pyrrole-to-Pyridine Molecular Editing

Brandon S. Martin^{a,†}, Donghui Ma,^{a,b†} Takeru Saito^a, Katelyn S. Gallagher^a, Mingji Dai^{*a,b}

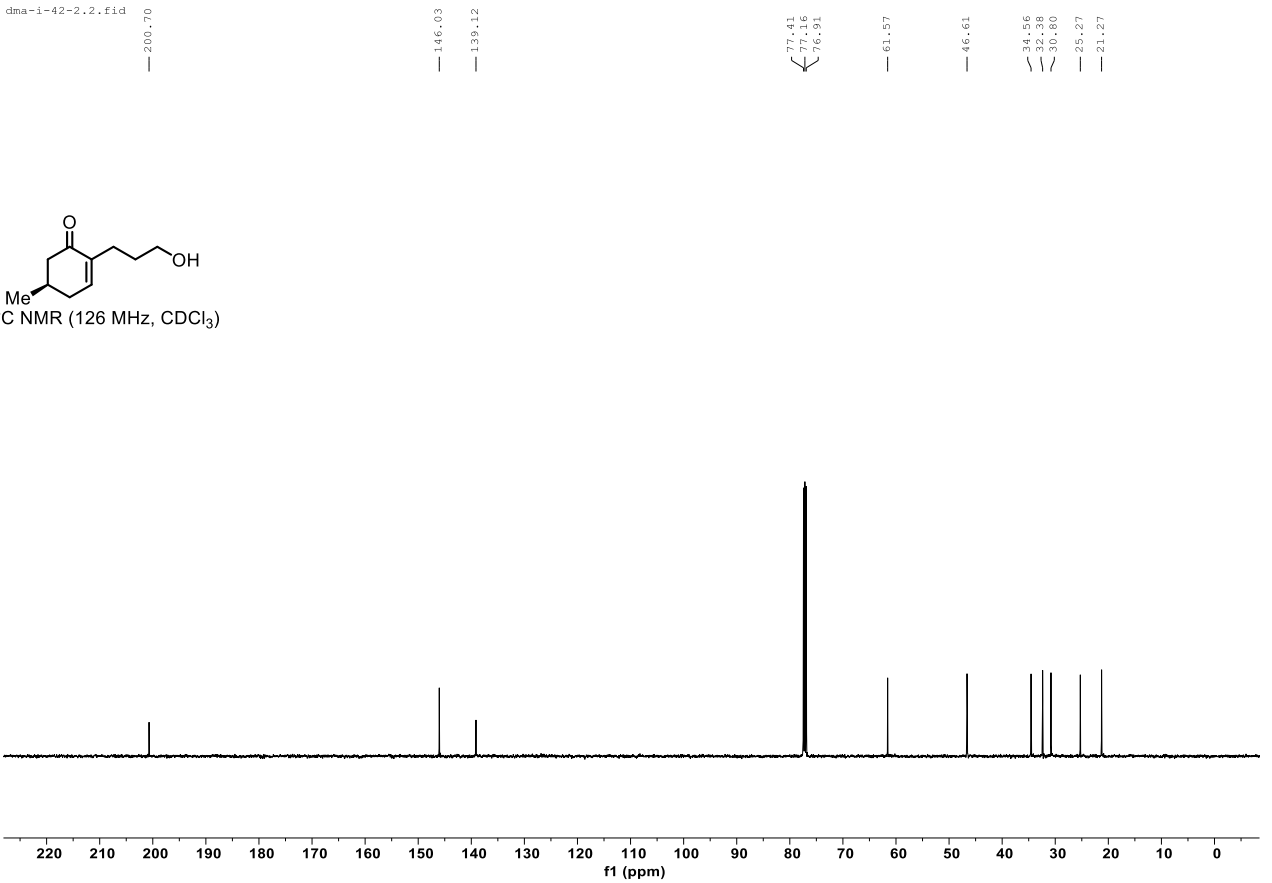
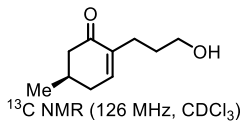
^aDepartment of Chemistry, Purdue University, West Lafayette, Indiana 47907, United States

^bDepartment of Chemistry, Emory University, Atlanta, Georgia 30322, United States

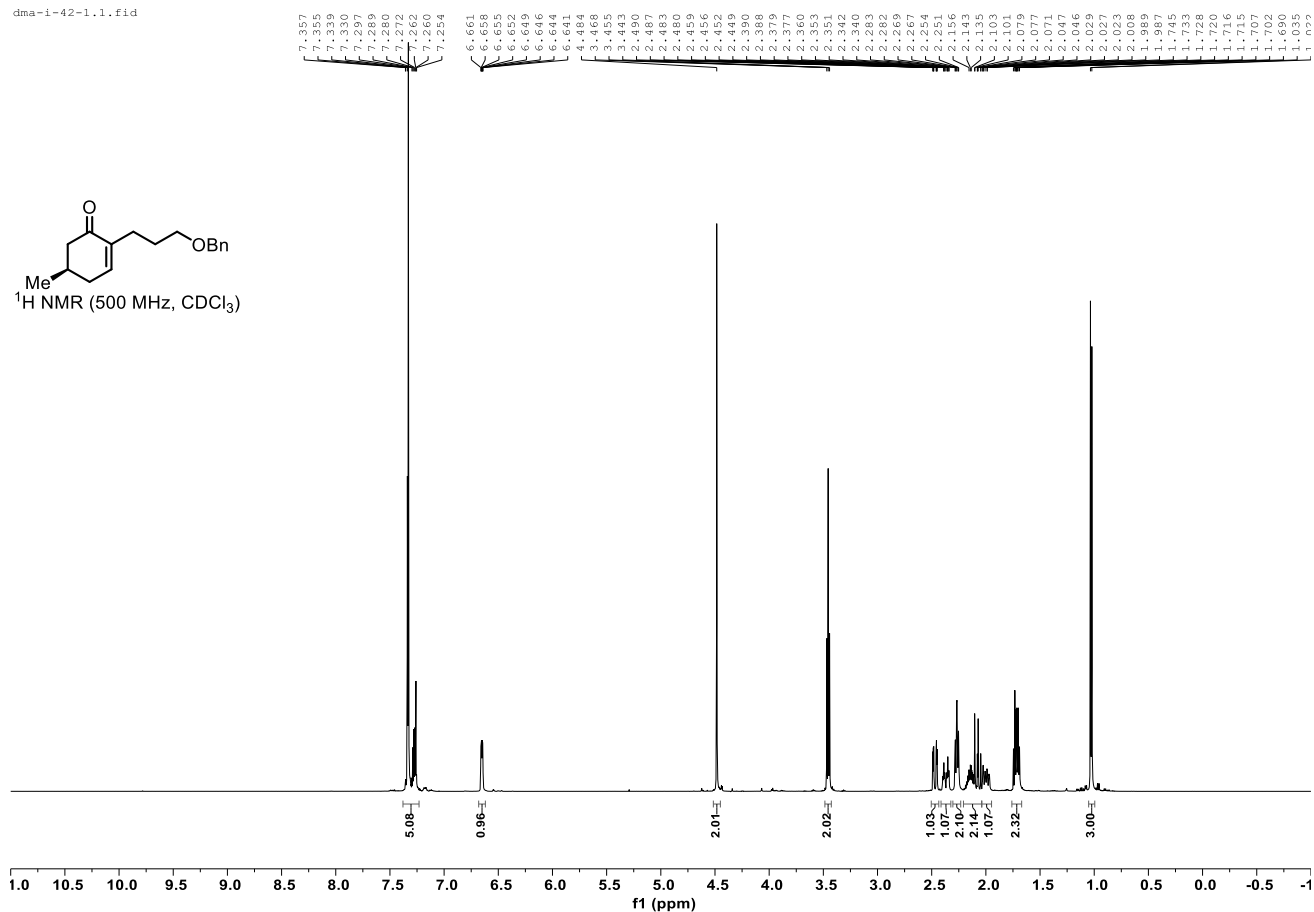
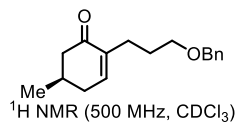
dma-1-42-2.1.fid



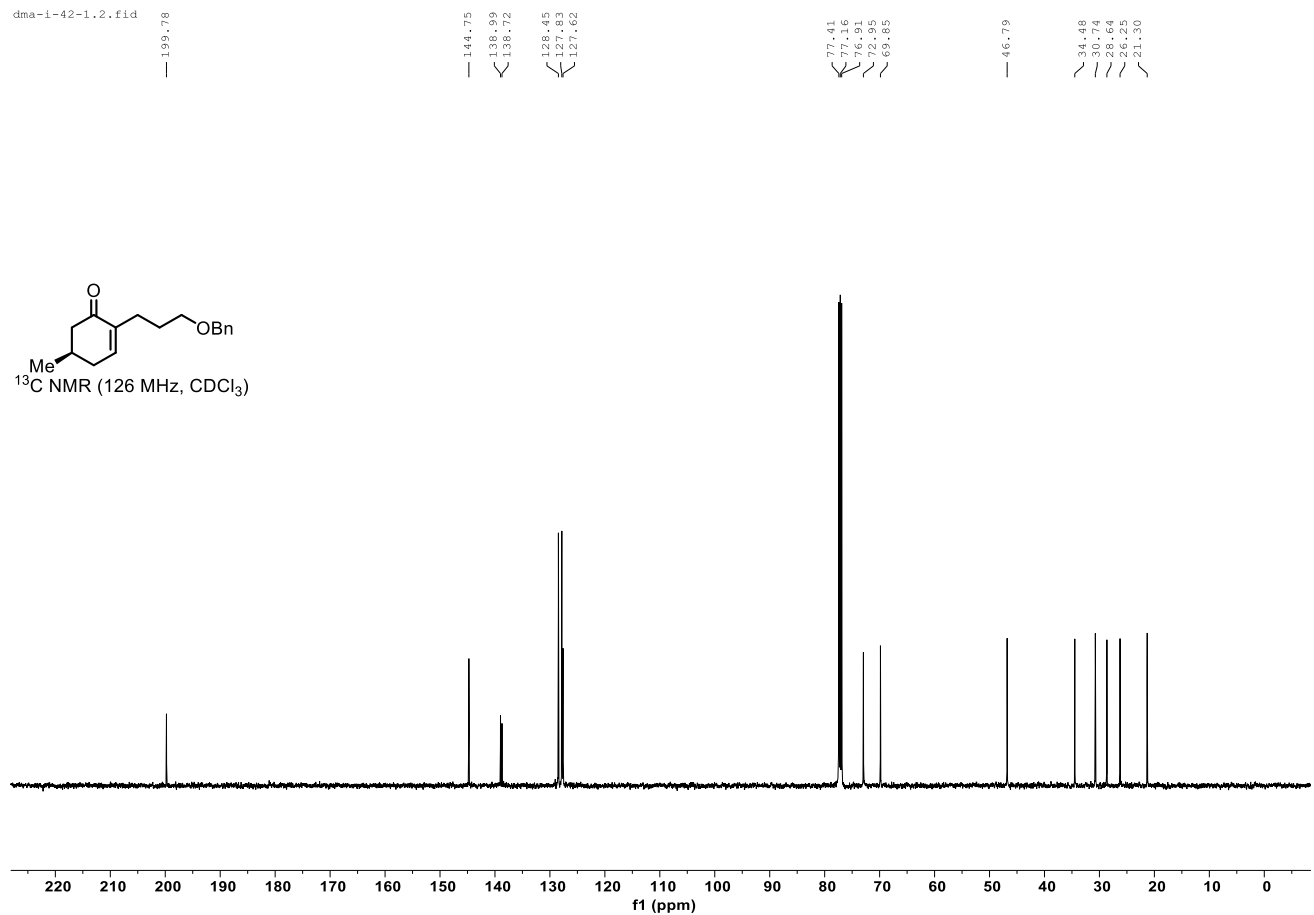
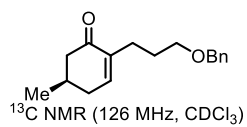
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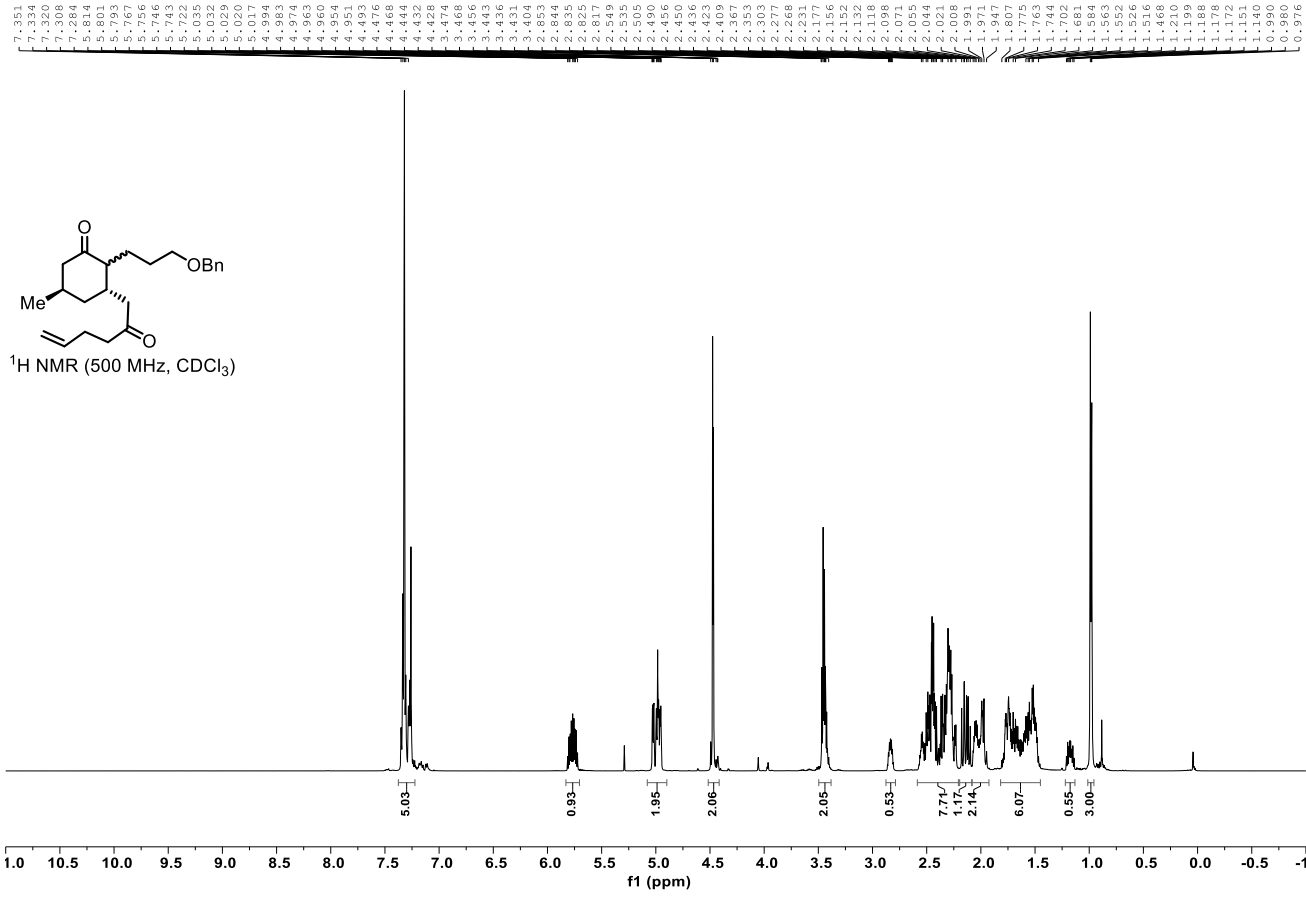
dma-i-42-1.1.fid



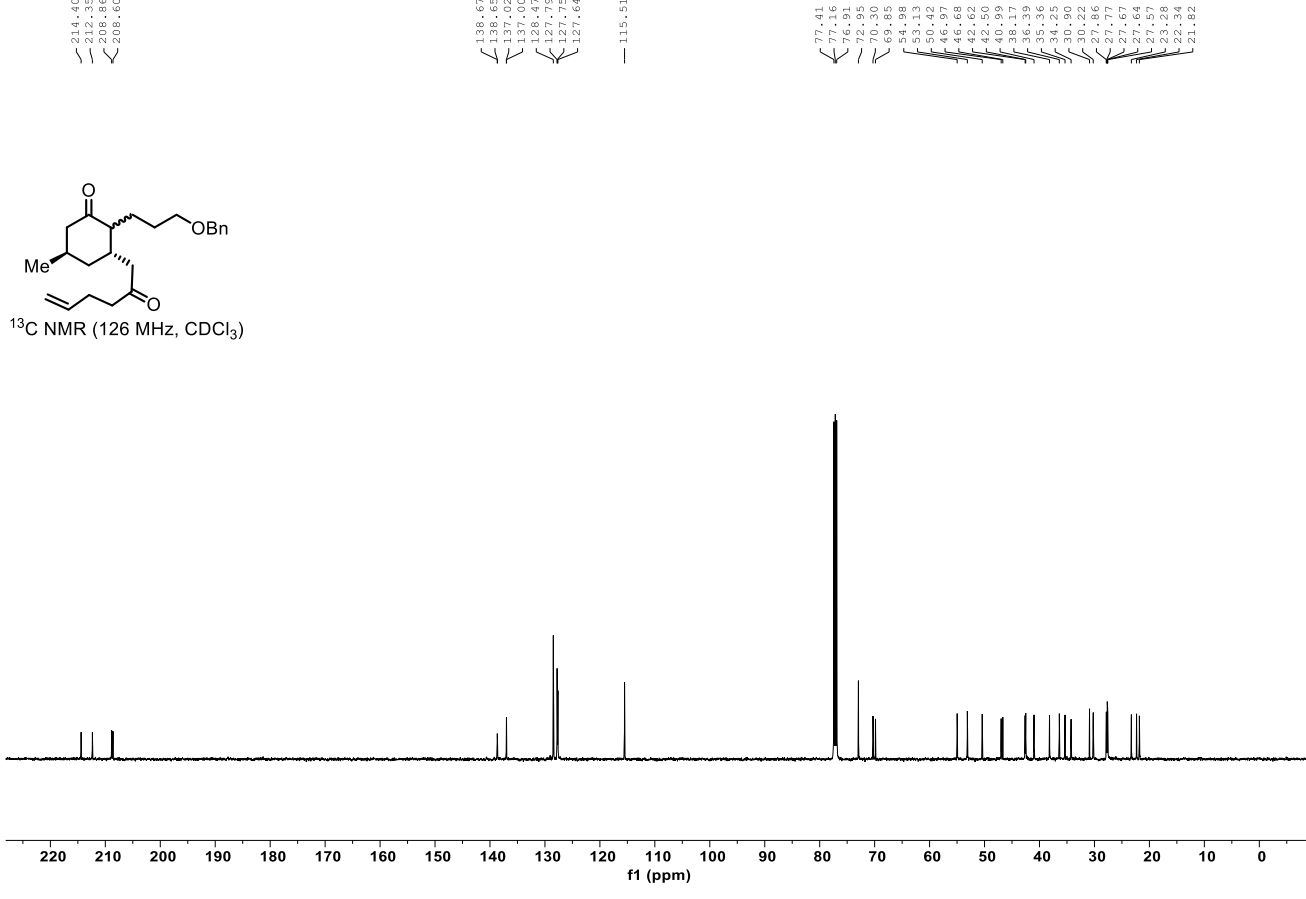
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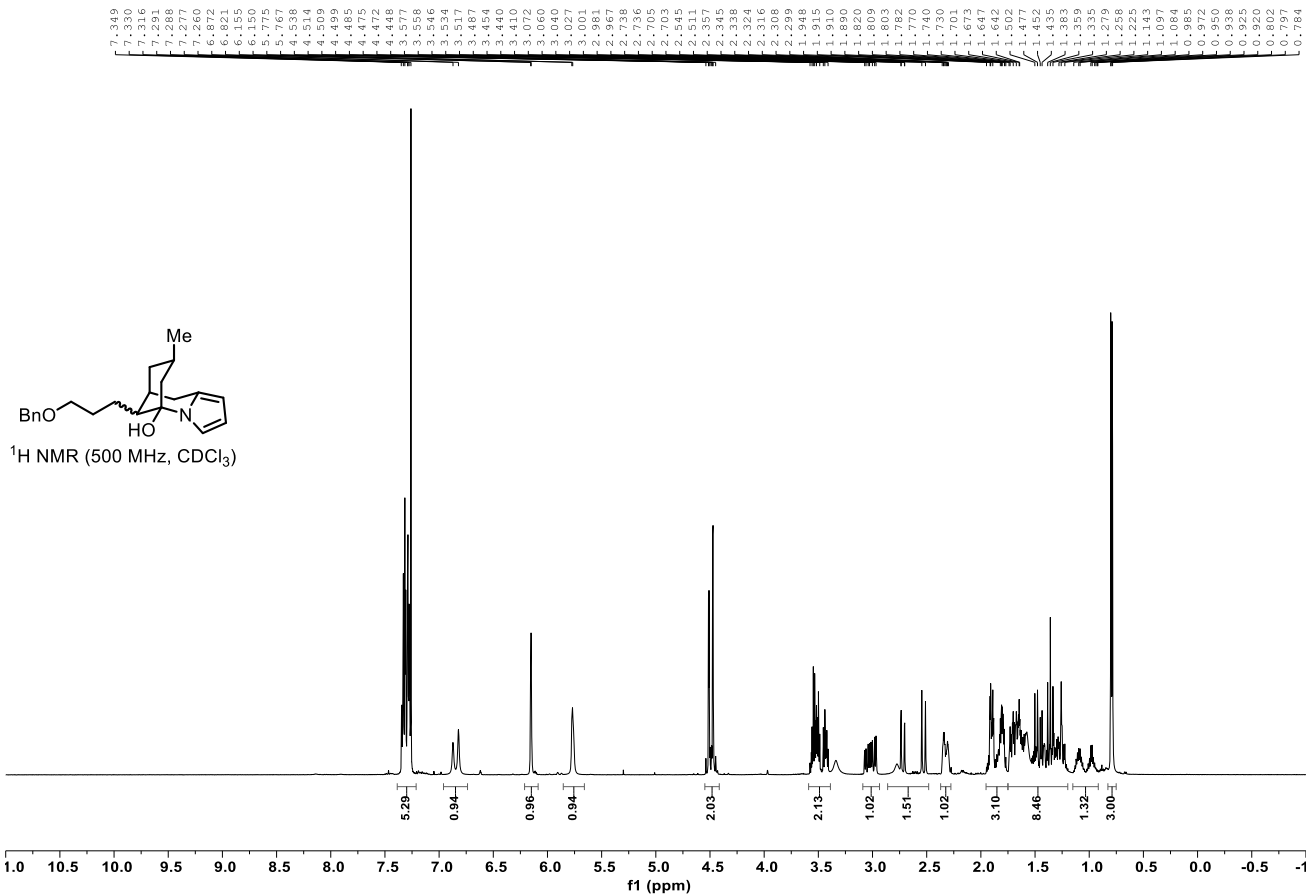
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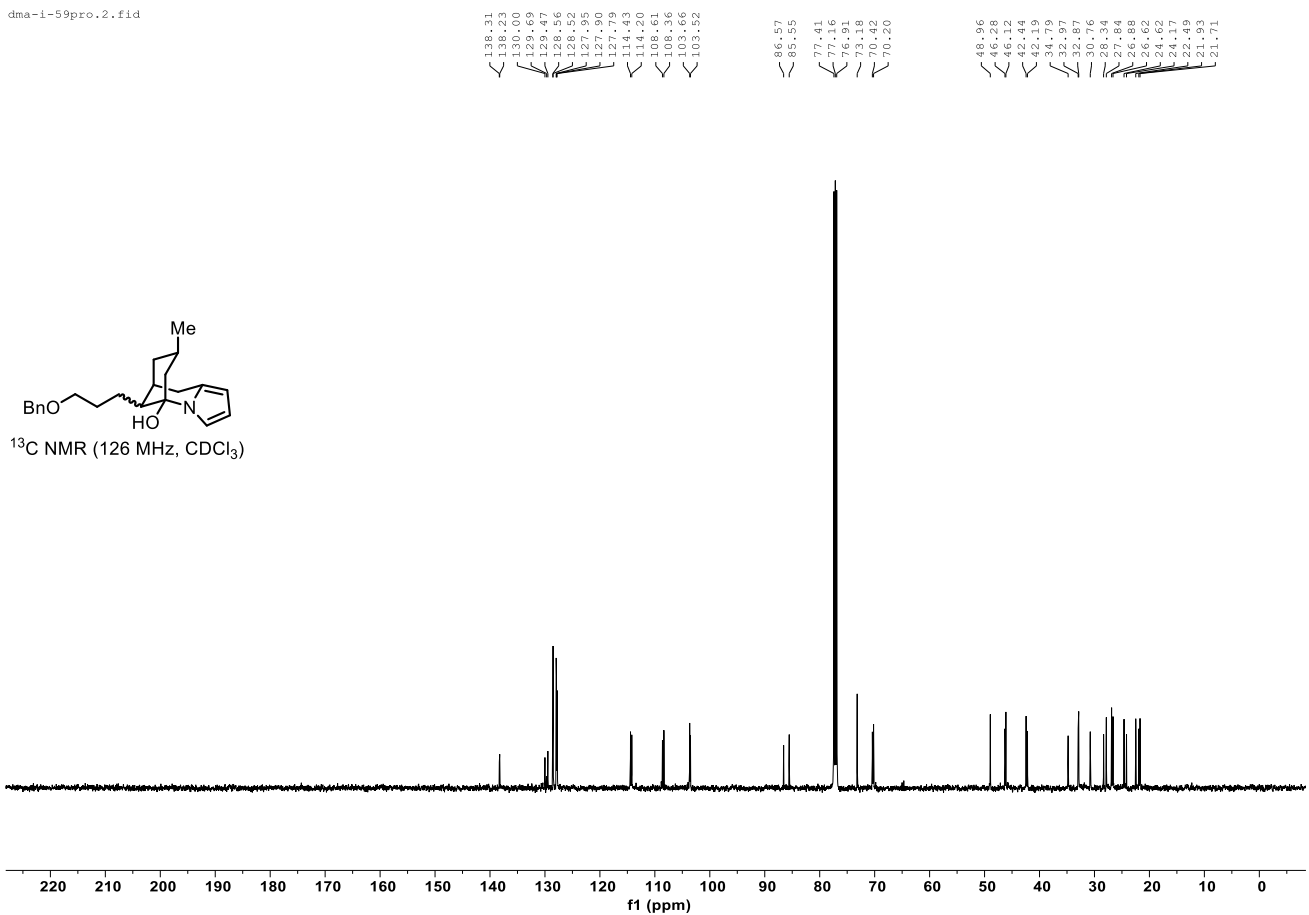
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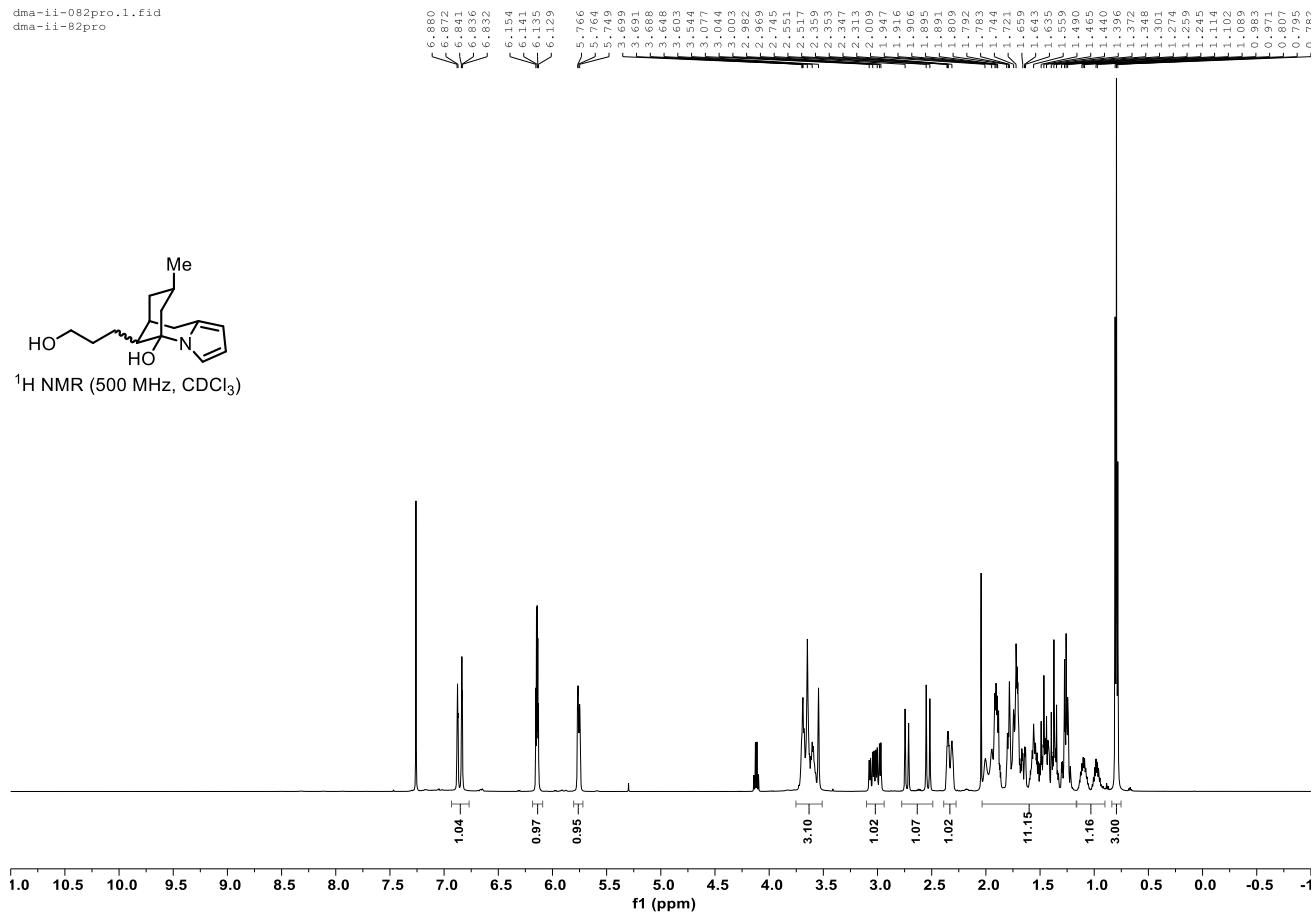
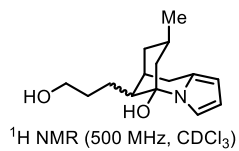
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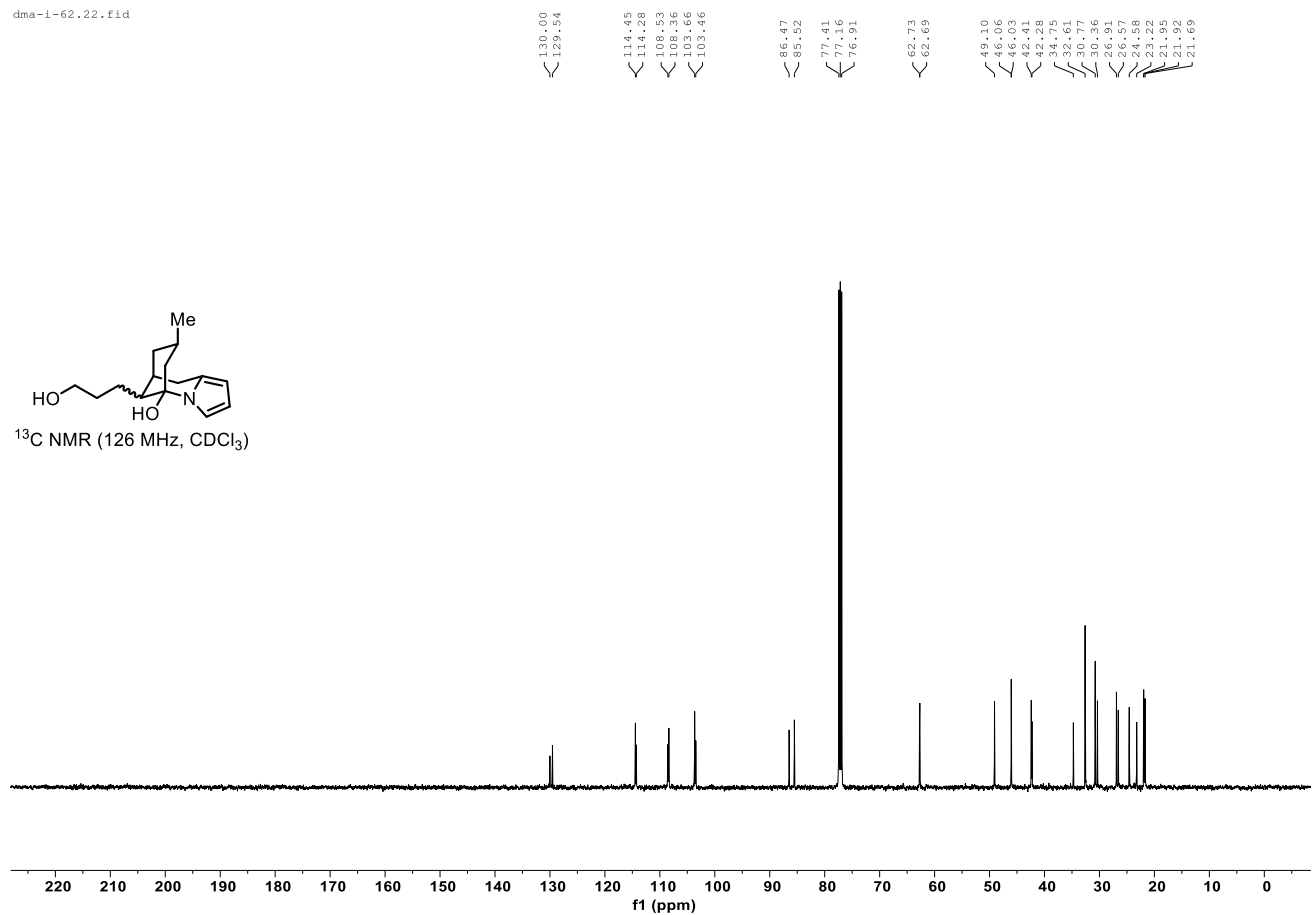
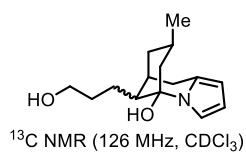
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dma-ii-082pro.1.fid
dma-ii-82pro



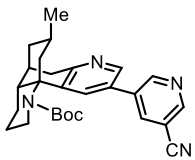
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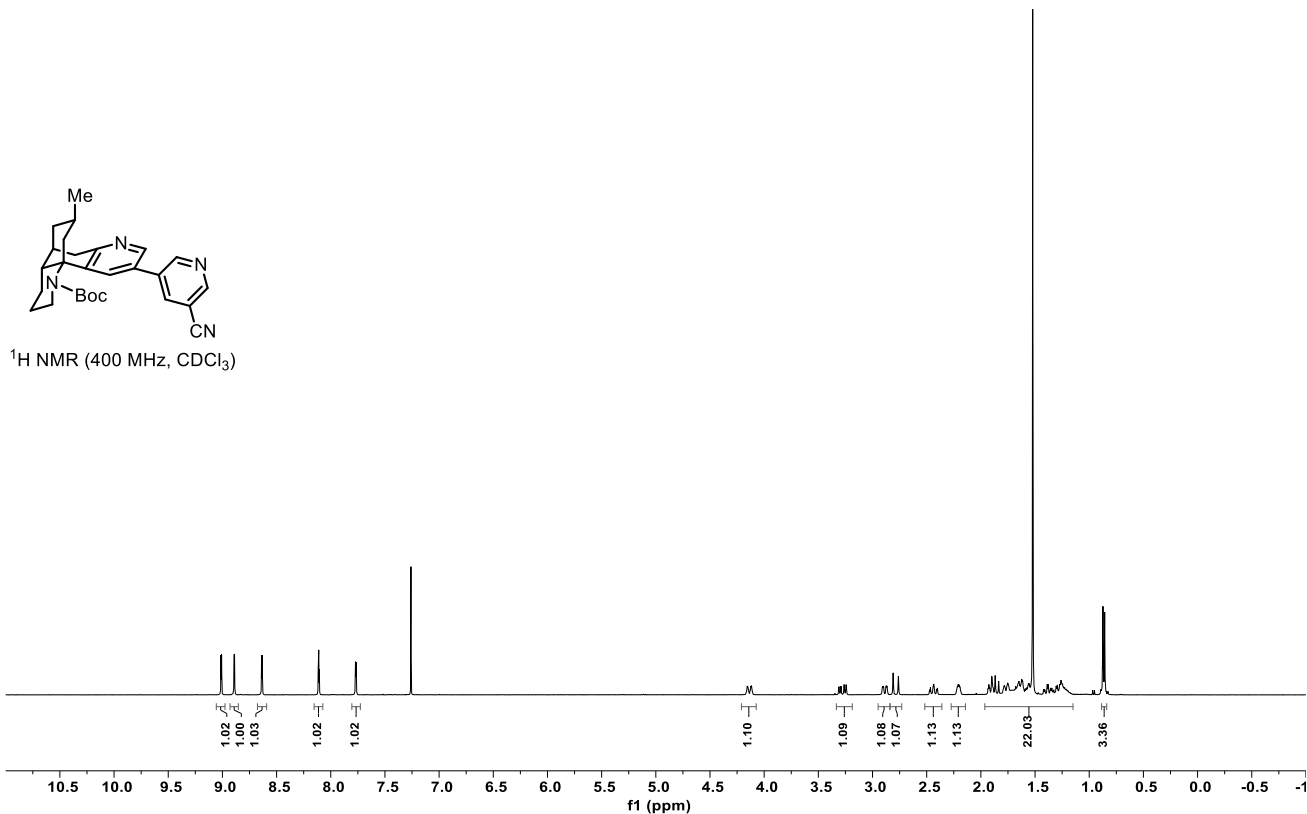
20230415-dma-iii-108pure.1.fid -

9.013
9.007
8.893
8.888
8.638
8.633
8.116
8.111
8.106
7.772
7.766
7.260

4.156
4.150
4.144
4.130
4.123
4.116
4.109
3.310
3.292
3.262
3.243
2.907
2.896
2.878
2.873
2.868
2.863
2.809
2.804
2.465
2.442
2.435
2.431
2.401
2.218
2.201
2.201
2.192
1.899
1.836
1.752
1.648
1.622
1.552
1.387
1.378
1.305
1.294
1.272
1.261
1.251
1.241
0.868



¹H NMR (400 MHz, CDCl₃)

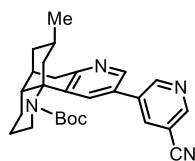


20230415-dma-iii-108pure.2.fid

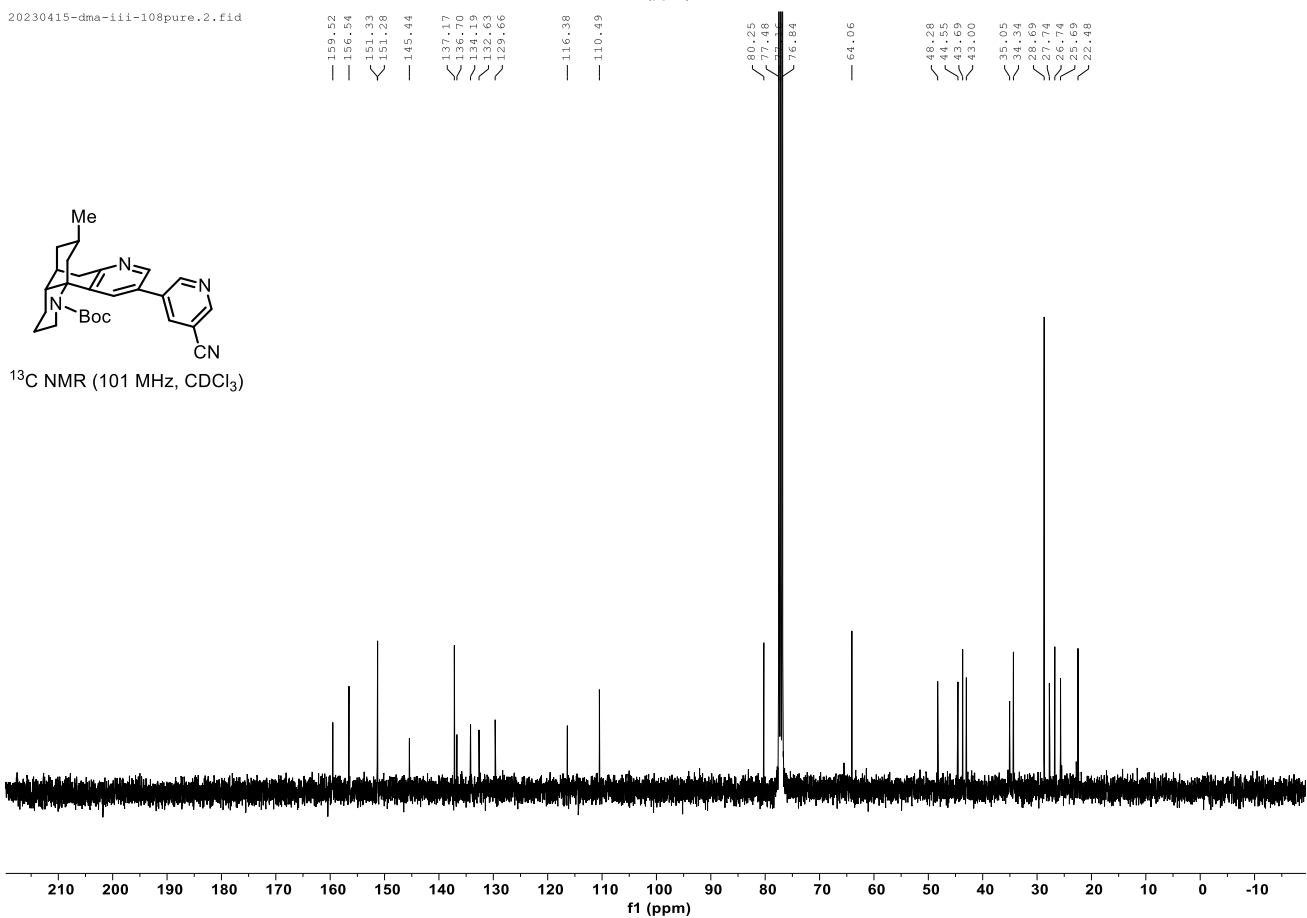
159.52
156.54
151.33
151.28
145.44
137.17
136.70
134.19
132.63
129.66
116.38
110.49

80.95
77.58
77.56
76.84
64.06

48.28
44.55
43.59
43.00
35.05
34.34
28.69
27.74
26.74
25.69
22.48



¹³C NMR (101 MHz, CDCl₃)



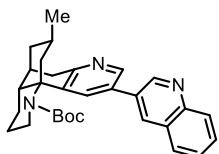
20230415-dma-iii-109.11.fid - dma-iii-109A

9.152
9.146
8.780
8.774
8.306
8.300
8.163
8.141
7.874
7.870
7.771
7.768
7.754
7.751
7.747
7.733
7.729
7.624
7.621
7.606
7.603
7.600
7.586
7.583
7.560

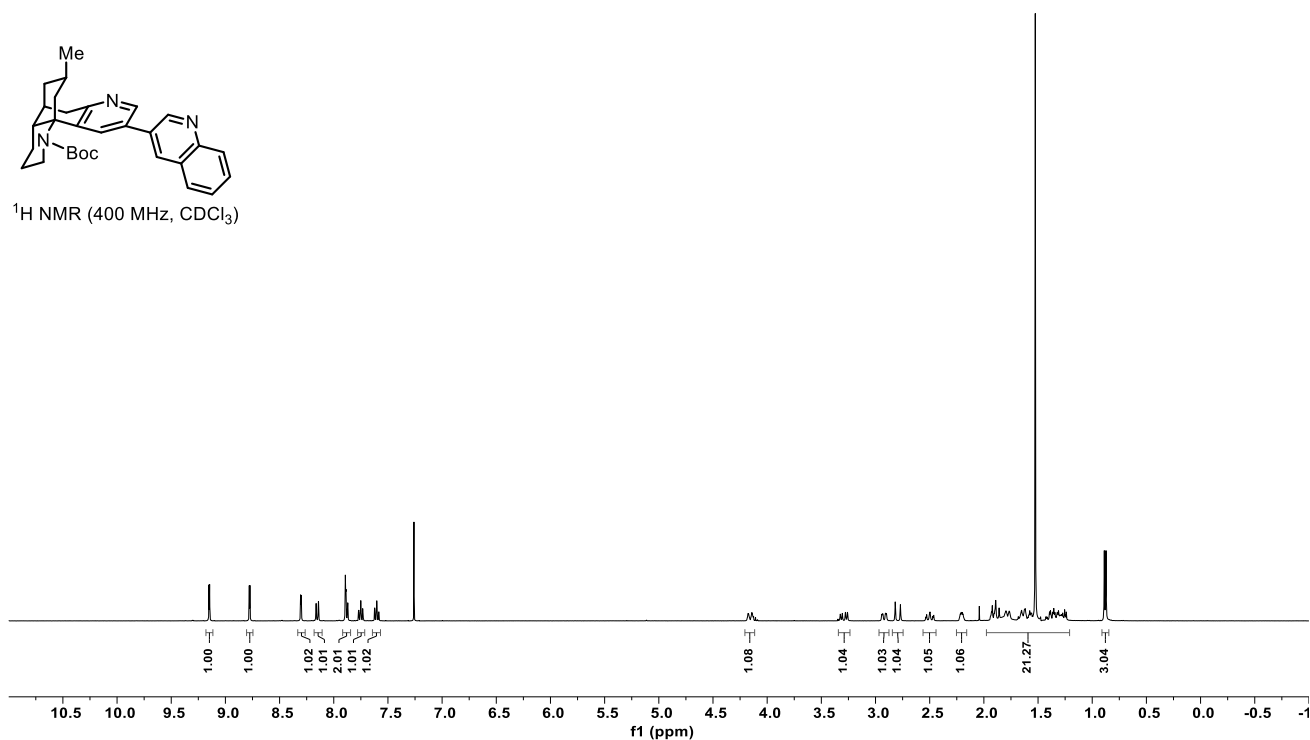
4.183
4.177
4.171
4.150
4.136

3.325
3.307
3.277
3.259

2.935
2.930
2.911
2.907
2.902
2.897
2.818
2.770
2.600
2.497
2.494
2.218
2.210
2.201
2.192
1.892
1.891
1.889
1.859
1.797
1.766
1.766
1.526
1.526
1.386
1.355
1.312
1.239
0.873



¹H NMR (400 MHz, CDCl₃)



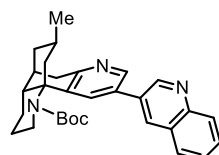
20230415-dma-iii-109.12.fid
dma-iii-109A

158.00
156.56
149.37
147.69
145.92
136.22
133.42
132.64
132.06
130.84
129.92
129.46
128.10
128.05
127.45

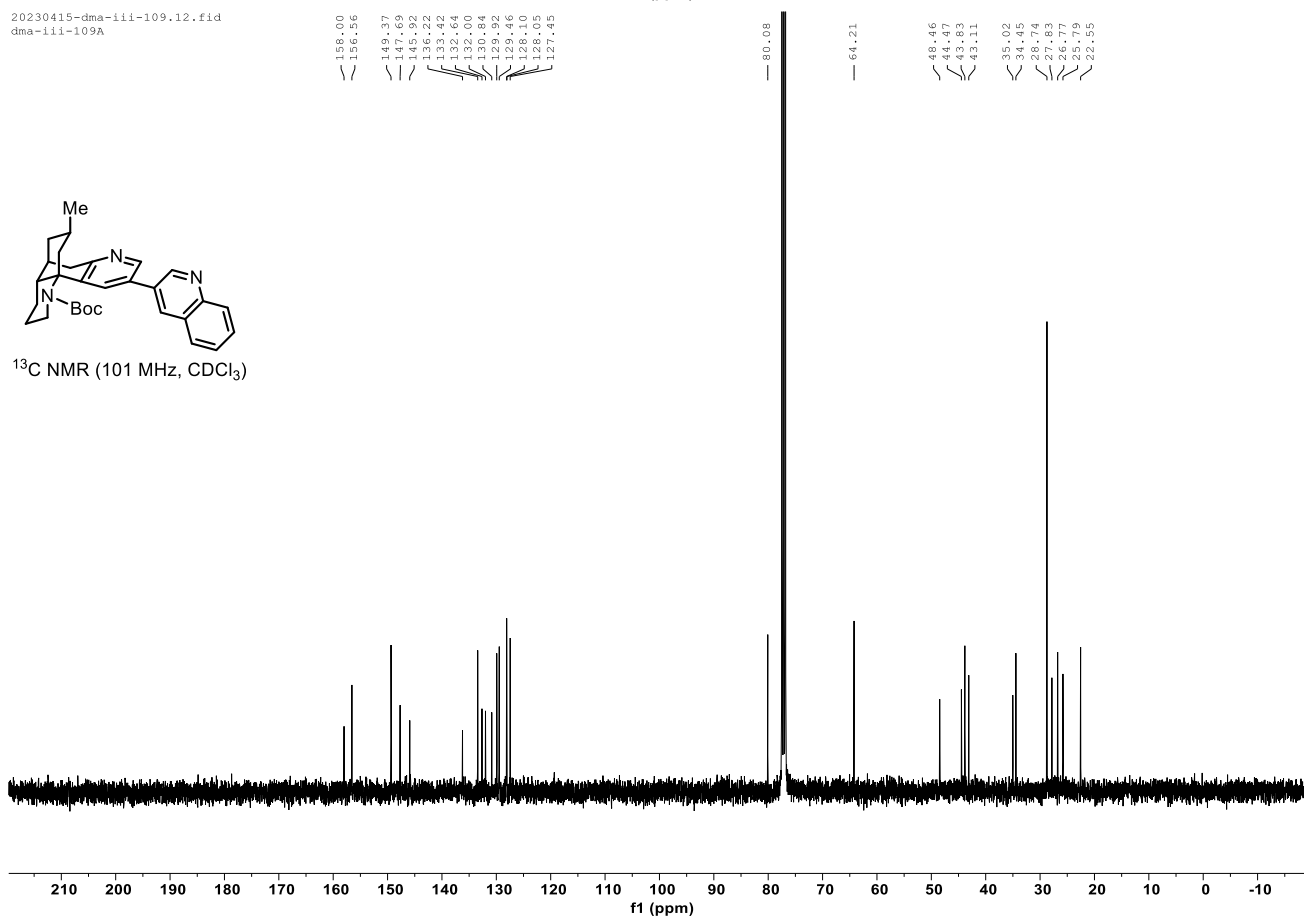
80.08

64.21

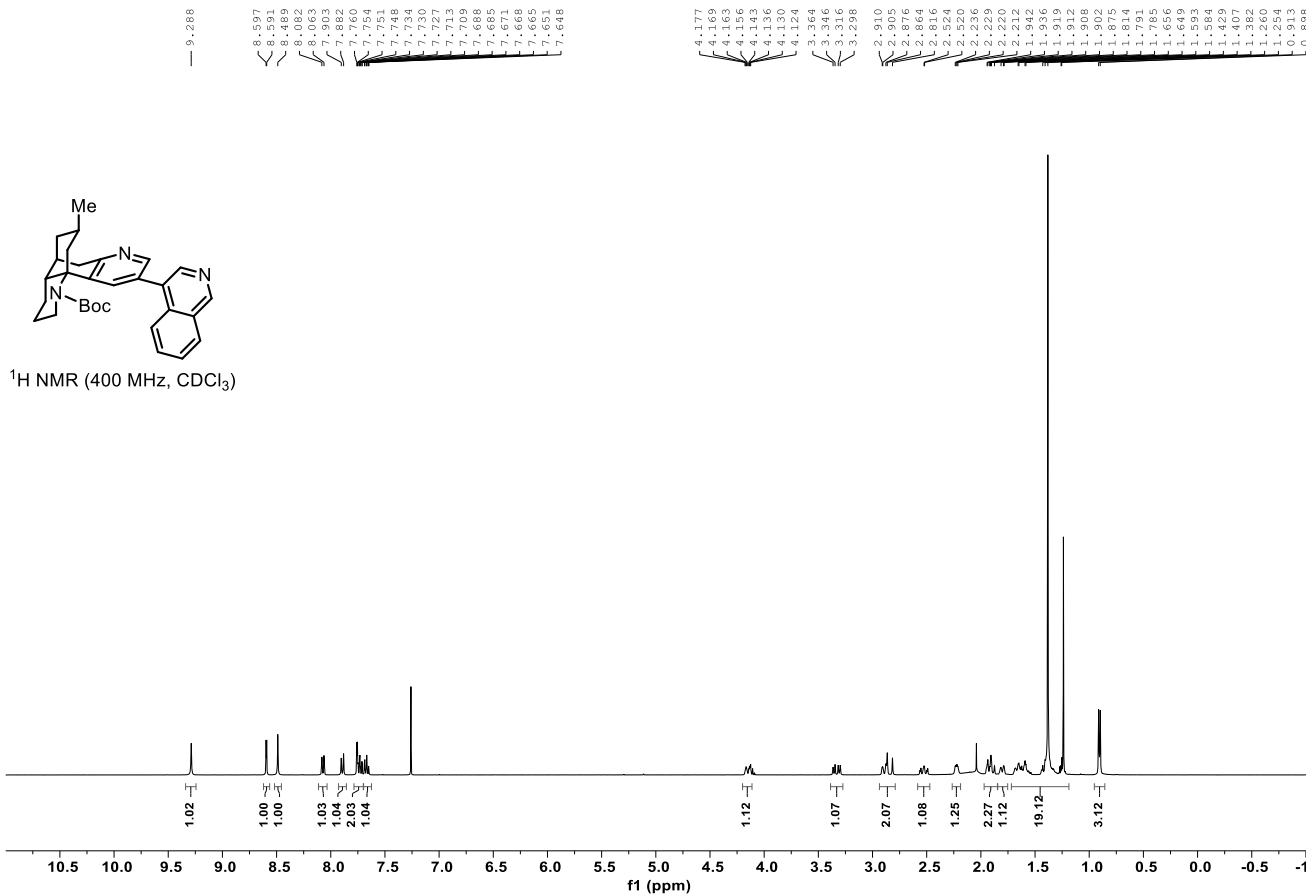
48.46
44.47
43.13
43.11
35.02
34.45
28.74
27.83
26.77
25.79
22.55



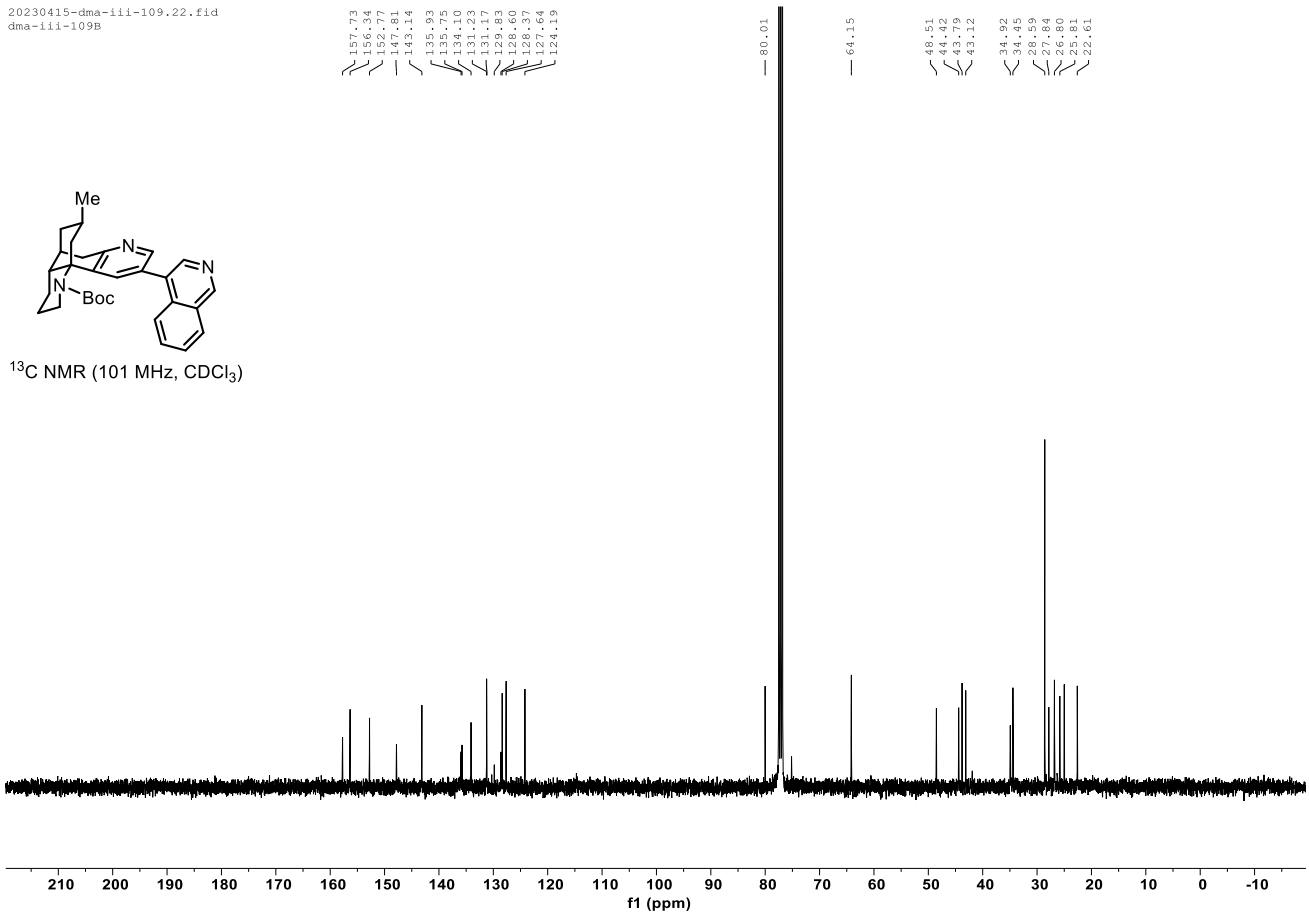
¹³C NMR (101 MHz, CDCl₃)



20230415-dma-iii-109.21.fid - dma-iii-109B



20230415-dma-iii-109.22.fid
dma-iii-109B



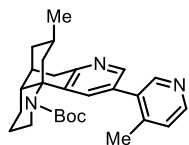
20230417-dma-iii-110.11.fid
dma-iii-110A

8.483
8.471
8.451
8.407
8.401

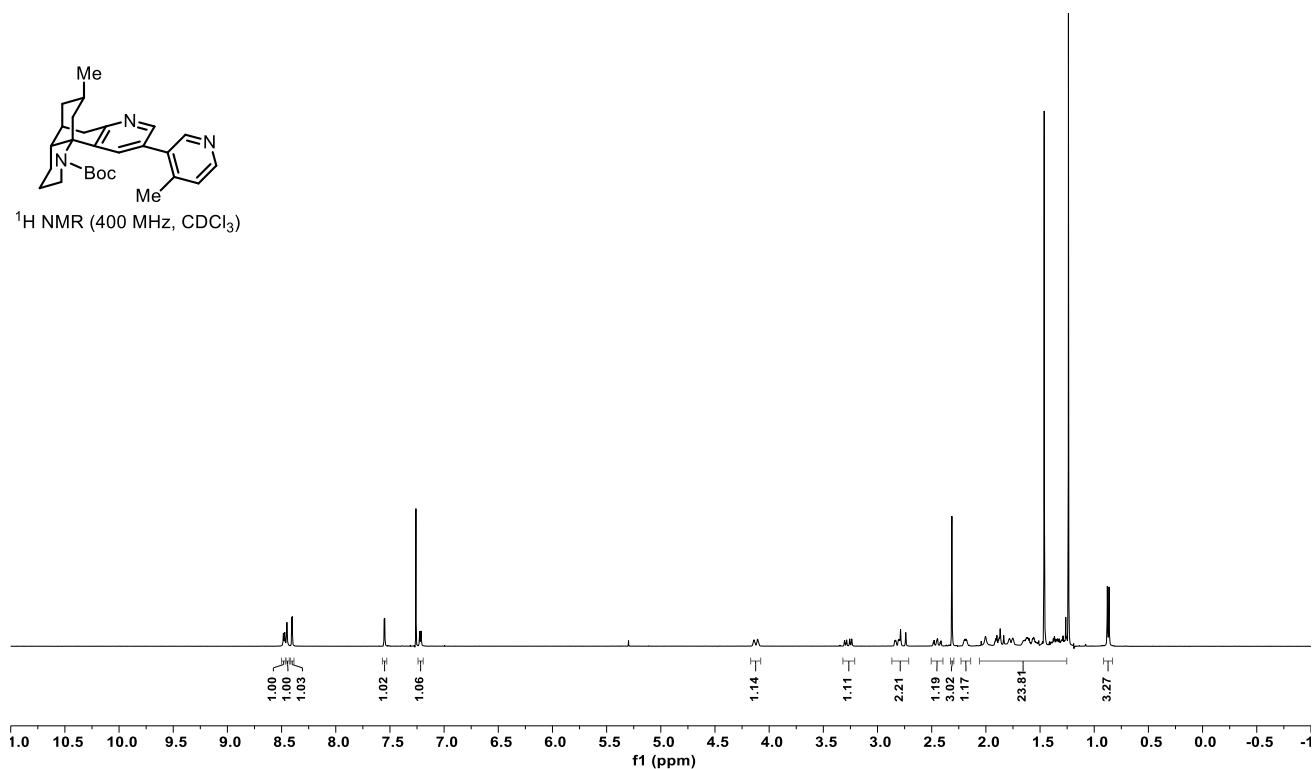
7.553
7.568
7.260
7.225
7.213

4.157
4.143
4.137
4.130
4.125
4.116
4.106
4.104
4.096
4.090
3.304
3.285
3.266
3.236

2.838
2.833
2.828
2.805
2.800
2.796
2.787
2.782
2.478
2.451
2.448
2.444
2.314
2.202
2.189
2.184
2.175
2.003
1.908
1.752
1.652
1.609
1.562
1.462
1.367
1.338
1.321
1.297
1.238
1.179
0.863



¹H NMR (400 MHz, CDCl₃)



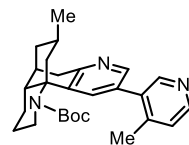
20230417-dma-iii-110.12.fid
dma-iii-110A

157.52
156.36
150.00
149.02
147.45
144.93
135.45
134.81
134.29
131.79
125.61

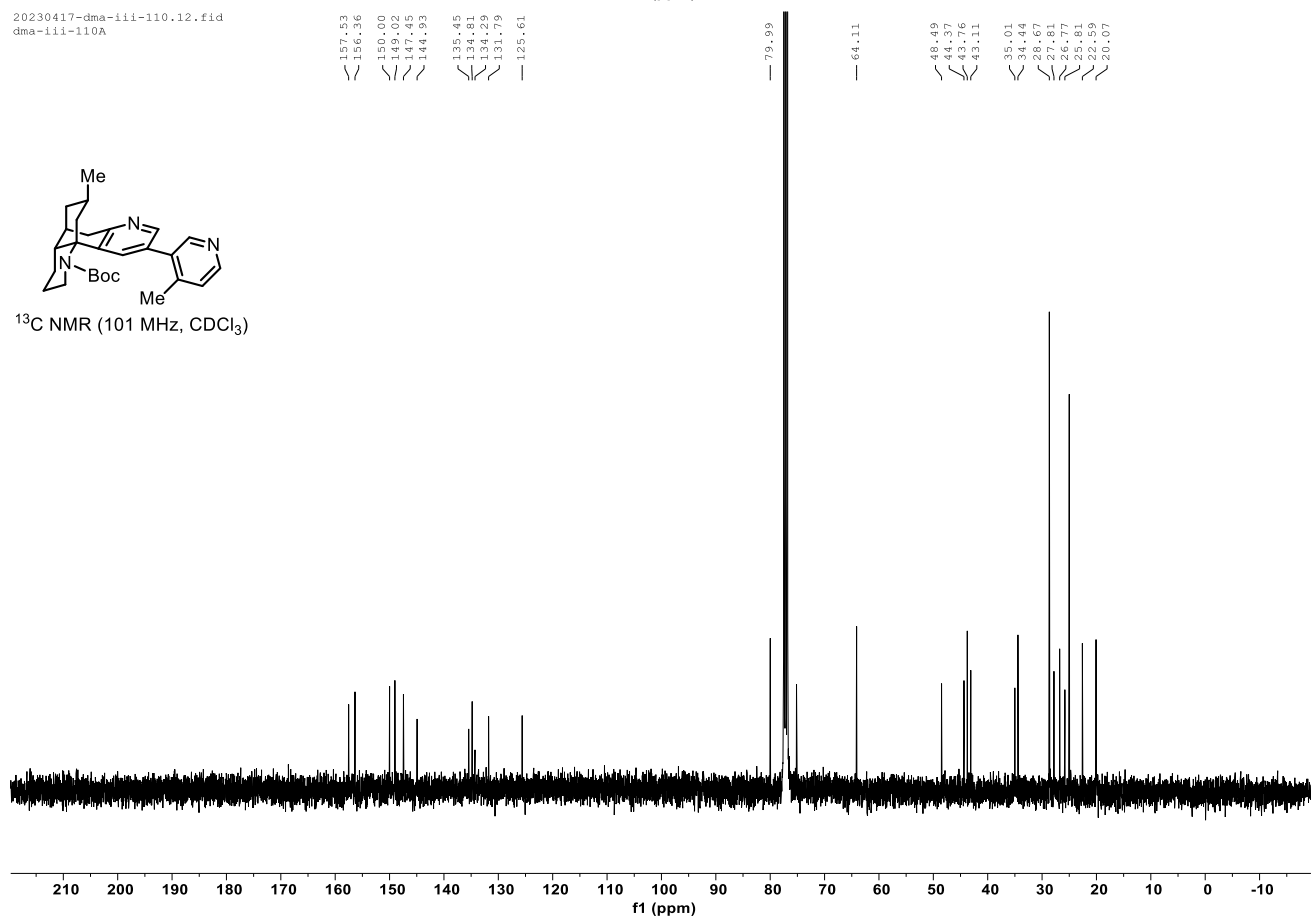
79.99

64.11

48.49
44.37
43.16
43.11
35.01
34.44
28.67
27.81
26.77
25.81
22.59
20.07



¹³C NMR (101 MHz, CDCl₃)

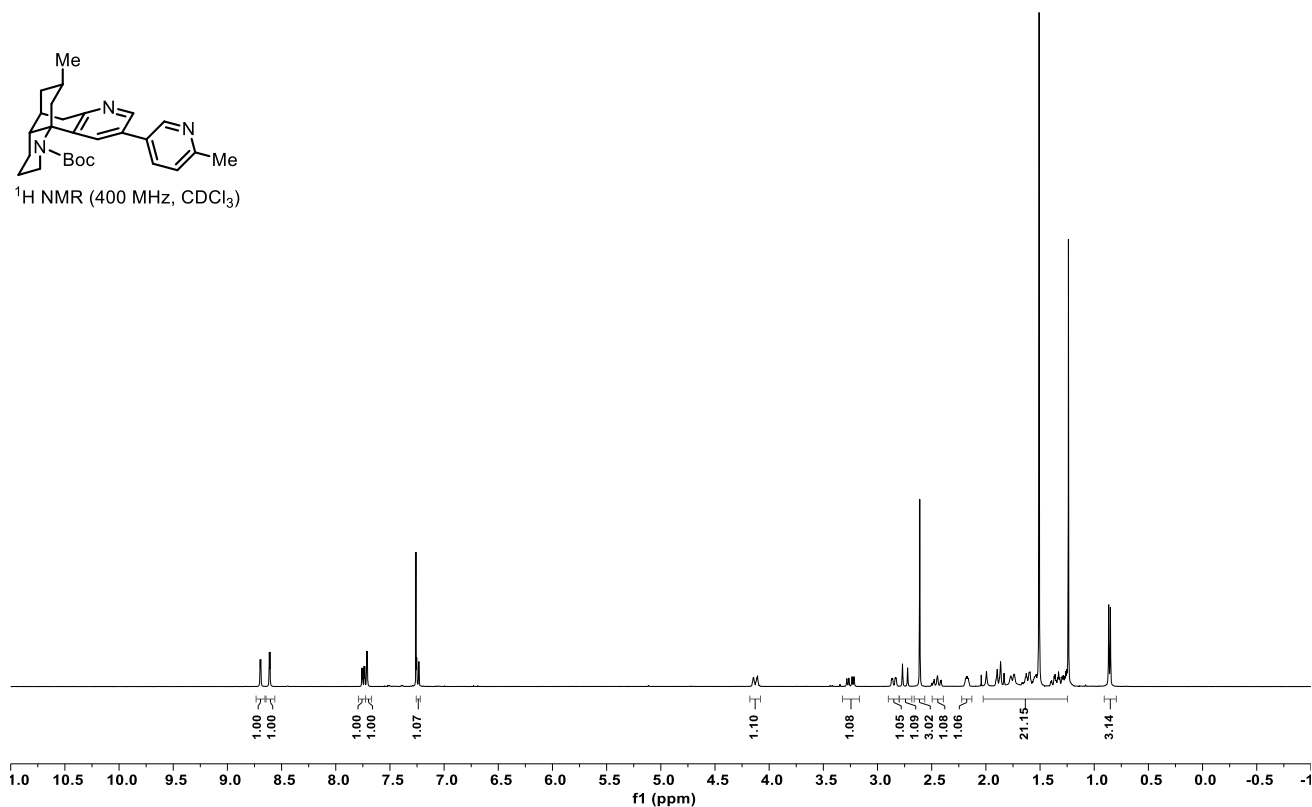
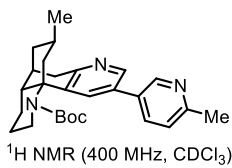


20230417-dma-iii-110.21.fid
dma-iii-110B

8.698
8.693
8.613
8.607

7.758
7.752
7.739
7.732
7.714
7.709
7.253
7.233

4.148
4.142
4.125
4.122
4.114
4.107
4.089
3.283
3.274
3.235
3.217
2.872
2.868
2.862
2.858
2.833
2.835
2.830
2.825
2.769
2.722
2.484
2.477
2.453
2.450
2.446
2.443
2.419
2.412
2.188
2.170
2.170
2.162
1.995
1.895
1.876
1.865
1.861
1.770
1.770
1.739
1.627
1.601
1.593
1.509
1.491
1.393
1.371
1.369
1.360
1.251
1.338
1.329
1.266
1.264
1.255
1.0866
0.851



20230417-dma-iii-110.22.fid
dma-iii-110B

158.06
157.67
156.48

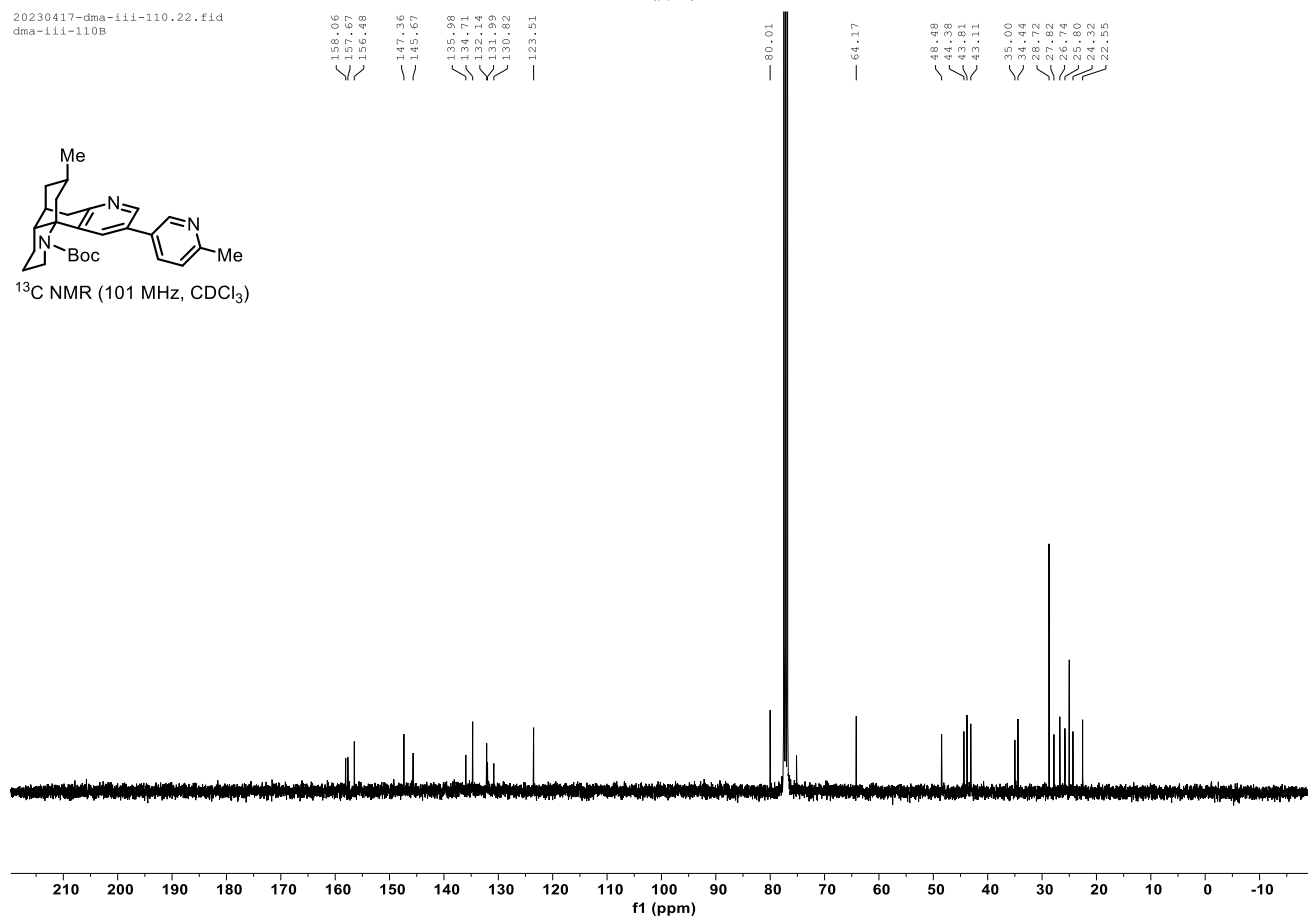
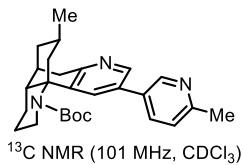
147.36
145.67

135.98
134.71
132.14
131.99
130.82
123.51

80.01

64.17

48.48
44.38
43.11
43.11
35.00
34.44
28.72
27.82
26.74
25.60
24.32
22.35

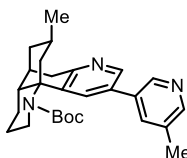


20230419-dma-iii-111.11.fid
dma-iii-111A

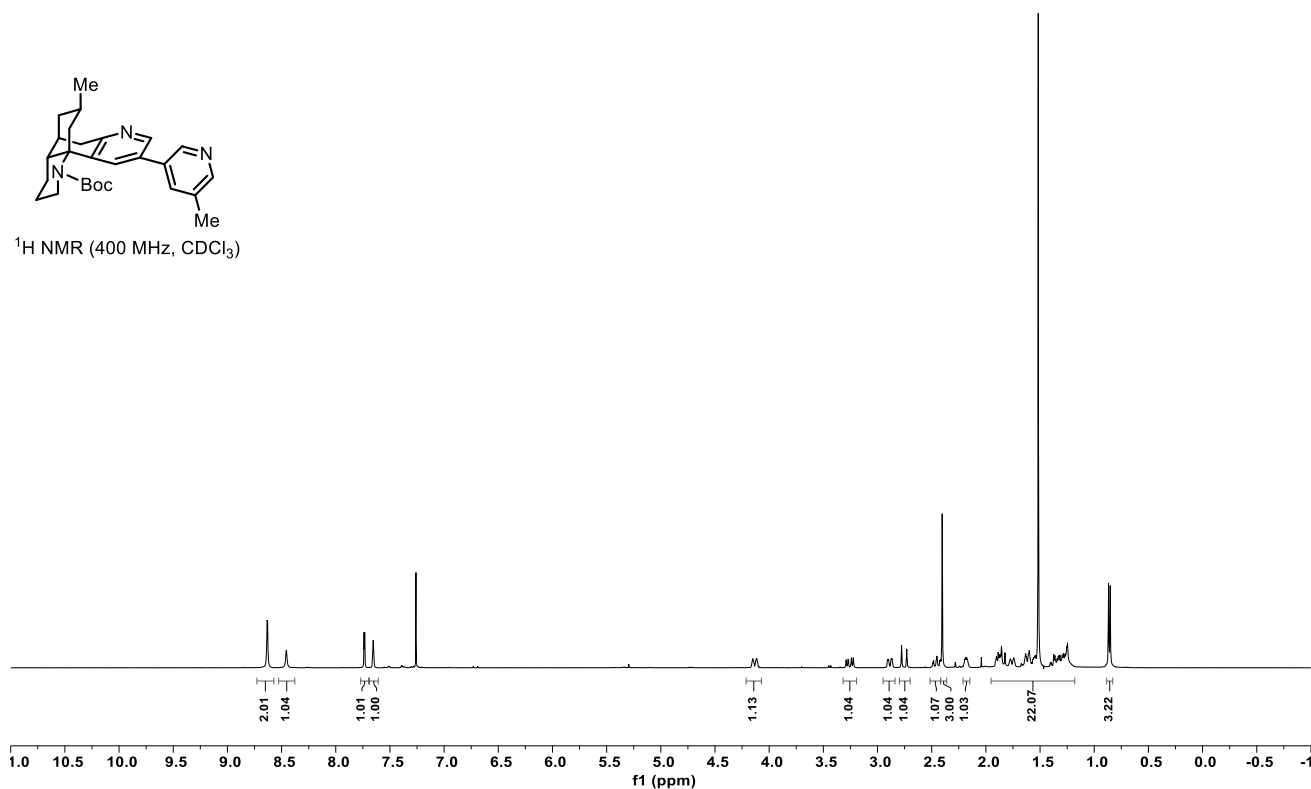
8.634
8.629
8.456

7.739
7.733
7.654

4.161
4.154
4.148
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4.126
4.120
4.114
4.107
3.289
3.271
3.265
3.253
2.909
2.905
2.900
2.895
2.877
2.871
2.865
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2.730
2.490
2.482
2.459
2.453
2.452
2.448
2.425
2.417
2.403
2.396
2.378
2.376
2.178
2.169
1.911
1.902
1.895
1.886
1.879
1.874
1.743
1.736
1.633
1.606
1.599
1.551
1.477
1.471
1.541
1.517
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1.266
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1.247
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0.868
0.852



¹H NMR (400 MHz, CDCl₃)



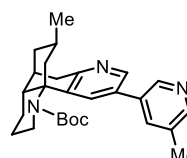
20230419-dma-iii-111.12.fid
dma-iii-111A

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156.57
149.68
145.69
145.29
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134.86
133.21
132.40
131.93

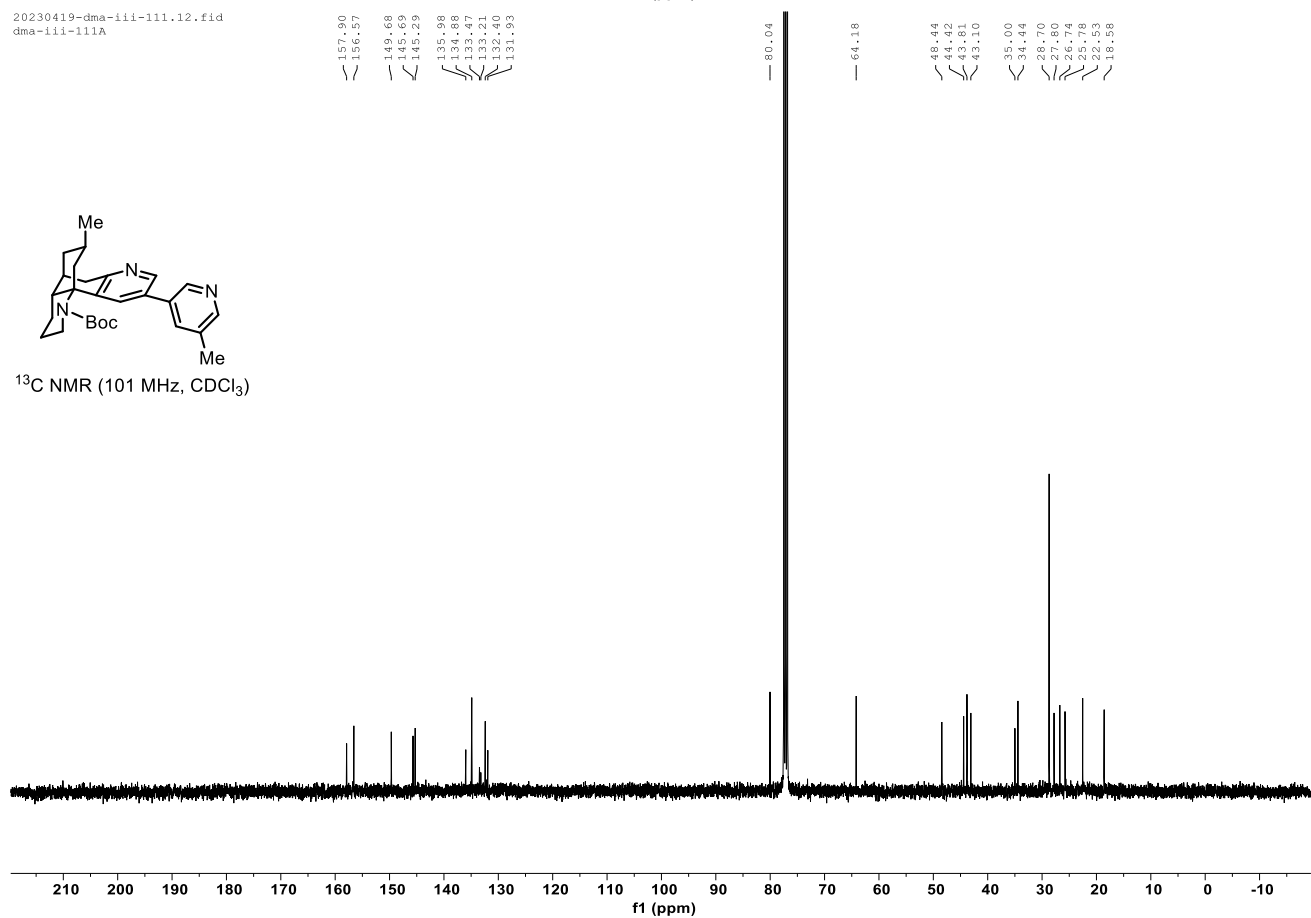
80.04

64.18

48.44
44.42
43.14
43.10
35.00
34.44
28.70
27.80
26.74
25.78
22.53
18.68



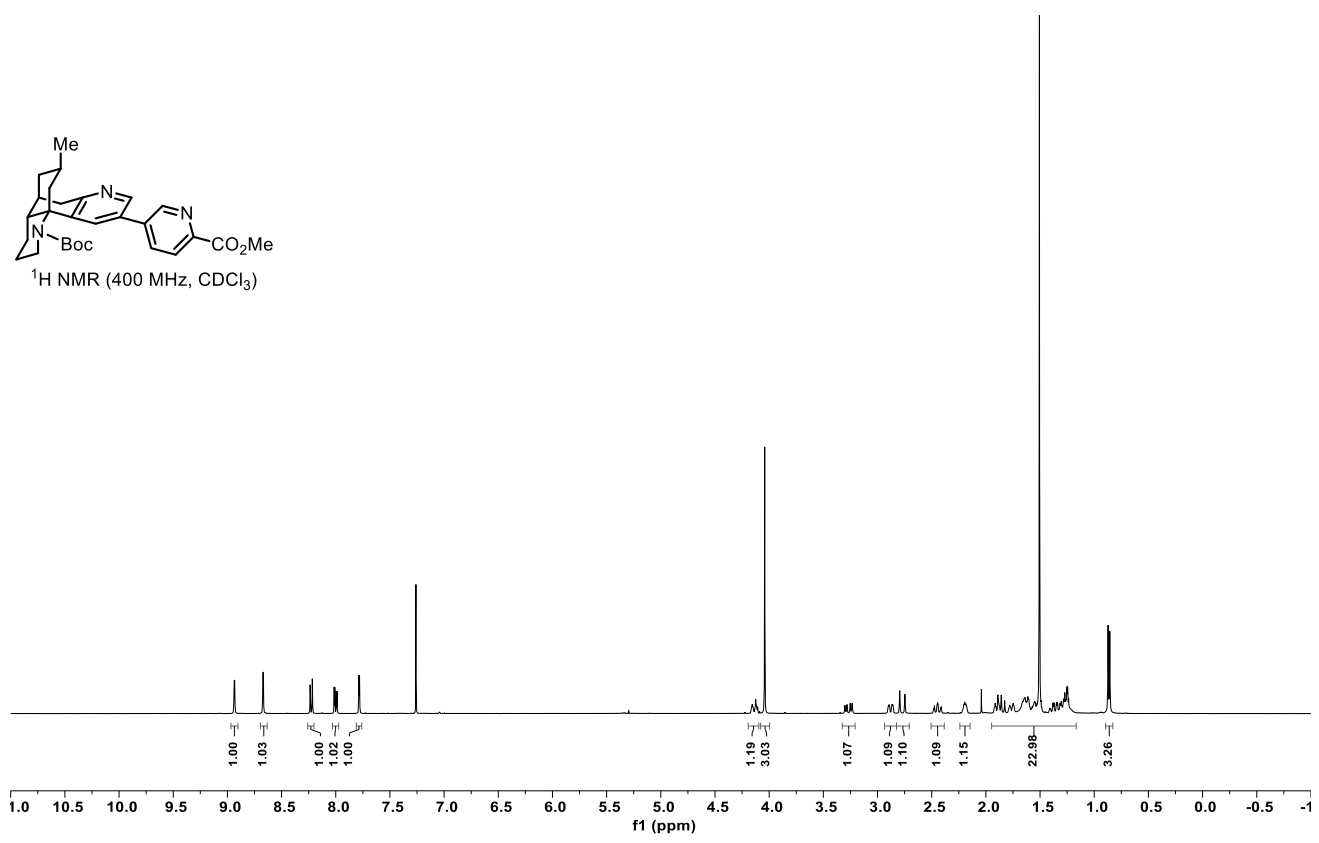
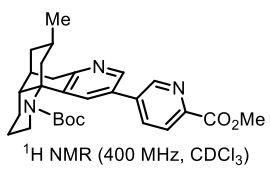
¹³C NMR (101 MHz, CDCl₃)



20230419-dma-iii-111.21.fid
 dma-iii-111B

8.931
 8.931
 8.931
 8.674
 8.668
 8.237
 8.237
 8.215
 8.215
 8.015
 8.009
 7.994
 7.786
 7.781

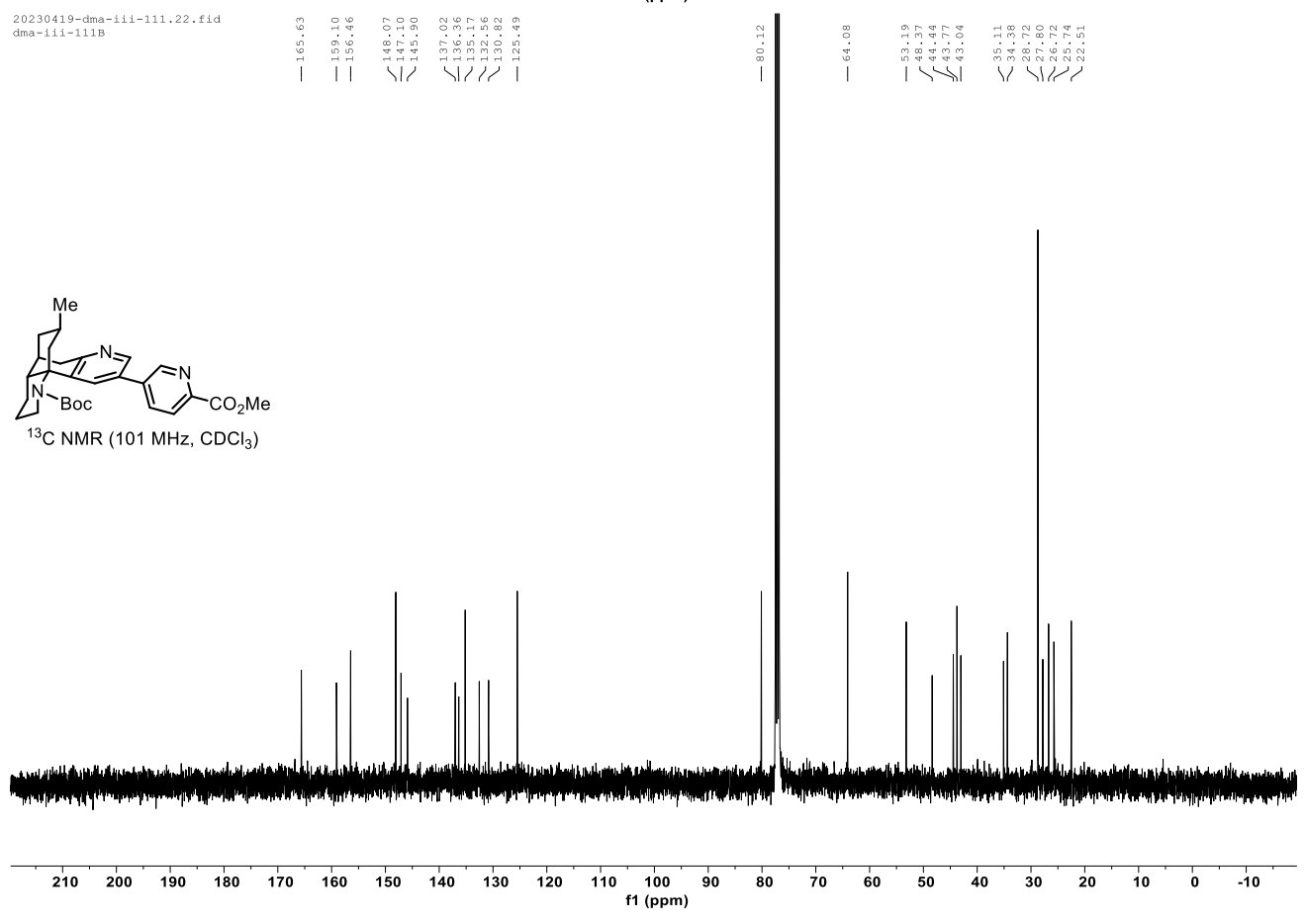
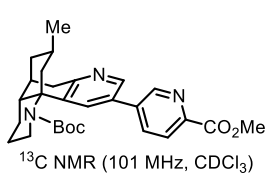
4.158
 4.142
 4.142
 4.132
 4.124
 4.119
 4.041
 3.900
 3.892
 3.852
 3.234
 2.903
 2.898
 2.893
 2.888
 2.885
 2.880
 2.855
 2.795
 2.747
 2.483
 2.475
 2.465
 2.445
 2.441
 2.418
 2.411
 2.204
 2.197
 2.180
 2.180
 1.923
 1.914
 1.907
 1.890
 1.882
 1.874
 1.866
 1.826
 1.780
 1.748
 1.639
 1.612
 1.603
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 1.246
 1.236
 0.872
 0.856



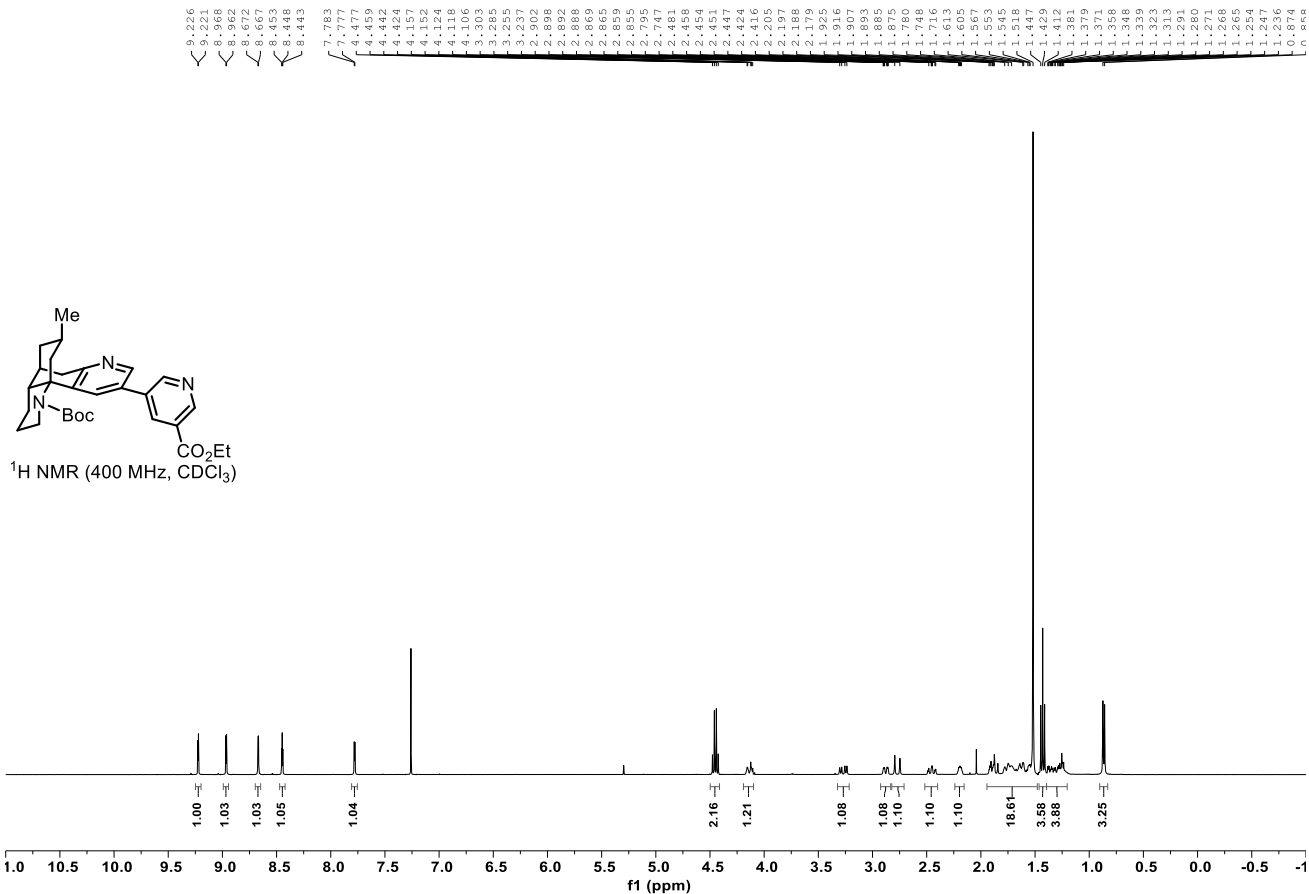
20230419-dma-iii-111.22.fid
 dma-iii-111B

165.63
 159.10
 156.46
 148.07
 147.10
 145.90
 137.02
 136.36
 135.17
 132.56
 130.82
 125.49

80.12
 64.08
 53.19
 48.37
 44.44
 43.77
 43.04
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 28.72
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 25.74
 22.51

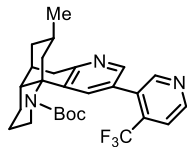


20230422-dma-iii-113.10.fid | dma-iii-113A

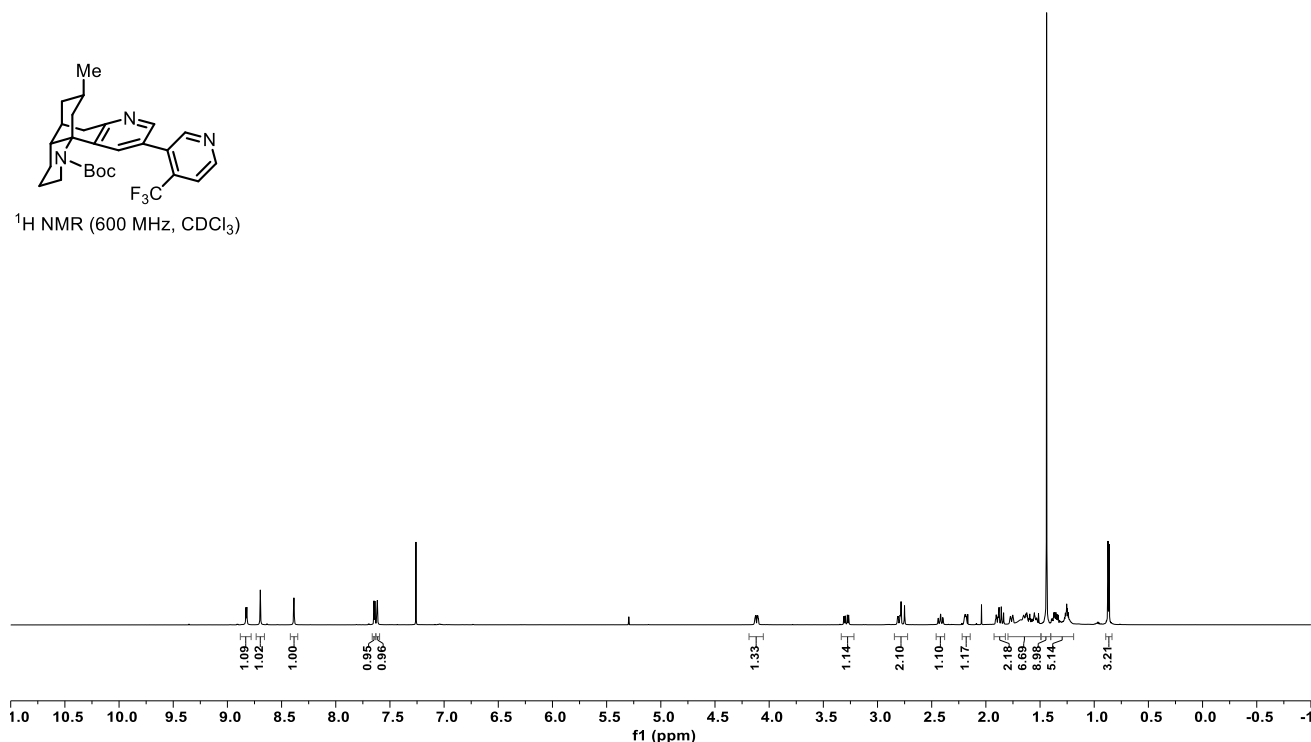


20230424-dma-iii-113B.10.fid

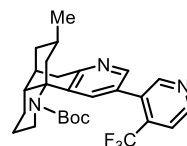
8.829 8.821 8.696 8.388 8.384 7.647 7.639 7.637 7.260 4.130 4.126 4.123 4.111 4.107 4.084 3.310 3.298 3.278 3.266 2.817 2.814 2.808 2.795 2.792 2.788 2.783 2.751 2.442 2.421 2.419 2.417 2.414 2.398 2.398 2.182 2.180 1.910 1.904 1.899 1.889 1.883 1.878 1.858 1.856 1.836 1.777 1.774 1.769 1.752 1.748 1.655 1.651 1.647 1.631 1.627 1.622 1.616 1.601 1.595 1.559 1.555 1.552 1.549 1.543 1.535 1.533 1.531 1.514 1.439 1.374 1.366 1.362 1.354 1.254 1.251 1.345 1.341 1.273 1.269 1.266 1.263 1.258 1.254 1.249 1.238 1.238 1.078 0.873 0.862



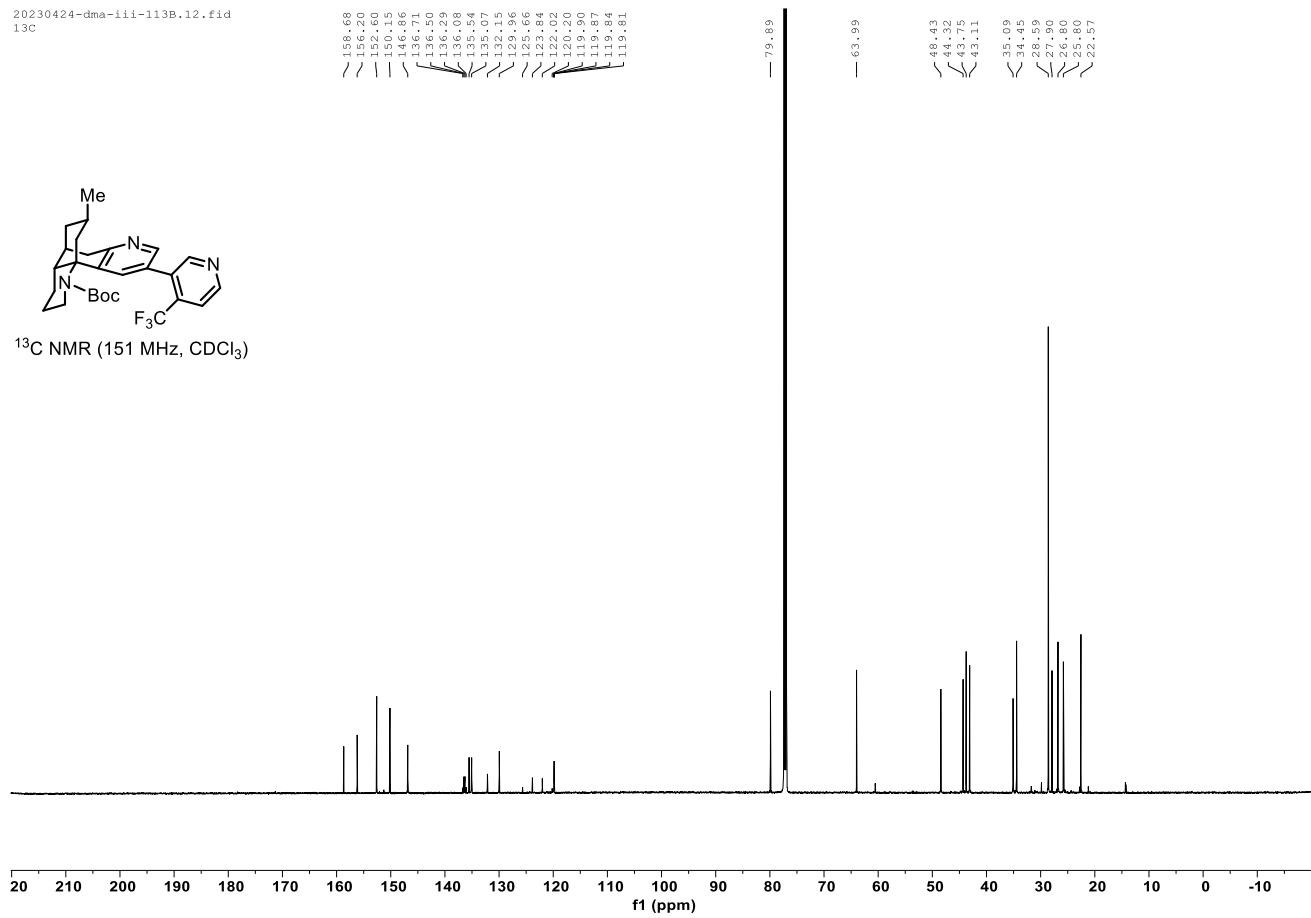
¹H NMR (600 MHz, CDCl₃)



20230424-dma-iii-113B.12.fid
13C

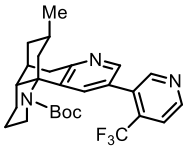


¹³C NMR (151 MHz, CDCl₃)



20230424-dma-iii-113B.11.fid
19F

-56.95



¹⁹F NMR (565 MHz, CDCl₃)

