

SUPPORTING INFORMATION

Exploiting the Nucleophilicity of the Nitrogen Atom of Imidazoles: One-pot Three-component Synthesis of Imidazopyperazines

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Ettore Novellino,^c Mariateresa Giustiniano,^{c*} and Gian Cesare Tron^{a*}

a) Dipartimento di Scienze del Farmaco, Università degli Studi del Piemonte Orientale “A. Avogadro”, Largo Donegani 2, 28100 Novara, Italy;

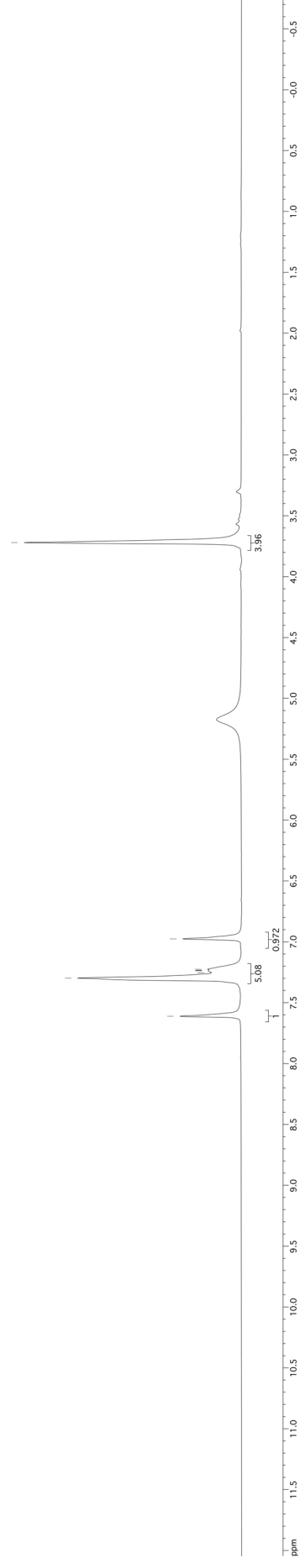
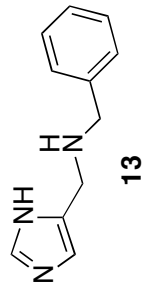
b) Dipartimento di Scienze Farmaceutiche, Università degli Studi di Milano, Via L. Mangiagalli 25, 20133 Milano, Italy;

c) Dipartimento di Farmacia, Università degli Studi di Napoli “Federico II”, via D. Montesano 49, 80131 Napoli, Italy.

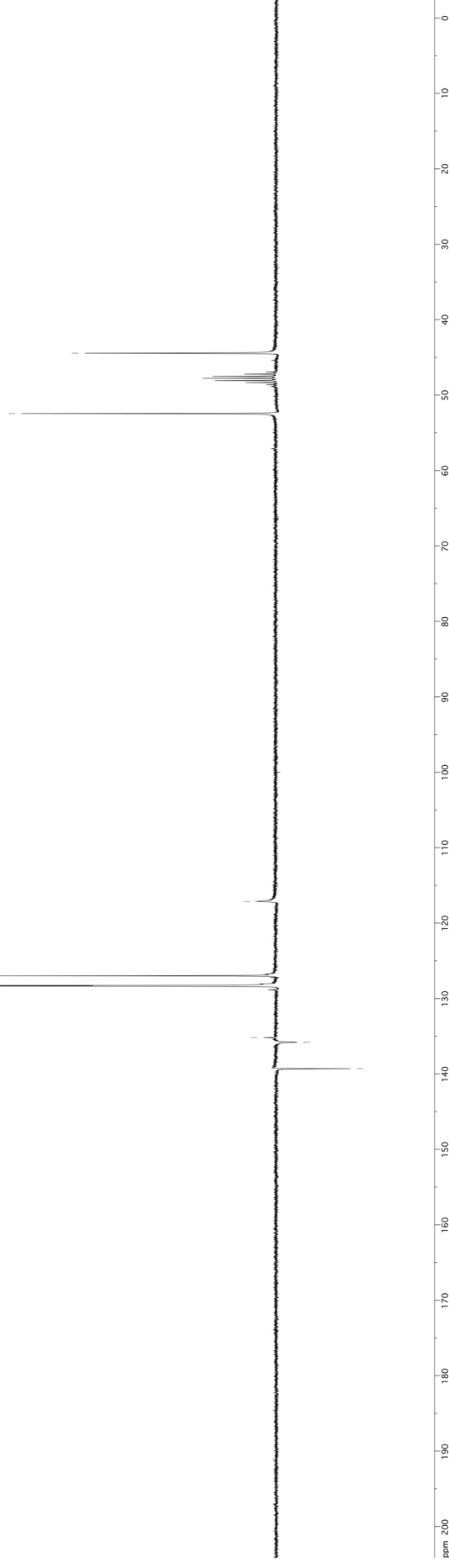
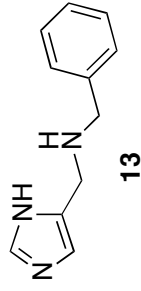
Contents:

- Copies of ^1H and ^{13}C spectra.....	S3
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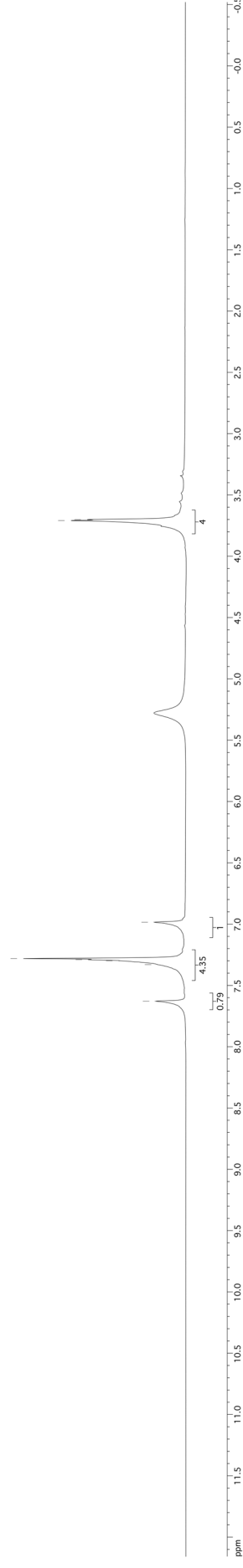
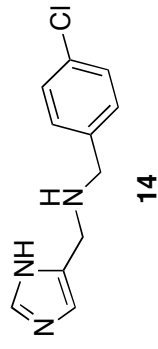
¹H NMR
300 MHz, CD₃OD



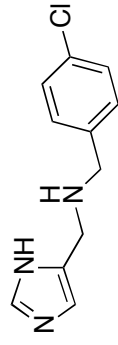
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75 MHz, CD₃OD



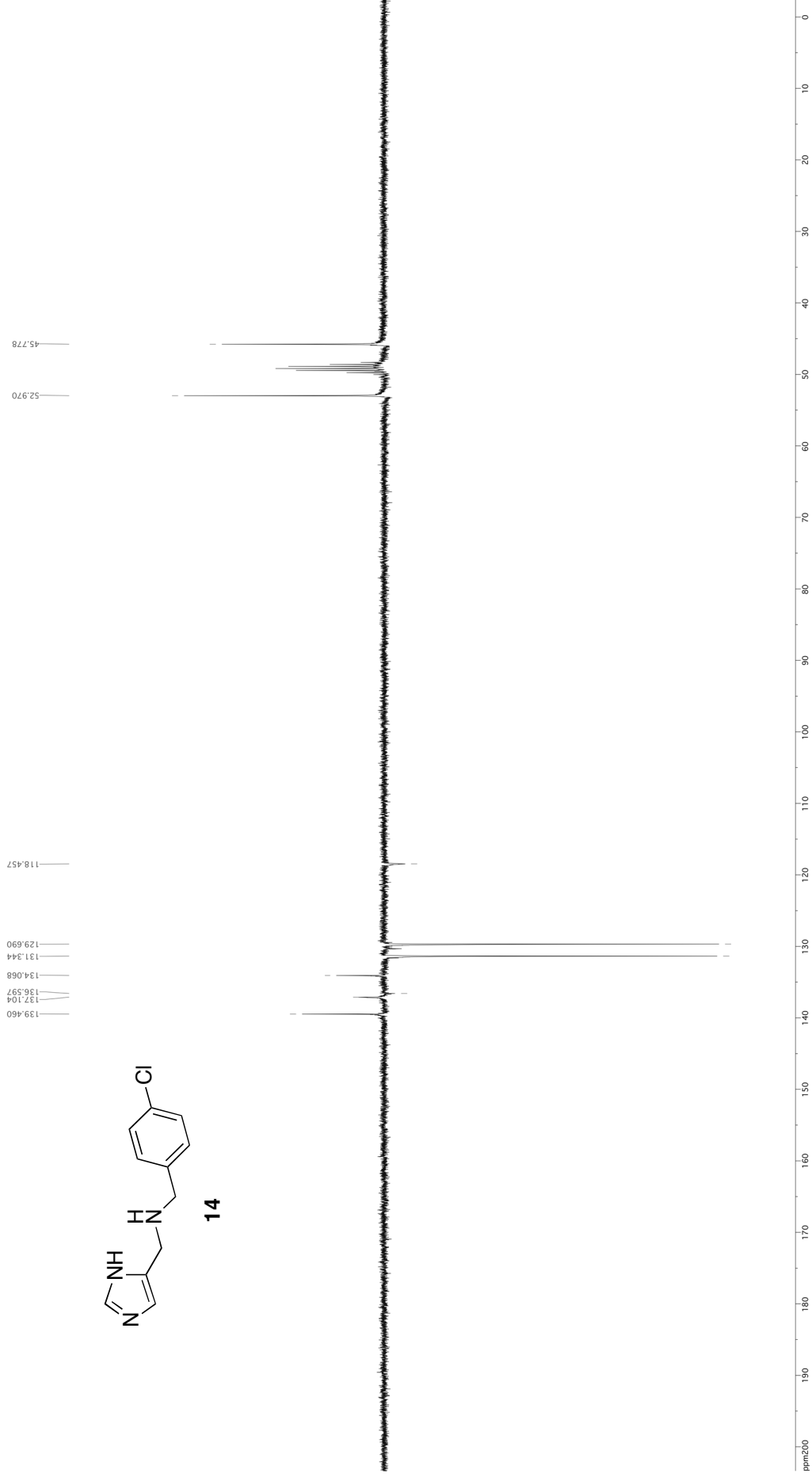
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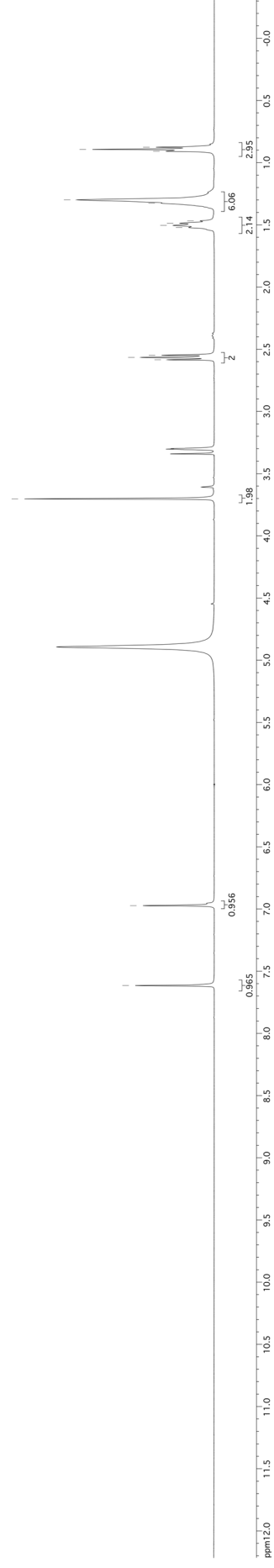
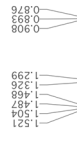
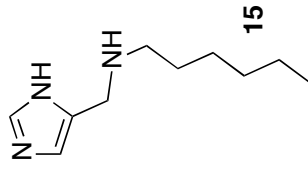
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75 MHz, CD₃OD



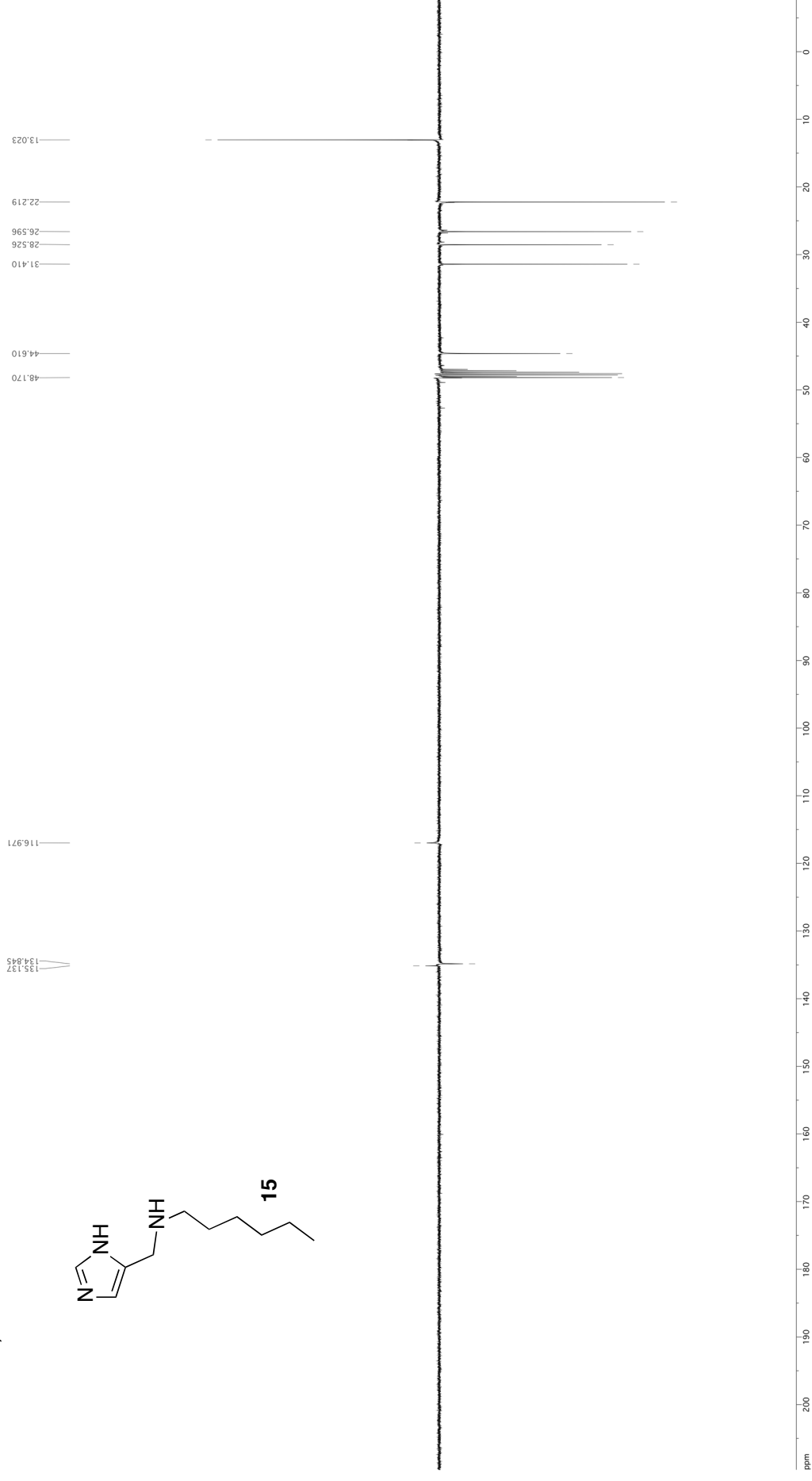
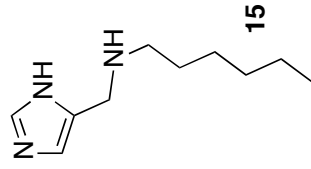
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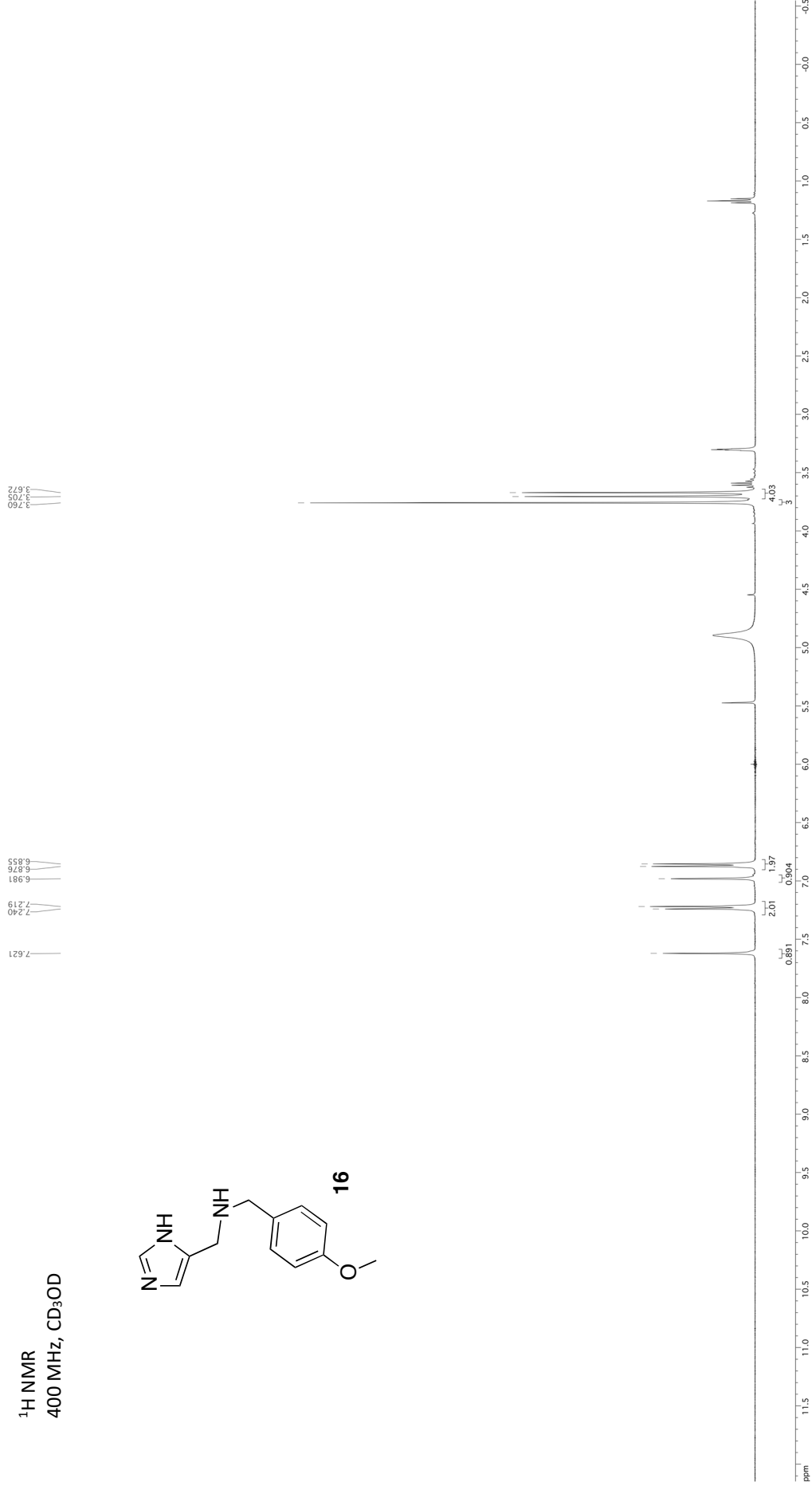
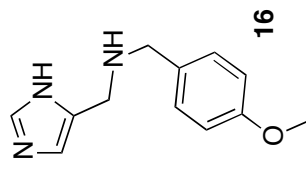
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400 MHz, CD₃OD



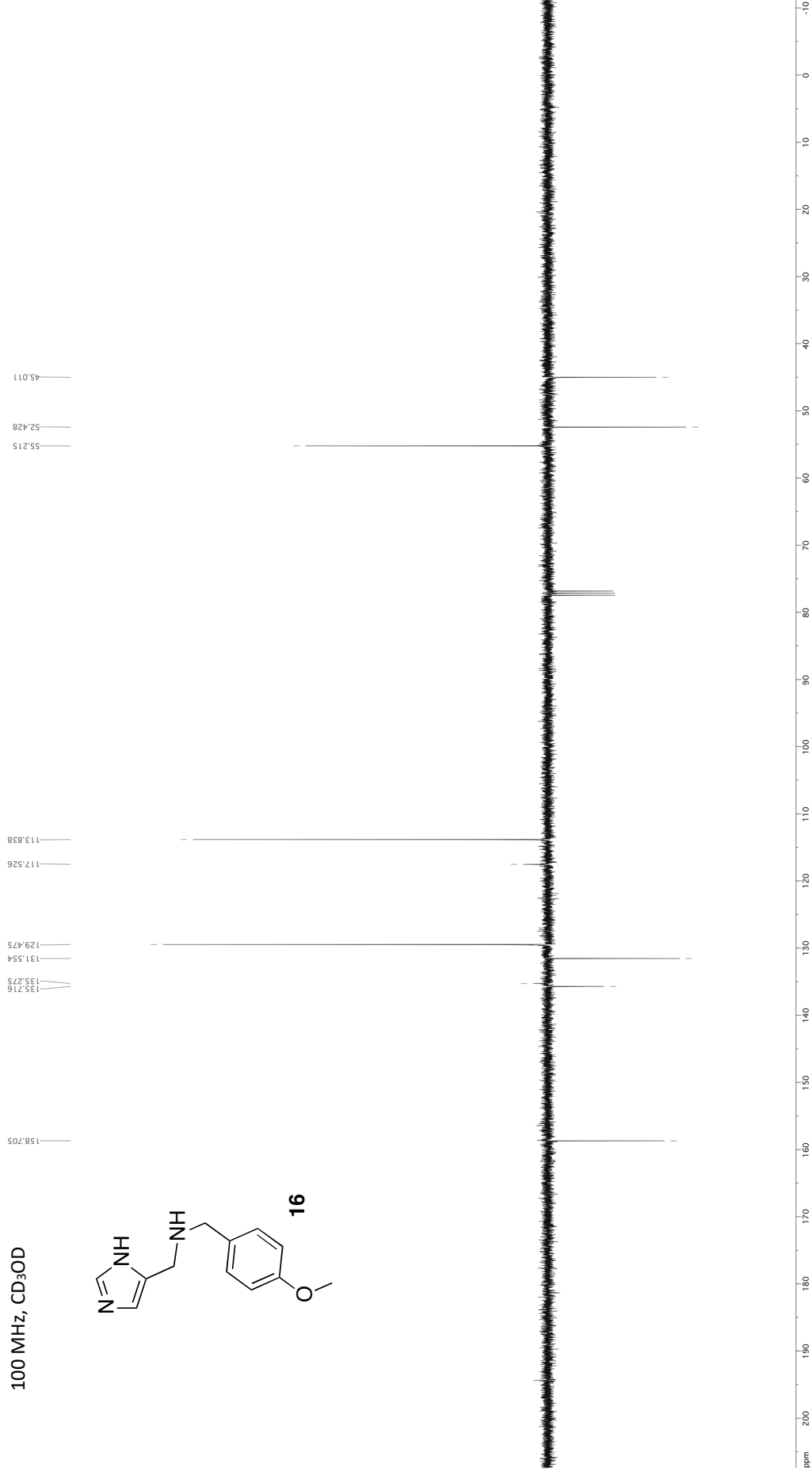
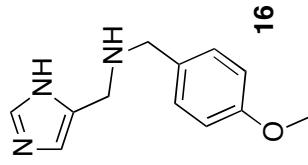
¹³C NMR
100 MHz, CD₃OD



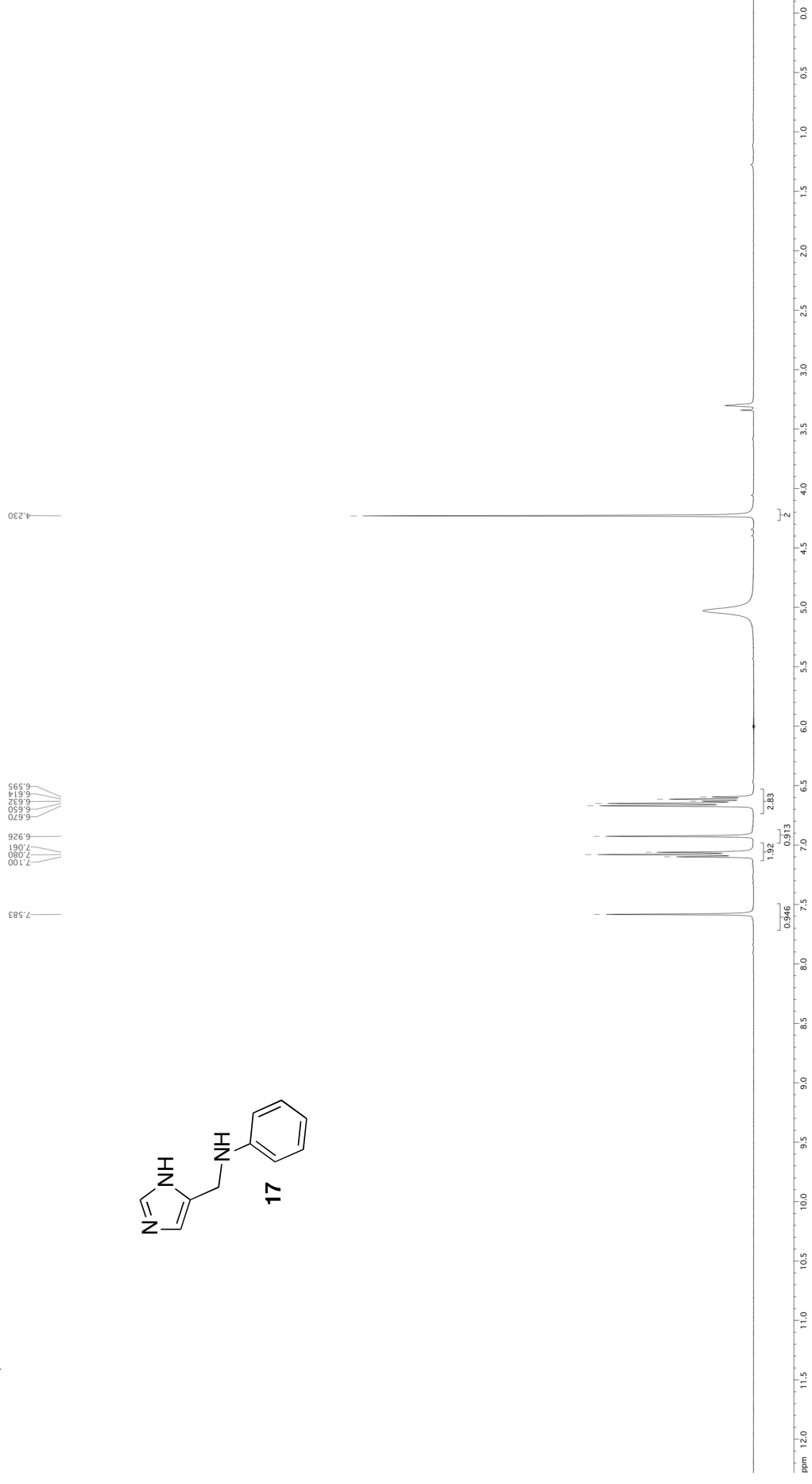
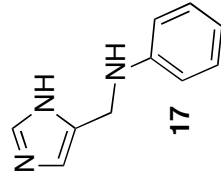
¹H NMR
400 MHz, CD₃OD



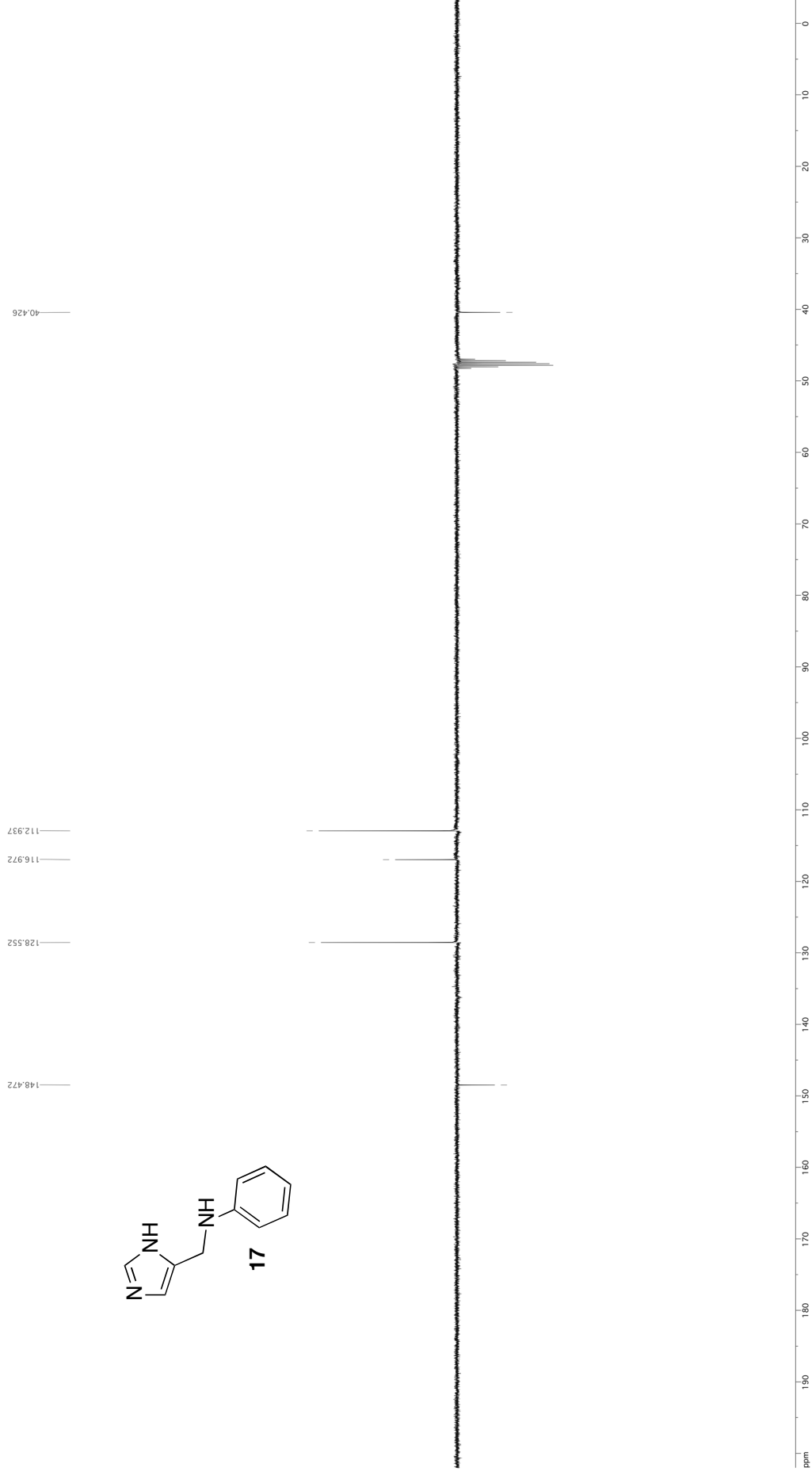
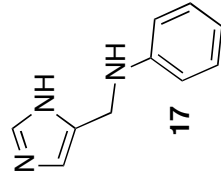
¹³C NMR
100 MHz, CD₃OD



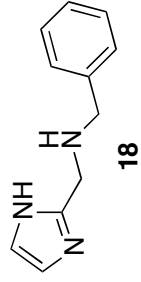
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400 MHz, CD₃OD



¹³C NMR
100 MHz, CD₃OD

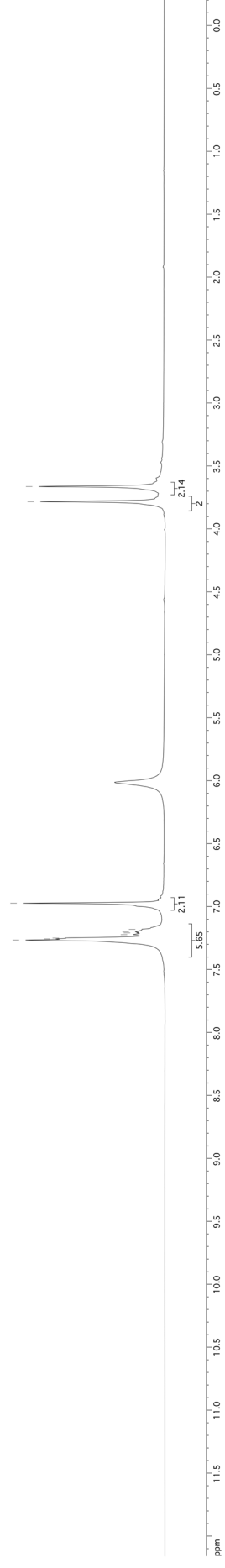


¹H NMR
300 MHz, CD₃OD

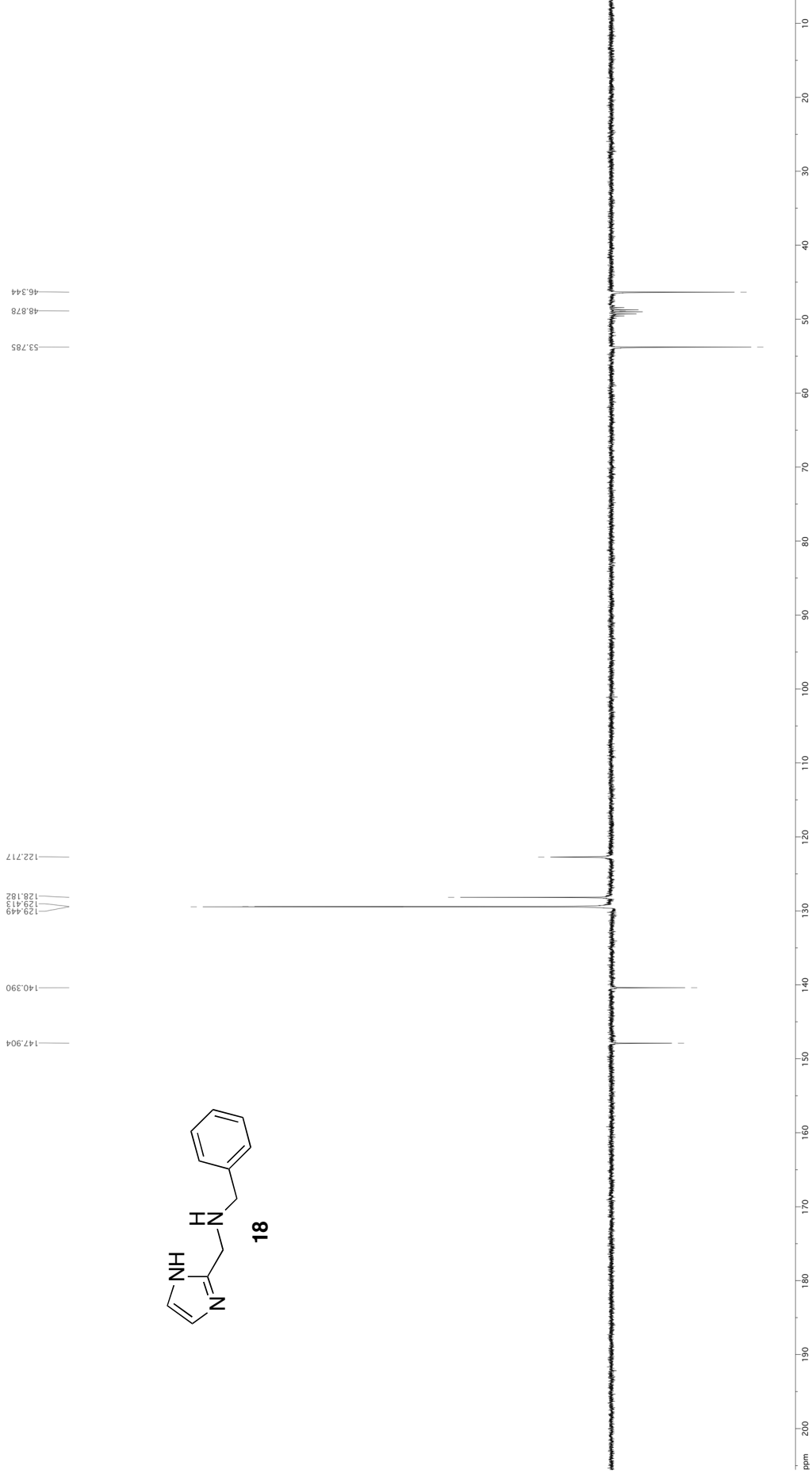
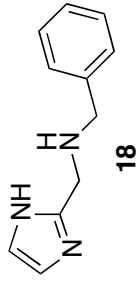


7.266
7.256
7.250
7.239
7.229
7.209
7.199
7.181
6.973

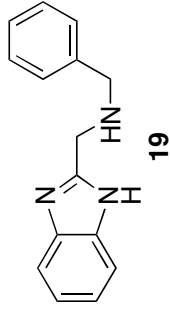
3.783
3.663



¹³C NMR
75 MHz, CD₃OD

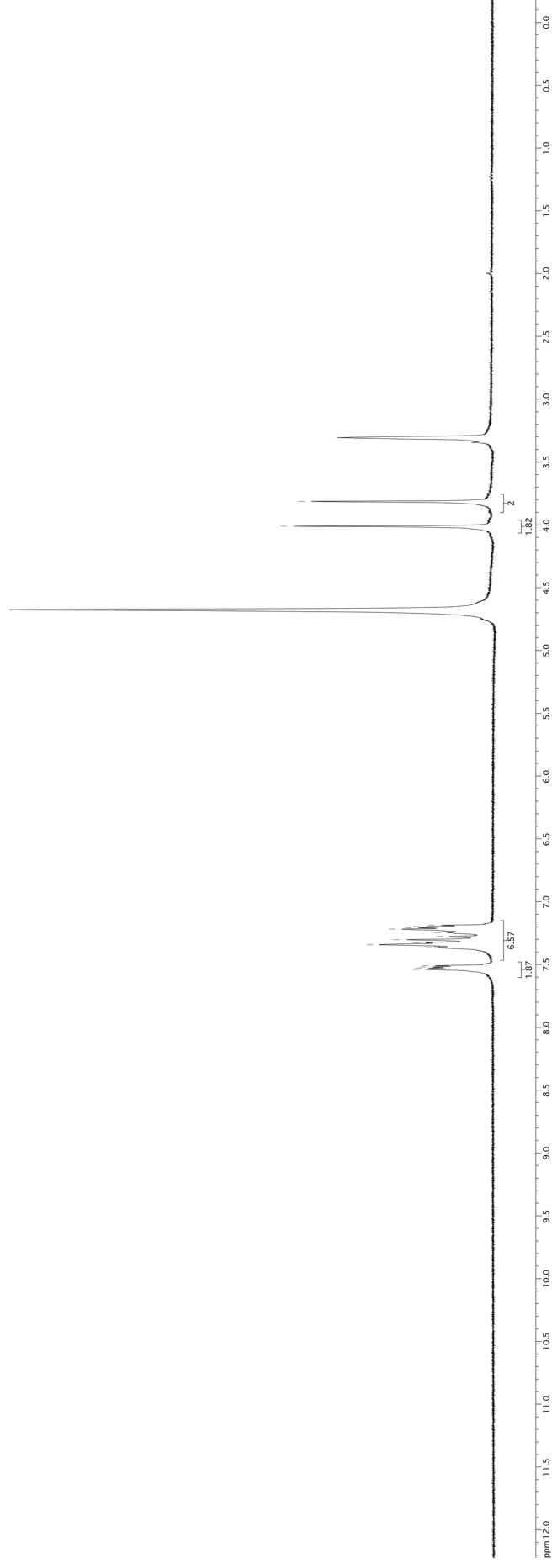


¹H NMR
300 MHz, CD₃OD

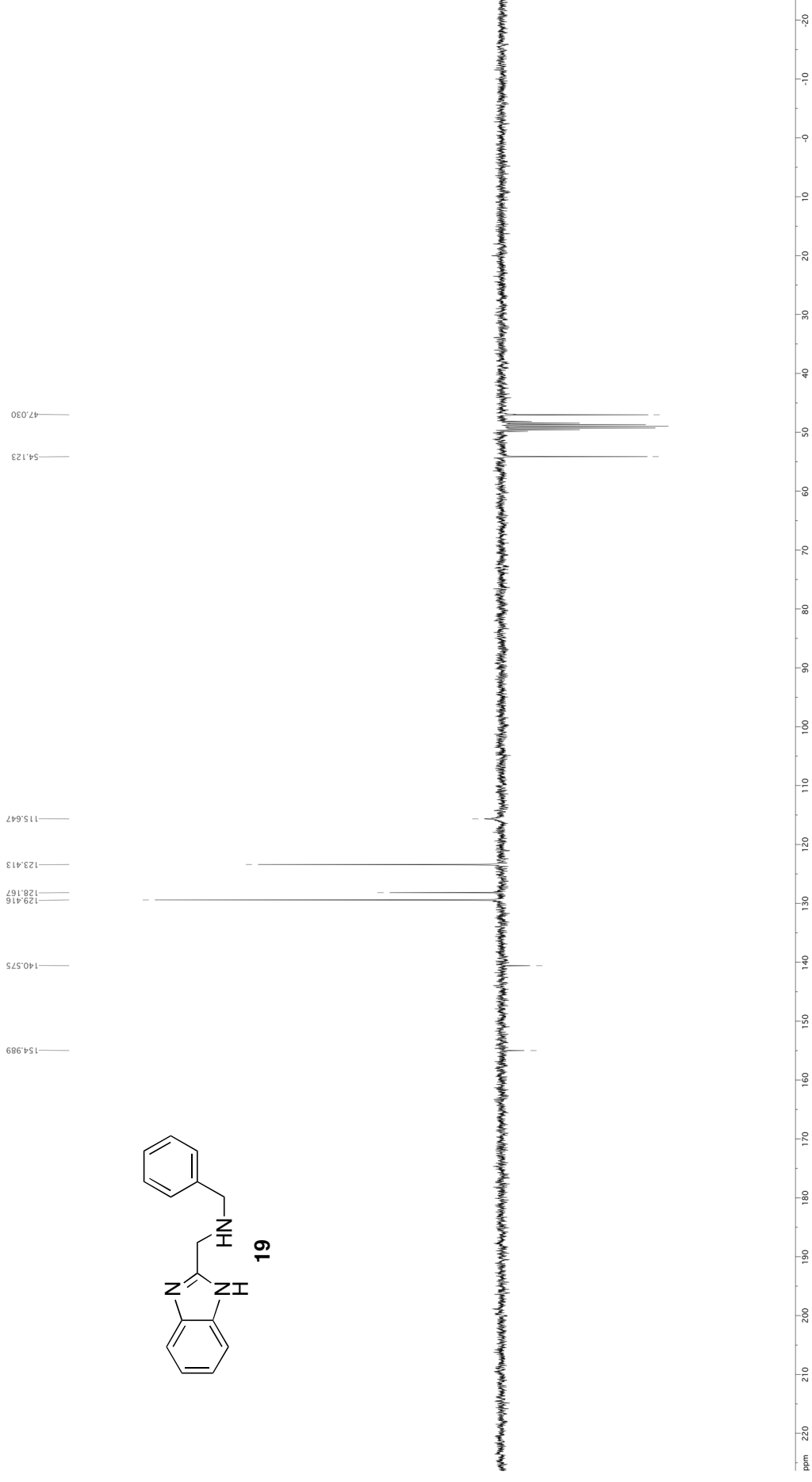
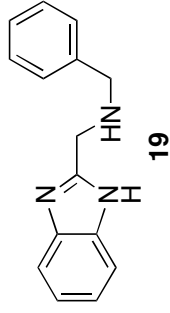


7.539
7.528
7.519
7.508
7.484
7.358
7.342
7.326
7.319
7.302
7.278
7.277
7.246
7.238
7.218
7.207
7.198
7.187

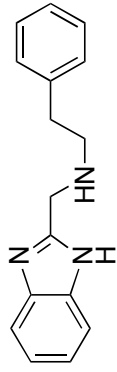
4.011
3.814



¹³C NMR
75 MHz, CD₃OD



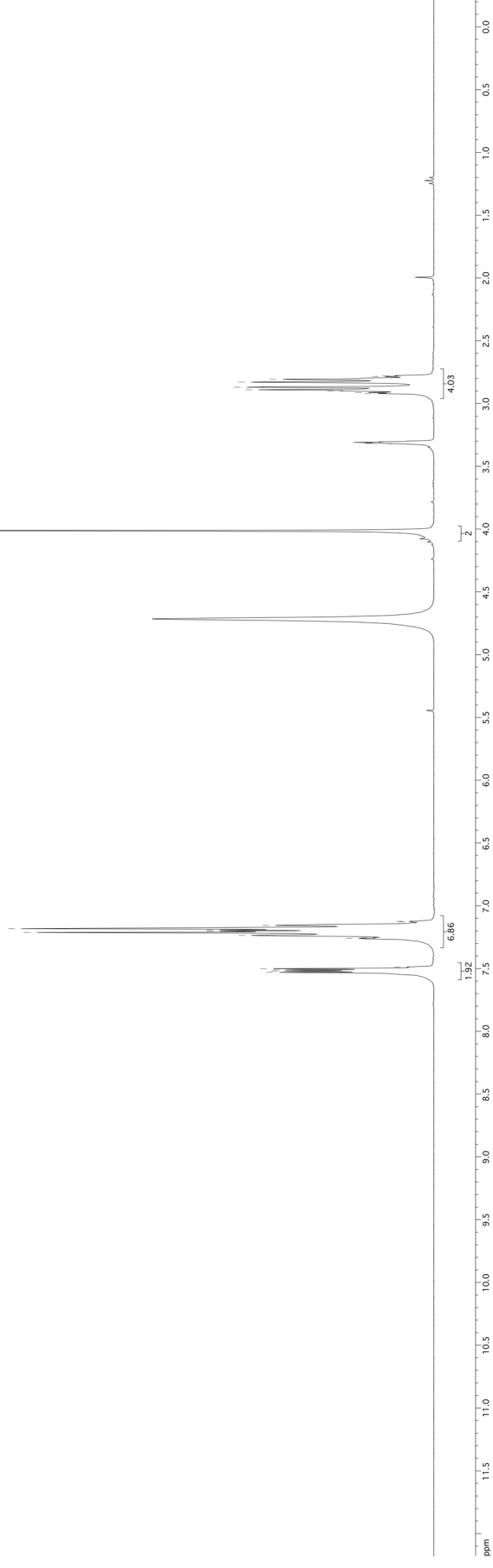
¹H NMR
300 MHz, CD₃OD



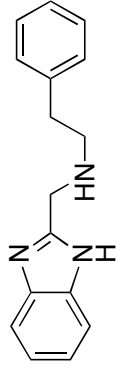
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7.531
7.530
7.511
7.500
7.489
7.461
7.255
7.236
7.219
7.202
7.182
7.162
7.156
7.129
7.124

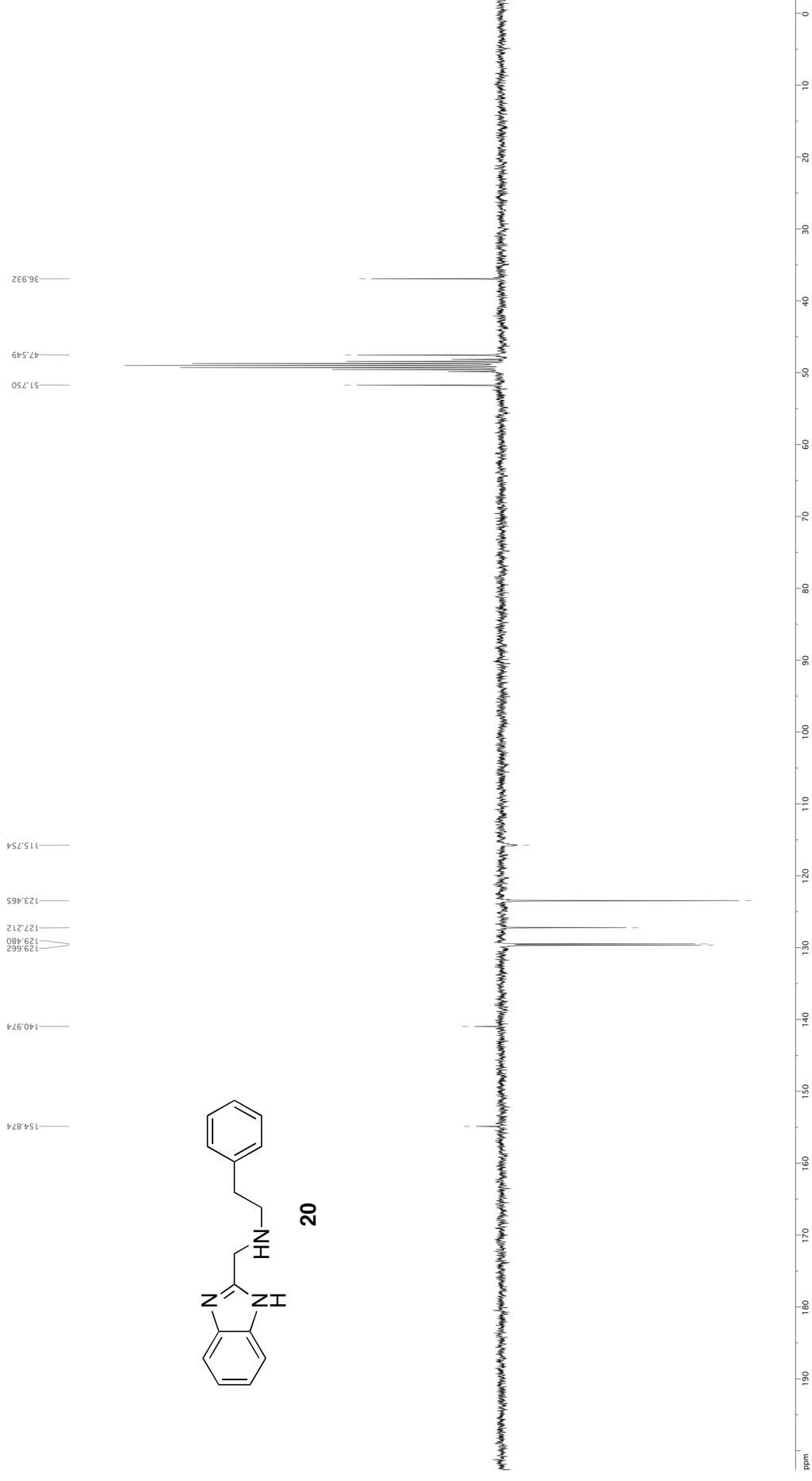
4.012



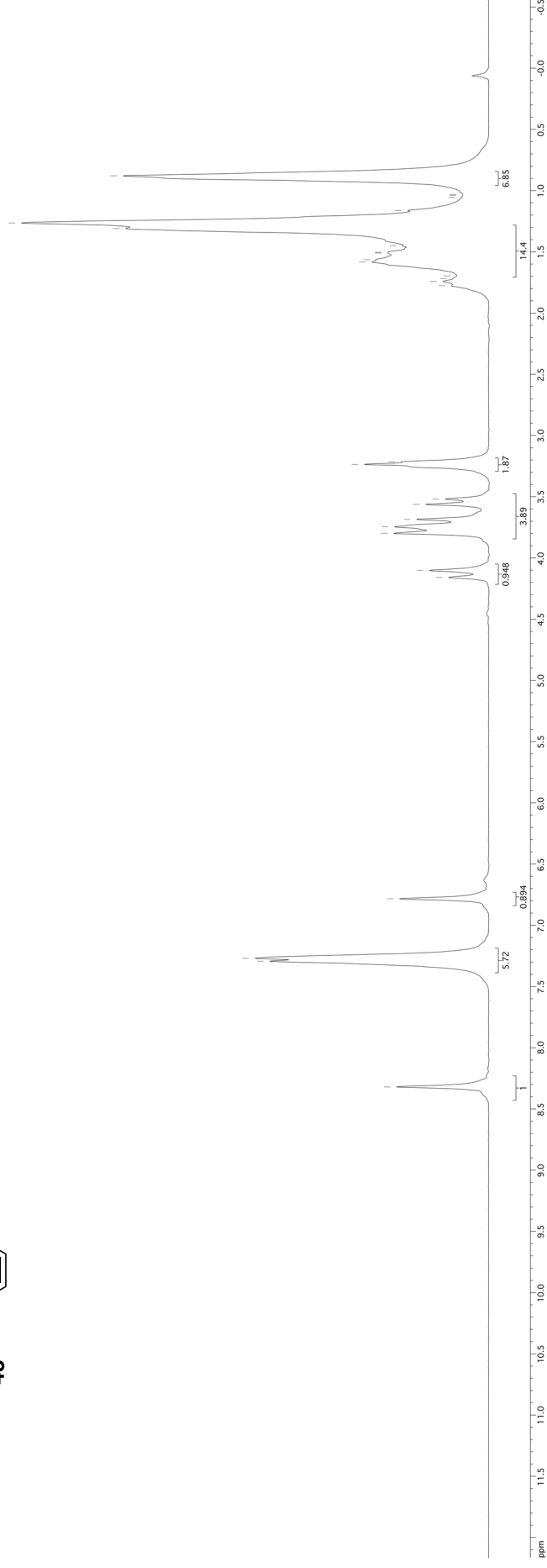
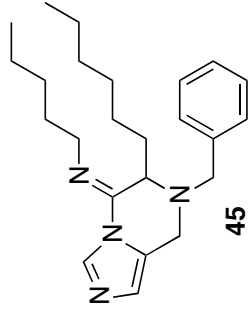
¹³C NMR
75 MHz, CD₃OD



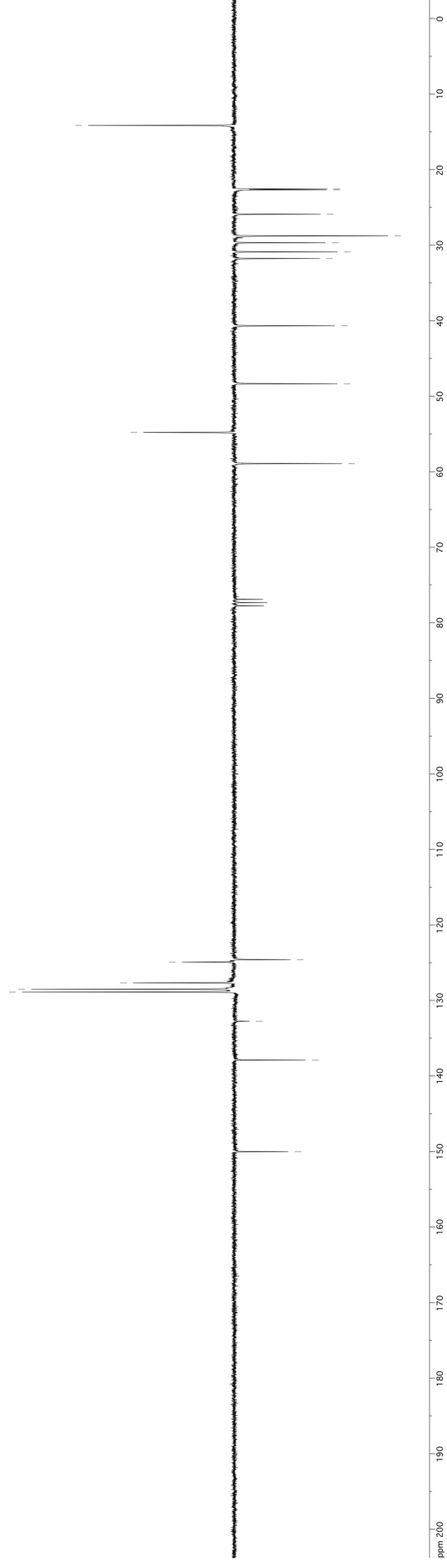
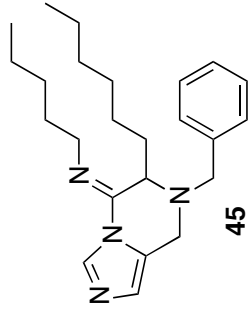
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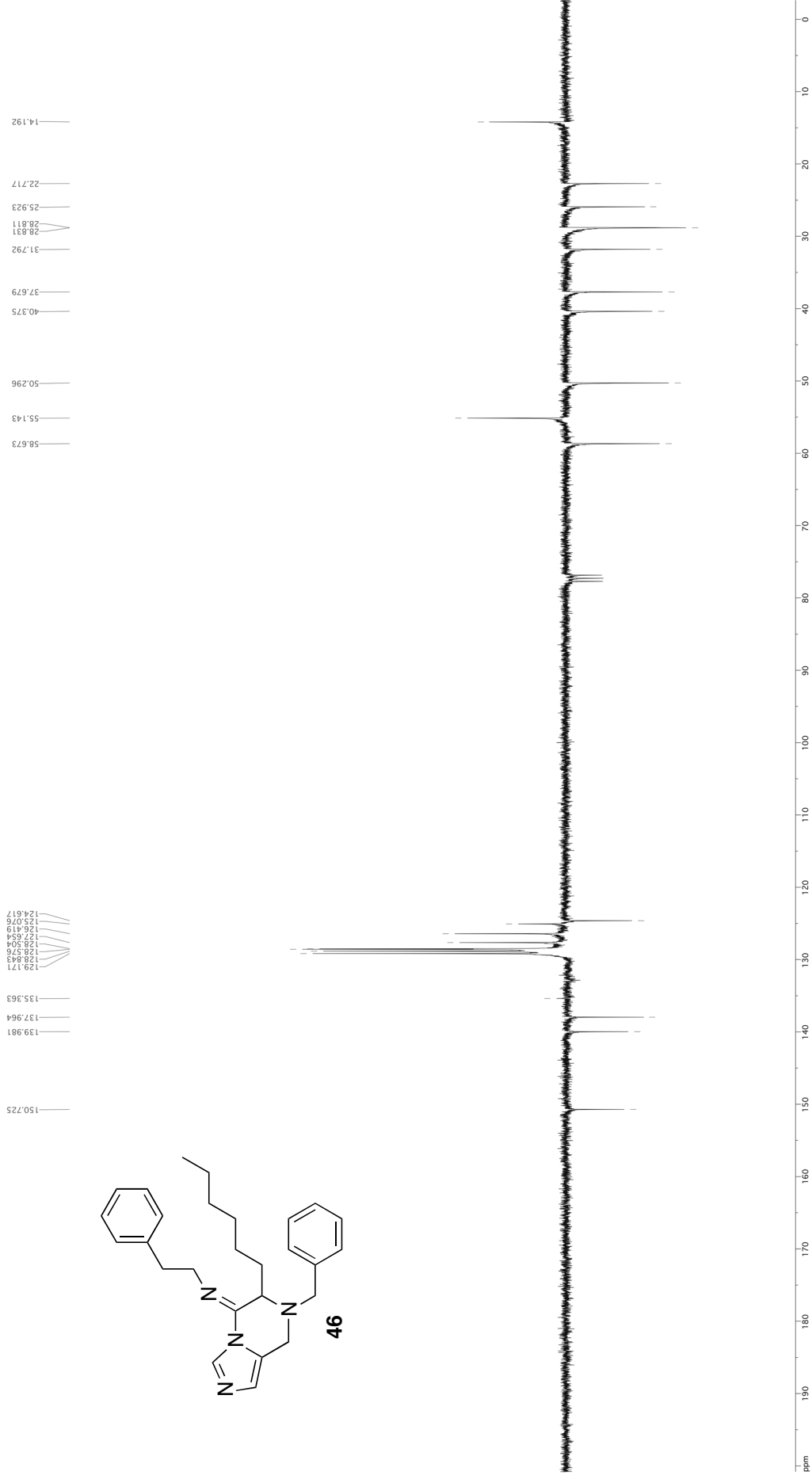
¹H NMR
300 MHz, CDCl₃

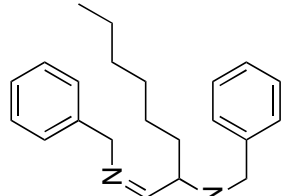


¹³C NMR
75 MHz, CDCl₃

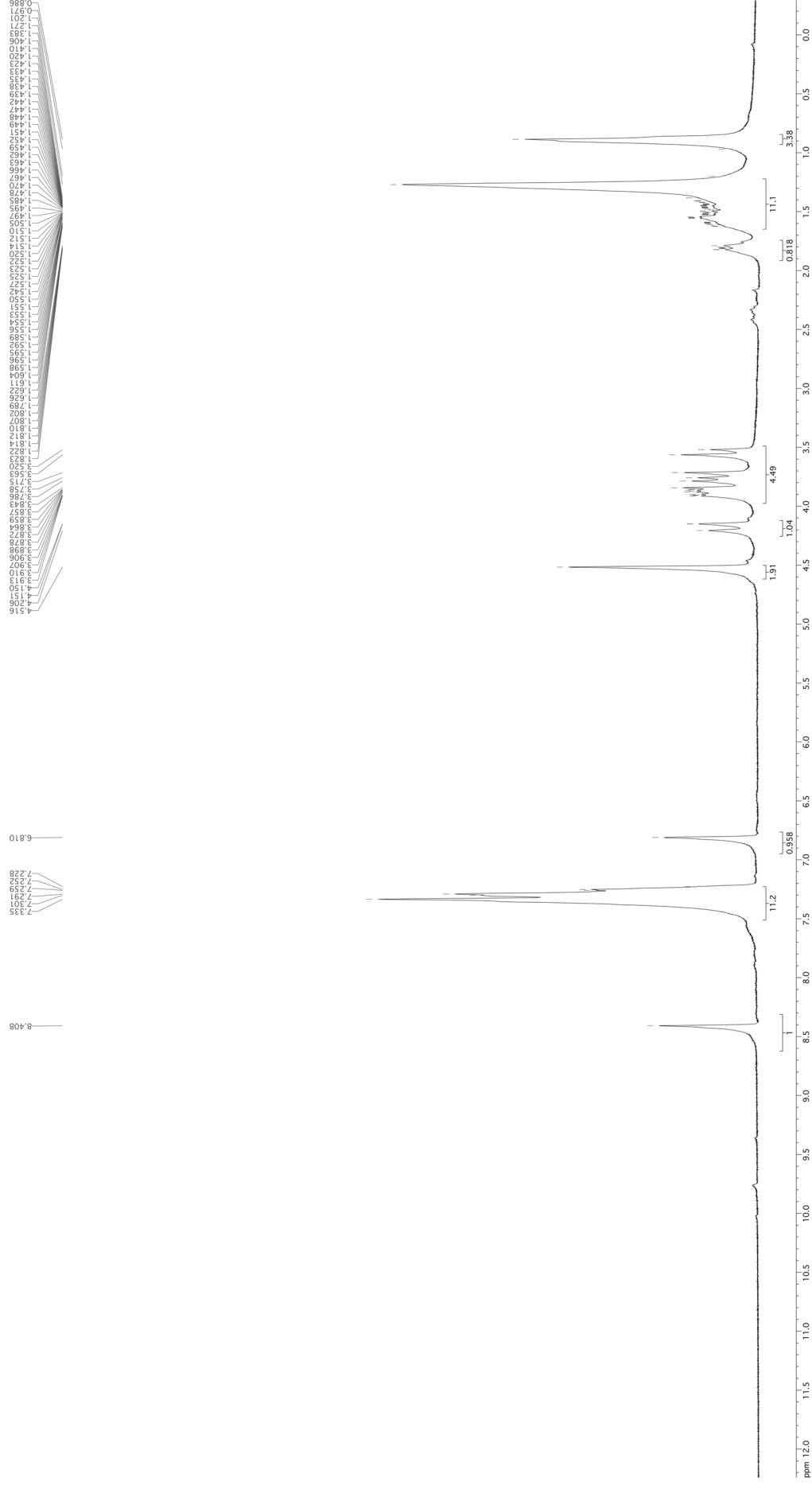


¹³C NMR
75 MHz, CDCl₃

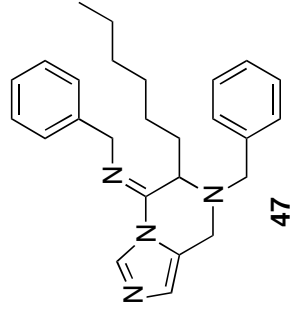




¹H NMR
300 MHz, CDCl₃

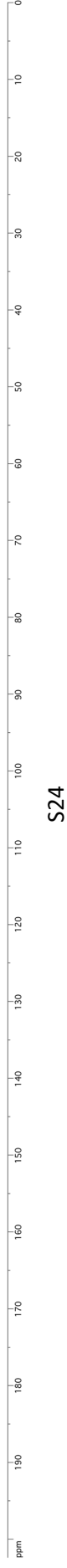


¹³C NMR
75 MHz, CDCl₃

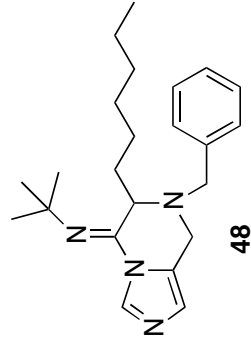


151.402
139.478
137.797
133.025
128.984
128.610
127.764
127.475
127.102
125.164
124.637

59.035
55.102
51.836
40.748
31.803
28.831
26.005
22.693
14.177



¹H NMR
300 MHz, CDCl₃



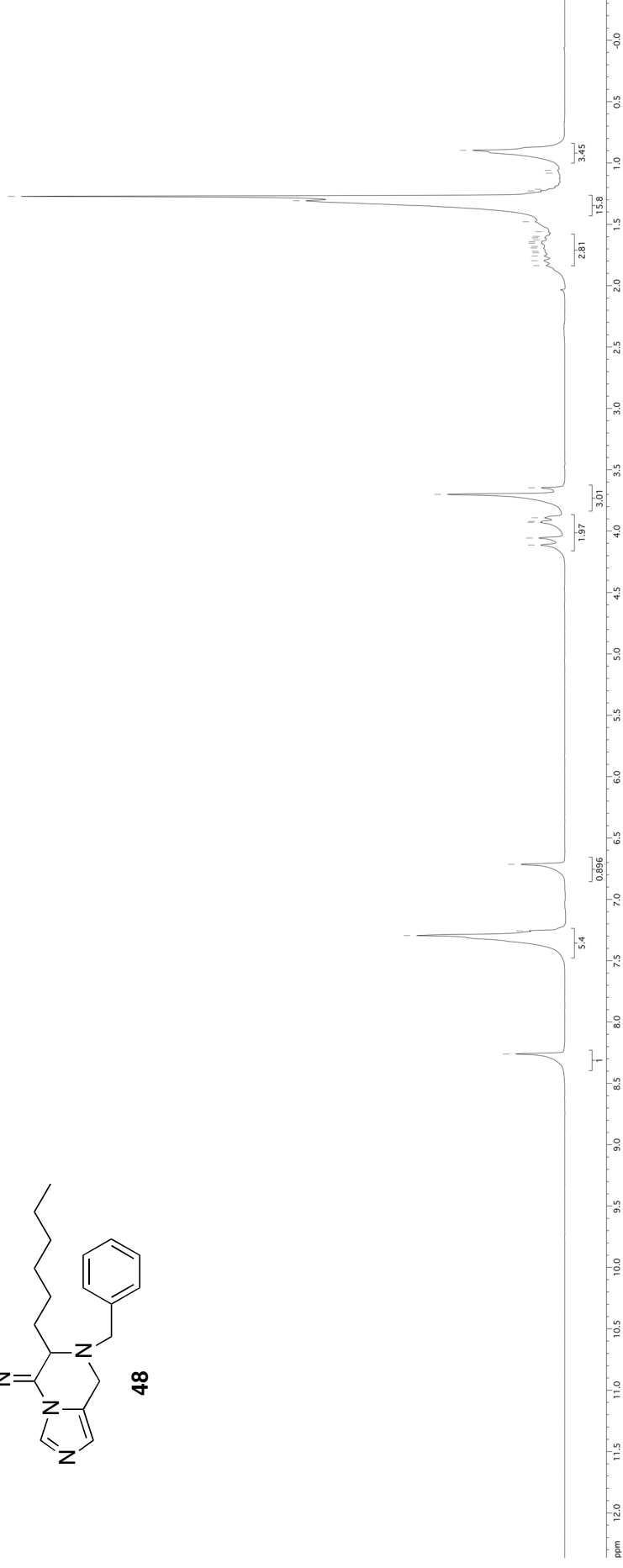
8.97
8.90
8.83
8.74
8.63
8.58
8.50
8.42
8.30
8.28
8.22
8.14
8.08
8.00
7.99
7.90
7.82
7.74
7.66
7.58
7.50
7.42
7.34
7.26
7.18
7.10
7.02
6.94
6.86
6.78
6.70
6.62
6.54
6.46
6.38
6.30
6.22
6.14
6.06
5.98
5.90
5.82
5.74
5.66
5.58
5.50
5.42
5.34
5.26
5.18
5.10
5.02
4.94
4.86
4.78
4.70
4.62
4.54
4.46
4.38
4.30
4.22
4.14
4.06
3.98
3.90
3.82
3.74
3.66
3.58
3.50
3.42
3.34
3.26
3.18
3.10
3.02
2.94
2.86
2.78
2.70
2.62
2.54
2.46
2.38
2.30
2.22
2.14
2.06
1.98
1.90
1.82
1.74
1.66
1.58
1.50
1.42
1.34
1.26
1.18
1.10
1.02
0.94
0.86
0.78
0.70
0.62
0.54
0.46
0.38
0.30
0.22
0.14
0.06
0.897

4.113
4.056
3.920
3.891
3.700
3.647

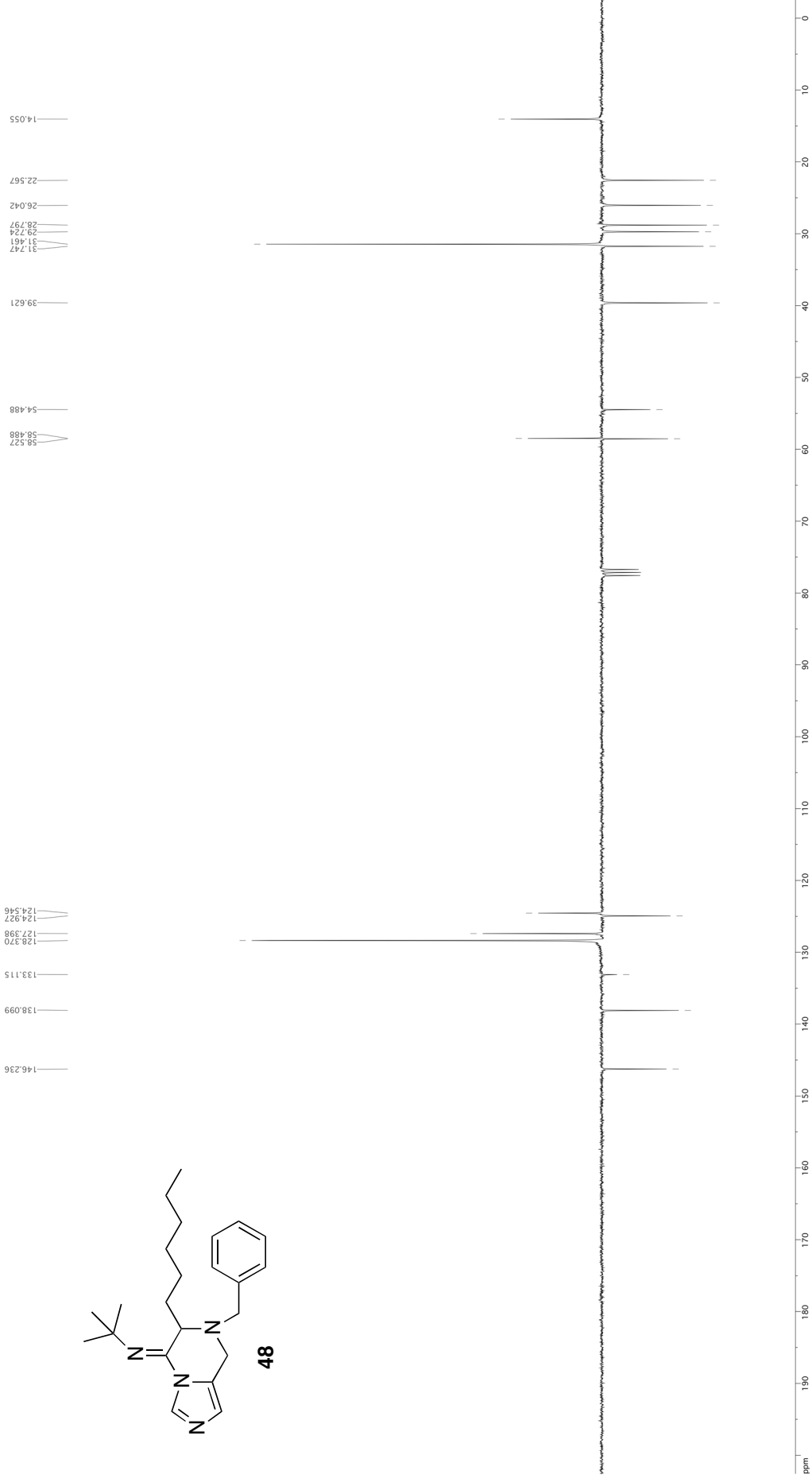
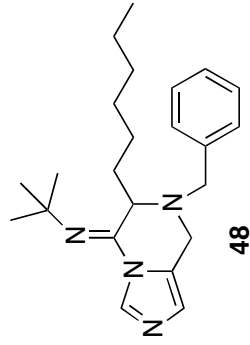
6.715

7.295
7.257

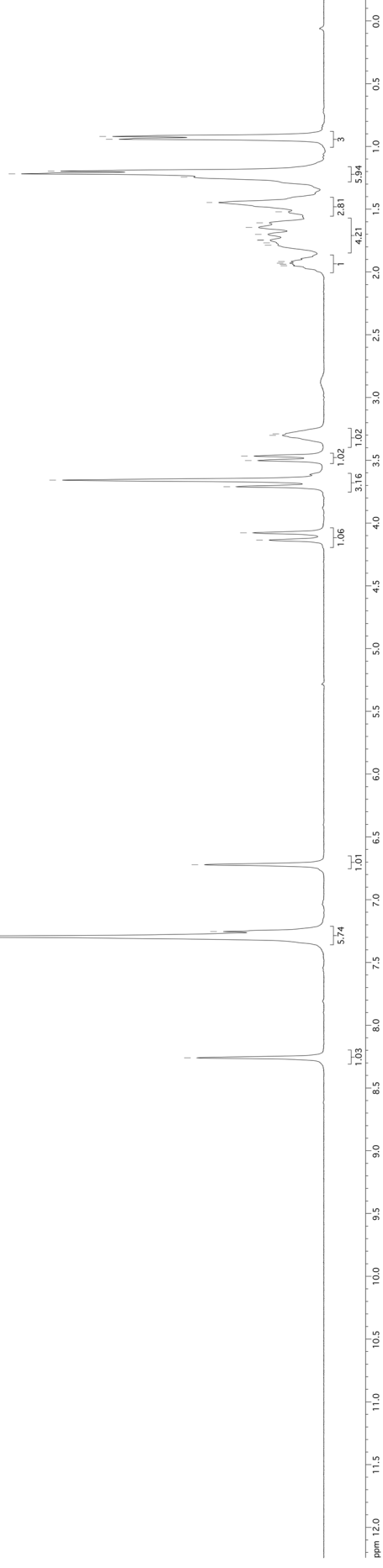
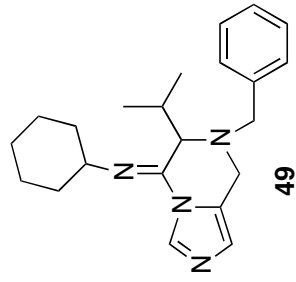
8.260

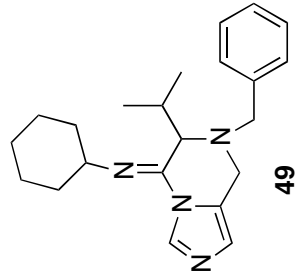


^{13}C NMR
75 MHz, CDCl_3



¹H NMR
300 MHz, CDCl₃





¹³C NMR
75 MHz, CDCl₃

146.612
138.237
132.924
128.512
127.553
125.313
124.522

62.473
58.993
57.405

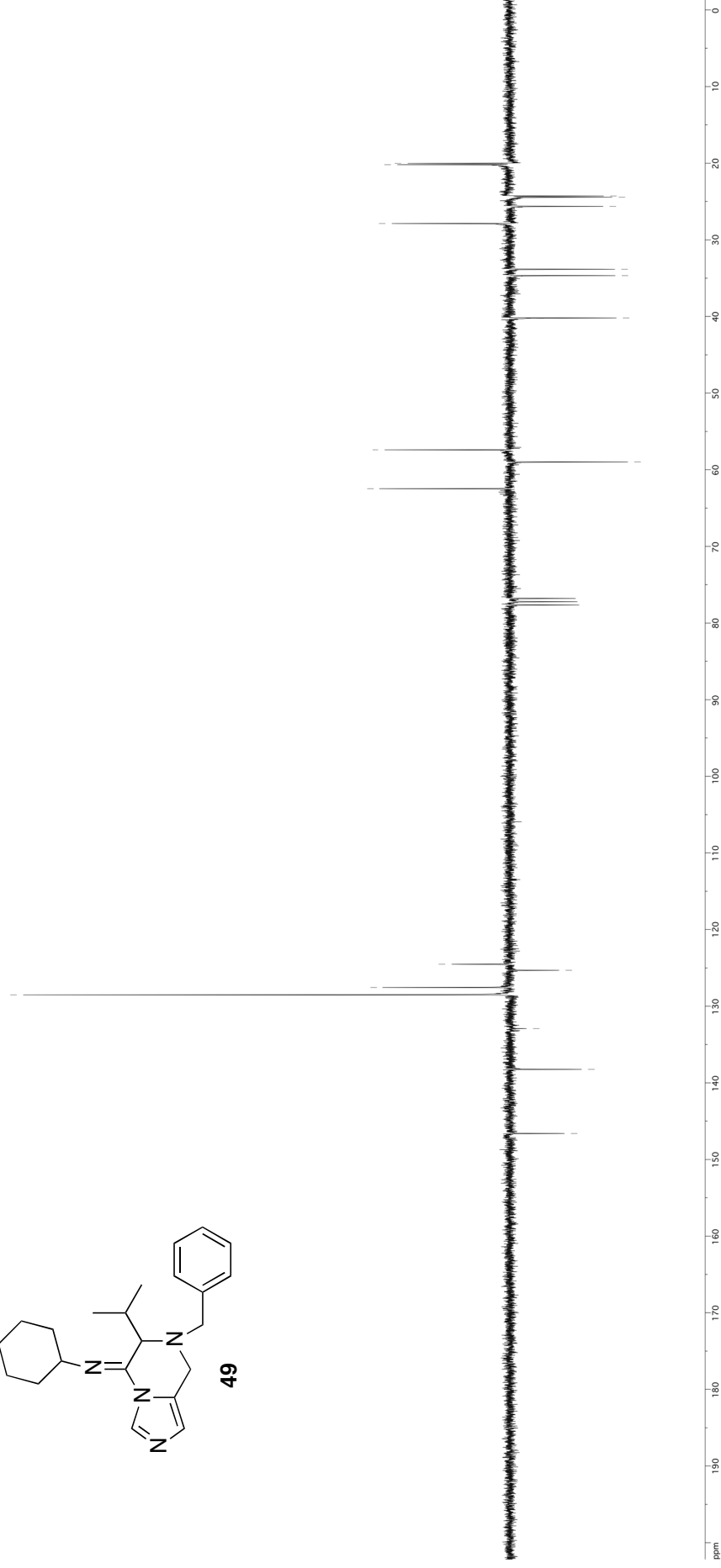
40.252
40.192

34.853
33.838

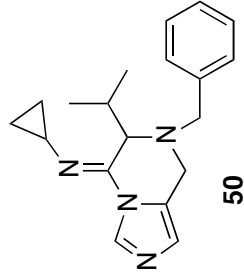
27.872

25.629
24.436
24.275

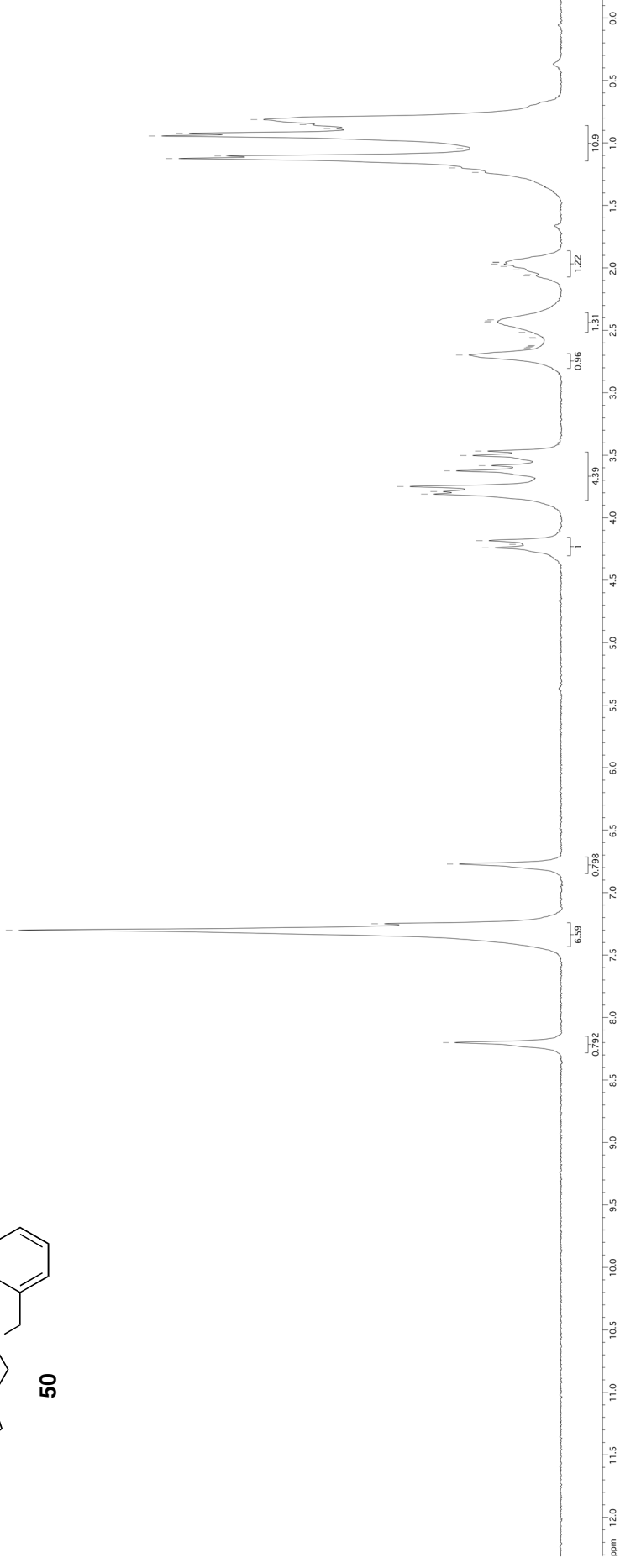
20.187
20.022



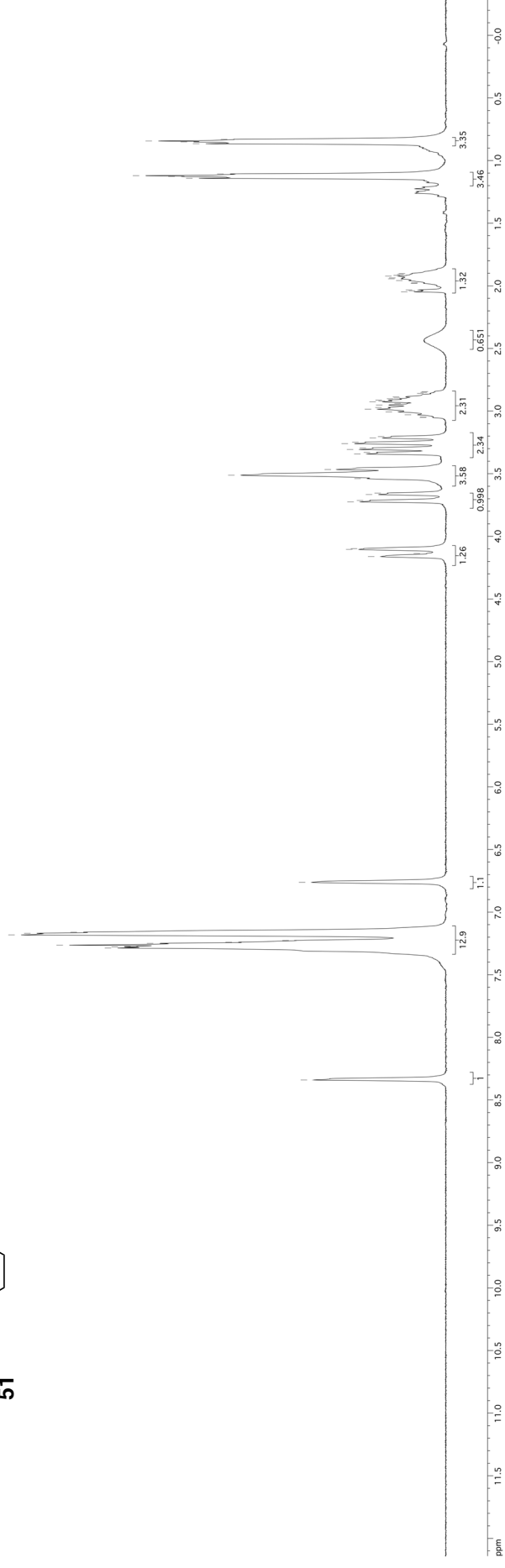
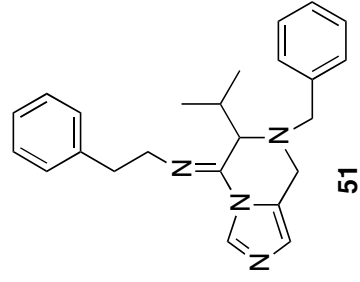
¹H NMR
300 MHz, CDCl₃



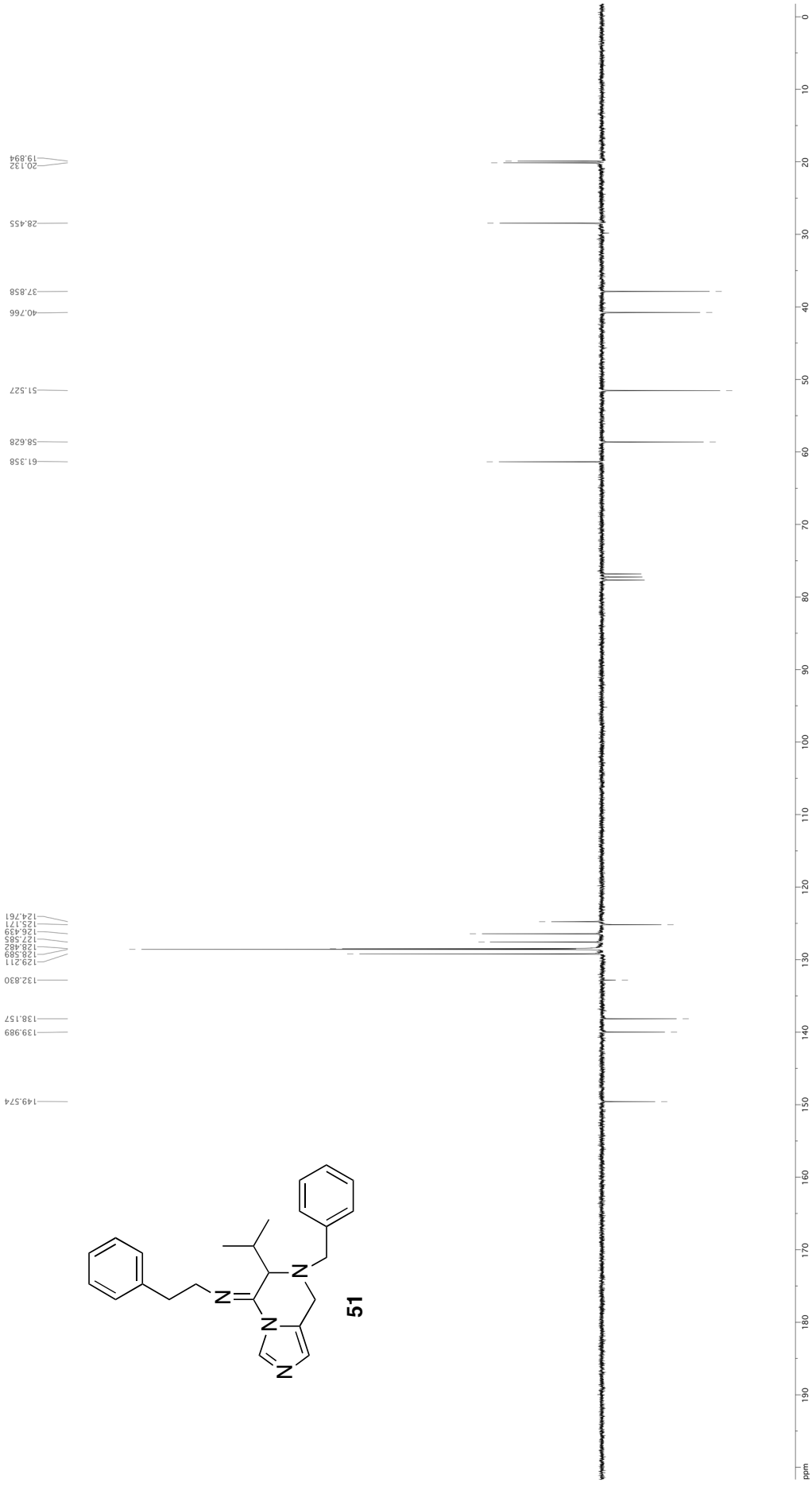
8.200
7.300
7.249
6.771
4.240
4.214
4.183
3.810
3.791
3.749
3.625
3.582
3.502
3.467
2.698
2.681
2.634
2.627
2.583
2.558
2.516
2.425
2.416
2.064
2.055
2.017
1.988
1.970
1.958
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1.045
0.944
0.923
0.885
0.854
0.813



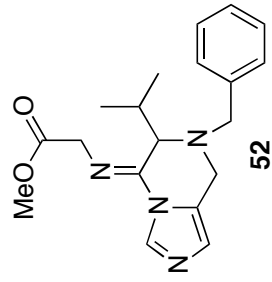
¹H NMR
300 MHz, CDCl₃

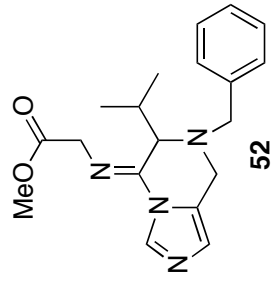


¹³C NMR
75 MHz, CDCl₃

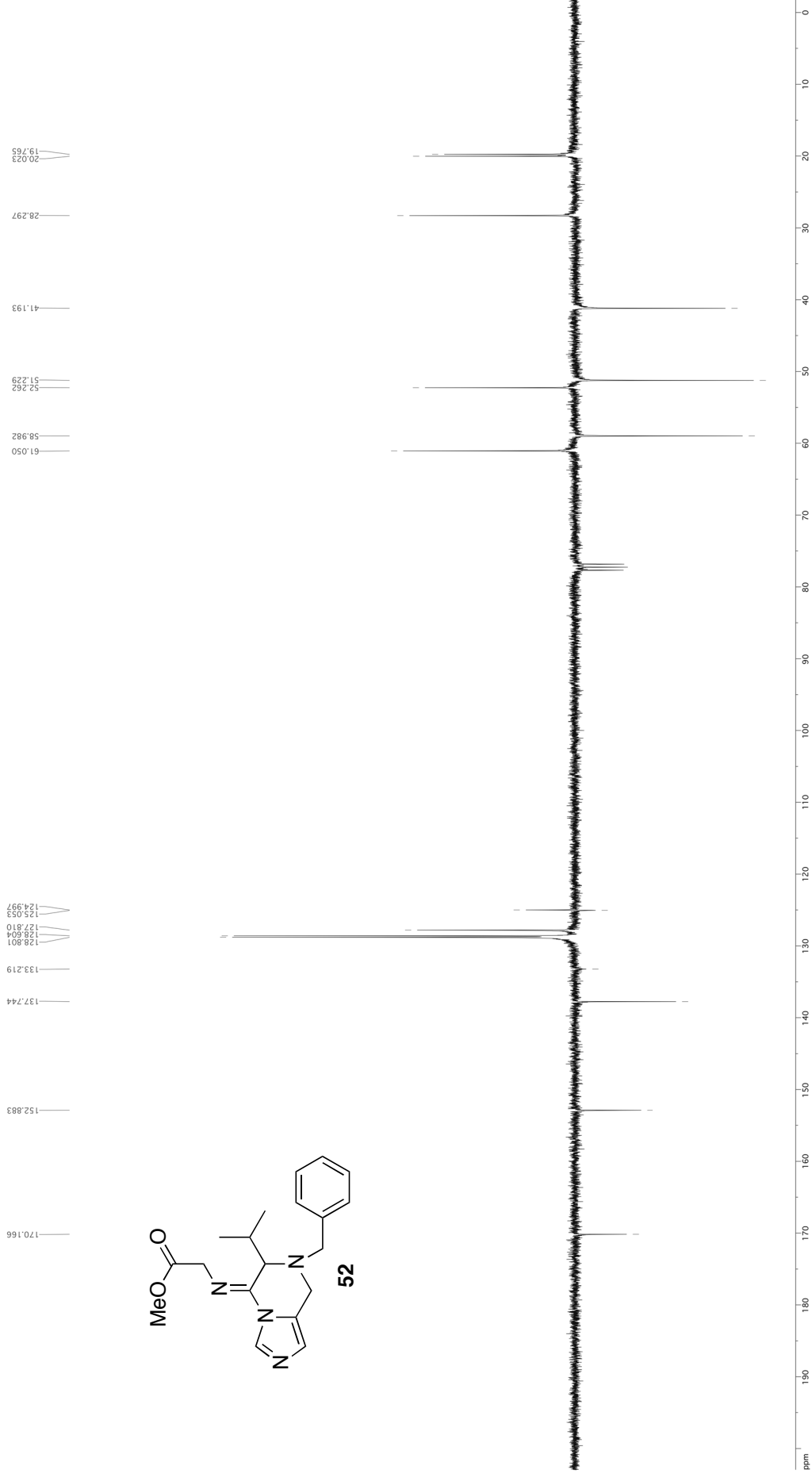


¹H NMR
300 MHz, CDCl₃

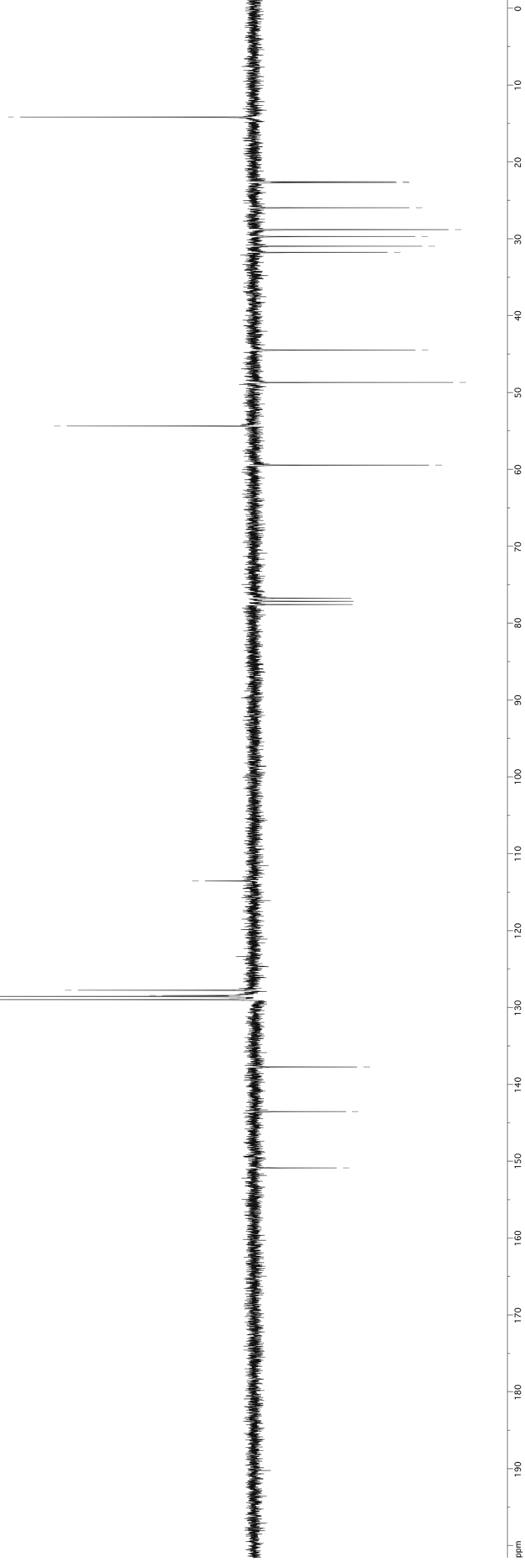
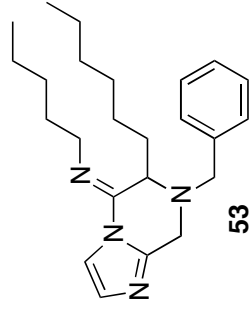




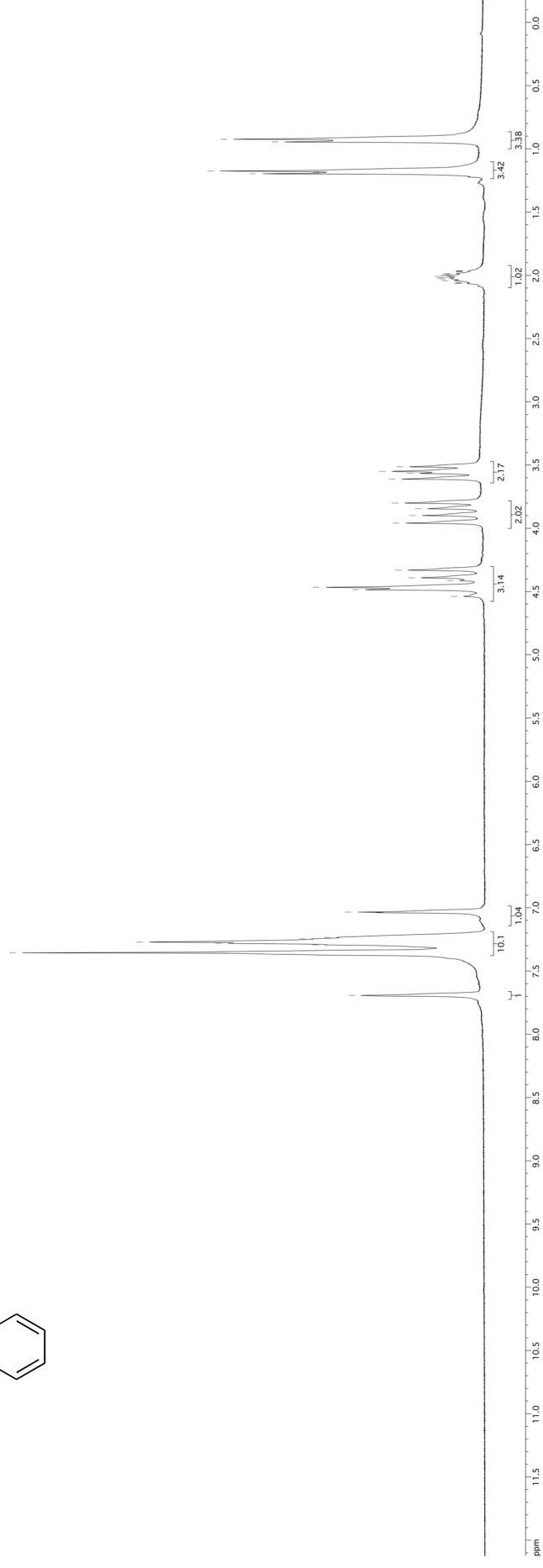
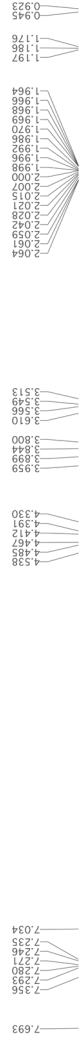
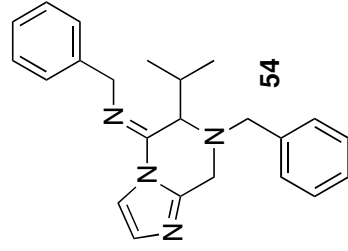
¹³C NMR
75 MHz, CDCl₃



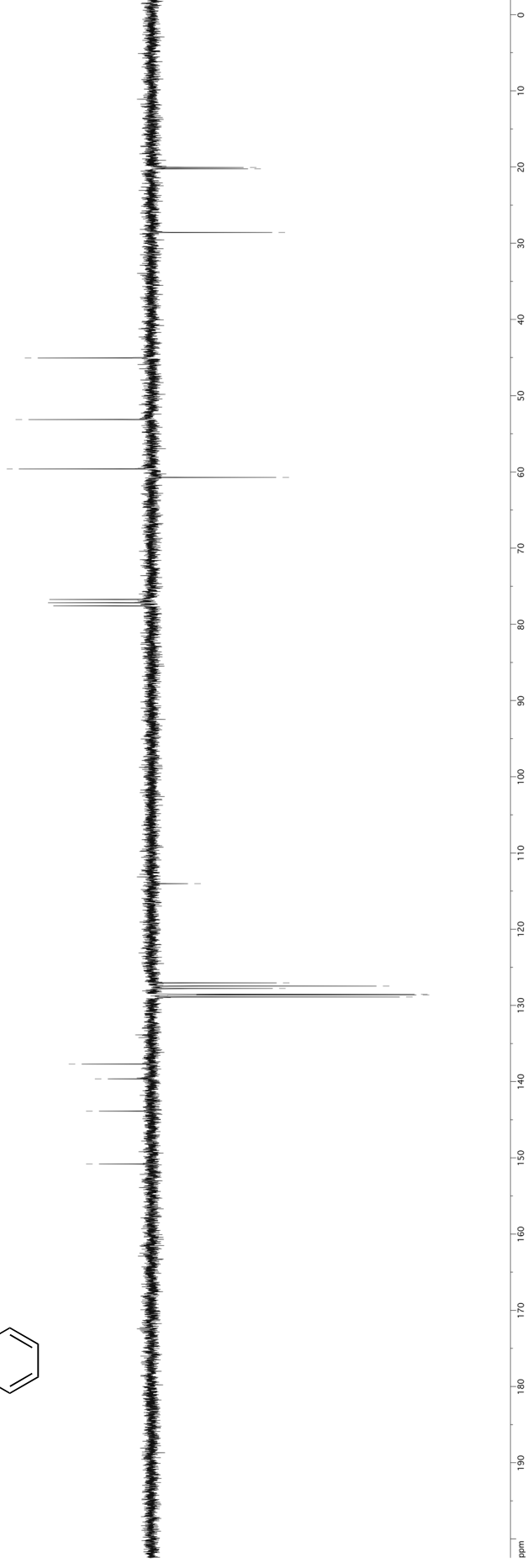
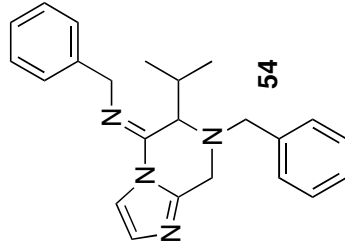
¹³C NMR
75 MHz, CDCl₃



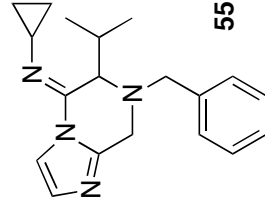
¹H NMR
300 MHz, CDCl₃



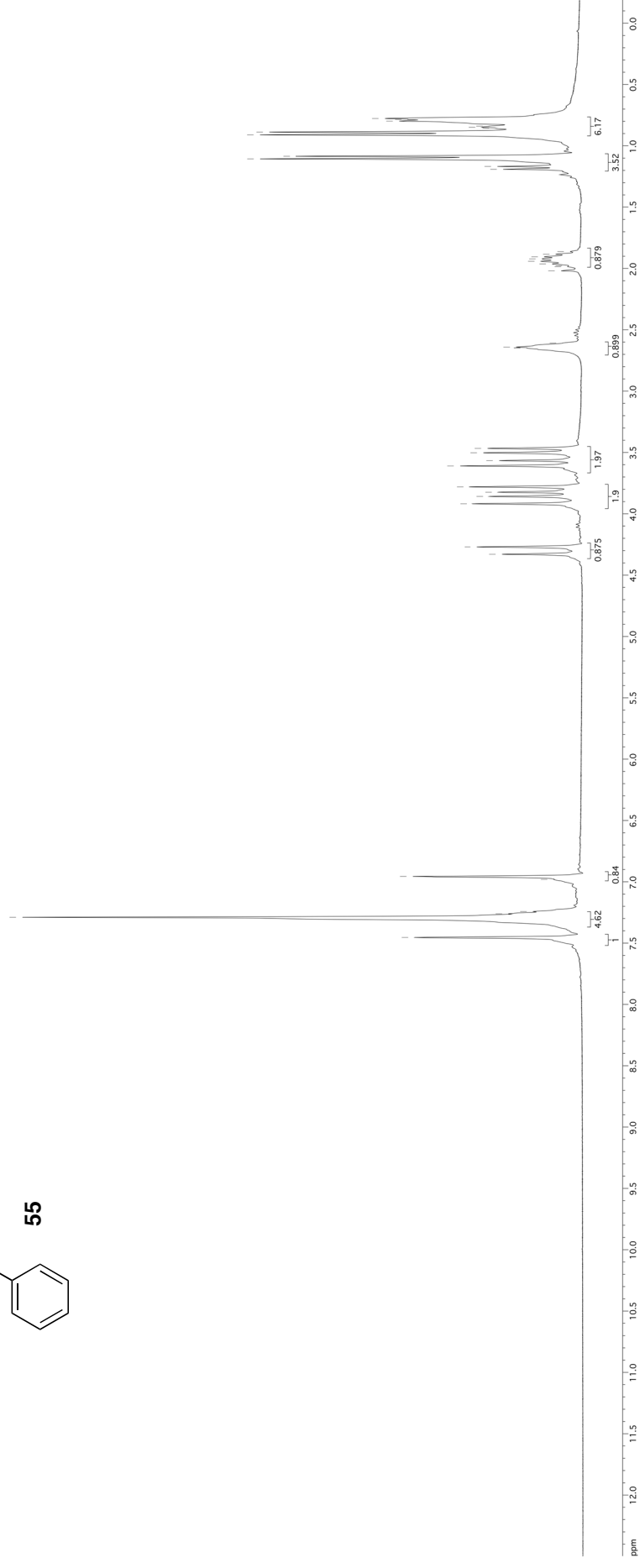
¹³C NMR
75 MHz, CDCl₃



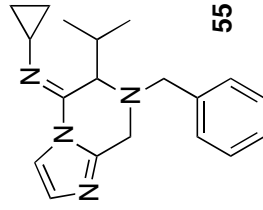
¹H NMR
300 MHz, CDCl₃



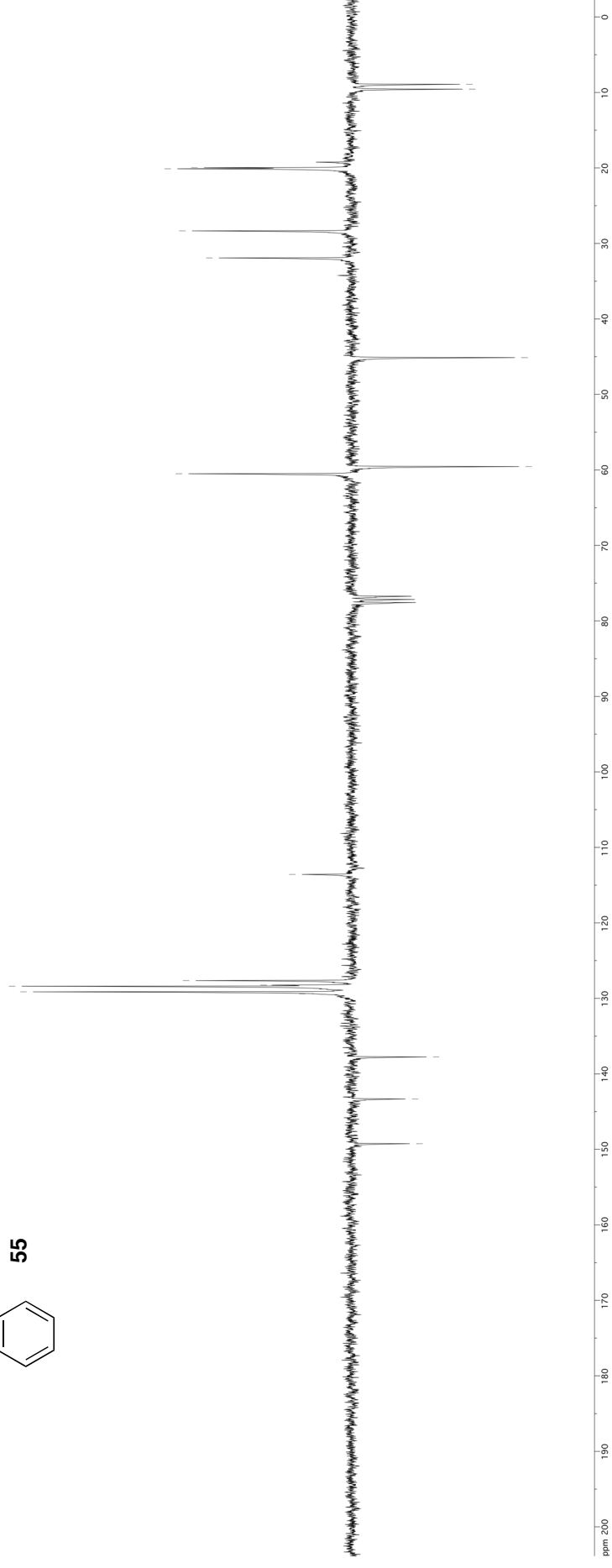
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7.290
7.243
6.981
6.956
4.330
4.270
3.918
3.859
3.824
3.781
3.610
3.567
3.503
3.467
2.648
2.647
2.640
2.608
2.018
1.977
1.984
1.963
1.941
1.921
1.905
1.883
1.861
1.191
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1.108
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0.856
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0.777



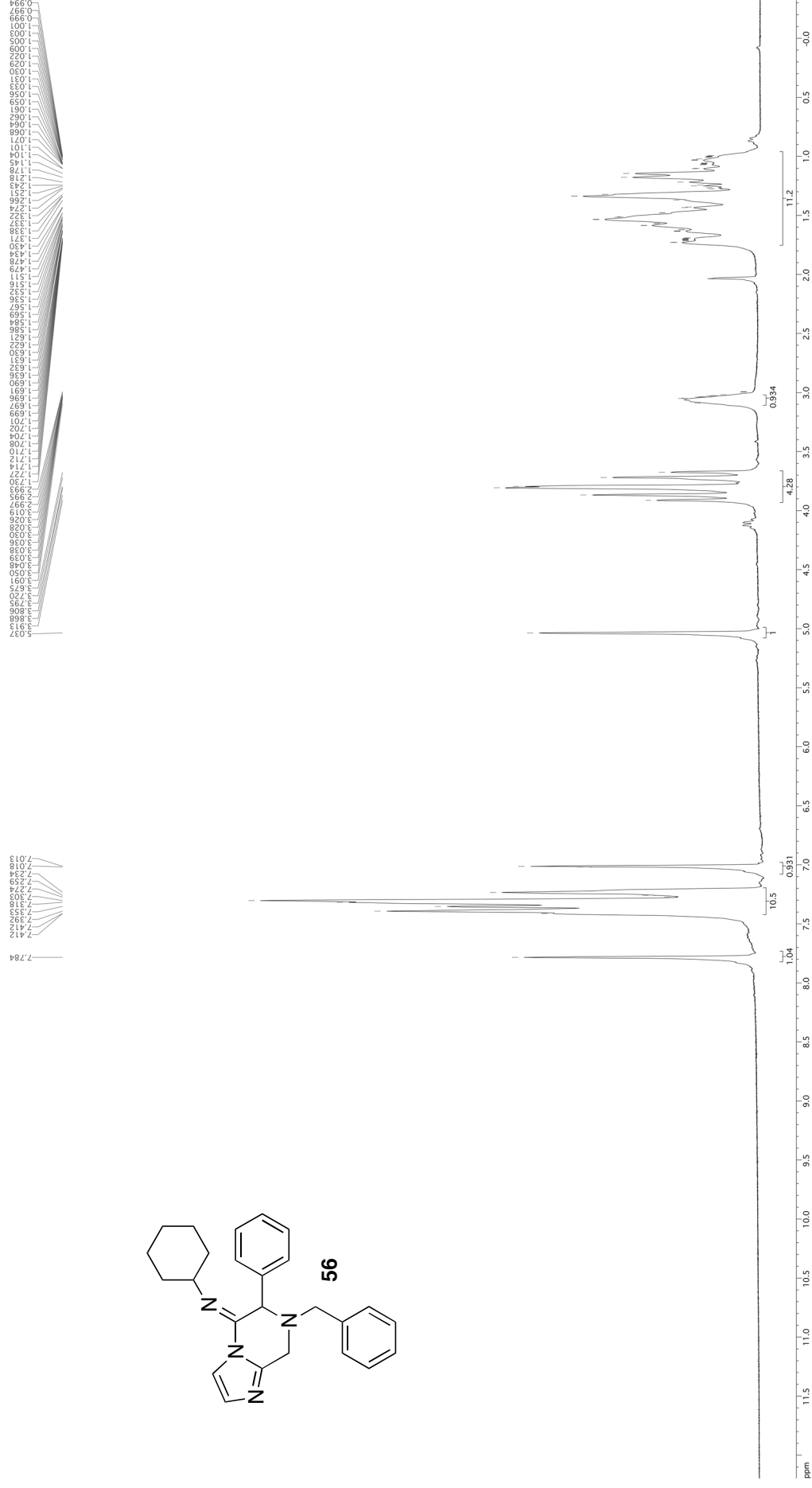
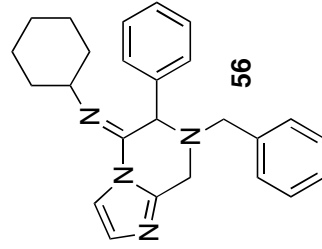
¹³C NMR
75 MHz, CDCl₃



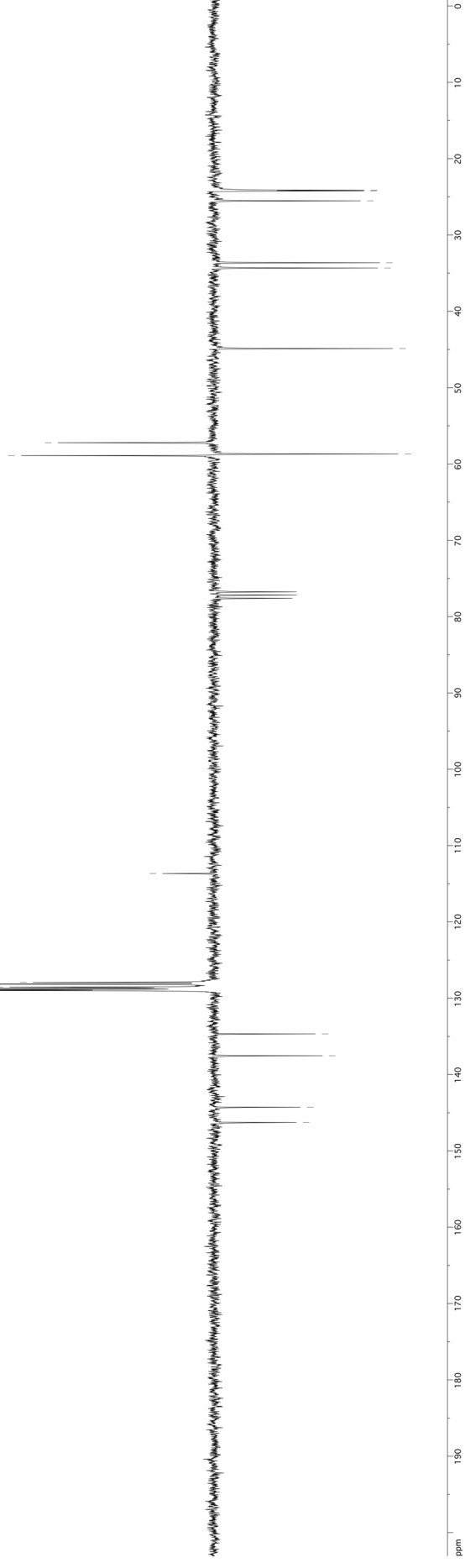
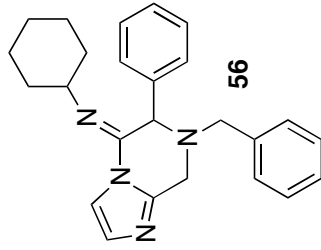
149.252
143.321
137.755
129.392
129.133
128.986
128.739
127.639
113.574
60.510
59.561
45.119
31.926
28.341
20.107
19.963
9.568
8.934

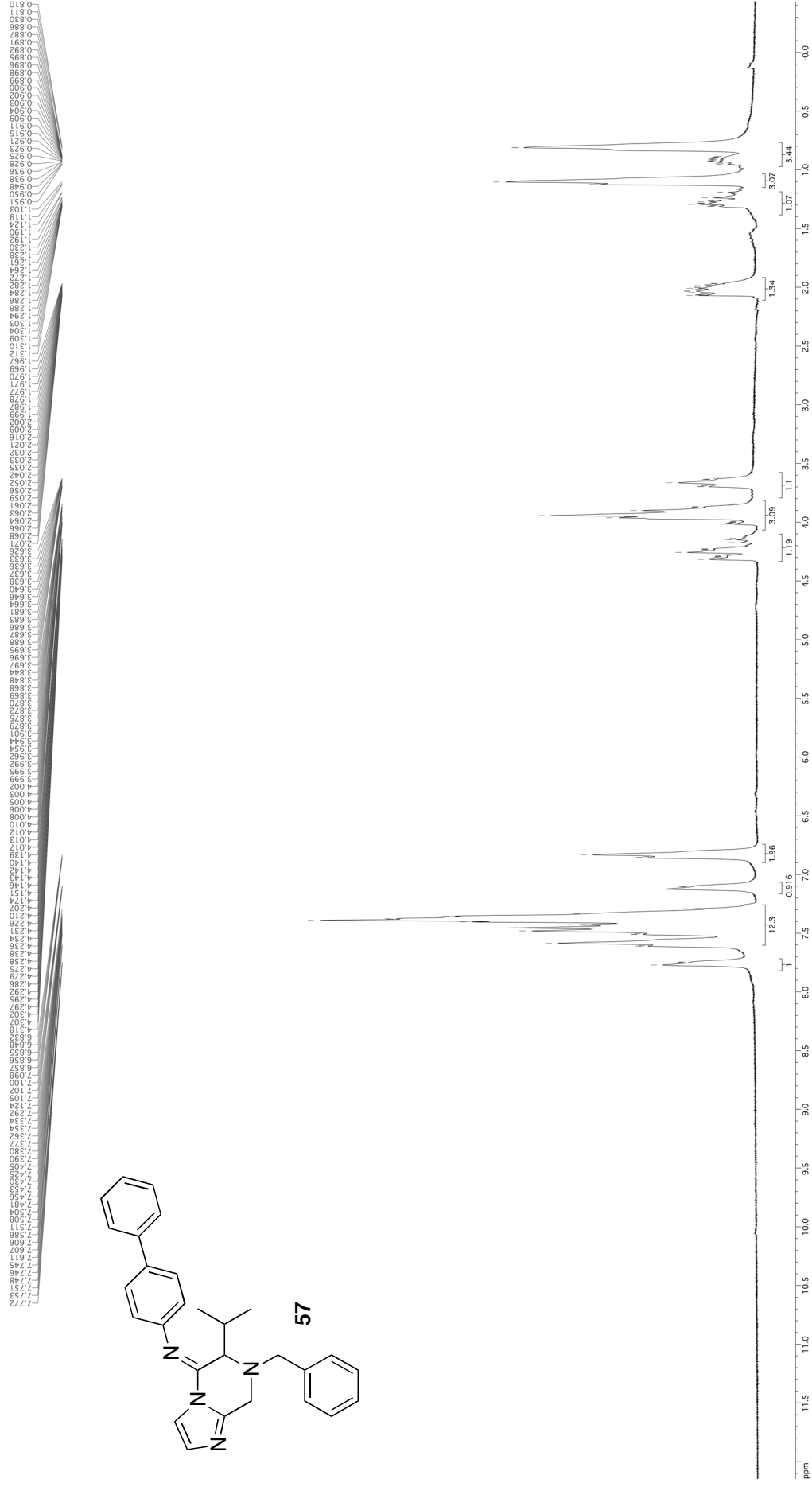


¹H NMR
300 MHz, CDCl₃

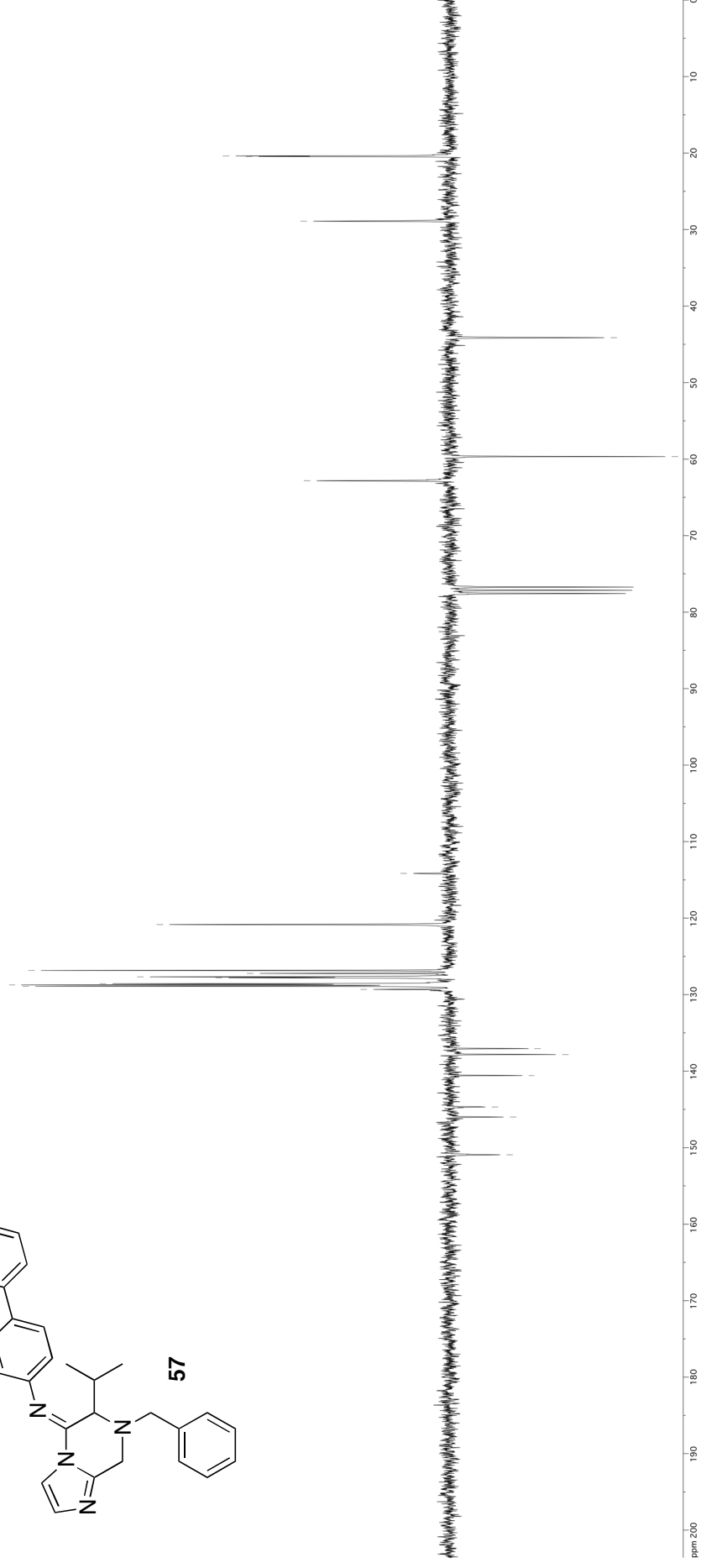
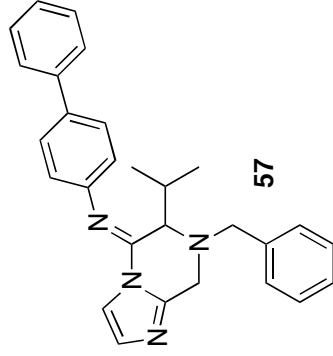


¹³C NMR
75 MHz, CDCl₃

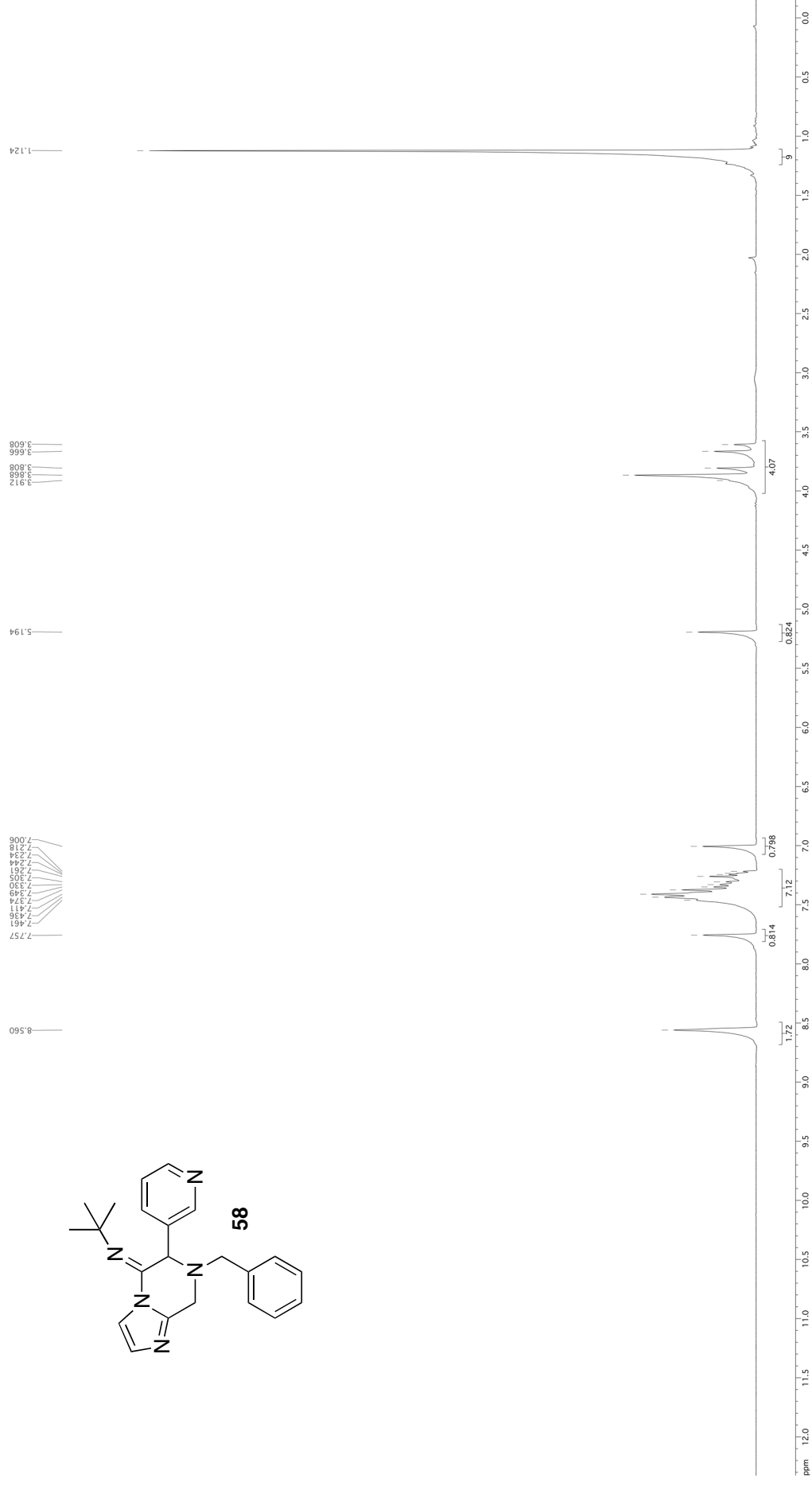
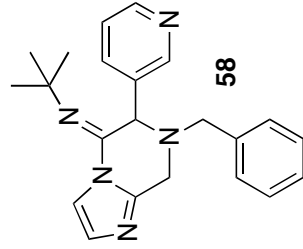


¹H NMR
300 MHz, CDCl₃

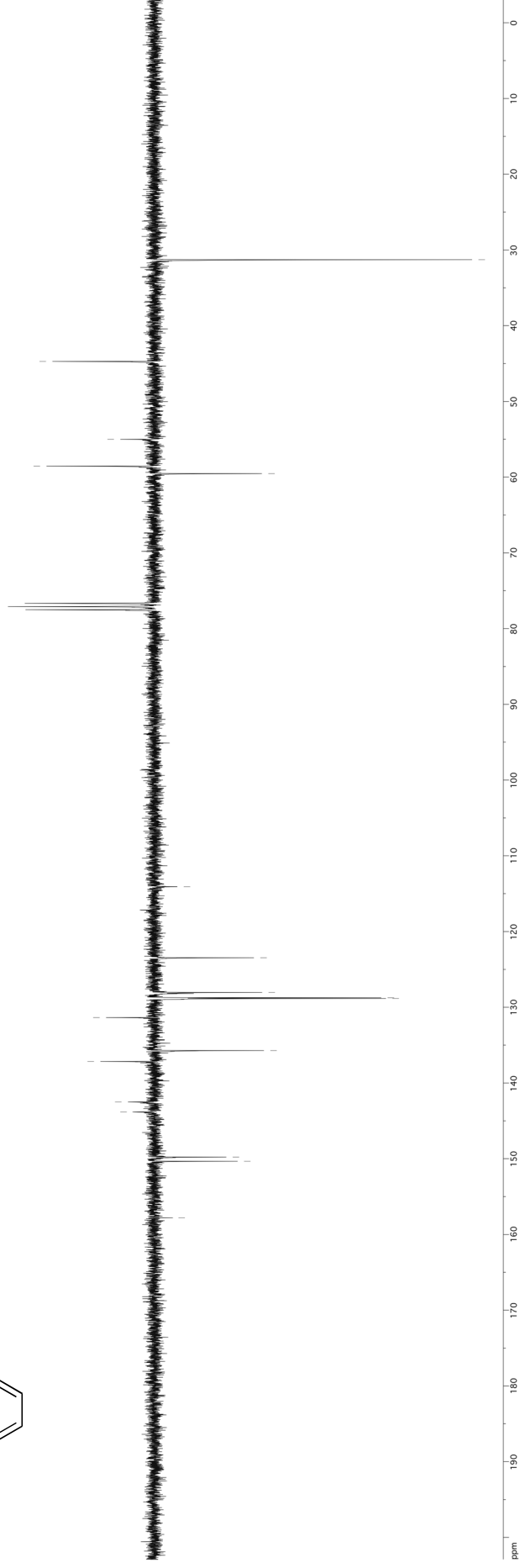
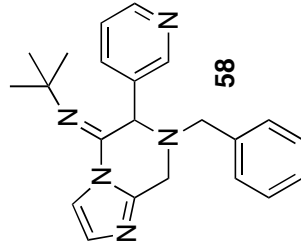
¹³C NMR
75 MHz, CDCl₃



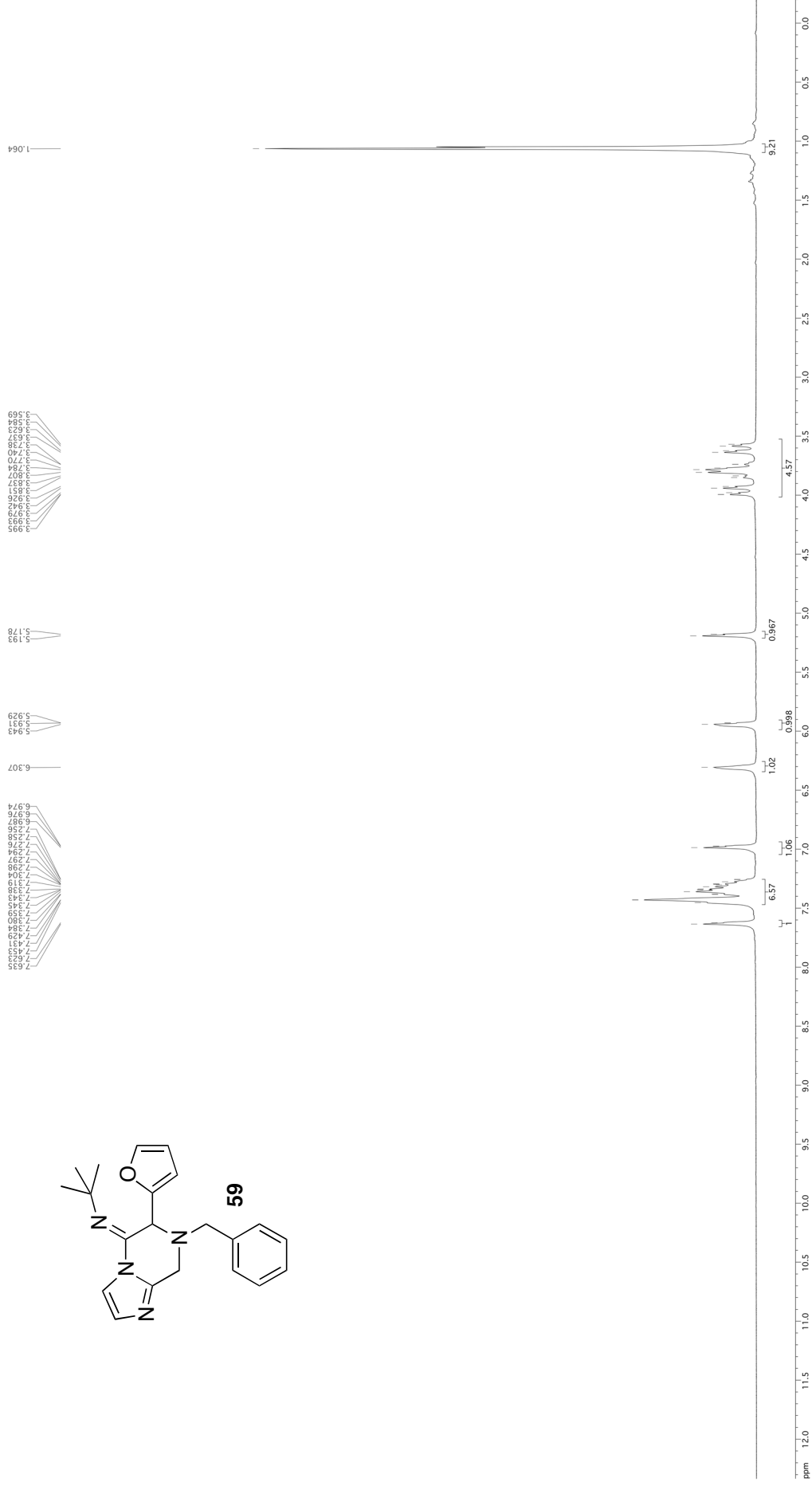
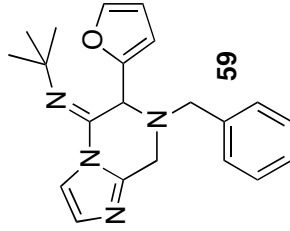
¹H NMR
300 MHz, CDCl₃



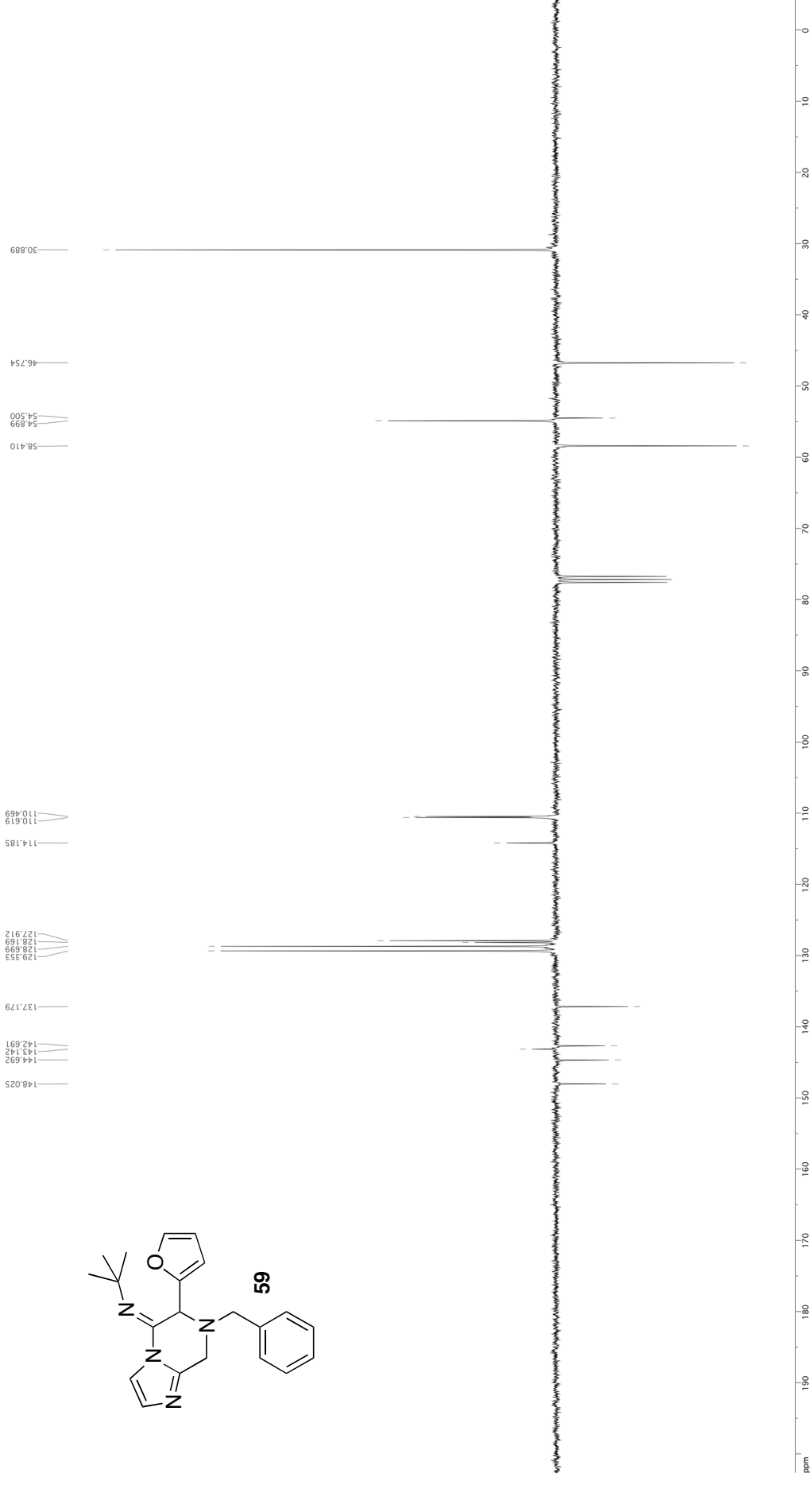
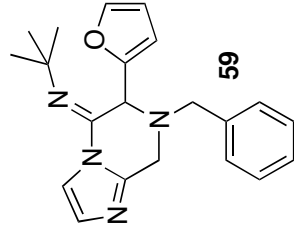
¹³C NMR
75 MHz, CDCl₃



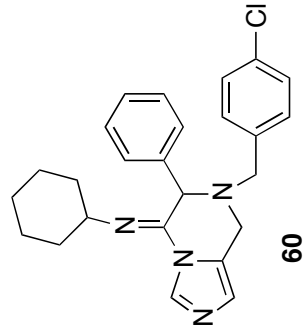
¹H NMR
300 MHz, CDCl₃



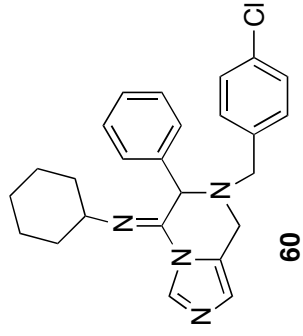
¹³C NMR
75 MHz, CDCl₃



¹H NMR
300 MHz, CDCl₃



¹³C NMR
75 MHz, CDCl₃

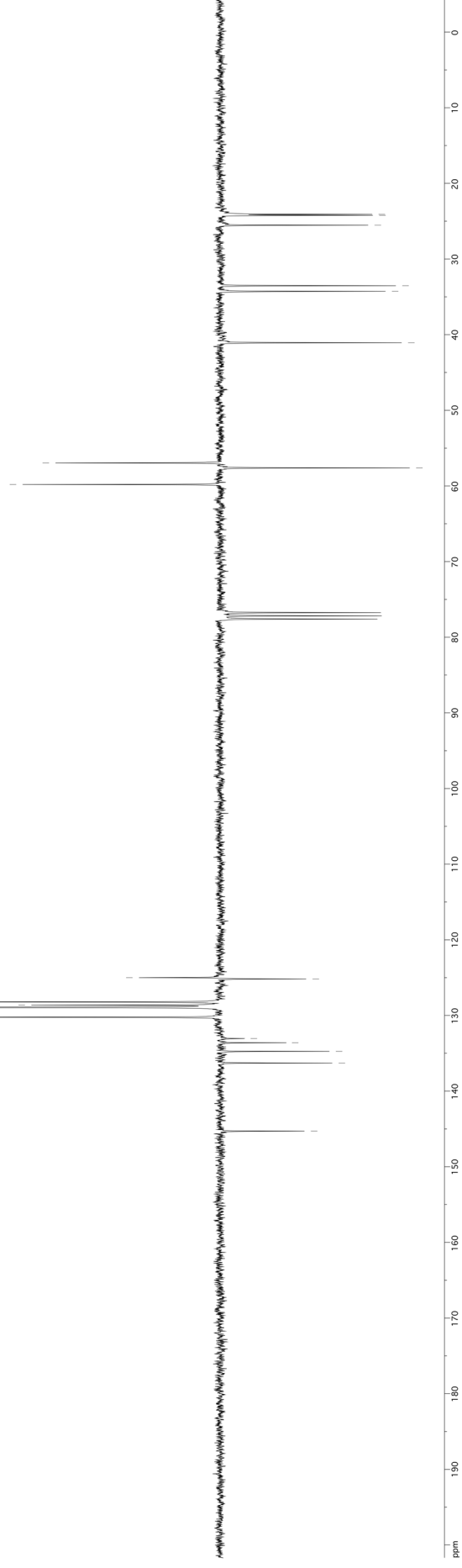


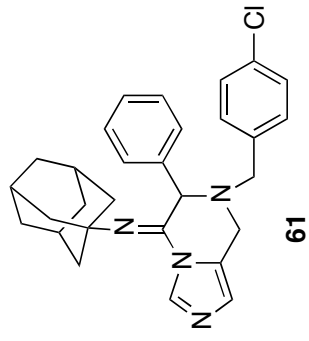
145.295
136.284
134.747
133.614
133.050
130.232
128.855
128.894
128.640
128.213
125.164
124.997

59.810
57.614
56.955

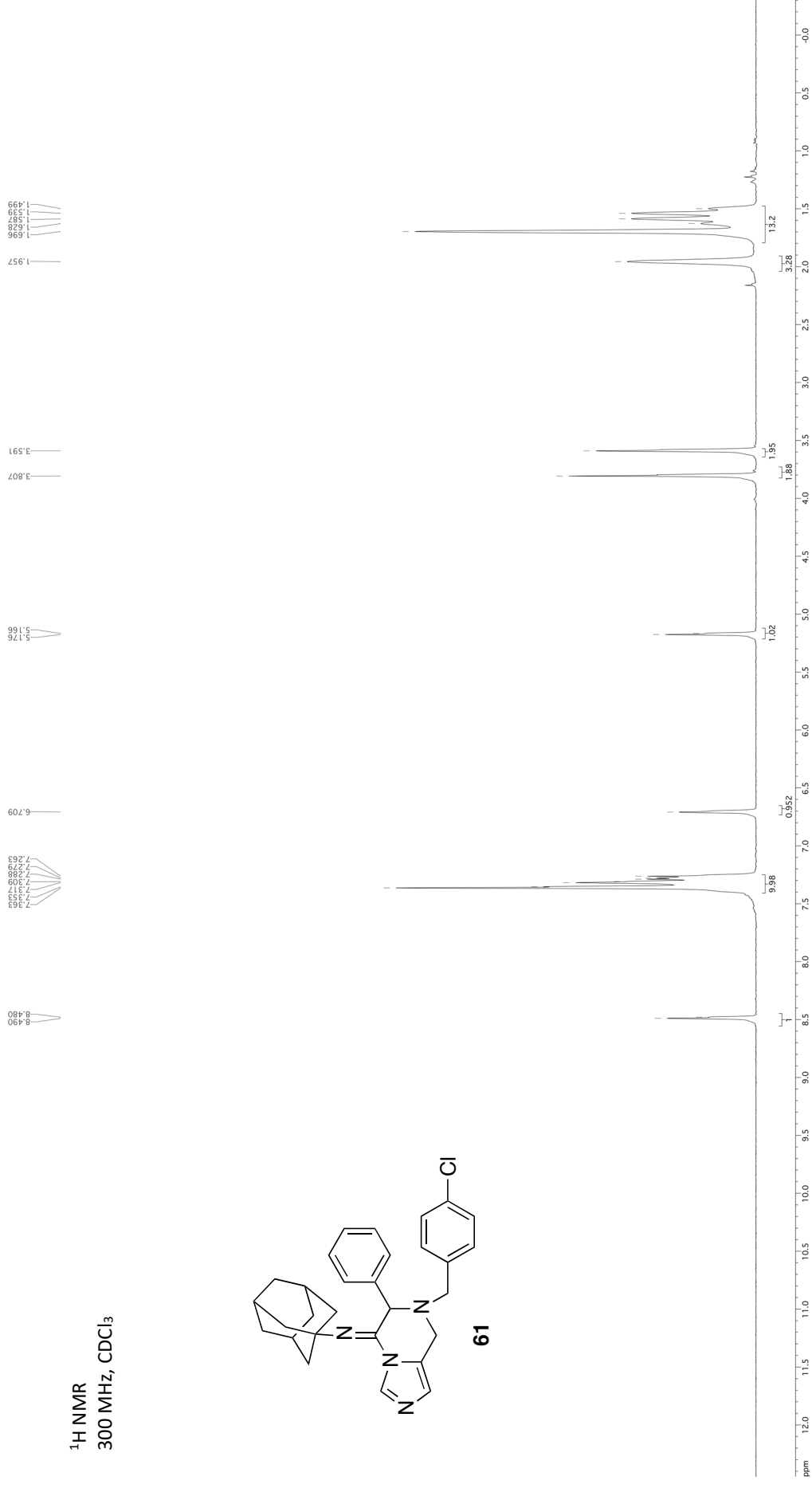
41.067
34.284
33.530

25.535
24.228
24.090

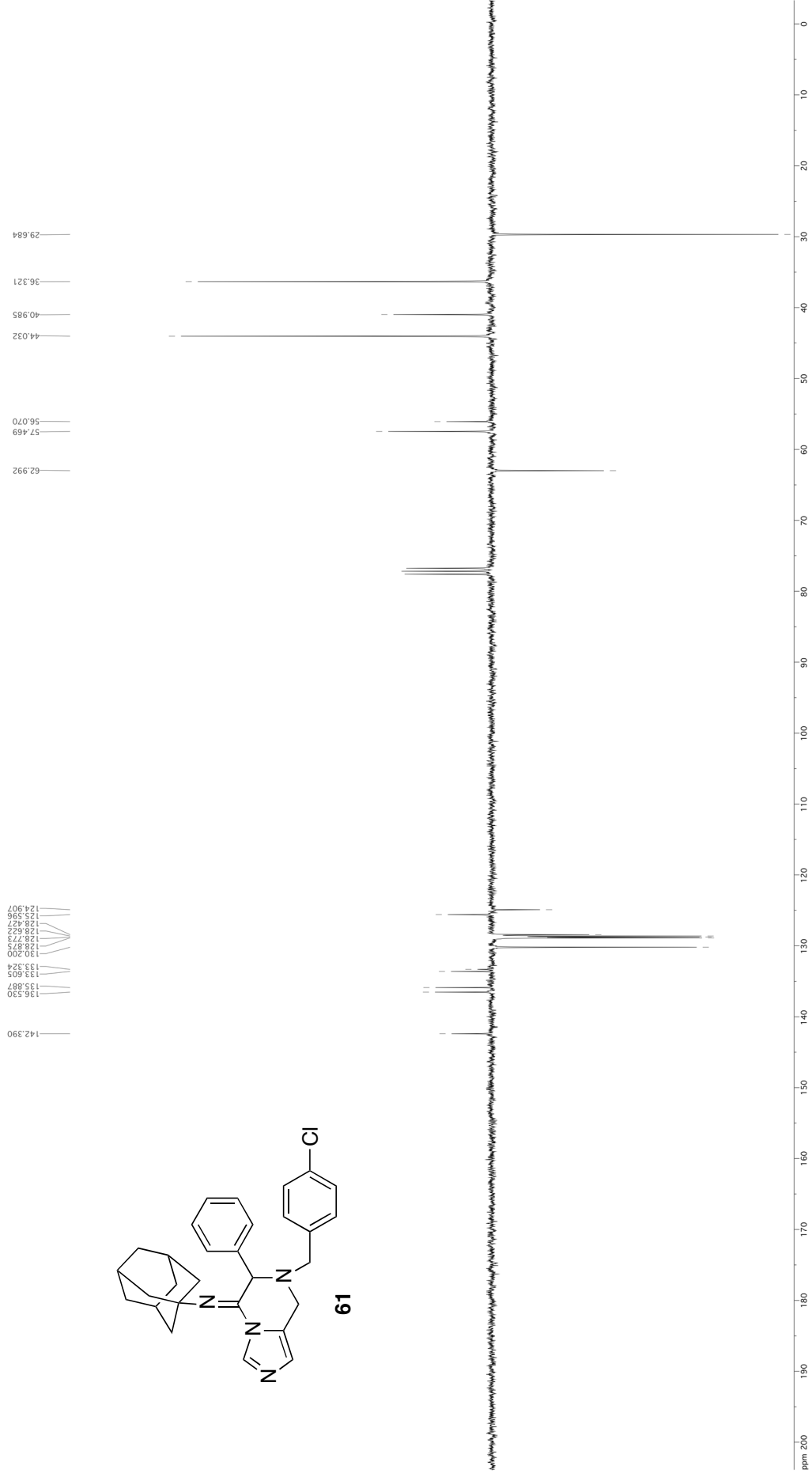
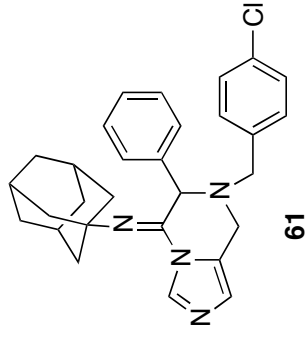




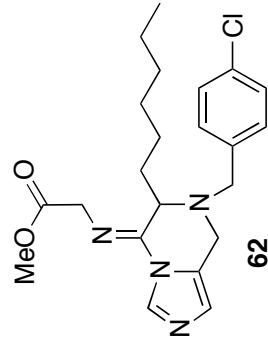
¹H NMR
300 MHz, CDCl₃



¹³C NMR
75 MHz, CDCl₃



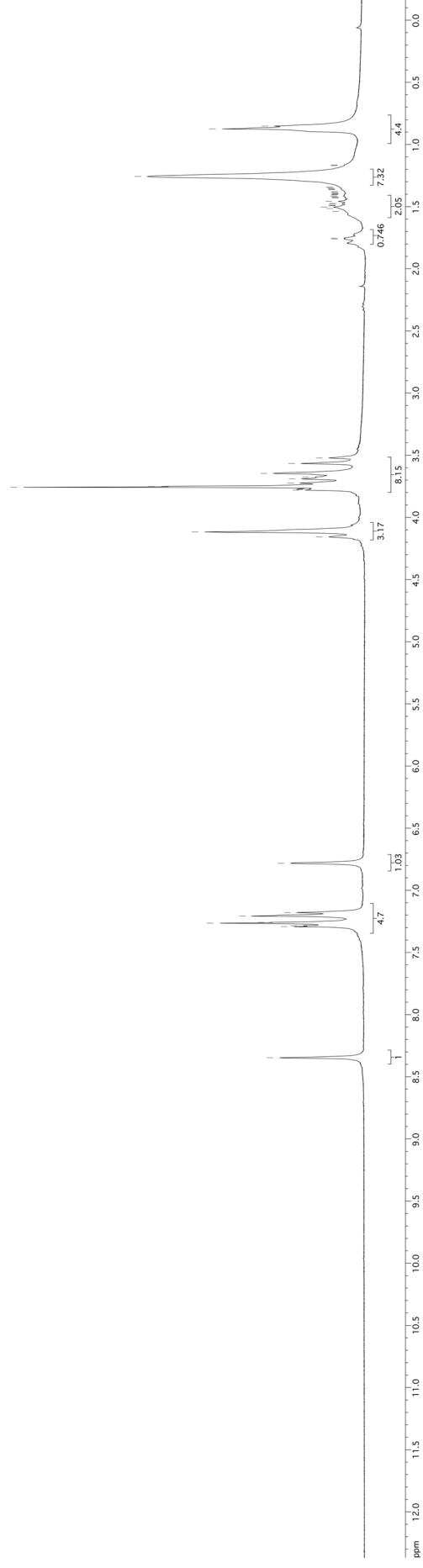
¹H NMR
300 MHz, CDCl₃



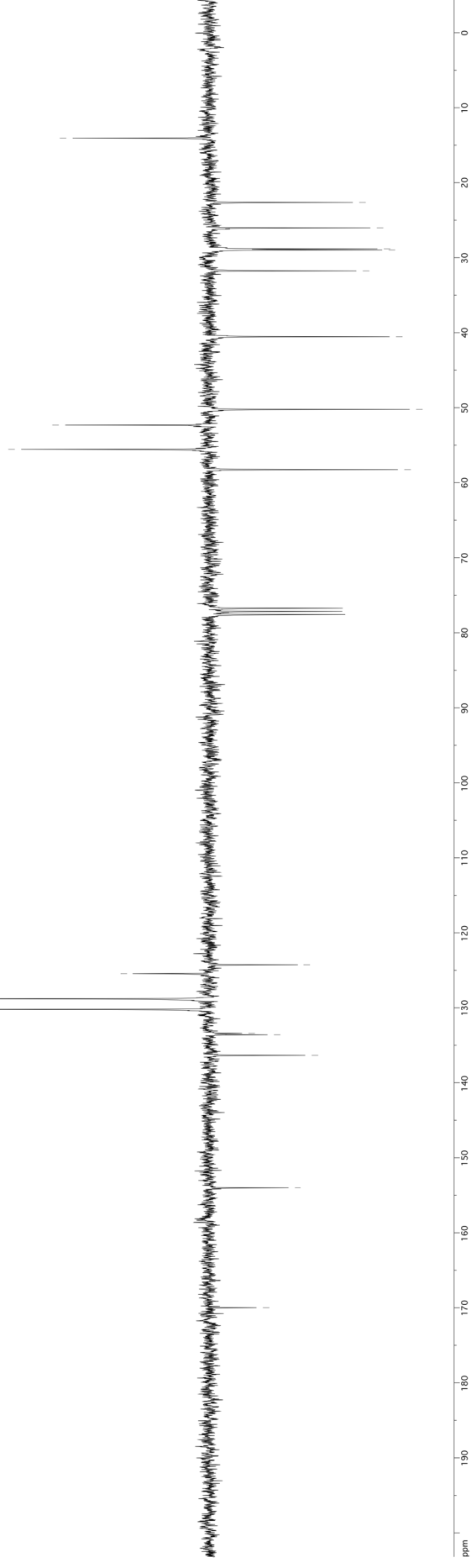
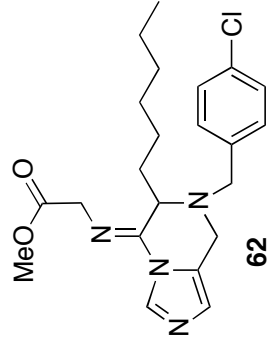
8.347
7.292
7.286
7.264
7.259
7.208
7.179

4.156
4.117
3.780
3.776
3.775
3.771
3.768
3.757
3.751
3.724
3.691
3.677
3.646
3.567
3.522

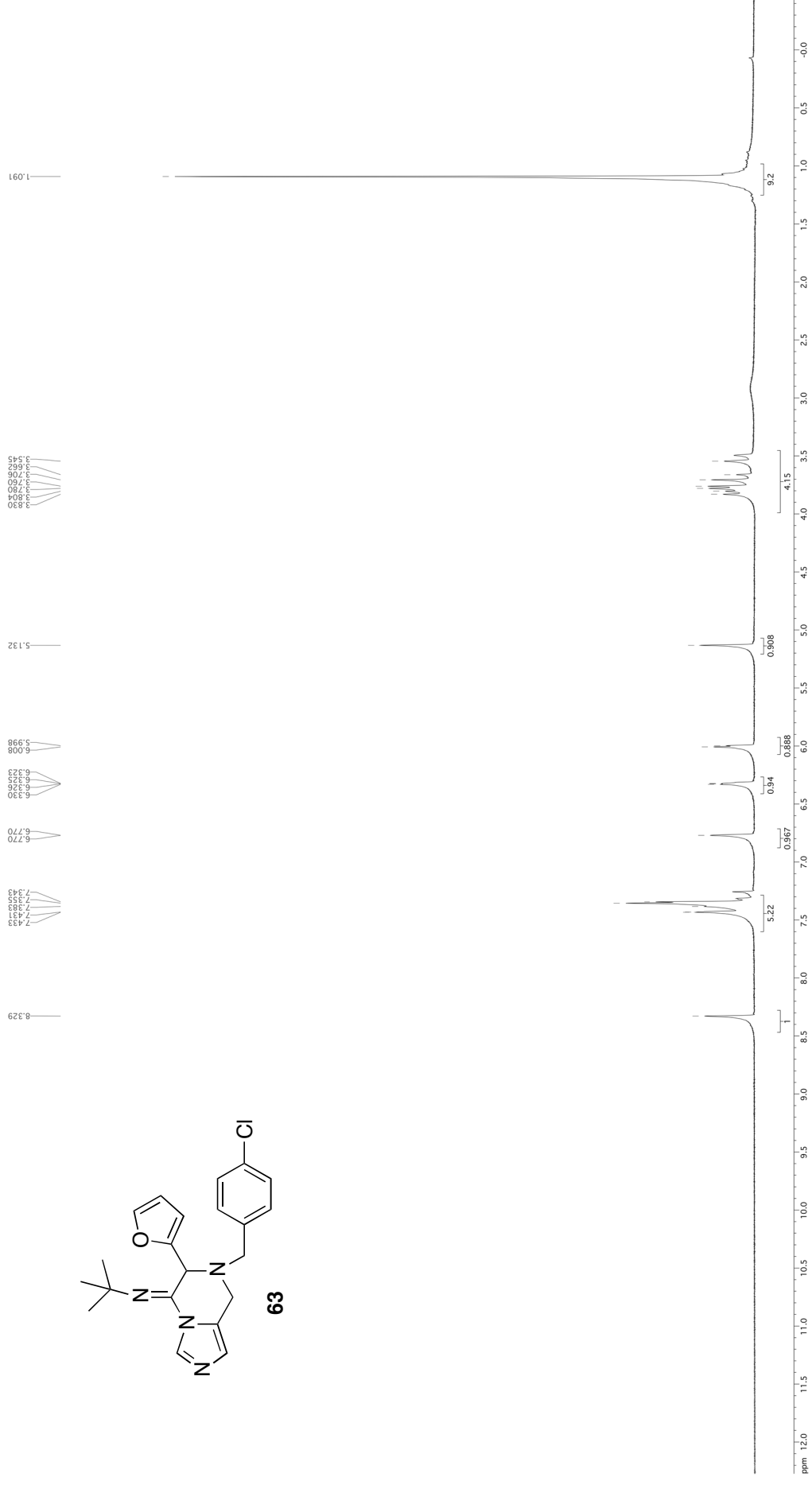
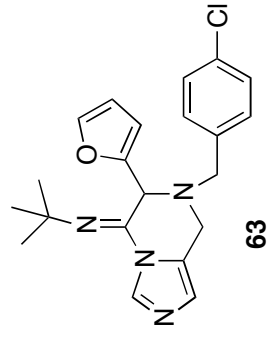
7.61
7.53
5.58
5.16
5.04
4.92
4.89
4.76
4.74
4.58
4.59
4.57
4.51
4.03
4.01
3.99
3.96
3.83
3.63
3.61
3.56
3.49
3.41
2.57
1.10
1.165
0.874
0.852



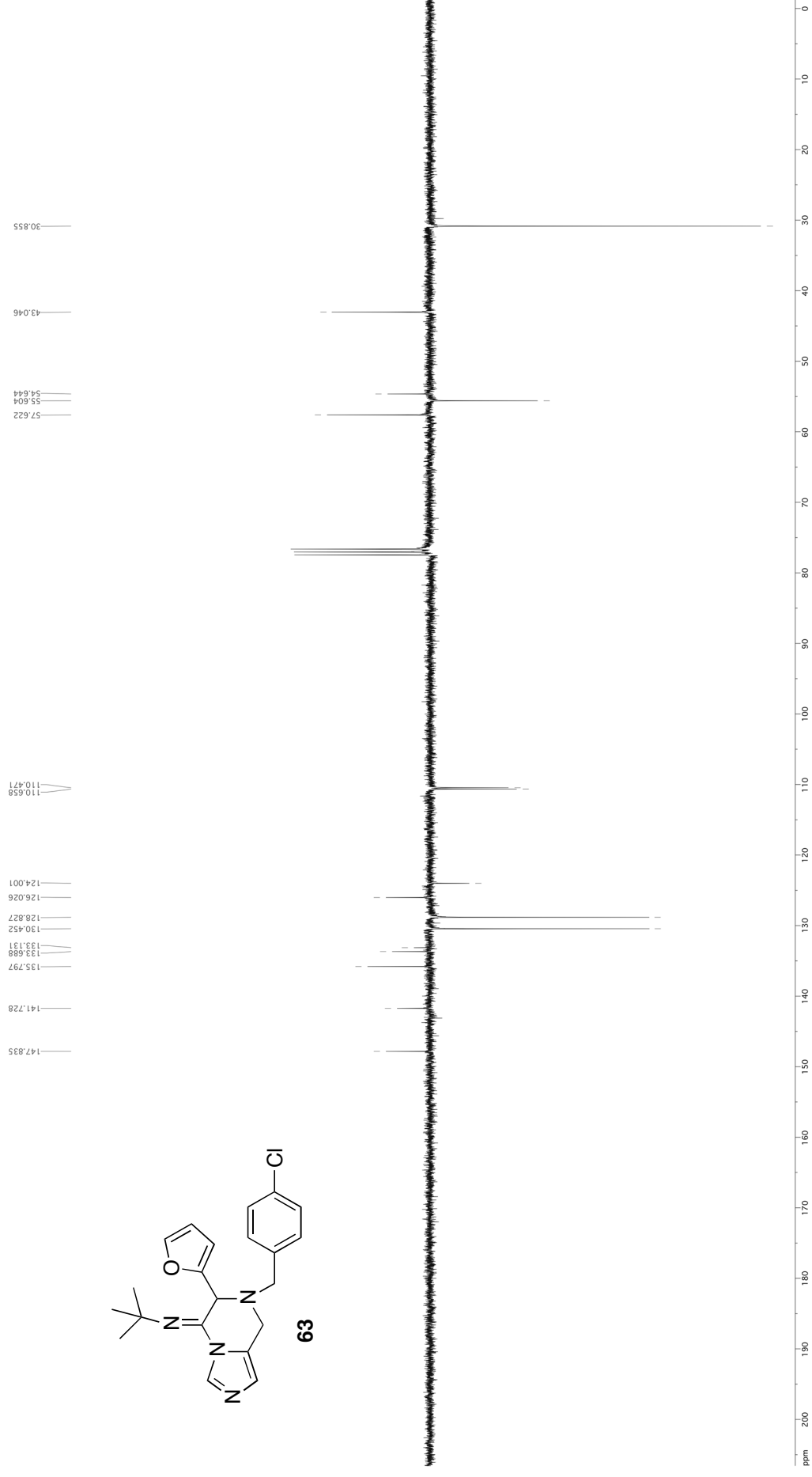
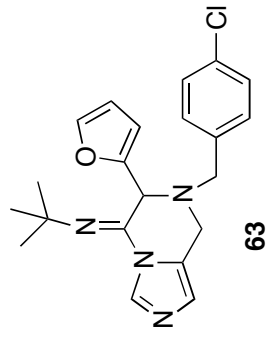
¹³C NMR
75 MHz, CDCl₃



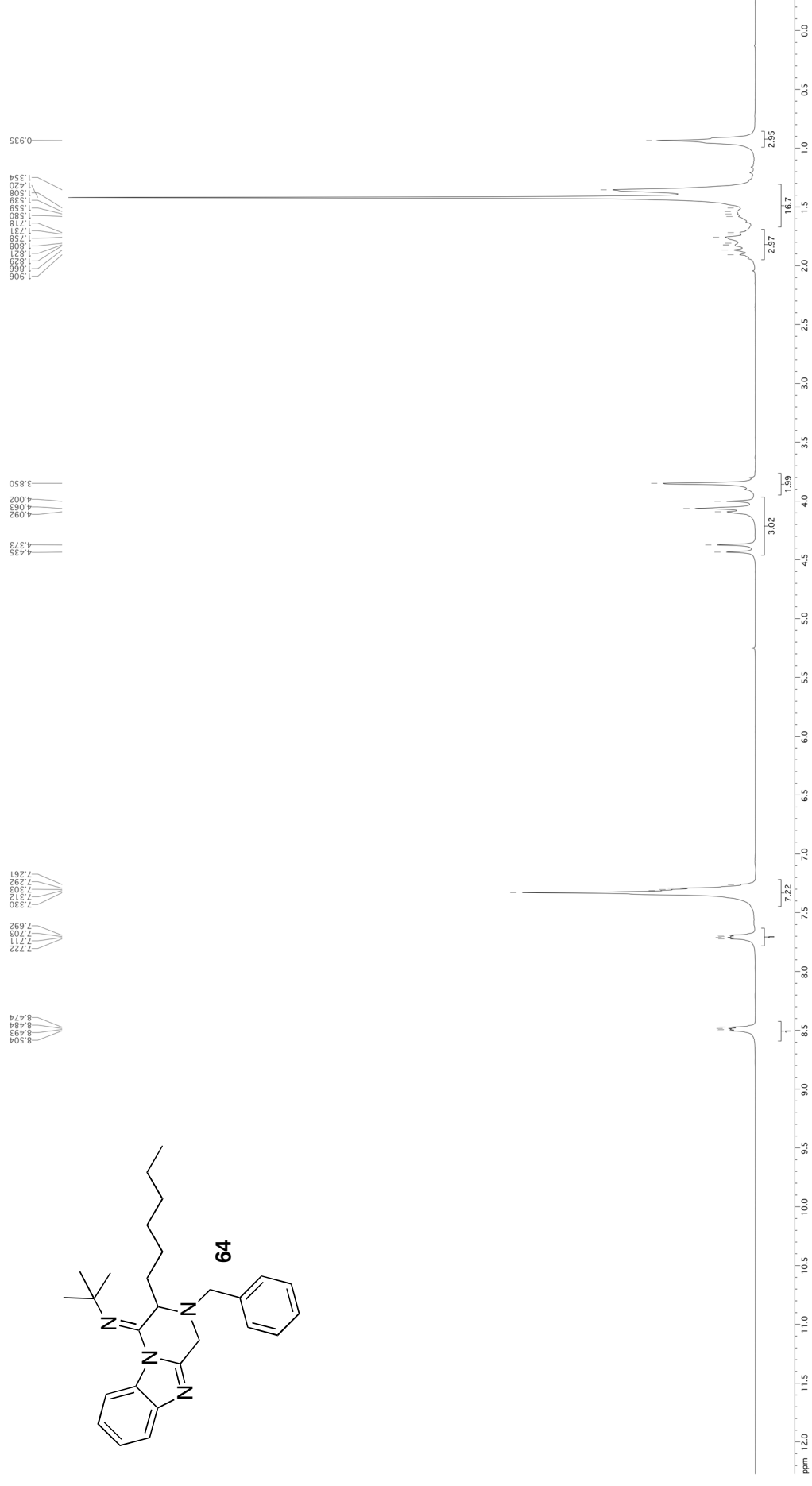
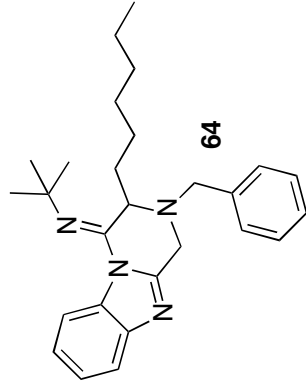
¹H NMR
300 MHz, CDCl₃



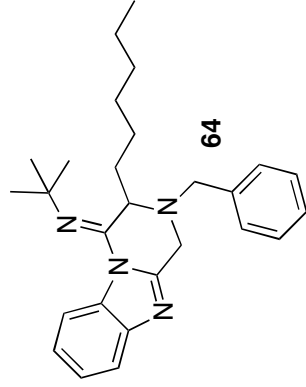
¹³C NMR
75 MHz, CDCl₃



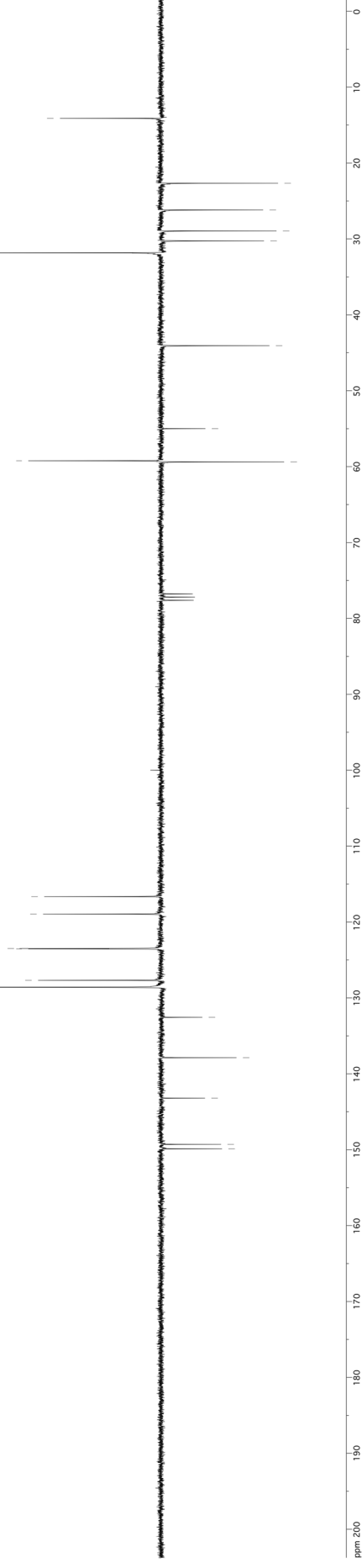
¹H NMR
300 MHz, CDCl₃



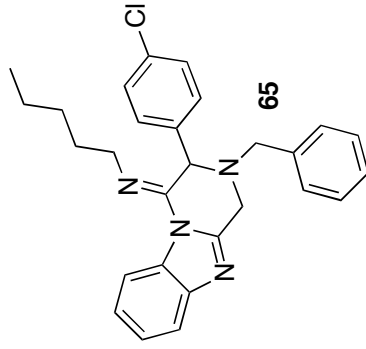
¹³C NMR
75 MHz, CDCl₃



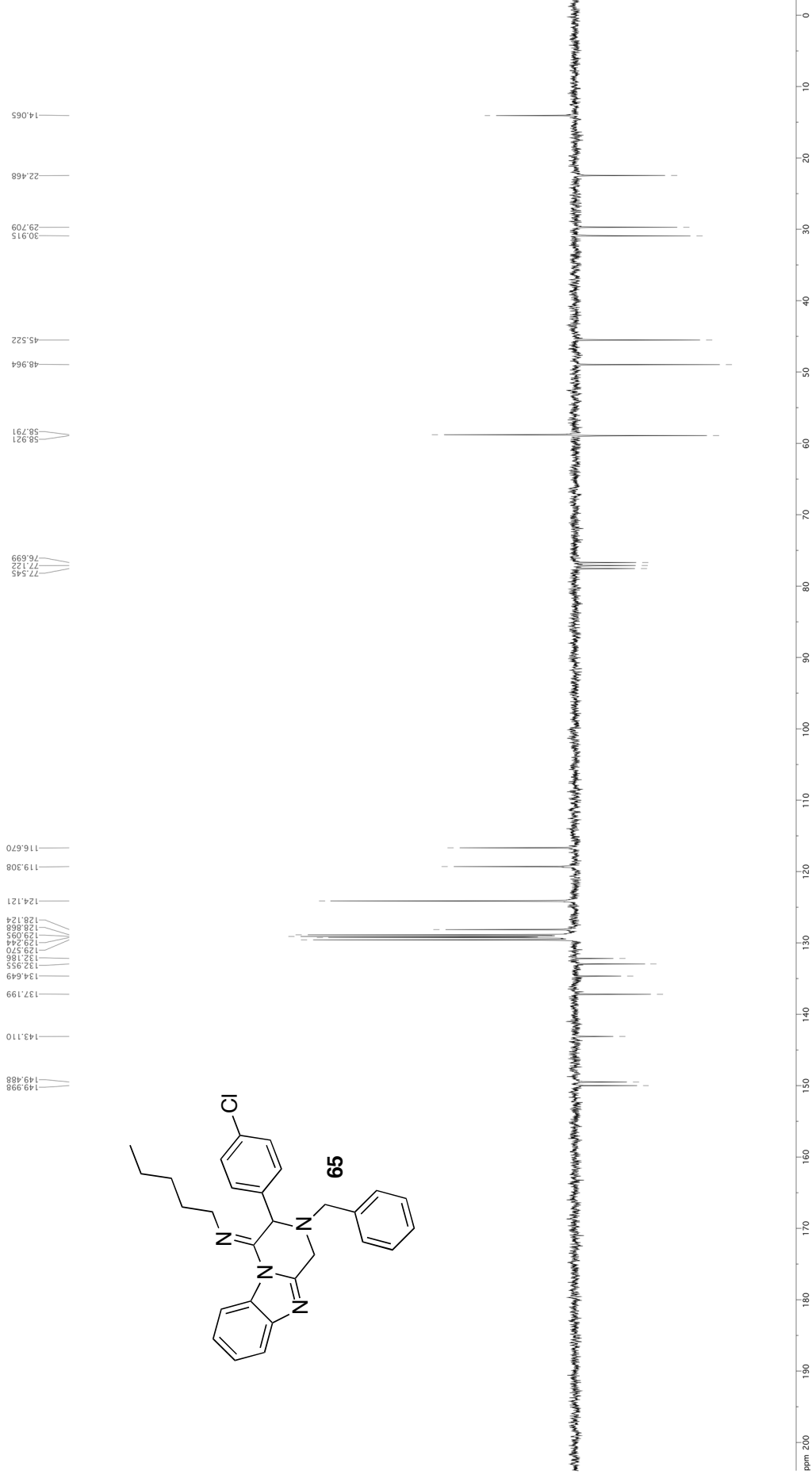
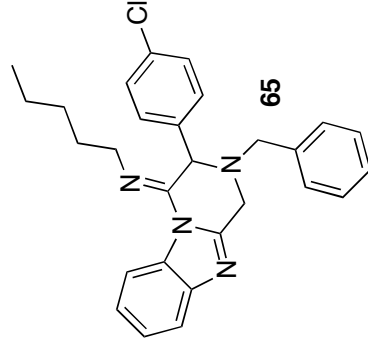
149.883
149.295
143.209
137.874
132.559
128.592
127.679
123.537
123.491
118.952
116.642
59.377
59.231
54.991
44.064
31.833
30.253
28.949
26.185
22.665
14.106



¹H NMR
300 MHz, CDCl₃



¹³C NMR
75 MHz, CDCl₃



¹H NMR
300 MHz, CDCl₃

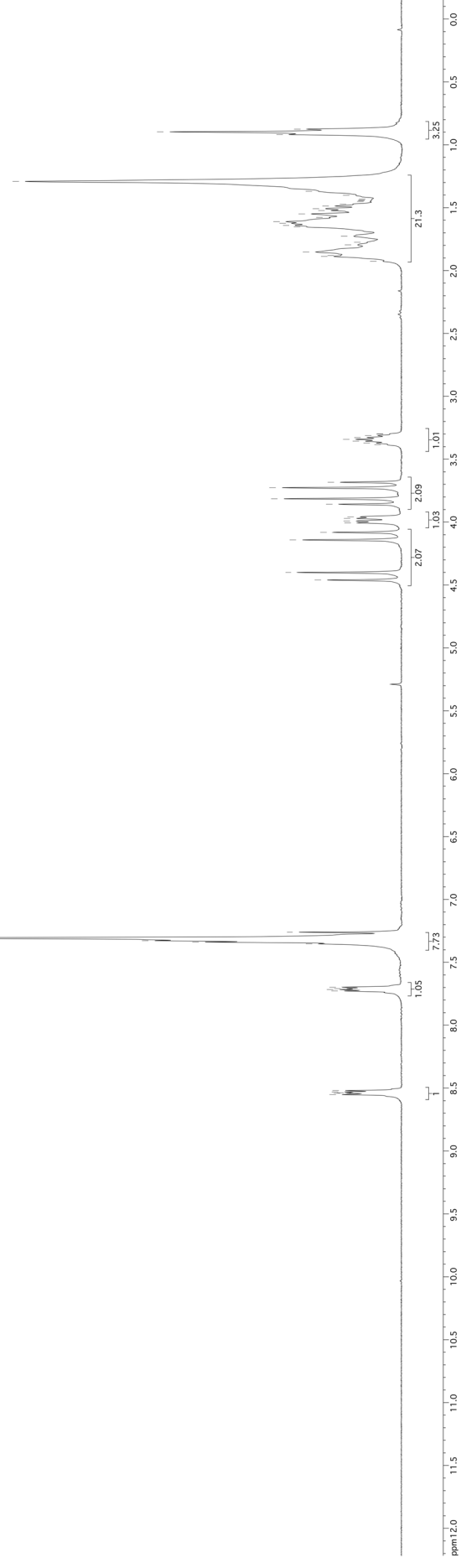
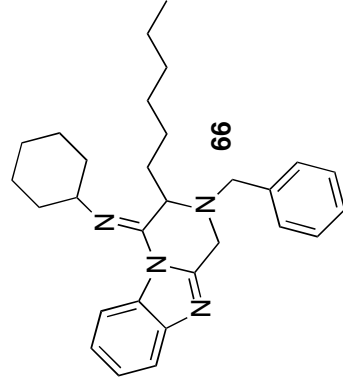
8.531
8.540
8.537
8.520

7.728
7.718
7.709
7.697

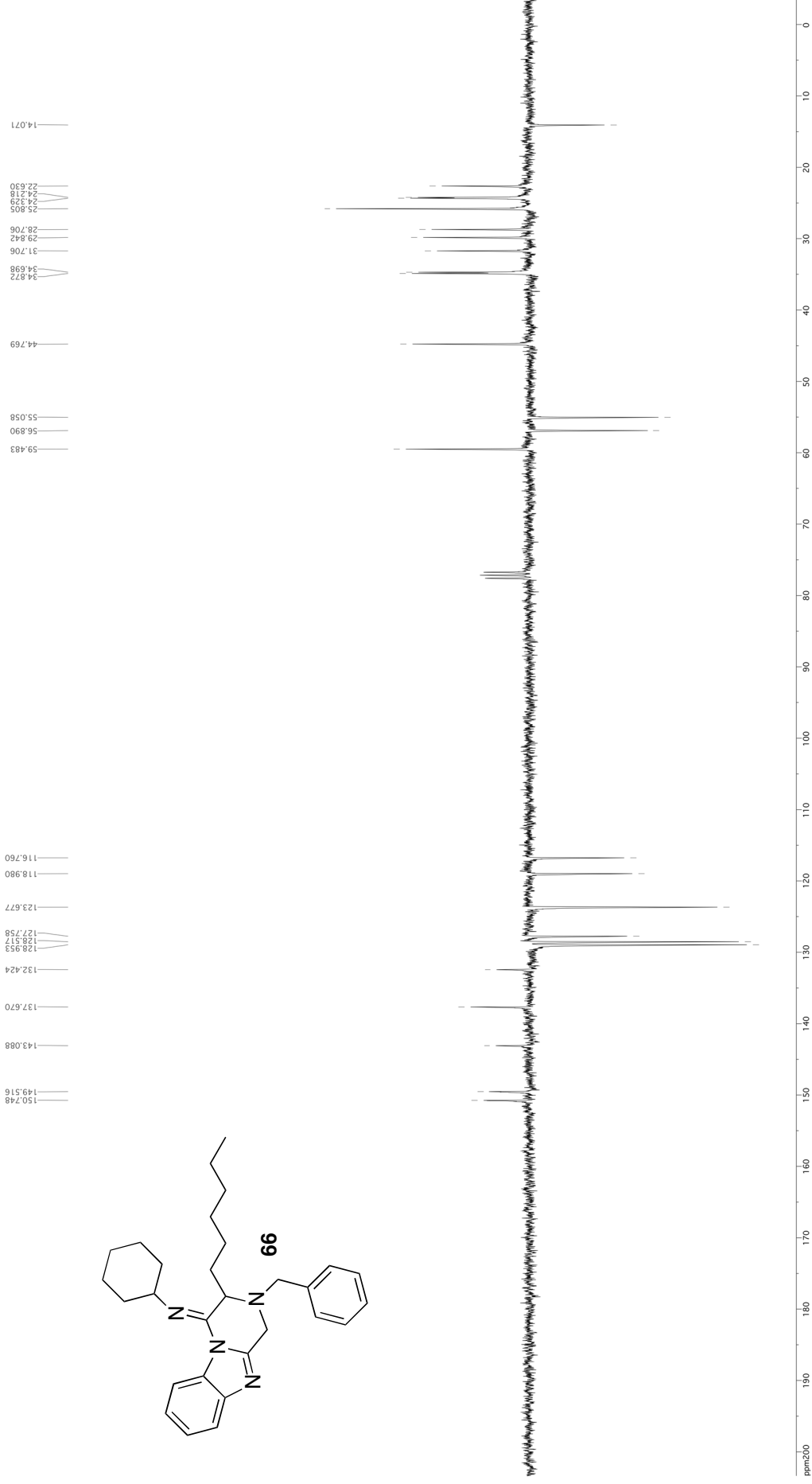
7.352
7.339
7.330
7.308
7.260

4.461
4.400
4.142
4.082
4.005
3.991
3.970
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3.984
3.772
3.358
3.342
3.329
3.301
3.298

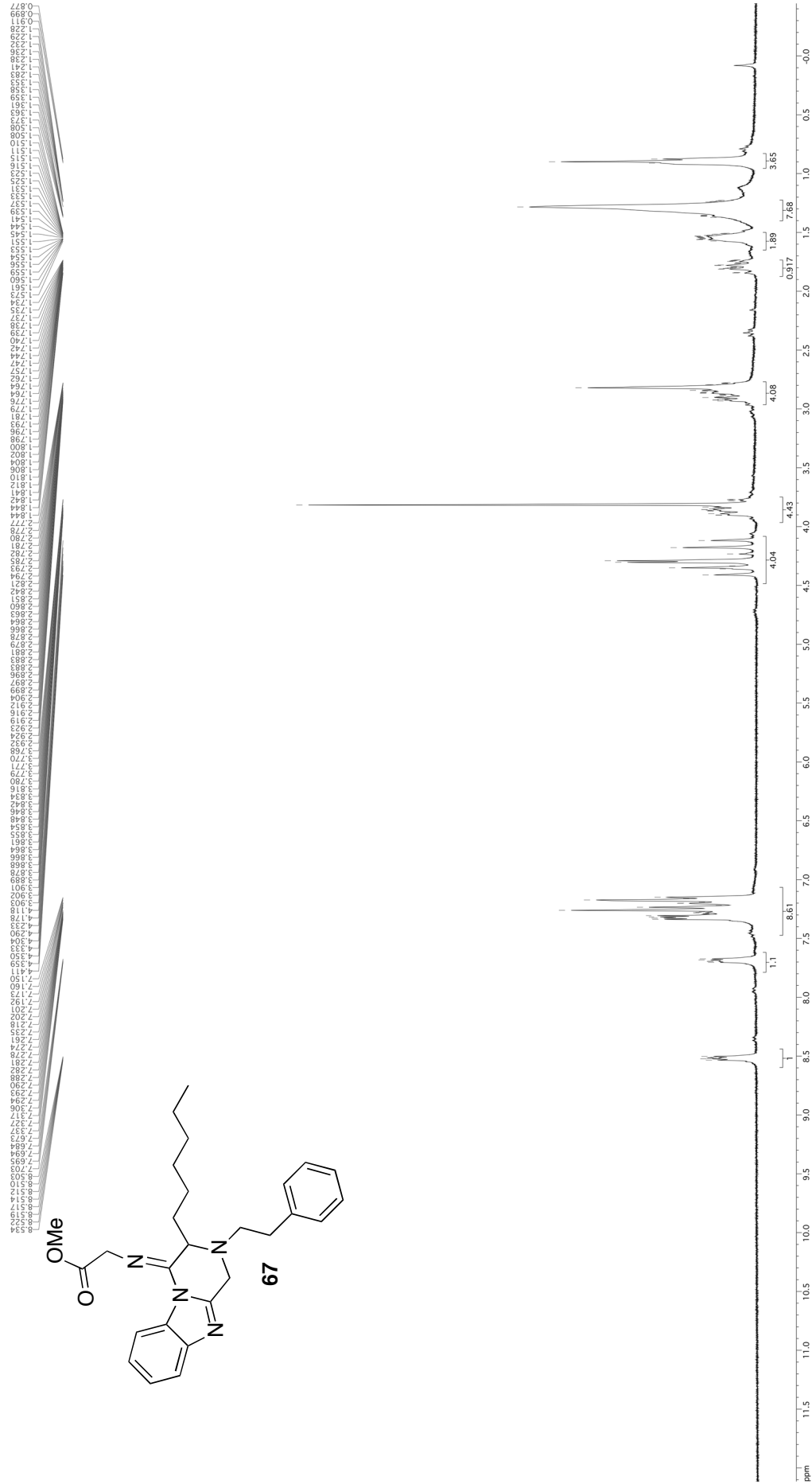
1.926
1.886
1.880
1.795
1.778
1.728
1.652
1.641
1.625
1.576
1.550
1.550
1.508
1.525
1.486
1.472
1.450
1.444
1.441
1.407
1.387
1.370
1.370
0.918
0.897
0.876



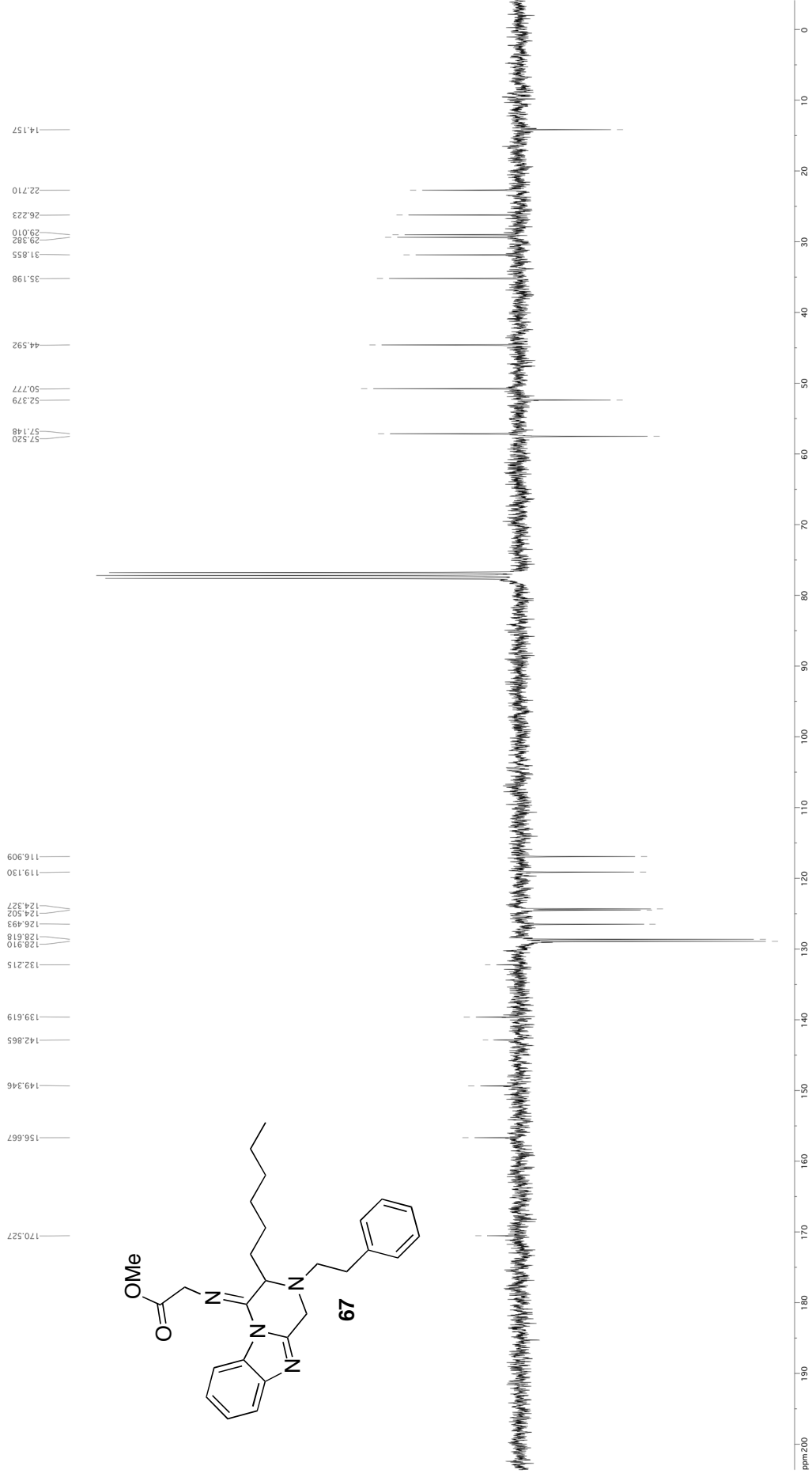
^{13}C NMR
75 MHz, CDCl_3



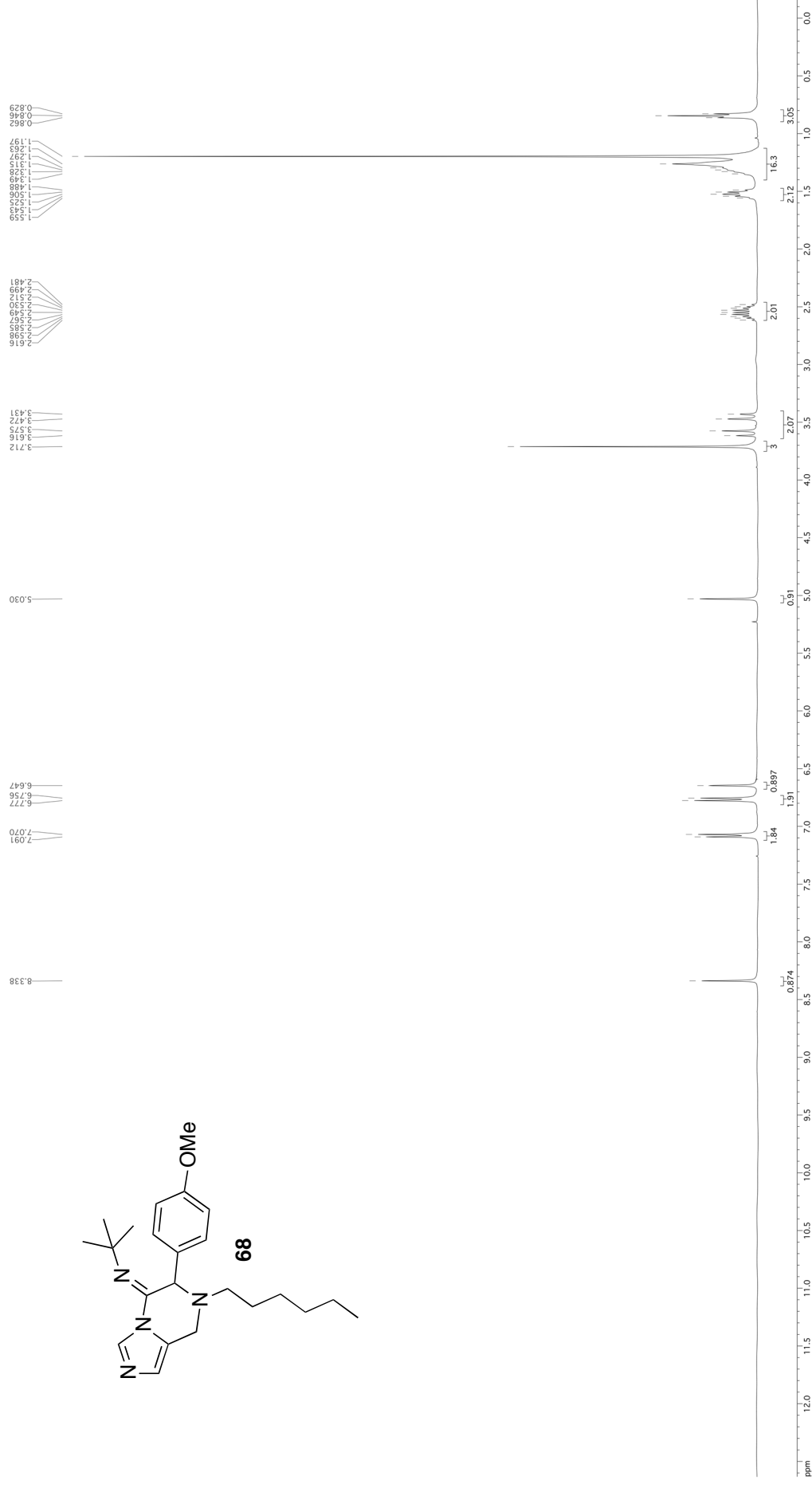
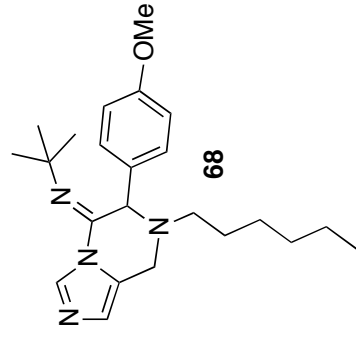
¹H NMR
300 MHz, CDCl₃



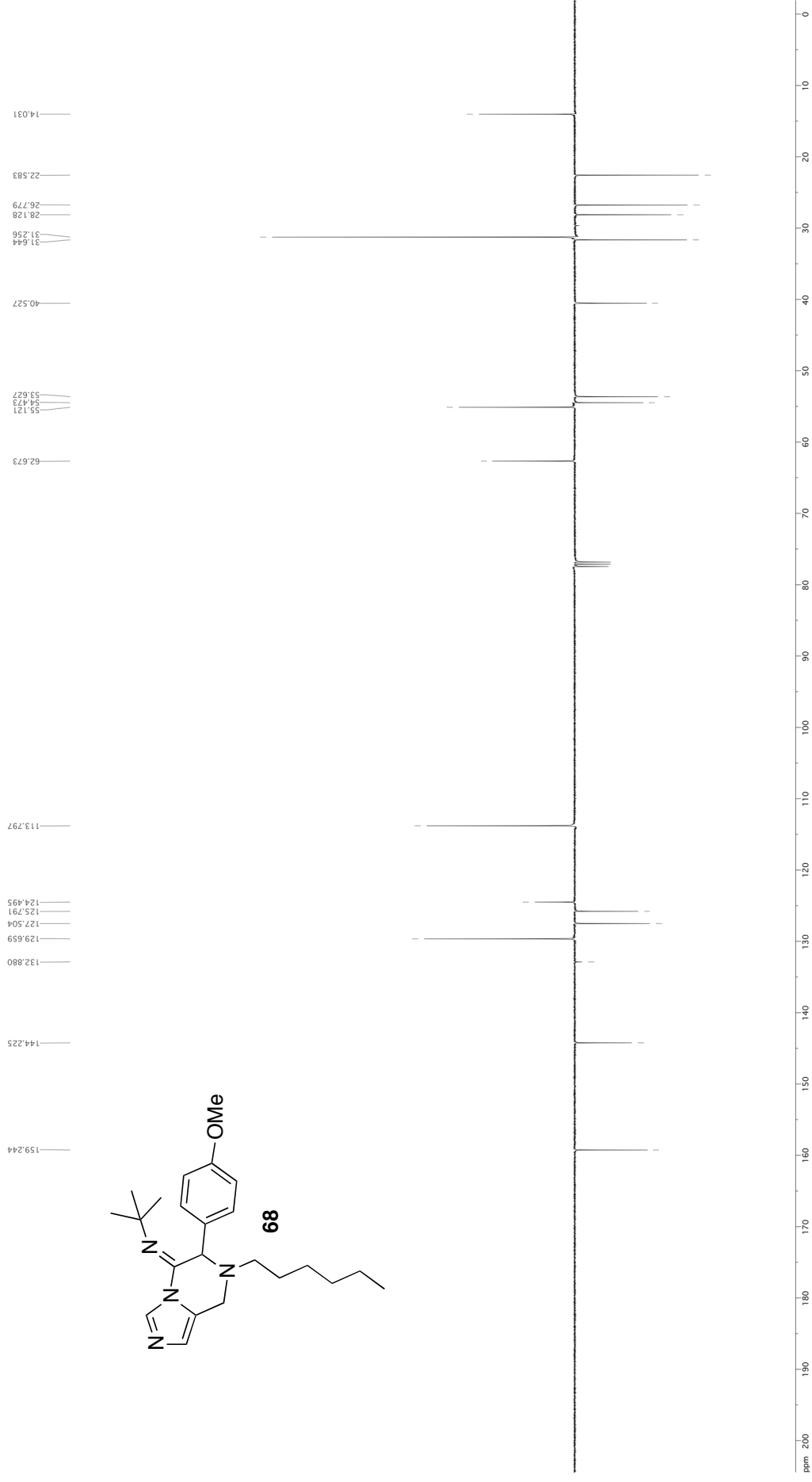
¹³C NMR
75 MHz, CDCl₃



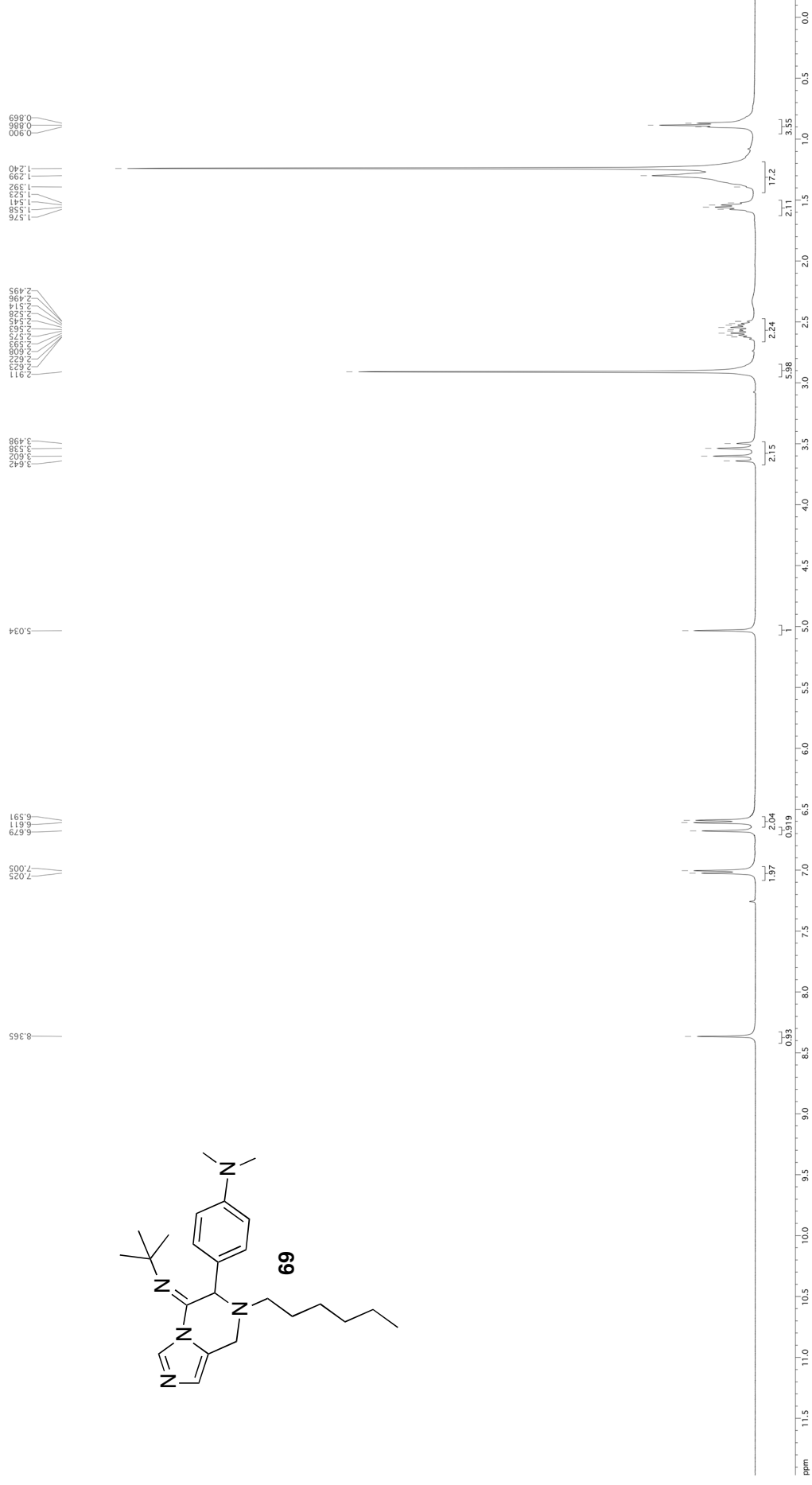
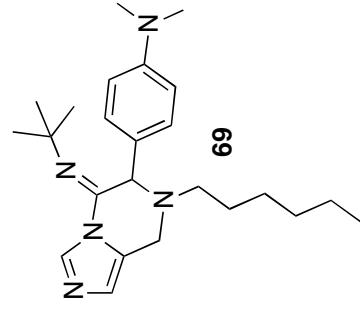
¹H NMR
400 MHz, CDCl₃

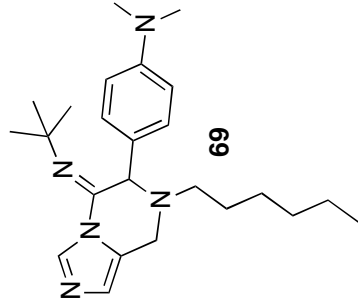


^{13}C NMR
100 MHz, CDCl_3

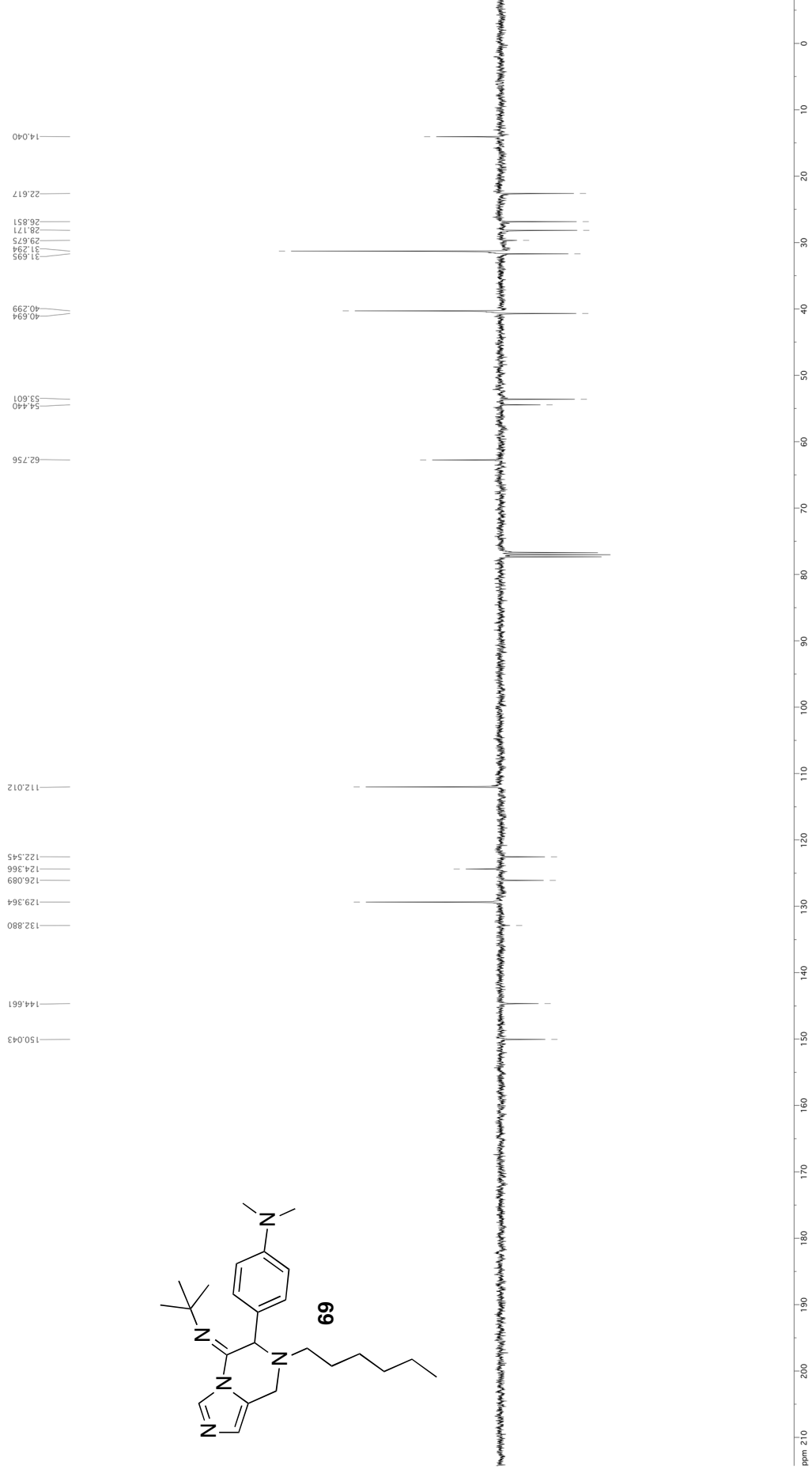


¹H NMR
400 MHz, CDCl₃

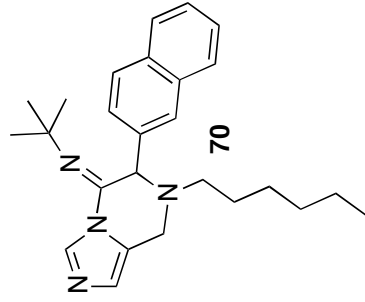




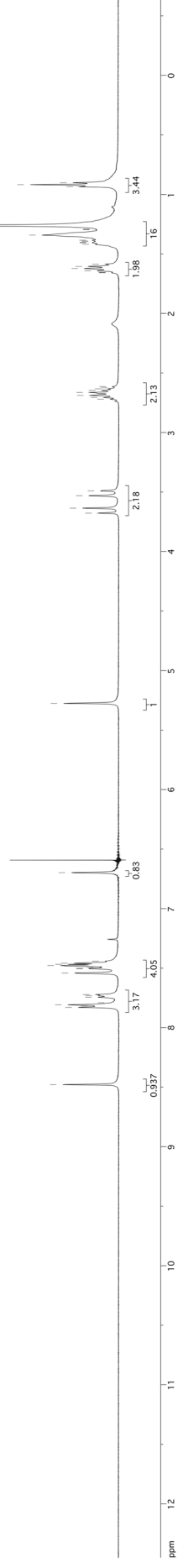
^{13}C NMR
100 MHz, CDCl_3



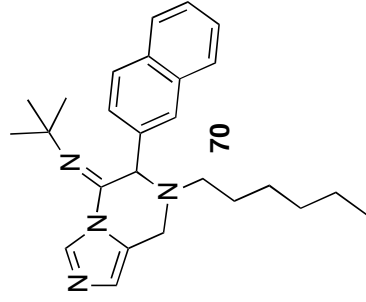
¹H NMR
400 MHz, CDCl₃



8.476
7.830
7.809
7.790
7.745
7.730
7.723
7.542
7.505
7.502
7.478
7.468
7.458
7.443
6.698
5.275
3.677
3.636
3.632
3.490
2.720
2.706
2.689
2.664
2.646
2.634
2.624
2.615
1.658
1.656
1.654
1.641
1.623
1.605
1.587
1.419
1.407
1.401
1.394
1.385
1.382
1.342
1.297
1.283
1.262
0.935
0.918
0.901

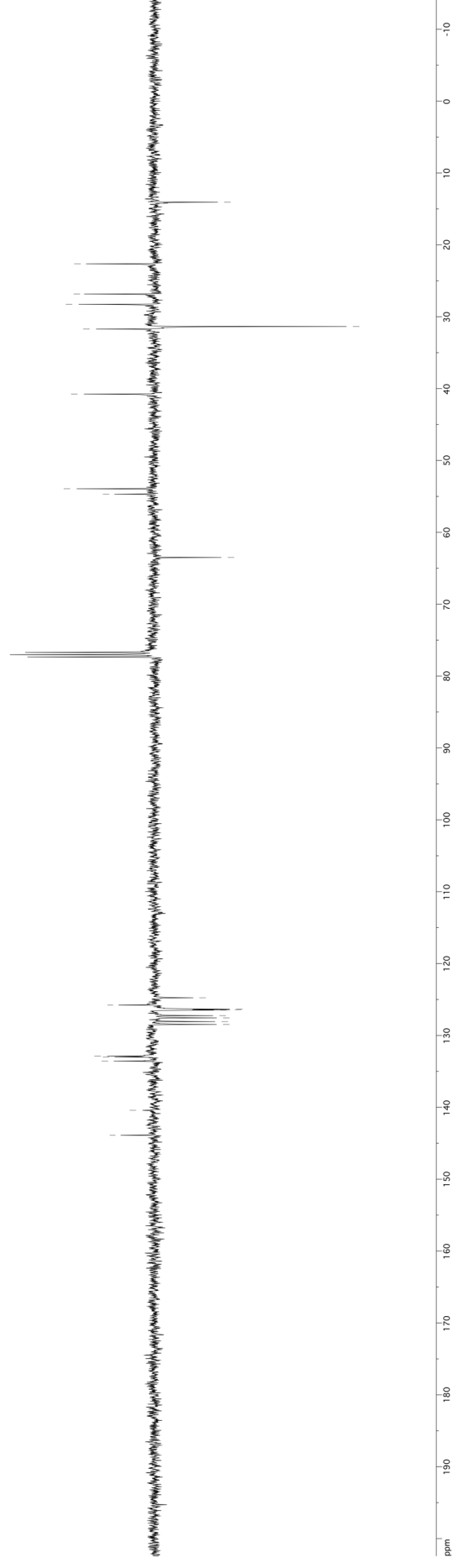


¹³C NMR
100 MHz, CDCl₃

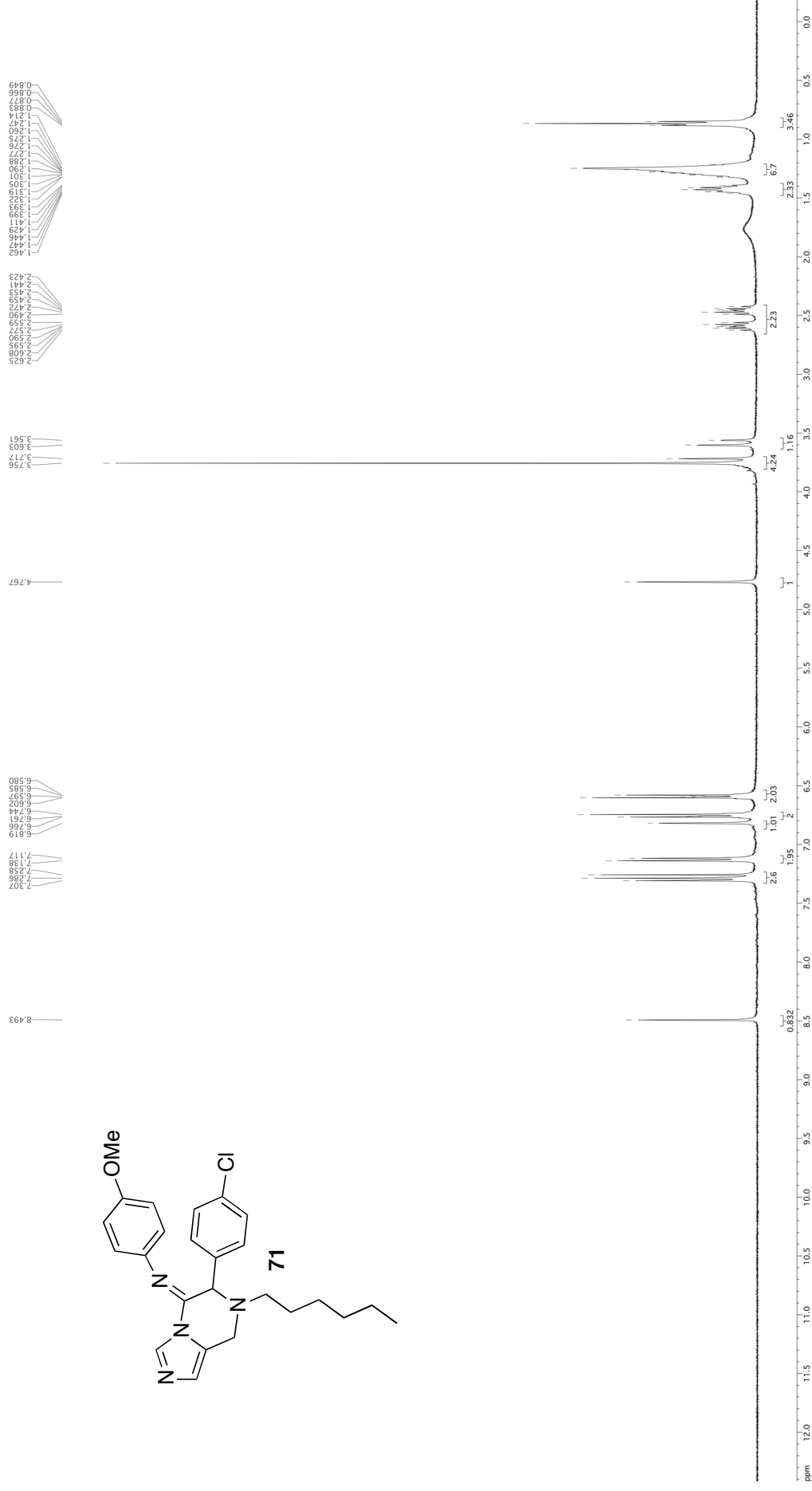
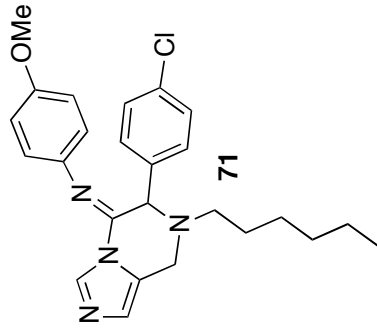


143.871
140.409
133.574
132.871
132.994
128.460
128.059
127.951
127.230
126.477
126.410
126.331
125.759
124.753

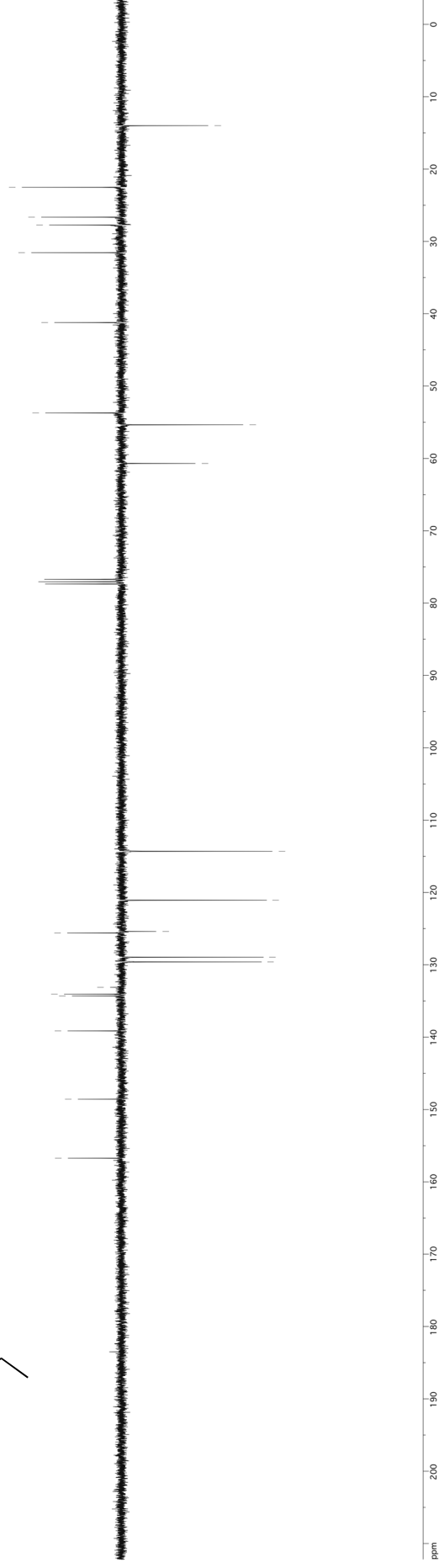
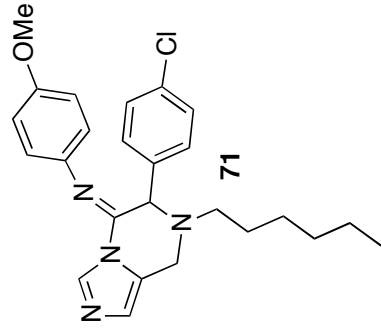
63.495
54.675
53.936
40.761
31.702
31.350
28.284
26.840
22.635
14.056



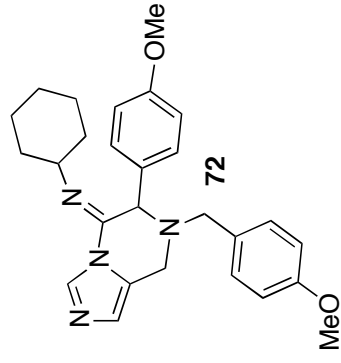
¹H NMR
400 MHz, CDCl₃



¹³C NMR
100 MHz, CDCl₃



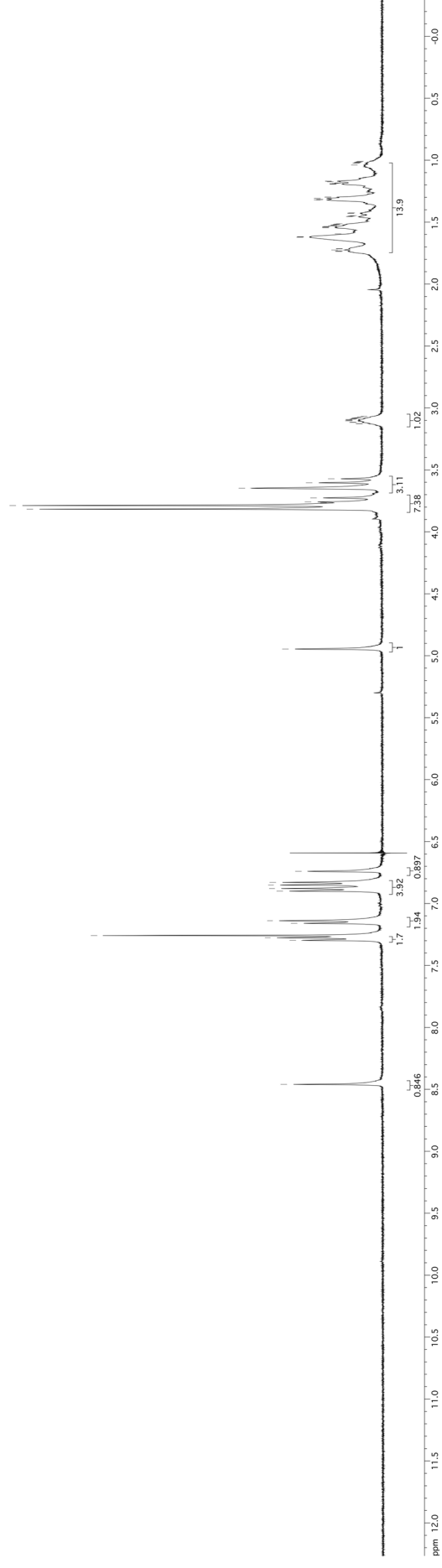
¹H NMR
400 MHz, CDCl₃



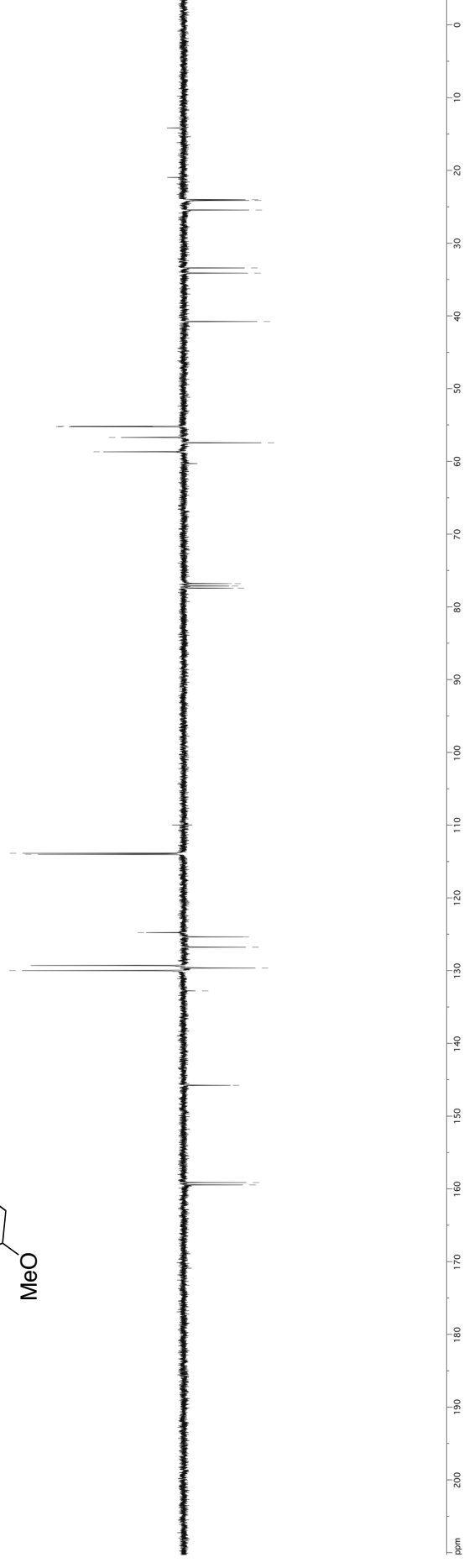
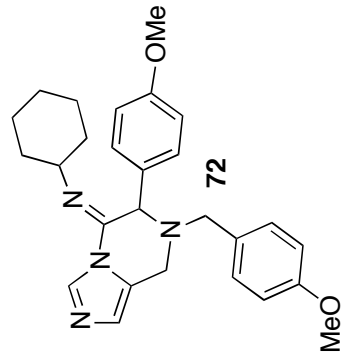
7.297
7.276
7.259
7.160
7.139
6.900
6.879
6.851
6.829
6.740

8.460

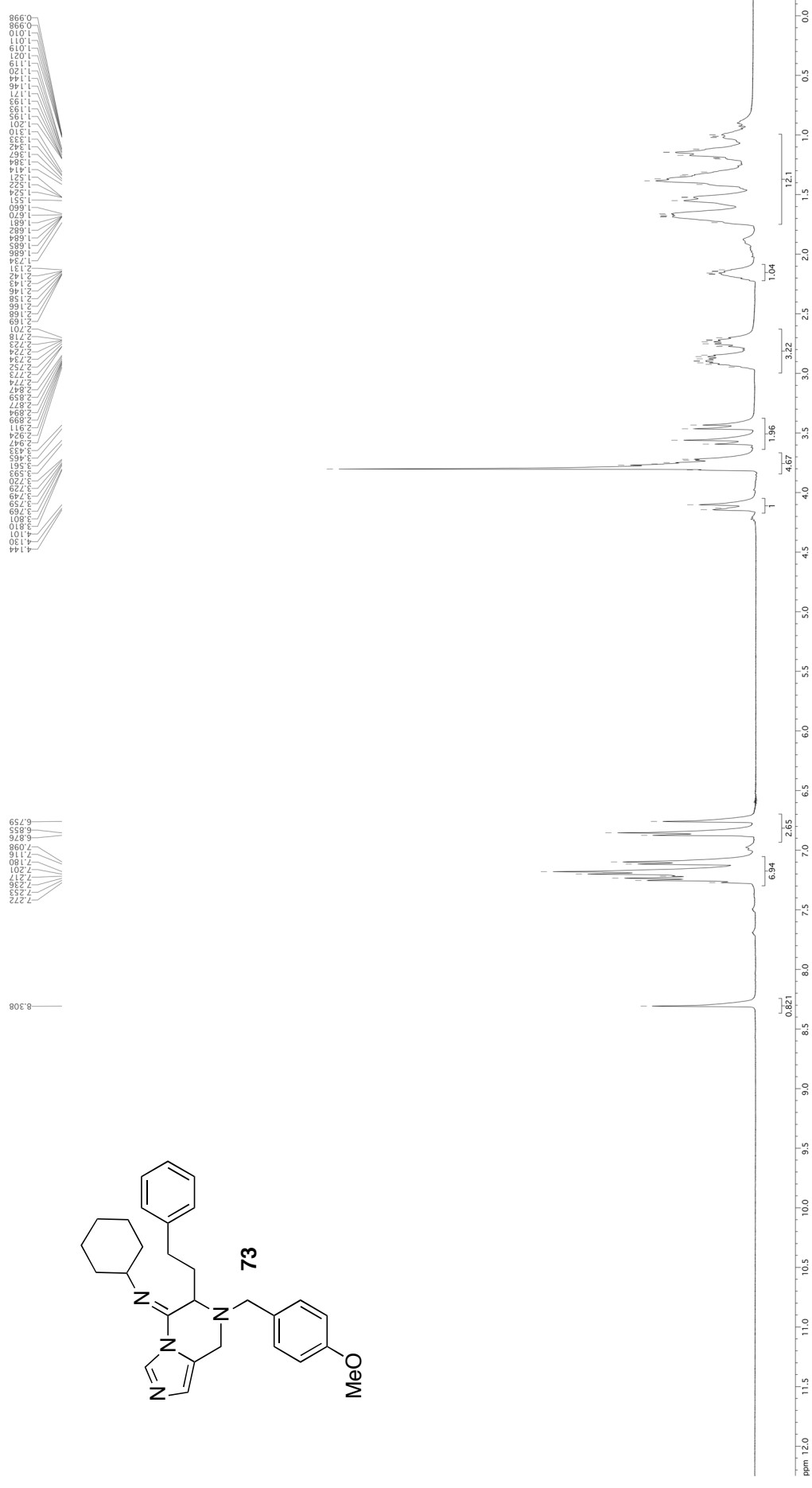
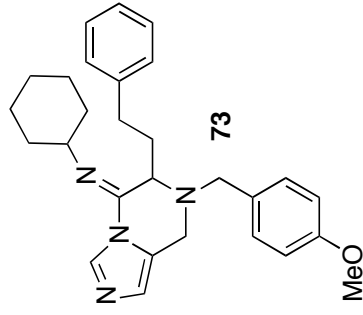
9.46
8.817
8.767
8.759
8.648
8.604
8.574
8.128
8.117
8.114
8.104
8.102
8.096
8.094
8.087
8.083
8.081
8.079
8.078
8.073
8.068
8.066
8.064
8.062
8.057
8.052
8.049
8.045
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8.018
8.014
8.012
8.010



¹³C NMR
100 MHz, CDCl₃

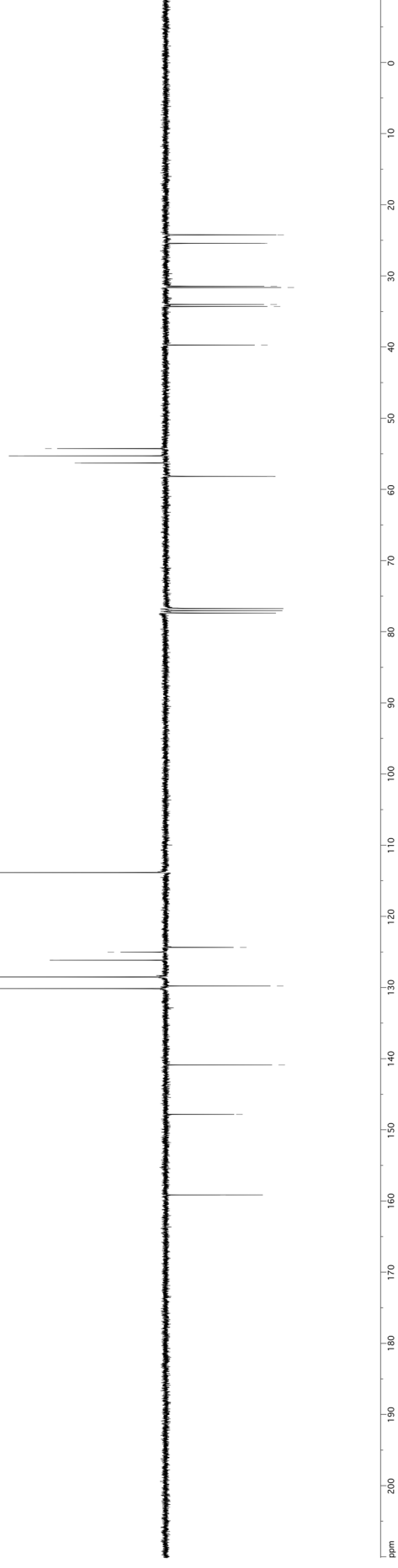
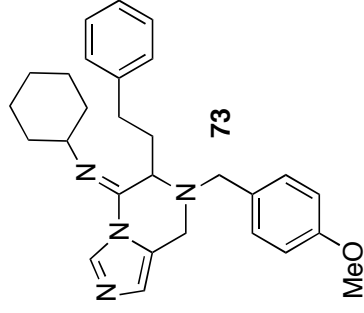


¹H NMR
400 MHz, CDCl₃

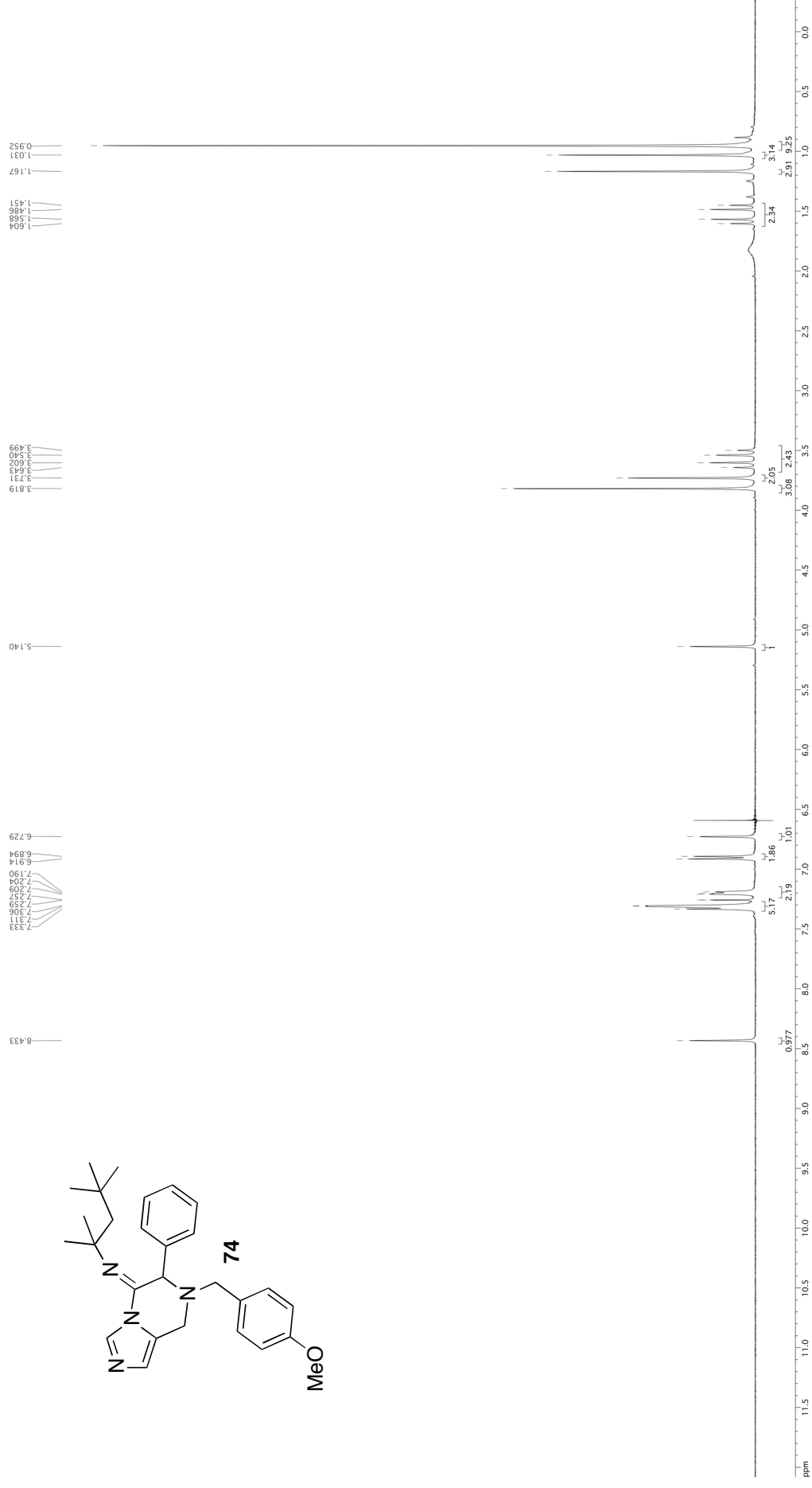
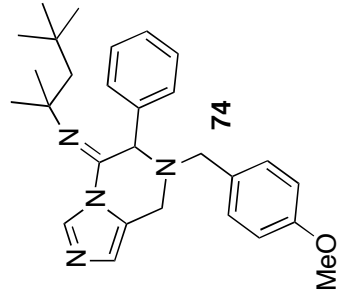


¹³C NMR
100 MHz, CDCl₃

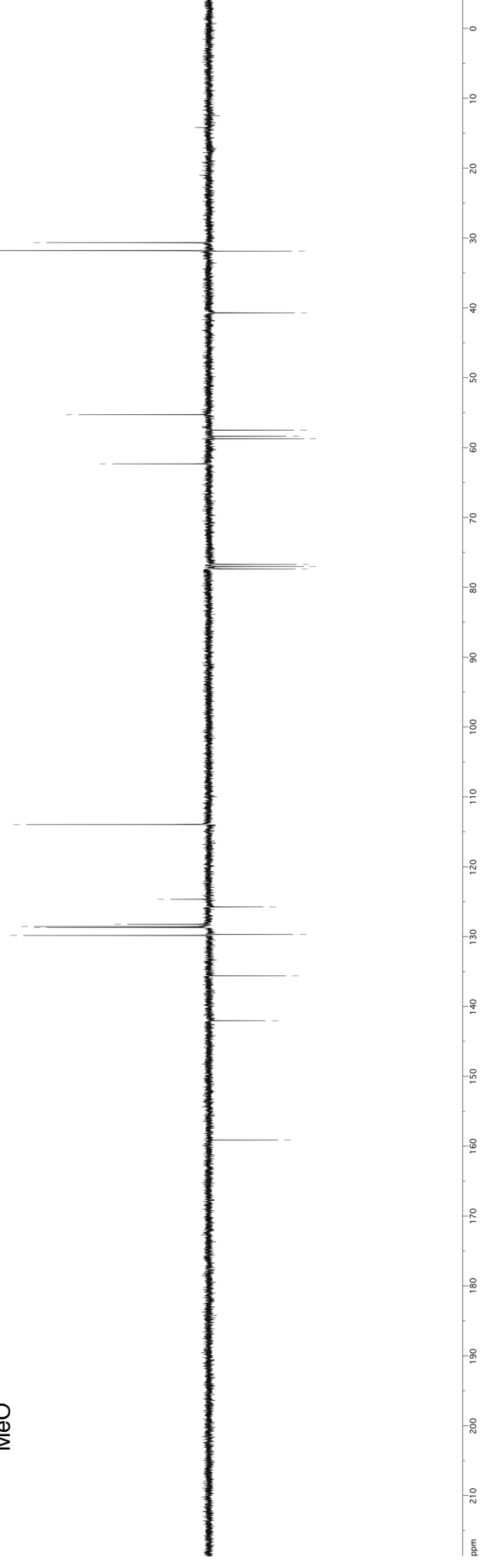
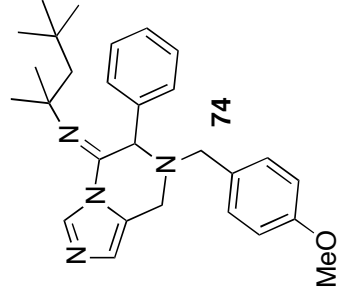
159.138
147.828
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130.156
129.787
128.518
126.170
124.356
113.846
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56.294
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54.277
39.733
34.307
34.012
31.450
25.441
24.235



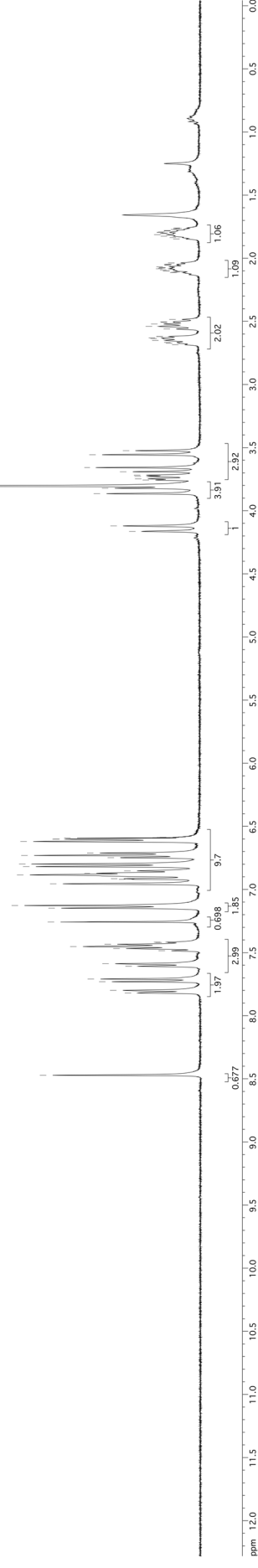
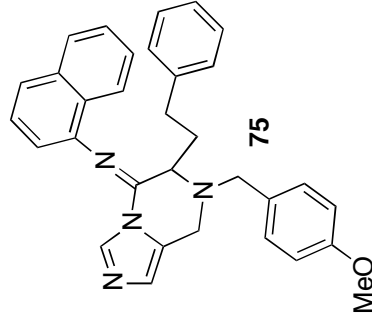
¹H NMR
400 MHz, CDCl₃



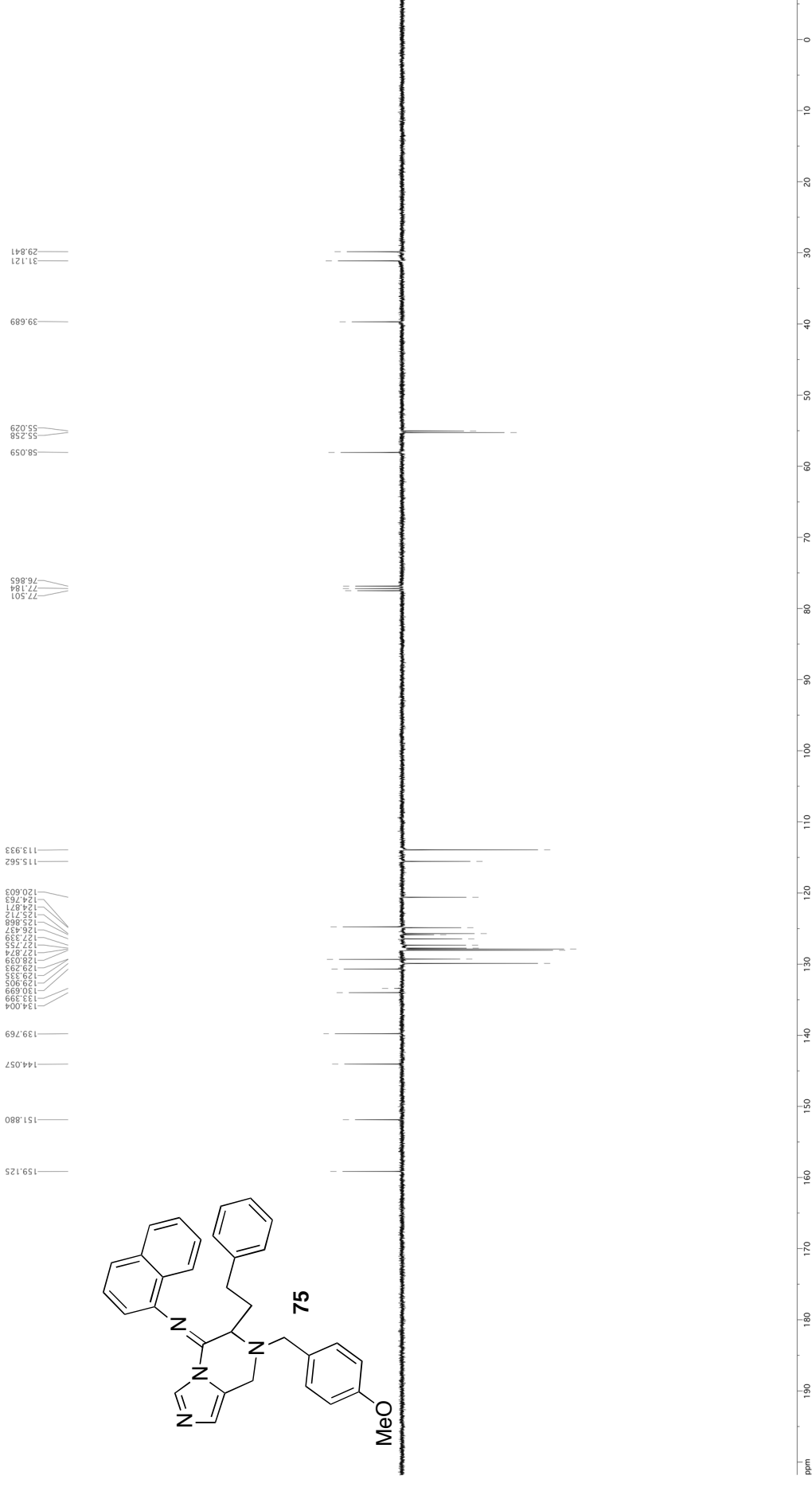
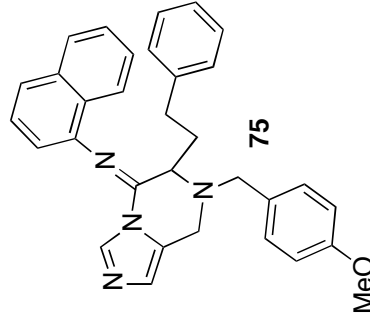
¹³C NMR
100 MHz, CDCl₃



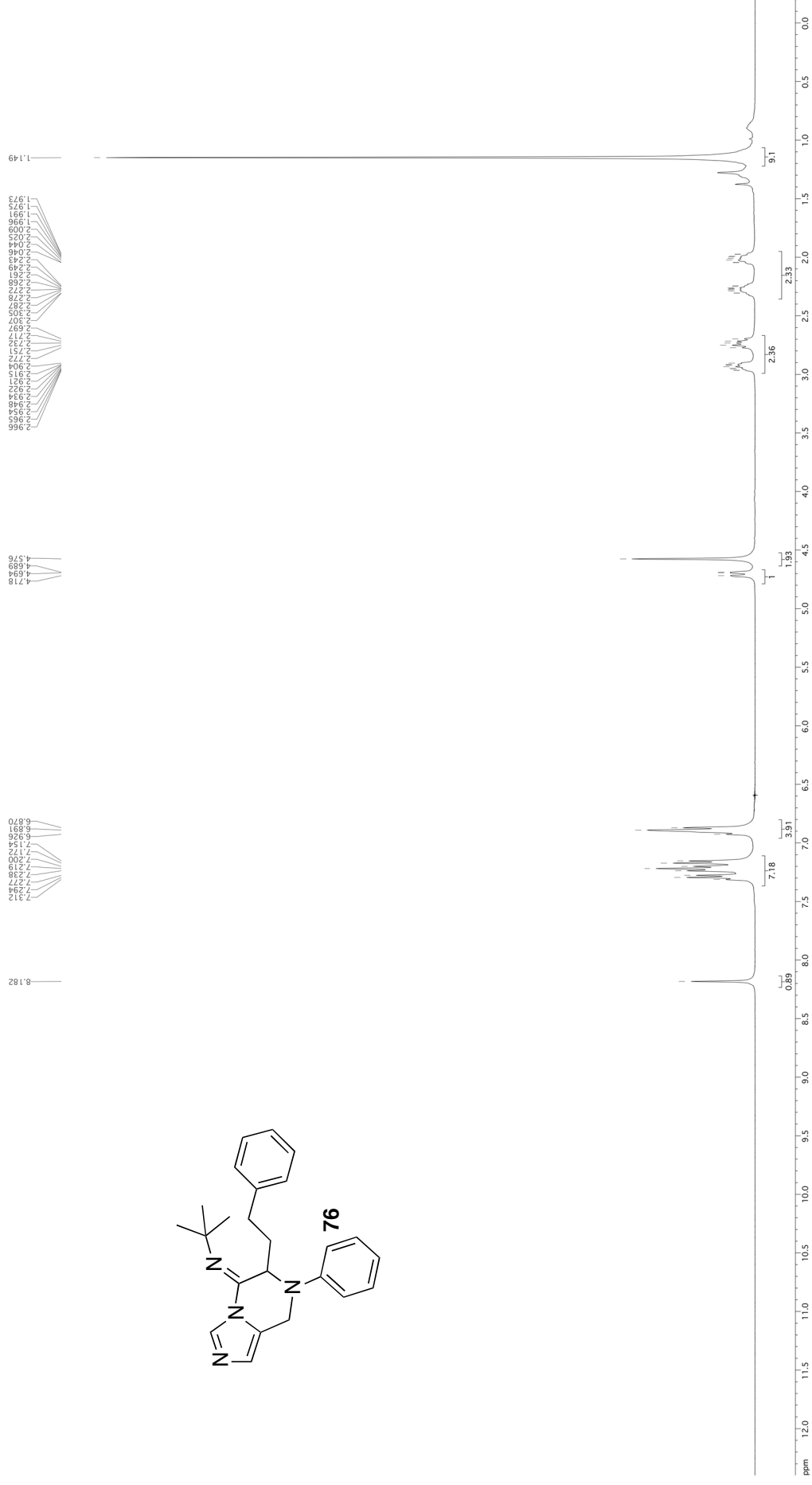
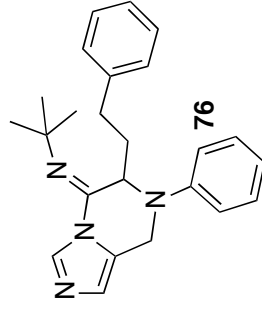
¹H NMR
400 MHz, CDCl₃



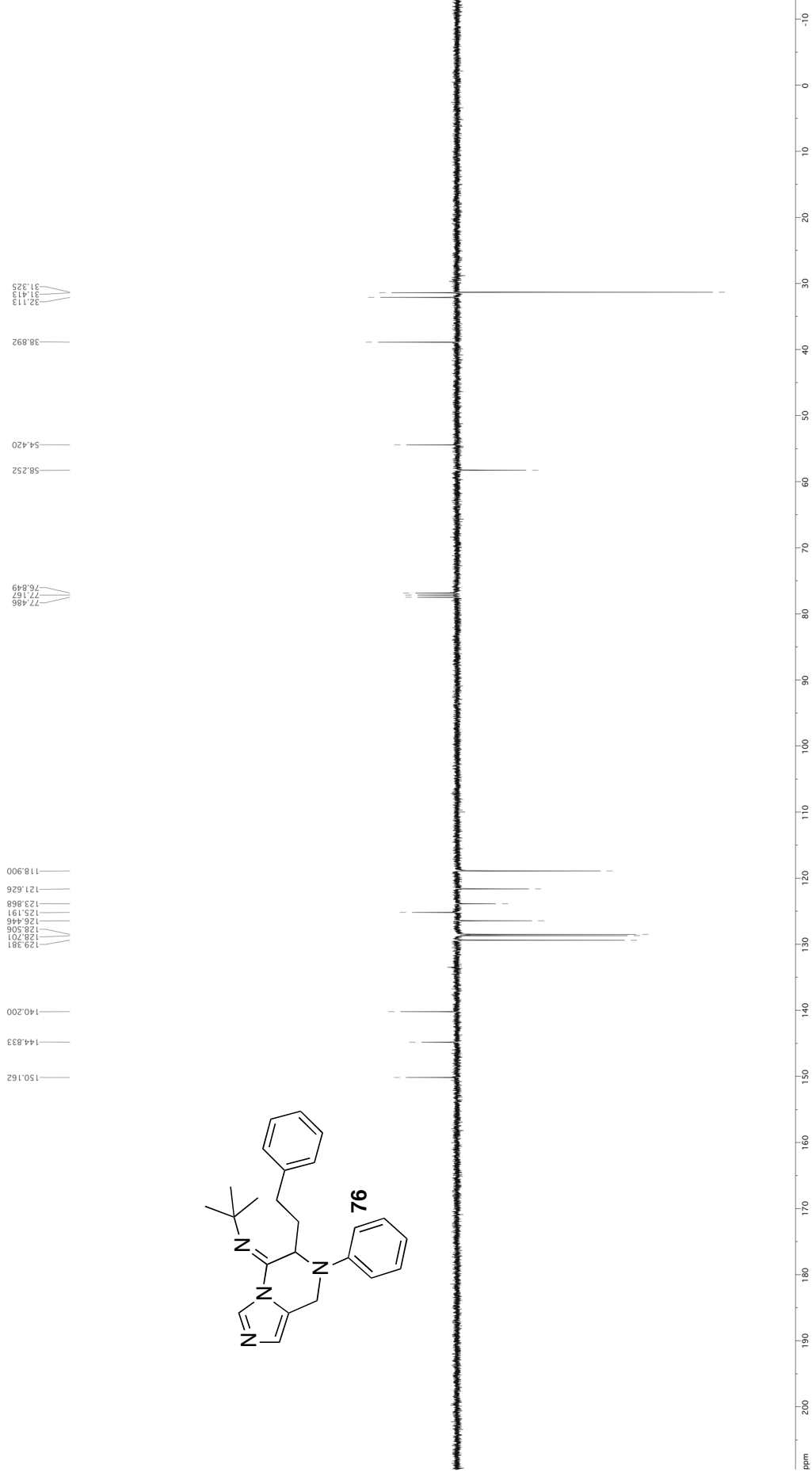
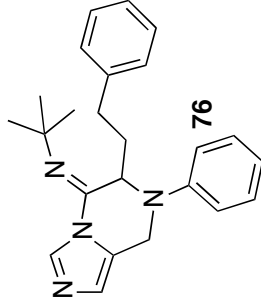
¹³C NMR
100 MHz, CDCl₃



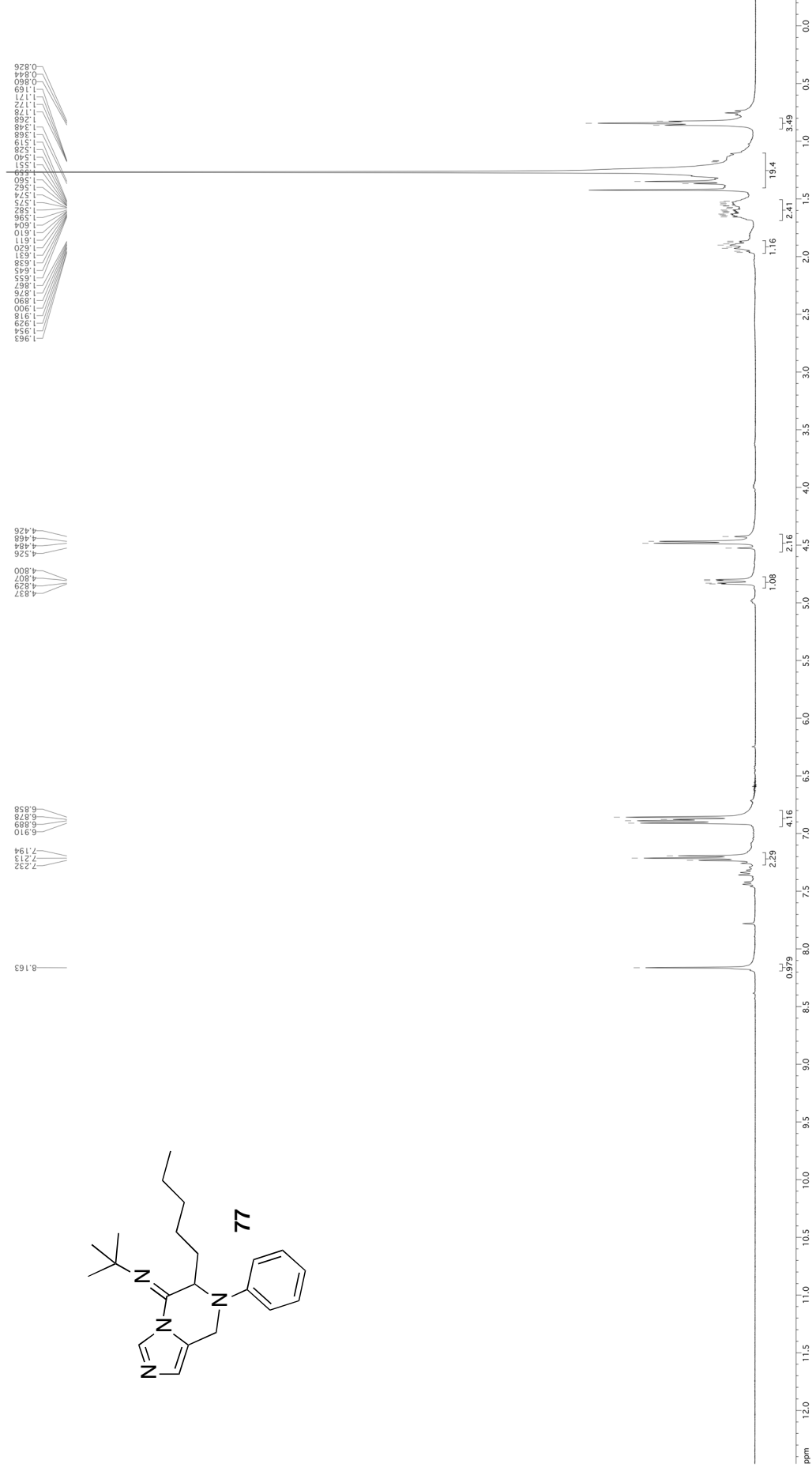
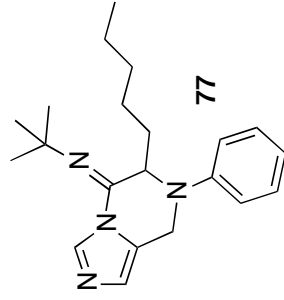
¹H NMR
400 MHz, CDCl₃



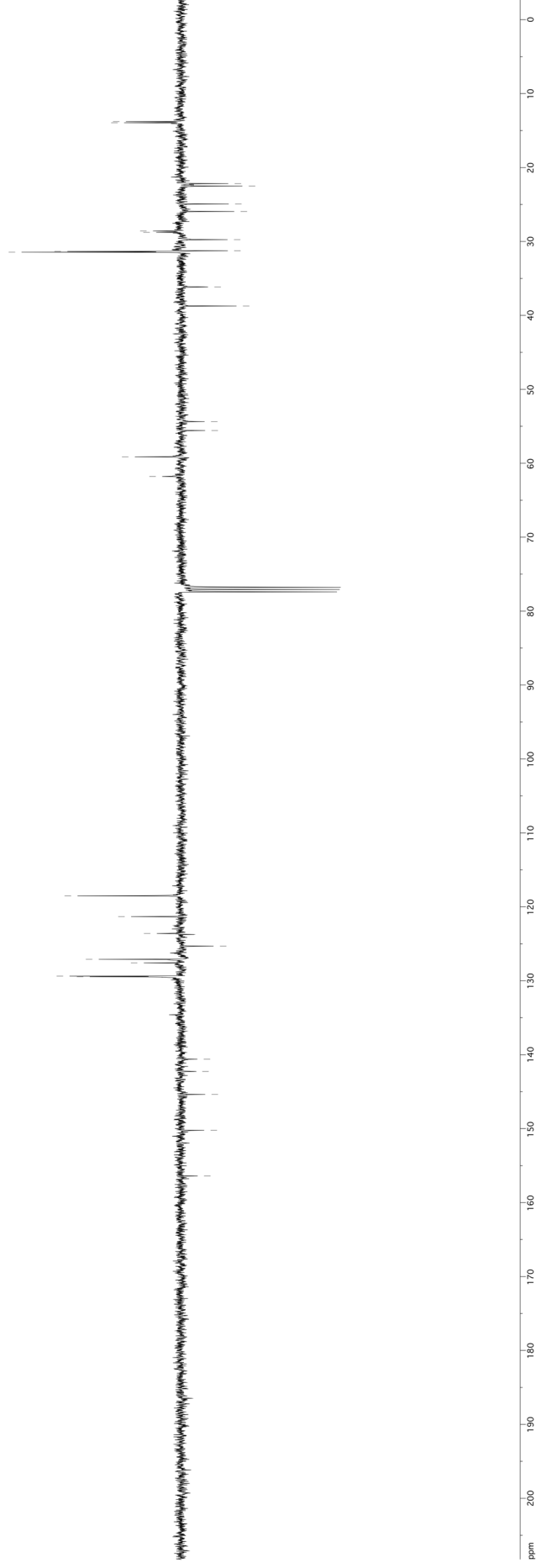
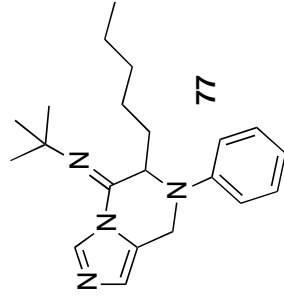
¹³C NMR
100 MHz, CDCl₃



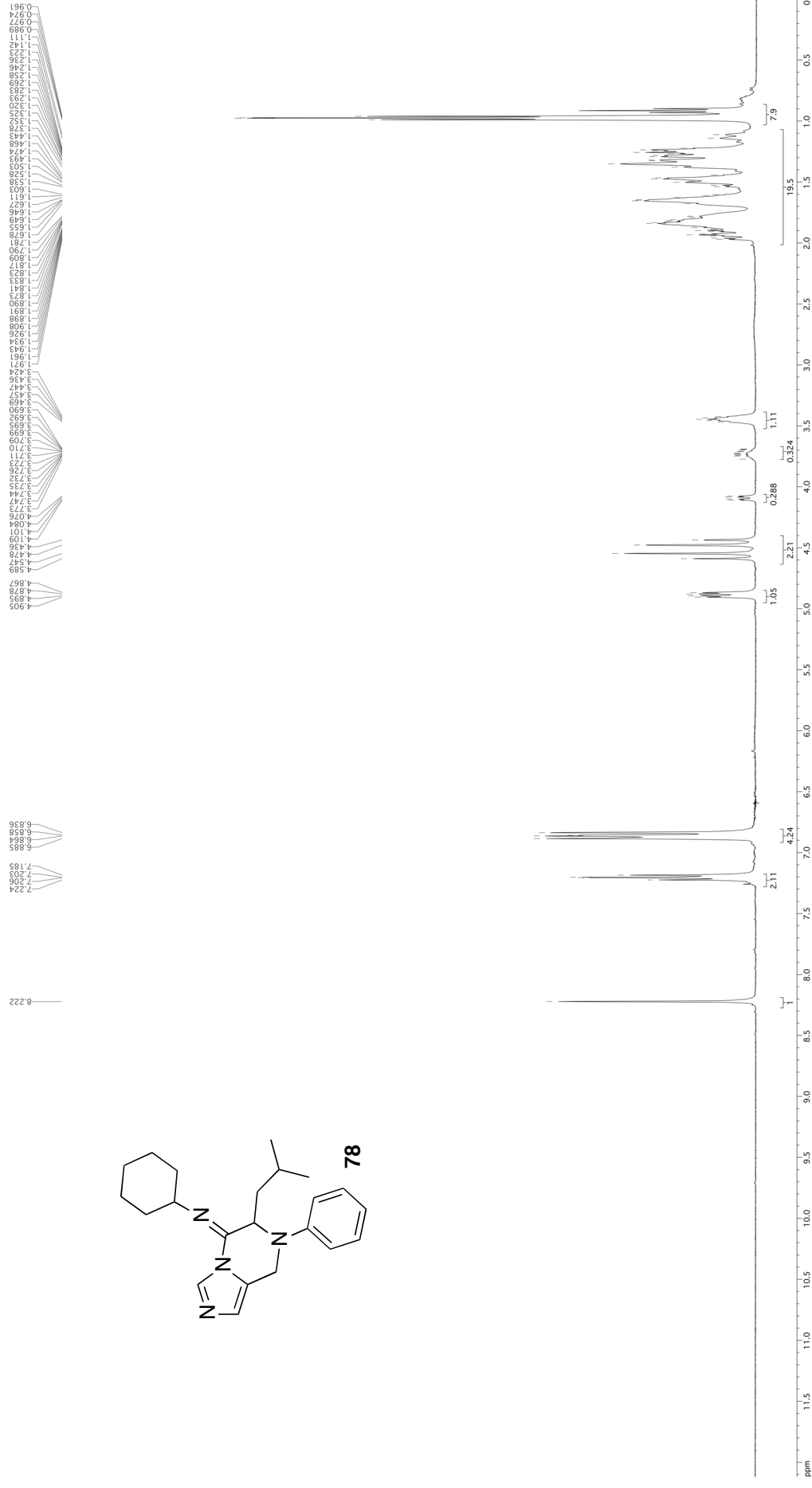
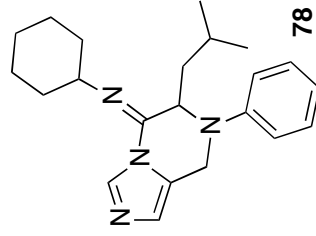
¹H NMR
400 MHz, CDCl₃

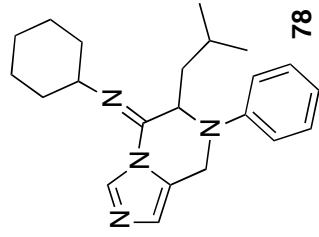


¹³C NMR
100 MHz, CDCl₃

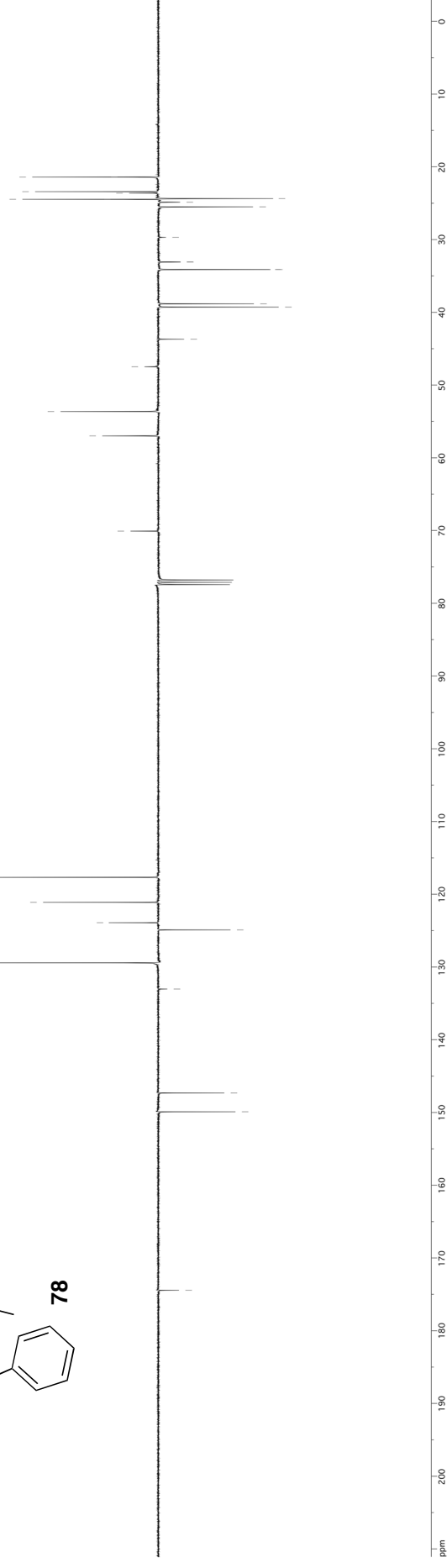


¹H NMR
400 MHz, CDCl₃

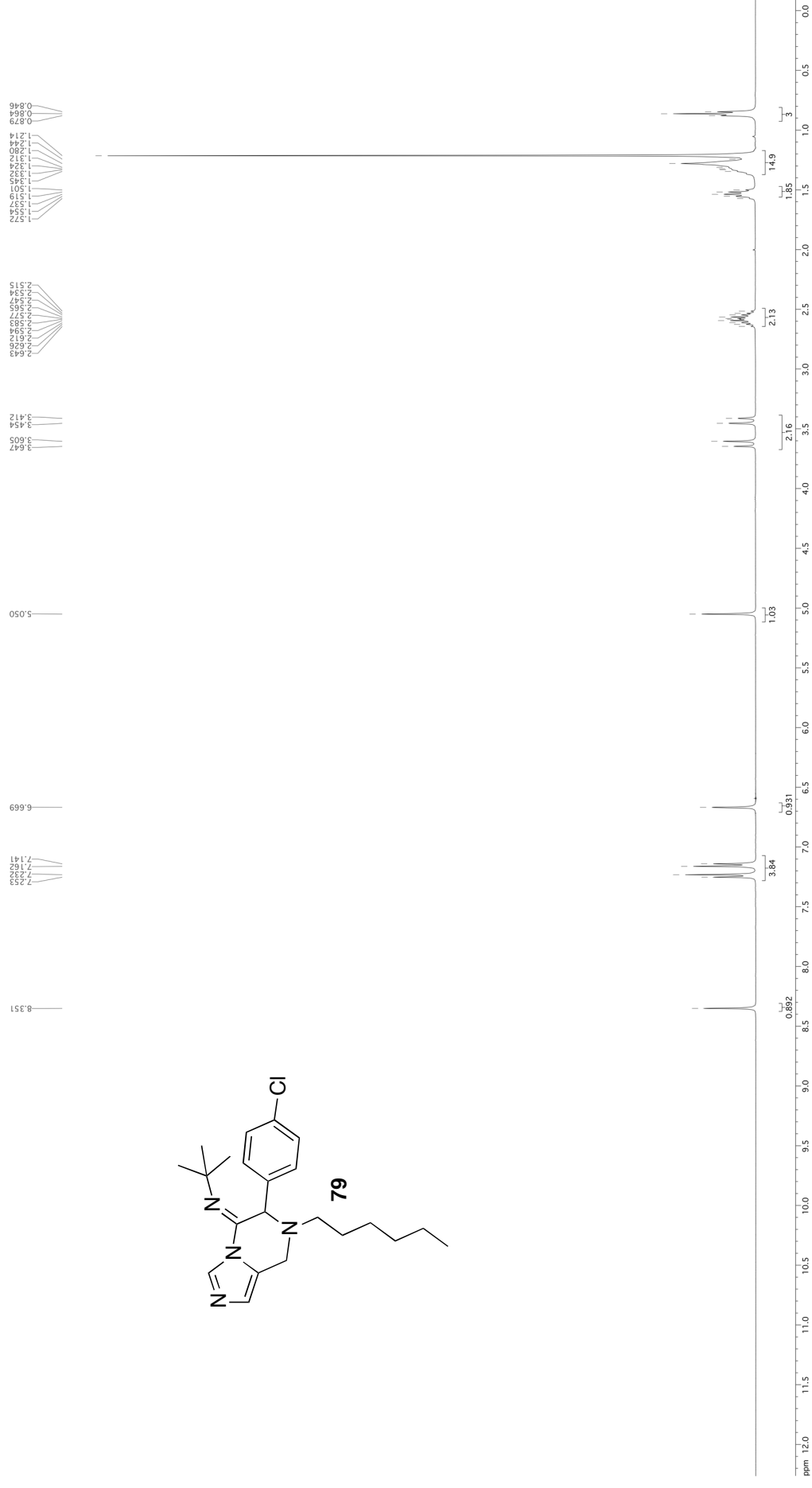
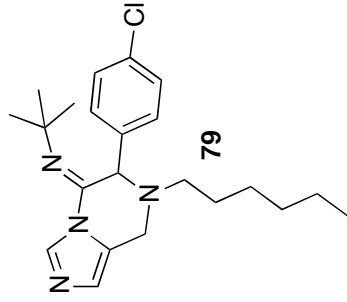




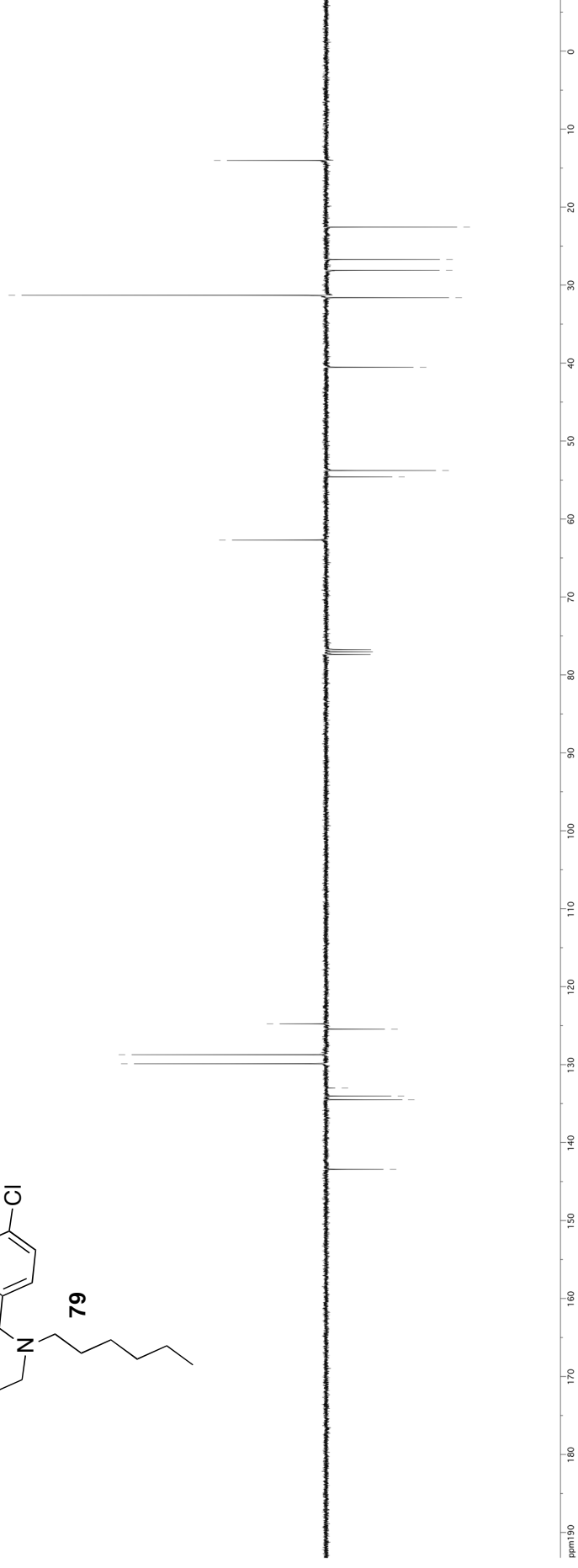
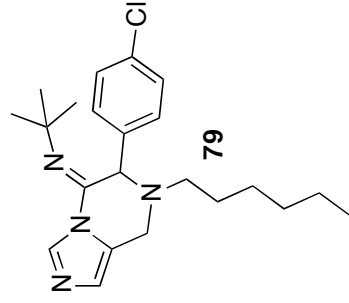
¹³C NMR
100 MHz, CDCl₃

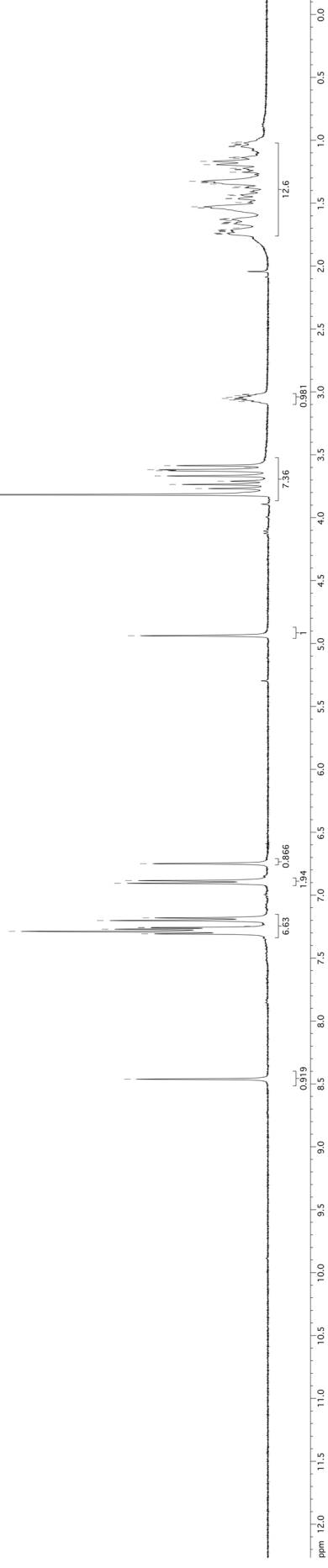
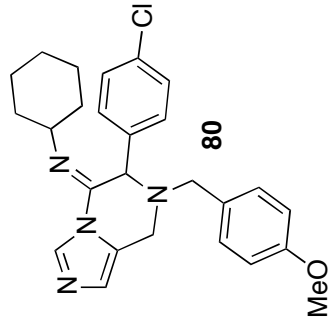


¹H NMR
400 MHz, CDCl₃



¹³C NMR
100 MHz, CDCl₃





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¹H NMR
400 MHz, CDCl₃



^{13}C NMR
100 MHz, CDCl_3

