

Supporting Information

A Concise Synthesis of (*E*)-3-aryl-2,3,4,5-tetrahydro-1*H*-3-benzazonines by Aryne induced [2,3] Stevens Rearrangement of 1,2,3,4-Tetrahydroisoquinolines

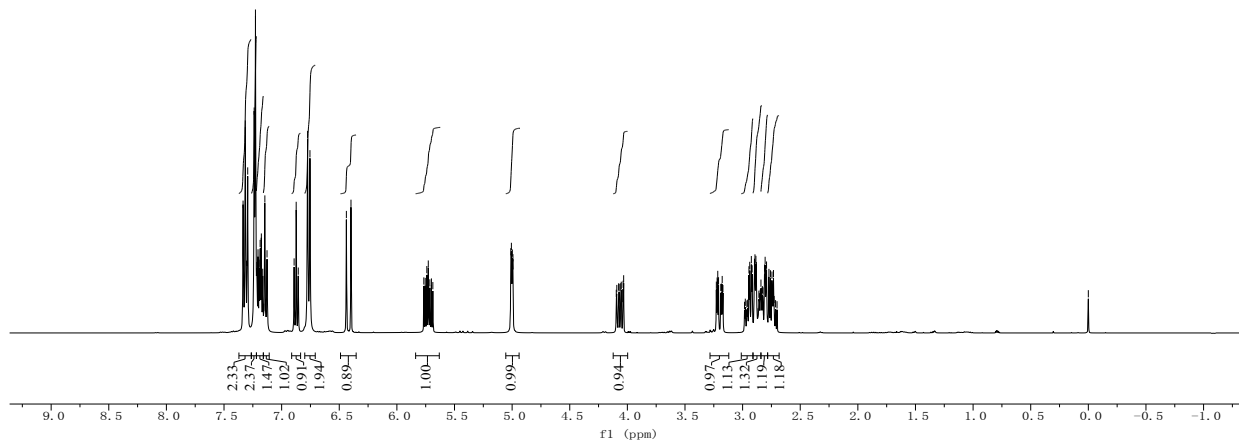
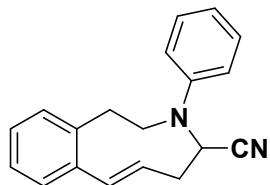
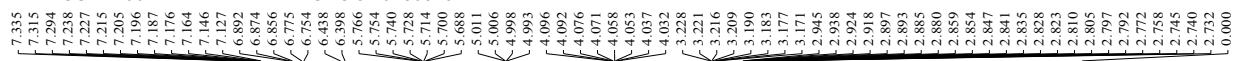
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^aState Key Laboratory of Bioactive Substances and Functions of Natural Medicines, Institute of Materia Medica, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing 100050, P. R. China

*E-mail: liuzhanzhu@imm.ac.cn

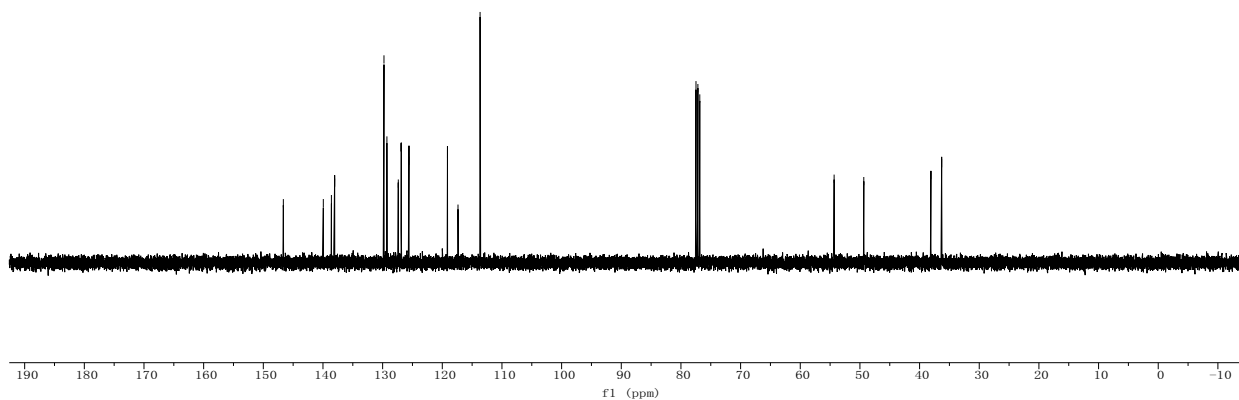
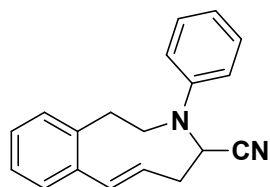
¹H NMR spectra of compound 3a

MERCURY400 HNMR MYT2-14-1 CDCl₃ 20180320



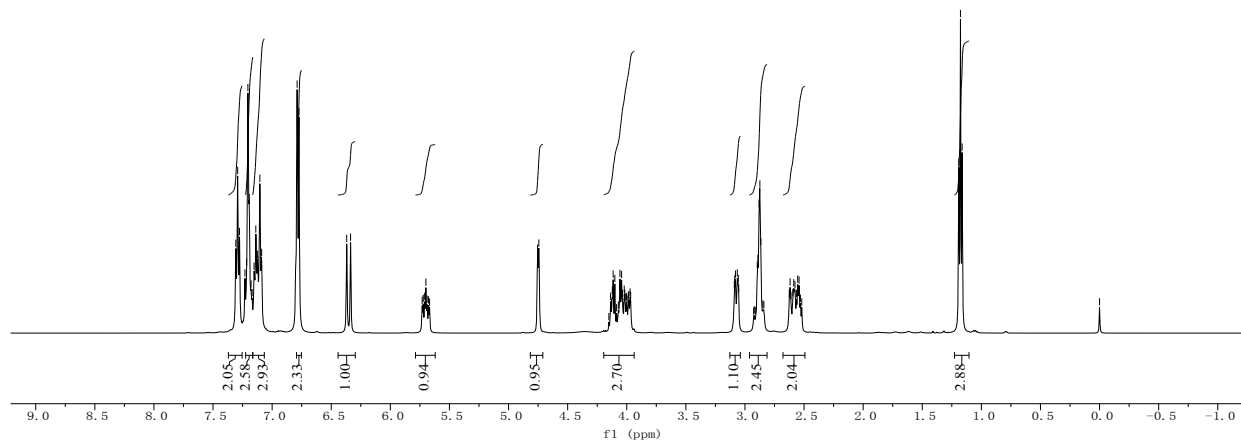
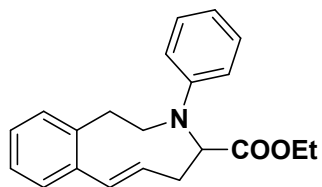
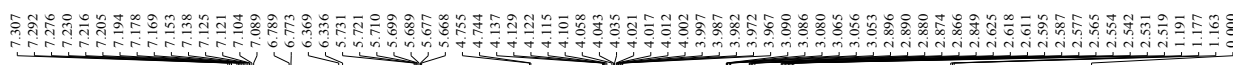
¹³C NMR spectra of compound 3a

MERCURY400 CNMR MYT2-14-1 CDCl₃ 20180323



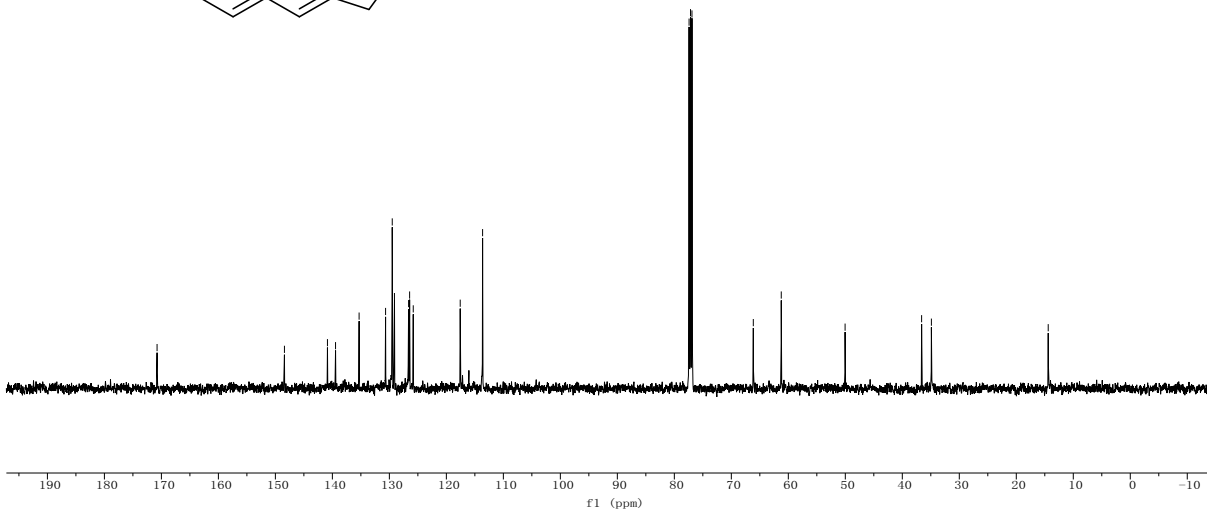
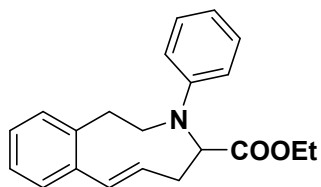
¹H NMR spectra of compound **3b**

MERCURY500 CNMR MYT1-40-2 CDCl3 20180408

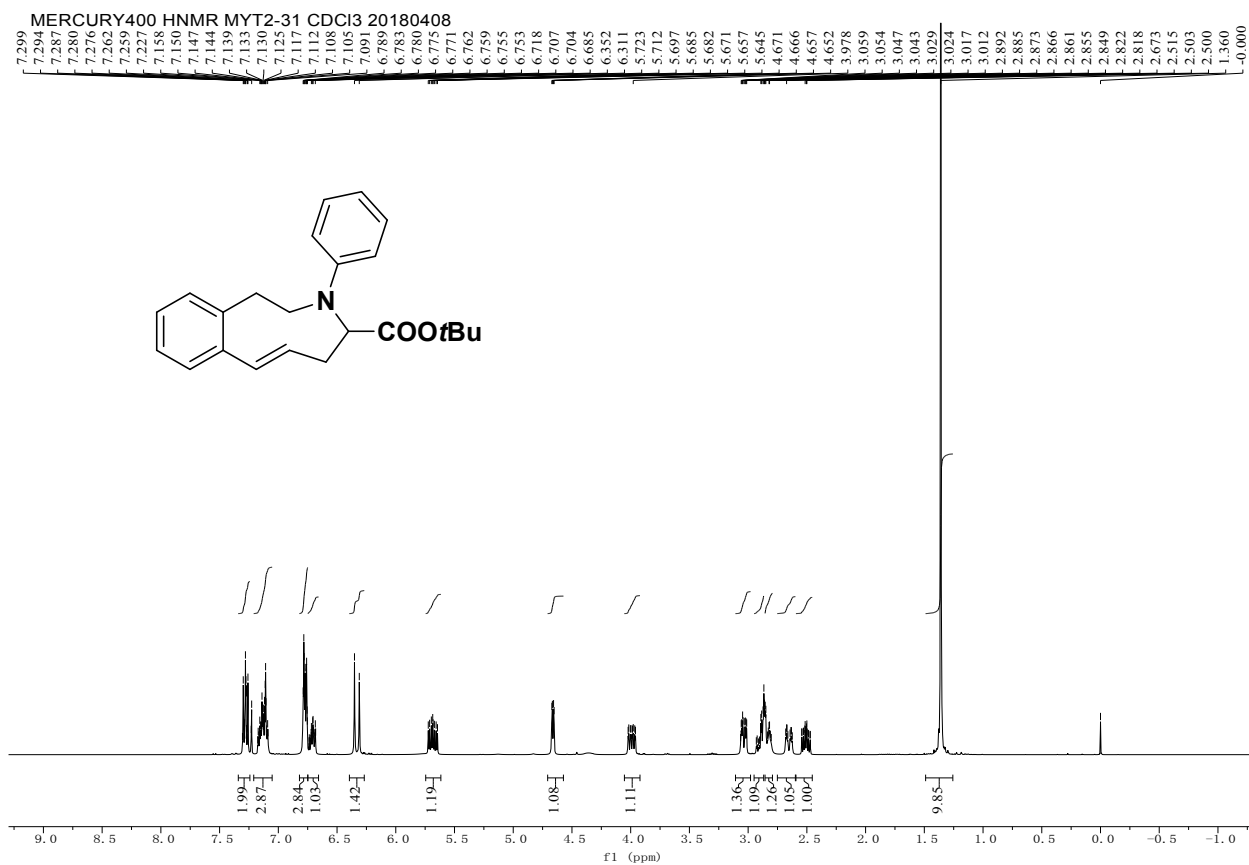


¹³C NMR spectra of compound **3b**

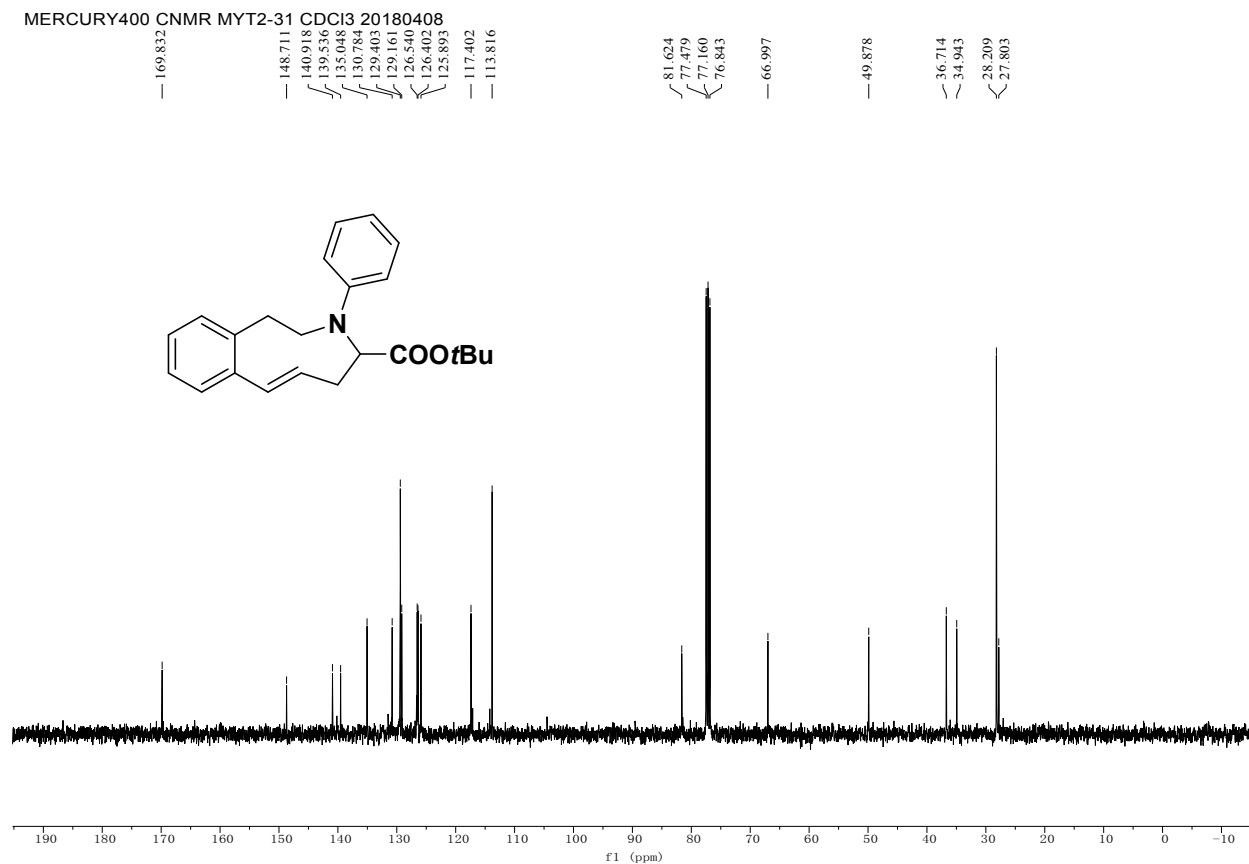
MERCURY500 CNMR MYT1-40-2 CDCl3 20180408



¹H NMR spectra of compound 3c



¹³C NMR spectra of compound 3c

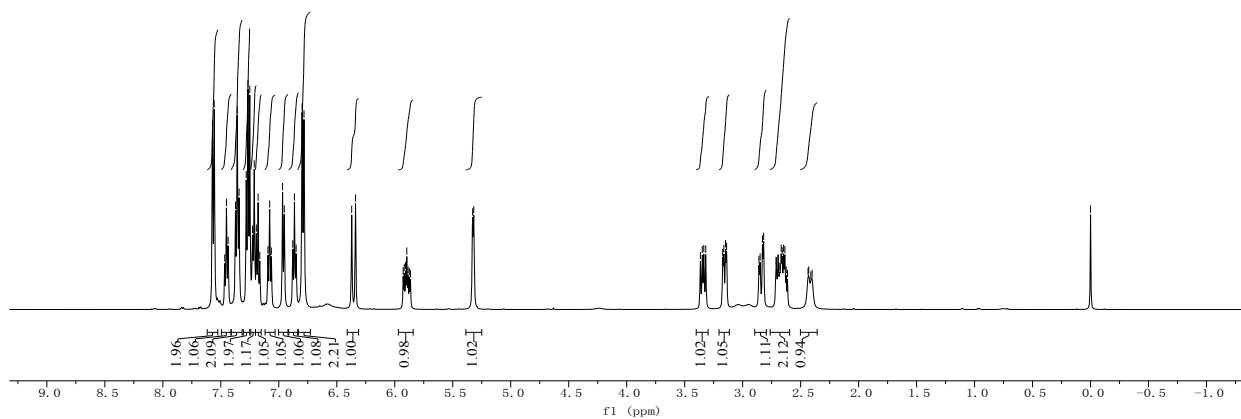
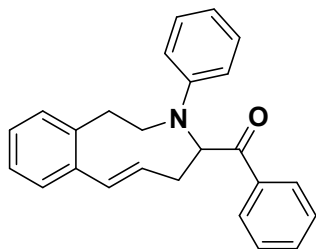


¹H NMR spectra of compound 3d

MERCURY500 HNMR MYT2-32 CDCI3 20180410

7.572
7.557
7.452
7.374
7.358
7.343
7.281
7.266
7.250
7.226
7.212
7.193
7.179
7.079
6.968
6.953
6.865
6.799
6.783
6.371
6.339
5.928
5.918
5.907
5.896
5.885
5.885
5.874
5.865
5.328
5.319
5.319
3.364
3.348
3.335
3.318
3.172
3.162
3.148
3.138
3.138
2.860
2.850
2.829
2.819
2.713
2.708
2.696
2.692
2.680
2.668
2.659
2.647
2.636
2.624
2.614
2.436
2.430
2.412
2.401

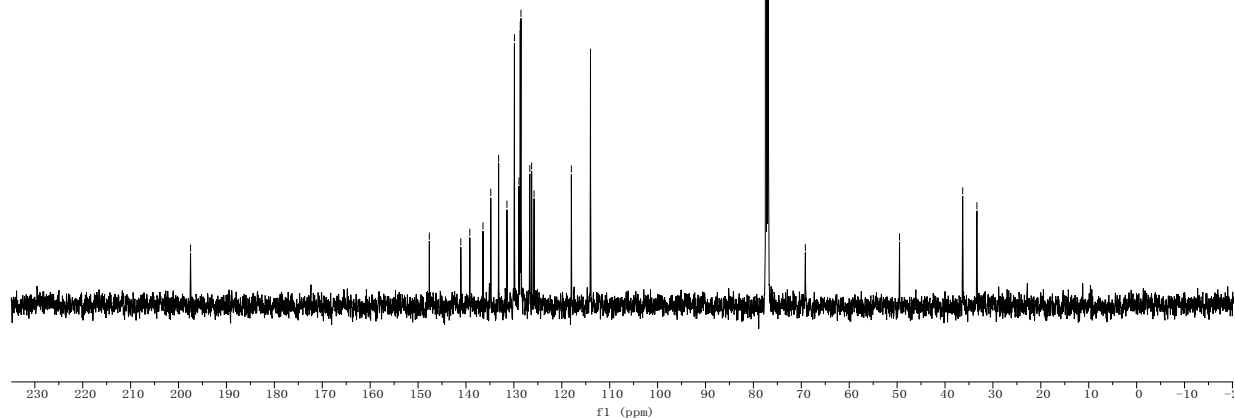
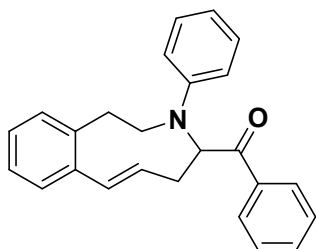
— -0.000



¹³C NMR spectra of compound 3d

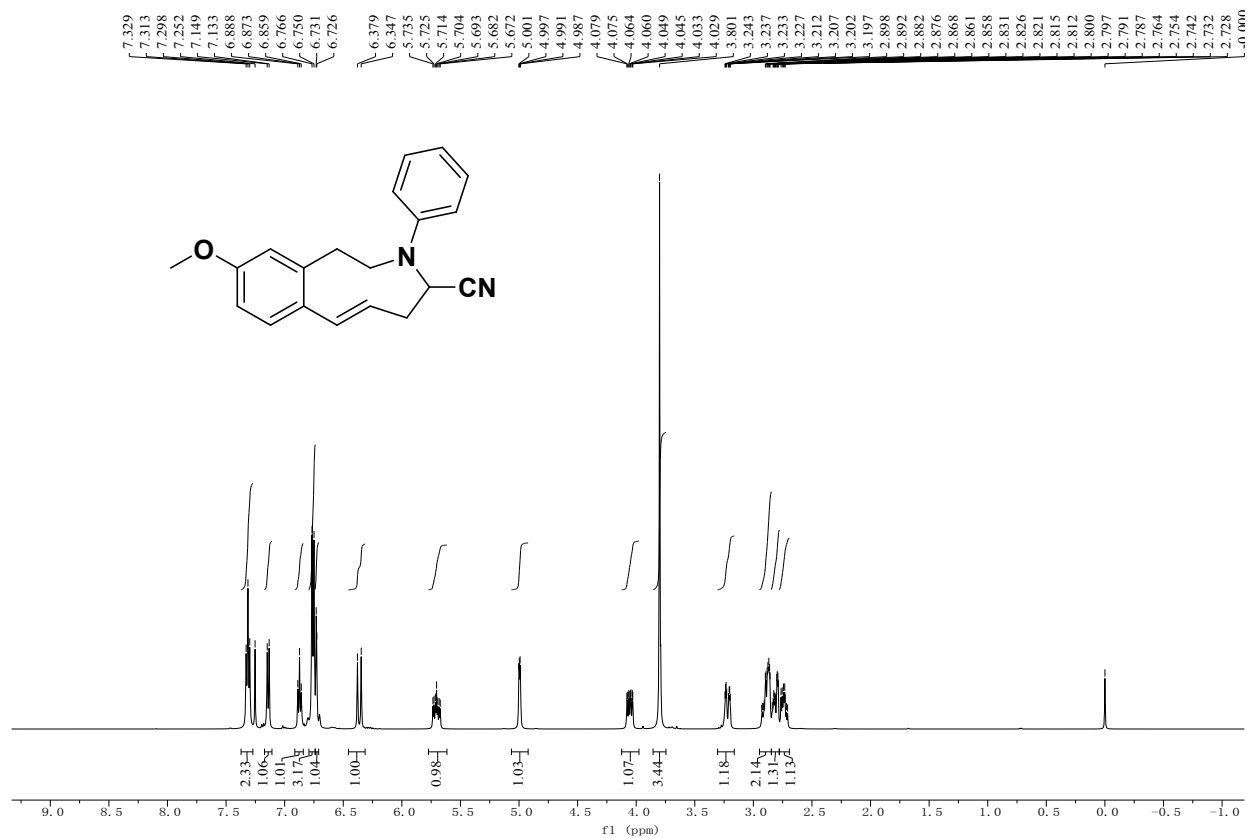
MERCURY500 CNMR MYT2-32 CDCI3 20180410

197.499
147.647
141.079
139.196
136.449
134.824
133.186
131.449
129.884
128.947
128.671
128.523
126.676
126.295
125.782
118.000
114.007
77.415
77.163
76.906
69.154
49.494
36.312
33.342



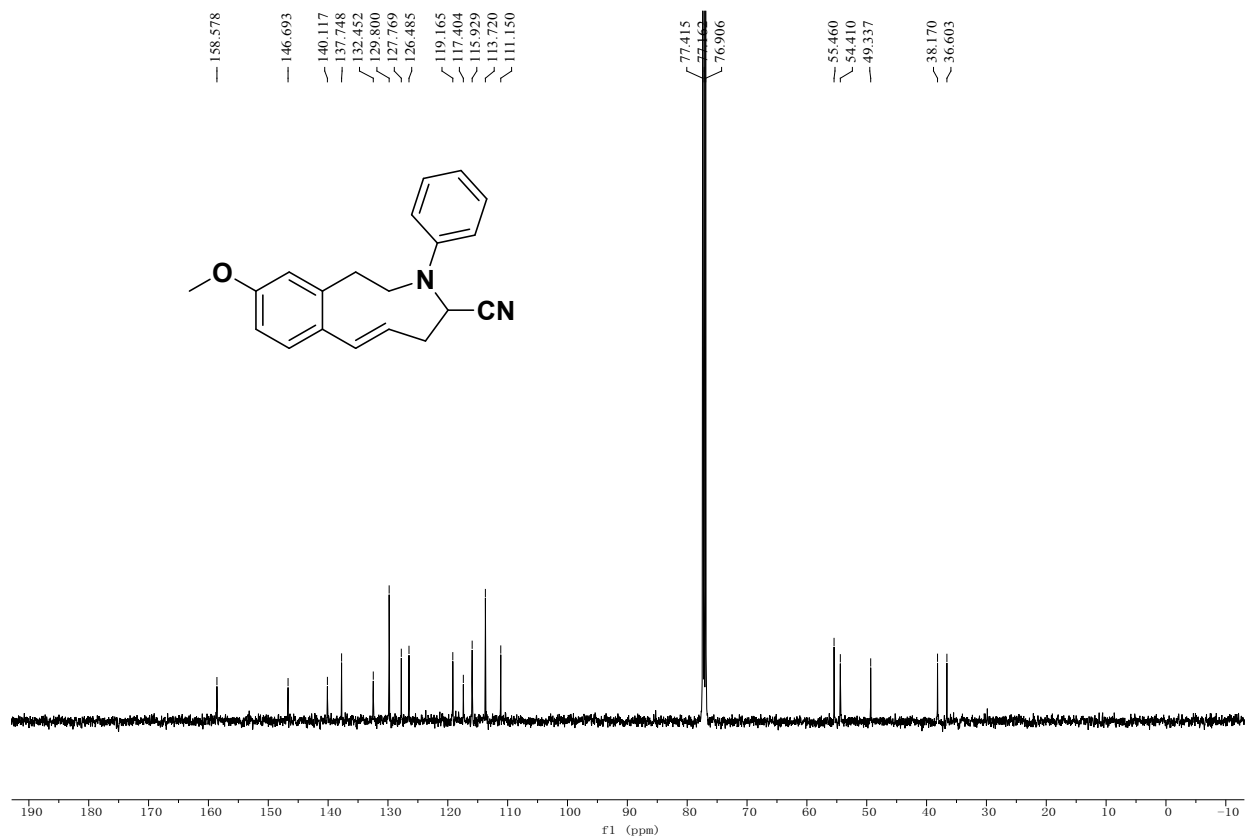
¹H NMR spectra of compound 3e

MERCURY500 HNMR MYT2-23 CDCl₃ 20180326



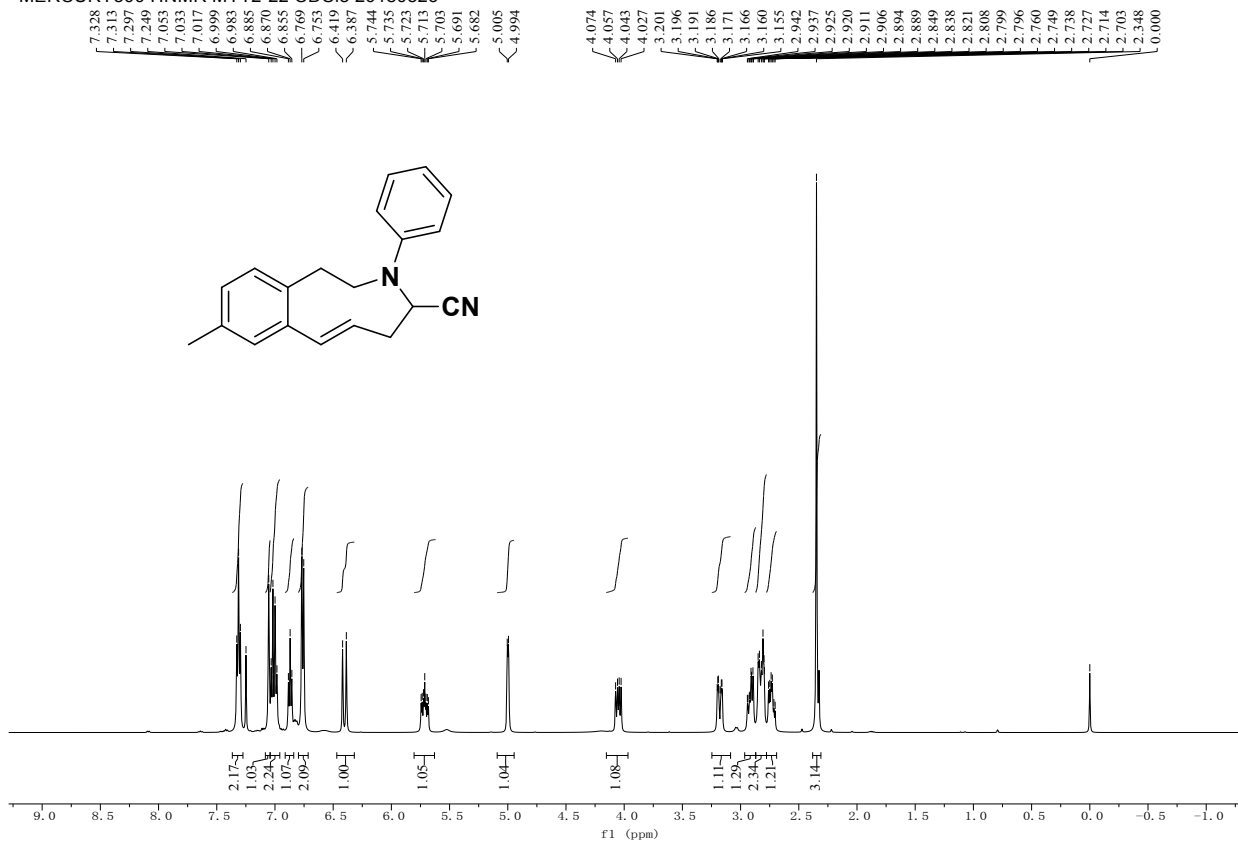
¹³C NMR spectra of compound 3e

MERCURY500 CNMR MYT2-23 CDCl₃ 20180323



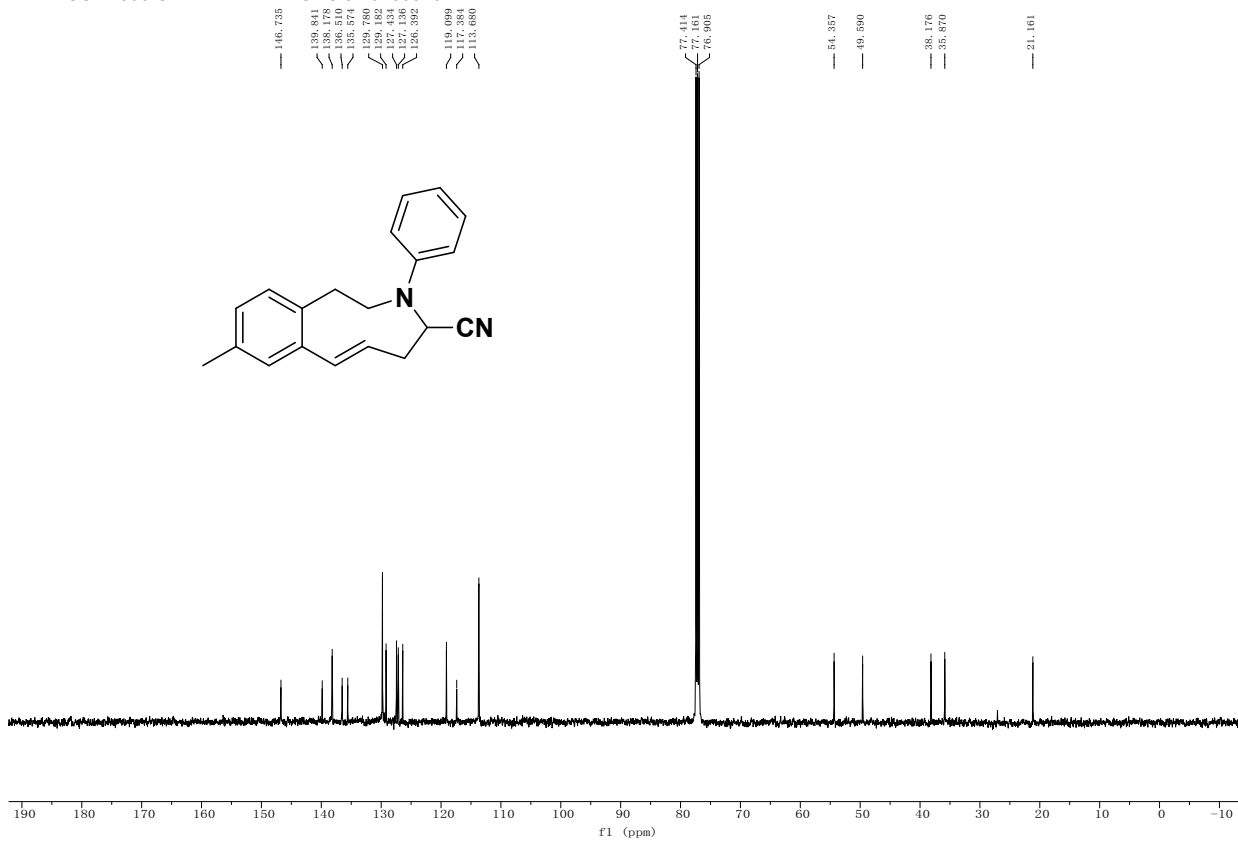
¹H NMR spectra of compound 3f

MERCURY500 HNMR MYT2-22 CDCl₃ 20180326



¹³C NMR spectra of compound 3f

MERCURY500 CNMR MYT2-22 CDCl₃ 20180326

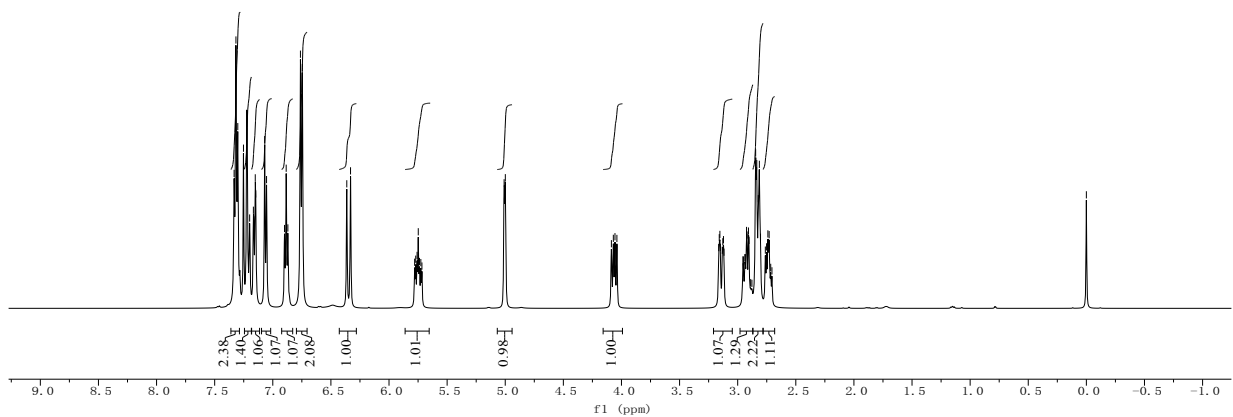
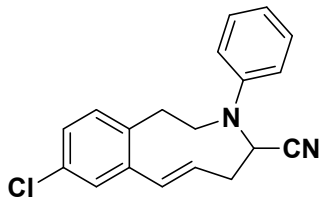


¹H NMR spectra of compound 3g

MERCURY500 HNMR MYT2-38 CDCl₃ 20180326

7.333
7.317
7.301
7.252
7.225
7.220
7.199
7.167
7.162
7.151
7.146
7.070
7.054
6.899
6.885
6.870
6.762
6.746
6.563
6.331
5.780
5.770
5.759
5.748
5.738
5.726
5.717
5.010
4.999

4.087
4.070
4.056
4.039
3.164
3.159
3.153
3.148
3.133
3.128
3.122
3.118
2.955
2.951
2.939
2.934
2.924
2.919
2.907
2.902
2.888
2.878
2.845
2.836
2.823
2.814
2.804
2.762
2.752
2.740
2.729
2.716
2.705
0.000



¹³C NMR spectra of compound 3g

MERCURY500 CNMR MYT2-38 CDCl₃ 20180326

146.514
141.464
137.169
136.764
132.450
130.548
129.853
128.152
126.865
125.834
119.368
117.239
113.725

77.414

77.160

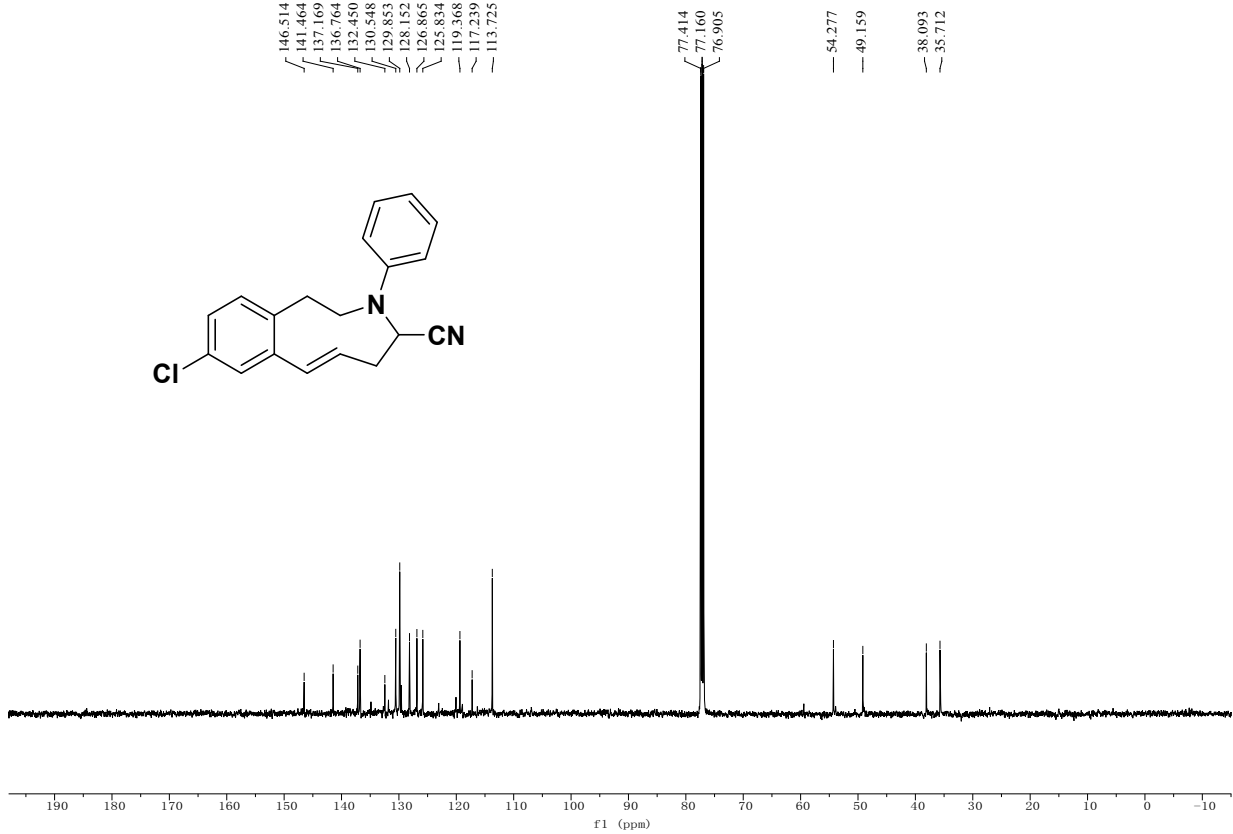
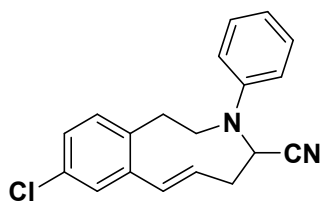
76.905

54.277

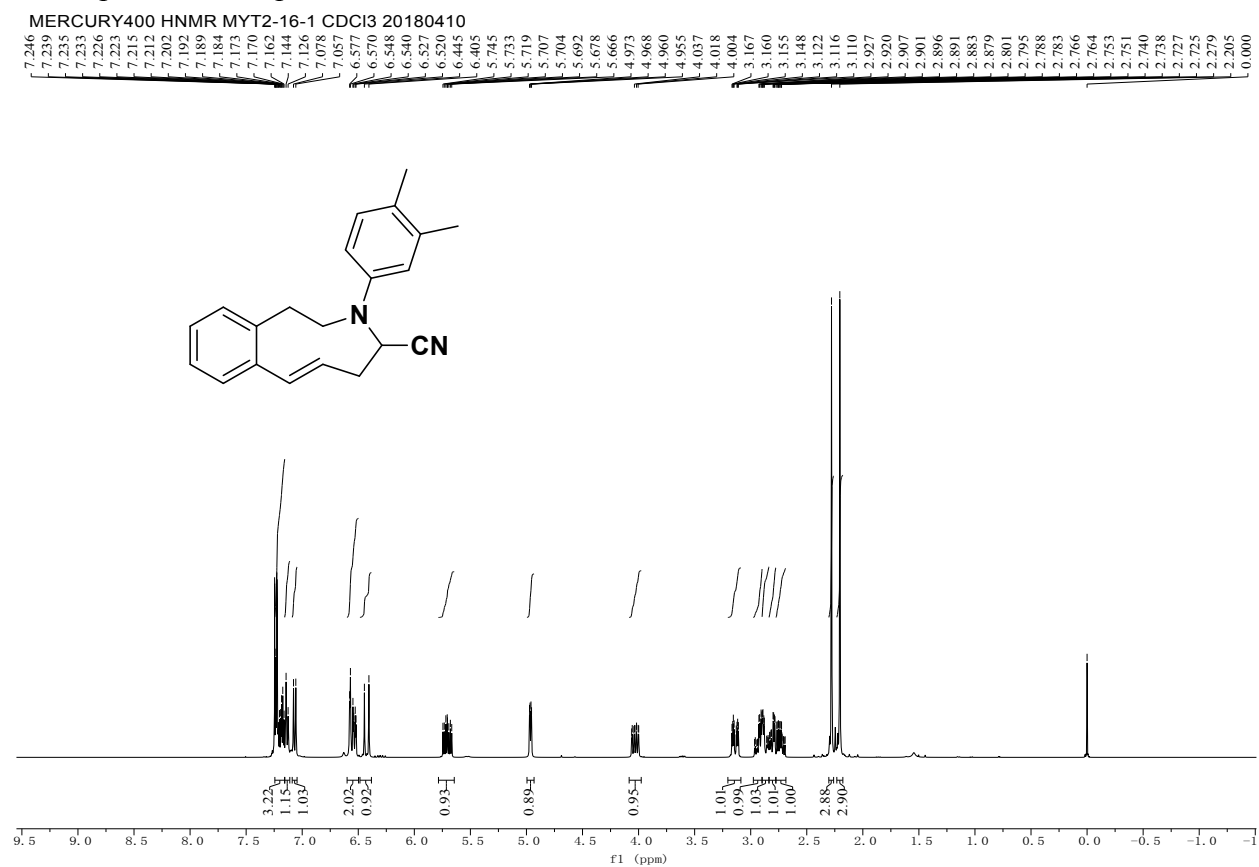
49.159

38.093

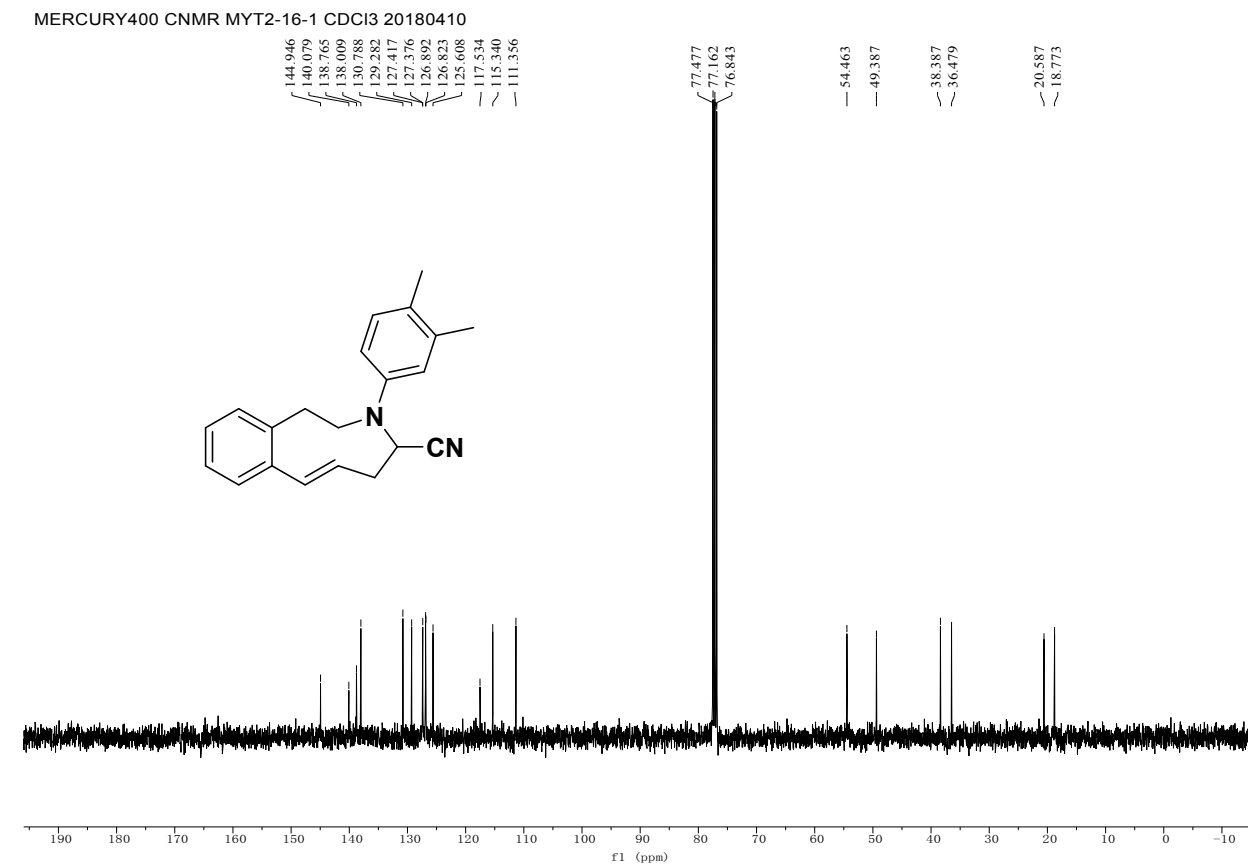
35.712



¹H NMR spectra of compound 3h

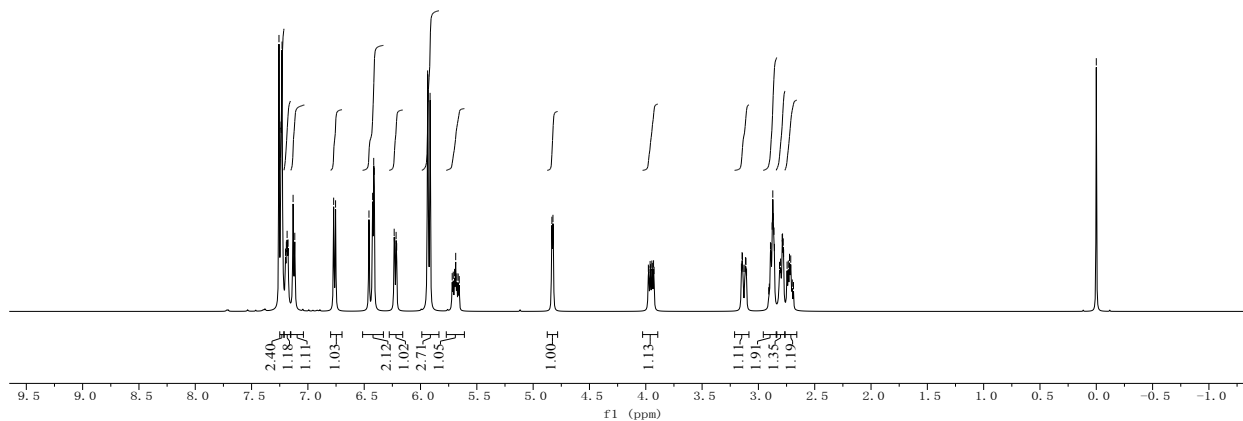
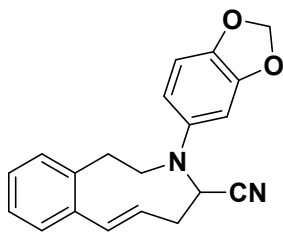
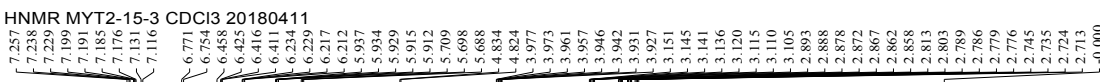


¹³C NMR spectra of compound 3h



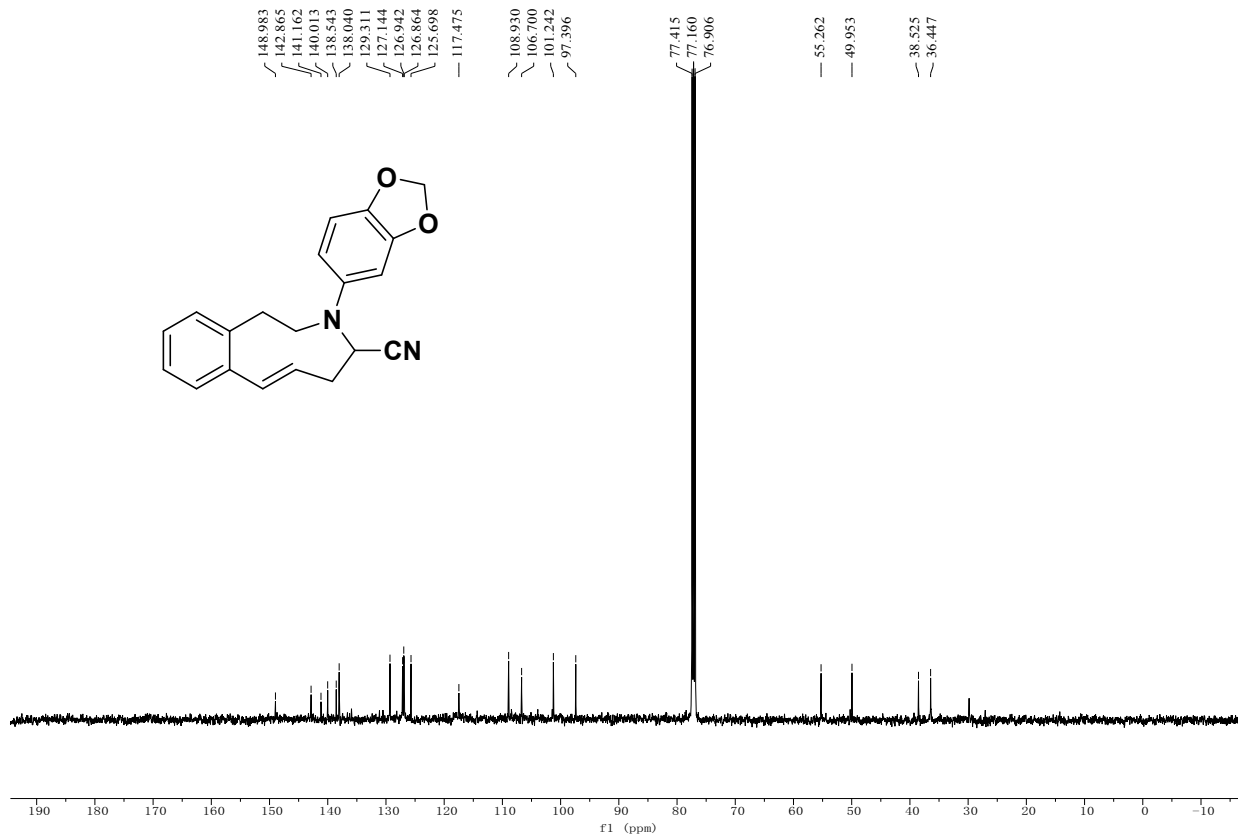
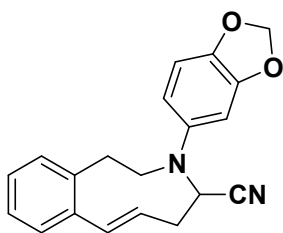
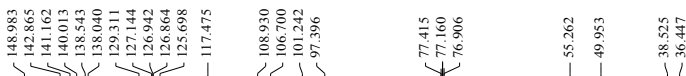
¹H NMR spectra of compound 3i

MERCURY500 HNMR MYT2-15-3 CDCl3 20180411



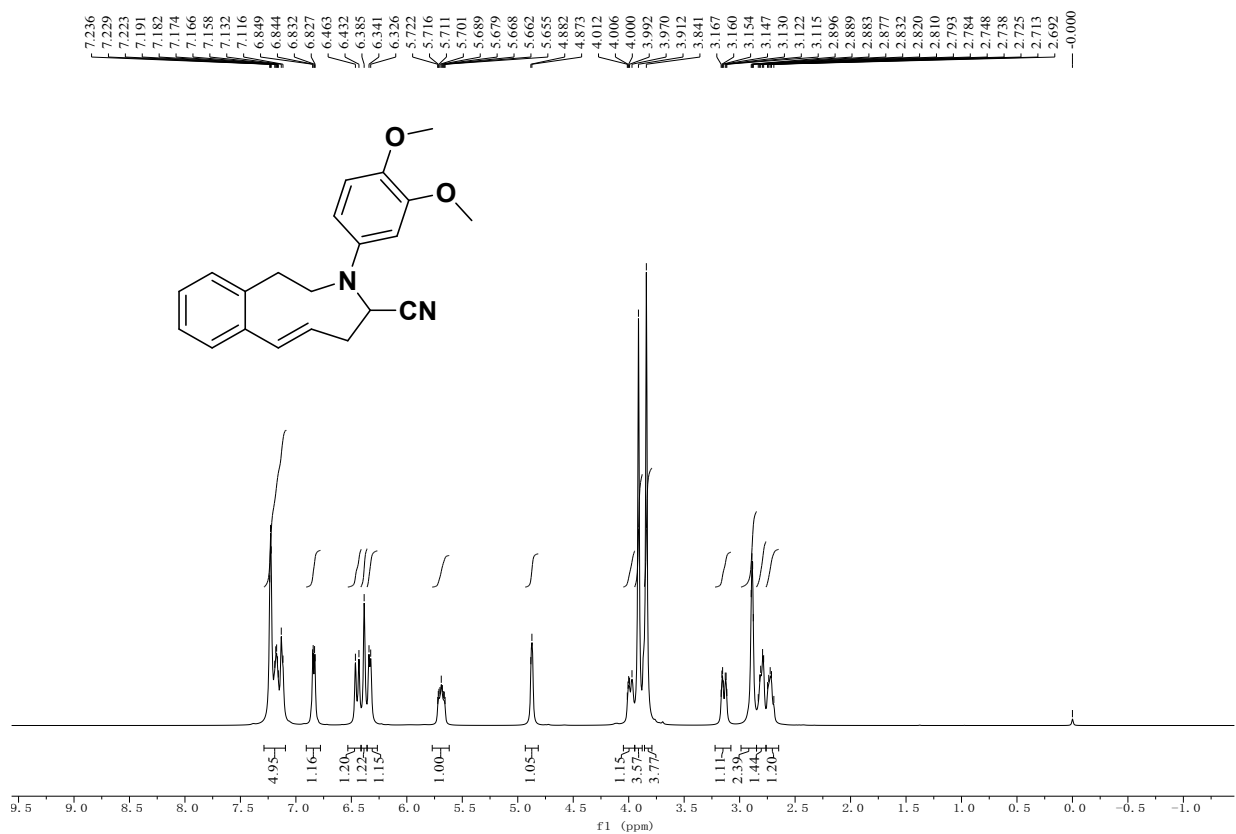
¹³C NMR spectra of compound 3i

MERCURY500 CNMR MYT2-15-3 CDCl3 20180411



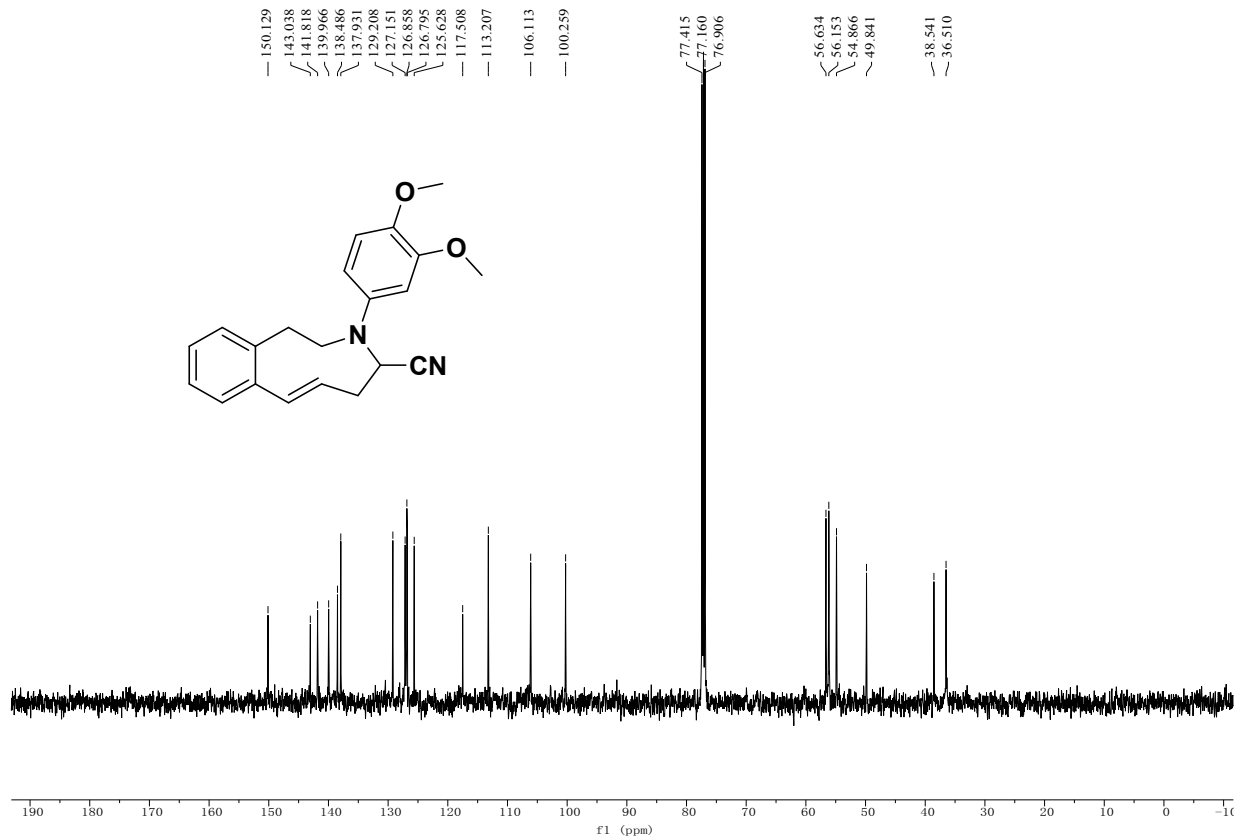
¹H NMR spectra of compound **3j**

MERCURY500 HNMR MYT3-44 CDCl₃ 20180918



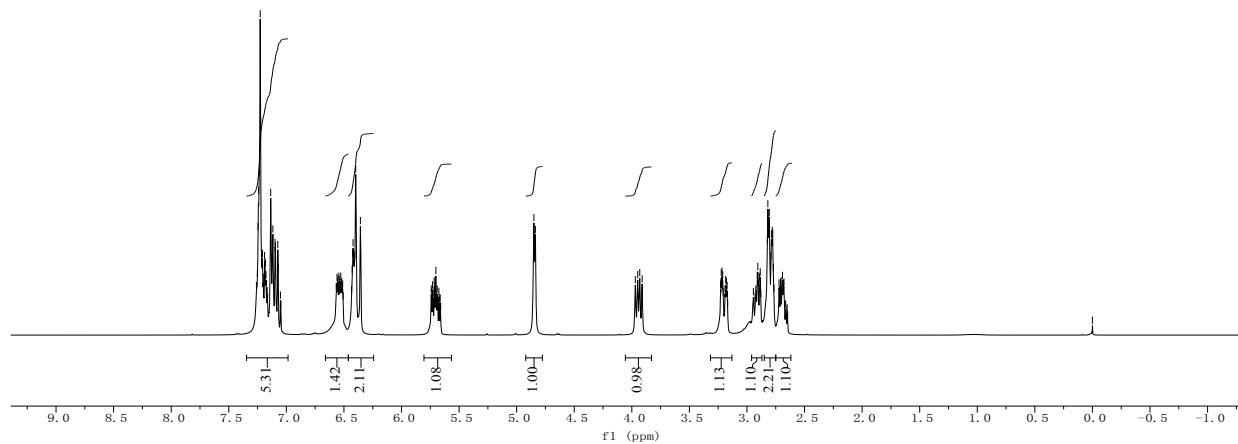
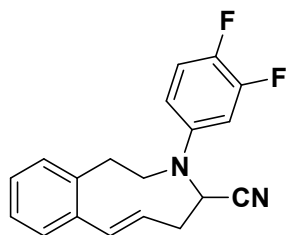
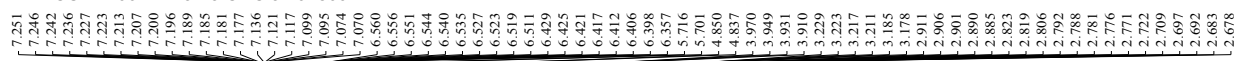
¹³C NMR spectra of compound **3j**

MERCURY500 CNMR MYT3-44 CDCl₃ 20180918



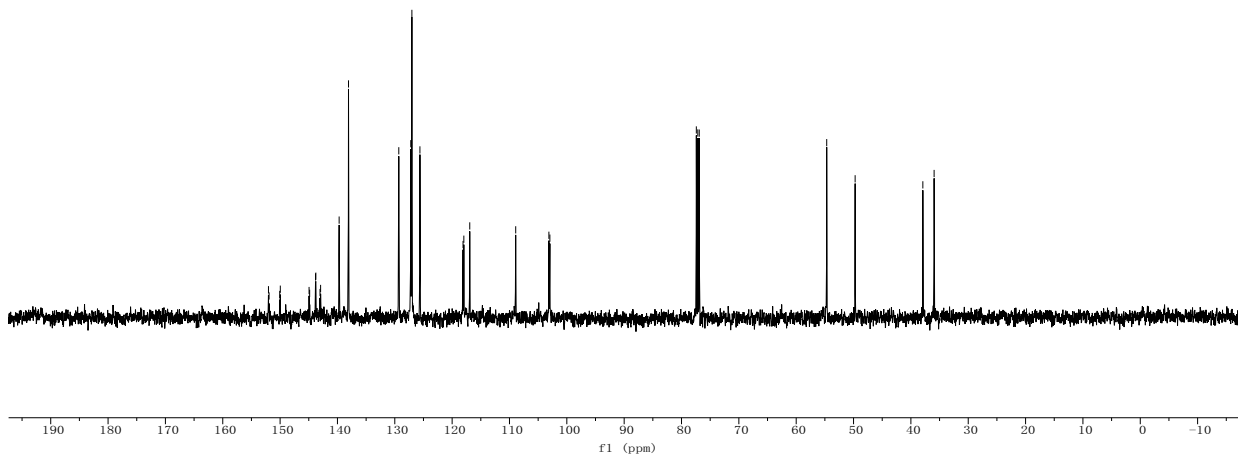
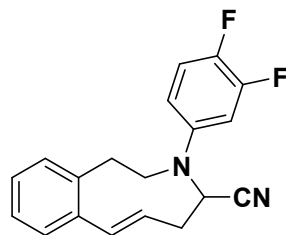
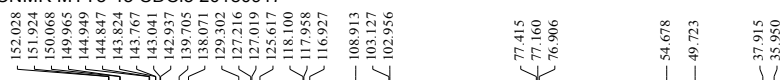
¹H NMR spectra of compound 3k

MERCURY400 MYT3-43 CDCl₃ 20180917

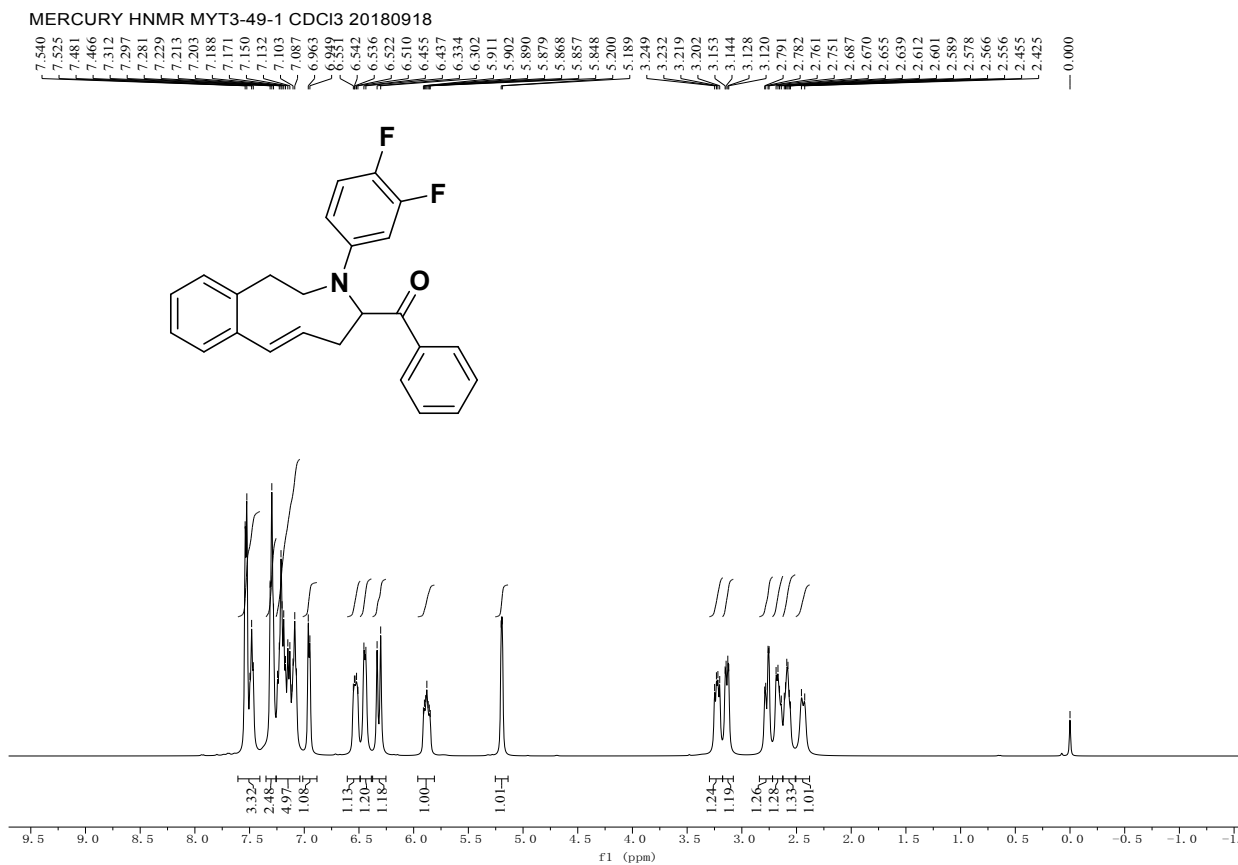


¹³C NMR spectra of compound 3k

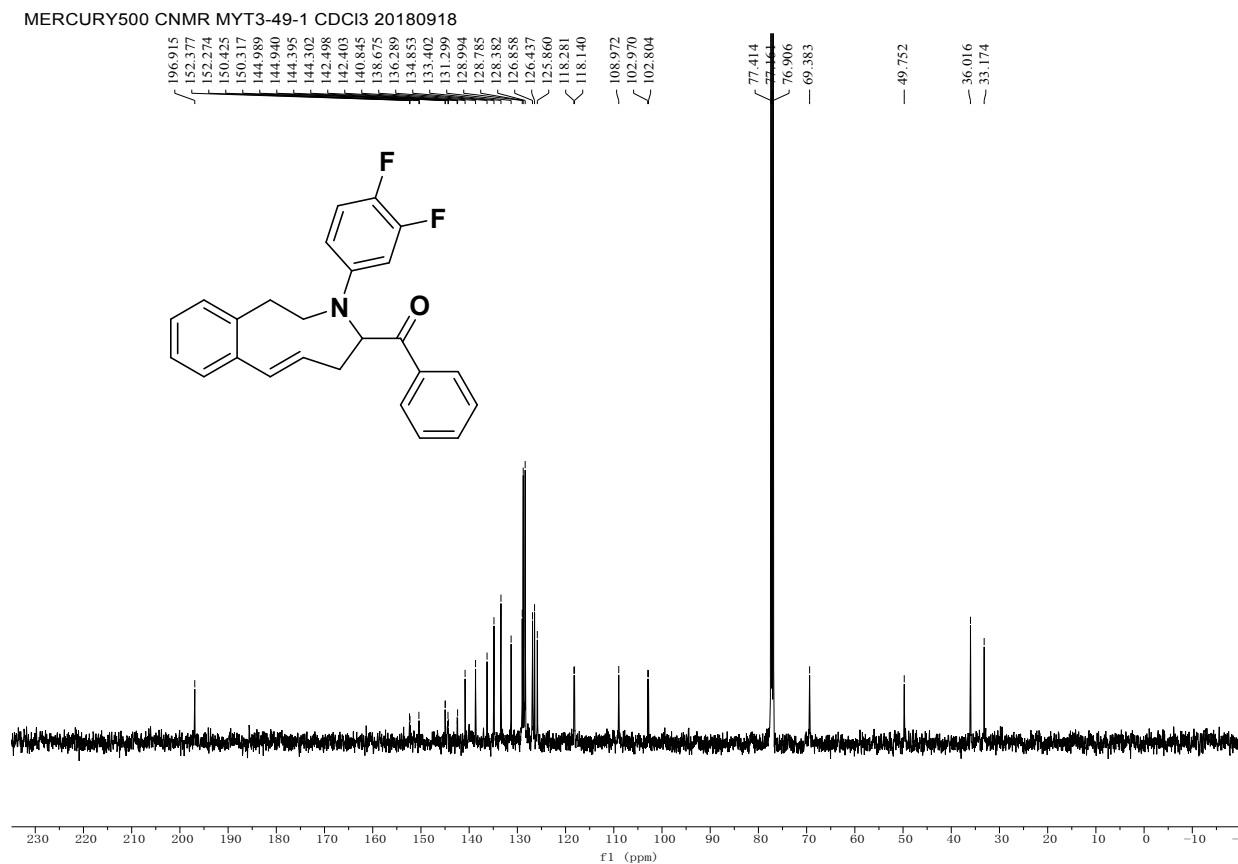
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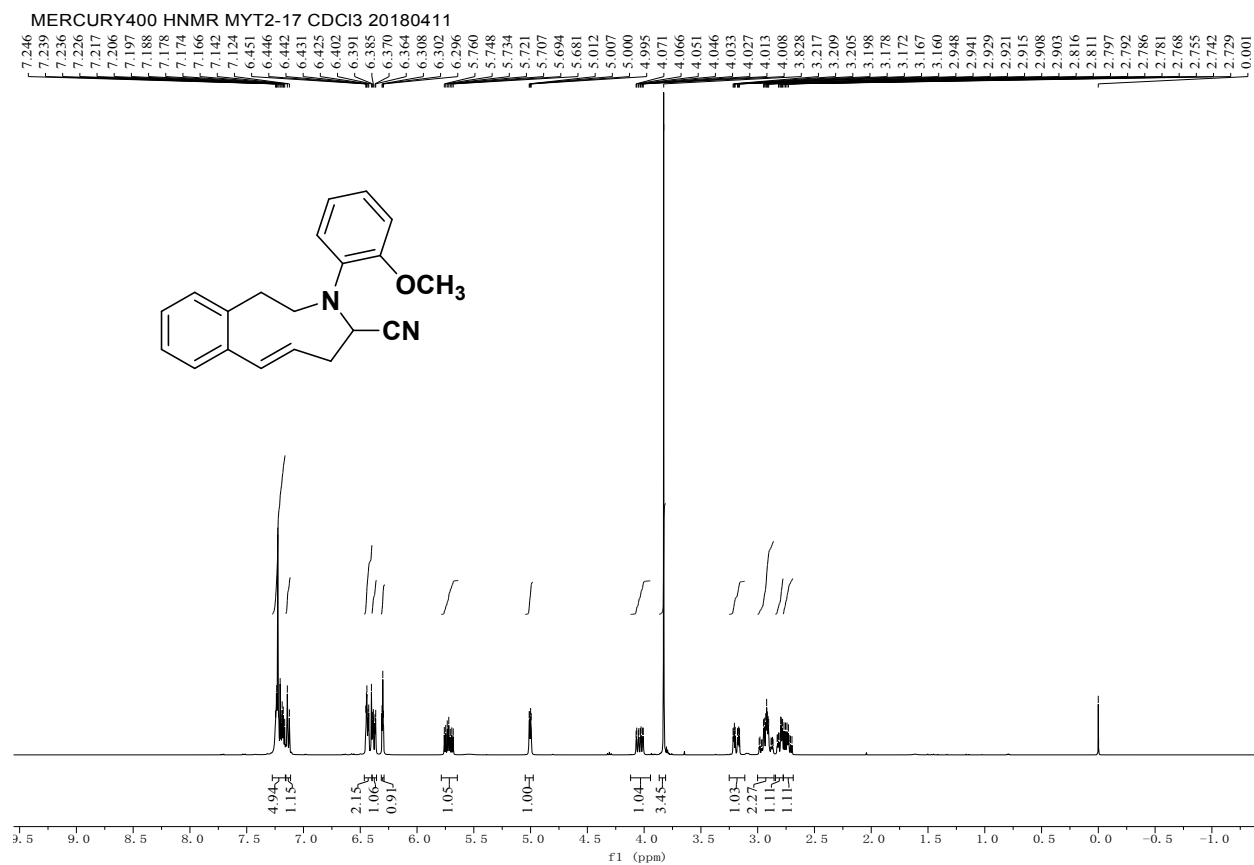
¹H NMR spectra of compound 31



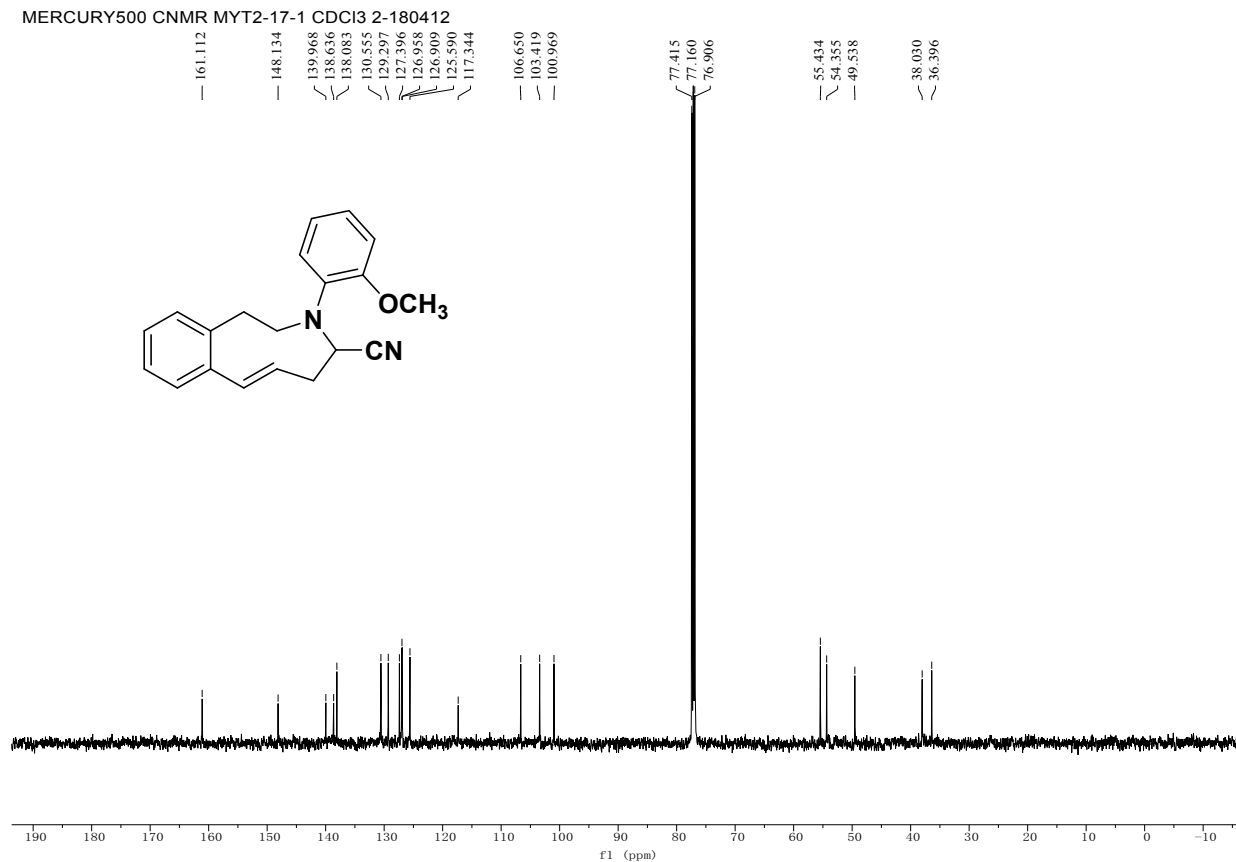
¹³C NMR spectra of compound 31



¹H NMR spectra of compound **3m**

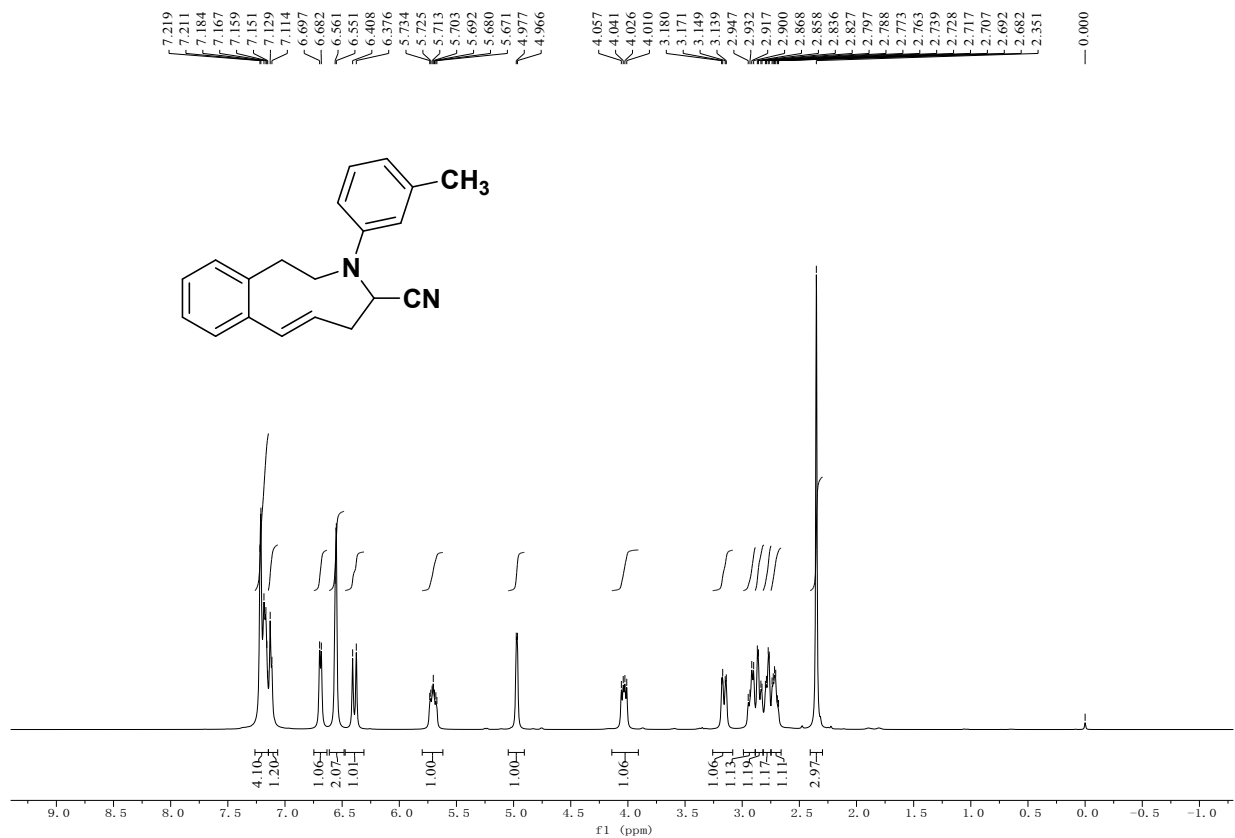


¹³C NMR spectra of compound **3m**



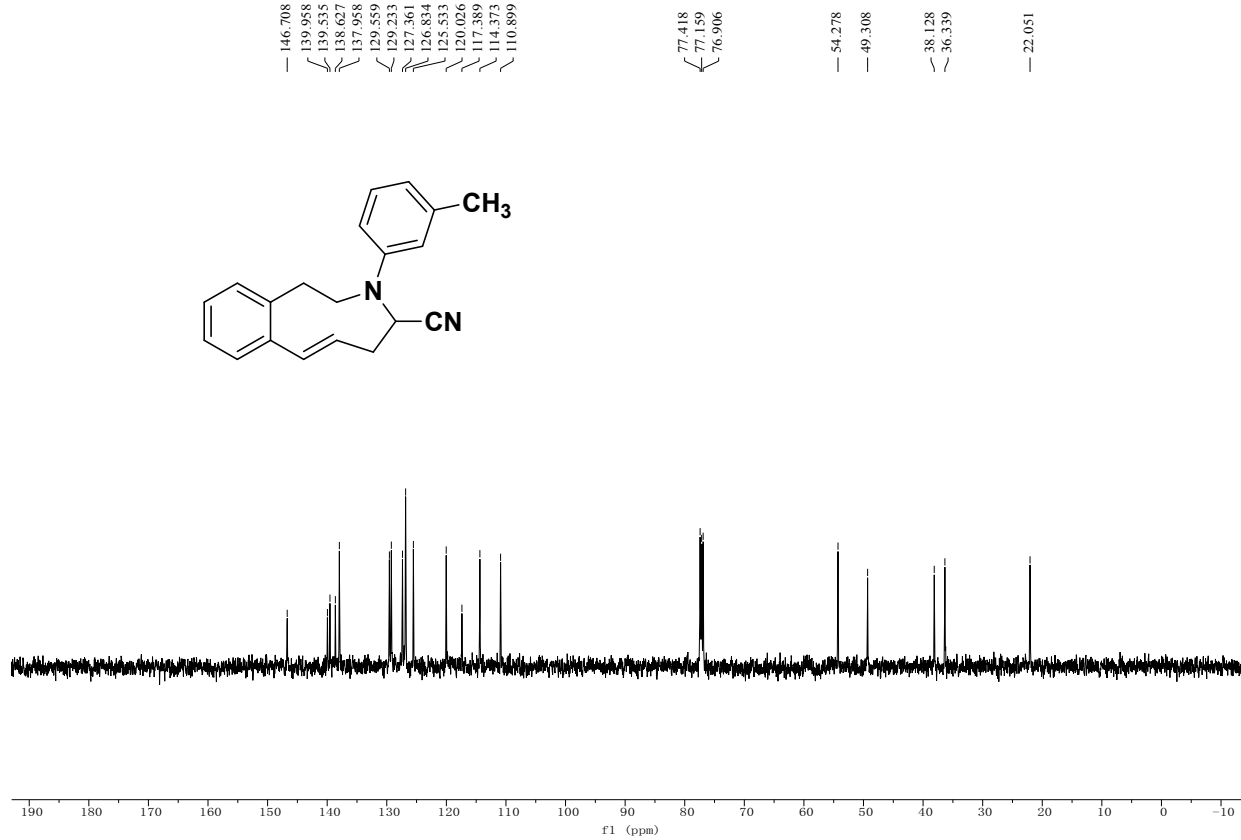
¹H NMR spectra of compound **3n**

MERCURY500 MYT3-46-3 CDCl₃ 20180914

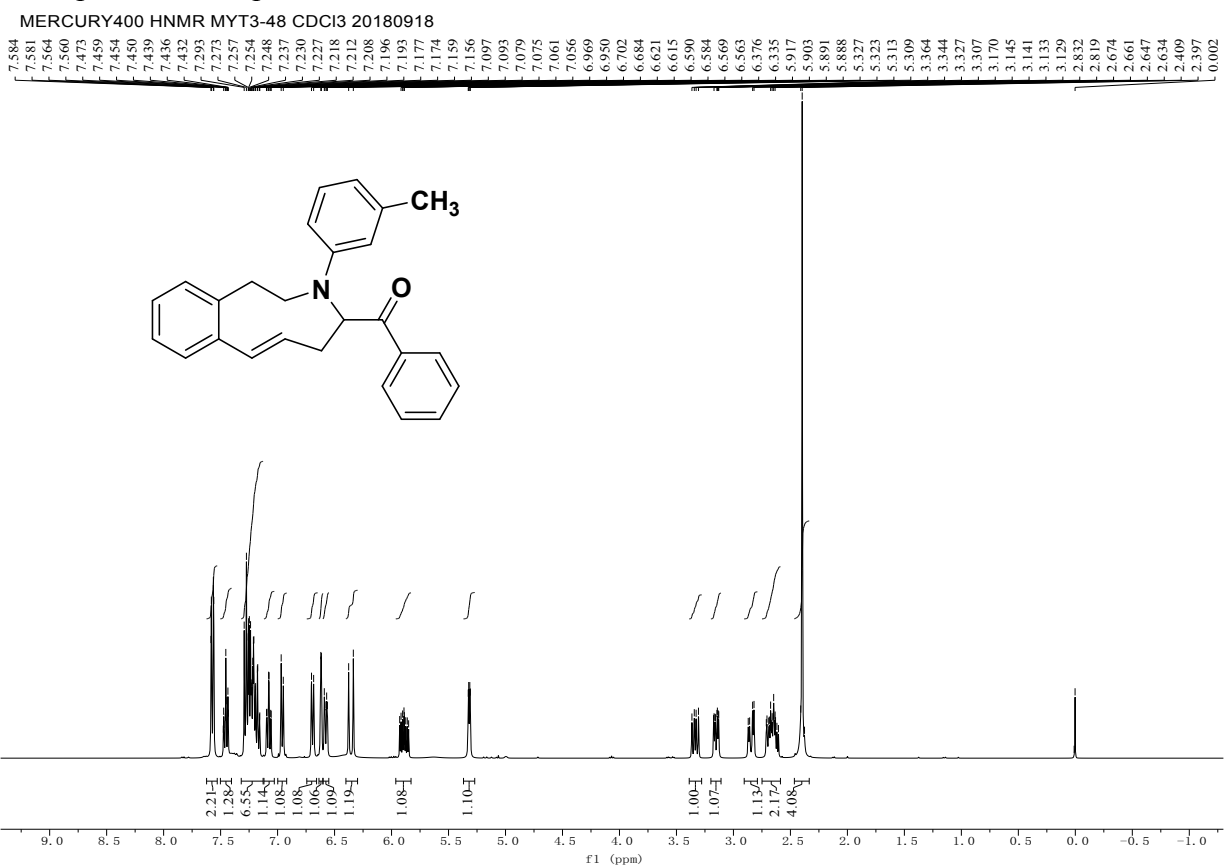


¹³C NMR spectra of compound **3n**

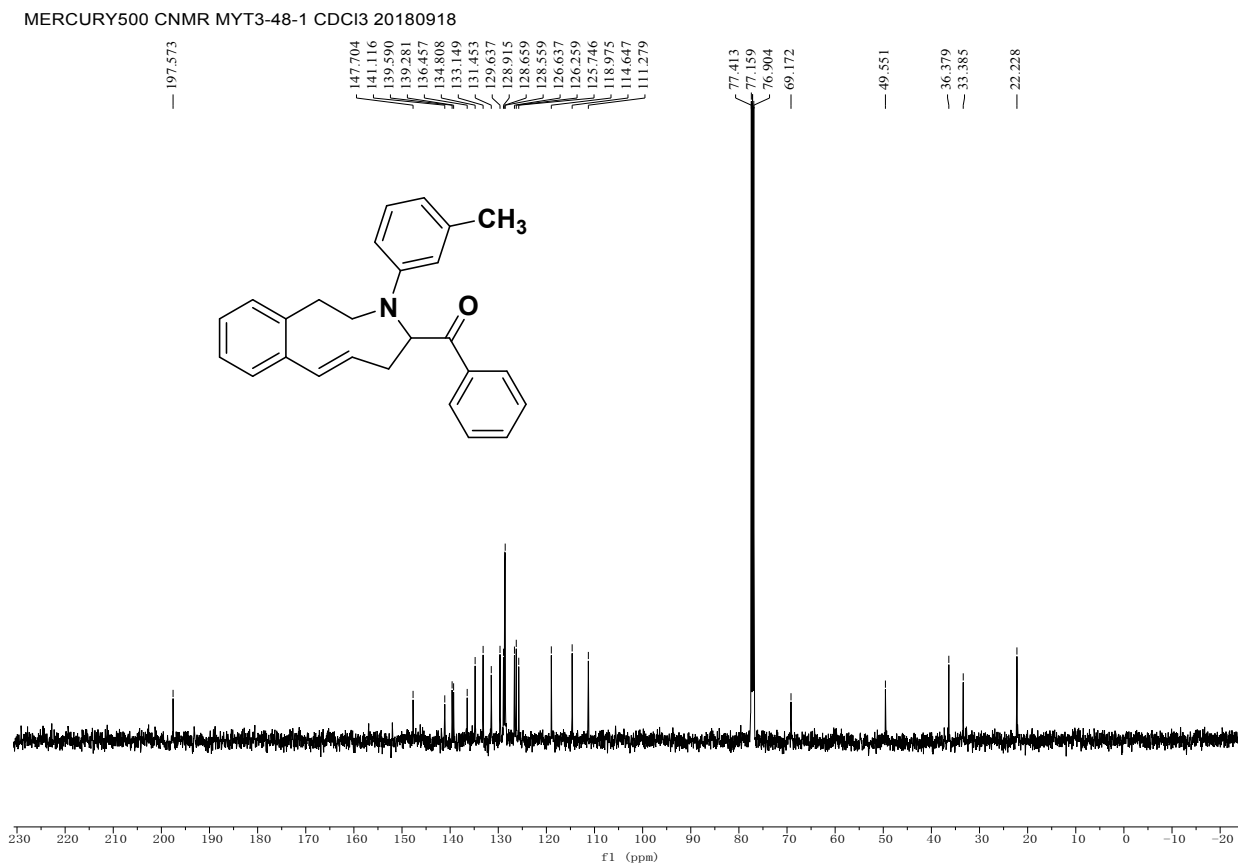
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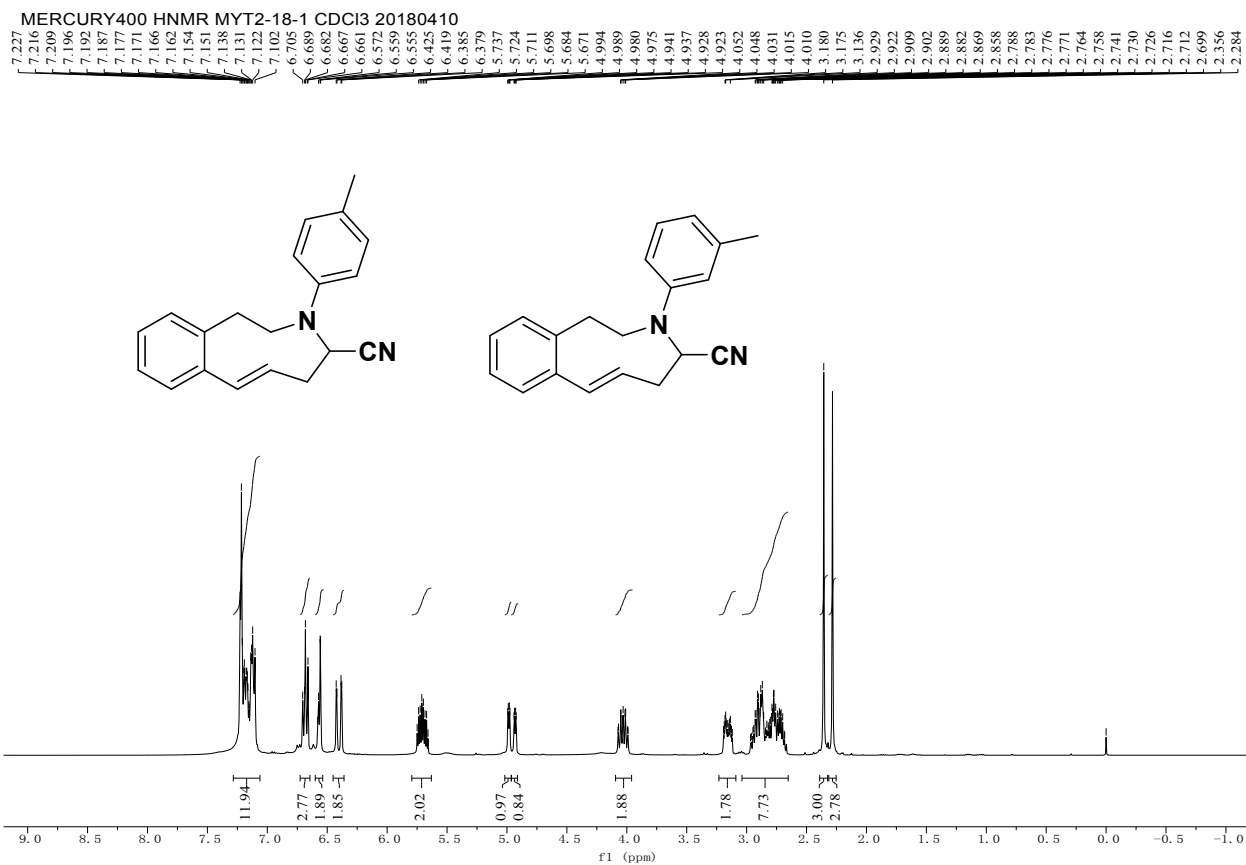
¹H NMR spectra of compound **3o**



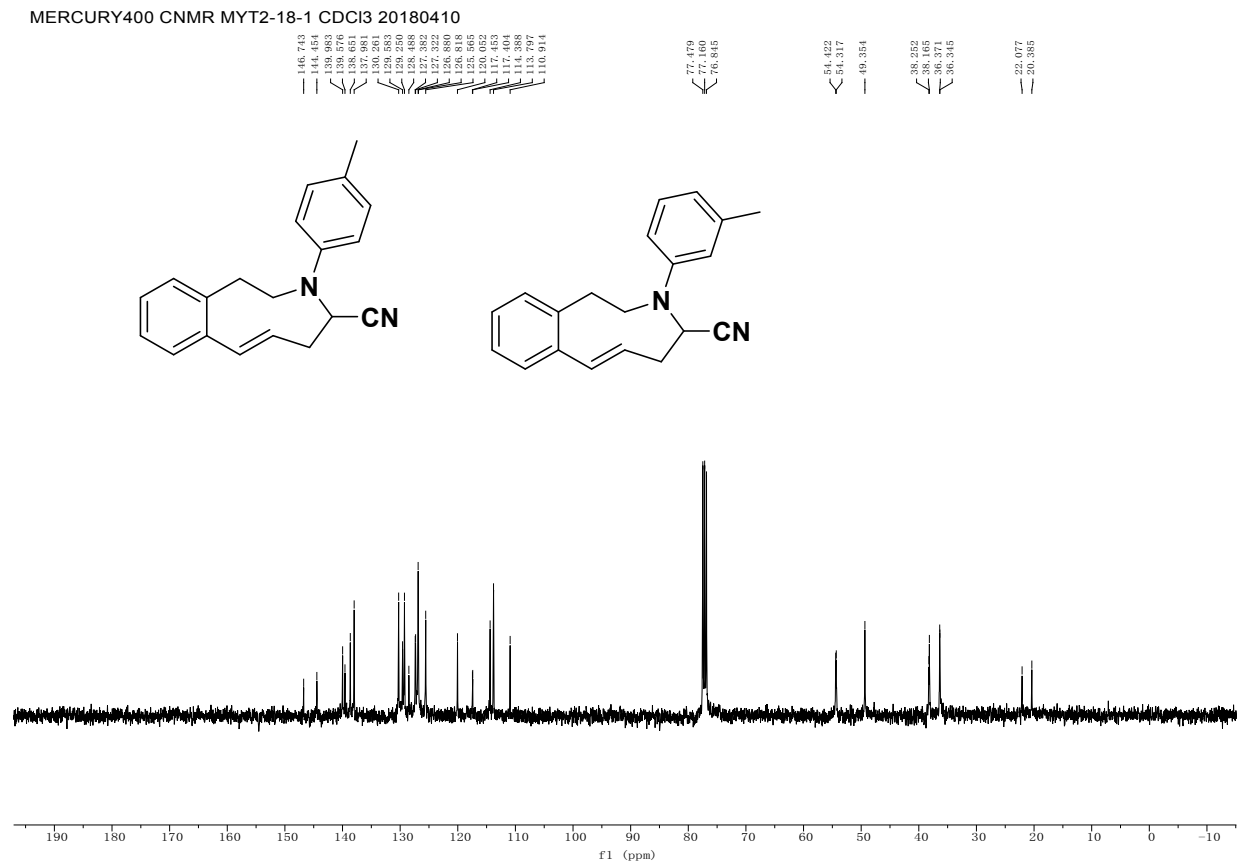
¹³C NMR spectra of compound **3o**



¹H NMR spectra of compounds **3pa** and **3pb**

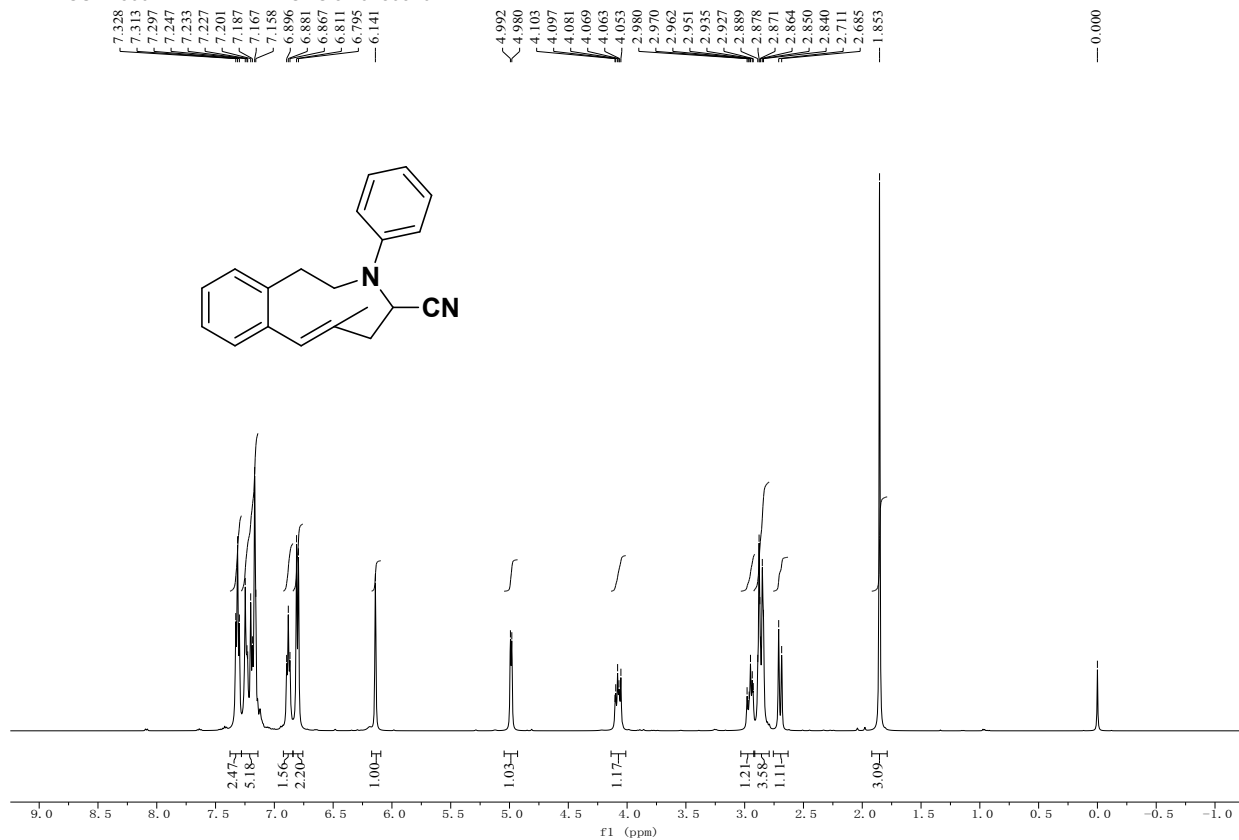


¹³C NMR spectra of compounds **3pa** and **3pb**



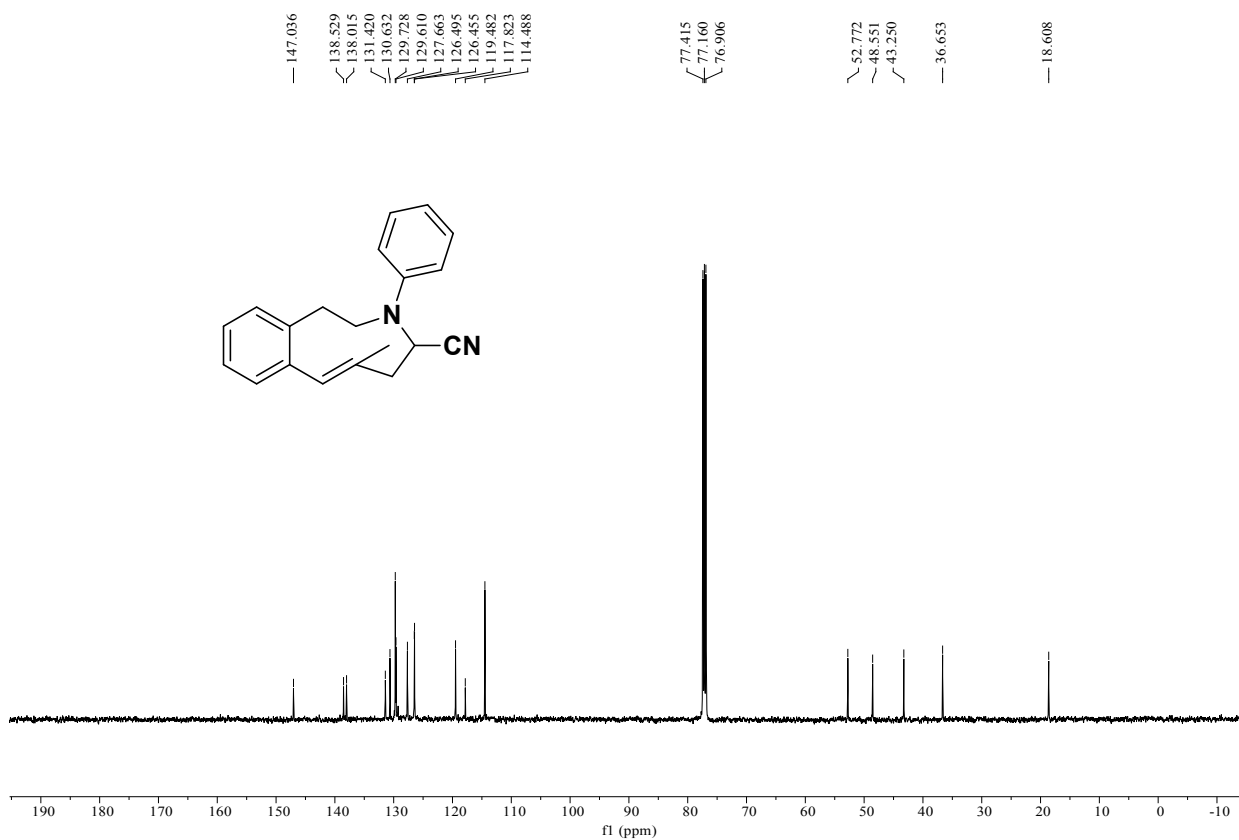
¹H NMR spectra of compound **3q**

MERCURY500 HNMR MYT2-4 CDCl₃ 20180326



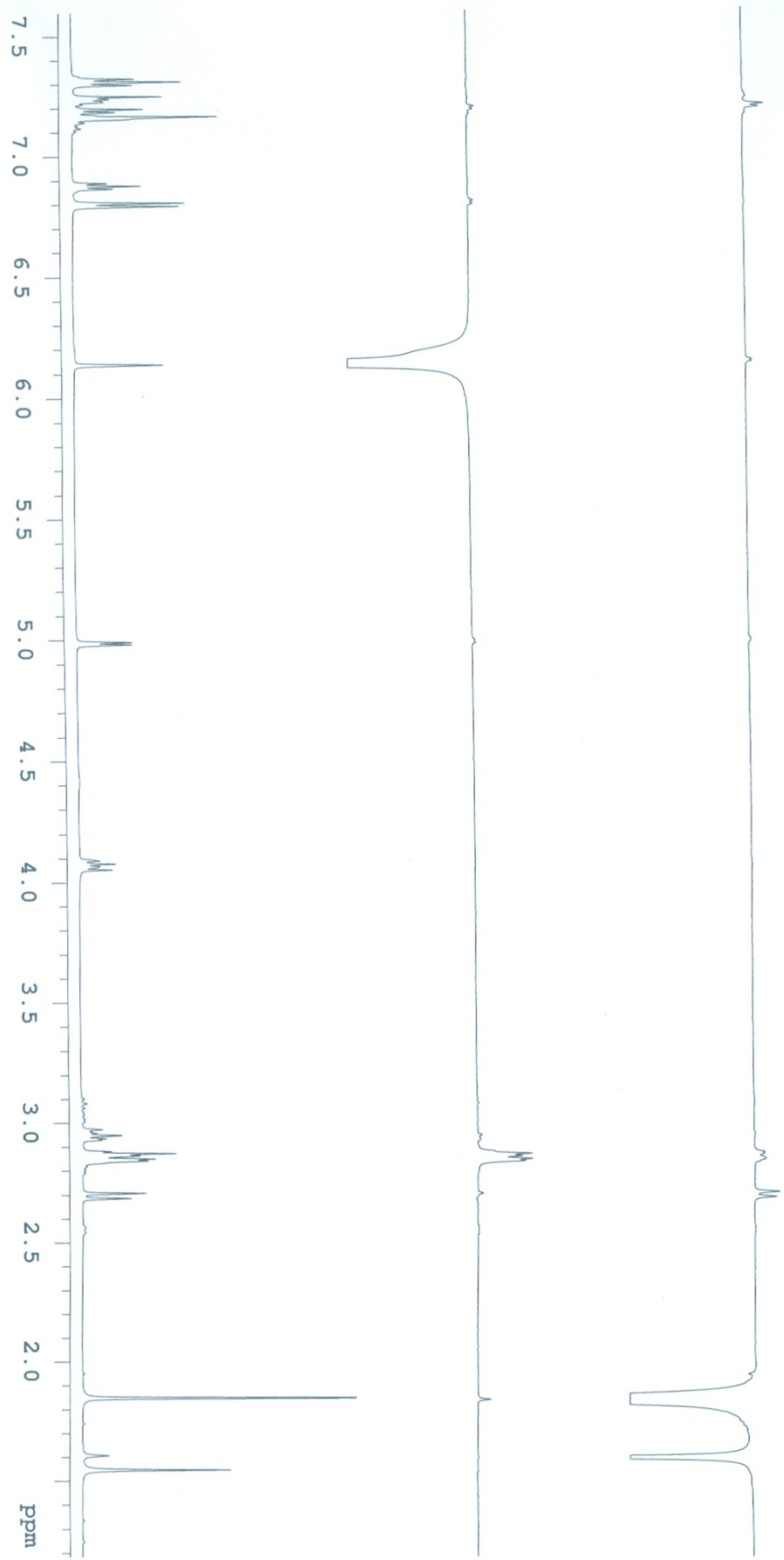
¹³C NMR spectra of compound **3q**

MERCURY500 CNMR MYT2-4 CDCl₃ 20180326



NOESY of compound **3q**

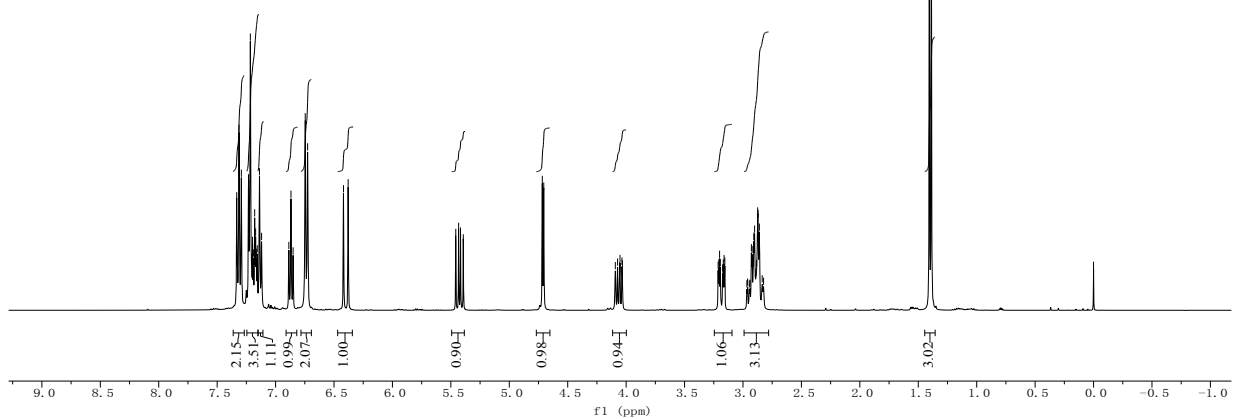
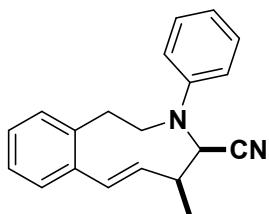
VNS-600 NOESY1D MVT2-4 IN cdcl3 Jul 23 2018



¹H NMR spectra of compound 3r

MERCURY400 HNMR MYT2-19 CDCl3 20180326

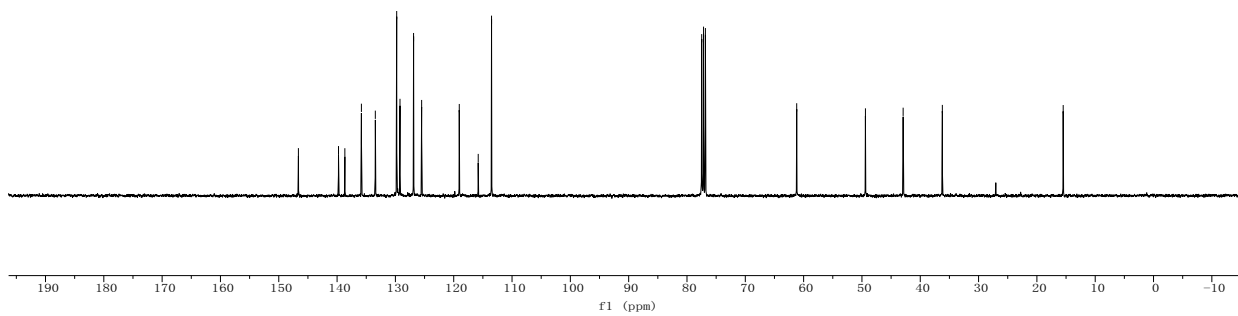
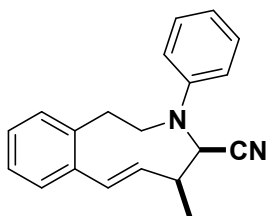
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¹³C NMR spectra of compound 3r

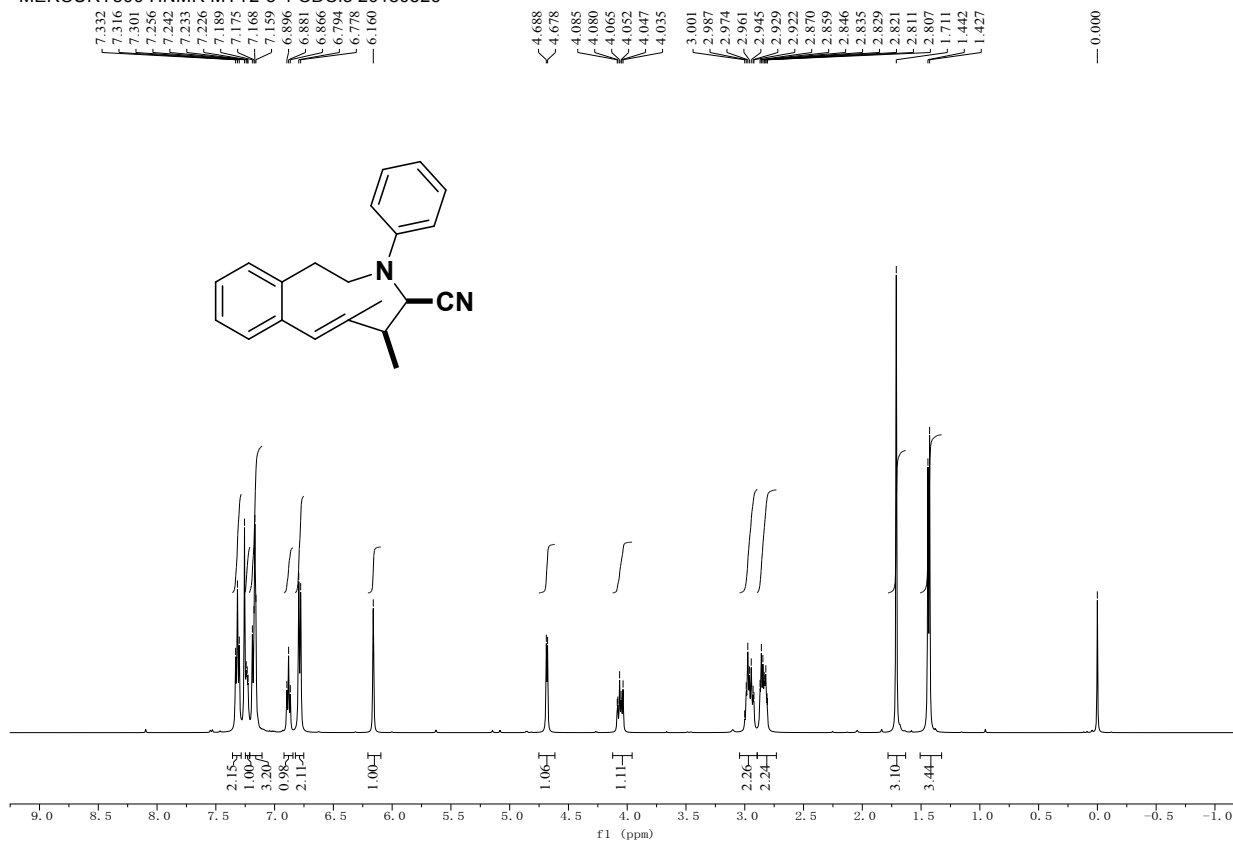
MERCURY400 CNMR MYT2-19 CDCl3 20180326

146.632 139.756 138.667 135.829 133.443 129.779 126.886 125.501 119.048 115.798 113.515 77.478 77.160 76.842 61.187 49.400 42.936 36.213 15.490



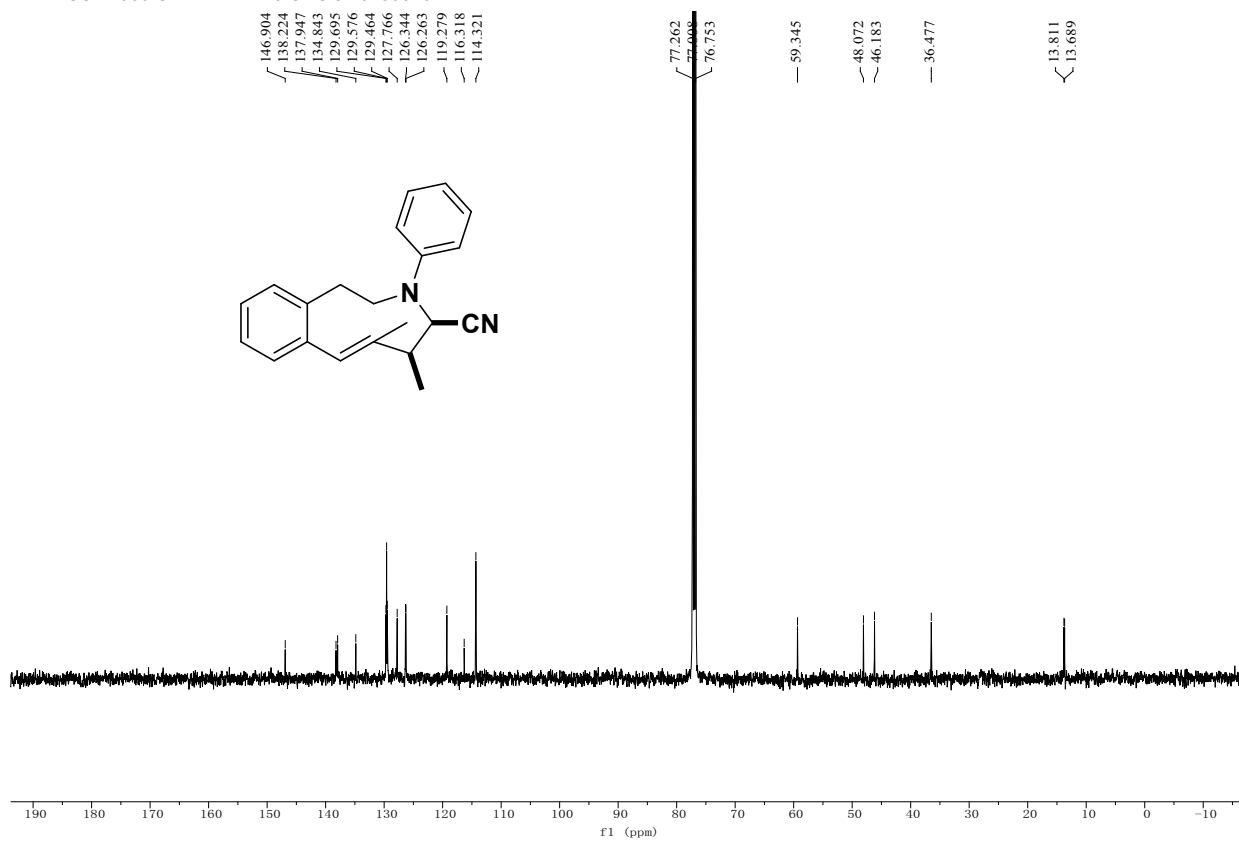
¹H NMR spectra of compound 3s

MERCURY500 HNMR MYT2-5-1 CDCl3 20180326



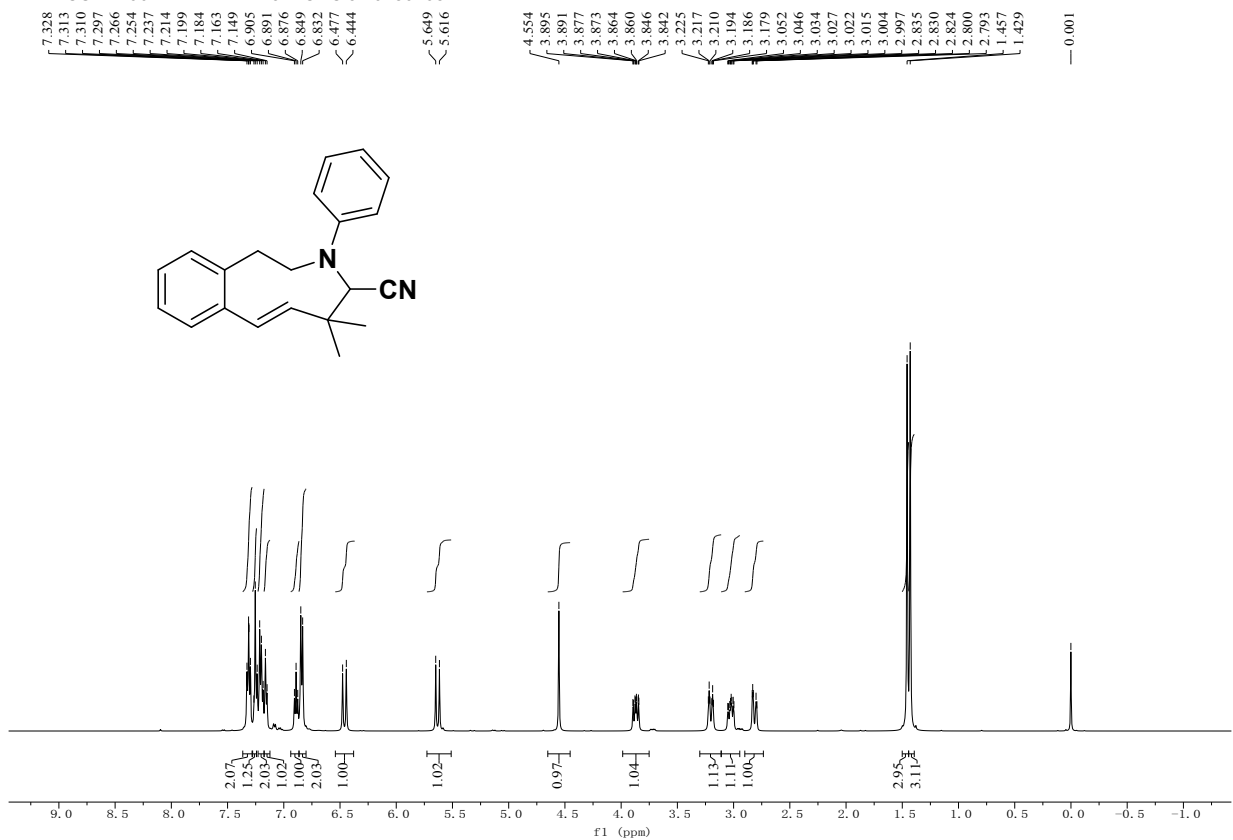
¹³C NMR spectra of compound 3s

MERCURY500 CNMR MYT2-5 CDCl3 20180326



¹H NMR spectra of compound 3t

MERCURY400 HNMR MYT2-3-1 CDCl₃ 20180408



¹³C NMR spectra of compound 3t

MERCURY500 CNMR MYT2-3-1 CDCl₃ 20180408

