

3-Cyanothiete 1,1-dioxide: synthesis and cycloaddition reactions

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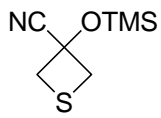
³ *Enamine Ltd.,
78 Winston Churchill St., Kyiv 02094, Ukraine*

Supplementary information

¹H NMR and ¹³C NMR data were acquired on Bruker spectrometers at 400 MHz for ¹H nuclei, and at 126 or 151 MHz for ¹³C nuclei. The residual solvent signals (CDCl₃: 7.26 ppm for ¹H nuclei and 77.2 ppm for ¹³C nuclei; DMSO-d₆: 2.50 ppm for ¹H nuclei and 39.5 ppm for ¹³C nuclei) served as internal standards.

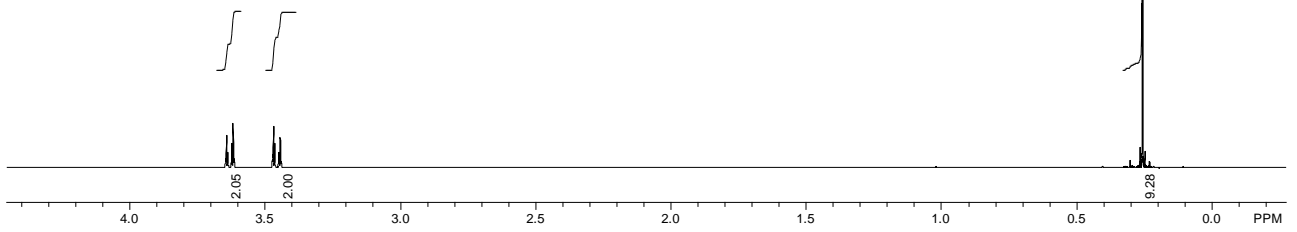
3.646
3.644
3.643
3.637
3.623
3.618
3.615
3.614
3.472
3.471
3.469
3.464
3.449
3.444
3.441
3.441

0.257
-0.000



2

¹HNMR (CDCl₃, 400 MHz)



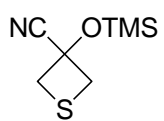
121.555

77.160

69.872

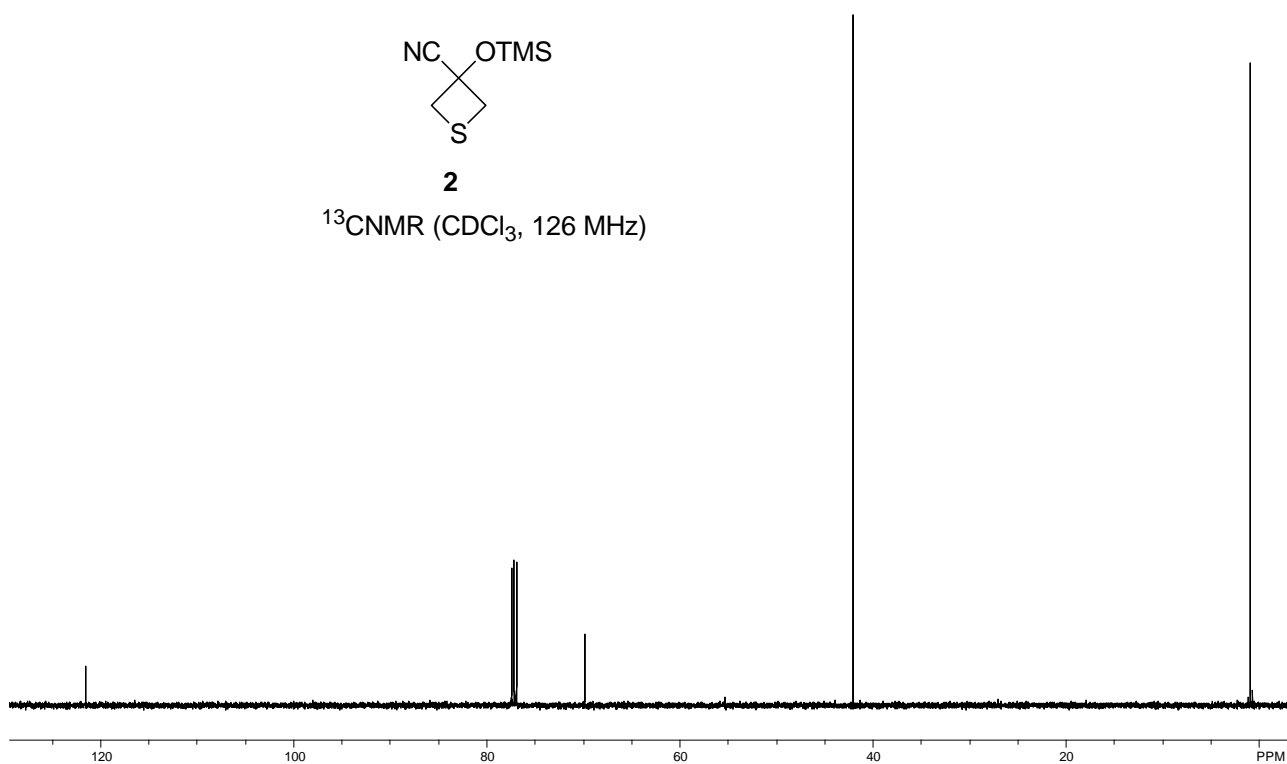
42.104

0.946



2

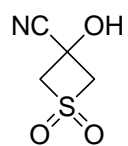
¹³CNMR (CDCl₃, 126 MHz)



8.031

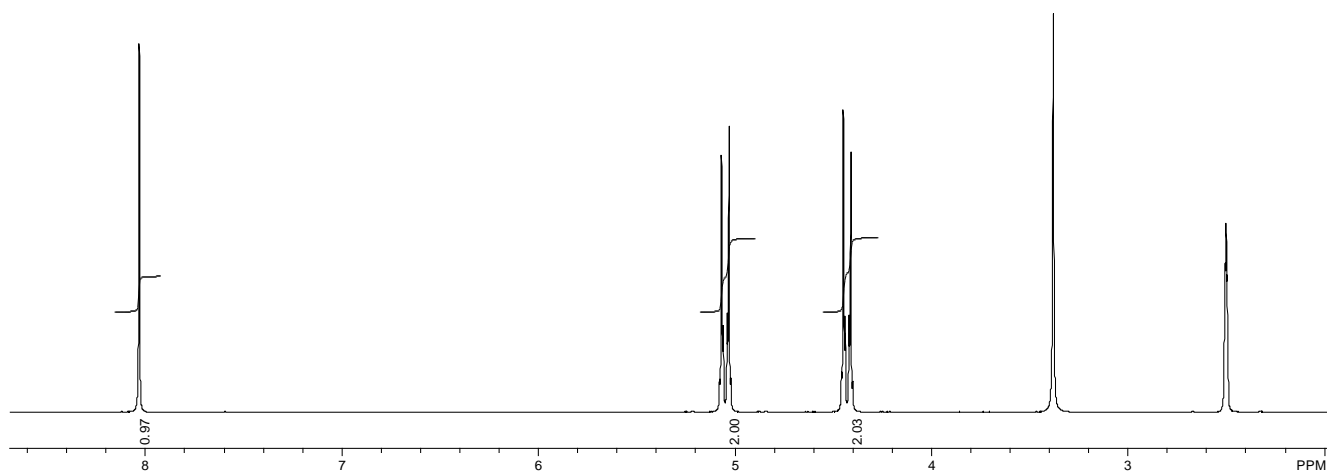
5.077
5.068
5.059
5.039
5.030
5.020
4.457
4.448
4.444
4.438
4.418
4.409
4.400

2.500



3

¹HNMR (DMSO-d₆, 400 MHz)

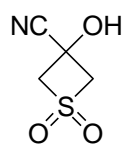


119.284

76.938

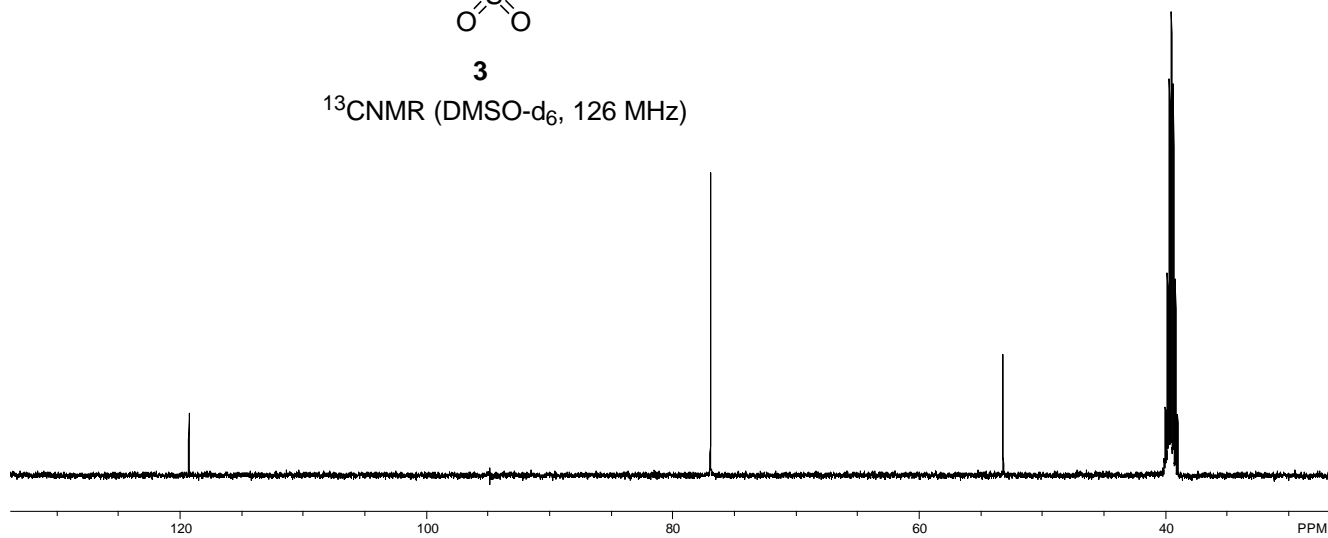
53.188

39.536



3

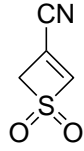
¹³CNMR (DMSO-d₆, 126 MHz)



8.088

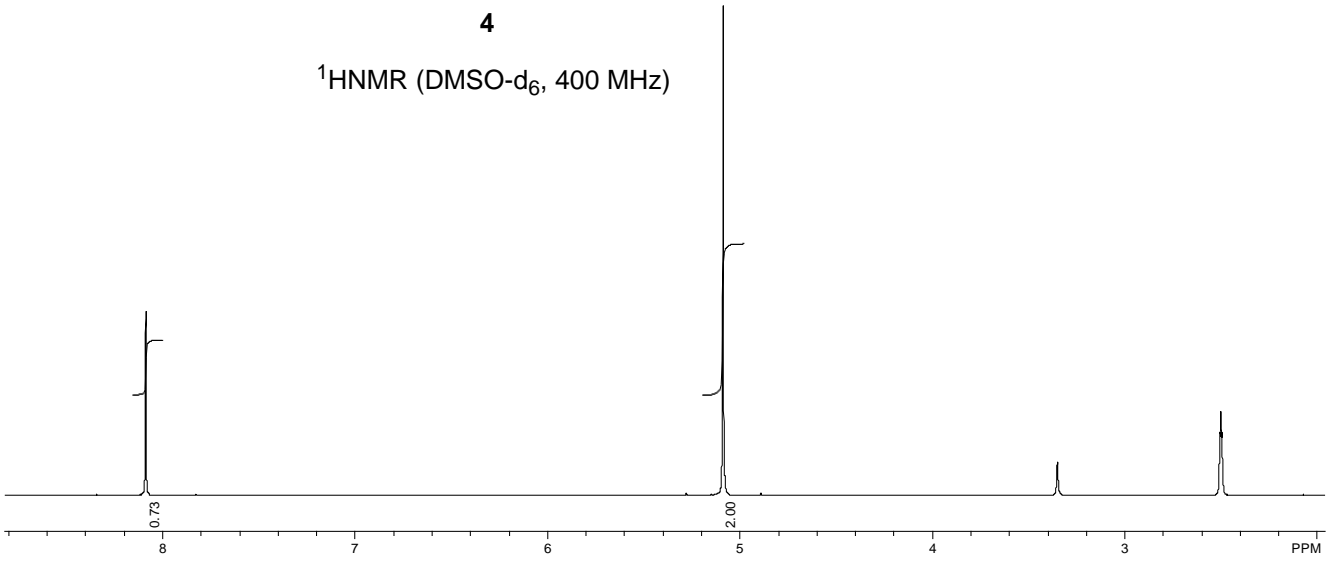
5.088

2.500



4

¹HNMR (DMSO-d₆, 400 MHz)



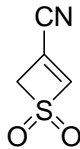
159.267

120.035

111.443

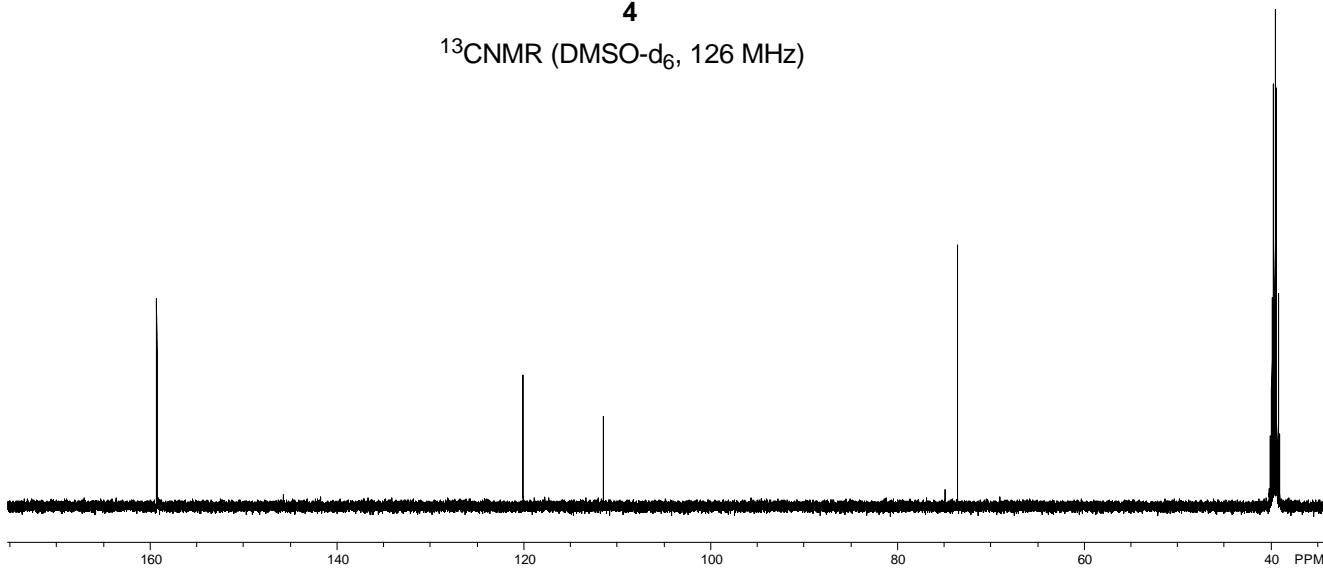
73.563

39.555



4

¹³CNMR (DMSO-d₆, 126 MHz)

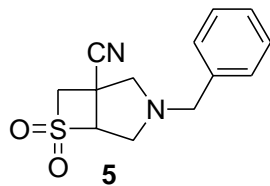


7.377
7.369
7.366
7.342
7.337
7.321
7.299
7.290
7.284
7.263

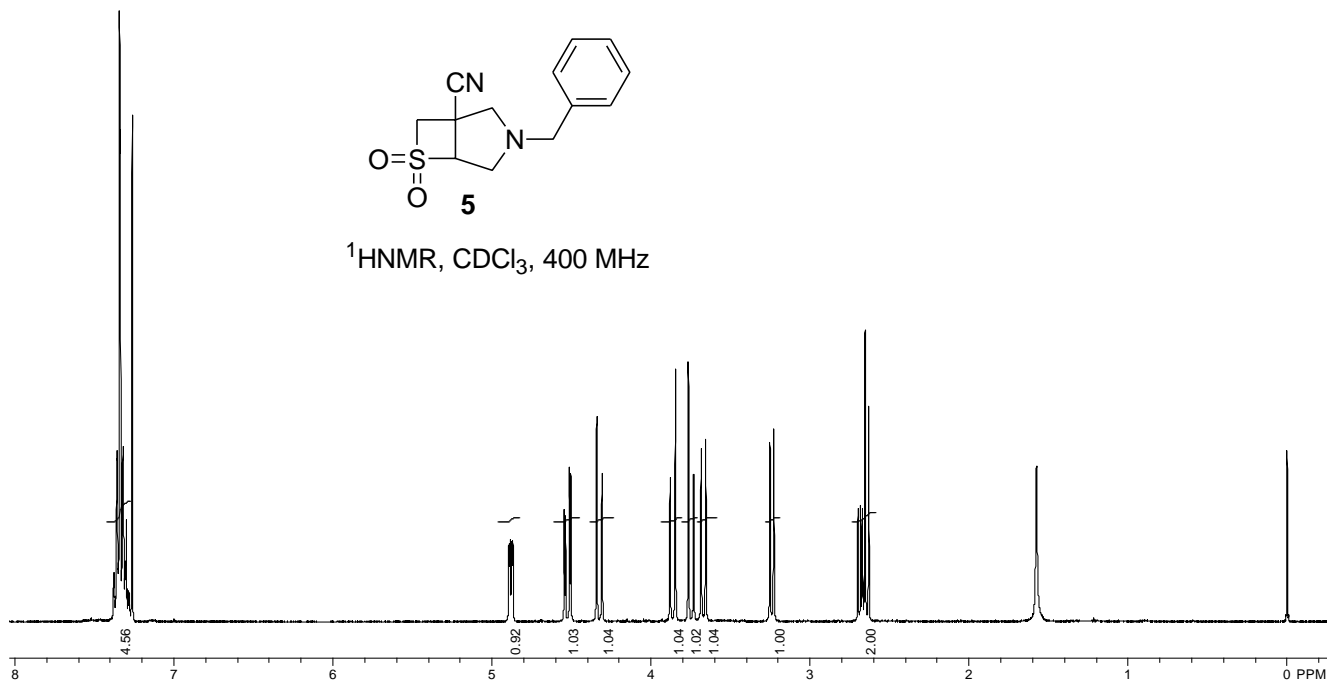
4.894
4.887
4.876
4.869
4.545
4.538
4.512
4.505
4.341
4.308
3.890
3.847
3.765
3.732
3.684
3.655
3.252
3.228

2.698
2.681
2.669
2.654
2.630

0.000



¹HNMR, CDCl₃, 400 MHz



7.349
7.340
7.278
7.268

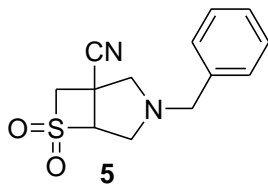
5.177
5.168

4.726
4.720
4.691
4.685
4.383
4.348

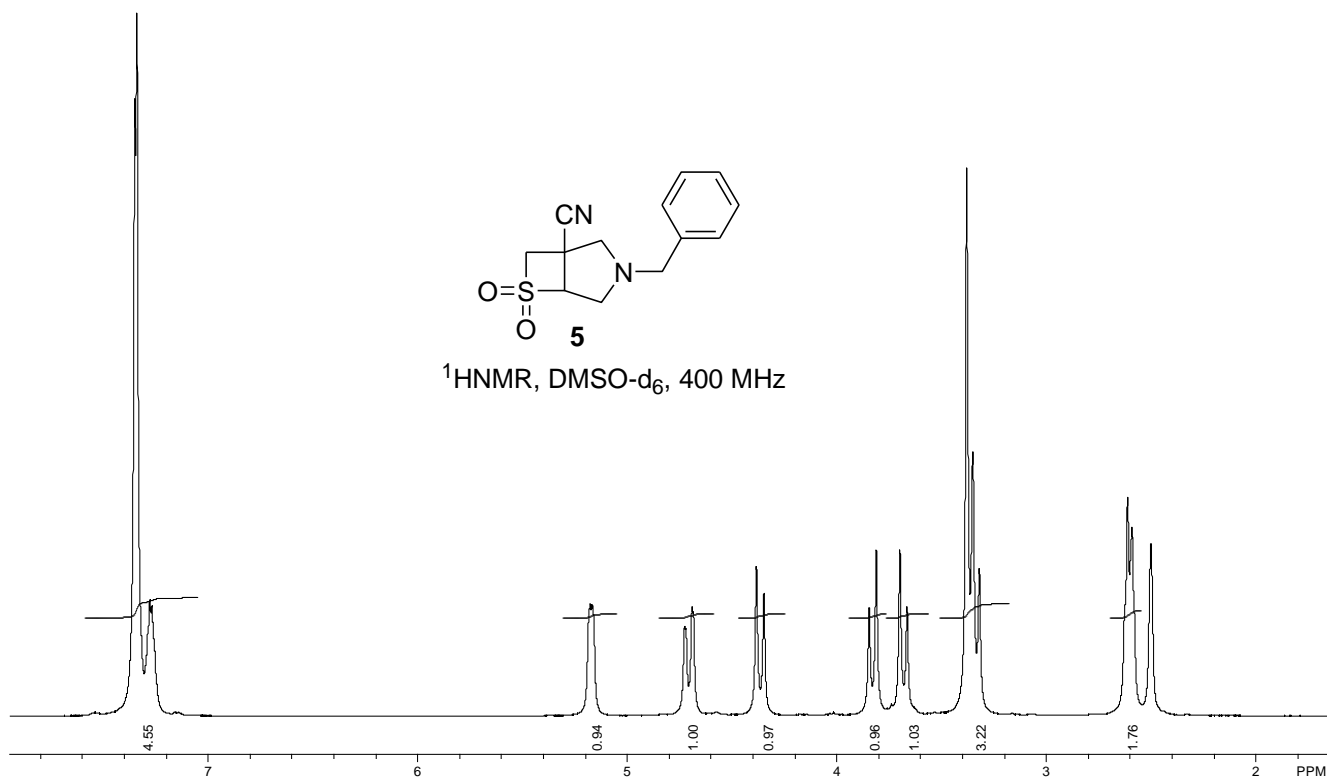
3.845
3.811
3.698
3.664

3.380
3.350
3.319

2.624
2.612
2.590
2.500



¹HNMR, DMSO-d₆, 400 MHz



137.475

128.338
128.229
127.167

119.248

85.768

73.705

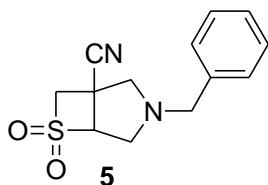
59.874

56.143

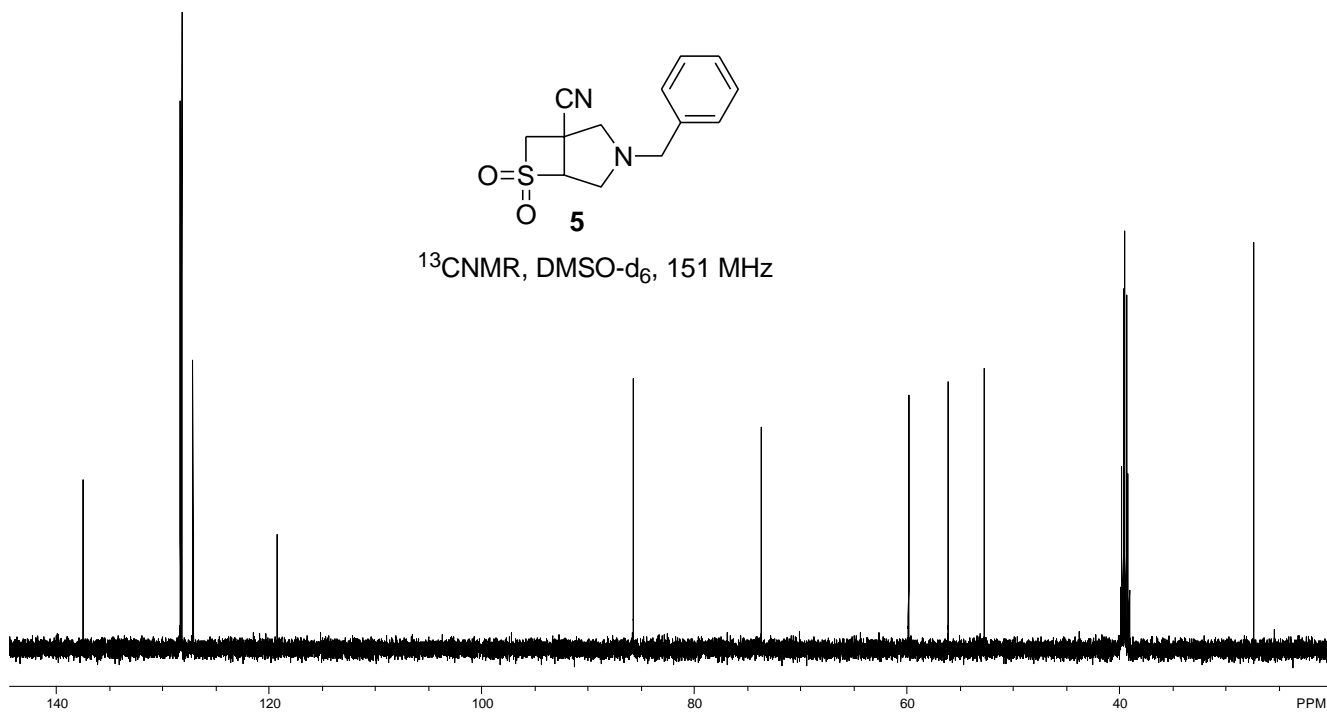
52.768

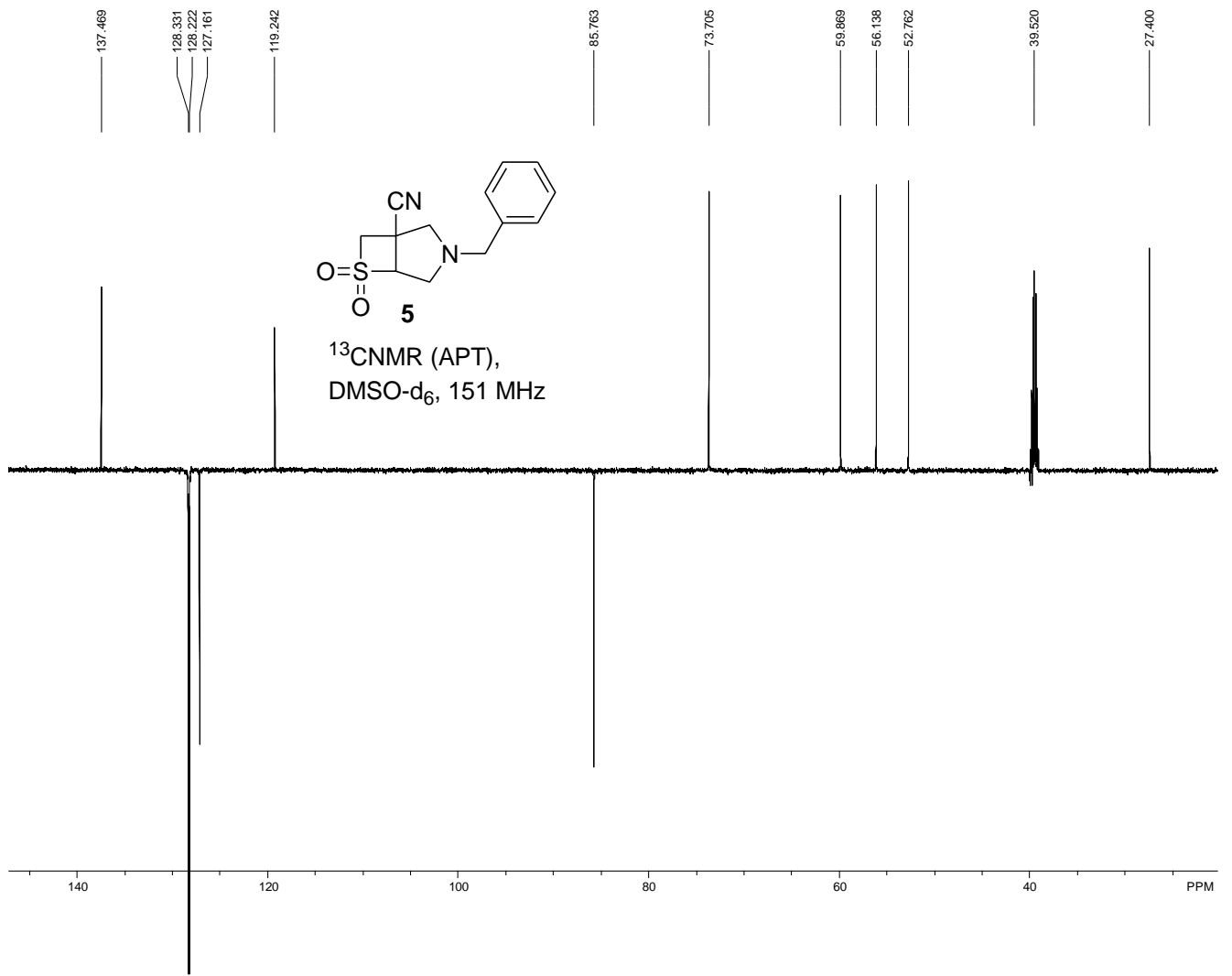
39.520

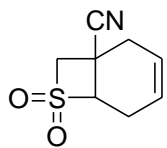
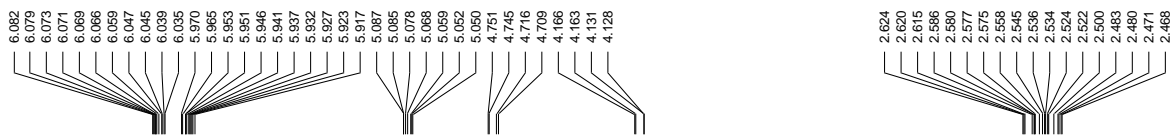
27.404



^{13}C NMR, DMSO- d_6 , 151 MHz

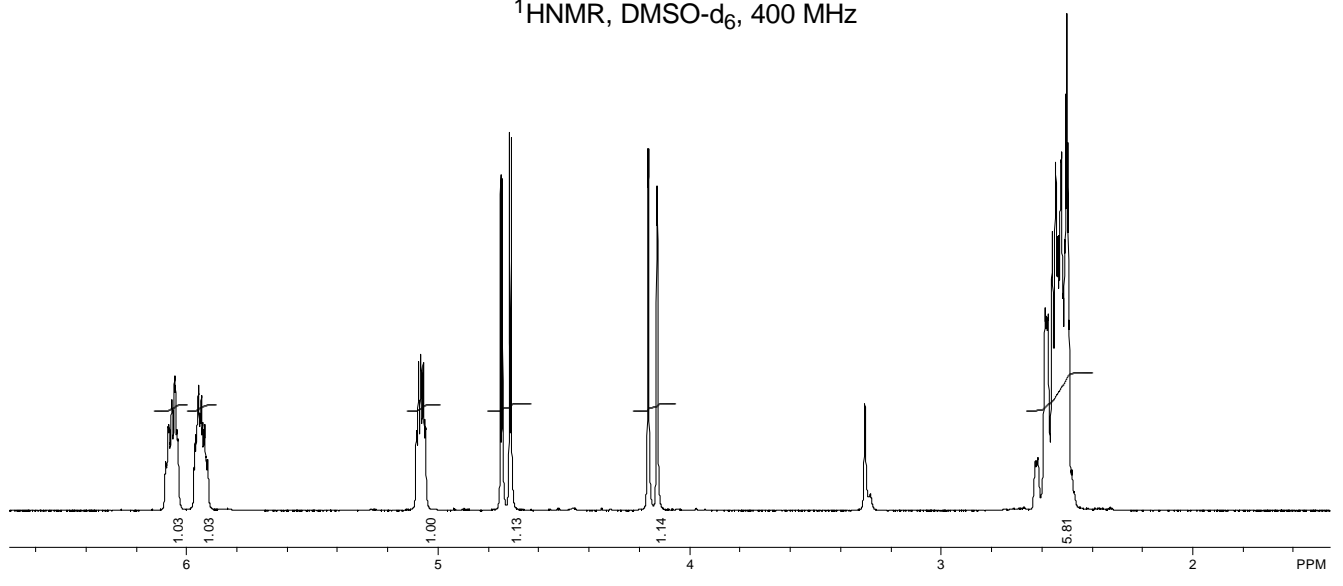






6

¹HNMR, DMSO-d₆, 400 MHz



127.208
123.971
121.653

79.453

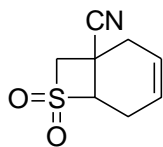
72.884

39.520

28.794

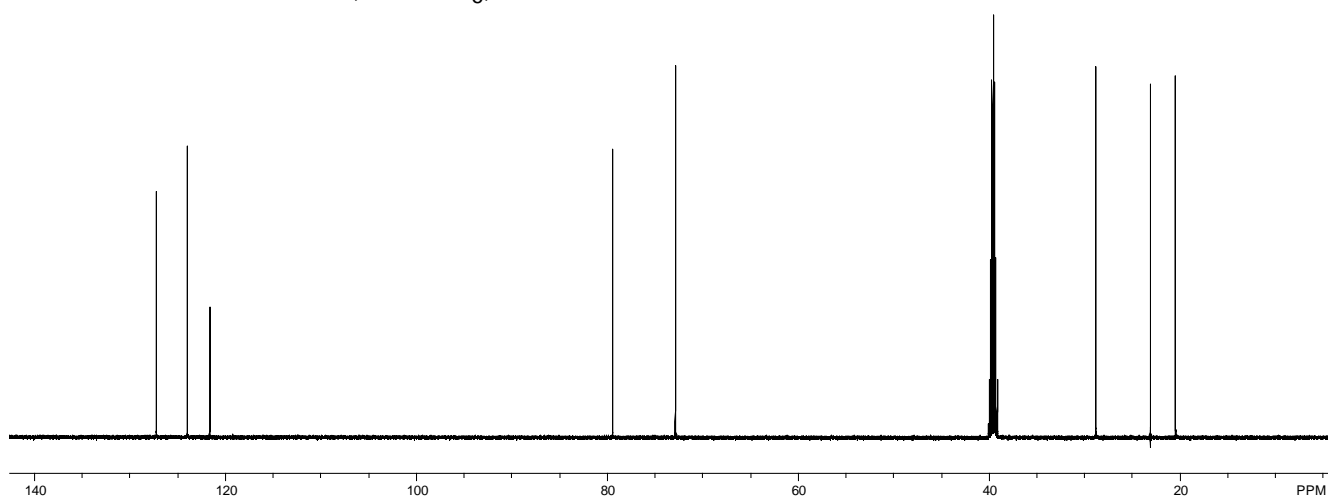
23.029

20.401



6

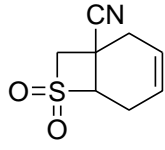
^{13}C NMR, DMSO- d_6 , 151 MHz



127.209
123.973
121.652

79.449
72.880

39.520
28.794
23.028
20.399



6

¹³CNMR (APT),
DMSO-d₆, 151 MHz

