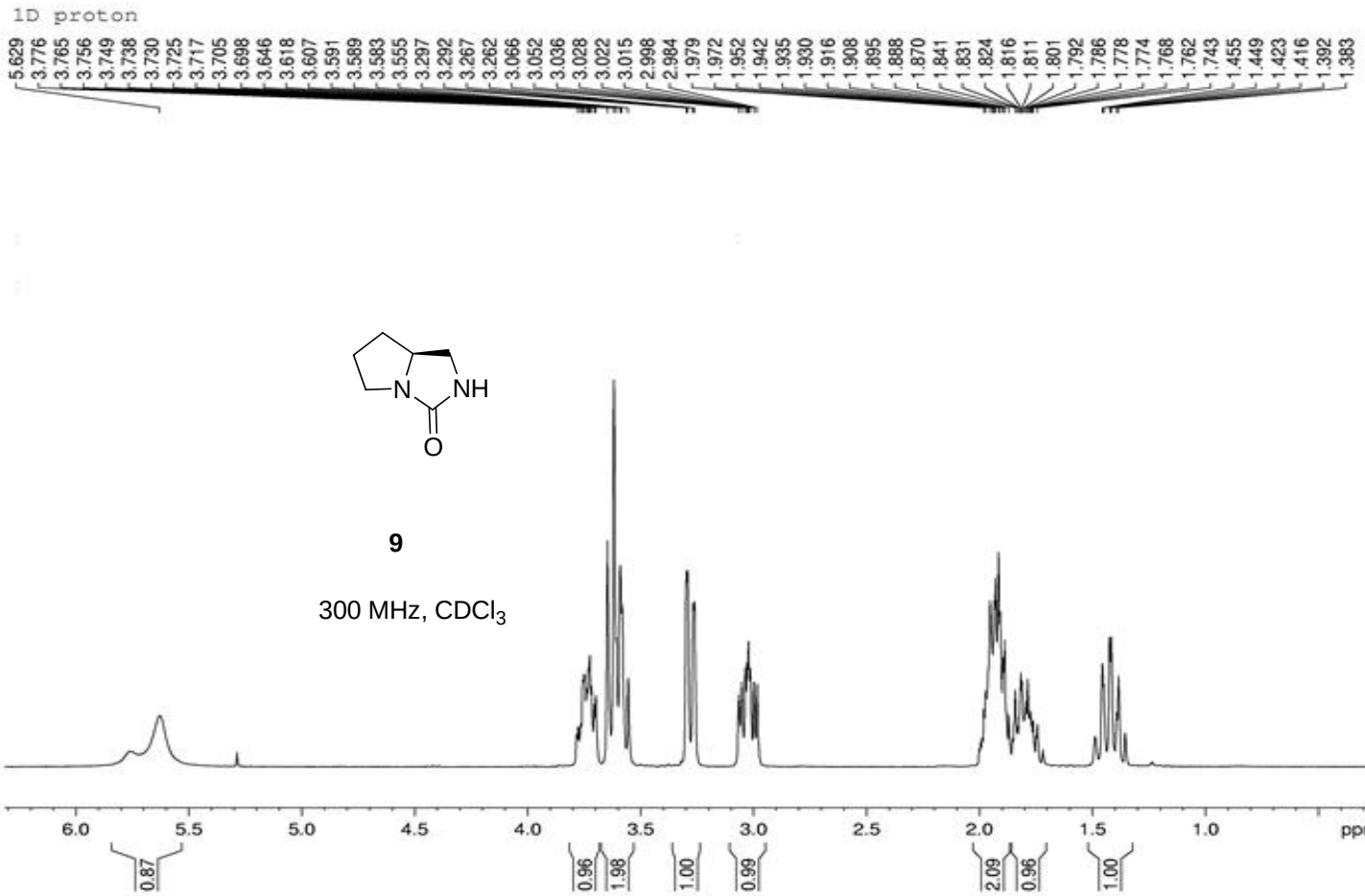
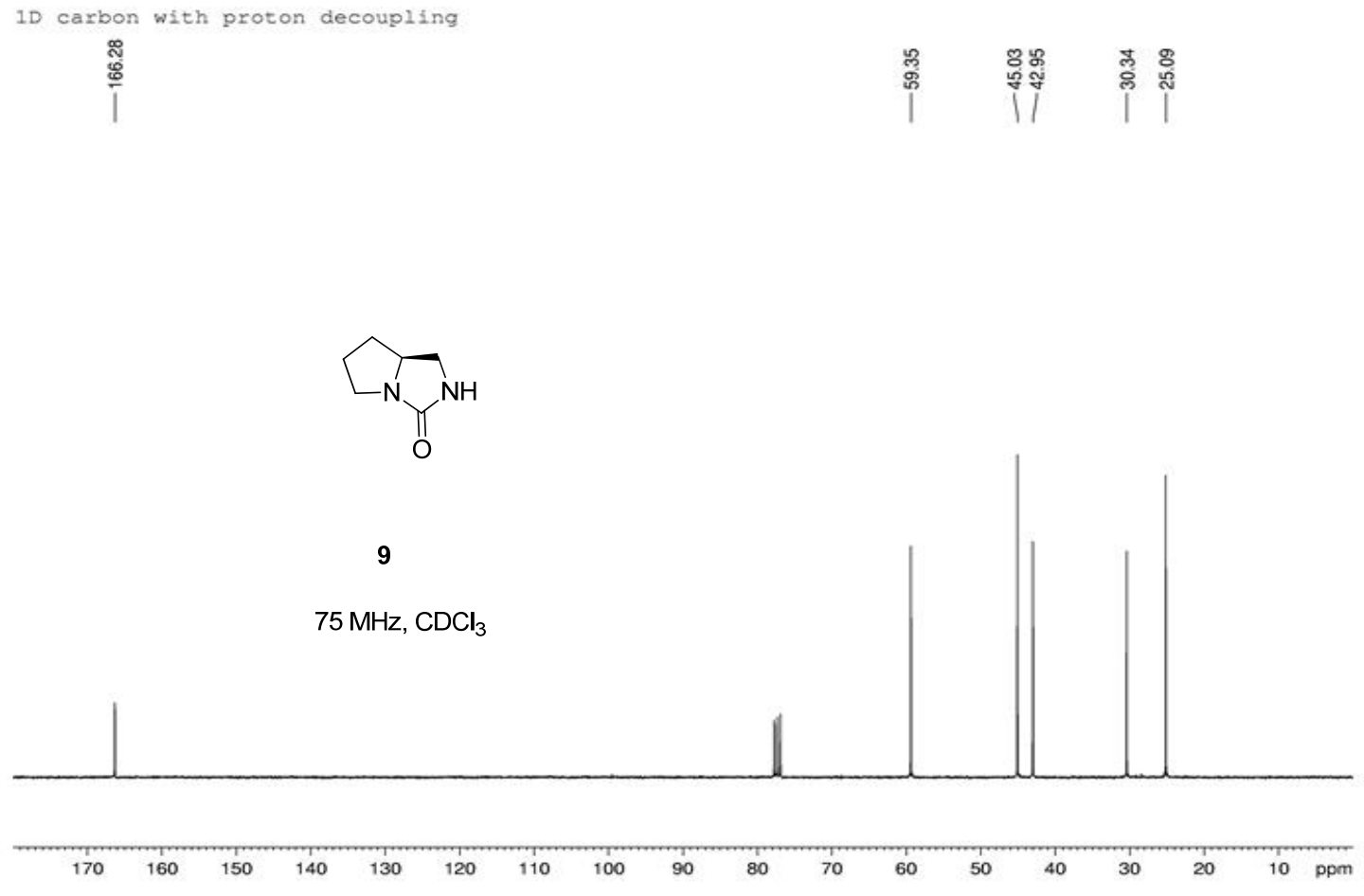
Supporting Information for

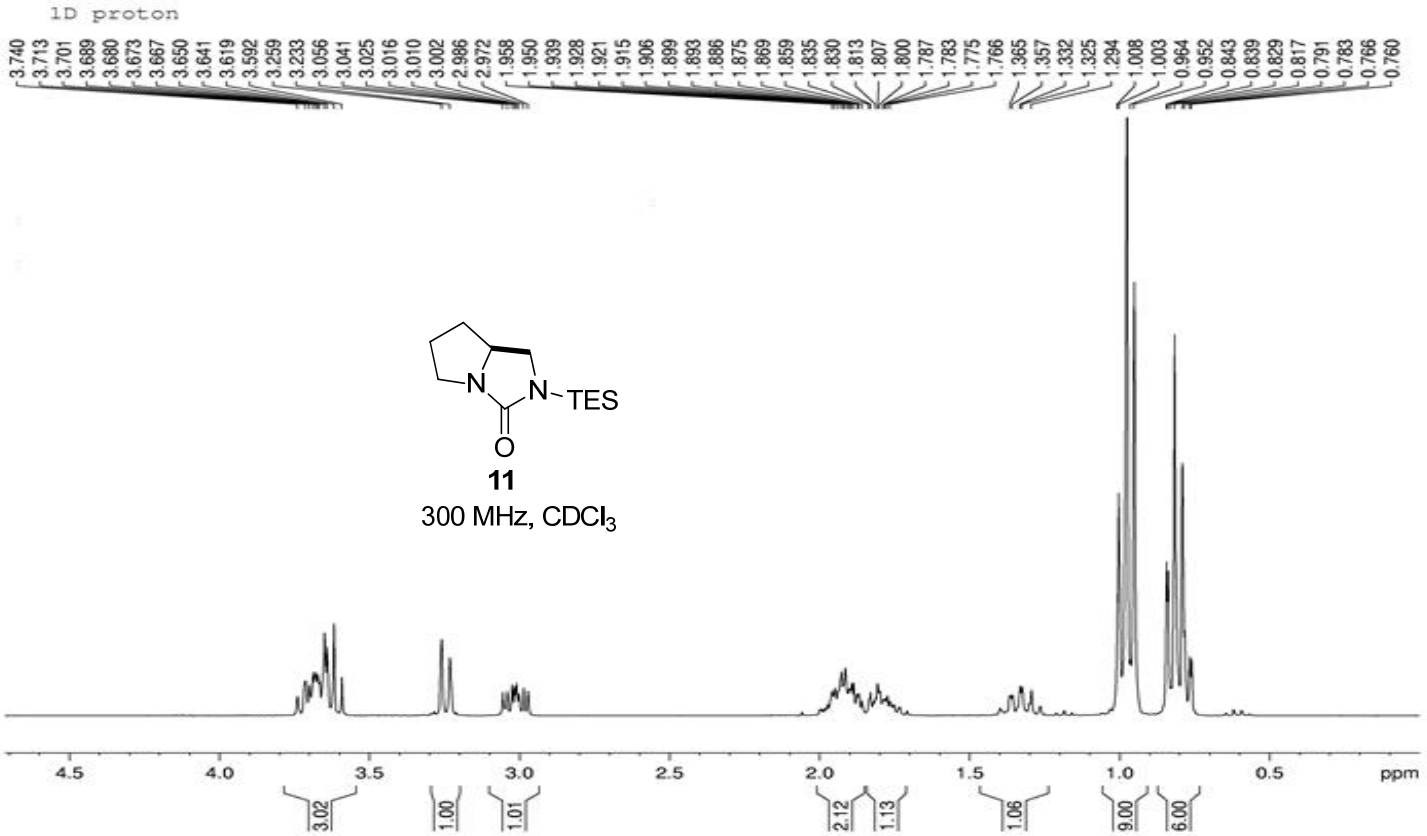
DIASTEREOSELECTIVE LITHIATION OF *N*-SILYL-PROTECTED (*S*)-TETRAHYDRO-1*H*-PYRROLO[1,2-*c*]IMIDAZOL-3(2*H*)-ONE

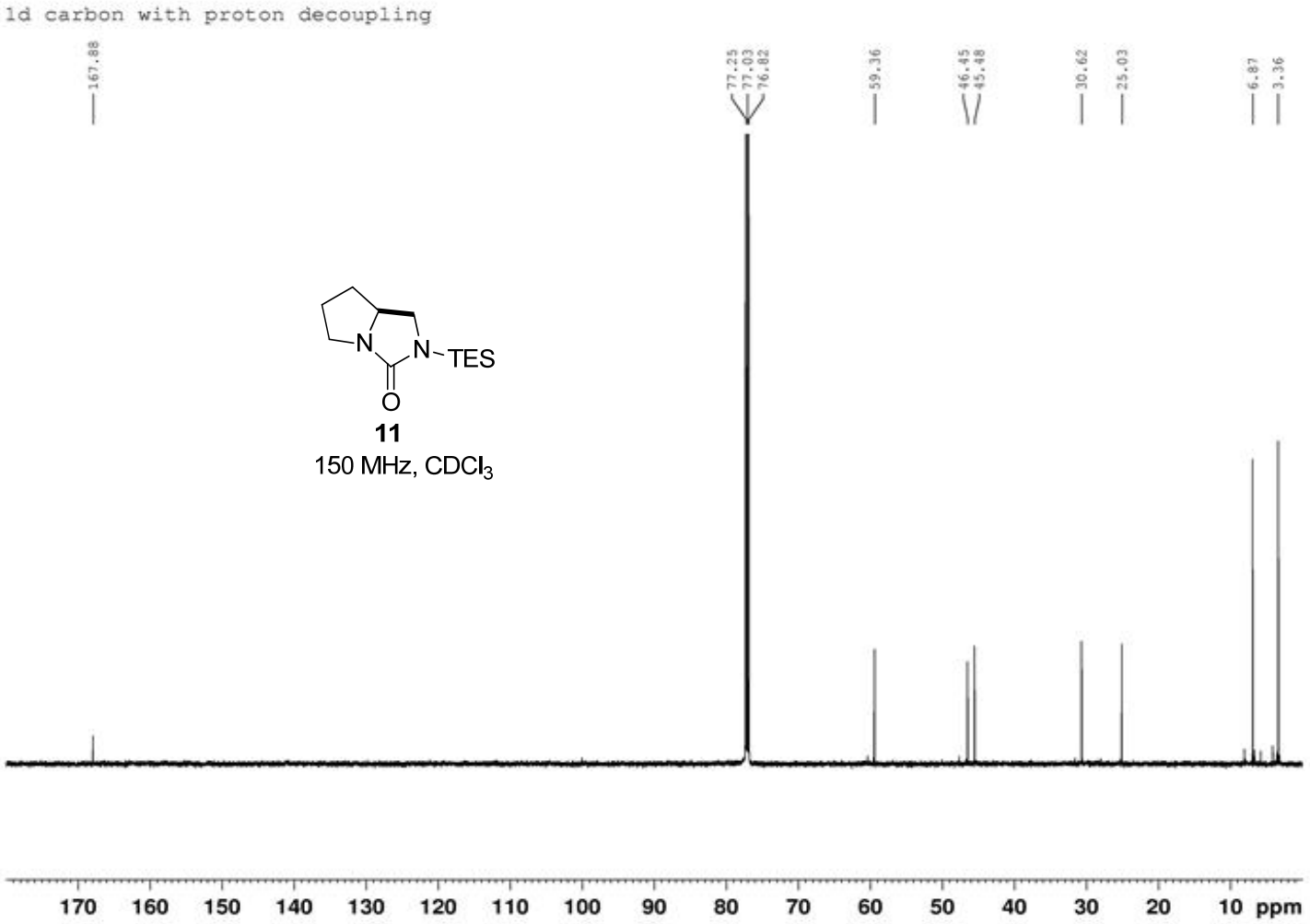
Costa Metallinos*, Seyed Iraj Sadraei, and Nadezda Zhukovskaya

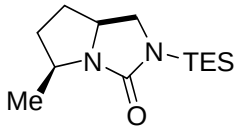
Department of Chemistry, Brock University, 500 Glenridge Avenue, St. Catharines, Ontario L2S 3A1, Canada


1D proton
5.629
3.776
3.765
3.756
3.749
3.738
3.730
3.725
3.717
3.705
3.698
3.646
3.618
3.607
3.591
3.589
3.583
3.555
3.297
3.292
3.267
3.262
3.066
3.052
3.036
3.028
3.022
3.015
2.998
2.984
1.979
1.972
1.952
1.942
1.935
1.930
1.916
1.908
1.895
1.888
1.870
1.841
1.831
1.824
1.816
1.811
1.801
1.792
1.786
1.778
1.774
1.768
1.762
1.743
1.455
1.449
1.423
1.416
1.392
1.383
NH
O
9
300 MHz, CDCl3
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.87
0.96
1.98
1.00
0.99
2.09
0.96
1.00


1D carbon with proton decoupling
166.28
59.35
45.03
42.95
30.34
25.09
NH
O
9
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

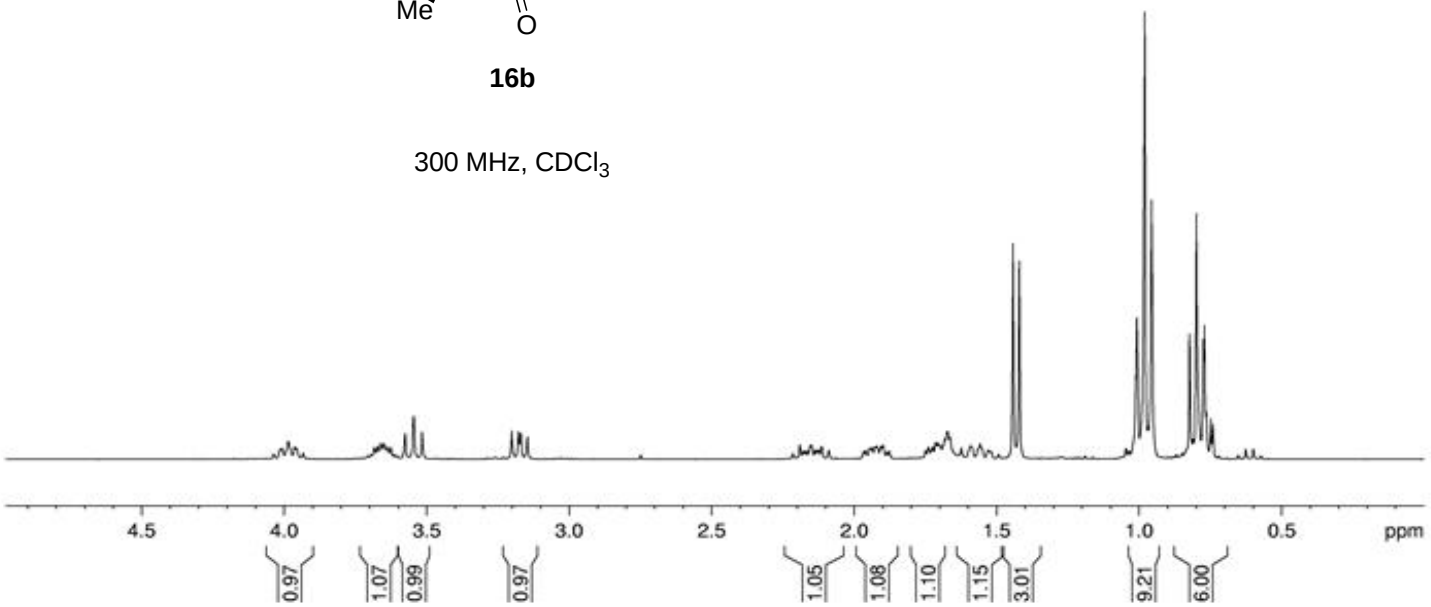

1D proton
3.740
3.713
3.701
3.689
3.680
3.673
3.667
3.650
3.641
3.619
3.592
3.259
3.233
3.056
3.041
3.025
3.016
3.010
3.002
2.986
2.972
1.958
1.950
1.939
1.928
1.921
1.915
1.906
1.899
1.893
1.886
1.875
1.869
1.859
1.835
1.830
1.813
1.807
1.800
1.787
1.783
1.775
1.766
1.365
1.357
1.332
1.325
1.294
1.008
1.003
0.964
0.952
0.843
0.839
0.829
0.817
0.791
0.783
0.766
0.760
N
N
TES
O
11
300 MHz, CDCl3
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.02
1.00
1.01
2.12
1.13
1.06
9.00
6.00

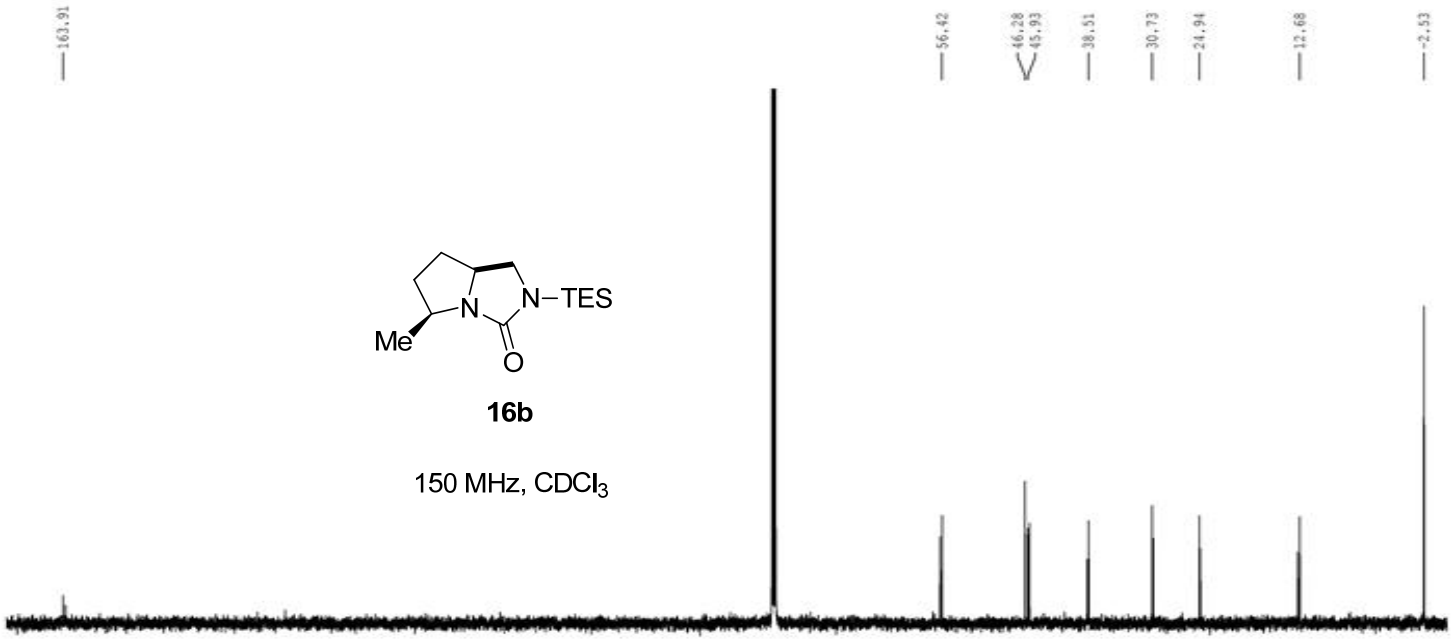

1d carbon with proton decoupling
167.88
77.25
77.03
76.82
59.36
46.45
45.48
30.62
25.03
6.87
3.36
N
N
TES
O
11
150 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



16b

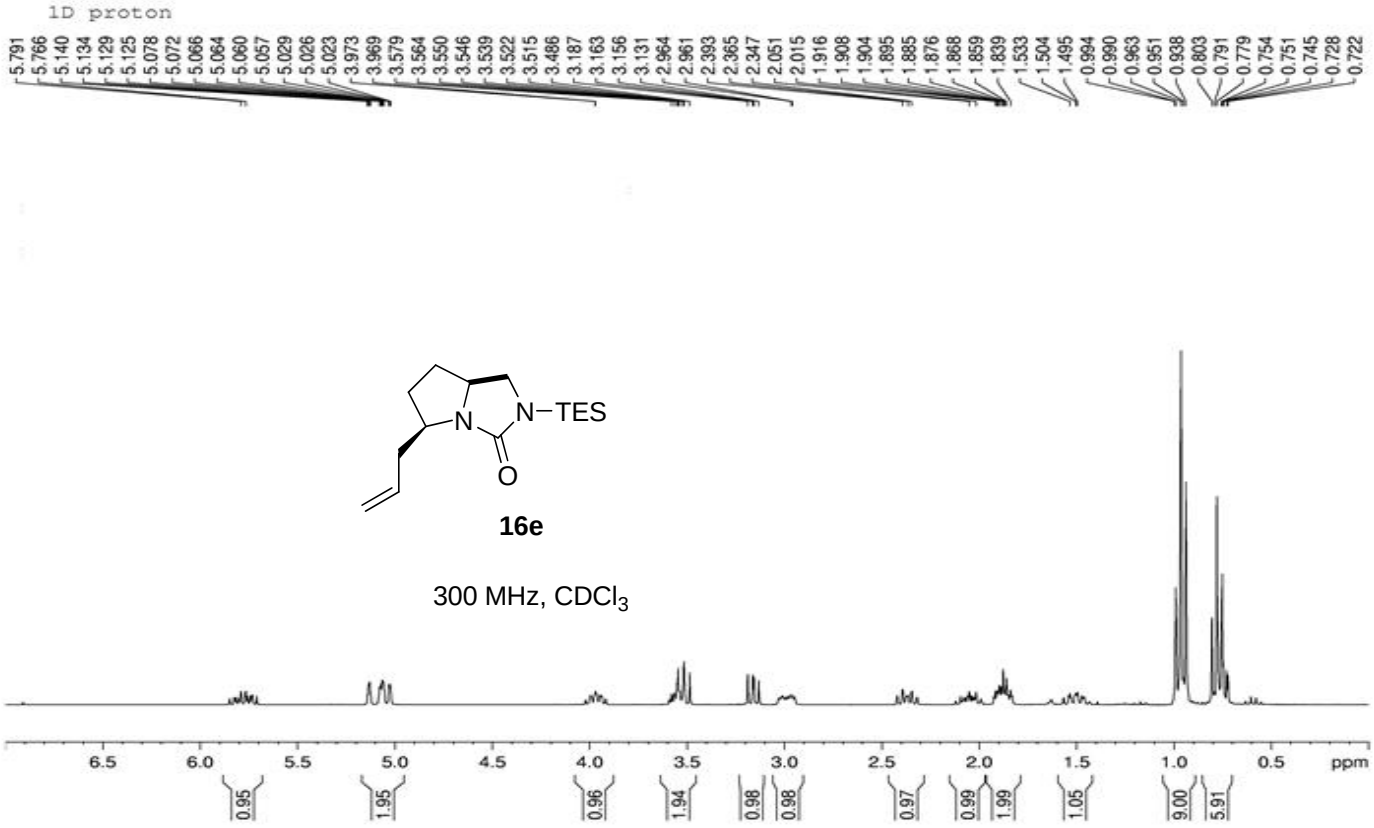
300 MHz, $CDCl_3$

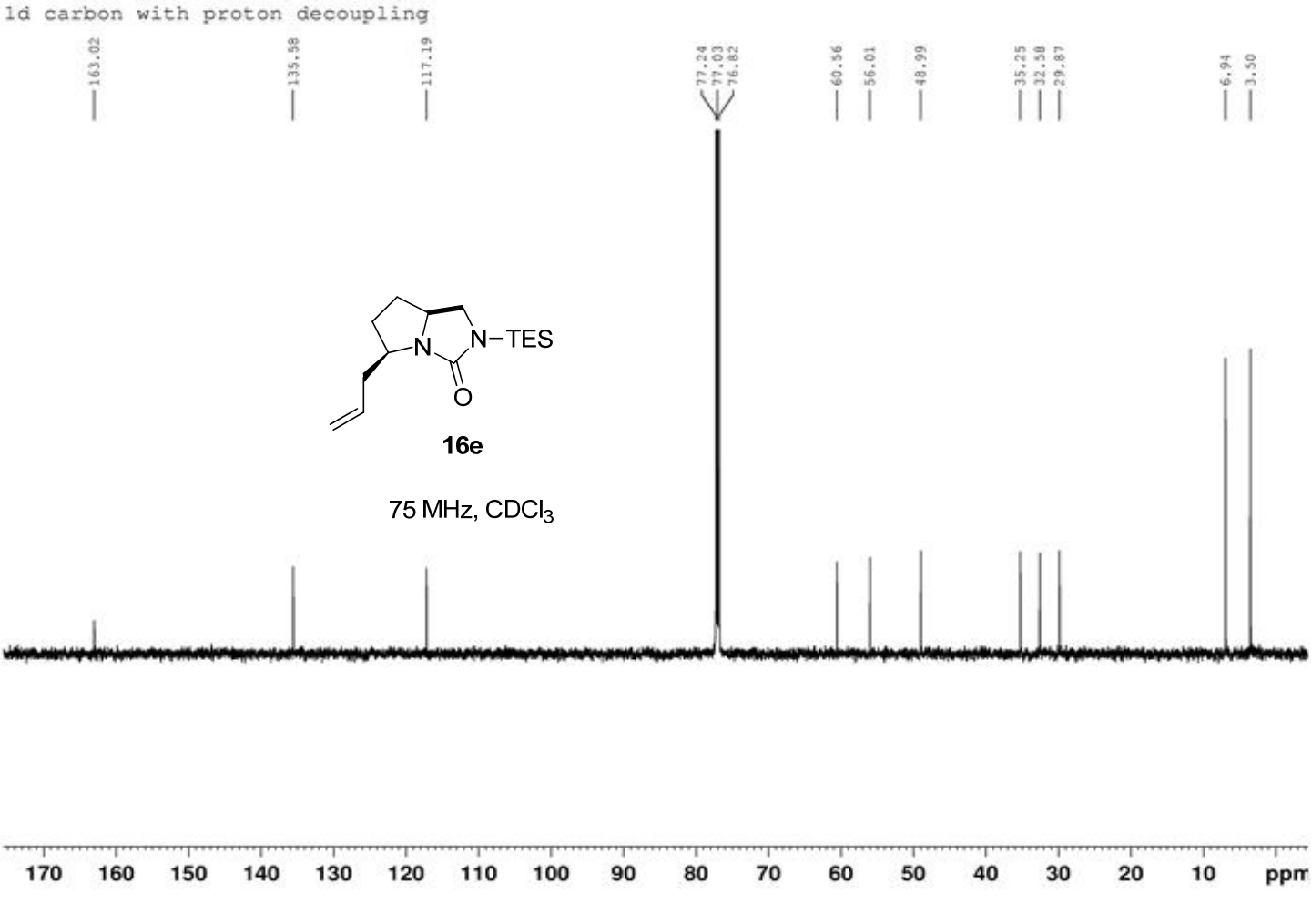




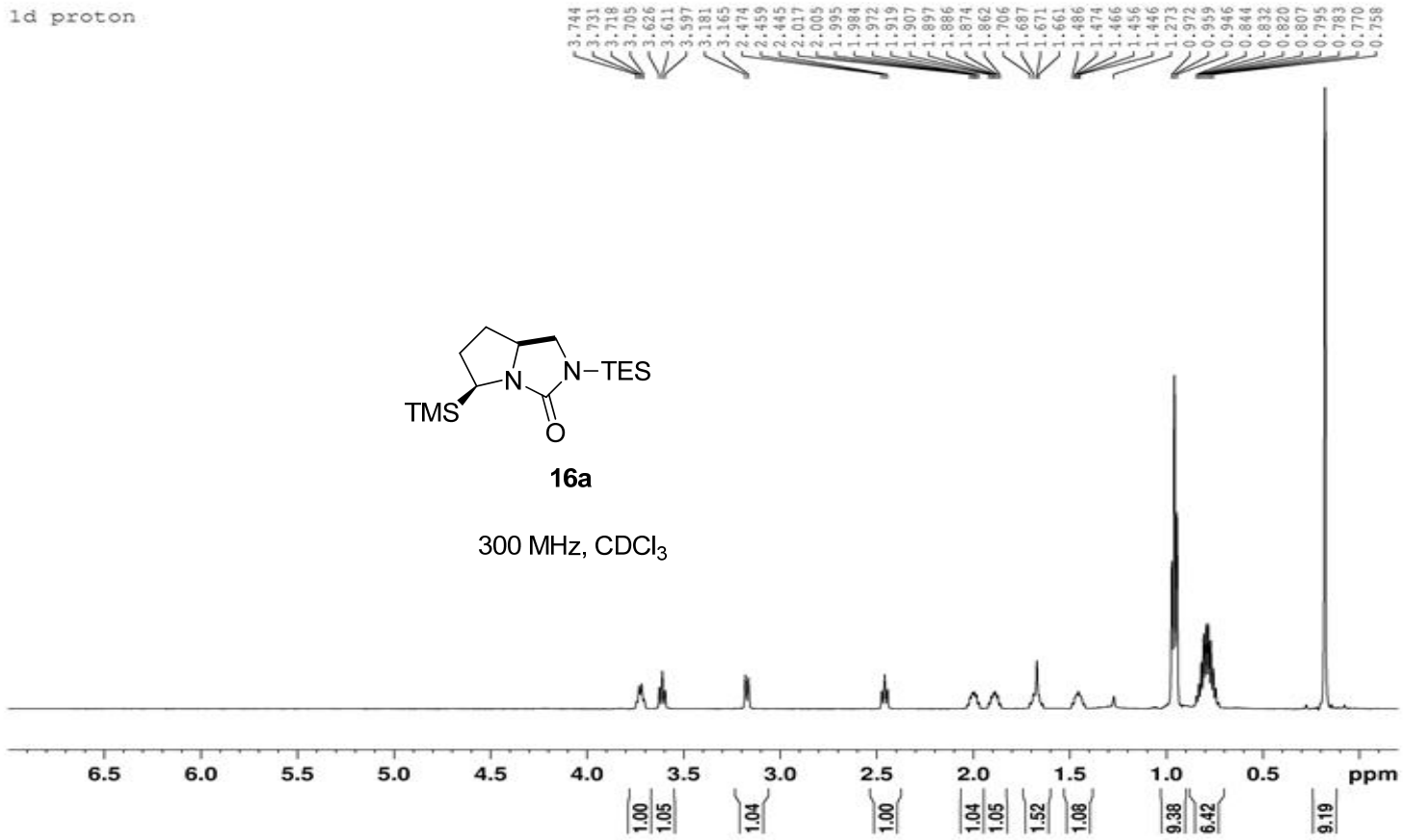
16b

150 MHz, $CDCl_3$


1D proton
5.791
5.766
5.140
5.134
5.129
5.125
5.078
5.072
5.066
5.064
5.060
5.057
5.029
5.026
5.023
3.973
3.969
3.579
3.564
3.550
3.546
3.539
3.522
3.515
3.486
3.187
3.163
3.156
3.131
2.964
2.961
2.393
2.365
2.347
2.051
2.015
1.916
1.908
1.904
1.895
1.885
1.876
1.868
1.859
1.839
1.533
1.504
1.495
0.994
0.990
0.963
0.951
0.938
0.803
0.791
0.779
0.754
0.751
0.745
0.728
0.722
N−TES
O
16e
300 MHz, CDCl3
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.95
1.95
0.96
1.94
0.98
0.98
0.97
0.99
1.99
1.05
9.00
5.91


1d carbon with proton decoupling
163.02
135.58
117.19
77.24
77.03
76.82
60.56
56.01
48.99
35.25
32.58
29.87
6.94
3.50
N−TES
O
16e
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

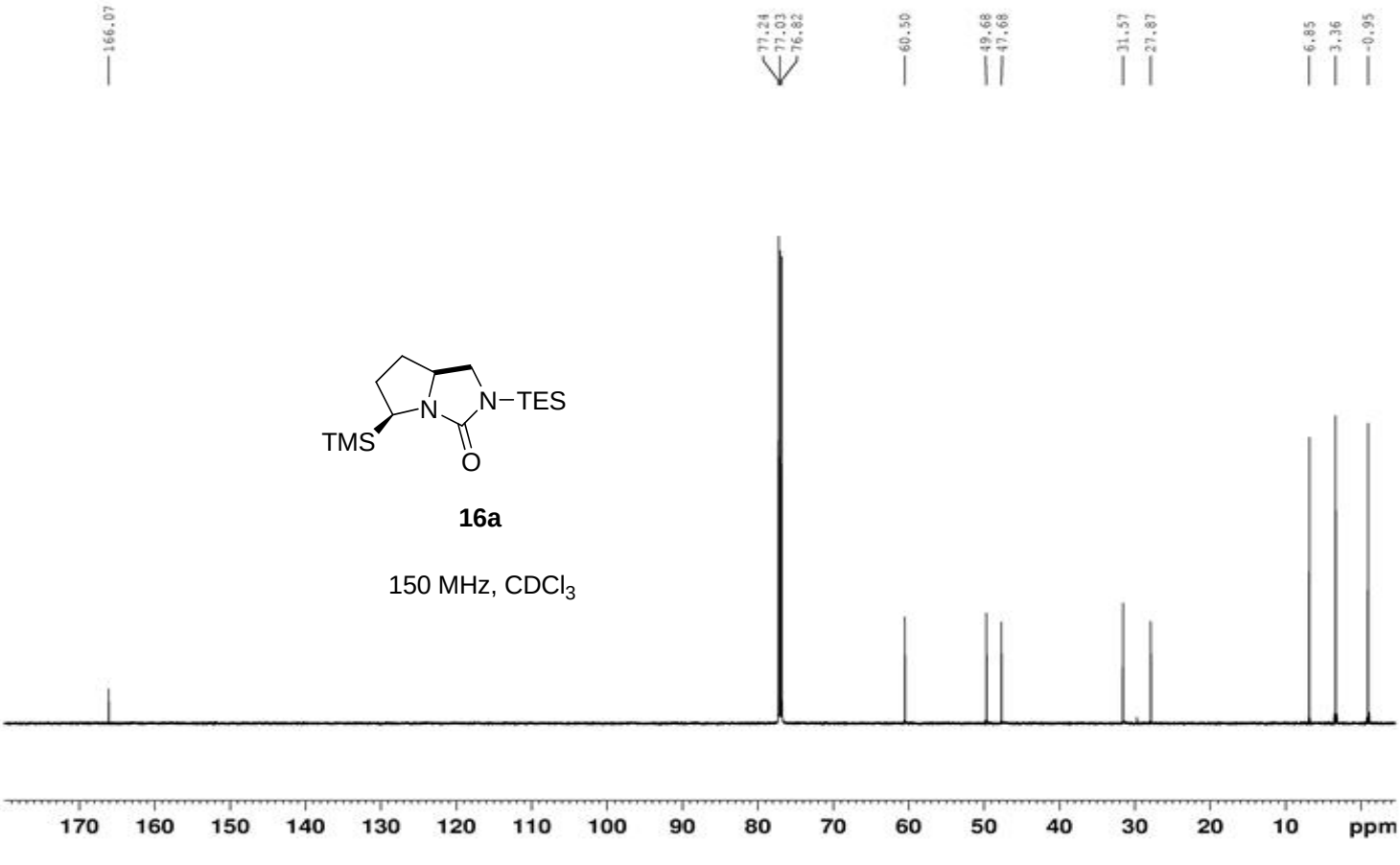
1d proton



16a

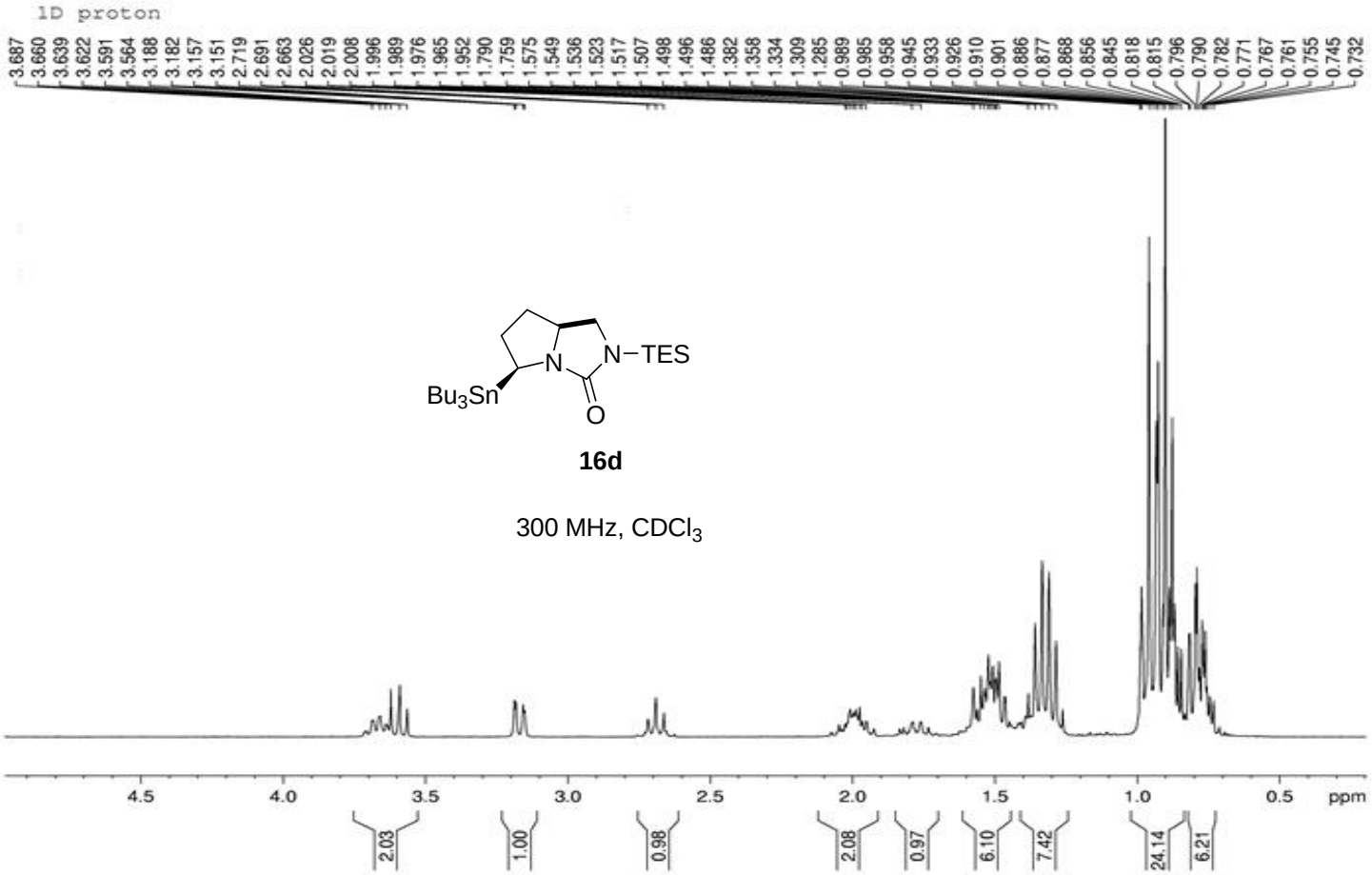
300 MHz, $CDCl_3$

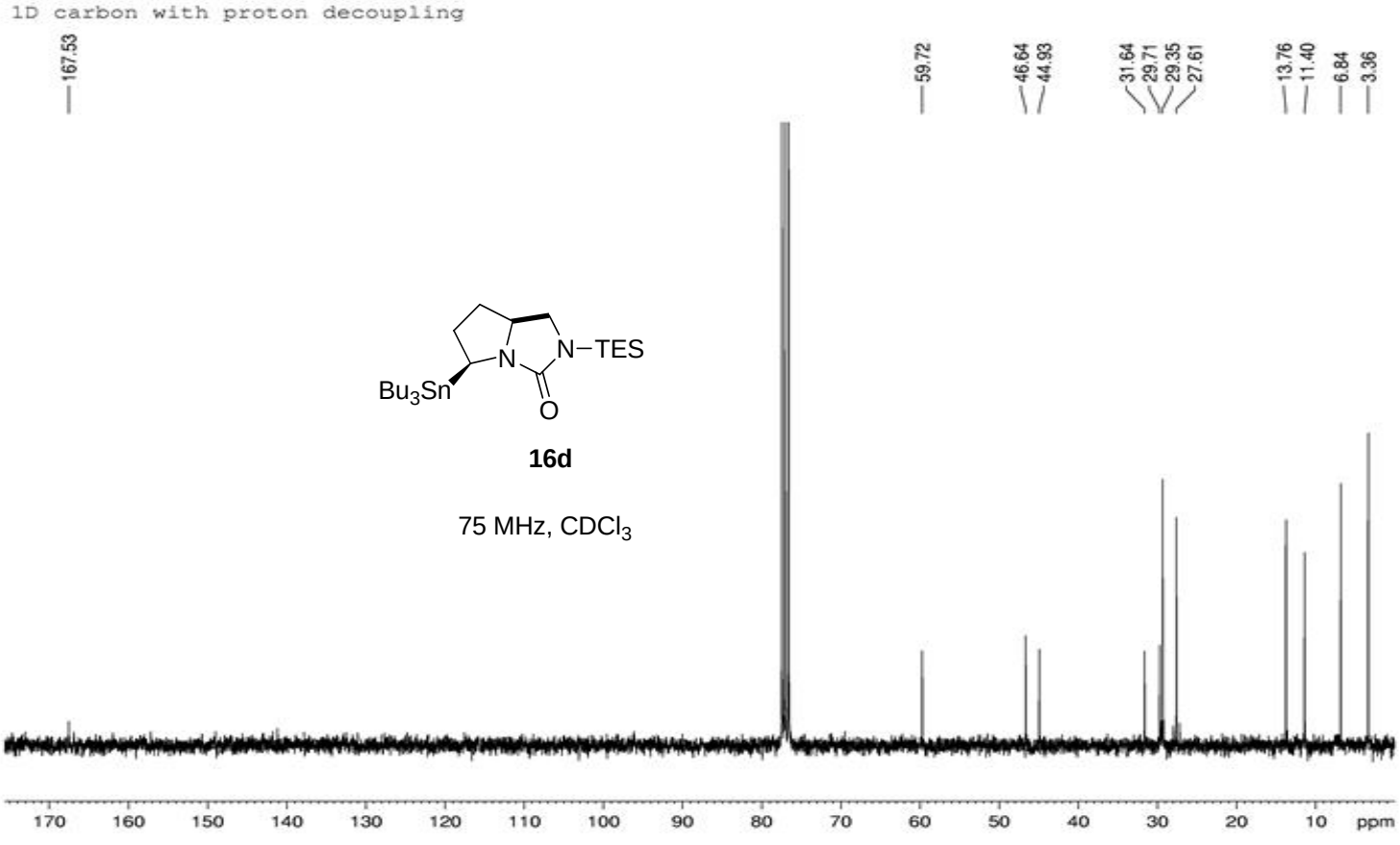
1d carbon with proton decoupling



16a

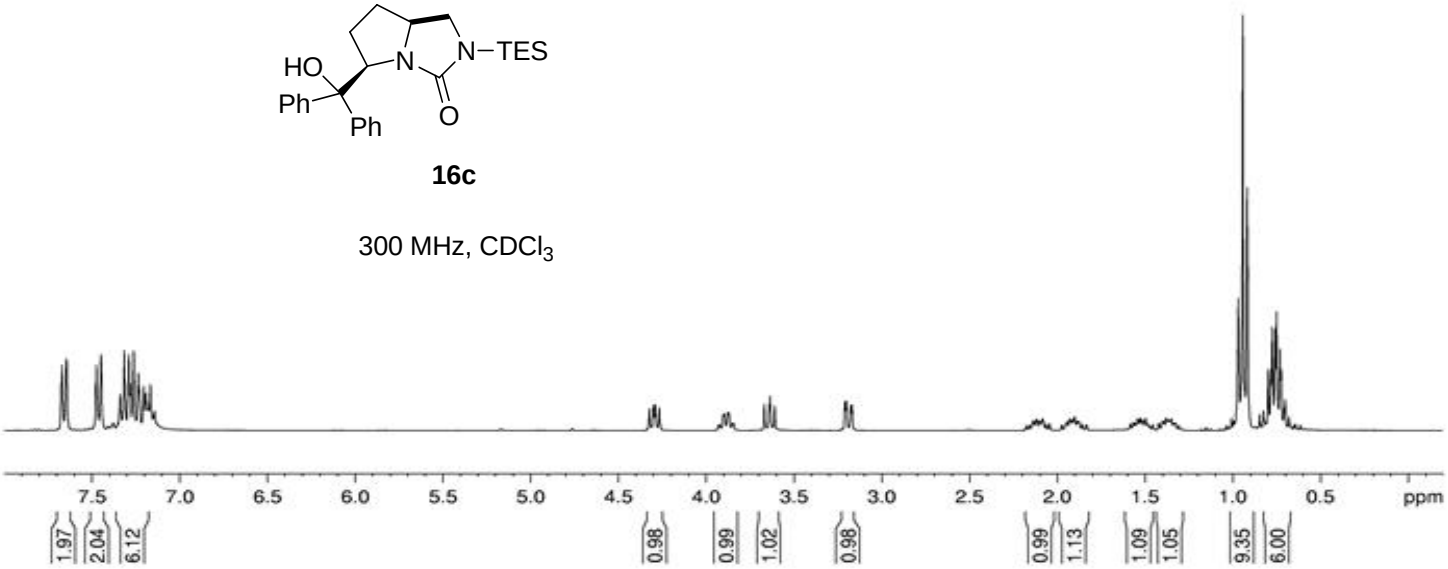
150 MHz, $CDCl_3$

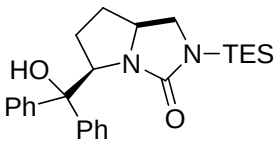

1D proton
3.687
3.660
3.639
3.622
3.591
3.564
3.188
3.182
3.157
3.151
2.719
2.691
2.663
2.026
2.019
2.008
1.996
1.989
1.976
1.965
1.952
1.790
1.759
1.575
1.549
1.536
1.523
1.517
1.507
1.498
1.496
1.486
1.382
1.358
1.334
1.309
1.285
0.989
0.985
0.958
0.945
0.933
0.926
0.910
0.901
0.886
0.877
0.868
0.856
0.845
0.818
0.815
0.796
0.790
0.782
0.771
0.767
0.761
0.755
0.745
0.732
N
N−TES
Bu3Sn
O
16d
300 MHz, CDCl3
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.03
1.00
0.98
2.08
0.97
6.10
7.42
24.14
6.21


1D carbon with proton decoupling
167.53
59.72
46.64
44.93
31.64
29.71
29.35
27.61
13.76
11.40
6.84
3.36
N
N−TES
Bu3Sn
O
16d
75 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

16c

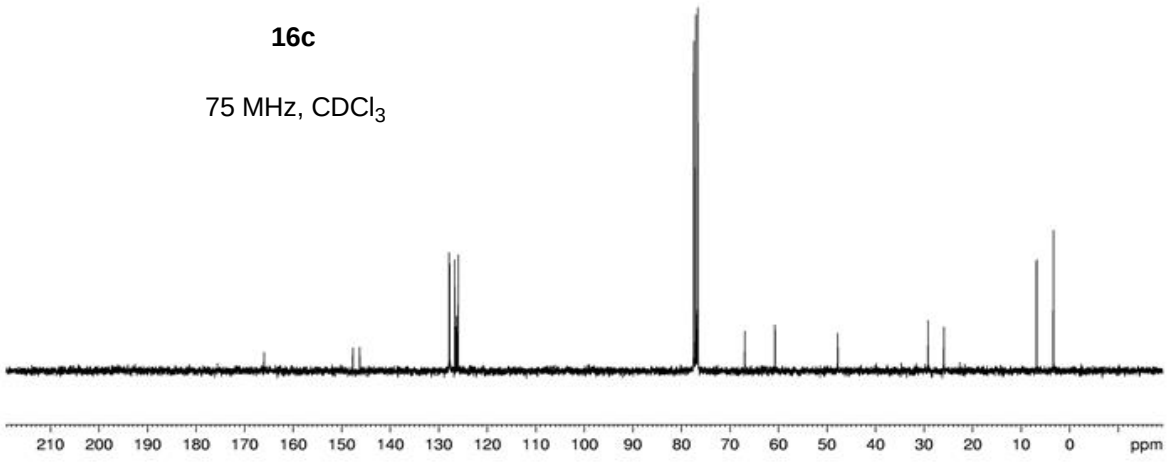
300 MHz, $CDCl_3$



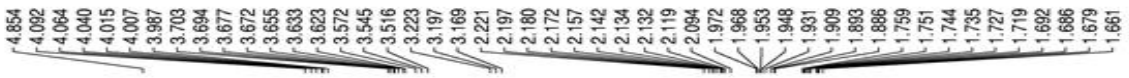


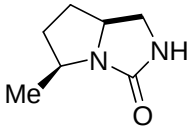
16c

75 MHz, $CDCl_3$



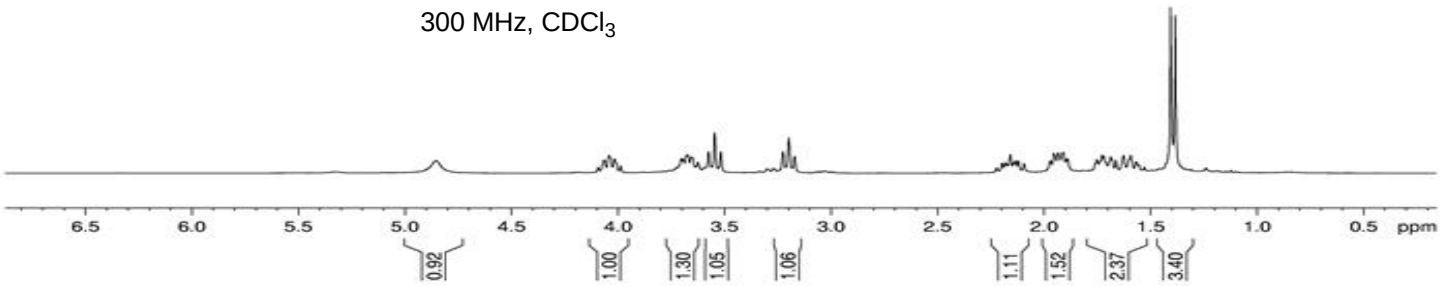
1D proton



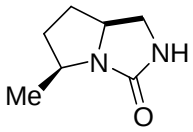


17b

300 MHz, $CDCl_3$

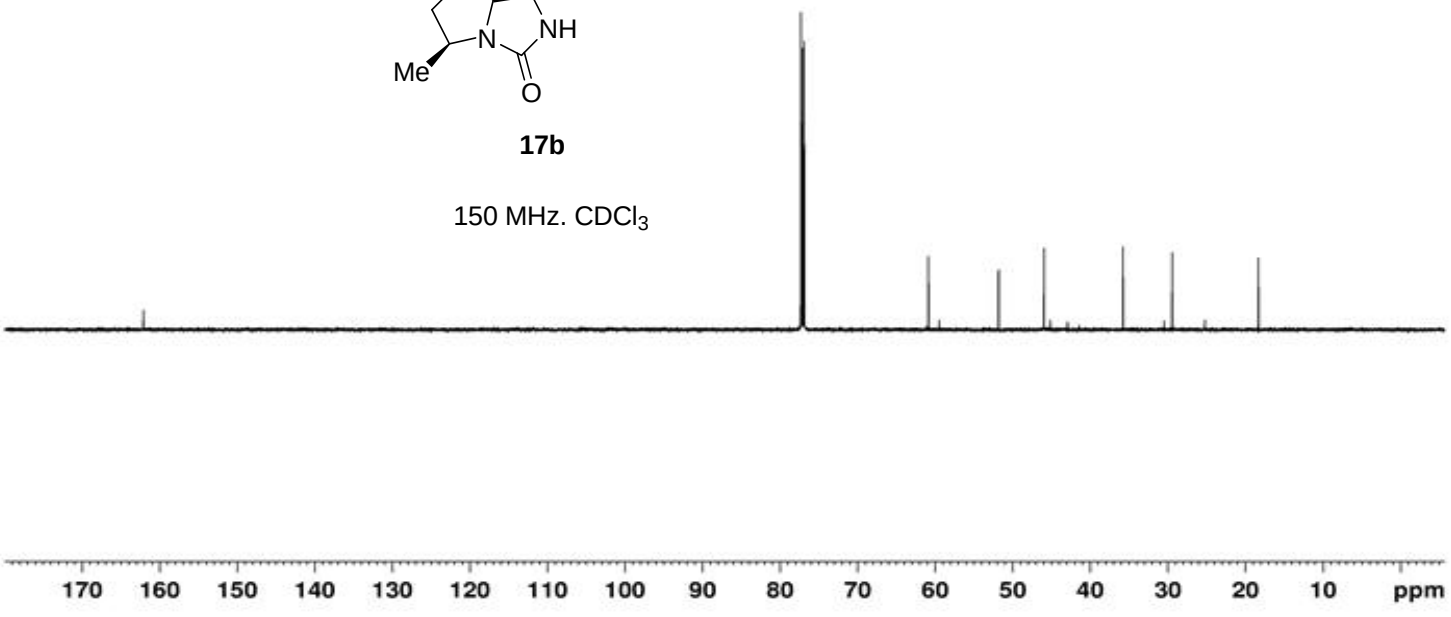


1d carbon with proton decoupling



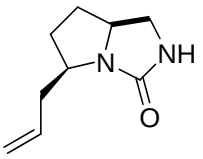
17b

150 MHz. $CDCl_3$



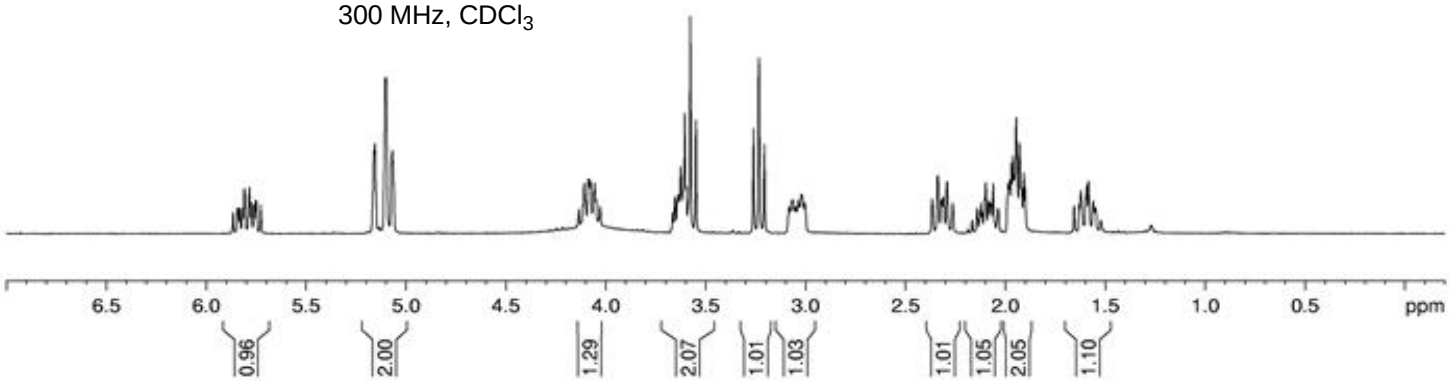
1D proton

5.809 5.784 5.774 5.761 5.754 5.748 5.160 5.156 5.104 5.101 5.068 4.115 4.108 4.088 4.082 4.075 4.061 4.056 4.048 3.637 3.625 3.605 3.597 3.585 3.576 3.549 3.261 3.233 3.206 3.066 3.036 3.030 3.020 3.010 3.003 2.366 2.337 2.320 2.310 2.291 2.263 2.123 2.104 2.097 2.085 2.077 2.073 2.060 1.978 1.969 1.962 1.956 1.945 1.928 1.907 1.631 1.622 1.593 1.584 1.560



17e

300 MHz, $CDCl_3$

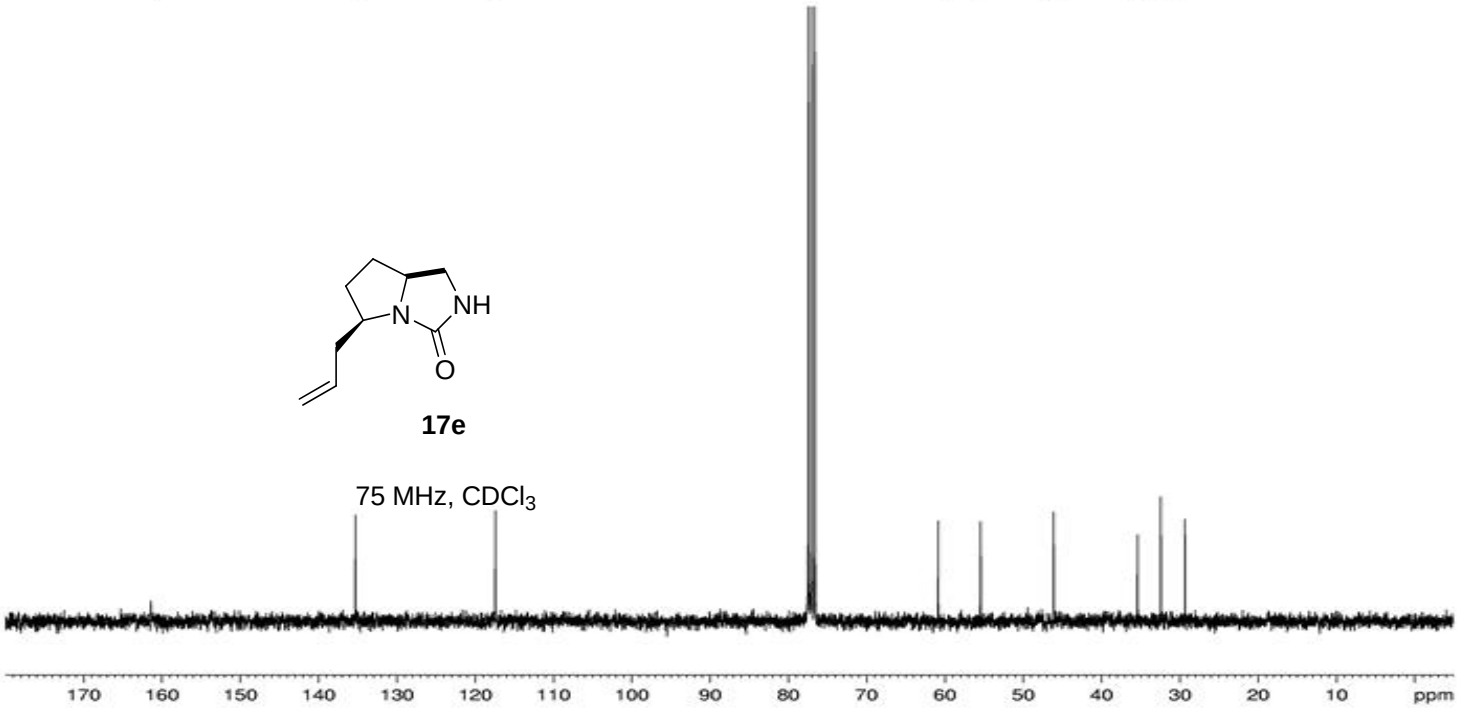


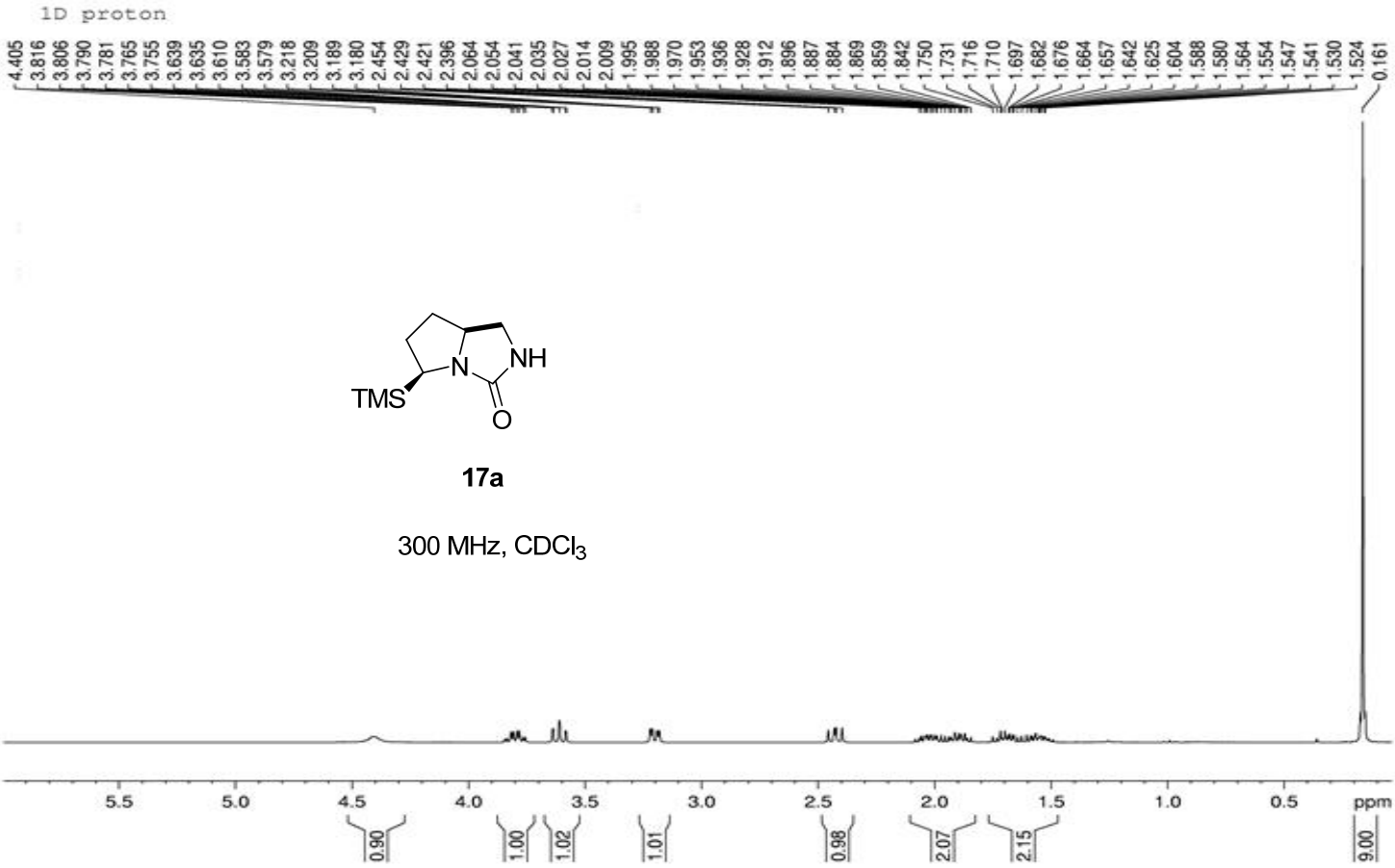
1D carbon with proton decoupling

161.40 135.29 117.39 60.84 55.44 46.09 35.38 32.42 29.32

17e

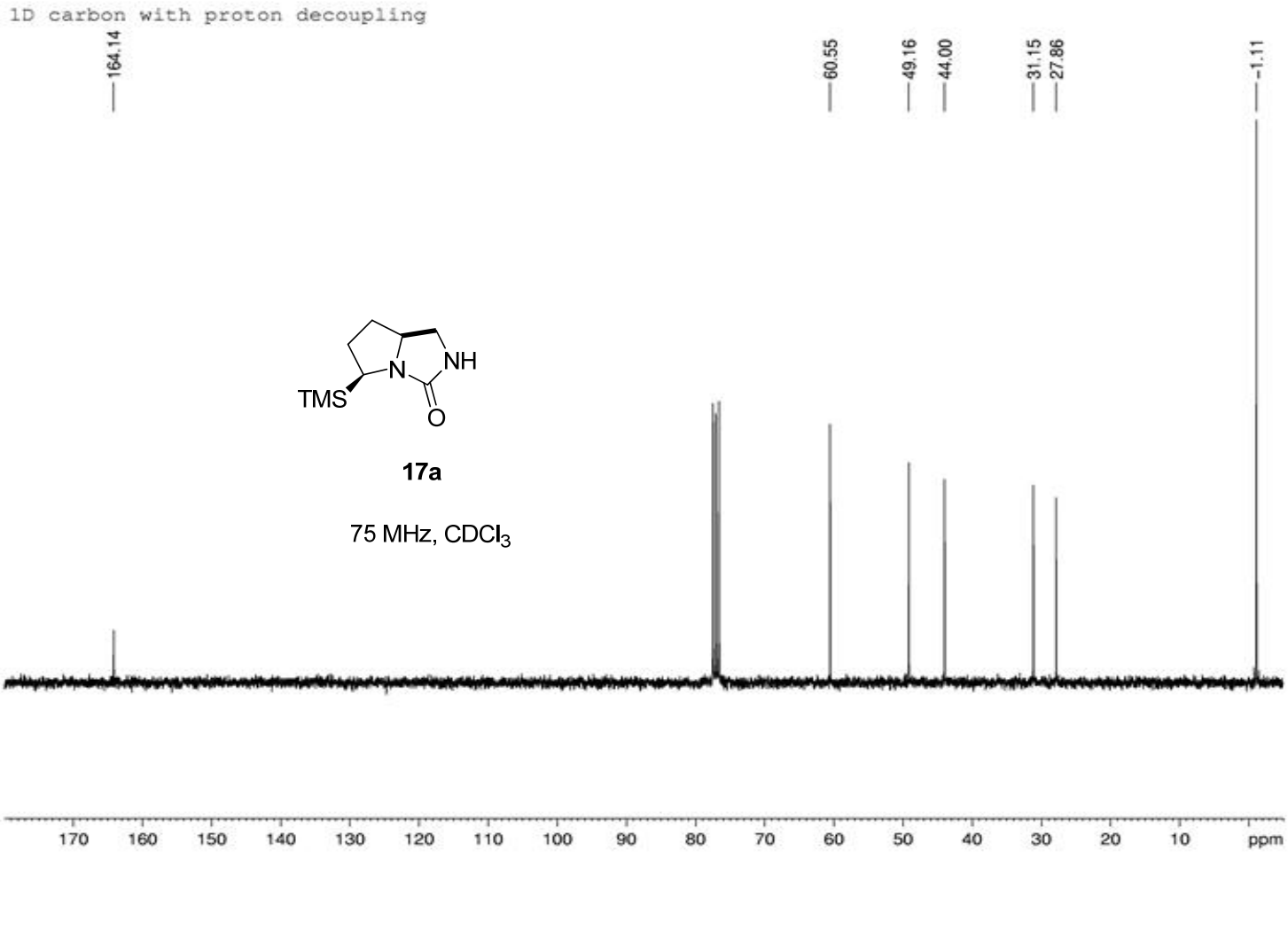
75 MHz, $CDCl_3$





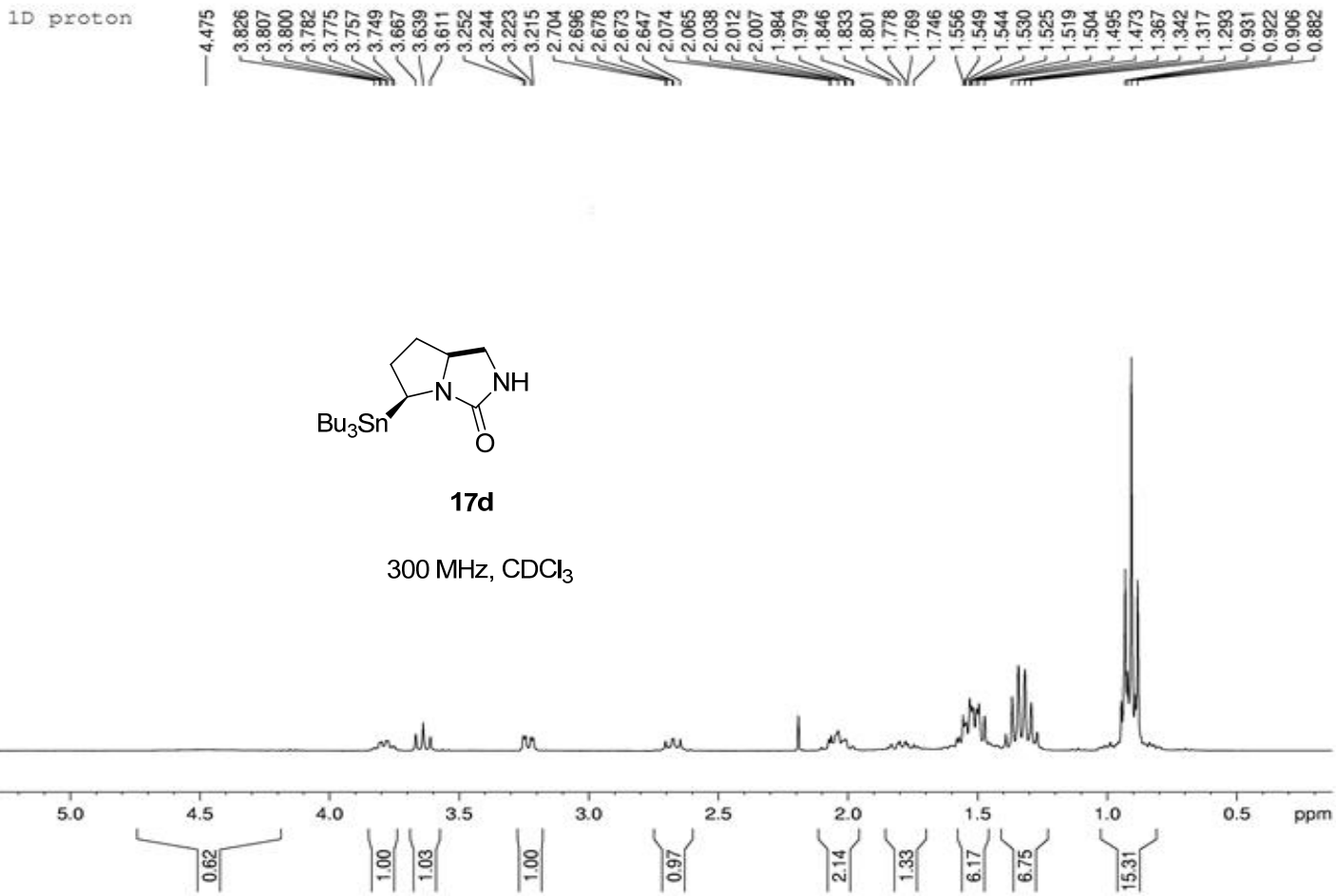
17a

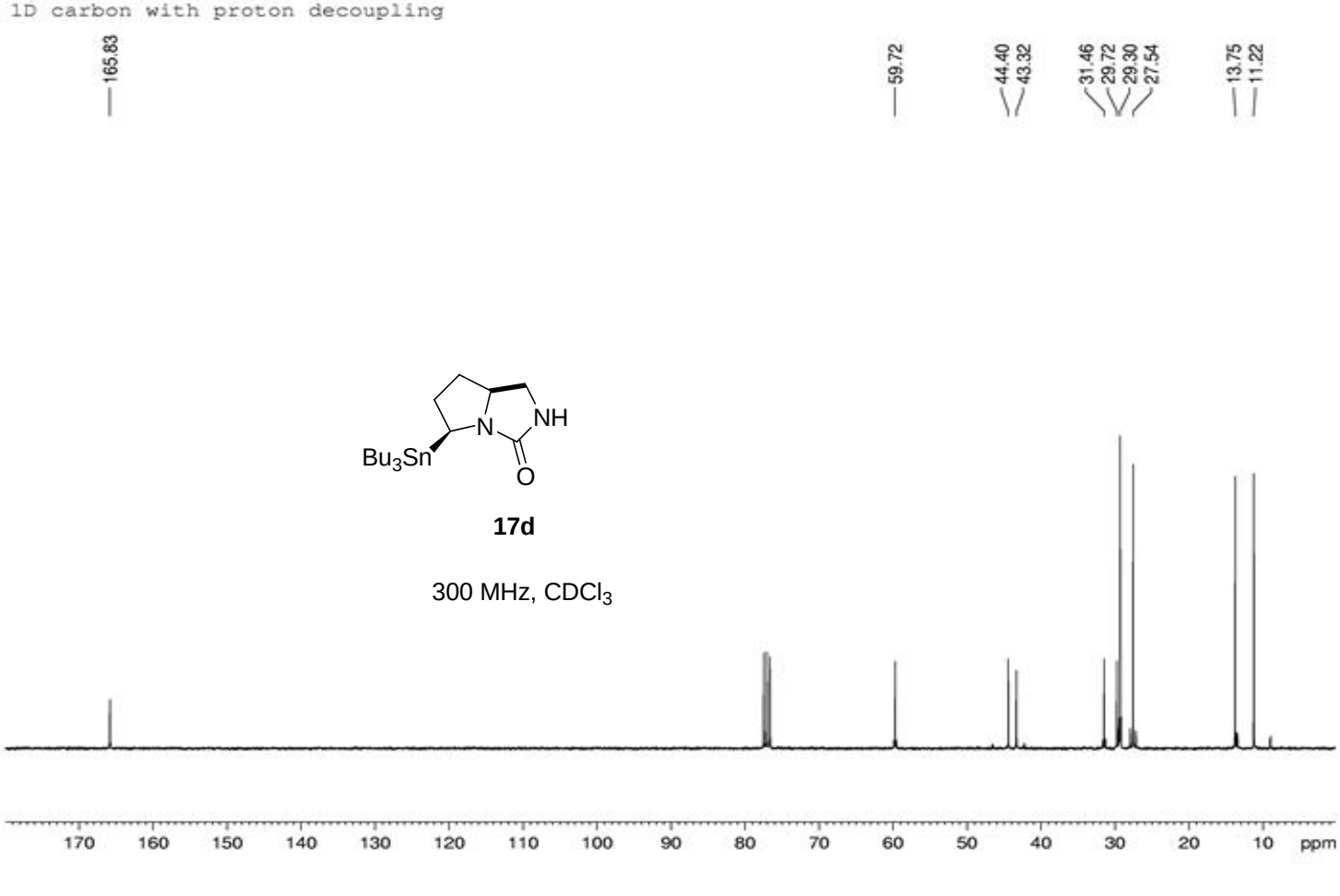
300 MHz, $CDCl_3$

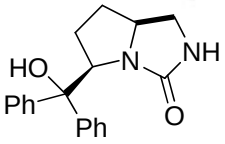


17a

75 MHz, $CDCl_3$

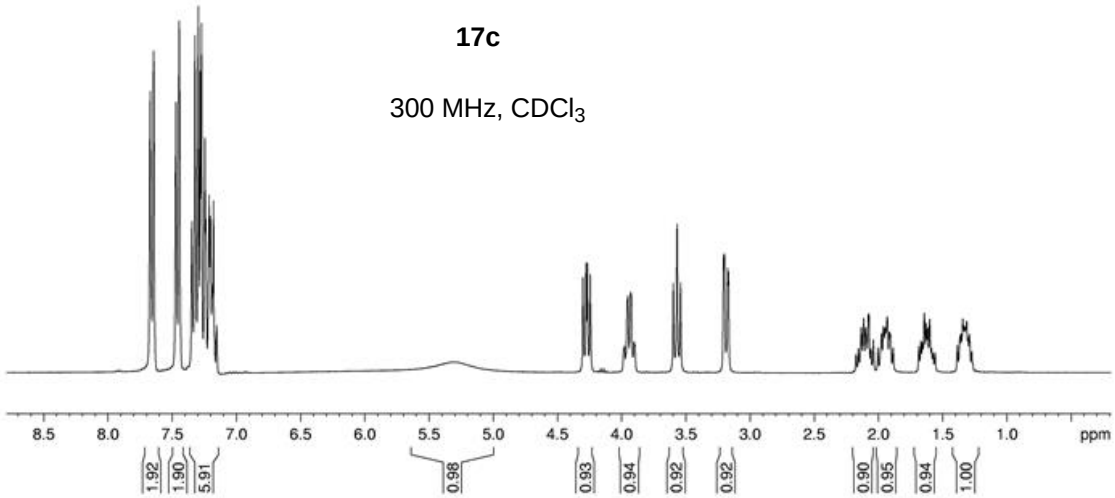

1D proton
4.475
3.826
3.807
3.800
3.782
3.775
3.757
3.749
3.667
3.639
3.611
3.252
3.244
3.223
3.215
2.704
2.696
2.678
2.673
2.647
2.074
2.065
2.038
2.012
2.007
1.984
1.979
1.846
1.833
1.801
1.778
1.769
1.746
1.556
1.549
1.544
1.530
1.525
1.519
1.504
1.495
1.473
1.367
1.342
1.317
1.293
0.931
0.922
0.906
0.882
NH
N
Bu3Sn
O
17d
300 MHz, CDCl3
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.62
1.00
1.03
1.00
0.97
2.14
1.33
6.17
6.75
15.31

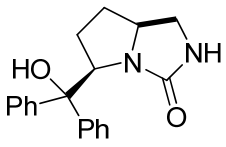

1D carbon with proton decoupling
165.83
59.72
44.40
43.32
31.46
29.72
29.30
27.54
13.75
11.22
NH
N
Bu3Sn
O
17d
300 MHz, CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



17c

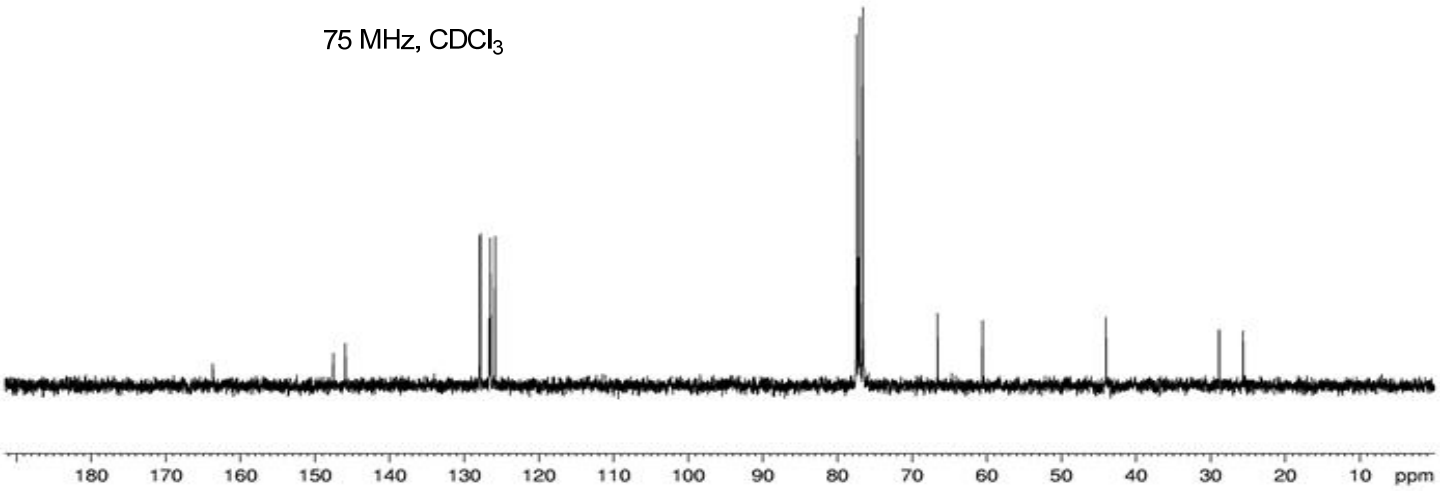
300 MHz, $CDCl_3$

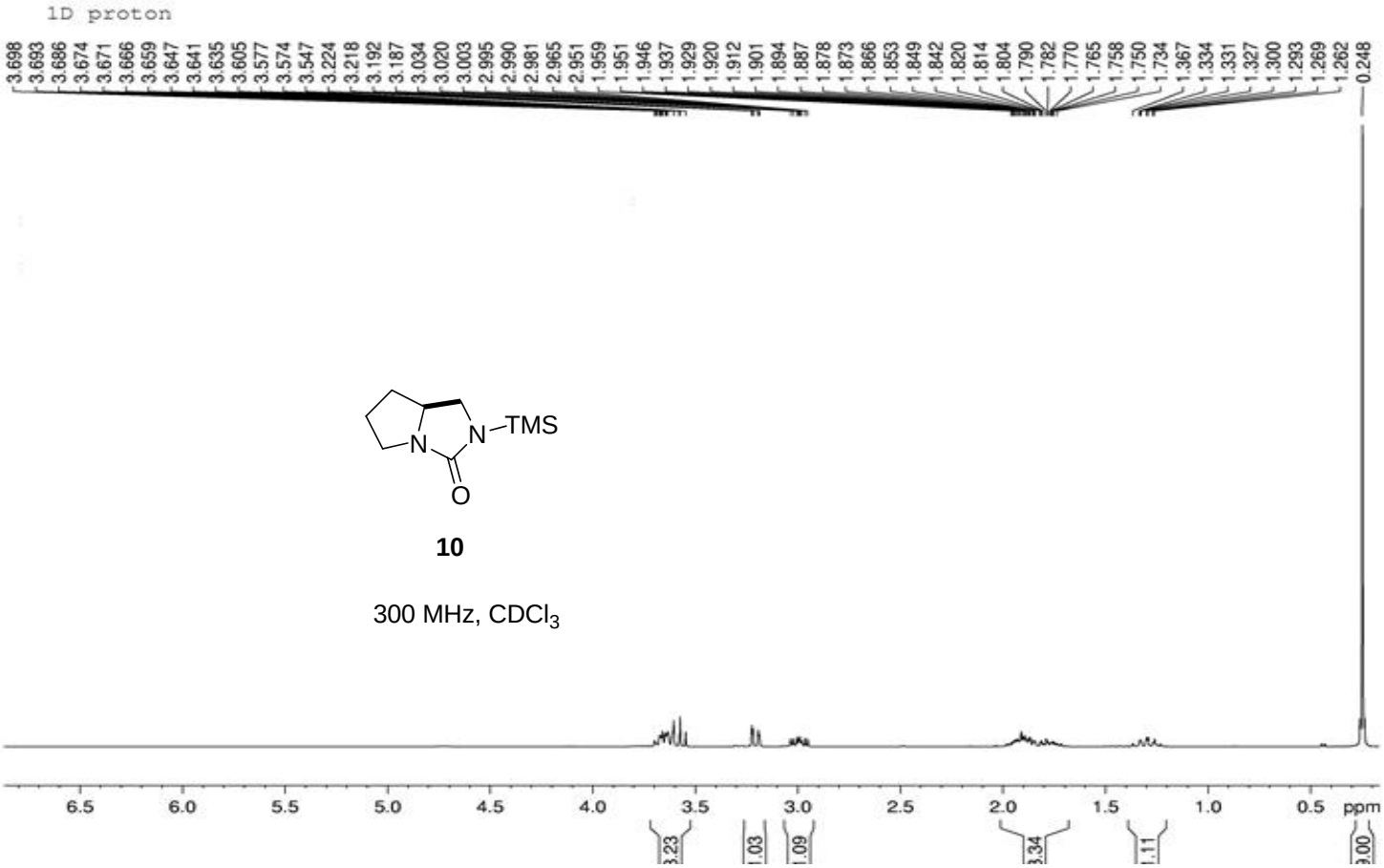




17c

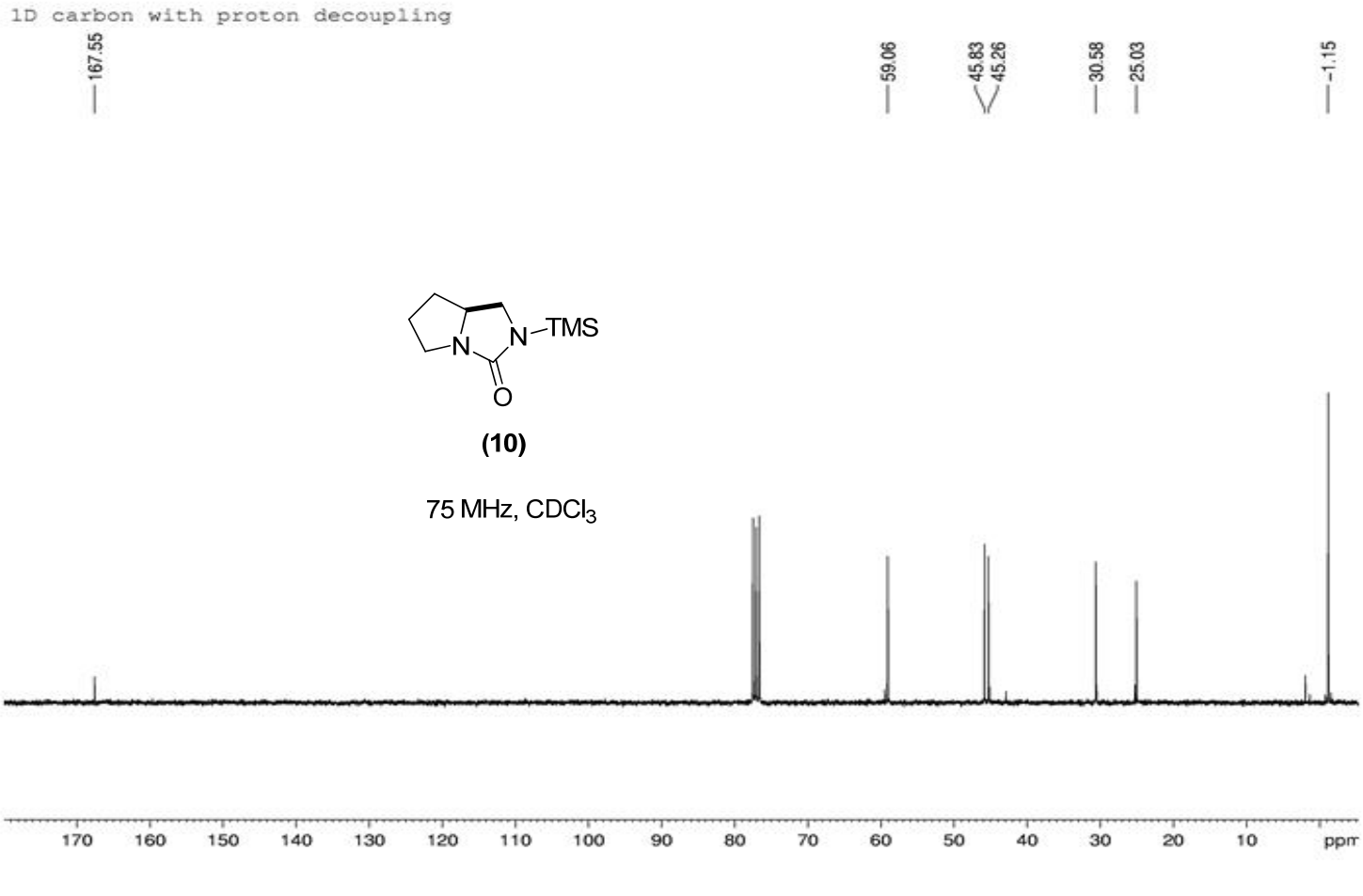
75 MHz, $CDCl_3$





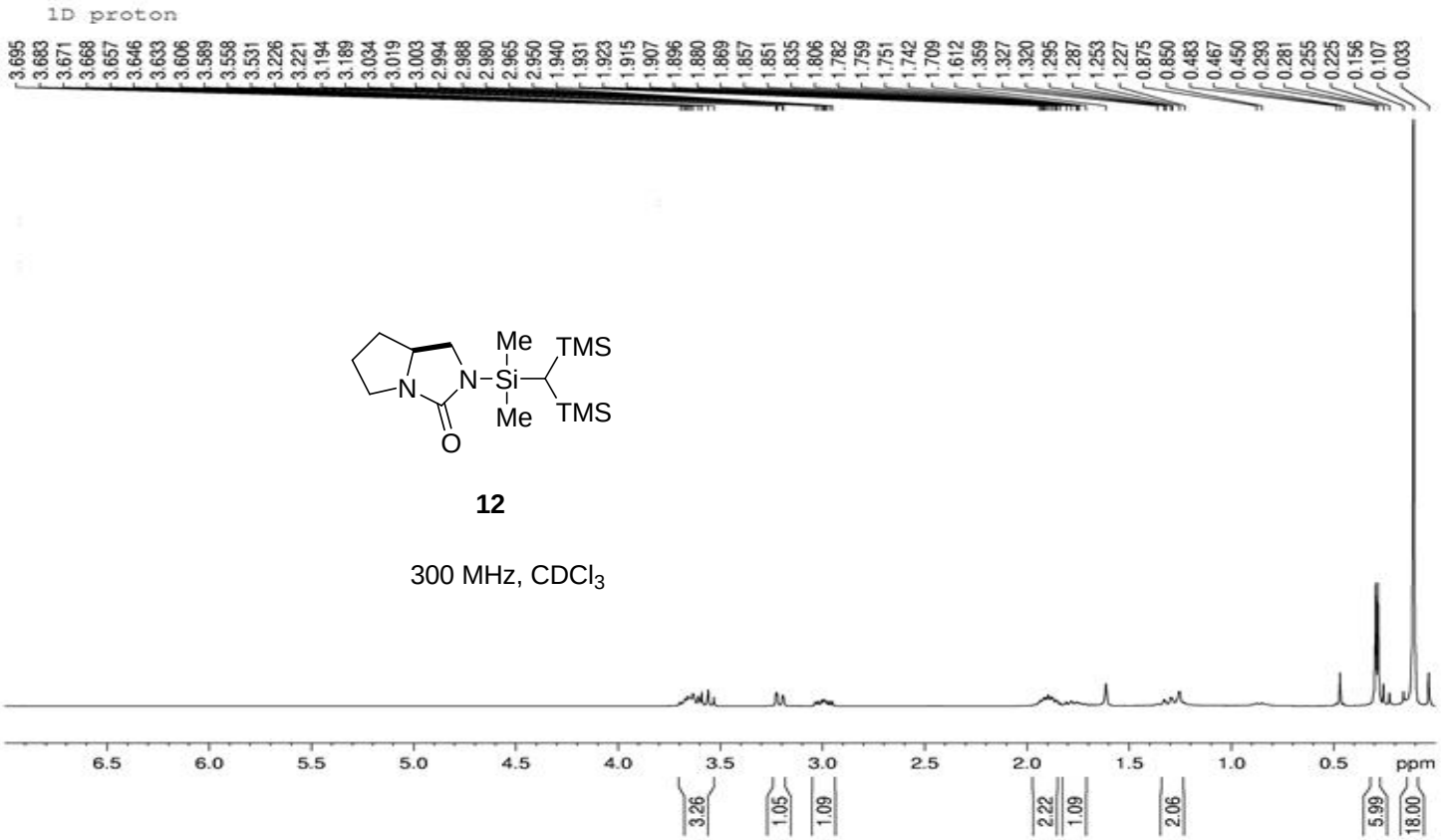
10

300 MHz, $CDCl_3$



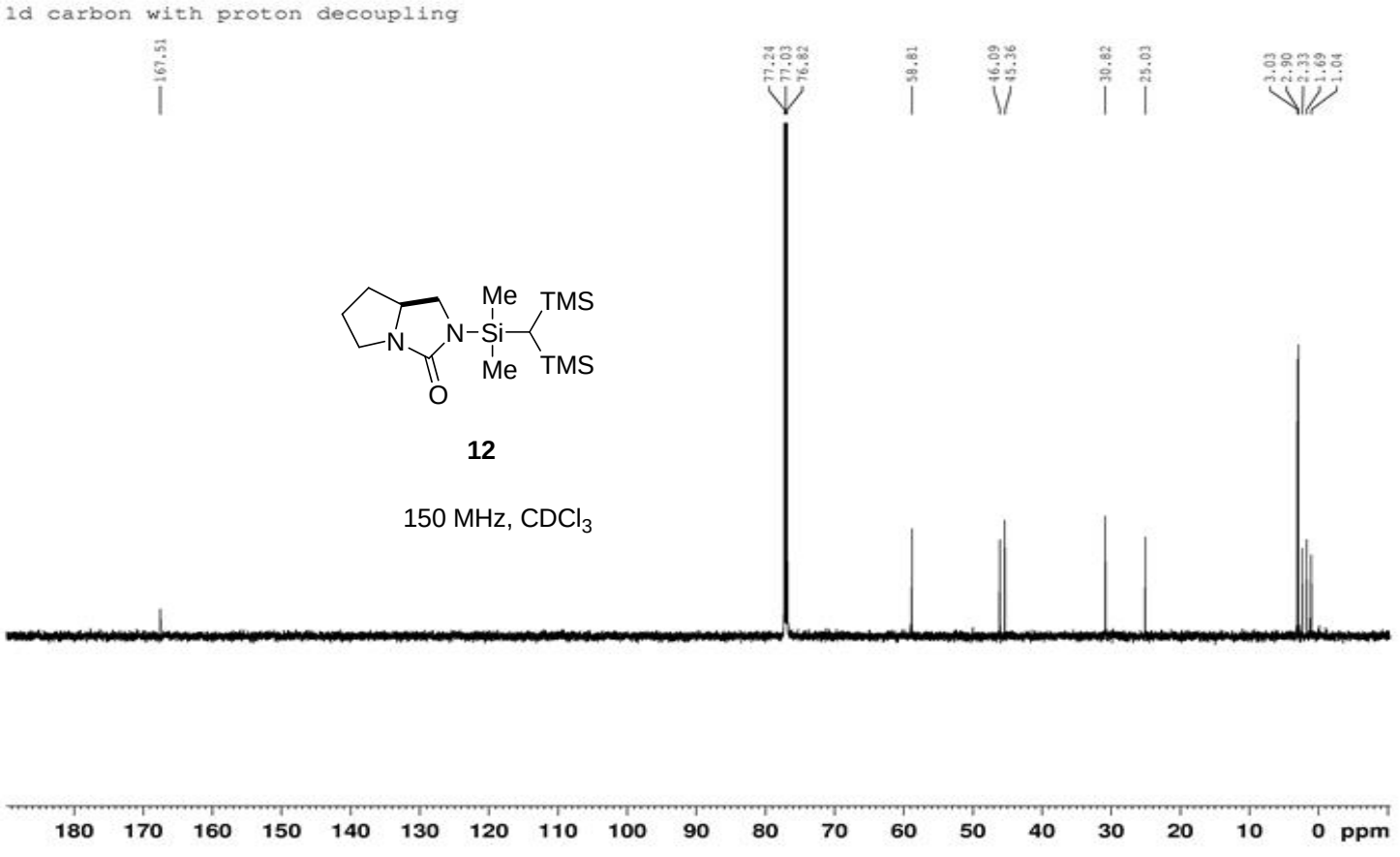
(10)

75 MHz, $CDCl_3$



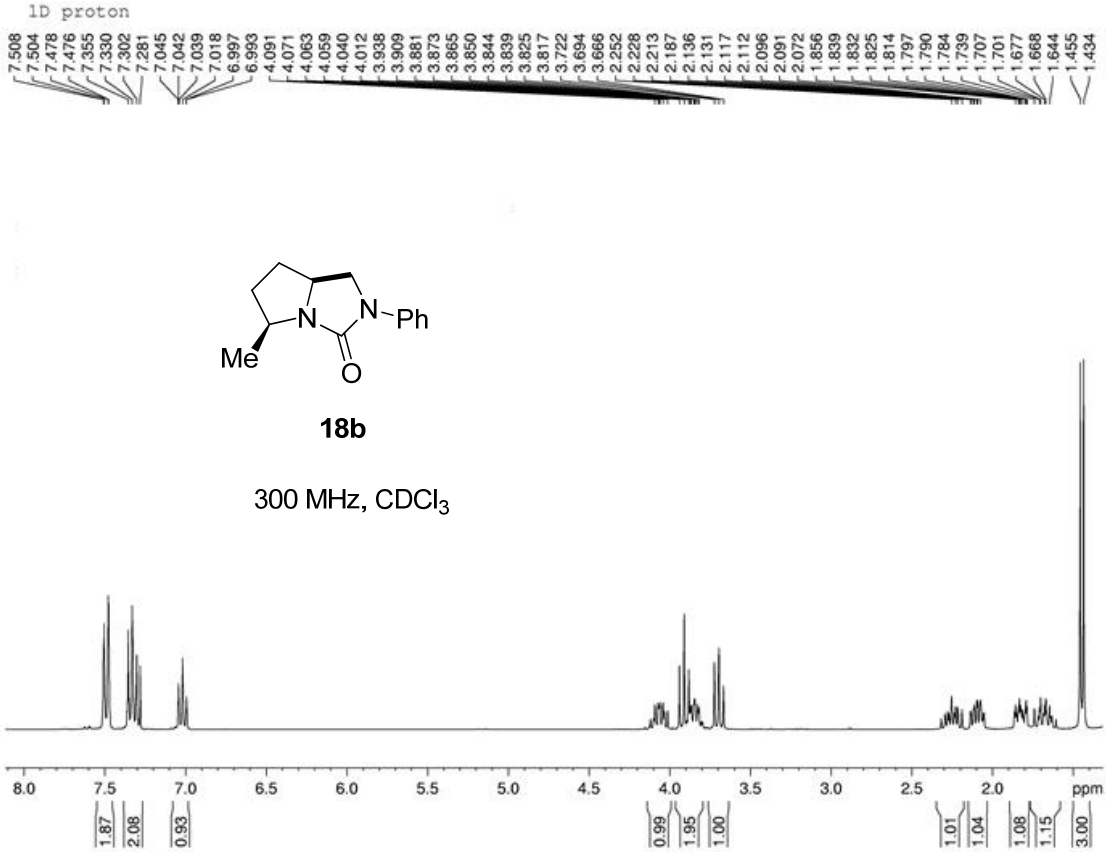
12

300 MHz, $CDCl_3$



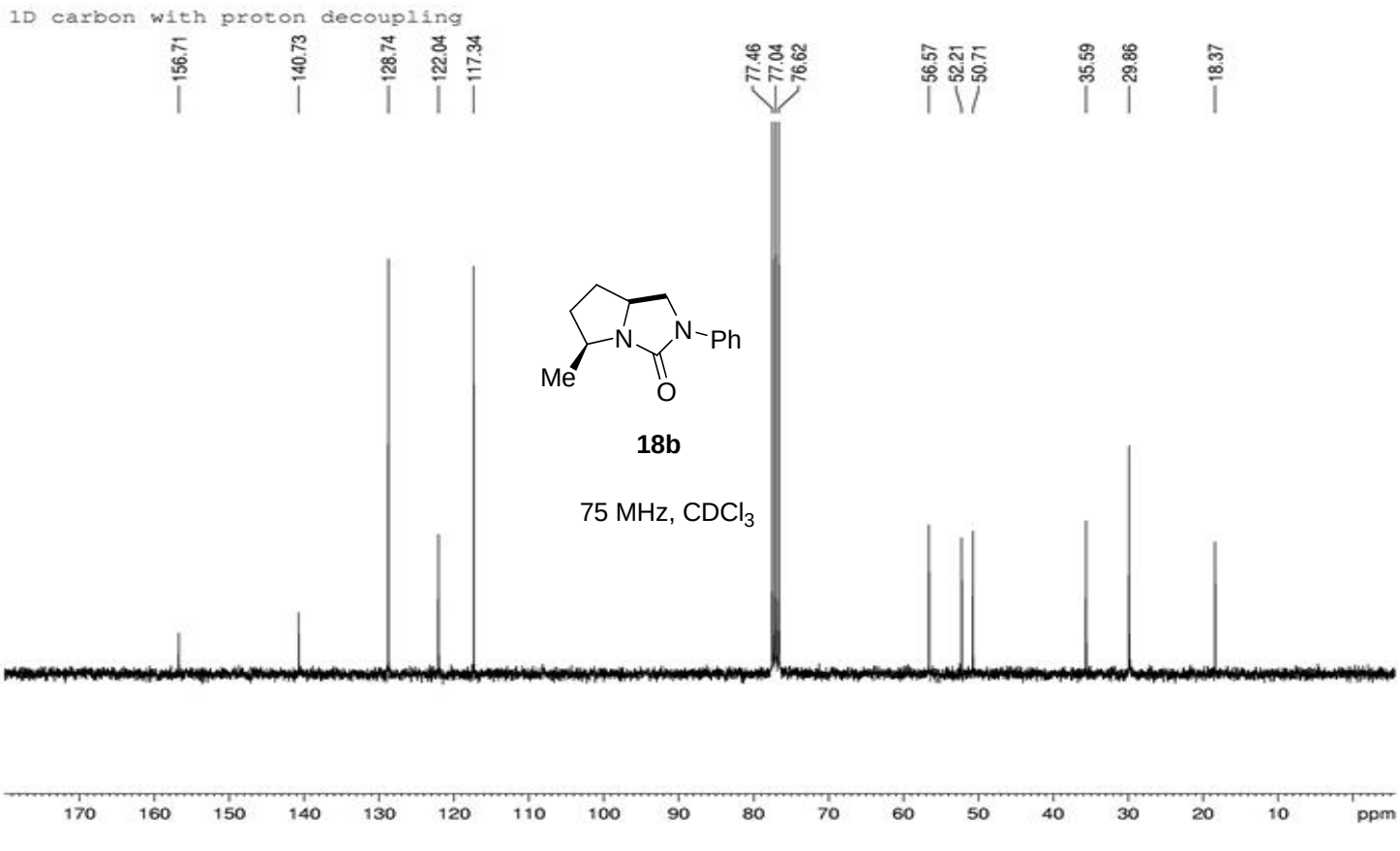
12

150 MHz, $CDCl_3$



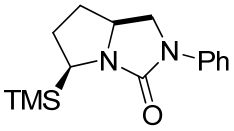
18b

300 MHz, $CDCl_3$



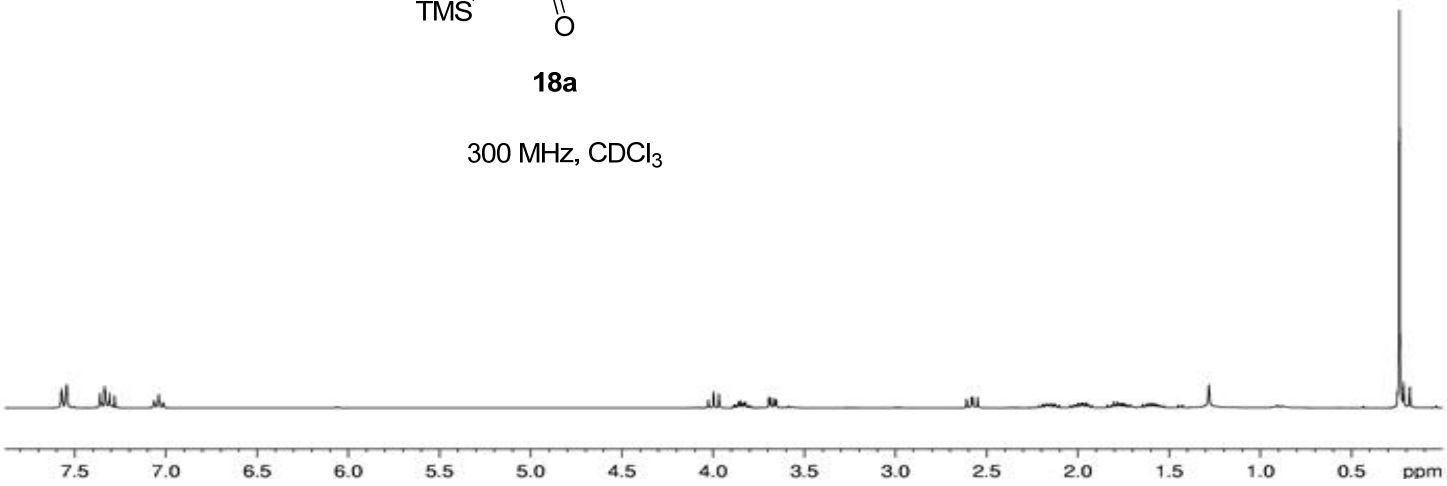
18b

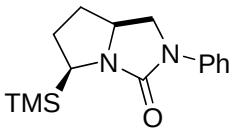
75 MHz, $CDCl_3$



18a

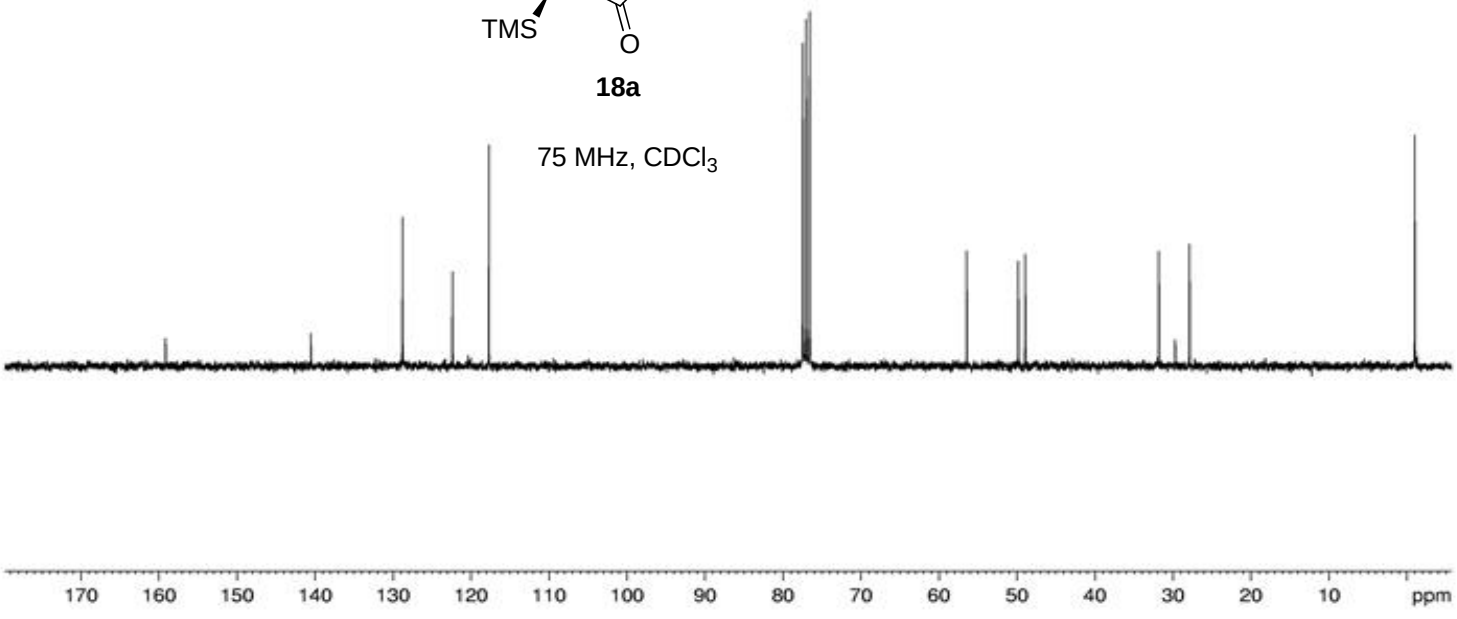
300 MHz, $CDCl_3$

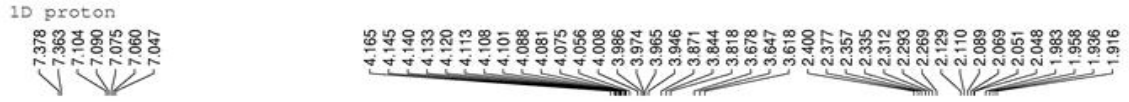


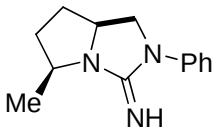


18a

75 MHz, $CDCl_3$

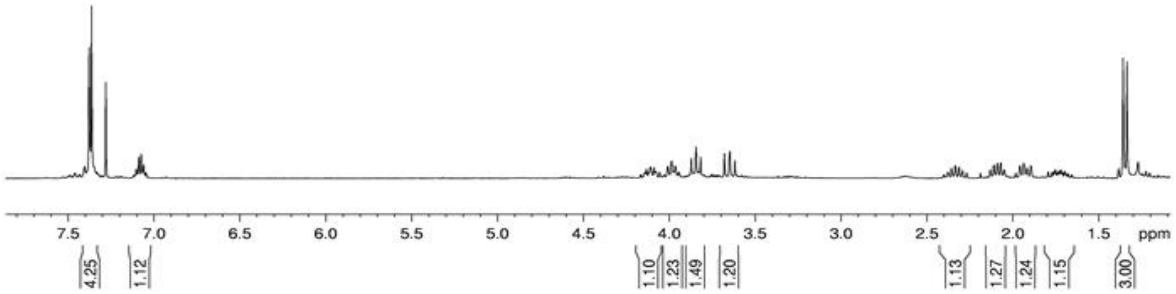


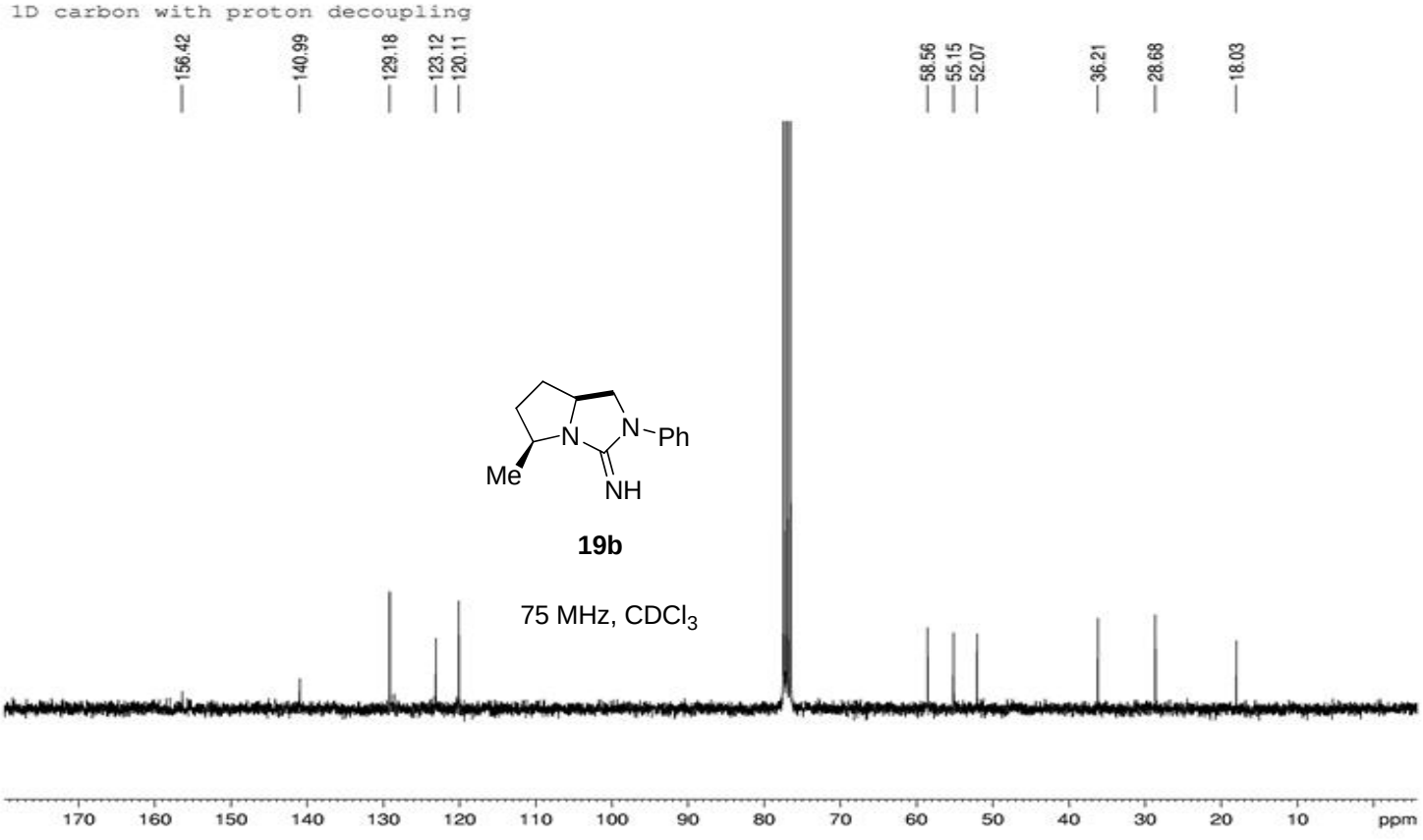




19b

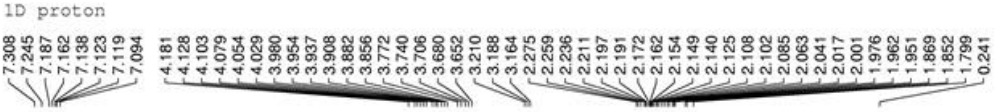
300 MHz, $CDCl_3$

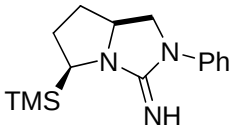




19b

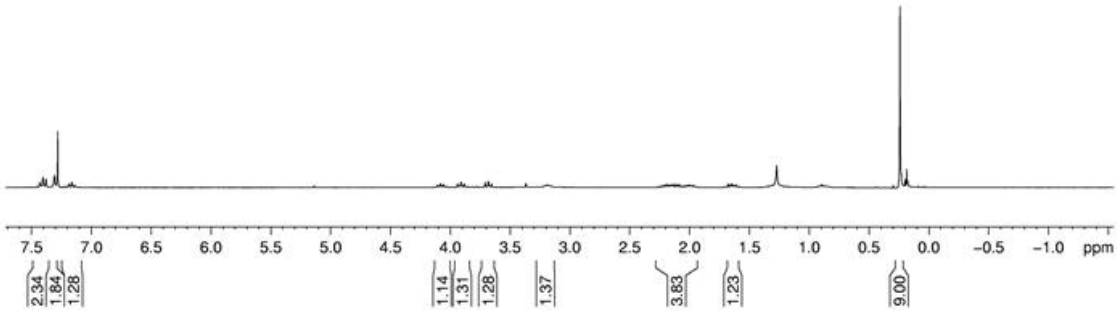
75 MHz, $CDCl_3$

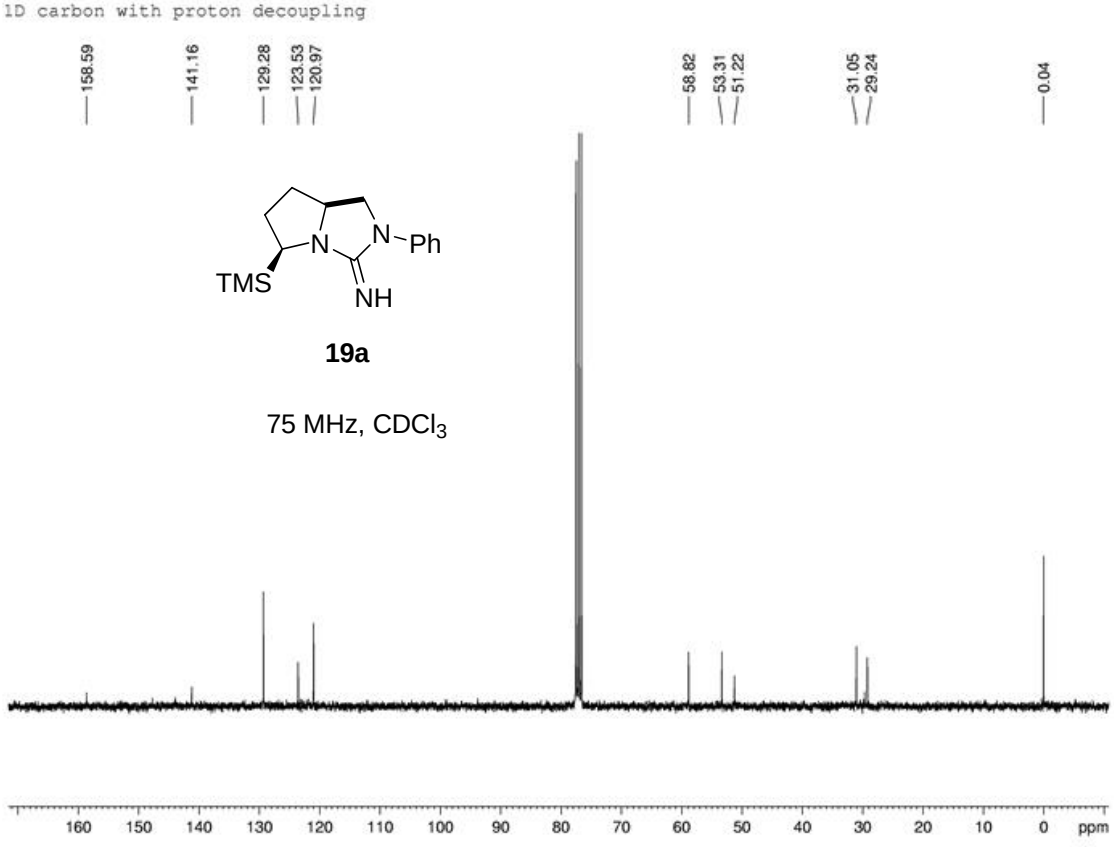




19a

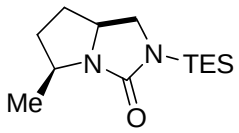
300 MHz, $CDCl_3$





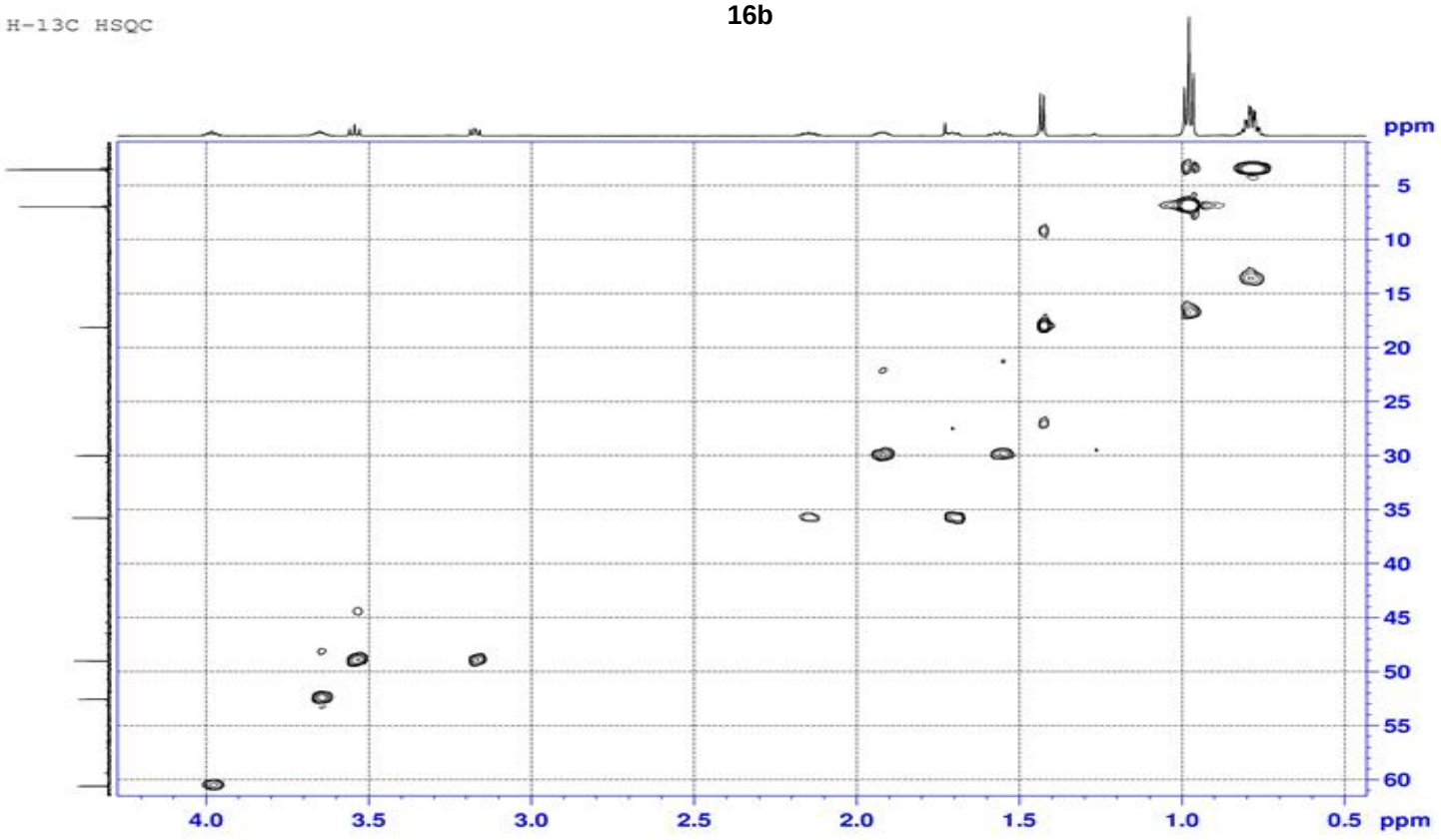
19a

75 MHz, $CDCl_3$

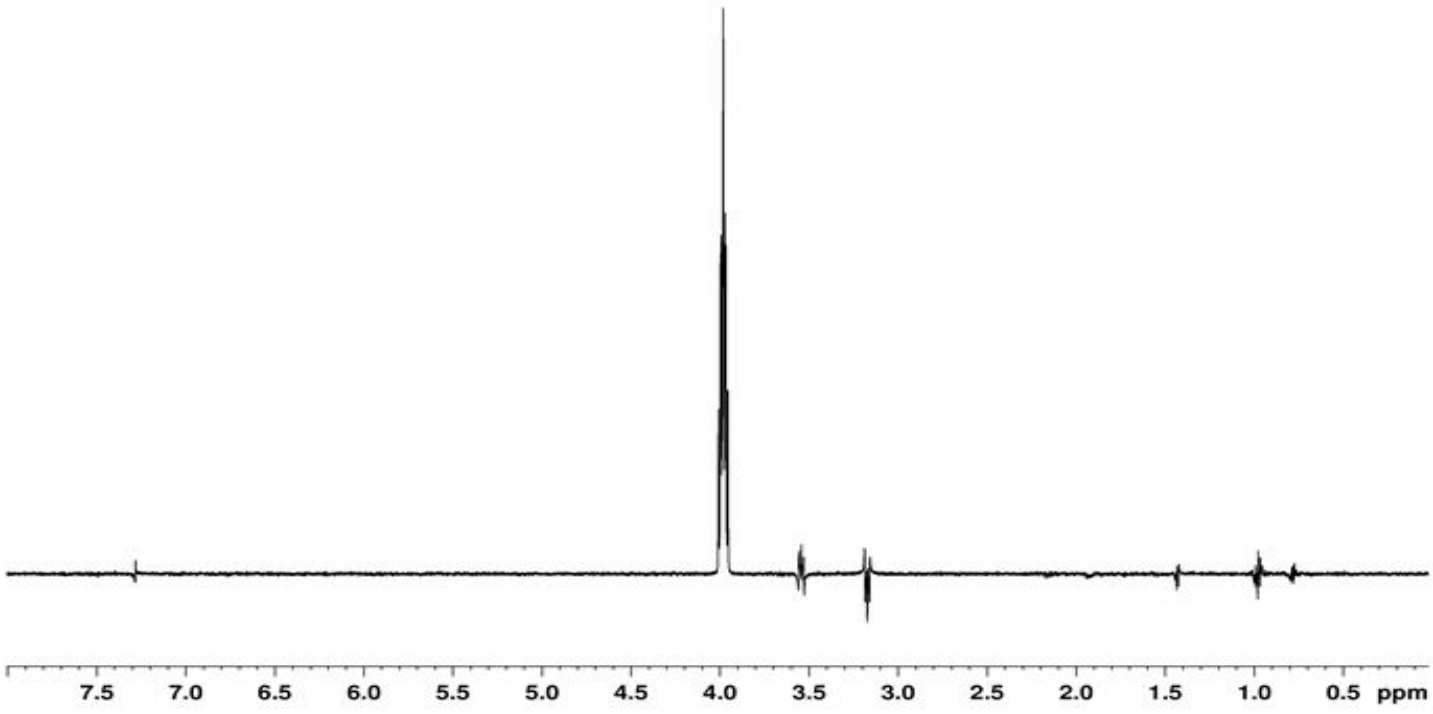


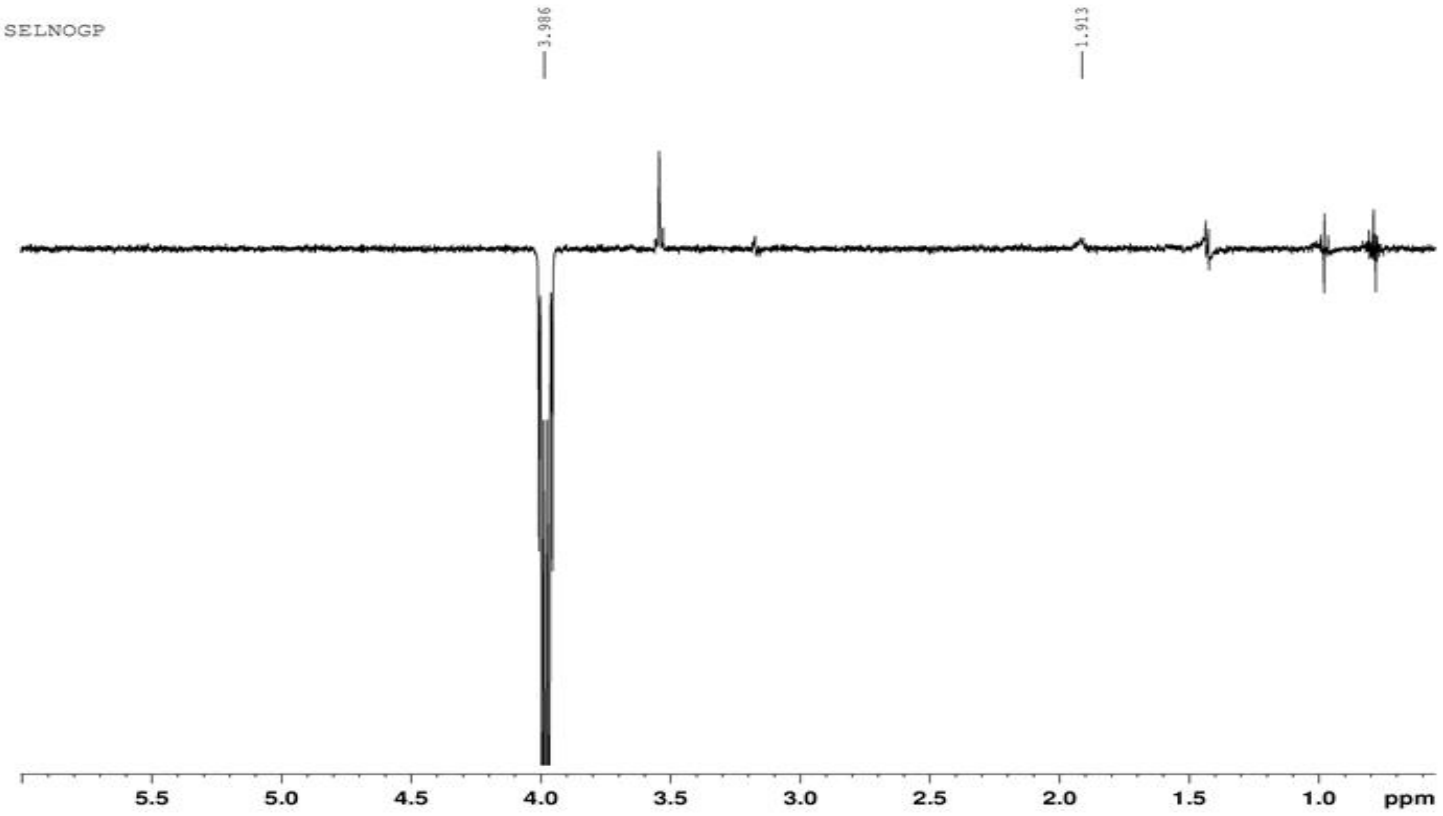
16b

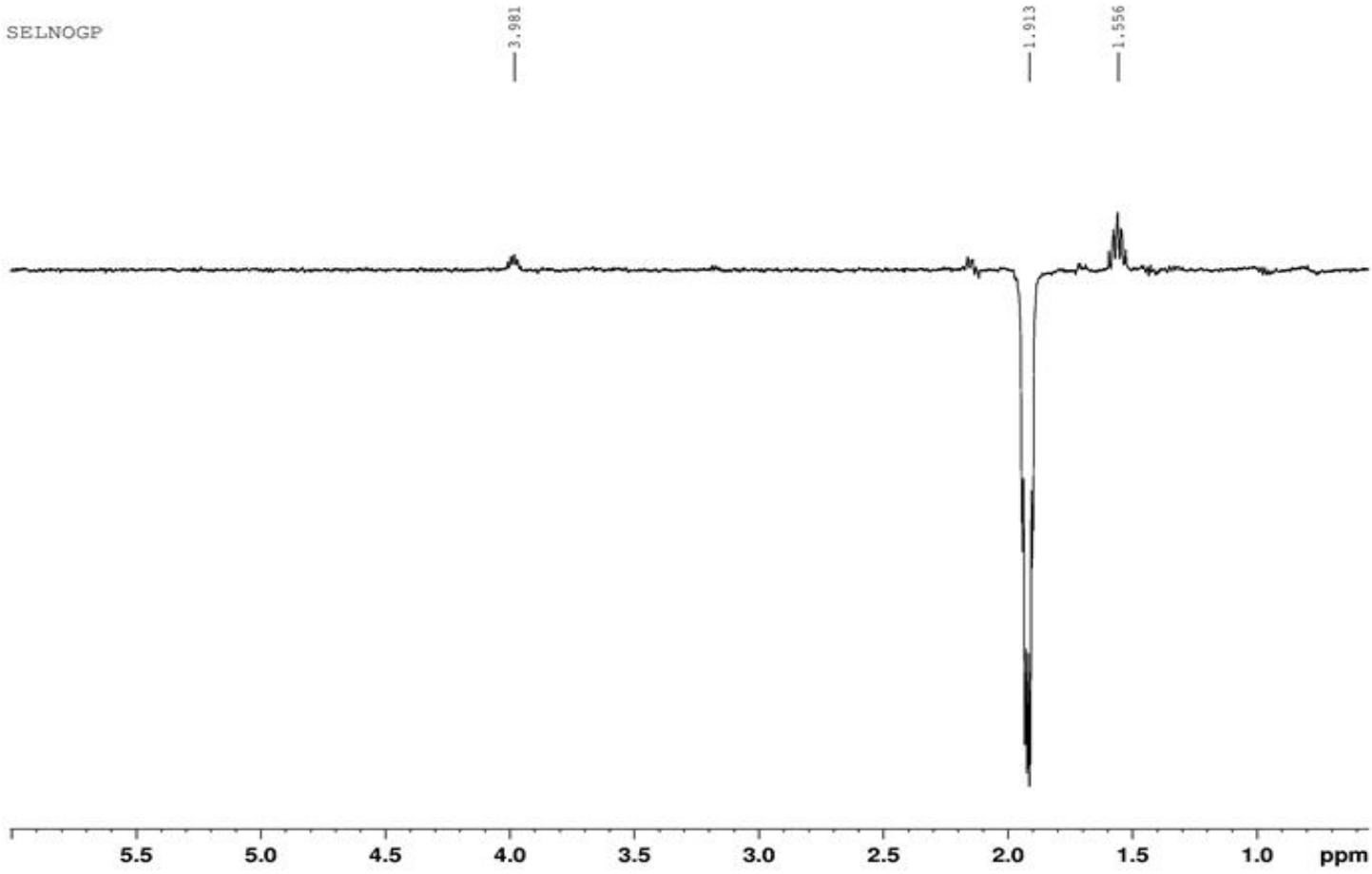
H-13C HSQC

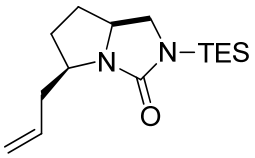


SELNOGP




SELNOGP
3.986
1.913
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

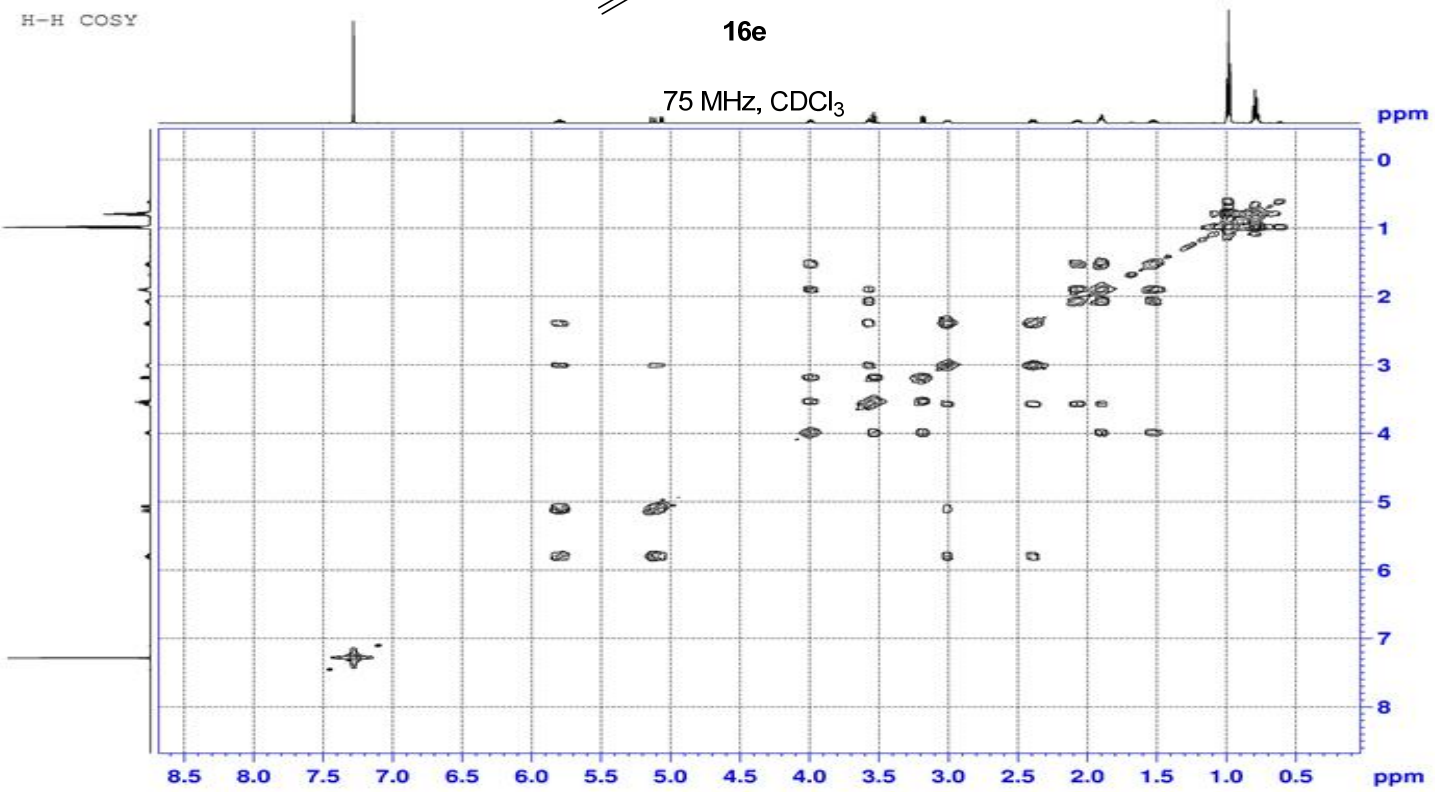

SELNOGP
3.981
1.913
1.556
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm



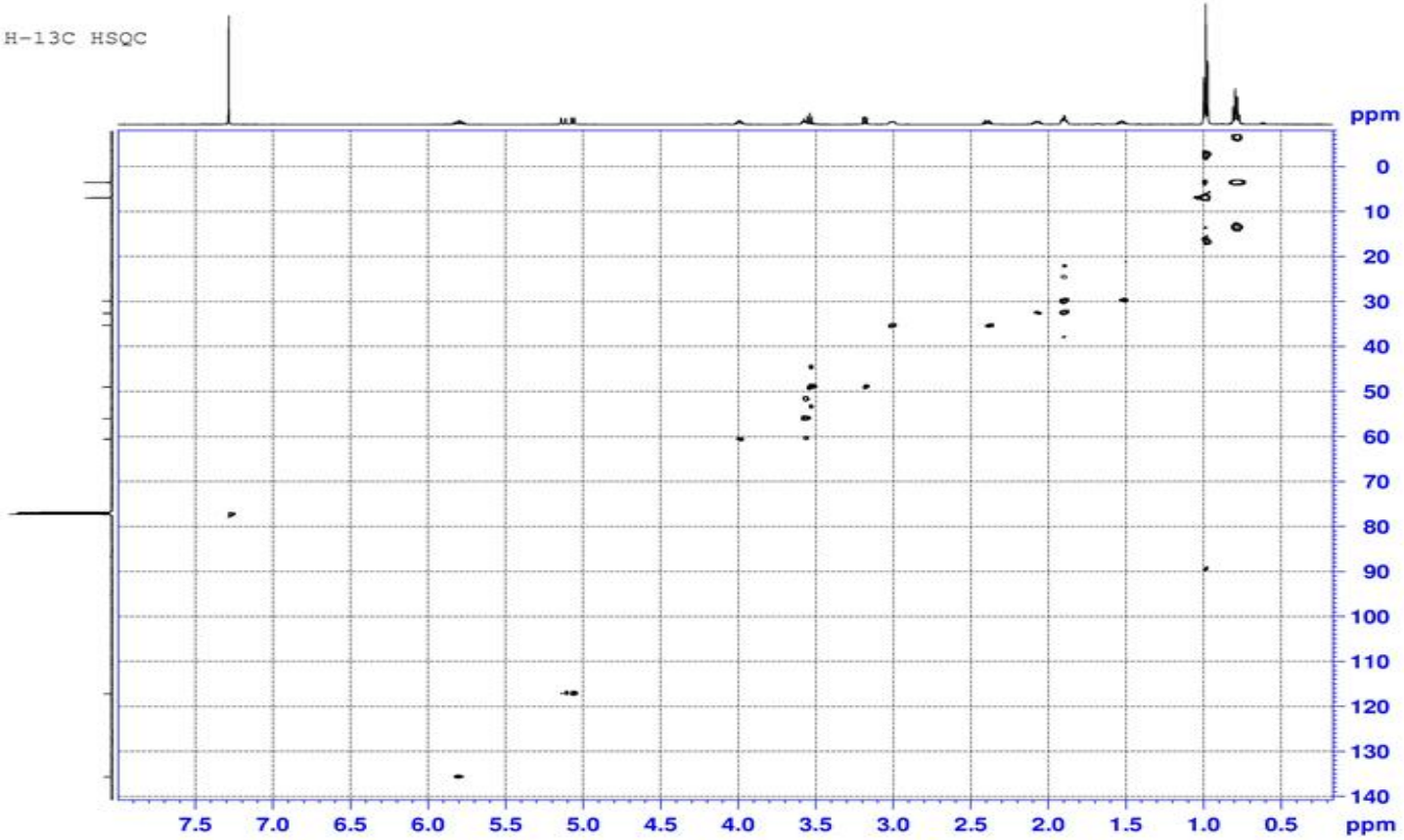
16e

H–H COSY

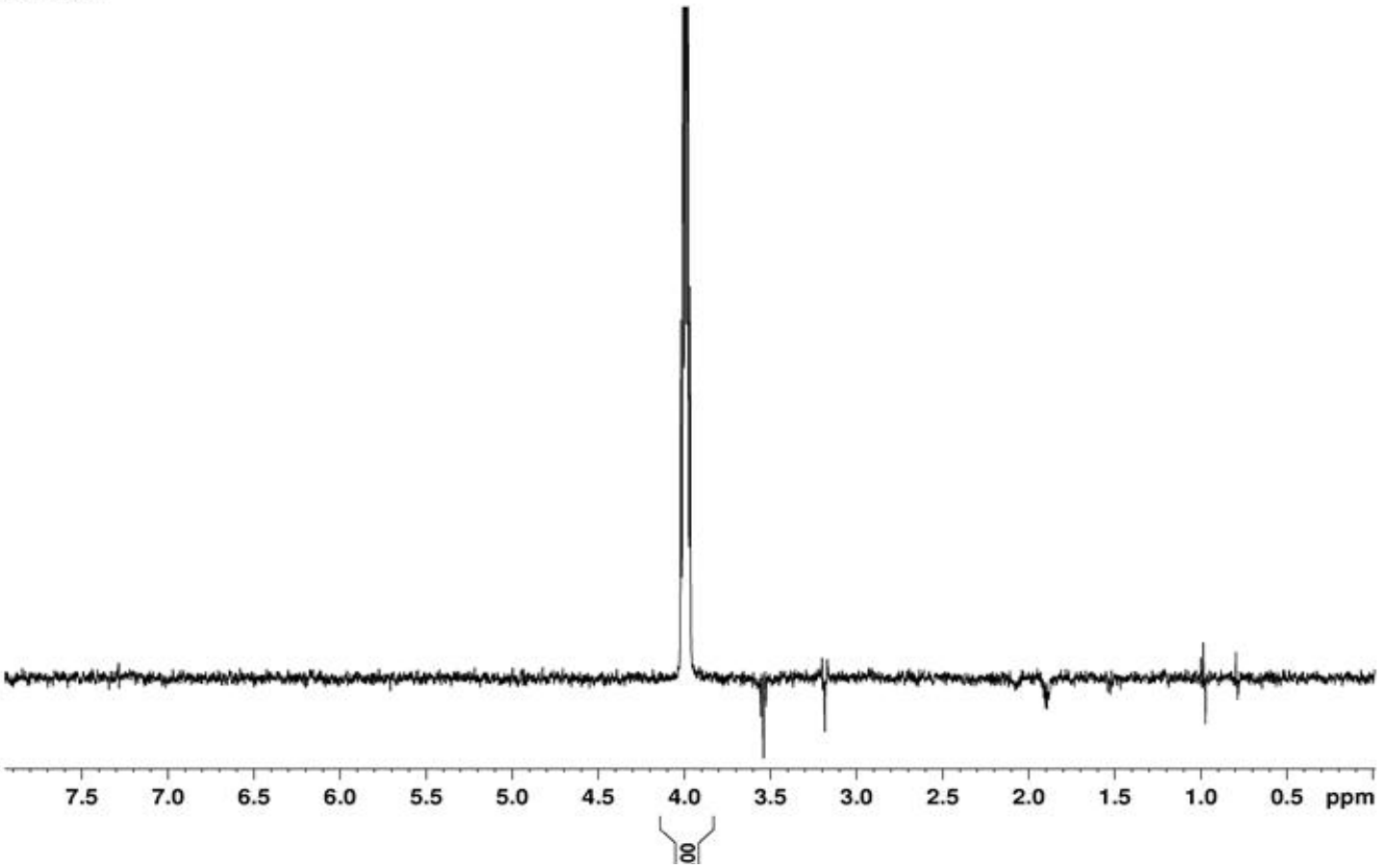
75 MHz, $CDCl_3$



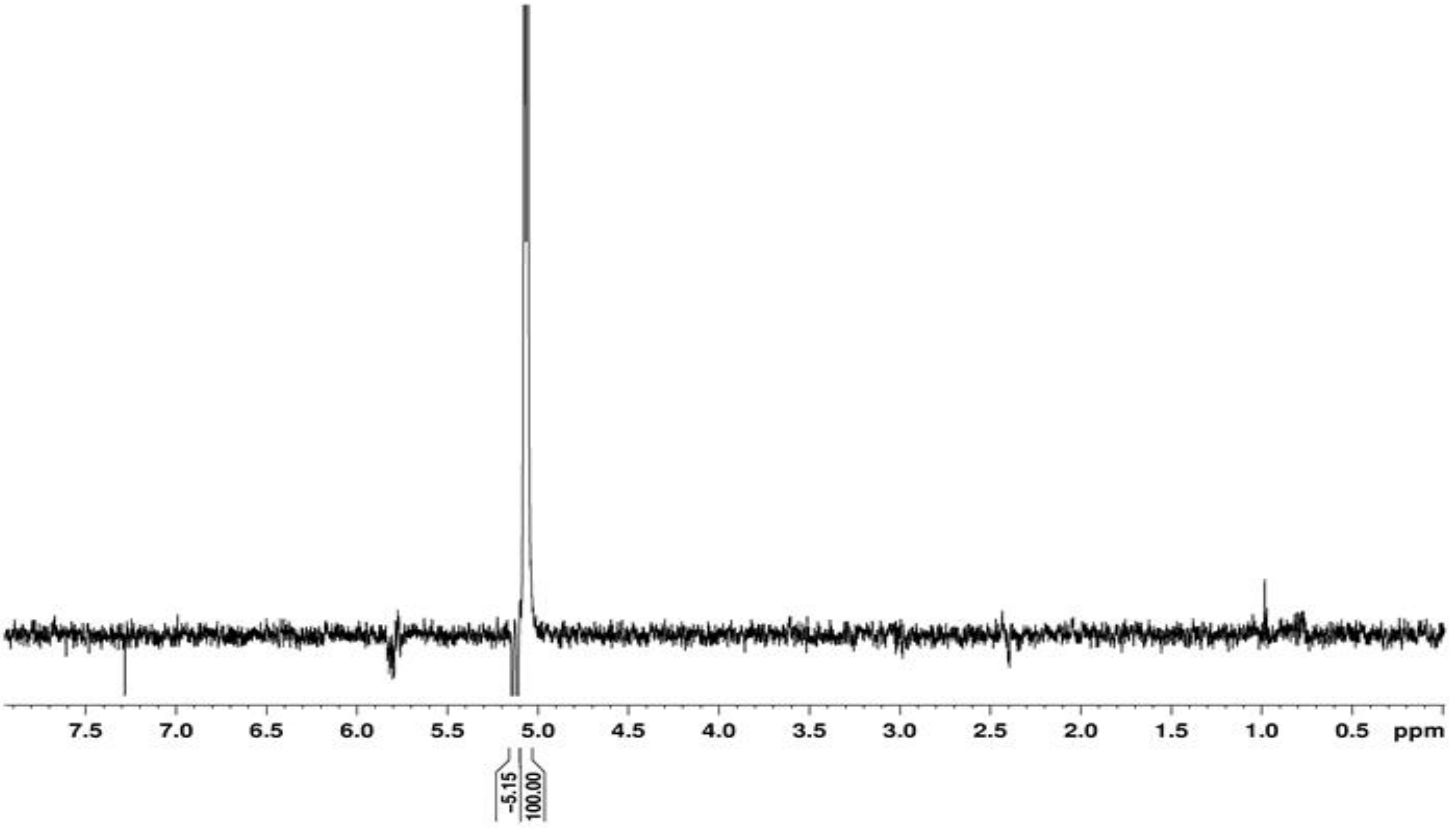
H–13C HSQC

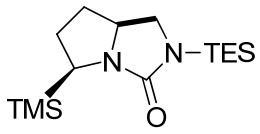


SELNOGP



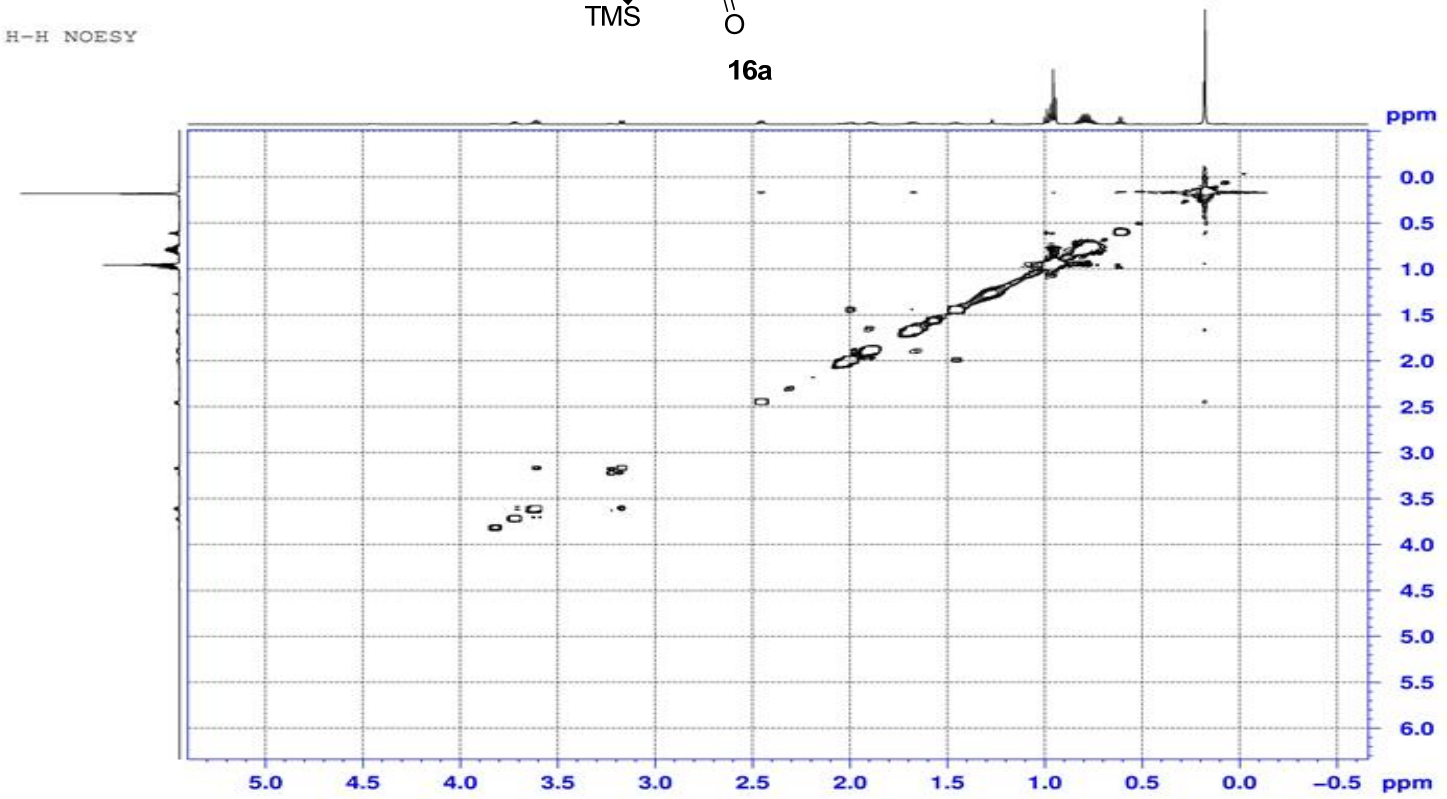
SELNOGP



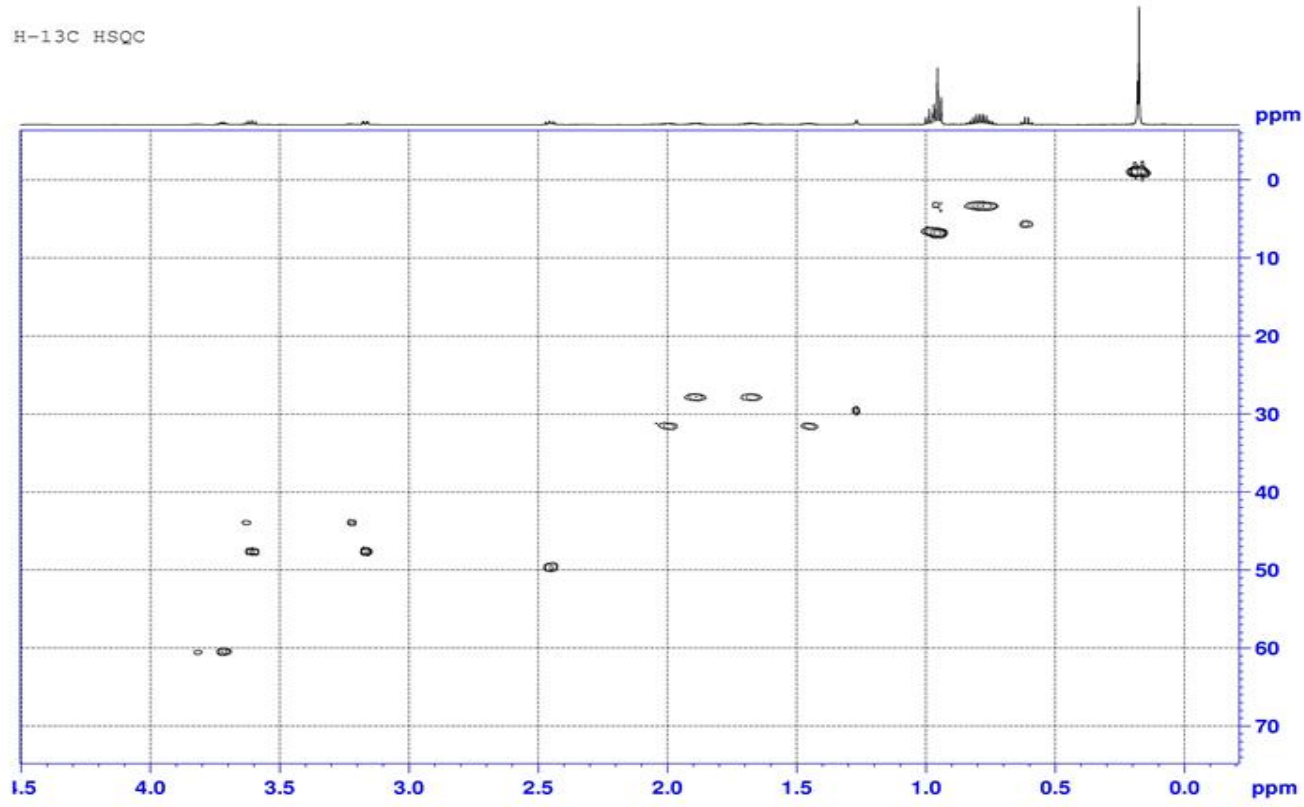


16a

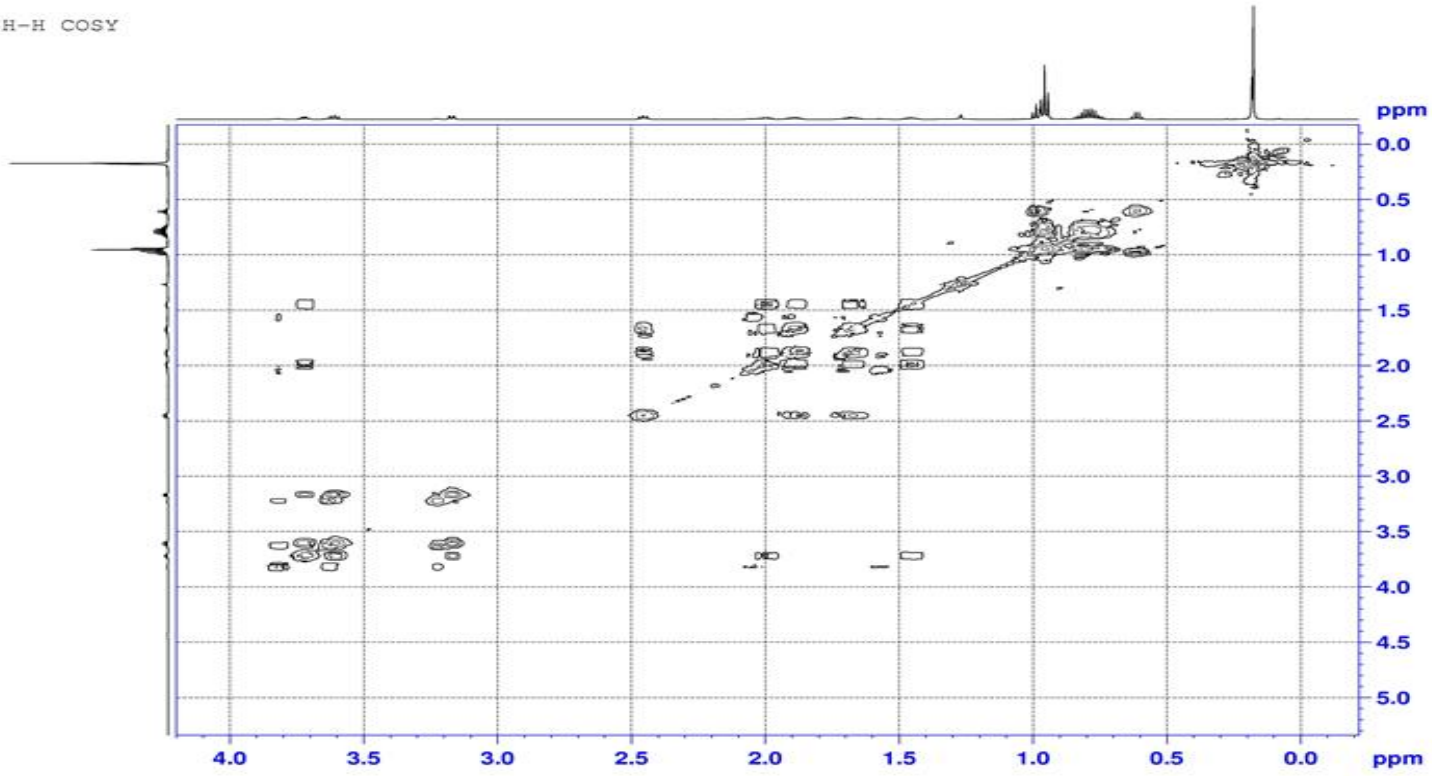
H–H NOESY

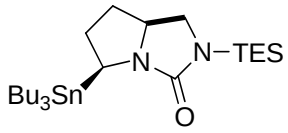


H–13C HSQC



H-H COSY

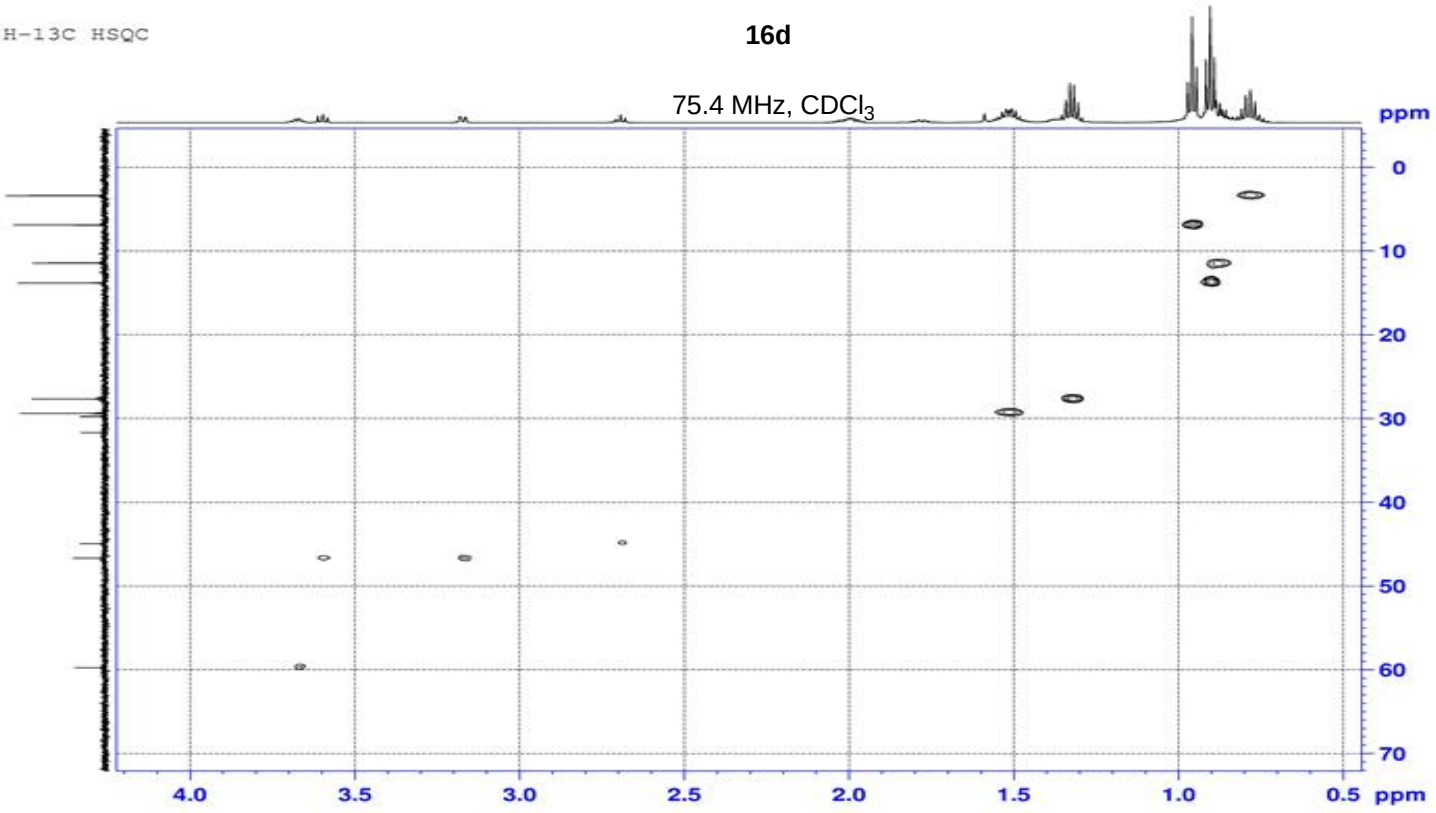




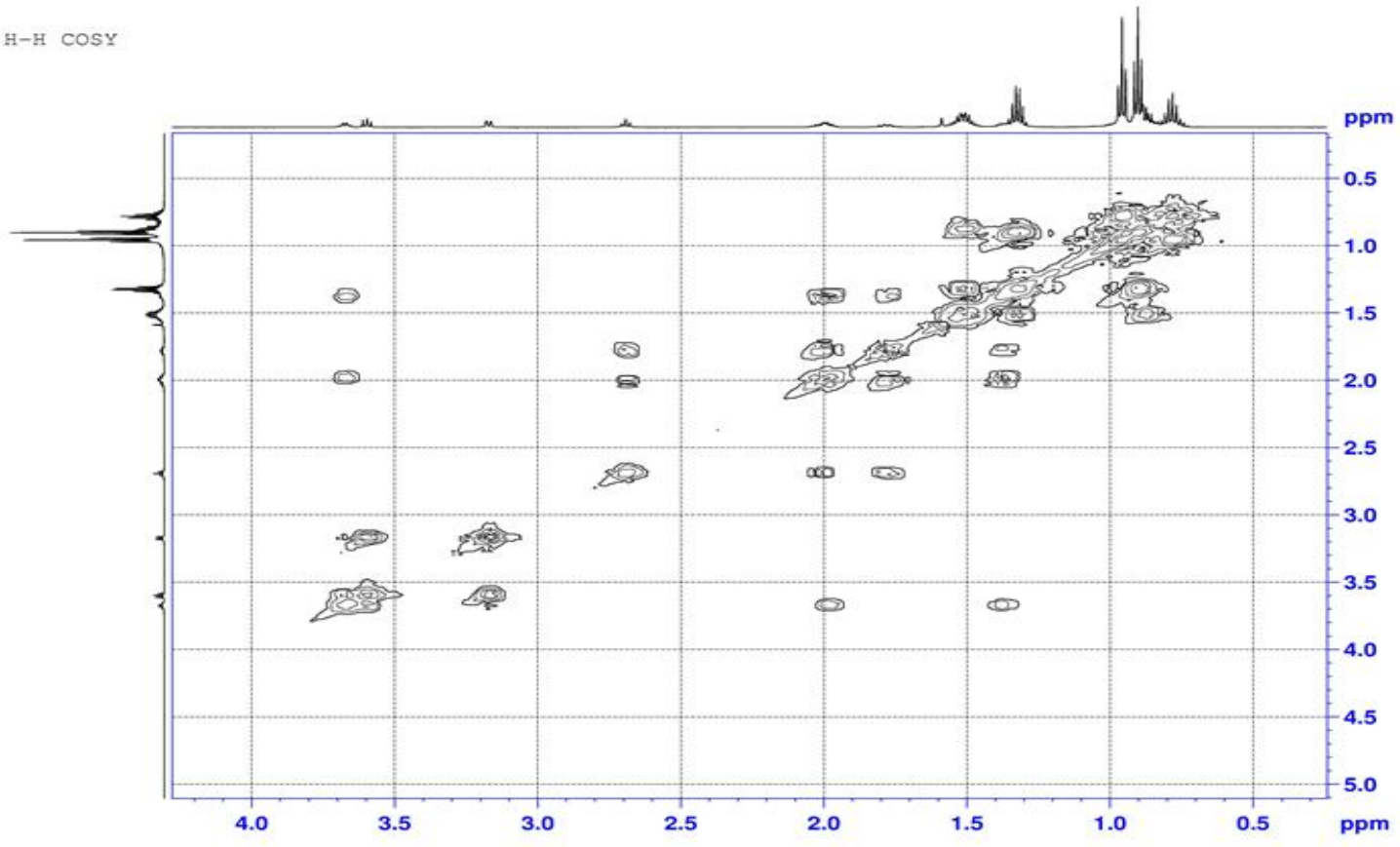
16d

H-13C HSQC

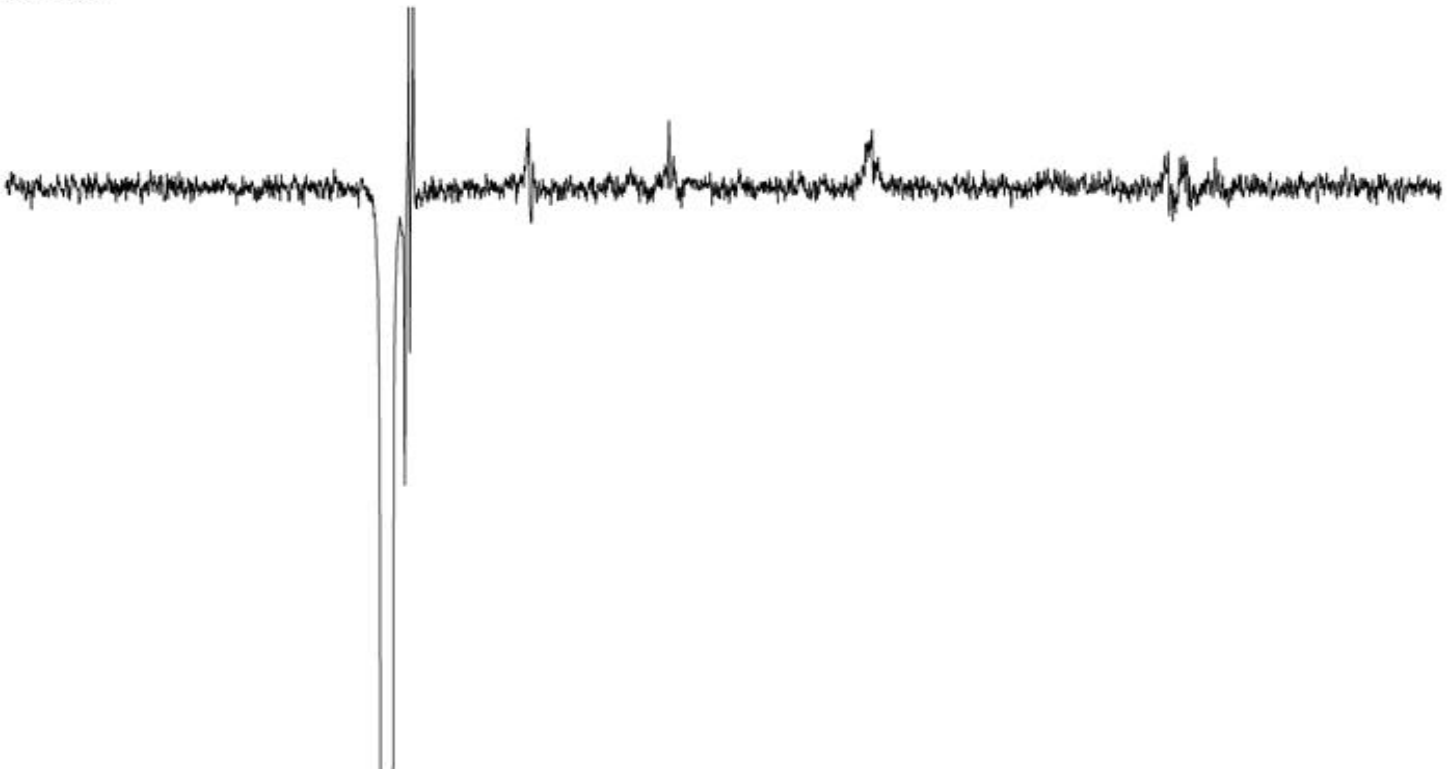
75.4 MHz, $CDCl_3$



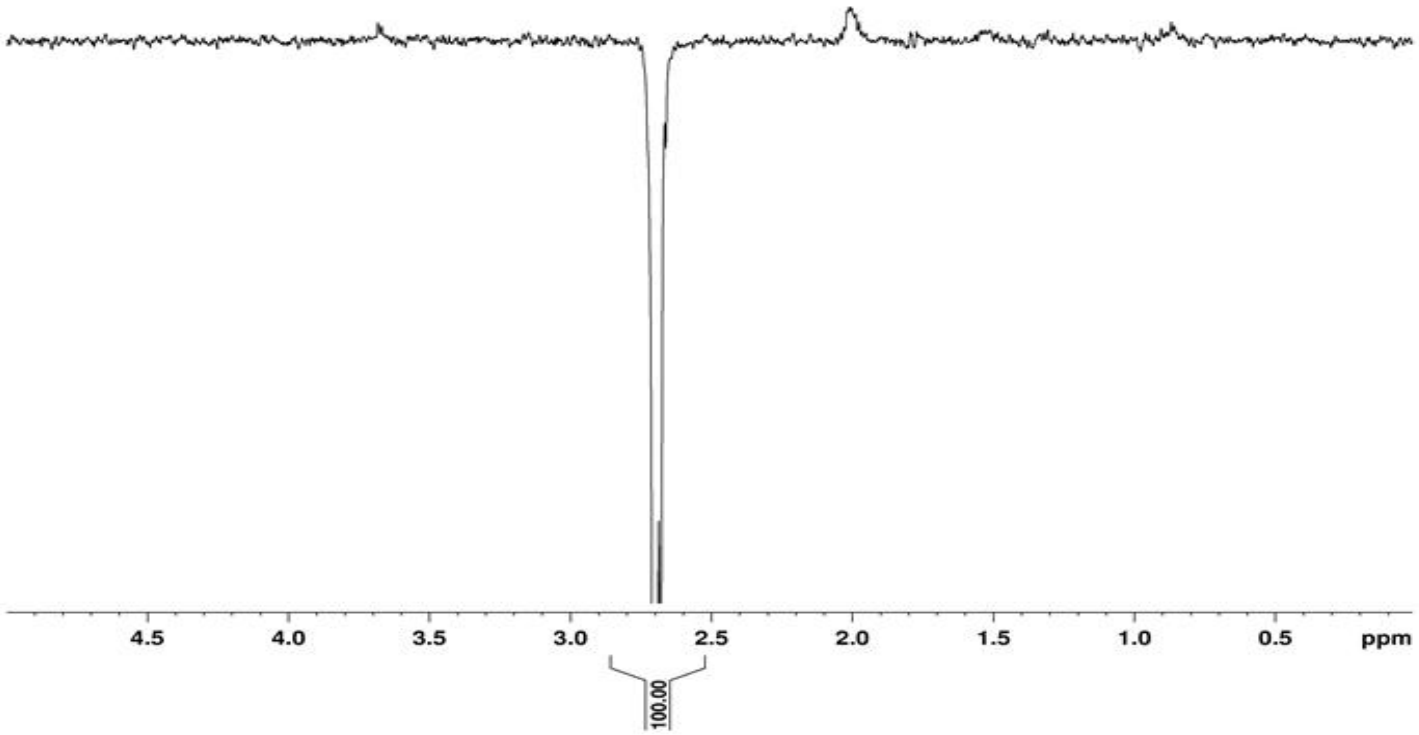
H-H COSY



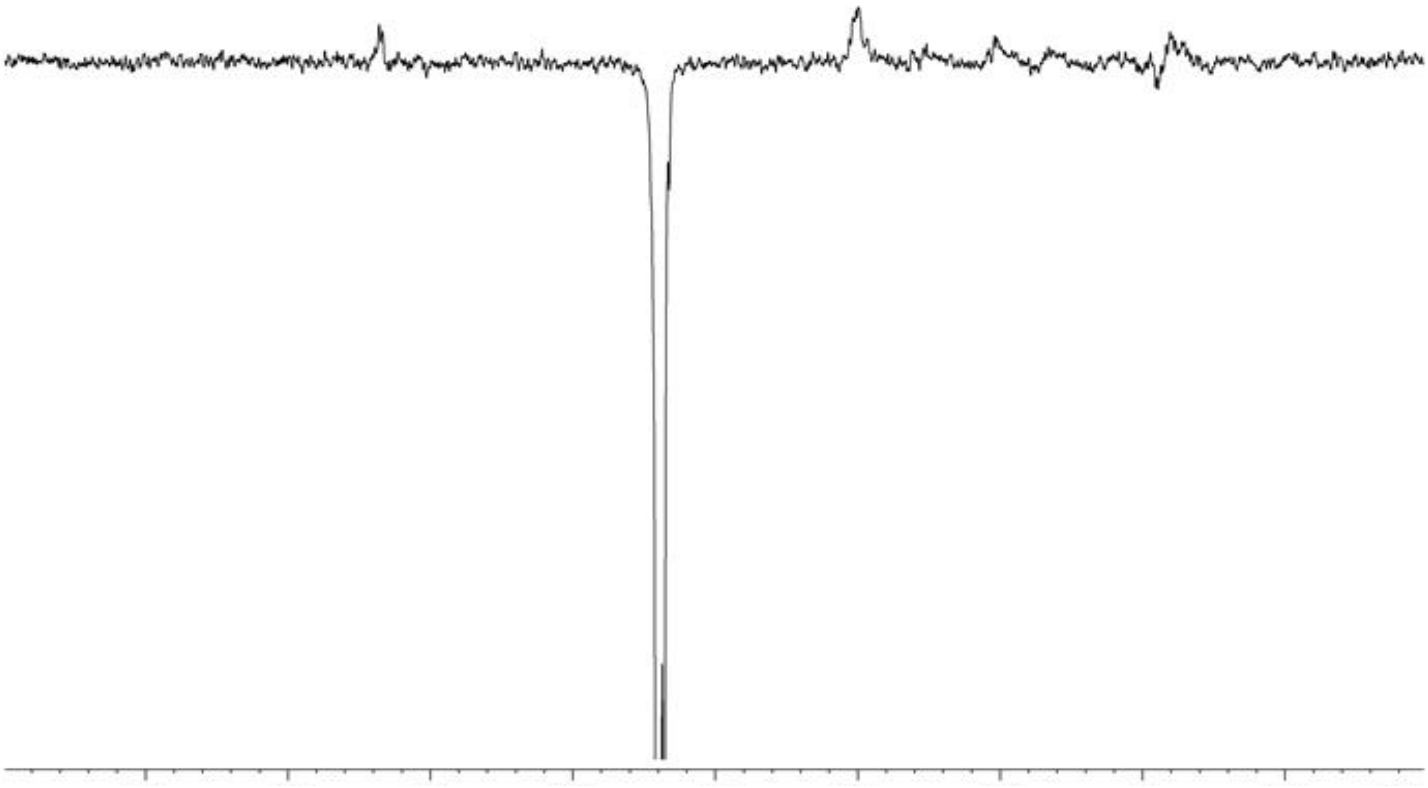
SELNOGP



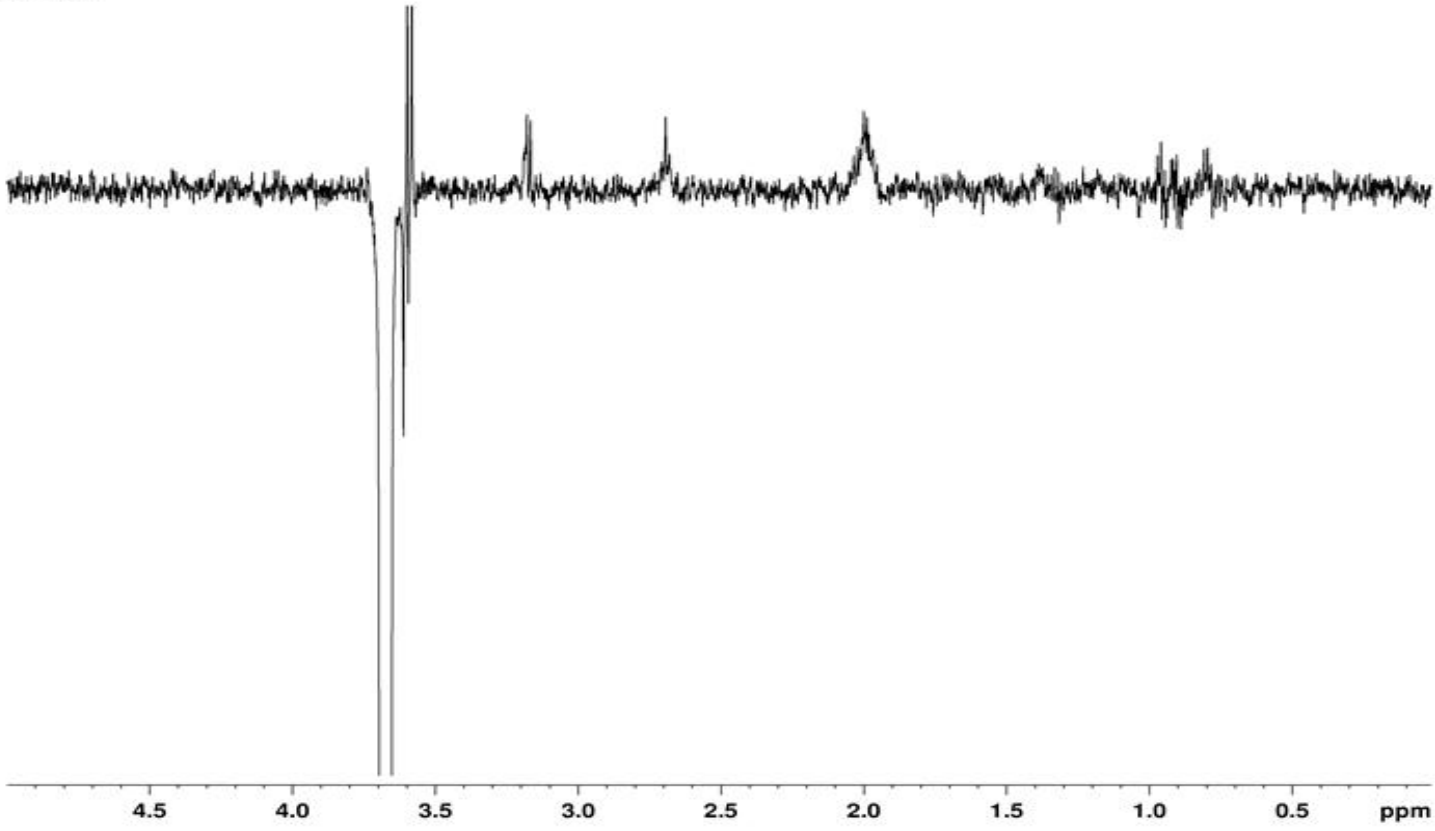
SELNOGP

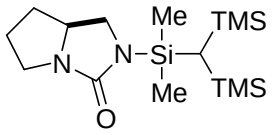


SELNOGP



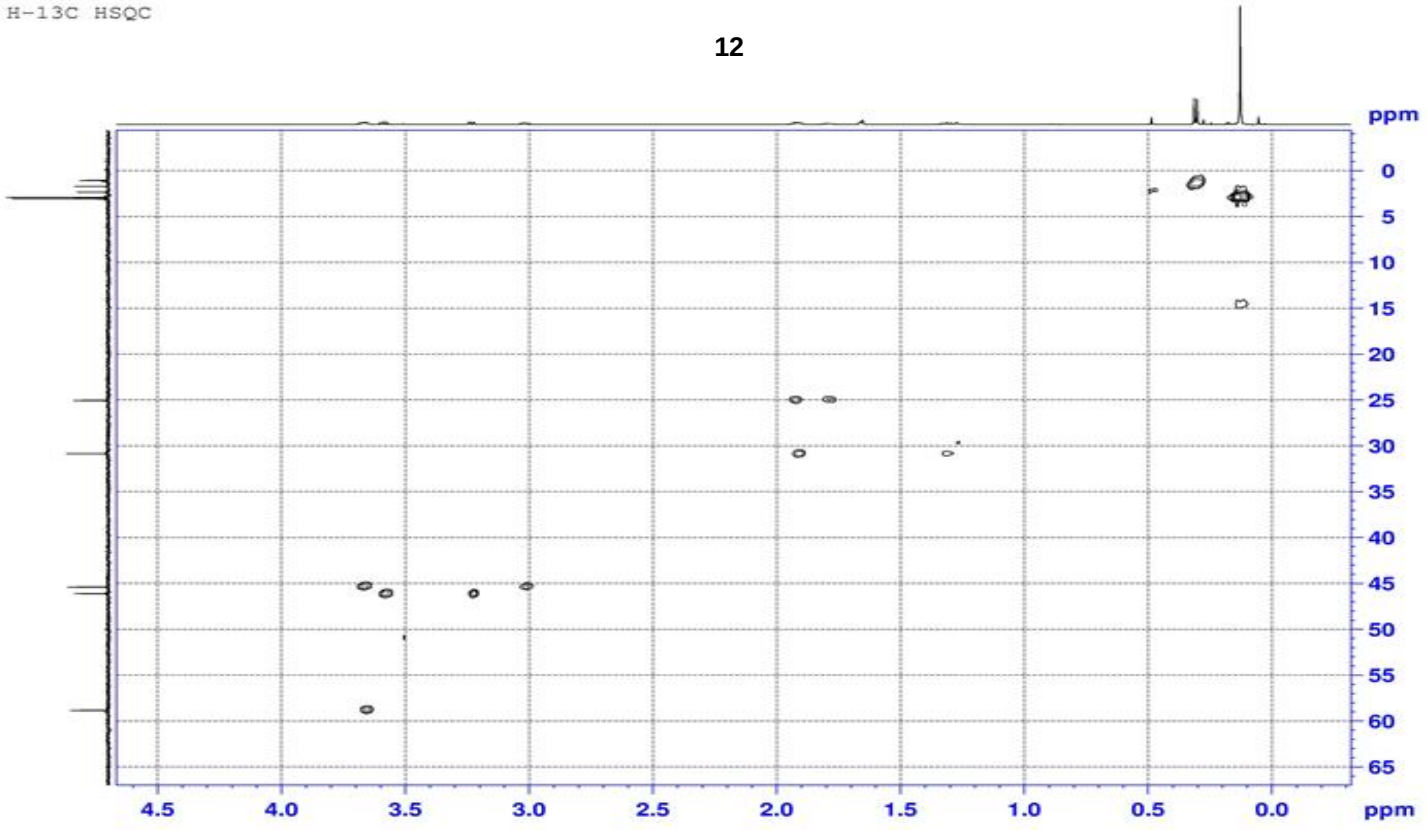
SELNOGP





12

H-13C HSQC



H-H COSY