Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

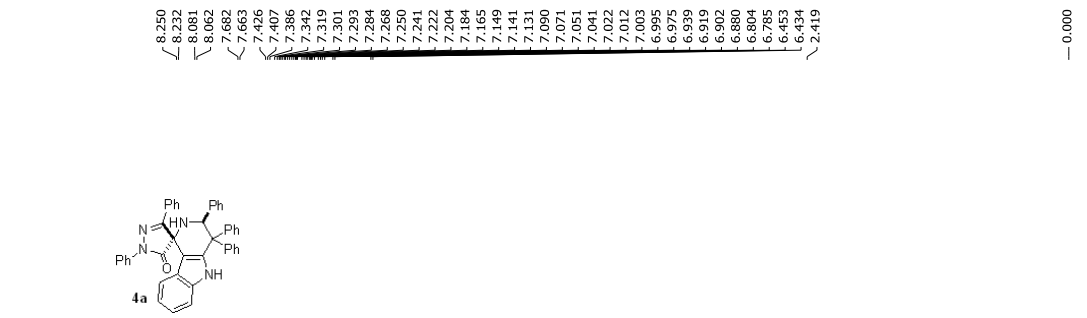
Construction of a spiro[pyrazolone-4,2'pyridoindole] scaffold through a [3+3] cycloaddition of 2-indolylmethanol with 4-aminopyrazolone-derived azomethine ylide.

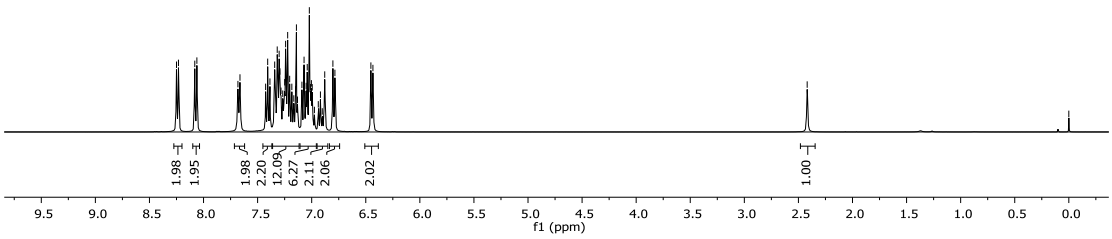
Shah Nawaz,[a,b] Yue Huang,[a] Xiaoze Bao,[a] Shiqiang Wei,[a] Xingfu Wei,[a] Jingping Qu[a] and Baomin Wang*[a]

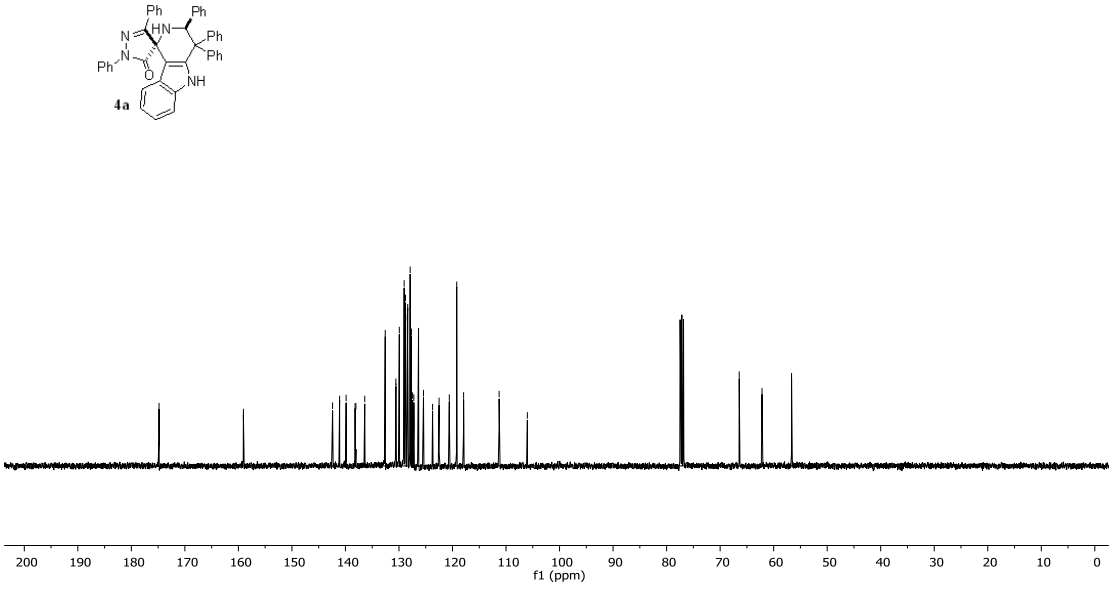
[a] State Key Laboratory of Fine Chemicals, Department of Pharmaceutical Sciences, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, P. R. China
E-mail: bmwang@dlut.edu.cn
[b] Department of Chemistry, Karakoram International University, Gilgit-Baltistan 15100, Pakistan

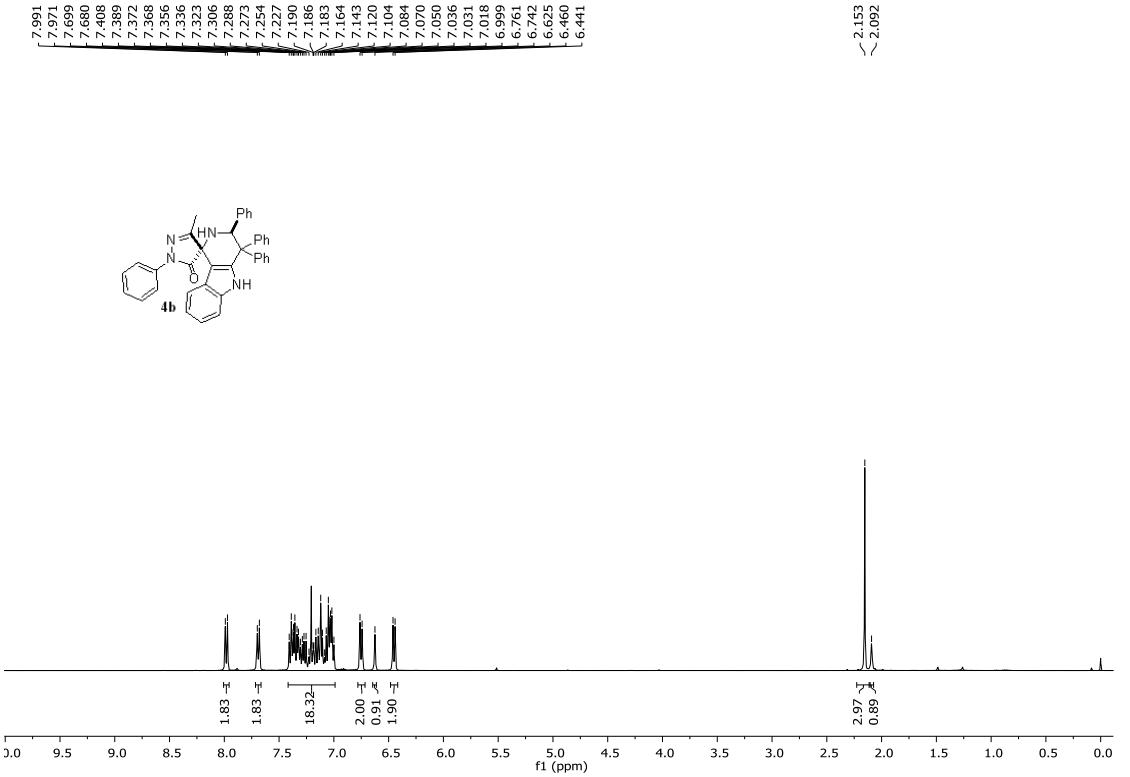
Contents

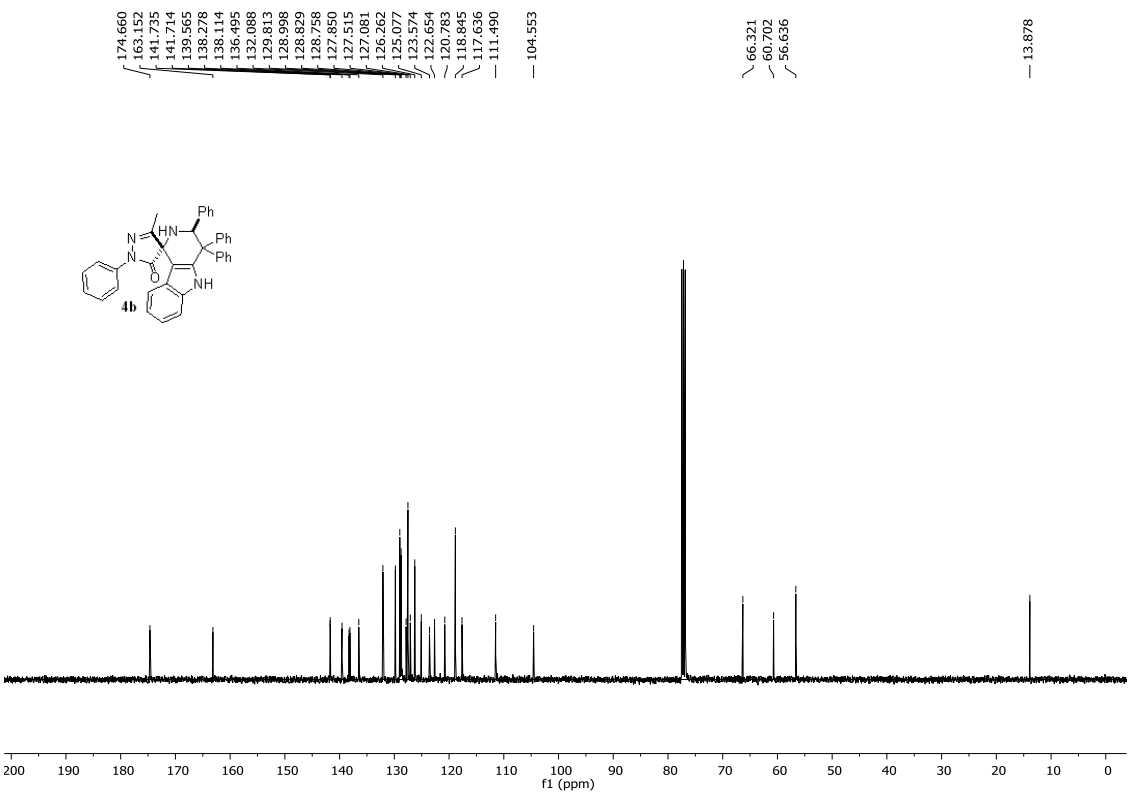
Copies of ^{1}H-NMR and ^{13}C-NMR spectra of compounds 4a-z, and 5.

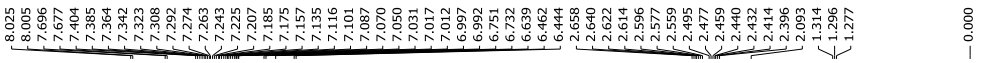


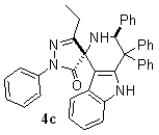




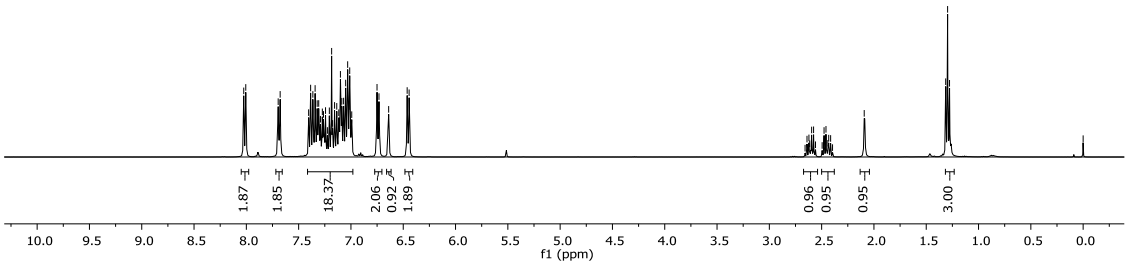

7.991
7.971
7.699
7.680
7.408
7.389
7.372
7.368
7.356
7.336
7.323
7.306
7.288
7.273
7.254
7.227
7.190
7.186
7.183
7.164
7.143
7.120
7.104
7.084
7.070
7.050
7.036
7.031
7.018
6.999
6.761
6.742
6.625
6.460
6.441
2.153
2.092
Ph
HN
N
N
O
Ph
Ph
NH
4b
1.83
1.83
18.32
2.00
0.91
1.90
2.97
0.89
f1 (ppm)


174.660
163.152
141.735
141.714
139.565
138.278
138.114
136.495
132.088
129.813
128.998
128.829
128.758
127.850
127.515
127.081
126.262
125.077
123.574
122.654
120.783
118.845
117.636
111.490
104.553
66.321
60.702
56.636
13.878
Ph
HN
N
N
O
Ph
Ph
NH
4b
f1 (ppm)

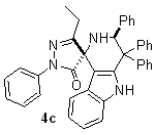

8.025
8.005
7.696
7.677
7.404
7.385
7.364
7.342
7.323
7.308
7.292
7.274
7.263
7.243
7.225
7.207
7.185
7.175
7.157
7.135
7.116
7.101
7.087
7.070
7.050
7.031
7.017
7.012
6.997
6.992
6.751
6.732
6.639
6.462
6.444
2.658
2.640
2.622
2.614
2.596
2.577
2.559
2.495
2.477
2.459
2.440
2.432
2.414
2.396
2.093
1.314
1.296
1.277
0.000


Ph
NH
Ph
Ph
N
N
O
NH

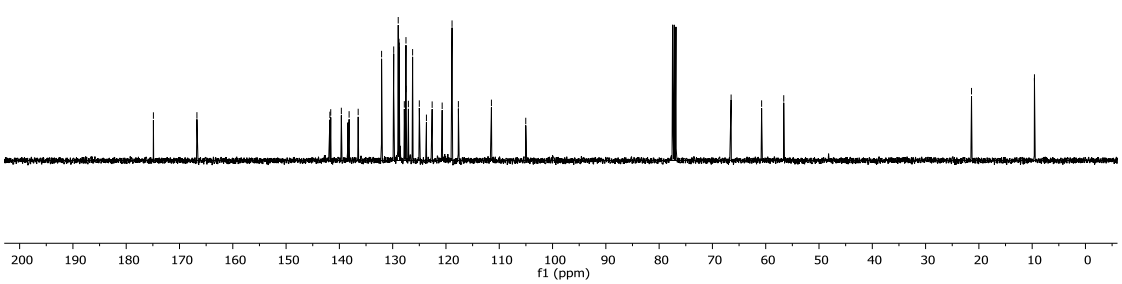
4c

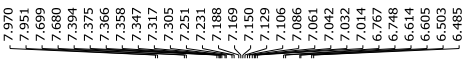

1.87
1.85
18.37
2.06
0.92
1.89
0.96
0.95
0.95
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

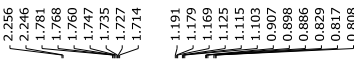

174.896
166.731
141.782
141.622
139.631
138.173
136.471
132.081
129.808
128.958
128.809
128.739
127.813
127.503
127.474
127.048
126.260
125.000
123.663
122.591
120.713
118.859
117.669
111.467
105.027
66.492
60.768
56.615
21.382
9.571

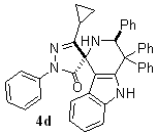

Ph
NH
Ph
Ph
N
N
O
NH

4c

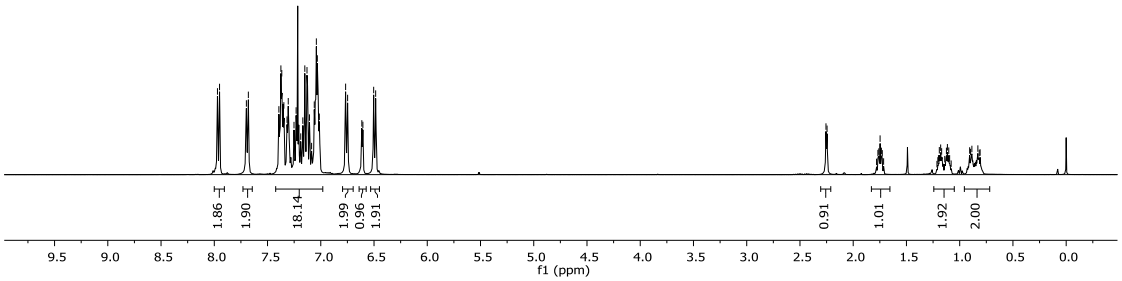

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

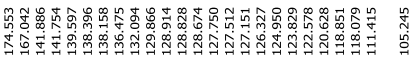

7.970
7.951
7.699
7.680
7.394
7.375
7.366
7.358
7.347
7.317
7.305
7.251
7.231
7.188
7.169
7.150
7.129
7.106
7.086
7.061
7.042
7.032
7.014
6.767
6.748
6.614
6.605
6.503
6.485


2.256
2.246
1.781
1.768
1.760
1.747
1.735
1.727
1.714
1.191
1.179
1.169
1.125
1.115
1.103
0.907
0.898
0.886
0.829
0.817


Ph
HN
N
N
O
Ph
Ph
NH

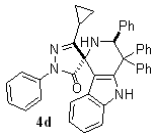
4d


1.86
1.90
18.14
1.99
0.96
1.91
0.91
1.01
1.92
2.00
9.5 9.0 8.5 8.0 7.5 7.0 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 0.0
f1 (ppm)

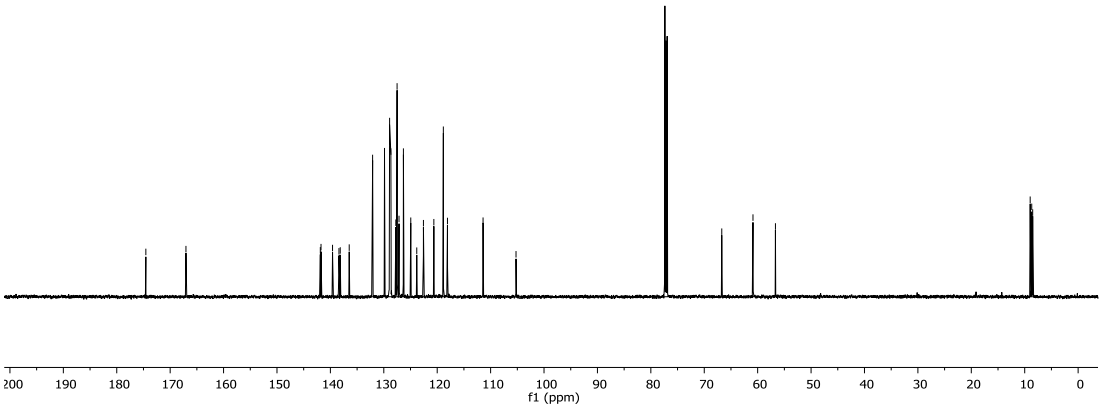

174.553
167.042
141.886
141.754
139.597
138.396
138.158
136.475
132.094
129.866
128.914
128.828
128.674
127.750
127.512
127.151
126.327
124.950
123.829
122.578
120.628
118.851
118.079
111.415
105.245

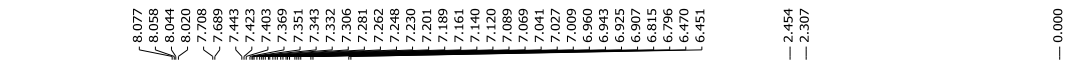

66.720
60.878
56.672

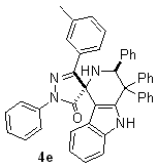

8.975
8.686
8.507


Ph
HN
N
N
O
Ph
Ph
NH

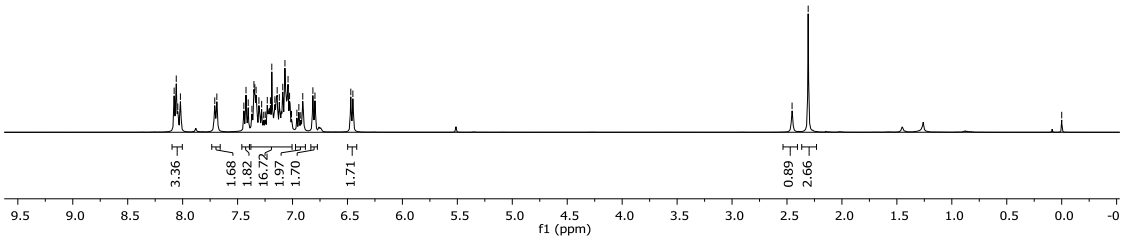
4d

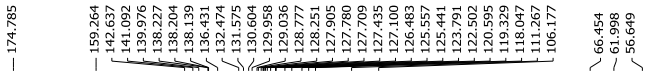

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

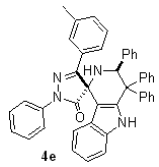

8.077
8.058
8.044
8.020
7.708
7.689
7.443
7.423
7.403
7.369
7.351
7.343
7.332
7.306
7.281
7.262
7.248
7.230
7.201
7.189
7.161
7.140
7.120
7.089
7.069
7.041
7.027
7.009
6.960
6.943
6.925
6.907
6.815
6.796
6.470
6.451
2.454
2.307
0.000


Ph
HN
Ph
Ph
N
N
O
NH

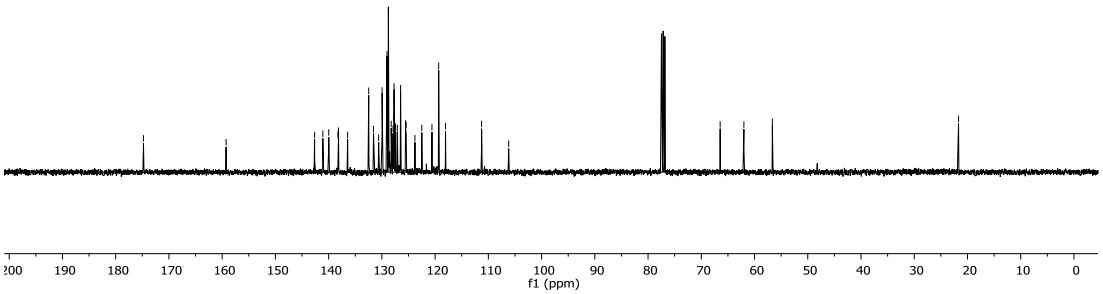
4e

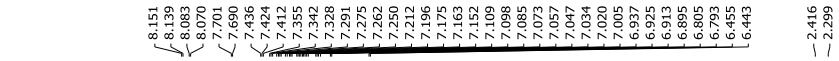

3.36
1.68
1.82
16.72
1.97
1.70
1.71
0.89
2.66
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

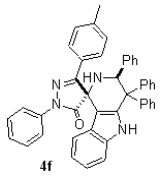

174.785
159.264
142.637
141.092
139.976
138.227
138.204
138.139
136.431
132.474
131.575
130.604
129.958
129.036
128.777
128.251
127.905
127.780
127.709
127.435
127.100
126.483
125.557
125.441
123.791
122.502
120.595
119.329
118.047
111.267
106.177
66.454
61.998
56.649
21.681


Ph
HN
Ph
Ph
N
N
O
NH

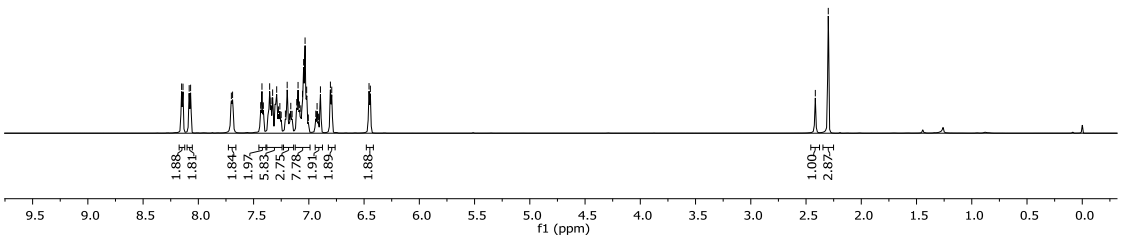
4e


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

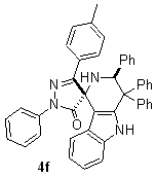

8.151
8.139
8.083
8.070
7.701
7.690
7.436
7.424
7.412
7.355
7.342
7.328
7.291
7.275
7.262
7.250
7.212
7.196
7.175
7.163
7.152
7.109
7.098
7.085
7.073
7.057
7.047
7.034
7.020
7.005
6.937
6.925
6.913
6.895
6.805
6.793
6.455
6.443
2.416
2.299


Ph
HN
N
Ph
N
Ph
O
NH

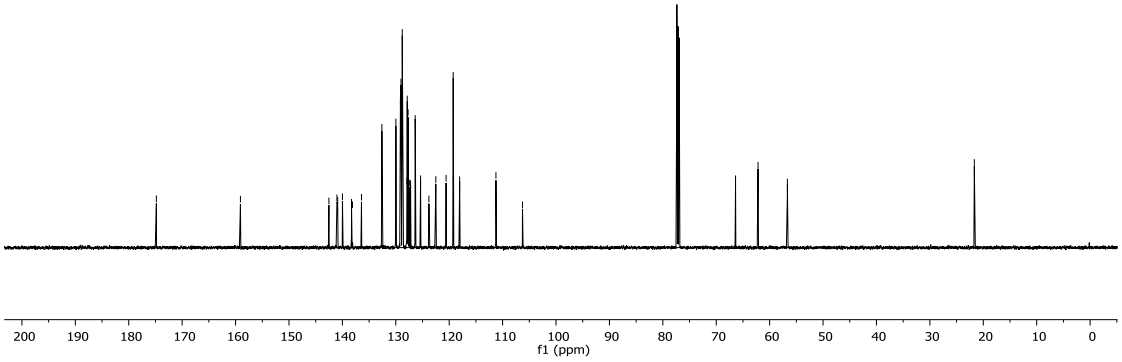
4f

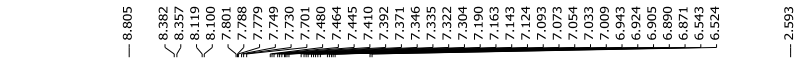

1.88
1.81
1.84
1.97
5.83
2.75
7.78
1.91
1.89
1.88
1.00
2.87
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

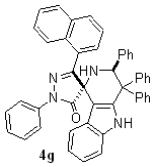

174.826
159.088
142.526
141.024
140.881
139.984
138.288
138.115
136.423
132.606
129.980
129.135
129.028
128.788
127.921
127.857
127.822
127.698
127.459
127.231
126.363
125.359
123.798
122.505
120.584
119.255
118.043
111.245
106.276
66.385
62.174
56.680
21.678


Ph
HN
N
Ph
N
Ph
O
NH

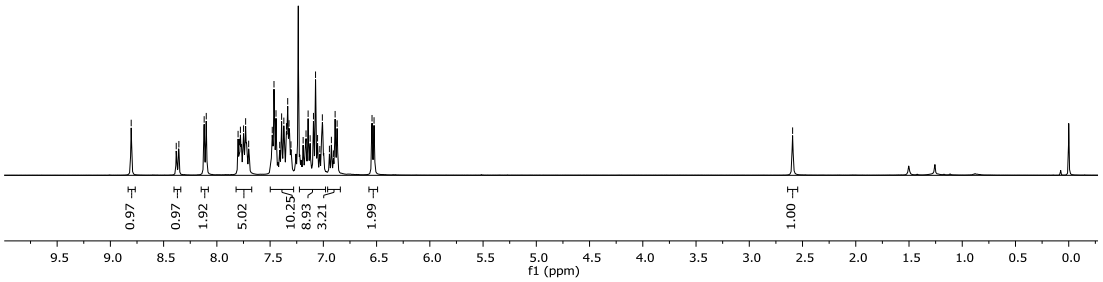
4f


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

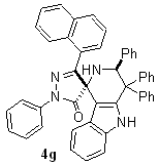

8.805
8.382
8.357
8.119
8.100
7.801
7.788
7.779
7.749
7.730
7.701
7.480
7.464
7.445
7.410
7.392
7.371
7.346
7.335
7.322
7.304
7.190
7.163
7.143
7.124
7.093
7.073
7.054
7.033
7.009
6.943
6.924
6.905
6.890
6.871
6.543
6.524
2.593


Ph
HN
N
N
Ph
Ph
O
NH

4g

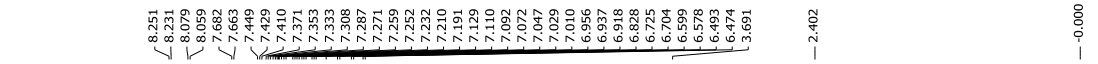

0.97
0.97
1.92
5.02
10.25
8.93
3.21
1.99
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

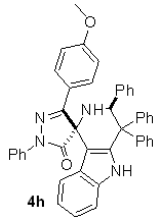

174.952
159.007
142.764
141.006
140.070
138.626
138.215
136.428
134.394
132.943
132.513
129.980
129.279
129.098
128.842
128.463
128.268
128.172
128.010
127.812
127.470
127.299
127.151
126.763
126.204
125.554
124.370
123.716
122.554
120.622
119.405
117.976
111.290
106.231
66.548
62.092
56.668


Ph
HN
N
N
Ph
Ph
O
NH

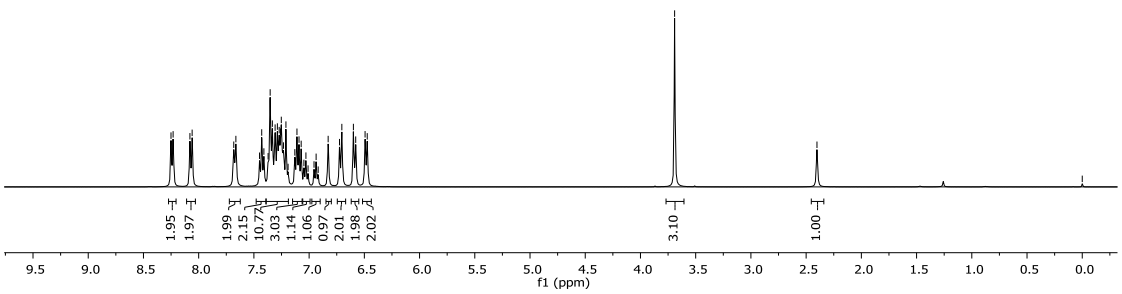
4g

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

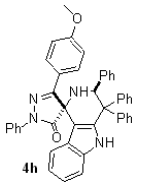

8.251
8.231
8.079
8.059
7.682
7.663
7.449
7.429
7.410
7.371
7.353
7.333
7.308
7.287
7.271
7.259
7.252
7.232
7.210
7.191
7.129
7.110
7.092
7.072
7.047
7.029
7.010
6.956
6.937
6.918
6.828
6.725
6.704
6.599
6.578
6.493
6.474
3.691
2.402
-0.000


O
Ph
NH
N
Ph
N
Ph
Ph
O
NH

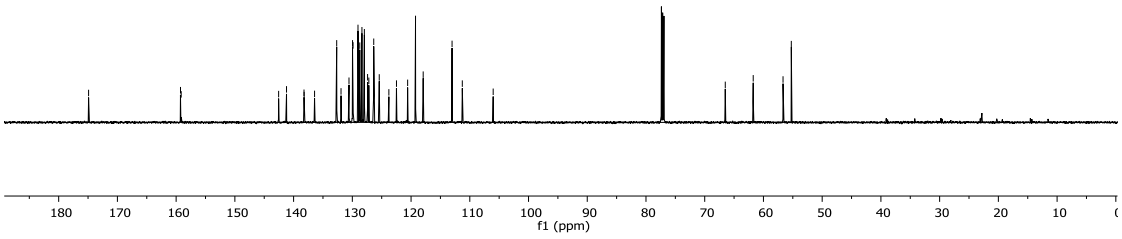
4h

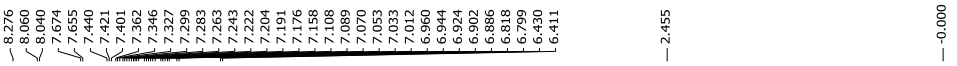

1.95
1.97
1.99
2.15
10.77
3.03
1.14
1.06
0.97
2.01
1.98
2.02
3.10
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

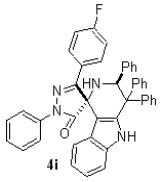

174.907
159.258
159.138
142.549
141.205
138.229
138.204
136.430
132.662
131.926
130.615
130.570
129.966
129.879
129.036
128.731
128.364
127.951
127.403
127.192
126.356
125.418
123.779
122.482
120.583
119.241
117.935
113.019
111.275
106.017
66.500
61.742
56.663
55.256


O
Ph
NH
N
Ph
N
Ph
Ph
O
NH

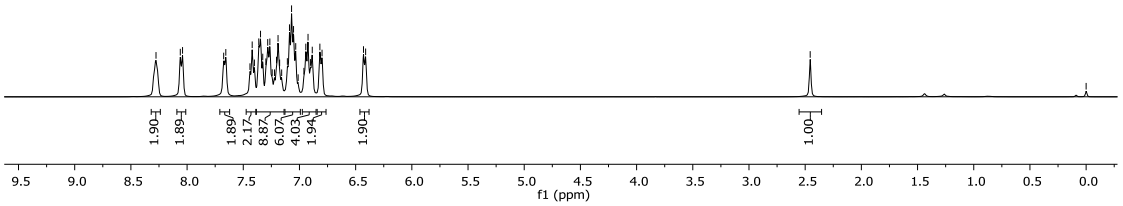
4h

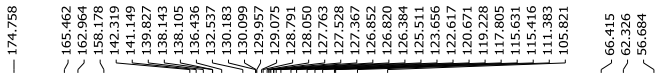

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

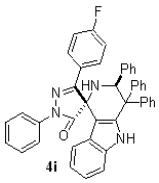

8.276
8.060
8.040
7.674
7.655
7.440
7.421
7.401
7.362
7.346
7.327
7.299
7.283
7.263
7.243
7.222
7.204
7.191
7.176
7.158
7.108
7.089
7.070
7.053
7.033
7.012
6.960
6.944
6.924
6.902
6.886
6.818
6.799
6.430
6.411
2.455
-0.000


F
Ph
HN
Ph
Ph
N
N
O
NH

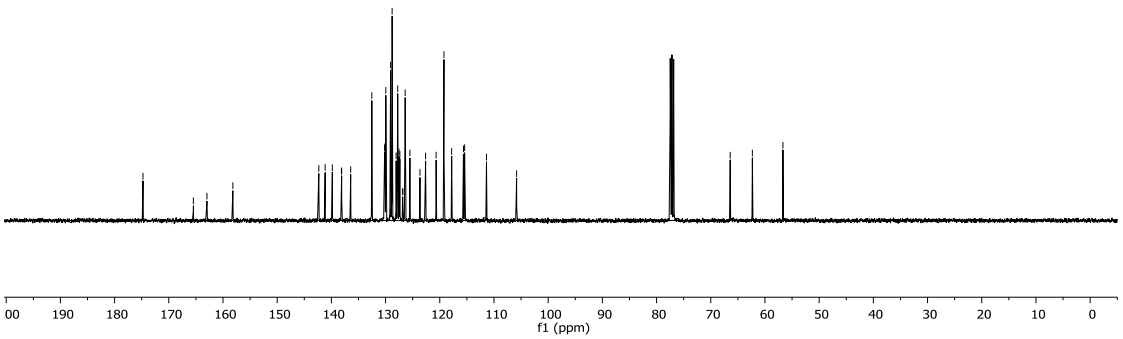
4i

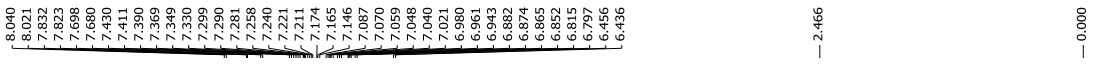

1.90
1.89
1.89
2.17
8.87
6.07
4.03
1.94
1.90
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

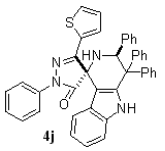

174.758
165.462
162.964
158.178
142.319
141.149
139.827
138.143
138.105
136.436
132.537
130.183
130.099
129.957
129.075
128.791
128.050
127.763
127.528
127.367
126.852
126.820
126.384
125.511
123.656
122.617
120.671
119.228
117.805
115.631
115.416
111.383
105.821
66.415
62.326
56.684


F
Ph
HN
Ph
Ph
N
N
O
NH

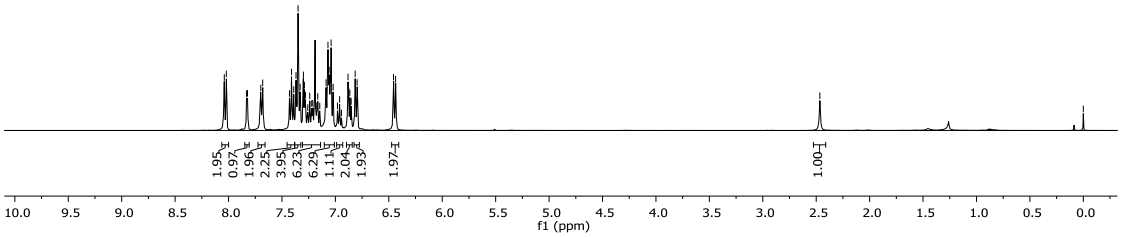
4i

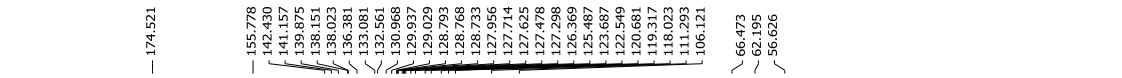

00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

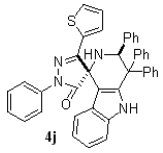

8.040
8.021
7.832
7.823
7.698
7.680
7.430
7.411
7.390
7.369
7.349
7.330
7.299
7.290
7.281
7.258
7.240
7.221
7.211
7.174
7.165
7.146
7.087
7.070
7.059
7.048
7.040
7.021
6.980
6.961
6.943
6.882
6.874
6.865
6.852
6.815
6.797
6.456
6.436
2.466
0.000


S
Ph
HN
Ph
Ph
N
N
O
NH

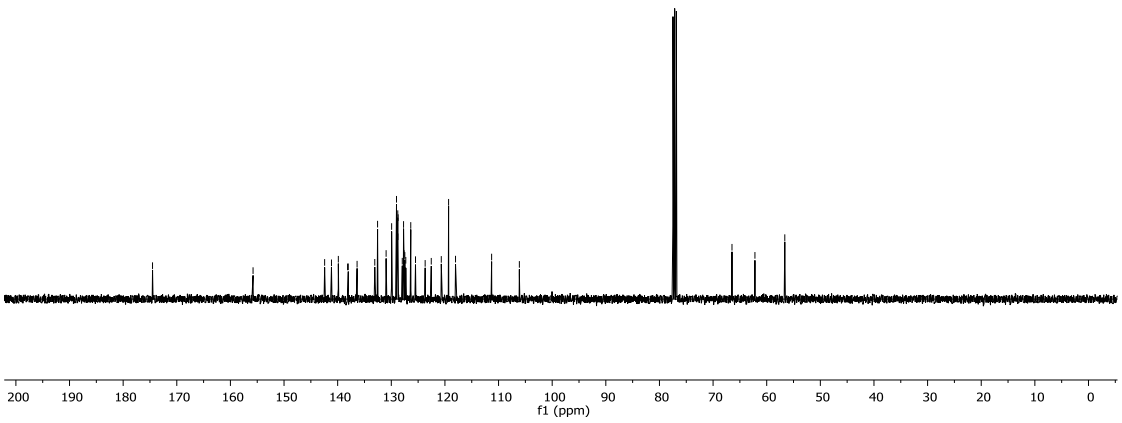
4j

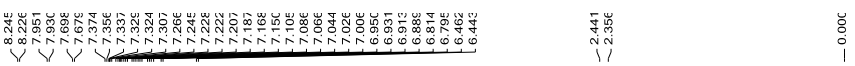

1.95
0.97
1.96
2.25
3.95
6.23
6.29
1.11
2.04
1.93
1.97
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

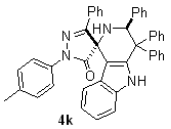

174.521
155.778
142.430
141.157
139.875
138.151
138.023
136.381
133.081
132.561
130.968
129.937
129.029
128.793
128.768
128.733
127.956
127.714
127.625
127.478
127.298
126.369
125.487
123.687
122.549
120.681
119.317
118.023
111.293
106.121
66.473
62.195
56.626


S
Ph
HN
Ph
Ph
N
N
O
NH

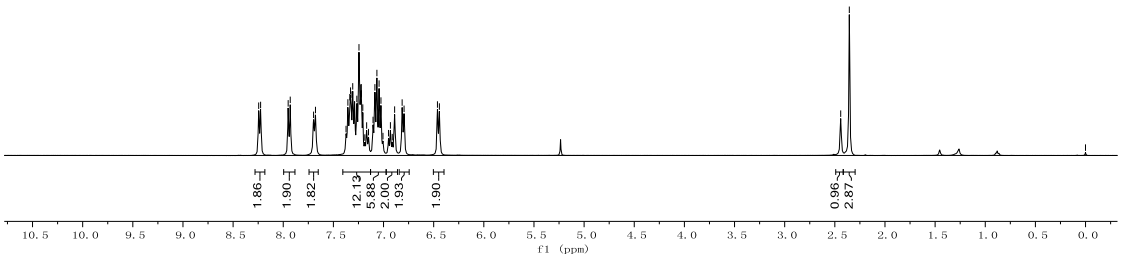
4j

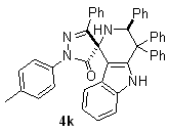

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



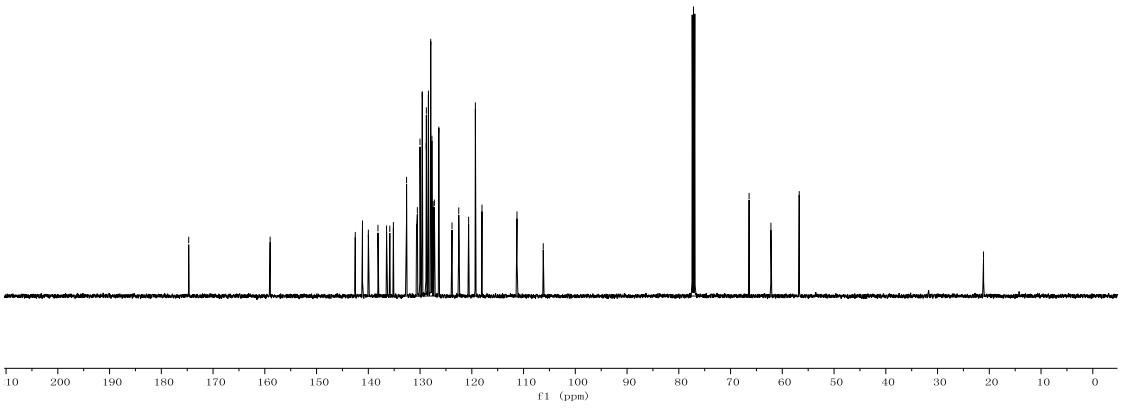

Ph
Ph
HN
N
N
Ph
Ph
O
NH

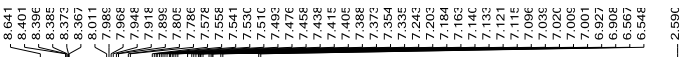
4k

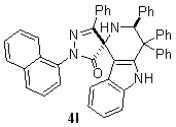

1.86
1.90
1.82
12.13
5.88
2.00
1.93
1.90
0.96
2.87
f1 (ppm)


Ph
Ph
HN
N
N
Ph
Ph
O
NH

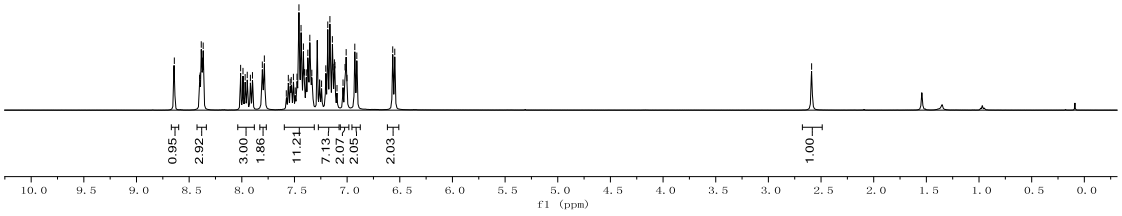
4k

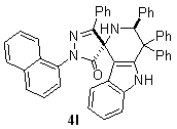

f1 (ppm)



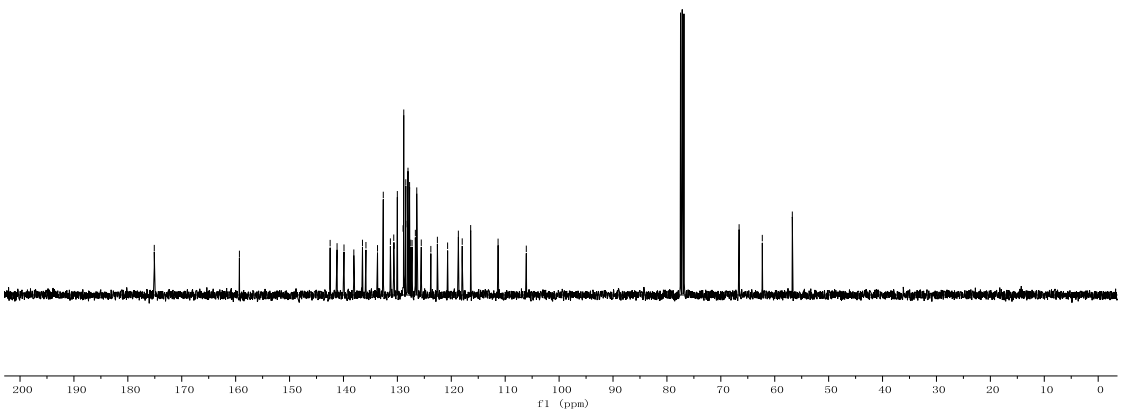


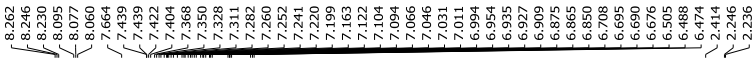
4l

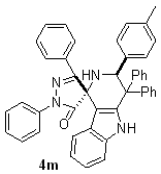




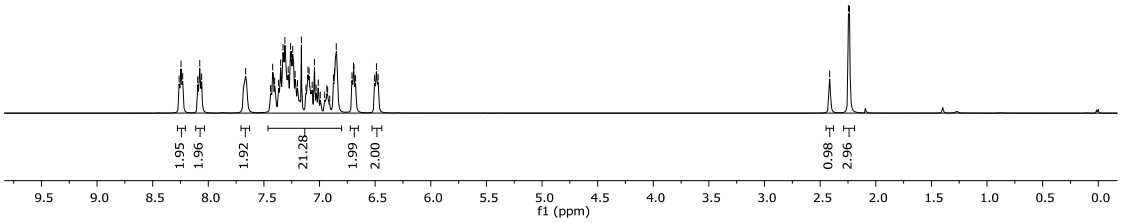
4l



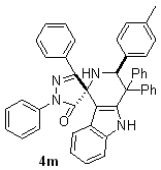

8.262
8.246
8.230
8.095
8.077
8.060
7.664
7.439
7.439
7.422
7.404
7.368
7.350
7.328
7.311
7.282
7.260
7.252
7.241
7.220
7.199
7.163
7.122
7.104
7.094
7.066
7.046
7.031
7.011
6.994
6.954
6.935
6.927
6.909
6.875
6.865
6.850
6.708
6.695
6.690
6.676
6.505
6.488
6.474
2.414
2.246
2.236


HN
N
N
O
Ph
Ph
NH

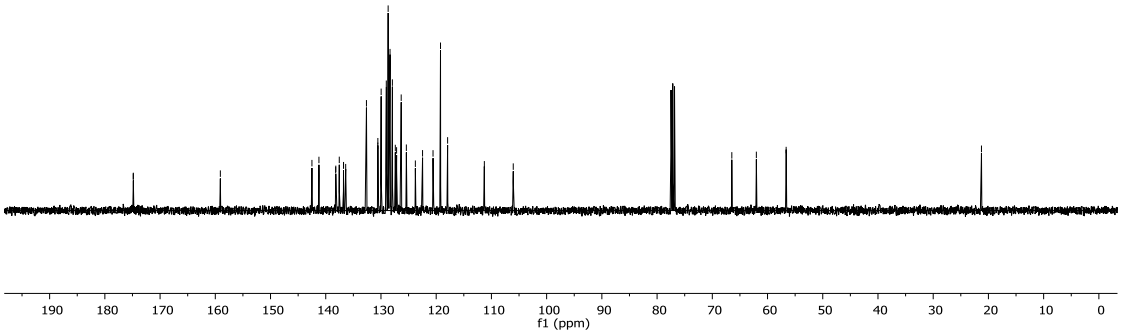
4m

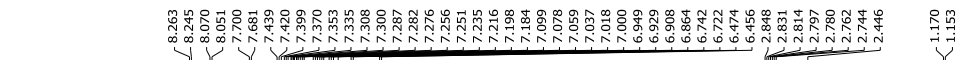

1.95
1.96
1.92
21.28
1.99
2.00
0.98
2.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

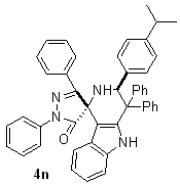

174.857
174.843
159.087
142.501
141.234
138.206
138.181
137.551
136.785
136.775
136.389
132.628
130.576
130.564
129.967
129.035
128.701
128.359
127.933
127.404
127.171
126.336
125.402
123.772
122.470
120.572
119.219
117.931
111.279
106.045
66.467
62.024
56.629
21.258


HN
N
N
O
Ph
Ph
NH

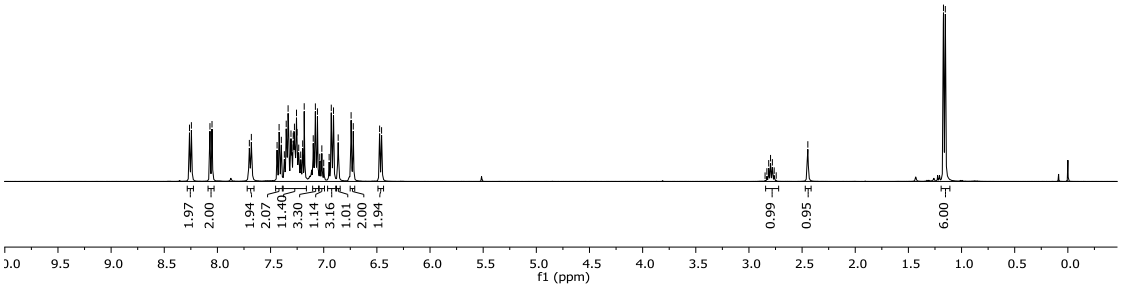
4m

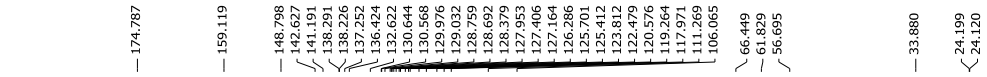

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

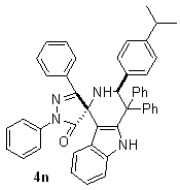

8.263
8.245
8.070
8.051
7.700
7.681
7.439
7.420
7.399
7.370
7.353
7.335
7.308
7.300
7.287
7.282
7.276
7.256
7.251
7.235
7.216
7.198
7.184
7.099
7.078
7.059
7.037
7.018
7.000
6.949
6.929
6.908
6.864
6.742
6.722
6.474
6.456
2.848
2.831
2.814
2.797
2.780
2.762
2.744
2.446
1.170
1.153


NH
Ph
Ph
N
N
O
NH

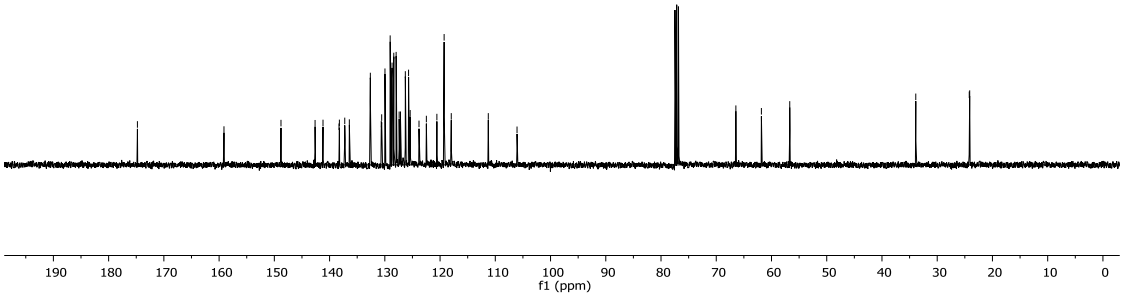
4n

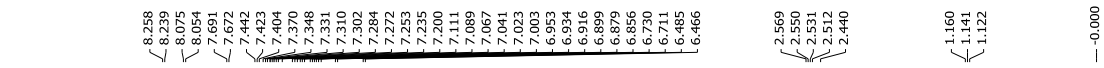

1.97
2.00
1.94
2.07
11.40
3.30
1.14
3.16
1.01
2.00
1.94
0.99
0.95
6.00
f1 (ppm)

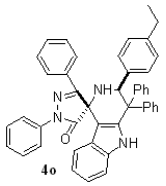

174.787
159.119
148.798
142.627
141.191
138.291
138.226
137.252
136.424
132.622
130.644
130.568
129.976
129.032
128.759
128.692
128.379
127.953
127.406
127.164
126.286
125.701
125.412
123.812
122.479
120.576
119.264
117.971
111.269
106.065
66.449
61.829
56.695
33.880
24.199
24.120

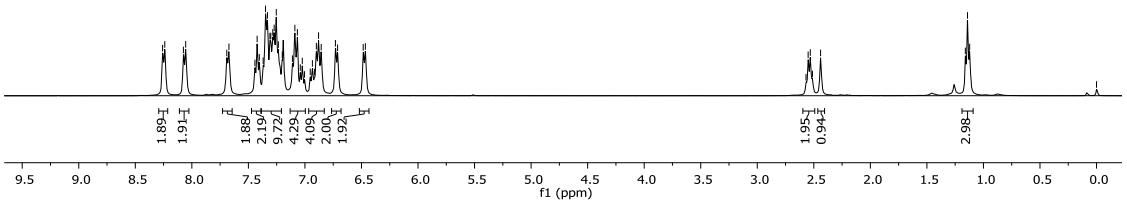

NH
Ph
Ph
N
N
O
NH

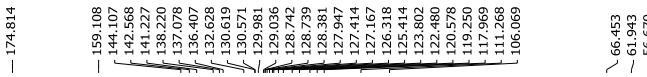
4n

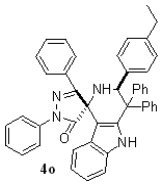

f1 (ppm)

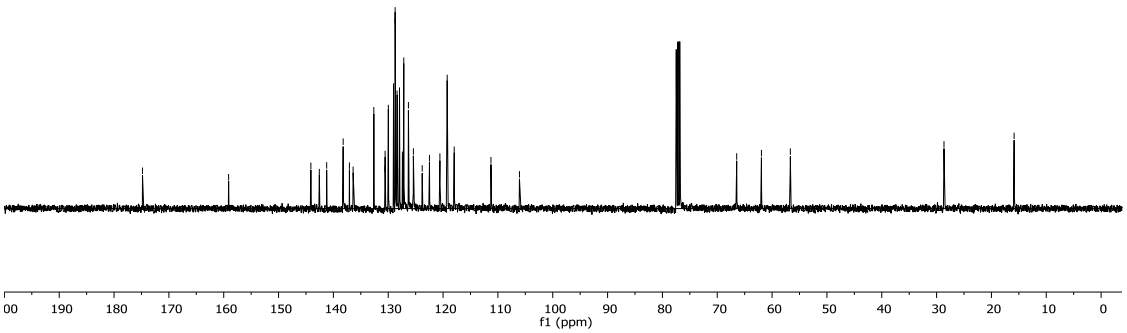

8.258
8.239
8.075
8.054
7.691
7.672
7.442
7.423
7.404
7.370
7.348
7.331
7.310
7.302
7.284
7.272
7.253
7.235
7.200
7.111
7.089
7.067
7.041
7.023
7.003
6.953
6.934
6.916
6.899
6.879
6.856
6.730
6.711
6.485
6.466
2.569
2.550
2.531
2.512
2.440
1.160
1.141
1.122
-0.000

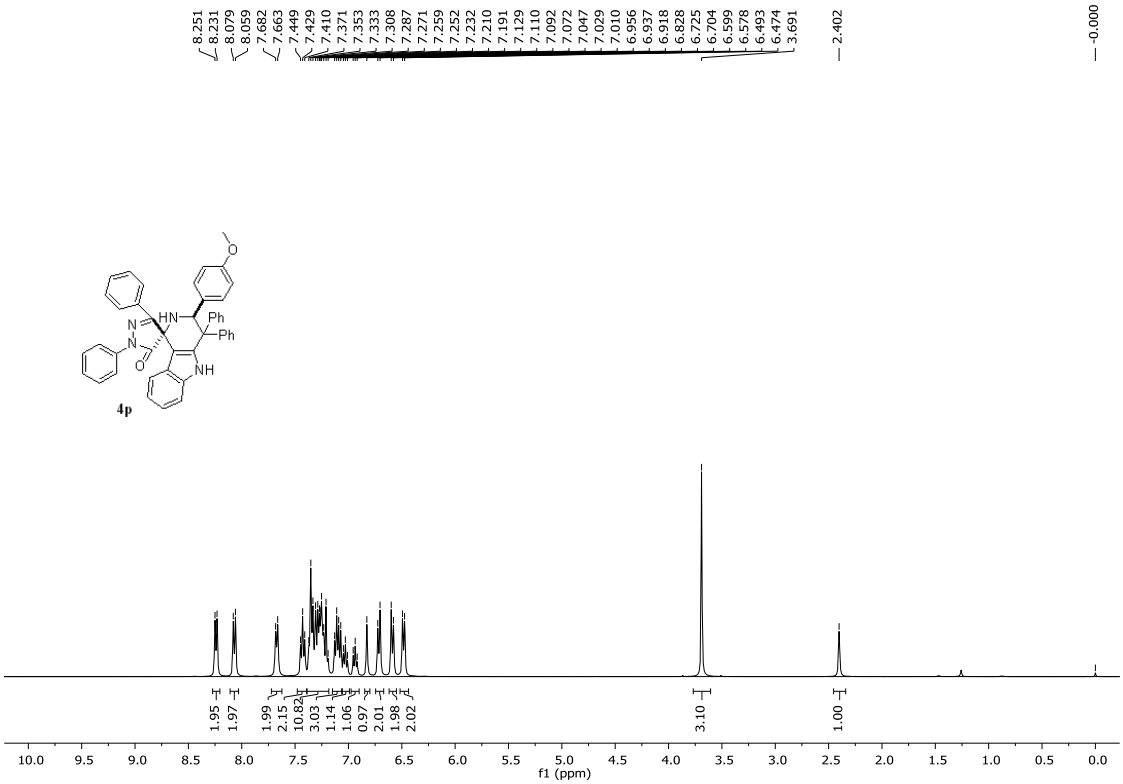

NH
Ph
Ph
N
N
O
NH
4o

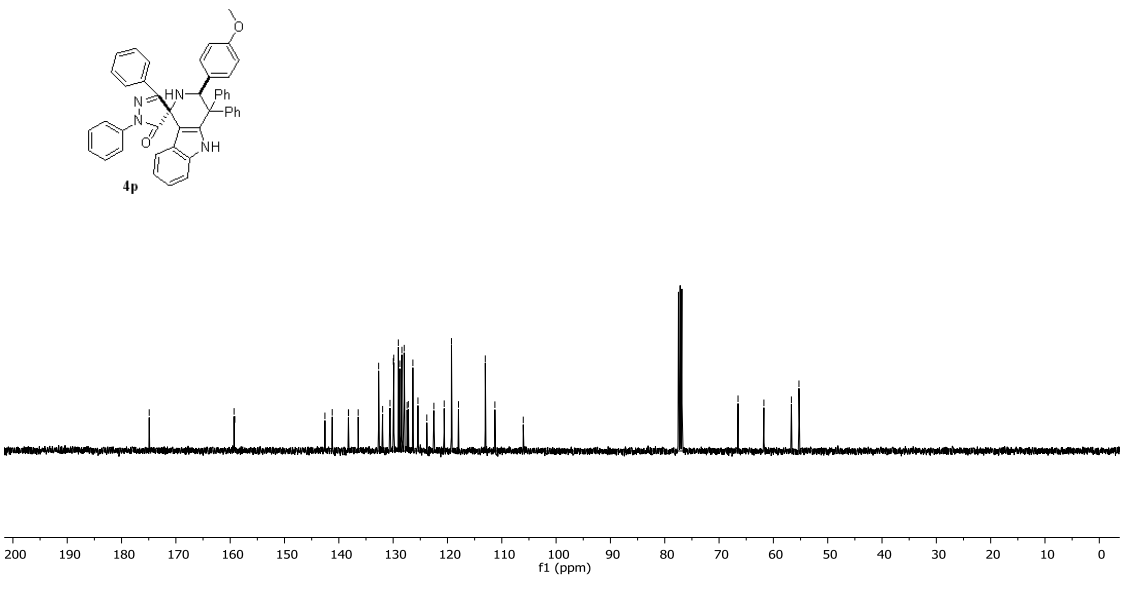

1.89
1.91
1.88
2.19
9.72
4.29
4.05
2.00
1.92
1.95
0.94
2.98
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

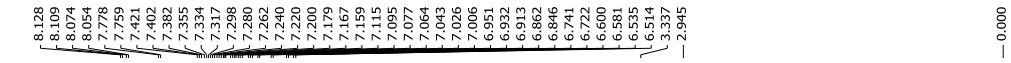

174.814
159.108
144.107
142.568
141.227
138.220
137.078
136.407
132.628
130.619
130.571
129.981
129.036
128.742
128.739
128.381
127.947
127.414
127.167
126.318
125.414
123.802
122.480
120.578
119.250
117.969
111.268
106.069
66.453
61.943
56.670
28.652
15.861

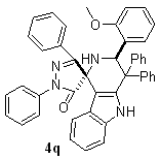

NH
Ph
Ph
N
N
O
NH
4o


00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

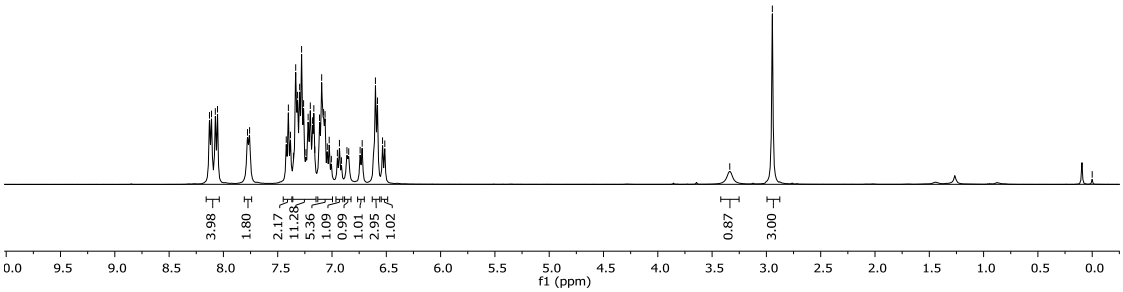

8.251
8.231
8.079
8.059
7.682
7.663
7.449
7.429
7.410
7.371
7.353
7.333
7.308
7.287
7.271
7.259
7.252
7.232
7.210
7.191
7.129
7.110
7.092
7.072
7.047
7.029
7.010
6.956
6.937
6.918
6.828
6.725
6.704
6.599
6.578
6.493
6.474
3.691
2.402
-0.000
4p
1.95
1.97
1.99
2.15
10.82
3.03
1.14
1.06
0.97
2.01
1.98
2.02
3.10
1.00
f1 (ppm)

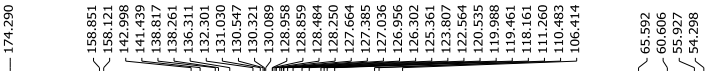

174.904
159.280
159.137
142.560
141.217
138.236
138.211
136.434
132.672
131.940
130.626
130.581
129.978
129.885
129.047
128.751
128.378
127.960
127.423
127.204
126.368
125.434
123.804
122.498
120.598
119.261
117.972
113.036
111.272
106.046
66.508
61.746
56.683
55.292
4p
f1 (ppm)

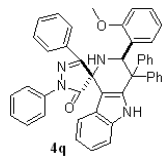

8.128
8.109
8.074
8.054
7.778
7.759
7.421
7.402
7.382
7.355
7.334
7.317
7.298
7.280
7.262
7.240
7.220
7.200
7.179
7.167
7.159
7.115
7.095
7.077
7.064
7.043
7.026
7.006
6.951
6.932
6.913
6.862
6.846
6.741
6.722
6.600
6.581
6.535
6.514
3.337
2.945
0.000


O
HN
Ph
Ph
N
N
O
NH

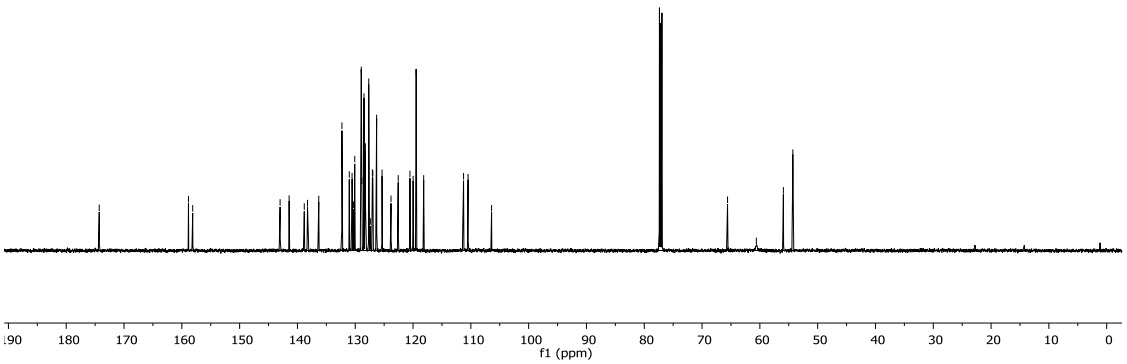
4q

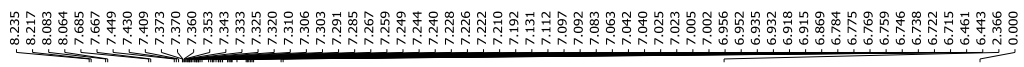

3.98
1.80
2.17
11.28
5.36
1.09
0.99
1.01
2.95
1.02
0.87
3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

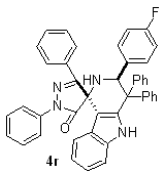

174.290
158.851
158.121
142.998
141.439
138.817
138.261
136.311
132.301
131.030
130.547
130.321
130.089
128.958
128.859
128.484
128.250
127.664
127.385
127.036
126.956
126.302
125.361
123.807
122.564
120.535
119.988
119.461
118.161
111.260
110.483
106.414
65.592
60.606
55.927
54.298


O
HN
Ph
Ph
N
N
O
NH

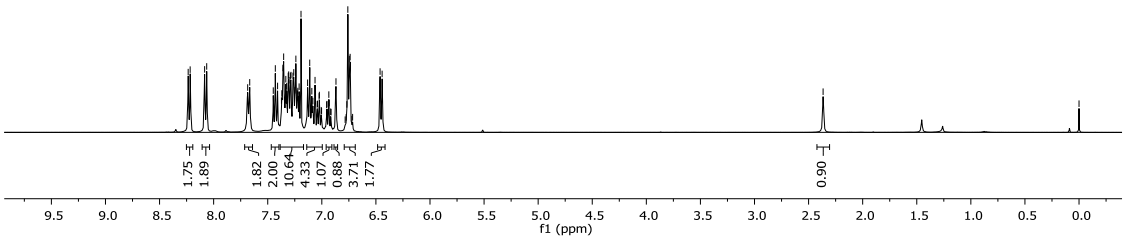
4q


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

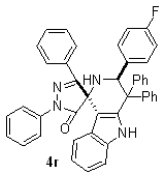

8.235
8.217
8.083
8.064
7.685
7.667
7.449
7.430
7.409
7.373
7.370
7.360
7.353
7.343
7.333
7.325
7.320
7.310
7.306
7.303
7.291
7.285
7.267
7.259
7.249
7.244
7.240
7.228
7.226
7.222
7.210
7.192
7.131
7.112
7.097
7.092
7.083
7.063
7.042
7.040
7.025
7.023
7.005
7.002
6.956
6.952
6.935
6.932
6.918
6.915
6.869
6.784
6.775
6.769
6.759
6.746
6.738
6.722
6.715
6.461
6.443
2.366
0.000


F
HN
Ph
Ph
N
N
O
NH

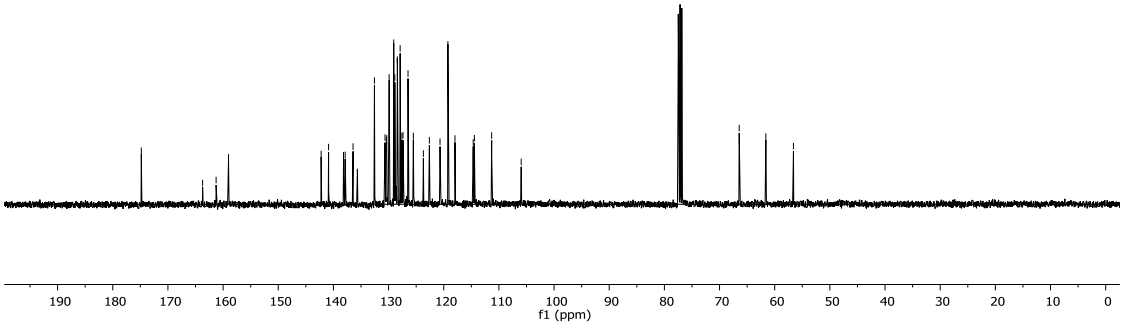
4r

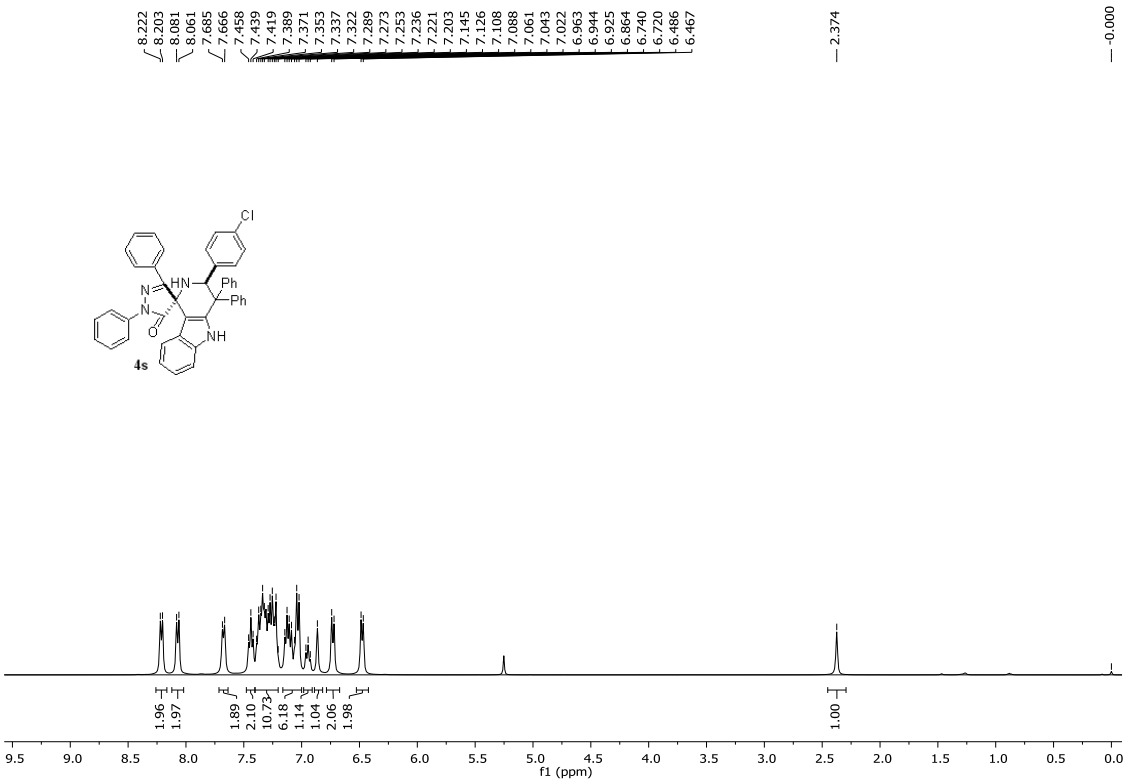

1.75
1.89
1.82
2.00
10.64
4.33
1.07
0.88
3.71
1.77
0.90
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

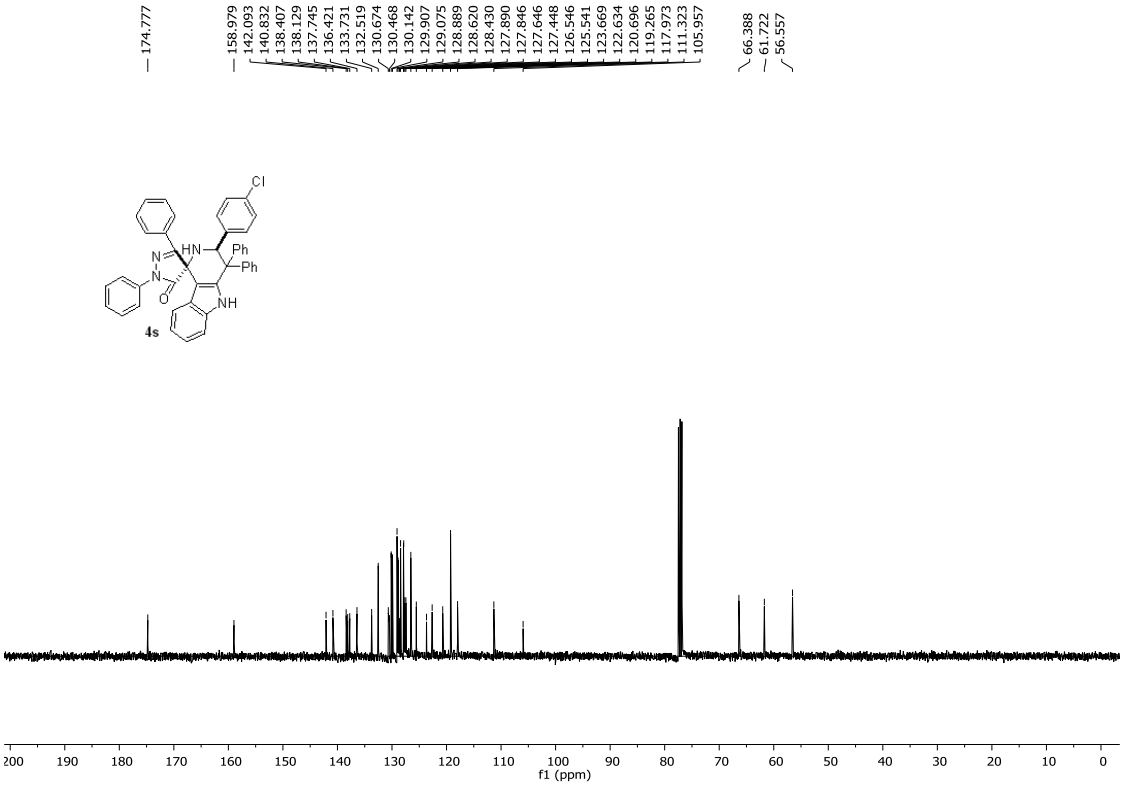

174.826
163.716
161.265
159.018
142.228
140.877
138.167
137.873
136.441
135.669
135.637
132.562
130.648
130.513
130.411
130.332
129.897
129.069
128.866
128.409
127.903
127.583
127.386
126.474
125.511
123.689
122.603
120.675
119.249
117.963
114.659
114.449
111.314
105.959
66.436
61.605
56.605


F
HN
Ph
Ph
N
N
O
NH

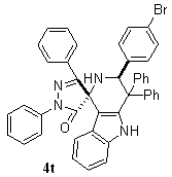
4r


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

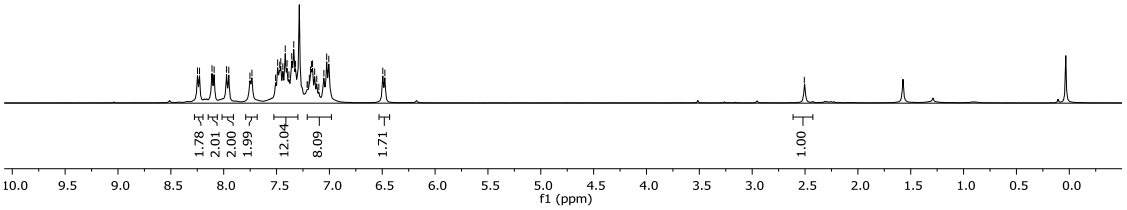

8.222
8.203
8.081
8.061
7.685
7.666
7.458
7.439
7.419
7.389
7.371
7.353
7.337
7.322
7.289
7.273
7.253
7.236
7.221
7.203
7.145
7.126
7.108
7.088
7.061
7.043
7.022
6.963
6.944
6.925
6.864
6.740
6.720
6.486
6.467
2.374
-0.000
Cl
HN
Ph
Ph
N
N
O
NH
4s
1.96
1.97
1.89
2.10
10.73
6.18
1.14
1.04
2.06
1.98
1.00
f1 (ppm)


174.777
158.979
142.093
140.832
138.407
138.129
137.745
136.421
133.731
132.519
130.674
130.468
130.142
129.907
129.075
128.889
128.620
128.430
127.890
127.846
127.646
127.448
126.546
125.541
123.669
122.634
120.696
119.265
117.973
111.323
105.957
66.388
61.722
56.557
Cl
HN
Ph
Ph
N
N
O
NH
4s
f1 (ppm)

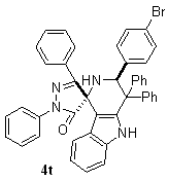

8.248
8.229
8.110
8.090
7.973
7.952
7.733
7.489
7.470
7.460
7.440
7.418
7.400
7.356
7.337
7.320
7.178
7.170
7.159
7.139
7.026
7.006
6.495
6.475
2.507


Br
HN
Ph
Ph
N
N
O
NH

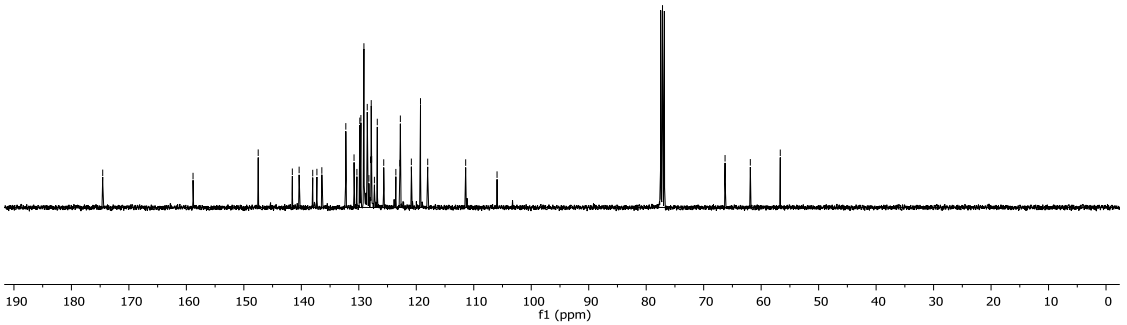
4t

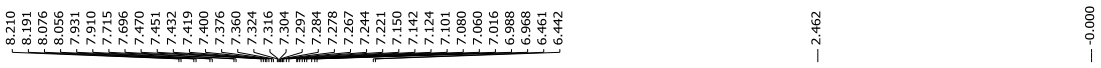

1.78
2.01
2.00
1.99
12.04
8.09
1.71
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

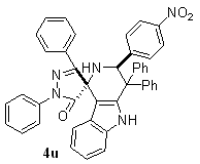

174.556
158.841
147.503
141.563
140.384
138.017
137.289
136.430
132.259
130.829
130.331
129.824
129.635
129.110
128.530
128.242
127.967
127.838
127.768
127.283
126.783
125.664
123.555
122.853
122.770
120.856
119.269
118.013
111.408
105.948
66.279
61.884
56.674


Br
HN
Ph
Ph
N
N
O
NH

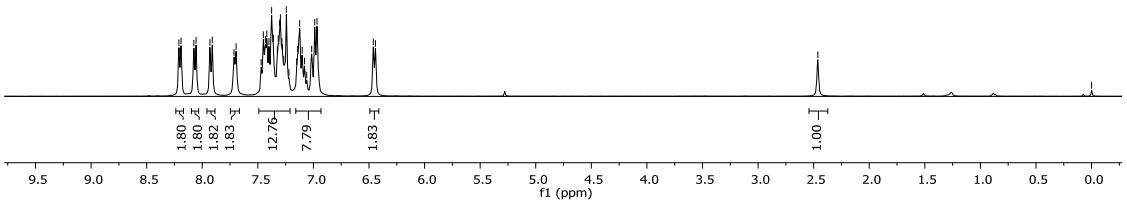
4t


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

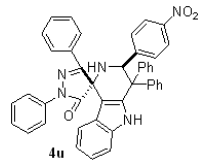

8.210
8.191
8.076
8.056
7.931
7.910
7.715
7.696
7.470
7.451
7.432
7.419
7.400
7.376
7.360
7.324
7.316
7.304
7.297
7.284
7.278
7.267
7.244
7.221
7.150
7.142
7.124
7.101
7.080
7.060
7.016
6.988
6.968
6.461
6.442
2.462
-0.000


NO2
HN
Ph
Ph
N
N
O
NH

4u

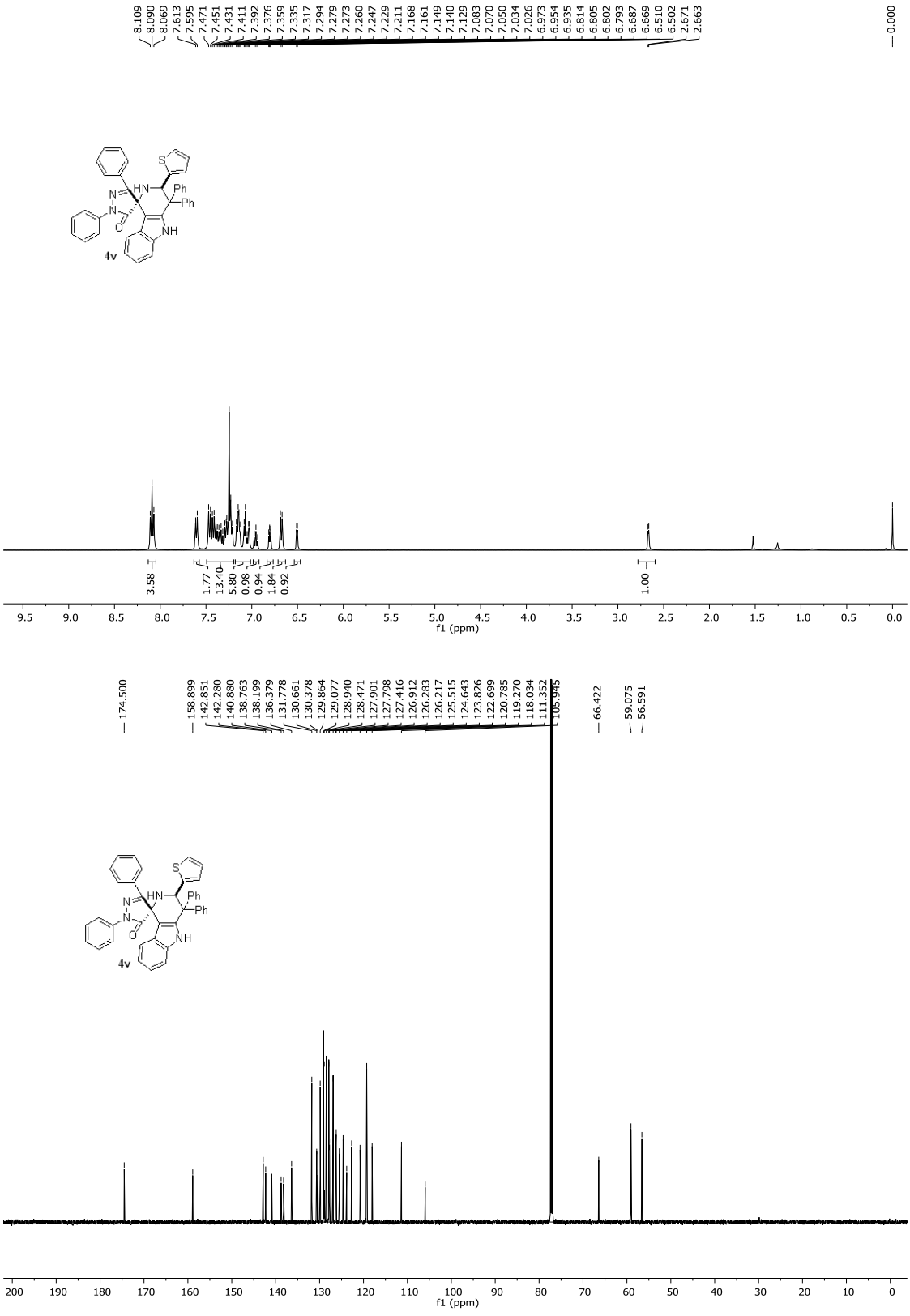

1.80
1.80
1.82
1.83
12.76
7.79
1.83
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

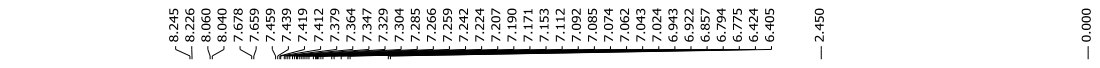

174.560
158.855
147.546
141.609
140.415
138.052
137.323
136.462
132.277
130.851
130.367
129.854
129.660
129.157
129.125
128.556
128.005
127.862
127.797
126.817
125.695
123.606
122.896
122.804
120.898
119.317
118.063
111.412
106.024
66.297
61.902
56.716

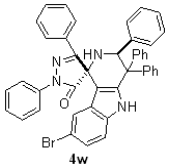

NO2
HN
Ph
Ph
N
N
O
NH

4u

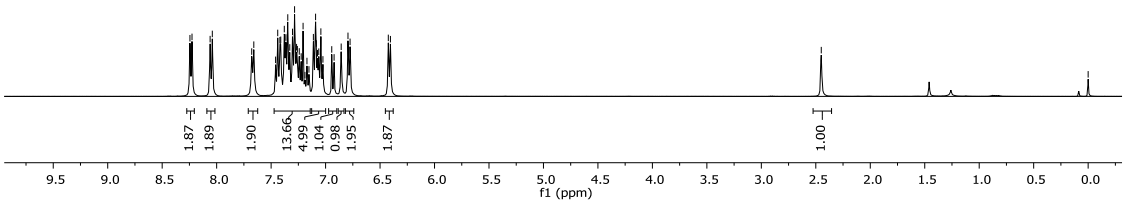
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.109
8.090
8.069
7.613
7.595
7.471
7.451
7.431
7.411
7.392
7.376
7.359
7.335
7.317
7.294
7.279
7.273
7.260
7.247
7.229
7.211
7.168
7.161
7.149
7.140
7.129
7.083
7.070
7.050
7.034
7.026
6.973
6.954
6.935
6.814
6.805
6.802
6.793
6.687
6.669
6.510
6.502
2.671
2.663
0.000
HN
Ph
Ph
S
N
N
O
NH
4v
3.58
1.77
13.40
5.80
0.98
0.94
1.84
0.92
1.00
f1 (ppm)
174.500
158.899
142.851
142.280
140.880
138.763
138.199
136.379
131.778
130.661
130.378
129.864
129.077
128.940
128.471
127.901
127.798
127.416
126.912
126.283
126.217
125.515
124.643
123.826
122.699
120.785
119.270
118.034
111.352
105.945
66.422
59.075
56.591
f1 (ppm)

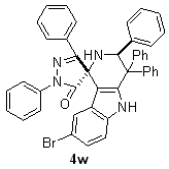

8.245
8.226
8.060
8.040
7.678
7.659
7.459
7.439
7.419
7.412
7.379
7.364
7.347
7.329
7.304
7.285
7.266
7.259
7.242
7.224
7.207
7.190
7.171
7.153
7.112
7.092
7.085
7.074
7.062
7.043
7.024
6.943
6.922
6.857
6.794
6.775
6.424
6.405
2.450
0.000


HN
Ph
Ph
N
N
O
NH
Br

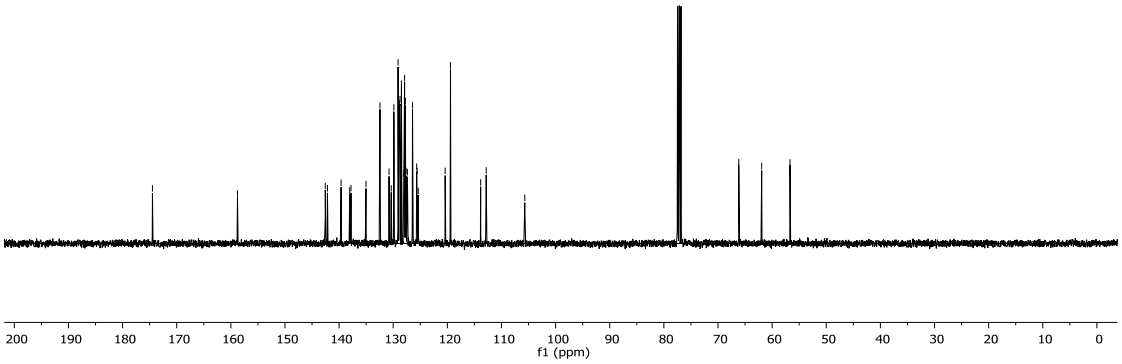
4w

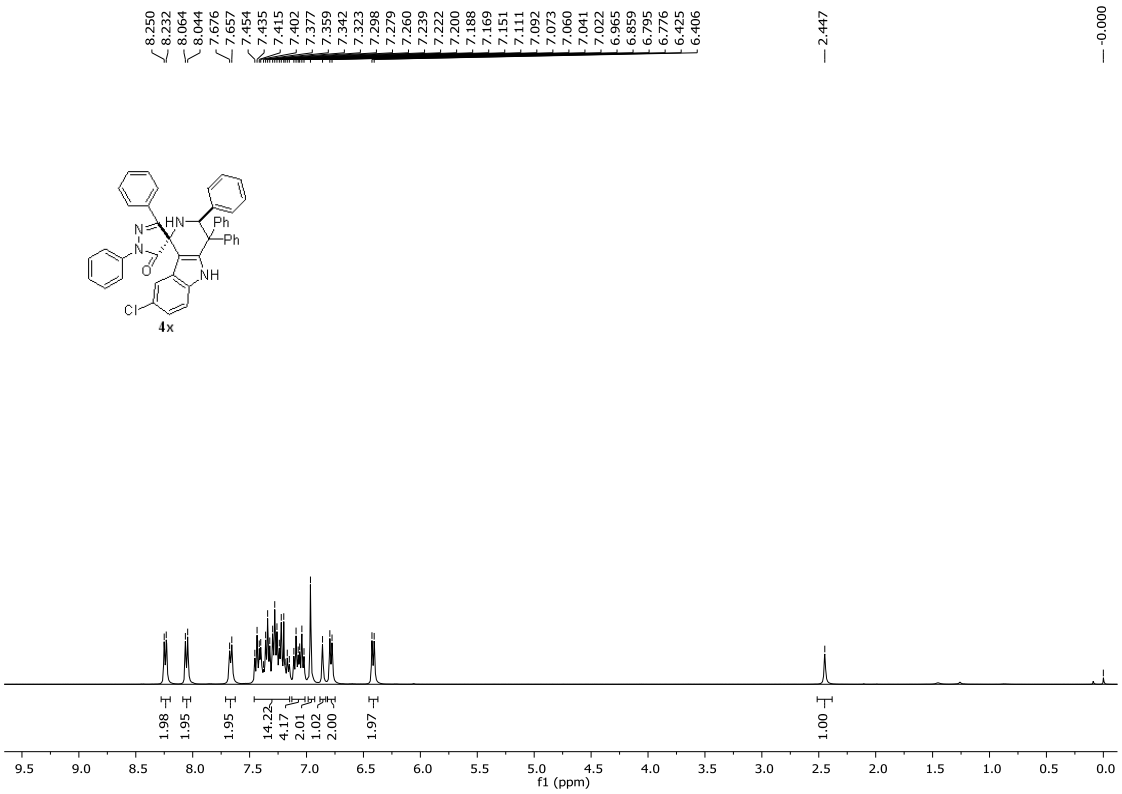

1.87
1.89
1.90
13.66
4.99
1.04
0.98
1.95
1.87
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

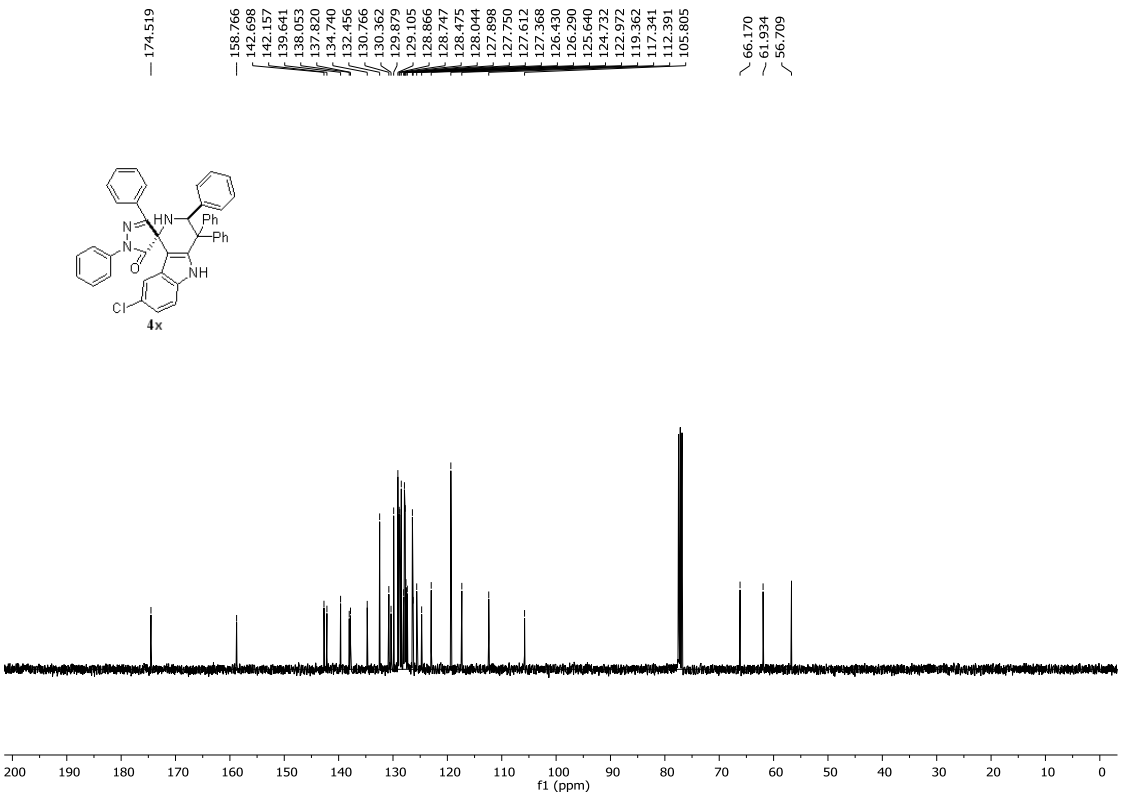

174.481
158.773
142.552
142.151
139.632
138.044
137.803
135.034
132.448
130.774
130.366
129.884
129.106
128.873
128.744
128.484
128.047
127.899
127.753
127.623
127.375
126.435
125.665
125.571
125.378
120.405
119.421
113.844
112.822
105.697
66.159
61.932
56.696

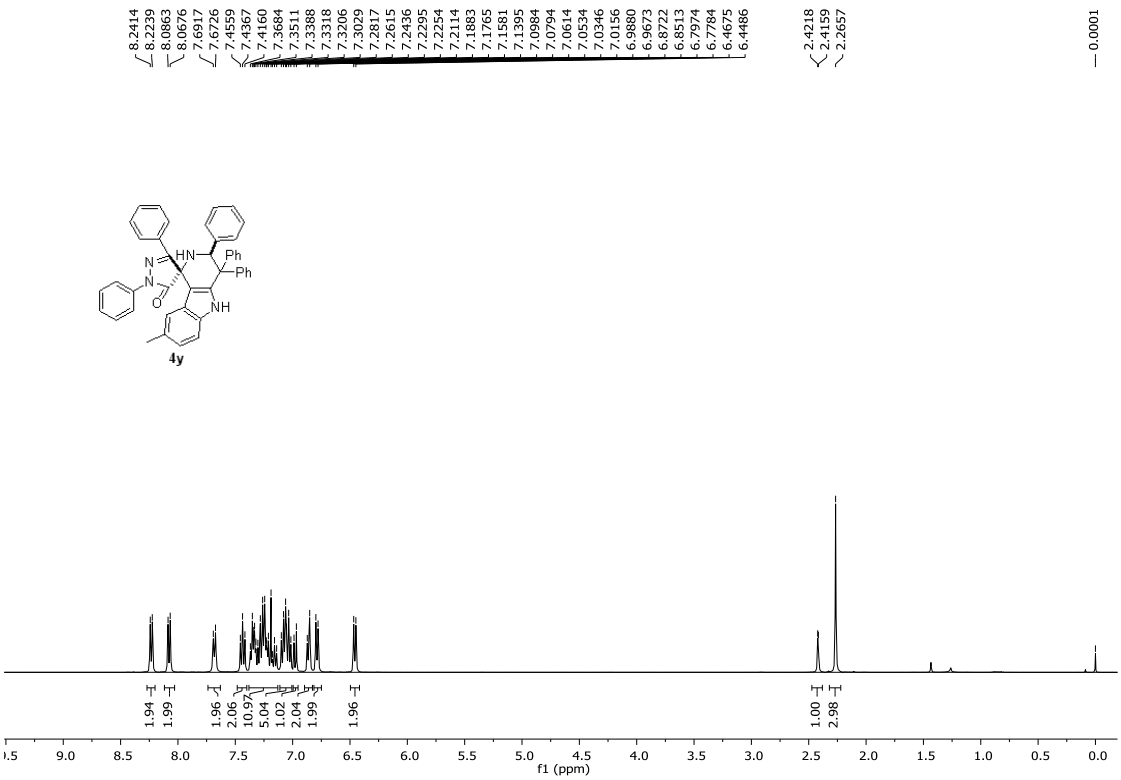

HN
Ph
Ph
N
N
O
NH
Br

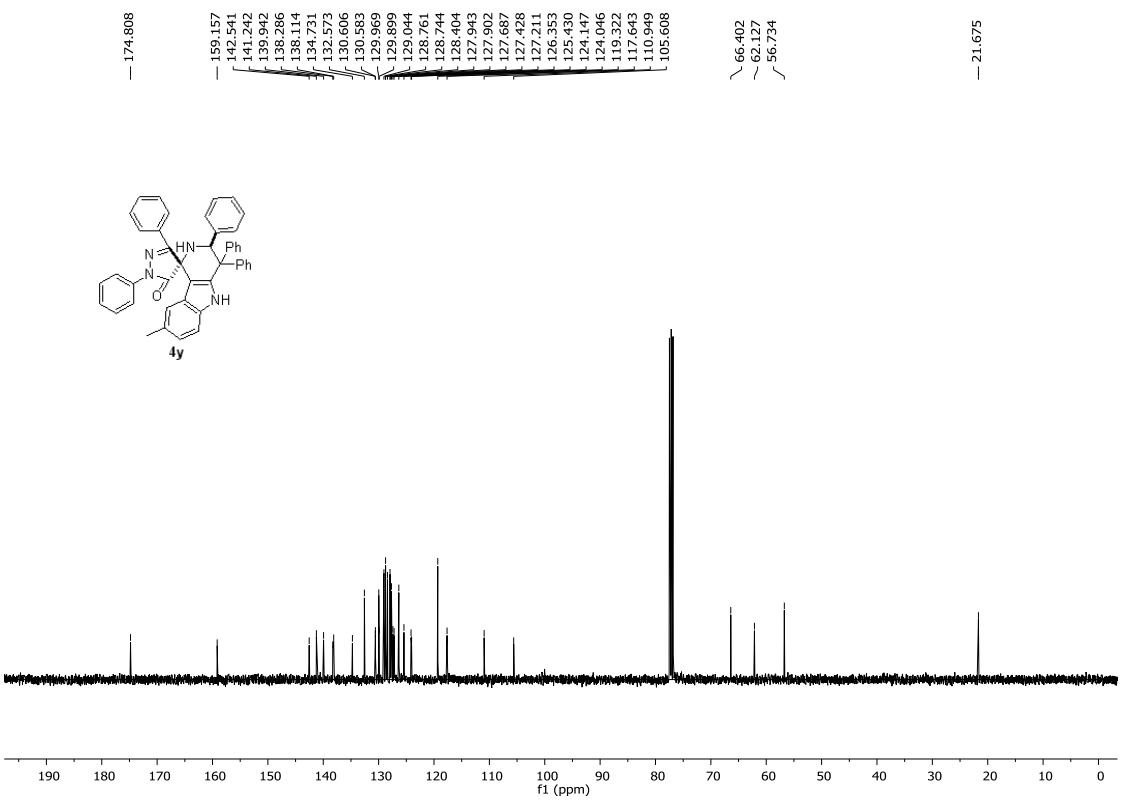
4w

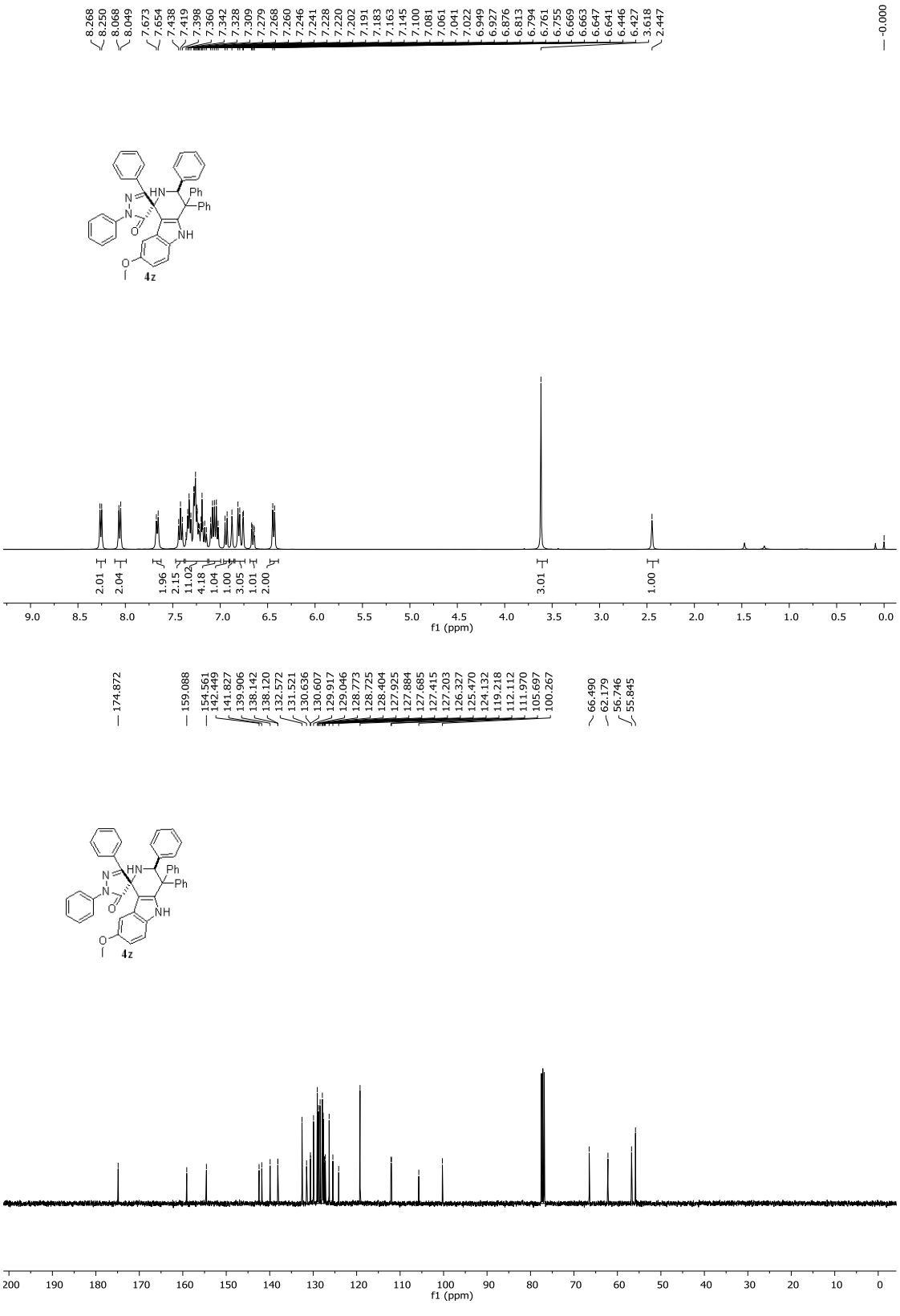

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

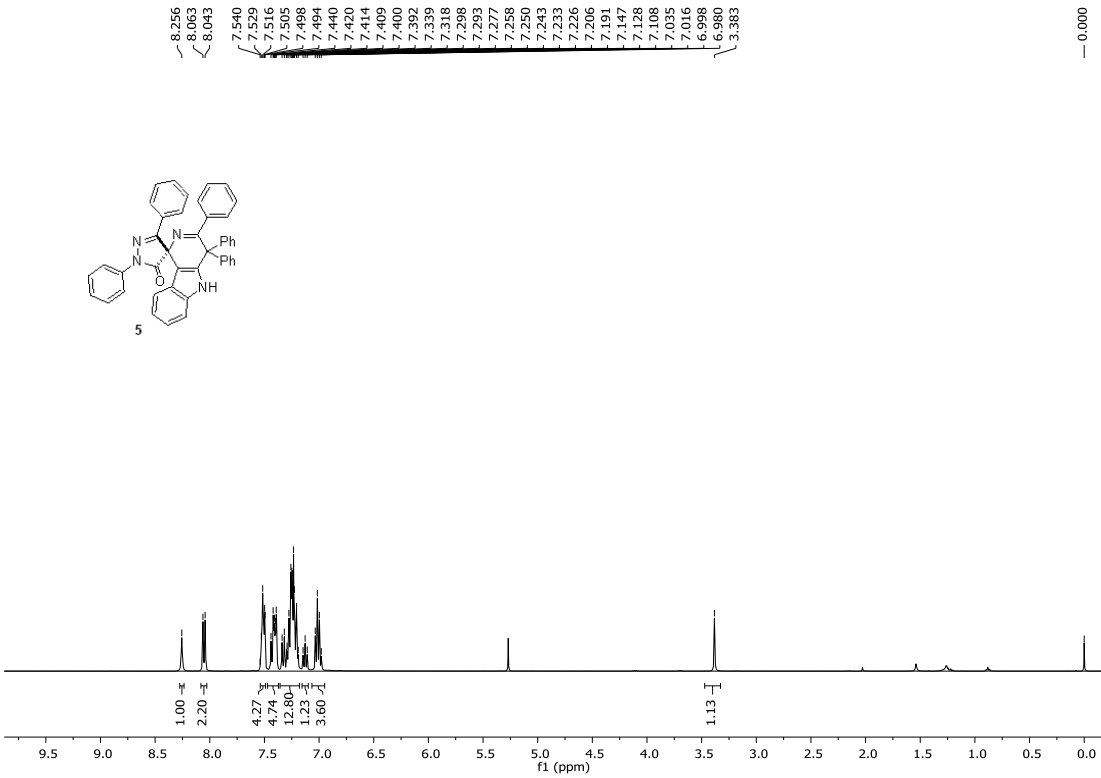

8.250
8.232
8.064
8.044
7.676
7.657
7.454
7.435
7.415
7.402
7.377
7.359
7.342
7.323
7.298
7.279
7.260
7.239
7.222
7.200
7.188
7.169
7.151
7.111
7.092
7.073
7.060
7.041
7.022
6.965
6.859
6.795
6.776
6.425
6.406
2.447
-0.000
HN
Ph
Ph
N
O
NH
Cl
4x
1.98
1.95
1.95
14.22
4.17
2.01
1.02
2.00
1.97
1.00
9.5
9.0
8.5
8.0
7.5
7.0
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
0.0
f1 (ppm)

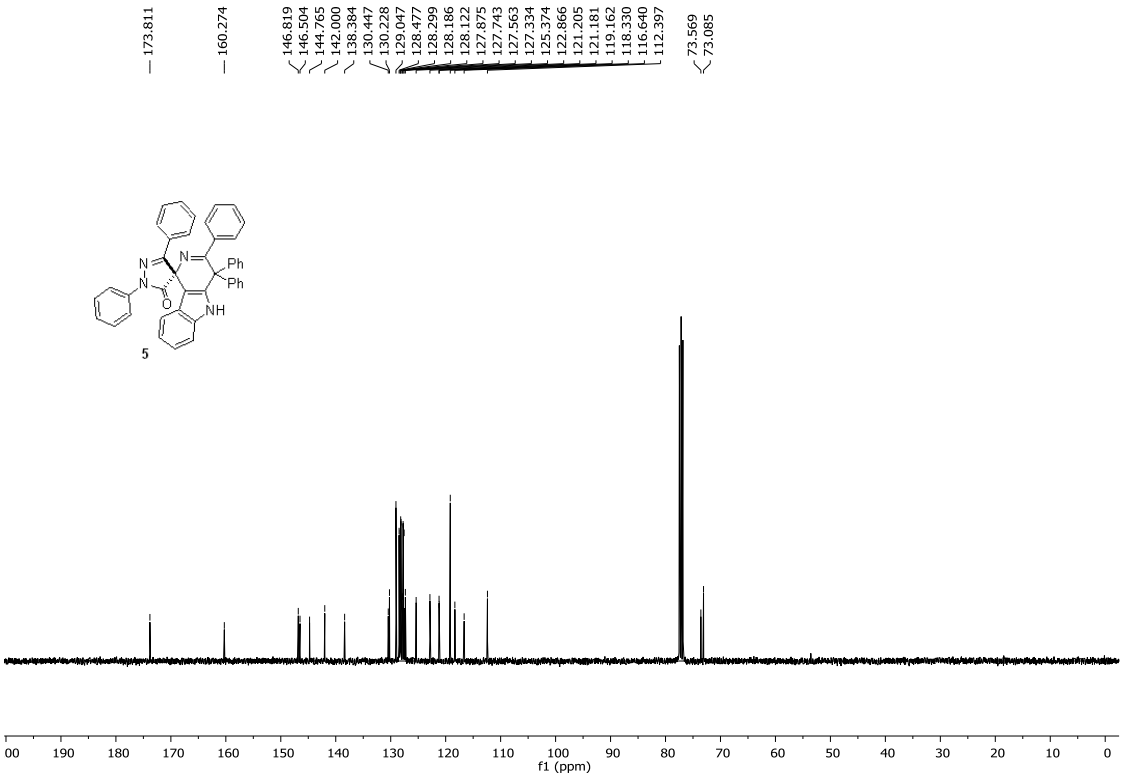

174.519
158.766
142.698
142.157
139.641
138.053
137.820
134.740
132.456
130.766
130.362
129.879
129.105
128.866
128.747
128.475
128.044
127.898
127.750
127.612
127.368
126.430
126.290
125.640
124.732
122.972
119.362
117.341
112.391
105.805
66.170
61.934
56.709
HN
Ph
Ph
N
O
NH
Cl
4x
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.2414
8.2239
8.0863
8.0676
7.6917
7.6726
7.4559
7.4367
7.4160
7.3684
7.3511
7.3388
7.3318
7.3206
7.3029
7.2817
7.2615
7.2436
7.2295
7.2254
7.2114
7.1883
7.1765
7.1581
7.1395
7.0984
7.0794
7.0614
7.0534
7.0346
7.0156
6.9880
6.9673
6.8722
6.8513
6.7974
6.7784
6.4675
6.4486
2.4218
2.4159
2.2657
0.0001
HN
Ph
Ph
N
N
O
NH
4y
1.94
1.99
1.96
2.06
10.97
5.04
1.02
2.04
1.99
1.96
1.00
2.98
f1 (ppm)

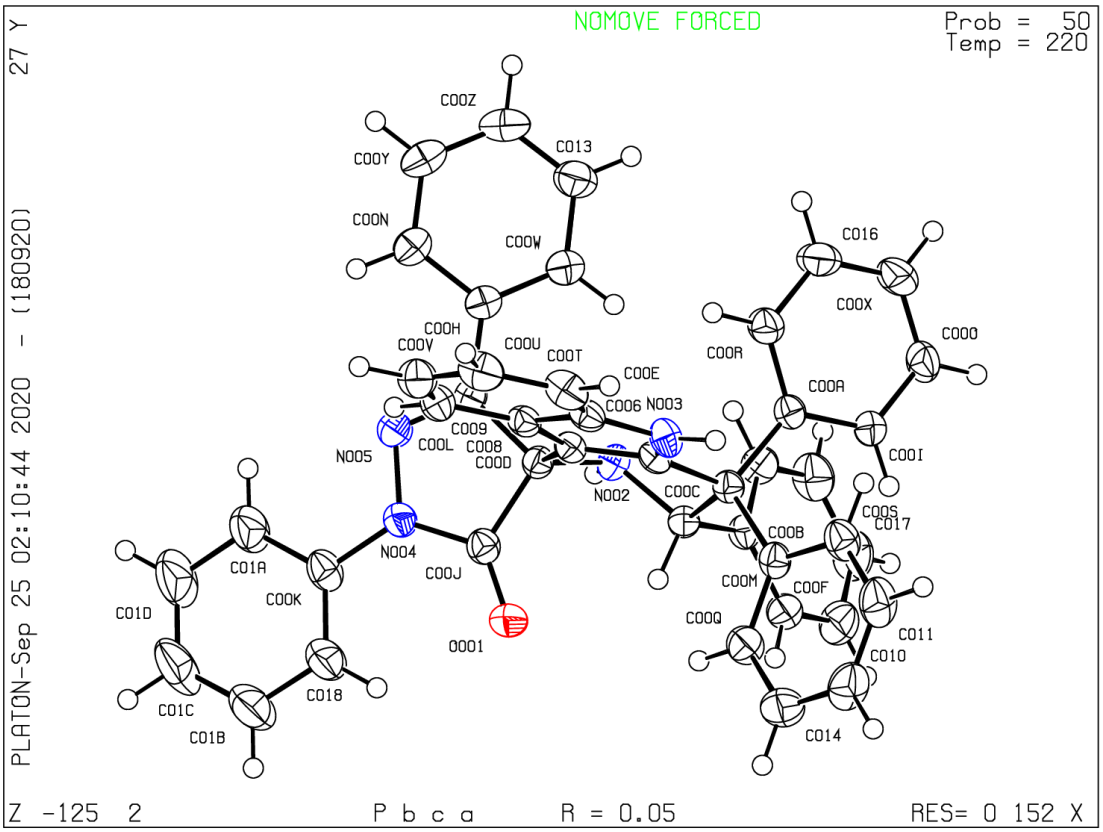

174.808
159.157
142.541
141.242
139.942
138.286
138.114
134.731
132.573
130.606
130.583
129.969
129.899
129.044
128.761
128.744
128.404
127.943
127.902
127.687
127.428
127.211
126.353
125.430
124.147
124.046
119.322
117.643
110.949
105.608
66.402
62.127
56.734
21.675
HN
Ph
Ph
N
N
O
NH
4y
f1 (ppm)


8.268
8.250
8.068
8.049
7.673
7.654
7.438
7.419
7.398
7.360
7.342
7.328
7.309
7.279
7.268
7.260
7.246
7.241
7.228
7.220
7.202
7.191
7.183
7.163
7.145
7.100
7.081
7.061
7.041
7.022
6.949
6.927
6.876
6.813
6.794
6.761
6.755
6.669
6.663
6.647
6.641
6.446
6.427
3.618
2.447
-0.000
HN
Ph
Ph
N
N
O
NH
O
4z
2.01
2.04
1.96
2.15
11.02
4.18
1.04
1.00
3.05
1.01
2.00
3.01
1.00
f1 (ppm)
174.872
159.088
154.561
142.449
141.827
139.906
138.142
138.120
132.572
131.521
130.636
130.607
129.917
129.046
128.773
128.725
128.404
127.925
127.884
127.685
127.415
127.203
126.327
125.470
124.132
119.218
112.112
111.970
105.697
100.267
66.490
62.179
56.746
55.845
HN
Ph
Ph
N
N
O
NH
O
4z
f1 (ppm)


8.256
8.063
8.043
7.540
7.529
7.516
7.505
7.498
7.494
7.440
7.420
7.414
7.409
7.400
7.392
7.339
7.318
7.298
7.293
7.277
7.258
7.250
7.243
7.233
7.226
7.206
7.191
7.147
7.128
7.108
7.035
7.016
6.998
6.980
3.383
0.000
Ph
Ph
NH
O
5
1.00
2.20
4.27
4.74
12.80
1.23
3.60
1.13
f1 (ppm)


173.811
160.274
146.819
146.504
144.765
142.000
138.384
130.447
130.228
129.047
128.477
128.299
128.186
128.122
127.875
127.743
127.563
127.334
125.374
122.866
121.205
121.181
119.162
118.330
116.640
112.397
73.569
73.085
Ph
Ph
NH
O
5
f1 (ppm)

Crystal data for 4a



Single crystal xray structure for compound **4a**

Empirical formula:	C43 H32 N4 O
Formula weight:	622.74
Temperature (K):	220
Crystal system:	Orthorhombic
Space group:	Pbca
Hall group:	-P 2ac 2ab
a (Å)	18.8089(13)
b (Å)	17.8043(12)
c (Å)	21.9597(15)
α(°)	90.00
β(°)	90.00
γ(°)	90.00

Volume (Å 3) = 7353.8 (9)

Z = 8

D calcd (g cm^{-3}) = 1.125

μ(mm^{-1}) = 0.068

F (000) = 2624.0

Crystal size/mm^3) = 0.26 × 0.24 × 0.22

Theta range for data collection = 4.296 to 55.08

Index ranges = -24 ≤ h ≤ 24, -23 ≤ k ≤ 23, -28 ≤ l ≤ 28

Reflections collected = 148677

Independent reflection = 8472

Data/restraints/parameters = 8472/0/441

GOF (on F2) = 1.069

Final R indexes [I>=2σ (I)] R1 = 0.0547, wR2 = 0.1451

Final R indexes [all data] R1 = 0.0889, wR2 = 0.1645

Largest diff. peak and hole (e Å 0.25/-0.24