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

SUPPORTING INFORMATION

Catalyst- and solvent-free thermal multicomponent approach for the construction of diverse and polysubstituted 2-aminopyrinides and their antibacterial activity

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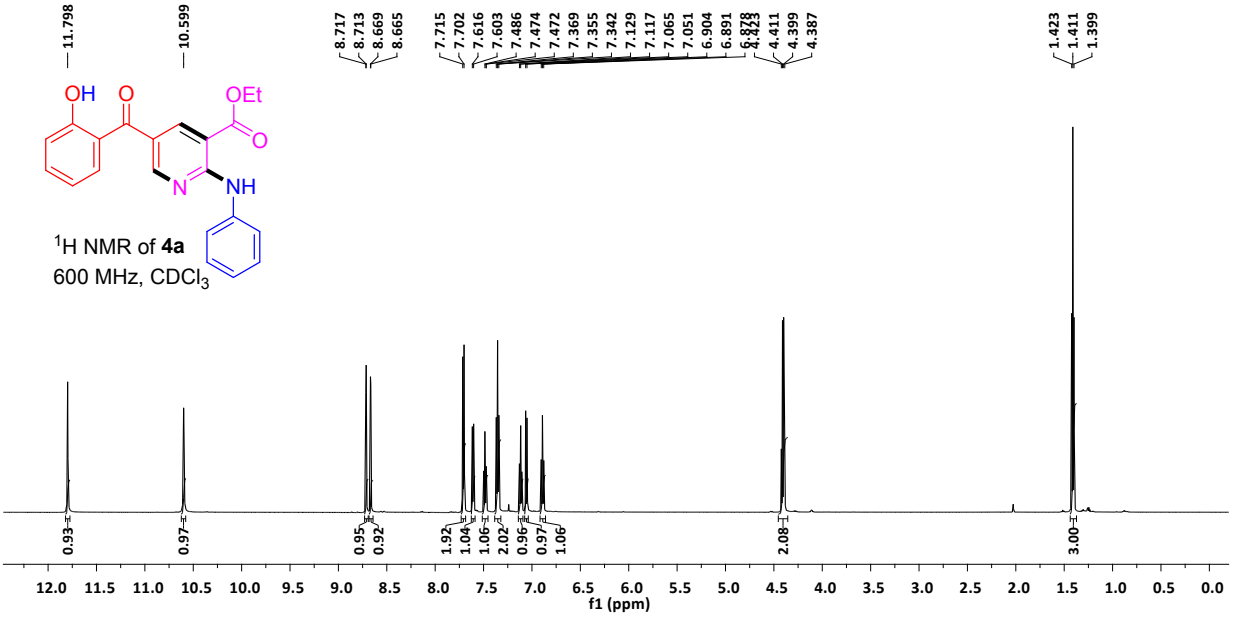
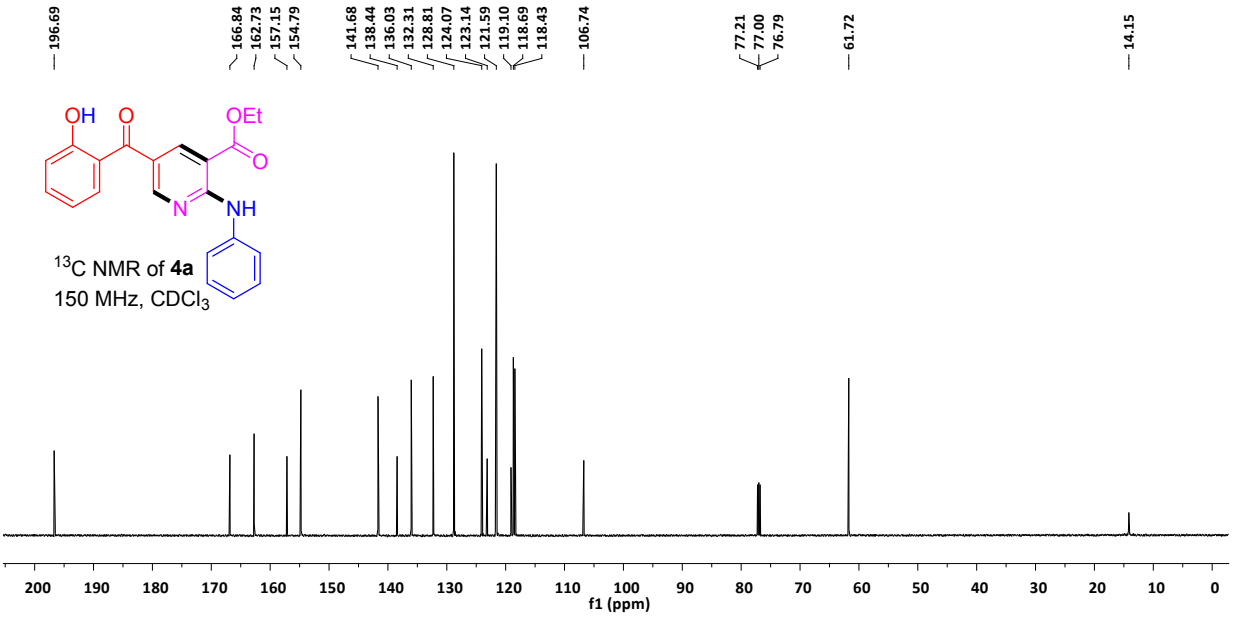
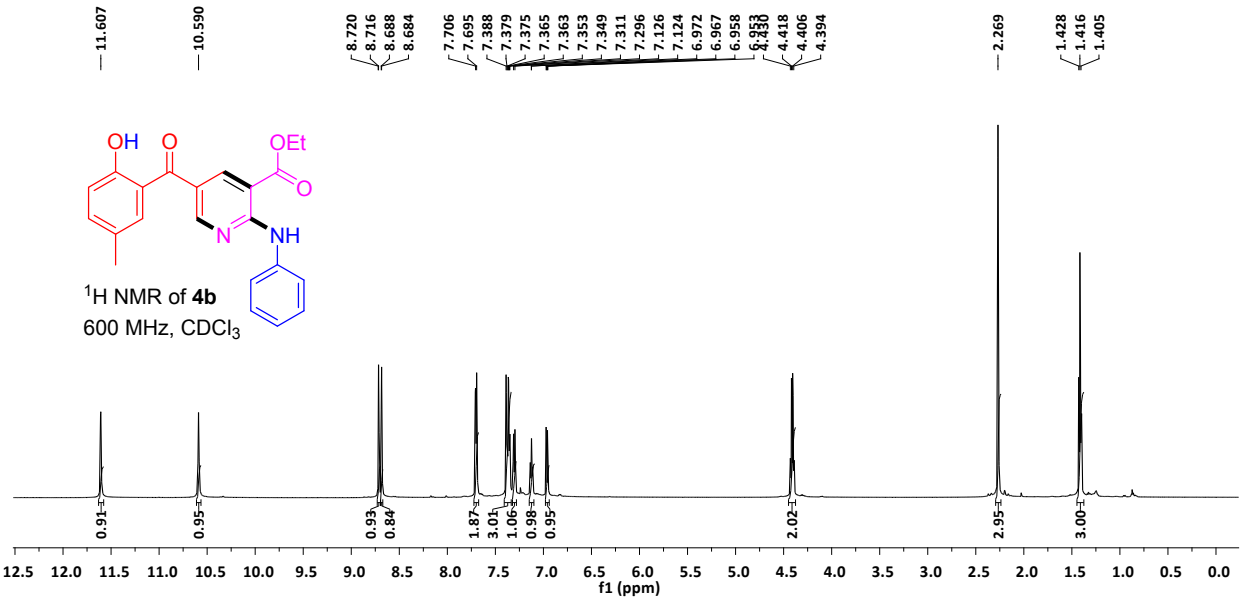
^{1}H NMR and ^{13}C NMR spectra of synthesized compounds



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6.958
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4.394
2.269
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1.416
1.405
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O
OEt
O
N
NH
1H NMR of 4b
600 MHz, CDCl3
0.91
0.95
0.93
0.84
1.87
3.01
1.06
0.98
0.95
2.02
2.95
3.00
12.5 12.0 11.5 11.0 10.5 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
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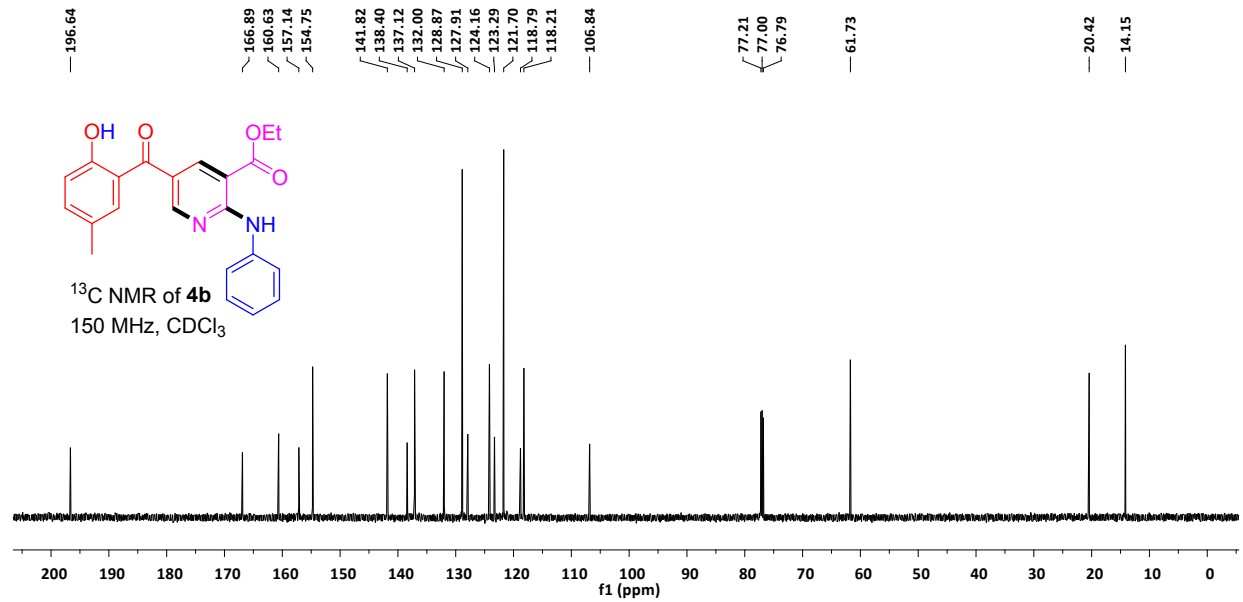
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123.29
121.70
118.79
118.21
106.84
77.21
77.00
76.79
61.73
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14.15
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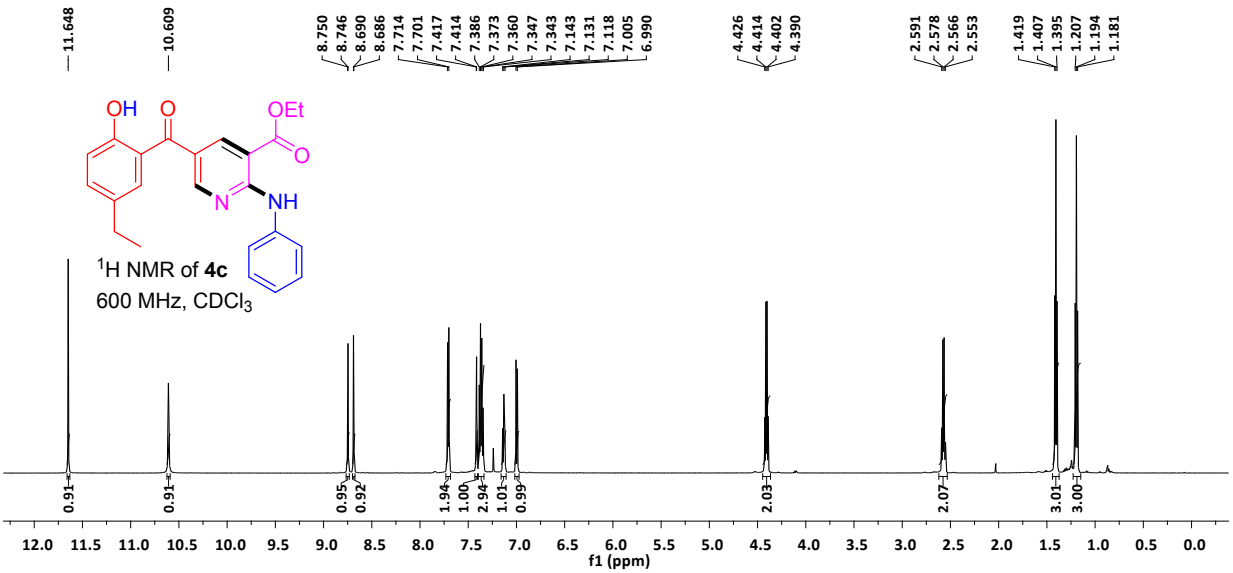
f1 (ppm)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4.414
4.402
4.390
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2.578
2.566
2.553
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1.407
1.395
1.207
1.194
1.181
OH
O
OEt
O
N
NH
1H NMR of 4c
600 MHz, CDCl3
0.91
0.91
0.95
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1.00
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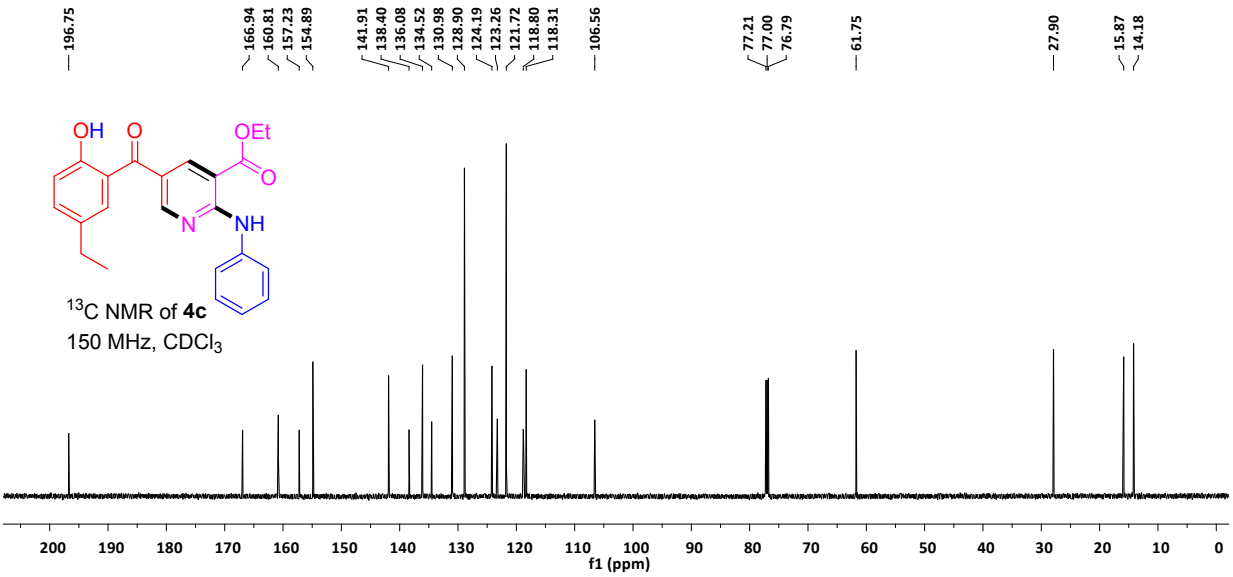
1.01
0.99
2.03
2.07
3.01
3.00
f1 (ppm)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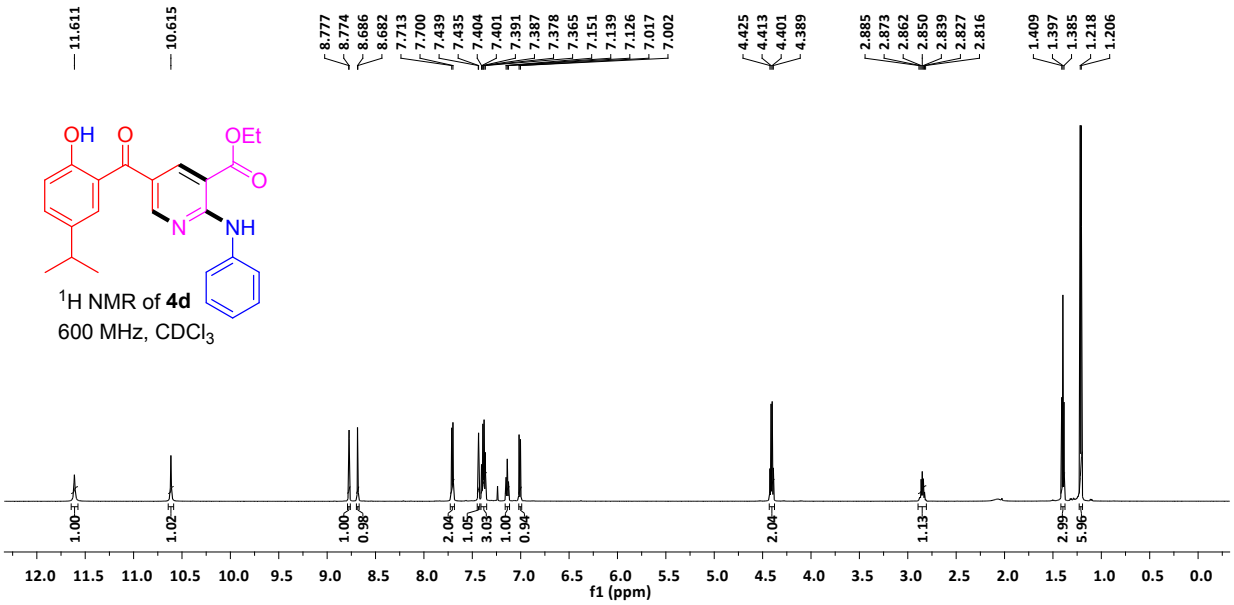
13C NMR of 4c
150 MHz, CDCl3
f1 (ppm)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7.139
7.126
7.017
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4.413
4.401
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2.862
2.850
2.839
2.827
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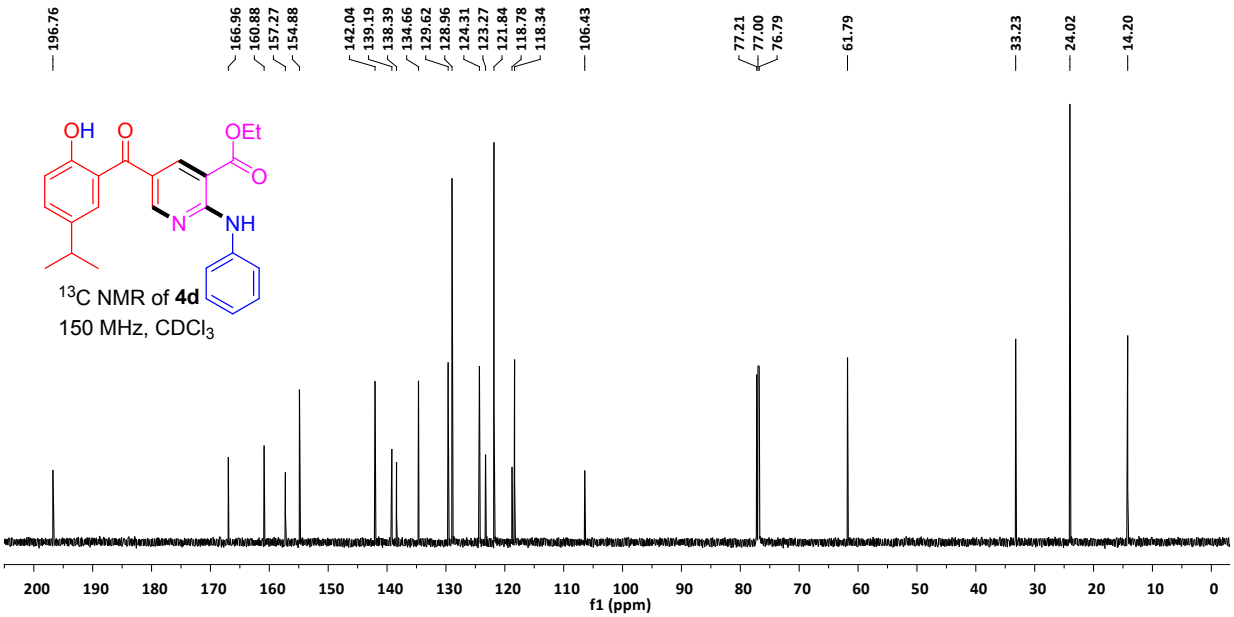
1.218
1.206
OH
O
OEt
O
N
NH
1H NMR of 4d
600 MHz, CDCl3
1.00
1.02
1.00
0.98
2.04
1.05
3.03
1.00
0.94
2.04
1.13
2.99
5.96
f1 (ppm)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118.34
106.43
77.21
77.00
76.79
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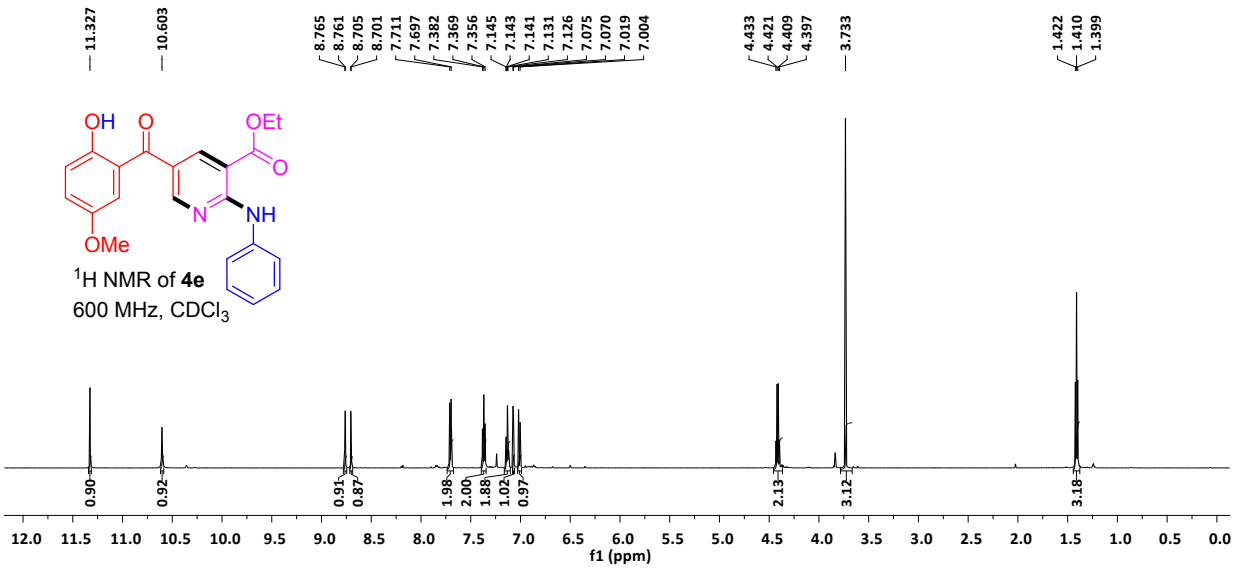
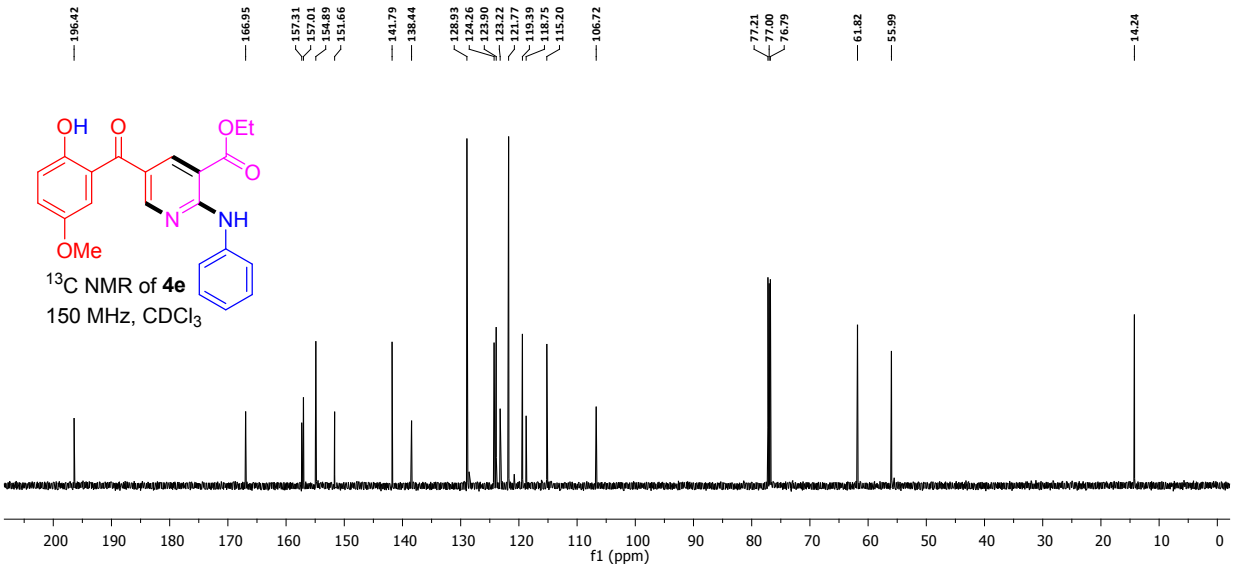
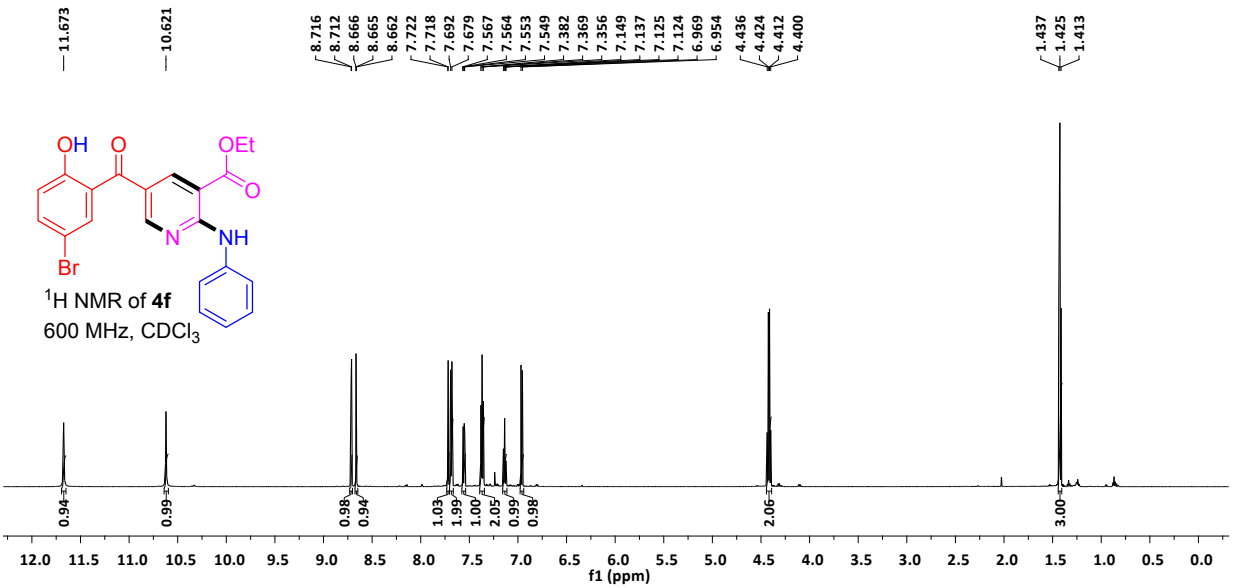
13C NMR of 4d
150 MHz, CDCl3
f1 (ppm)



^{1}H NMR of **4e**
600 MHz, $CDCl_3$



^{13}C NMR of **4e**
150 MHz, $CDCl_3$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7.137
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7.124
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6.954
4.436
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4.412
4.400
1.437
1.425
1.413
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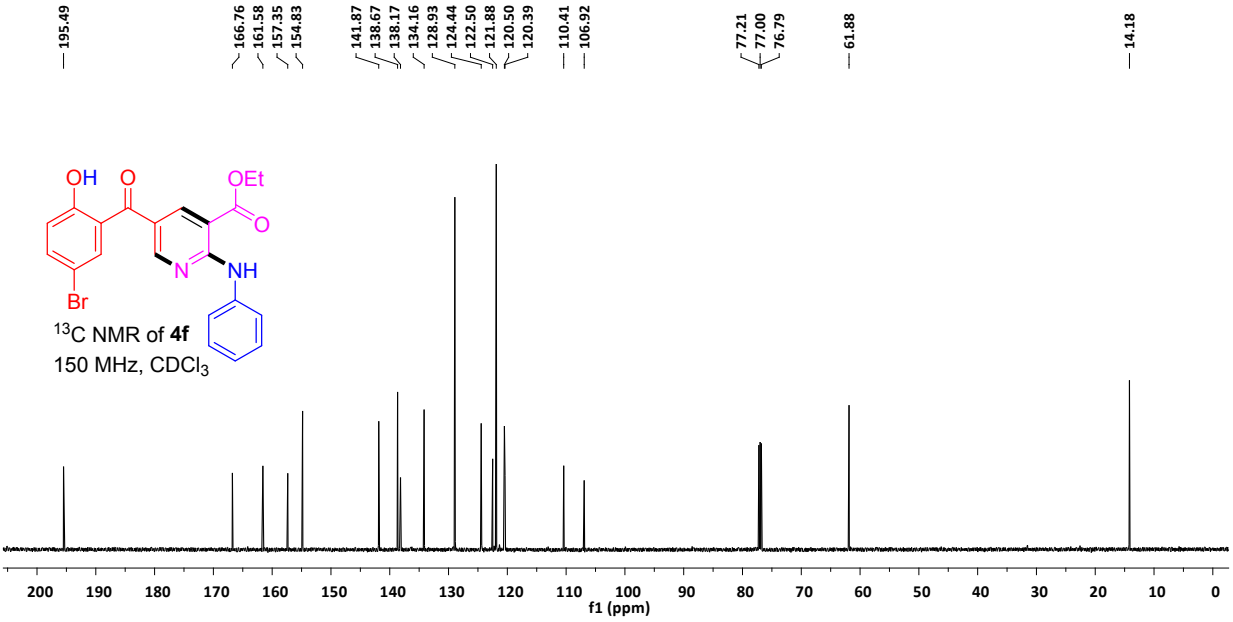
O
OEt
O
N
NH
Br
1H NMR of 4f
600 MHz, CDCl3
0.94
0.99
0.98
0.94
1.03
1.99
1.00
2.05
0.99
0.98
2.06
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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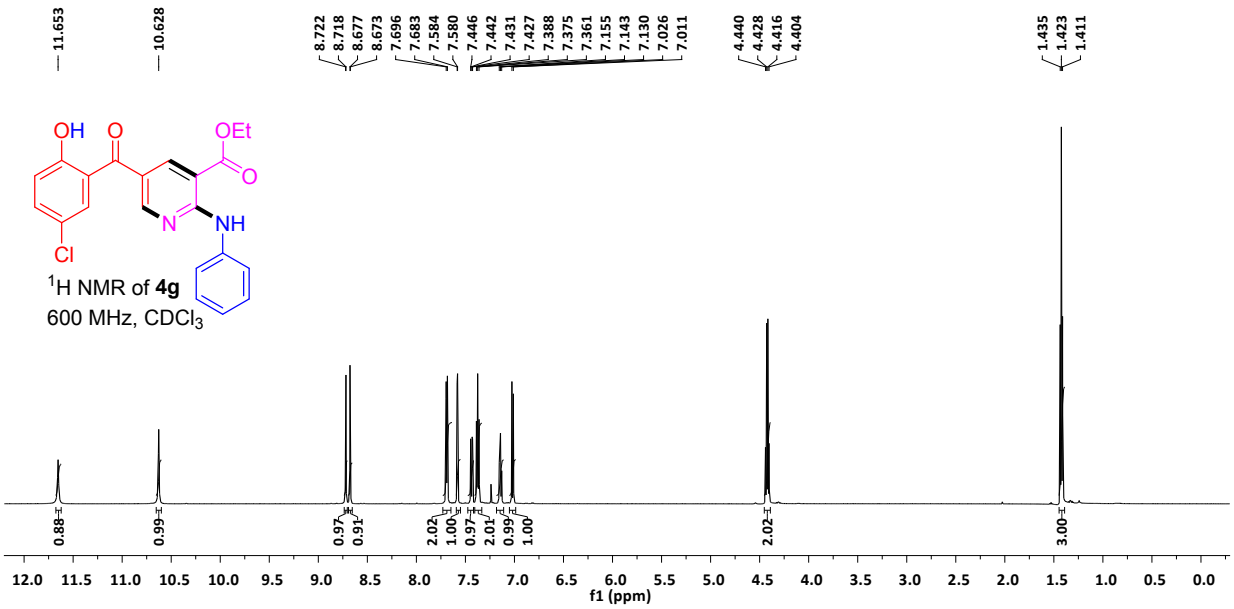
120.50
120.39
110.41
106.92
77.21
77.00
76.79
61.88
14.18
OH
O
OEt
O
N
NH
Br
13C NMR of 4f
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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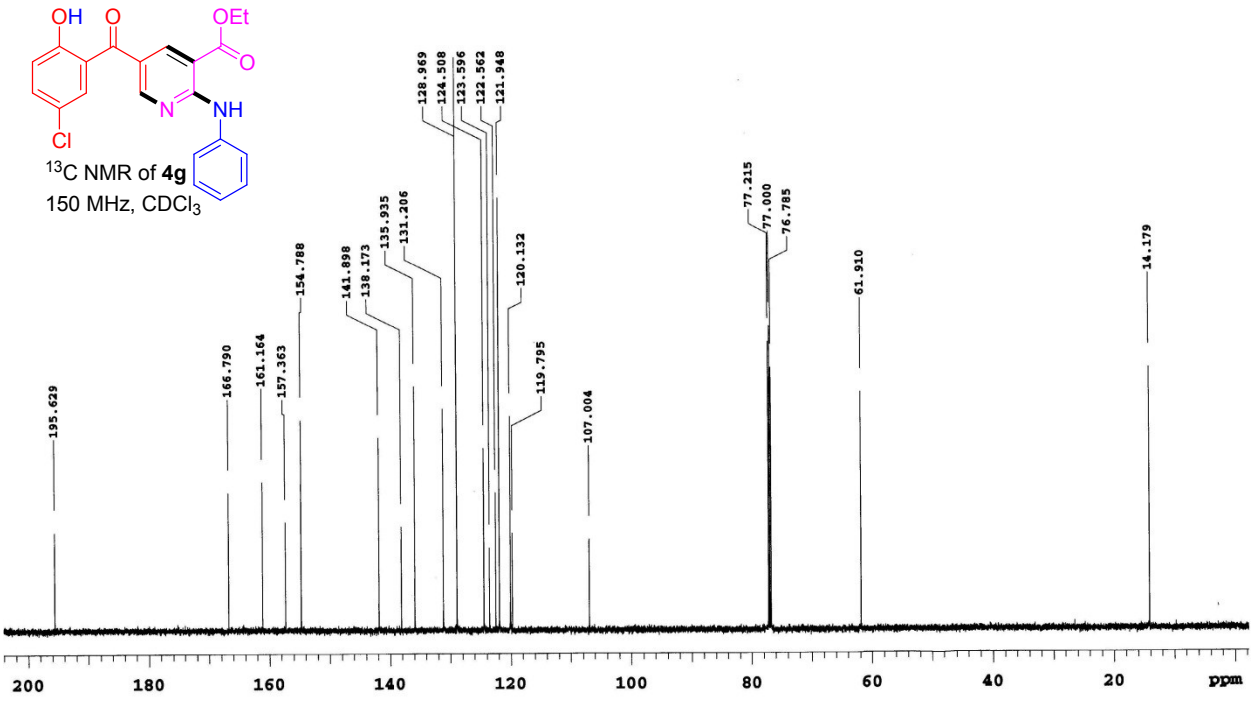
7.026
7.011
4.440
4.428
4.416
4.404
1.435
1.423
1.411
OH
O
OEt
O
N
NH
Cl
1H NMR of 4g
600 MHz, CDCl3
0.88
0.99
0.97
0.91
2.02
1.00
0.97
2.01
0.99
1.00
2.02
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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OEt
O
N
NH
Cl
13C NMR of 4g
150 MHz, CDCl3
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154.788
141.898
138.173
135.935
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128.969
124.508
123.596
122.562
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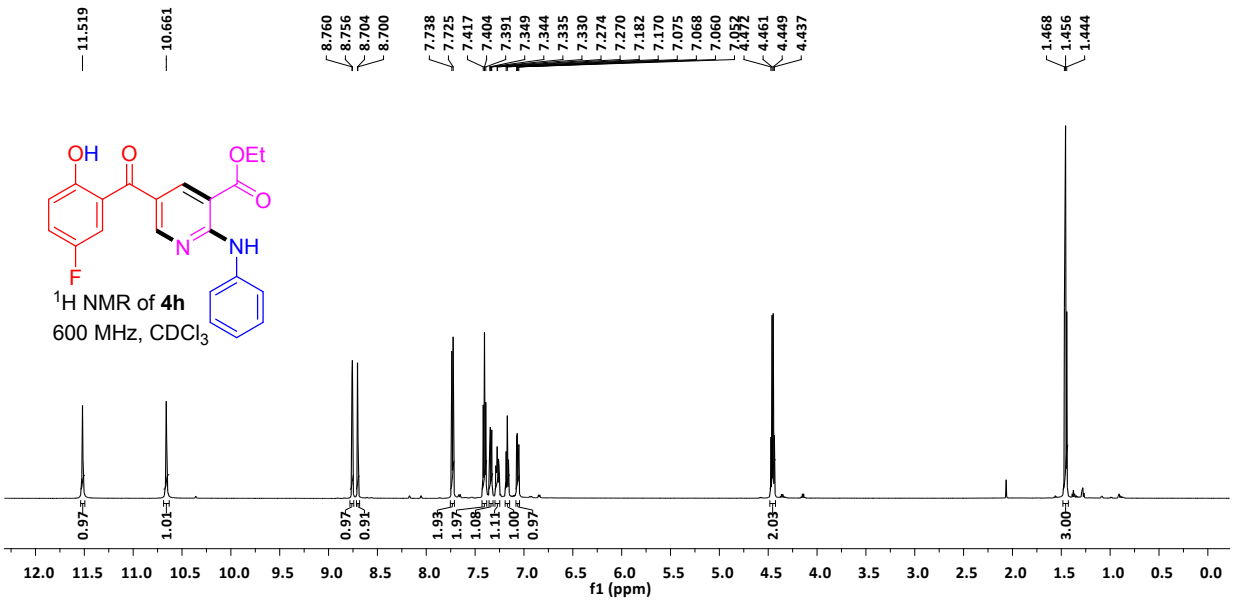
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7.344
7.335
7.330
7.274
7.270
7.182
7.170
7.075
7.068
7.060
7.052
4.472
4.461
4.449
4.437
1.468
1.456
1.444
OH
O
OEt
O
N
NH
F
1H NMR of 4h
600 MHz, CDCl3
0.97
1.01
0.97
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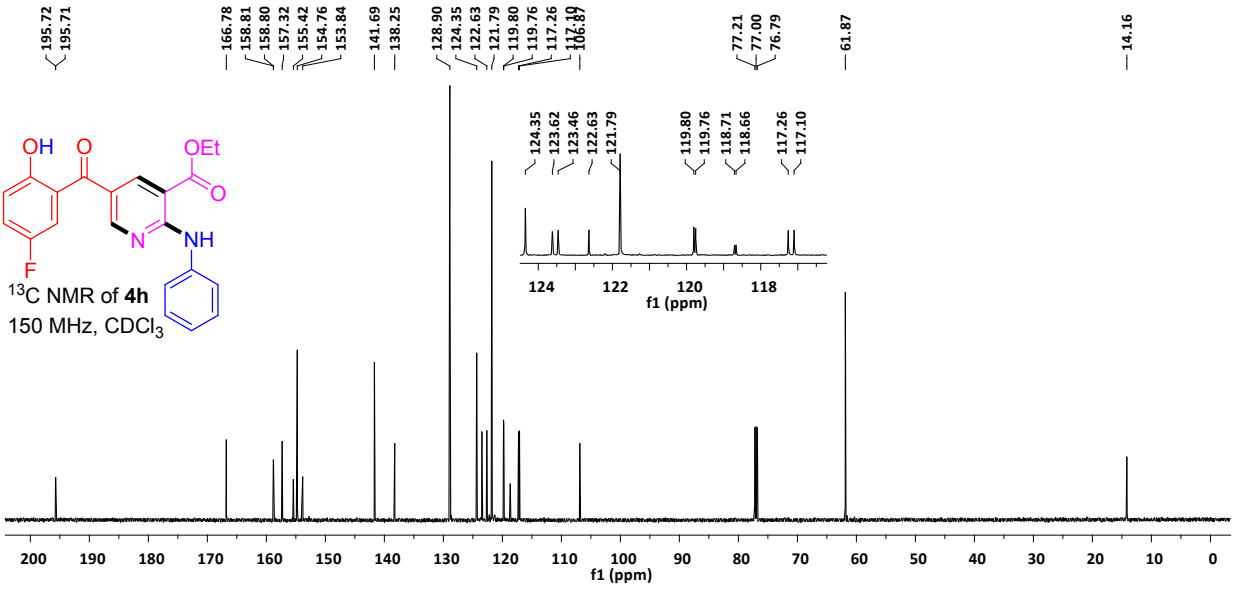
1.08
1.11
1.00
0.97
2.03
3.00
f1 (ppm)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122.63
121.79
119.80
119.76
117.26
77.21
77.00
76.79
61.87
14.16
124.35
123.62
123.46
122.63
121.79
119.80
119.76
118.71
118.66
117.26
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OH
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OEt
O
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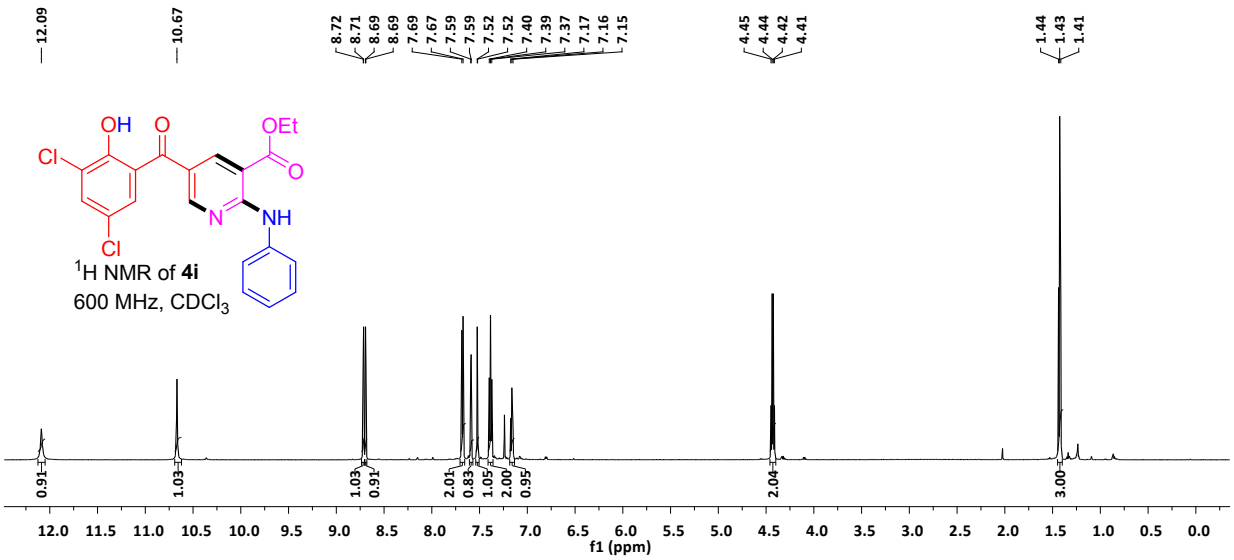
NH
F
13C NMR of 4h
150 MHz, CDCl3
f1 (ppm)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Cl
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600 MHz, CDCl3
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1.03
0.91
2.01
0.83
1.05
2.00
0.95
2.04
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 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
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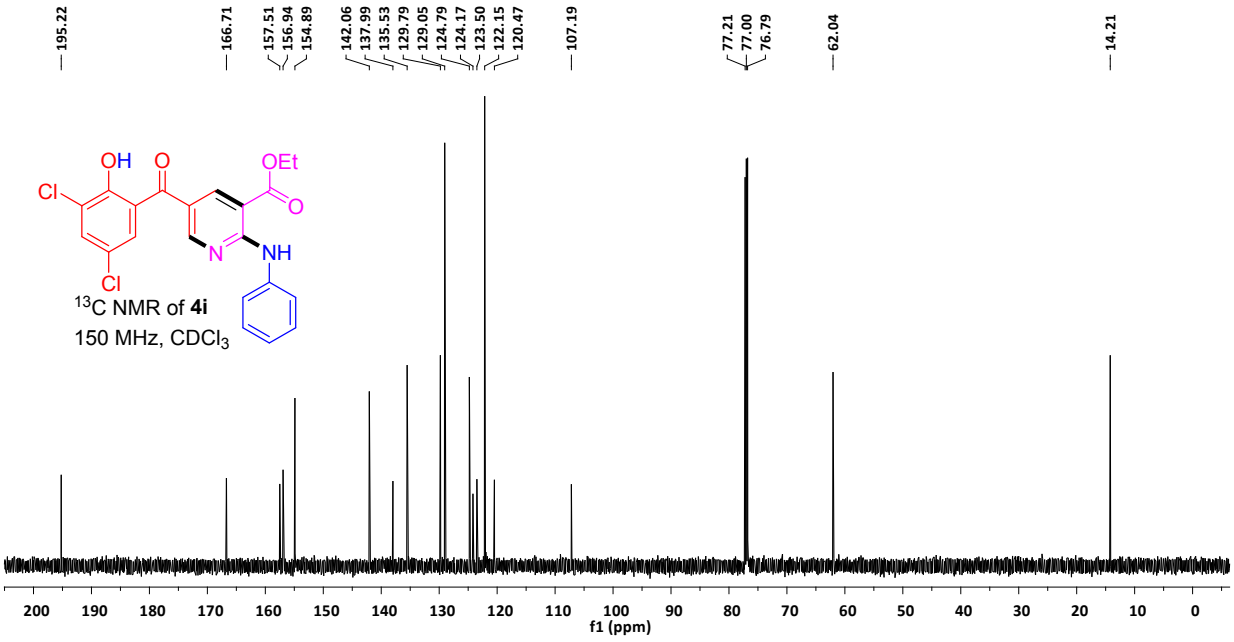
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122.15
120.47
107.19
77.21
77.00
76.79
62.04
14.21
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O
OEt
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Cl
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150 MHz, CDCl3
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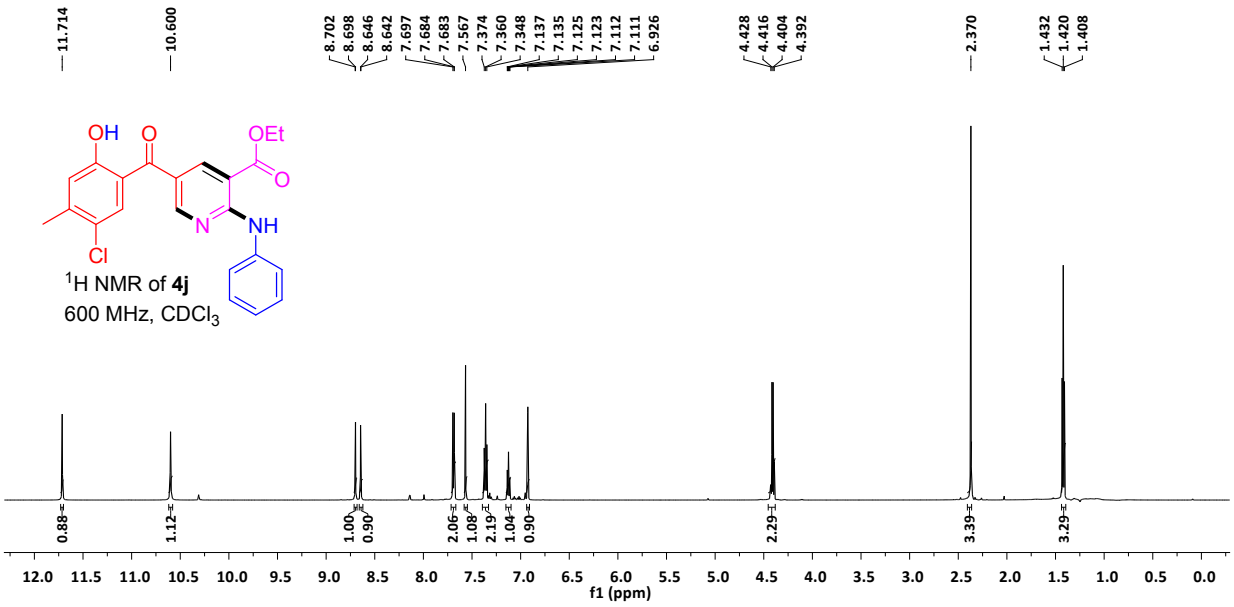
f1 (ppm)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7.137
7.135
7.125
7.123
7.112
7.111
6.926
4.428
4.416
4.404
4.392
2.370
1.432
1.420
1.408
OH
O
OEt
O
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NH
Cl
1H NMR of 4j
600 MHz, CDCl3
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2.29
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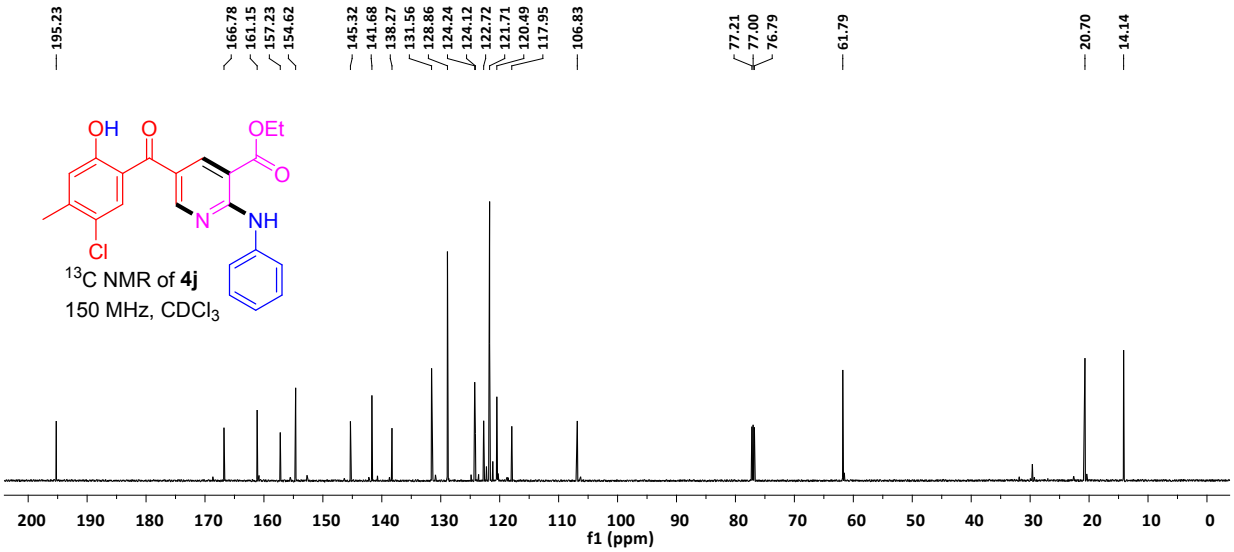
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121.71
120.49
117.95
106.83
77.21
77.00
76.79
61.79
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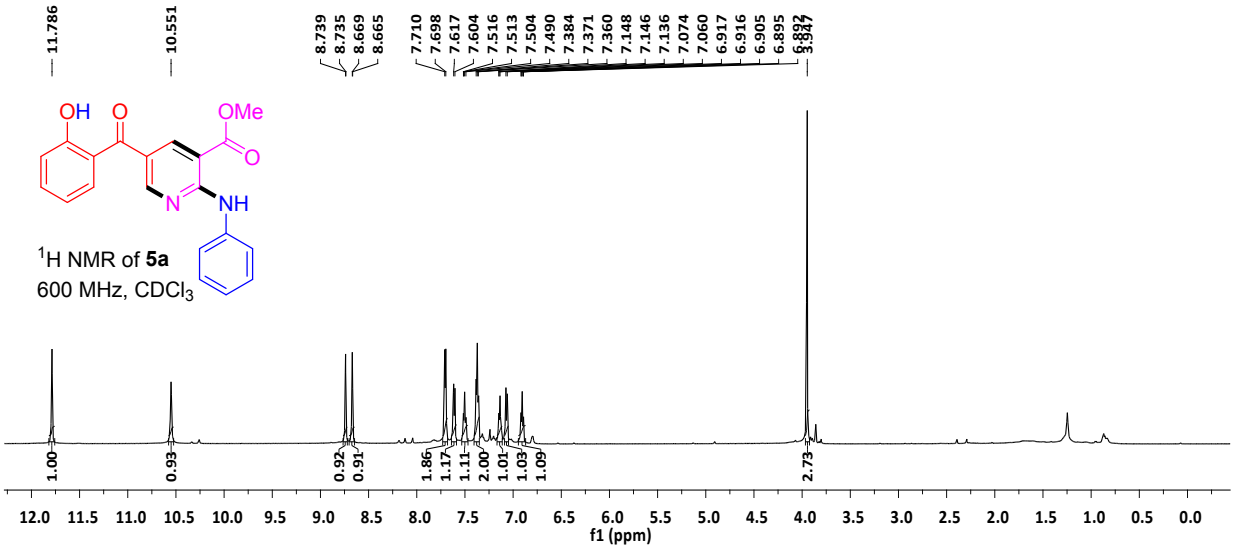
OEt
O
N
NH
Cl
13C NMR of 4j
150 MHz, CDCl3
f1 (ppm)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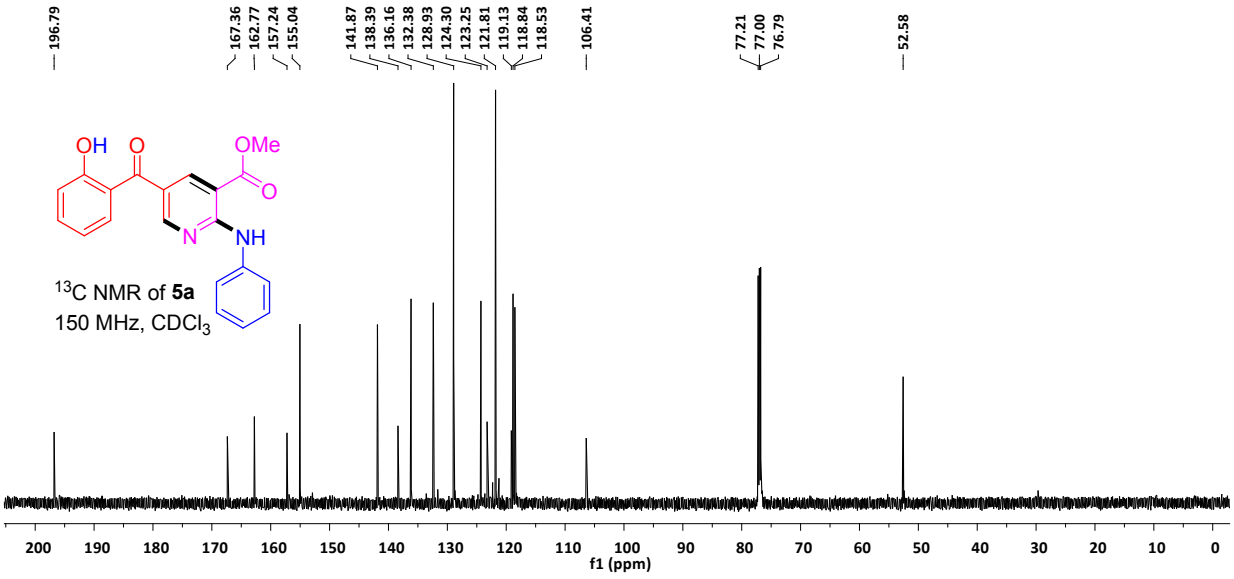
7.371
7.360
7.148
7.146
7.136
7.074
7.060
6.917
6.916
6.905
6.895
3.947
OH
O
OMe
O
N
NH
1H NMR of 5a
600 MHz, CDCl3
1.00
0.93
0.92
0.91
1.86
1.17
1.11
2.00
1.01
1.03
1.09
2.73
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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167.36
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123.25
121.81
119.13
118.84
118.53
106.41
77.21
77.00
76.79
52.58
OH
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OMe
O
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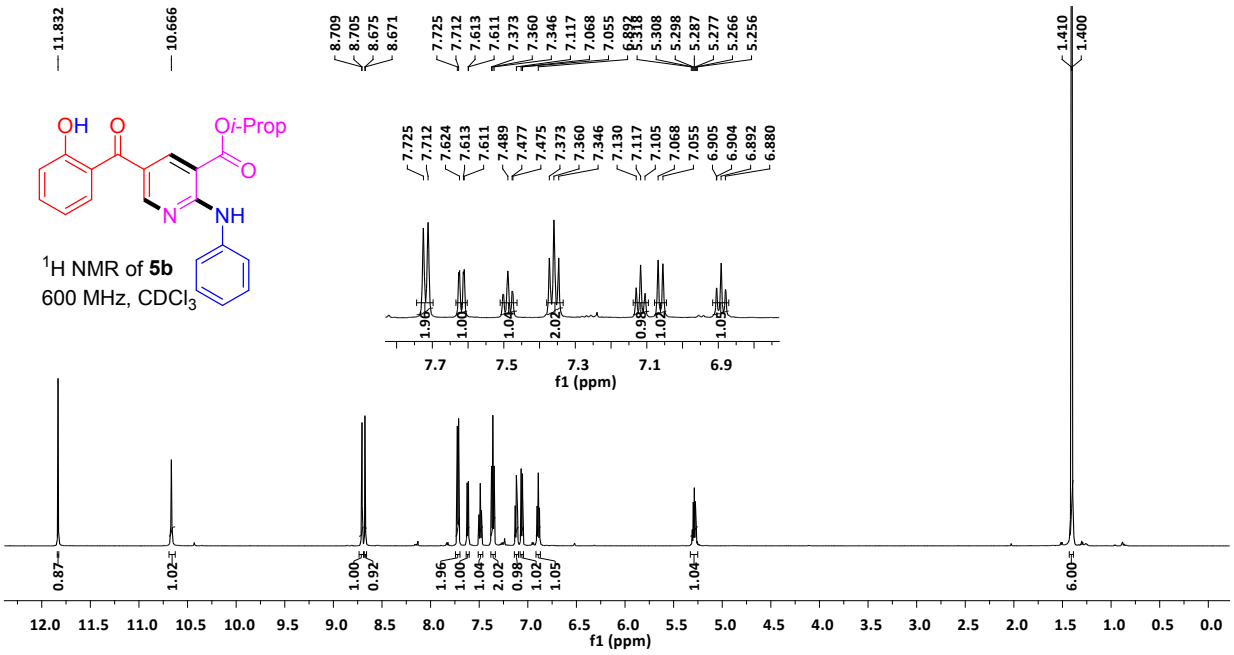
NH
13C NMR of 5a
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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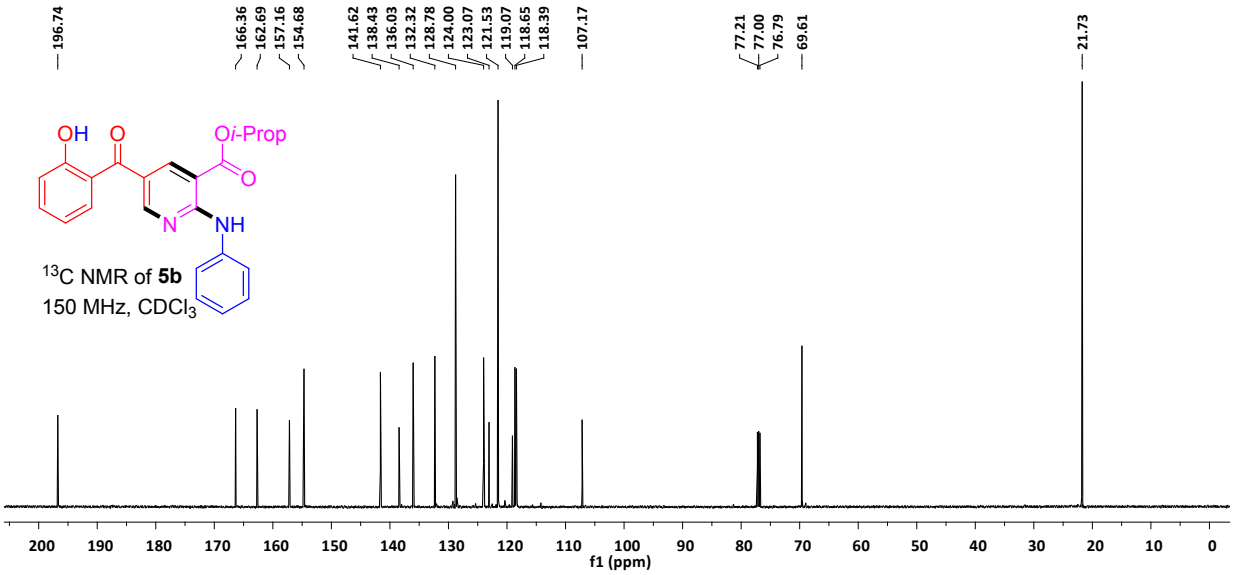
O*i*-Prop
O
N
NH
^{1}H NMR of **5b**
600 MHz, $CDCl_3$
f1 (ppm)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NH
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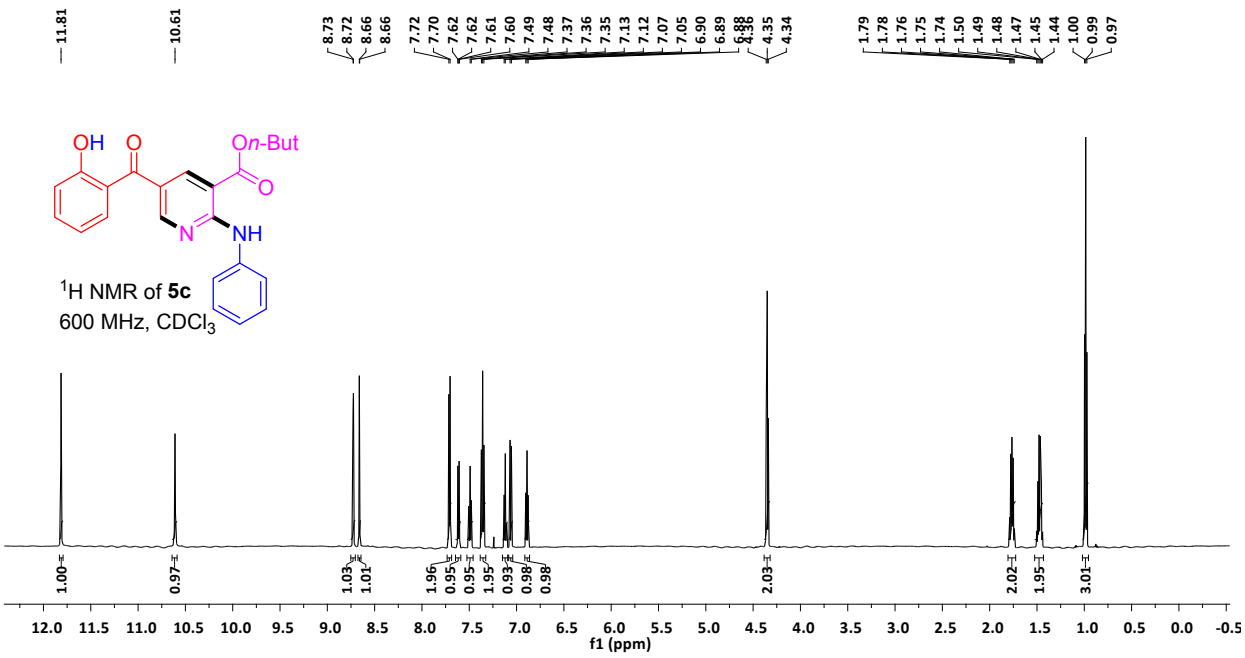
150 MHz, $CDCl_3$
f1 (ppm)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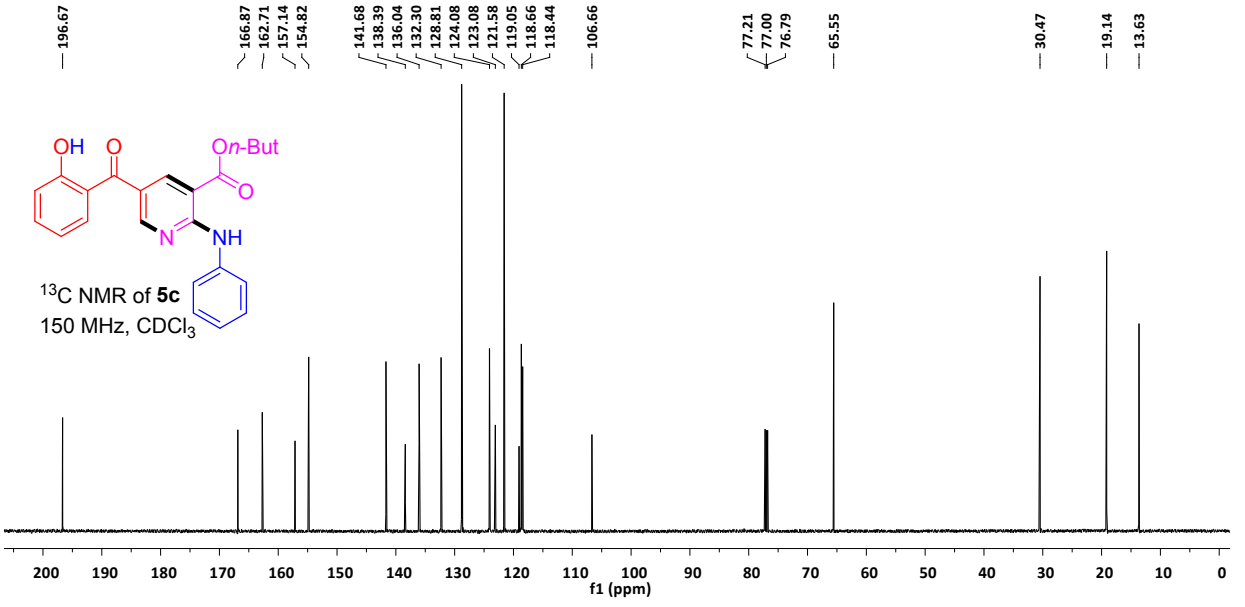
O
On-But
O
N
NH
1H NMR of 5c
600 MHz, CDCl3
f1 (ppm)


OH
O
On-But
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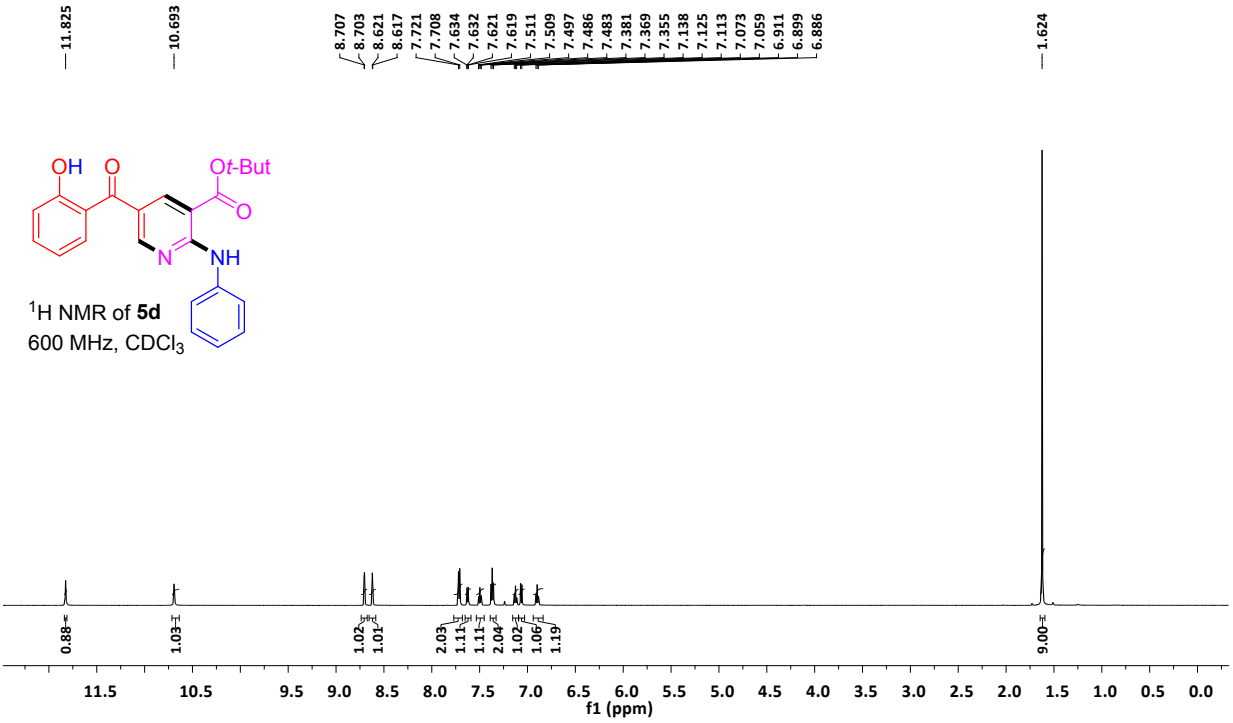
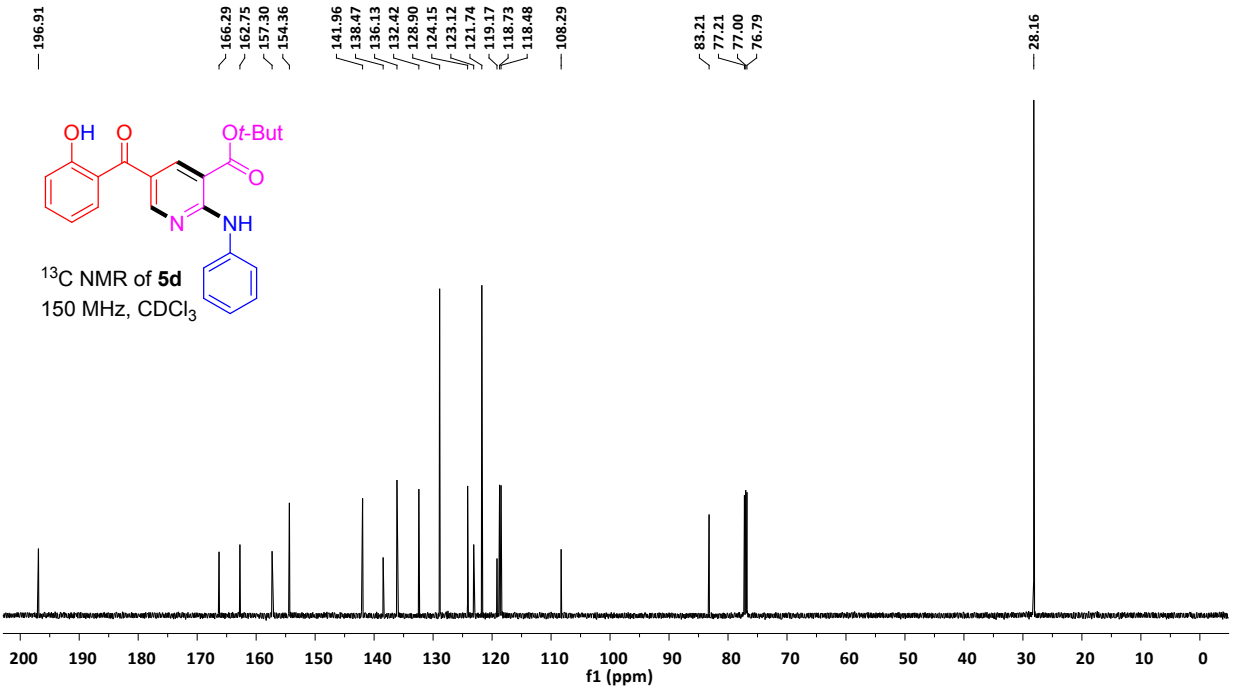
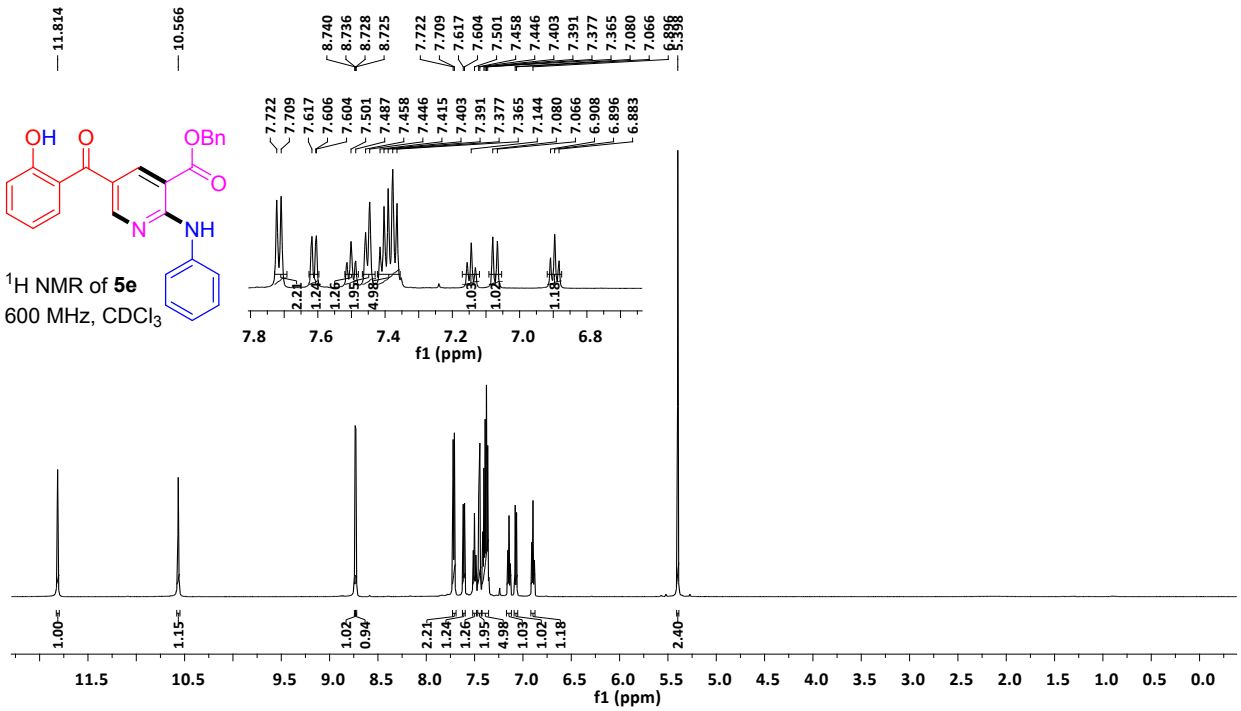
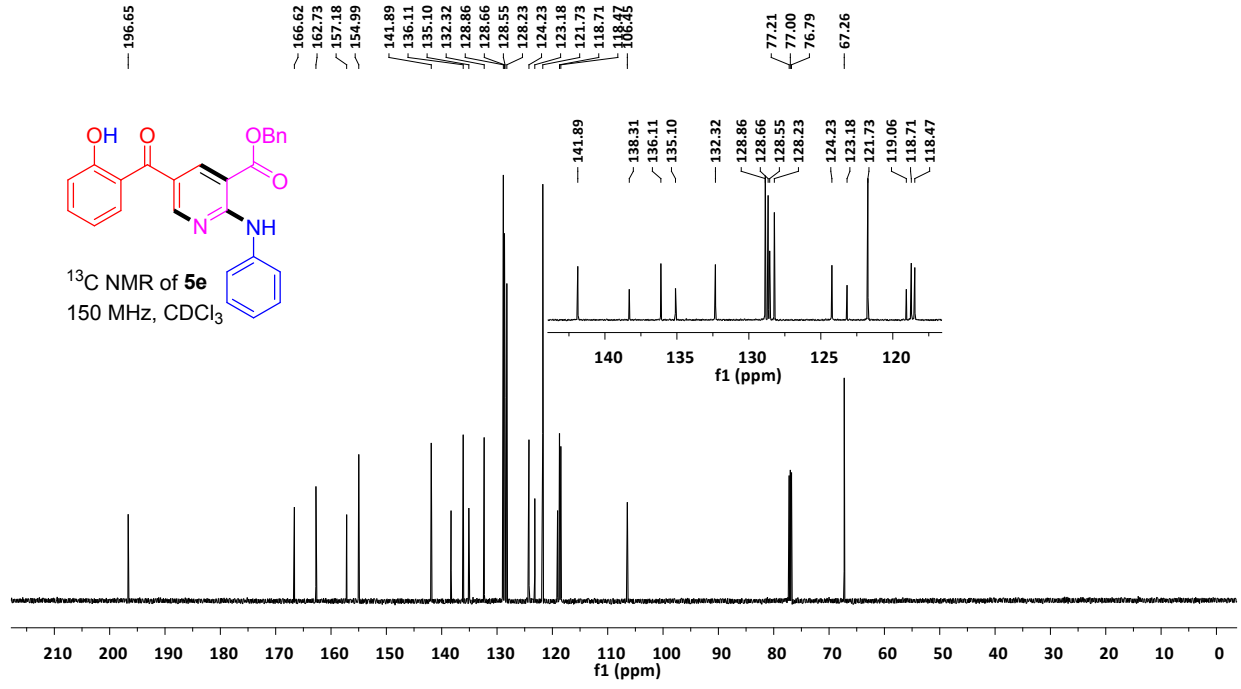
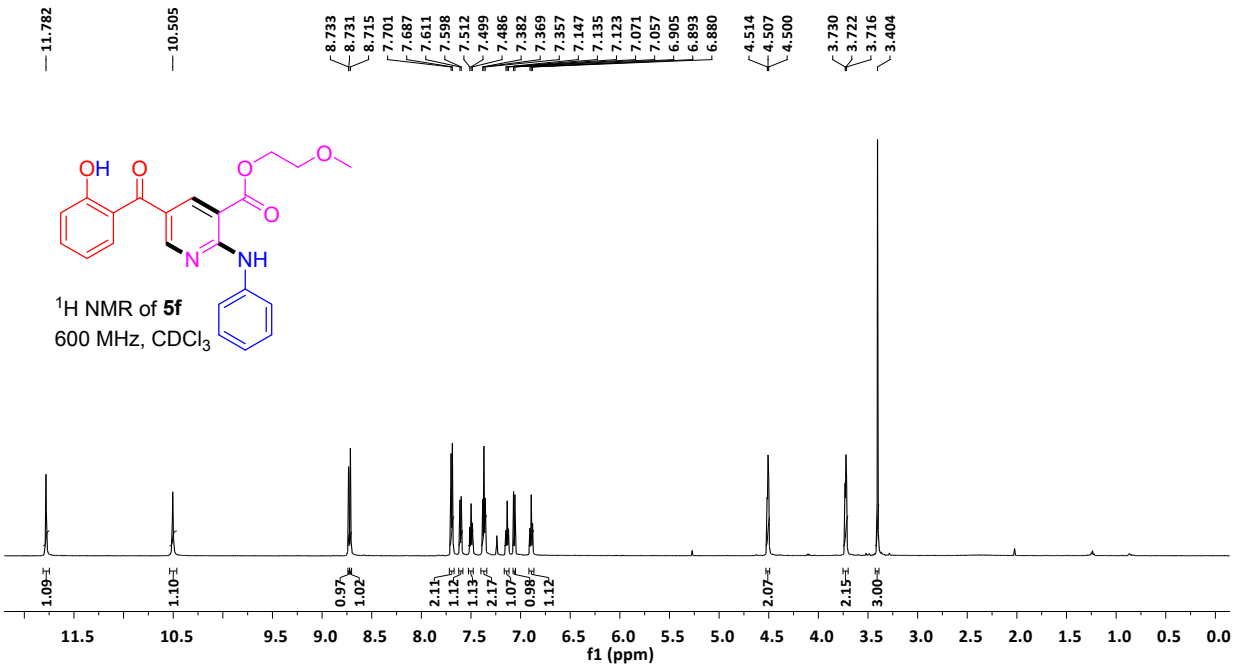
N
NH
13C NMR of 5c
150 MHz, CDCl3
f1 (ppm)

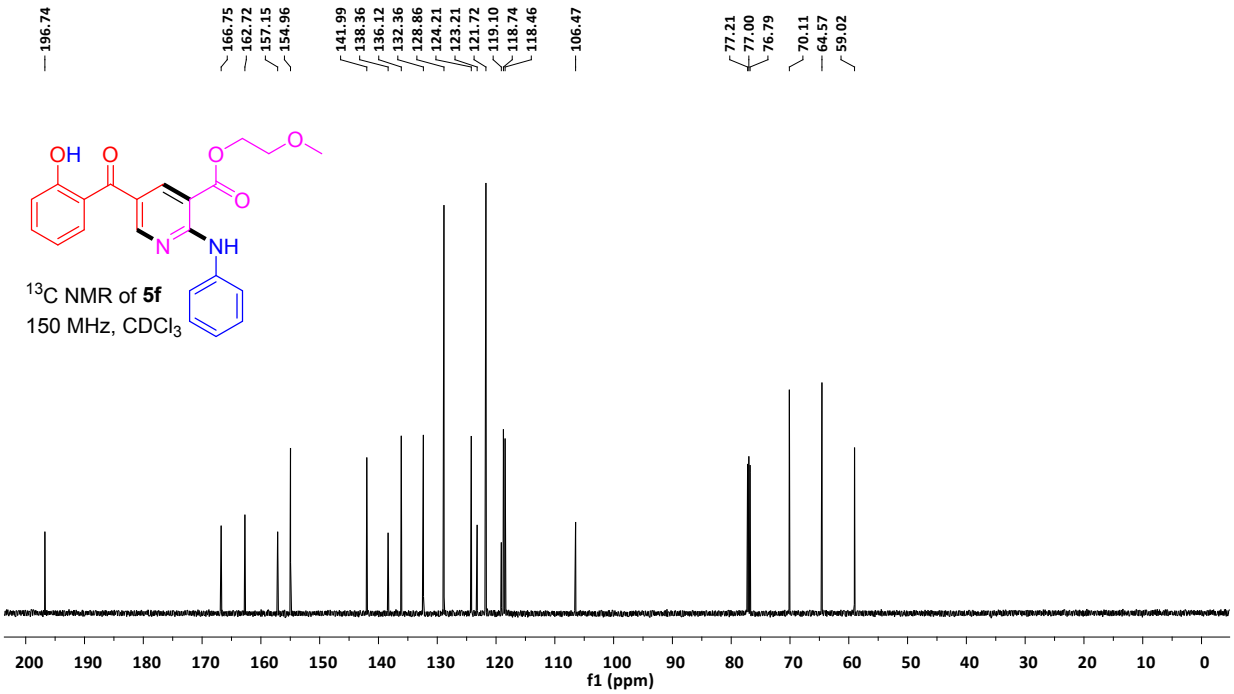

11.825
10.693
8.707
8.703
8.621
8.617
7.721
7.708
7.634
7.632
7.621
7.619
7.511
7.509
7.497
7.486
7.483
7.381
7.369
7.355
7.138
7.125
7.113
7.073
7.059
6.911
6.899
6.886
1.624
OH
O
Ot-But
O
N
NH
1H NMR of 5d
600 MHz, CDCl3
0.88
1.03
1.02
1.01
2.03
1.15
1.11
2.04
1.02
1.06
1.19
9.00
11.5
10.5
9.5
9.0
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)

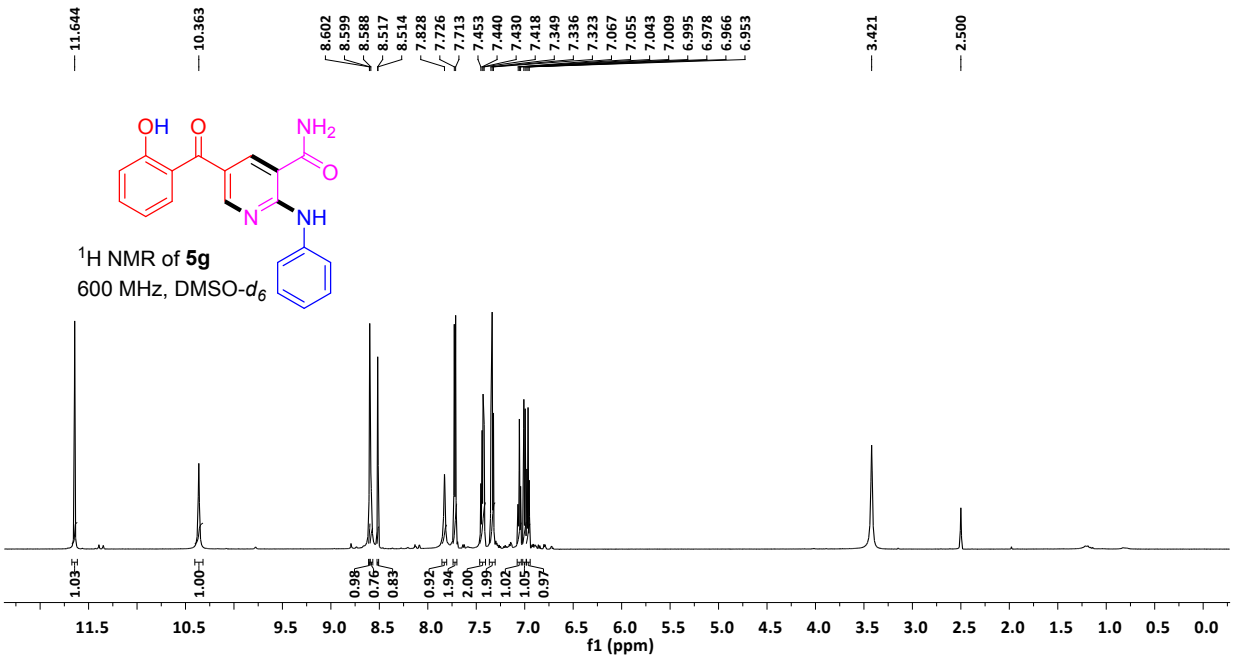

196.91
166.29
162.75
157.30
154.36
141.96
138.47
136.13
132.42
128.90
124.15
123.12
121.74
119.17
118.73
118.48
108.29
83.21
77.21
77.00
76.79
28.16
OH
O
Ot-But
O
N
NH
13C NMR of 5d
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

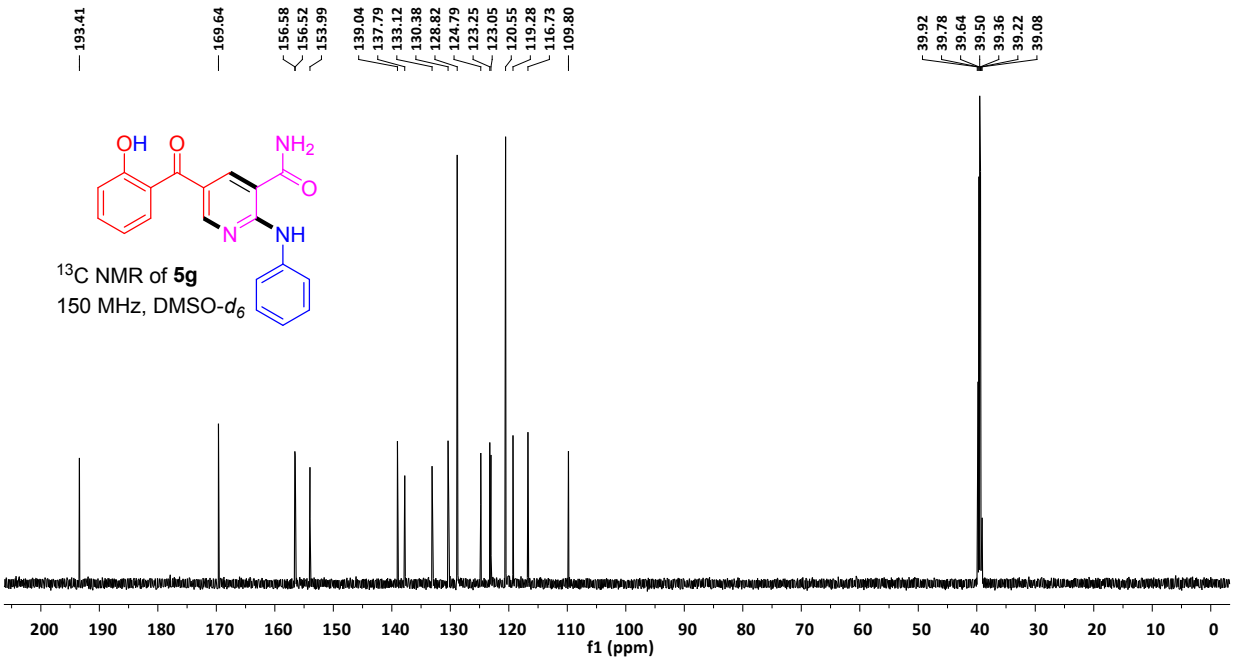

11.814
10.566
8.740
8.736
8.728
8.725
7.722
7.709
7.617
7.604
7.501
7.458
7.446
7.403
7.391
7.377
7.365
7.080
7.066
6.896
6.883
5.398
OH
O
OBn
O
N
NH
1H NMR of 5e
600 MHz, CDCl3
7.8
7.6
7.4
7.2
7.0
6.8
f1 (ppm)
1.00
1.15
1.02
0.94
2.21
1.24
1.26
1.95
4.98
1.03
1.02
1.18
2.40
11.5
10.5
9.5
9.0
8.5
8.0
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)

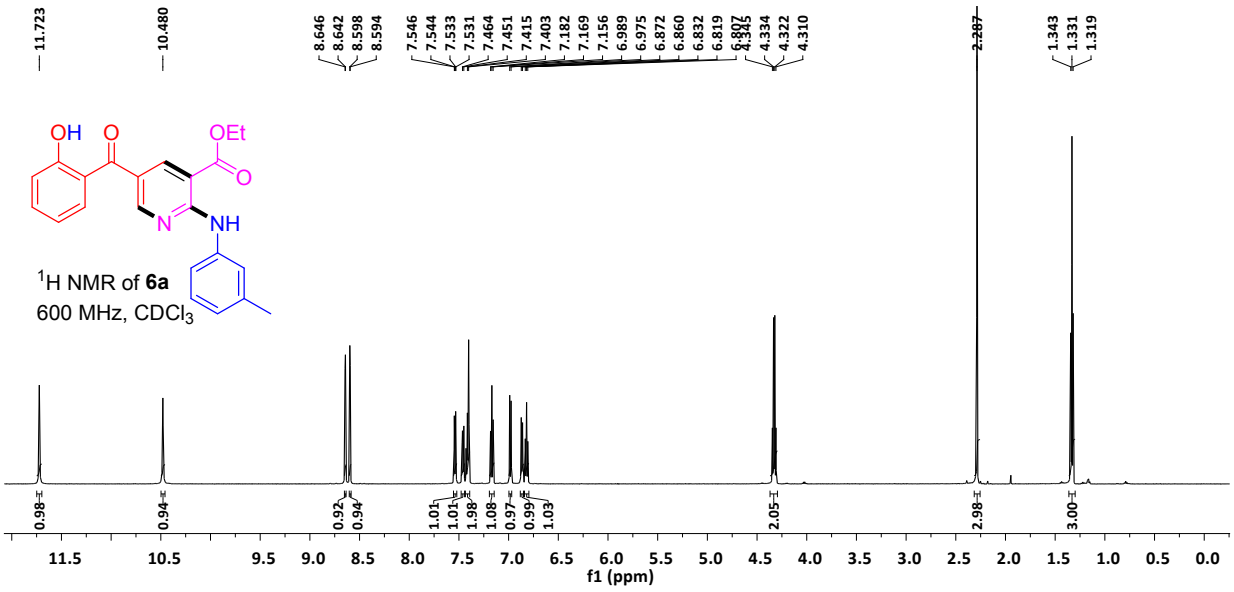

196.65
166.62
162.73
157.18
154.99
141.89
136.11
135.10
132.32
128.86
128.66
128.55
128.23
124.23
123.18
121.73
118.71
118.47
77.21
77.00
76.79
67.26
OH
O
OBn
O
N
NH
13C NMR of 5e
150 MHz, CDCl3
140
135
130
125
120
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

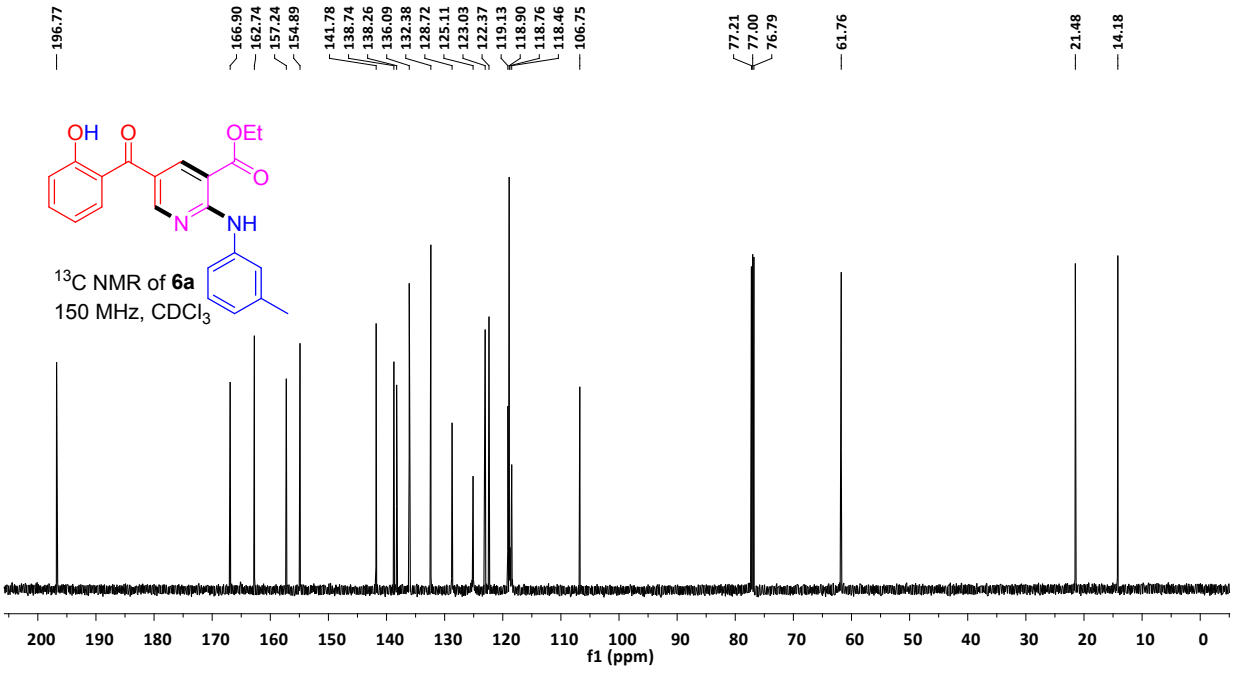

11.782
10.505
8.733
8.731
8.715
7.701
7.687
7.611
7.598
7.512
7.499
7.486
7.382
7.369
7.357
7.147
7.135
7.123
7.071
7.057
6.905
6.893
6.880
4.514
4.507
4.500
3.730
3.722
3.716
3.404
OH
O
O
O
N
NH
1H NMR of 5f
600 MHz, CDCl3
1.09
1.10
0.97
1.02
2.11
1.12
1.13
2.17
1.07
0.98
1.12
2.07
2.15
3.00
11.5
10.5
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)

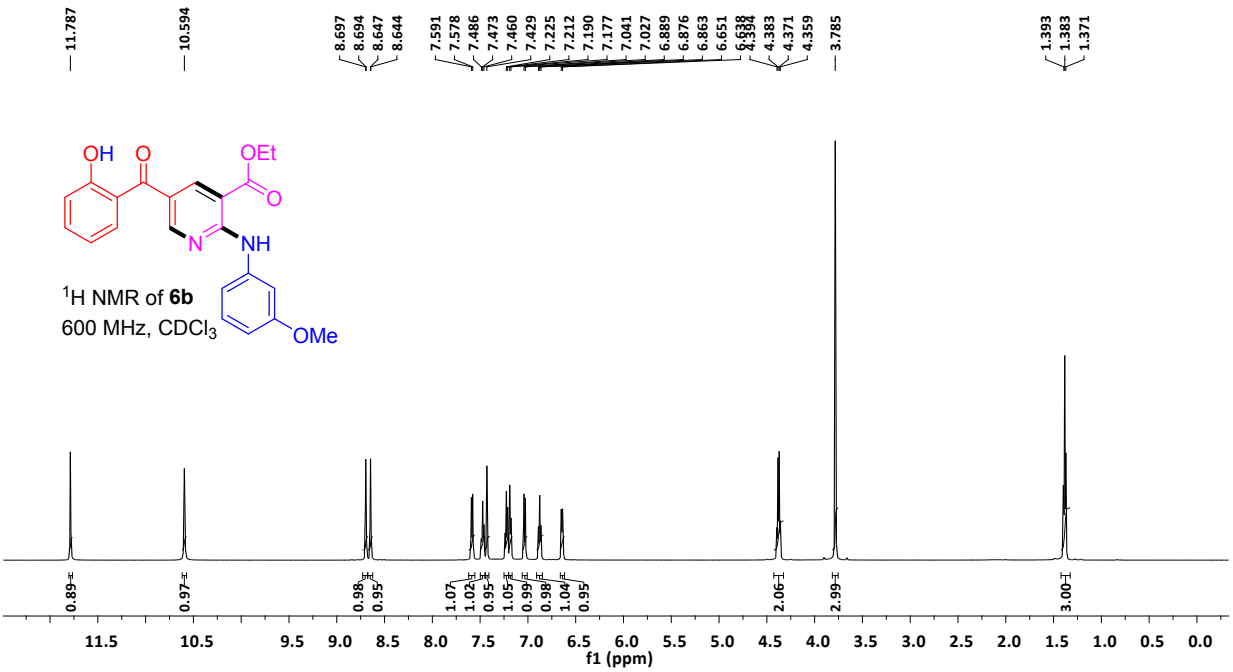

196.74
166.75
162.72
157.15
154.96
141.99
138.36
136.12
132.36
128.86
124.21
123.21
121.72
119.10
118.74
118.46
106.47
77.21
77.00
76.79
70.11
64.57
59.02
OH
O
O
O
N
NH
13C NMR of 5f
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

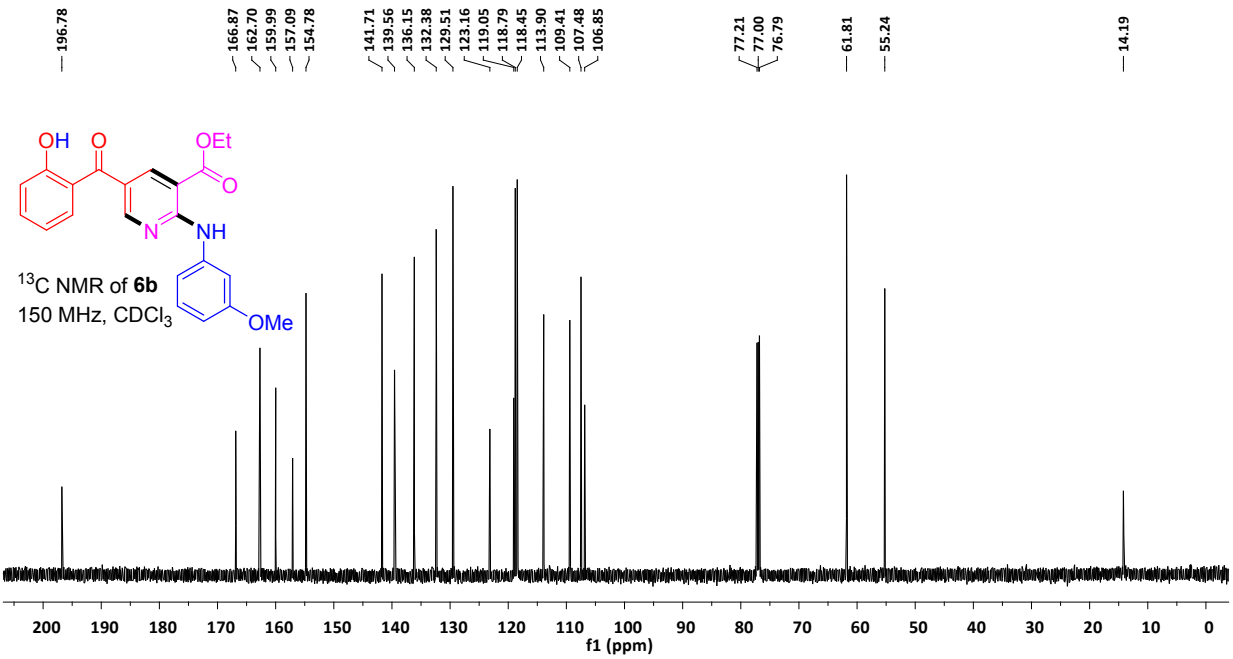

11.644
10.363
8.602
8.599
8.588
8.517
8.514
7.828
7.726
7.713
7.453
7.440
7.430
7.418
7.349
7.336
7.323
7.067
7.055
7.043
7.009
6.995
6.978
6.966
6.953
3.421
2.500
OH
O
NH2
O
N
NH
1H NMR of 5g
600 MHz, DMSO-d6
1.03
1.00
0.98
0.76
0.83
0.92
1.94
2.00
1.99
1.02
1.05
0.97
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
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)


193.41
169.64
156.58
156.52
153.99
139.04
137.79
133.12
130.38
128.82
124.79
123.25
123.05
120.55
119.28
116.73
109.80
39.92
39.78
39.64
39.50
39.36
39.22
39.08
OH
O
NH2
O
N
NH
13C NMR of 5g
150 MHz, DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.723
10.480
8.646
8.642
8.598
8.594
7.546
7.544
7.533
7.531
7.464
7.451
7.415
7.403
7.182
7.169
7.156
6.989
6.975
6.872
6.860
6.832
6.819
6.807
4.345
4.334
4.322
4.310
2.287
1.343
1.331
1.319
OH
O
OEt
O
N
NH
1H NMR of 6a
600 MHz, CDCl3
0.98
0.94
0.92
0.94
1.01
1.01
1.98
1.08
0.97
0.99
1.03
2.05
2.98
3.00
11.5
10.5
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)


196.77
166.90
162.74
157.24
154.89
141.78
138.74
138.26
136.09
132.38
128.72
125.11
123.03
122.37
119.13
118.90
118.76
118.46
106.75
77.21
77.00
76.79
61.76
21.48
14.18
OH
O
OEt
O
N
NH
13C NMR of 6a
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.787
10.594
8.697
8.694
8.647
8.644
7.591
7.578
7.486
7.473
7.460
7.429
7.225
7.212
7.190
7.177
7.041
7.027
6.889
6.876
6.863
6.651
4.383
4.371
4.359
3.785
1.393
1.383
1.371
OH
O
OEt
O
N
NH
OMe
1H NMR of 6b
600 MHz, CDCl3
0.89
0.97
0.98
0.95
1.07
1.02
0.95
1.05
0.99
0.98
1.04
0.95
2.06
2.99
3.00
11.5
10.5
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)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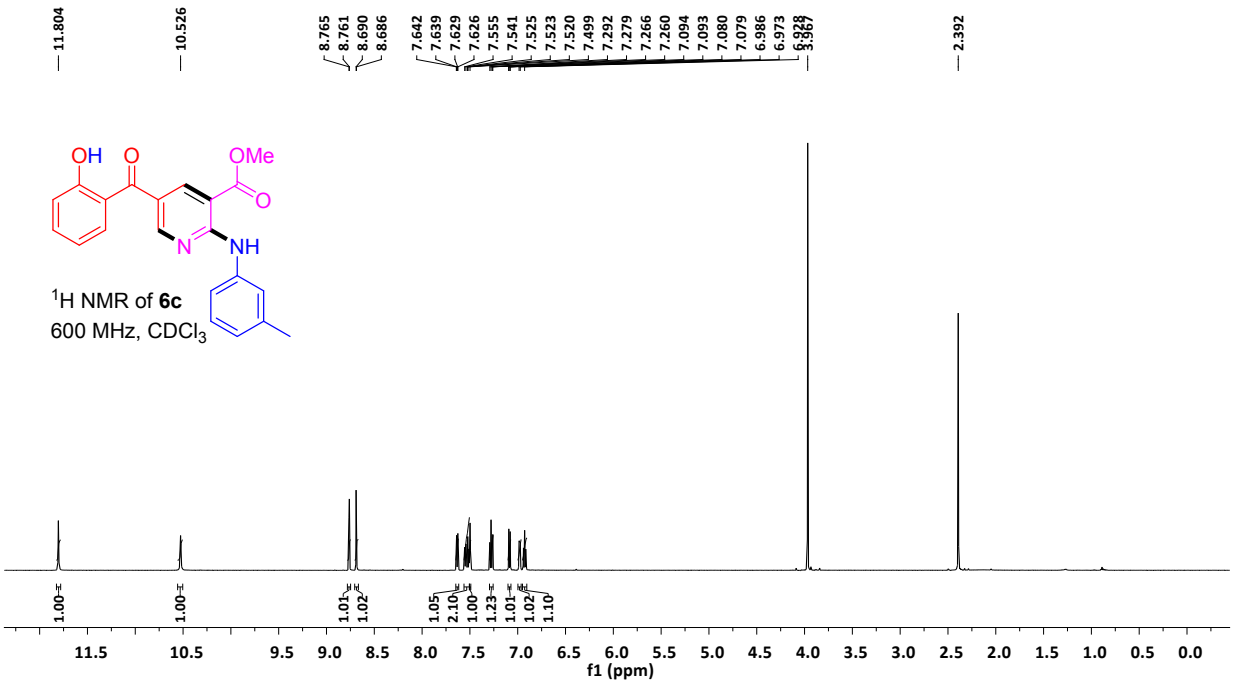
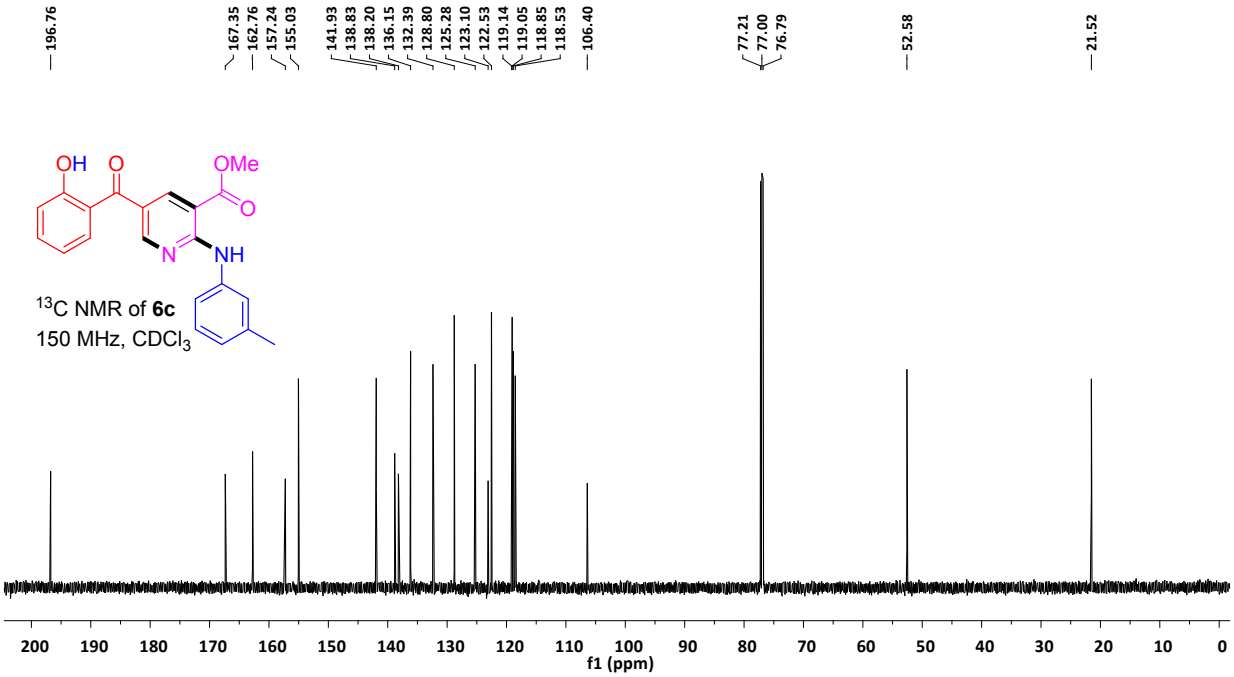
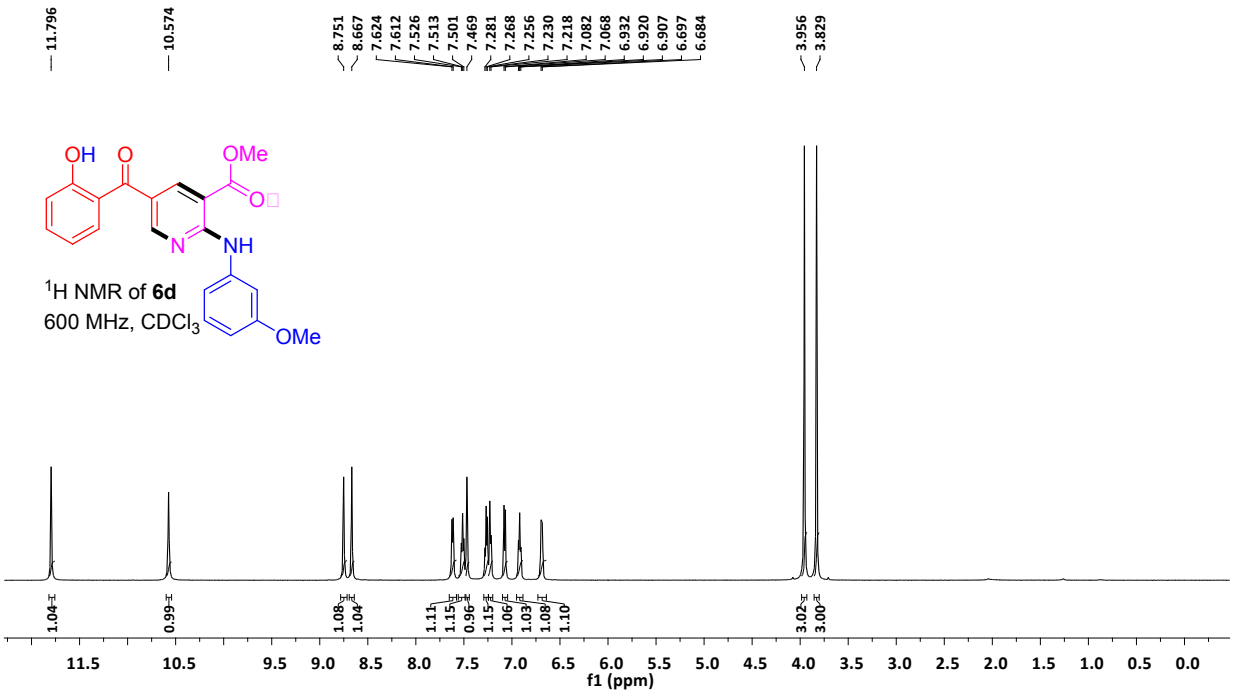
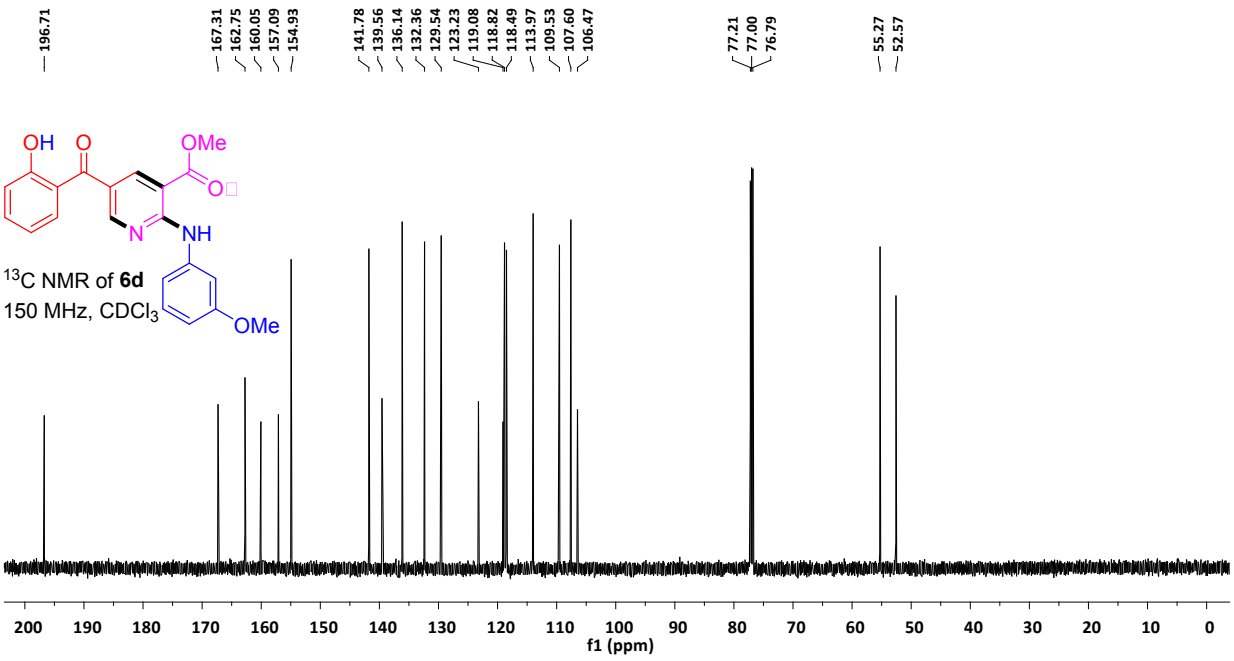
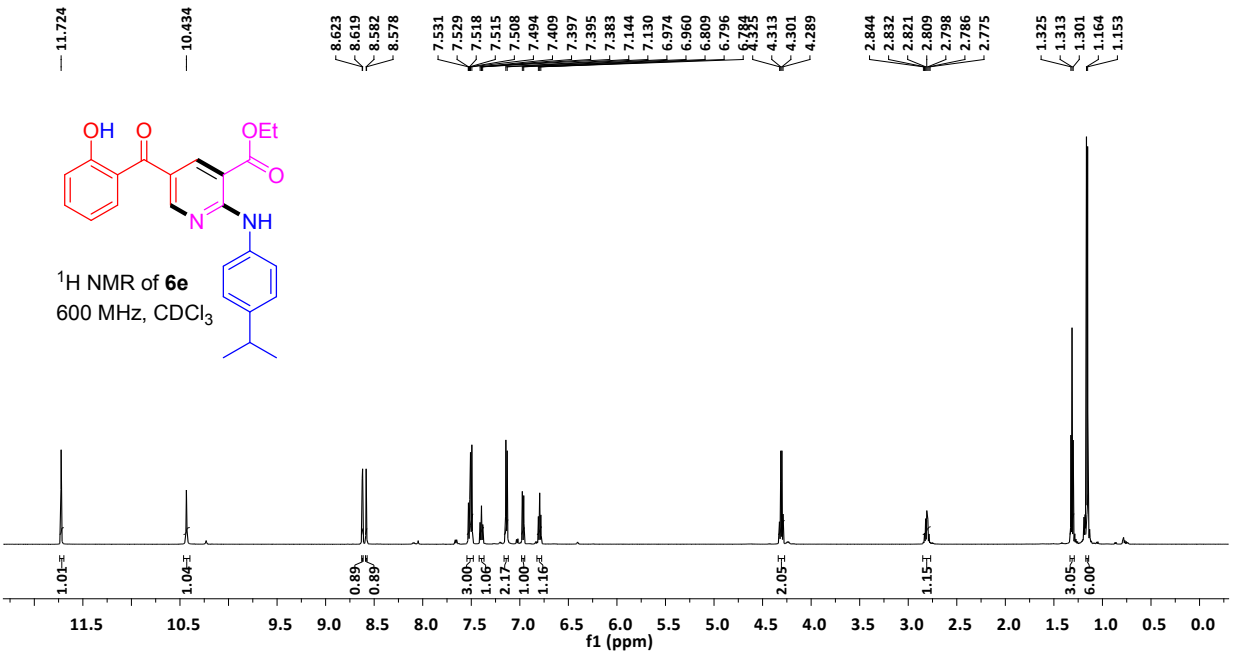
166.87
162.70
159.99
157.09
154.78
141.71
139.56
136.15
132.38
129.51
123.16
119.05
118.79
118.45
113.90
109.41
107.48
106.85
77.21
77.00
76.79
61.81
55.24
14.19
OH
O
OEt
O
N
NH
OMe
13C NMR of 6b
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

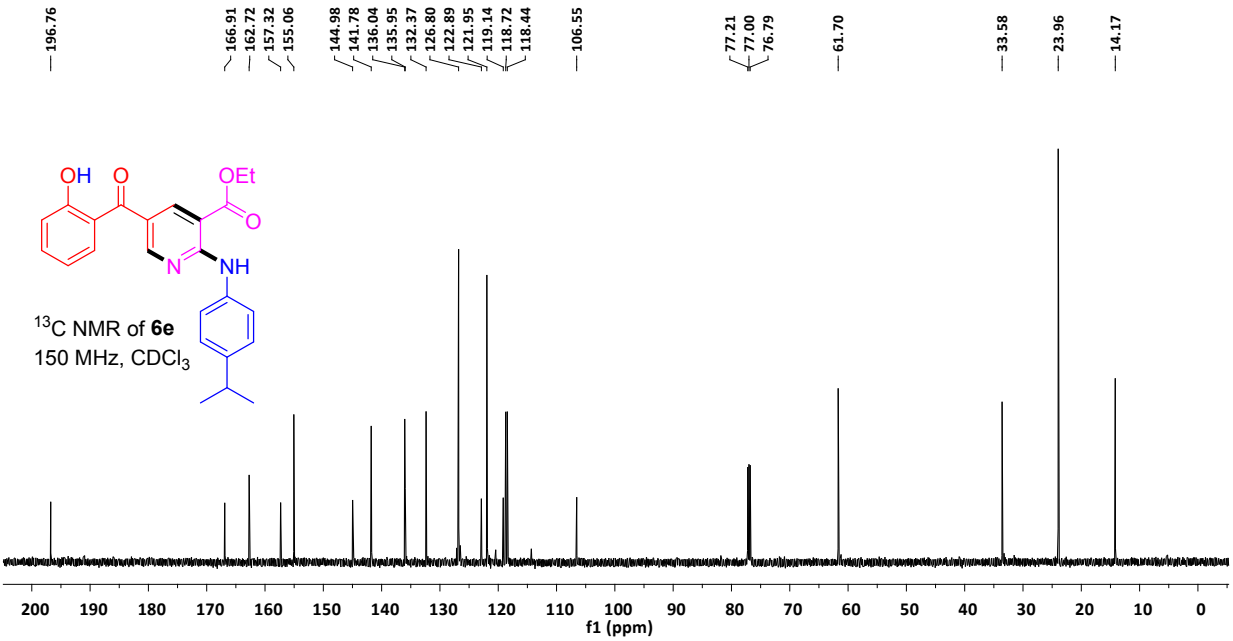

11.804
10.526
8.765
8.761
8.690
8.686
7.642
7.639
7.629
7.626
7.555
7.541
7.525
7.523
7.520
7.499
7.292
7.279
7.266
7.260
7.094
7.093
7.080
7.079
6.986
6.973
3.987
2.392
OH
O
OMe
O
N
NH
1H NMR of 6c
600 MHz, CDCl3
1.00
1.00
1.01
1.02
1.05
2.10
1.00
1.23
1.01
1.02
1.10
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
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)

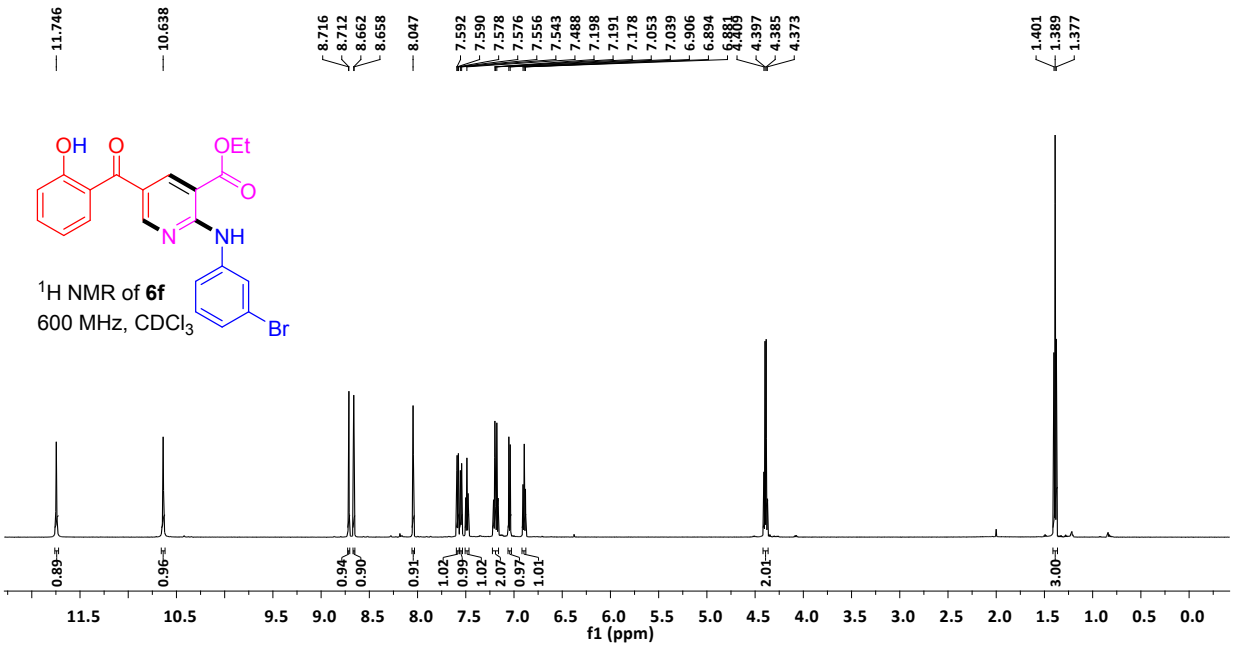

196.76
167.35
162.76
157.24
155.03
141.93
138.83
138.20
136.15
132.39
128.80
125.28
123.10
122.53
119.14
119.05
118.85
118.53
106.40
77.21
77.00
76.79
52.58
21.52
OH
O
OMe
O
N
NH
13C NMR of 6c
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

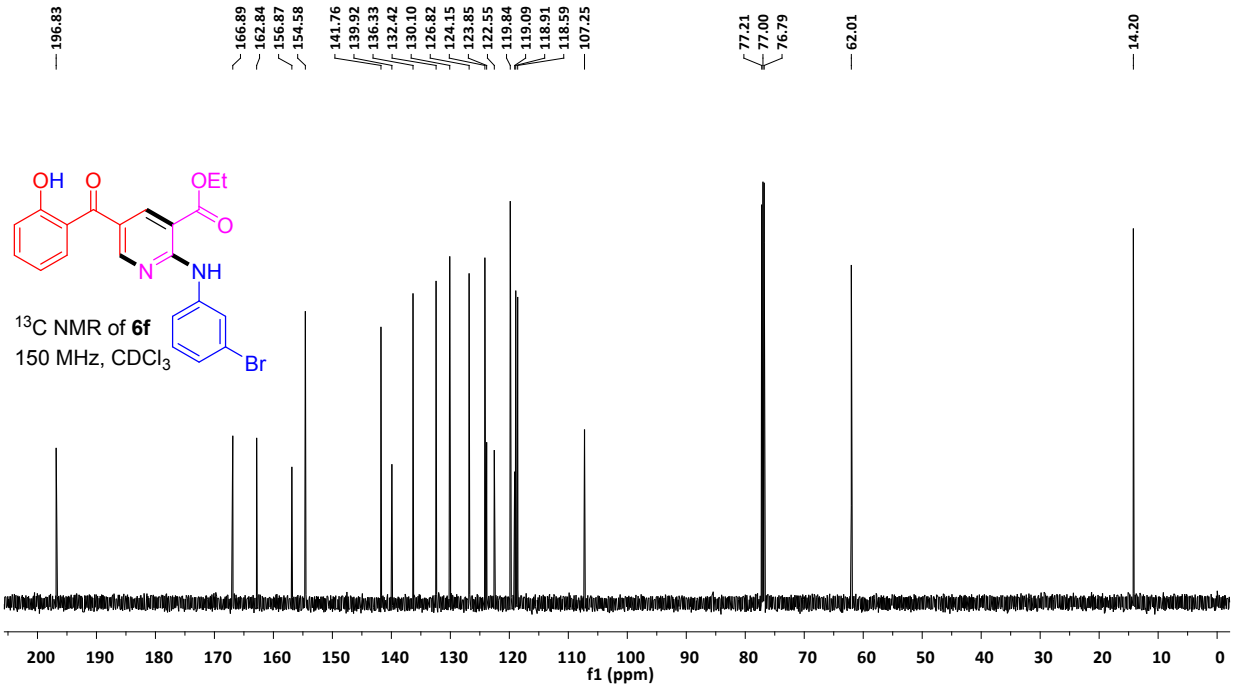

11.796
10.574
8.751
8.667
7.624
7.612
7.526
7.513
7.501
7.469
7.281
7.268
7.256
7.230
7.218
7.082
7.068
6.932
6.920
6.907
6.697
6.684
3.956
3.829
OH
O
OMe
O
N
NH
OMe
1H NMR of 6d
600 MHz, CDCl3
1.04
0.99
1.08
1.04
1.11
1.15
0.96
1.15
1.06
1.03
1.08
1.10
3.02
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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)

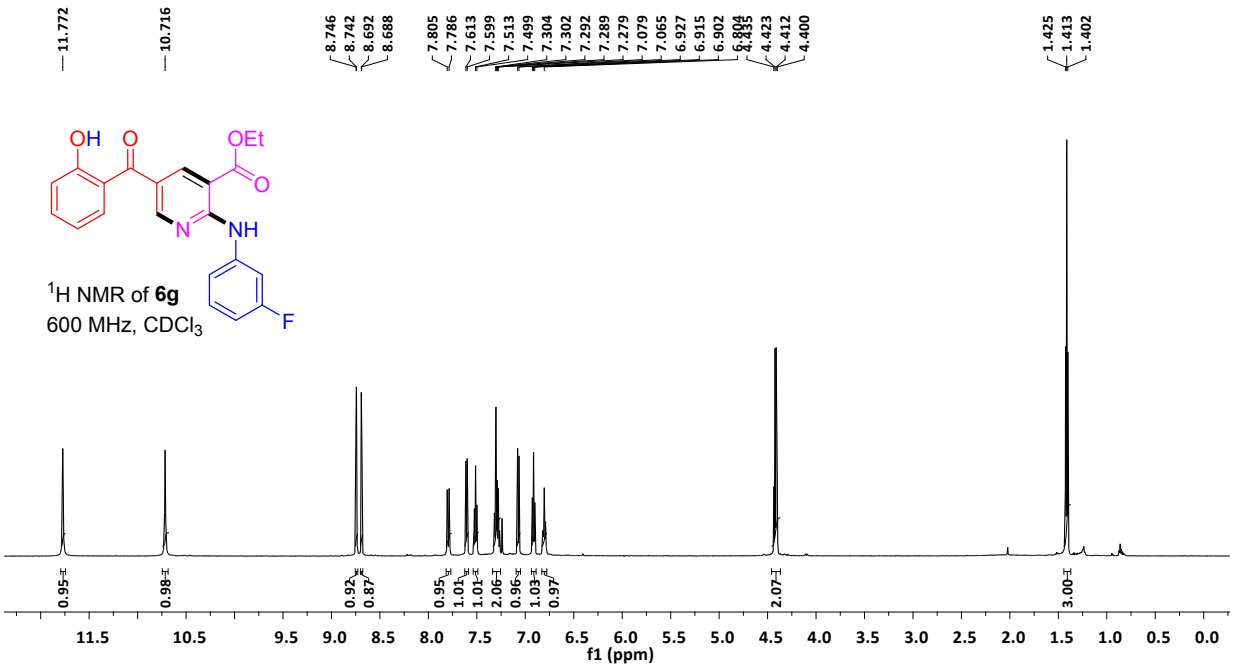

196.71
167.31
162.75
160.05
157.09
154.93
141.78
139.56
136.14
132.36
129.54
123.23
119.08
118.82
118.49
113.97
109.53
107.60
106.47
77.21
77.00
76.79
55.27
52.57
OH
O
OMe
O
N
NH
OMe
13C NMR of 6d
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

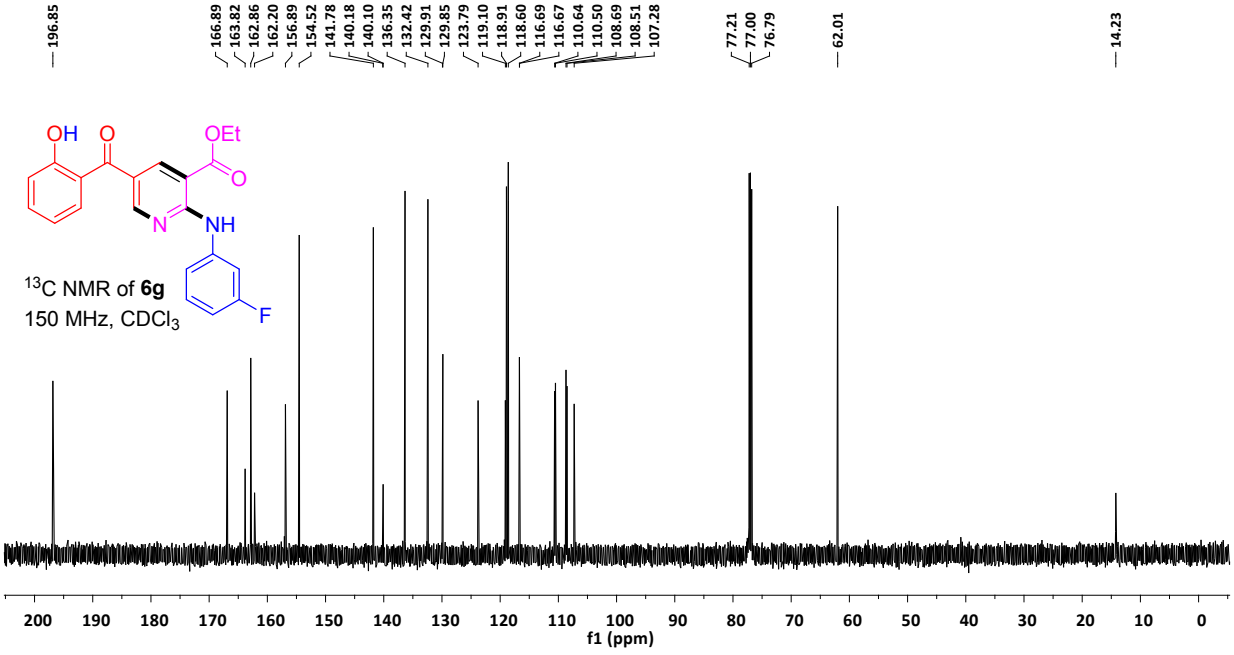

11.724
10.434
8.623
8.619
8.582
8.578
7.531
7.529
7.518
7.515
7.508
7.494
7.409
7.397
7.395
7.383
7.144
7.130
6.974
6.960
6.809
6.796
4.313
4.301
4.289
2.844
2.832
2.821
2.809
2.798
2.786
2.775
1.325
1.313
1.301
1.164
1.153
OH
O
OEt
O
N
NH
1H NMR of 6e
600 MHz, CDCl3
1.01
1.04
0.89
0.89
3.00
1.06
2.17
1.00
1.16
2.05
1.15
3.05
6.00
11.5
10.5
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)


196.76
166.91
162.72
157.32
155.06
144.98
141.78
136.04
135.95
132.37
126.80
122.89
121.95
119.14
118.72
118.44
106.55
77.21
77.00
76.79
61.70
33.58
23.96
14.17
OH
O
OEt
O
N
NH
13C NMR of 6e
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.746
10.638
8.716
8.712
8.662
8.658
8.047
7.592
7.590
7.578
7.576
7.556
7.543
7.488
7.198
7.191
7.178
7.053
7.039
6.906
6.894
4.397
4.385
4.373
1.401
1.389
1.377
OH
O
OEt
O
N
NH
Br
1H NMR of 6f
600 MHz, CDCl3
0.89
0.96
0.94
0.90
0.91
1.02
0.99
1.02
2.07
0.97
1.01
2.01
3.00
f1 (ppm)


196.83
166.89
162.84
156.87
154.58
141.76
139.92
136.33
132.42
130.10
126.82
124.15
123.85
122.55
119.84
119.09
118.91
118.59
107.25
77.21
77.00
76.79
62.01
14.20
OH
O
OEt
O
N
NH
Br
13C NMR of 6f
150 MHz, CDCl3
f1 (ppm)


11.772
10.716
8.746
8.742
8.692
8.688
7.805
7.786
7.613
7.599
7.513
7.499
7.304
7.302
7.292
7.289
7.279
7.079
7.065
6.927
6.915
6.902
6.804
4.423
4.412
4.400
1.425
1.413
1.402
OH
O
OEt
O
N
NH
F
1H NMR of 6g
600 MHz, CDCl3
0.95
0.98
0.92
0.87
0.95
1.01
1.01
2.06
0.96
1.03
0.97
2.07
3.00
11.5
10.5
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)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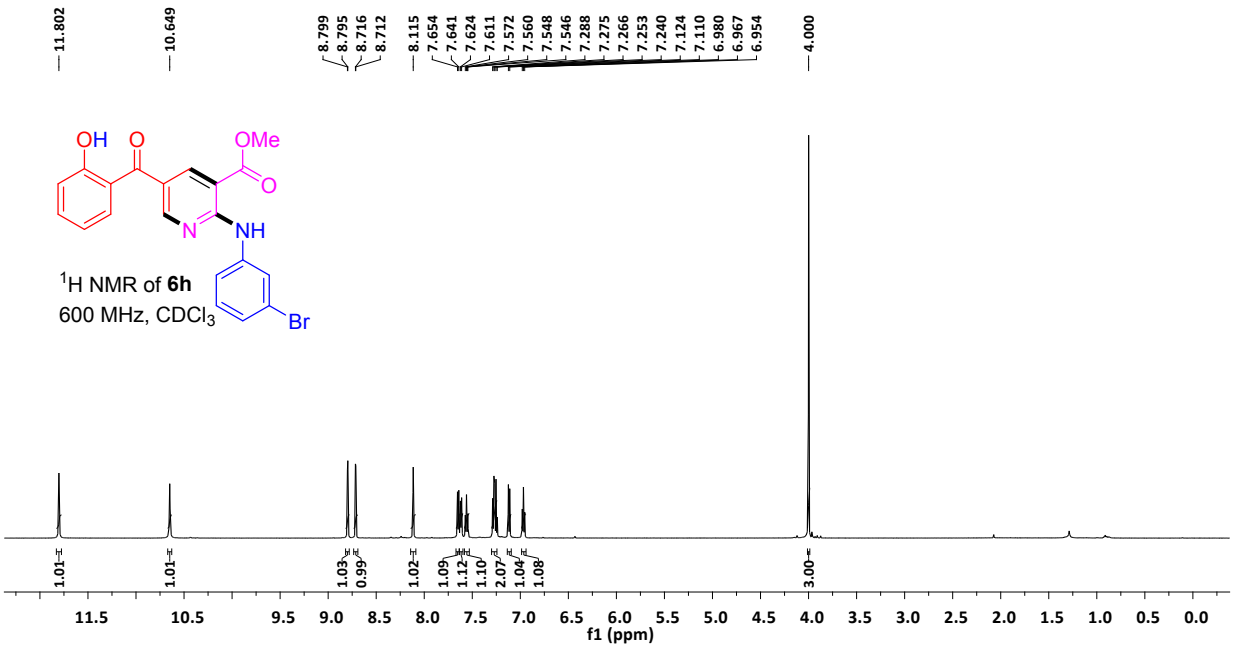
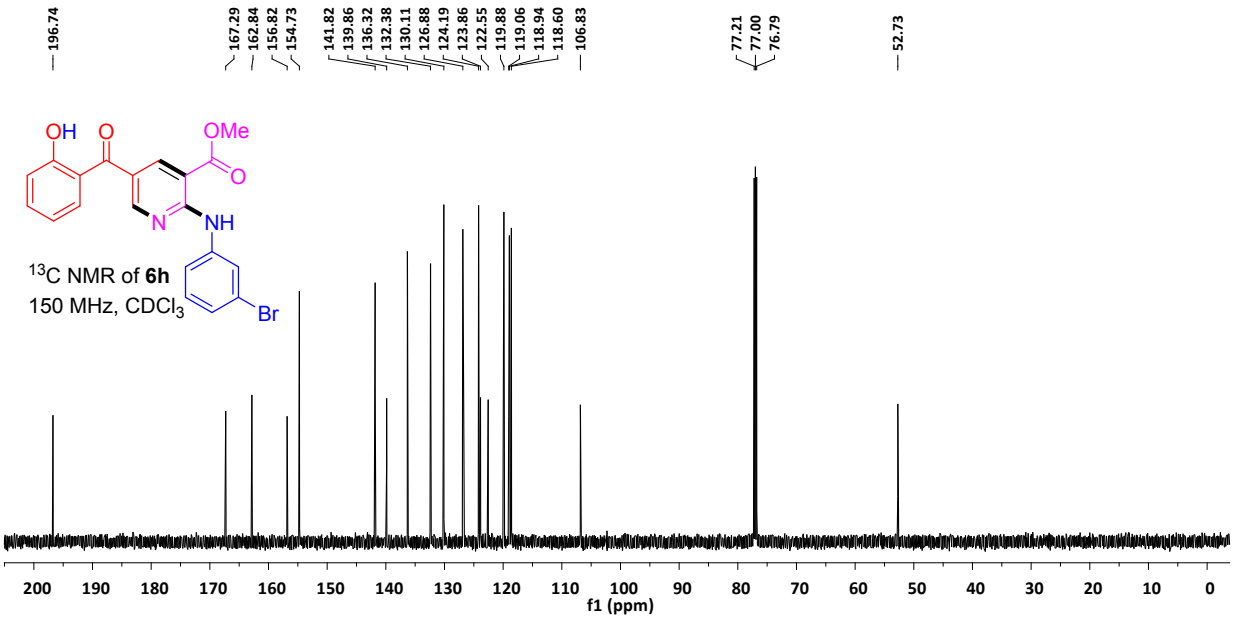
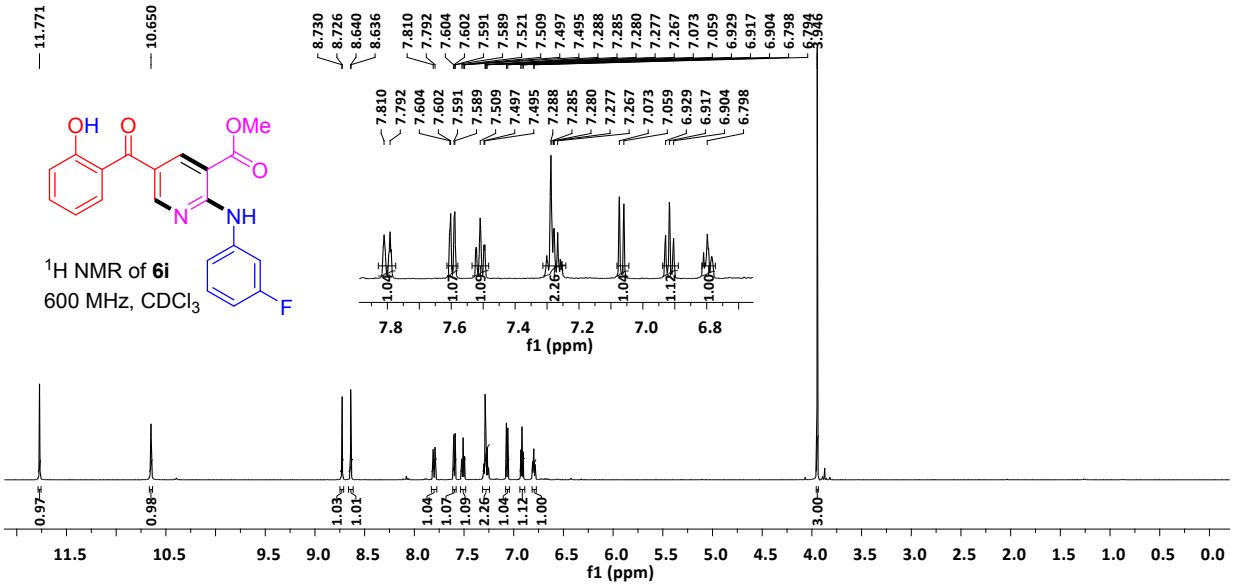
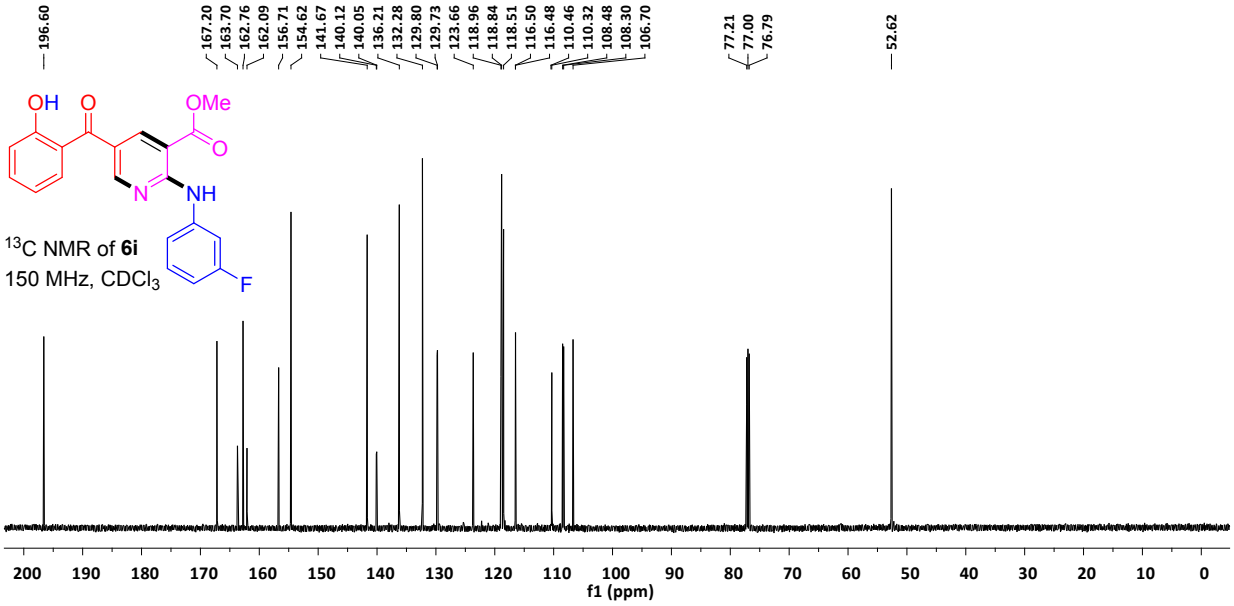
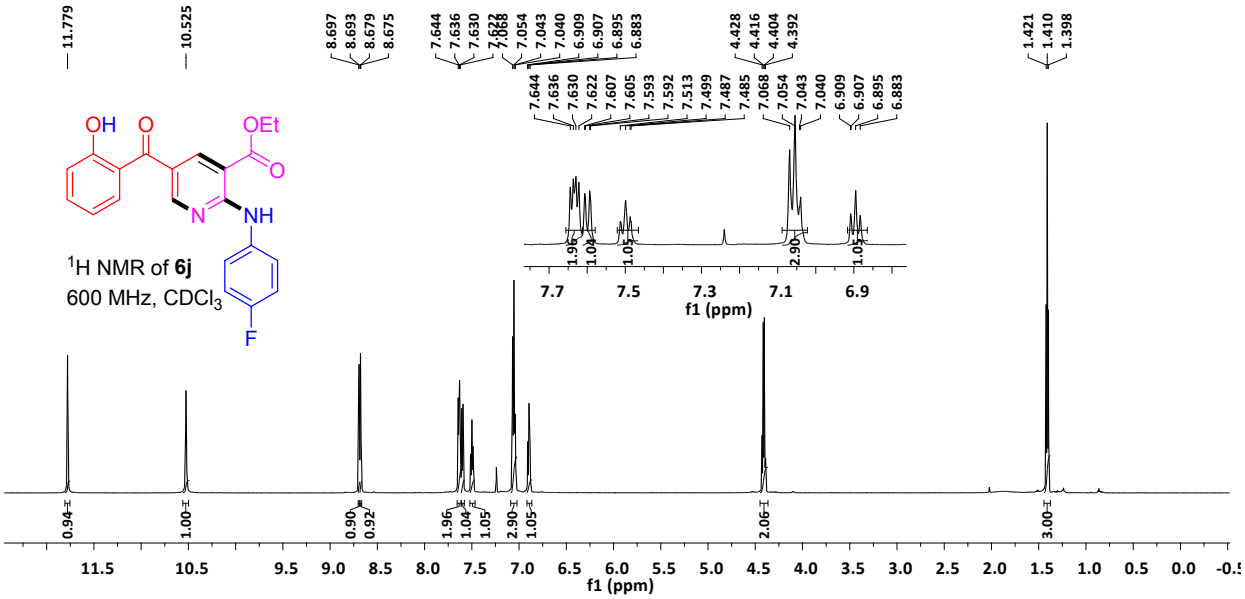
166.89
163.82
162.86
162.20
156.89
154.52
141.78
140.18
140.10
136.35
132.42
129.91
129.85
123.79
119.10
118.91
118.60
116.69
116.67
110.64
110.50
108.69
108.51
107.28
77.21
77.00
76.79
62.01
14.23
OH
O
OEt
O
N
NH
F
13C NMR of 6g
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

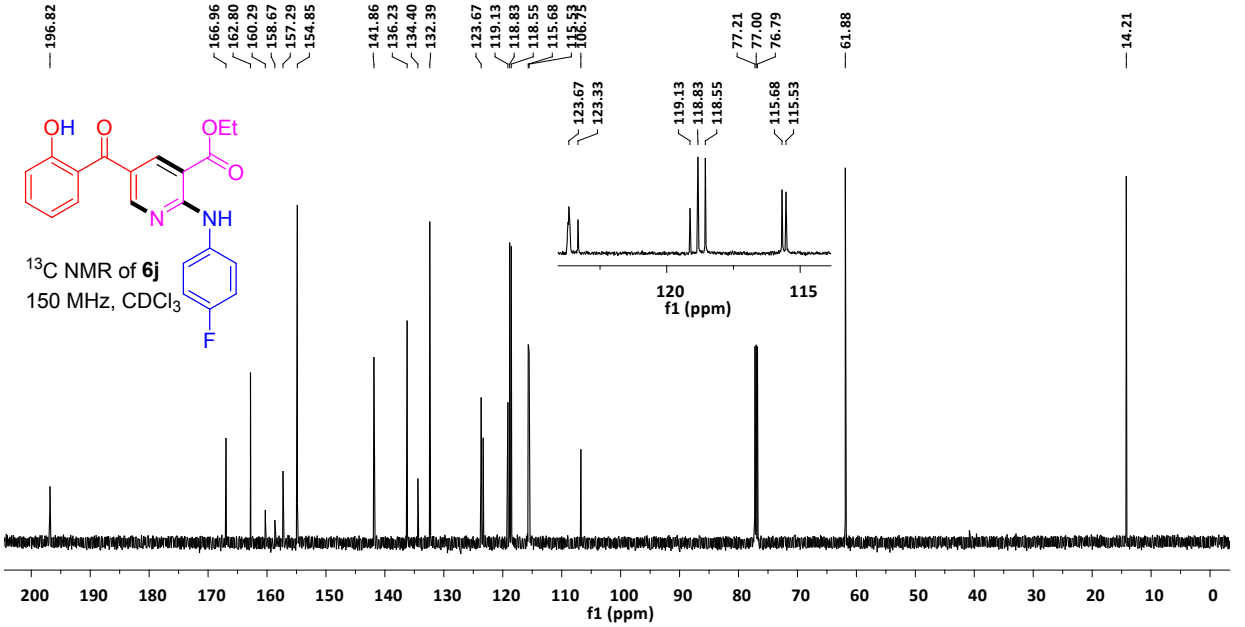

11.802
10.649
8.799
8.795
8.716
8.712
8.115
7.654
7.641
7.624
7.611
7.572
7.560
7.548
7.546
7.288
7.275
7.266
7.253
7.240
7.124
7.110
6.980
6.967
6.954
4.000
OH
O
OMe
O
N
NH
Br
1H NMR of 6h
600 MHz, CDCl3
1.01
1.01
1.03
0.99
1.02
1.09
1.12
1.10
2.07
1.04
1.08
3.00
f1 (ppm)

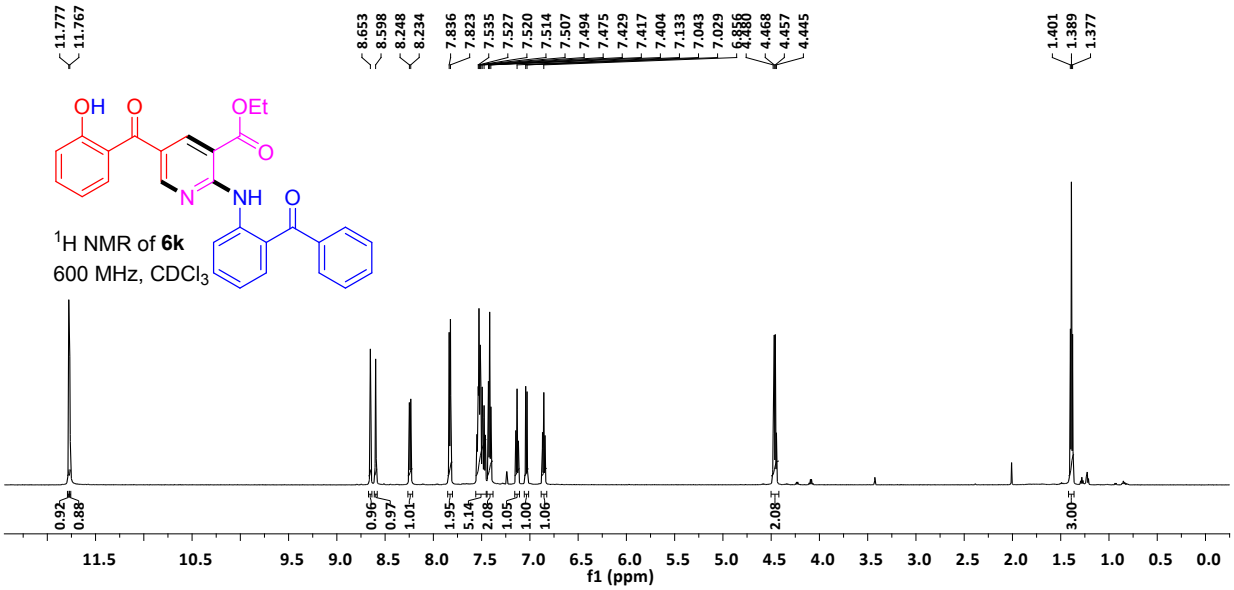

196.74
167.29
162.84
156.82
154.73
141.82
139.86
136.32
132.38
130.11
126.88
124.19
123.86
122.55
119.88
119.06
118.94
118.60
106.83
77.21
77.00
76.79
52.73
OH
O
OMe
O
N
NH
Br
13C NMR of 6h
150 MHz, CDCl3
f1 (ppm)

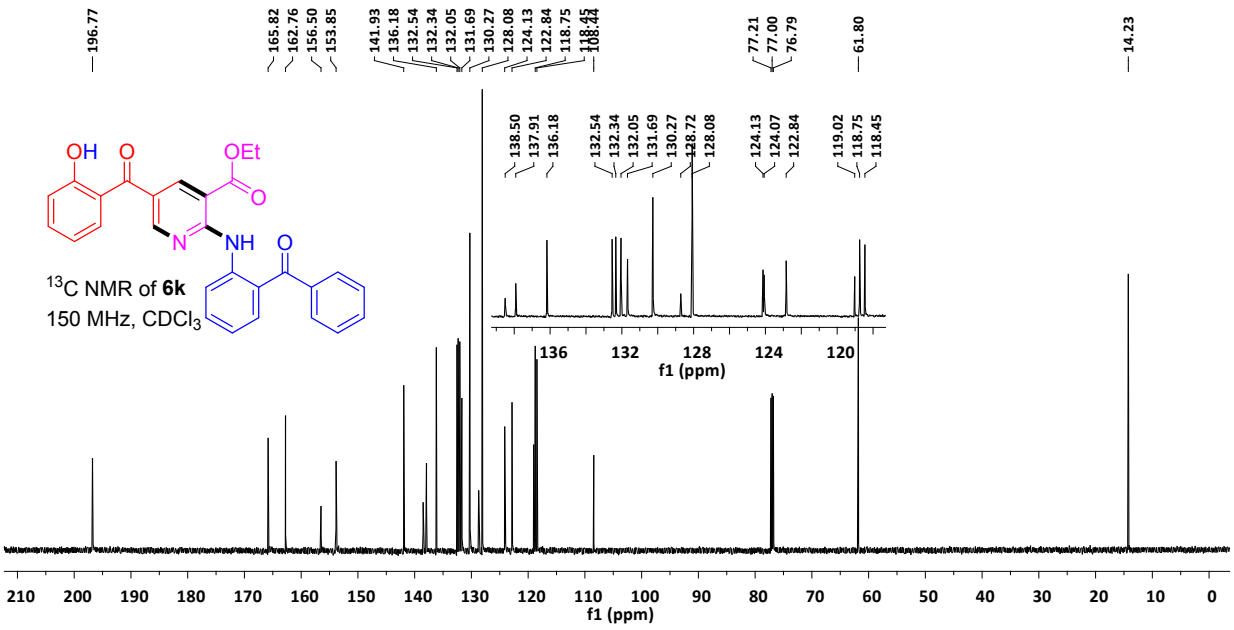

11.771
10.650
8.730
8.726
8.640
8.636
7.810
7.792
7.604
7.602
7.591
7.589
7.521
7.509
7.497
7.495
7.288
7.285
7.280
7.277
7.267
7.073
7.059
6.929
6.917
6.904
6.798
6.794
3.946
OH
O
OMe
O
N
NH
F
1H NMR of 6i
600 MHz, CDCl3
0.97
0.98
1.03
1.01
1.04
1.07
1.09
2.26
1.04
1.12
1.00
3.00
f1 (ppm)

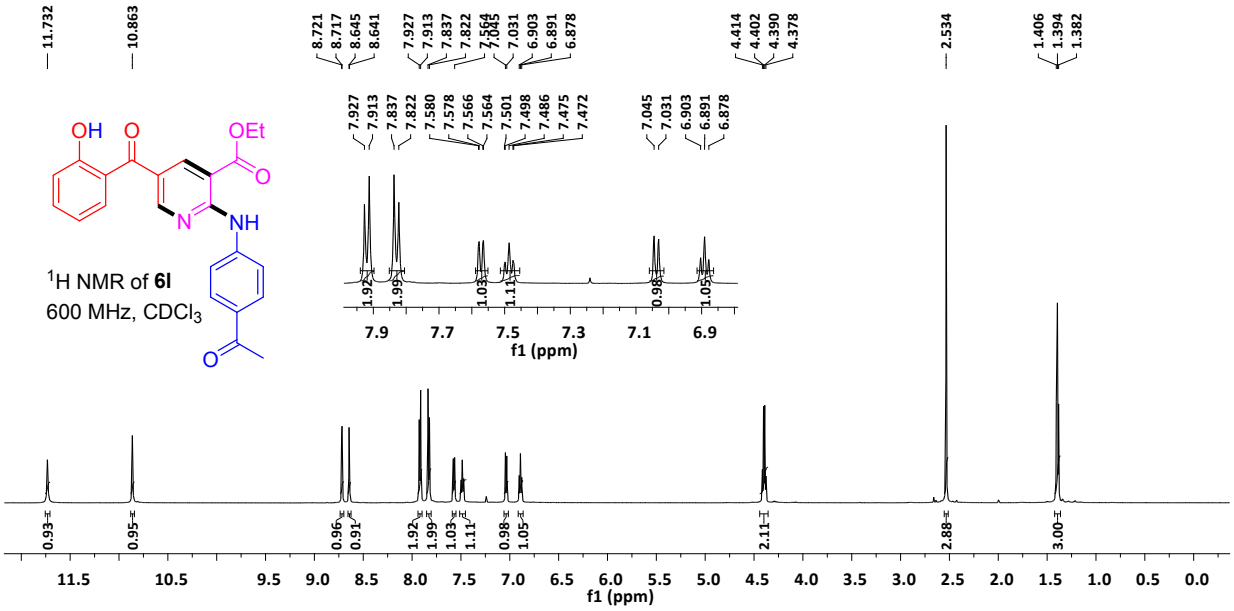

196.60
167.20
163.70
162.76
162.09
156.71
154.62
141.67
140.12
140.05
136.21
132.28
129.80
129.73
123.66
118.96
118.84
118.51
116.50
116.48
110.46
110.32
108.48
108.30
106.70
77.21
77.00
76.79
52.62
OH
O
OMe
O
N
NH
F
13C NMR of 6i
150 MHz, CDCl3
f1 (ppm)

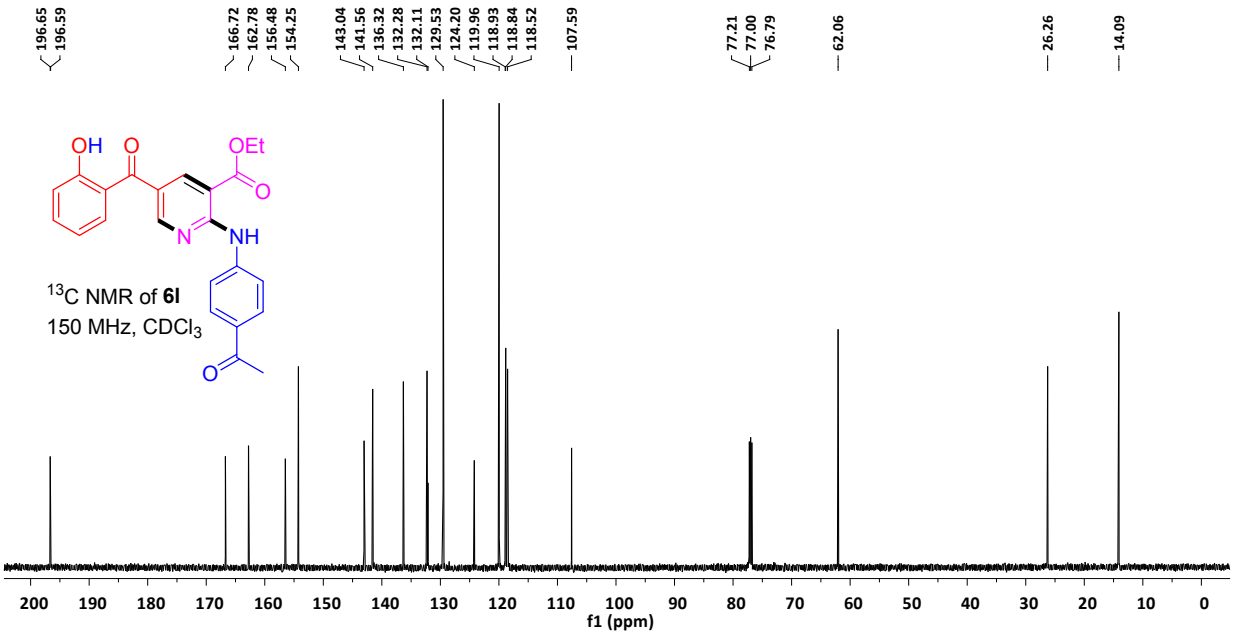

11.779
10.525
8.697
8.693
8.679
8.675
7.644
7.636
7.630
7.622
7.607
7.605
7.593
7.592
7.513
7.499
7.487
7.485
7.068
7.054
7.043
7.040
6.909
6.907
6.895
6.883
4.428
4.416
4.404
4.392
1.421
1.410
1.398
OH
O
OEt
O
N
NH
F
1H NMR of 6j
600 MHz, CDCl3
0.94
1.00
0.90
0.92
1.96
1.04
1.05
2.90
1.05
2.06
3.00
f1 (ppm)

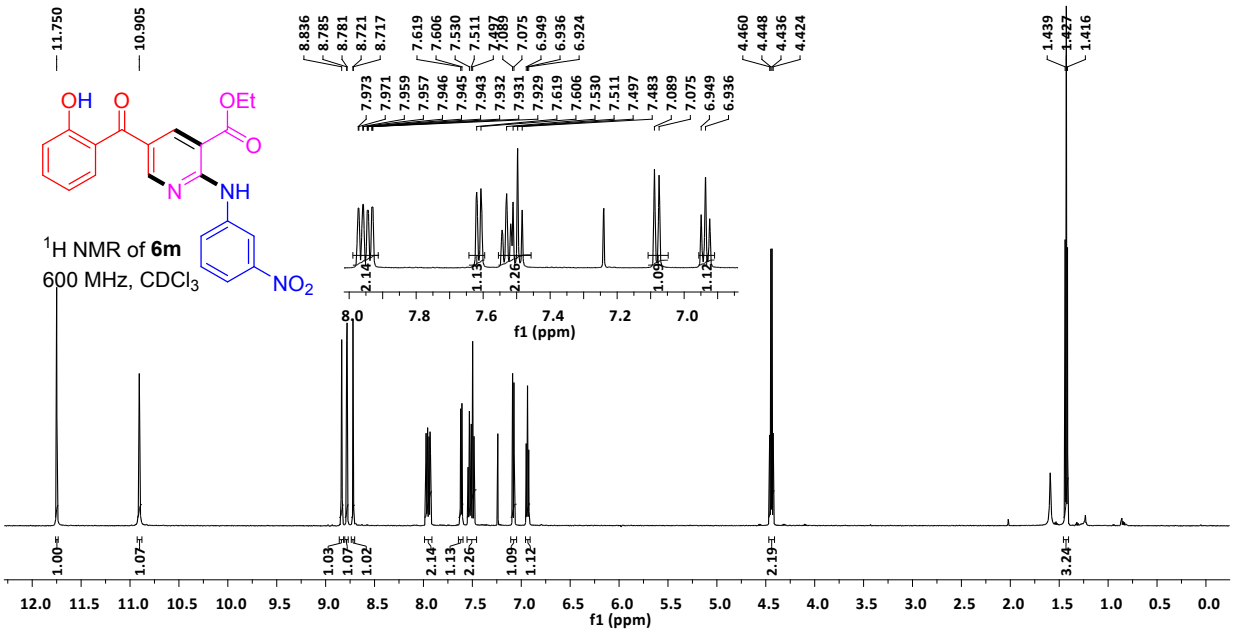

196.82
166.96
162.80
160.29
158.67
157.29
154.85
141.86
136.23
134.40
132.39
123.67
119.13
118.83
118.55
115.68
115.53
77.21
77.00
76.79
61.88
14.21
OH
O
OEt
O
N
NH
F
13C NMR of 6j
150 MHz, CDCl3
f1 (ppm)

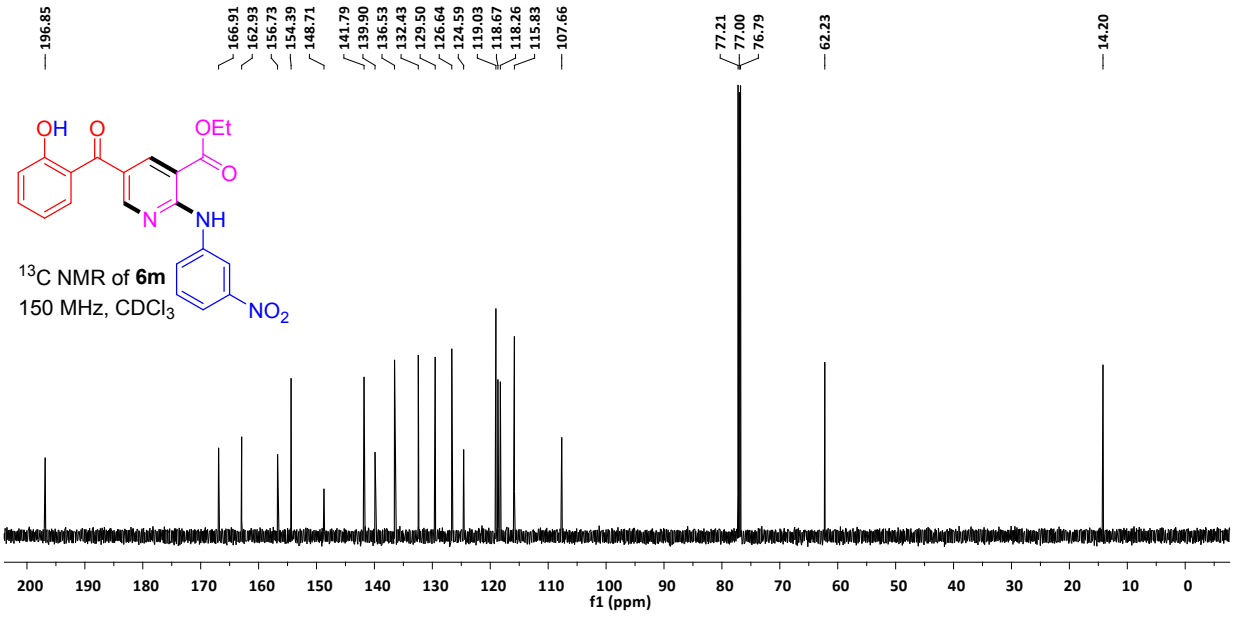

11.777
11.767
8.653
8.598
8.248
8.234
7.836
7.823
7.535
7.527
7.520
7.514
7.507
7.494
7.475
7.429
7.417
7.404
7.133
7.043
7.029
6.856
4.468
4.457
4.445
1.401
1.389
1.377
OH
O
OEt
O
N
NH
O
1H NMR of 6k
600 MHz, CDCl3
0.92
0.88
0.96
0.97
1.01
1.95
5.14
2.08
1.05
1.00
1.06
2.08
3.00
11.5
10.5
9.5
9.0
8.5
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)

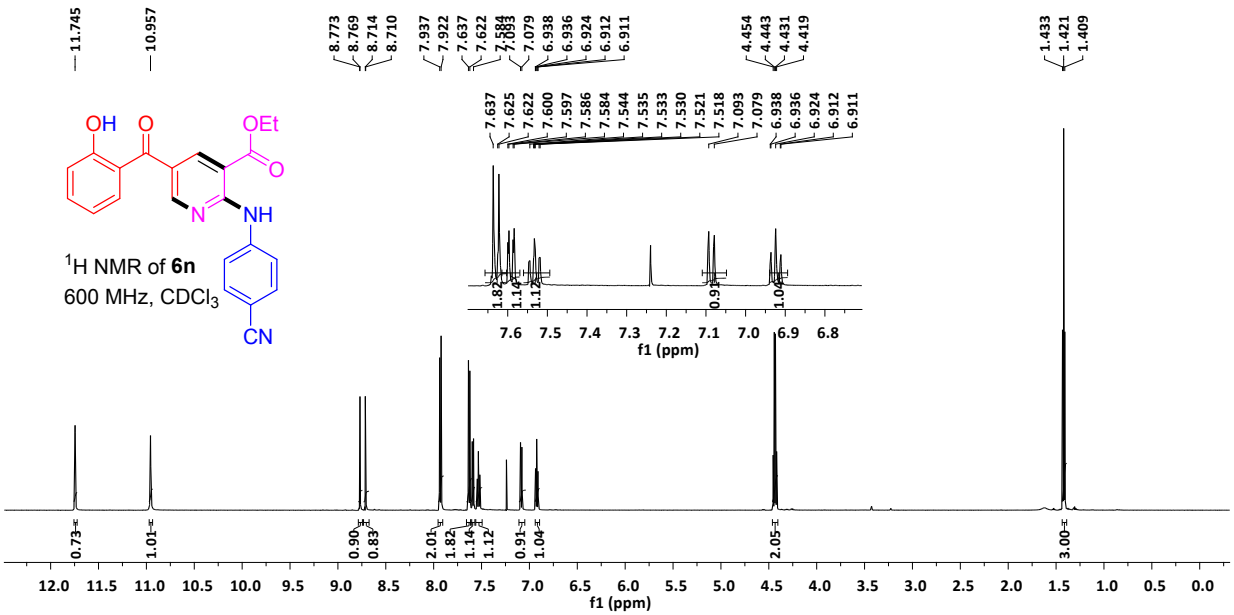

196.77
165.82
162.76
156.50
153.85
141.93
136.18
132.54
132.34
132.05
131.69
130.27
128.08
124.13
122.84
118.75
77.21
77.00
76.79
61.80
14.23
138.50
137.91
136.18
132.54
132.34
132.05
131.69
130.27
128.72
128.08
124.13
124.07
122.84
119.02
118.75
118.45
OH
O
OEt
O
N
NH
O
13C NMR of 6k
150 MHz, CDCl3
136
132
128
124
120
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

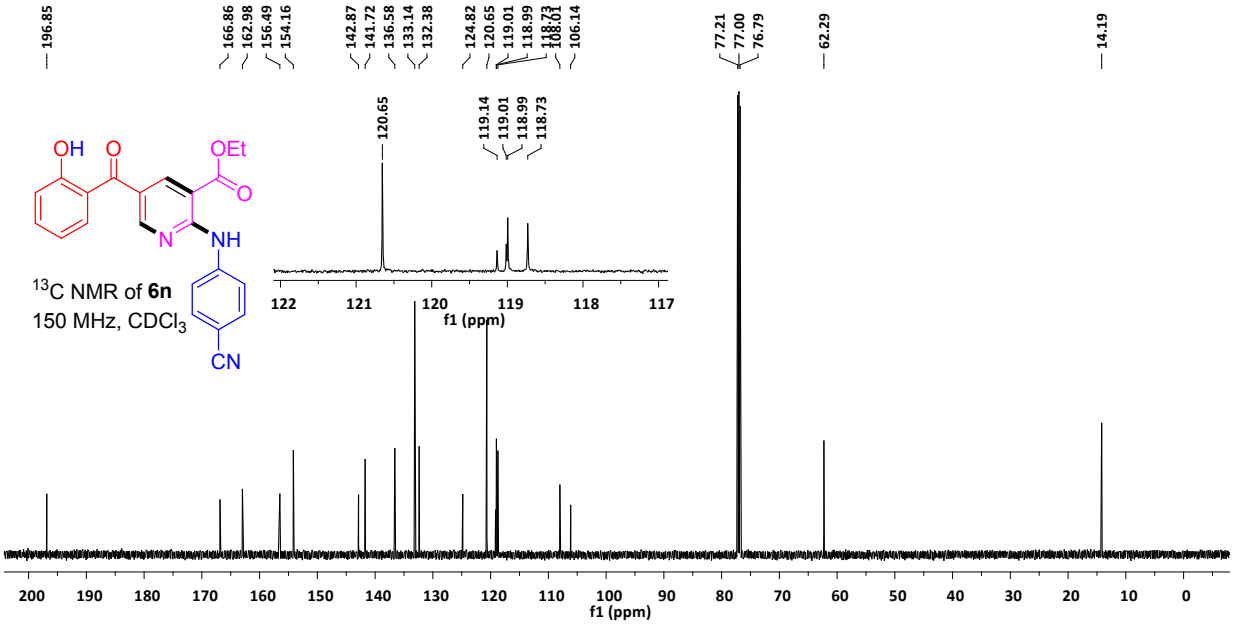

11.732
10.863
8.721
8.717
8.645
8.641
7.927
7.913
7.837
7.822
7.580
7.578
7.566
7.564
7.501
7.498
7.486
7.475
7.472
7.045
7.031
6.903
6.891
6.878
4.414
4.402
4.390
4.378
2.534
1.406
1.394
1.382
OH
O
OEt
O
N
NH
O
^{1}H NMR of **6l**
600 MHz, $CDCl_3$
1.92
1.99
1.03
1.11
0.98
1.05
7.9
7.7
7.5
7.3
7.1
6.9
f1 (ppm)
0.93
0.95
0.96
0.91
1.92
1.99
1.03
1.11
0.98
1.05
2.11
2.88
3.00
11.5
10.5
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)

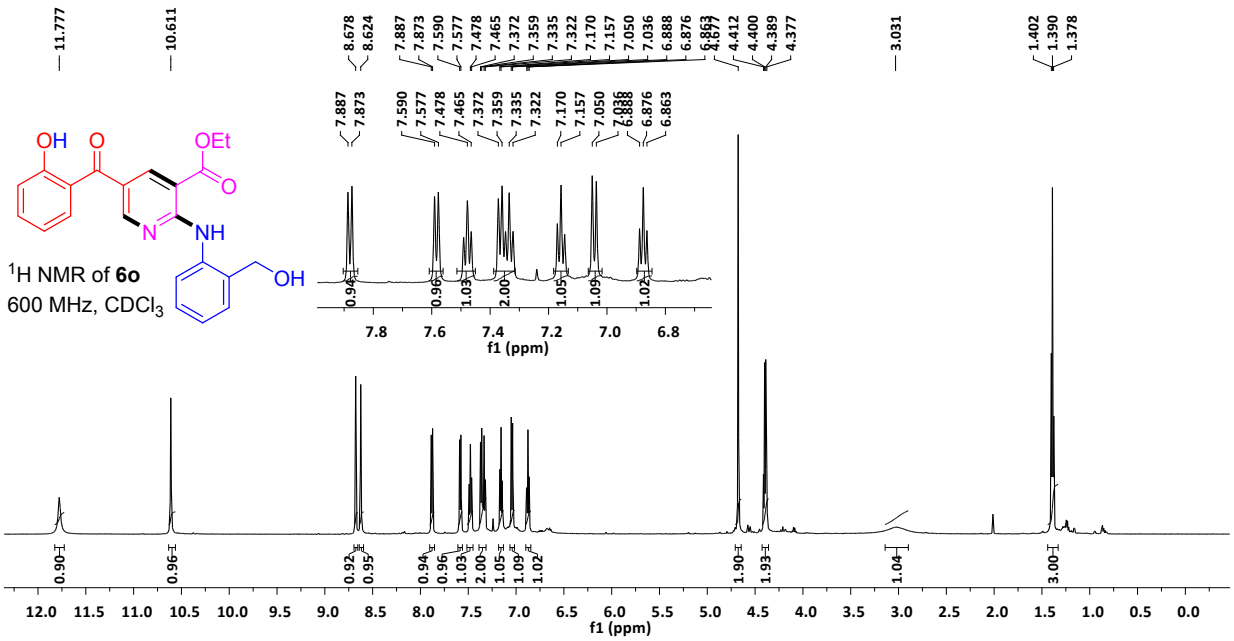

196.65
196.59
166.72
162.78
156.48
154.25
143.04
141.56
136.32
132.28
132.11
129.53
124.20
119.96
118.93
118.84
118.52
107.59
77.21
77.00
76.79
62.06
26.26
14.09
OH
O
OEt
O
N
NH
O
^{13}C NMR of **6l**
150 MHz, $CDCl_3$
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

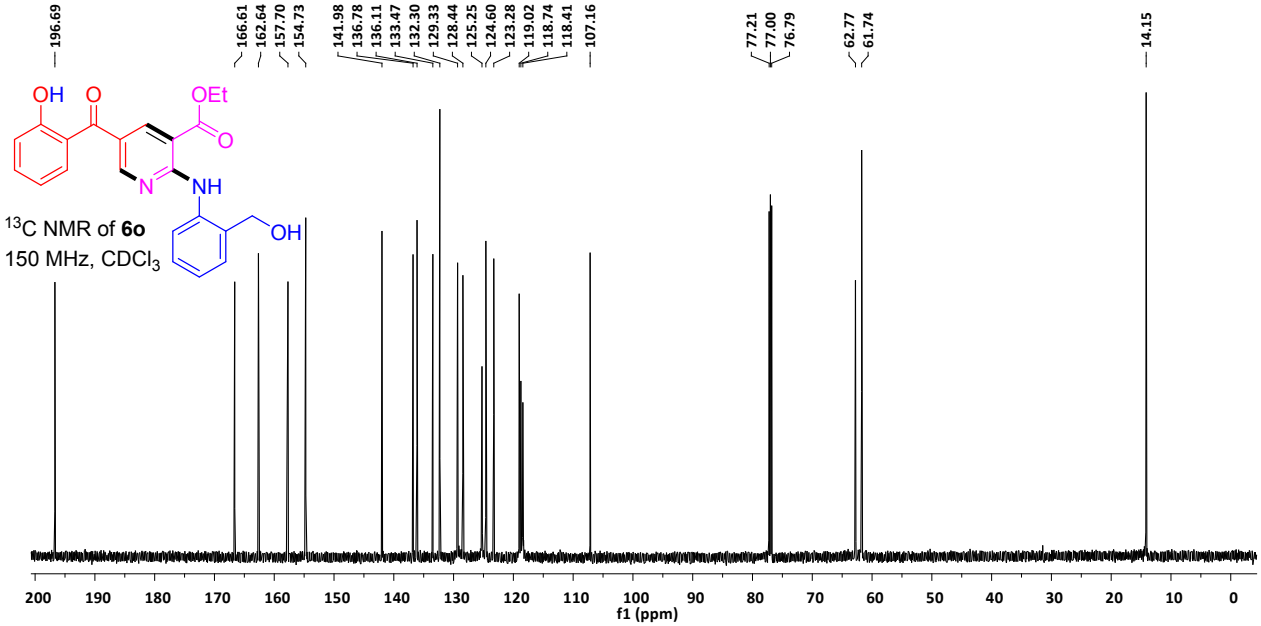

OH
O
OEt
O
N
NH
NO2
1H NMR of 6m
600 MHz, CDCl3
f1 (ppm)

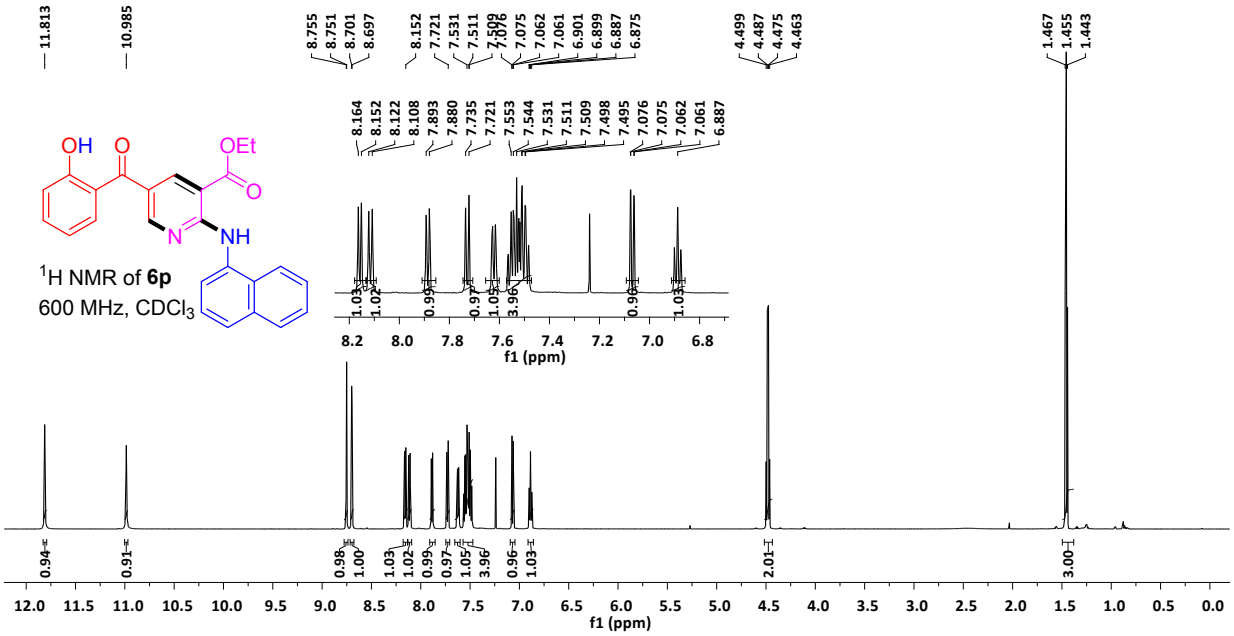

OH
O
OEt
O
N
NH
NO2
13C NMR of 6m
150 MHz, CDCl3
f1 (ppm)

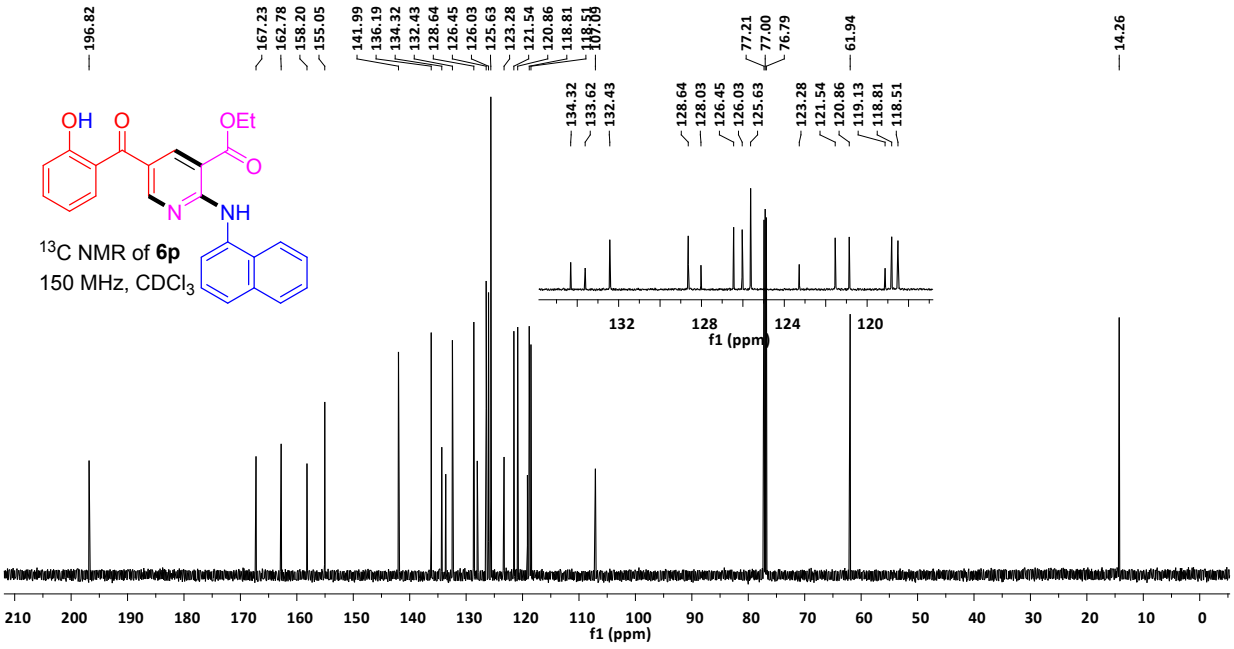

OH
O
OEt
O
N
NH
CN
^{1}H NMR of **6n**
600 MHz, CDCl$_3$
f1 (ppm)

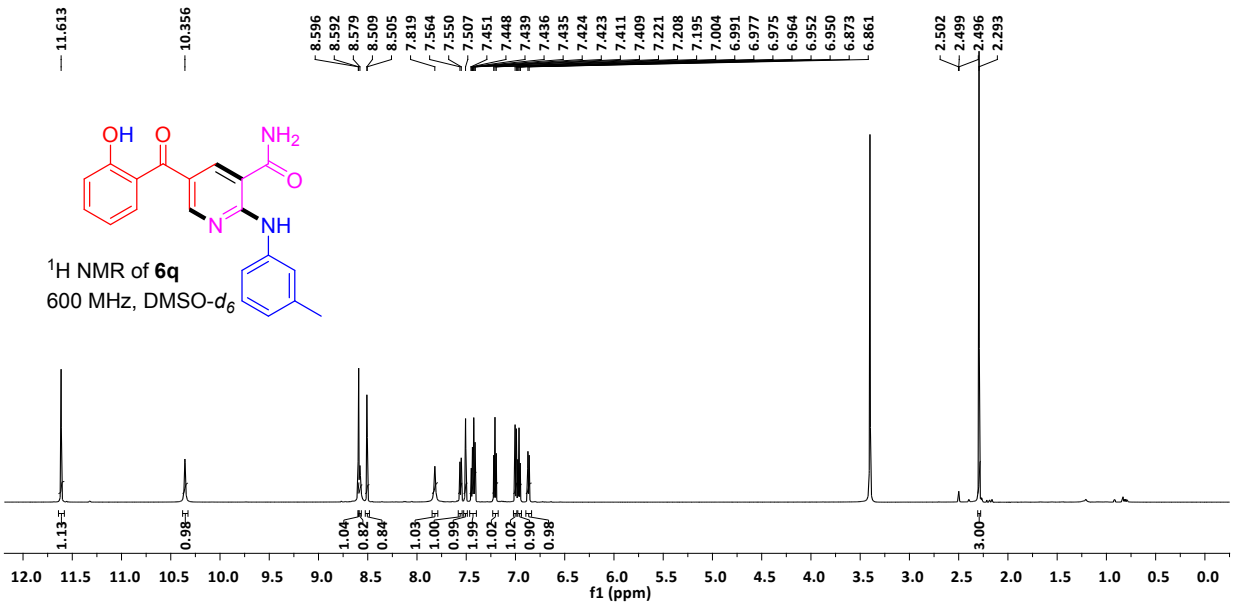

OH
O
OEt
O
N
NH
CN
^{13}C NMR of **6n**
150 MHz, CDCl$_3$
f1 (ppm)

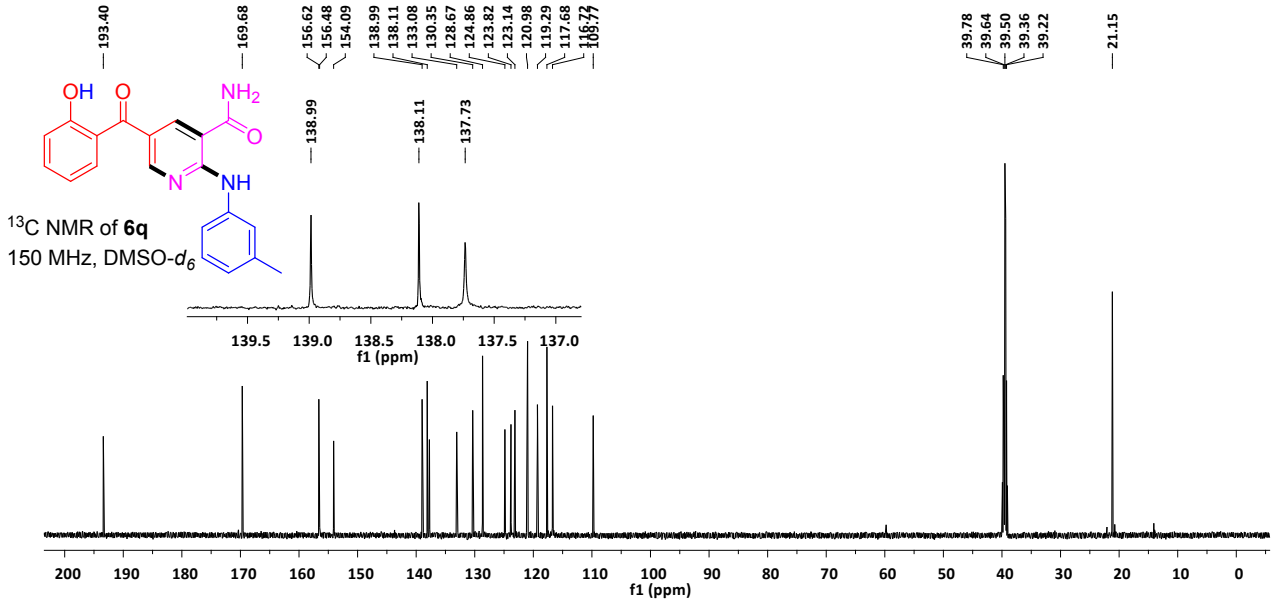

11.777
10.611
8.678
8.624
7.887
7.873
7.590
7.577
7.478
7.465
7.372
7.359
7.335
7.322
7.170
7.157
7.050
6.888
6.876
6.863
4.412
4.400
4.389
4.377
3.031
1.402
1.390
1.378
OH
O
OEt
O
N
NH
OH
1H NMR of 6o
600 MHz, CDCl3
f1 (ppm)

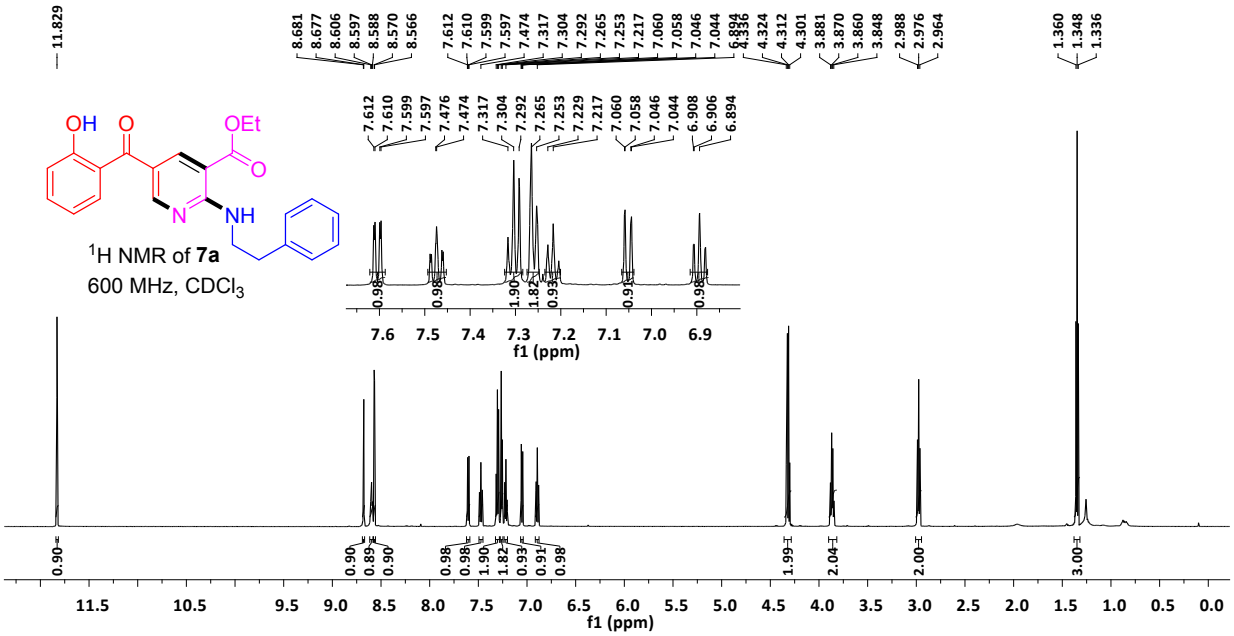

196.69
166.61
162.64
157.70
154.73
141.98
136.78
136.11
133.47
132.30
129.33
128.44
125.25
124.60
123.28
119.02
118.74
118.41
107.16
77.21
77.00
76.79
62.77
61.74
14.15
OH
O
OEt
O
N
NH
OH
13C NMR of 6o
150 MHz, CDCl3
f1 (ppm)

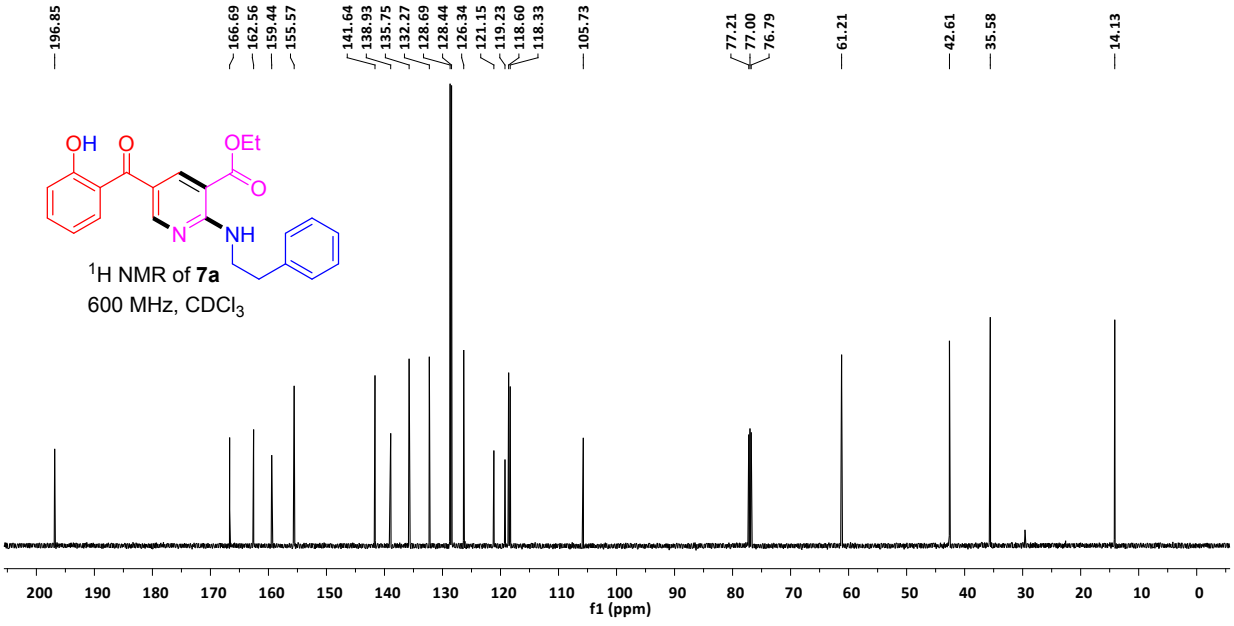

OH
O
OEt
O
N
NH
^{1}H NMR of **6p**
600 MHz, CDCl$_3$
f1 (ppm)

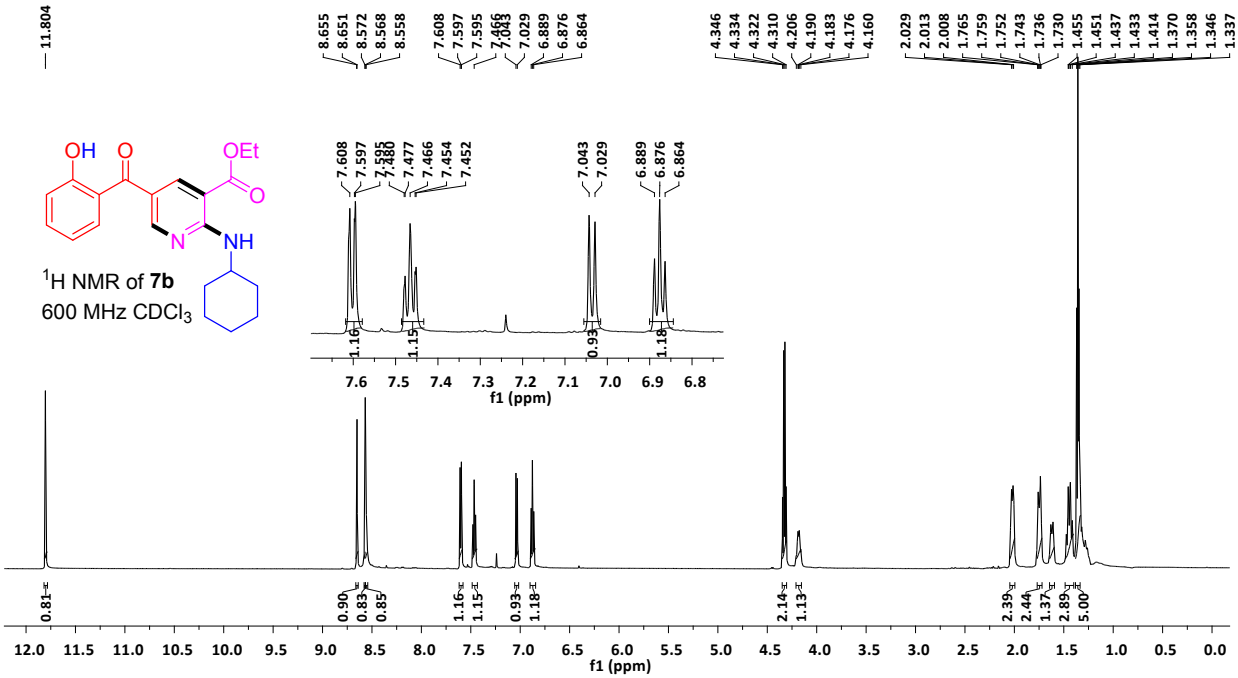

OH
O
OEt
O
N
NH
^{13}C NMR of **6p**
150 MHz, CDCl$_3$
f1 (ppm)

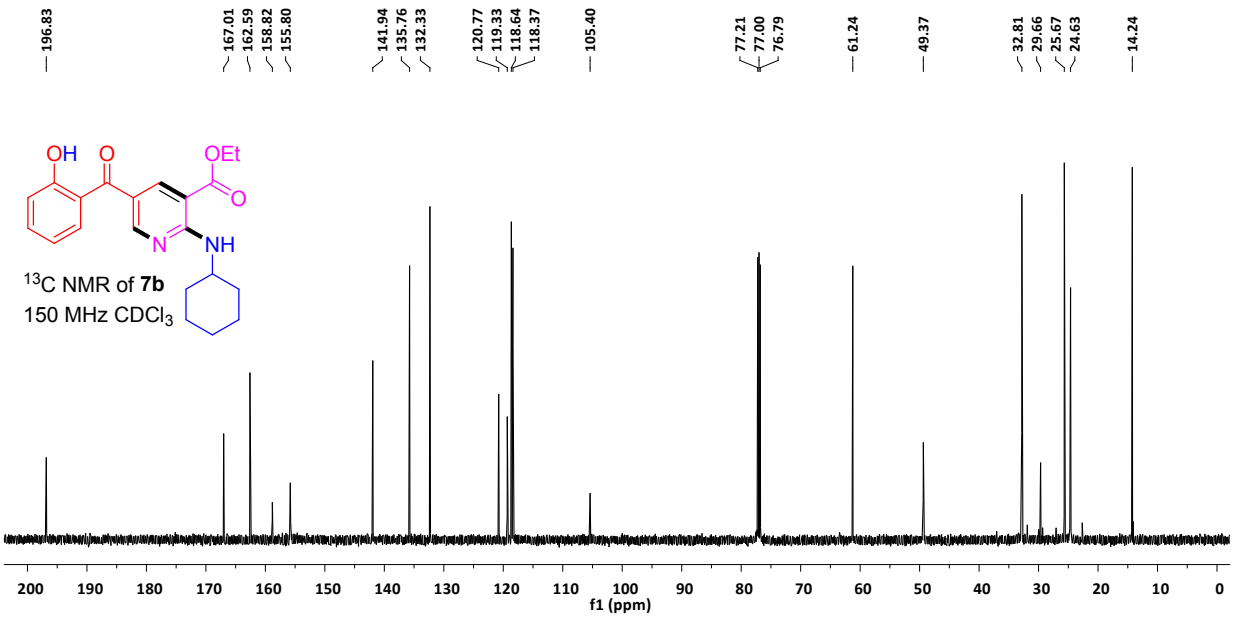

11.613
10.356
8.596
8.592
8.579
8.509
8.505
7.819
7.564
7.550
7.507
7.451
7.448
7.439
7.436
7.435
7.424
7.423
7.411
7.409
7.221
7.208
7.195
7.004
6.991
6.977
6.975
6.964
6.952
6.950
6.873
6.861
2.502
2.499
2.496
2.293
OH
O
NH2
O
N
NH
1H NMR of 6q
600 MHz, DMSO-d6
1.13
0.98
1.04
0.82
0.84
1.03
1.00
0.99
1.99
1.02
1.02
0.90
0.98
3.00
12.0 11.5 11.0 10.5 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)

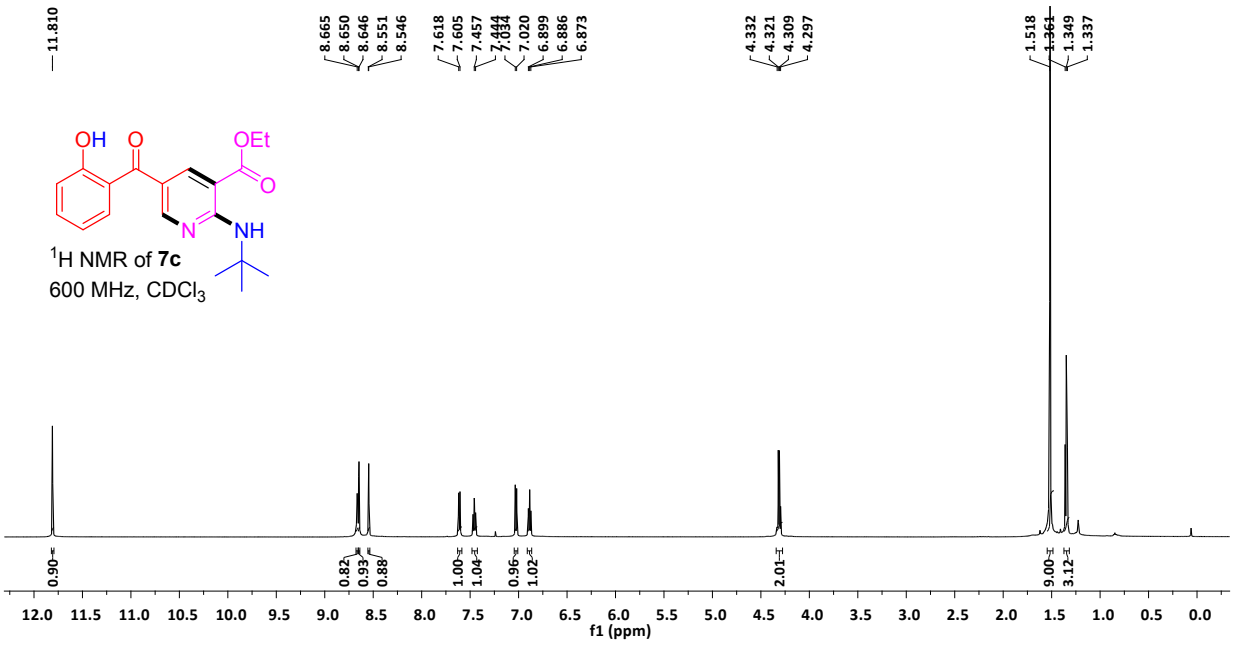

193.40
169.68
156.62
156.48
154.09
138.99
138.11
133.08
130.35
128.67
124.86
123.82
123.14
120.98
119.29
117.68
39.78
39.64
39.50
39.36
39.22
21.15
OH
O
NH2
O
N
NH
13C NMR of 6q
150 MHz, DMSO-d6
138.99
138.11
137.73
139.5 139.0 138.5 138.0 137.5 137.0
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OH
O
OEt
O
N
NH
^{1}H NMR of **7a**
600 MHz, $CDCl_3$
f1 (ppm)

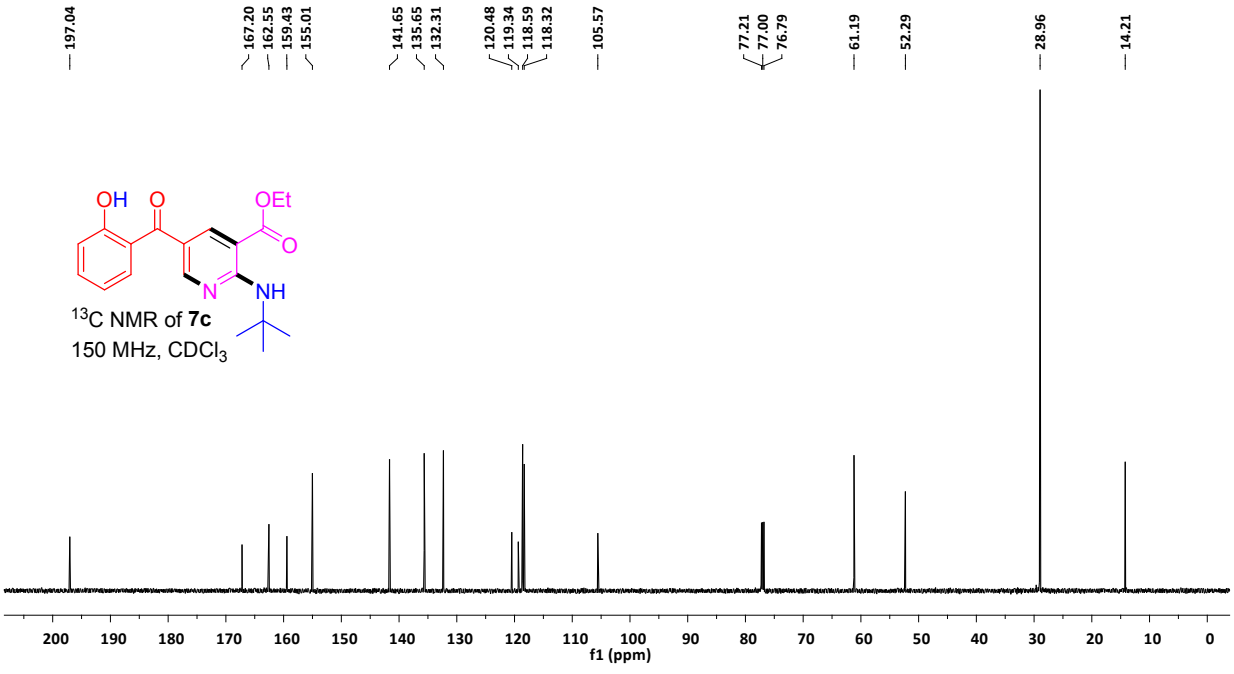

OH
O
OEt
O
N
NH
^{1}H NMR of **7a**
600 MHz, $CDCl_3$
f1 (ppm)


OH
O
OEt
O
N
NH
^{1}H NMR of **7b**
600 MHz $CDCl_3$
f1 (ppm)

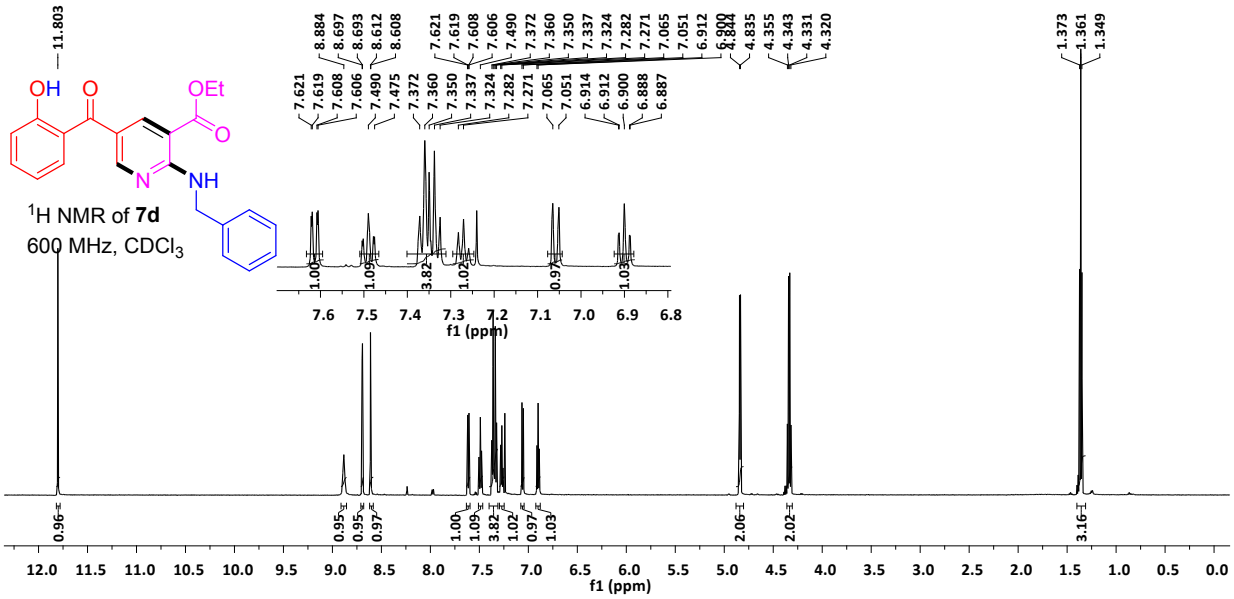

OH
O
OEt
O
N
NH
^{13}C NMR of **7b**
150 MHz $CDCl_3$
f1 (ppm)

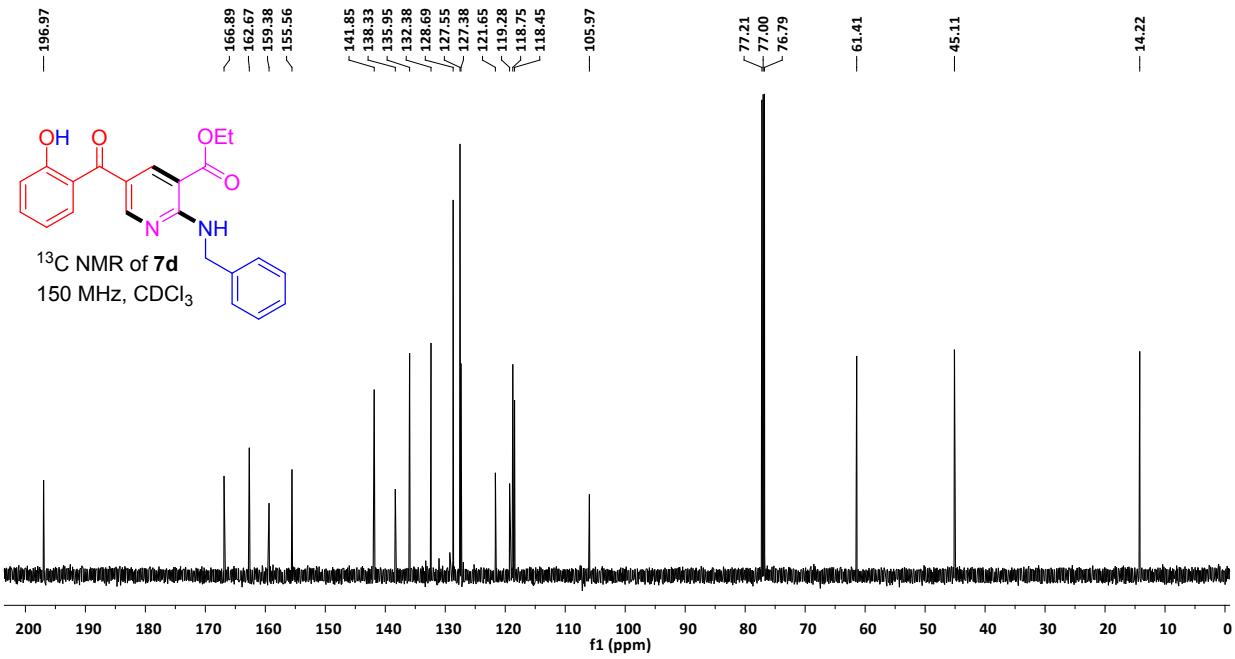


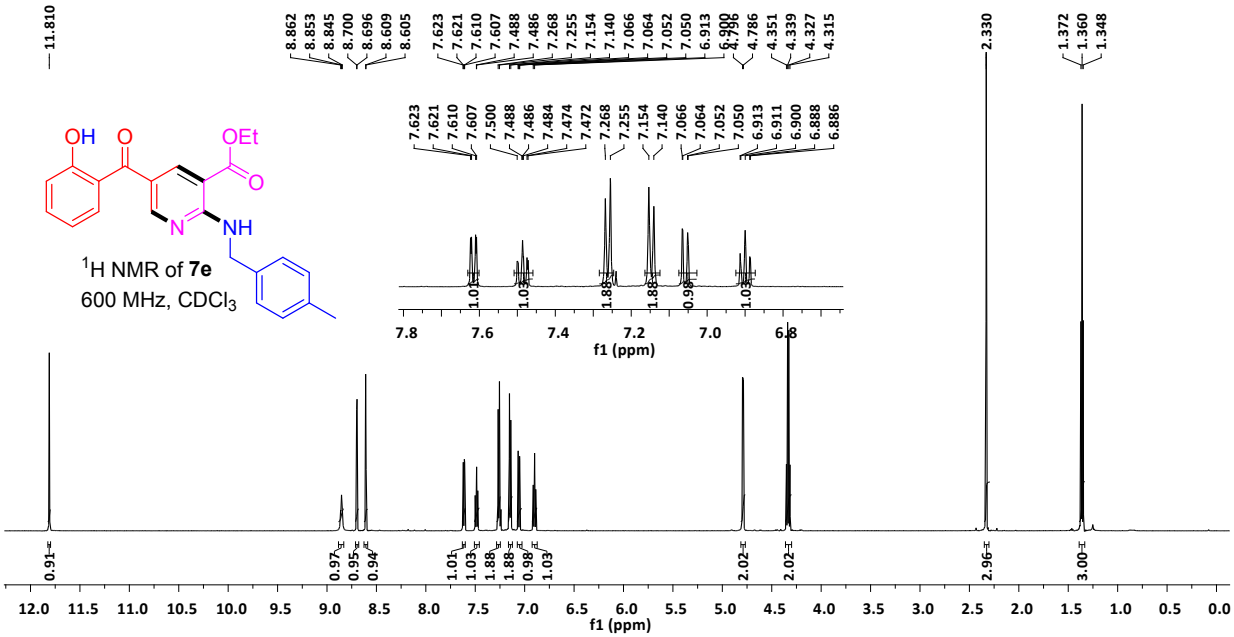
^{1}H NMR of **7c**
600 MHz, $CDCl_3$

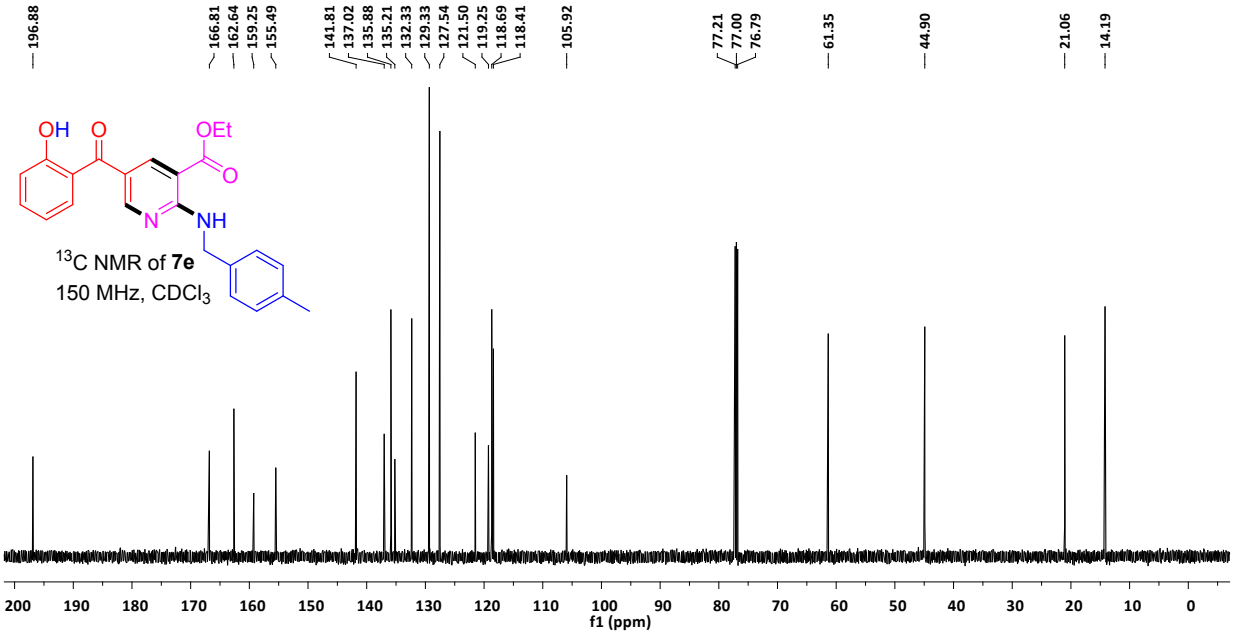


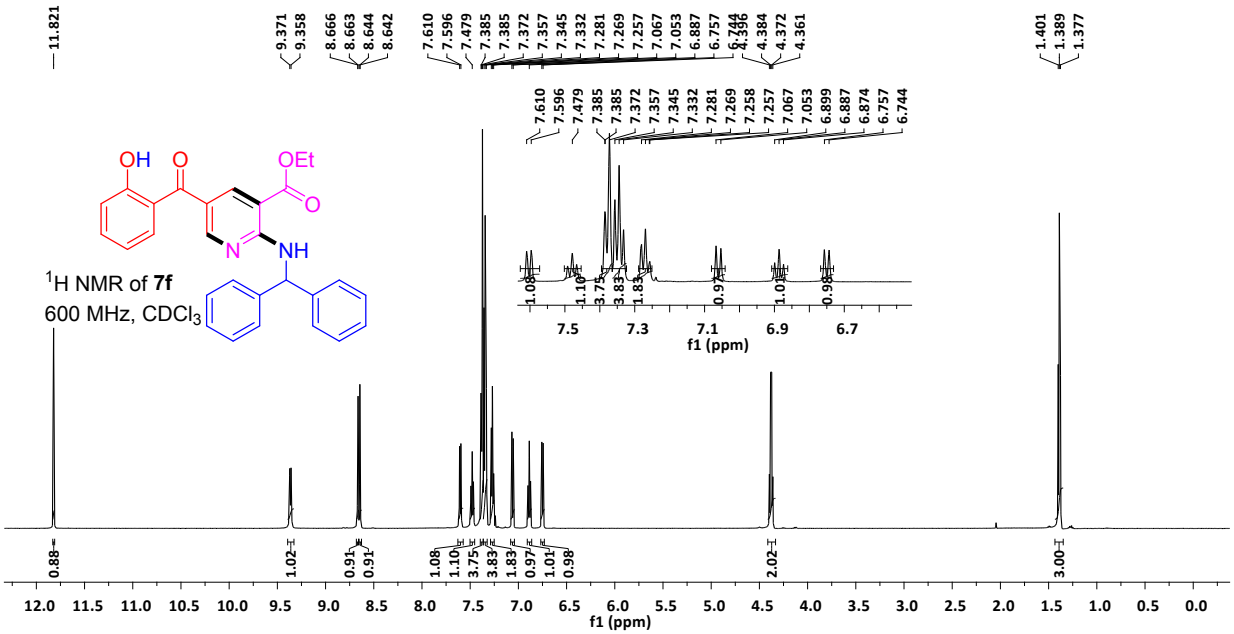
^{13}C NMR of **7c**
150 MHz, $CDCl_3$

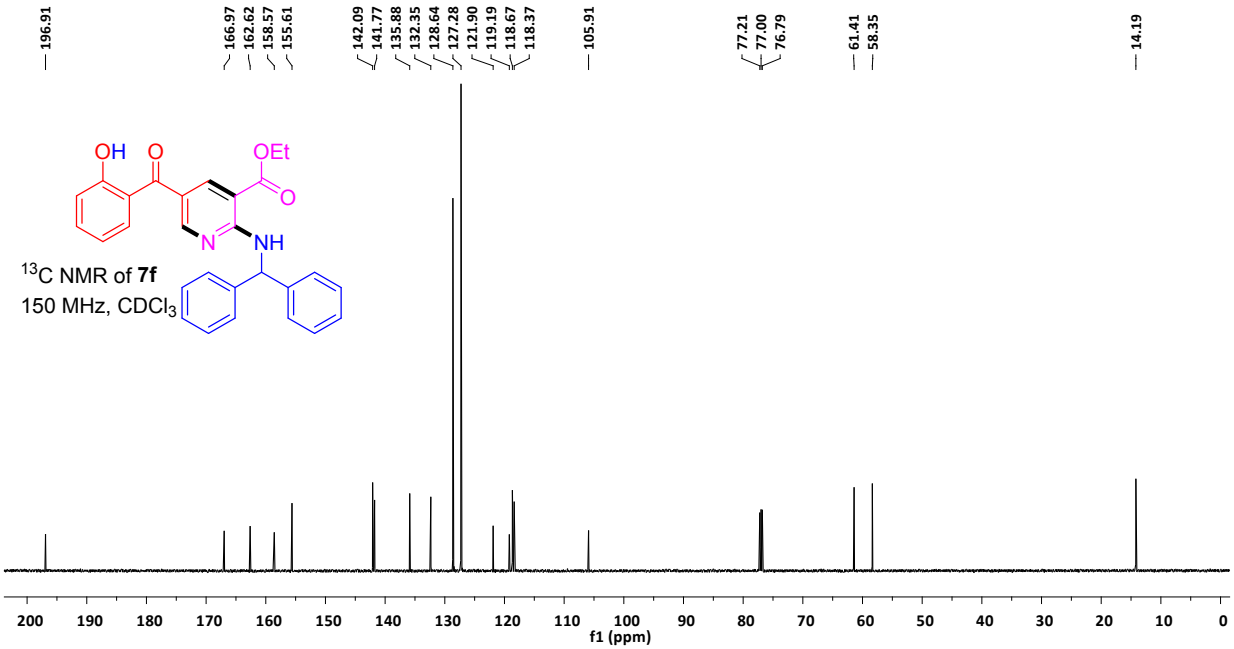

OH
O
OEt
O
N
NH
^{1}H NMR of **7d**
600 MHz, $CDCl_3$
f1 (ppm)

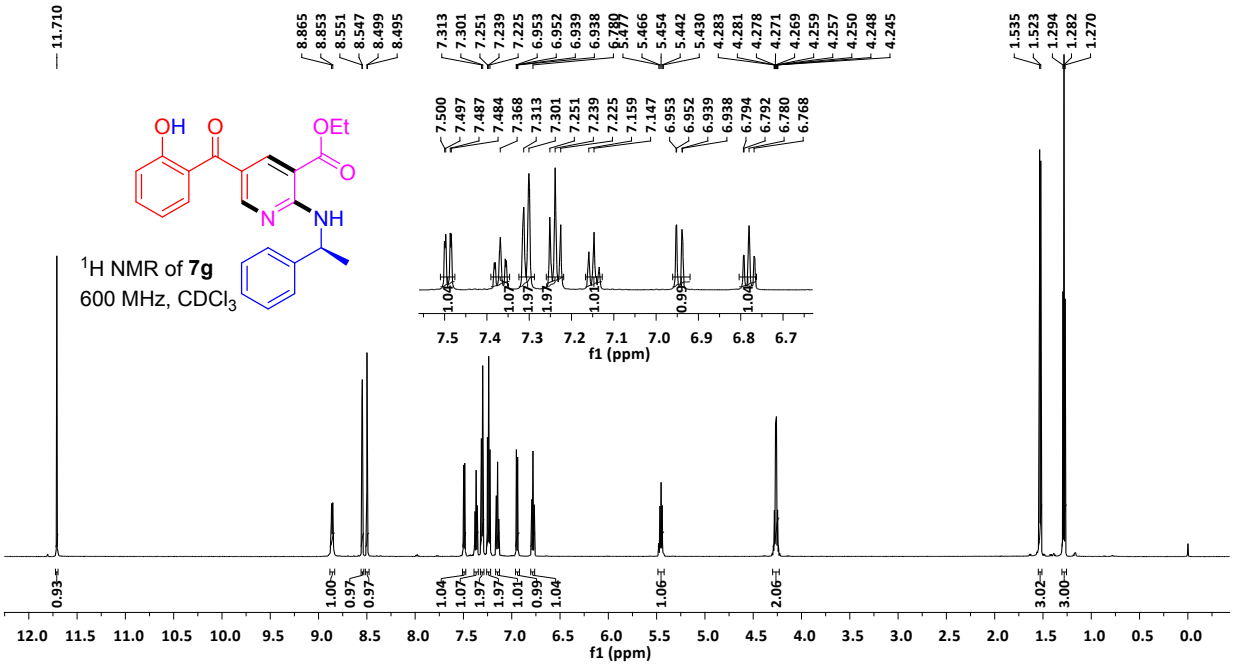

OH
O
OEt
O
N
NH
^{13}C NMR of **7d**
150 MHz, $CDCl_3$
f1 (ppm)

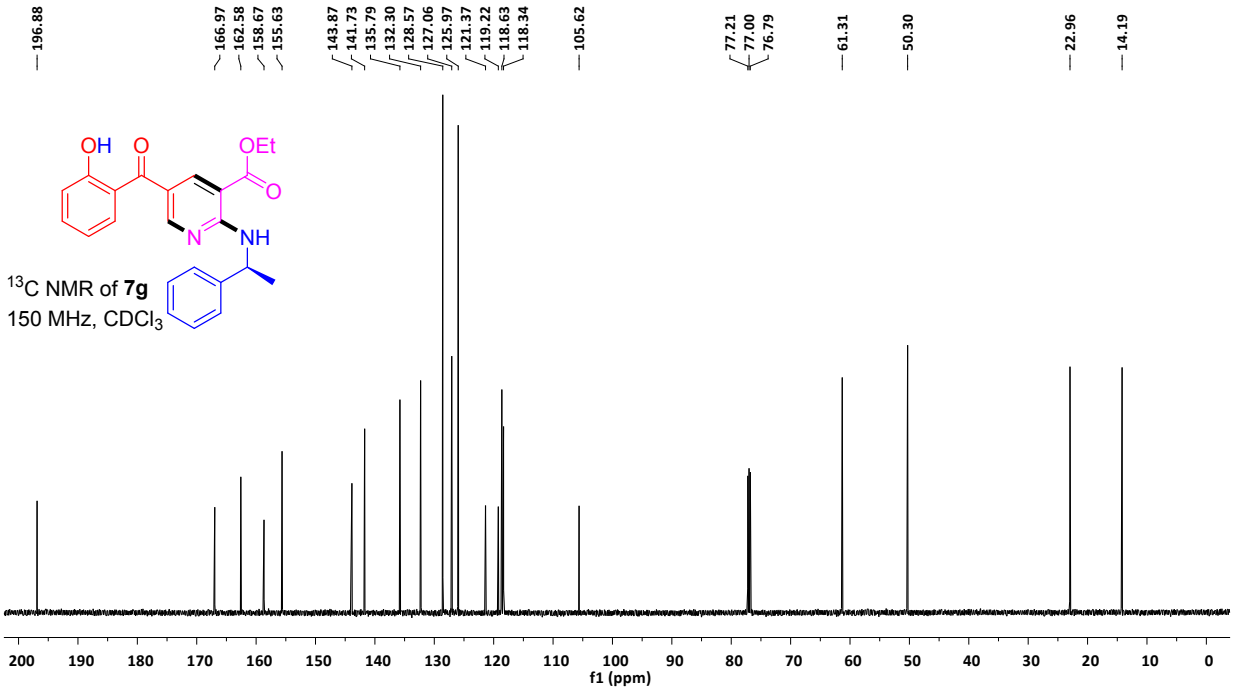

OH
O
OEt
O
N
NH
^{1}H NMR of **7e**
600 MHz, $CDCl_3$
f1 (ppm)

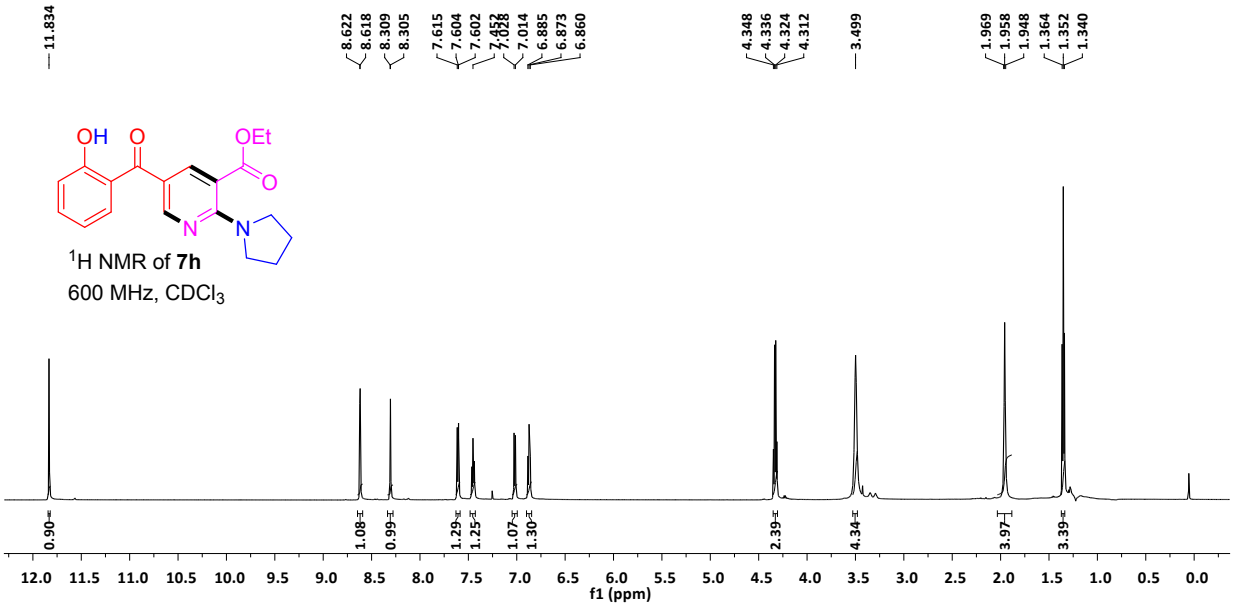

OH
O
OEt
O
N
NH
^{13}C NMR of **7e**
150 MHz, $CDCl_3$
f1 (ppm)


11.821
9.371
9.358
8.666
8.663
8.644
8.642
7.610
7.596
7.479
7.385
7.385
7.372
7.357
7.345
7.332
7.281
7.269
7.257
7.067
7.053
6.887
6.757
6.744
4.396
4.384
4.372
4.361
1.401
1.389
1.377
OH
O
OEt
O
N
NH
1H NMR of 7f
600 MHz, CDCl3
f1 (ppm)
f1 (ppm)

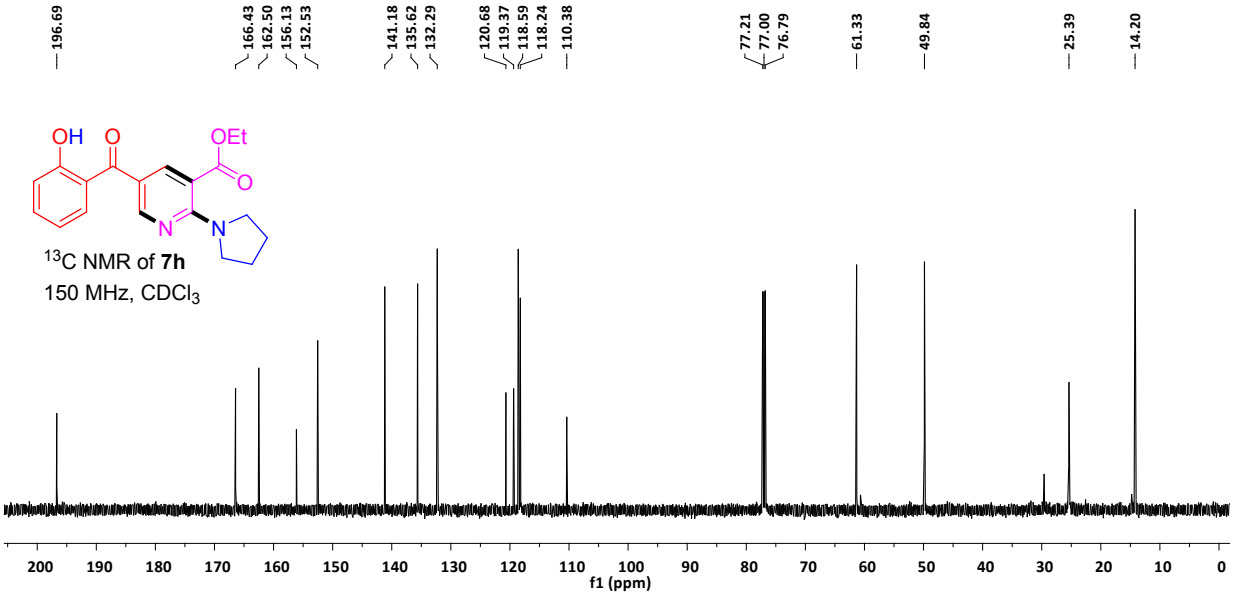

196.91
166.97
162.62
158.57
155.61
142.09
141.77
135.88
132.35
128.64
127.28
121.90
119.19
118.67
118.37
105.91
77.21
77.00
76.79
61.41
58.35
14.19
OH
O
OEt
O
N
NH
13C NMR of 7f
150 MHz, CDCl3
f1 (ppm)


OH
O
OEt
O
N
NH
^{1}H NMR of **7g**
600 MHz, $CDCl_3$
f1 (ppm)

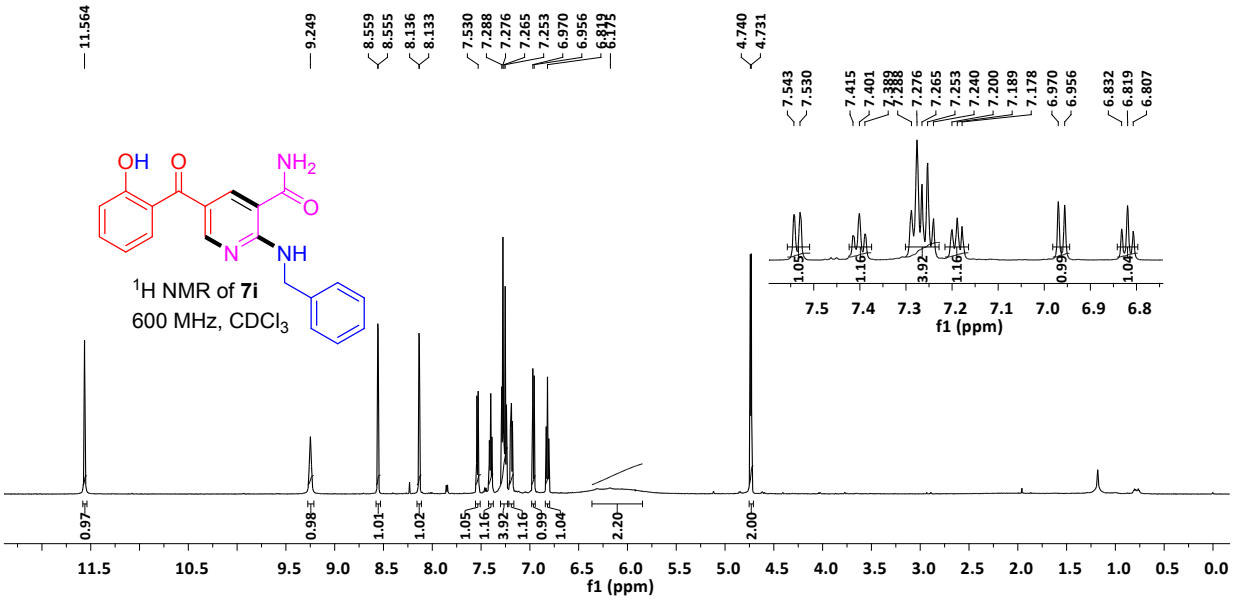

OH
O
OEt
O
N
NH
^{13}C NMR of **7g**
150 MHz, $CDCl_3$
f1 (ppm)

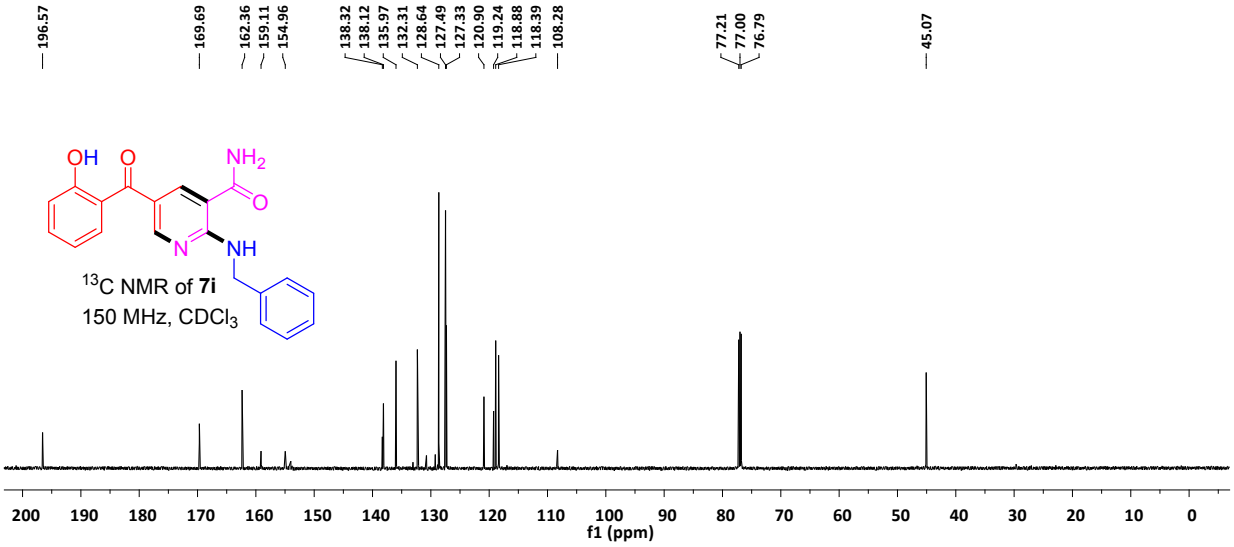


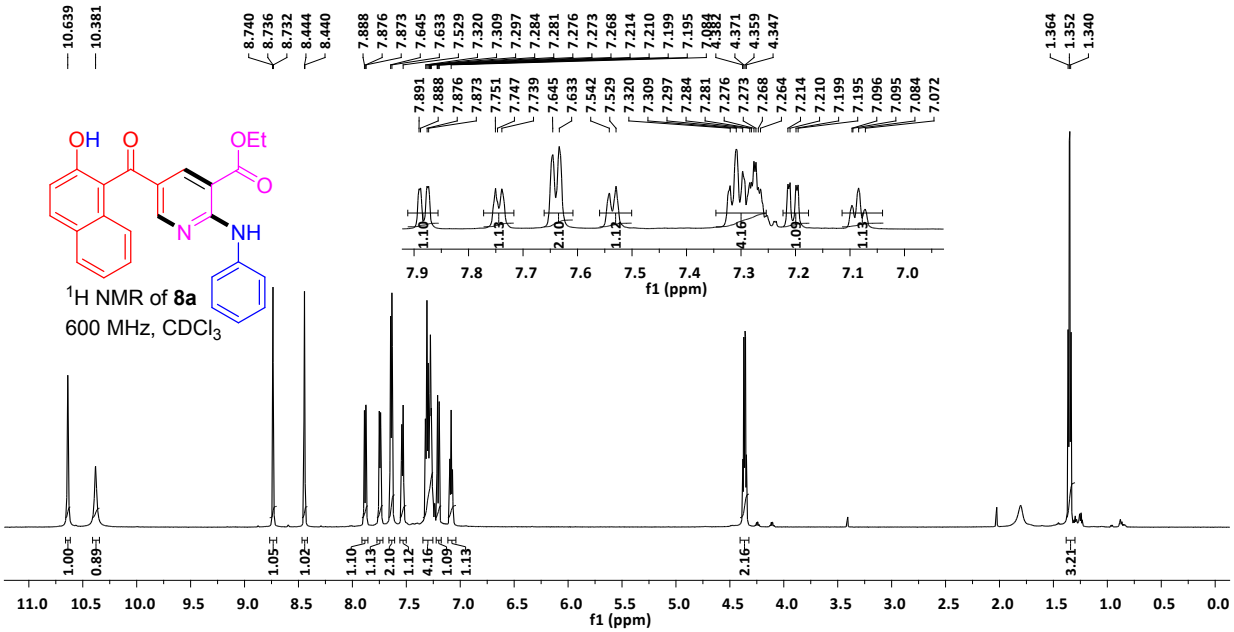
^{1}H NMR of **7h**
600 MHz, $CDCl_3$

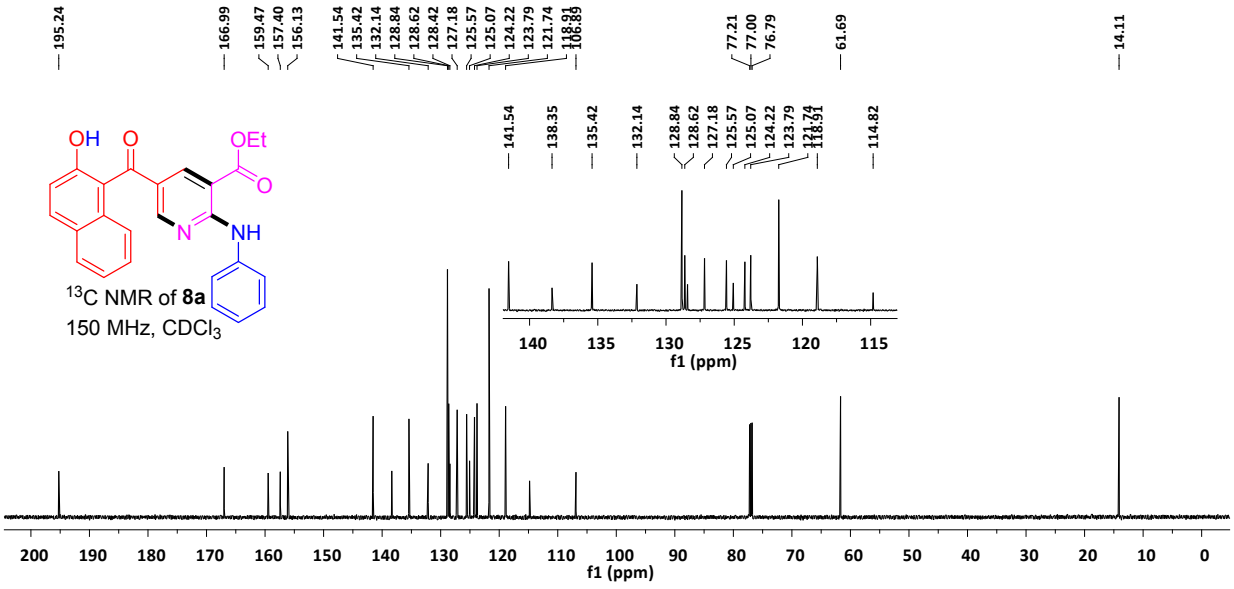


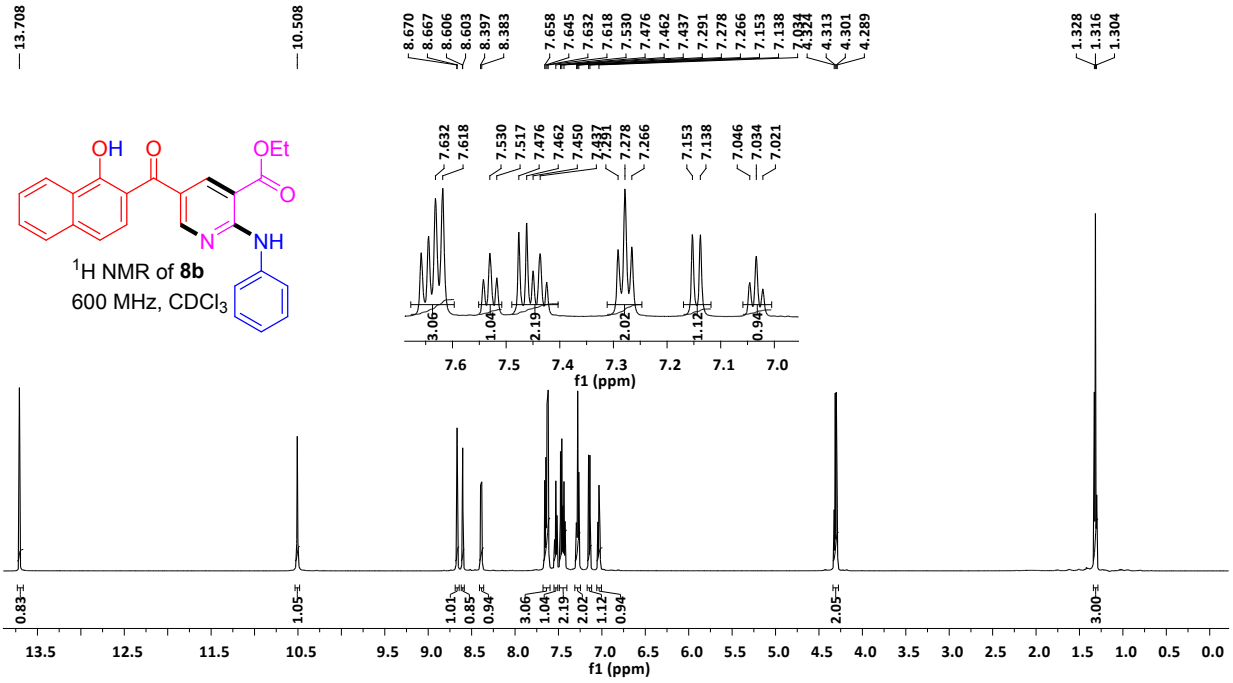
^{13}C NMR of **7h**
150 MHz, $CDCl_3$

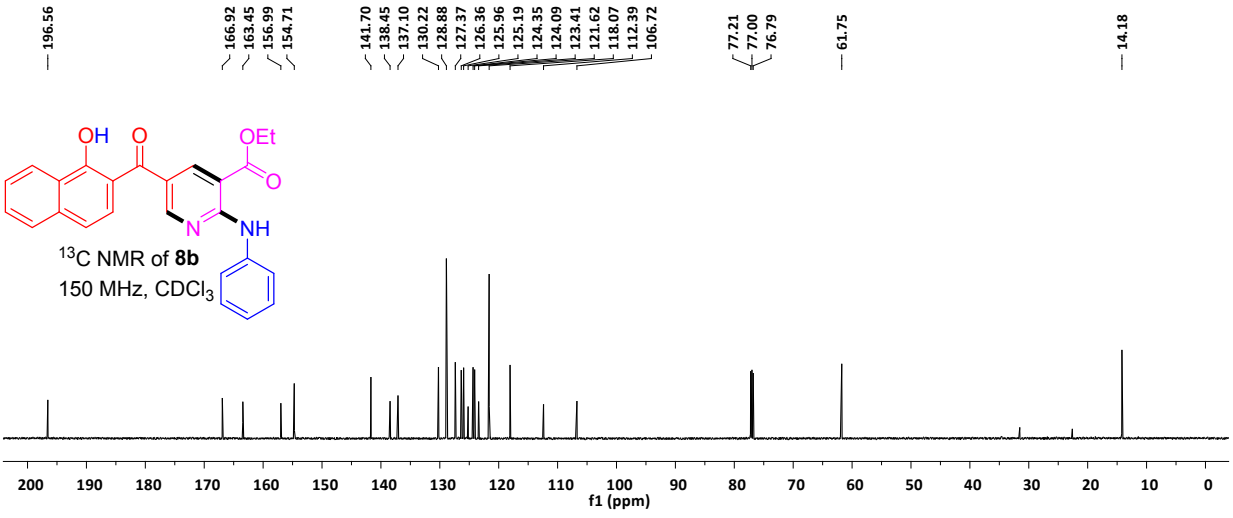

11.564
9.249
8.559
8.555
8.136
8.133
7.530
7.288
7.276
7.265
7.253
6.970
6.956
4.740
4.731
7.543
7.530
7.415
7.401
7.276
7.265
7.253
7.240
7.200
7.189
7.178
6.970
6.956
6.832
6.819
6.807
OH
O
NH2
O
N
NH
1H NMR of 7i
600 MHz, CDCl3
f1 (ppm)


196.57
169.69
162.36
159.11
154.96
138.32
138.12
135.97
132.31
128.64
127.49
127.33
120.90
119.24
118.88
118.39
108.28
77.21
77.00
76.79
45.07
OH
O
NH2
O
N
NH
13C NMR of 7i
150 MHz, CDCl3
f1 (ppm)


OH
O
OEt
O
N
NH
^{1}H NMR of **8a**
600 MHz, $CDCl_3$
f1 (ppm)


OH
O
OEt
O
N
NH
^{13}C NMR of **8a**
150 MHz, $CDCl_3$
f1 (ppm)


13.708
10.508
8.670
8.667
8.606
8.603
8.397
8.383
7.658
7.645
7.632
7.618
7.530
7.517
7.476
7.462
7.450
7.437
7.291
7.278
7.266
7.153
7.138
7.046
7.034
7.021
4.313
4.301
4.289
1.328
1.316
1.304
OH
O
OEt
O
N
NH
1H NMR of 8b
600 MHz, CDCl3
3.06
1.04
2.19
2.02
1.12
0.94
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
0.83
1.05
1.01
0.85
0.94
3.06
1.04
2.19
2.02
1.12
0.94
2.05
3.00
13.5
12.5
11.5
10.5
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)


196.56
166.92
163.45
156.99
154.71
141.70
138.45
137.10
130.22
128.88
127.37
126.36
125.96
125.19
124.35
124.09
123.41
121.62
118.07
112.39
106.72
77.21
77.00
76.79
61.75
14.18
OH
O
OEt
O
N
NH
13C NMR of 8b
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

X-Ray crystallographic data of compound 5c: Empirical Formula- C_{23} H_{22} N_2 O_4, M = 390.43, Monoclinic, Space group P2(1)/c, a = 12.1869(5) Å, b = 14.4300(6) Å, c = 12.8949(5) Å, V = 2039.18(14) $Å^3$, Z = 4, T = 296(2) K, ρ_{calcd} = 1.272 Mg/m^3, $2\Theta_{max.}$ = 28.35^0, Refinement of 264 parameters on 5091 independent reflections out of 73769 collected reflections (R_{int} = 0.0800) led to R_1 = 0.0471 [I >2σ(I)], wR_2 = 0.1242 (all data) and S = 1.024 with the largest difference peak and hole of 0.255 and -0.214 e. $Å^{-3}$ respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1501115). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

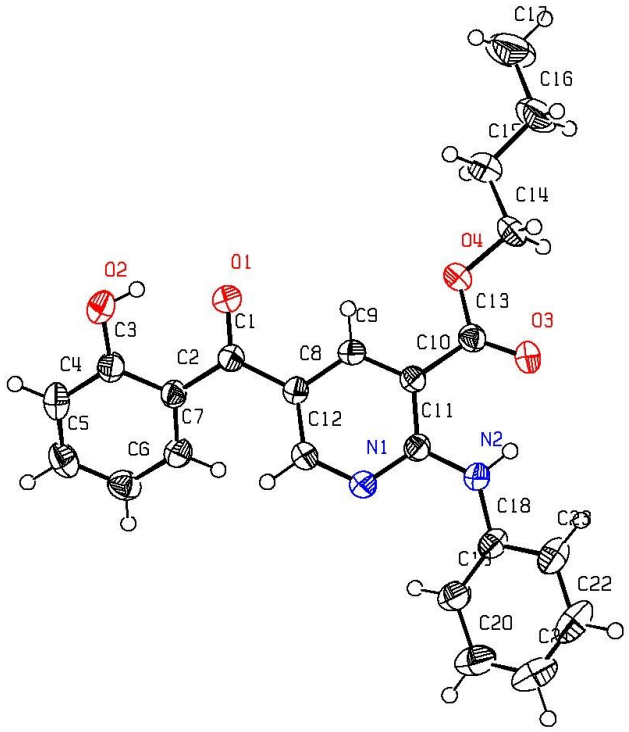


Fig. S1 X-Ray Structure of Compound **5c**.

X-Ray Data of Compound 5c

Table S1 Crystal data and structure refinement for **5c**.

Identification code	**5c**	
Empirical formula	$C_{23}\ H_{22}\ N_2\ O_4$	
Formula weight	390.43	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.1869(5) Å	α= 90°.
	b = 14.4300(6) Å	β= 115.9411(17)°.
	c = 12.8949(5) Å	γ = 90°.
Volume	2039.18(14) $Å^3$	
Z	4	
Density (calculated)	1.272 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	824	
Crystal size	0.21 x 0.18 x 0.07 mm^3	
Theta range for data collection	2.25 to 28.35°.	
Index ranges	-16<=h<=16, -19<=k<=19, -17<=l<=17	
Reflections collected	73769	
Independent reflections	5091 [R(int) = 0.0800]	
Completeness to theta = 28.35°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9939 and 0.9818	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5091 / 0 / 264	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1063	
R indices (all data)	R1 = 0.0866, wR2 = 0.1242	
Largest diff. peak and hole	0.255 and -0.214 e.$Å^{-3}$	

Table S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5c**

	x	y	z	U(eq)
C(1)	10493(1)	6132(1)	3712(1)	34(1)
O(1)	11608(1)	5993(1)	4145(1)	46(1)
C(2)	9880(1)	6329(1)	4447(1)	32(1)
C(3)	10496(1)	6138(1)	5638(1)	37(1)
O(2)	11649(1)	5812(1)	6140(1)	49(1)
C(4)	9913(2)	6275(1)	6338(1)	45(1)
C(5)	8752(2)	6624(1)	5884(2)	48(1)
C(6)	8147(2)	6862(1)	4727(2)	44(1)
C(7)	8712(1)	6717(1)	4025(1)	38(1)
C(8)	9807(1)	6075(1)	2440(1)	32(1)
C(9)	10417(1)	6266(1)	1767(1)	32(1)
C(10)	9846(1)	6159(1)	591(1)	31(1)
C(11)	8610(1)	5845(1)	81(1)	31(1)
N(1)	8026(1)	5638(1)	724(1)	34(1)
C(12)	8619(1)	5748(1)	1860(1)	34(1)
C(13)	10510(1)	6343(1)	-111(1)	33(1)
O(3)	10084(1)	6234(1)	-1148(1)	45(1)
O(4)	11640(1)	6632(1)	520(1)	41(1)
C(14)	12409(1)	6747(1)	-75(1)	42(1)
C(15)	13625(2)	7088(1)	789(2)	47(1)
C(16)	14525(2)	7150(2)	279(2)	74(1)
C(17)	15775(2)	7448(2)	1129(2)	94(1)
N(2)	8005(1)	5725(1)	-1076(1)	38(1)
C(18)	6798(1)	5424(1)	-1755(1)	38(1)
C(19)	5840(2)	5590(1)	-1480(2)	51(1)
C(20)	4677(2)	5307(2)	-2222(2)	65(1)
C(21)	4455(2)	4853(2)	-3226(2)	67(1)
C(22)	5402(2)	4689(1)	-3505(2)	61(1)
C(23)	6575(2)	4977(1)	-2779(1)	47(1)

Table S3 Bond lengths [Å] and angles [°] for **5c**.

C(1)-O(1)#1	1.2384(17)
C(1)-O(1)	1.2384(17)
C(1)-C(2)	1.469(2)
C(1)-C(8)	1.4821(19)
C(2)-C(7)	1.399(2)
C(2)-C(3)	1.411(2)
C(3)-O(2)	1.3489(19)
C(3)-C(4)	1.385(2)
O(2)-H(2)	0.8200
C(4)-C(5)	1.369(2)
C(4)-H(4)	0.9300
C(5)-C(6)	1.387(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.373(2)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(12)	1.389(2)
C(8)-C(9)	1.3943(19)
C(9)-C(10)	1.3729(19)
C(9)-H(9)	0.9300
C(10)-C(11)	1.4286(19)
C(10)-C(13)	1.4781(19)
C(11)-N(1)	1.3415(18)
C(11)-N(2)	1.3548(18)
N(1)-C(12)	1.3295(18)
C(12)-H(12)	0.9300
C(13)-O(3)#1	1.2139(17)
C(13)-O(3)	1.2139(17)
C(13)-O(4)	1.3240(17)
O(4)-C(14)	1.4571(17)
C(14)-C(15)	1.496(2)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.508(2)

C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.498(3)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
N(2)-C(18)	1.4115(19)
N(2)-H(2N)	0.8600
C(18)-C(19)	1.381(2)
C(18)-C(23)	1.386(2)
C(19)-C(20)	1.381(2)
C(19)-H(19)	0.9300
C(20)-C(21)	1.368(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.371(3)
C(21)-H(21)	0.9300
C(22)-C(23)	1.387(2)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300

O(1)#1-C(1)-C(2)	120.49(13)
O(1)-C(1)-C(2)	120.49(13)
O(1)#1-C(1)-C(8)	117.85(13)
O(1)-C(1)-C(8)	117.85(13)
C(2)-C(1)-C(8)	121.65(13)
C(7)-C(2)-C(3)	117.88(13)
C(7)-C(2)-C(1)	123.00(13)
C(3)-C(2)-C(1)	119.11(13)
O(2)-C(3)-C(4)	117.44(14)
O(2)-C(3)-C(2)	122.45(13)
C(4)-C(3)-C(2)	120.11(15)
C(3)-O(2)-H(2)	109.5
C(5)-C(4)-C(3)	120.15(15)
C(5)-C(4)-H(4)	119.9

C(3)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	121.03(15)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(7)-C(6)-C(5)	119.13(16)
C(7)-C(6)-H(6)	120.4
C(5)-C(6)-H(6)	120.4
C(6)-C(7)-C(2)	121.56(15)
C(6)-C(7)-H(7)	119.2
C(2)-C(7)-H(7)	119.2
C(12)-C(8)-C(9)	116.50(13)
C(12)-C(8)-C(1)	124.40(13)
C(9)-C(8)-C(1)	118.74(13)
C(10)-C(9)-C(8)	120.92(13)
C(10)-C(9)-H(9)	119.5
C(8)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	117.89(12)
C(9)-C(10)-C(13)	120.52(13)
C(11)-C(10)-C(13)	121.57(13)
N(1)-C(11)-N(2)	118.15(13)
N(1)-C(11)-C(10)	121.54(12)
N(2)-C(11)-C(10)	120.29(13)
C(12)-N(1)-C(11)	118.35(12)
N(1)-C(12)-C(8)	124.74(13)
N(1)-C(12)-H(12)	117.6
C(8)-C(12)-H(12)	117.6
O(3)#1-C(13)-O(4)	123.12(13)
O(3)-C(13)-O(4)	123.12(13)
O(3)#1-C(13)-C(10)	124.51(14)
O(3)-C(13)-C(10)	124.51(14)
O(4)-C(13)-C(10)	112.36(12)
C(13)-O(4)-C(14)	116.58(12)
O(4)-C(14)-C(15)	107.55(13)
O(4)-C(14)-H(14A)	110.2
C(15)-C(14)-H(14A)	110.2
O(4)-C(14)-H(14B)	110.2

C(15)-C(14)-H(14B)	110.2
H(14A)-C(14)-H(14B)	108.5
C(14)-C(15)-C(16)	111.60(15)
C(14)-C(15)-H(15A)	109.3
C(16)-C(15)-H(15A)	109.3
C(14)-C(15)-H(15B)	109.3
C(16)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	108.0
C(17)-C(16)-C(15)	113.48(19)
C(17)-C(16)-H(16A)	108.9
C(15)-C(16)-H(16A)	108.9
C(17)-C(16)-H(16B)	108.9
C(15)-C(16)-H(16B)	108.9
H(16A)-C(16)-H(16B)	107.7
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(11)-N(2)-C(18)	129.75(13)
C(11)-N(2)-H(2N)	115.1
C(18)-N(2)-H(2N)	115.1
C(19)-C(18)-C(23)	119.36(15)
C(19)-C(18)-N(2)	123.78(14)
C(23)-C(18)-N(2)	116.79(14)
C(20)-C(19)-C(18)	119.84(17)
C(20)-C(19)-H(19)	120.1
C(18)-C(19)-H(19)	120.1
C(21)-C(20)-C(19)	121.00(19)
C(21)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(20)-C(21)-C(22)	119.40(18)
C(20)-C(21)-H(21)	120.3
C(22)-C(21)-H(21)	120.3
C(21)-C(22)-C(23)	120.56(18)

C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(18)-C(23)-C(22)	119.83(17)
C(18)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(1)	39(1)	30(1)	0(1)	13(1)	-4(1)
O(1)	31(1)	72(1)	34(1)	0(1)	13(1)	0(1)
C(2)	35(1)	35(1)	28(1)	-3(1)	14(1)	-5(1)
C(3)	40(1)	37(1)	31(1)	0(1)	15(1)	-5(1)
O(2)	44(1)	67(1)	31(1)	8(1)	13(1)	7(1)
C(4)	62(1)	44(1)	33(1)	0(1)	25(1)	-2(1)
C(5)	60(1)	48(1)	50(1)	-7(1)	37(1)	-4(1)
C(6)	40(1)	44(1)	51(1)	-8(1)	23(1)	-1(1)
C(7)	38(1)	41(1)	33(1)	-5(1)	14(1)	-3(1)
C(8)	31(1)	36(1)	27(1)	0(1)	12(1)	1(1)
C(9)	26(1)	36(1)	32(1)	-1(1)	12(1)	1(1)
C(10)	30(1)	35(1)	30(1)	-1(1)	14(1)	2(1)
C(11)	30(1)	34(1)	29(1)	-2(1)	12(1)	4(1)
N(1)	30(1)	41(1)	31(1)	-4(1)	14(1)	-3(1)
C(12)	33(1)	41(1)	32(1)	-1(1)	17(1)	-1(1)
C(13)	33(1)	35(1)	34(1)	2(1)	16(1)	5(1)
O(3)	45(1)	63(1)	32(1)	-4(1)	21(1)	-3(1)
O(4)	34(1)	56(1)	38(1)	2(1)	20(1)	-3(1)
C(14)	41(1)	49(1)	46(1)	2(1)	30(1)	-1(1)
C(15)	41(1)	51(1)	56(1)	0(1)	26(1)	-2(1)
C(16)	56(1)	98(2)	86(2)	-17(1)	47(1)	-24(1)
C(17)	54(1)	119(2)	118(2)	-29(2)	48(1)	-29(1)
N(2)	32(1)	53(1)	28(1)	-5(1)	13(1)	-1(1)
C(18)	35(1)	41(1)	30(1)	-1(1)	8(1)	4(1)
C(19)	35(1)	71(1)	41(1)	-10(1)	11(1)	1(1)
C(20)	36(1)	86(2)	60(1)	-4(1)	9(1)	-1(1)
C(21)	45(1)	66(1)	61(1)	-5(1)	-4(1)	-6(1)
C(22)	68(1)	53(1)	38(1)	-10(1)	-1(1)	3(1)
C(23)	50(1)	48(1)	32(1)	-3(1)	9(1)	7(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **5c.**

	x	y	z	U(eq)
H(2)	11931	5809	5668	73
H(4)	10312	6131	7119	54
H(5)	8363	6702	6358	58
H(6)	7368	7117	4431	53
H(7)	8310	6881	3250	46
H(9)	11222	6469	2121	38
H(12)	8209	5596	2298	41
H(14A)	12044	7190	-699	50
H(14B)	12499	6160	-396	50
H(15A)	13941	6671	1445	57
H(15B)	13530	7695	1062	57
H(16A)	14584	6549	-29	89
H(16B)	14220	7587	-357	89
H(17A)	15739	8070	1378	140
H(17B)	16319	7427	771	140
H(17C)	16067	7040	1782	140
H(2N)	8419	5851	-1454	45
H(19)	5979	5892	-796	61
H(20)	4033	5426	-2037	78
H(21)	3670	4658	-3716	80
H(22)	5256	4382	-4187	74
H(23)	7211	4870	-2979	56

Table S6. Torsion angles [°] for **5c**.

C(2)-C(1)-O(1)-O(1)#1	0.00(11)
C(8)-C(1)-O(1)-O(1)#1	0.00(11)
O(1)#1-C(1)-C(2)-C(7)	163.29(15)
O(1)-C(1)-C(2)-C(7)	163.29(15)
C(8)-C(1)-C(2)-C(7)	-17.9(2)
O(1)#1-C(1)-C(2)-C(3)	-15.4(2)
O(1)-C(1)-C(2)-C(3)	-15.4(2)
C(8)-C(1)-C(2)-C(3)	163.44(14)
C(7)-C(2)-C(3)-O(2)	-176.20(14)
C(1)-C(2)-C(3)-O(2)	2.6(2)
C(7)-C(2)-C(3)-C(4)	4.4(2)
C(1)-C(2)-C(3)-C(4)	-176.89(14)
O(2)-C(3)-C(4)-C(5)	178.54(16)
C(2)-C(3)-C(4)-C(5)	-2.0(2)
C(3)-C(4)-C(5)-C(6)	-1.3(3)
C(4)-C(5)-C(6)-C(7)	2.1(3)
C(5)-C(6)-C(7)-C(2)	0.5(2)
C(3)-C(2)-C(7)-C(6)	-3.6(2)
C(1)-C(2)-C(7)-C(6)	177.68(15)
O(1)#1-C(1)-C(8)-C(12)	145.74(16)
O(1)-C(1)-C(8)-C(12)	145.74(16)
C(2)-C(1)-C(8)-C(12)	-33.1(2)
O(1)#1-C(1)-C(8)-C(9)	-27.1(2)
O(1)-C(1)-C(8)-C(9)	-27.1(2)
C(2)-C(1)-C(8)-C(9)	154.03(14)
C(12)-C(8)-C(9)-C(10)	1.9(2)
C(1)-C(8)-C(9)-C(10)	175.29(14)
C(8)-C(9)-C(10)-C(11)	-0.1(2)
C(8)-C(9)-C(10)-C(13)	-178.65(14)
C(9)-C(10)-C(11)-N(1)	-1.6(2)
C(13)-C(10)-C(11)-N(1)	176.99(13)
C(9)-C(10)-C(11)-N(2)	-179.83(14)
C(13)-C(10)-C(11)-N(2)	-1.3(2)
N(2)-C(11)-N(1)-C(12)	179.55(14)

C(10)-C(11)-N(1)-C(12)	1.2(2)
C(11)-N(1)-C(12)-C(8)	0.8(2)
C(9)-C(8)-C(12)-N(1)	-2.3(2)
C(1)-C(8)-C(12)-N(1)	-175.32(15)
C(9)-C(10)-C(13)-O(3)#1	177.33(15)
C(11)-C(10)-C(13)-O(3)#1	-1.2(2)
C(9)-C(10)-C(13)-O(3)	177.33(15)
C(11)-C(10)-C(13)-O(3)	-1.2(2)
C(9)-C(10)-C(13)-O(4)	-1.8(2)
C(11)-C(10)-C(13)-O(4)	179.71(13)
O(4)-C(13)-O(3)-O(3)#1	0.00(9)
C(10)-C(13)-O(3)-O(3)#1	0.00(5)
O(3)#1-C(13)-O(4)-C(14)	-4.9(2)
O(3)-C(13)-O(4)-C(14)	-4.9(2)
C(10)-C(13)-O(4)-C(14)	174.20(13)
C(13)-O(4)-C(14)-C(15)	179.14(14)
O(4)-C(14)-C(15)-C(16)	175.08(16)
C(14)-C(15)-C(16)-C(17)	-177.4(2)
N(1)-C(11)-N(2)-C(18)	1.6(2)
C(10)-C(11)-N(2)-C(18)	179.92(14)
C(11)-N(2)-C(18)-C(19)	31.3(3)
C(11)-N(2)-C(18)-C(23)	-151.97(16)
C(23)-C(18)-C(19)-C(20)	0.3(3)
N(2)-C(18)-C(19)-C(20)	176.97(18)
C(18)-C(19)-C(20)-C(21)	0.7(3)
C(19)-C(20)-C(21)-C(22)	-0.8(3)
C(20)-C(21)-C(22)-C(23)	0.1(3)
C(19)-C(18)-C(23)-C(22)	-1.1(3)
N(2)-C(18)-C(23)-C(22)	-177.96(16)
C(21)-C(22)-C(23)-C(18)	0.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z

Table S7. Hydrogen bonds for **5c** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)#1	0.82	1.84	2.5637(15)	145.7
N(2)-H(2N)...O(3)#1	0.86	1.97	2.6778(16)	139.0

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z