A Multi-component Synthesis of *N*-Substituted 2-Amino-3-Cyano Pyrroles *via* Ring-opening of Nitroepoxides

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Supporting Information

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General information

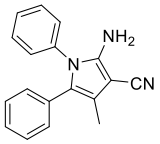
Unless otherwise noted, all reagents were obtained from commercial suppliers and used without any purification. All solvents were purified according to standard methods prior to use. Purifications of final products were carried out by chromatography using silica gel (200-300 mesh). Melting points were recorded on a melting point apparatus. NMR spectra were recorded for ^{1}H NMR at 500 MHz and for ^{13}C NMR at 125 MHz. For ^{1}H NMR, tetramethylsilane (TMS) served as internal standard (δ=0) and data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constant(s) in Hz. For ^{13}C NMR, TMS (δ=0) or $CDCl_3$ (δ=77.26) was used as internal standard and spectra were obtained with complete proton decoupling. HRMS of all final products were confirmed on a HPLC- Time of Fight Mass Spectrometer.

General procedure for the synthesis of 4

A solution of nitroepoxides **1** (1.0 mmol), amine **2** (1.0 mmol), malononitrile **3** (1.2 mmol), K_2CO_3 (1.0 mmol) in methanol was stirred at 60 °C for 3.0 h. Then, water was added (10 mL), and extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over $MgSO_4$ and concentrated under vacuum to afford a residue which was purified by silica gel chromatography (hexanes : ethyl acetate, 15:1) to give the pure product **4**.

Characterization Data of 4:

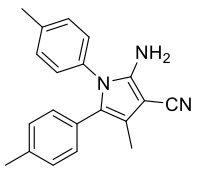
2-amino-4-methyl-1, 5-diphenyl-1H-pyrrole-3-carbonitrile (**4a**)



4a,88%

Yellow solid, mp 186.3-187.6 °C, yield 88%. ^{1}H NMR (500 MHz, DMSO) δ 7.39-7.31 (m, 3H), 7.19-7.05 (m, 5H), 7.00-6.93 (m, 2H), 5.65 (s, 2H), 2.04 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ148.1, 136.4, 131.6, 129.9, 129.7, 128.8, 128.5, 128.4, 126.6, 123.7, 118.0, 116.4, 73.6, 11.1. HRMS (ESI): m/z calcd for $(C_{18}H_{15}N_3+H)^+$: 274.1339; found: 274.1340.

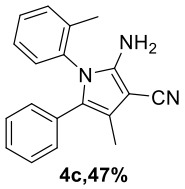
2-amino-4-methyl-1, 5-di-p-tolyl-1H-pyrrole-3-carbonitrile (**4b**)



4b,83%

Yellow solid, mp 171.0-172.1 °C, yield 83%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.16 (d, *J* = 8.0 Hz, 2H), 7.00-6.98 (m, 4H), 6.86 (d, *J* = 8.0 Hz, 2H), 4.03 (s, 2H), 2.34 (s, 3H), 2.27 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.3, 138.4, 136.2, 133.2, 130.3, 129.6, 128.7, 128.1, 127.7, 124.6, 117.5, 116.3, 75.3, 21.2, 10.8. HRMS (ESI): m/z calcd for $(C_{20}H_{19}N_3+H)^+$: 302.1652; found: 302.1655.

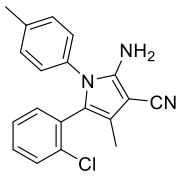
2-amino-4-methyl-5-phenyl-1-(*o*-tolyl)-1H-pyrrole-3-carbonitrile (**4c**)



4c,47%

Yellow solid, mp 97.8-98.4 °C, yield 47%. ^{1}H NMR (500 MHz, DMSO) δ 7.32-7.28 (m, 1H), 7.26-7.24 (m, 3H), 7.17 (t, *J* = 7.4 Hz, 2H), 7.10 (t, *J* = 7.3 Hz, 1H), 6.99 (d, *J* = 8 Hz, 2H), 5.56 (s, 2H), 2.07 (s, 3H), 1.91 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.2, 137.1, 134.6, 131.5, 131.0, 129.5, 129.4, 129.3, 127.9, 127.1, 126.6, 124.7, 117.5, 116.6, 75.1, 17.51, 10.9. HRMS (ESI): m/z calcd for $(C_{19}H_{17}N_3+H)^+$: 288.1495; found: 288.1499.

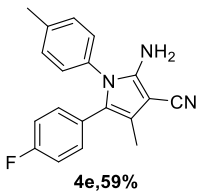
2-amino-5-(2-chlorophenyl)-4-methyl-1-(*p*-tolyl)-1H-pyrrole-3-carbonitrile (**4d**)



4d,56%

Yellow solid, mp 114.8-115.1 °C, yield 56%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.18-7.15 (m, 1H), 7.12-7.06 (m, 4H), 6.99 (d, *J* = 8.3 Hz, 2H), 4.05 (s, 2H), 2.29 (s, 3H), 2.00 (s, 3H). ^{13}C NMR (125MHz, DMSO) δ 147.7, 137.9, 135.0, 134.3, 133.3, 130.8, 130.1, 129.6, 128.0, 127.2, 120.9, 117.9, 117.1, 112.6, 73.1, 21.1, 10.8. HRMS (ESI): m/z calcd for $(C_{19}H_{16}ClN_3+H)^+$: 322.1106; found: 322.1104.

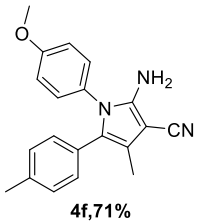
2-amino-5-(4-fluorophenyl)-4-methyl-1-(p-tolyl)-1H-pyrrole-3-carbonitrile (**4e**)



4e,59%

Yellow solid, mp 178.0-179.1 °C, yield 59%. ^{1}H NMR (500 MHz, DMSO) δ 7.18 (d, *J* = 7.9 Hz, 2H), 7.06-6.96 (m, 6H), 5.62 (s, 2H), 2.29 (s, 3H), 2.00 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 160.5(d, *J* = 240.3 Hz), 147.4, 137.4, 133.0, 131.3(d, *J* = 8.0 Hz), 129.8, 128.0, 122.2, 117.4, 115.7, 114.8(d, *J* = 21.5Hz), 72.8, 20.5, 10.4. HRMS (ESI): m/z calcd for $(C_{19}H_{16}FN_3+H)^+$: 306.1401; found: 306.1402.

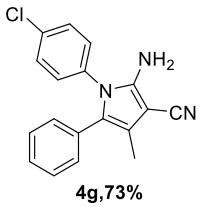
2-amino-1-(4-methoxyphenyl)-4-methyl-5-(p-tolyl)-1H-pyrrole-3-carbonitrile (**4f**)



4f,71%

Yellow solid, mp 162.9-163.1 °C, yield 71%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.04 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 7.9 Hz, 2H), 6.89 -6.84 (m, 4H), 4.02 (s, 2H), 3.80 (s, 3H), 2.27 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 159.3, 145.4, 136.2, 129.7, 129.2, 128.7, 128.4, 128.1, 124.7, 117.5, 116.1, 114.8, 75.1, 55.5, 21.2, 10.8. HRMS (ESI): m/z calcd for $(C_{20}H_{19}N_3O+H)^+$: 318.1601; found: 318.1605.

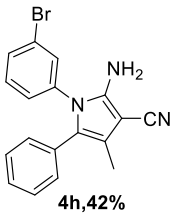
2-amino-1-(4-chlorophenyl)-4-methyl-5-phenyl-1H-pyrrole-3-carbonitrile (**4g**)



4g,73%

Yellow solid, mp 165.3-166.1 °C, yield 73%. ^{1}H NMR (500 MHz, DMSO) δ 7.43 (d, *J* = 8.6 Hz, 2H), 7.22-7.11 (m, 5H), 6.97 (d, *J* = 7.3 Hz, 2H), 5.80 (s, 2H), 2.02 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.7, 139.5, 134.4, 130.7, 129.9, 129.8, 129.2, 128.2, 126.8, 124.4, 117.3, 117.0, 76.2, 10.7. HRMS (ESI): m/z calcd for $(C_{18}H_{14}ClN_3+H)^+$: 308.0949; found: 308.0950.

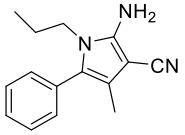
2-amino-1-(3-bromophenyl)-4-methyl-5-phenyl-1H-pyrrole-3-carbonitrile (**4h**)



4h,42%

Yellow solid, mp 168.8-169.6 °C, yield 42%. ^{1}H NMR (500 MHz, DMSO) δ 7.52 (d, *J* = 8.0 Hz, 1H), 7.40 (s, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 2H), 7.12 (m, 2H), 6.98 (d, *J* = 7.3 Hz, 2H), 5.84 (s, 2H), 2.02 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 148.3, 137.9, 131.6, 131.5, 129.9, 128.5, 128.1, 126.9, 124.6, 123.8, 122.1, 117.8, 116.6, 88.9, 77.1, 11.0. HRMS (ESI): m/z calcd for $(C_{18}H_{14}BrN_3+H)^+$: 352.0444; found: 352.0449.

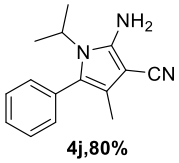
2-amino-4-methyl-5-phenyl-1-propyl-1H-pyrrole-3-carbonitrile (**4i**)



4i,89%

Yellow solid, mp 90.8-91.4 ºC, yield 89%. ^{1}H NMR (500 MHz, DMSO) δ 7.42 (t, *J* = 7.5 Hz, 2H), 7.33 (d, *J* = 7.3 Hz, 1H), 7.24 (d, *J* = 7.4 Hz, 2H), 5.92 (s, 2H), 3.65-3.58 (m, 2H), 1.88 (s, 3H), 1.37-1.26 (m, 2H), 0.59 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 147.8, 132.0, 130.4, 128.9, 127.5, 123.5, 118.6, 115.1, 72.5, 44.2, 22.5, 11.1, 10.8. HRMS (ESI): m/z calcd for $(C_{15}H_{17}N_3+H)^+$: 240.1495; found: 240.1499.

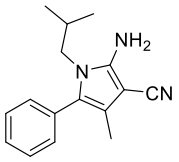
2-amino-1-isopropyl-4-methyl-5-phenyl-1H-pyrrole-3-carbonitrile (**4j**)



4j,80%

Yellow solid, mp 126.8-127.1 ºC, yield 80%. ^{1}H NMR (500 MHz, DMSO) δ 7.43 (t, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 7.1 Hz, 2H), 5.60 (s, 2H), 4.17-4.07 (m, 1H), 1.81 (s, 3H), 1.28 (d, *J* = 7.1 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.9, 132.5, 131.1, 128.9, 127.8, 124.1, 118.4, 115.1, 74.4, 47.7, 21.0, 10.8. HRMS (ESI): m/z calcd for $(C_{15}H_{17}N_3+H)^+$: 240.1495; found: 240.1494.

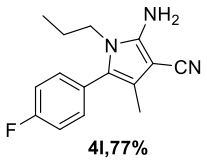
2-amino-1-isobutyl-4-methyl-5-phenyl-1H-pyrrole-3-carbonitrile (**4k**)



4k,86%

Yellow solid, mp 104.5-105.1 ºC, yield 86%. ^{1}H NMR (500 MHz, DMSO) δ 7.41 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 7.0 Hz, 2H), 5.93 (s, 2H), 3.55 (d, *J* = 7.6 Hz, 2H), 1.89 (s, 3H), 1.63-1.58 (m, 1H), 0.54 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (125 MHz, DMSO) δ 148.2, 132.3, 130.4, 128.9, 127.3, 123.8, 118.6, 115.2, 72.4, 49.6, 28.0, 19.8, 10.8. HRMS (ESI): m/z calcd for $(C_{16}H_{19}N_3+H)^+$: 254.1652; found: 254.1657.

2-amino-5-(4-fluorophenyl)-4-methyl-1-propyl-1H-pyrrole-3-carbonitrile (**4l**)

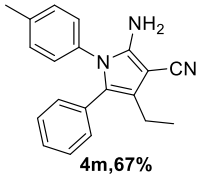


4l,77%

Yellow solid, mp 176.8-177.1 ºC, yield 77%. ^{1}H NMR (500 MHz, DMSO) δ 7.39-7.21 (m, 4H), 5.93 (s, 2H), 3.65-3.53 (m, 2H), 1.86 (s, 3H), 1.31 (d, *J* = 7.4 Hz, 2H), 0.60 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, DMSO) δ 161.7(d, *J* = 242.9 Hz), 147.7,

132.6(d, *J* = 8 Hz), 128.4, 122.3, 118.5, 115.9 (d, *J* = 21.1 Hz), 115.3, 72.4, 44.1, 22.5, 11.1, 10.7. HRMS (ESI): m/z calcd for $(C_{15}H_{16}FN_3+H)^+$: 258.1401; found: 258.1404.

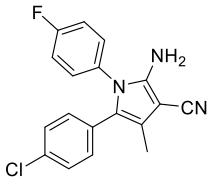
2-amino-4-ethyl-5-phenyl-1-(p-tolyl)-1H-pyrrole-3-carbonitrile (**4m**)



4m,67%

Yellow solid, mp 118.0-119.1 ºC, yield 67%. ^{1}H NMR (500 MHz, DMSO) δ 7.21-7.11 (m, 5H), 7.01 (d, *J* = 8.1 Hz, 2H), 6.97 (d, *J* = 7.3 Hz, 2H), 5.58 (s, 2H), 2.40-2.36 (m, 2H), 2.27 (s, 3H), 1.14 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (125MHz, DMSO) δ 148.3, 137.8, 133.7, 131.6, 130.3, 130.0, 129.9, 128.5, 128.4, 126.9, 122.2, 118.1, 72.0, 21.1, 18.9, 15.8. HRMS (ESI): m/z calcd for $(C_{20}H_{19}N_3+H)^+$: 302.1652; found: 302.1654.

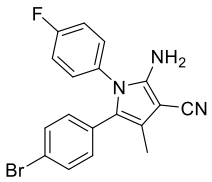
2-amino-5-(4-chlorophenyl)-1-(4-fluorophenyl)-4-methyl-1H-pyrrole-3-carbonitrile (**4n**)



4n,78%

White solid, mp 163.2-164.1 ºC, yield 78%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.11-7.07 (m, 2H), 7.03-7.01 (m, 4H), 6.84-6.78 (m, 2H), 4.01 (s, 2H), 2.08 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.1(d, *J* = 249.1 Hz), 144.6, 131.6, 130.5, 129.9, 128.8(d, *J* = 8.5 Hz), 128.2, 127.4, 122.4, 116.6, 116.0(d, *J* = 23.0 Hz), 115.9, 74.9, 9.7. HRMS (ESI): m/z calcd for $(C_{18}H_{13}ClFN_3+H)^+$: 326.0855; found: 326.0857.

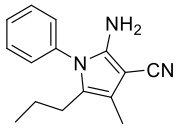
2-amino-5-(4-bromophenyl)-1-(4-fluorophenyl)-4-methyl-1H-pyrrole-3-carbonitrile (**4o**)



4o,64%

White solid, mp 208.2-209.3 ºC, yield 64%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.5 Hz, 2H), 7.03-7.01 (m, 4H), 6.75 (d, *J* = 8.5 Hz, 2H), 4.01 (s, 2H), 2.08 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.3(d, *J* = 248.75 Hz), 145.7, 131.7, 131.6, 131.5, 131.3, 129.9(d, *J* = 8.75 Hz), 123.5, 120.9, 117.8, 117.1 (d, *J* = 22.5 Hz), 76.2, 10.9. HRMS (ESI): m/z calcd for $(C_{18}H_{13}BrFN_3+H)$+: 370.0350; found: 370.0356.

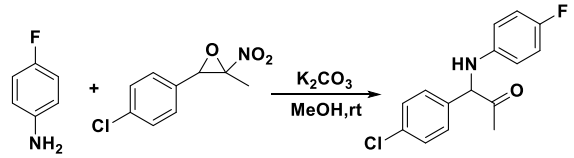
2-amino-4-methyl-1-phenyl-5-propyl-1H-pyrrole-3-carbonitrile(**4p**)



4p,57%

Tan liquid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53-7.48 (m, 3H), 7.25 (d, *J* = 5.7 Hz, 2H), 3.79 (s, 2H), 2.25 (t, *J* = 6.0 Hz, 2H), 2.07 (s, 3H), 1.19-1.15 (m, 2H), 0.71 (t, *J* = 5.9 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.3, 135.6, 129.9, 129.2, 128.4, 123.8, 117.7, 114.1, 74.2, 26.1, 22.9, 13.5, 10.0. HRMS (ESI): m/z calcd for $(C_{15}H_{17}N_3+H)^+$: 240.1495; found: 240.1497.

General procedure for the synthesis of 5

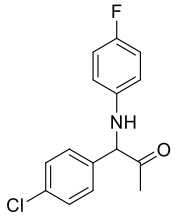


2n **1n** **aminoketone II (5)**

A solution of nitroepoxides **1n** (1.0 mmol), amine **2n** (1.0 mmol) and K_2CO_3 (1.0 mmol) in methanol was stirred at 25 °C for 1.0 h. Then, water was added (10 mL), and extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over $MgSO_4$ and concentrated under vacuum to afford a residue which was purified by silica gel chromatography (hexanes : ethyl acetate, 20:1) to give the pure product **5**.

Characterization Data of 5

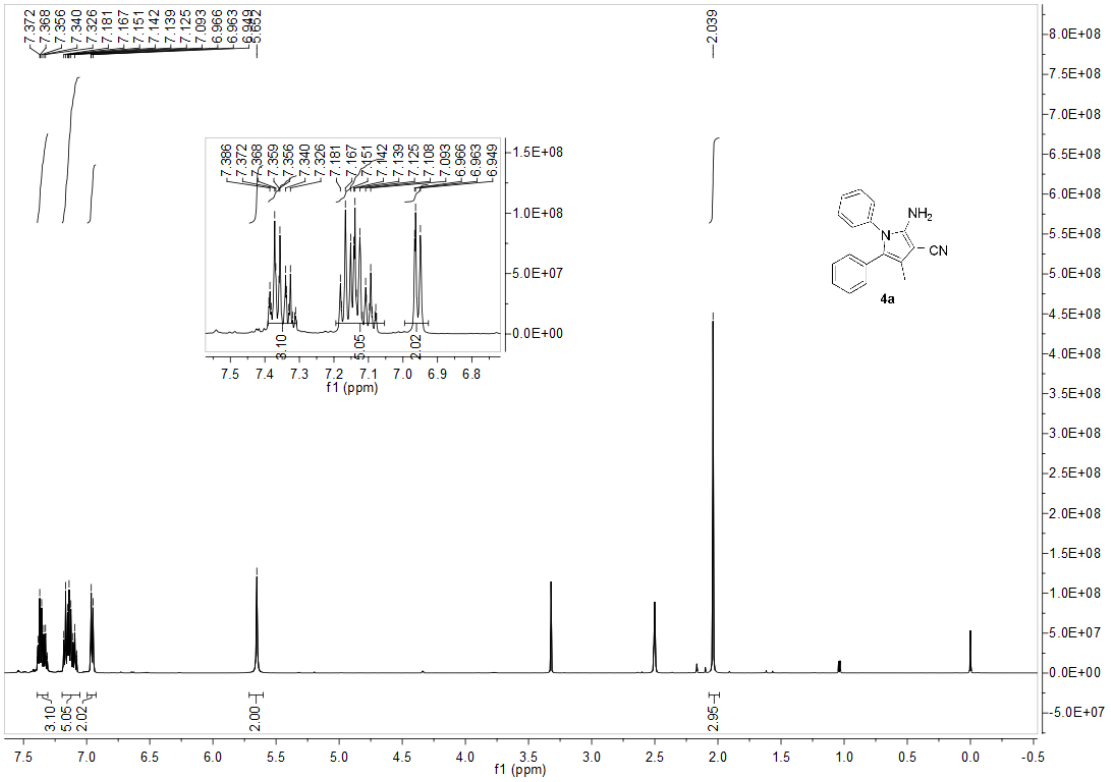
1-(4-chlorophenyl)-1-((4-fluorophenyl)amino)propan-2-one (**5**)

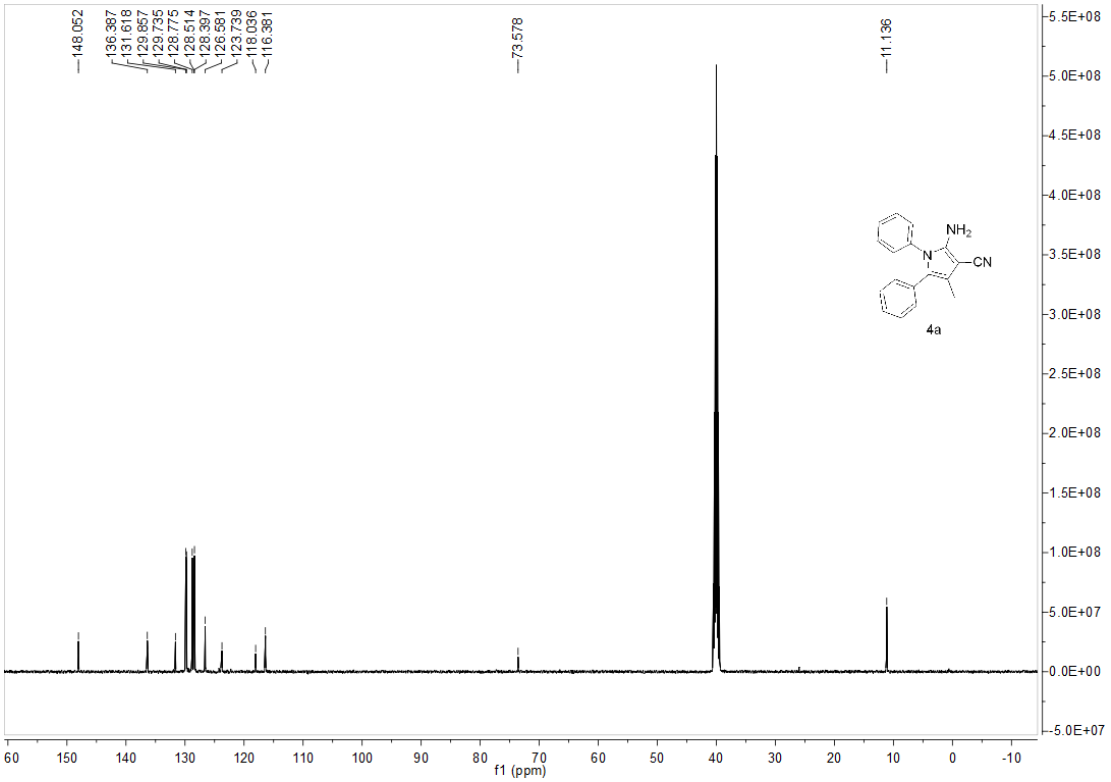


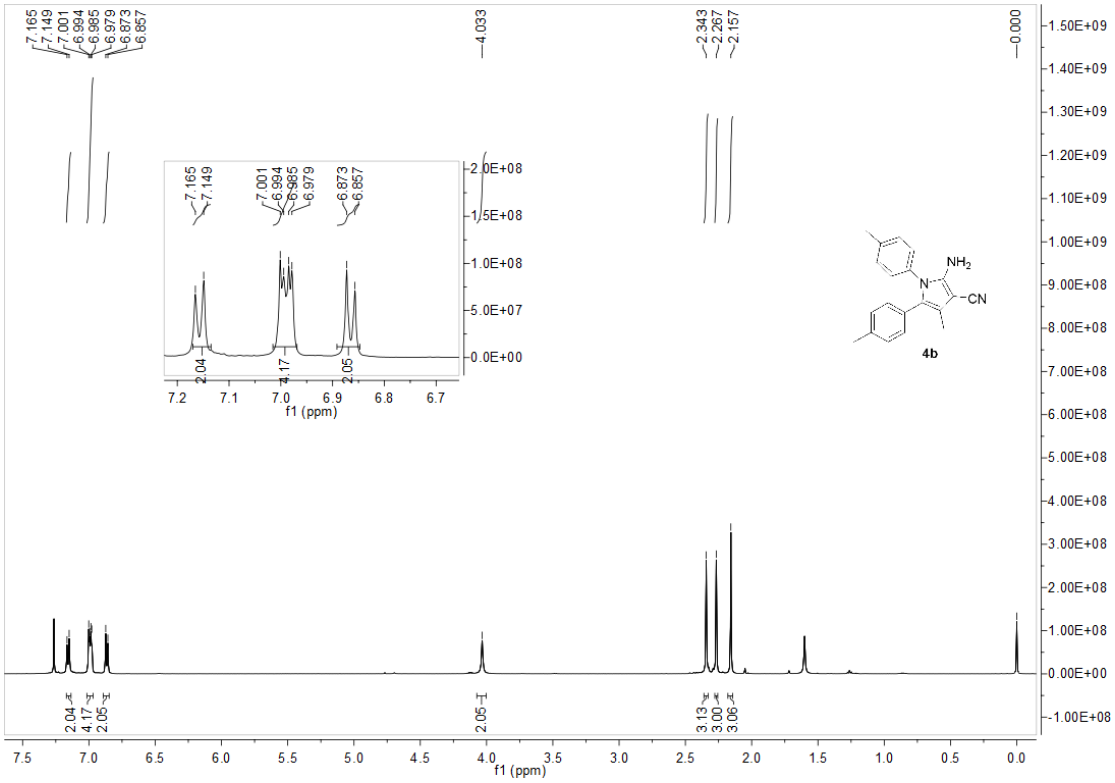
5

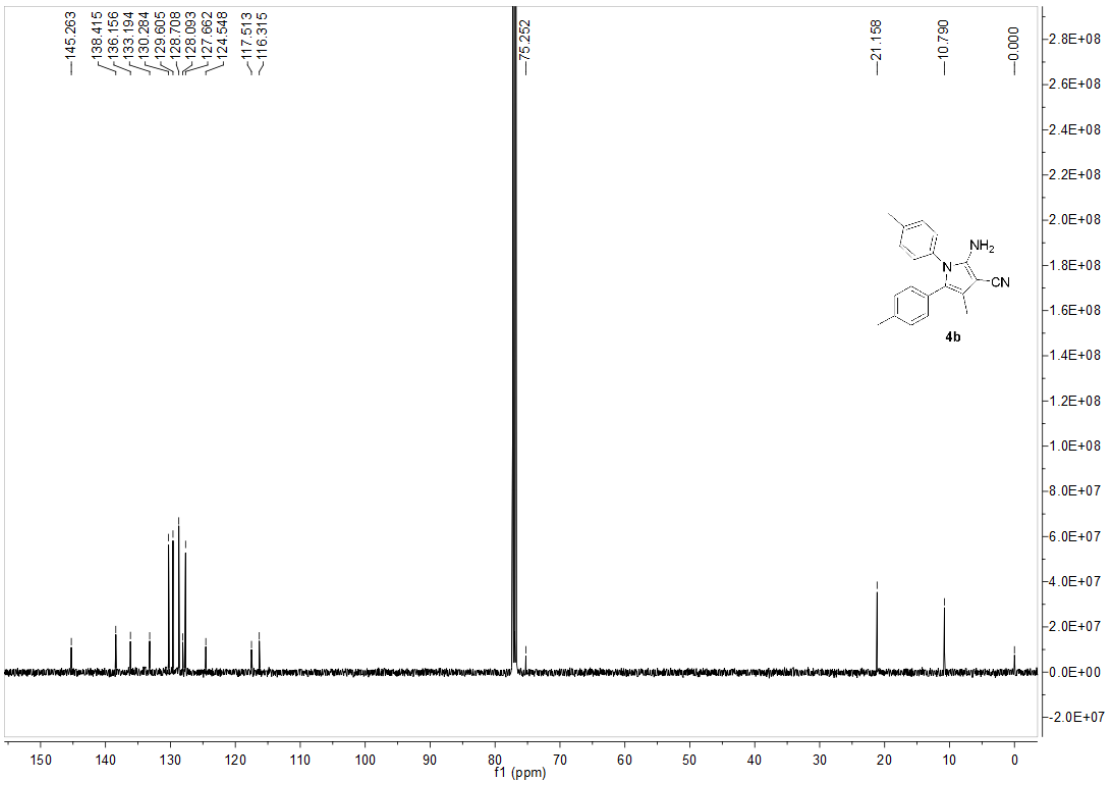
Yellow liquid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.26 (m, 4H), 6.77-6.64 (m, 2H), 6.46-6.26 (m, 2H), 5.25 (s, 1H), 4.84 (s, 1H), 2.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 202.1, 155.0(d, *J* = 234.4 Hz), 141.0, 135.5, 133.4, 128.5, 128.1, 114.7 (d, *J* = 22.3 Hz), 113.1(d, *J* = 7.4 Hz), 67.0, 25.6. HRMS (ESI): m/z calcd for $(C_{15}H_{13}ClFNO+H)^+$: 278.0742; found: 278.0745.

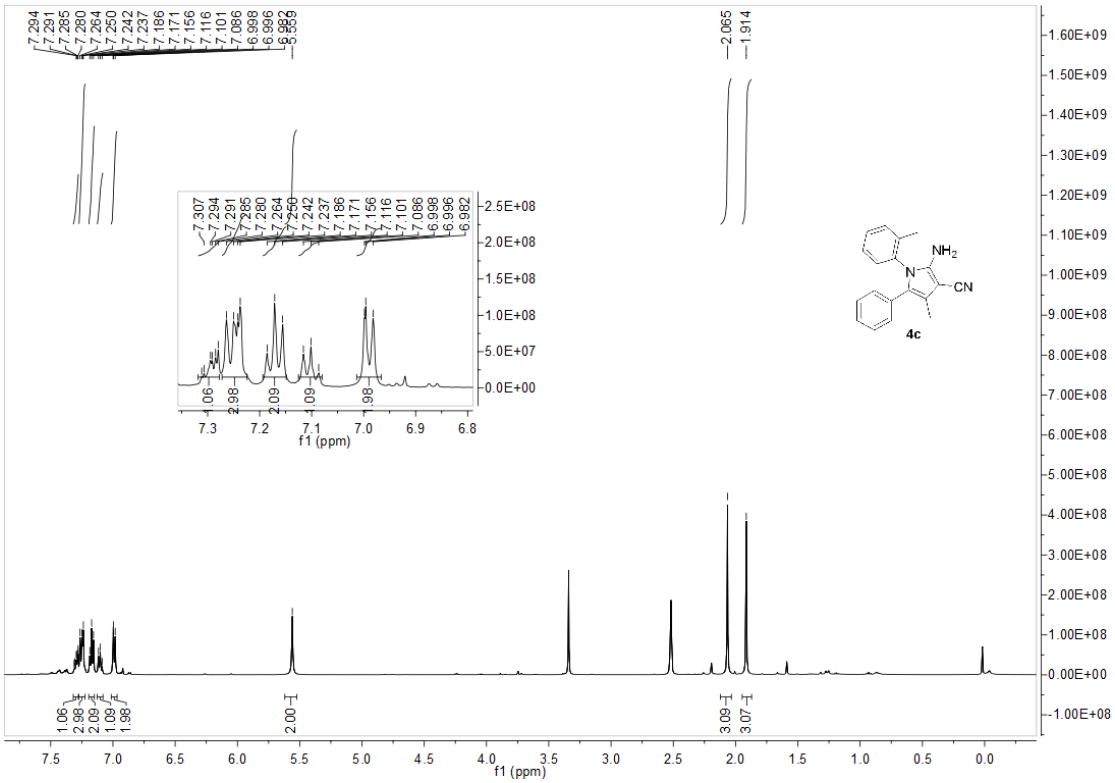
^{1}H NMR and ^{13}C NMR spectrum

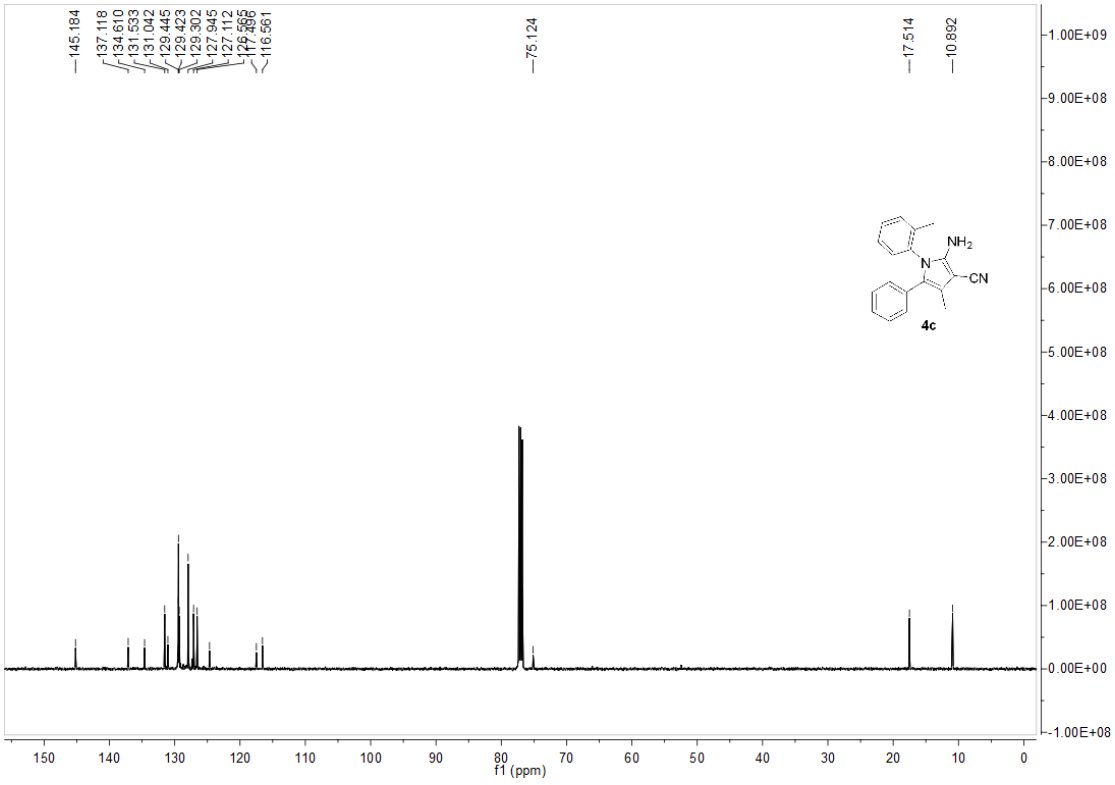


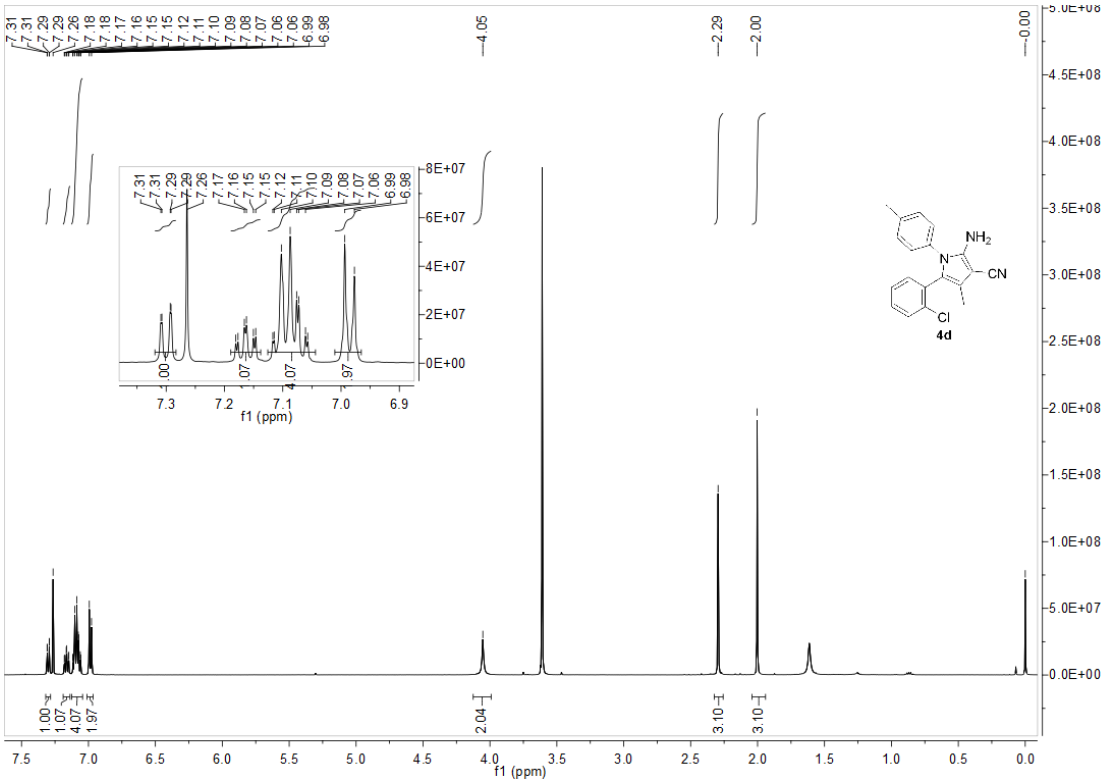


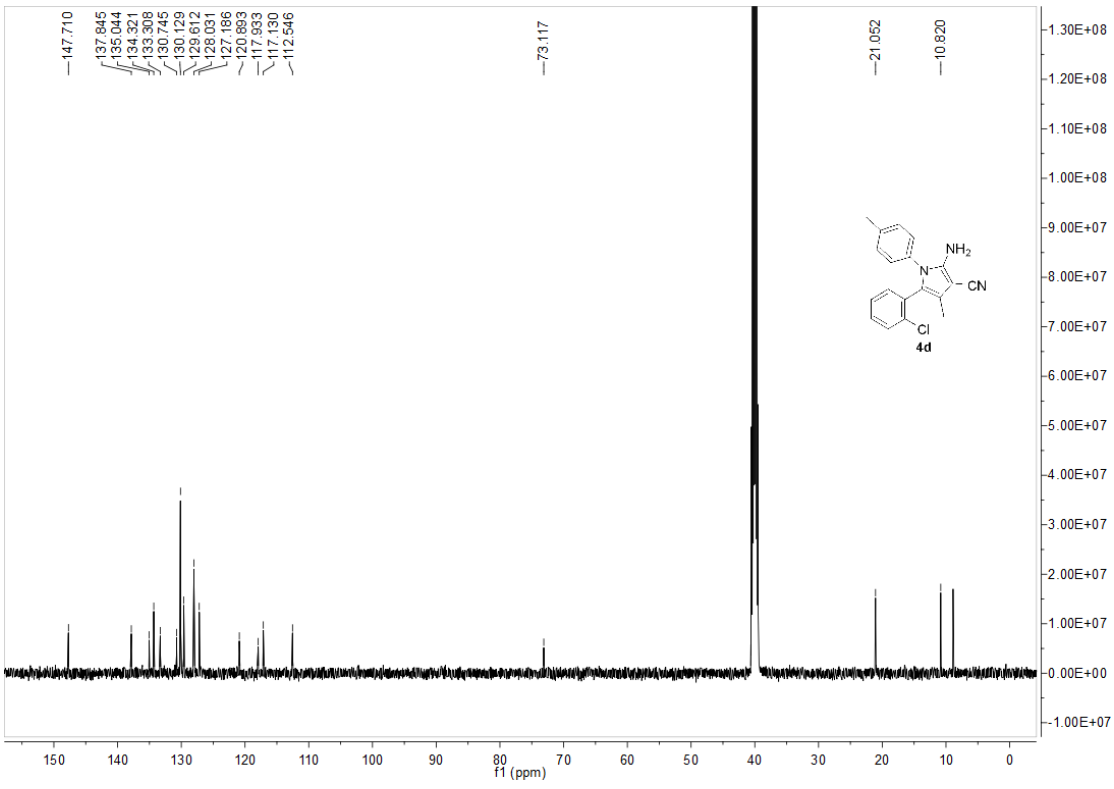

7.165
7.149
7.001
6.994
6.985
6.979
6.873
6.857
4.033
2.343
2.267
2.157
0.000
NH2
CN
4b
f1 (ppm)

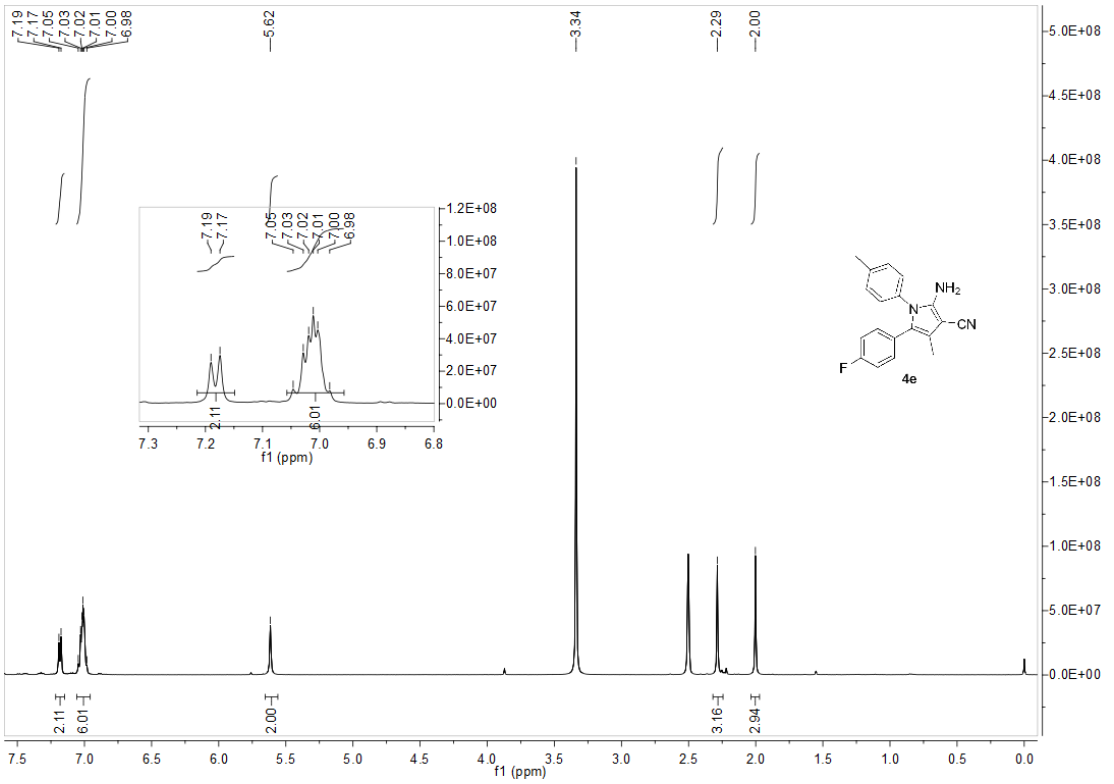

145.263
138.415
136.156
133.194
130.284
129.605
128.708
128.093
127.662
124.548
117.513
116.315
75.252
21.158
10.790
0.000
NH2
CN
4b
f1 (ppm)

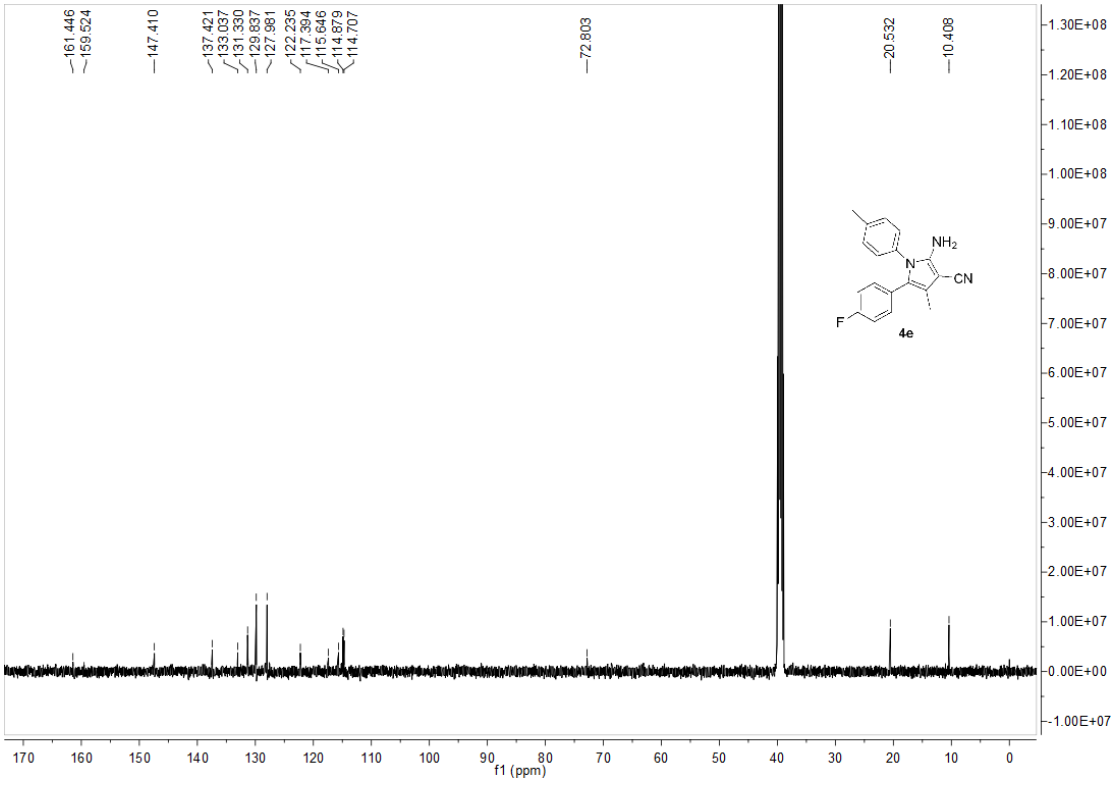

7.294
7.291
7.285
7.280
7.264
7.250
7.242
7.237
7.186
7.171
7.156
7.116
7.101
7.086
6.998
6.996
6.982
2.065
1.914
NH2
N
CN
4c
1.06
2.98
2.09
1.09
1.98
2.00
3.09
3.07
f1 (ppm)

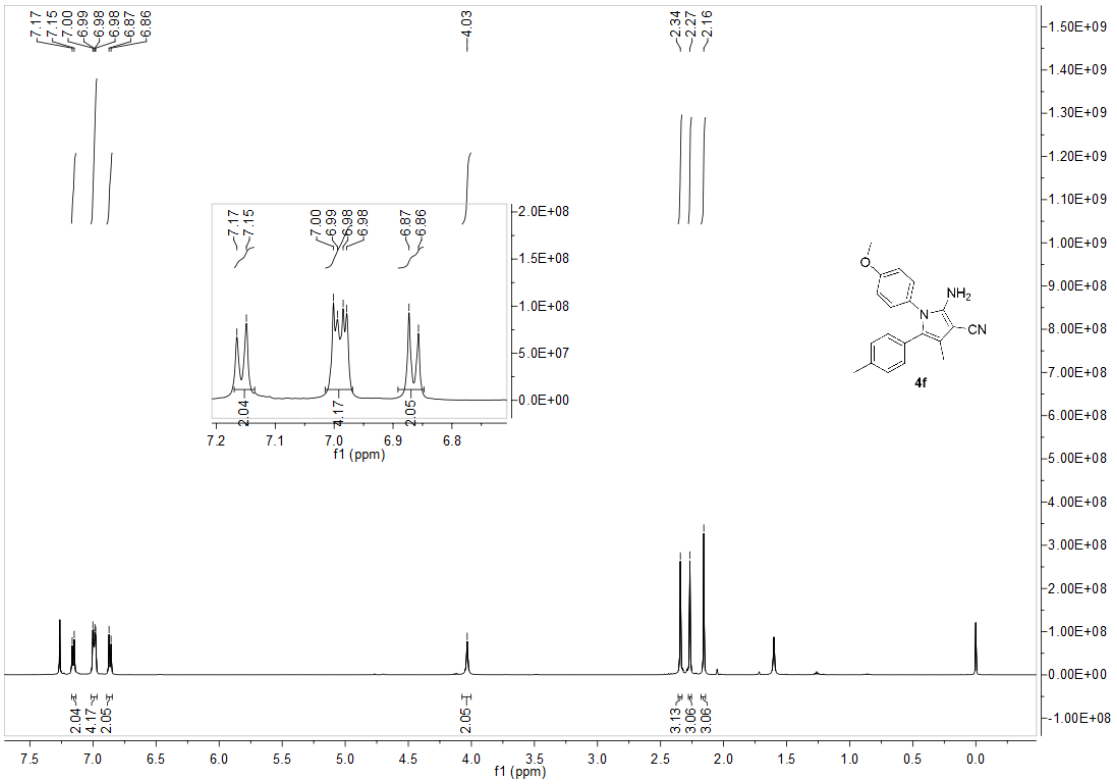

145.184
137.118
134.610
131.533
131.042
129.445
129.423
129.302
127.945
127.112
116.561
75.124
17.514
10.892
NH2
N
CN
4c
f1 (ppm)

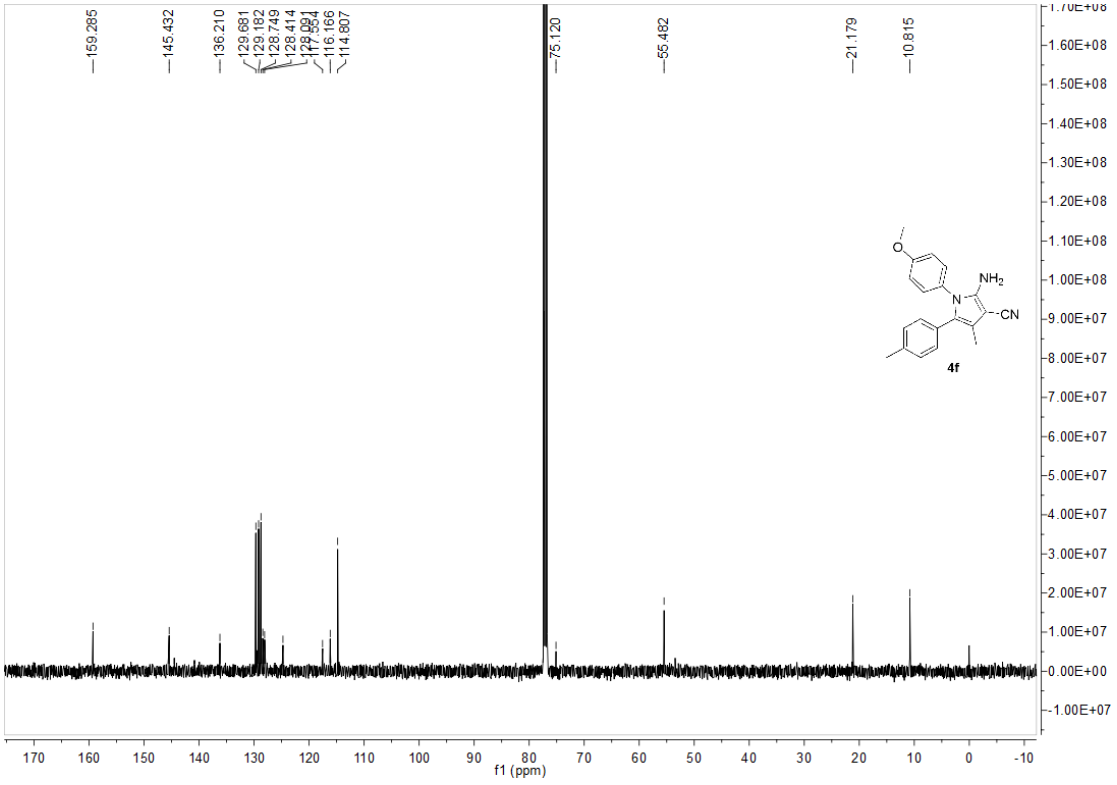

7.31
7.29
7.26
7.18
7.17
7.16
7.15
7.12
7.11
7.10
7.09
7.08
7.07
7.06
6.99
6.98
4.05
2.29
2.00
0.00
1.00
1.07
4.07
1.97
2.04
3.10
3.10
f1 (ppm)
NH2
CN
Cl
4d

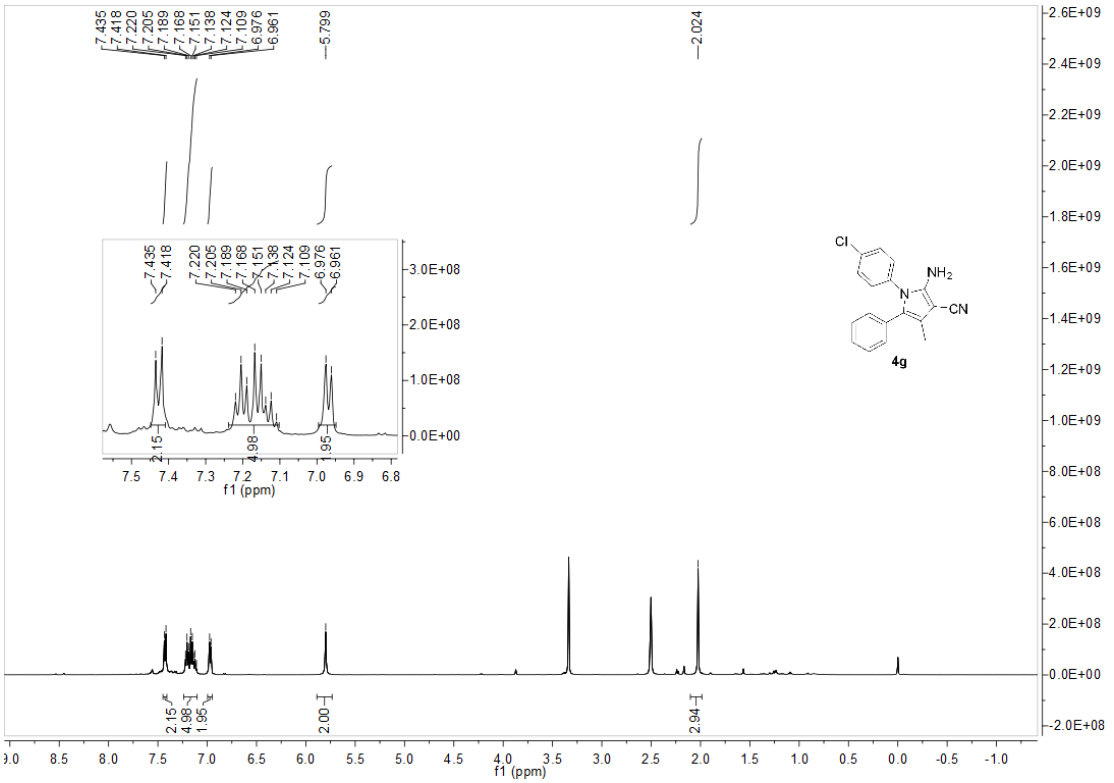

147.710
137.845
135.044
134.321
133.308
130.745
130.129
129.612
128.031
127.186
120.693
117.933
117.130
112.546
73.117
21.052
10.820
f1 (ppm)
NH2
CN
Cl
4d

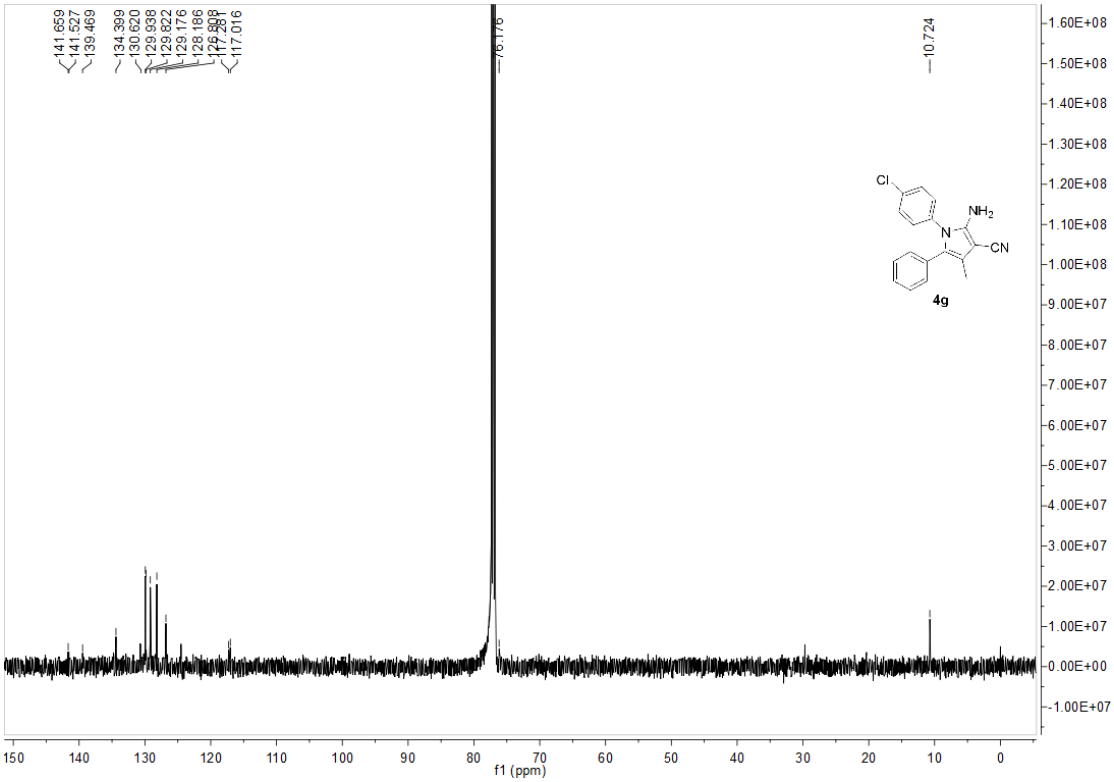

7.19
7.17
7.05
7.03
7.02
7.01
7.00
6.98
5.62
3.34
2.29
2.00
2.11
6.01
2.00
3.16
2.94
f1 (ppm)
NH2
CN
F
4e

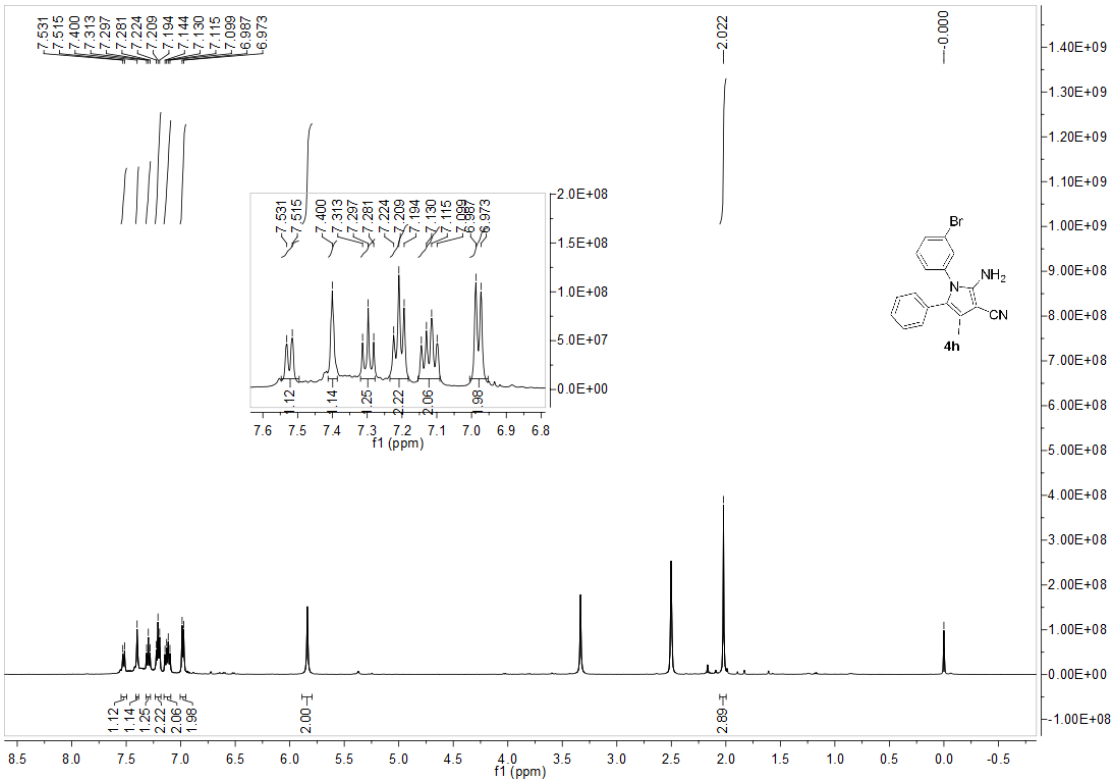

161.446
159.524
147.410
137.421
133.037
131.330
129.837
127.981
122.235
117.394
115.646
114.879
114.707
72.803
20.532
10.408
f1 (ppm)
NH2
CN
F
4e

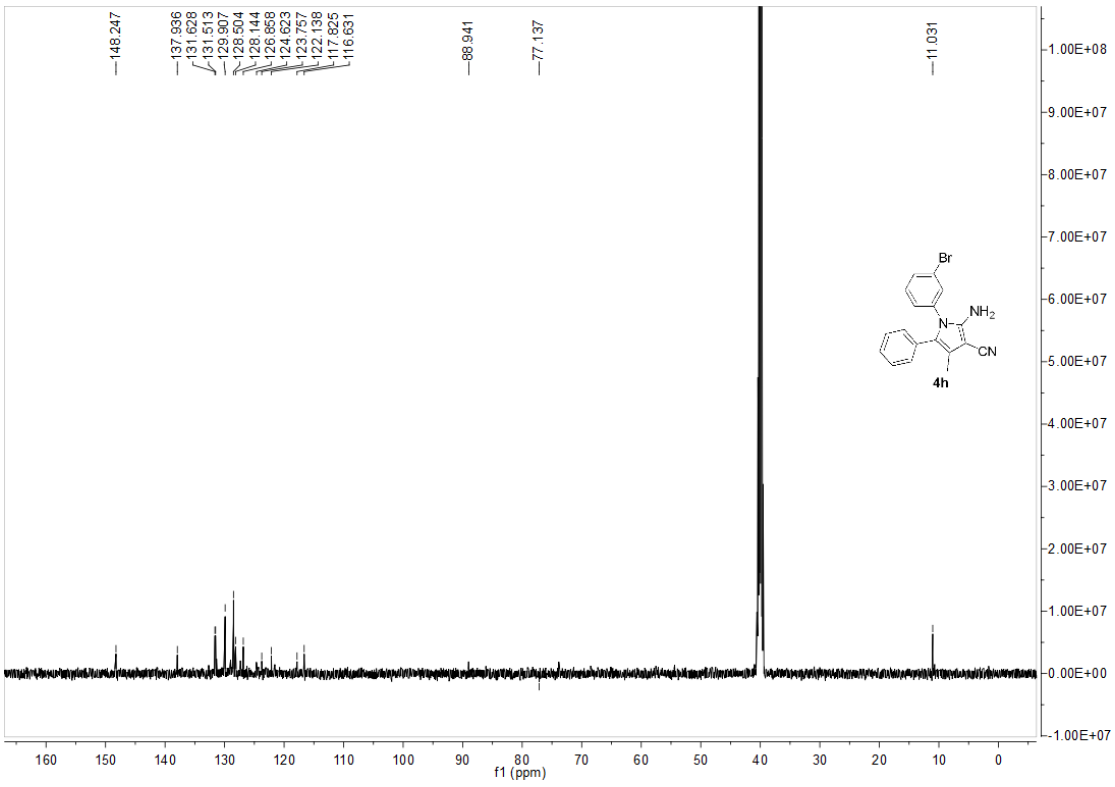

7.17
7.15
7.00
6.99
6.98
6.98
6.87
6.86
4.03
2.34
2.27
2.16
NH2
CN
O
N
4f
f1 (ppm)


159.285
145.432
136.210
129.681
129.182
128.749
128.414
116.166
114.807
75.120
55.482
21.179
10.815
NH2
CN
O
N
4f
f1 (ppm)


7.435
7.418
7.220
7.205
7.189
7.168
7.151
7.138
7.124
7.109
6.976
6.961
5.799
2.024
Cl
NH2
N
CN
4g
2.15
4.98
1.95
2.00
2.94
f1 (ppm)


141.659
141.527
139.469
134.399
130.620
129.938
129.822
129.176
128.186
117.016
76.176
10.724
Cl
NH2
N
CN
4g
f1 (ppm)


7.531
7.515
7.400
7.313
7.297
7.281
7.224
7.209
7.194
7.144
7.130
7.115
7.099
6.987
6.973
2.022
0.000
1.12
1.14
1.25
2.22
2.06
1.98
2.00
2.89
Br
NH2
N
CN
4h
f1 (ppm)


148.247
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131.628
131.513
129.907
128.504
128.144
126.858
124.623
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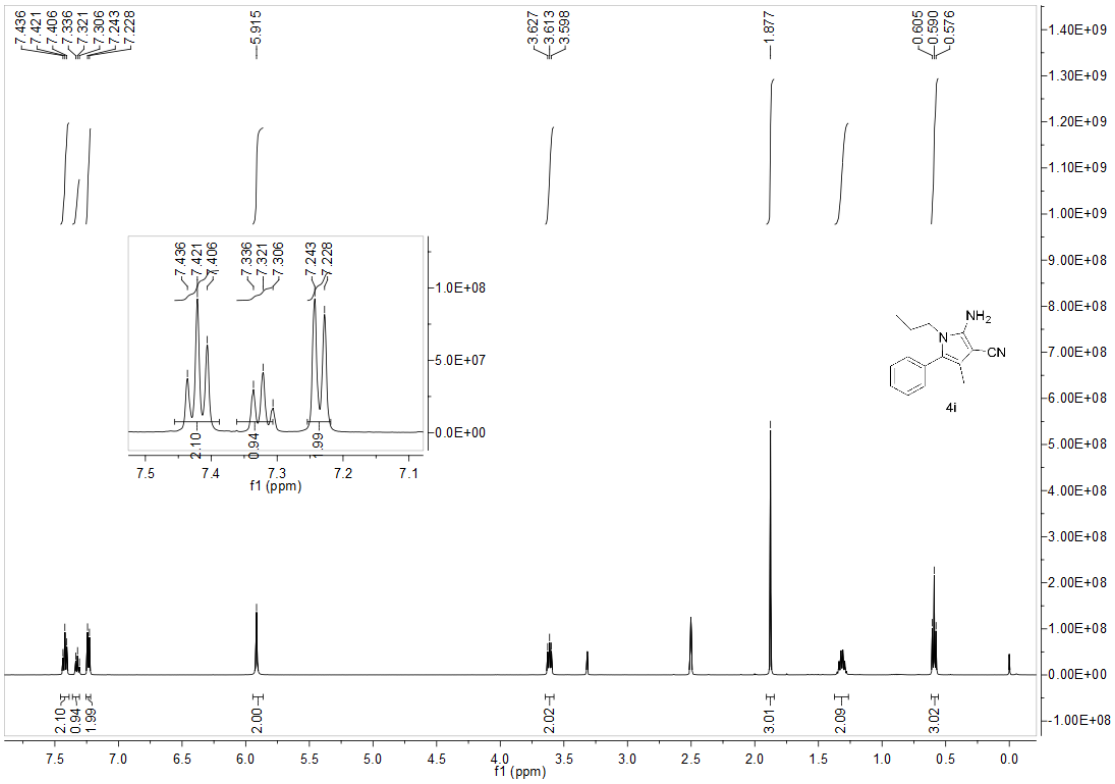
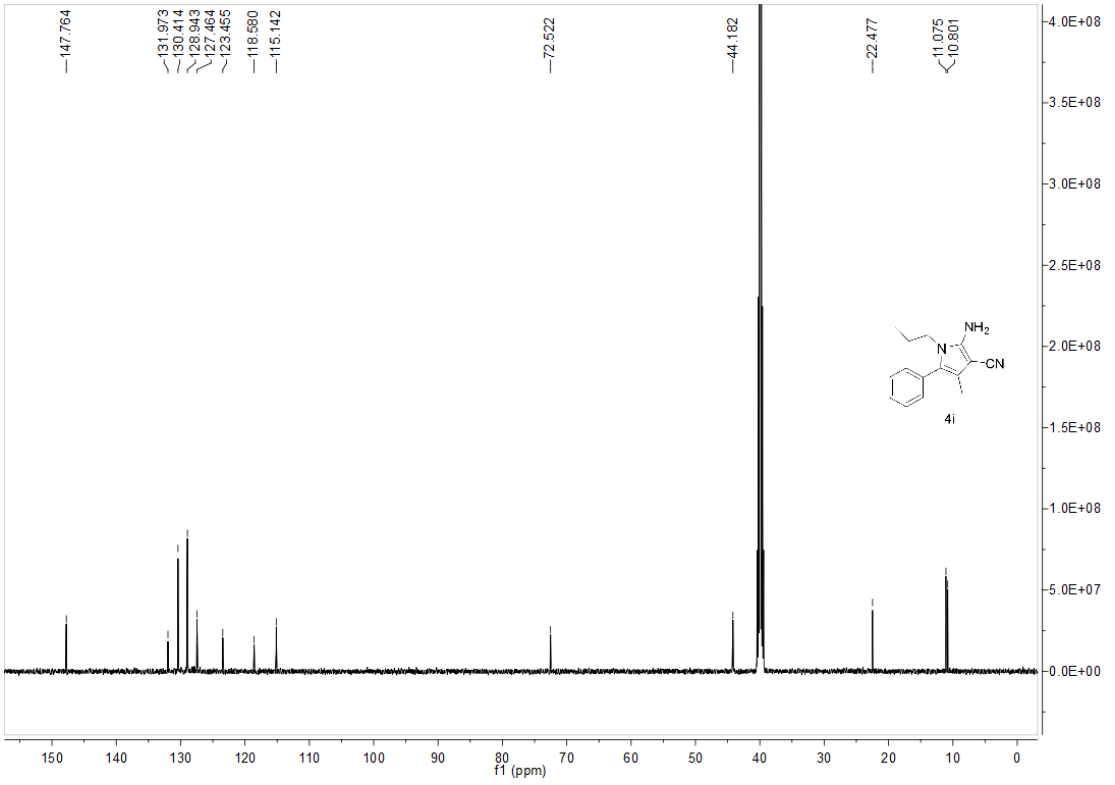
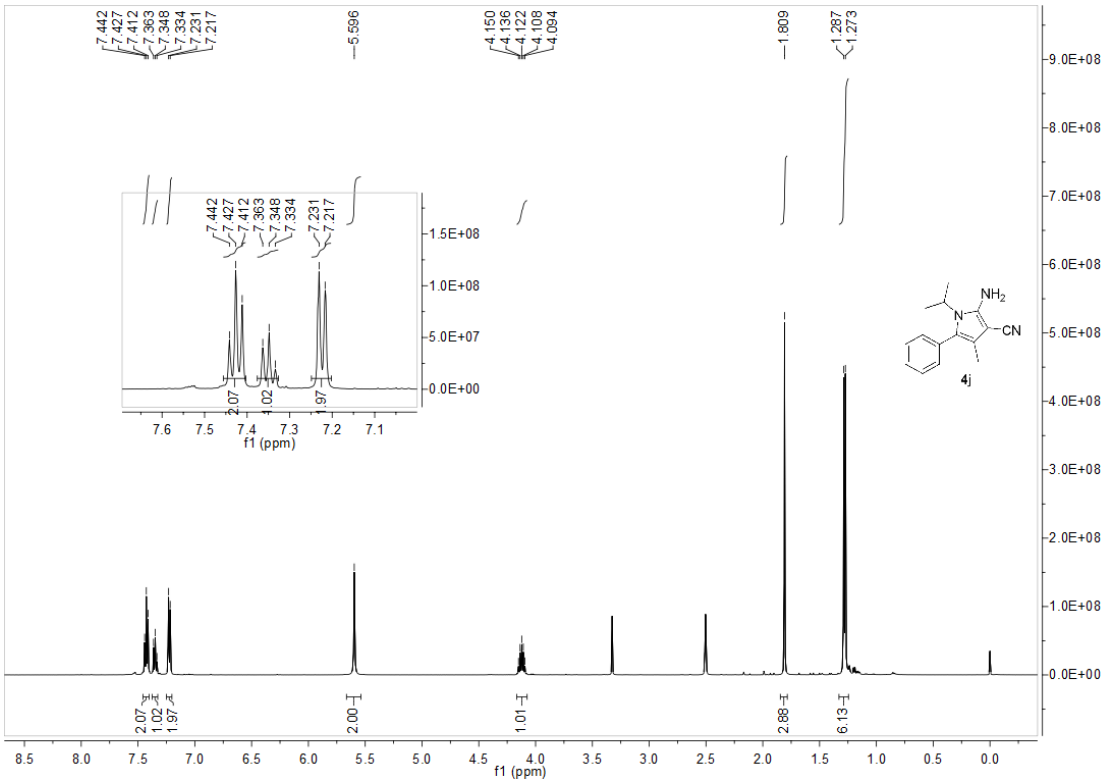
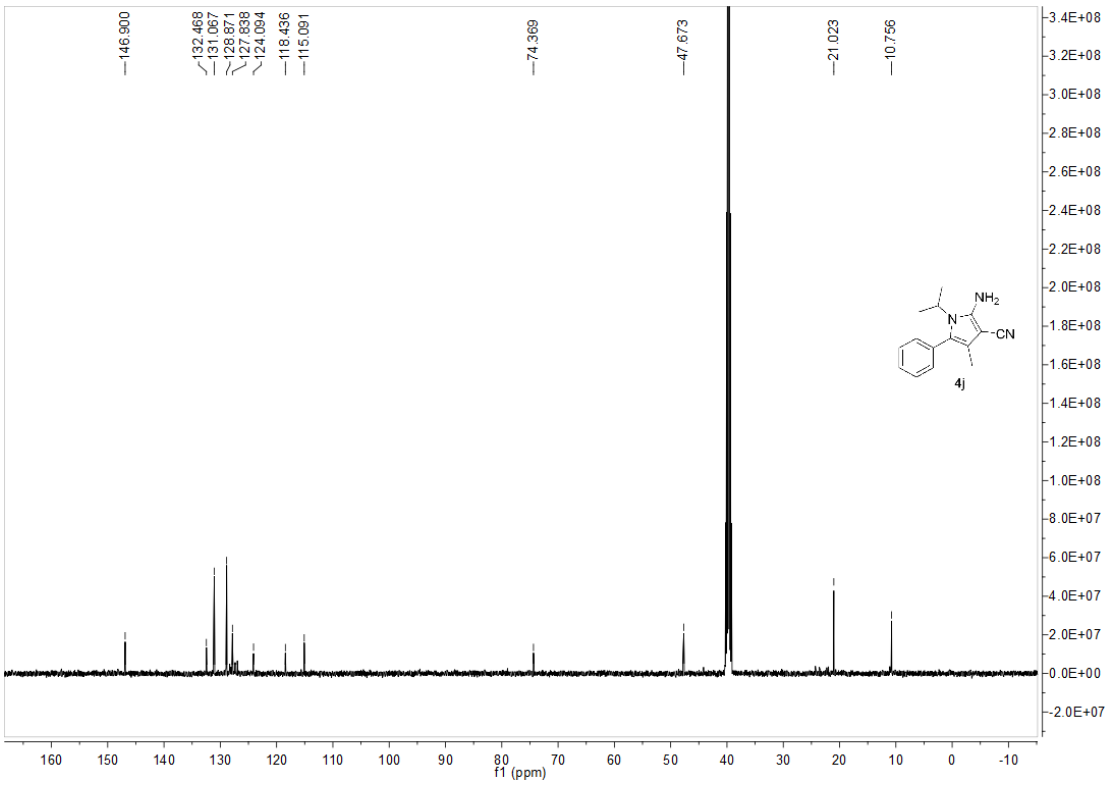
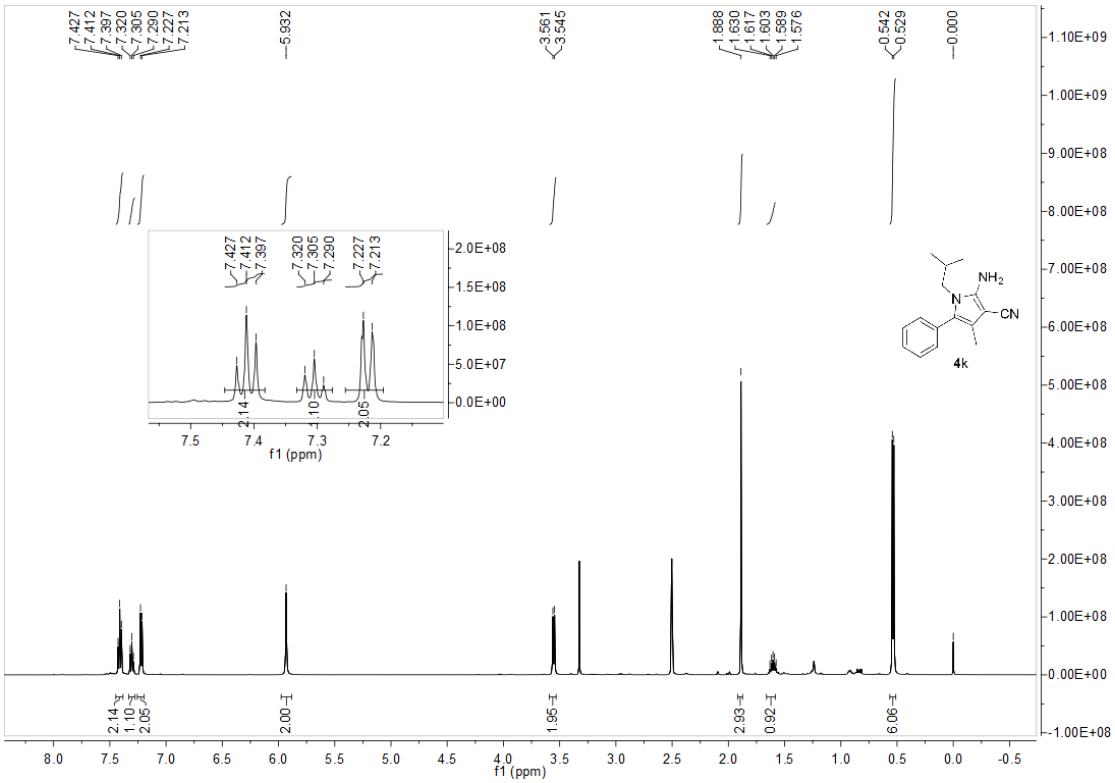
122.138
117.825
116.631
88.941
77.137
11.031
Br
NH2
N
CN
4h
f1 (ppm)

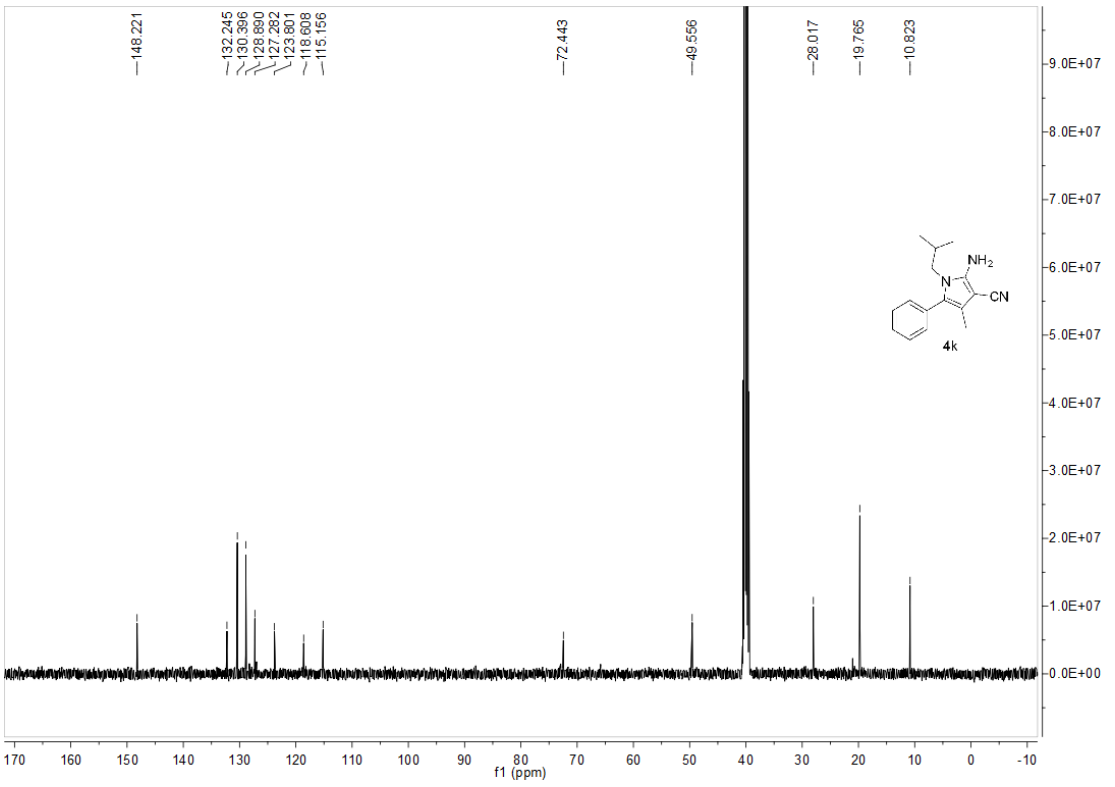

7.436
7.421
7.406
7.336
7.321
7.306
7.243
7.228
5.915
3.627
3.613
3.598
1.877
0.605
0.590
0.576
NH2
N
CN
4i
f1 (ppm)


147.764
131.973
130.414
128.943
127.464
123.455
118.580
115.142
72.522
44.182
22.477
11.075
10.801
NH2
N
CN
4i
f1 (ppm)


7.442
7.427
7.412
7.363
7.348
7.334
7.231
7.217
5.596
4.150
4.136
4.122
4.108
4.094
1.809
1.287
1.273
2.07
1.02
1.97
2.00
1.01
2.88
6.13
f1 (ppm)
NH2
CN
4j


146.900
132.468
131.067
128.871
127.838
124.094
118.436
115.091
74.369
47.673
21.023
10.756
f1 (ppm)
NH2
CN
4j


7.427
7.412
7.397
7.320
7.305
7.290
7.227
7.213
5.932
3.561
3.545
1.888
1.630
1.617
1.603
1.589
1.576
0.542
0.529
0.000
NH2
CN
4k
f1 (ppm)


148.221
132.245
130.396
128.890
127.282
123.801
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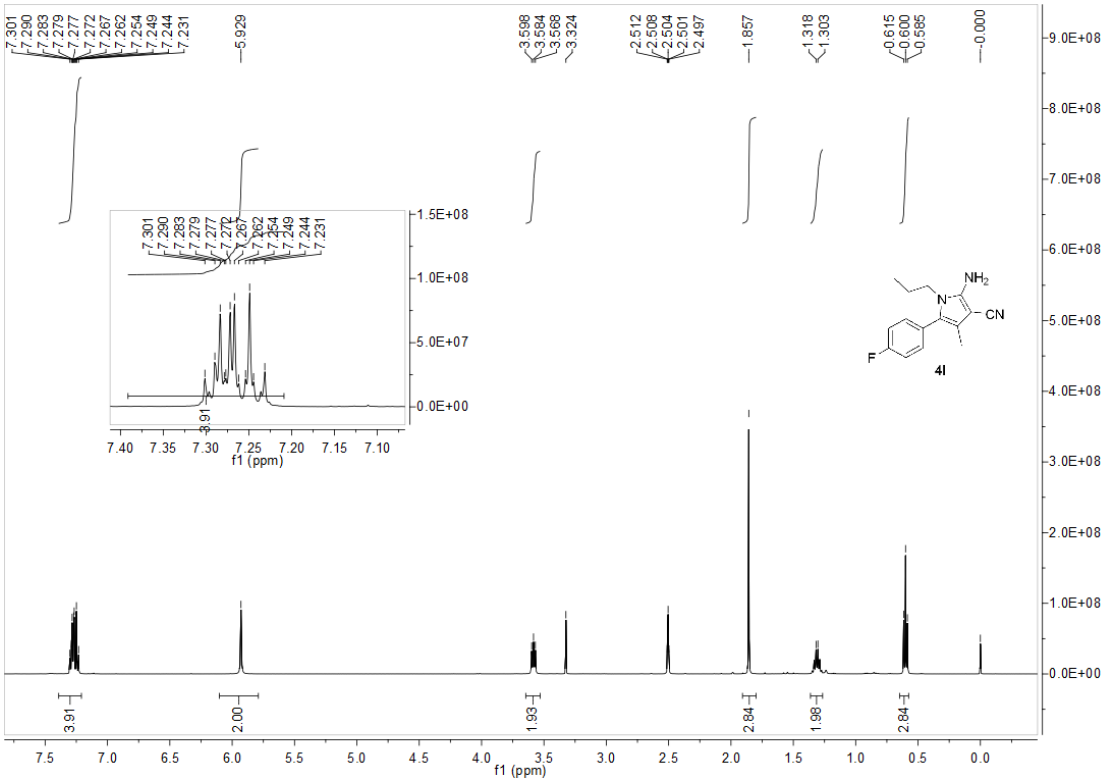
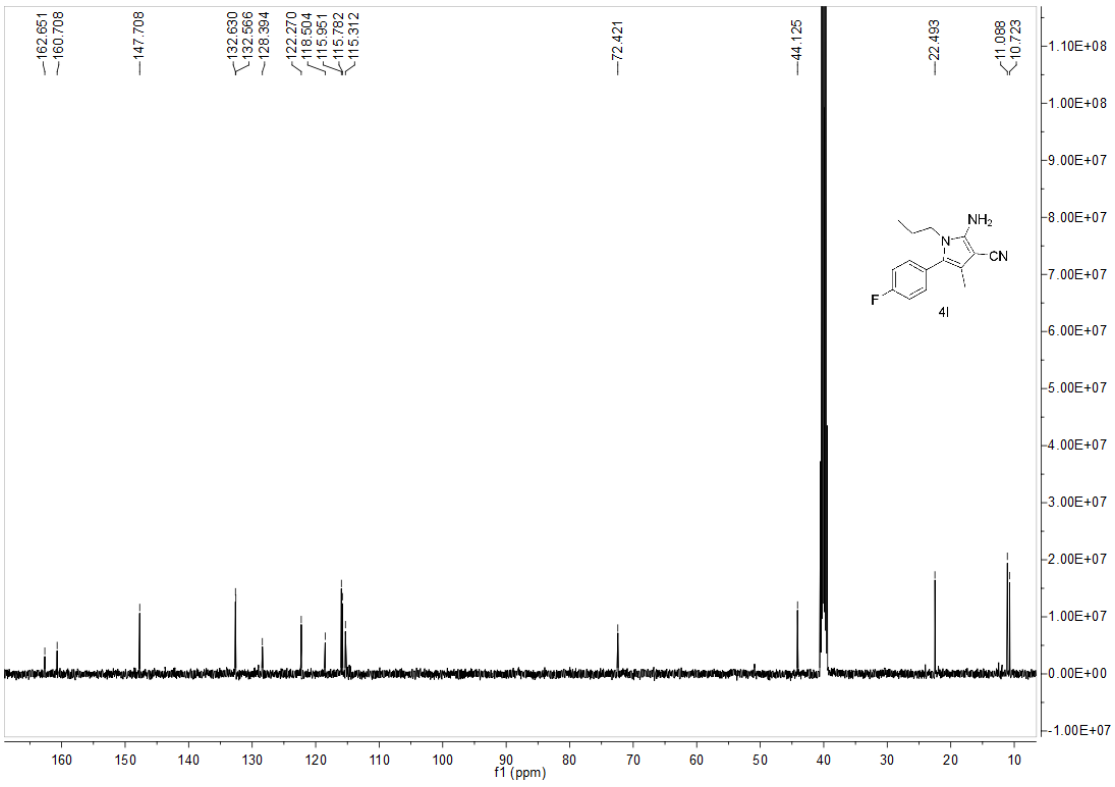
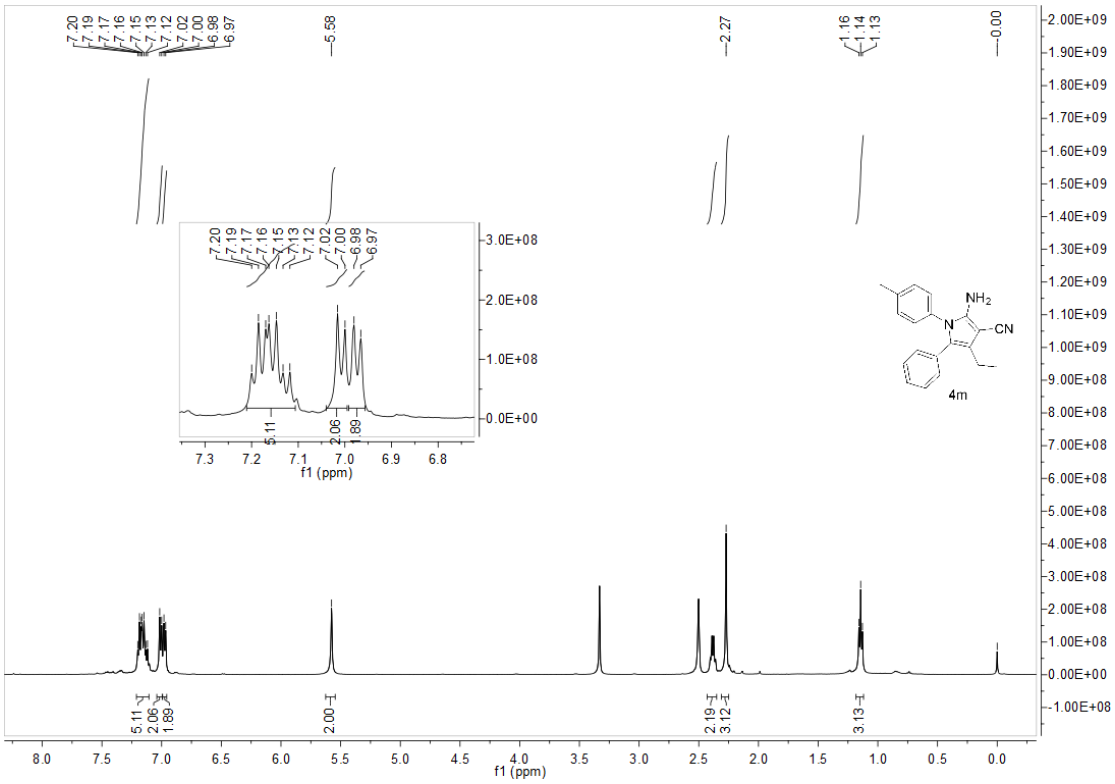
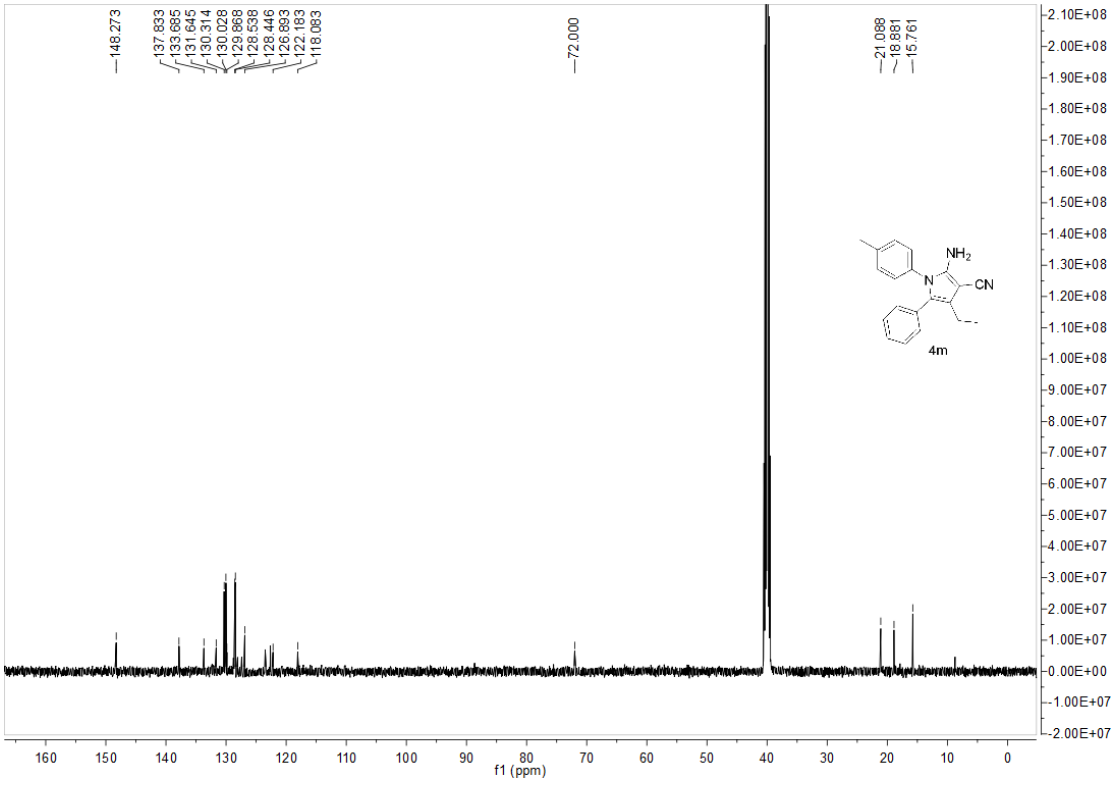
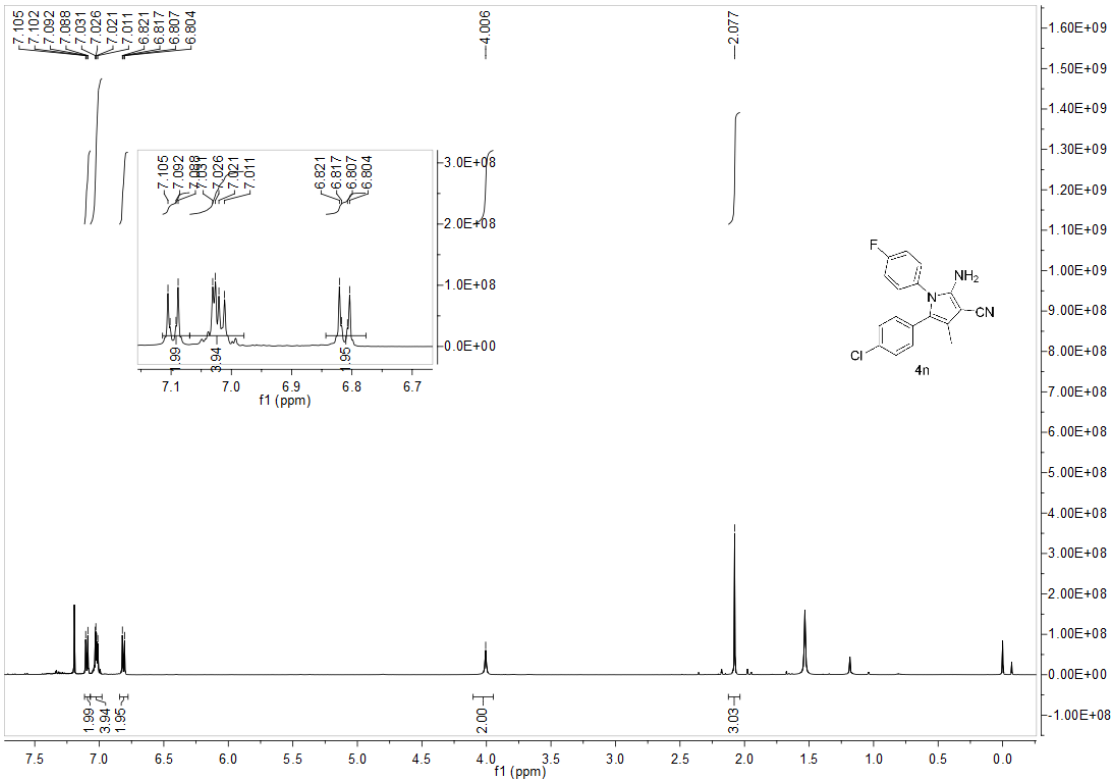
115.156
72.443
49.556
28.017
19.765
10.823
NH2
CN
4k
f1 (ppm)

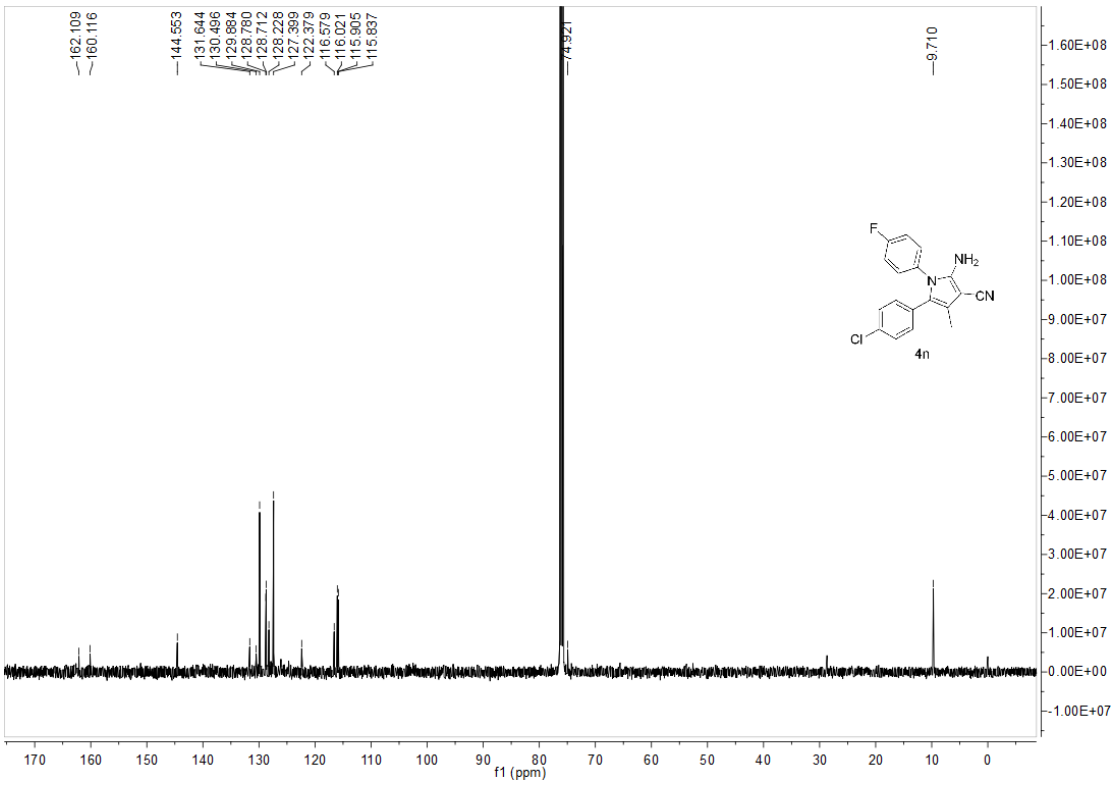

7.301
7.290
7.283
7.279
7.277
7.272
7.267
7.262
7.254
7.249
7.244
7.231
5.929
3.598
3.584
3.568
3.324
2.512
2.508
2.504
2.501
2.497
1.857
1.318
1.303
0.615
0.600
0.585
0.000
3.91
2.00
1.93
2.84
1.98
2.84
f1 (ppm)
NH2
CN
F
4l

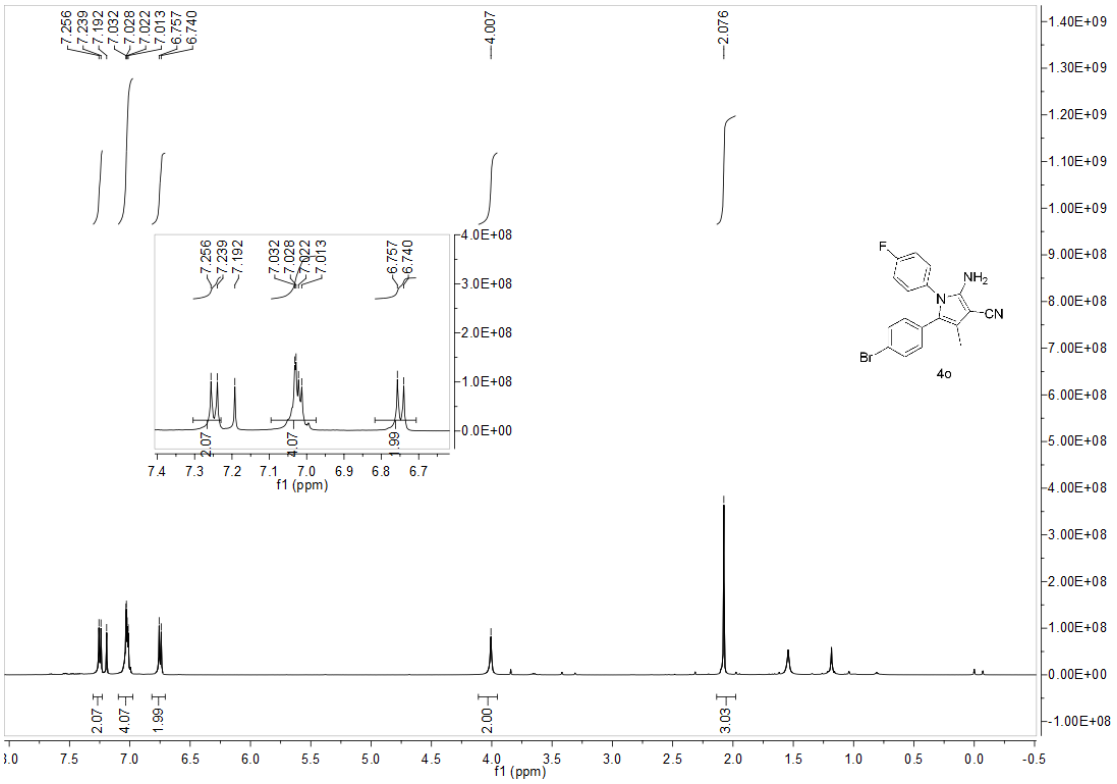

162.651
160.708
147.708
132.630
132.566
128.394
122.270
118.504
115.951
115.782
115.312
72.421
44.125
22.493
11.088
10.723
f1 (ppm)
NH2
CN
F
4l

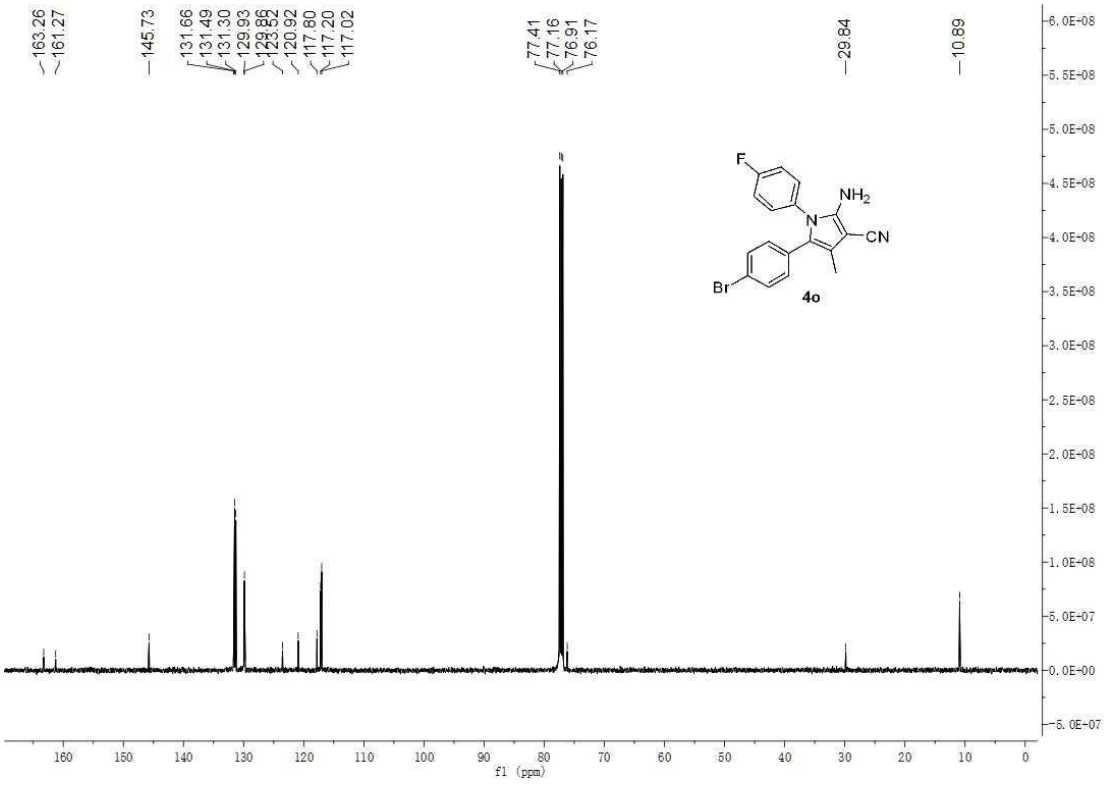

7.20
7.19
7.17
7.16
7.15
7.13
7.12
7.02
7.00
6.98
6.97
5.58
2.27
1.16
1.14
1.13
0.00
NH2
CN
4m
5.11
2.06
1.89
2.00
2.19
3.12
3.13
f1 (ppm)

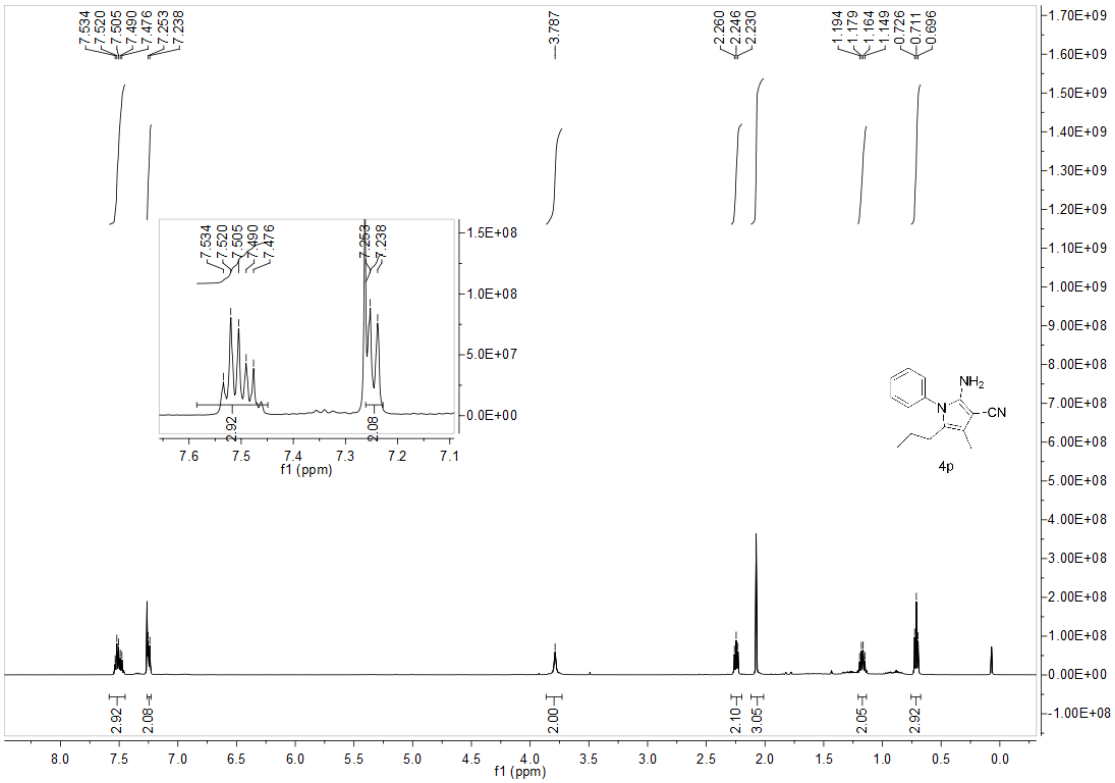

148.273
137.833
133.685
131.645
130.314
130.028
129.868
128.538
128.446
126.693
122.183
118.083
72.000
21.088
18.881
15.761
NH2
CN
4m
f1 (ppm)

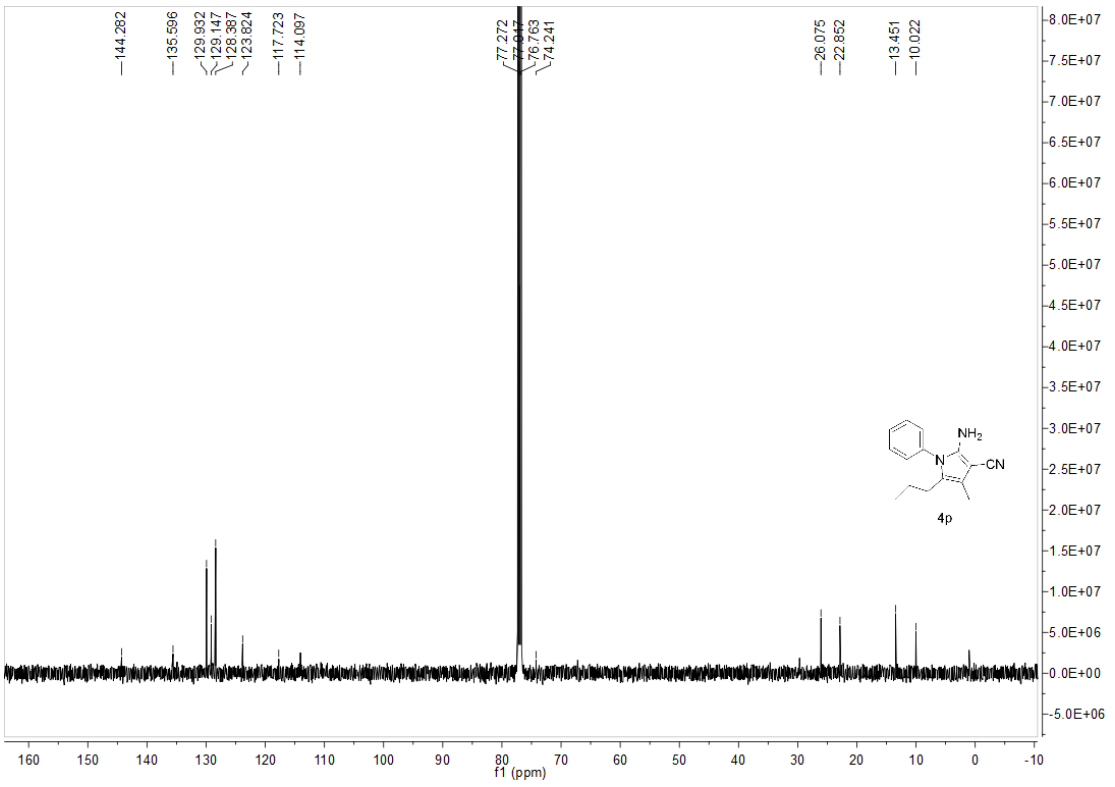

7.105
7.102
7.092
7.088
7.031
7.026
7.021
7.011
6.821
6.817
6.807
6.804
4.006
2.077
1.99
3.94
1.95
2.00
3.03
f1 (ppm)
F
NH2
N
CN
Cl
4n

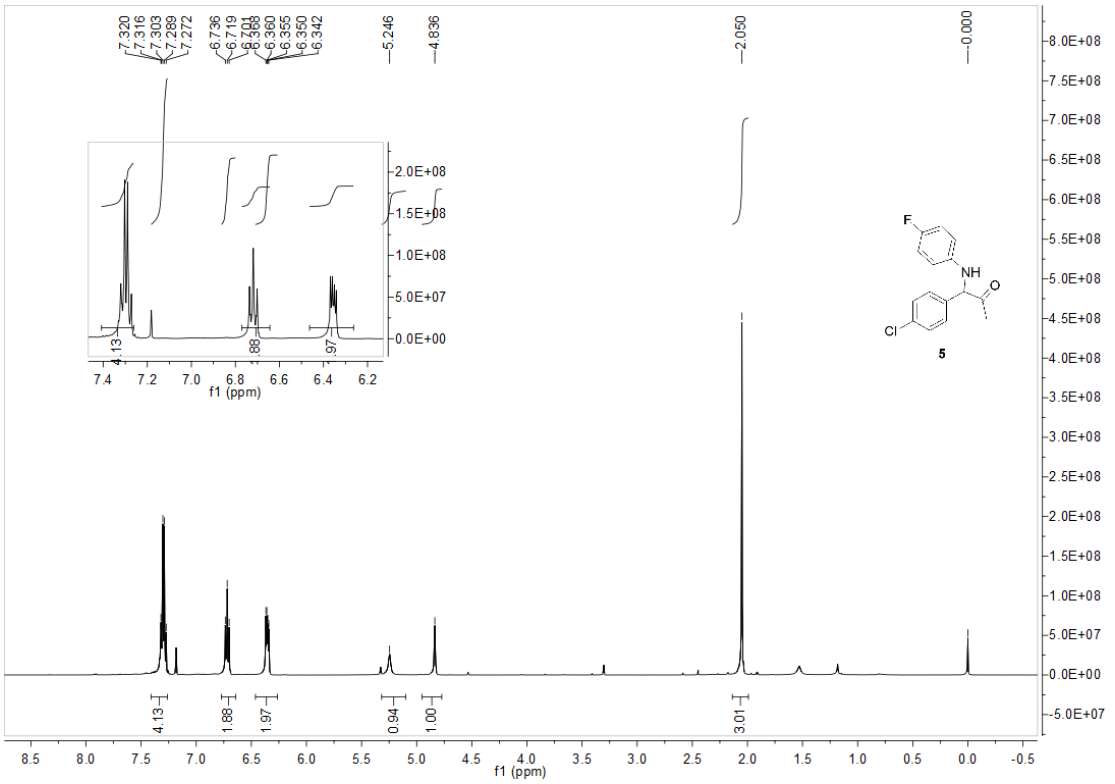

162.109
160.116
144.553
131.644
130.496
129.884
128.780
128.712
128.228
127.399
122.379
116.579
116.021
115.905
115.837
74.921
9.710
f1 (ppm)
F
NH2
N
CN
Cl
4n

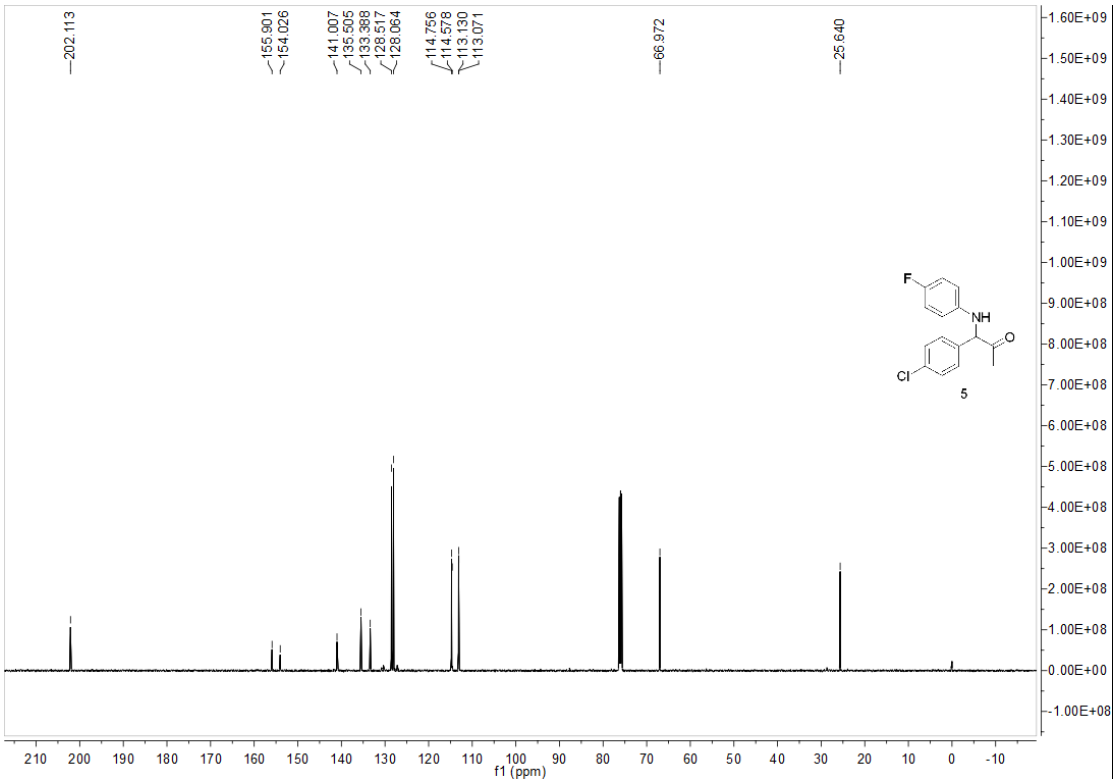

7.256
7.239
7.192
7.032
7.028
7.022
7.013
6.757
6.740
4.007
2.076
2.07
4.07
1.99
2.00
3.03
f1 (ppm)
F
NH2
N
CN
Br
4o


163.26
161.27
145.73
131.66
131.49
131.30
129.93
129.86
123.52
120.92
117.80
117.20
117.02
77.41
77.16
76.91
76.17
29.84
10.89
f1 (ppm)
F
NH2
N
CN
Br
4o

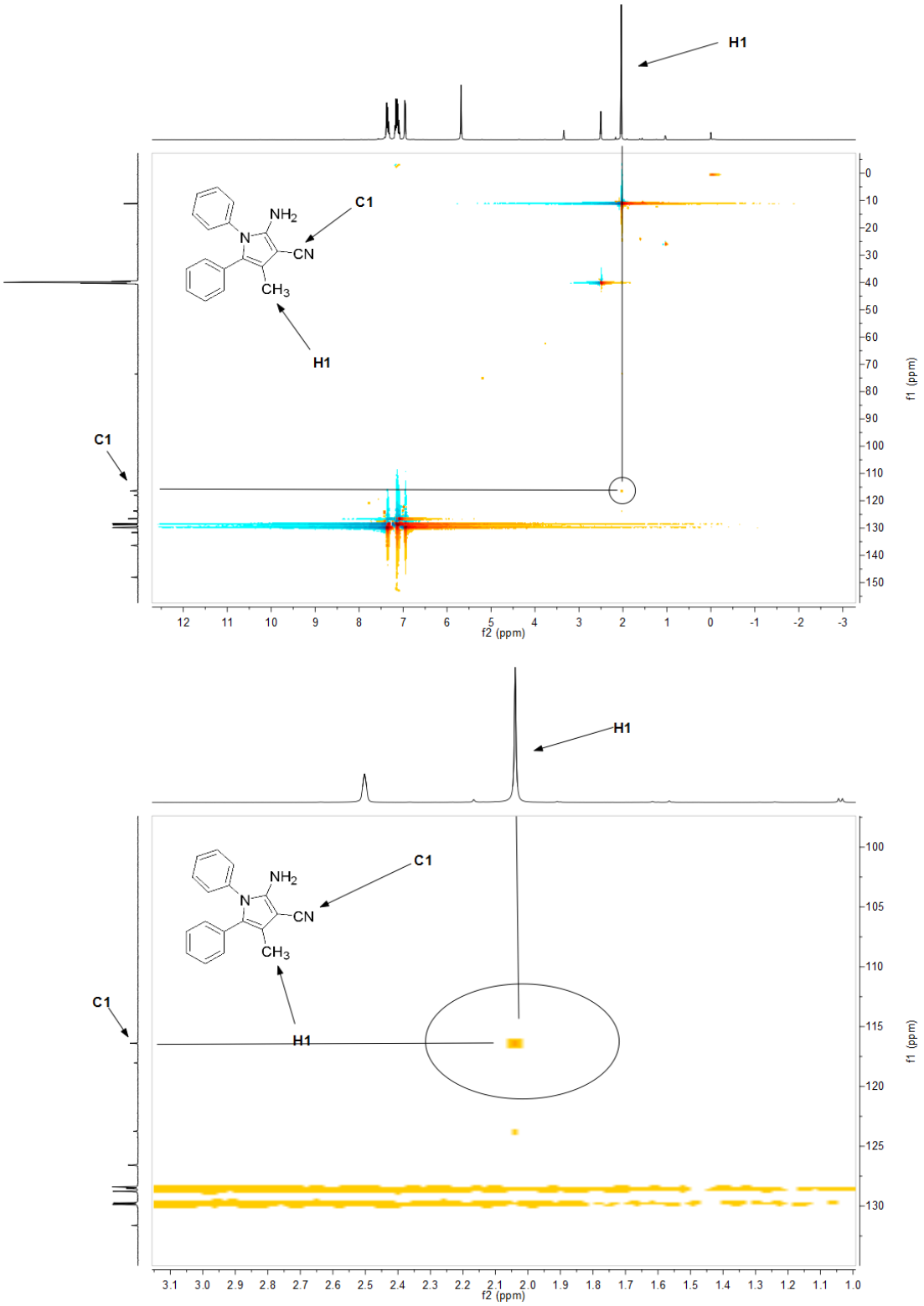

7.534
7.520
7.505
7.490
7.476
7.253
7.238
3.787
2.260
2.246
2.230
1.194
1.179
1.164
1.149
0.726
0.711
0.696
2.92
2.08
2.00
2.10
3.05
2.05
2.92
f1 (ppm)
NH2
CN
4p


144.282
135.596
129.932
129.147
128.387
123.824
117.723
114.097
77.272
76.763
74.241
26.075
22.852
13.451
10.022
f1 (ppm)
NH2
CN
4p


7.320
7.316
7.303
7.289
7.272
6.736
6.719
6.388
6.360
6.355
6.350
6.342
5.246
4.836
2.050
0.000
4.13
1.88
1.97
0.94
1.00
3.01
f1 (ppm)
F
NH
O
Cl
5


202.113
155.901
154.026
141.007
135.505
133.388
128.517
128.064
114.756
114.578
113.130
113.071
66.972
25.640
f1 (ppm)
F
NH
O
Cl
5

2D ^{1}H-^{13}C HSQC



2D ^{1}H-^{13}C HMBC