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

Supporting Information

Domino reaction of cyclic sulfamidate imines with Morita-Baylis-Hillman acetates promoted by DABCO: a metal-free approach to functionalized nicotinic acid derivatives

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Crystallographic data: Single crystal X-ray structural of **3ai** was collected at 150(2) K using graphite monochromated Mo Kα radiation (λα = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structure was solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on *F2*. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally 1.2*Ueq* of their parent atoms. The crystal data are summarized in Table 1. The CCDC number of **3ai** (**1522097)** can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre,12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

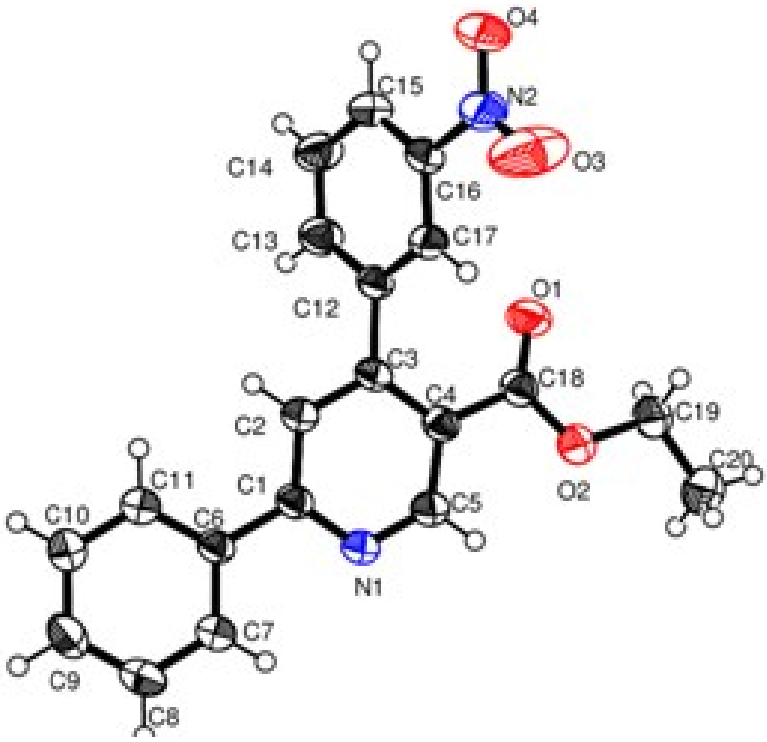
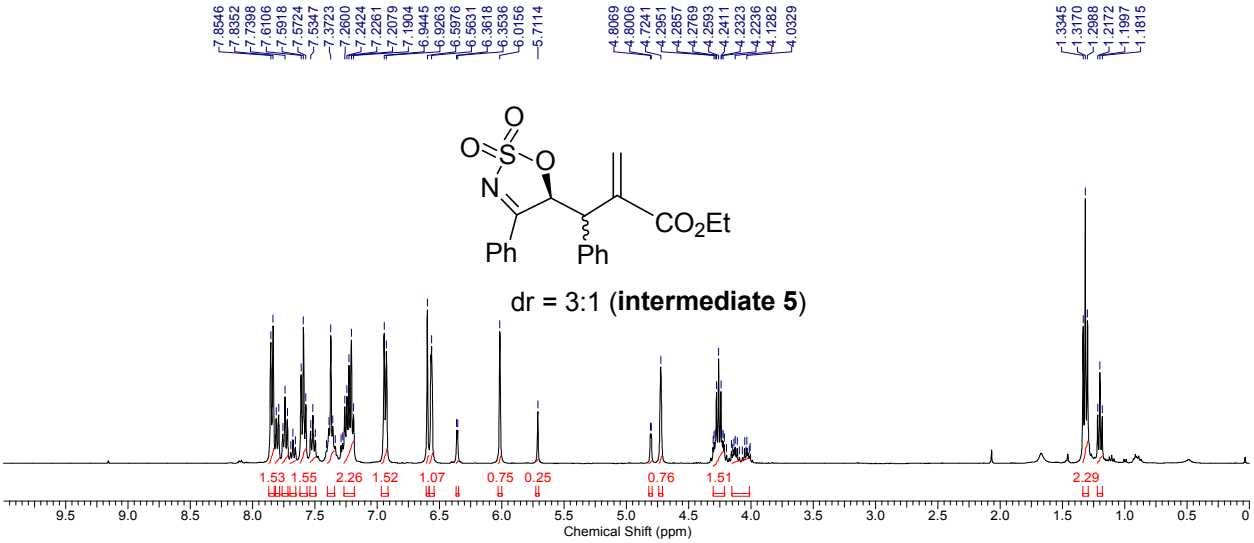


Figure 1. ORTEP diagram of compound **3ai (CCDC** 1522097**),** thermal ellipsoids drawn at the 50% probability level.

Table 1. Crystal data for compound 3ai.

Compound	**3ai**
Empirical formula	C20 H16 N2 O4
Formula weight	348.35
Temperatute	293(2) K
Wave length (Å)	0.71073 A
Crystal system, space group	Triclinic, P-1
a (Å) *b* (Å) *c* (Å) *α* (°) *β* (°) *γ* (°)	a =8.1889(3) A b = 10.3419(5) A c = 10.9166(4) A alpha = 105.058(4) deg. beta =.98.466(3) deg. gamma = 99.563(3) deg
Volume ($Å^3$)	862.59(6) A^3
Z, Calculated density (mg/m^3)	2, 1.341 Mg/m^3
Absorption coefficient (mm^{-1})	0.095 mm^-1
F(000)	364
Crystal size (mm)	0.230 x 0.180 x 0.130 mm
Θ range (deg)	2.947 to 32.231 deg.
Limiting indices	-12<=h<=12, -15<=k<=15, -15<=l<=16
Reflections collected / unique	10763 / 5548 [R(int) = 0.0262]
Completeness to Θ = 25.242	99.8 %
Max. and min. transmission	1.00000 and 0.77304
Absorption correction	Semi-empirical from equivalents
Refined method	Full-matrix least-squares on F^2
Data / restrains / parameters	5548 / 0 / 236
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0624, wR2 = 0.1619
R indices (all data)	R1 = 0.0967, wR2 = 0.1867
Largest diff. peak and hole ($e.A^{-3}$)	0.260 and -0.234 e.A^-3
CCDC	**1522097**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4.2593
4.2411
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4.2236
4.1282
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1.1997
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O
O
S
O
N
Ph
Ph
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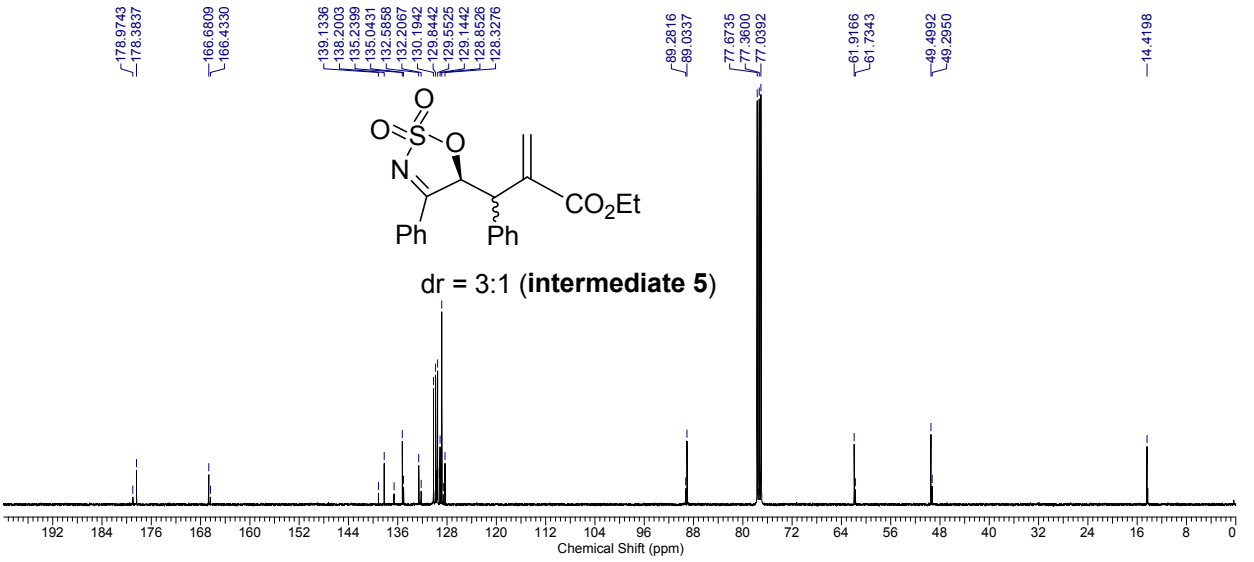
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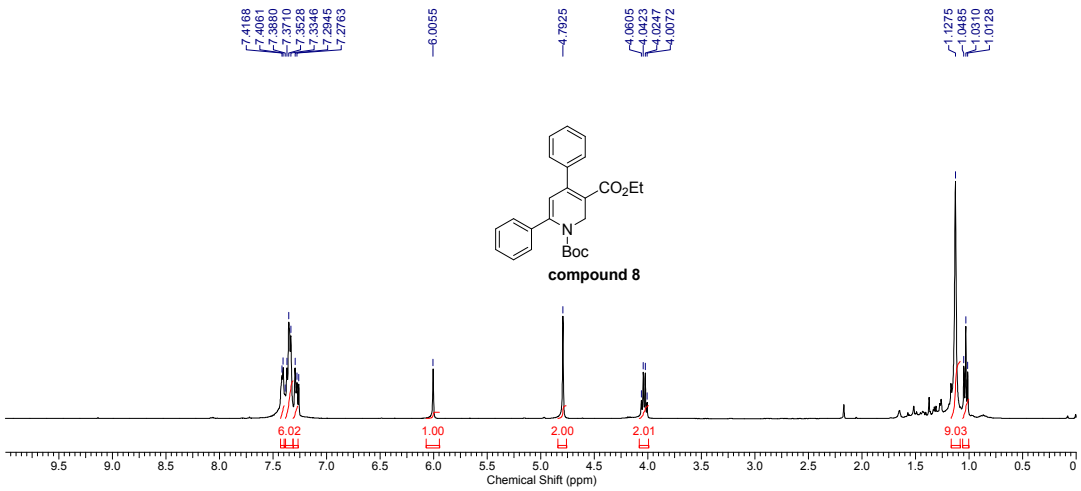
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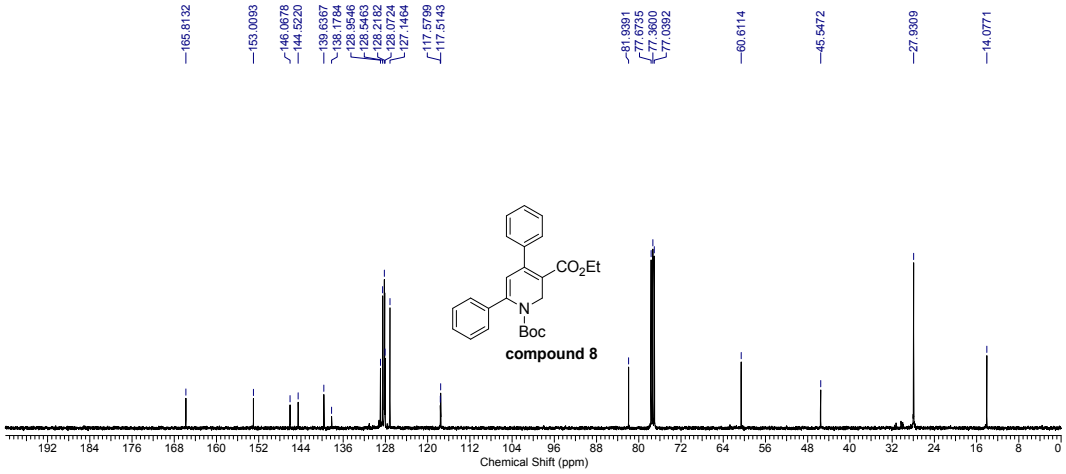
9.03
Chemical Shift (ppm)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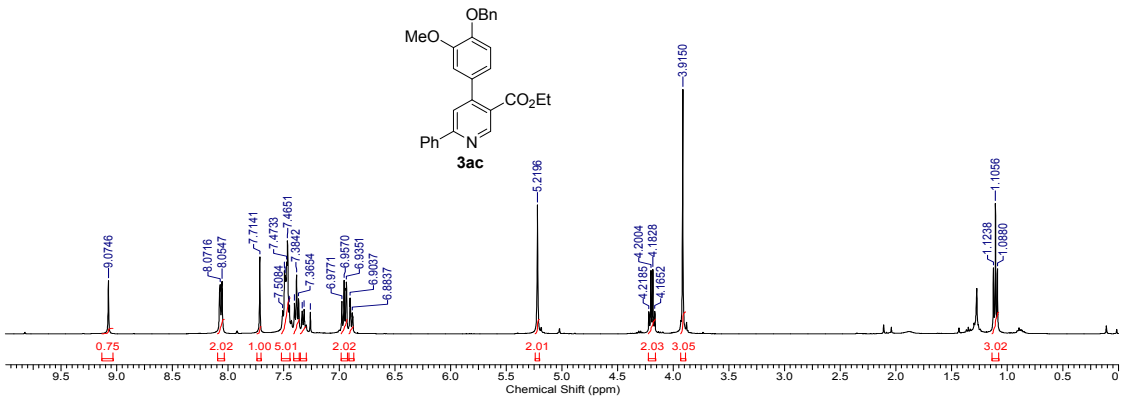
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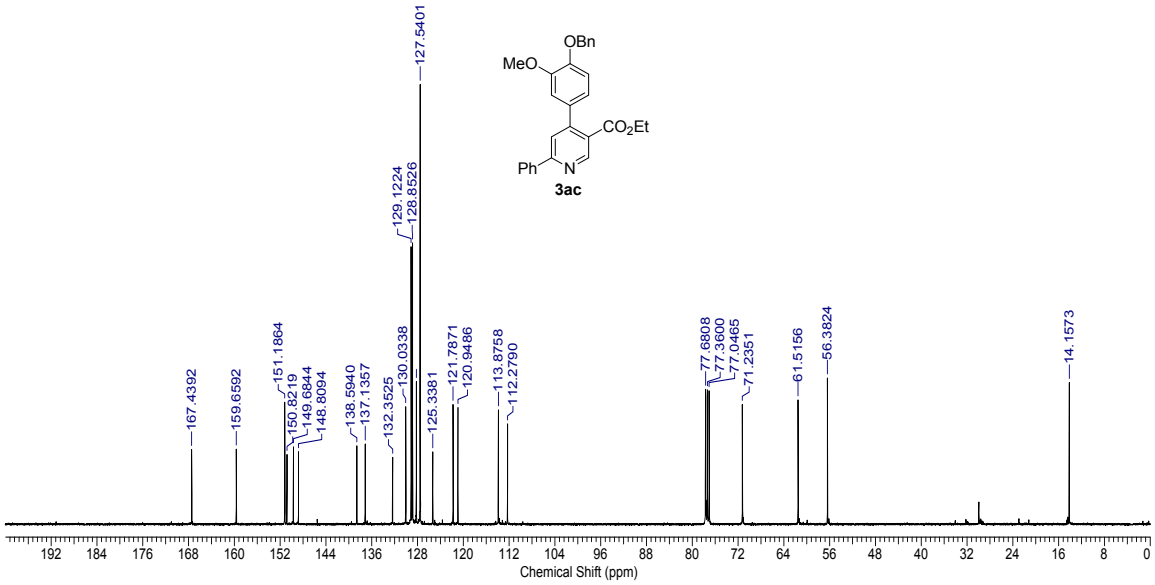
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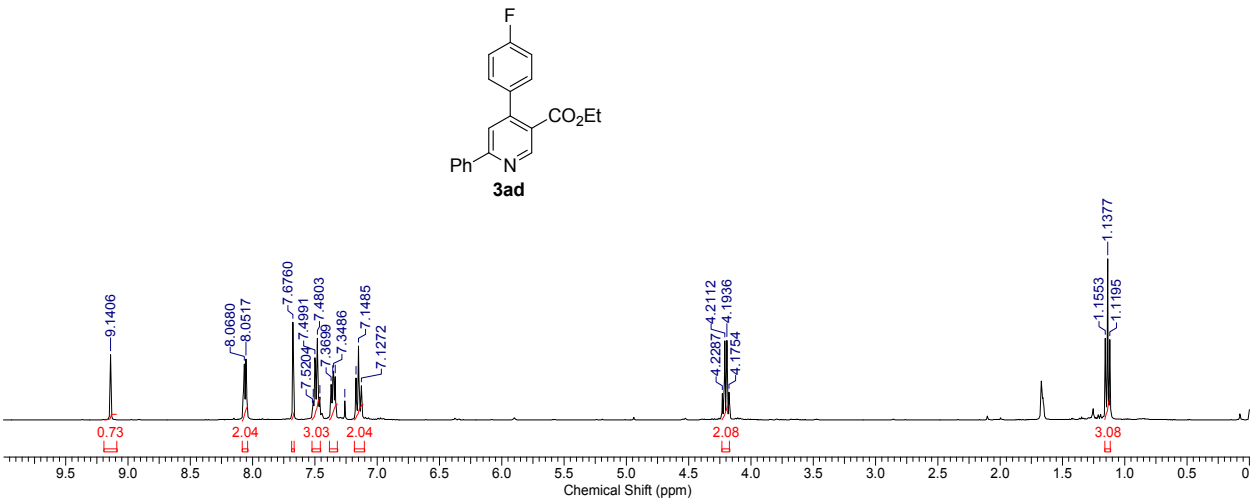
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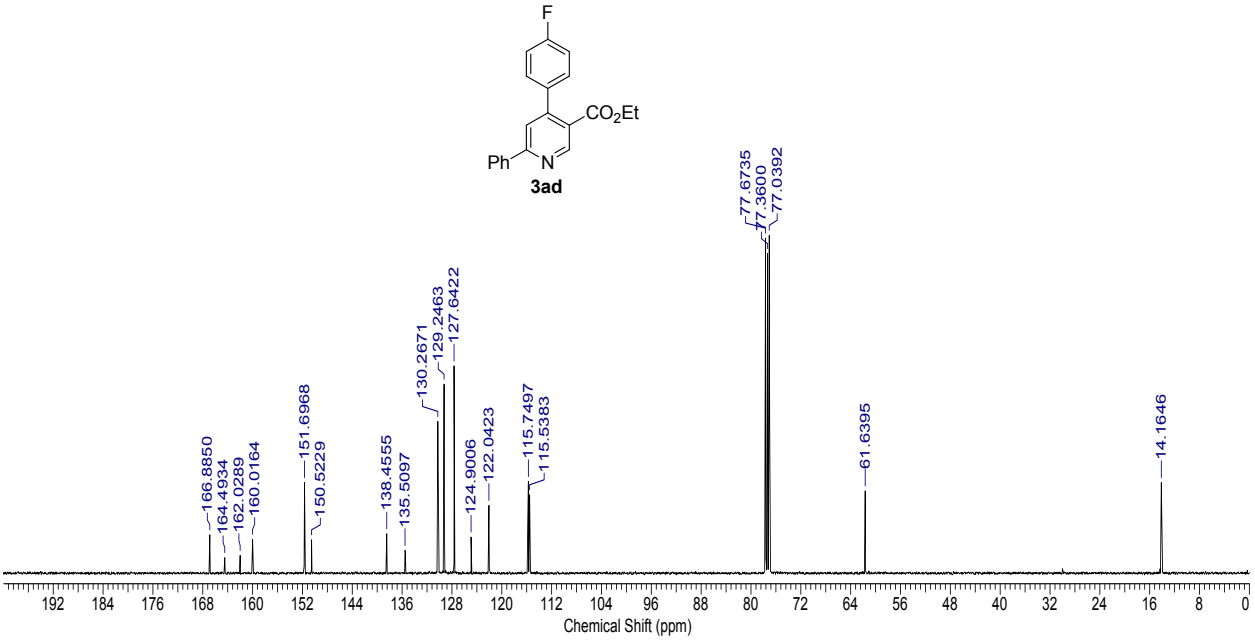
Chemical Shift (ppm)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127.6422
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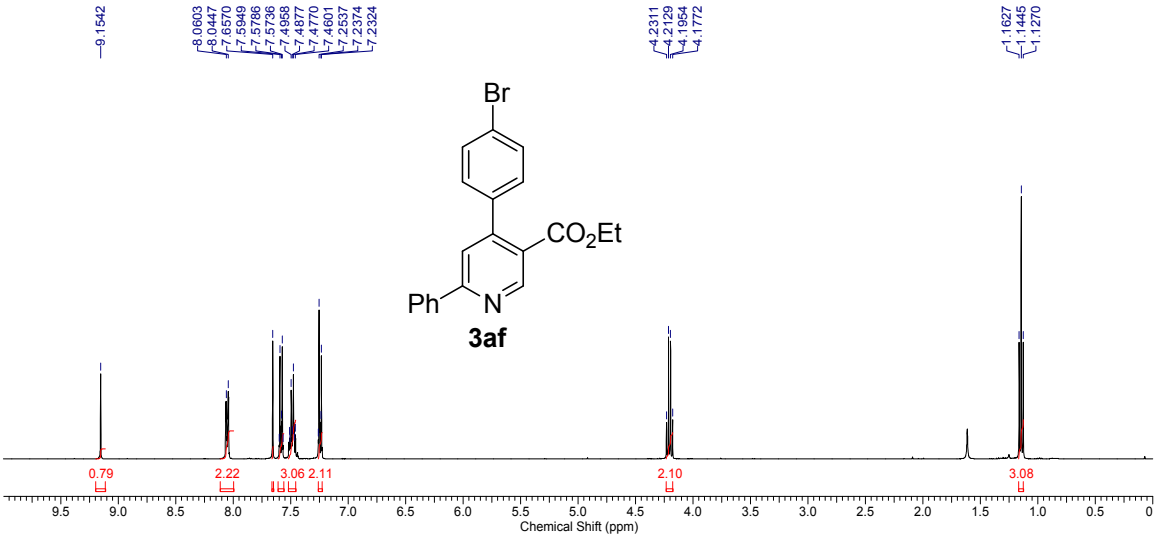
Chemical Shift (ppm)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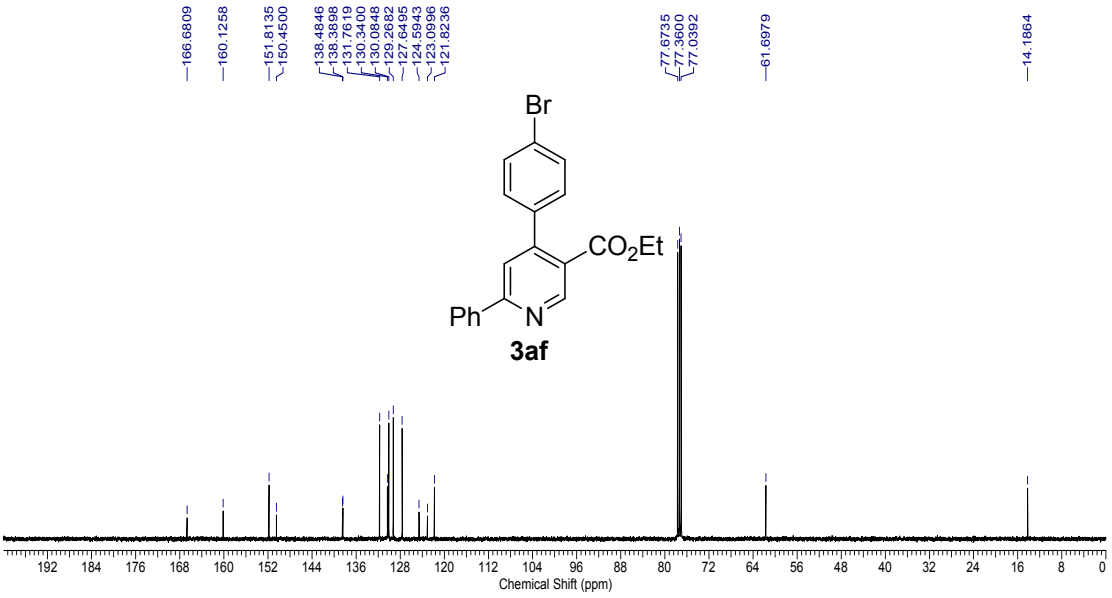
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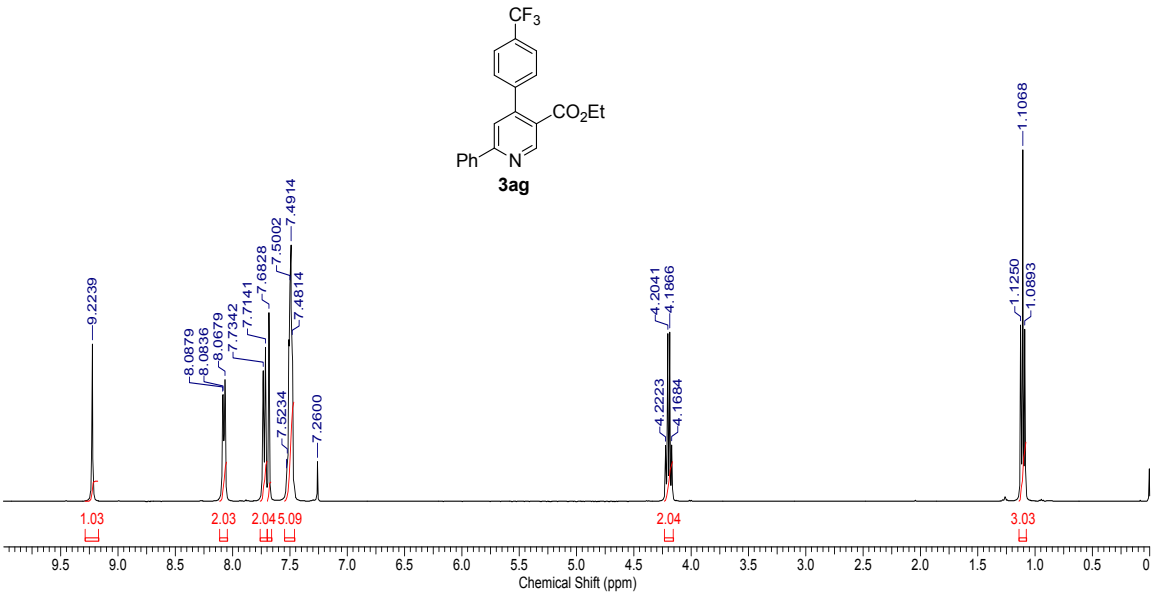
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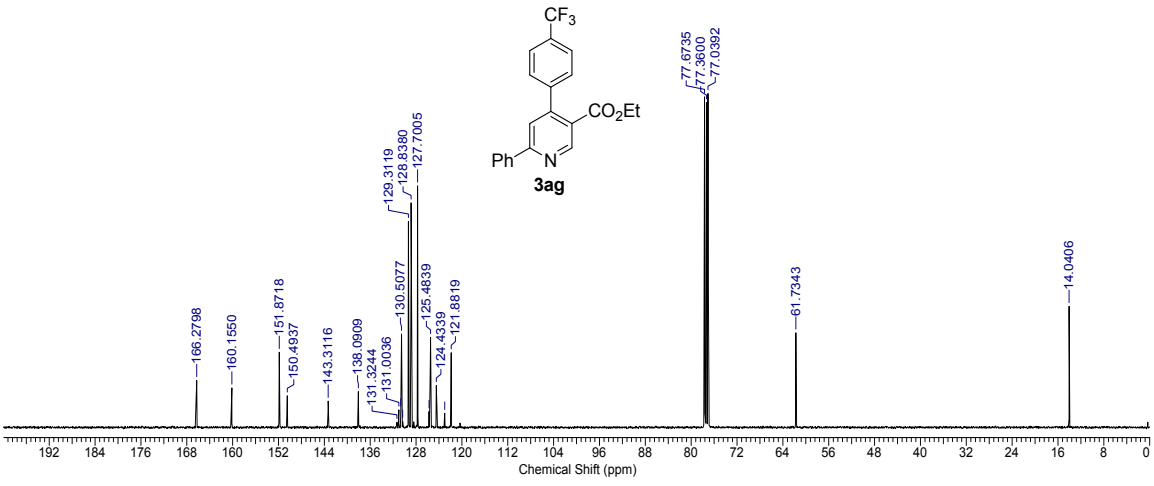
Chemical Shift (ppm)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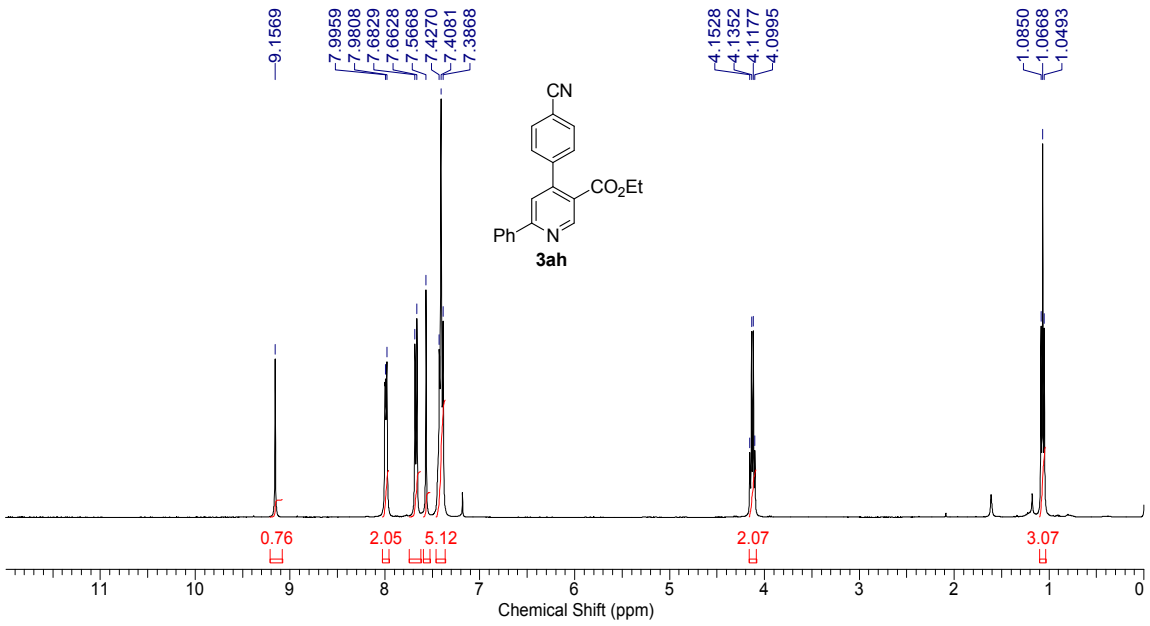
Chemical Shift (ppm)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Ph
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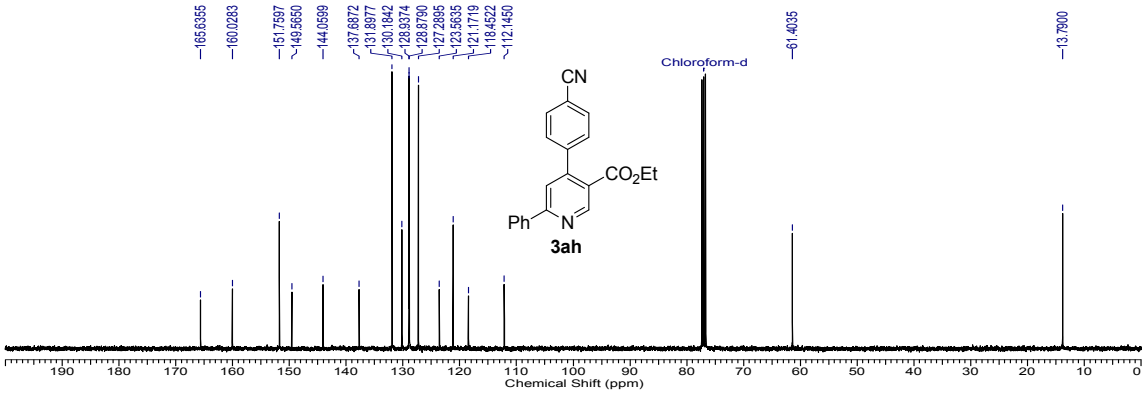
Chemical Shift (ppm)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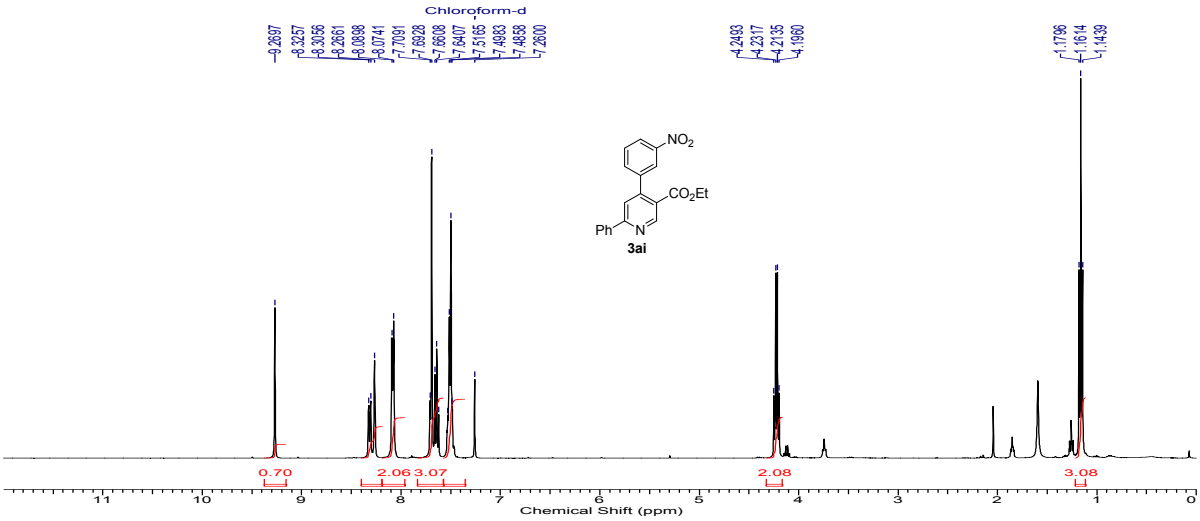
CN
CO2Et
Ph
N
3ah
Chemical Shift (ppm)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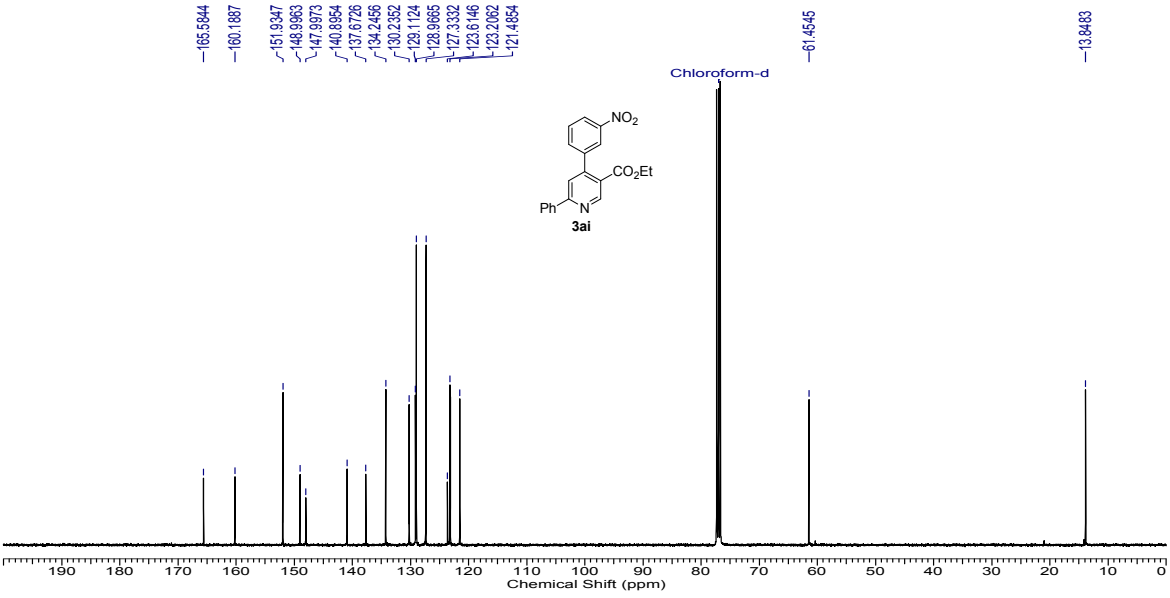
Chemical Shift (ppm)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Ph
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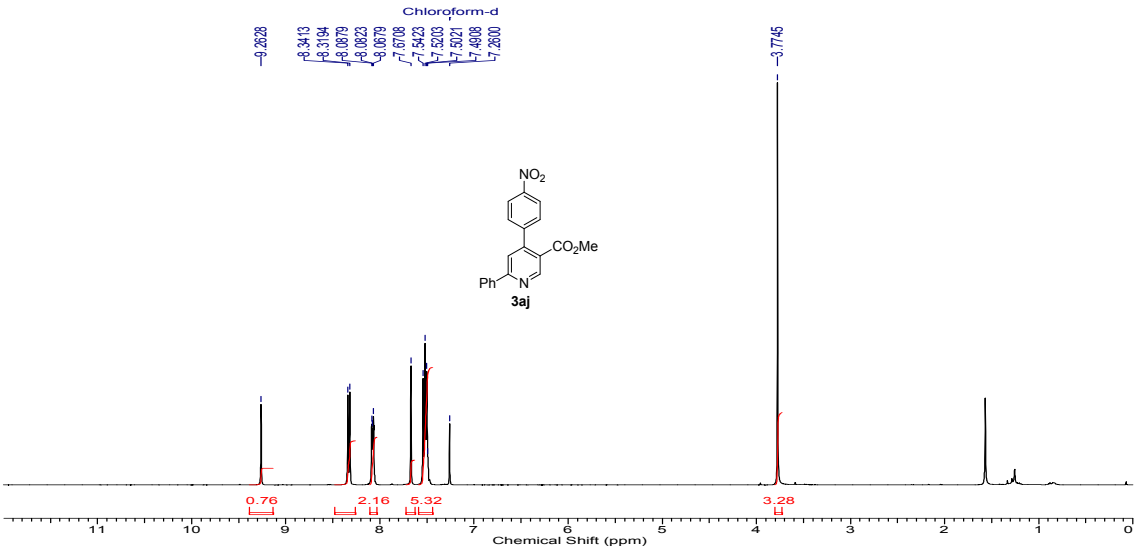
Chemical Shift (ppm)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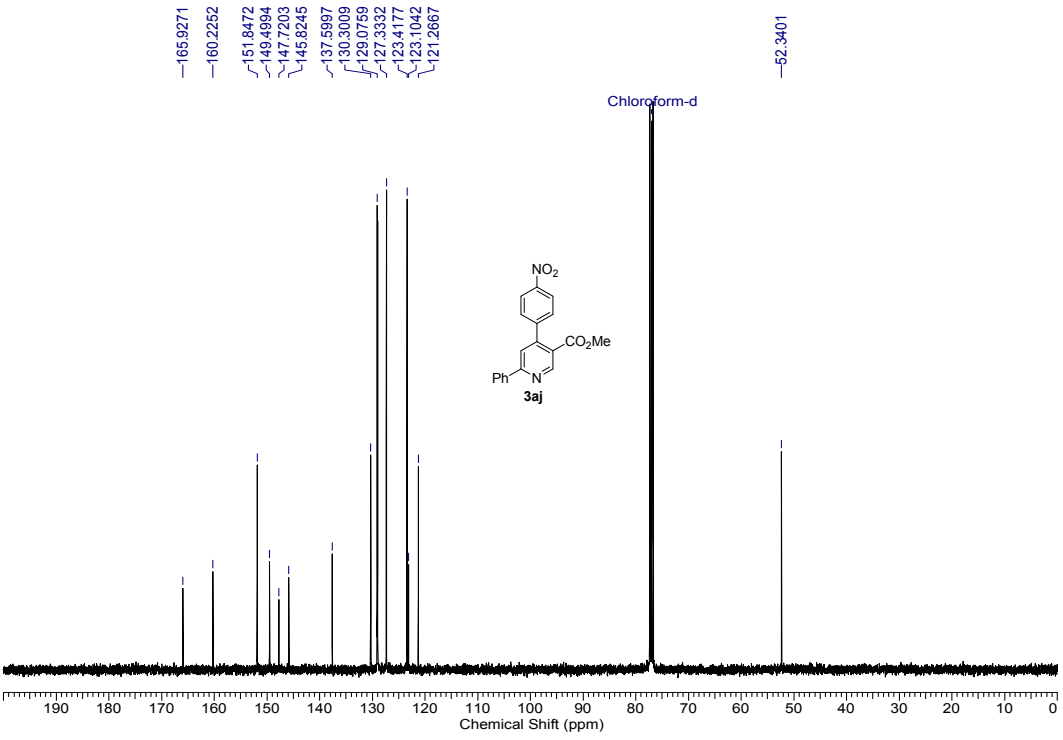
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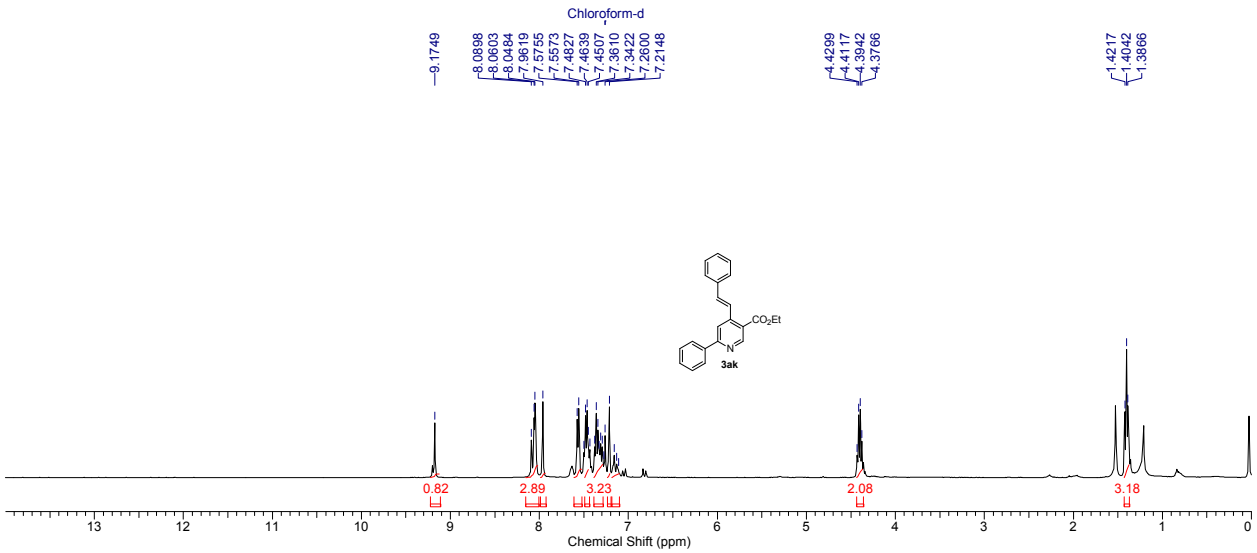
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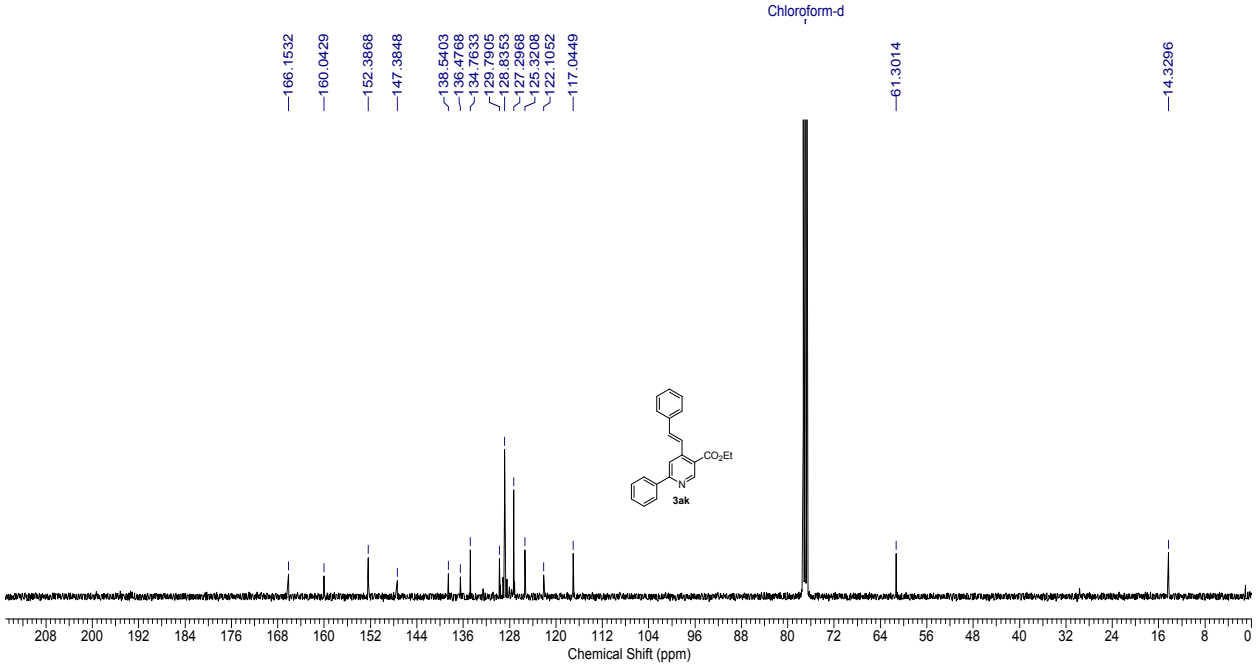
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192
184
176
168
160
152
144
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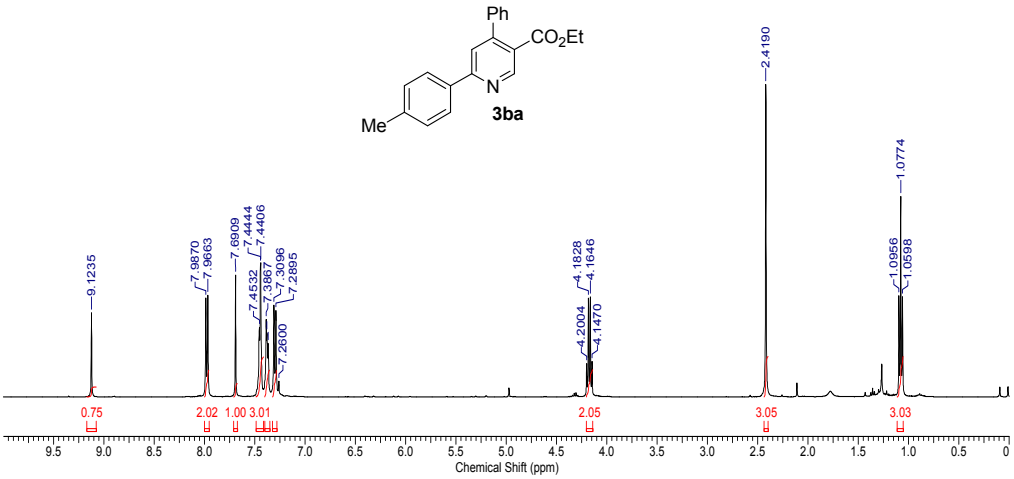
Chemical Shift (ppm)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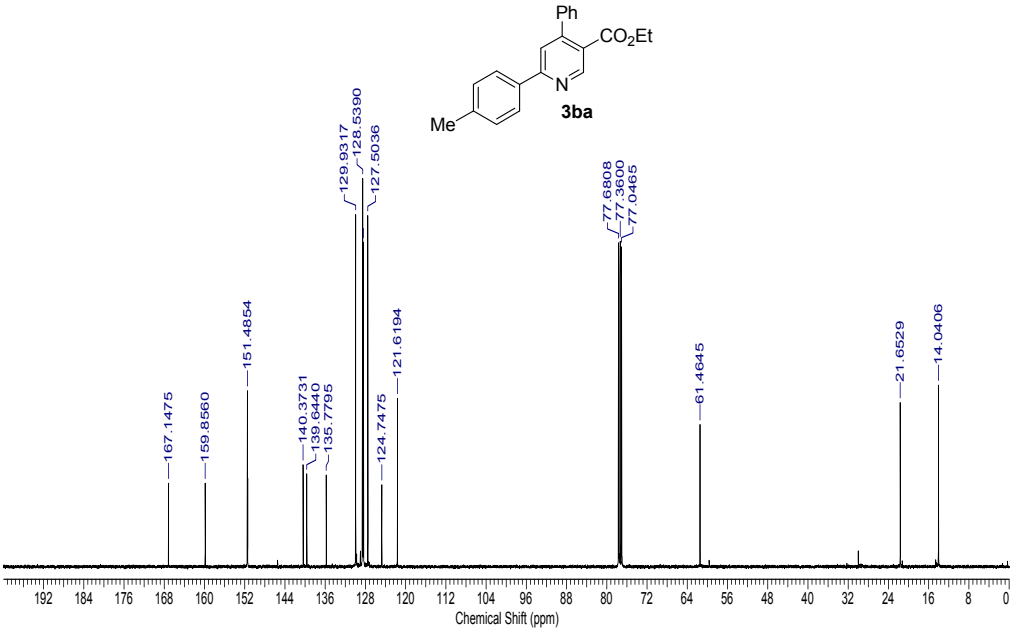
2.05
3.05
3.03
Chemical Shift (ppm)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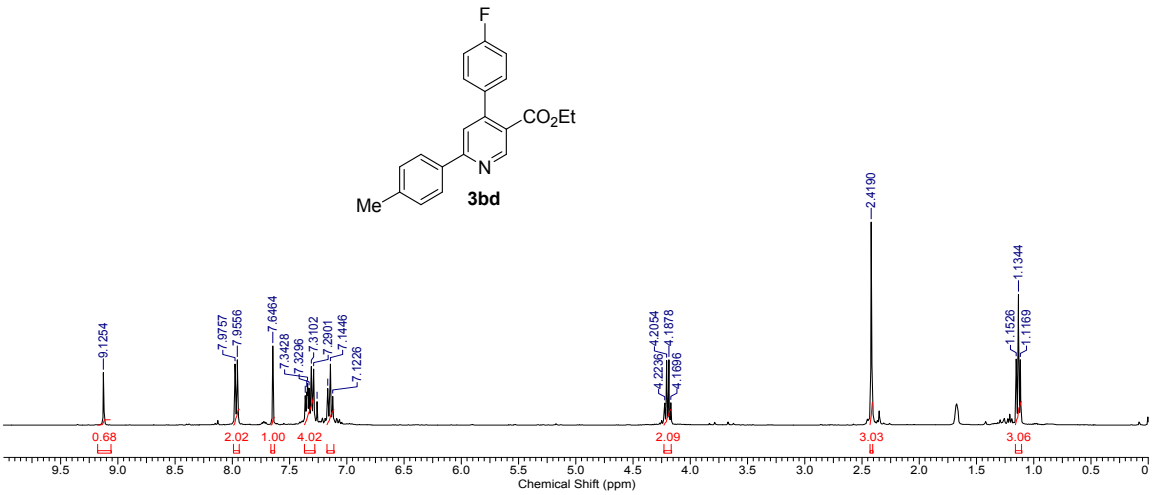
Chemical Shift (ppm)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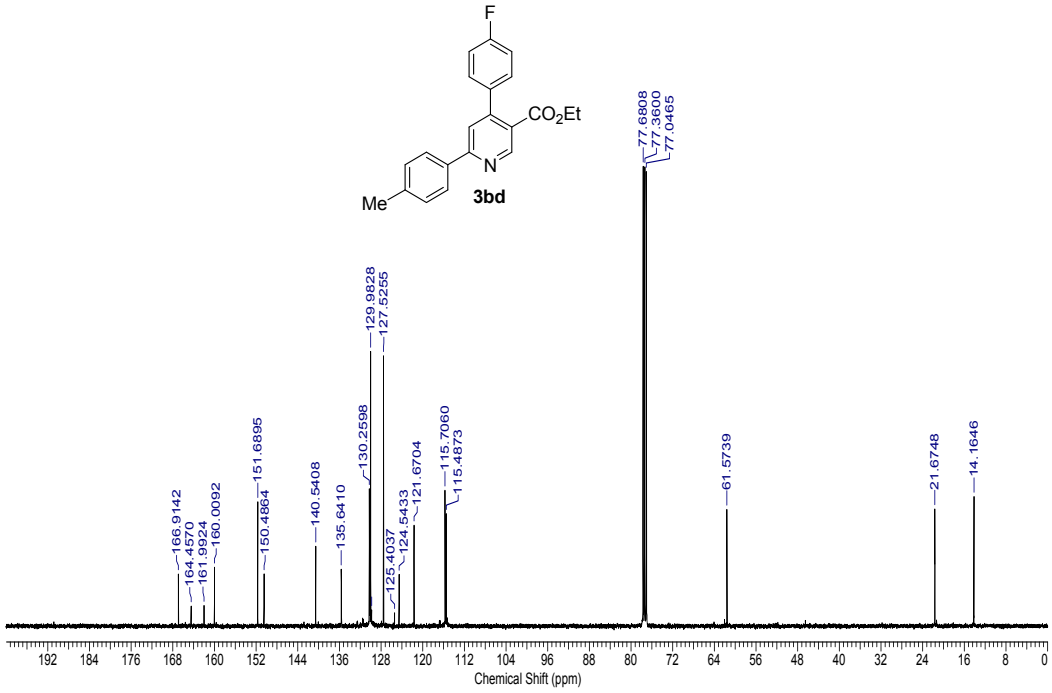
Chemical Shift (ppm)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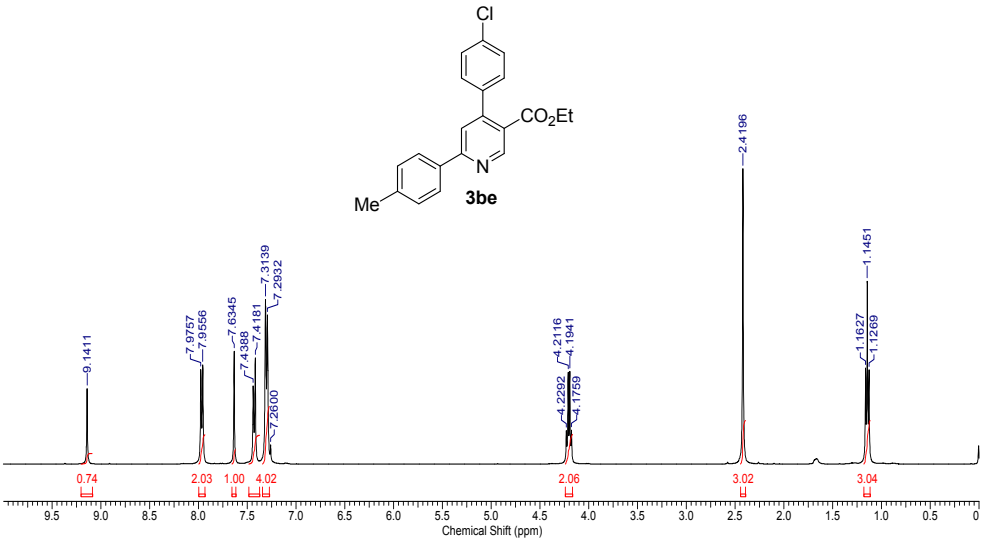
160.0092
151.6895
150.4864
140.5408
135.6410
130.2598
129.9828
127.5255
125.4037
124.5433
121.6704
115.7060
115.4873
77.6808
77.3600
77.0465
61.5739
21.6748
14.1646
Chemical Shift (ppm)


Cl
CO2Et
N
Me
3be
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7.9556
7.6345
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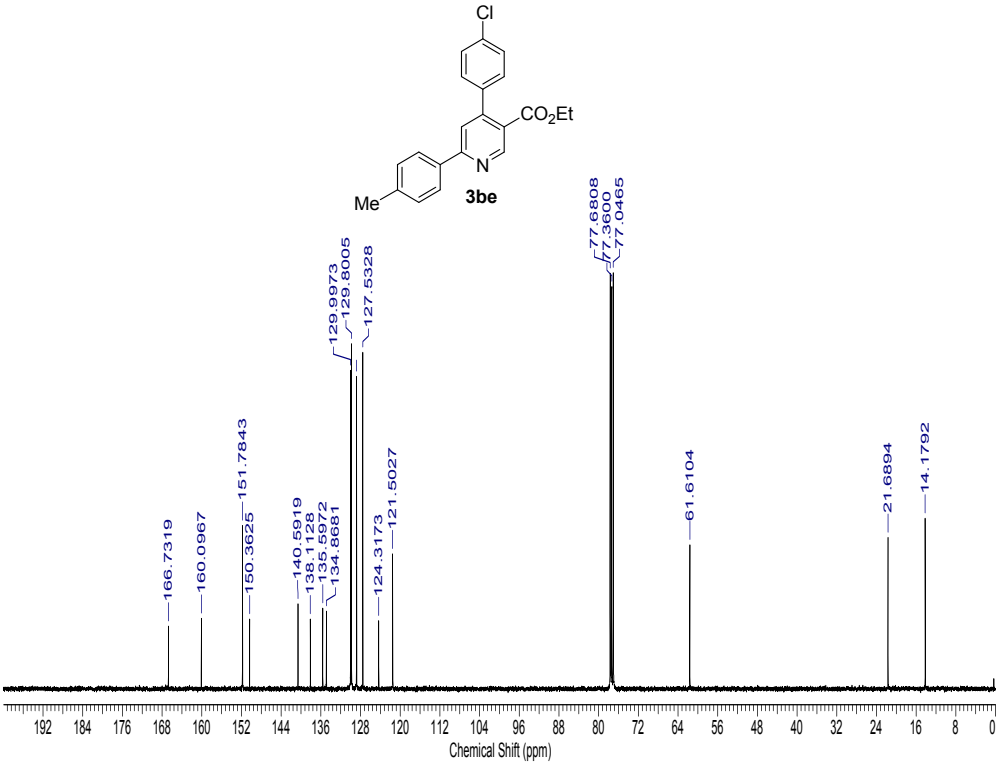
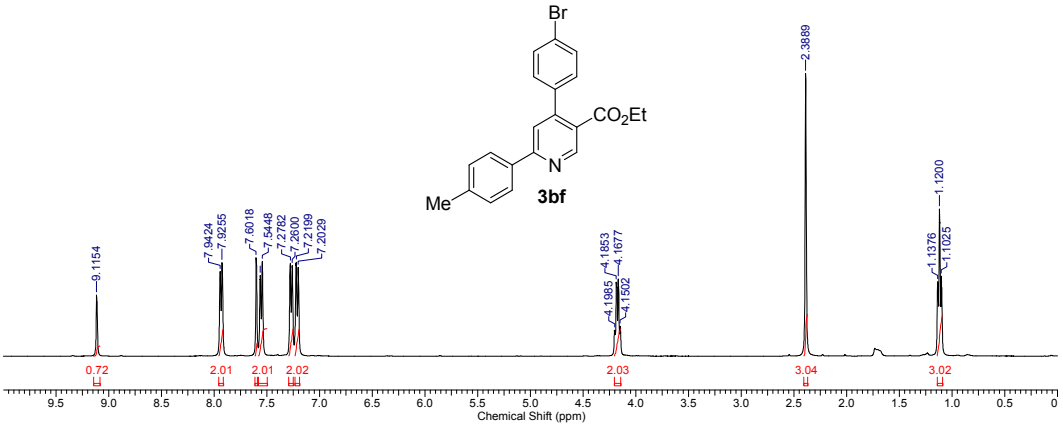
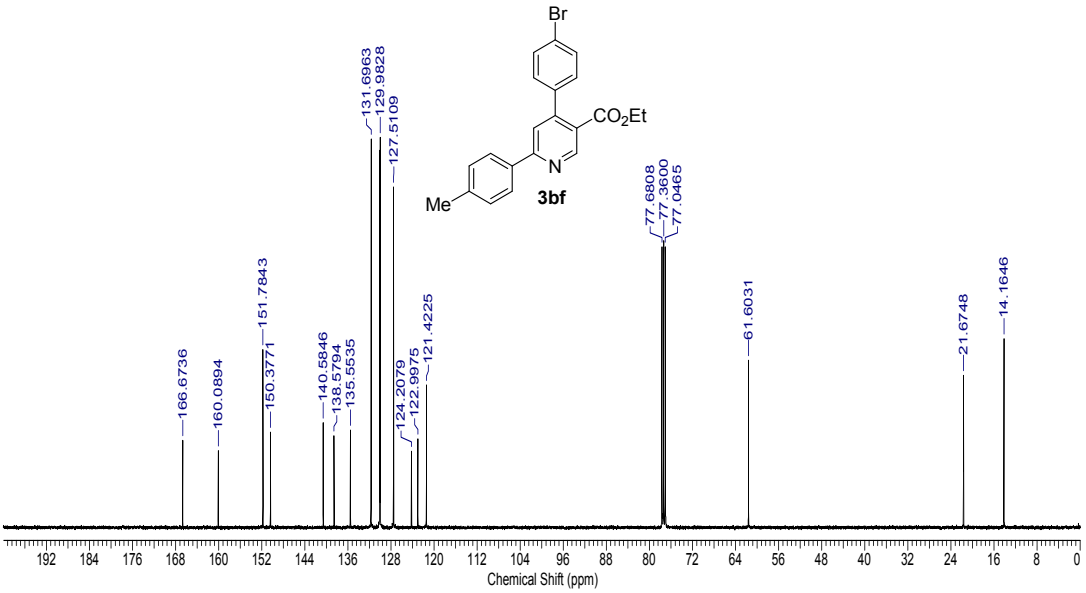
7.4181
7.3139
7.2932
7.2600
4.2292
4.2116
4.1941
4.1759
2.4196
1.1627
1.1451
1.1269
0.74
2.03
1.00
4.02
2.06
3.02
3.04
Chemical Shift (ppm)


Cl
CO2Et
N
Me
3be
166.7319
160.0967
151.7843
150.3625
140.5919
138.1128
135.5972
134.8681
129.9973
129.8005
127.5328
124.3173
121.5027
77.6808
77.3600
77.0465
61.6104
21.6894
14.1792
Chemical Shift (ppm)


Br
CO2Et
N
Me
3bf
9.1154
7.9424
7.9255
7.6018
7.5448
7.2782
7.2600
7.2199
7.2029
4.1985
4.1853
4.1677
4.1502
2.3889
1.1376
1.1200
1.1025
0.72
2.01
2.01
2.02
2.03
3.04
3.02
Chemical Shift (ppm)


Br
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N
Me
3bf
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151.7843
150.3771
140.5846
138.5794
135.5535
131.6963
129.9828
127.5109
124.2079
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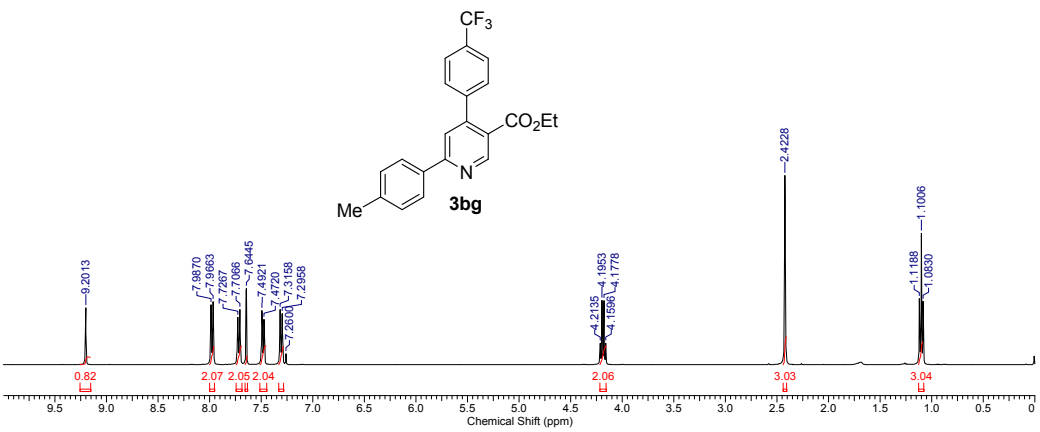
121.4225
77.6808
77.3600
77.0465
61.6031
21.6748
14.1646
Chemical Shift (ppm)


CF3
CO2Et
N
Me
3bg
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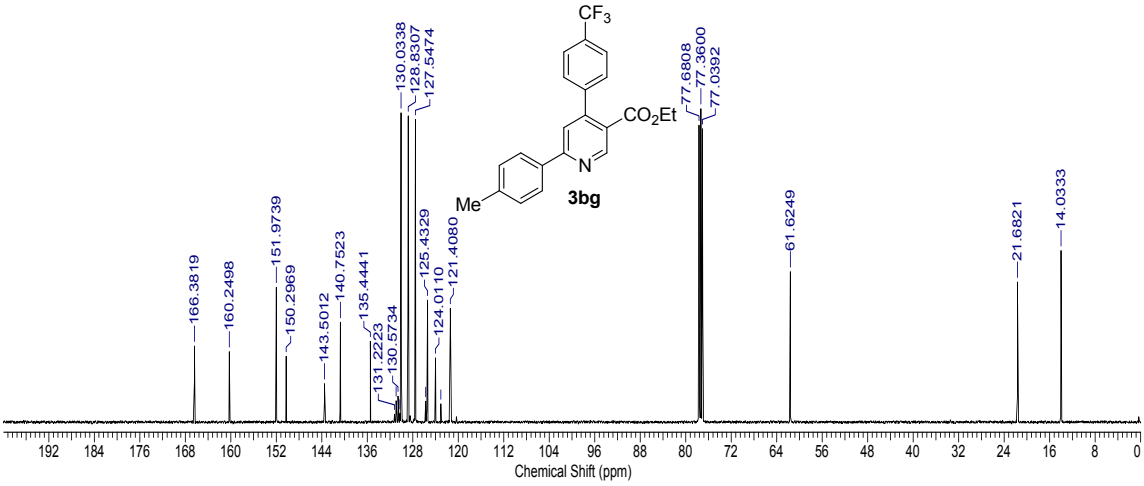
7.9870
7.9663
7.7267
7.7066
7.6445
7.4921
7.4720
7.3158
7.2958
7.2600
4.2135
4.1953
4.1586
4.1778
2.4228
1.1188
1.1006
1.0830
0.82
2.07
2.05
2.04
2.06
3.03
3.04
Chemical Shift (ppm)


CF3
CO2Et
N
Me
3bg
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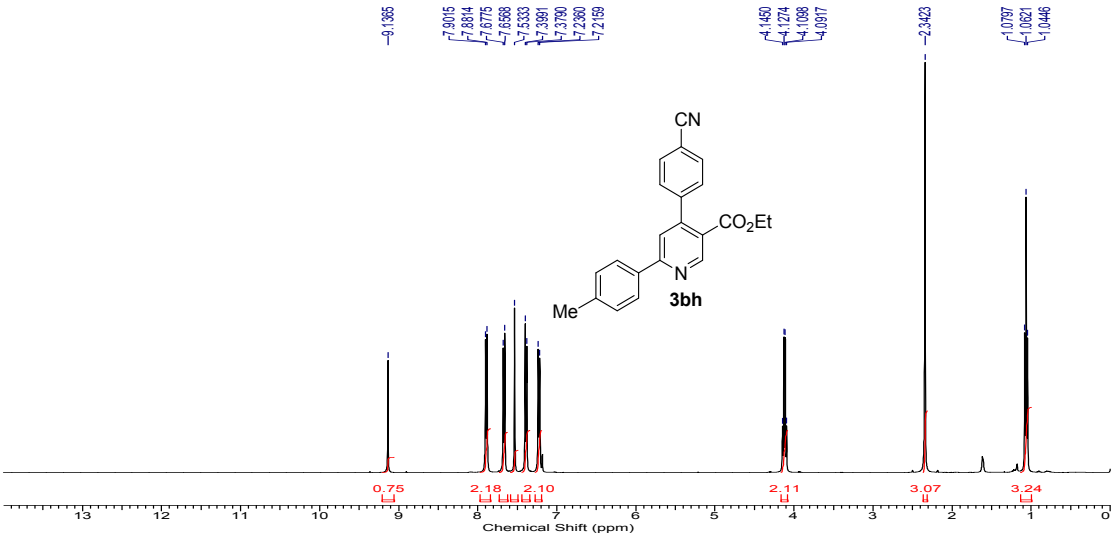
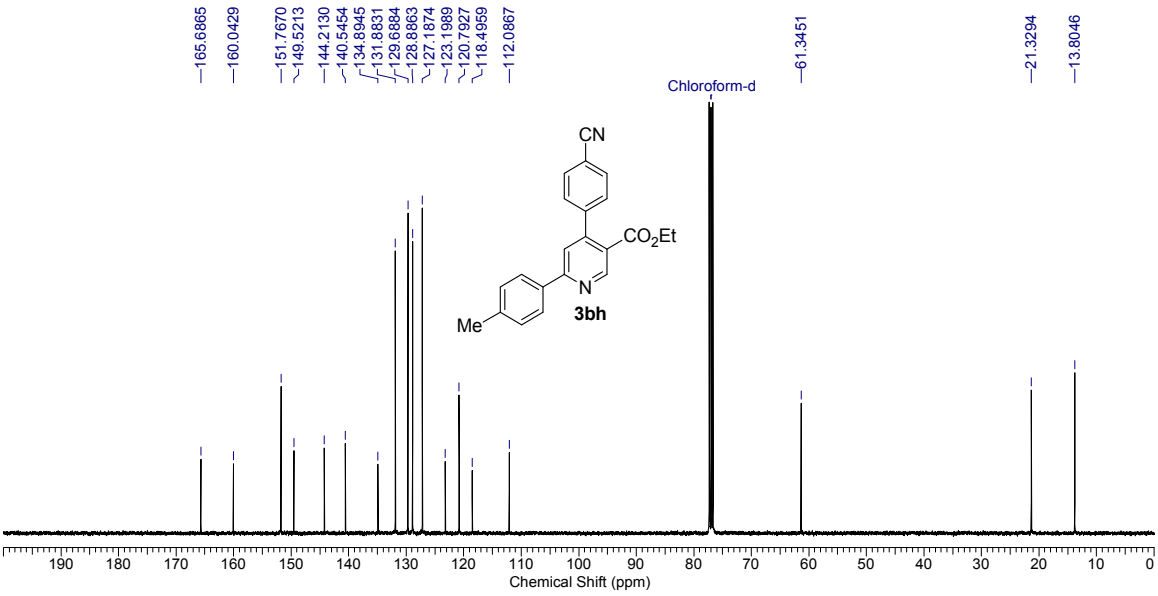
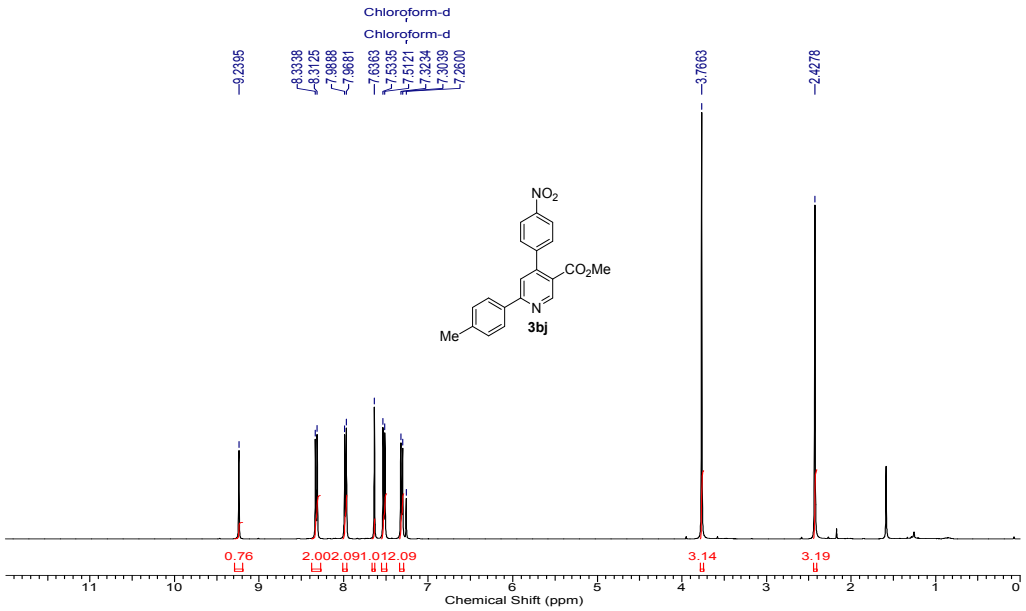
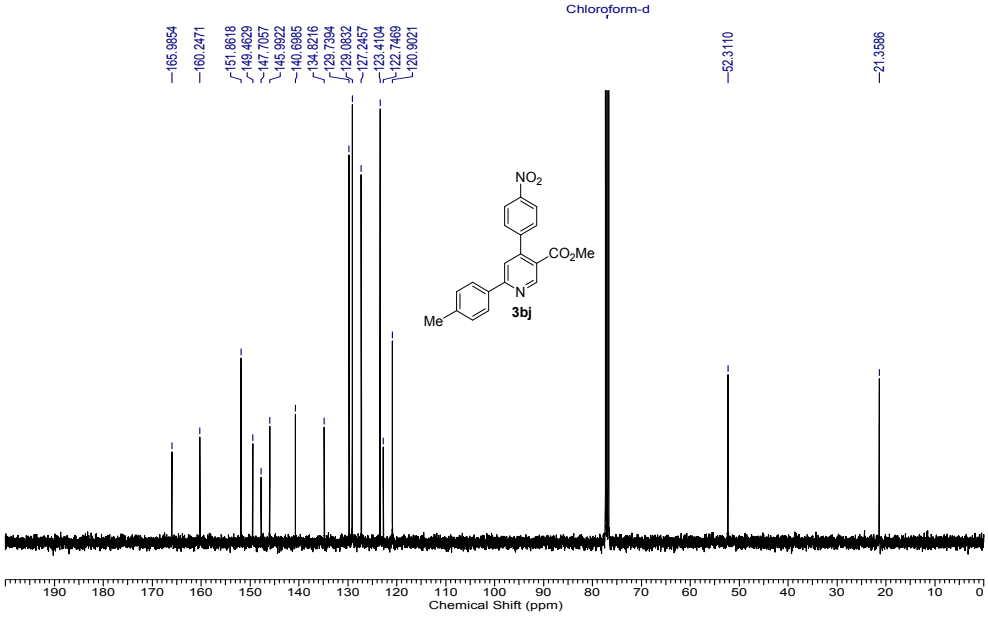
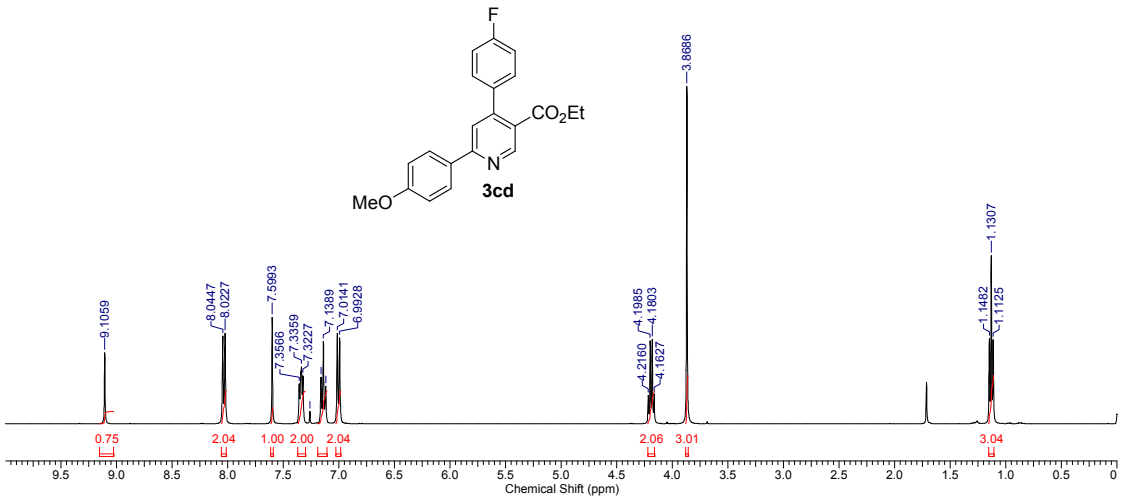
160.2498
151.9739
150.2969
143.5012
140.7523
135.4441
131.2223
130.5734
130.0338
128.8307
127.5474
125.4329
124.0110
121.4080
77.6808
77.3600
77.0392
61.6249
21.6821
14.0333
Chemical Shift (ppm)

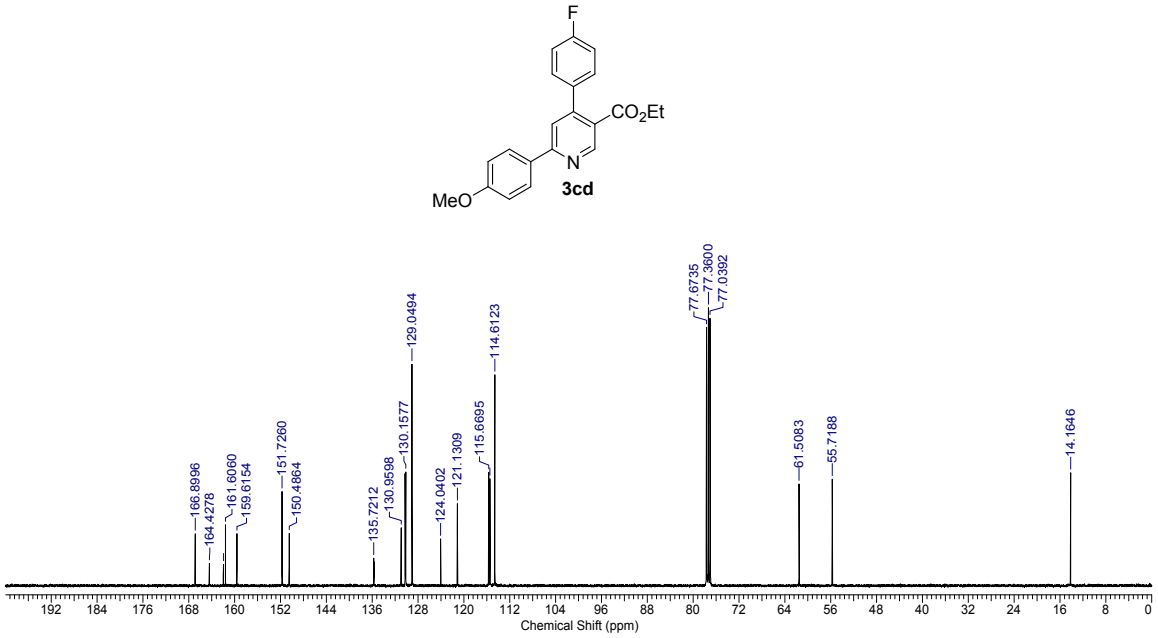

9.1365
7.9015
7.8814
7.6775
7.6568
7.5333
7.3991
7.3790
7.2360
7.2159
4.1450
4.1274
4.1098
4.0917
2.3423
1.0797
1.0621
1.0446
CN
CO2Et
N
Me
3bh
0.75
2.18
2.10
2.11
3.07
3.24
Chemical Shift (ppm)

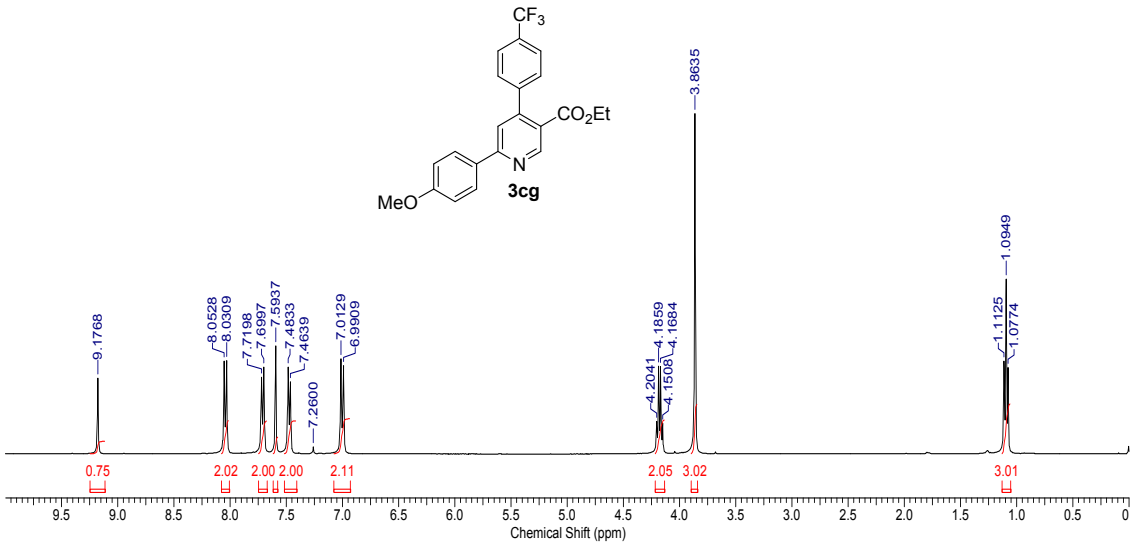

165.6865
160.0429
151.7670
149.5213
144.2130
140.5454
134.8945
131.8831
129.6884
128.8863
127.1874
123.1989
120.7927
118.4959
112.0867
Chloroform-d
61.3451
21.3294
13.8046
CN
CO2Et
N
Me
3bh
Chemical Shift (ppm)

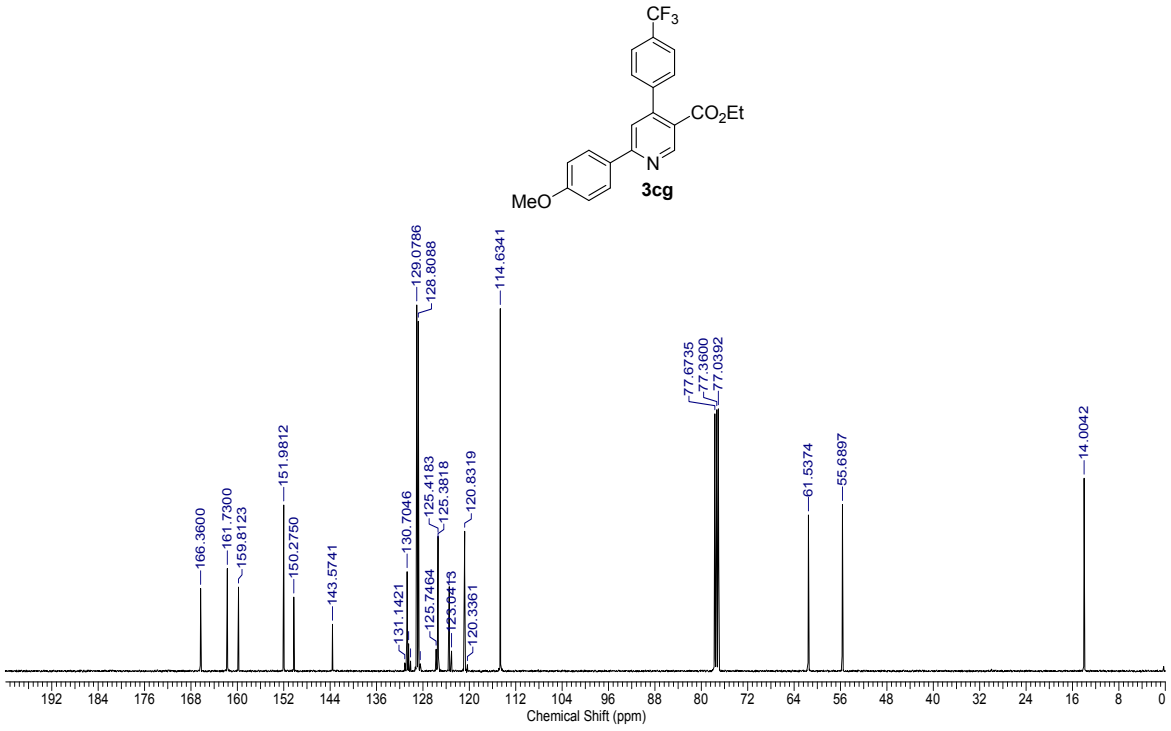

Chloroform-d
Chloroform-d
9.2395
8.3338
8.3125
7.9988
7.9681
7.6363
7.5335
7.5121
7.3234
7.3039
7.2600
3.7663
2.4278
NO2
CO2Me
N
Me
3bj
0.76
2.00
2.09
1.01
2.09
3.14
3.19
Chemical Shift (ppm)

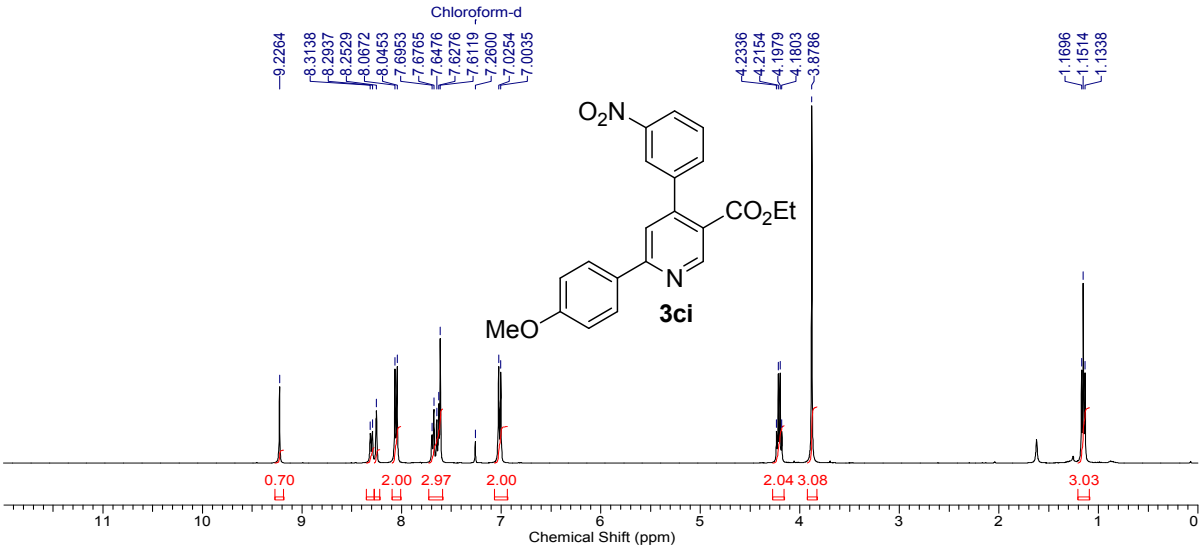

Chloroform-d
165.9854
160.2471
151.8618
149.4629
147.7057
145.9922
140.6985
134.8216
129.7394
129.0832
127.2457
123.4104
122.7469
120.9021
52.3110
21.3586
NO2
CO2Me
N
Me
3bj
Chemical Shift (ppm)

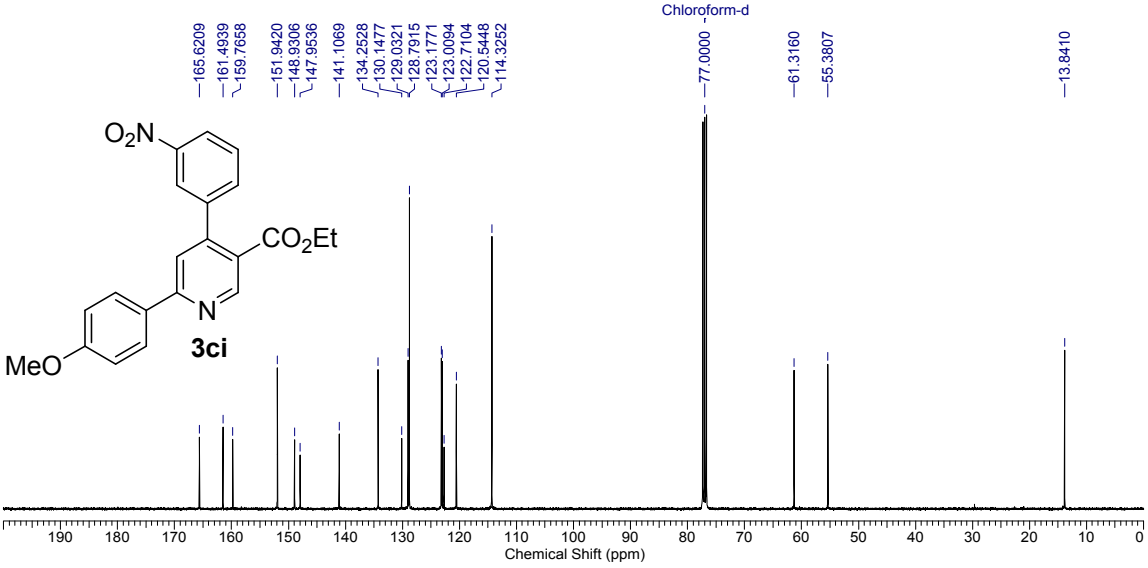

F
CO2Et
N
MeO
3cd
9.1059
8.0447
8.0227
7.5993
7.3566
7.3359
7.3227
7.1389
7.0141
6.9928
4.1985
4.1803
4.2160
4.1627
3.8686
1.1307
1.1482
1.1125
0.75
2.04
1.00
2.00
2.04
2.06
3.01
3.04
Chemical Shift (ppm)

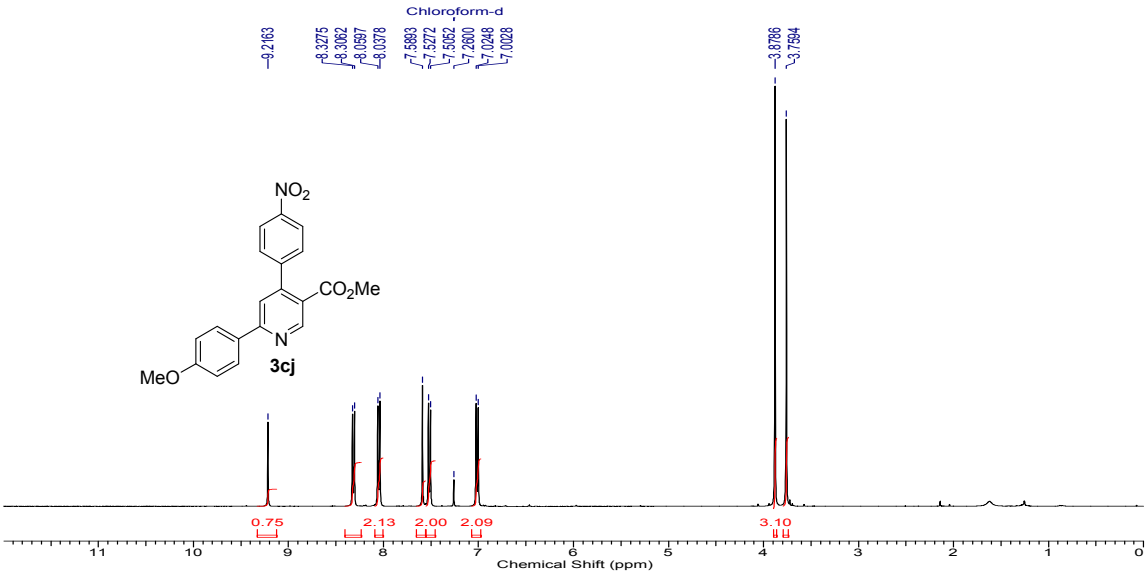

F
CO2Et
N
MeO
3cd
166.8996
164.4278
161.6060
159.6154
151.7260
150.4864
135.7212
130.9598
130.1577
129.0494
124.0402
121.1309
115.6695
114.6123
77.6735
77.3600
77.0392
61.5083
55.7188
14.1646
Chemical Shift (ppm)

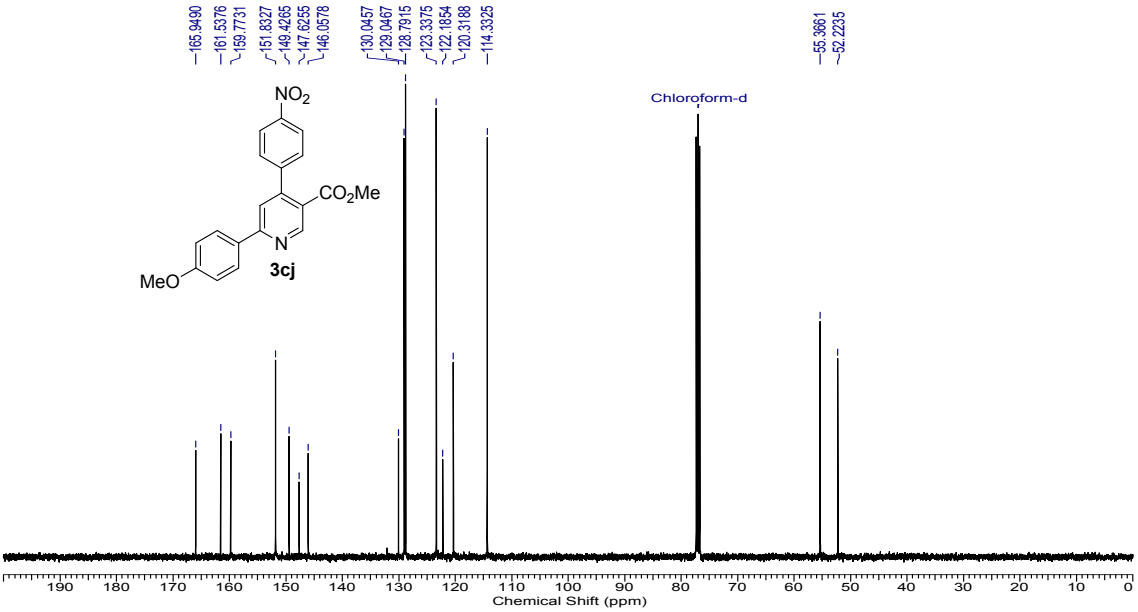

CF3
CO2Et
N
MeO
3cg
9.1768
8.0528
8.0309
7.7198
7.6997
7.5937
7.4833
7.4639
7.2600
7.0129
6.9909
4.2041
4.1859
4.1508
4.1684
3.8635
1.1125
1.0949
1.0774
0.75
2.02
2.00
2.00
2.11
2.05
3.02
3.01
Chemical Shift (ppm)

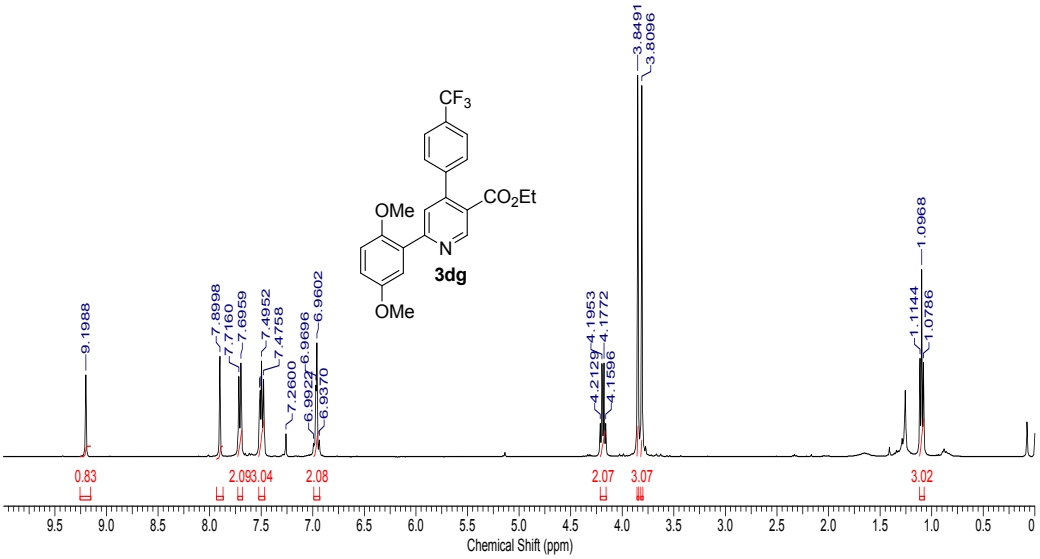

CF3
CO2Et
N
MeO
3cg
166.3600
161.7300
159.8123
151.9812
150.2750
143.5741
131.1421
130.7046
129.0786
128.8088
125.7464
125.4183
125.3818
123.0413
120.8319
120.3361
114.6341
77.6735
77.3600
77.0392
61.5374
55.6897
14.0042
Chemical Shift (ppm)


Chloroform-d
9.2264
8.3138
8.2937
8.2529
8.0672
8.0453
7.6953
7.6765
7.6476
7.6276
7.6119
7.2600
7.0254
7.0035
4.2336
4.2154
4.1979
4.1803
3.8786
1.1696
1.1514
1.1338
O2N
CO2Et
N
MeO
3ci
0.70
2.00
2.97
2.00
2.04
3.08
3.03
Chemical Shift (ppm)


Chloroform-d
165.6209
161.4939
159.7658
151.9420
148.9306
147.9536
141.1069
134.2528
130.1477
129.0321
128.7915
123.1771
123.0094
122.7104
120.5448
114.3252
77.0000
61.3160
55.3807
13.8410
O2N
CO2Et
N
MeO
3ci
Chemical Shift (ppm)


Chloroform-d
9.2163
8.3275
8.3062
8.0597
8.0378
7.5883
7.5272
7.5052
7.2800
7.0248
7.0028
3.8786
3.7594
NO2
CO2Me
N
MeO
3cj
0.75
2.13
2.00
2.09
3.10
Chemical Shift (ppm)


165.9490
161.5376
159.7731
151.8327
149.4265
147.6255
146.0578
130.0457
129.0467
128.7915
123.3375
122.1654
120.3188
114.3325
55.3661
52.2235
Chloroform-d
NO2
CO2Me
N
MeO
3cj
Chemical Shift (ppm)


CF3
CO2Et
OMe
N
OMe
3dg
9.1988
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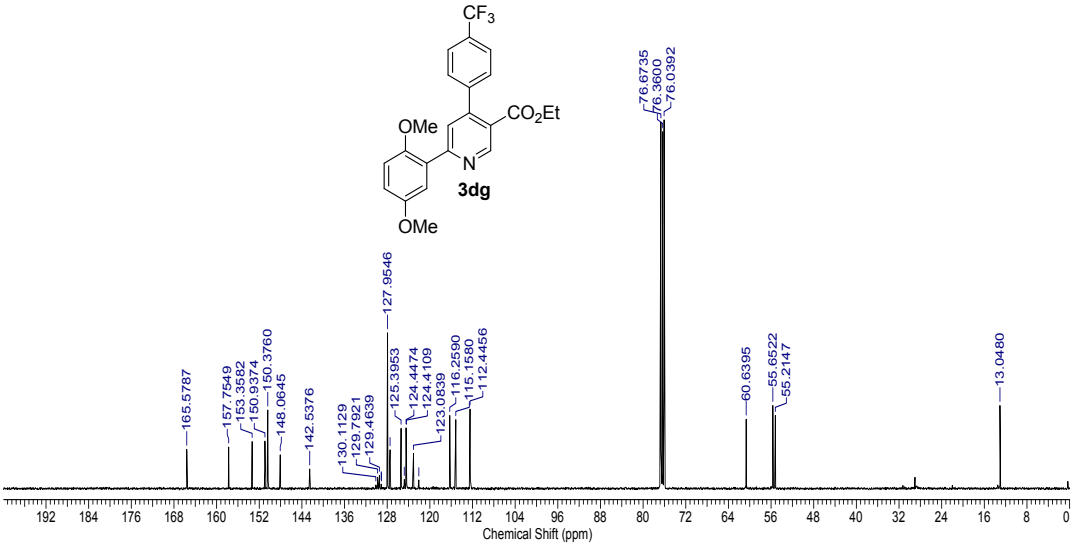
7.7160
7.6959
7.4952
7.4758
7.2600
6.9922
6.9696
6.9370
6.9602
4.2129
4.1953
4.1772
4.1596
3.8491
3.8096
1.1144
1.0968
1.0786
0.83
2.09
3.04
2.08
2.07
3.07
3.02
Chemical Shift (ppm)


CF3
CO2Et
OMe
N
OMe
3dg
165.5787
157.7549
153.3582
150.9374
150.3760
148.0645
142.5376
130.1129
129.7921
129.4639
127.9546
125.3953
124.4474
124.4109
123.0838
116.2590
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112.4456
76.6735
76.3600
76.0392
60.6395
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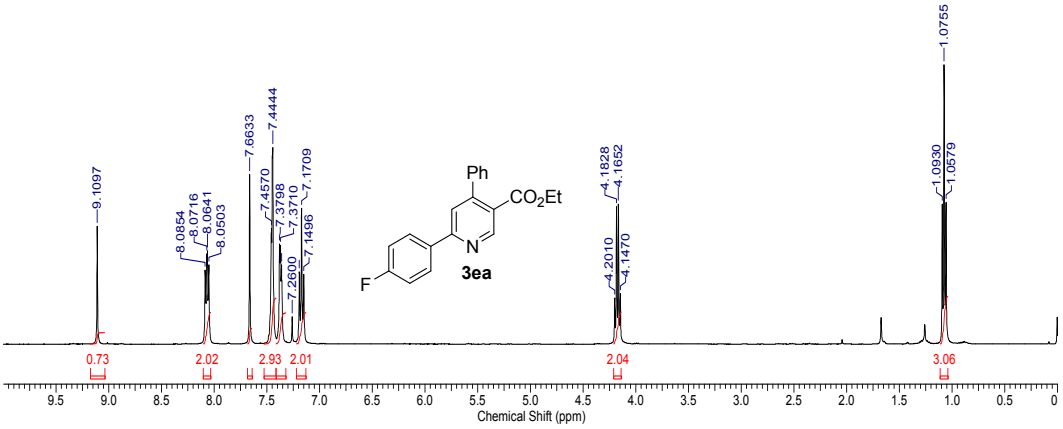
13.0480
Chemical Shift (ppm)


9.1097
8.0854
8.0716
8.0641
8.0503
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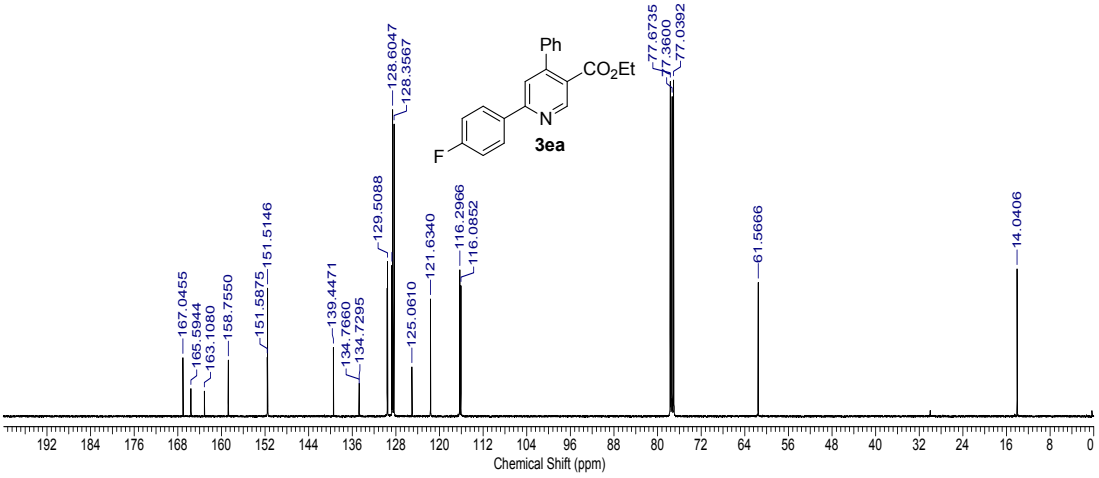
7.4570
7.4444
7.3798
7.3710
7.2600
7.1709
7.1496
4.1828
4.1652
4.2010
4.1470
1.0930
1.0579
1.0755
Ph
CO2Et
N
F
3ea
0.73
2.02
2.93
2.01
2.04
3.06
Chemical Shift (ppm)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165.5944
163.1080
158.7550
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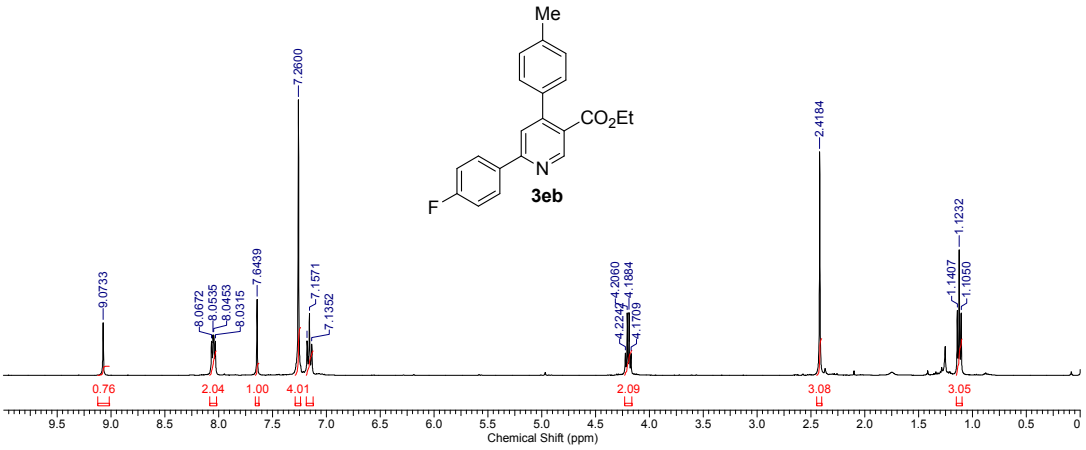
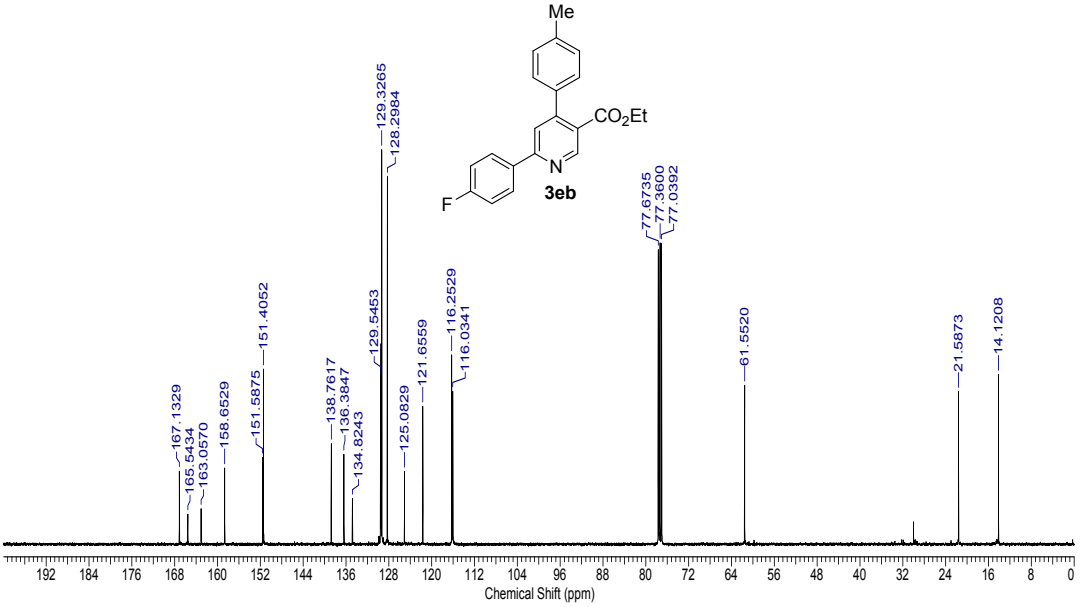
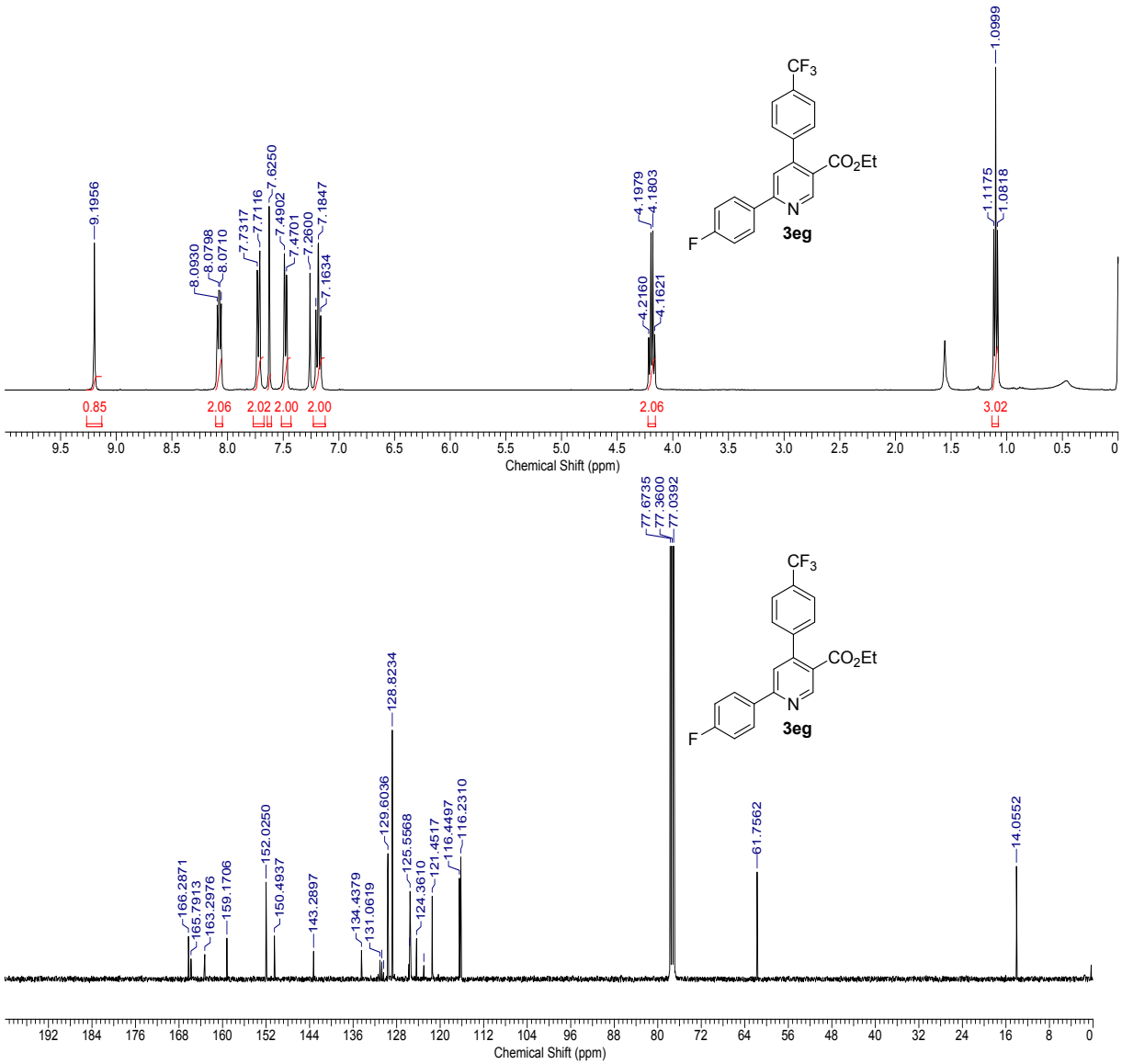
139.4471
134.7660
134.7295
129.5088
128.6047
128.3567
125.0610
121.6340
116.2966
116.0852
77.6735
77.3600
77.0392
61.5666
14.0406
Ph
CO2Et
N
F
3ea
Chemical Shift (ppm)


Me
CO2Et
N
F
3eb
9.0733
8.0672
8.0535
8.0453
8.0315
7.6439
7.2600
7.1571
7.1352
4.2247
4.2060
4.1884
4.1709
2.4184
1.1407
1.1232
1.1050
0.76
2.04
1.00
4.01
2.09
3.08
3.05
Chemical Shift (ppm)


Me
CO2Et
N
F
3eb
167.1329
165.5434
163.0570
158.6529
151.5875
151.4052
138.7617
136.3847
134.8243
129.5453
129.3265
128.2984
125.0829
121.6559
116.2529
116.0341
77.6735
77.3600
77.0392
61.5520
21.5873
14.1208
Chemical Shift (ppm)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8.0710
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7.7116
7.6250
7.4902
7.4701
7.2600
7.1847
7.1634
4.2160
4.1979
4.1803
4.1621
1.1175
1.0818
1.0999
0.85
2.06
2.02
2.00
2.00
2.06
3.02
Chemical Shift (ppm)
CF3
CO2Et
N
F
3eg
77.6735
77.3600
77.0392
166.2871
165.7913
163.2976
159.1706
152.0250
150.4937
143.2897
134.4379
131.0619
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128.8234
125.5568
124.3610
121.4517
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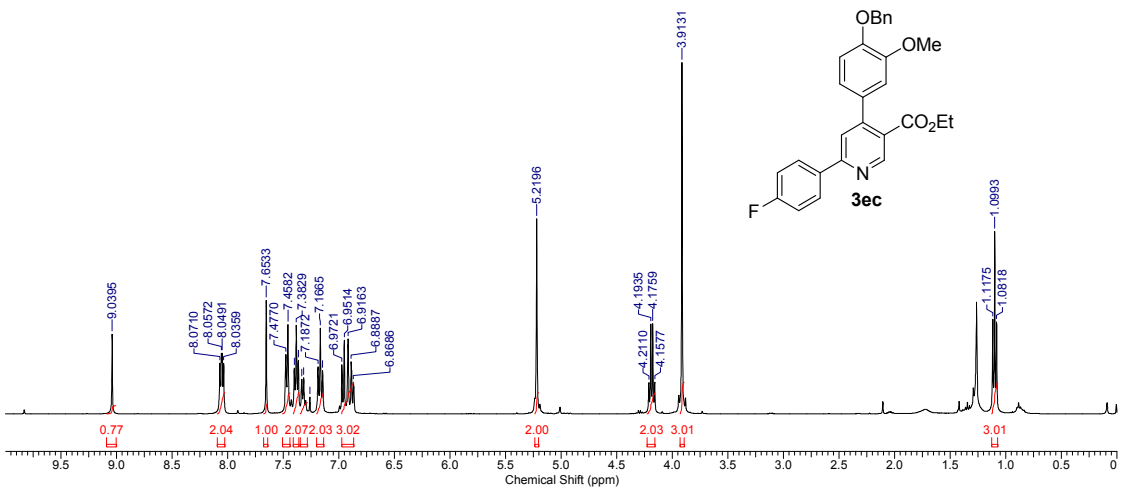
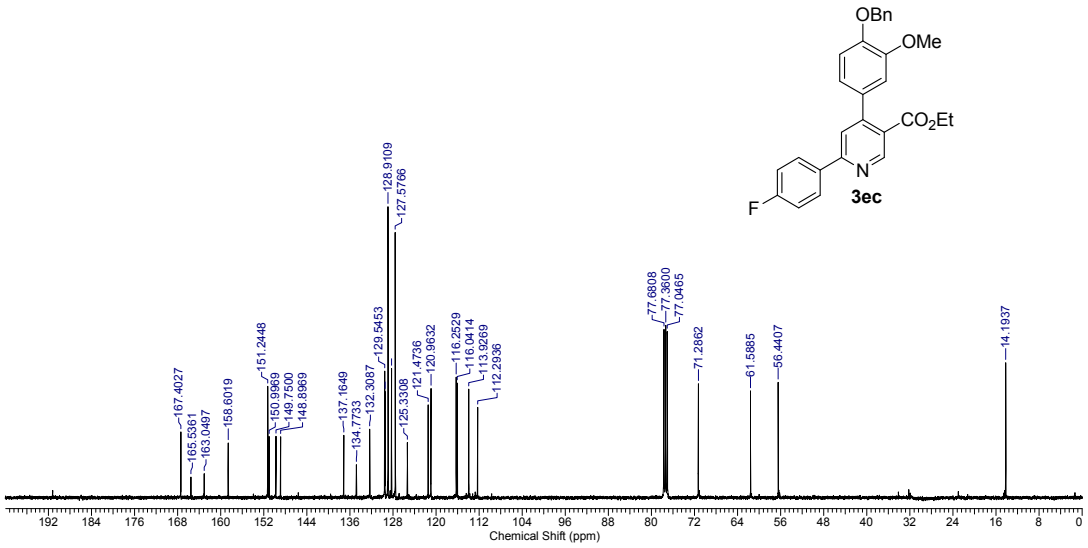
116.2310
61.7562
14.0552
Chemical Shift (ppm)


OBn
OMe
CO2Et
N
F
3ec
9.0395
8.0710
8.0572
8.0491
8.0359
7.6533
7.4770
7.4582
7.3829
7.1872
7.1665
6.9721
6.9514
6.9163
6.8887
6.8686
5.2196
4.1935
4.1759
4.2110
4.1577
3.9131
1.0993
1.1175
1.0818
0.77
2.04
1.00
2.07
2.03
3.02
2.00
2.03
3.01
3.01
Chemical Shift (ppm)


OBn
OMe
CO2Et
N
F
3ec
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150.9960
149.7500
148.8969
137.1649
134.7733
132.3087
125.3308
121.4736
120.9632
116.2529
116.0414
113.9289
112.2936
167.4027
165.5361
163.0497
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77.0465
71.2862
61.5885
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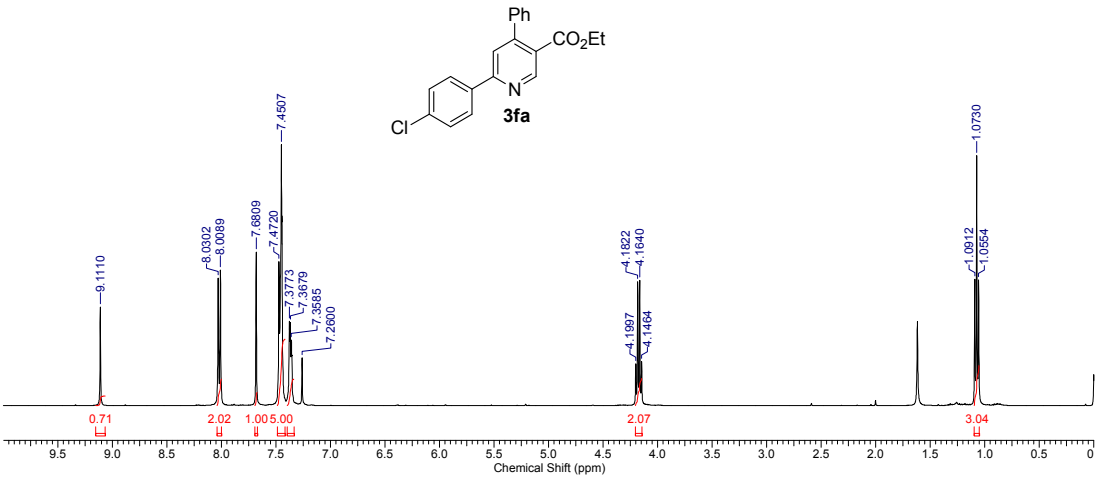
14.1937
Chemical Shift (ppm)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Cl
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7.6809
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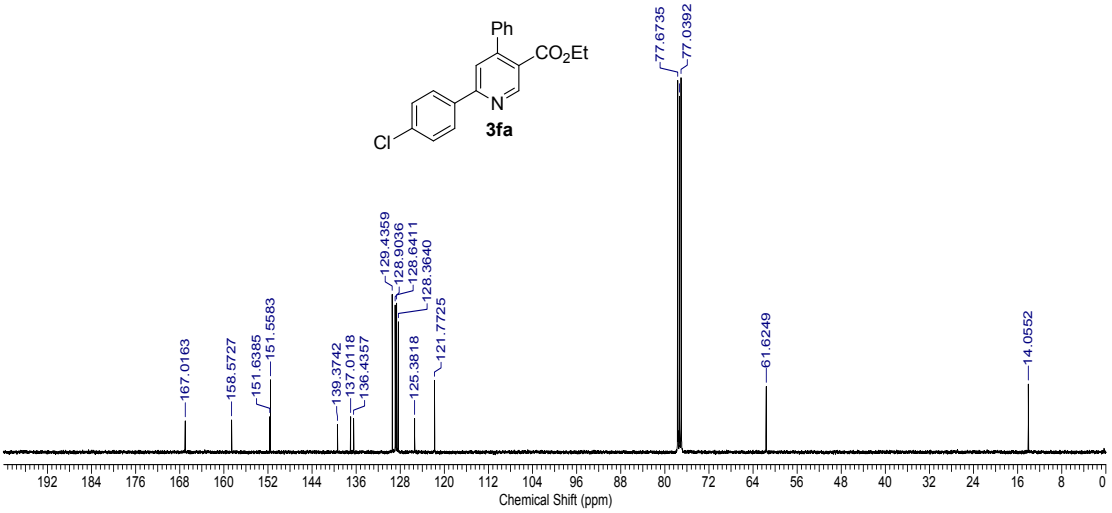
7.4507
7.3773
7.3679
7.3585
7.2600
4.1997
4.1822
4.1640
4.1464
1.0912
1.0730
1.0554
0.71
2.02
1.00
5.00
2.07
3.04
Chemical Shift (ppm)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CO2Et
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Cl
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158.5727
151.6385
151.5583
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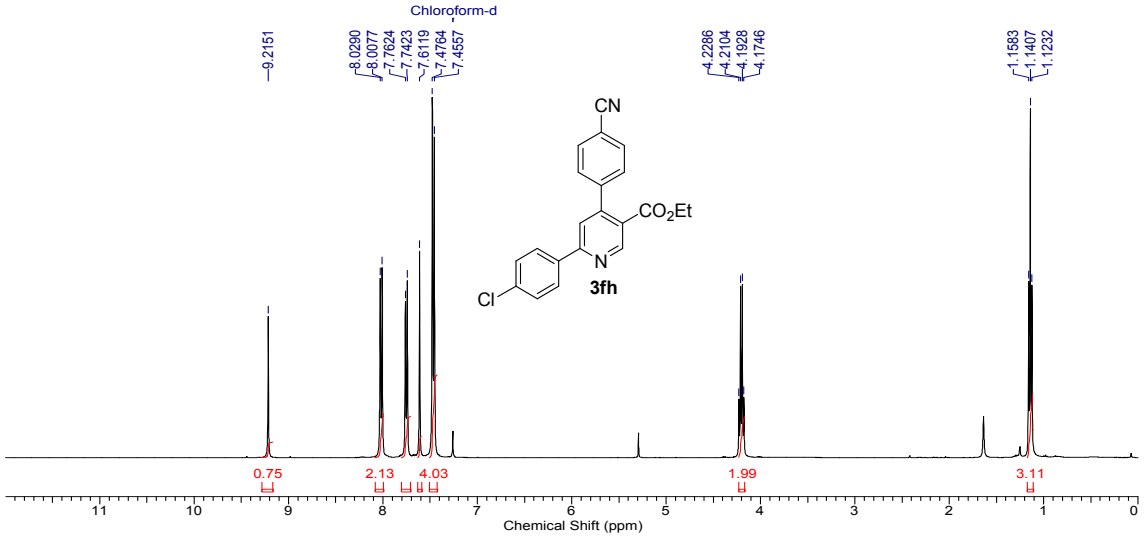
137.0118
136.4357
129.4359
129.0036
128.6411
128.3640
125.3818
121.7725
77.6735
77.0392
61.6249
14.0552
Chemical Shift (ppm)


Chloroform-d
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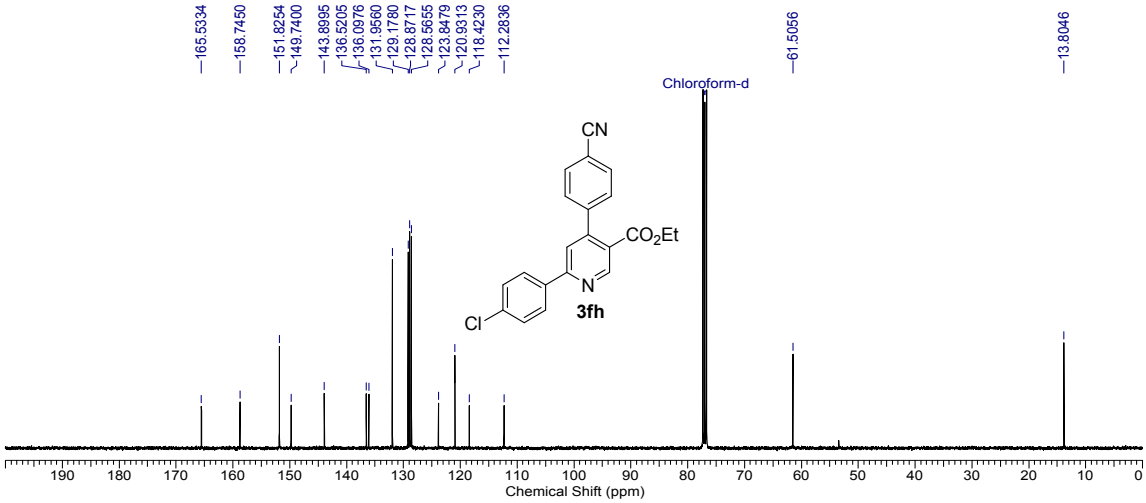
8.0290
8.0077
7.7624
7.7423
7.6119
7.4764
7.4557
4.2286
4.2104
4.1928
4.1746
1.1583
1.1407
1.1232
CN
CO2Et
N
Cl
3fh
0.75
2.13
4.03
1.99
3.11
Chemical Shift (ppm)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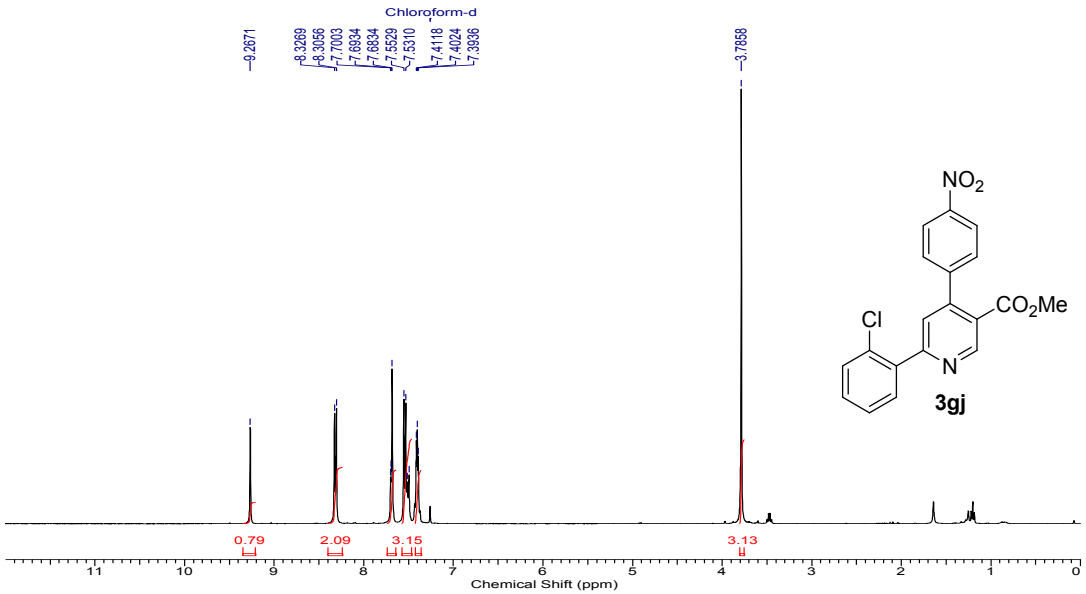
151.8254
149.7400
143.8995
136.5205
136.0976
131.9560
129.1780
128.8717
128.5655
123.8479
120.9313
118.4230
112.2836
61.5056
13.8046
Chloroform-d
CN
CO2Et
N
Cl
3fh
Chemical Shift (ppm)


Chloroform-d
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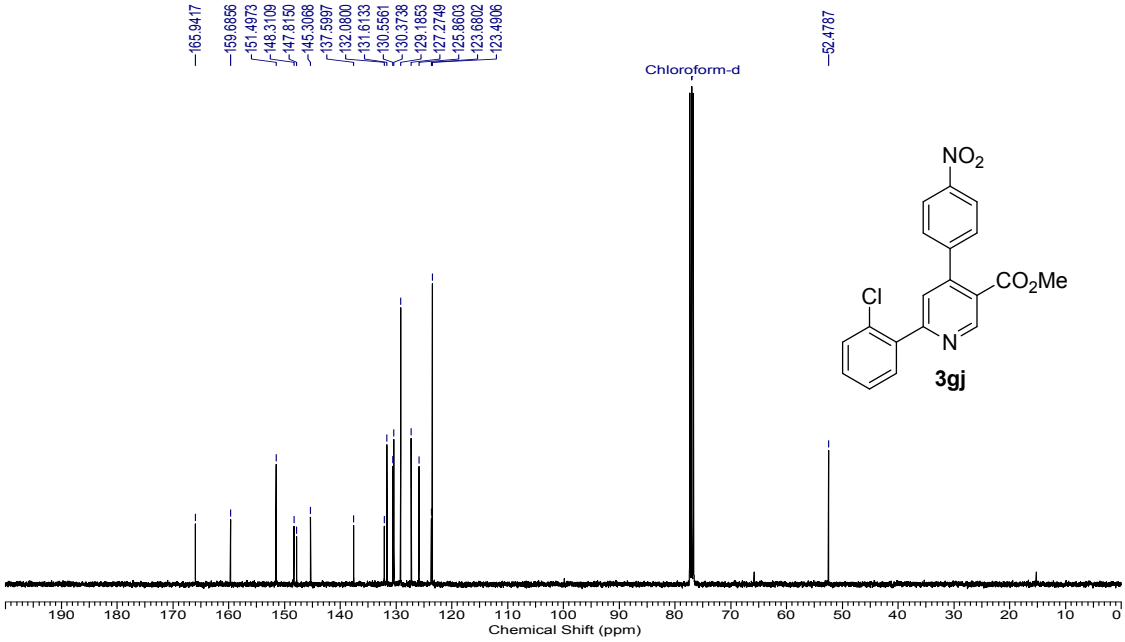
8.3269
8.3056
7.7003
7.6934
7.6834
7.5529
7.5310
7.4118
7.4024
7.3936
3.7858
NO2
CO2Me
Cl
N
3gj
0.79
2.09
3.15
3.13
Chemical Shift (ppm)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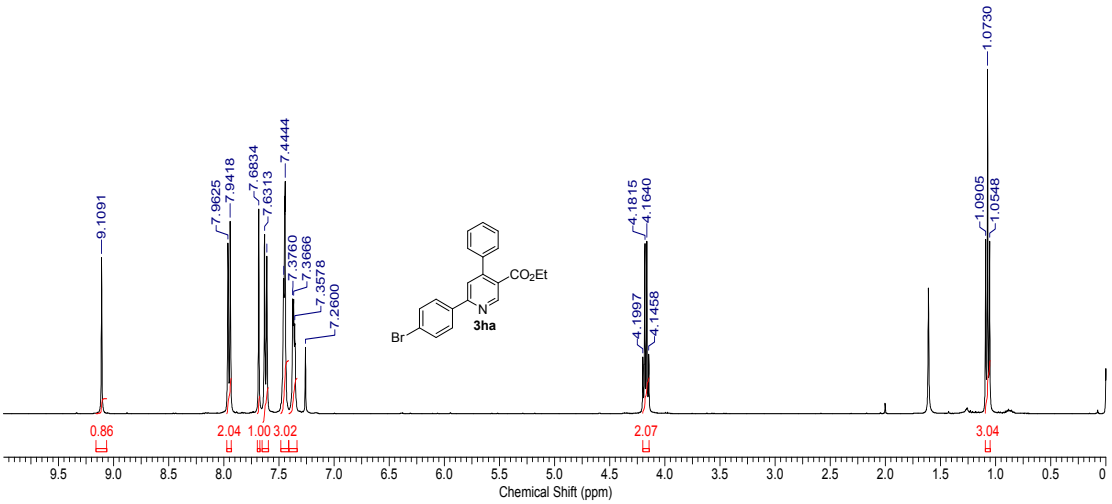
159.6856
151.4973
148.3109
147.8150
145.3068
137.5997
132.0800
131.6133
130.5561
130.3738
129.1853
127.2749
125.8603
123.6802
123.4906
52.4787
Chloroform-d
NO2
CO2Me
Cl
N
3gj
Chemical Shift (ppm)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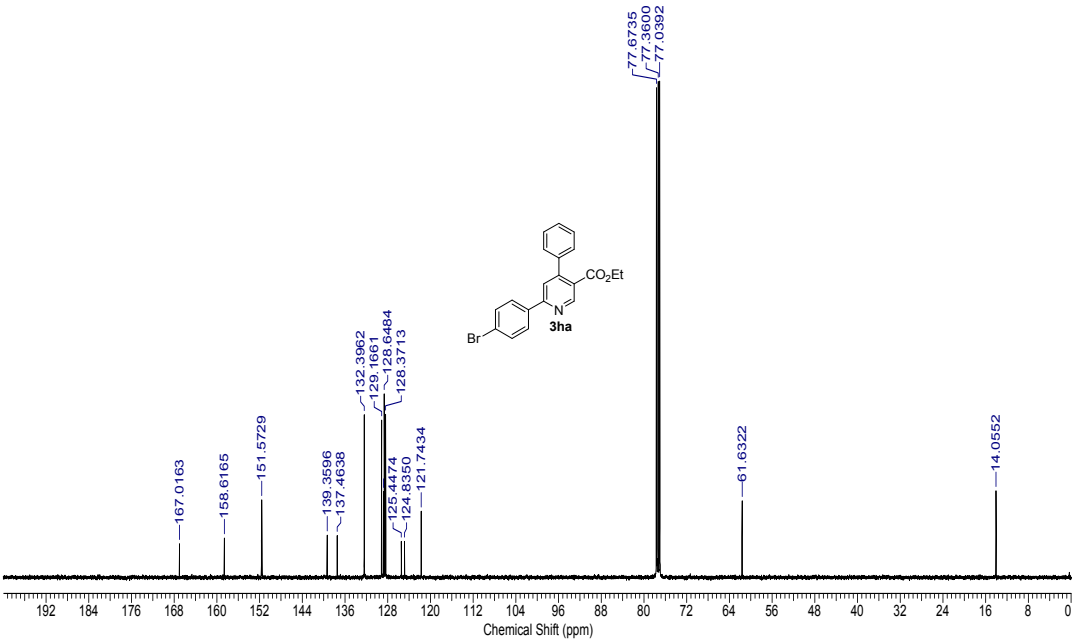
7.9418
7.6834
7.6313
7.4444
7.3760
7.3666
7.3578
7.2600
4.1815
4.1640
4.1997
4.1458
1.0730
1.0905
1.0548
CO2Et
N
Br
3ha
0.86
2.04
1.00
3.02
2.07
3.04
Chemical Shift (ppm)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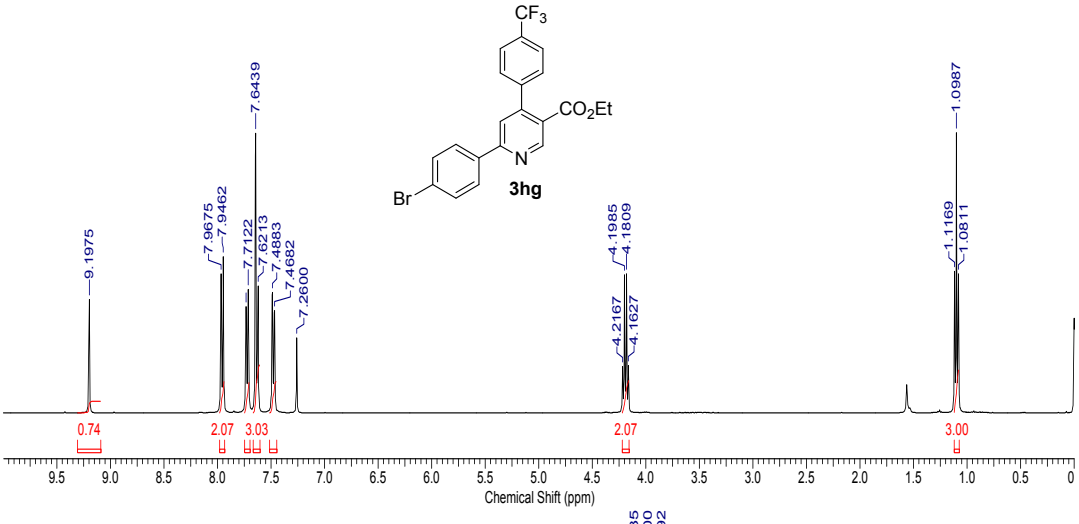
77.3600
77.0392
132.3962
129.1661
128.6484
128.3713
167.0163
158.6165
151.5729
139.3596
137.4638
125.4474
124.8350
121.7434
61.6322
14.0552
CO2Et
N
Br
3ha
Chemical Shift (ppm)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CO2Et
N
Br
3hg
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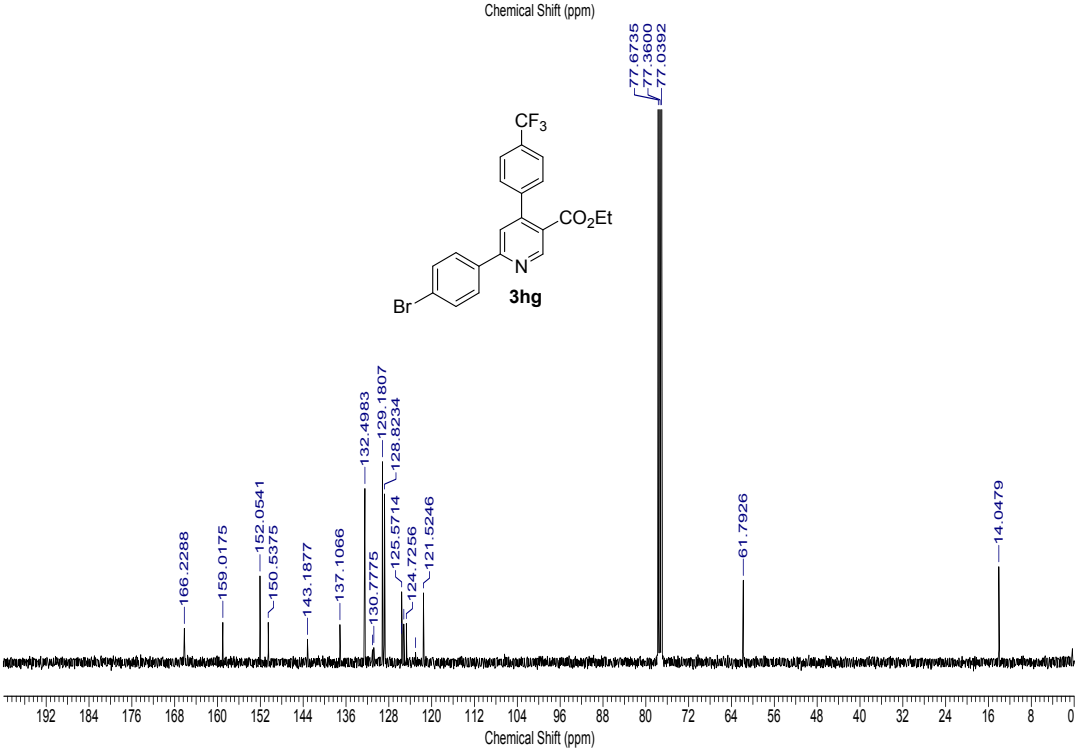
7.9675
7.9462
7.7122
7.6439
7.6213
7.4883
7.4682
7.2600
4.1985
4.1809
4.2167
4.1627
1.1169
1.0987
1.0811
0.74
2.07
3.03
2.07
3.00
Chemical Shift (ppm)


CF3
CO2Et
N
Br
3hg
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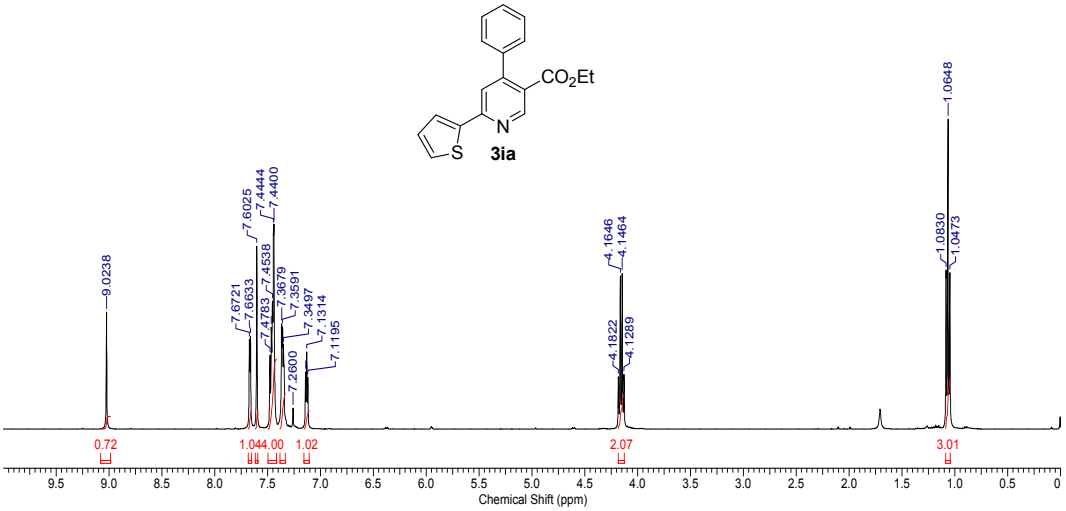
77.3600
77.0392
166.2288
159.0175
152.0541
150.5375
143.1877
137.1066
132.4983
130.7775
129.1807
128.8234
125.5714
124.7256
121.5246
61.7926
14.0479
Chemical Shift (ppm)


CO2Et
N
S
3ia
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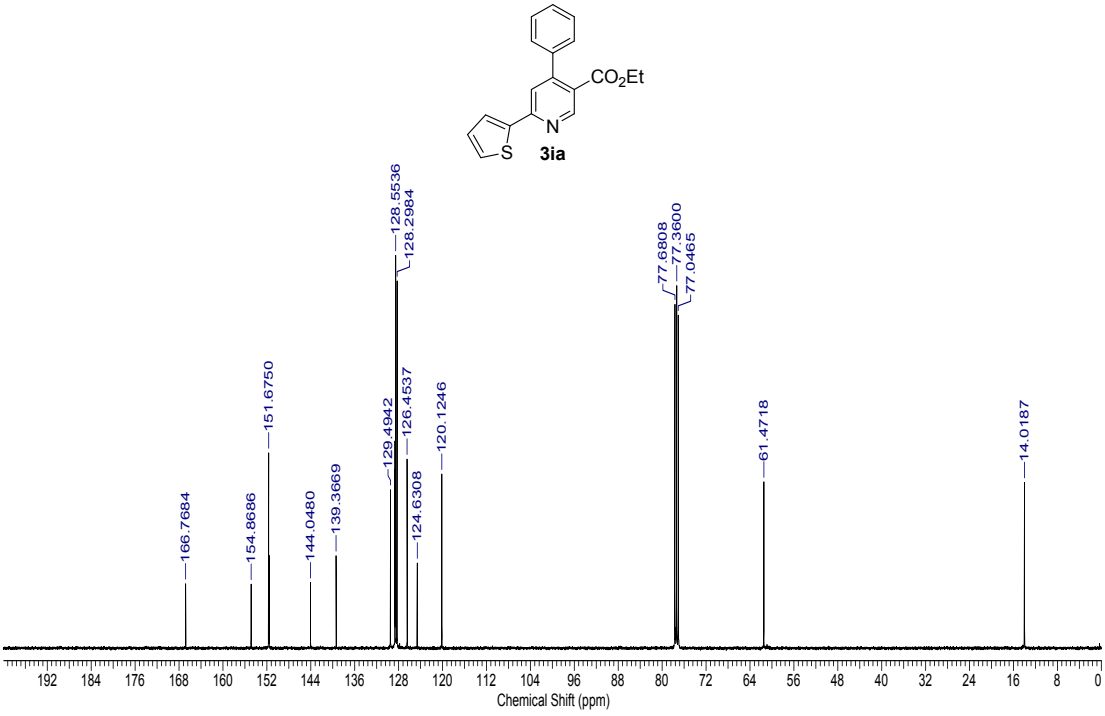
7.6721
7.6633
7.6025
7.4783
7.4538
7.4444
7.4400
7.3679
7.3591
7.3497
7.2600
7.1314
7.1195
4.1822
4.1646
4.1464
4.1289
1.0830
1.0648
1.0473
0.72
1.04
4.00
1.02
2.07
3.01
Chemical Shift (ppm)


CO2Et
N
S
3ia
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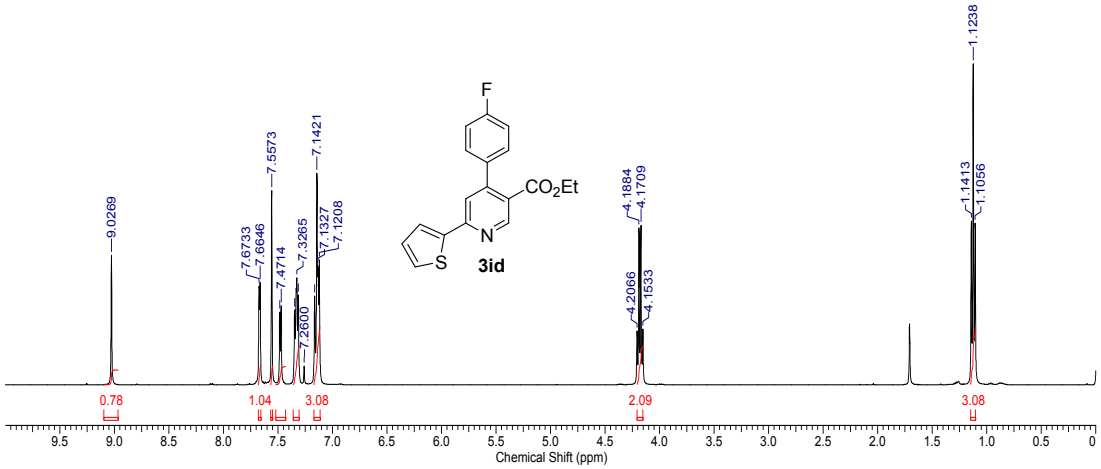
154.8686
151.6750
144.0480
139.3669
129.4942
128.5536
128.2984
126.4537
124.6308
120.1246
77.6808
77.3600
77.0465
61.4718
14.0187
Chemical Shift (ppm)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CO2Et
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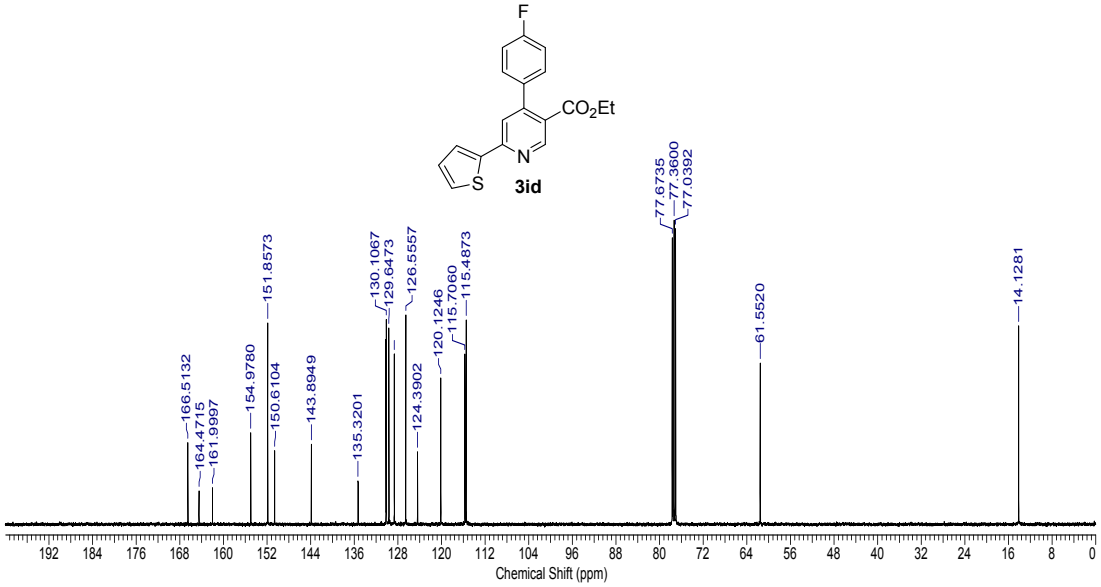
S
3id
9.0269
7.6733
7.6646
7.5573
7.4714
7.3265
7.2600
7.1421
7.1327
7.1208
4.1884
4.1709
4.2066
4.1533
1.1238
1.1413
1.1056
0.78
1.04
3.08
2.09
3.08
Chemical Shift (ppm)


F
CO2Et
N
S
3id
166.5132
164.4715
161.9997
154.9780
151.8573
150.6104
143.8949
135.3201
130.1067
129.6473
126.5557
124.3902
120.1246
115.7060
115.4873
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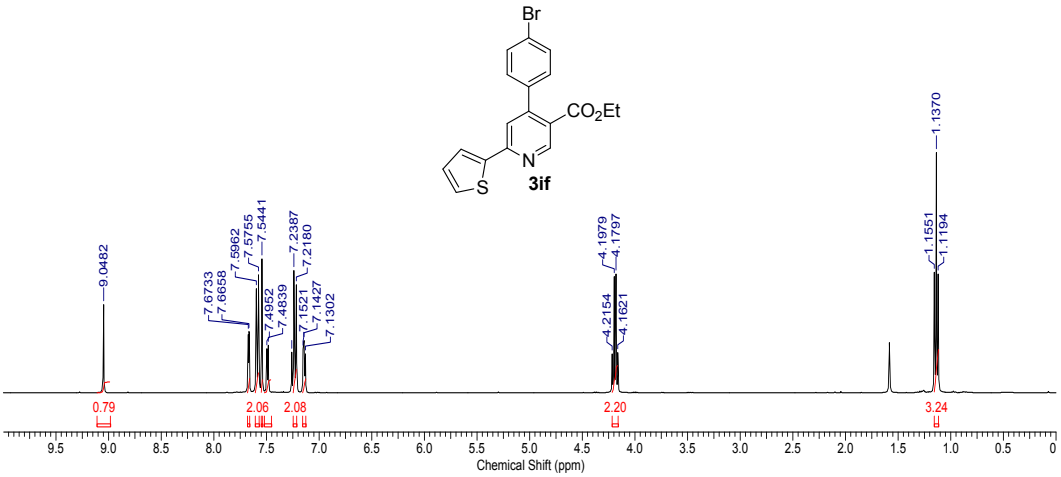
77.3600
77.0392
61.5520
14.1281
Chemical Shift (ppm)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CO2Et
N
S
3if
9.0482
7.6733
7.6658
7.5962
7.5755
7.5441
7.4952
7.4839
7.2387
7.2180
7.1521
7.1427
7.1302
4.1979
4.1797
4.2154
4.1621
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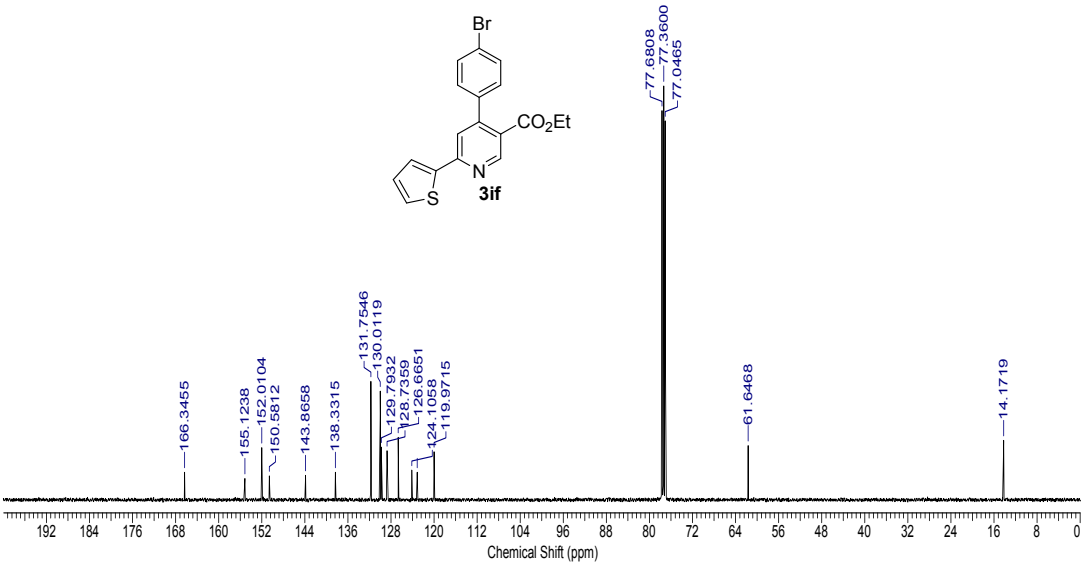
1.1370
1.1194
0.79
2.06
2.08
2.20
3.24
Chemical Shift (ppm)


Br
CO2Et
N
S
3if
77.6808
77.3600
77.0465
166.3455
155.1238
152.0104
150.5812
143.8658
138.3315
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129.7932
128.7359
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124.1058
119.9715
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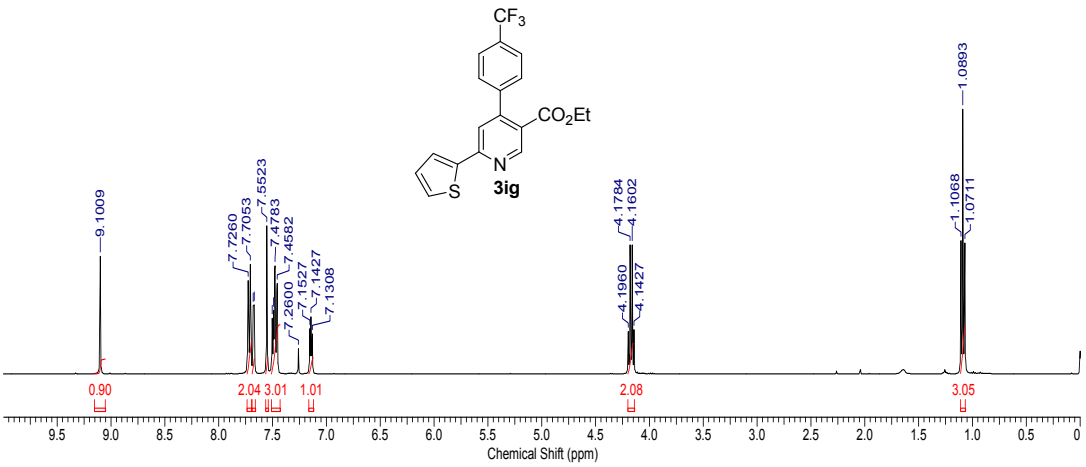
14.1719
Chemical Shift (ppm)


CF3
CO2Et
N
S
3ig
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7.5523
7.4783
7.4582
7.2600
7.1527
7.1427
7.1308
4.1784
4.1602
4.1960
4.1427
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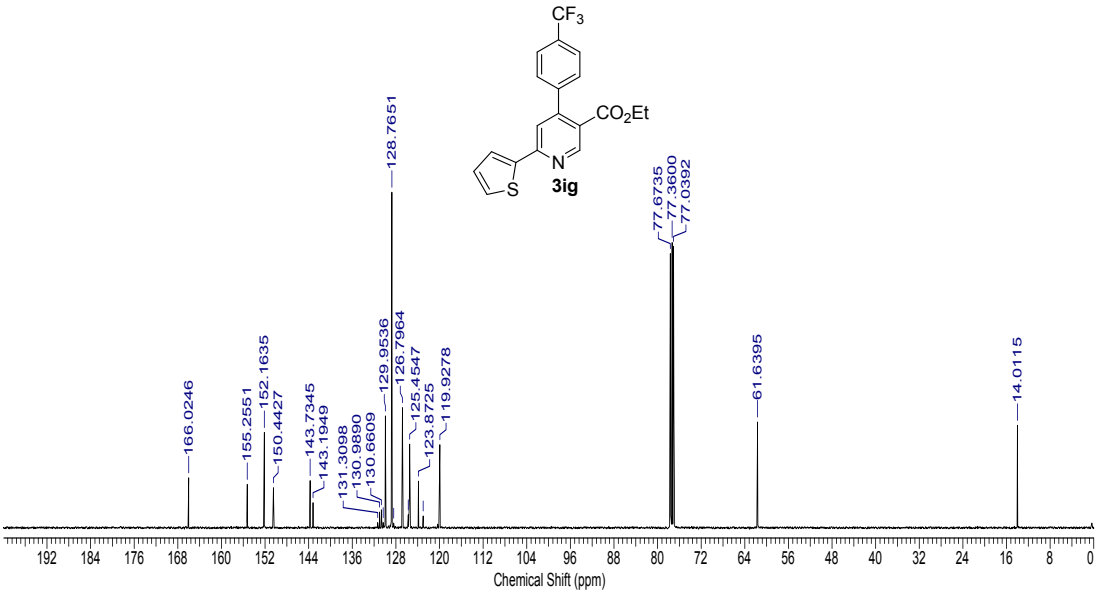
1.0711
0.90
2.04
3.01
1.01
2.08
3.05
Chemical Shift (ppm)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CO2Et
N
S
3ig
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150.4427
143.7345
143.1949
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130.6609
129.9536
128.7651
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123.8725
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77.0392
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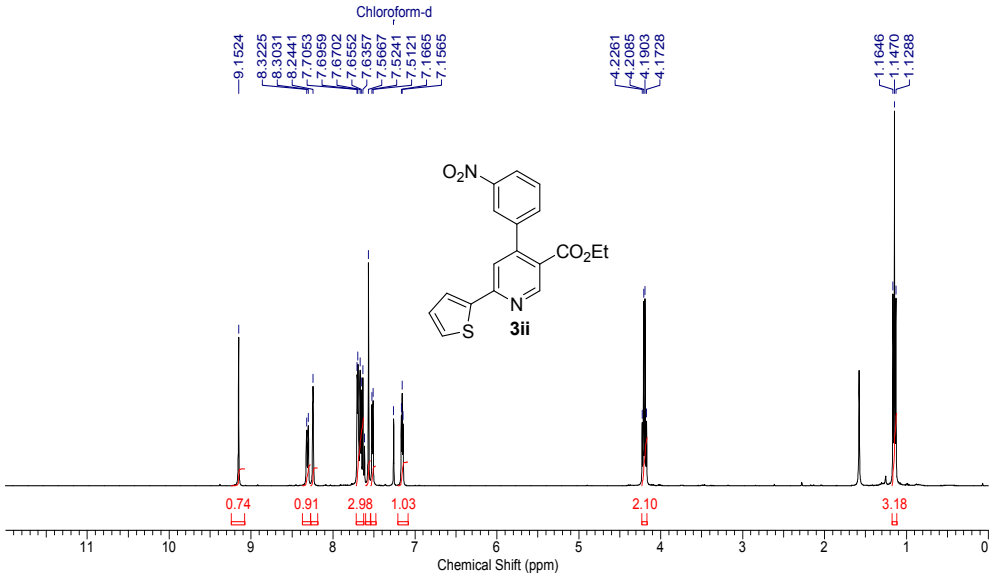
14.0115
Chemical Shift (ppm)


Chloroform-d
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8.3031
8.2441
7.7053
7.6959
7.6702
7.6552
7.6357
7.5667
7.5241
7.5121
7.1665
7.1565
4.2261
4.2085
4.1903
4.1728
1.1646
1.1470
1.1288
O2N
CO2Et
N
S
3ii
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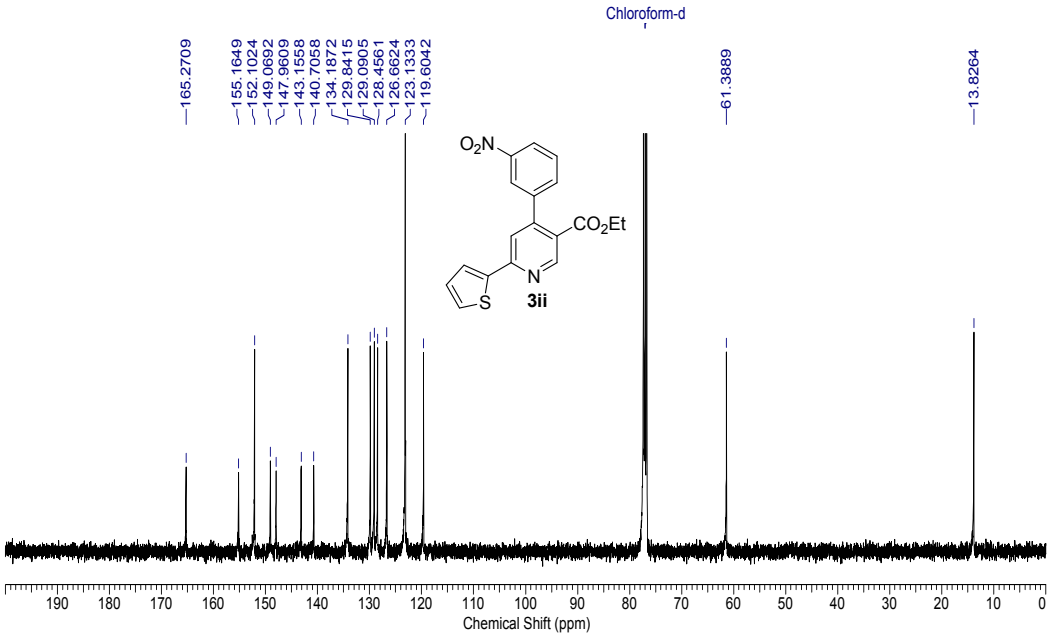
1.03
2.10
3.18
Chemical Shift (ppm)


Chloroform-d
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149.0692
147.9609
143.1558
140.7058
134.1872
129.8415
129.0905
128.4561
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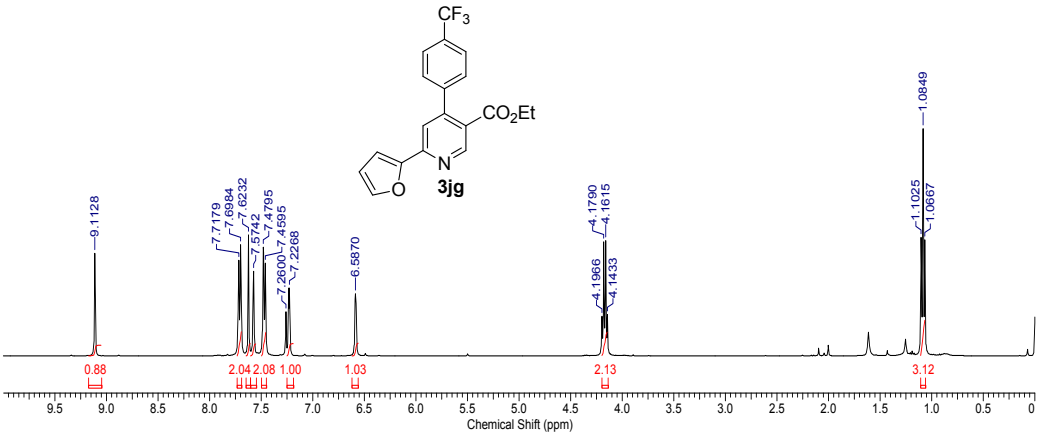
CO2Et
N
S
3ii
Chemical Shift (ppm)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O
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7.6232
7.5742
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7.2600
7.2268
6.5870
4.1966
4.1790
4.1615
4.1433
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1.03
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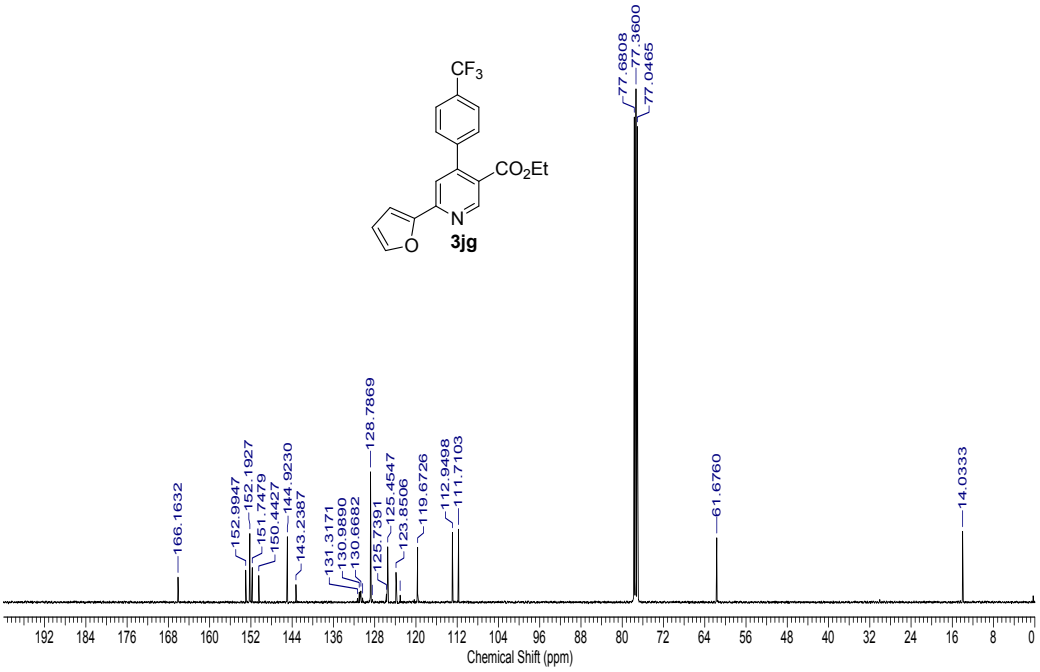
3.12
Chemical Shift (ppm)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O
3jg
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166.1632
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152.1927
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150.4427
144.9230
143.2387
131.3171
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130.6682
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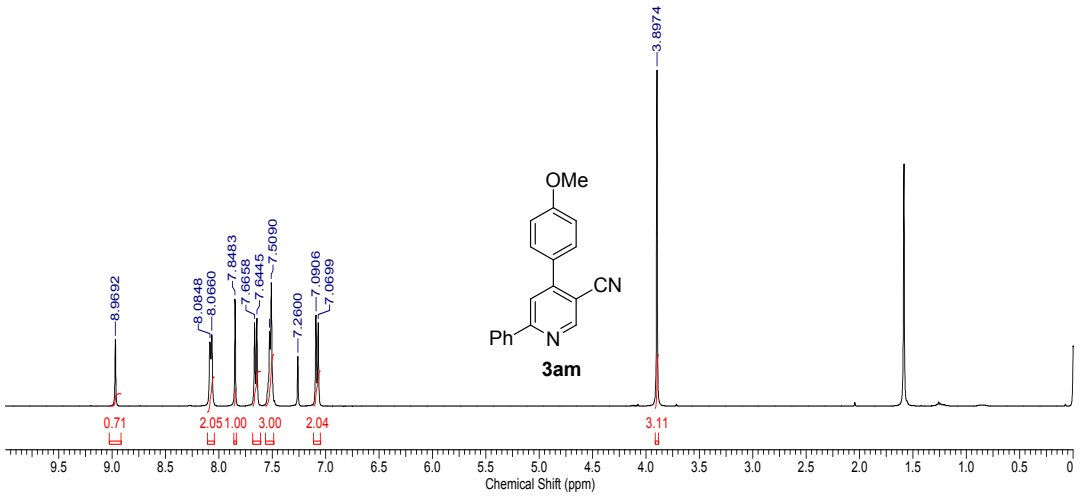
Chemical Shift (ppm)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7.6658
7.6445
7.5090
7.2600
7.0906
7.0699
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OMe
CN
Ph
N
3am
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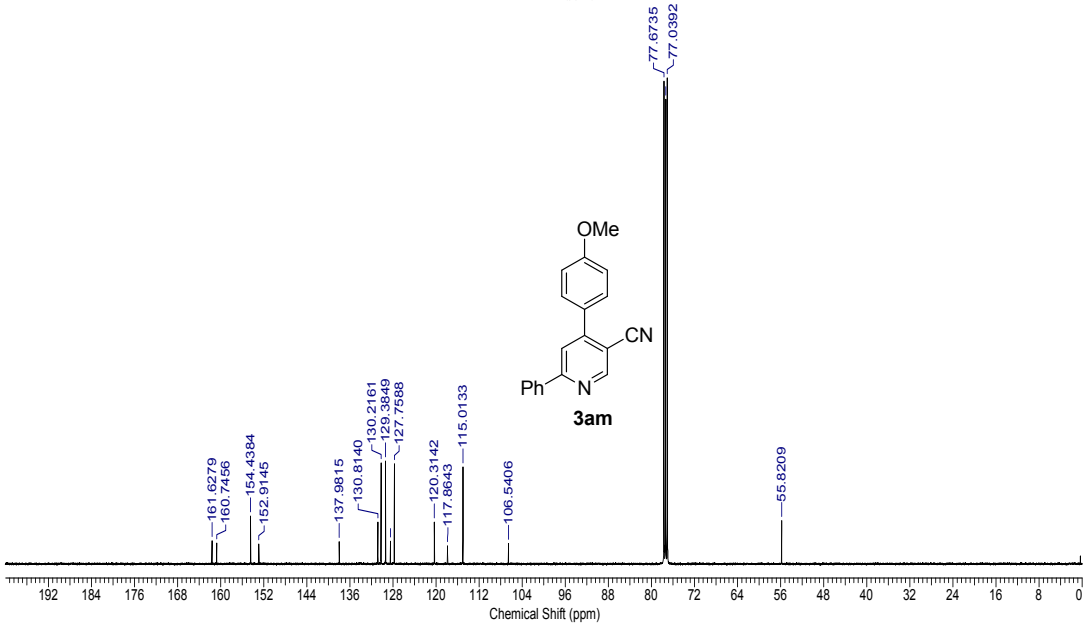
2.05
1.00
3.00
2.04
3.11
Chemical Shift (ppm)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130.8140
130.2161
129.3849
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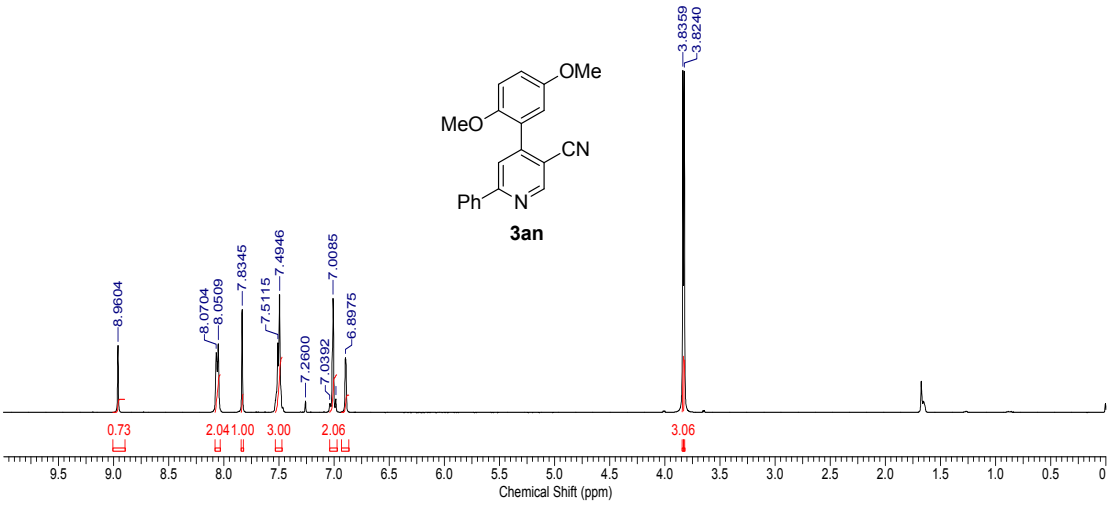
115.0133
106.5406
55.8209
OMe
CN
Ph
N
3am
Chemical Shift (ppm)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MeO
CN
Ph
N
3an
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8.0509
7.8345
7.5115
7.4946
7.2600
7.0392
7.0085
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3.8240
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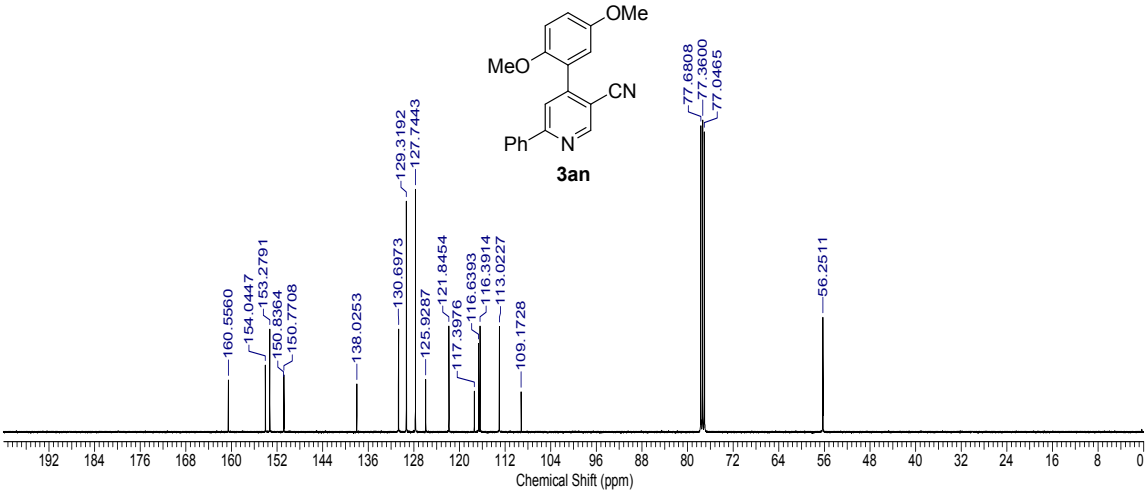
1.00
3.00
2.06
3.06
Chemical Shift (ppm)


OMe
MeO
CN
Ph
N
3an
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129.3192
127.7443
125.9287
121.8454
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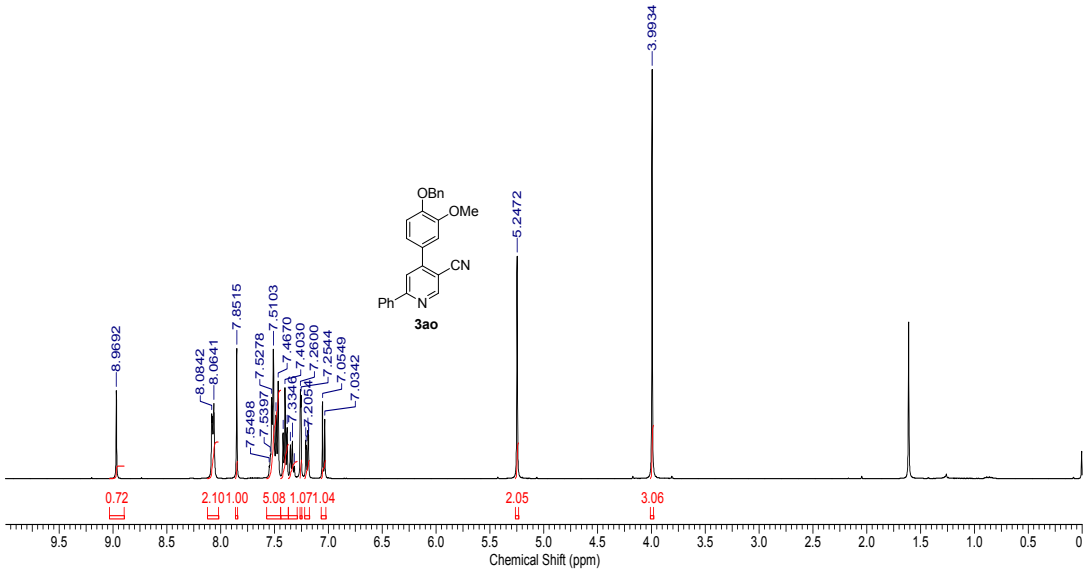
56.2511
Chemical Shift (ppm)


OBn
OMe
CN
Ph
N
3ao
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7.5103
7.4670
7.4030
7.3348
7.2600
7.2544
7.2054
7.0549
7.0342
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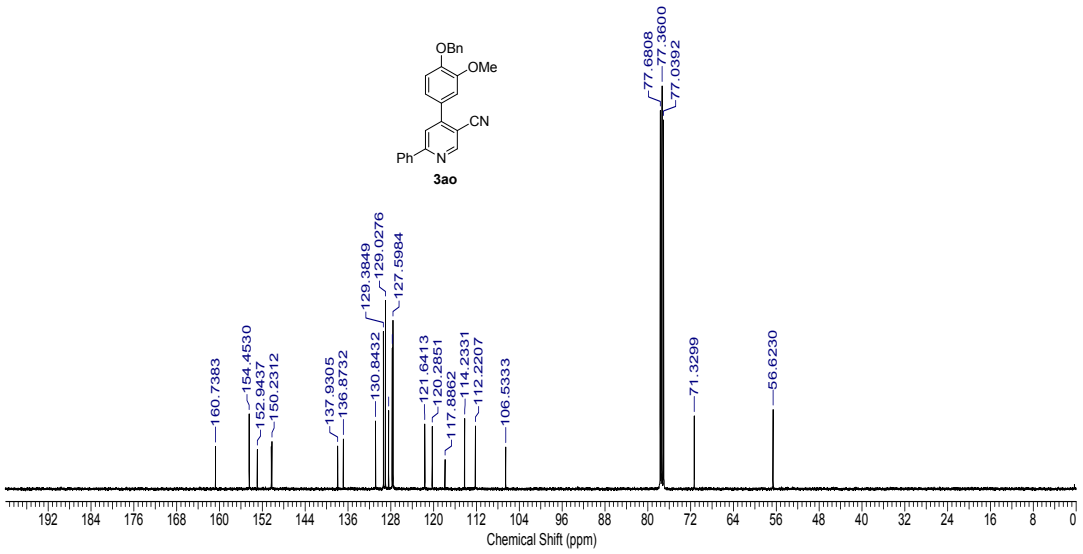
1.00
5.08
1.07
1.04
2.05
3.06
Chemical Shift (ppm)


OBn
OMe
CN
Ph
N
3ao
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129.3849
129.0276
127.5984
121.6413
120.2851
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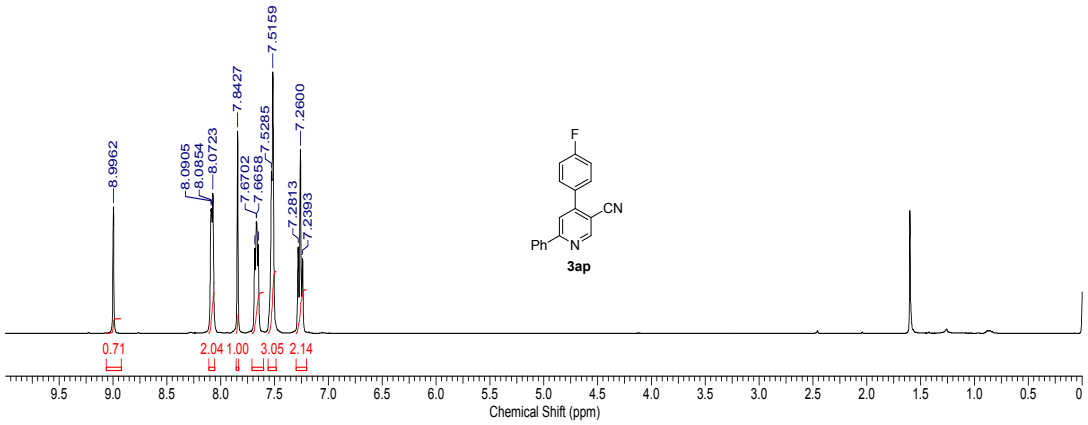
106.5333
77.6808
77.3600
77.0392
71.3299
56.6230
Chemical Shift (ppm)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8.0854
8.0723
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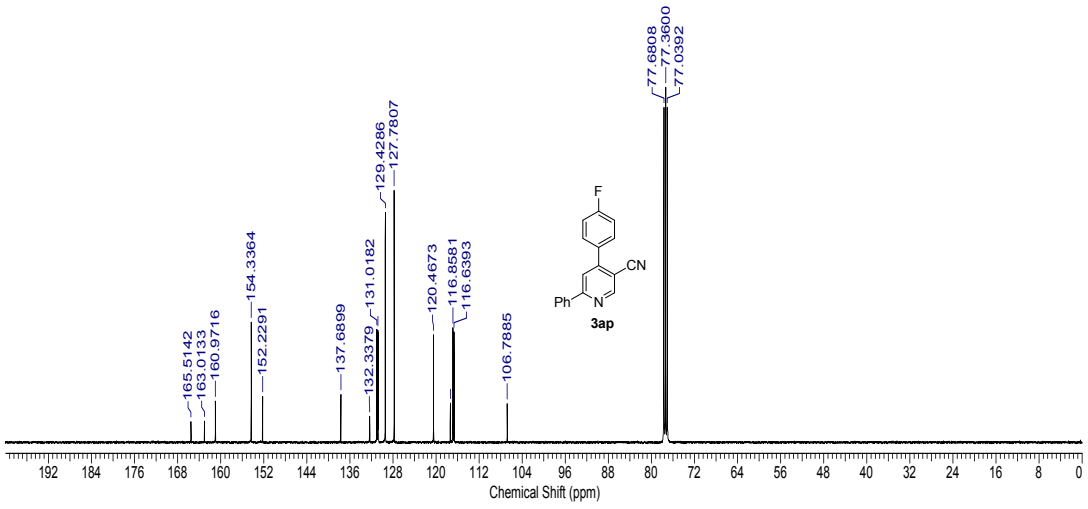
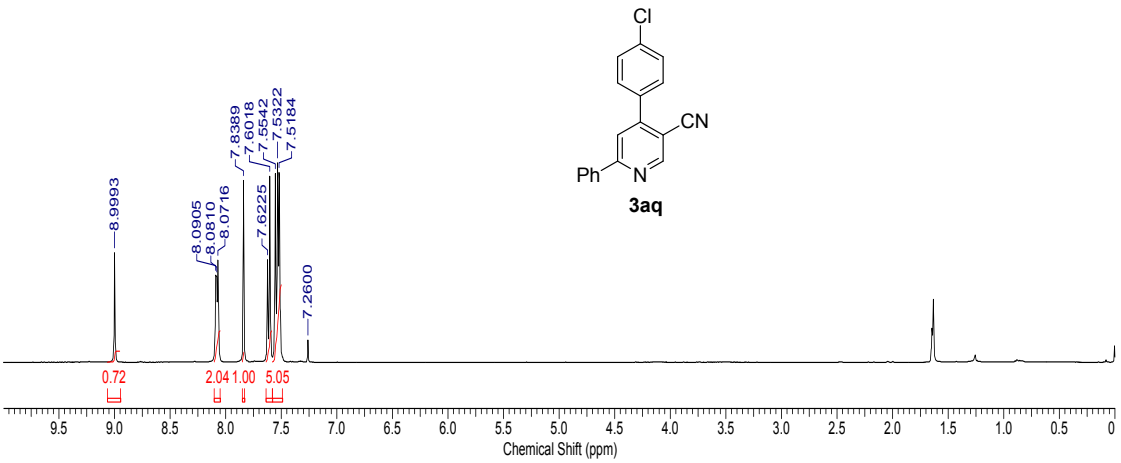
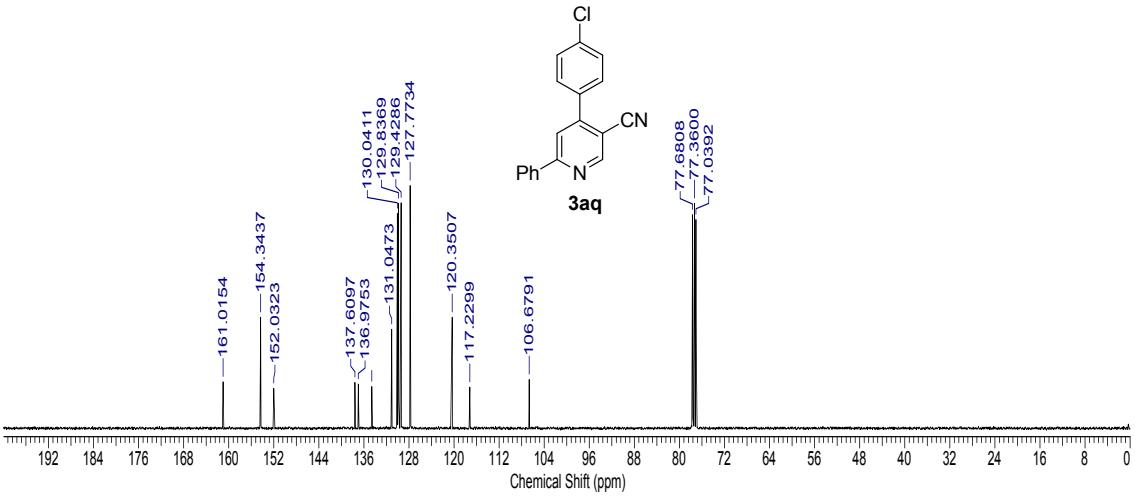
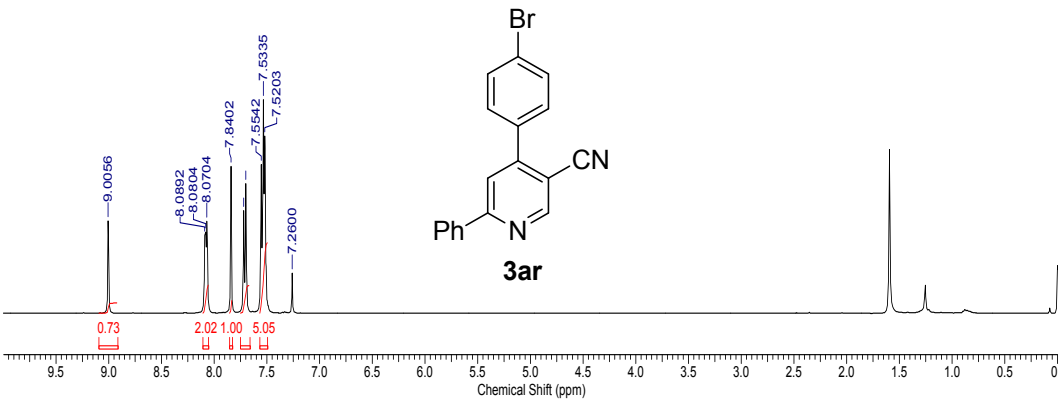
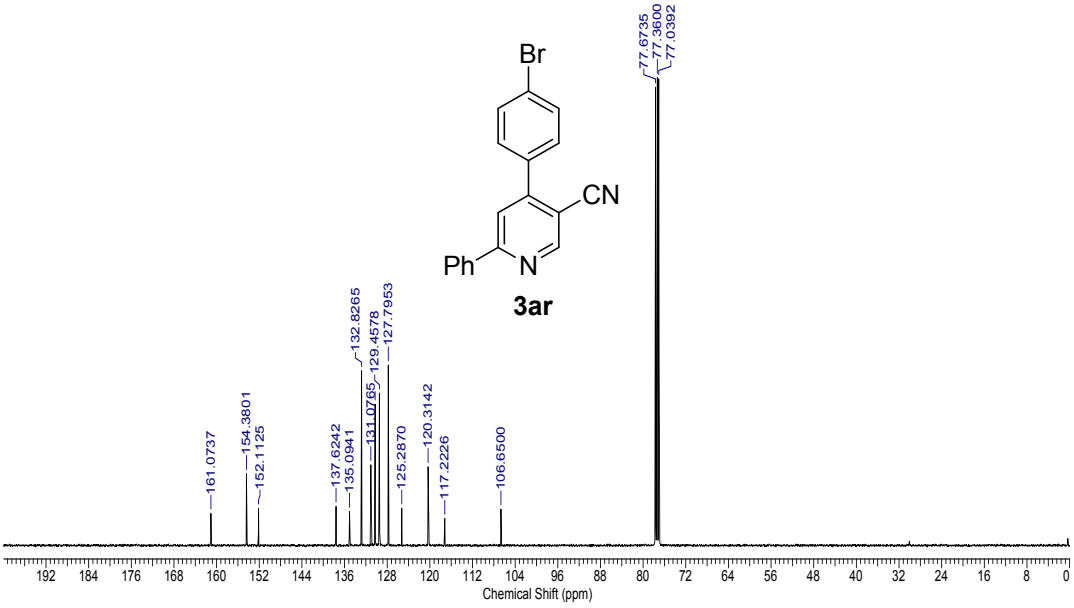
7.6702
7.6658
7.5285
7.5159
7.2813
7.2600
7.2393
0.71
2.04
1.00
3.05
2.14
F
CN
Ph
N
3ap
Chemical Shift (ppm)

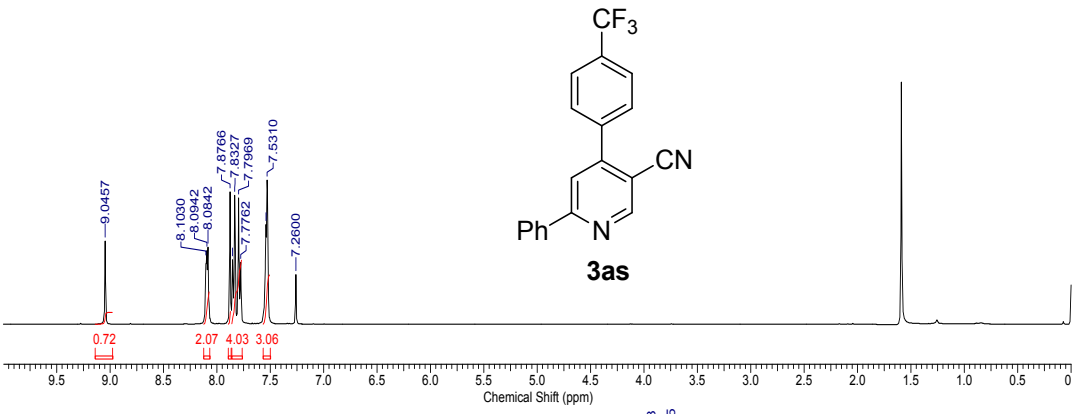

165.5142
163.0133
160.9716
154.3364
152.2291
137.6899
132.3379
131.0182
129.4286
127.7807
120.4673
116.8581
116.6393
106.7885
77.6808
77.3600
77.0392
F
CN
Ph
N
3ap
Chemical Shift (ppm)

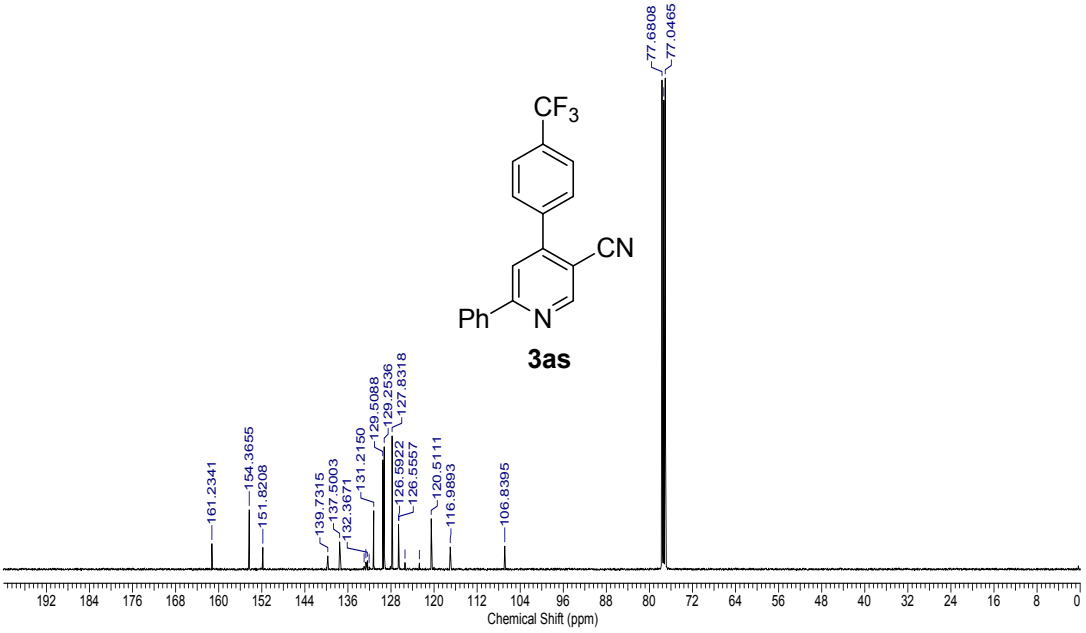

Cl
CN
Ph
N
3aq
8.9993
8.0905
8.0810
8.0716
7.8389
7.6018
7.5542
7.5322
7.5184
7.6225
7.2600
0.72
2.04
1.00
5.05
Chemical Shift (ppm)

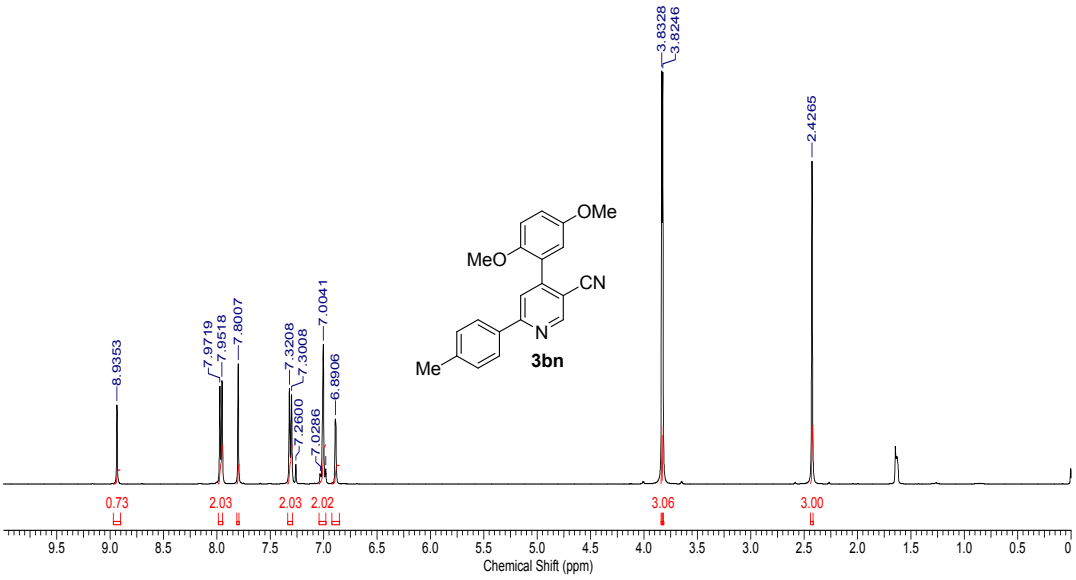

Cl
CN
Ph
N
3aq
161.0154
154.3437
152.0323
137.6097
136.9753
131.0473
130.0411
129.8369
129.4286
127.7734
120.3507
117.2299
106.6791
77.6808
77.3600
77.0392
Chemical Shift (ppm)

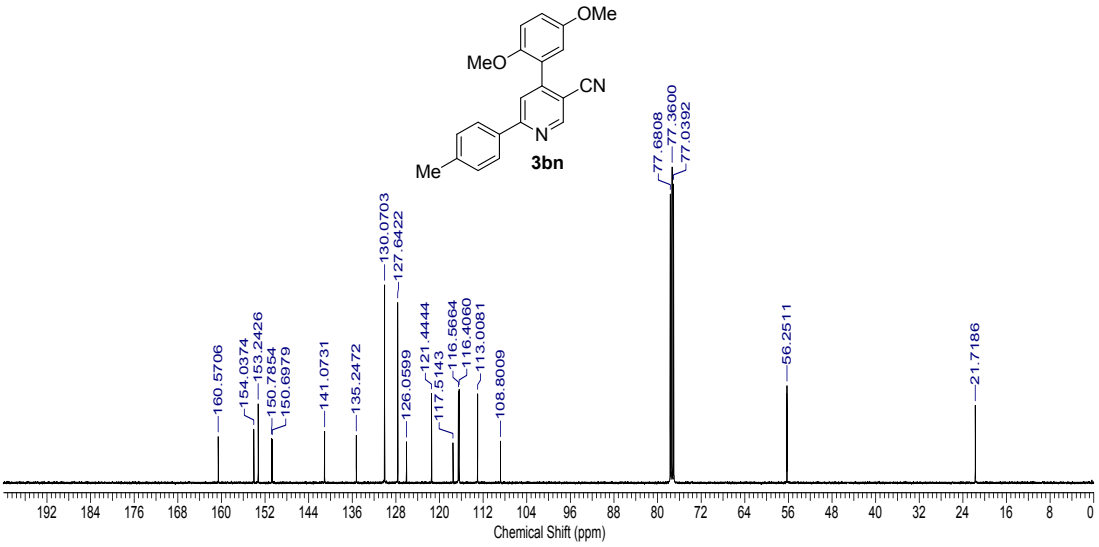

Br
CN
Ph
N
3ar
9.0056
8.0892
8.0804
8.0704
7.8402
7.5542
7.5335
7.5203
7.2600
0.73
2.02
1.00
5.05
Chemical Shift (ppm)

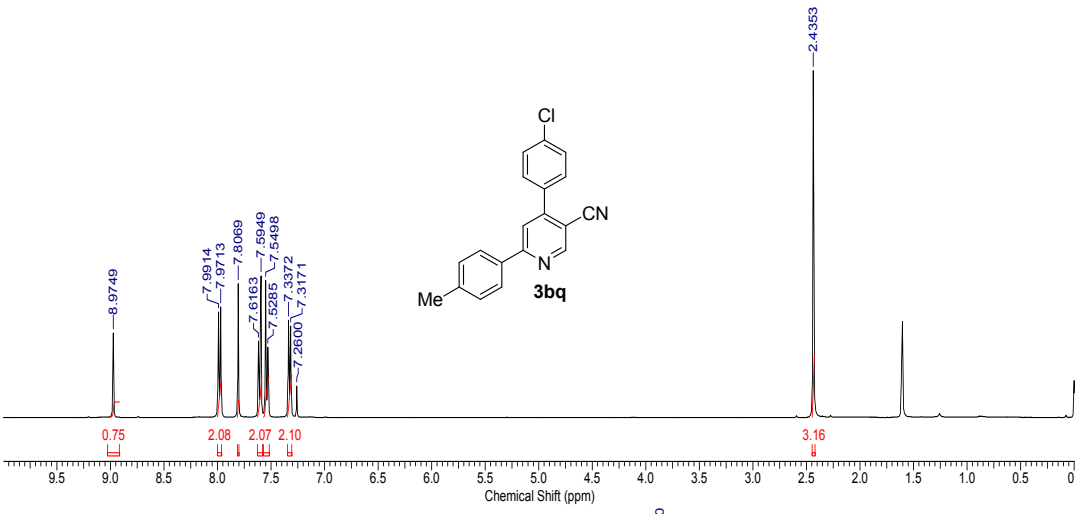

Br
CN
Ph
N
3ar
77.6735
77.3600
77.0392
161.0737
154.3801
152.1125
137.6242
135.0941
132.8265
131.0765
129.4578
127.7953
125.2870
120.3142
117.2226
106.6500
Chemical Shift (ppm)

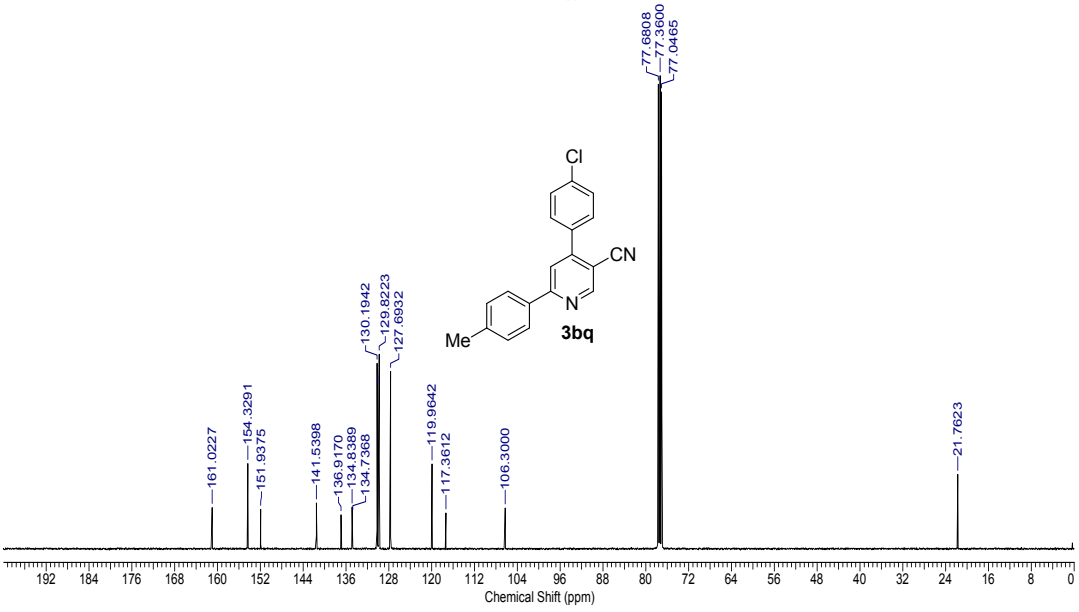

CF3
CN
Ph
N
3as
9.0457
8.1030
8.0942
8.0842
7.8766
7.8327
7.7969
7.7762
7.5310
7.2600
0.72
2.07
4.03
3.06
Chemical Shift (ppm)

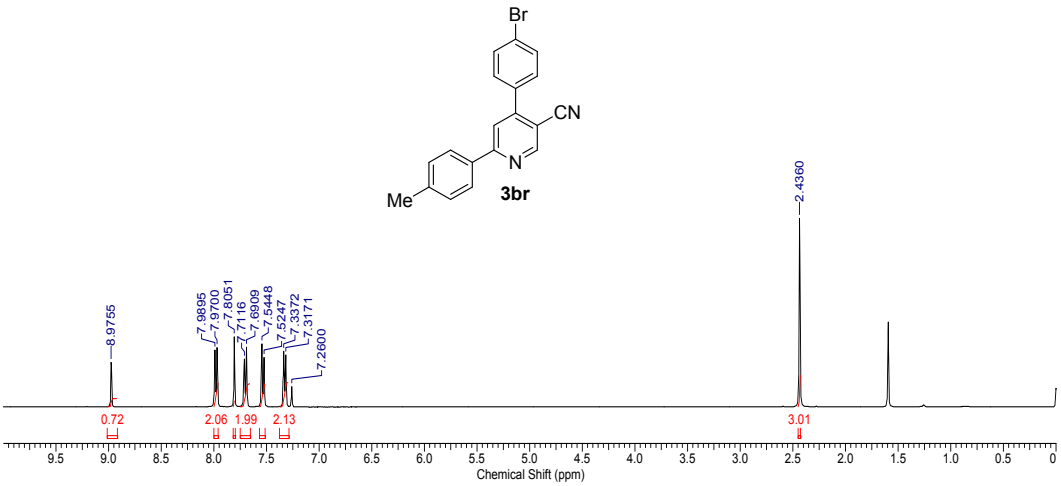

CF3
CN
Ph
N
3as
77.6808
77.0465
161.2341
154.3655
151.8208
139.7315
137.5003
132.3671
131.2150
129.5088
129.2536
127.8318
126.5922
126.5557
120.5111
116.9893
106.8395
Chemical Shift (ppm)

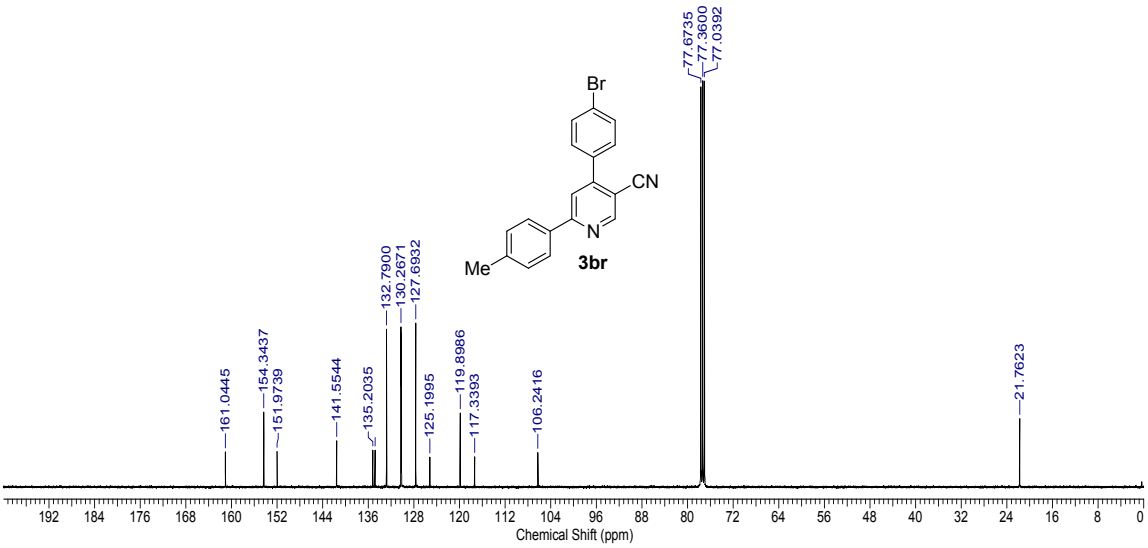

8.9353
7.9719
7.9518
7.8007
7.3208
7.3008
7.2600
7.0286
7.0041
6.8906
3.8328
3.8246
2.4265
OMe
MeO
CN
N
Me
3bn
0.73
2.03
2.03
2.02
3.06
3.00
Chemical Shift (ppm)

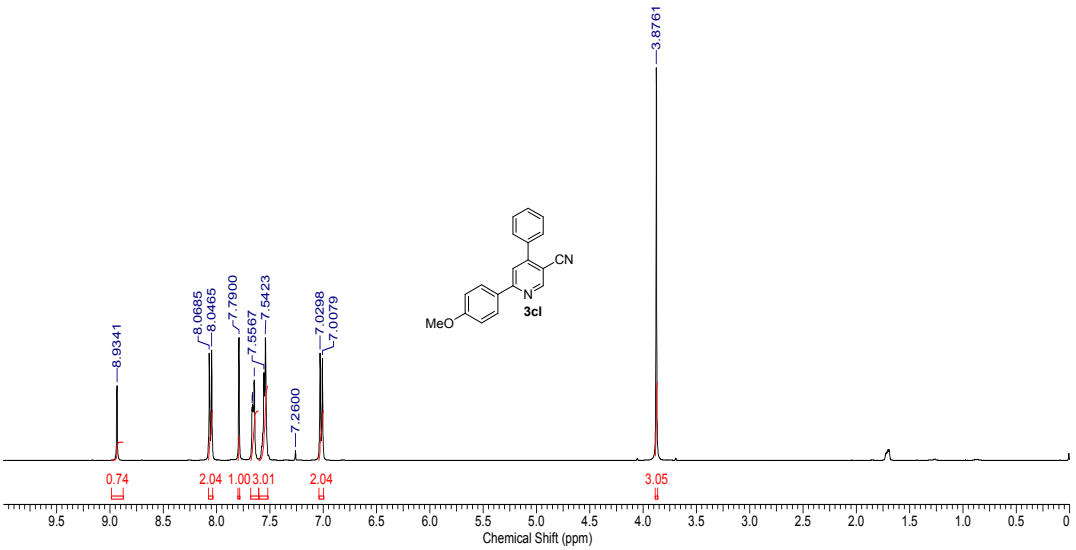

OMe
MeO
CN
N
Me
3bn
160.5706
154.0374
153.2426
150.7854
150.6979
141.0731
135.2472
130.0703
127.6422
126.0599
121.4444
117.5143
116.5664
116.4060
113.0081
108.8009
77.6808
77.3600
77.0392
56.2511
21.7186
Chemical Shift (ppm)

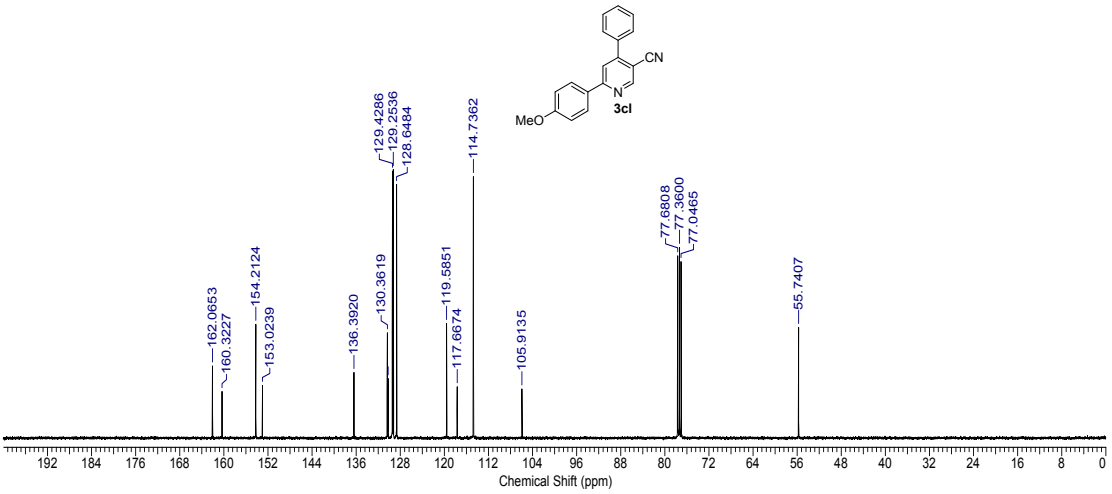

8.9749
7.9914
7.9713
7.8069
7.6163
7.5949
7.5498
7.5285
7.3372
7.3171
7.2600
2.4353
0.75
2.08
2.07
2.10
3.16
Cl
CN
N
Me
3bq
Chemical Shift (ppm)

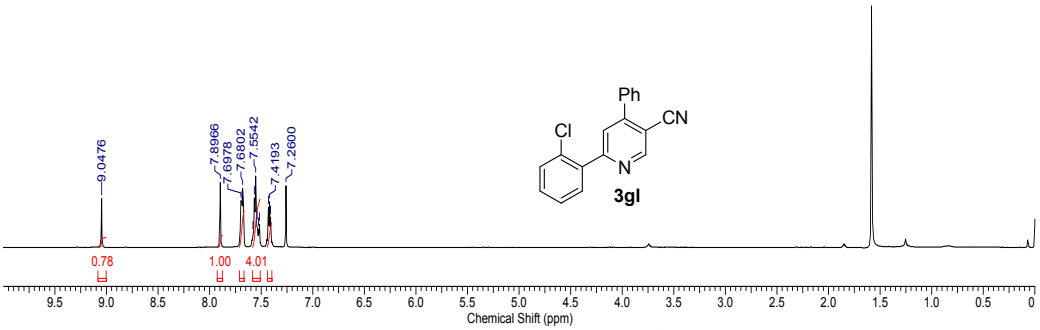

161.0227
154.3291
151.9375
141.5398
136.9170
134.8389
134.7368
130.1942
129.8223
127.6932
119.9642
117.3612
106.3000
77.6808
77.3600
77.0465
21.7623
Cl
CN
N
Me
3bq
Chemical Shift (ppm)

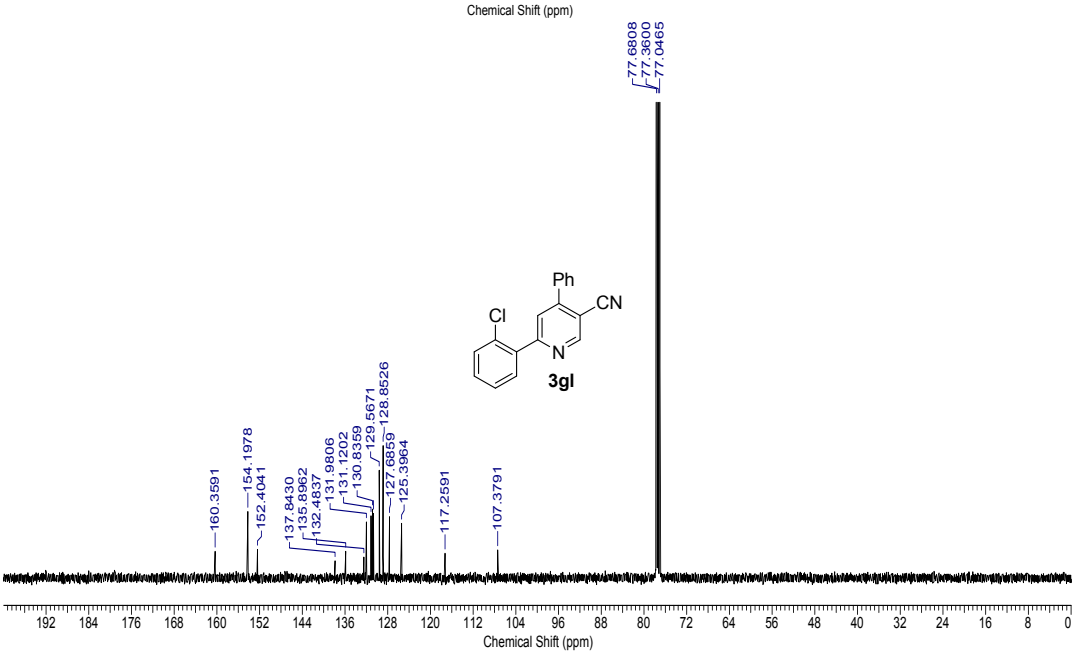

Br
CN
N
Me
3br
8.9755
7.9895
7.9700
7.8051
7.7116
7.6909
7.5448
7.5247
7.3372
7.3171
7.2600
2.4360
0.72
2.06
1.99
2.13
3.01
Chemical Shift (ppm)

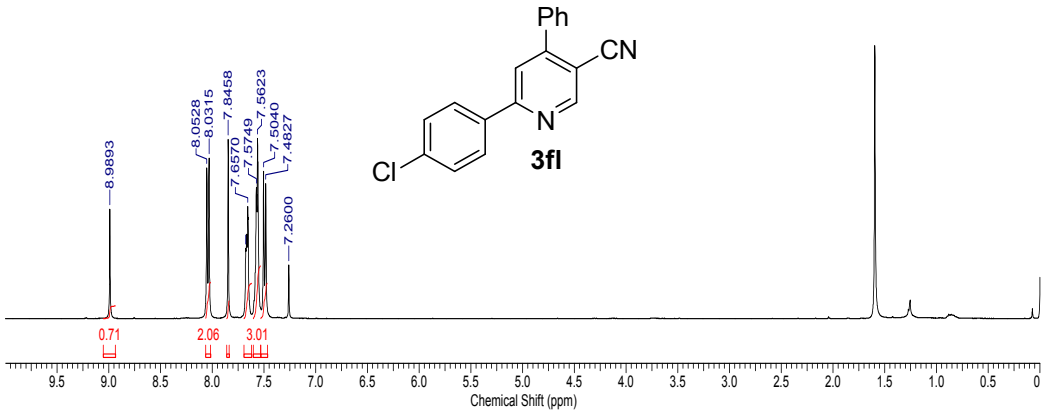

Br
CN
N
Me
3br
77.6735
77.3600
77.0392
161.0445
154.3437
151.9739
141.5544
135.2035
132.7900
130.2671
127.6932
125.1995
119.8986
117.3393
106.2416
21.7623
Chemical Shift (ppm)

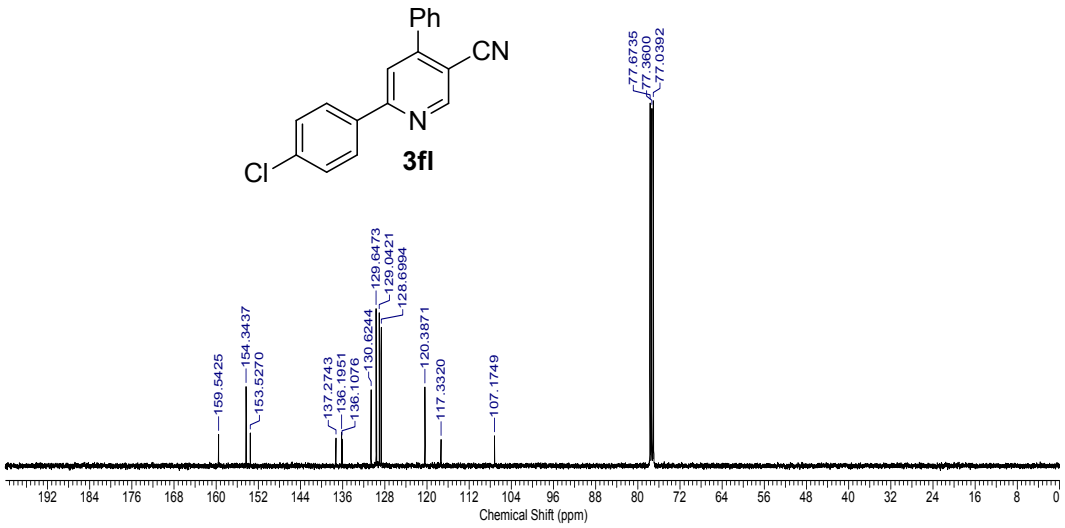

3.8761
8.9341
8.0685
8.0465
7.7900
7.5567
7.5423
7.2600
7.0298
7.0079
CN
N
MeO
3cl
0.74
2.04
1.00
3.01
2.04
3.05
Chemical Shift (ppm)

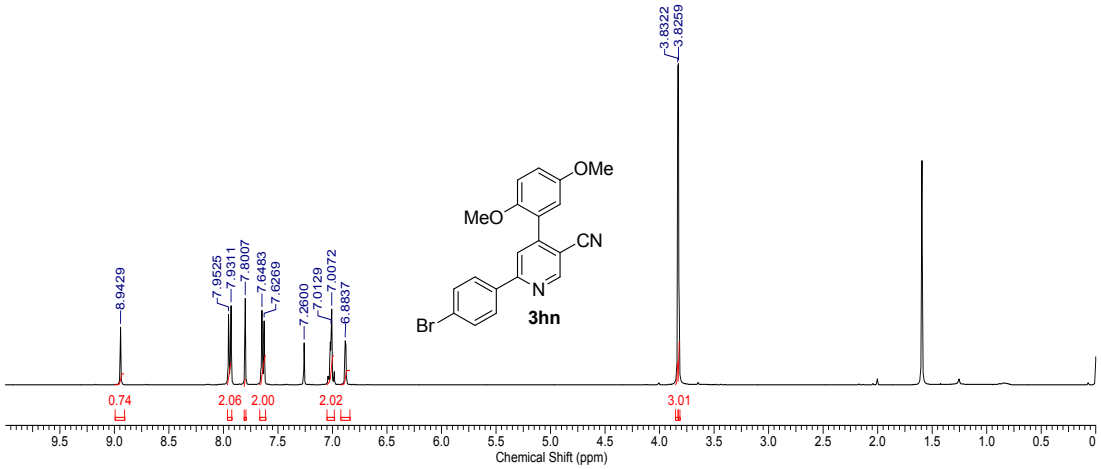

CN
N
MeO
3cl
129.4286
129.2536
128.6484
114.7362
77.6808
77.3600
77.0465
162.0653
160.3227
154.2124
153.0239
136.3920
130.3619
119.5851
117.6674
105.9135
55.7407
Chemical Shift (ppm)

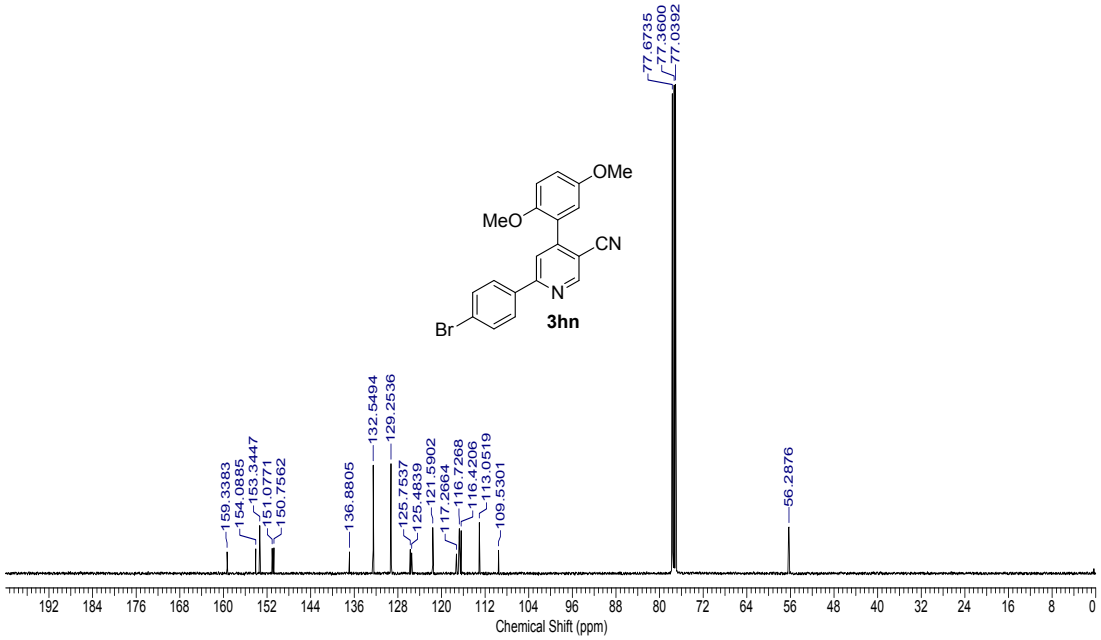

9.0476
7.8966
7.6978
7.6802
7.5542
7.4193
7.2600
0.78
1.00
4.01
Ph
Cl
CN
N
3gl
Chemical Shift (ppm)

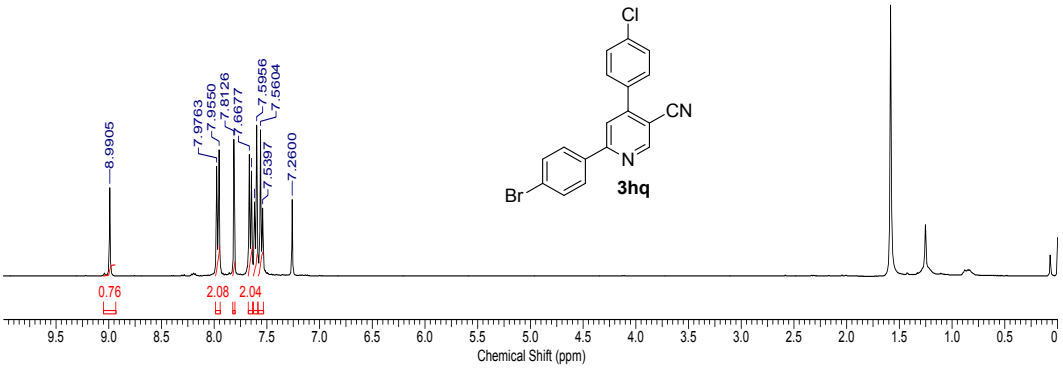

77.6808
77.3600
77.0465
Ph
Cl
CN
N
3gl
160.3591
154.1978
152.4041
137.8430
135.8962
132.4837
131.9806
131.1205
130.8359
129.5671
128.8526
127.6859
125.3964
117.2591
107.3791
Chemical Shift (ppm)

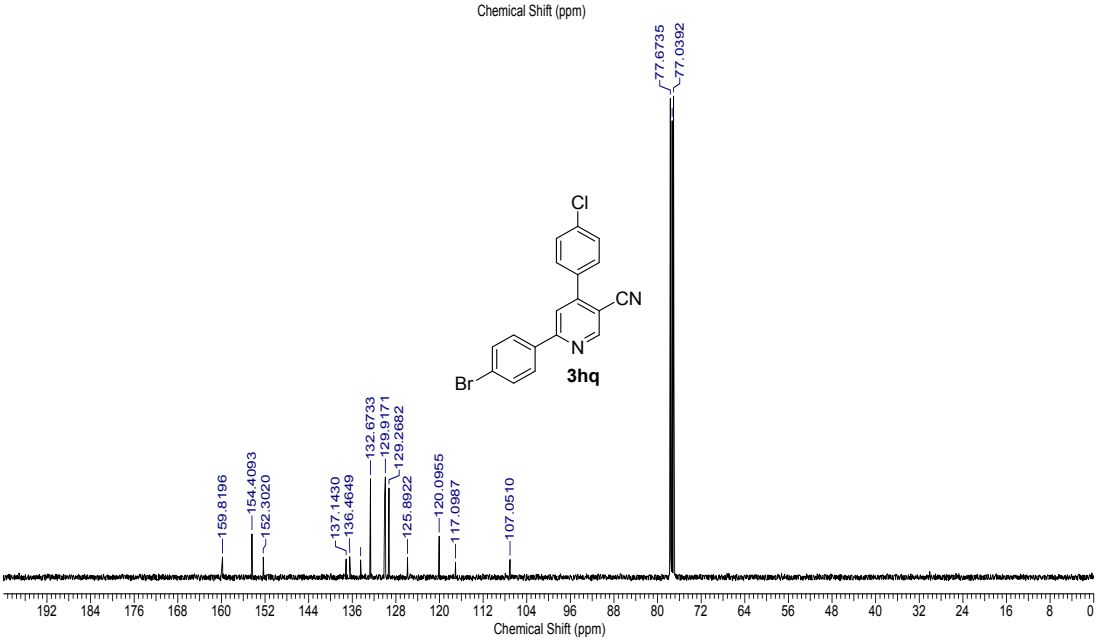

Ph
CN
N
Cl
3fl
8.9893
8.0528
8.0315
7.8458
7.6570
7.5749
7.5623
7.5040
7.4827
7.2600
0.71
2.06
3.01
Chemical Shift (ppm)

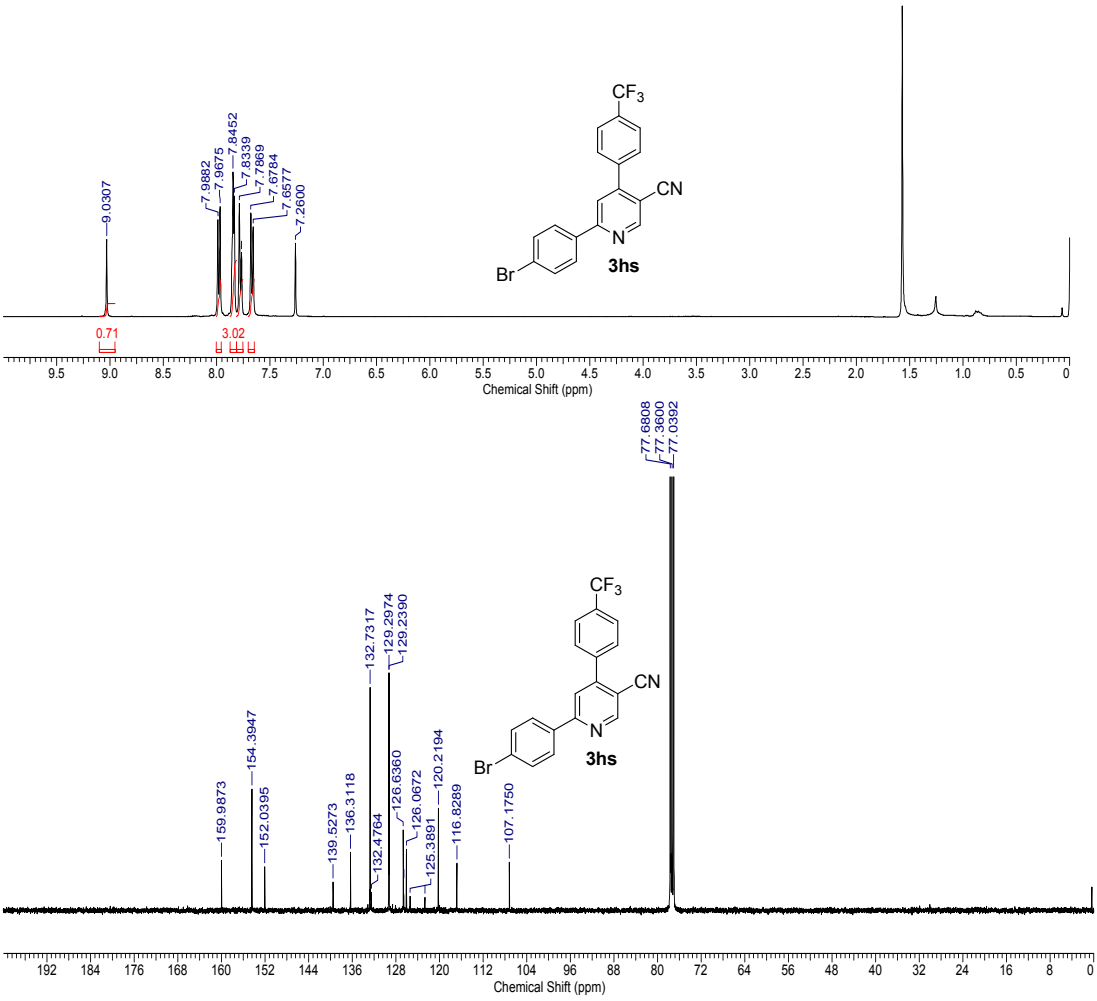

Ph
CN
N
Cl
3fl
77.6735
77.3600
77.0392
159.5425
154.3437
153.5270
137.2743
136.1951
136.1076
130.6244
129.6473
129.0421
128.6994
120.3871
117.3320
107.1749
Chemical Shift (ppm)

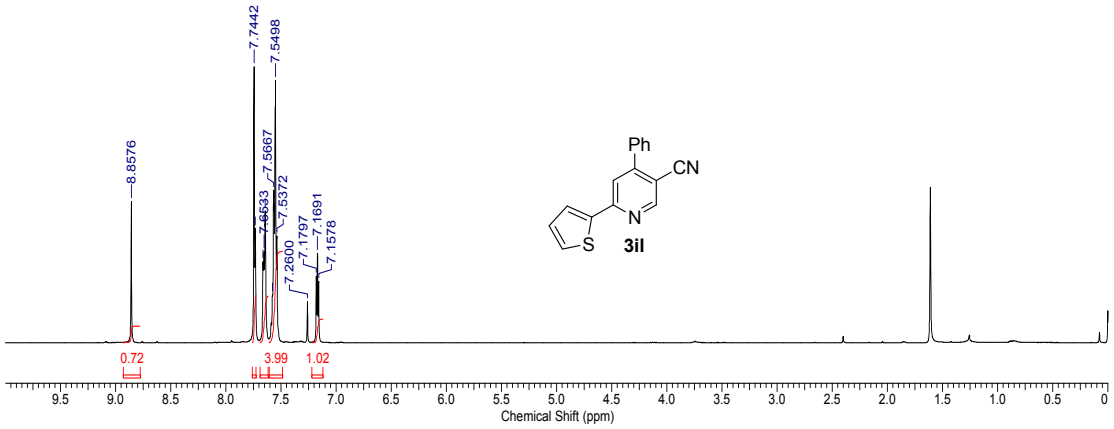

8.9429
7.9525
7.9311
7.8007
7.6483
7.6269
7.2600
7.0129
7.0072
6.8837
3.8322
3.8259
0.74
2.06
2.00
2.02
3.01
OMe
MeO
CN
N
Br
3hn
Chemical Shift (ppm)

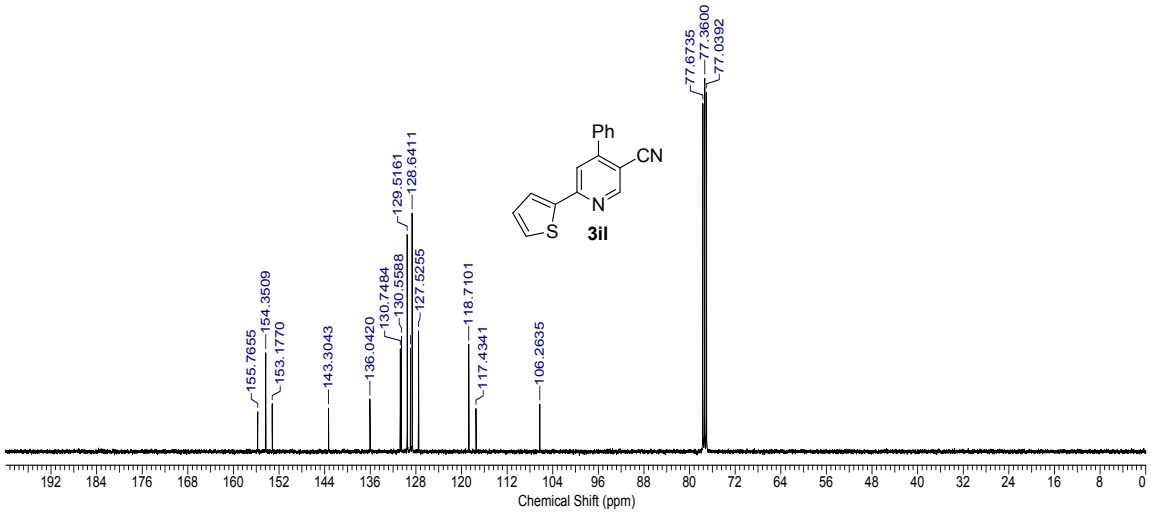

77.6735
77.3600
77.0392
159.3383
154.0885
153.3447
151.0771
150.7562
136.8805
132.5494
129.2536
125.7537
125.4839
121.5902
117.2664
116.7268
116.4206
113.0519
109.5301
56.2876
OMe
MeO
CN
N
Br
3hn
Chemical Shift (ppm)

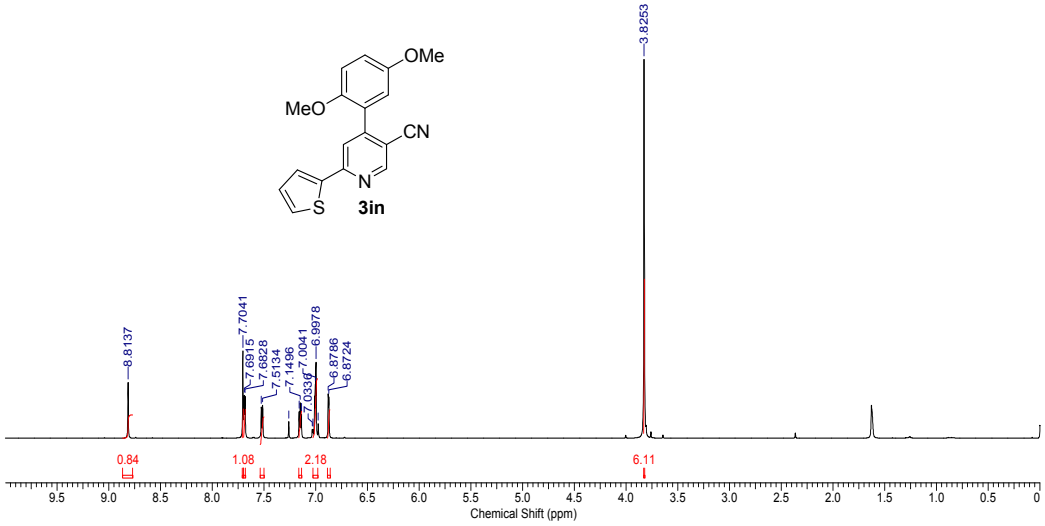

Cl
CN
N
Br
3hq
8.9905
7.9763
7.9550
7.8126
7.6677
7.5956
7.5604
7.5397
7.2600
0.76
2.08
2.04
Chemical Shift (ppm)

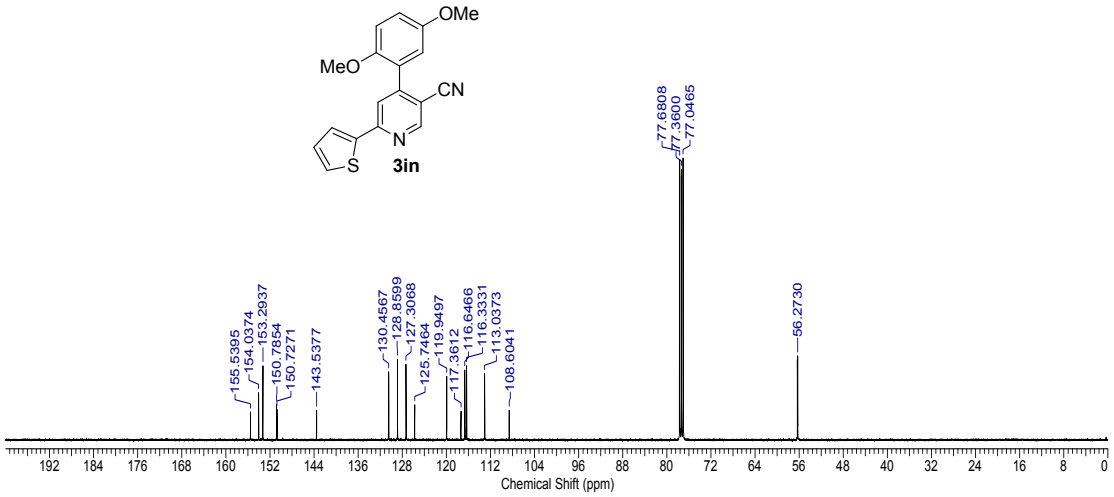

Cl
CN
N
Br
3hq
77.6735
77.0392
159.8196
154.4093
152.3020
137.1430
136.4649
132.6733
129.9171
129.2682
125.8922
120.0955
117.0987
107.0510
Chemical Shift (ppm)

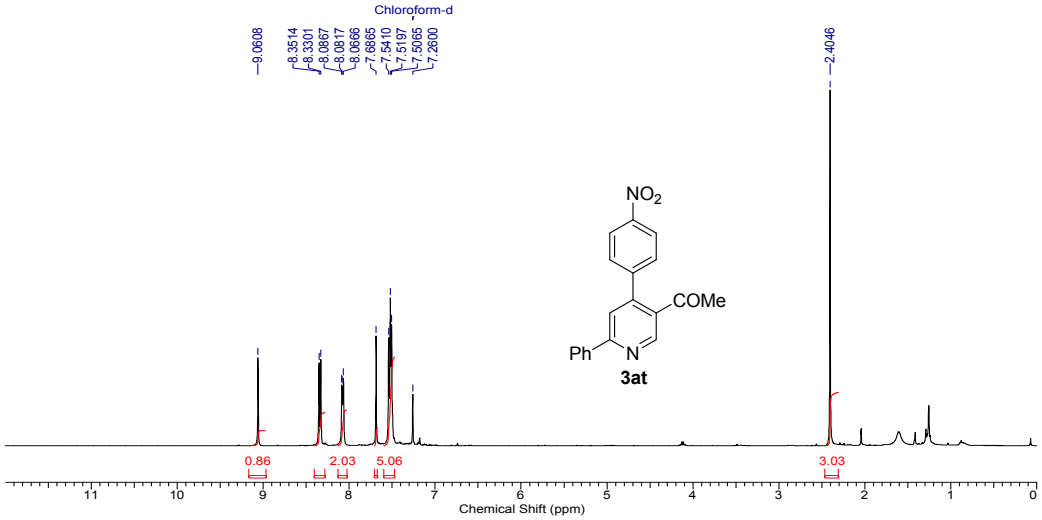

9.0307
7.9882
7.9675
7.8452
7.8339
7.7869
7.6784
7.6577
7.2600
0.71
3.02
CF3
CN
N
Br
3hs
Chemical Shift (ppm)
77.6808
77.3600
77.0392
159.9873
154.3947
152.0395
139.5273
136.3118
132.7317
132.4764
129.2974
129.2390
126.6360
126.0672
125.3891
120.2194
116.8289
107.1750
Chemical Shift (ppm)

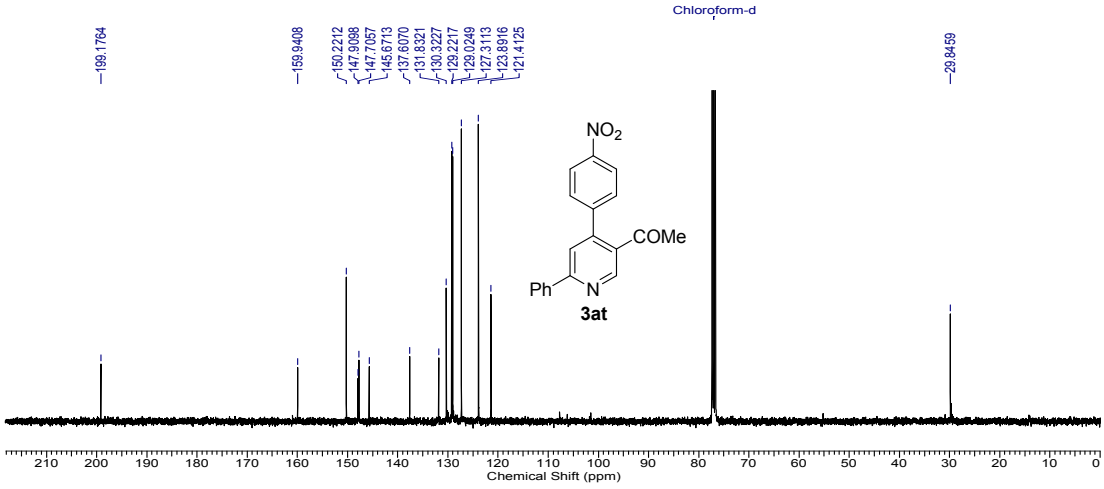

8.8576
7.7442
7.5498
7.5667
7.5633
7.5372
7.2600
7.1797
7.1691
7.1578
Ph
CN
N
S
3il
0.72
3.99
1.02
Chemical Shift (ppm)

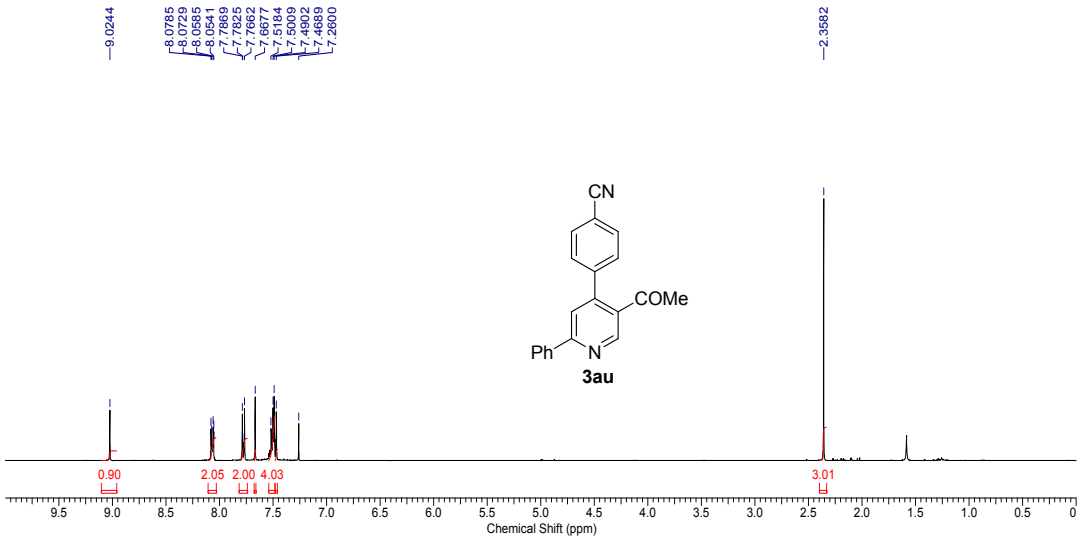

77.6735
77.3600
77.0392
Ph
CN
N
S
3il
129.5161
128.6411
130.7484
130.5588
127.5255
118.7101
117.4341
155.7655
154.3509
153.1770
143.3043
136.0420
106.2635
Chemical Shift (ppm)

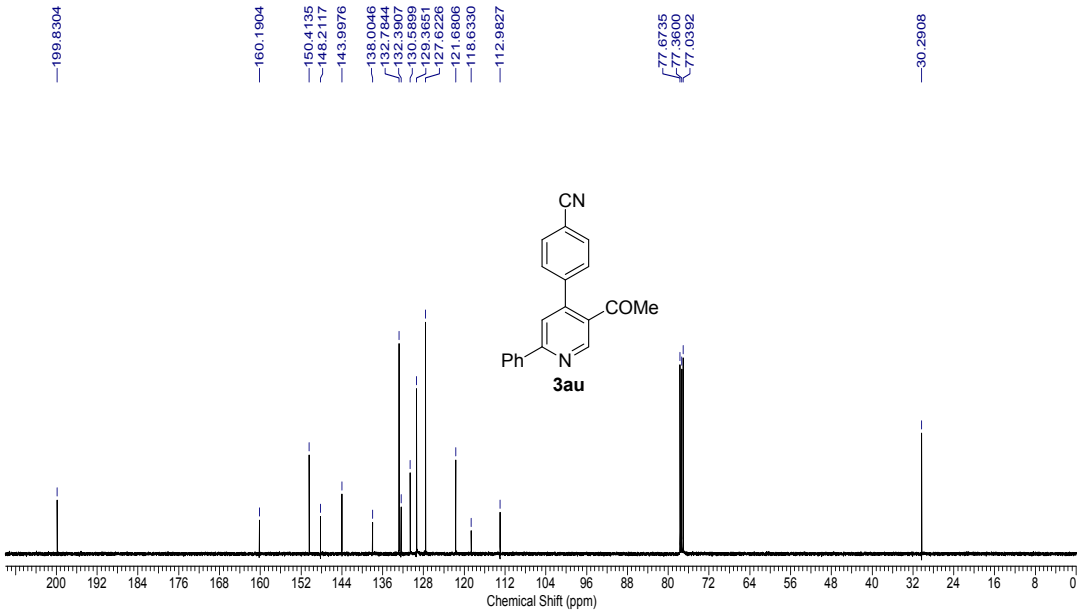

OMe
MeO
CN
N
S
3in
8.8137
7.7041
7.6915
7.6828
7.5134
7.1486
7.0336
7.0041
6.9978
6.8786
6.8724
3.8253
0.84
1.08
2.18
6.11
Chemical Shift (ppm)

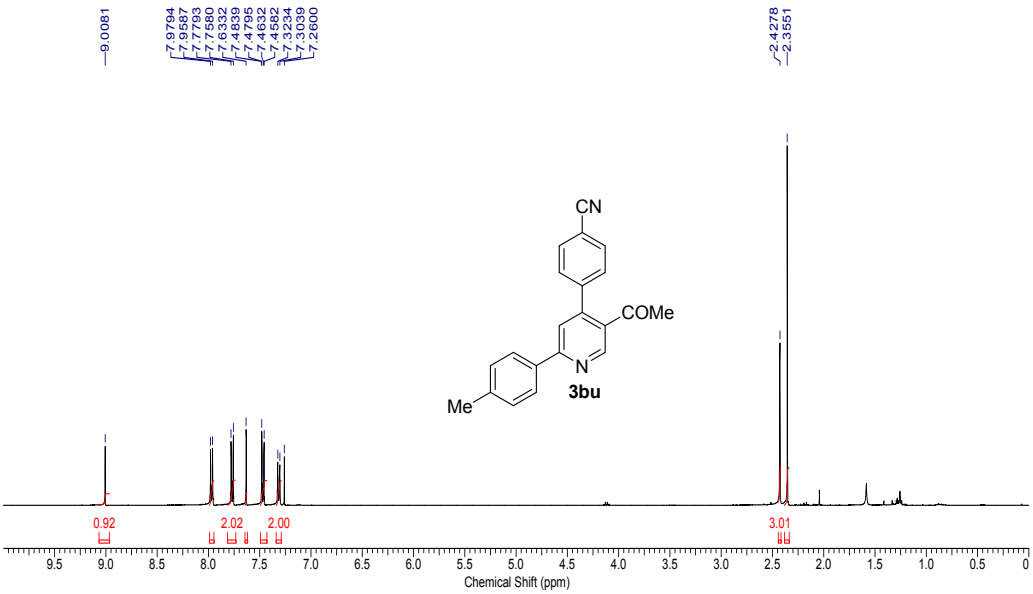

OMe
MeO
CN
N
S
3in
155.5395
154.0374
153.2937
150.7854
150.7271
143.5377
130.4567
128.8599
127.3068
125.7464
119.9497
117.3612
116.6466
116.3331
113.0373
108.6041
77.6808
77.3600
77.0465
56.2730
Chemical Shift (ppm)


Chloroform-d
9.0608
8.3514
8.3301
8.0867
8.0817
8.0666
7.6865
7.5410
7.5197
7.5065
7.2600
2.4046
NO2
COMe
Ph
N
3at
0.86
2.03
5.06
3.03
Chemical Shift (ppm)


Chloroform-d
199.1764
159.9408
150.2212
147.9098
147.7057
145.6713
137.6070
131.8321
130.3227
129.2217
129.0249
127.3113
123.8916
121.4125
29.8459
NO2
COMe
Ph
N
3at
Chemical Shift (ppm)


9.0244
8.0785
8.0729
8.0585
8.0541
7.7869
7.7825
7.7662
7.6677
7.5184
7.5009
7.4902
7.4689
7.2600
2.3582
CN
COMe
Ph
N
3au
0.90
2.05
2.00
4.03
3.01
Chemical Shift (ppm)


199.8304
160.1904
150.4135
148.2117
143.9976
138.0046
132.7844
132.3907
130.5899
129.3651
127.6226
121.6806
118.6330
112.9827
77.6735
77.3600
77.0392
30.2908
CN
COMe
Ph
N
3au
Chemical Shift (ppm)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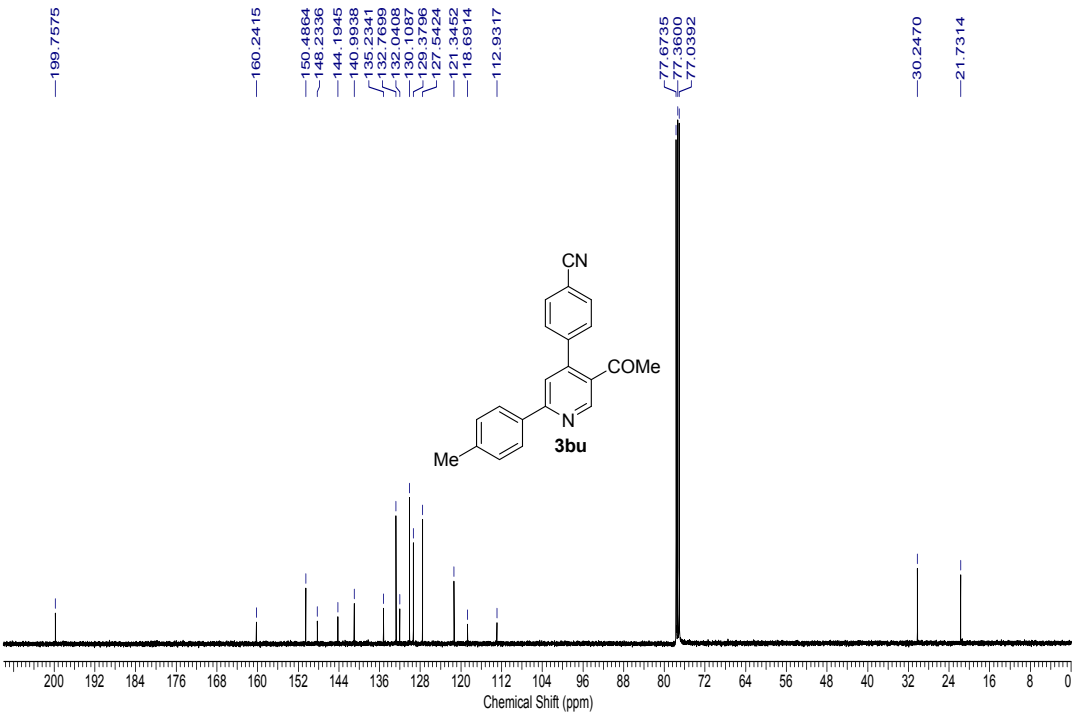
7.9794
7.9587
7.7793
7.7580
7.6332
7.4839
7.4795
7.4632
7.4582
7.3234
7.3039
7.2600
2.4278
2.3551
CN
COMe
N
Me
3bu
0.92
2.02
2.00
3.01
Chemical Shift (ppm)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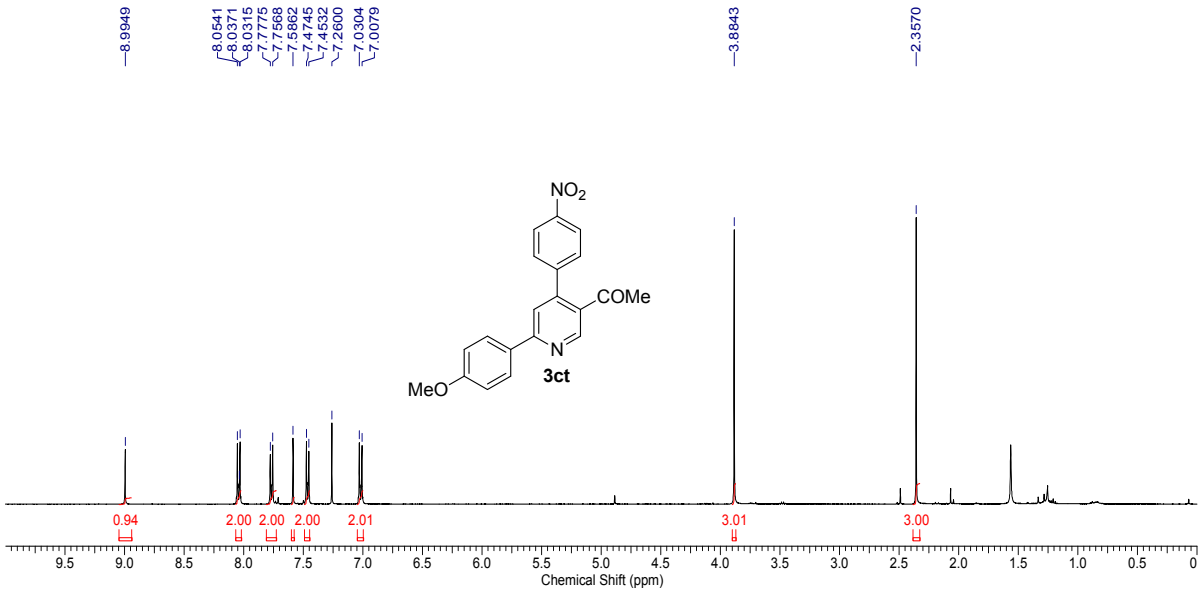
160.2415
150.4864
148.2336
144.1945
140.9938
135.2341
132.7699
132.0408
130.1087
129.3796
127.5424
121.3452
118.6914
112.9317
77.6735
77.3600
77.0392
30.2470
21.7314
CN
COMe
N
Me
3bu
Chemical Shift (ppm)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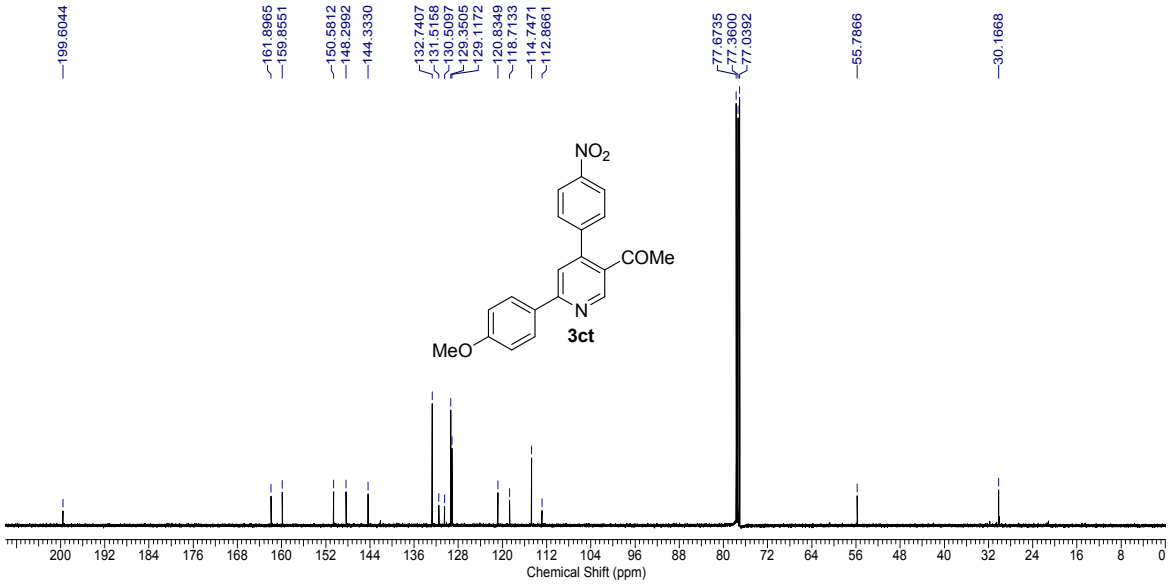
8.0541
8.0371
8.0315
7.7775
7.7568
7.5862
7.4745
7.4532
7.2600
7.0304
7.0079
3.8843
2.3570
NO2
COMe
N
MeO
3ct
0.94
2.00
2.00
2.00
2.01
3.01
3.00
Chemical Shift (ppm)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161.8965
159.8551
150.5812
148.2992
144.3330
132.7407
131.5158
130.5097
129.3505
129.1172
120.8349
118.7133
114.7471
112.8661
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77.3600
77.0392
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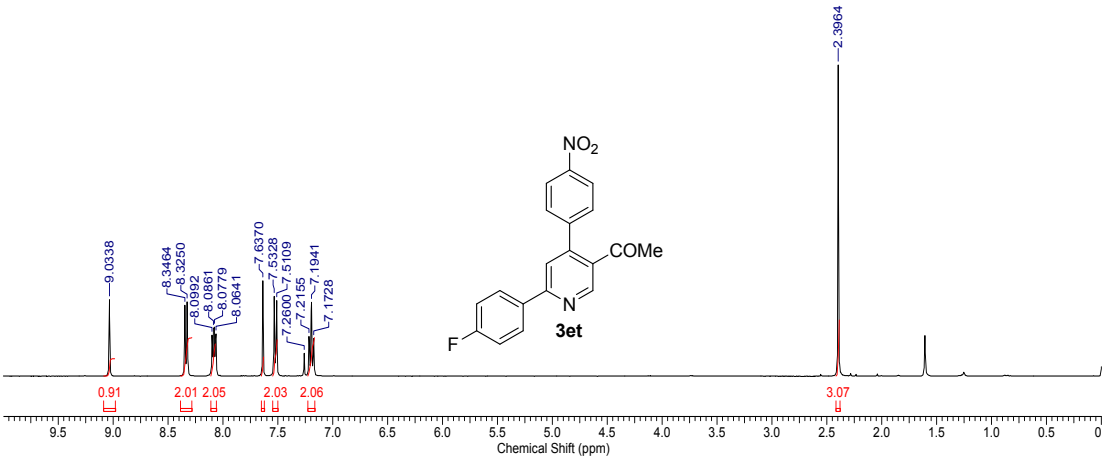
30.1668
NO2
COMe
N
MeO
3ct
Chemical Shift (ppm)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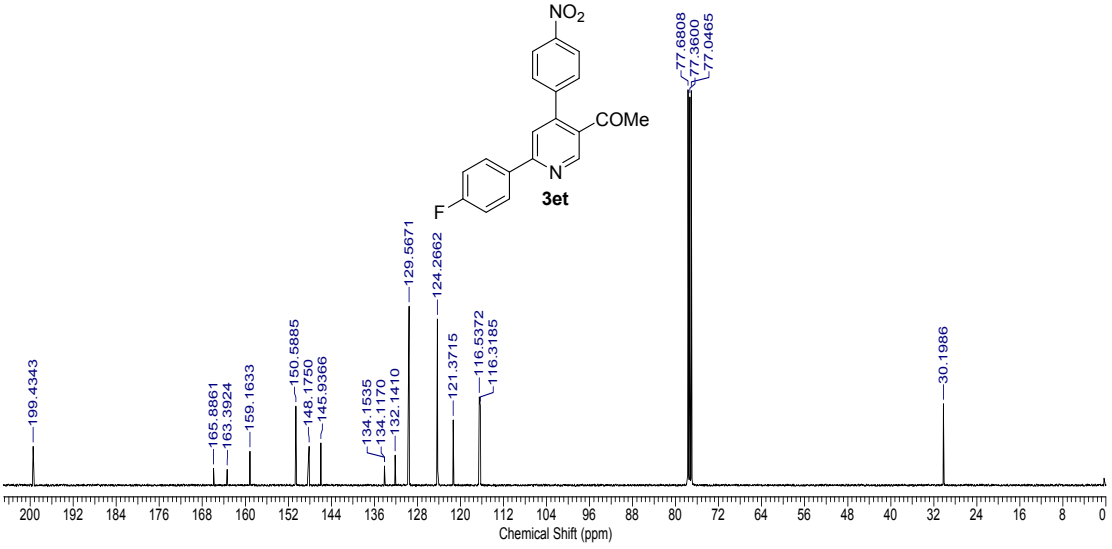
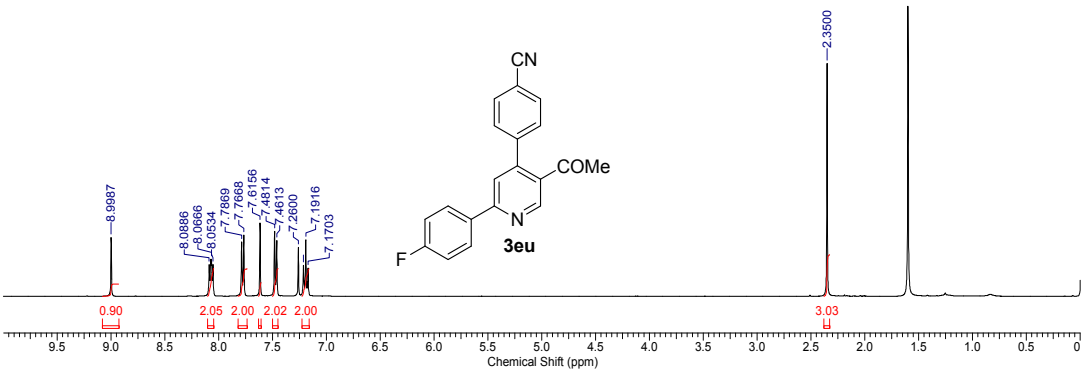
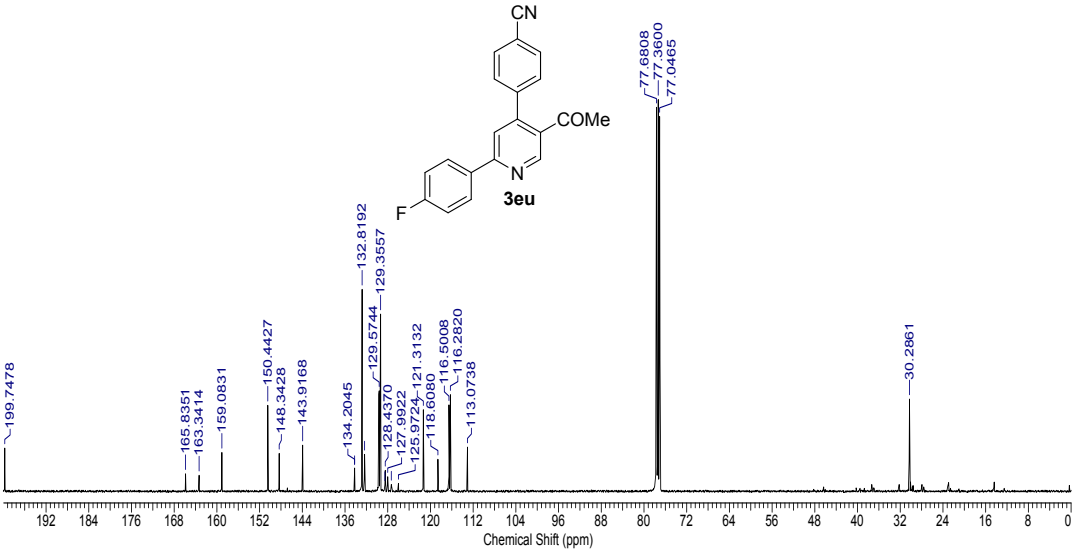
8.3464
8.3250
8.0992
8.0861
8.0779
8.0641
7.6370
7.5328
7.5109
7.2600
7.2155
7.1941
7.1728
2.3964
NO2
COMe
N
F
3et
0.91
2.01
2.05
2.03
2.06
3.07
Chemical Shift (ppm)


NO2
COMe
N
F
3et
77.6808
77.3600
77.0465
199.4343
165.8861
163.3924
159.1633
150.5885
148.1750
145.9366
134.1535
134.1170
132.1410
129.5671
124.2662
121.3715
116.5372
116.3185
30.1986
Chemical Shift (ppm)


CN
COMe
N
F
3eu
8.9987
8.0886
8.0666
8.0534
7.7869
7.7668
7.6156
7.4814
7.4613
7.2600
7.1916
7.1703
2.3500
0.90
2.05
2.00
2.02
2.00
3.03
Chemical Shift (ppm)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COMe
N
F
3eu
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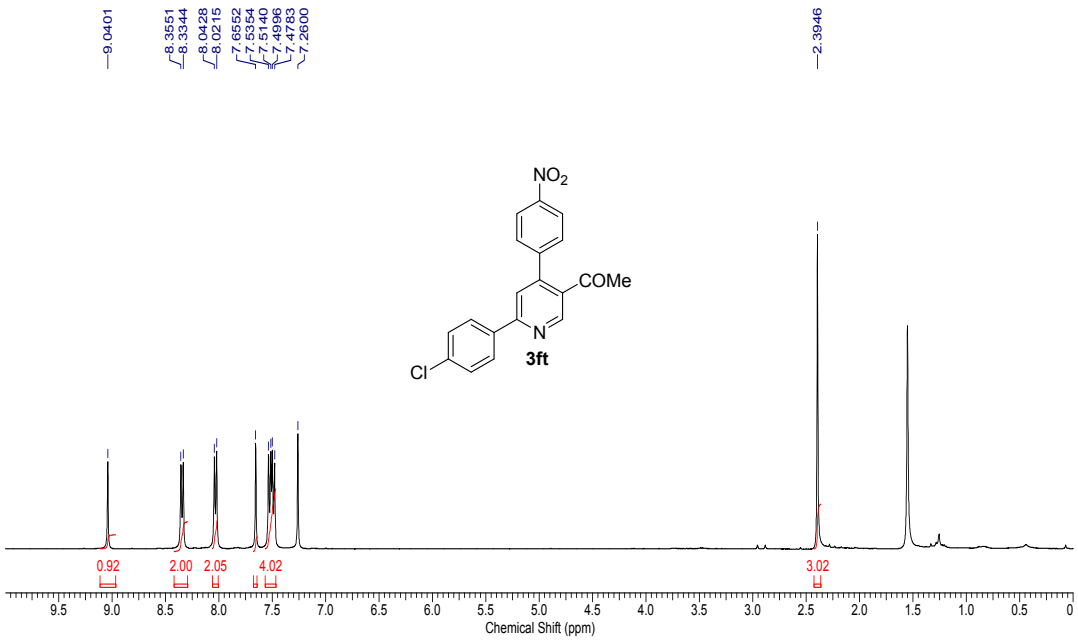
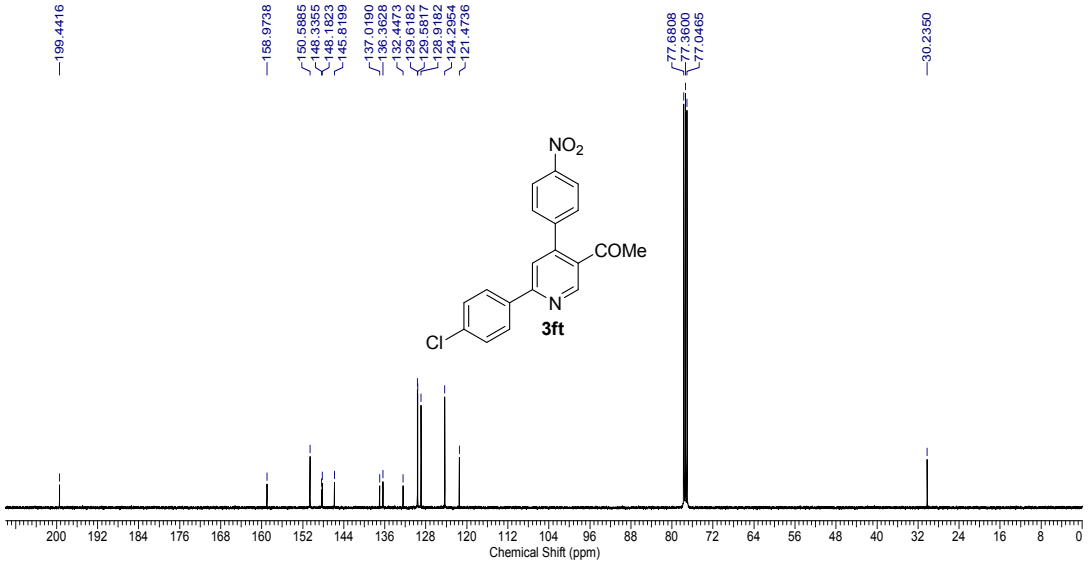
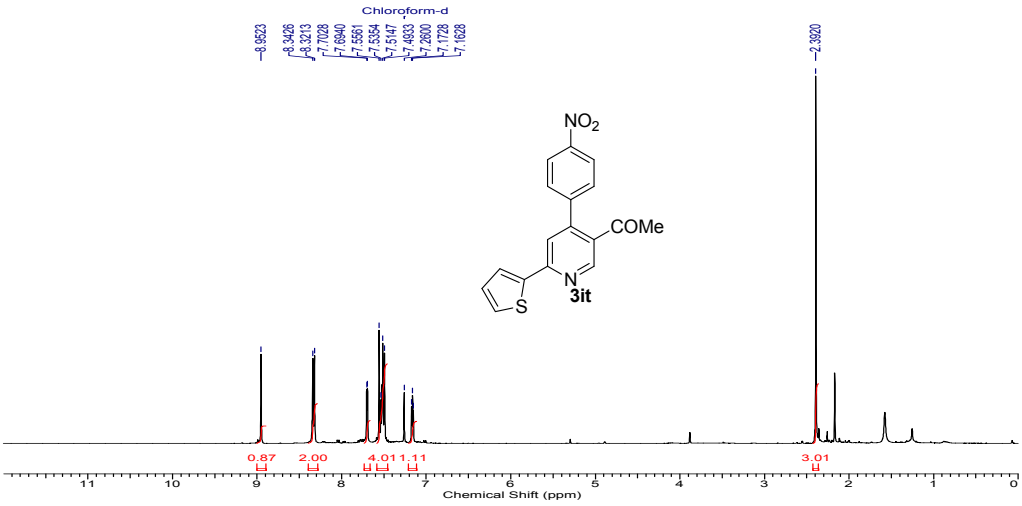
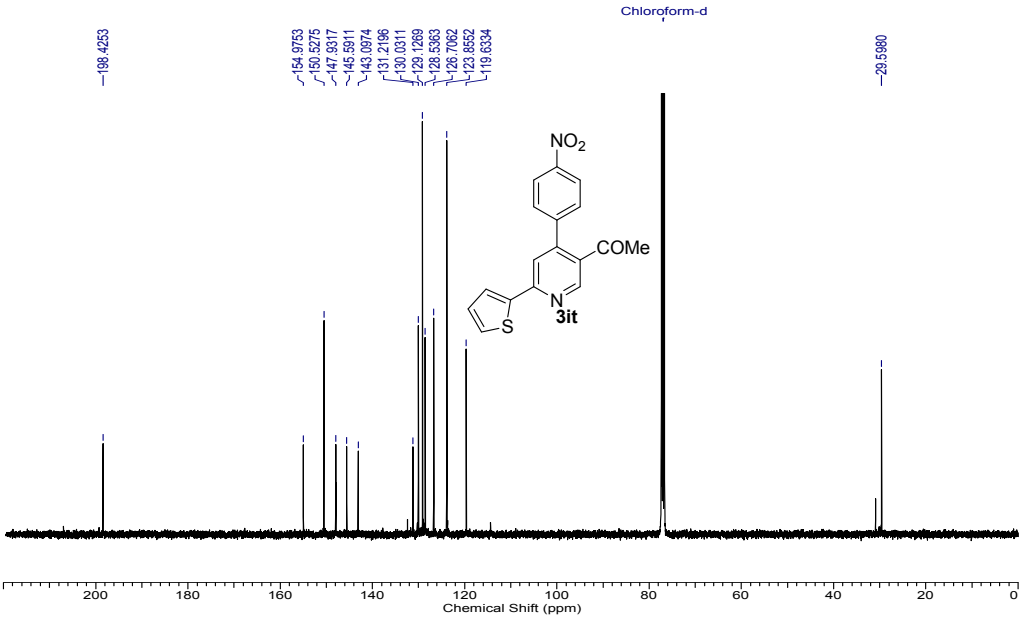
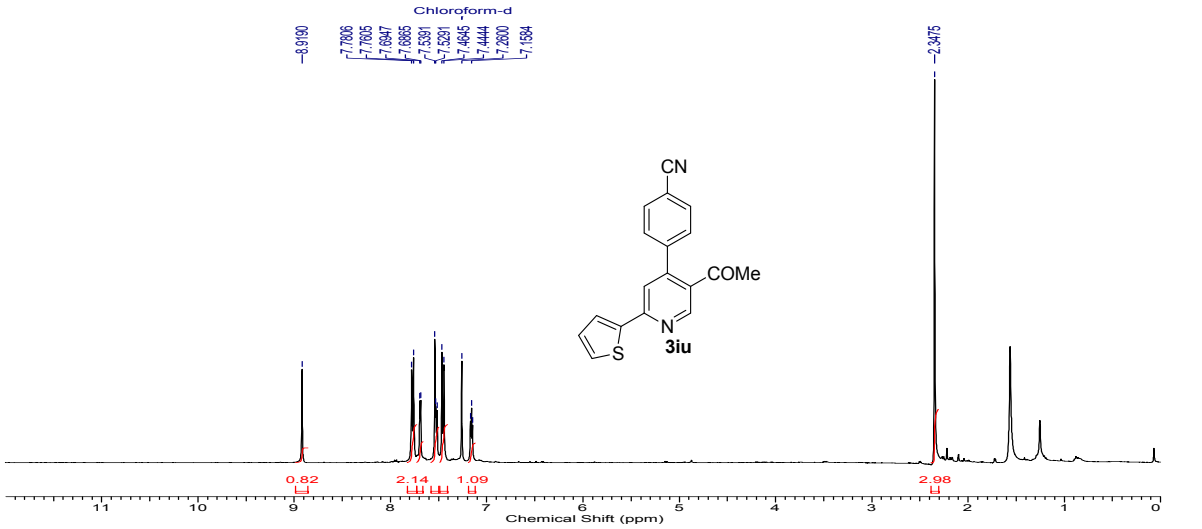
163.3414
159.0831
150.4427
148.3428
143.9168
134.2045
132.8192
129.5744
129.3557
128.4370
127.9922
125.9724
121.3132
118.6080
116.5008
116.2820
113.0738
77.6808
77.3600
77.0465
30.2861
Chemical Shift (ppm)

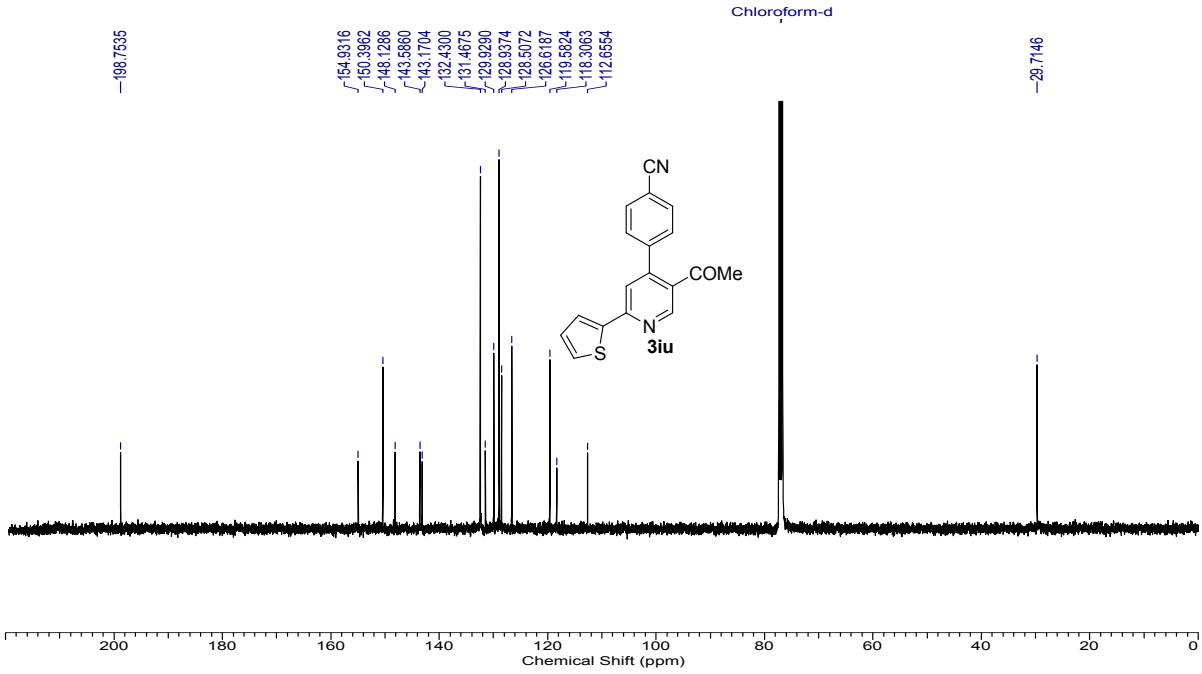

9.0401
8.3551
8.3344
8.0428
8.0215
7.6552
7.5354
7.5140
7.4996
7.4783
7.2600
2.3946
NO2
COMe
N
Cl
3ft
0.92
2.00
2.05
4.02
3.02
Chemical Shift (ppm)


199.4416
158.9738
150.5885
148.3355
148.1823
145.8199
137.0190
136.3628
132.4473
129.6182
129.5817
128.9182
124.2954
121.4736
77.6808
77.3600
77.0465
30.2350
NO2
COMe
N
Cl
3ft
Chemical Shift (ppm)


Chloroform-d
8.9523
8.3426
8.3213
7.7028
7.6940
7.5561
7.5354
7.5147
7.4933
7.2600
7.1728
7.1628
2.3920
NO2
COMe
N
S
3it
0.87
2.00
4.01
1.11
3.01
Chemical Shift (ppm)


Chloroform-d
198.4253
154.9753
150.5275
147.9317
145.5911
143.0974
131.2196
130.0311
129.1269
128.5363
126.7062
123.8552
119.6334
29.5980
NO2
COMe
N
S
3it
Chemical Shift (ppm)


Chloroform-d
8.9190
7.7806
7.7605
7.6947
7.6865
7.5391
7.5291
7.4945
7.4444
7.2600
7.1584
2.3475
CN
COMe
N
S
3iu
0.82
2.14
1.09
2.98
Chemical Shift (ppm)


Chloroform-d
198.7535
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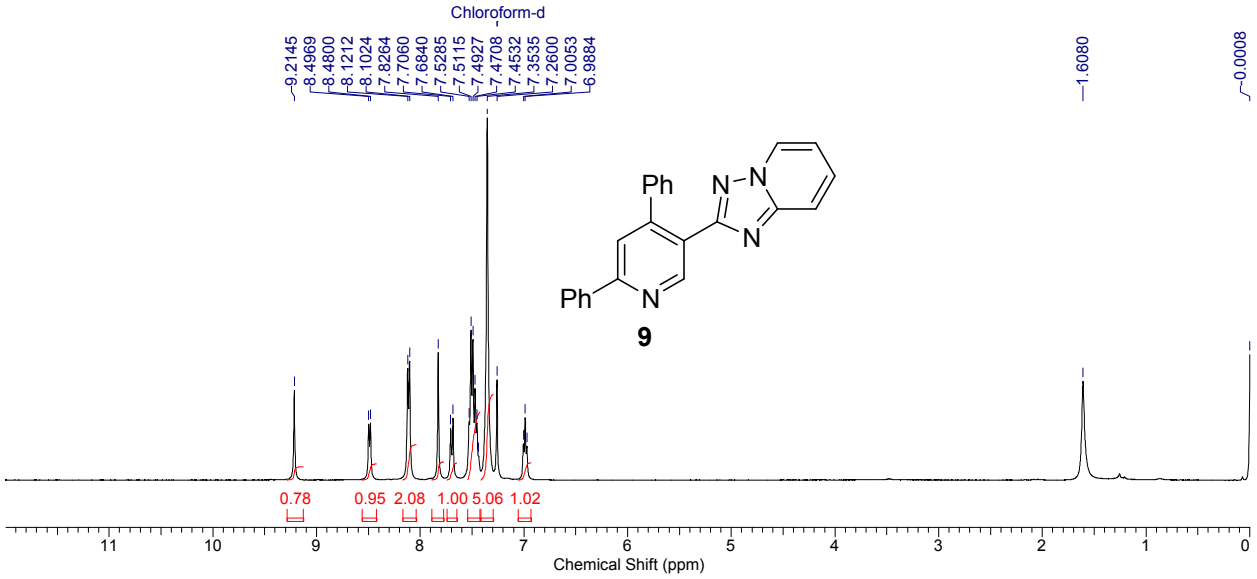
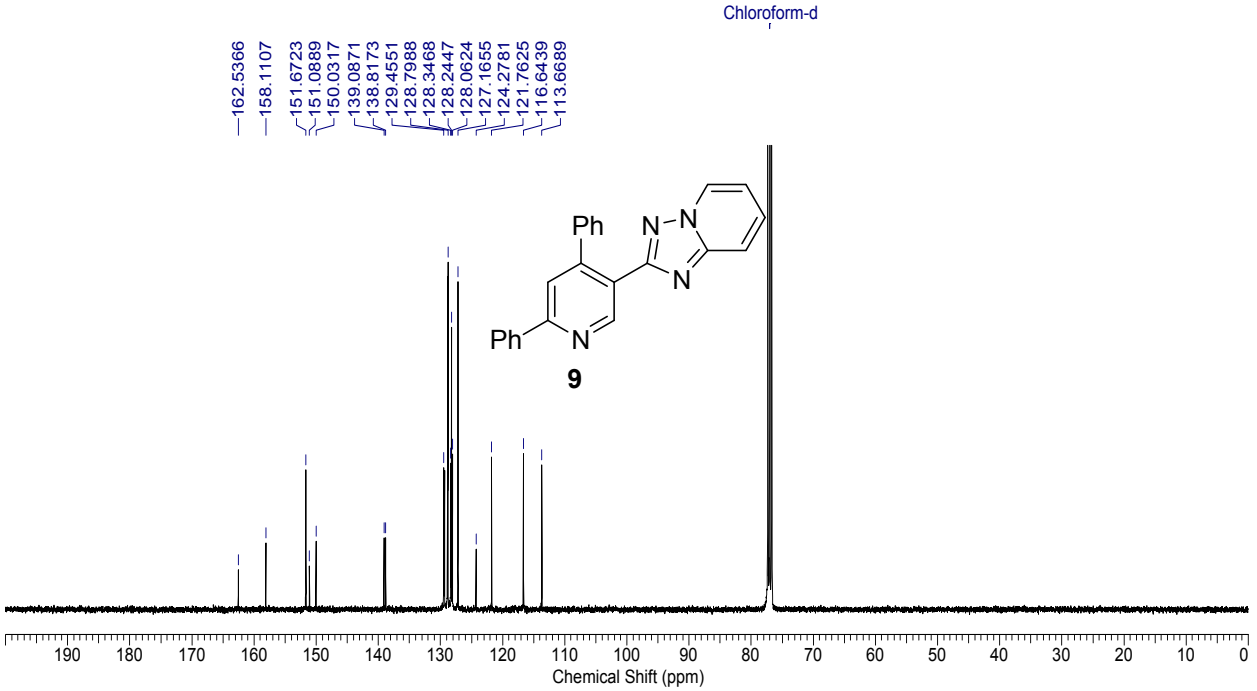
150.3962
148.1286
143.5860
143.1704
132.4300
131.4675
129.9290
128.9374
128.5072
126.6187
119.5824
118.3063
112.6554
29.7146
CN
COMe
N
S
3iu
Chemical Shift (ppm)


Chloroform-d
9.2145
8.4969
8.4800
8.1212
8.1024
7.8264
7.7060
7.6840
7.5285
7.5115
7.4927
7.4708
7.4532
7.3535
7.2600
7.0053
6.9884
1.6080
0.0008
Ph
N
N
N
Ph
N
9
0.78
0.95
2.08
1.00
5.06
1.02
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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158.1107
151.6723
151.0889
150.0317
139.0871
138.8173
129.4551
128.7988
128.3468
128.2447
128.0624
127.1655
124.2781
121.7625
116.6439
113.6689
Ph
N
N
N
Ph
N
9
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)