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Supporting Information

An expedient approach to fluorescent 3-substituted 4*H*-quinolizin-4 ones *via* (η^4-vinylketene)-$Fe(CO)_3$ complexes

Alfredo Rosas-Sánchez,[†] Rubén A. Toscano,[‡] José G. López-Cortés[‡] and M. Carmen Ortega-Alfaro [†,*]

[†]*Instituto de Ciencias Nucleares, UNAM, Circuito Exterior, Ciudad Universitaria, Coyoacán, C.P. 04510, México D.F., México.*

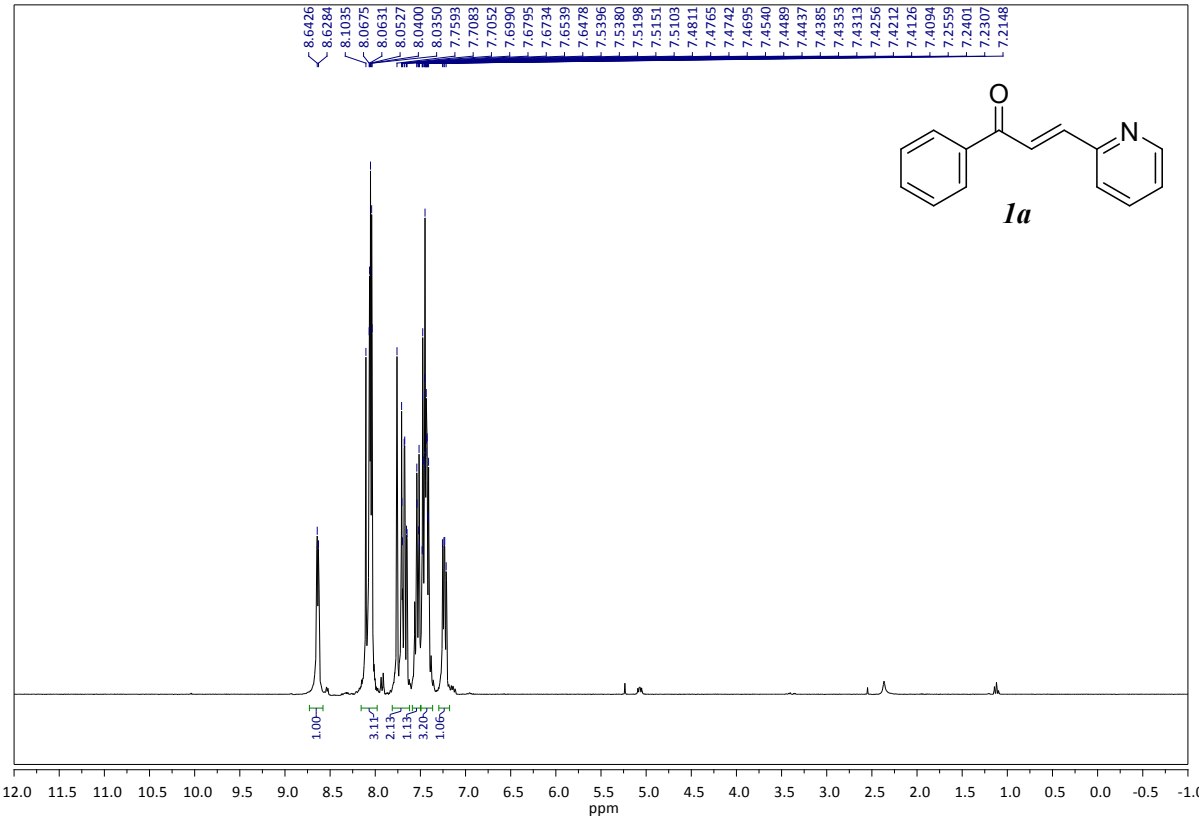
[‡]*Instituto de Química, UNAM, Circuito Exterior, Ciudad Universitaria, Coyoacán, C.P. 04510, México D.F., México.*

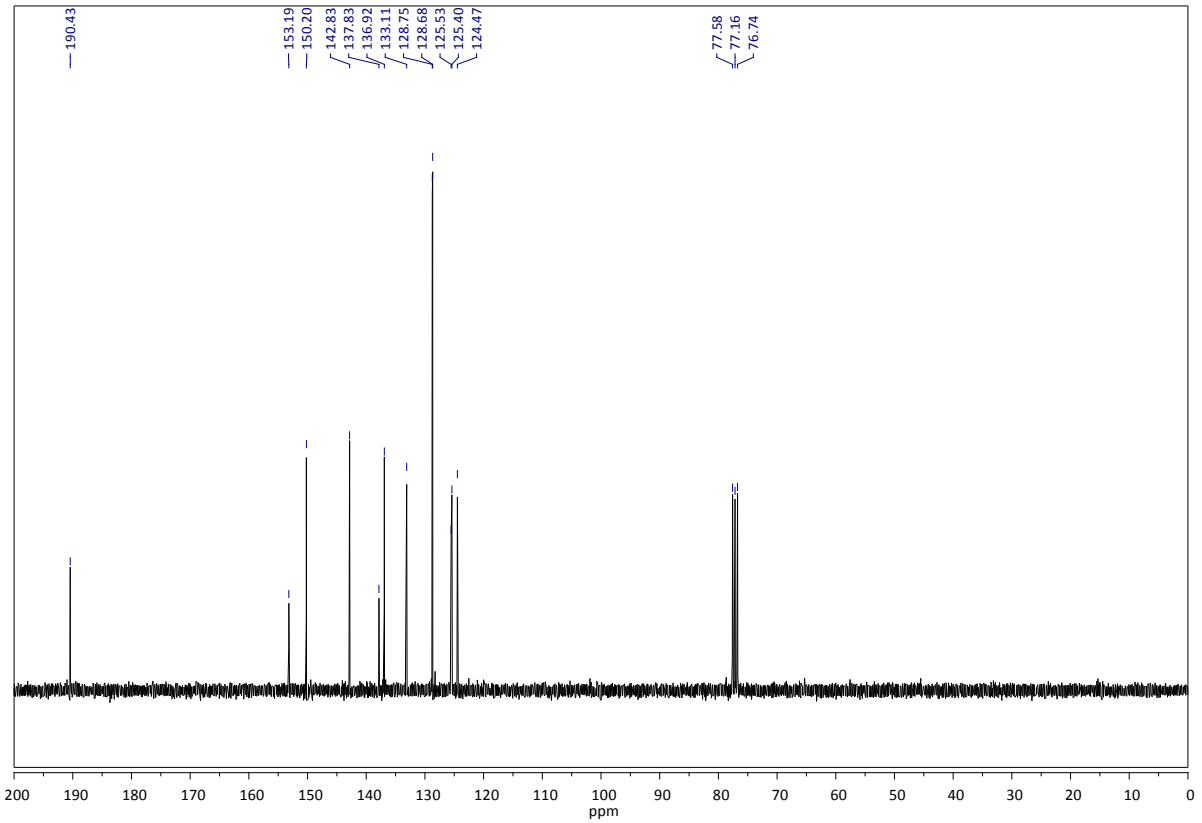
carmen.ortega@nucleares.unam.mx

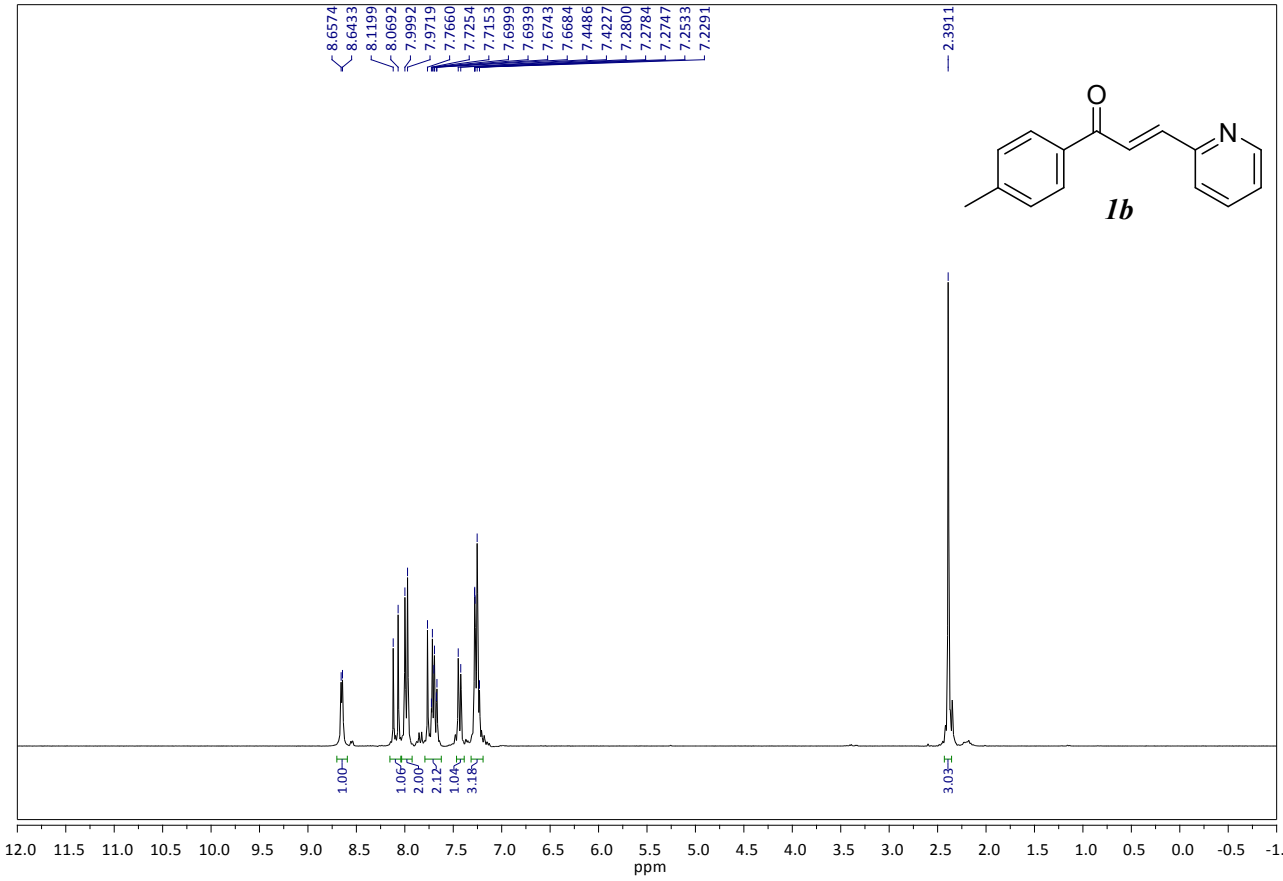
Contents

1. ^{1}H and ^{13}C NMR Spectra

1.1 Spectra of compounds 1a-l.



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7.6743
7.6684
7.4486
7.4227
7.2800
7.2784
7.2747
7.2533
7.2291
2.3911
O
N
1b
1.00
1.06
2.00
2.12
1.04
3.18
3.03
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 -0.5
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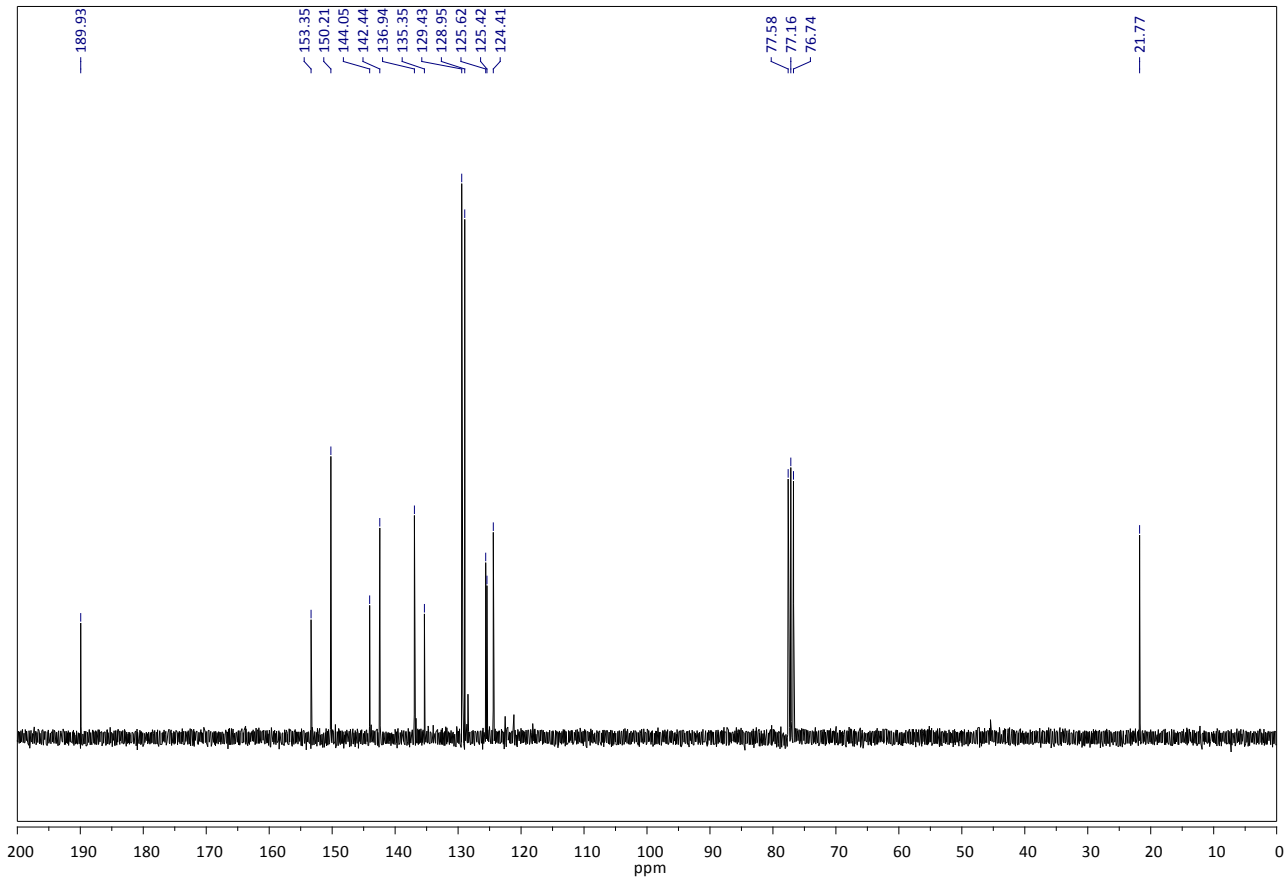
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76.74
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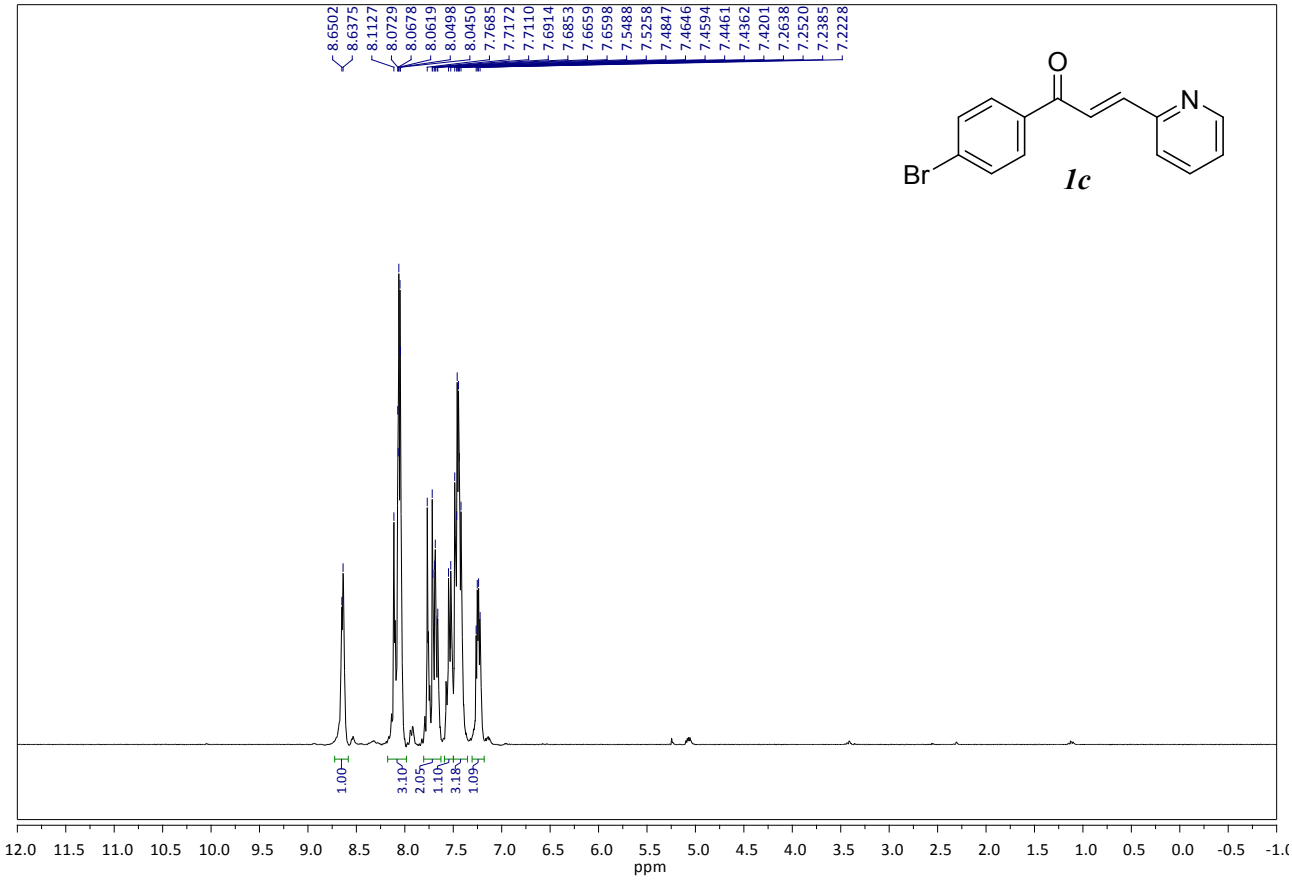
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Br
1c
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3.10
2.05
1.10
3.18
1.09
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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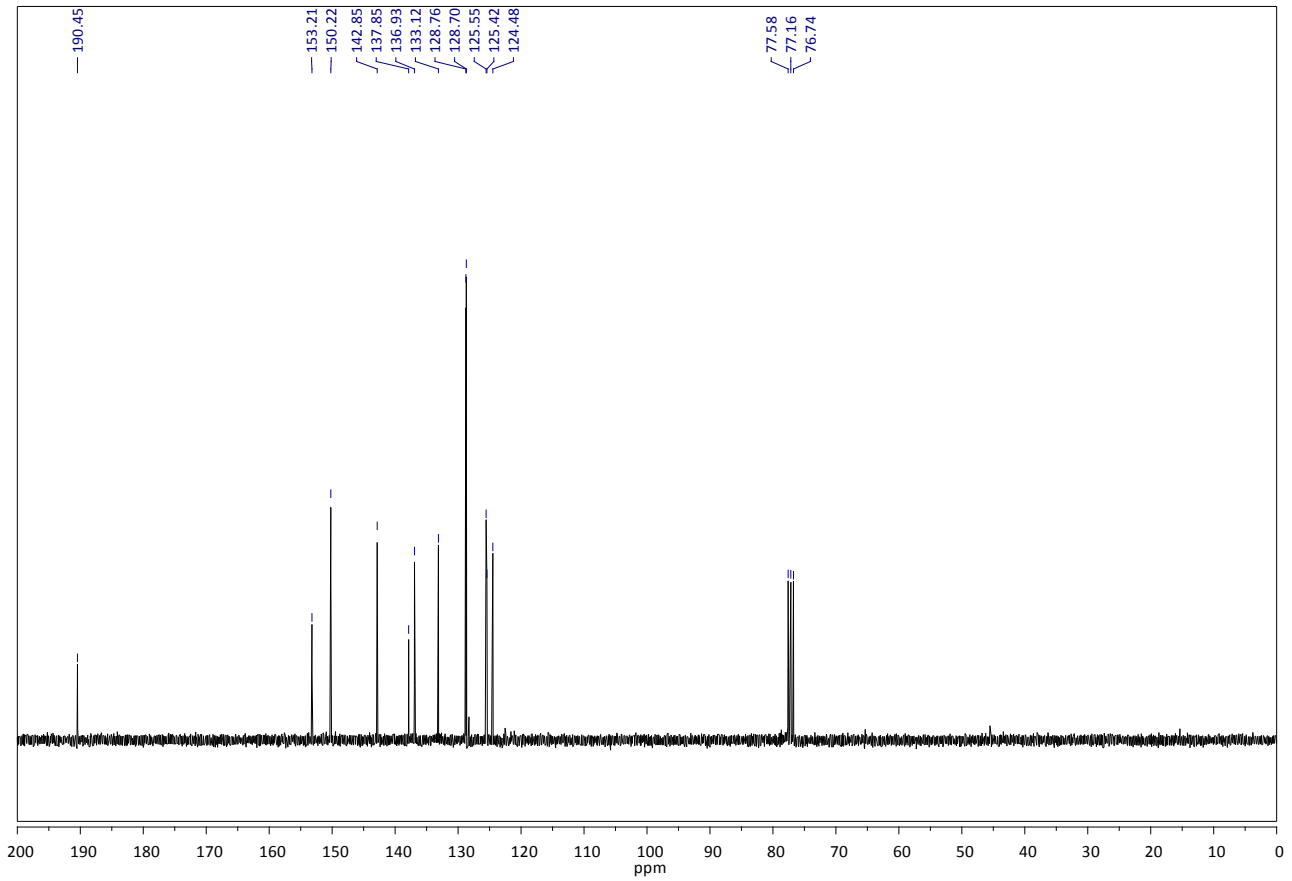
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77.16
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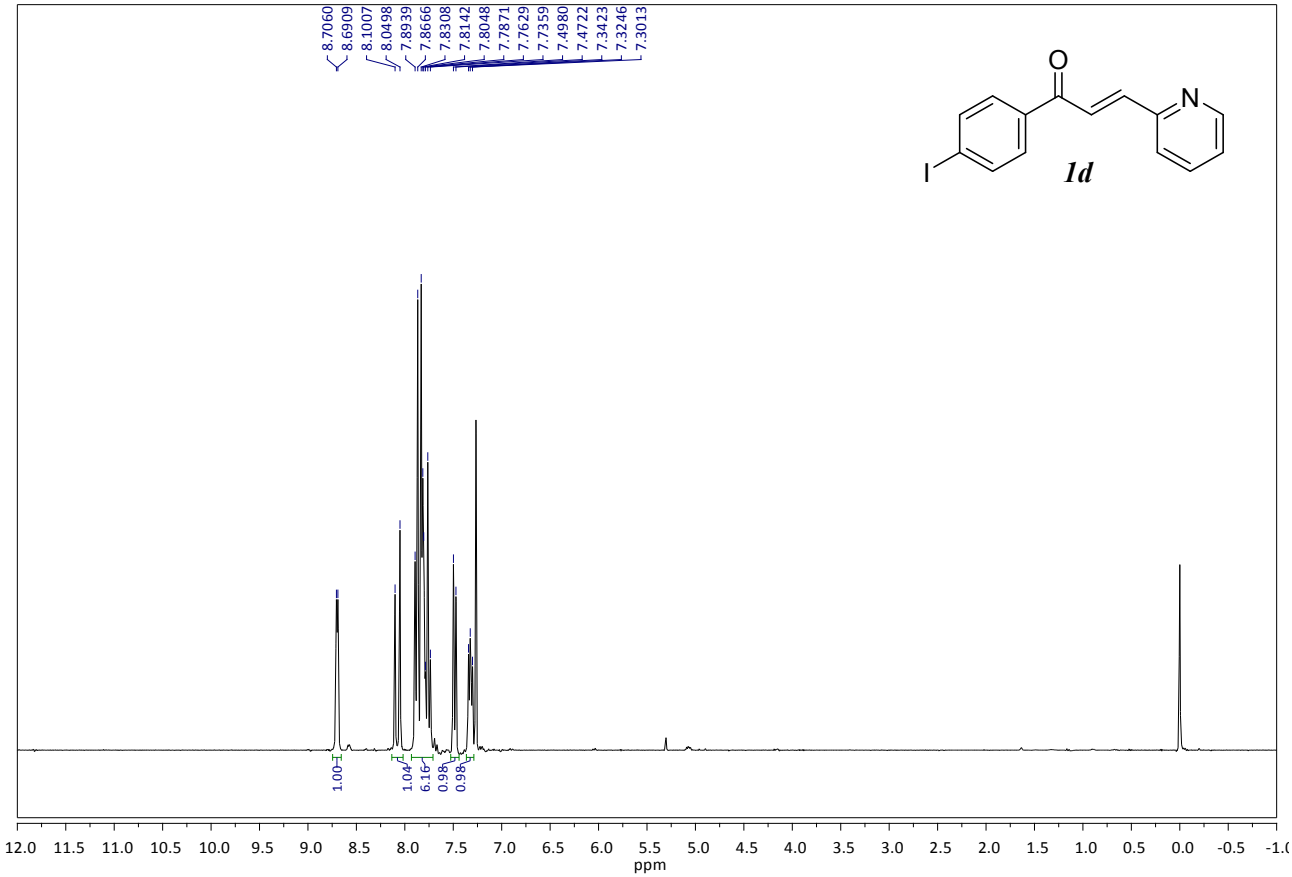
ppm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N
I
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1.04
6.16
0.98
0.98
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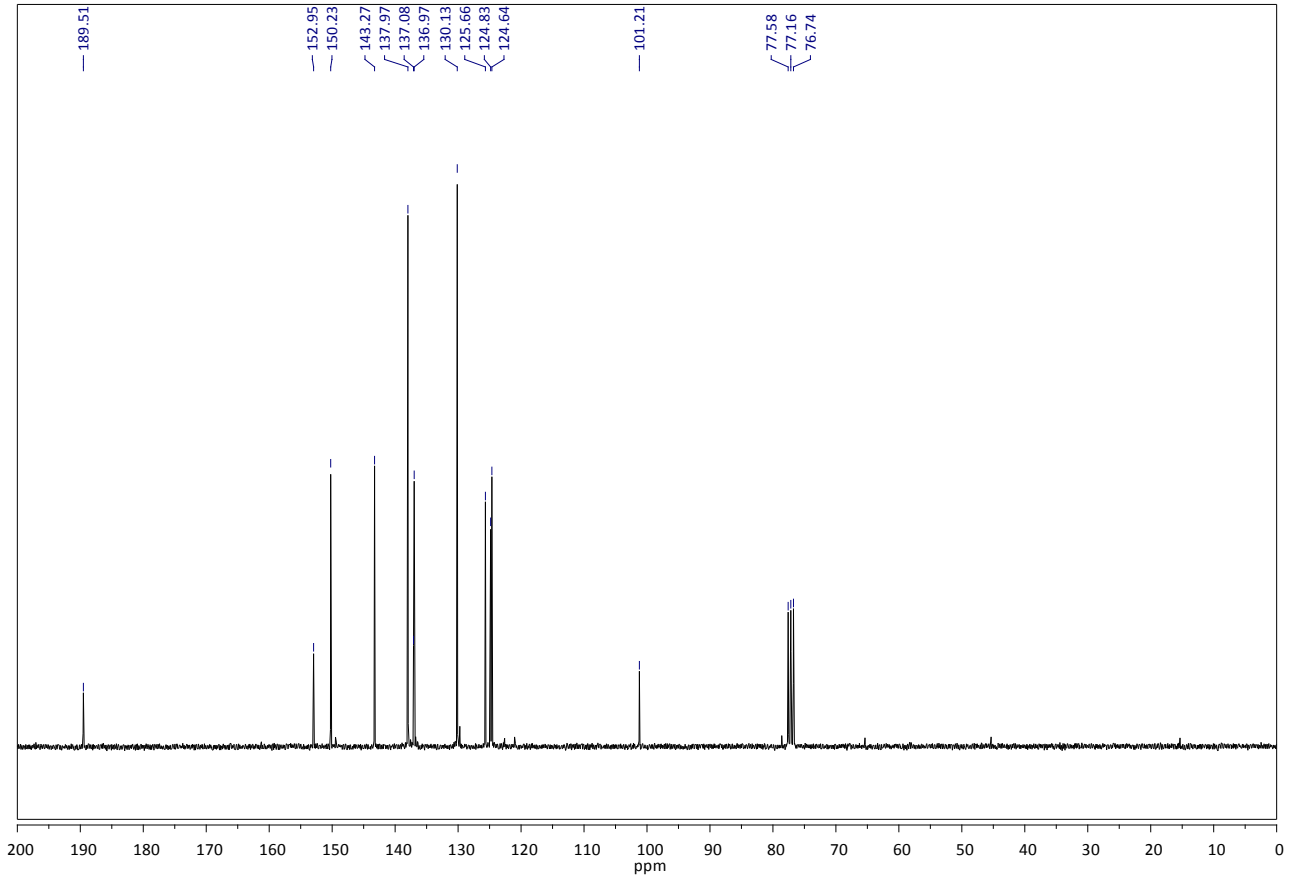
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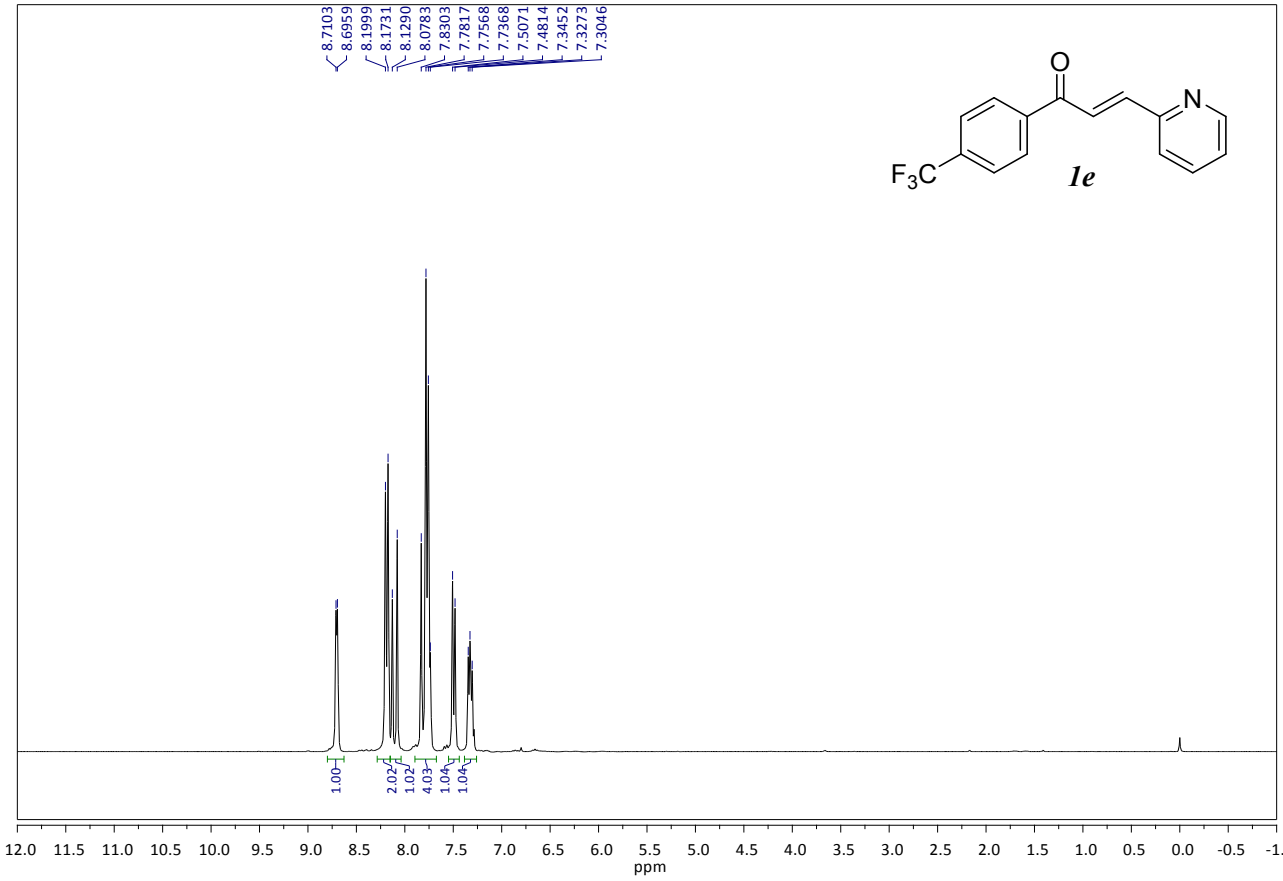
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7.3046
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N
F3C
1e
1.00
2.02
1.02
4.03
1.04
1.04
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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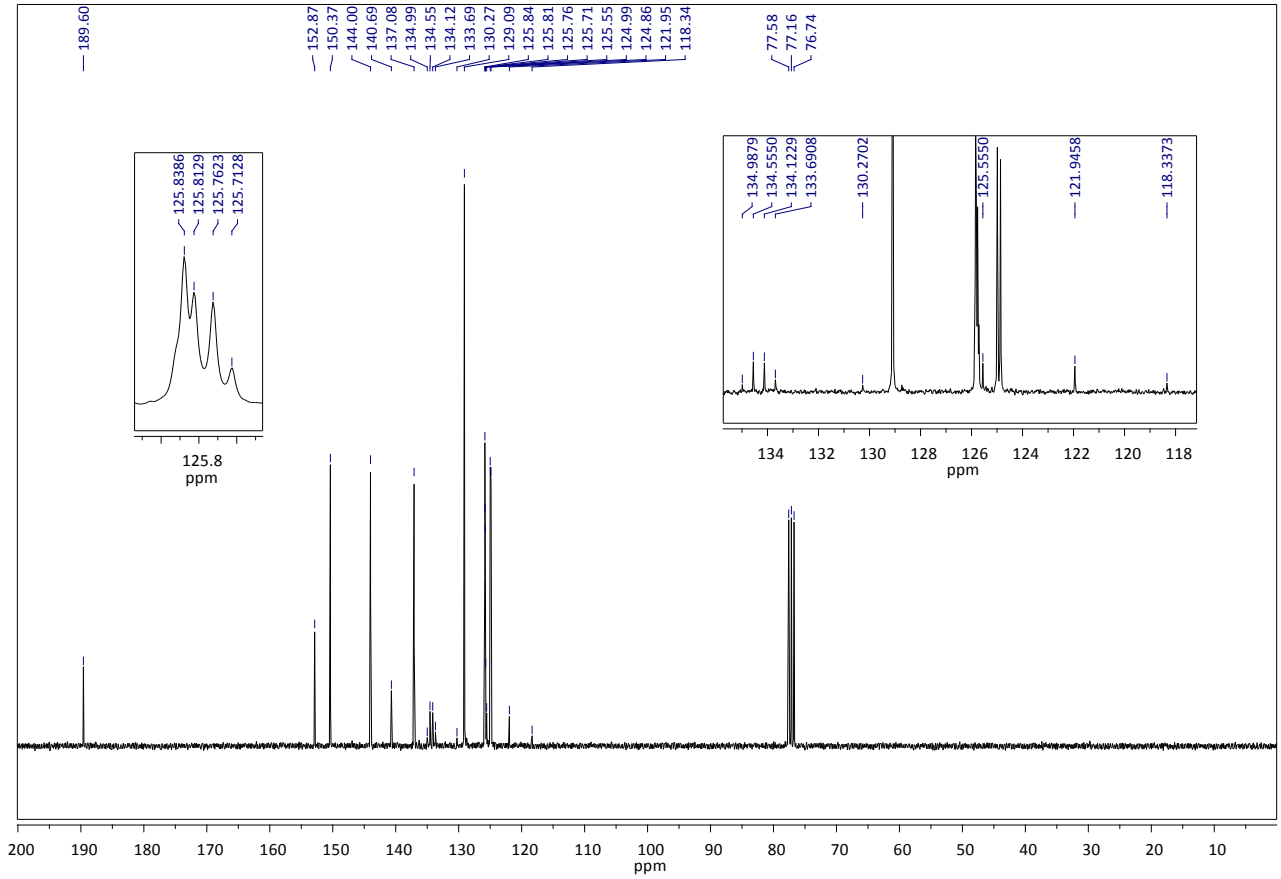
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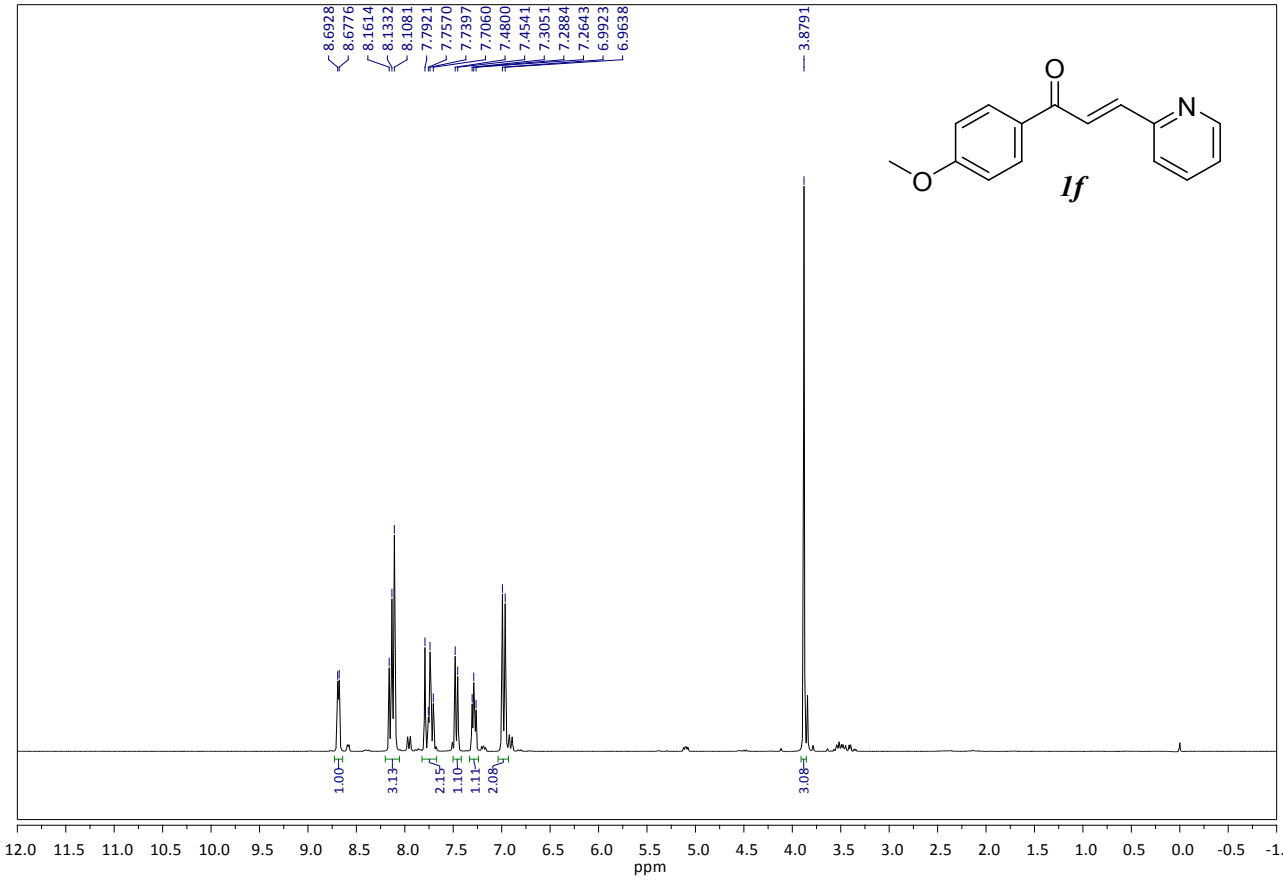
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N
O
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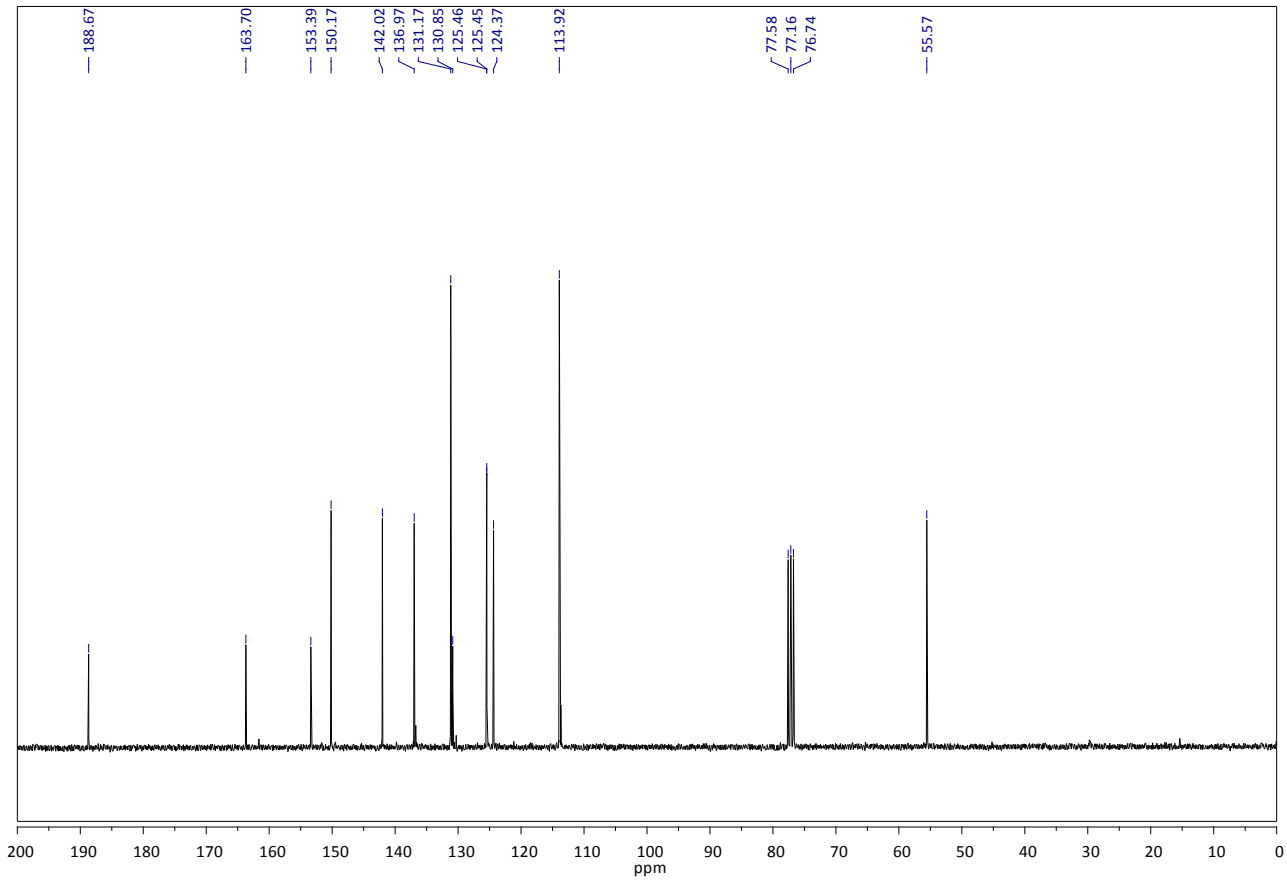
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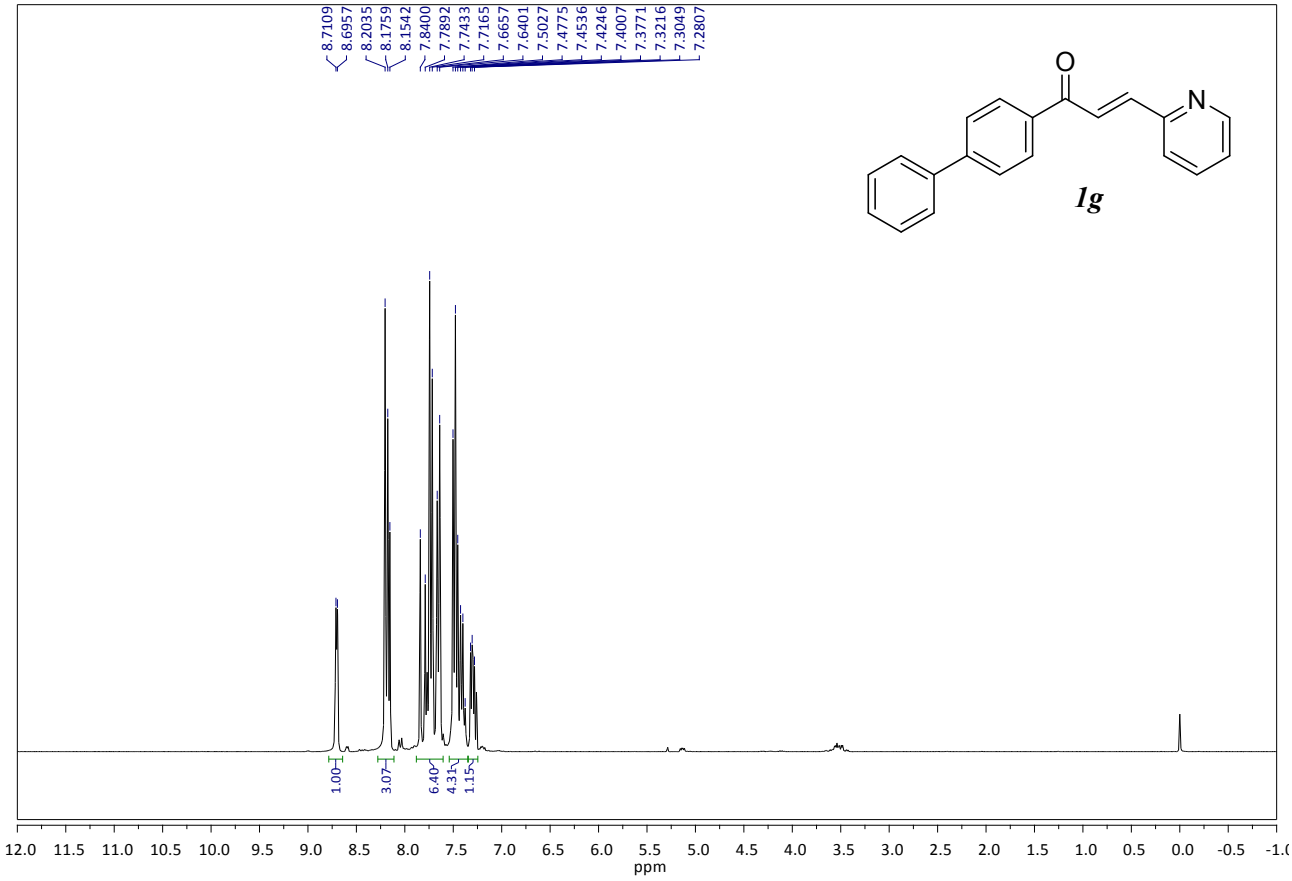
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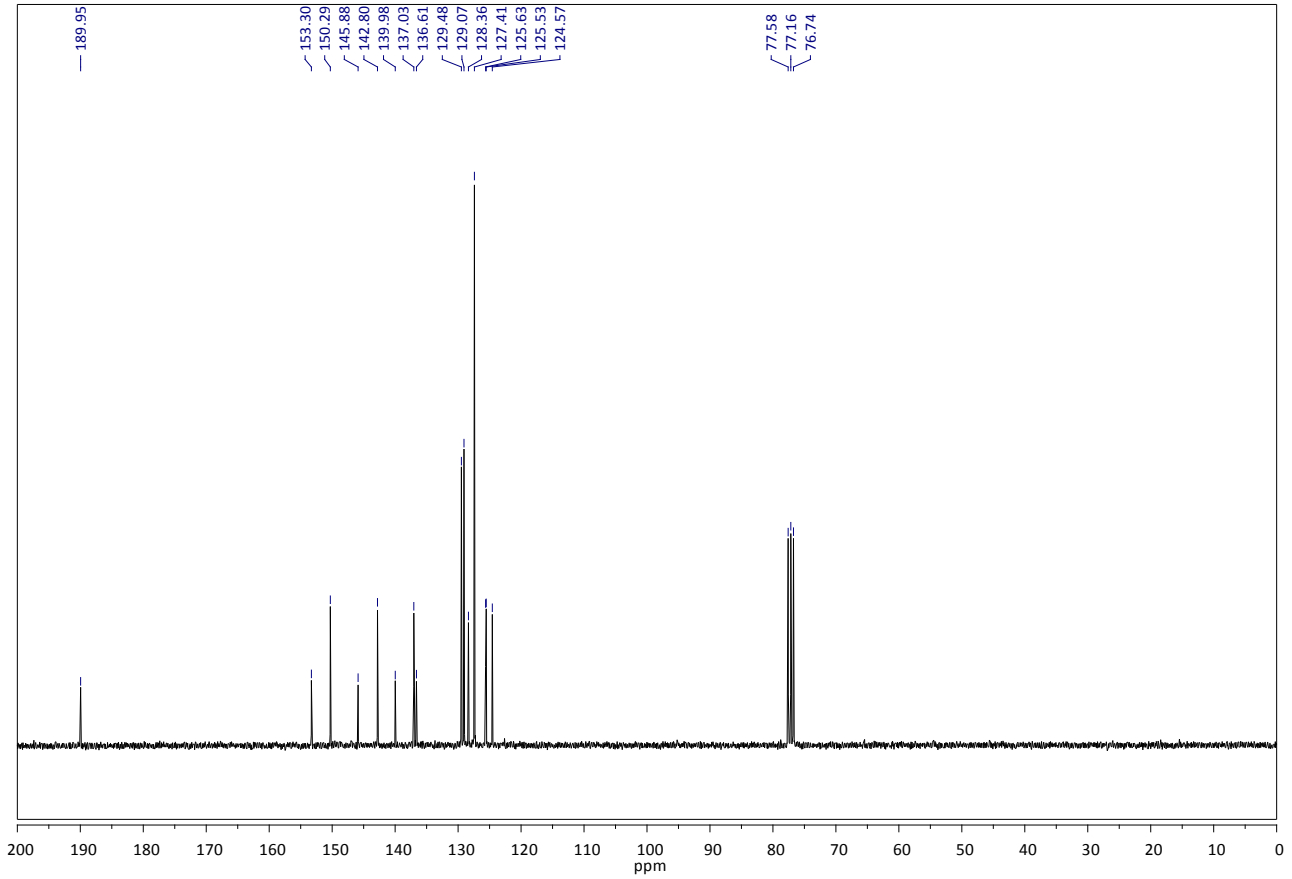
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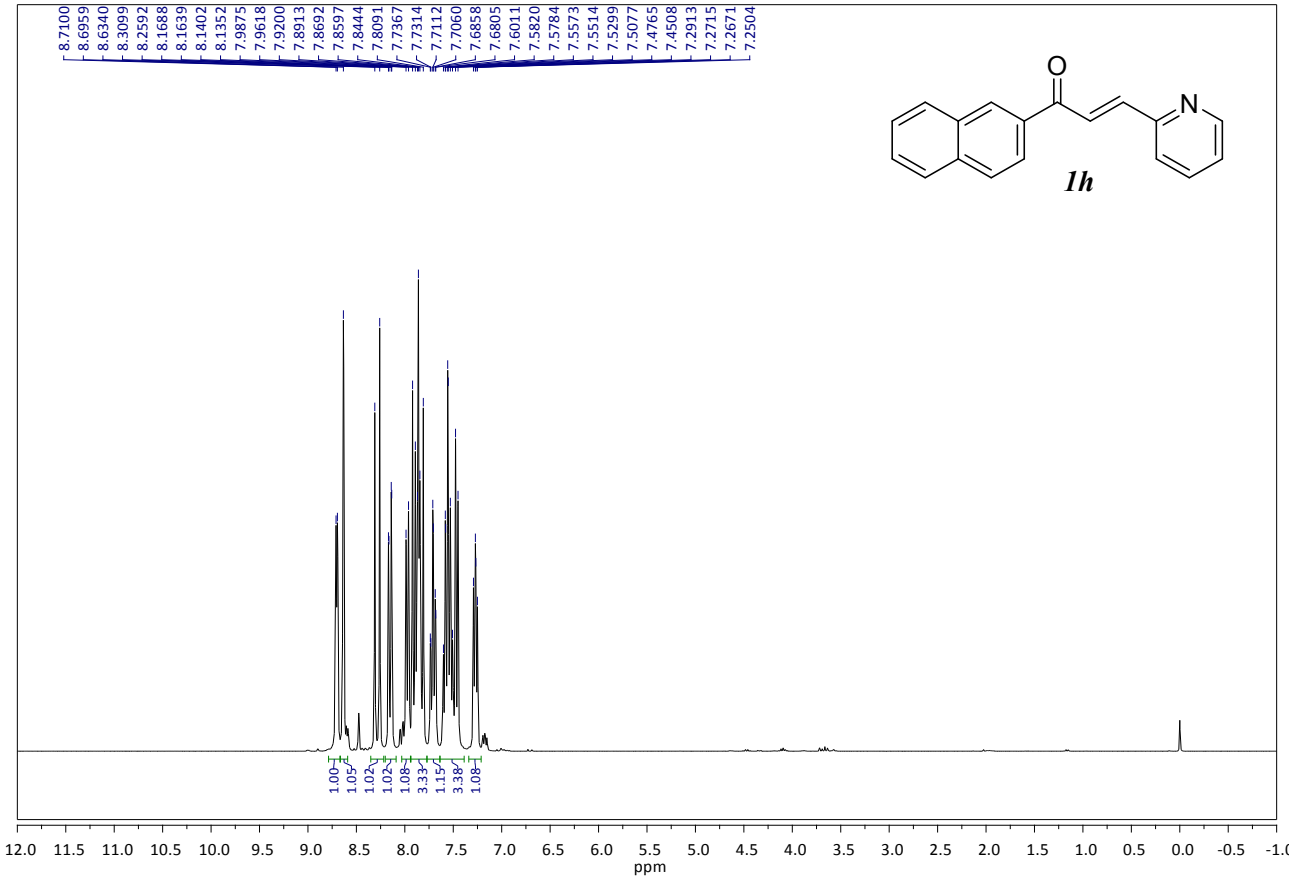
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1.02
1.08
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1.15
3.38
1.08
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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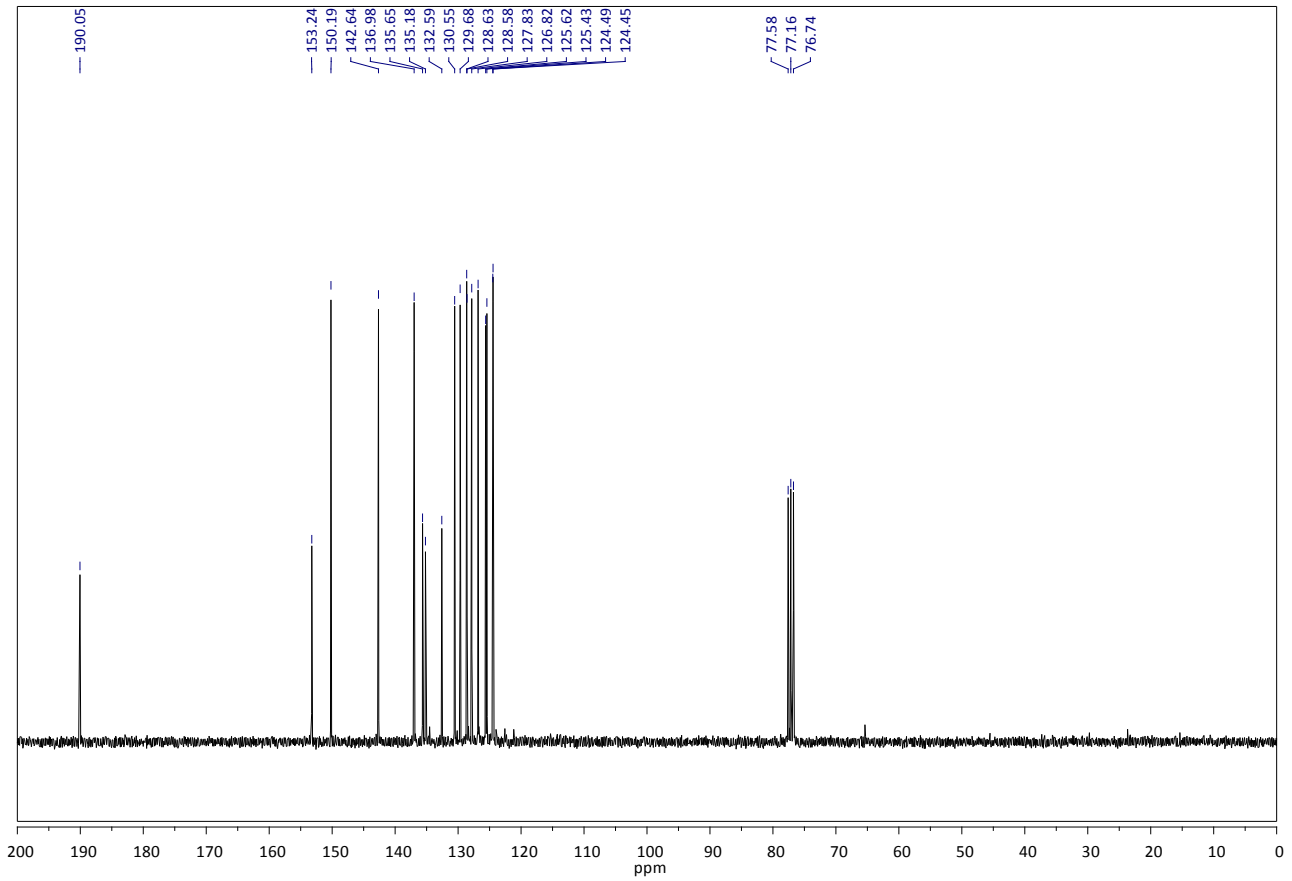
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77.16
76.74
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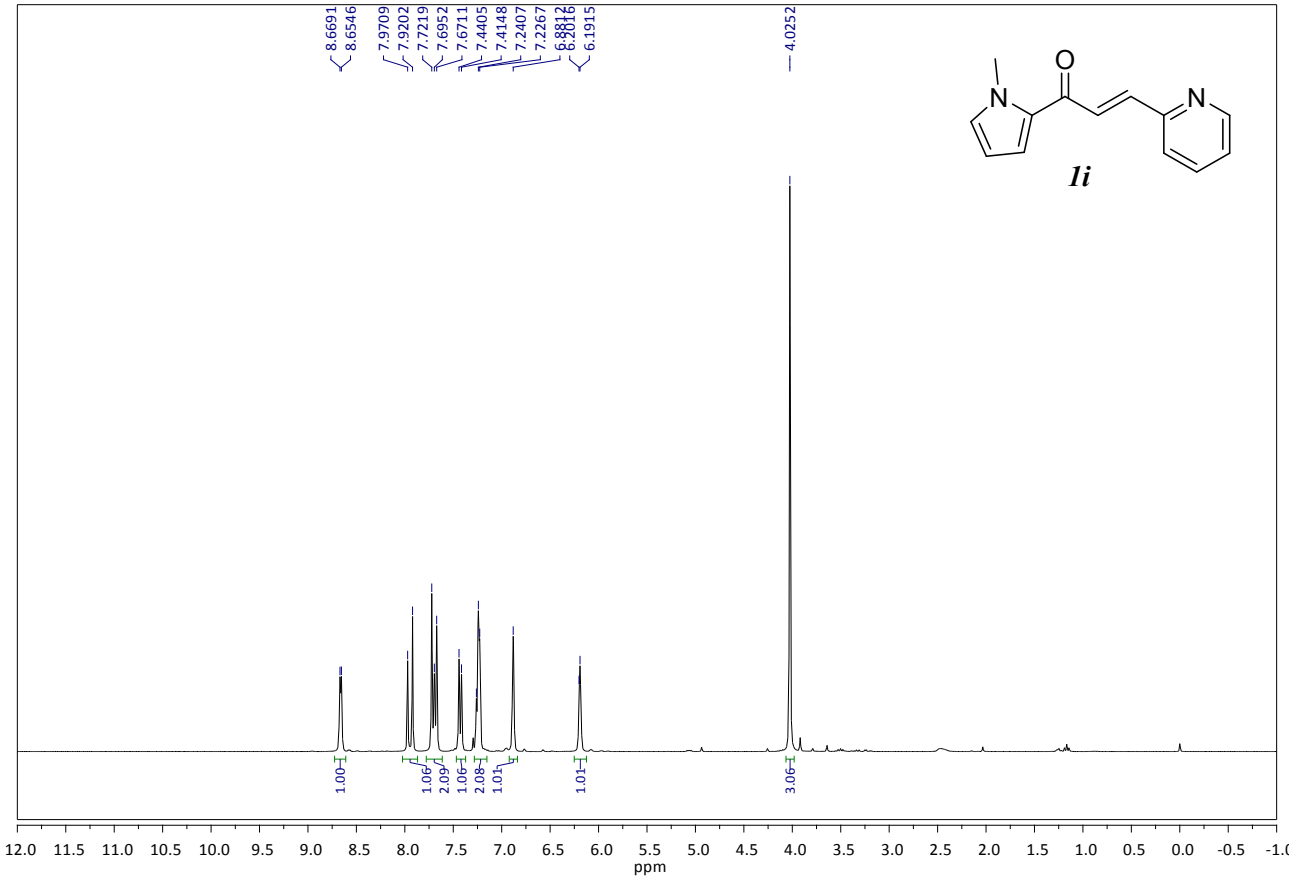
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6.8616
6.1915
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1.01
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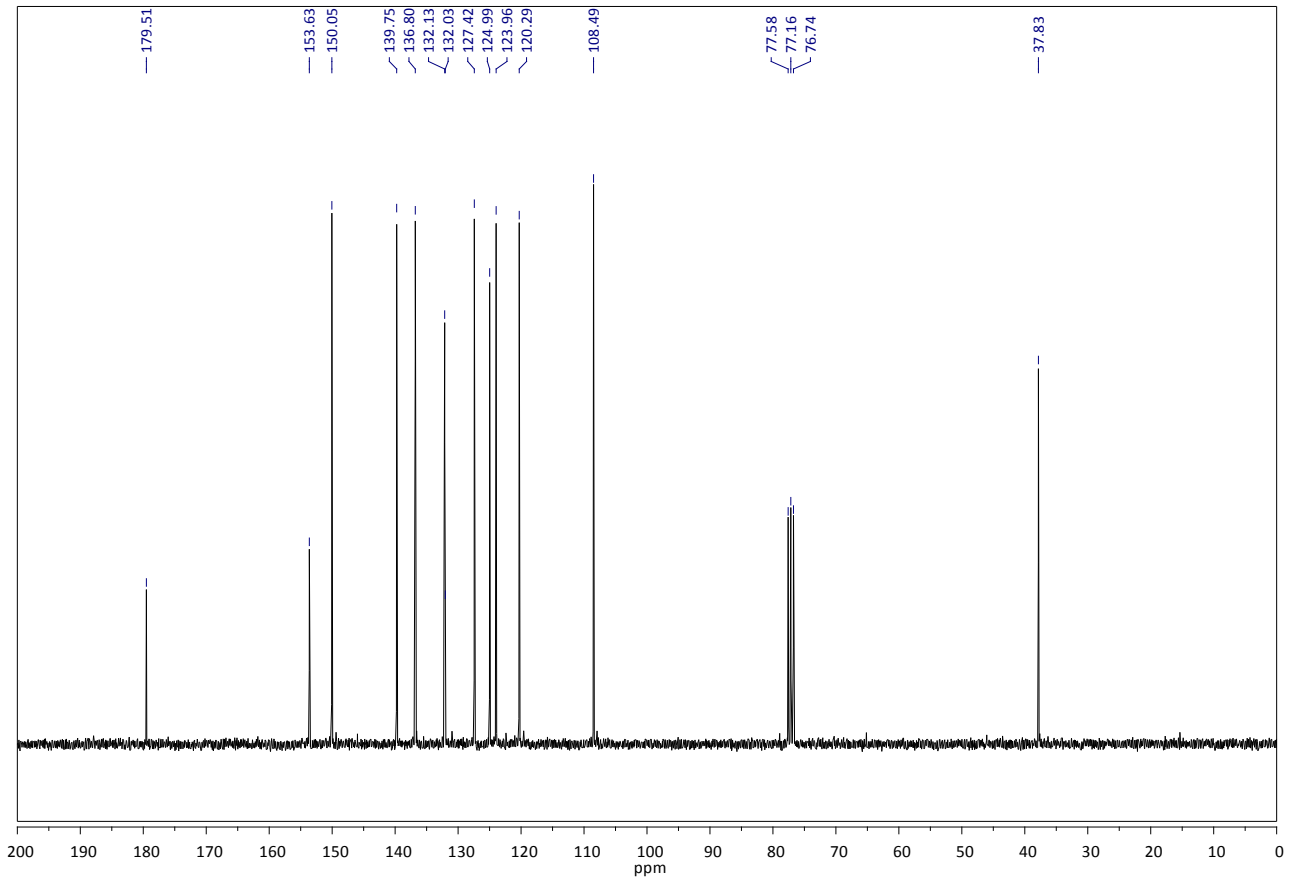
N
N
ppm

1i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37.83
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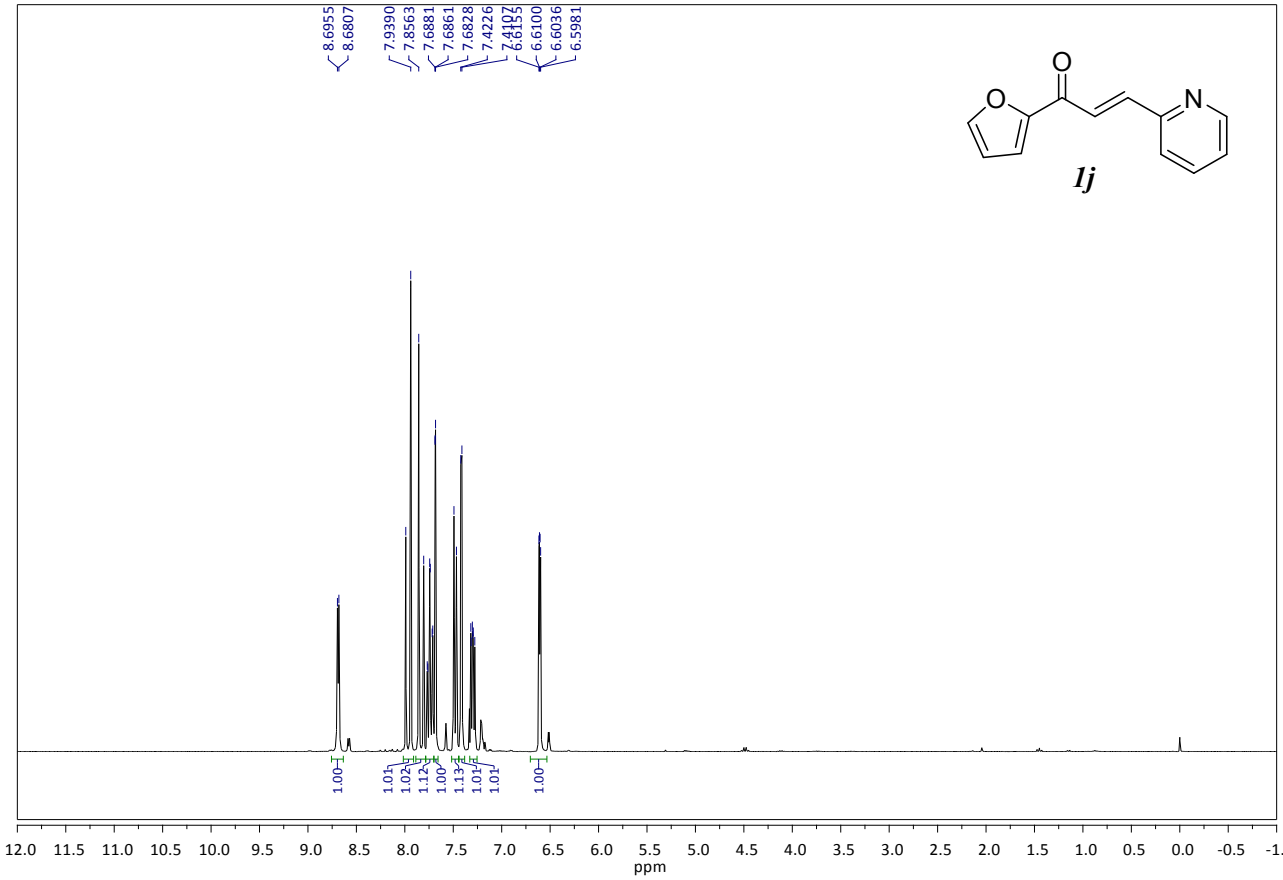
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1.12
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1.01
1.01
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O
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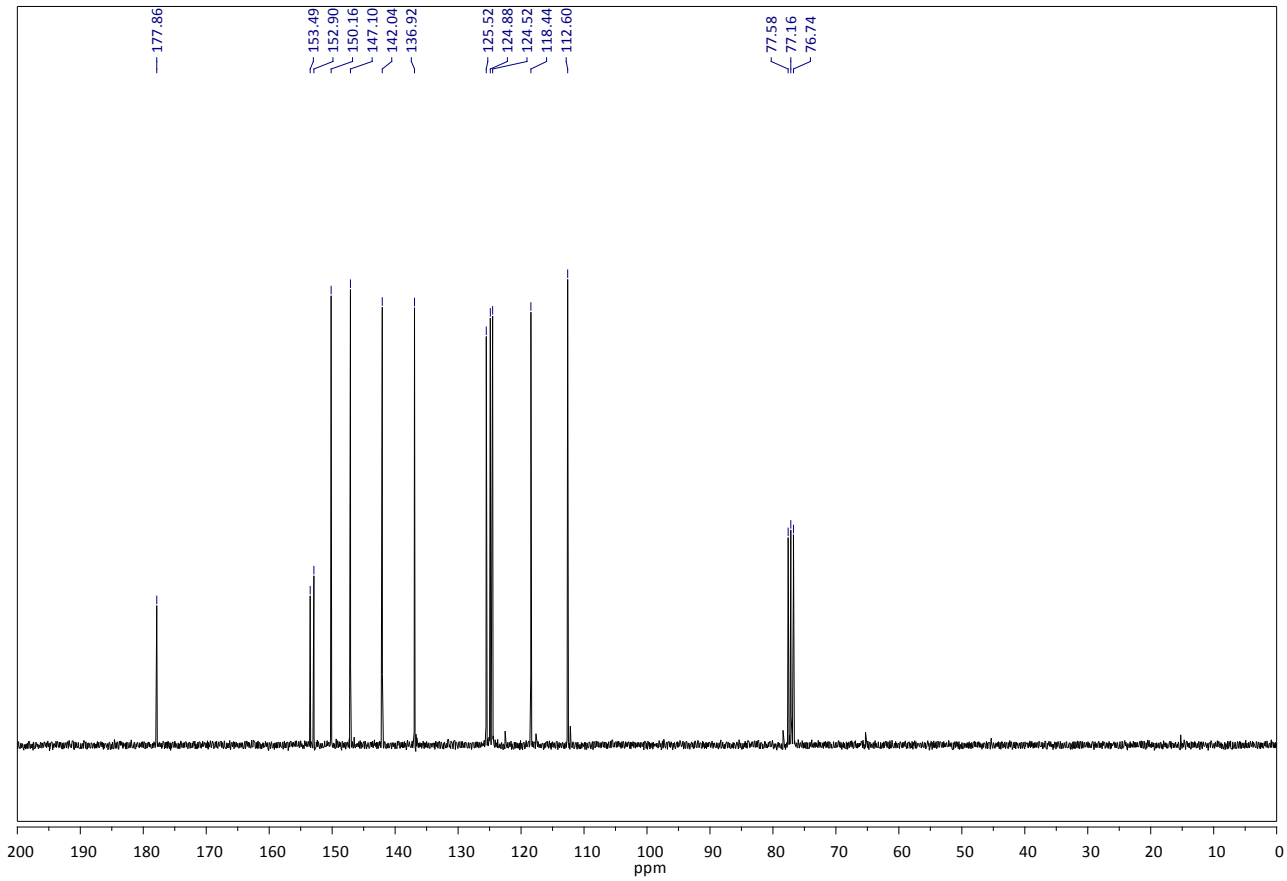
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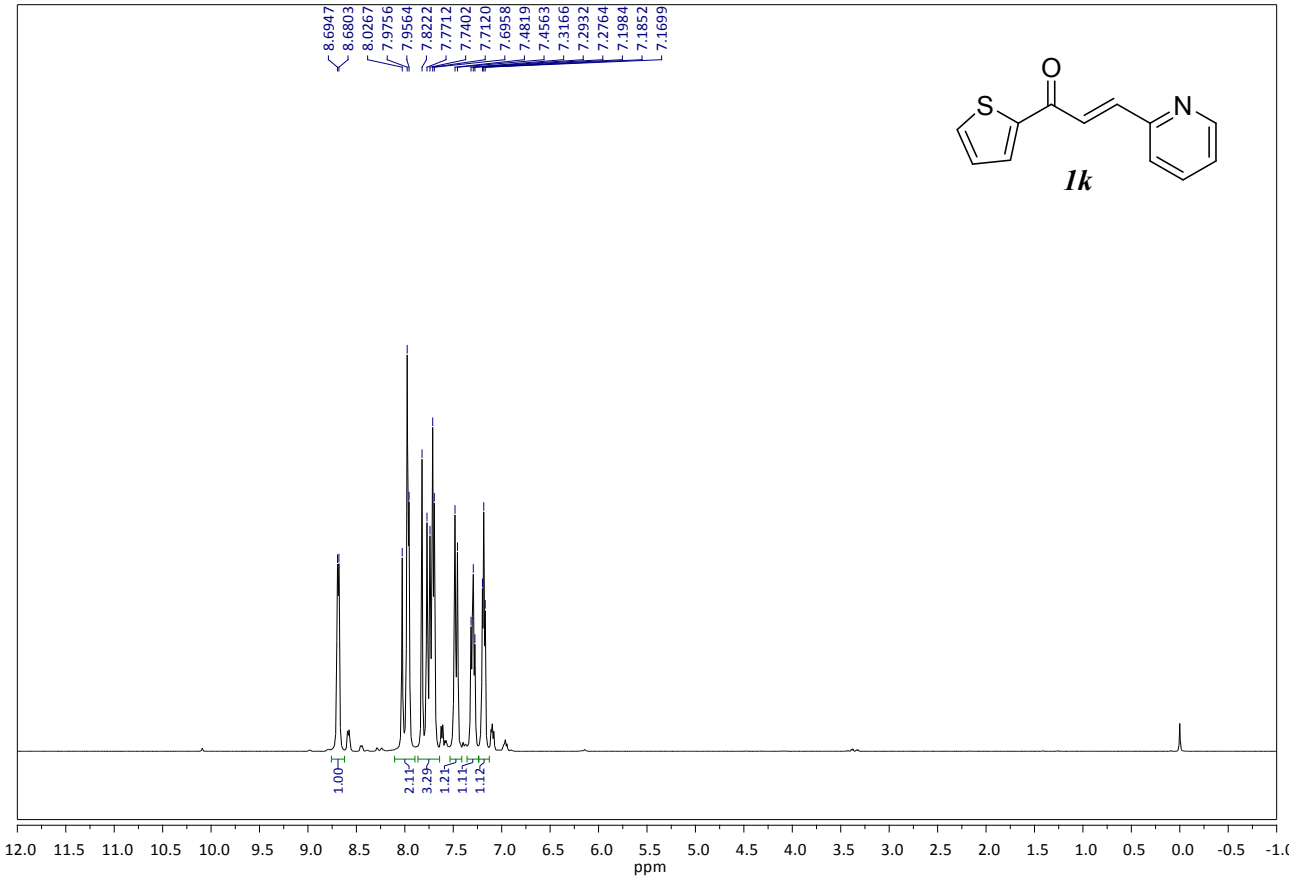
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7.1984
7.1852
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S
N
1k
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2.11
3.29
1.21
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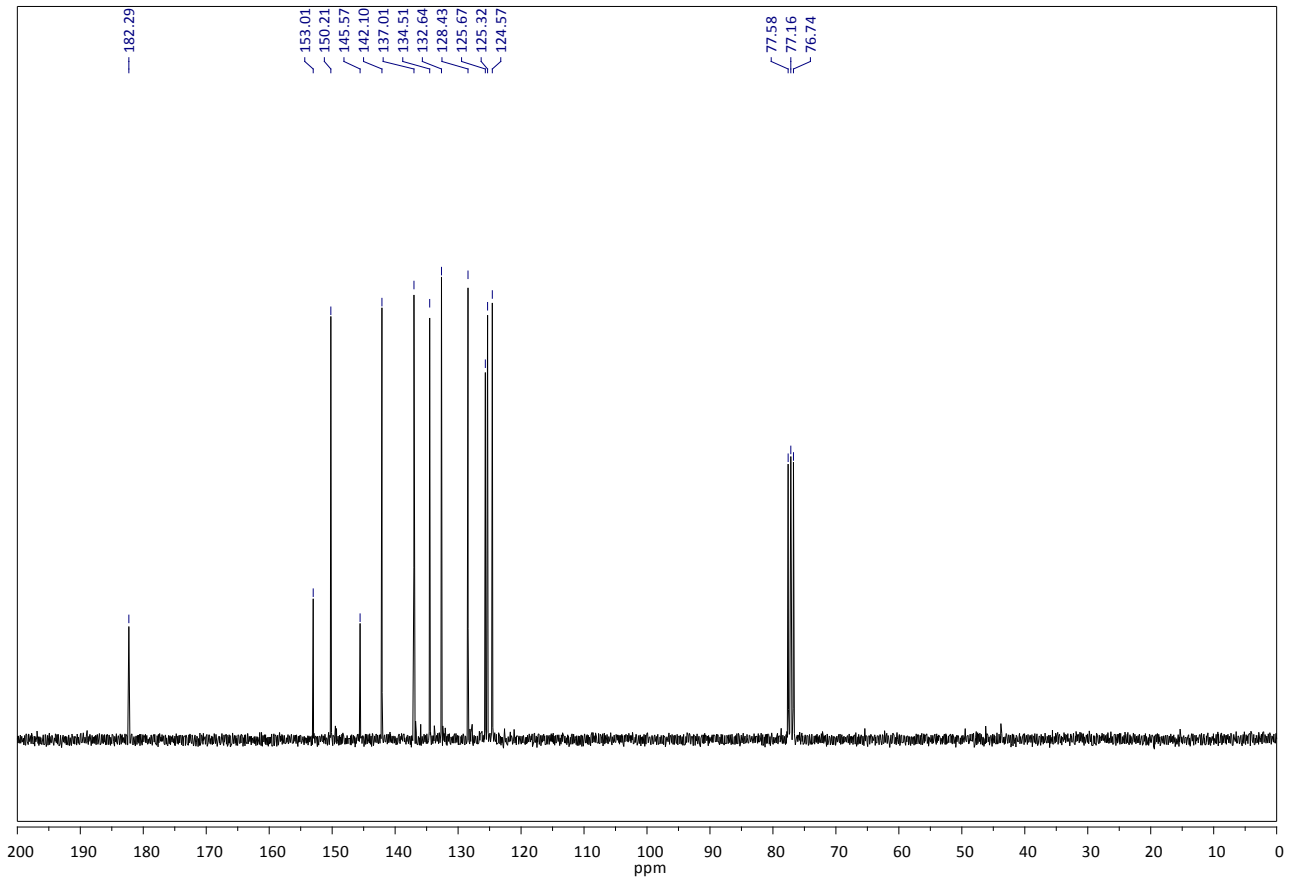
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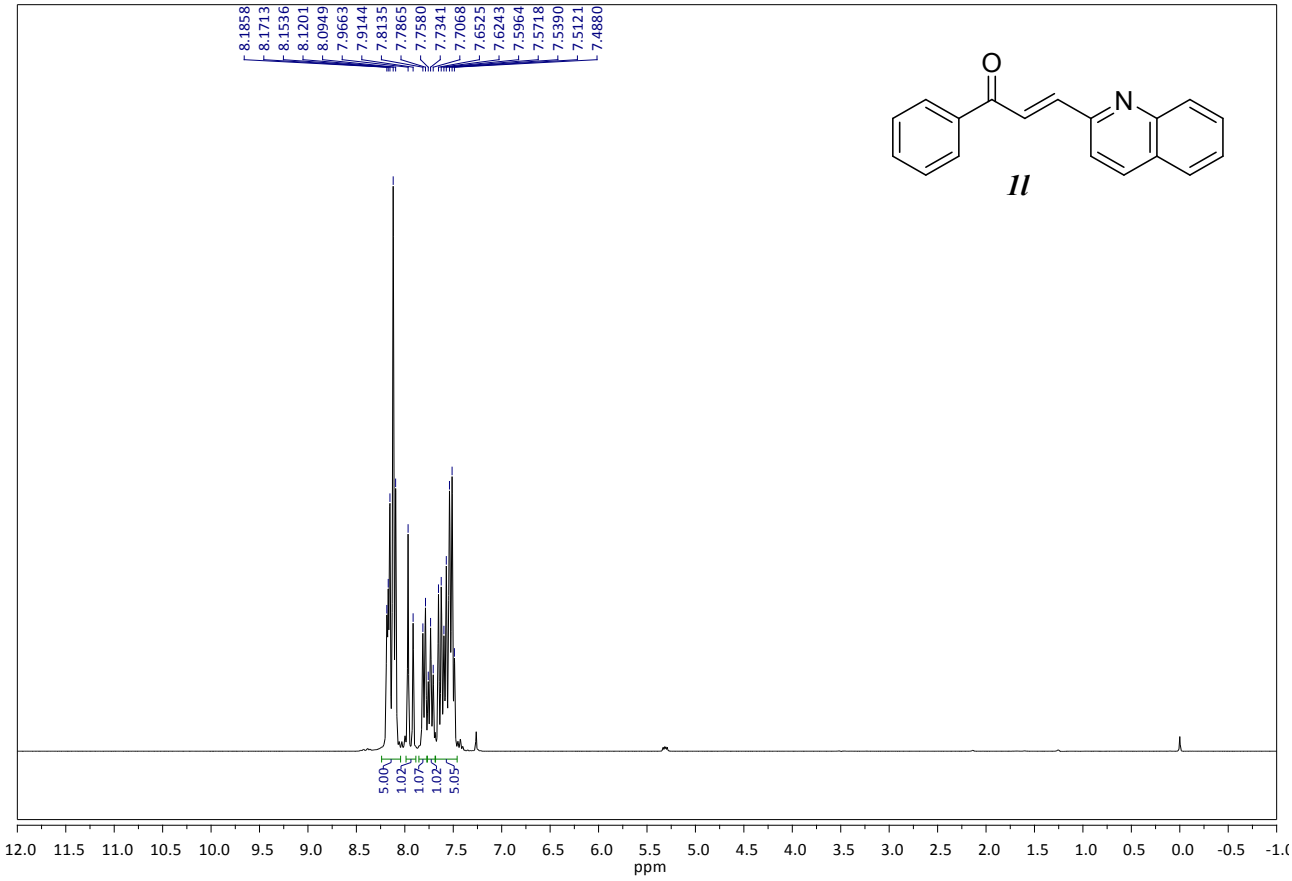
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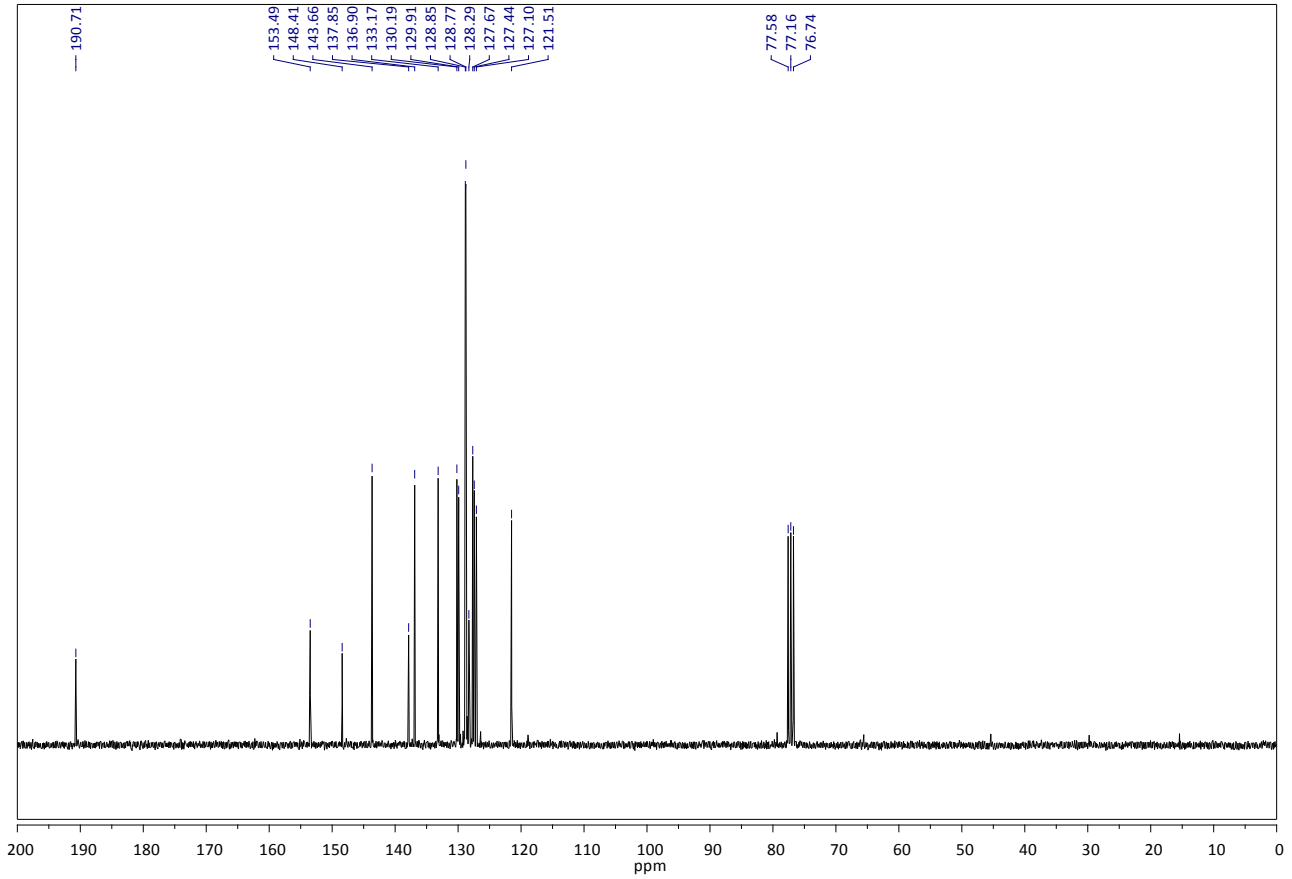
N
ppm

11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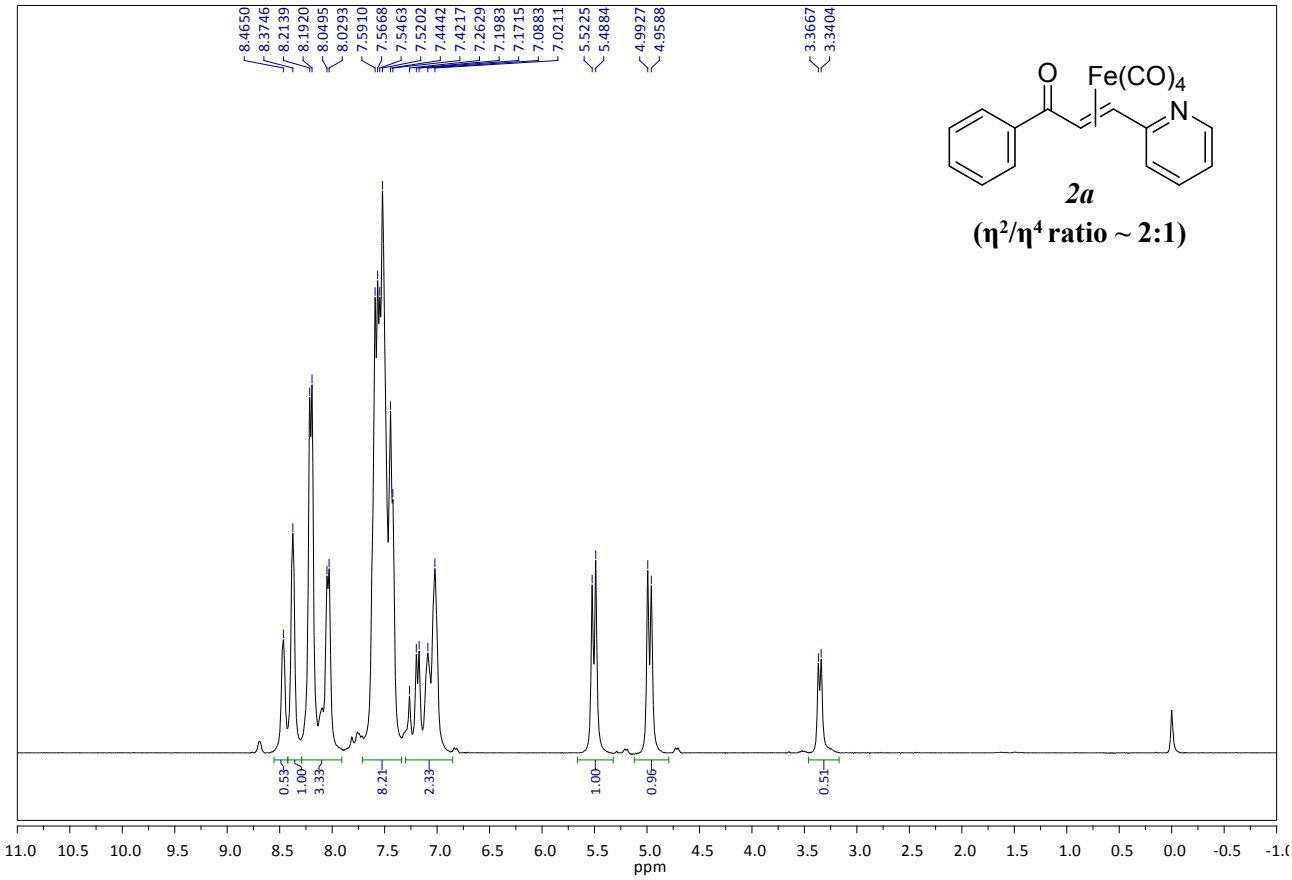
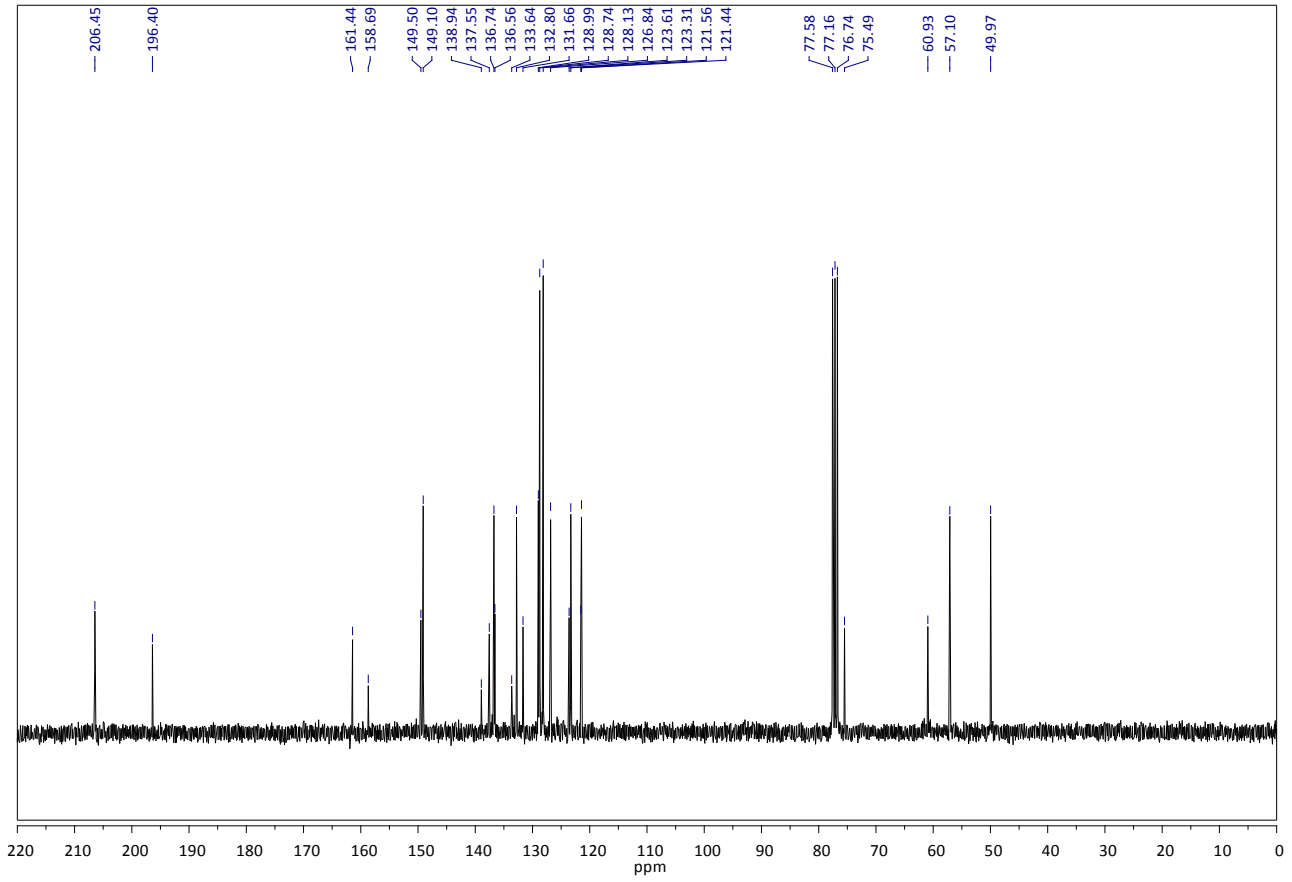
76.74
ppm

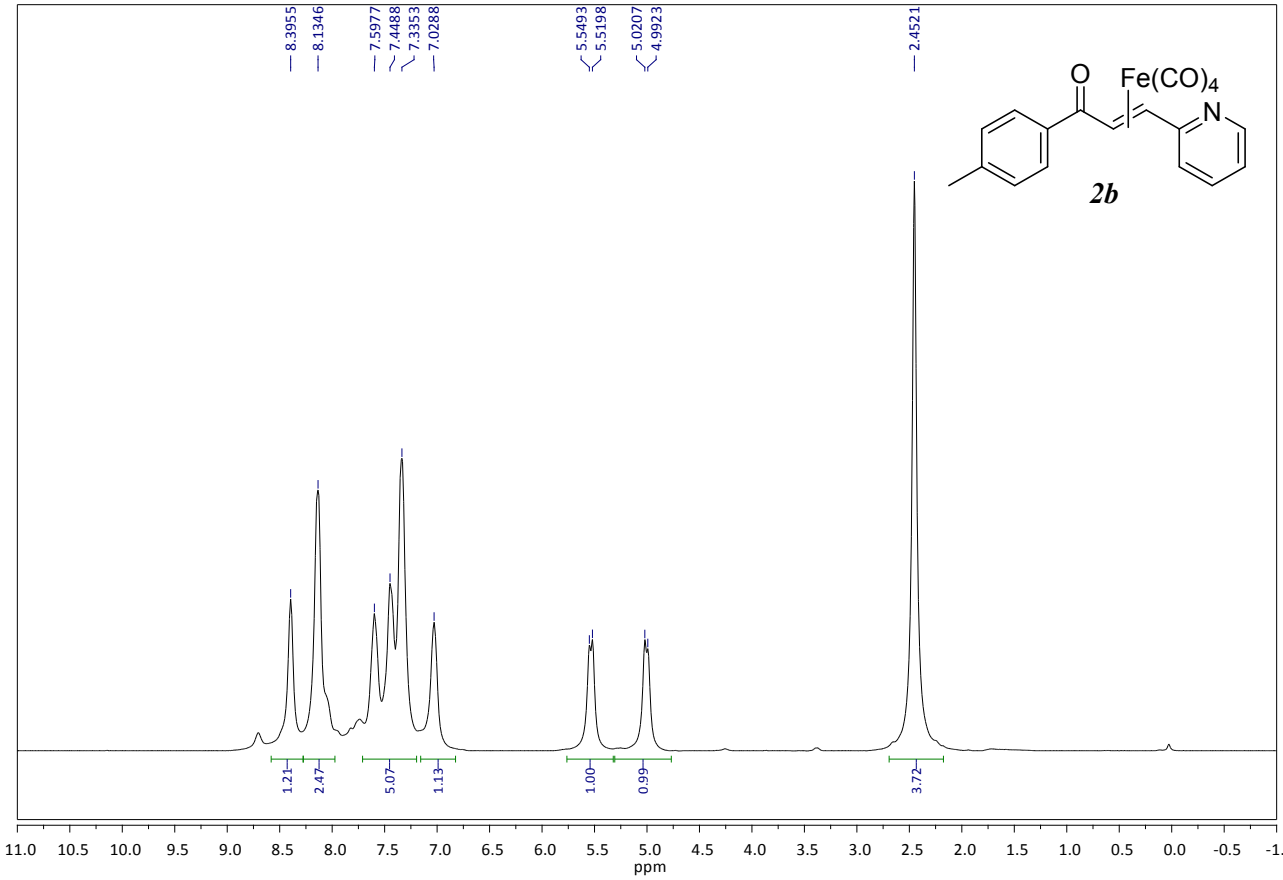
1.2 Spectra of compounds 2a-l.



2a

(η^2/η^4 ratio ~ 2:1)

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Fe(CO)4
N
2b
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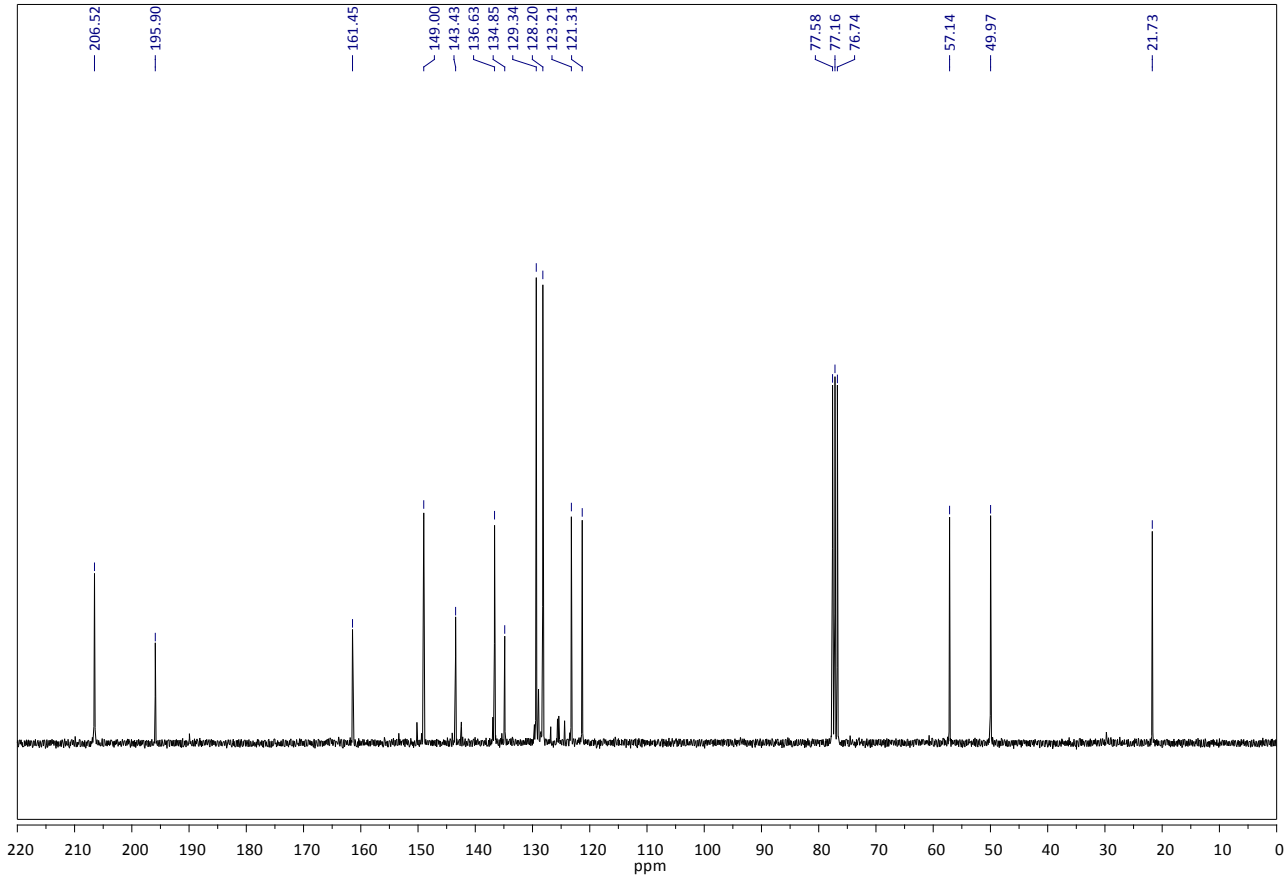
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77.16
76.74
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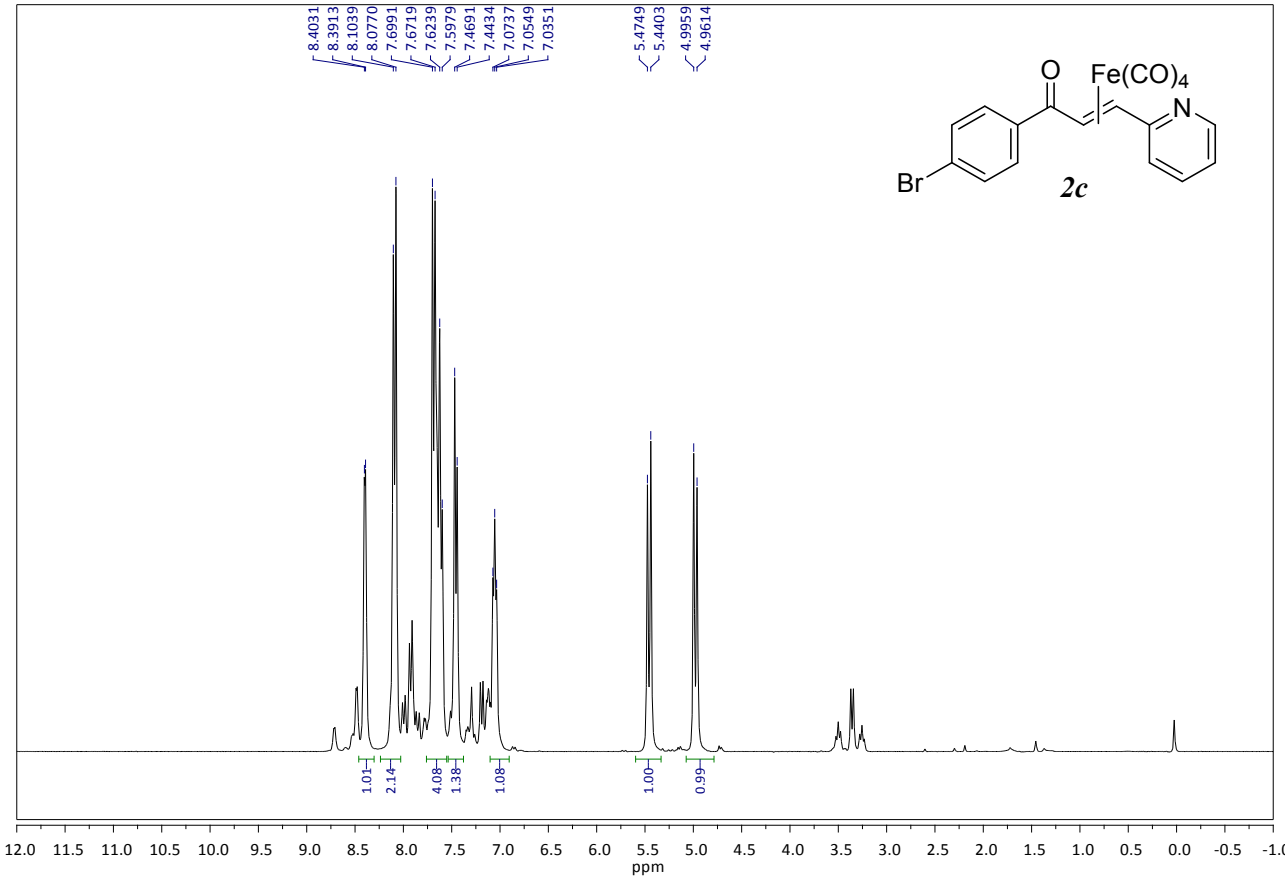
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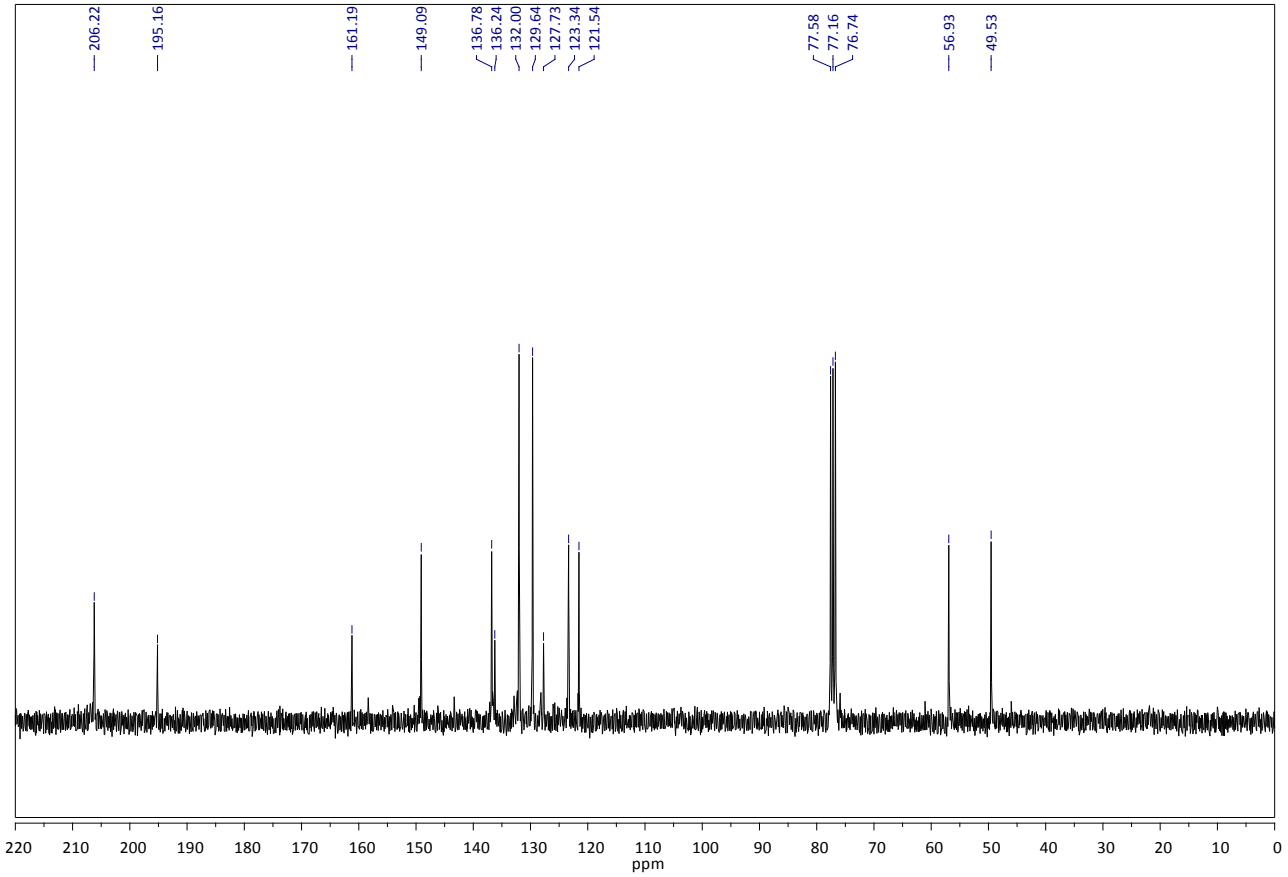
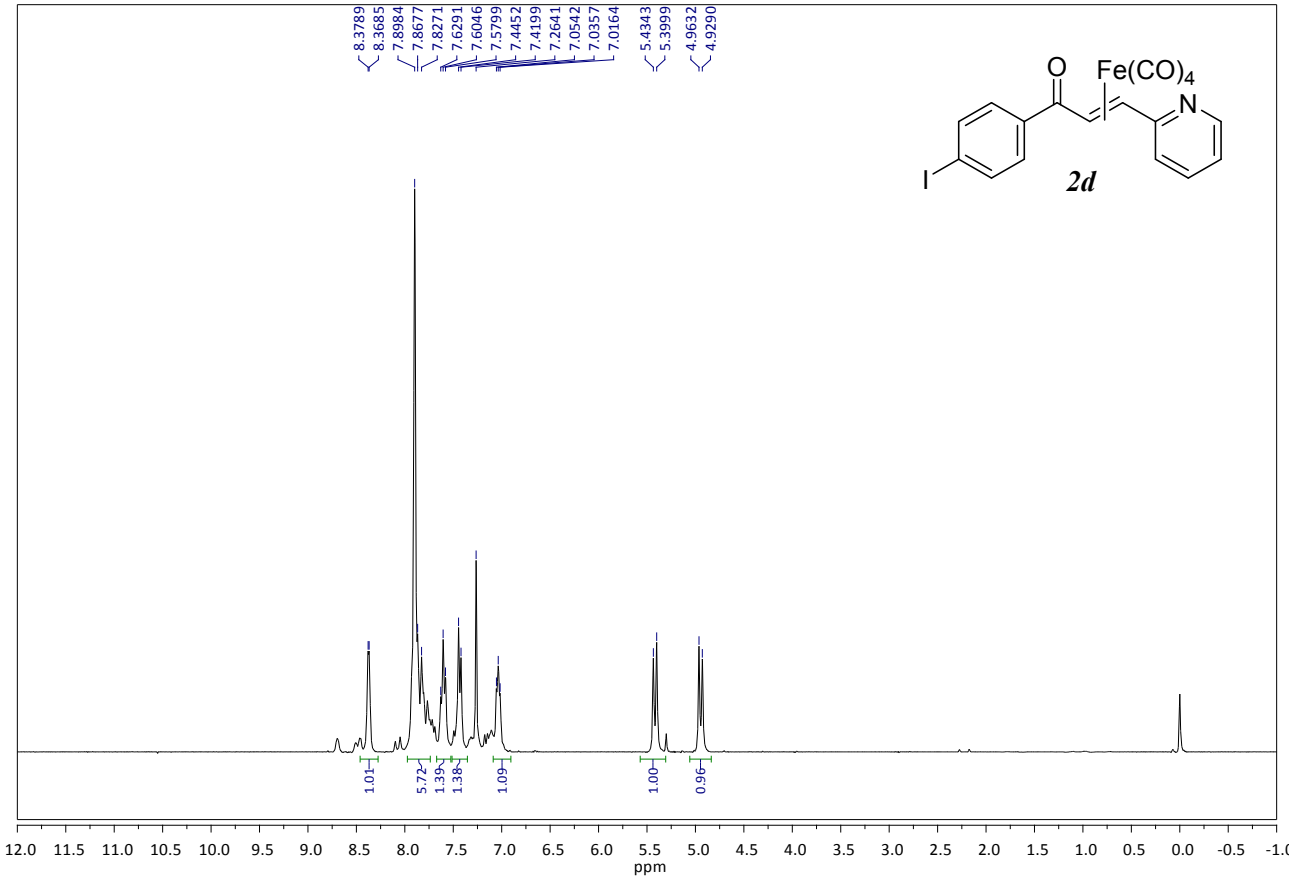
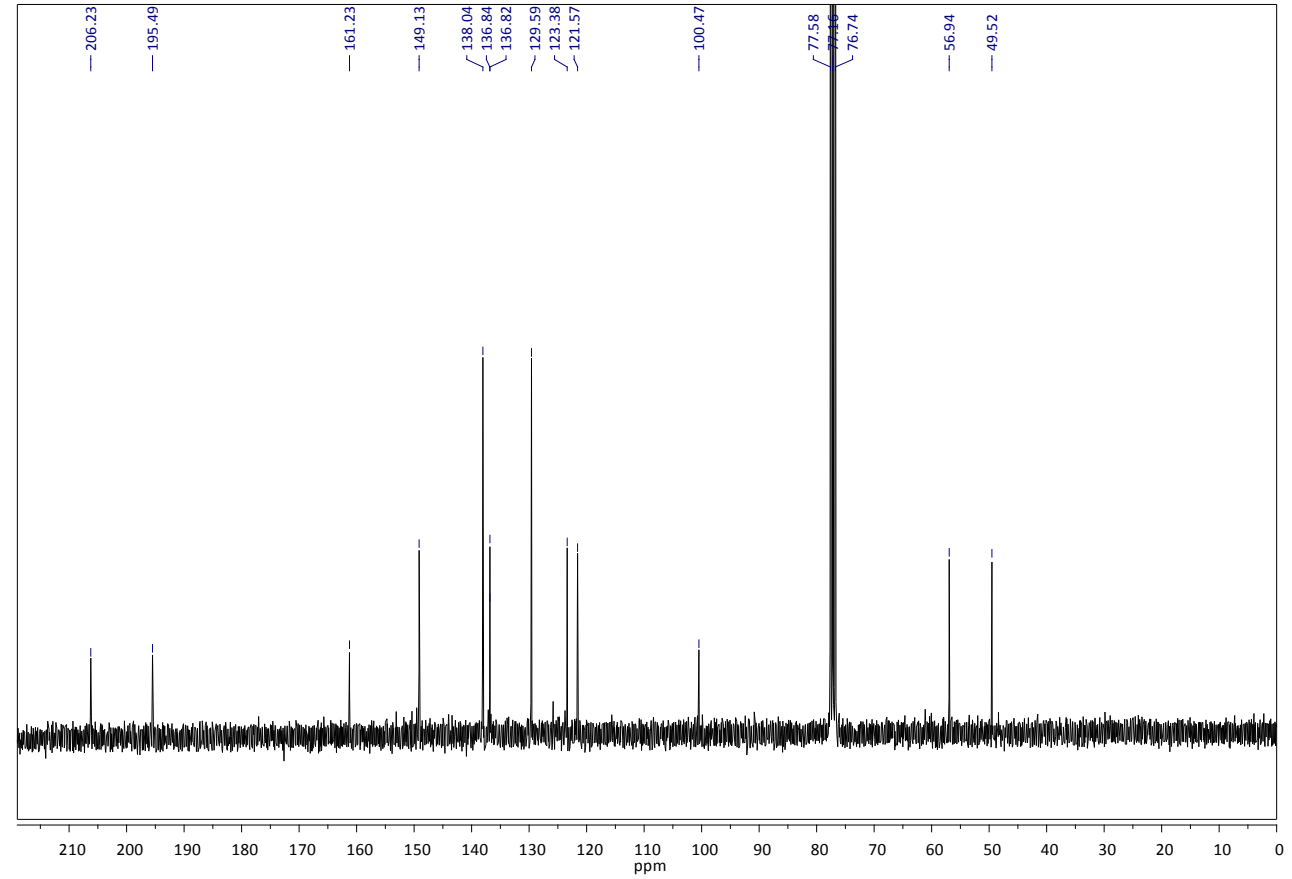
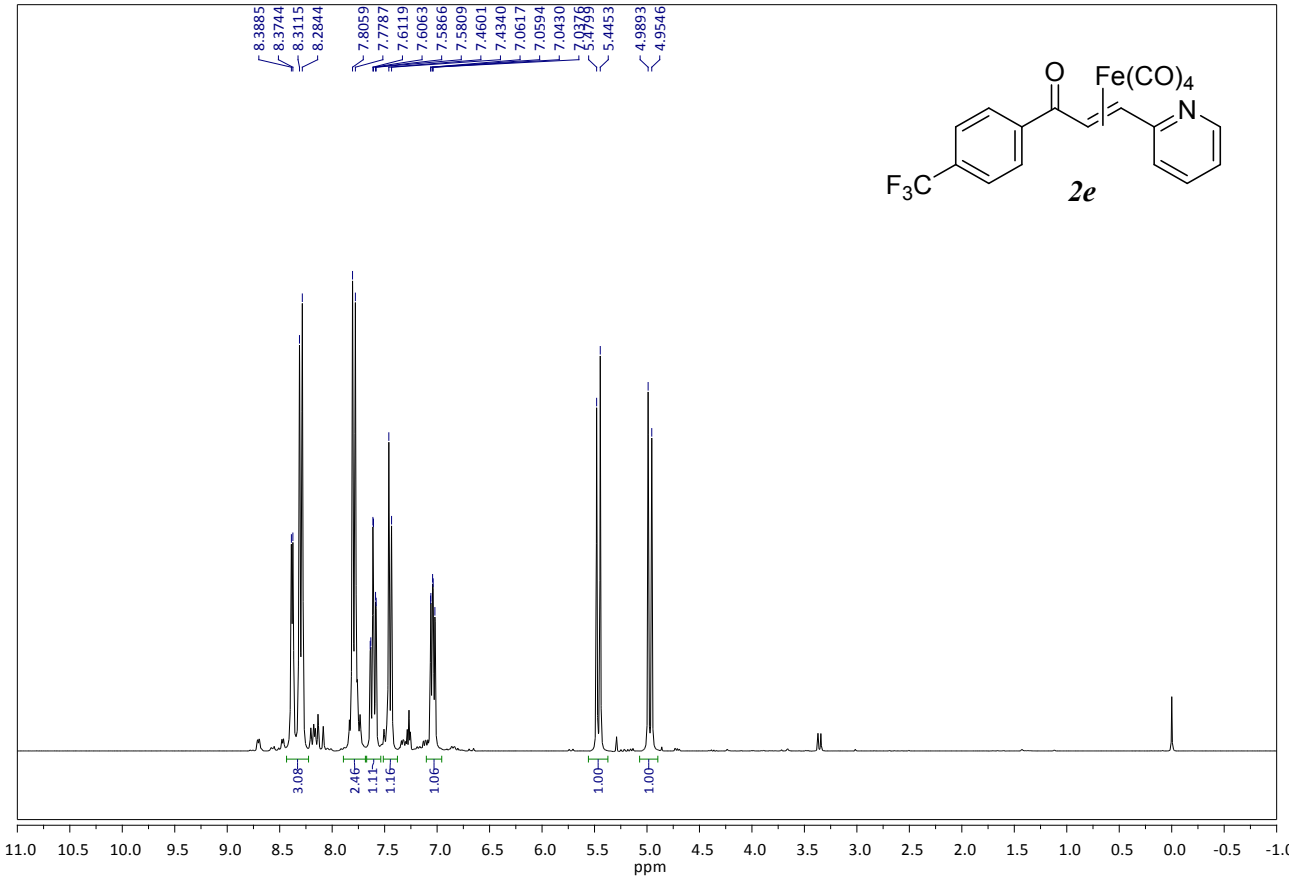
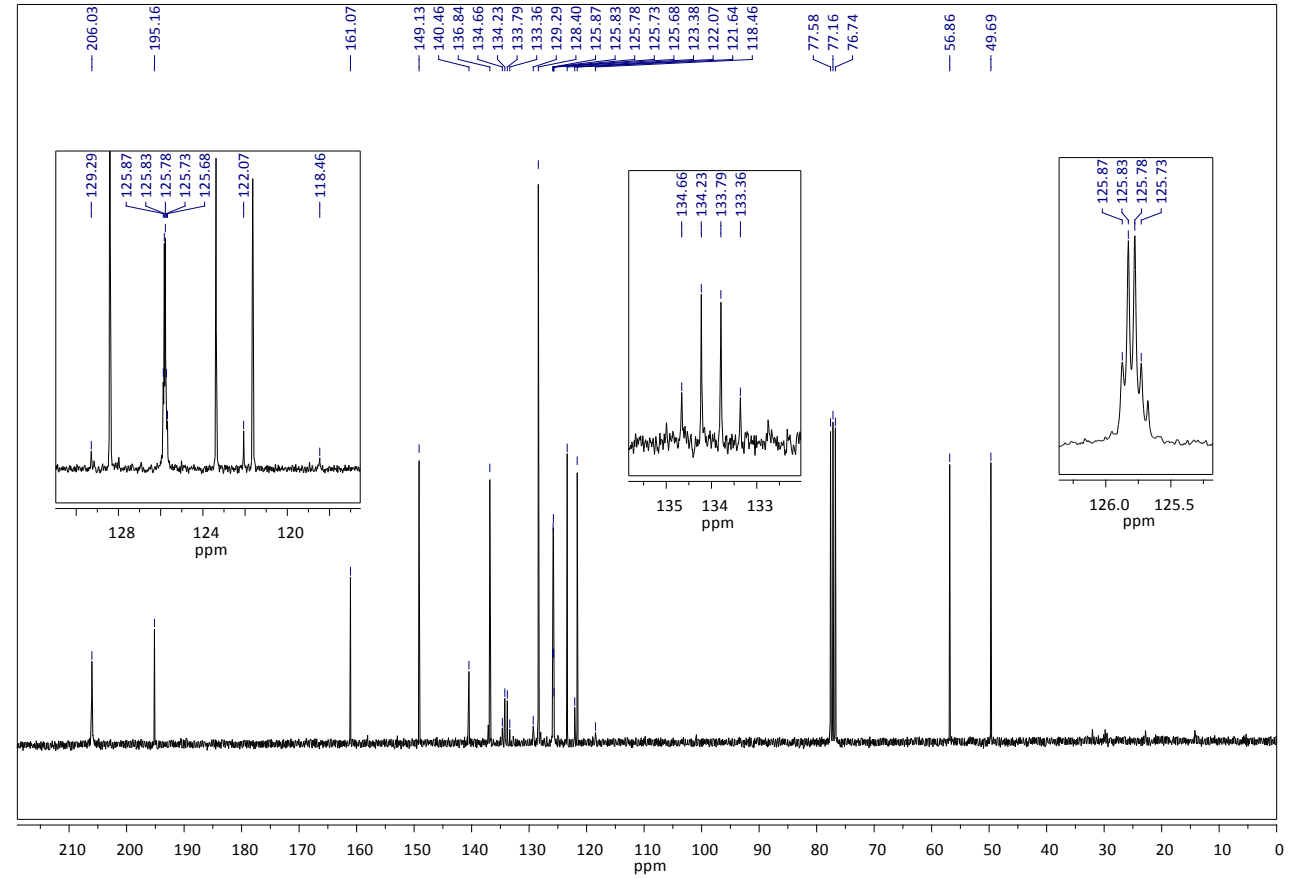
Fe(CO)4
N
Br
2c
ppm

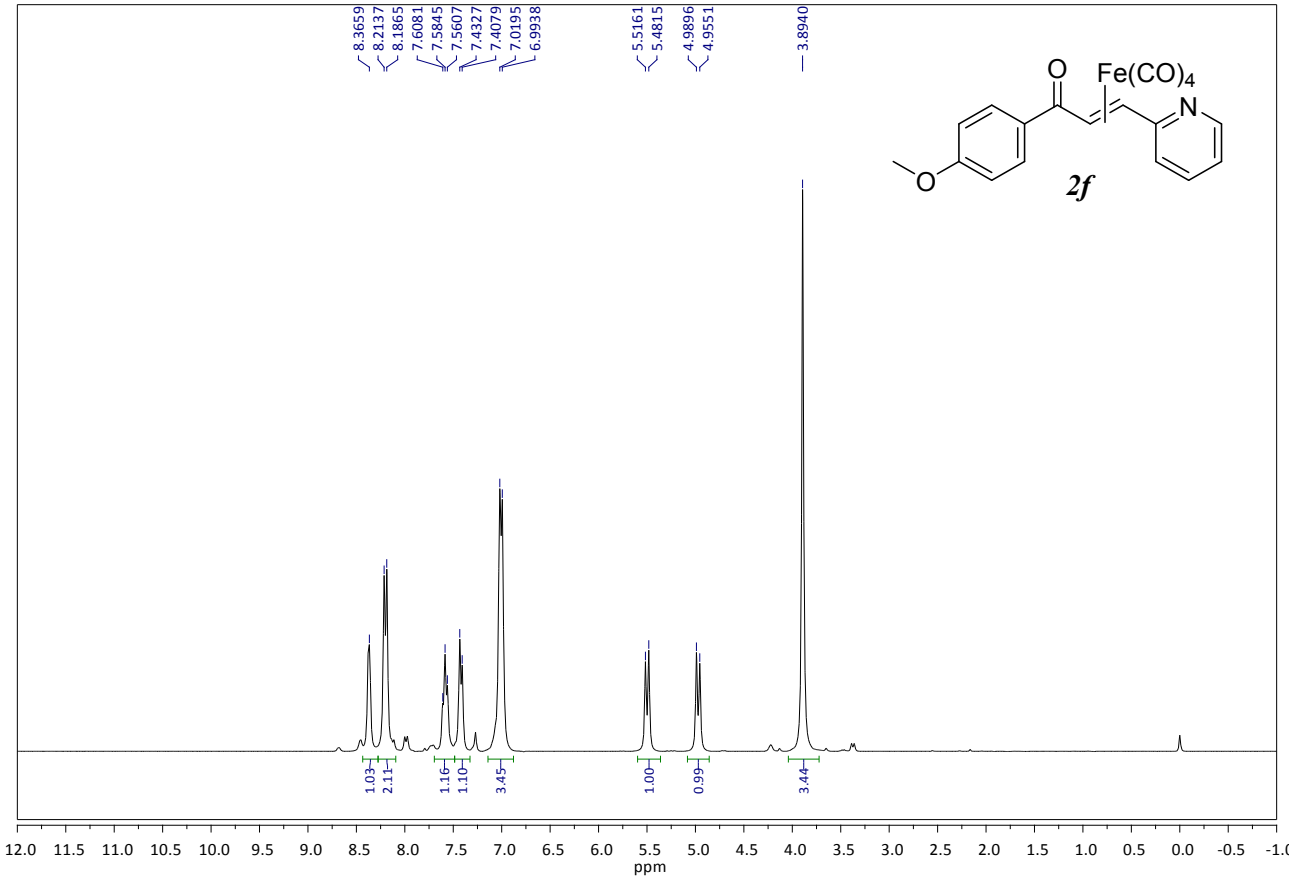

206.22
195.16
161.19
149.09
136.78
136.24
132.00
129.64
127.73
123.34
121.54
77.58
77.16
76.74
56.93
49.53
ppm

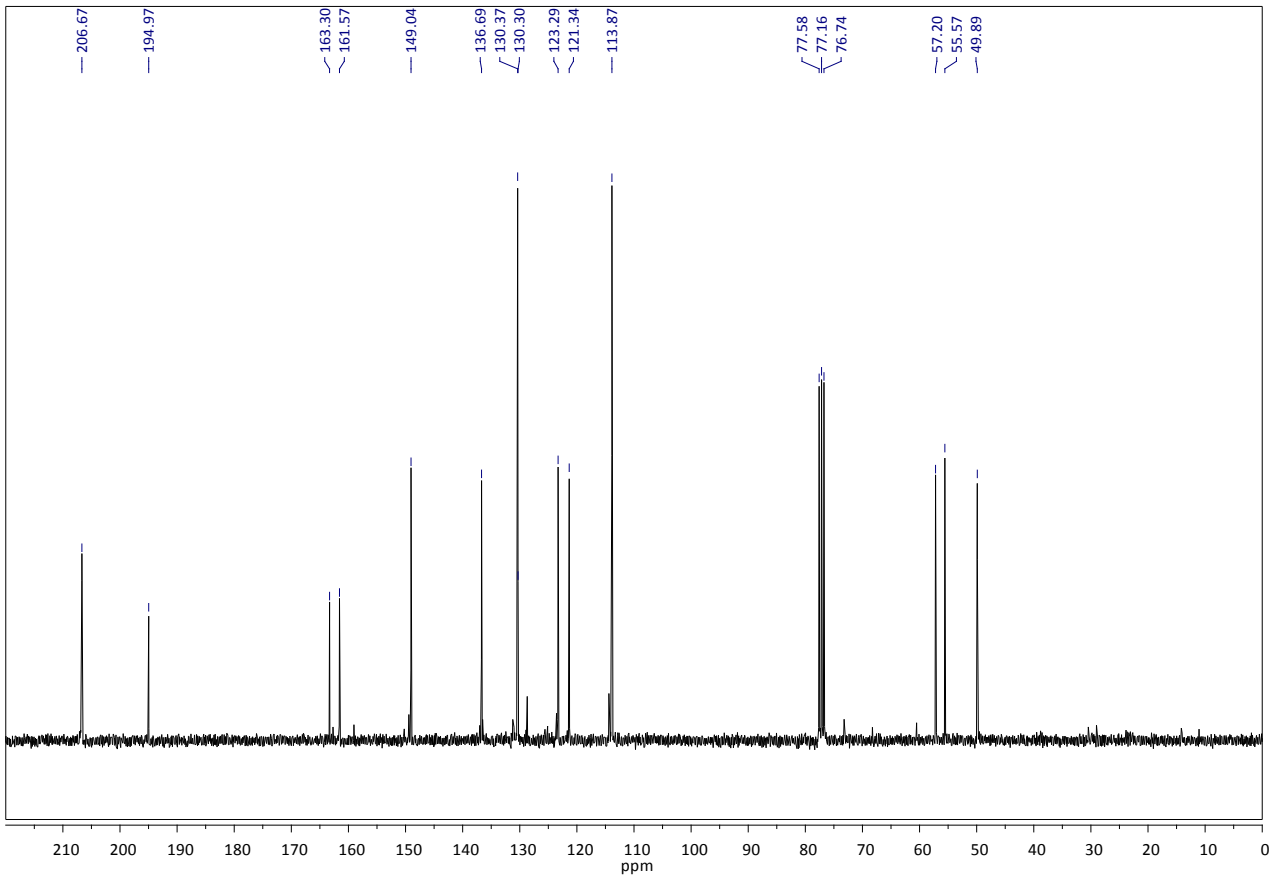

8.3789
8.3685
7.8984
7.8677
7.8271
7.6291
7.6046
7.5799
7.4452
7.4199
7.2641
7.0542
7.0357
7.0164
5.4343
5.3999
4.9632
4.9290
1.01
5.72
1.39
1.38
1.09
1.00
0.96
O
Fe(CO)4
N
I
2d
ppm

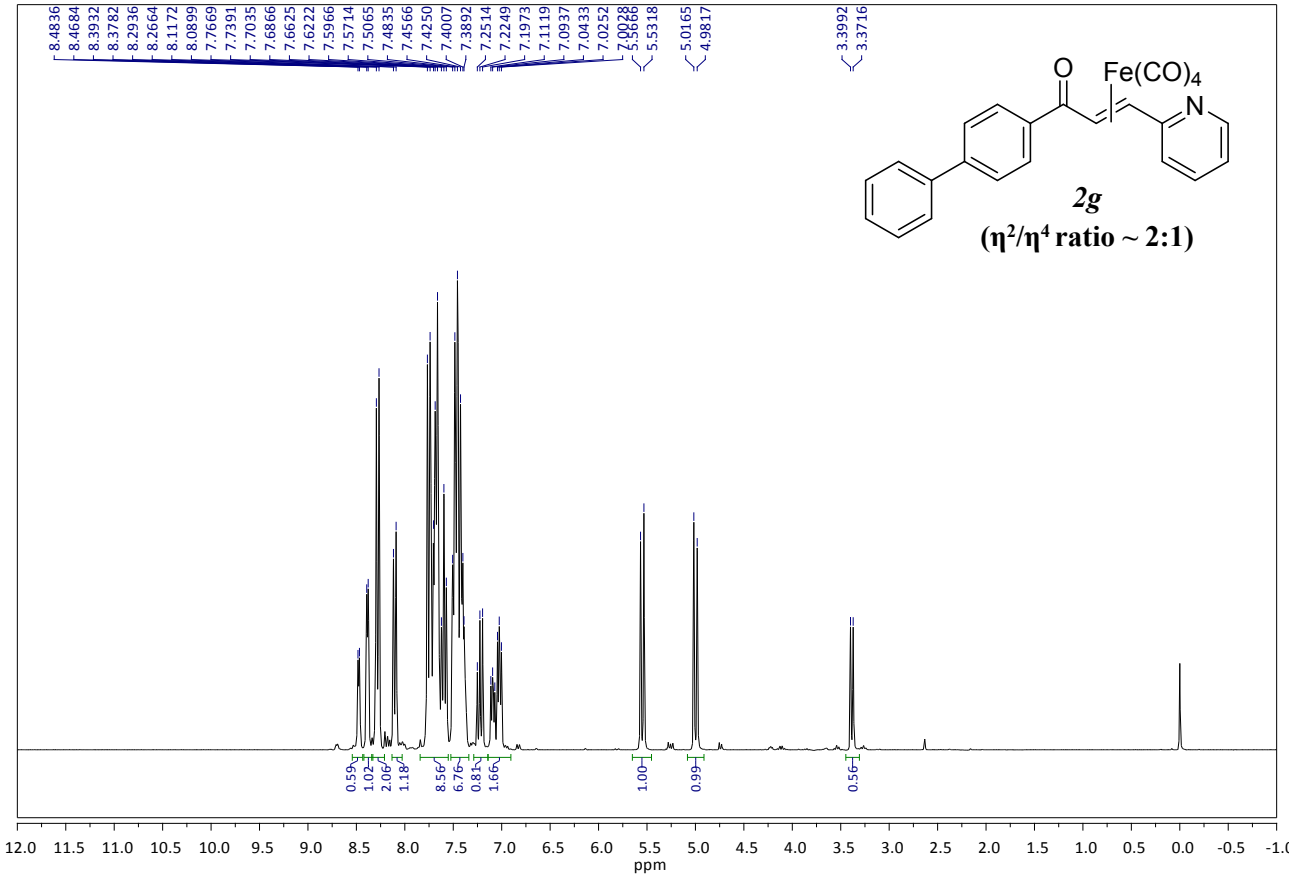

206.23
195.49
161.23
149.13
138.04
136.84
136.82
129.59
123.38
121.57
100.47
77.58
77.16
76.74
56.94
49.52
ppm

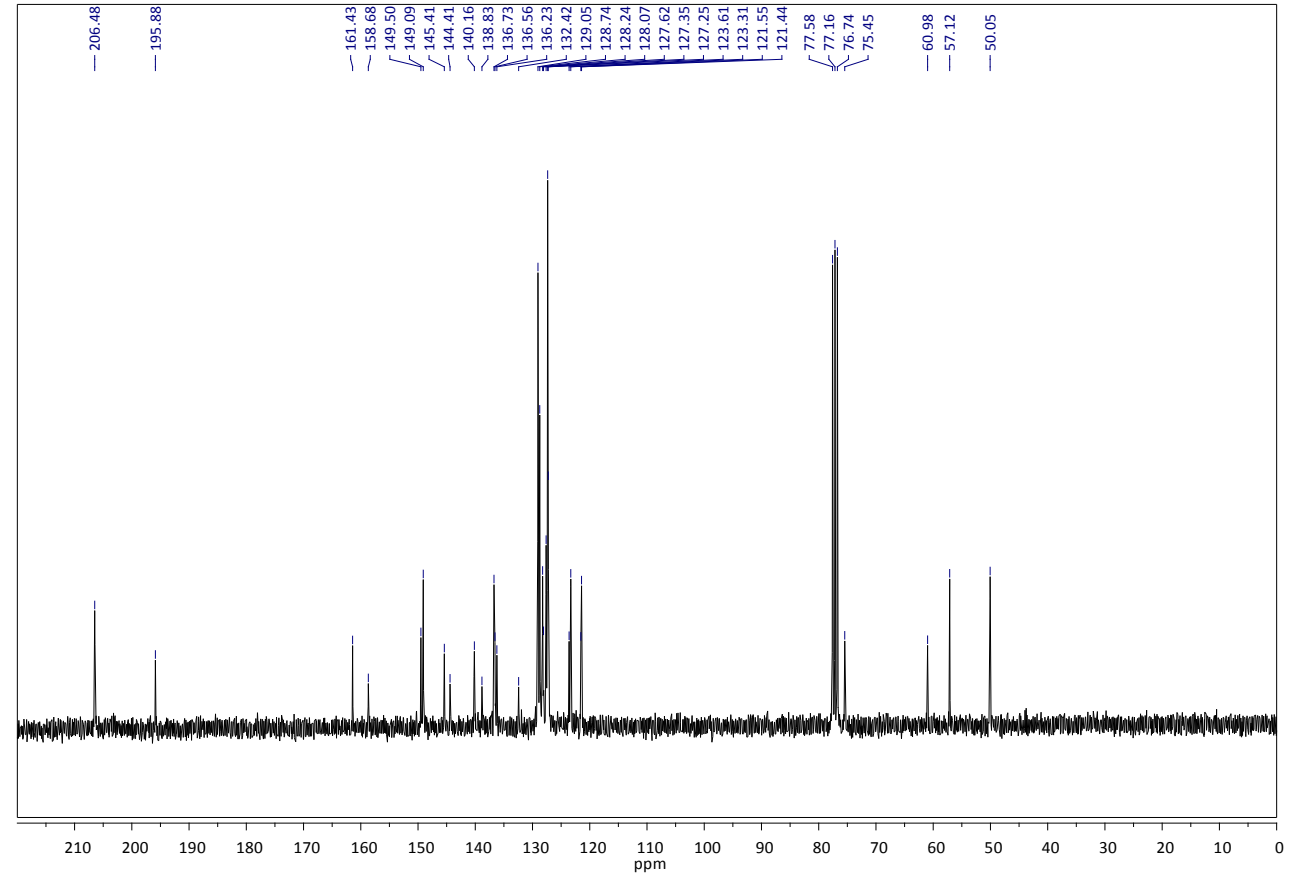

8.3885
8.3744
8.3115
8.2844
7.8059
7.7787
7.6119
7.6063
7.5866
7.5809
7.4601
7.4340
7.0617
7.0594
7.0430
5.4799
5.4453
4.9893
4.9546
3.08
2.46
1.11
1.16
1.06
1.00
1.00
O
Fe(CO)4
N
F3C
2e
ppm

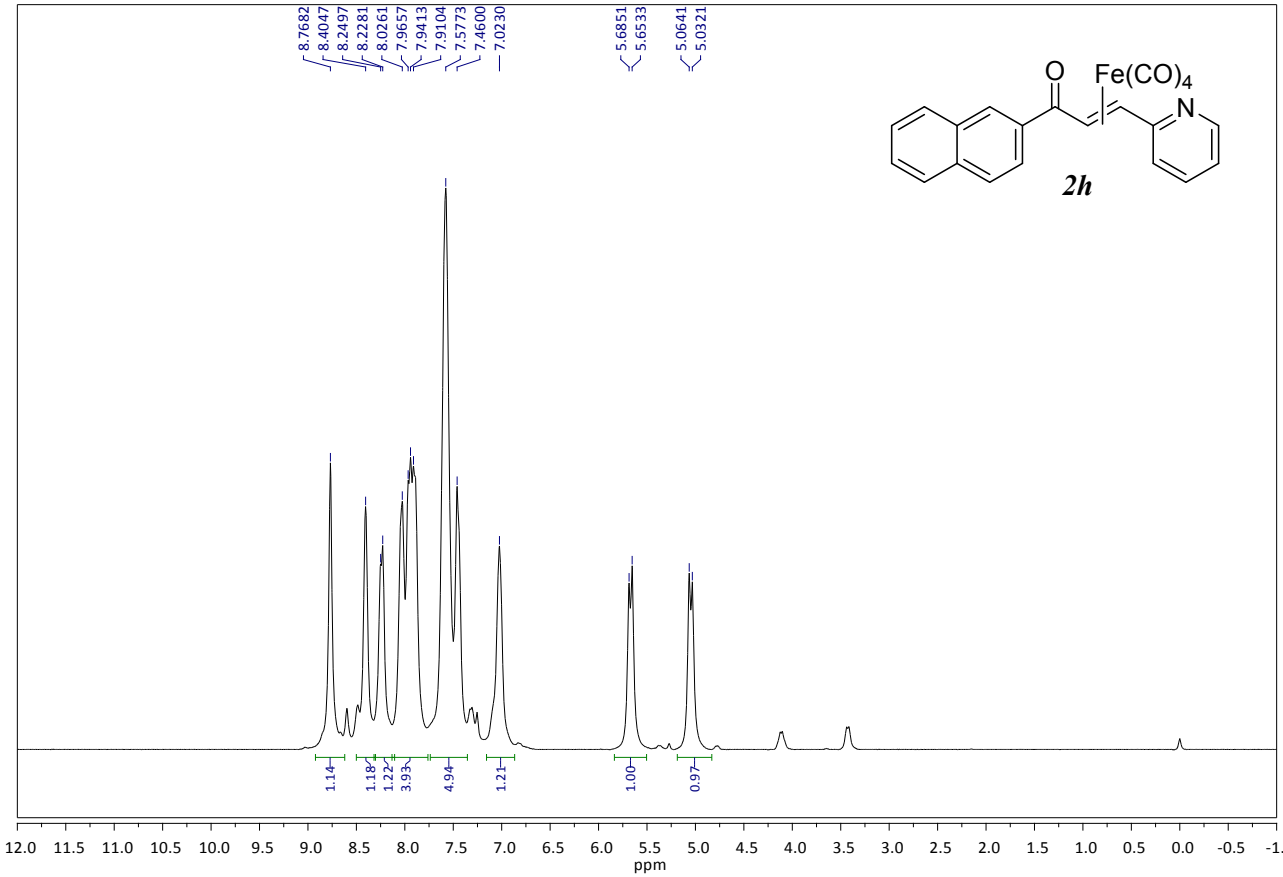

206.03
195.16
161.07
149.13
140.46
136.84
134.66
134.23
133.79
133.36
129.29
128.40
125.87
125.83
125.78
125.73
125.68
123.38
122.07
121.64
118.46
77.58
77.16
76.74
56.86
49.69
ppm

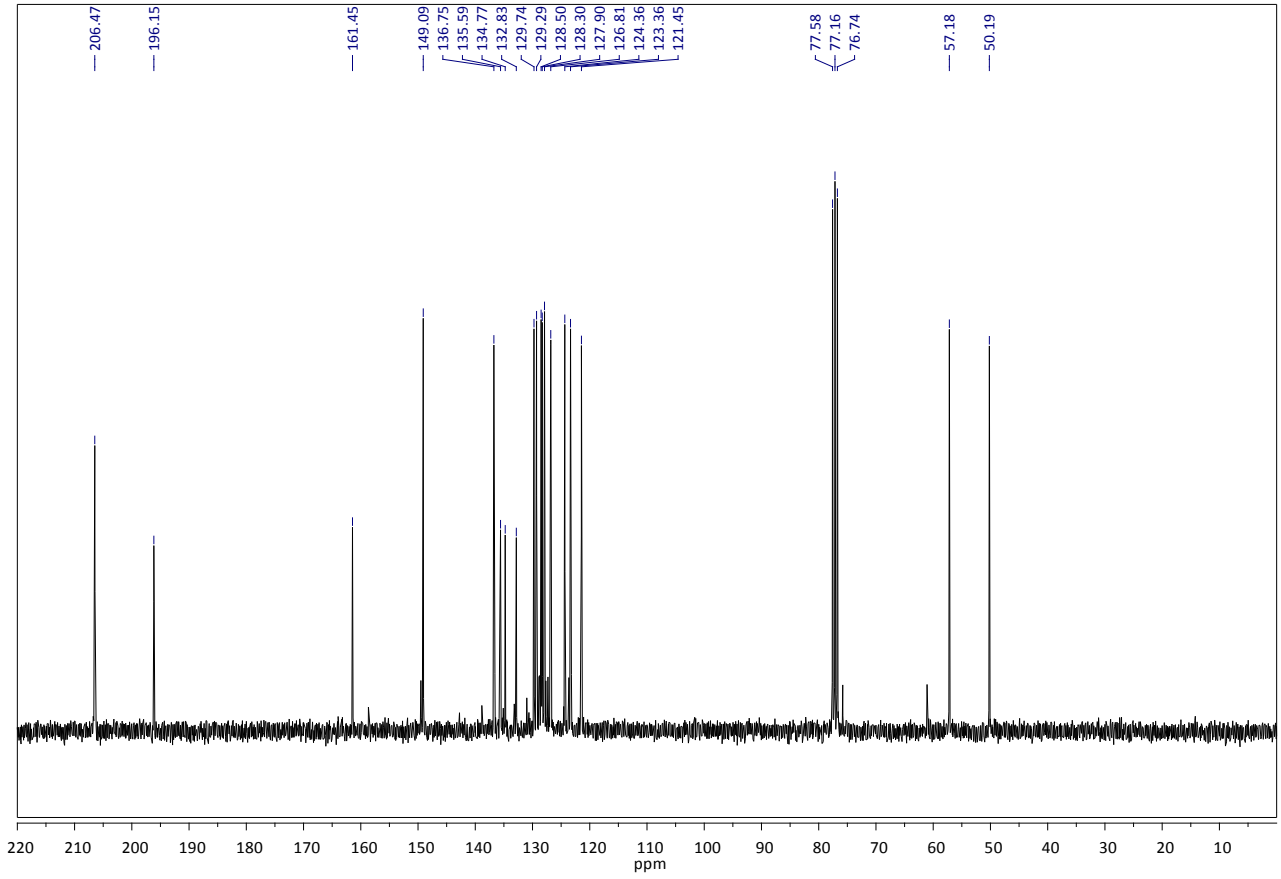

8.3659
8.2137
8.1865
7.6081
7.5845
7.5607
7.4327
7.4079
7.0195
6.9938
5.5161
5.4815
4.9896
4.9551
3.8940
1.03
2.11
1.16
1.10
3.45
1.00
0.99
3.44
O
Fe(CO)4
N
O
2f
ppm

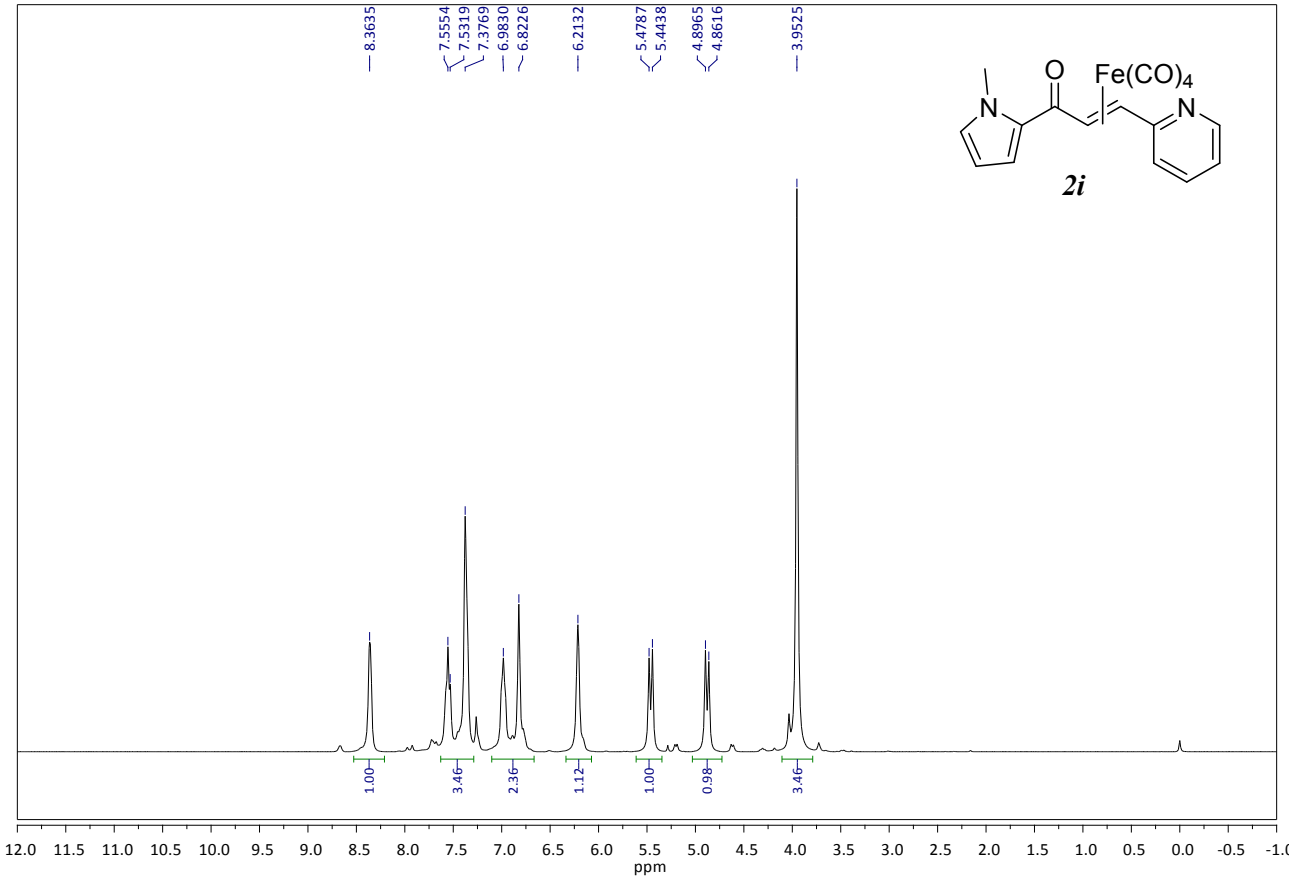

206.67
194.97
163.30
161.57
149.04
136.69
130.37
130.30
123.29
121.34
113.87
77.58
77.16
76.74
57.20
55.57
49.89
ppm

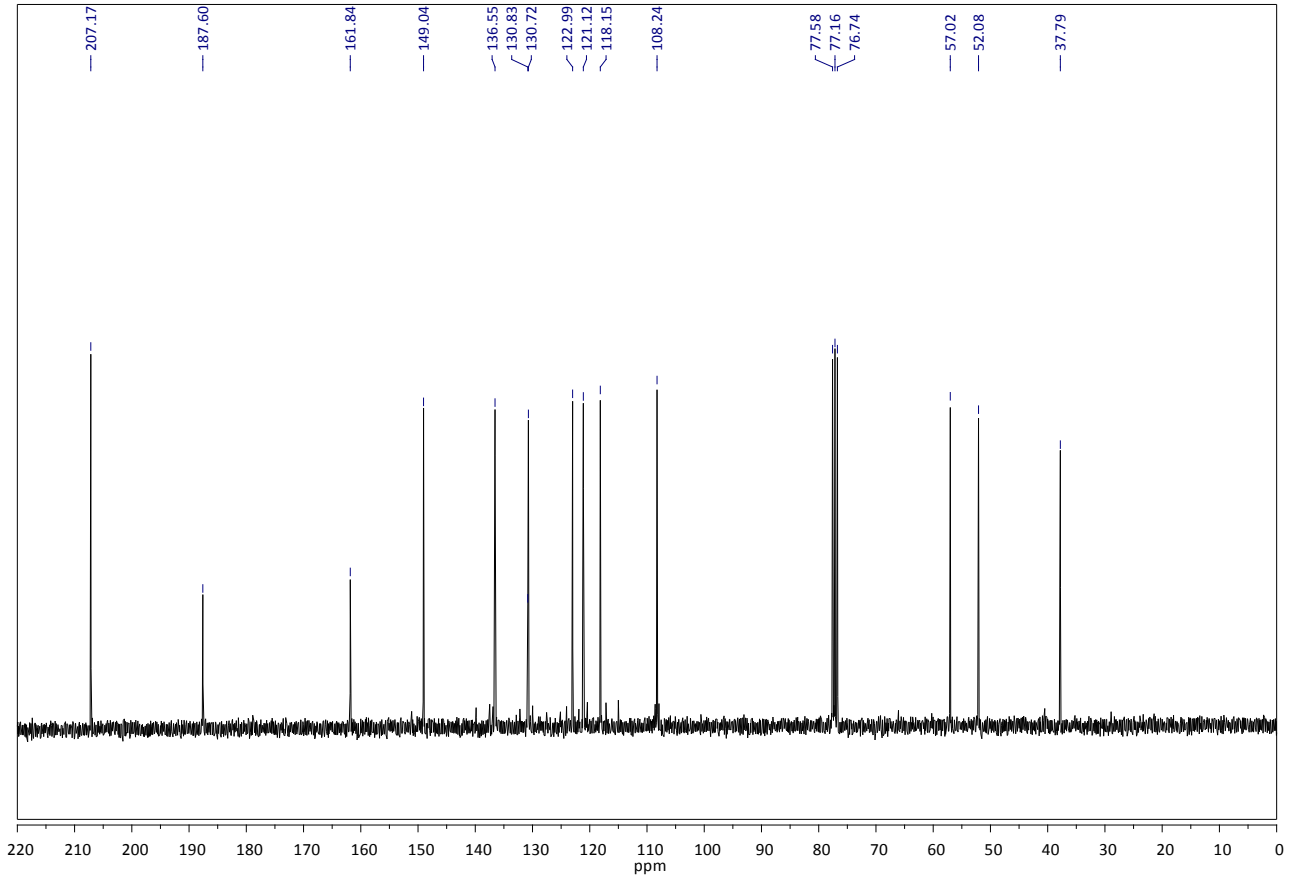

8.4836
8.4684
8.3932
8.3782
8.2936
8.2664
8.1172
8.0899
7.7669
7.7391
7.7035
7.6866
7.6625
7.6222
7.5966
7.5714
7.5065
7.4835
7.4566
7.4250
7.4007
7.3892
7.2514
7.2249
7.1973
7.1119
7.0937
7.0433
7.0252
7.0028
5.5666
5.5318
5.0165
4.9817
3.3992
3.3716
O
Fe(CO)4
N
2g
(η2/η4 ratio ~ 2:1)
0.59
1.02
2.06
1.18
8.56
6.76
0.81
1.66
1.00
0.99
0.56
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 -0.5
ppm

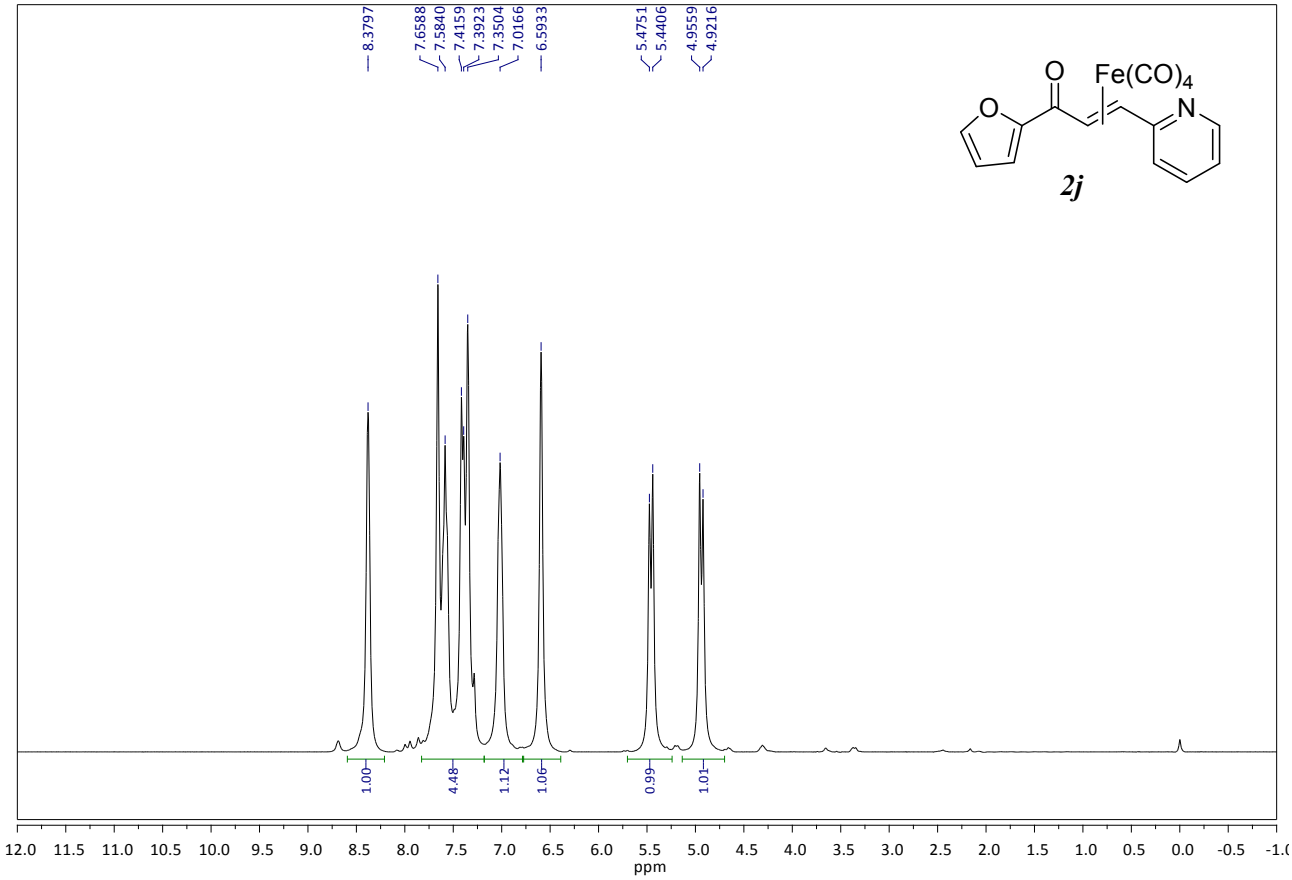

206.48
195.88
161.43
158.68
149.50
149.09
145.41
144.41
140.16
138.83
136.73
136.56
136.23
132.42
129.05
128.74
128.24
128.07
127.62
127.35
127.25
123.61
123.31
121.55
121.44
77.58
77.16
76.74
75.45
60.98
57.12
50.05
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


8.7682
8.4047
8.2497
8.2281
8.0261
7.9657
7.9413
7.9104
7.5773
7.4600
7.0230
5.6851
5.6533
5.0641
5.0321
O
Fe(CO)4
N
2h
1.14
1.18
1.22
3.93
4.94
1.21
1.00
0.97
ppm


206.47
196.15
161.45
149.09
136.75
135.59
134.77
132.83
129.74
129.29
128.50
128.30
127.90
126.81
124.36
123.36
121.45
77.58
77.16
76.74
57.18
50.19
ppm

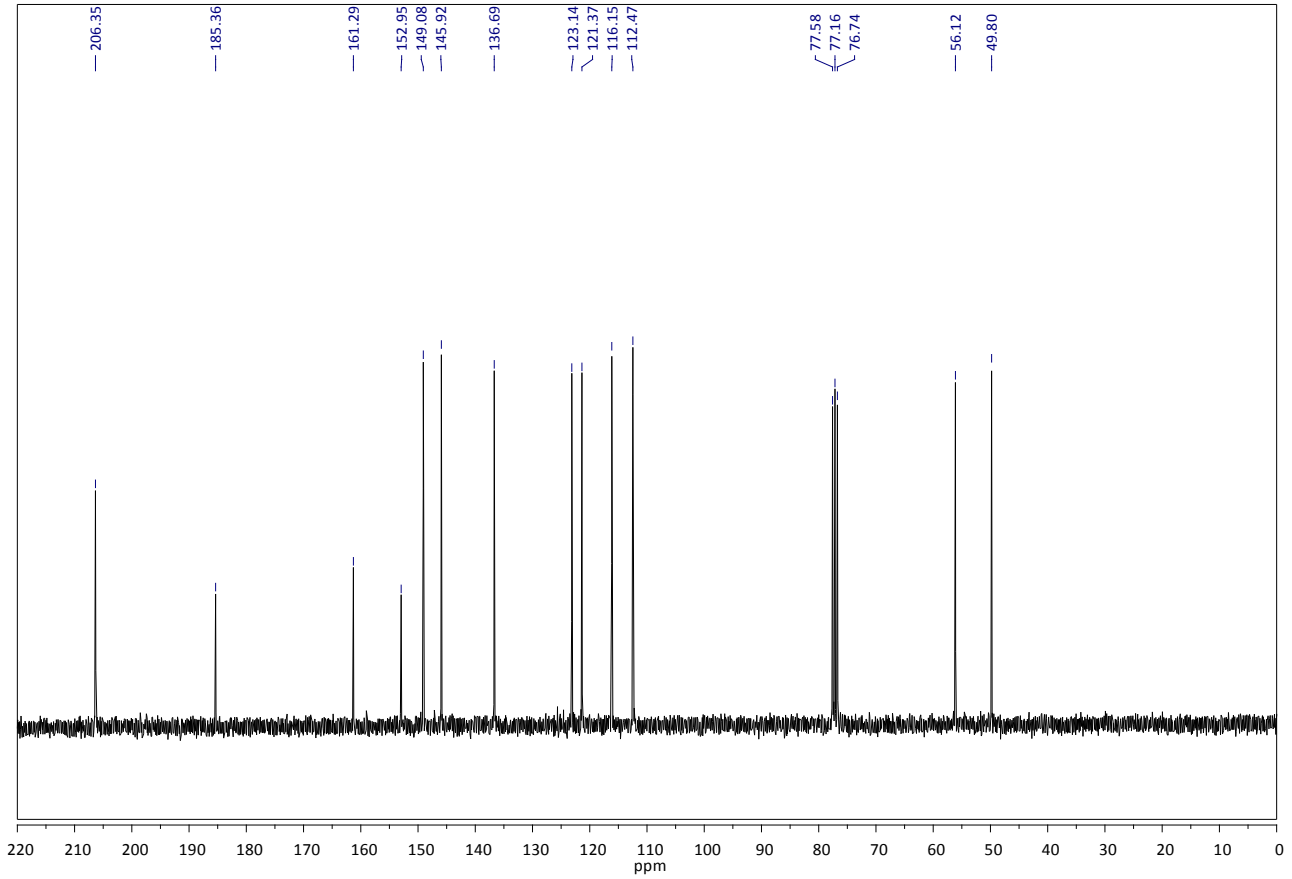

8.3635
7.5554
7.5319
7.3769
6.9830
6.8226
6.2132
5.4787
5.4438
4.8965
4.8616
3.9525
1.00
3.46
2.36
1.12
1.00
0.98
3.46
O
Fe(CO)4
N
N
2i
ppm

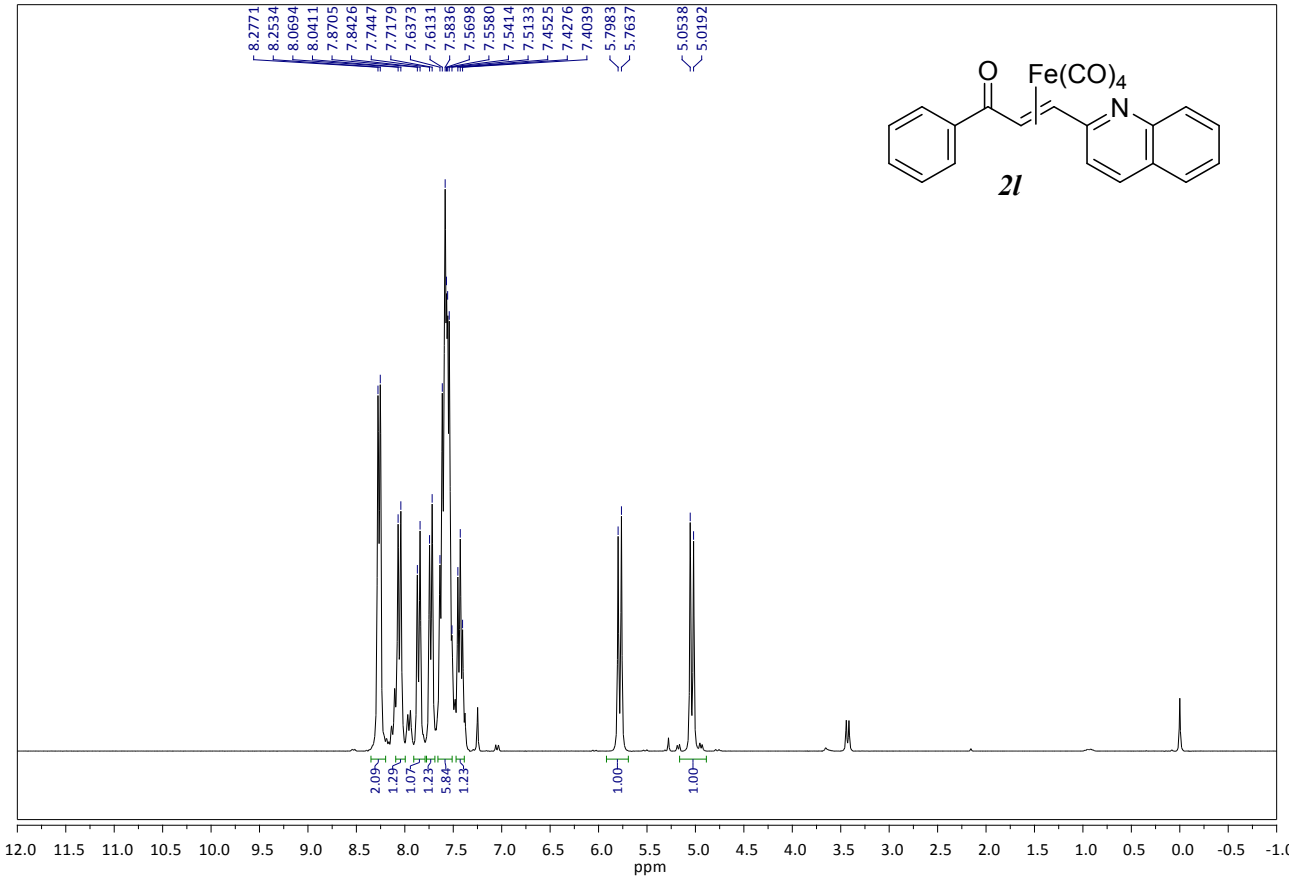

207.17
187.60
161.84
149.04
136.55
130.83
130.72
122.99
121.12
118.15
108.24
77.58
77.16
76.74
57.02
52.08
37.79
ppm

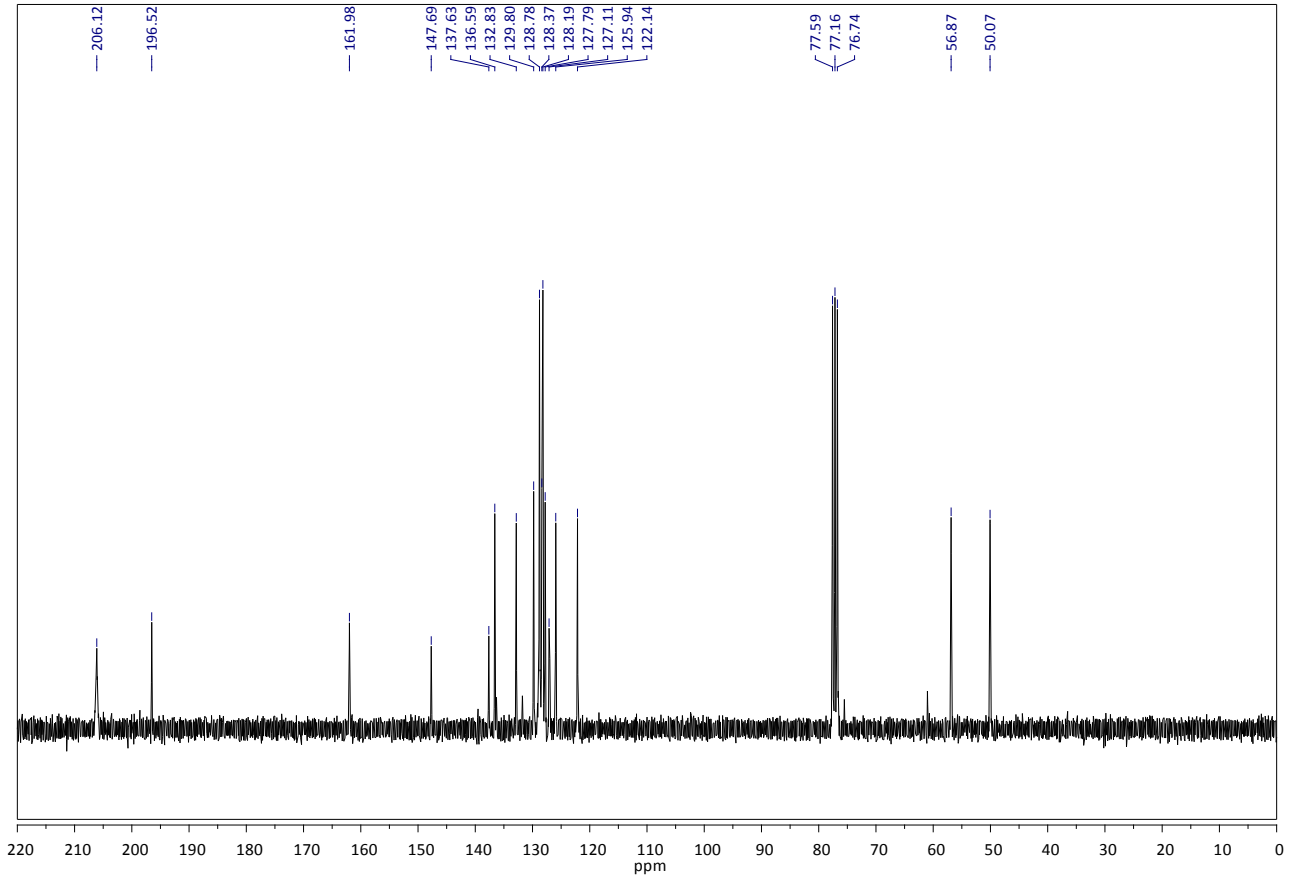

8.3797
7.6588
7.5840
7.4159
7.3923
7.3504
7.0166
6.5933
5.4751
5.4406
4.9559
4.9216
1.00
4.48
1.12
1.06
0.99
1.01
ppm

O
Fe(CO)4
O
N

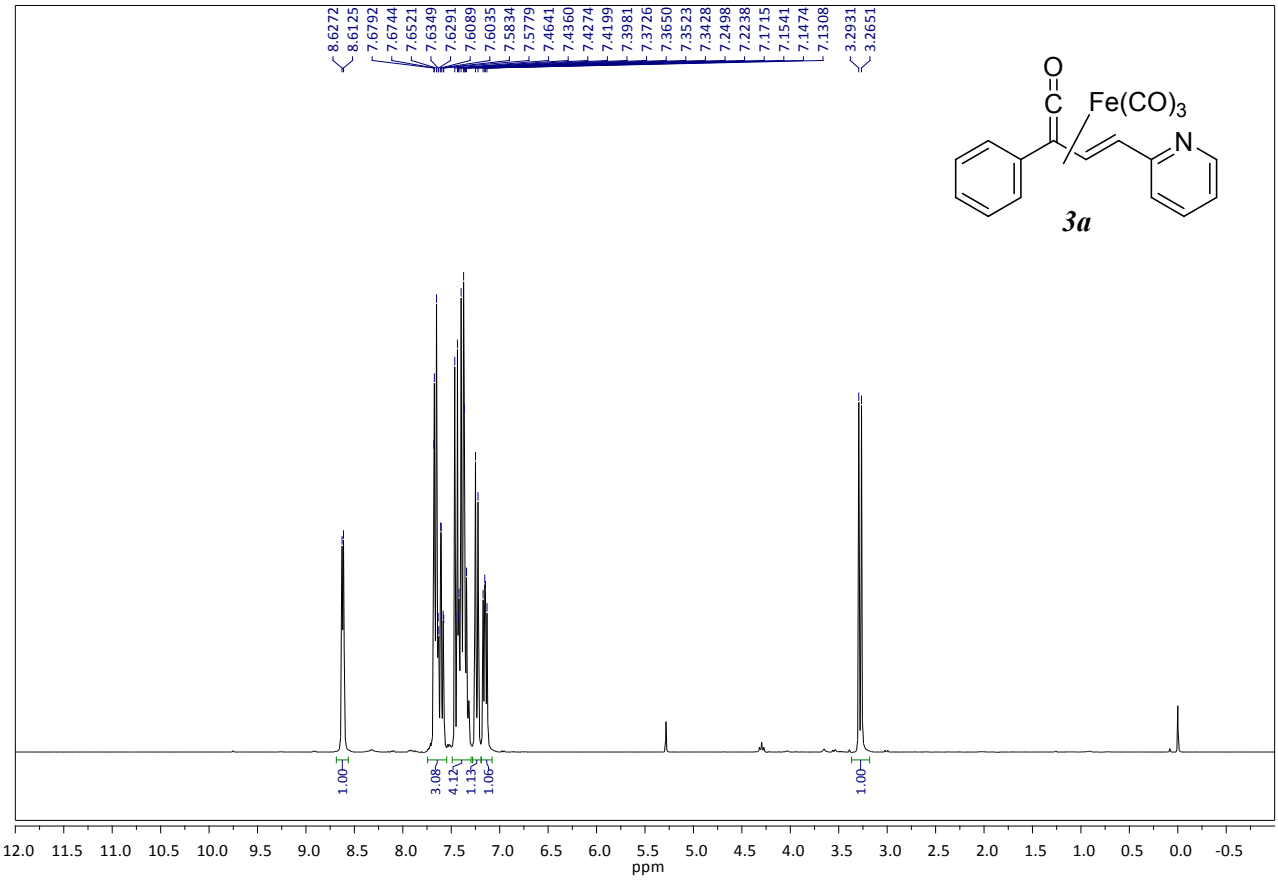
2j

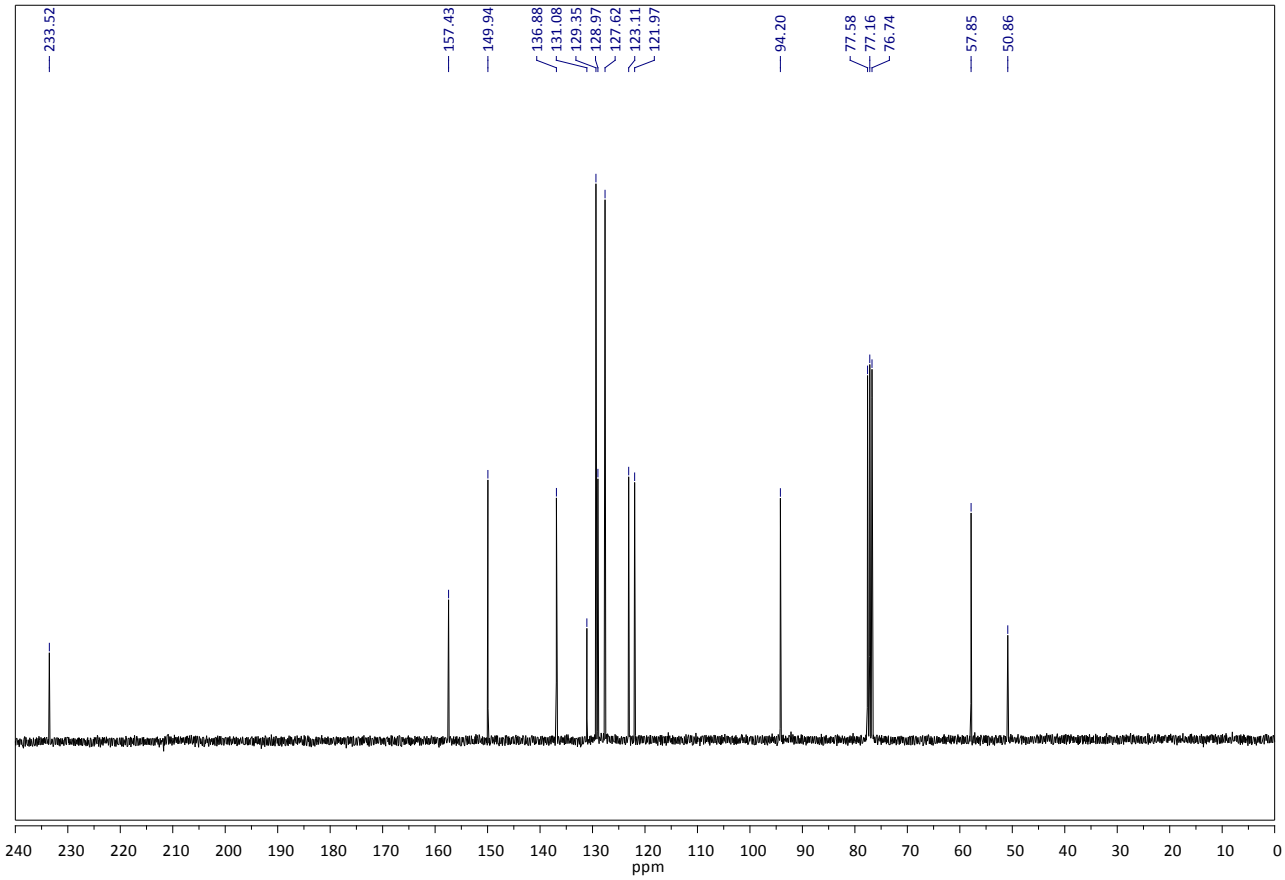

206.35
185.36
161.29
152.95
149.08
145.92
136.69
123.14
121.37
116.15
112.47
77.58
77.16
76.74
56.12
49.80
ppm

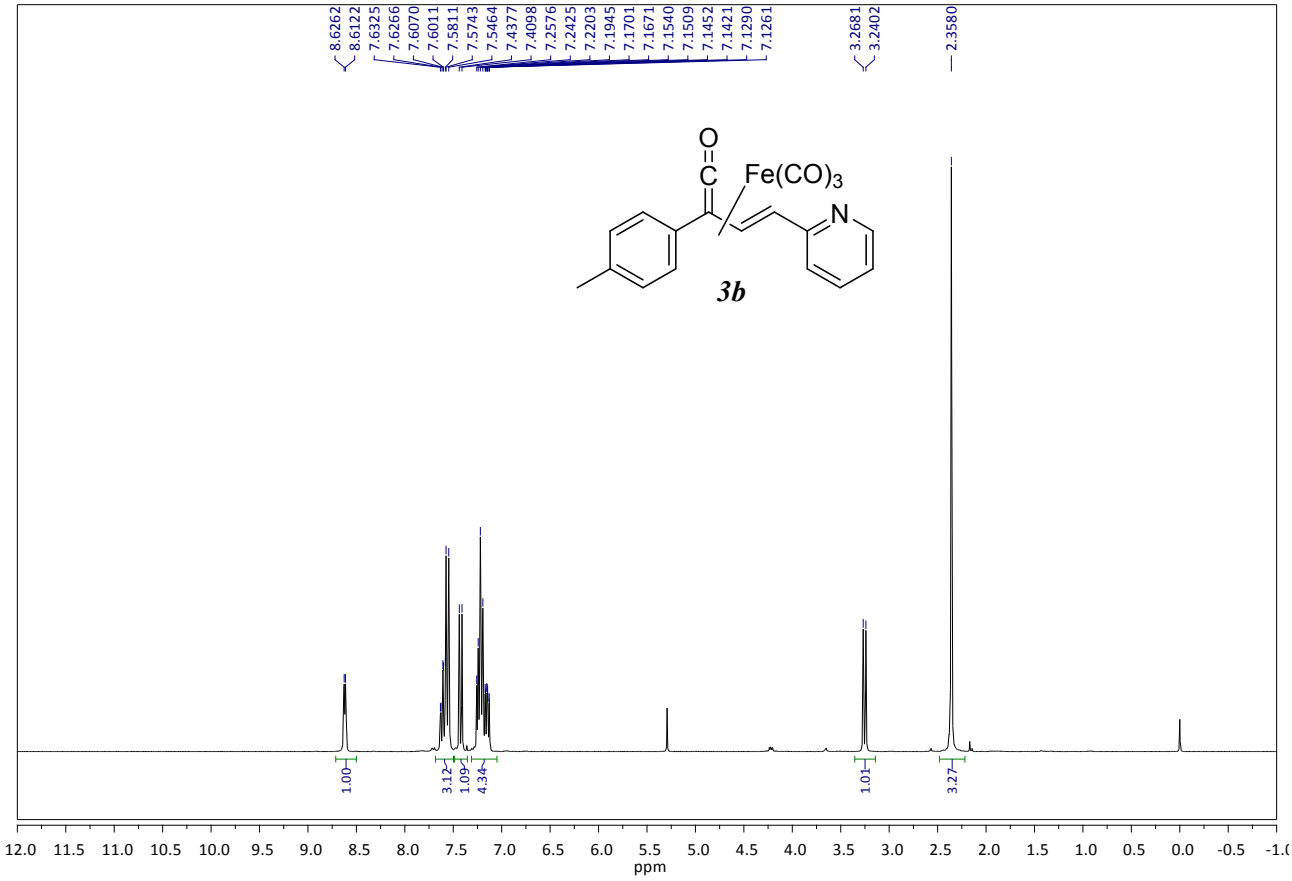

8.2771
8.2534
8.0694
8.0411
7.8705
7.8426
7.7447
7.7179
7.6373
7.6131
7.5836
7.5698
7.5580
7.5414
7.5133
7.4525
7.4276
7.4039
5.7983
5.7637
5.0538
5.0192
O
Fe(CO)4
N
2l
2.09
1.29
1.07
1.23
5.84
1.23
1.00
1.00
ppm

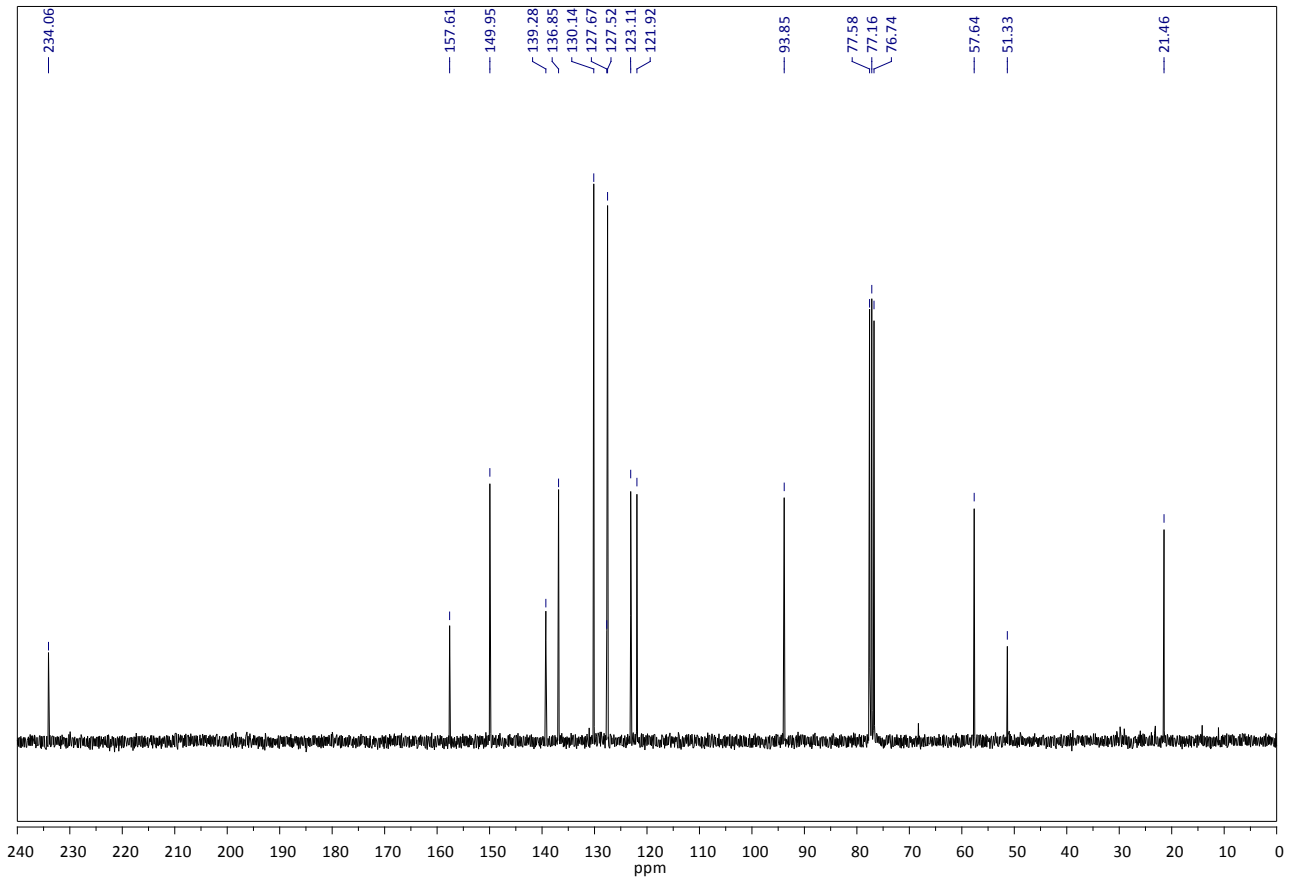

206.12
196.52
161.98
147.69
137.63
136.59
132.83
129.80
128.78
128.37
128.19
127.79
127.11
125.94
122.14
77.59
77.16
76.74
56.87
50.07
ppm

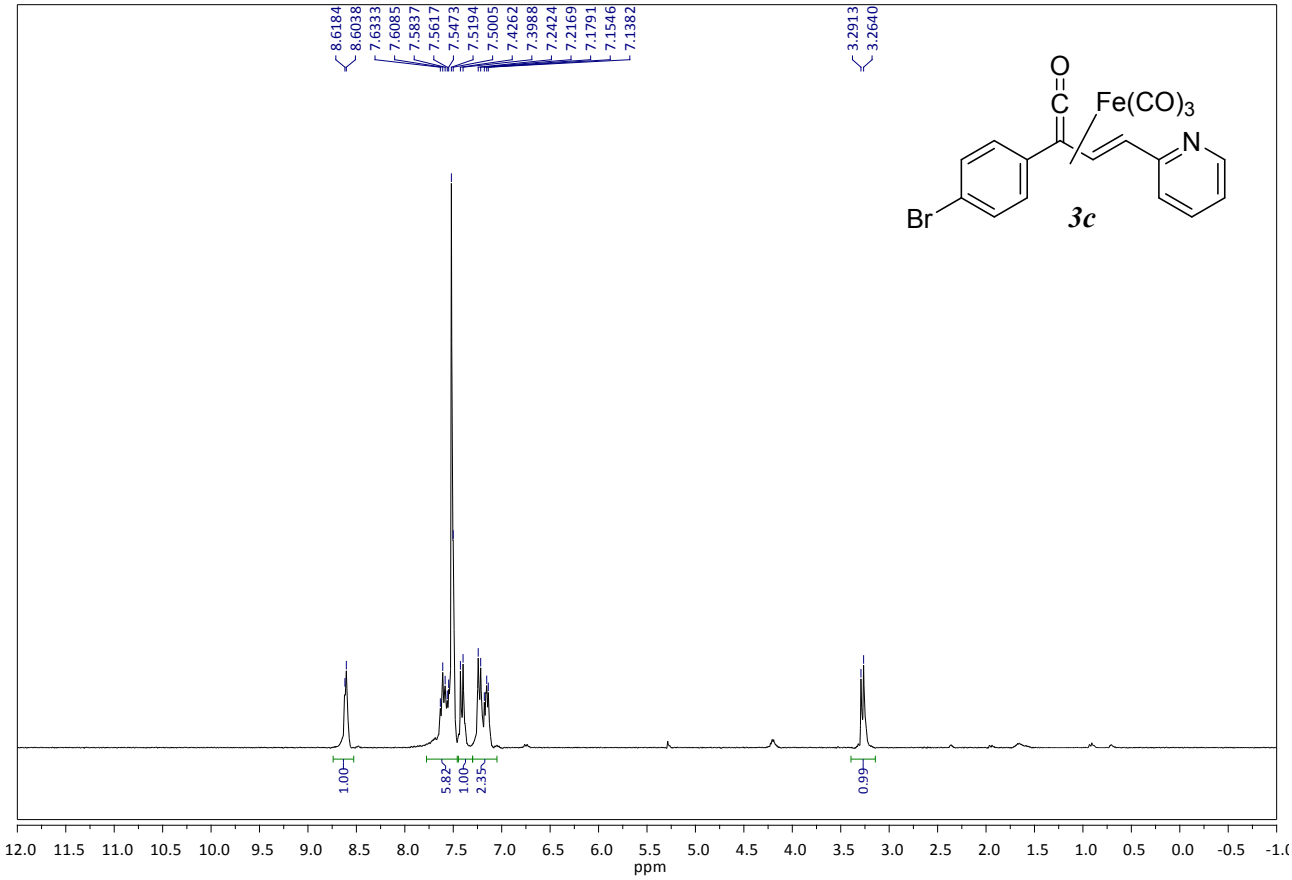
1.3 Spectra of compounds 3a-l.

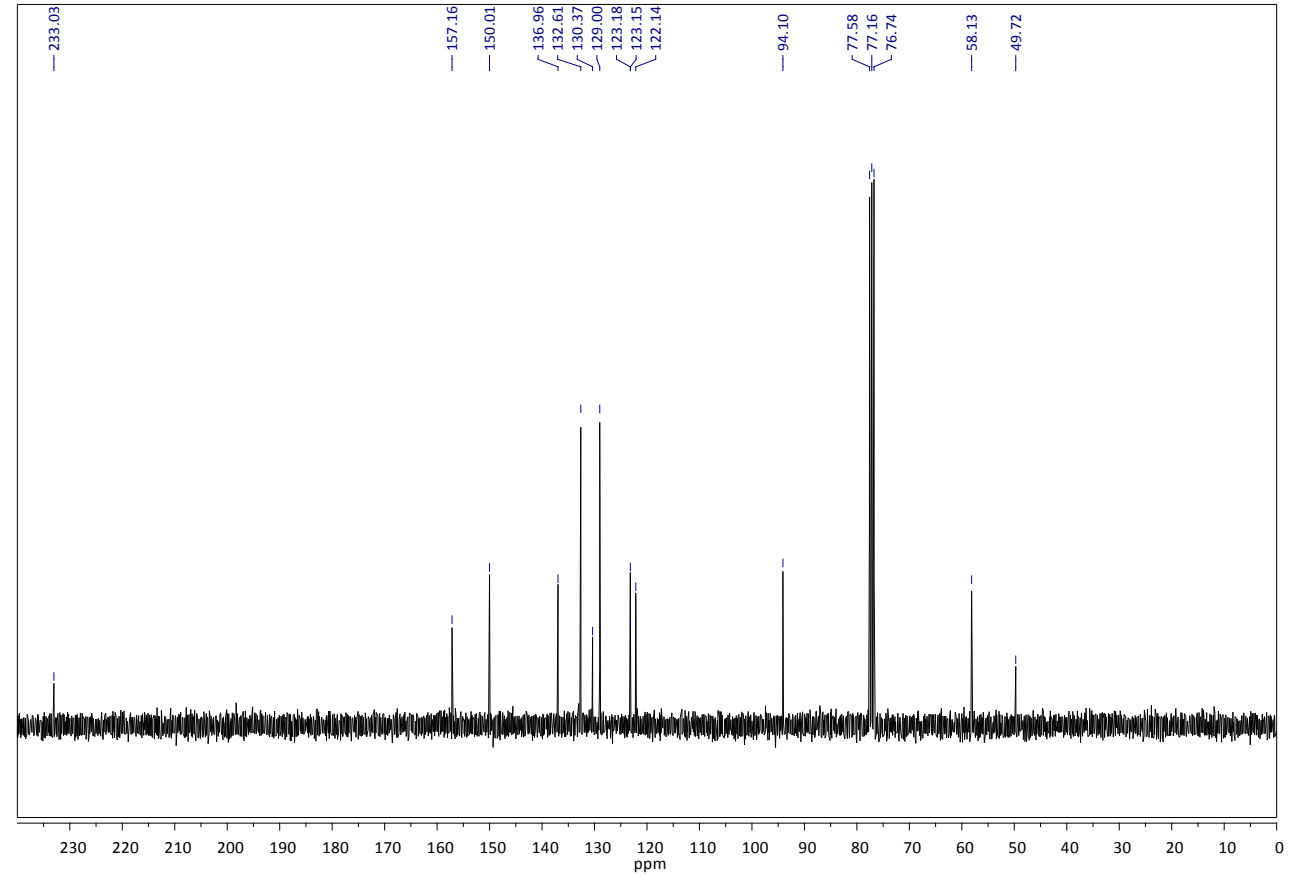


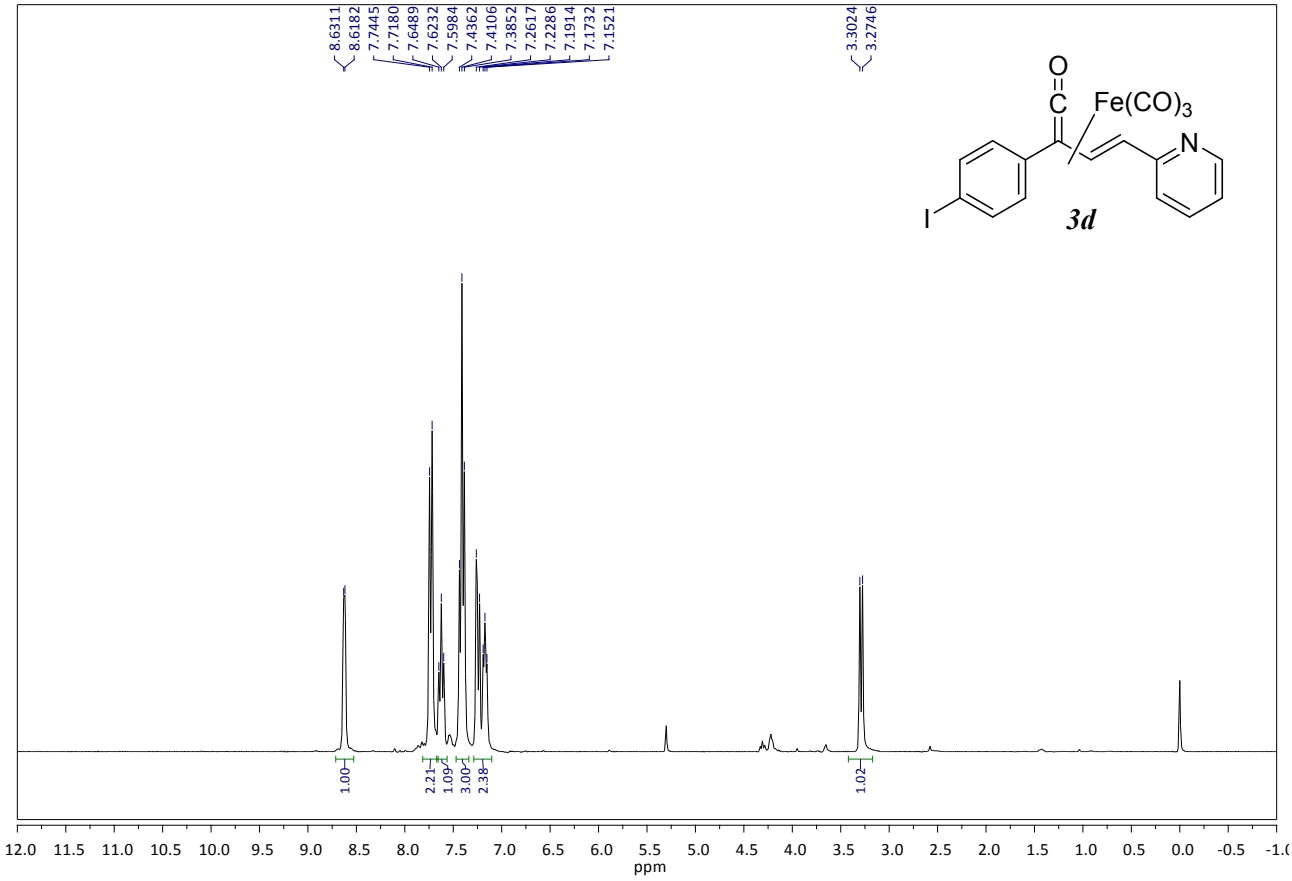


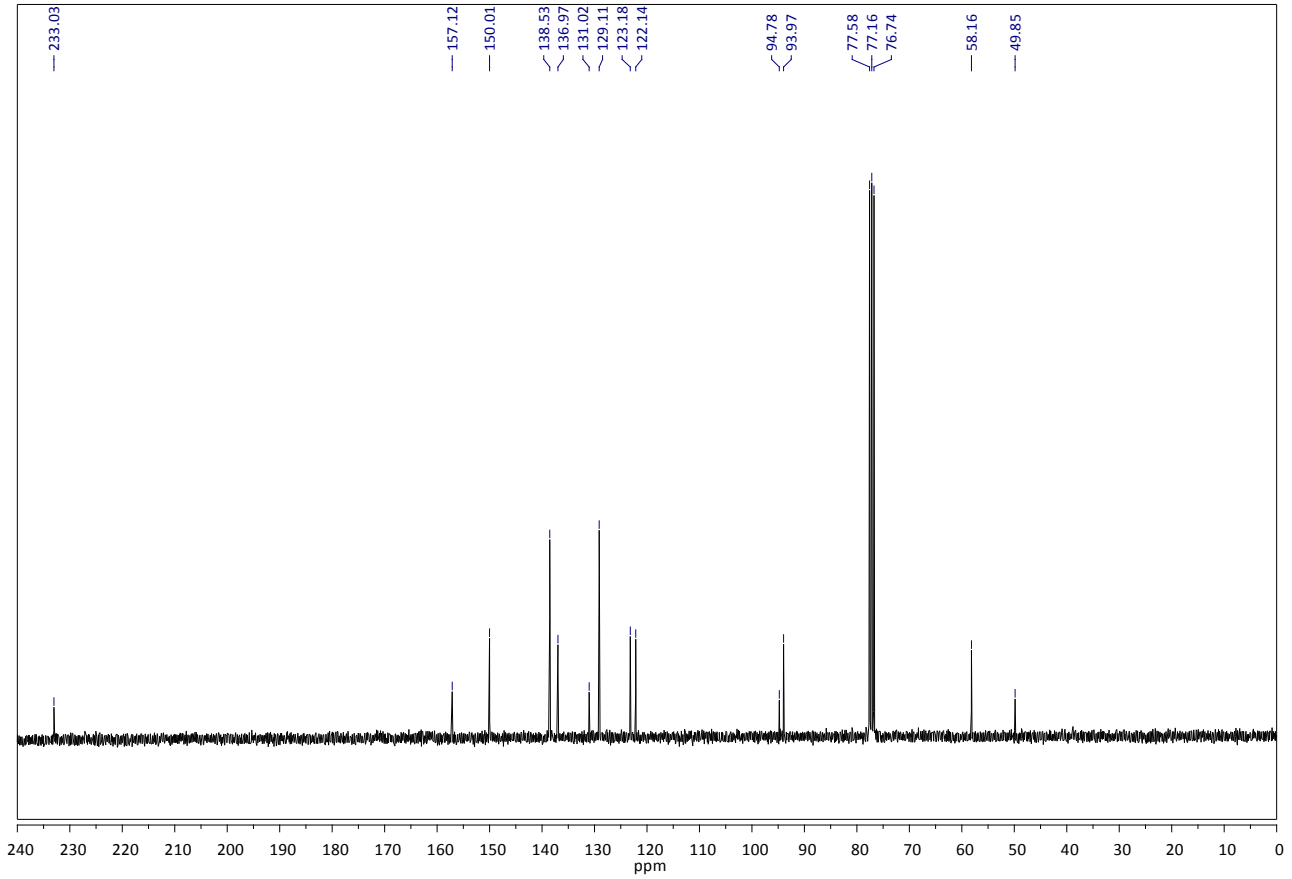

8.6262
8.6122
7.6325
7.6266
7.6070
7.6011
7.5811
7.5743
7.5464
7.4377
7.4098
7.2576
7.2425
7.2203
7.1945
7.1701
7.1671
7.1540
7.1509
7.1452
7.1421
7.1290
7.1261
3.2681
3.2402
2.3580
O
C
Fe(CO)3
N
3b
1.00
3.12
1.09
4.34
1.01
3.27
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

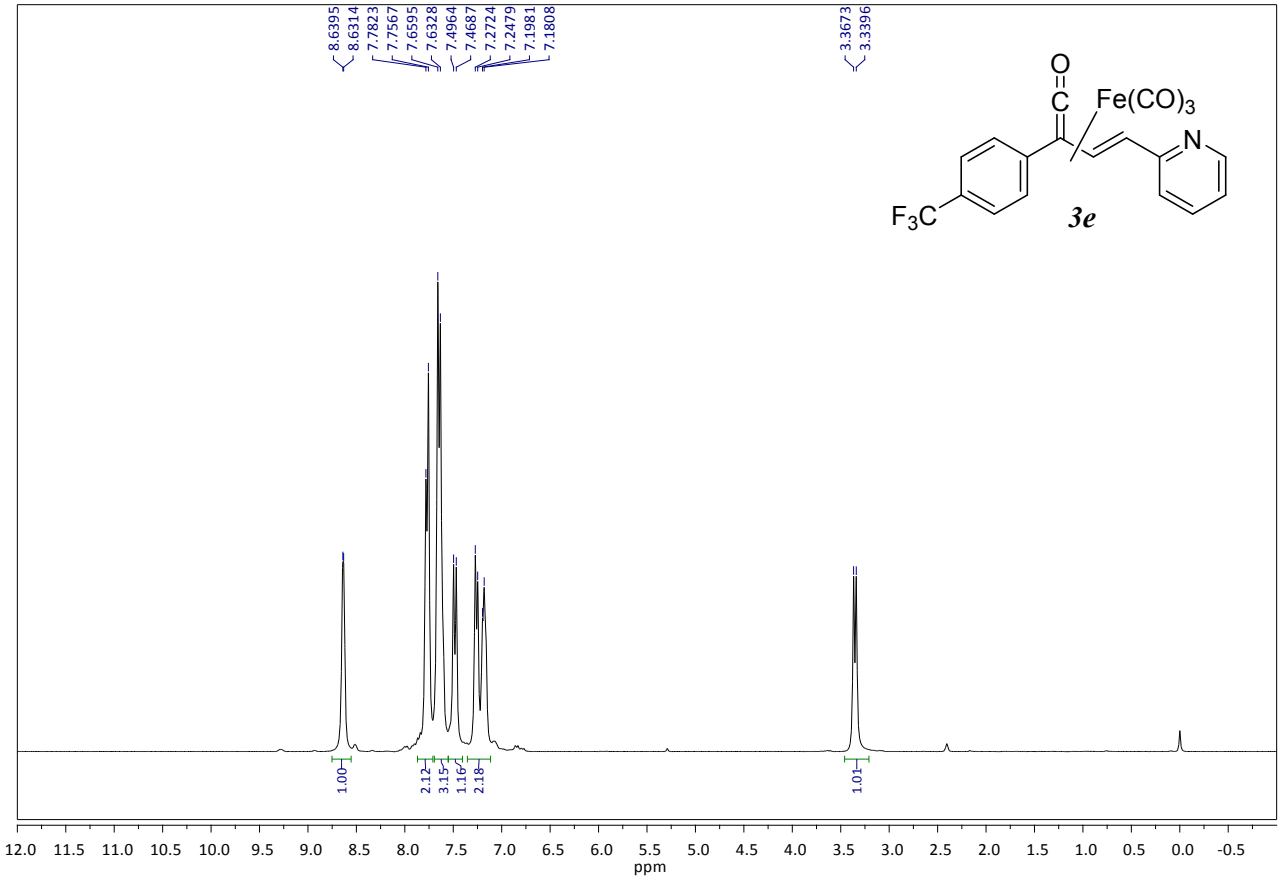

234.06
157.61
149.95
139.28
136.85
130.14
127.67
127.52
123.11
121.92
93.85
77.58
77.16
76.74
57.64
51.33
21.46
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

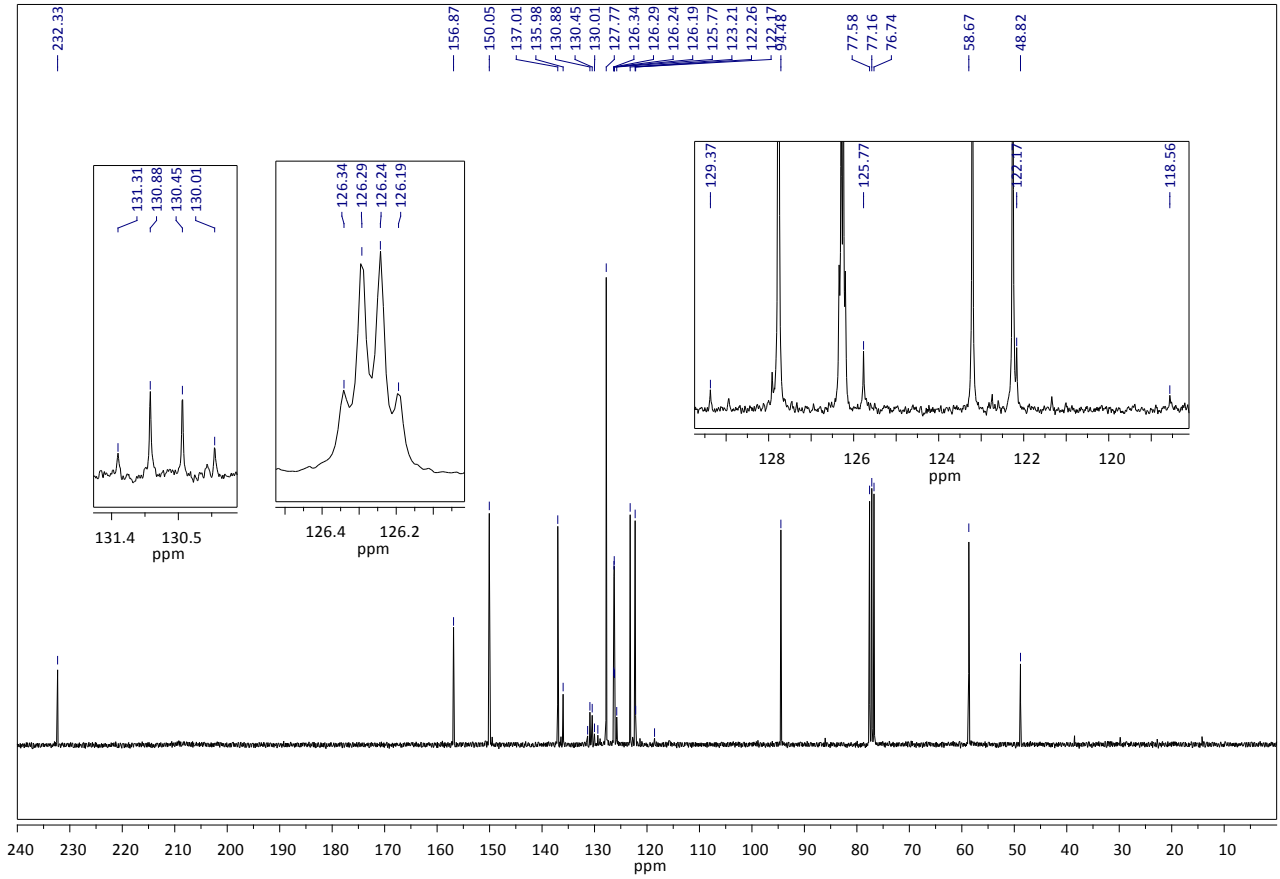

8.6184
8.6038
7.6333
7.6085
7.5837
7.5617
7.5473
7.5194
7.5005
7.4262
7.3988
7.2424
7.2169
7.1791
7.1546
7.1382
3.2913
3.2640
O
C
Fe(CO)3
N
Br
3c
1.00
5.82
1.00
2.35
0.99
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

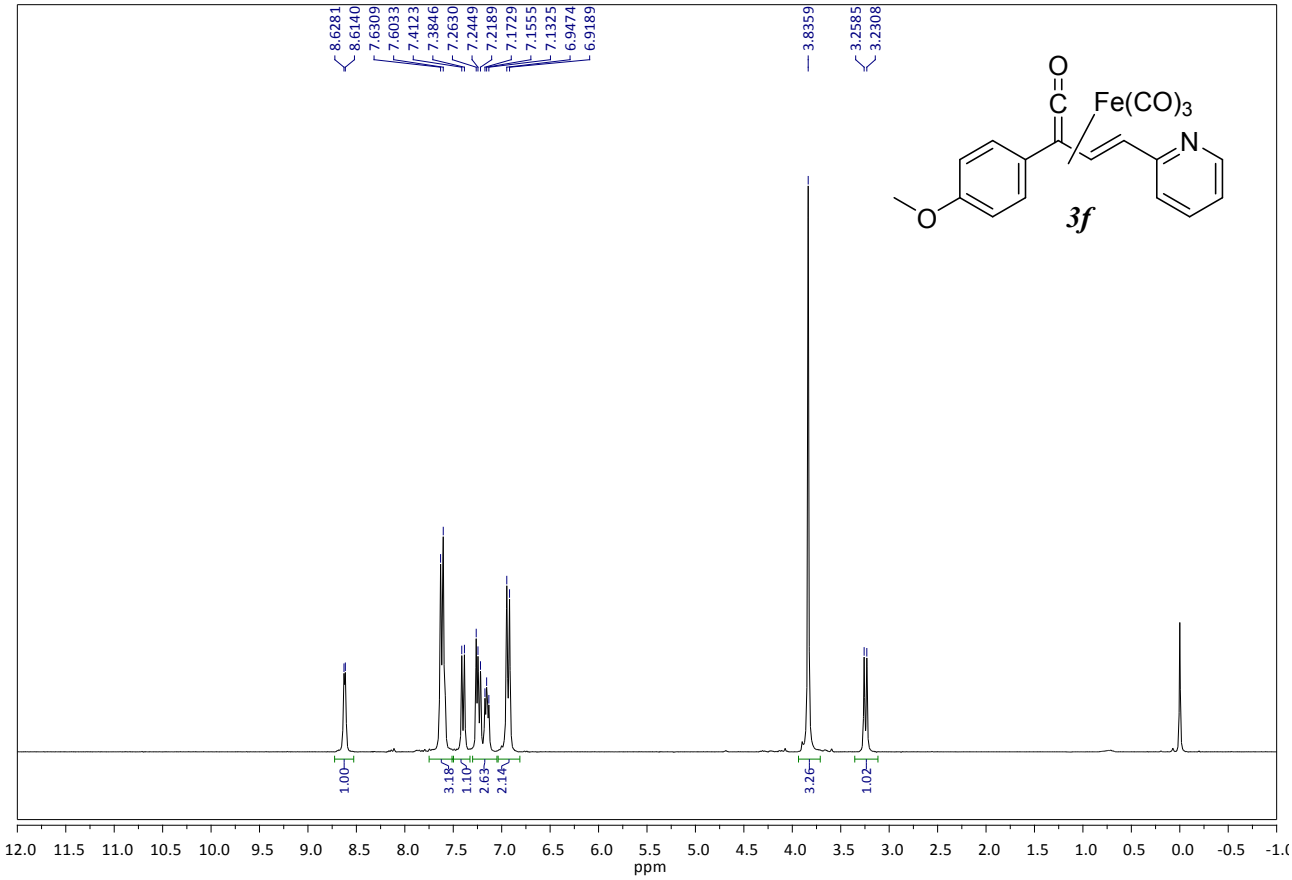

233.03
157.16
150.01
136.96
132.61
130.37
129.00
123.18
123.15
122.14
94.10
77.58
77.16
76.74
58.13
49.72
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

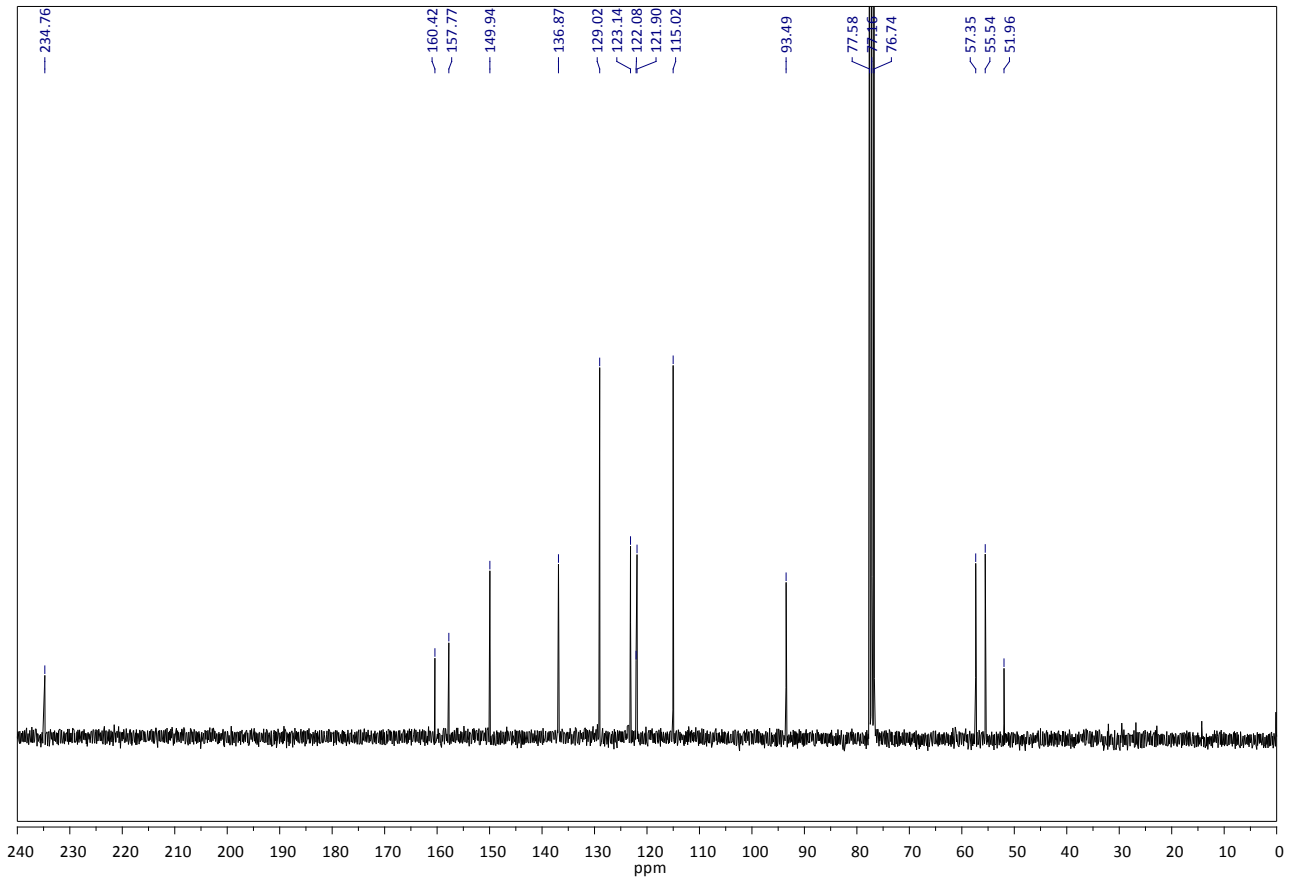

8.6311
8.6182
7.7445
7.7180
7.6489
7.6232
7.5984
7.4362
7.4106
7.3852
7.2617
7.2286
7.1914
7.1732
7.1521
3.3024
3.2746
O
C
Fe(CO)3
N
I
3d
1.00
2.21
1.09
3.00
2.38
1.02
ppm

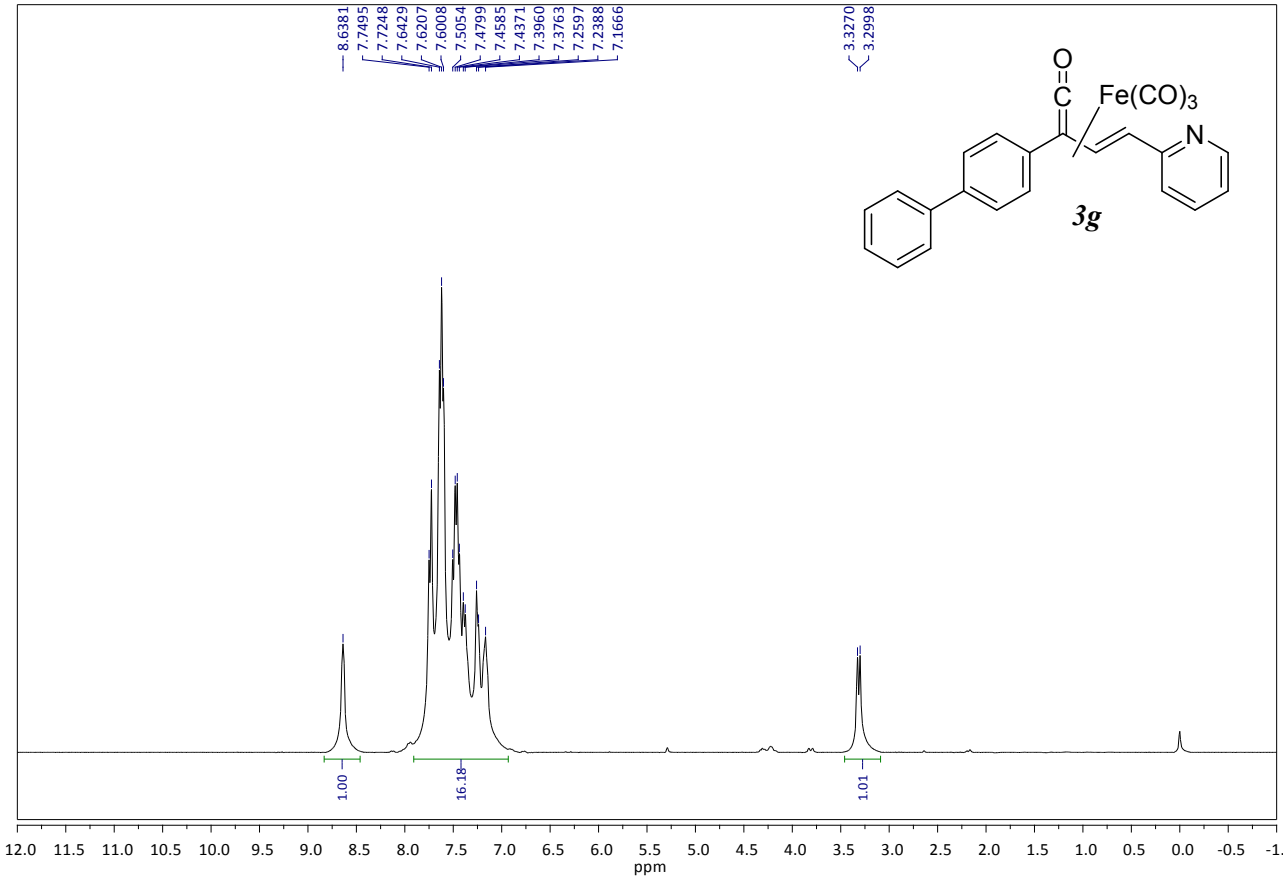

233.03
157.12
150.01
138.53
136.97
131.02
129.11
123.18
122.14
94.78
93.97
77.58
77.16
76.74
58.16
49.85
ppm

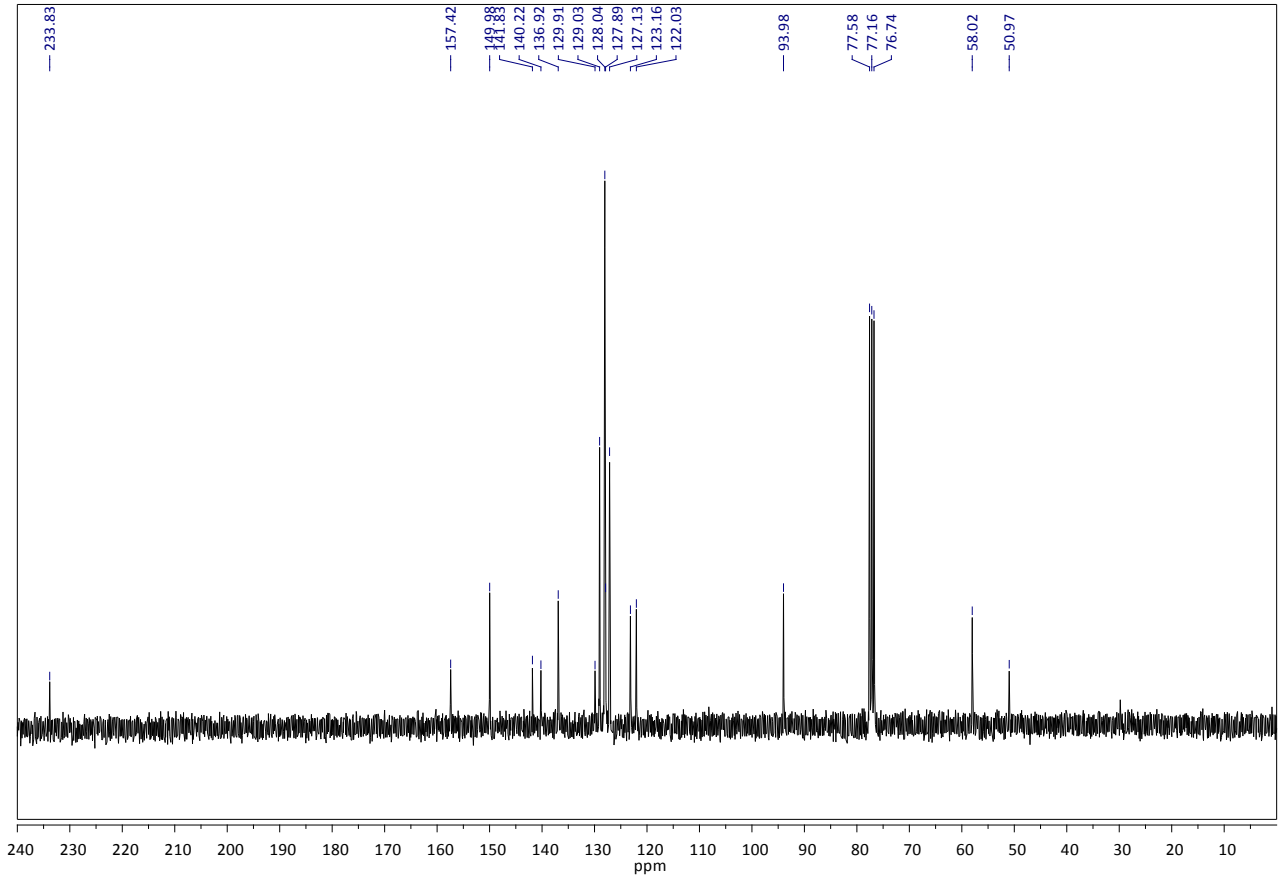

8.6395
8.6314
7.7823
7.7567
7.6595
7.6328
7.4964
7.4687
7.2724
7.2479
7.1981
7.1808
3.3673
3.3396
O
C
Fe(CO)3
N
F3C
3e
1.00
2.12
3.15
1.16
2.18
1.01
ppm

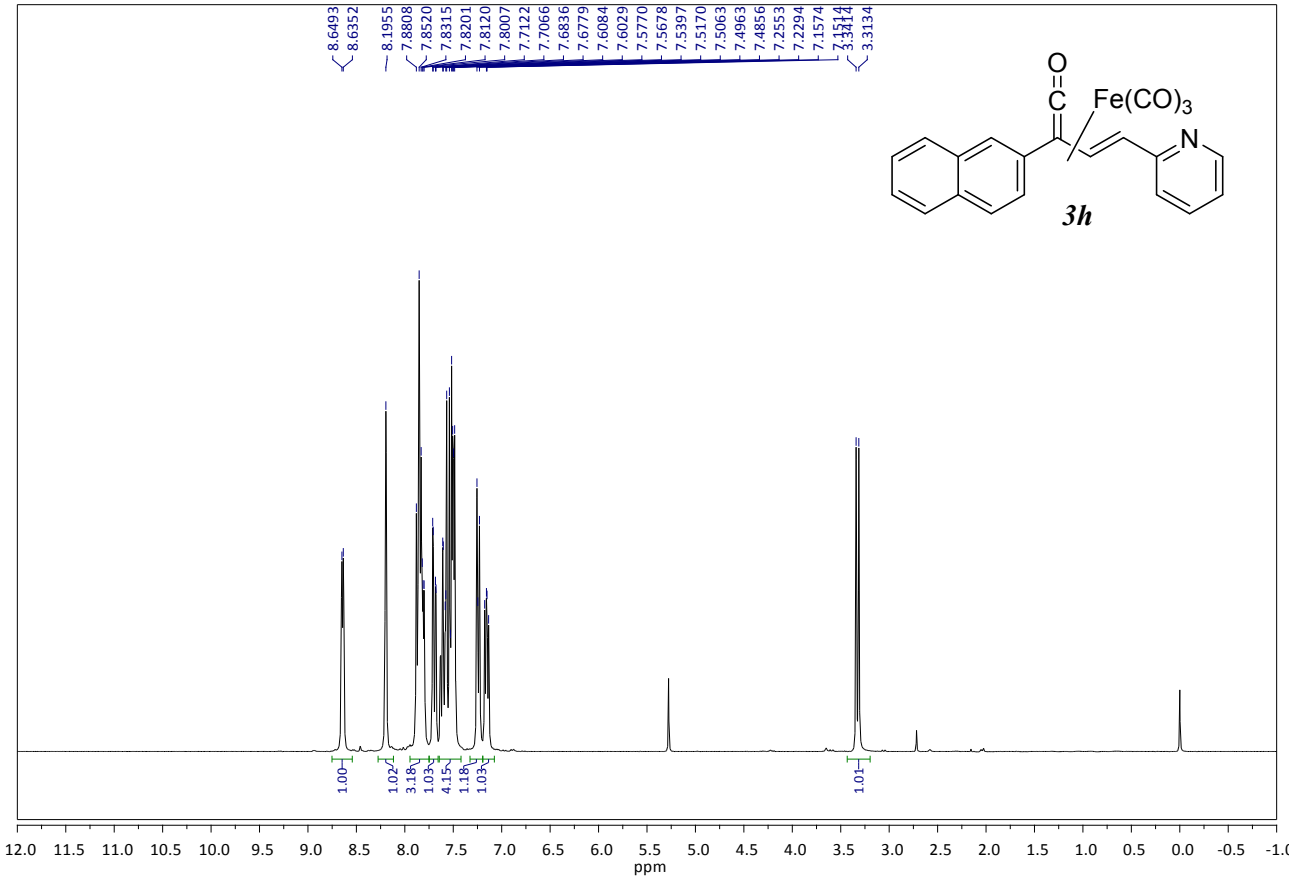

232.33
156.87
150.05
137.01
135.98
130.88
130.45
130.01
127.77
126.34
126.29
126.24
126.19
125.77
123.21
122.26
122.17
94.48
77.58
77.16
76.74
58.67
48.82
131.31
130.88
130.45
130.01
126.34
126.29
126.24
126.19
129.37
125.77
122.17
118.56
131.4
130.5
126.4
126.2
128
126
124
122
120
ppm

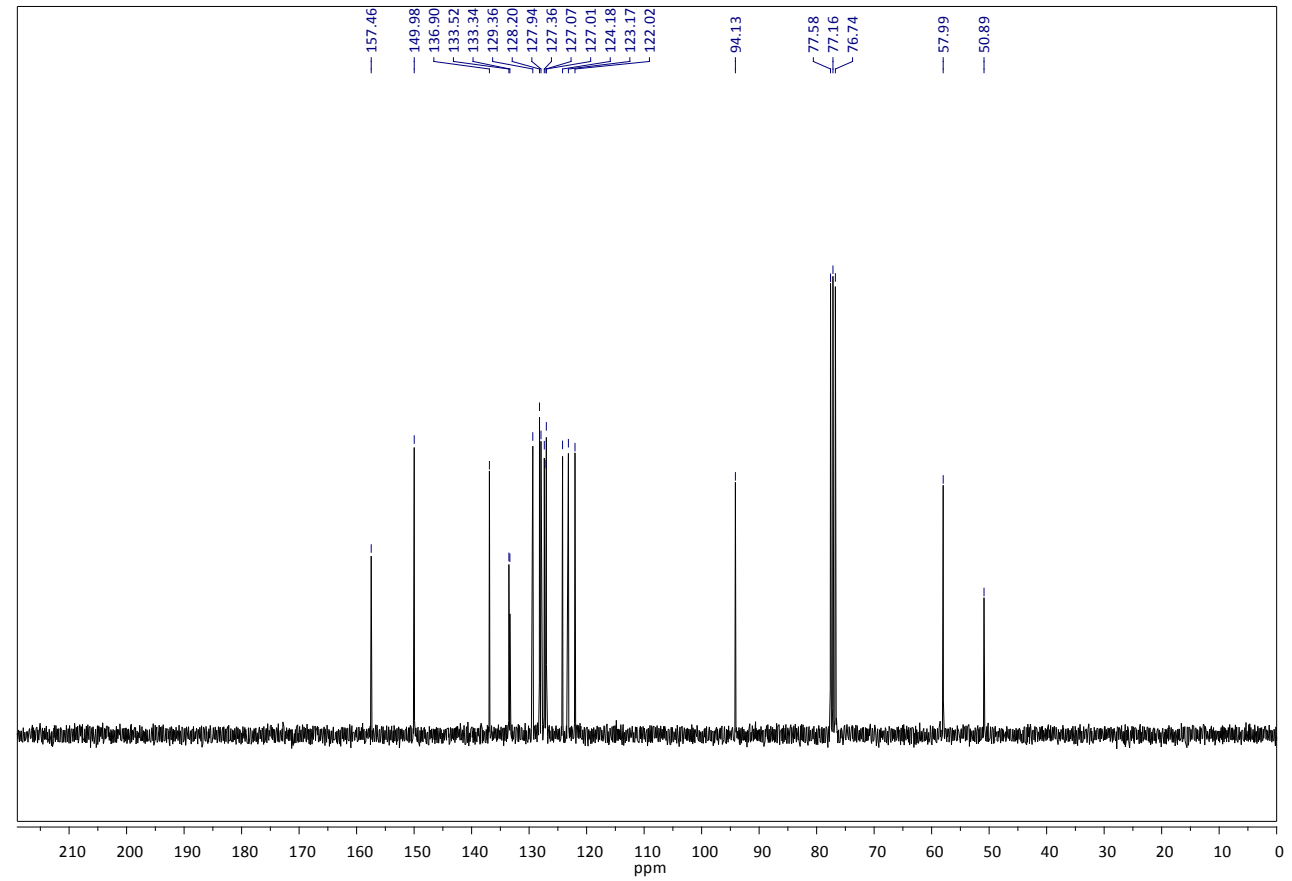

8.6281
8.6140
7.6309
7.6033
7.4123
7.3846
7.2630
7.2449
7.2189
7.1729
7.1555
7.1325
6.9474
6.9189
3.8359
3.2585
3.2308
O
C
Fe(CO)3
N
O
3f
1.00
3.18
1.10
2.63
2.14
3.26
1.02
ppm

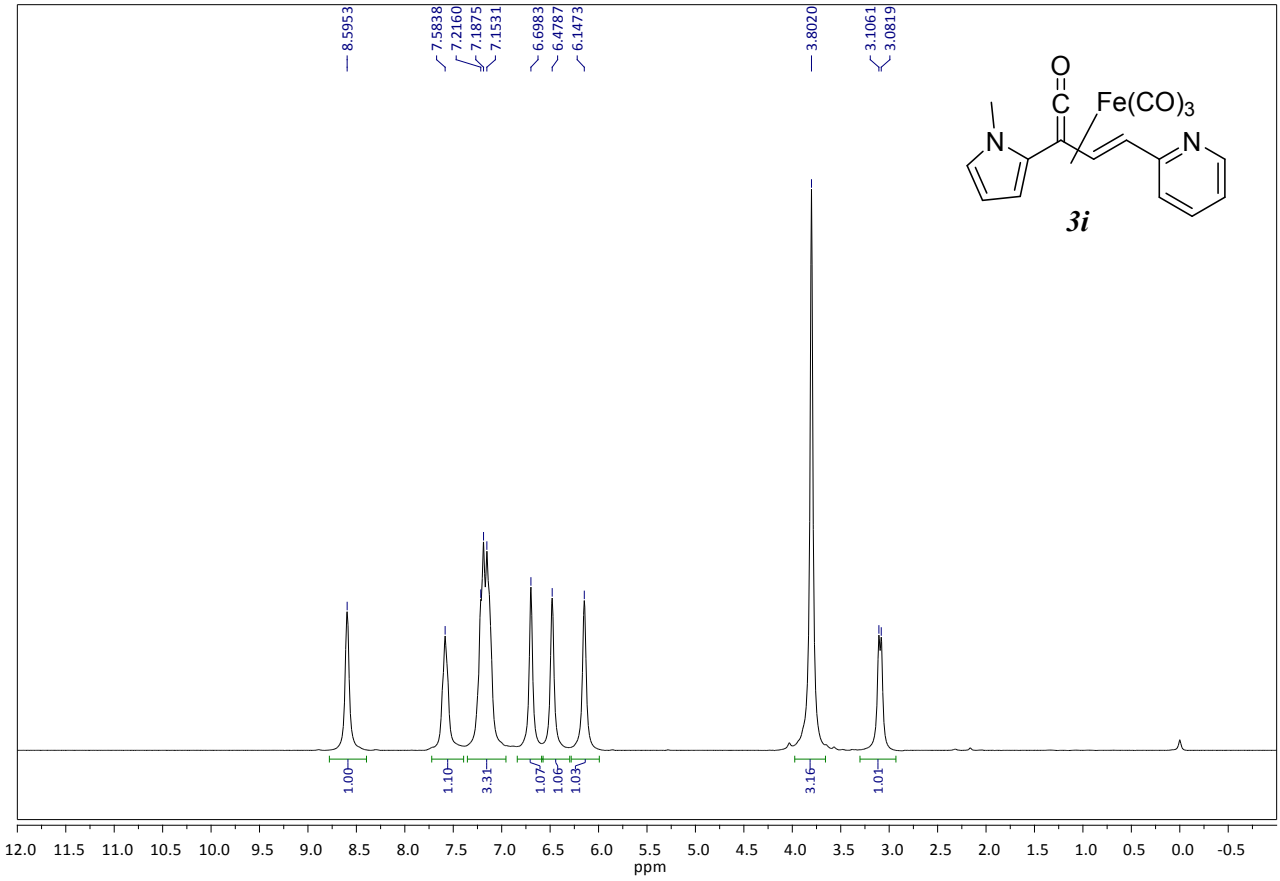

234.76
160.42
157.77
149.94
136.87
129.02
123.14
122.08
121.90
115.02
93.49
77.58
77.16
76.74
57.35
55.54
51.96
ppm

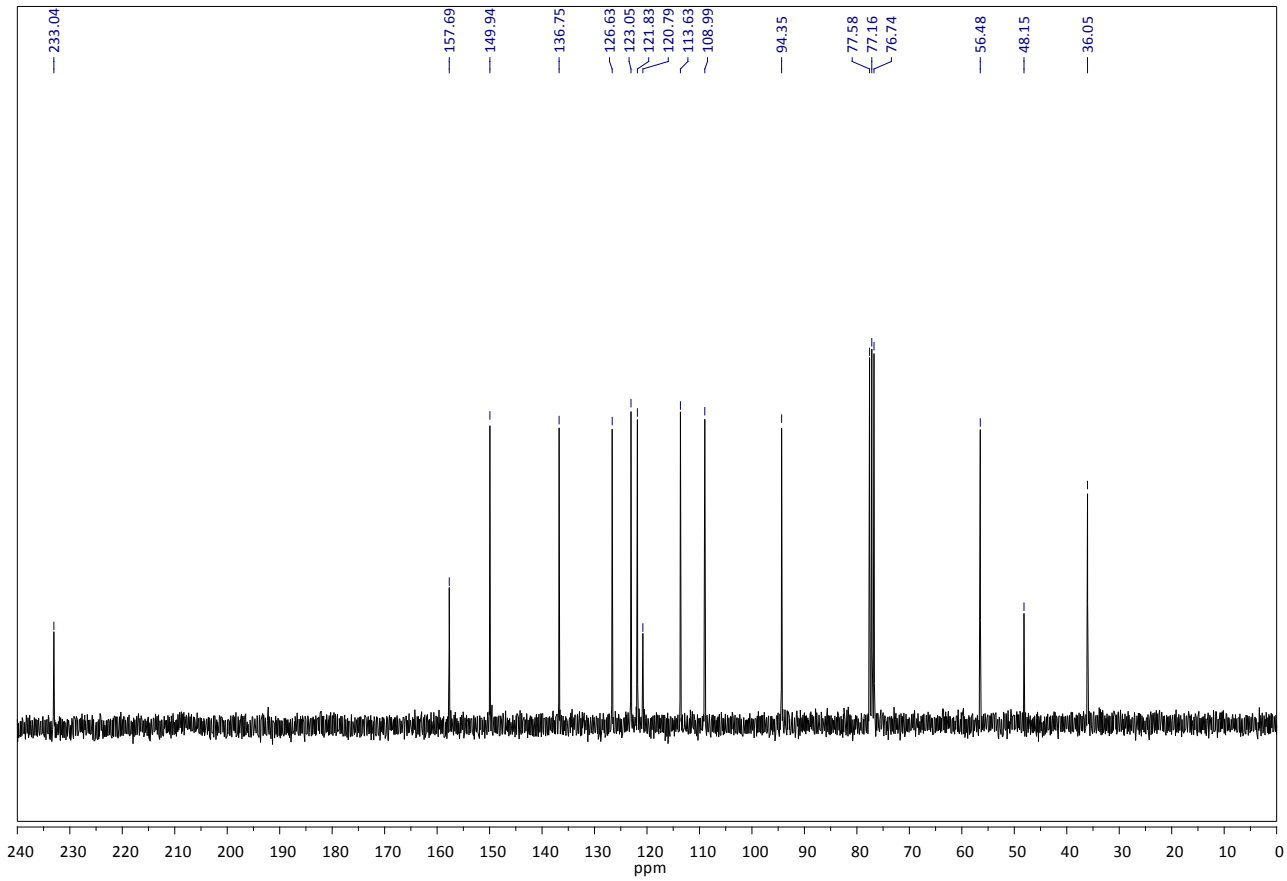

8.6381
7.7495
7.7248
7.6429
7.6207
7.6008
7.5054
7.4799
7.4585
7.4371
7.3960
7.3763
7.2597
7.2388
7.1666
3.3270
3.2998
O
C
Fe(CO)3
N
3g
1.00
16.18
1.01
ppm

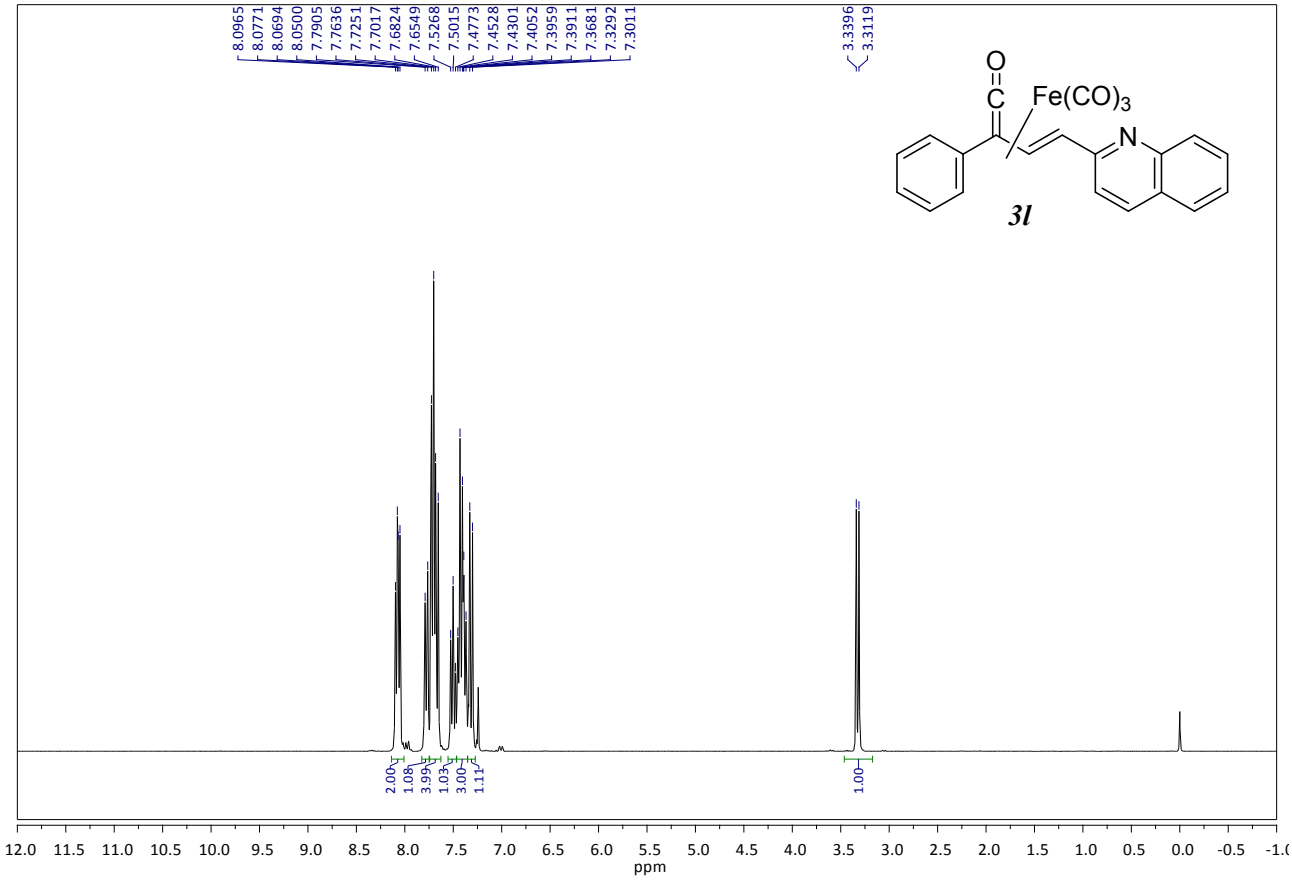

233.83
157.42
149.98
141.83
140.22
136.92
129.91
129.03
128.04
127.89
127.13
123.16
122.03
93.98
77.58
77.16
76.74
58.02
50.97
ppm

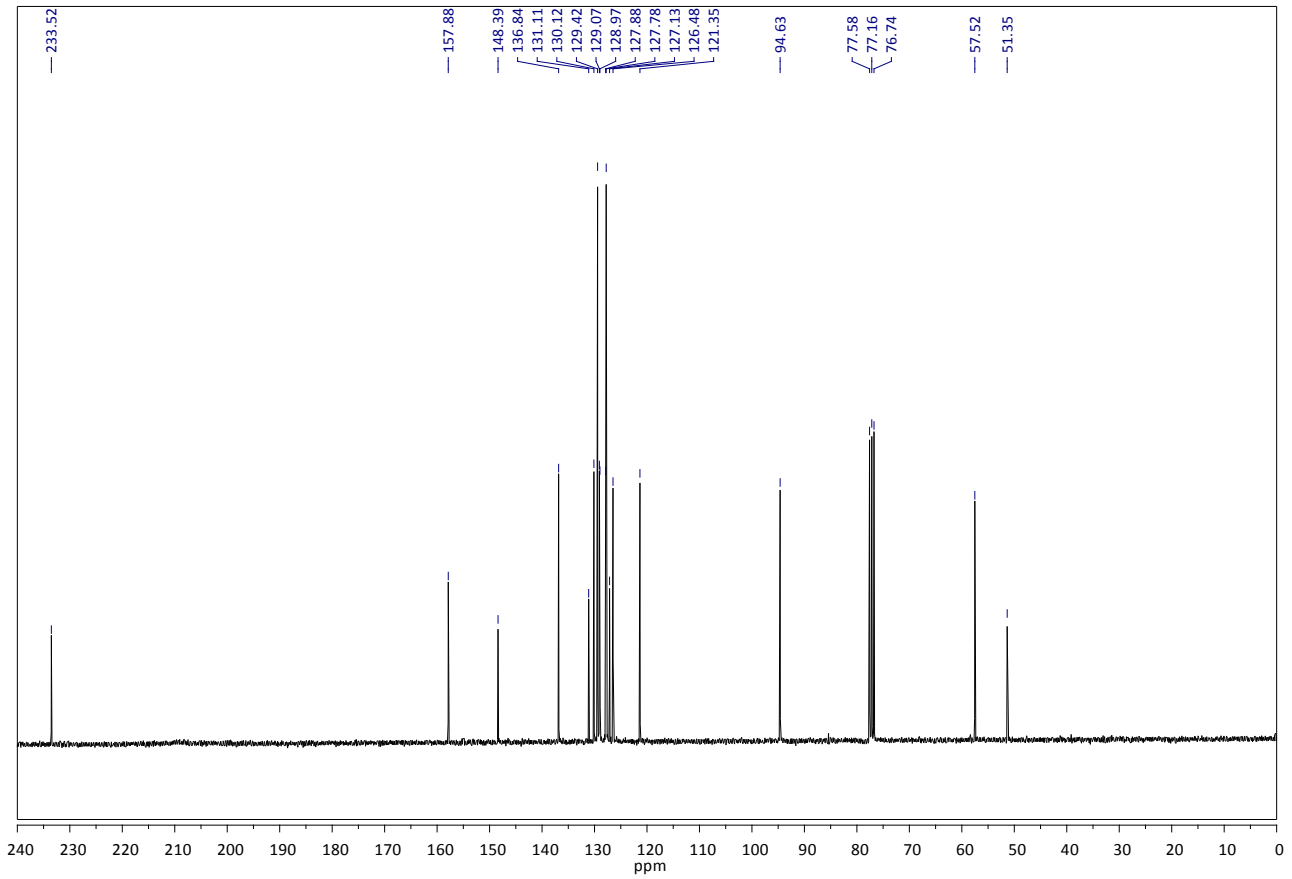

8.6493
8.6352
8.1955
7.8808
7.8520
7.8315
7.8201
7.8120
7.8007
7.7122
7.7066
7.6836
7.6779
7.6084
7.6029
7.5770
7.5678
7.5397
7.5170
7.5063
7.4963
7.4856
7.2553
7.2294
7.1574
3.3134
O
C
Fe(CO)3
N
3h
1.00
1.02
3.18
1.03
4.15
1.18
1.03
1.01
ppm


157.46
149.98
136.90
133.52
133.34
129.36
128.20
127.94
127.36
127.07
127.01
124.18
123.17
122.02
94.13
77.58
77.16
76.74
57.99
50.89
ppm

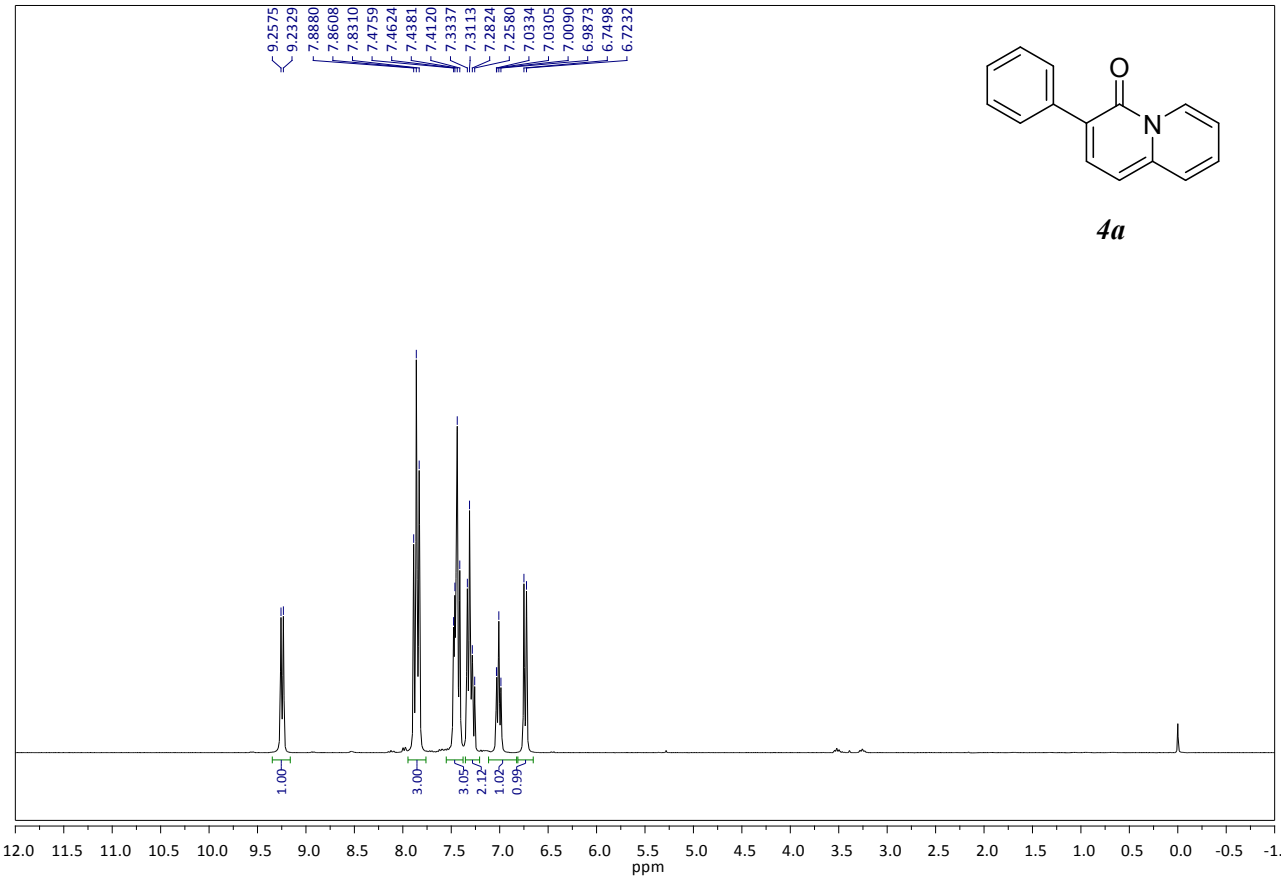

8.5953
7.5838
7.2160
7.1875
7.1531
6.6983
6.4787
6.1473
3.8020
3.1061
3.0819
1.00
1.10
3.31
1.07
1.06
1.03
3.16
1.01
O
C
Fe(CO)3
N
N
3i
ppm


233.04
157.69
149.94
136.75
126.63
123.05
121.83
120.79
113.63
108.99
94.35
77.58
77.16
76.74
56.48
48.15
36.05
ppm

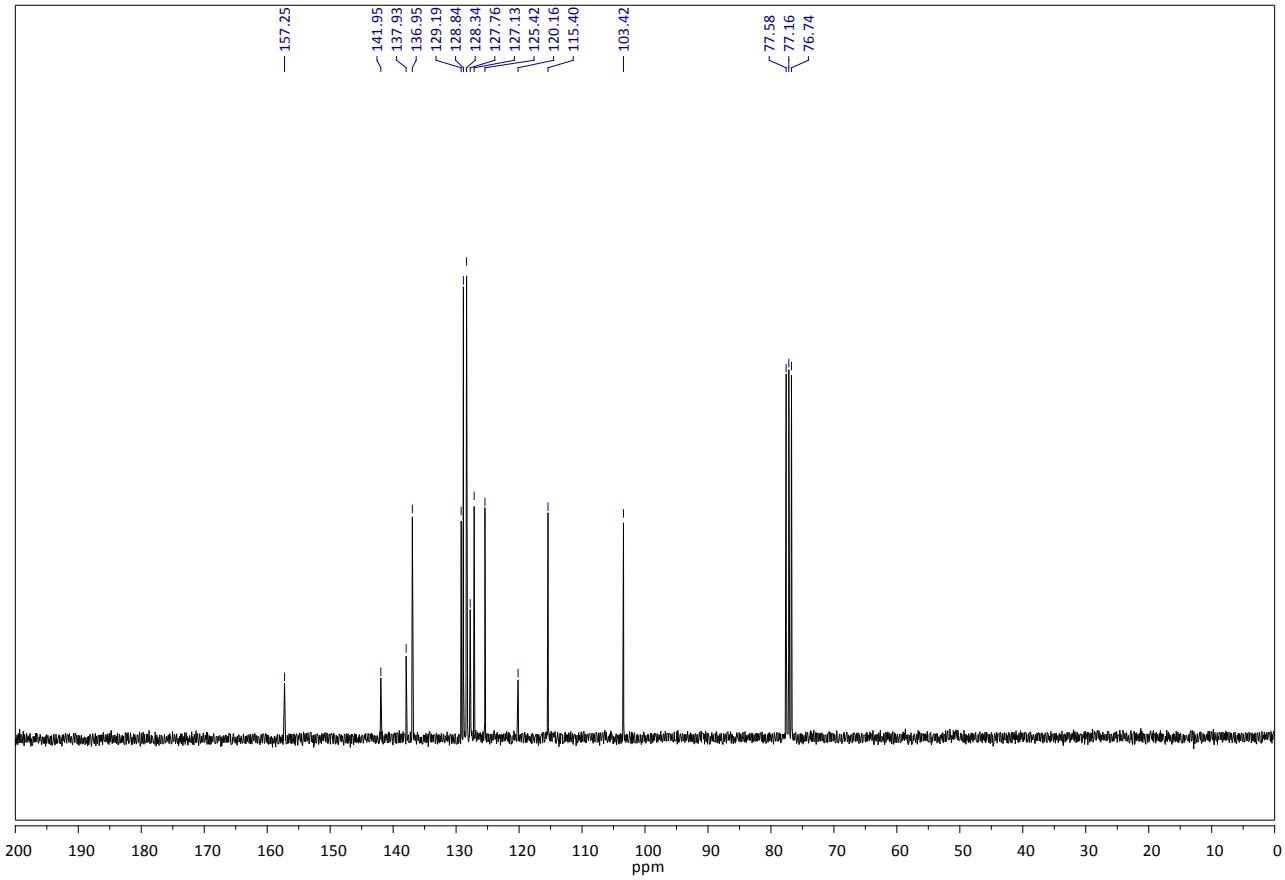

8.0965
8.0771
8.0694
8.0500
7.7905
7.7636
7.7251
7.7017
7.6824
7.6549
7.5268
7.5015
7.4773
7.4528
7.4301
7.4052
7.3959
7.3911
7.3681
7.3292
7.3011
3.3396
3.3119
O
C
Fe(CO)3
N
3l
2.00
1.08
3.99
1.03
3.00
1.11
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

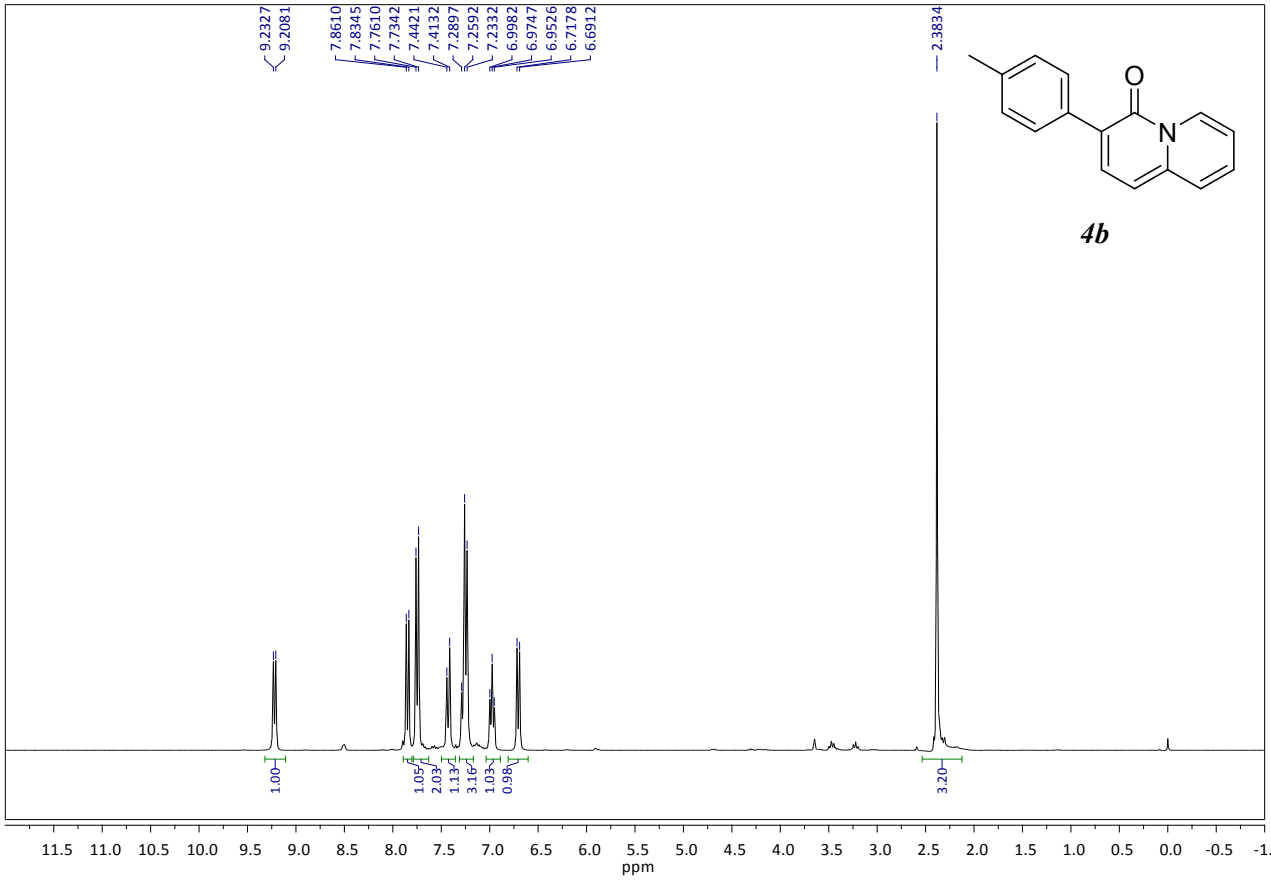

233.52
157.88
148.39
136.84
131.11
130.12
129.42
129.07
128.97
127.88
127.78
127.13
126.48
121.35
94.63
77.58
77.16
76.74
57.52
51.35
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

1.4 Spectra of compounds 4a-l.

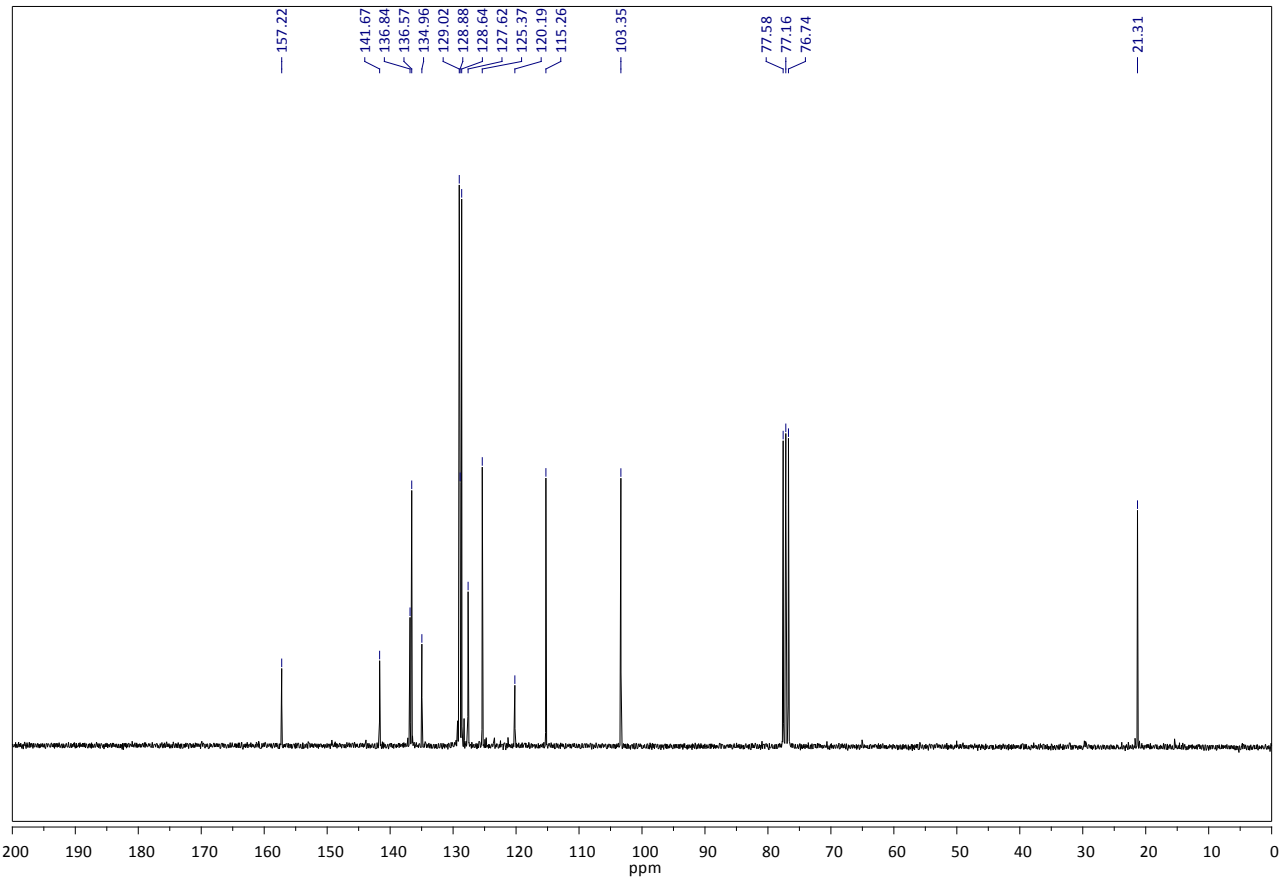


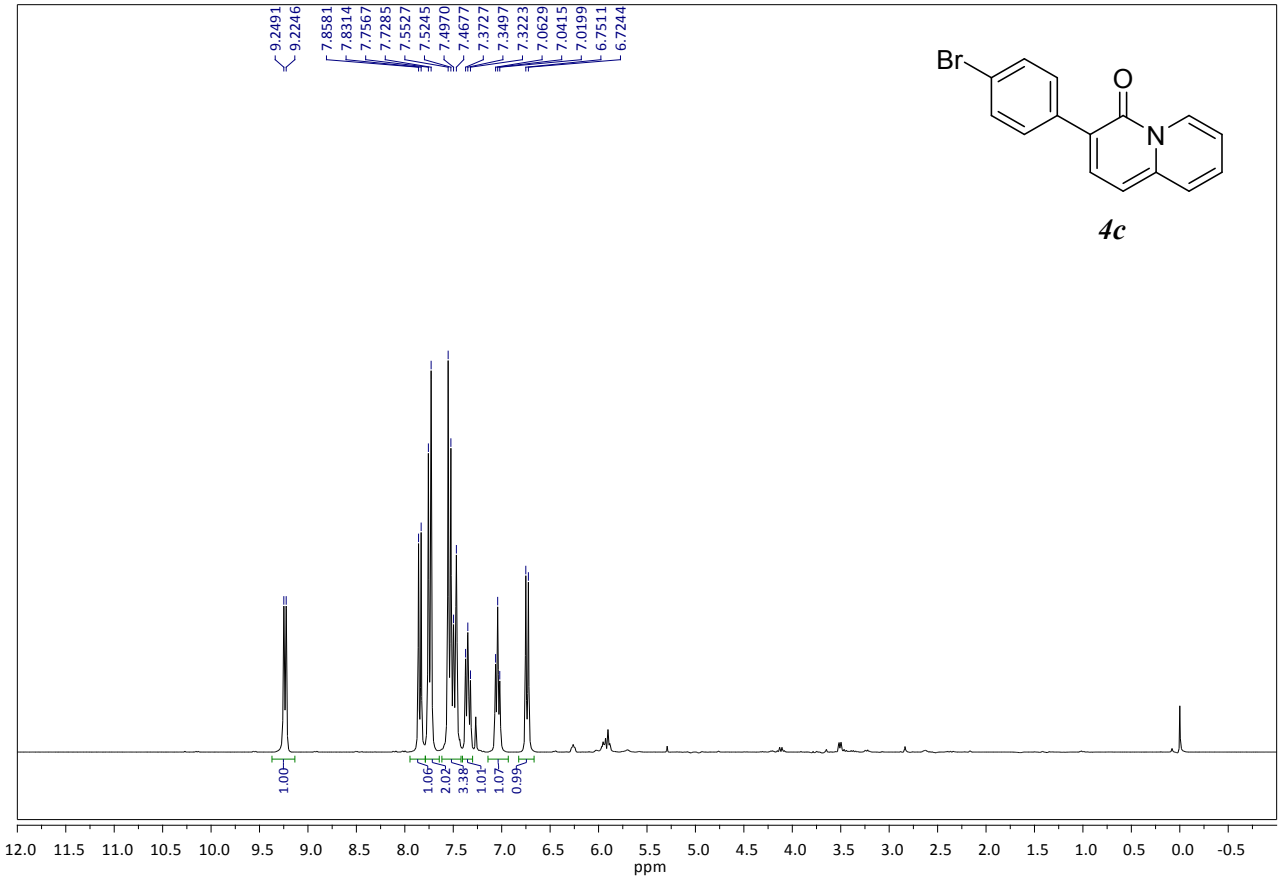
4a



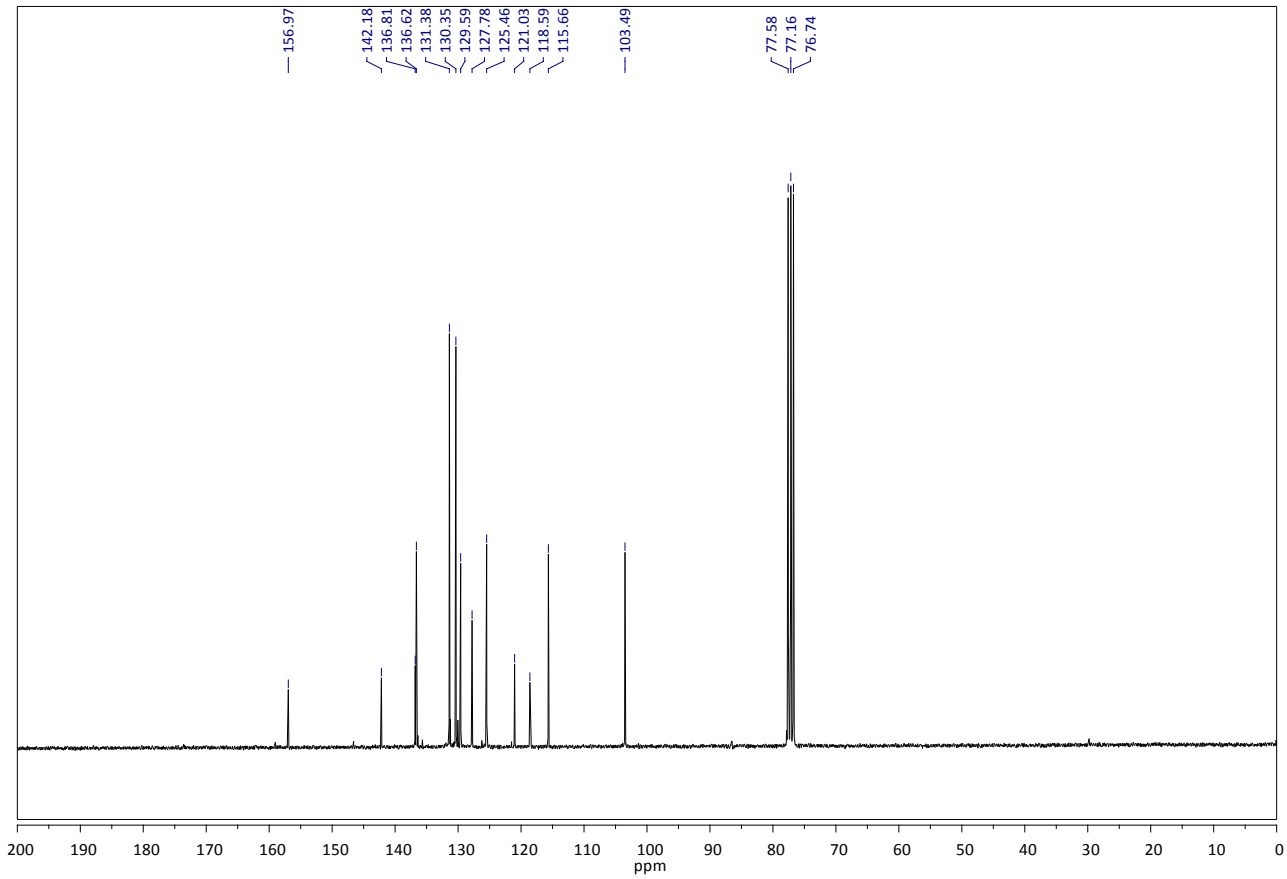

9.2327
9.2081
7.8610
7.8345
7.7610
7.7342
7.4421
7.4132
7.2897
7.2592
7.2332
6.9982
6.9747
6.9526
6.7178
6.6912
2.3834
O
N
1.00
1.05
2.03
1.13
3.16
1.03
0.98
3.20
ppm

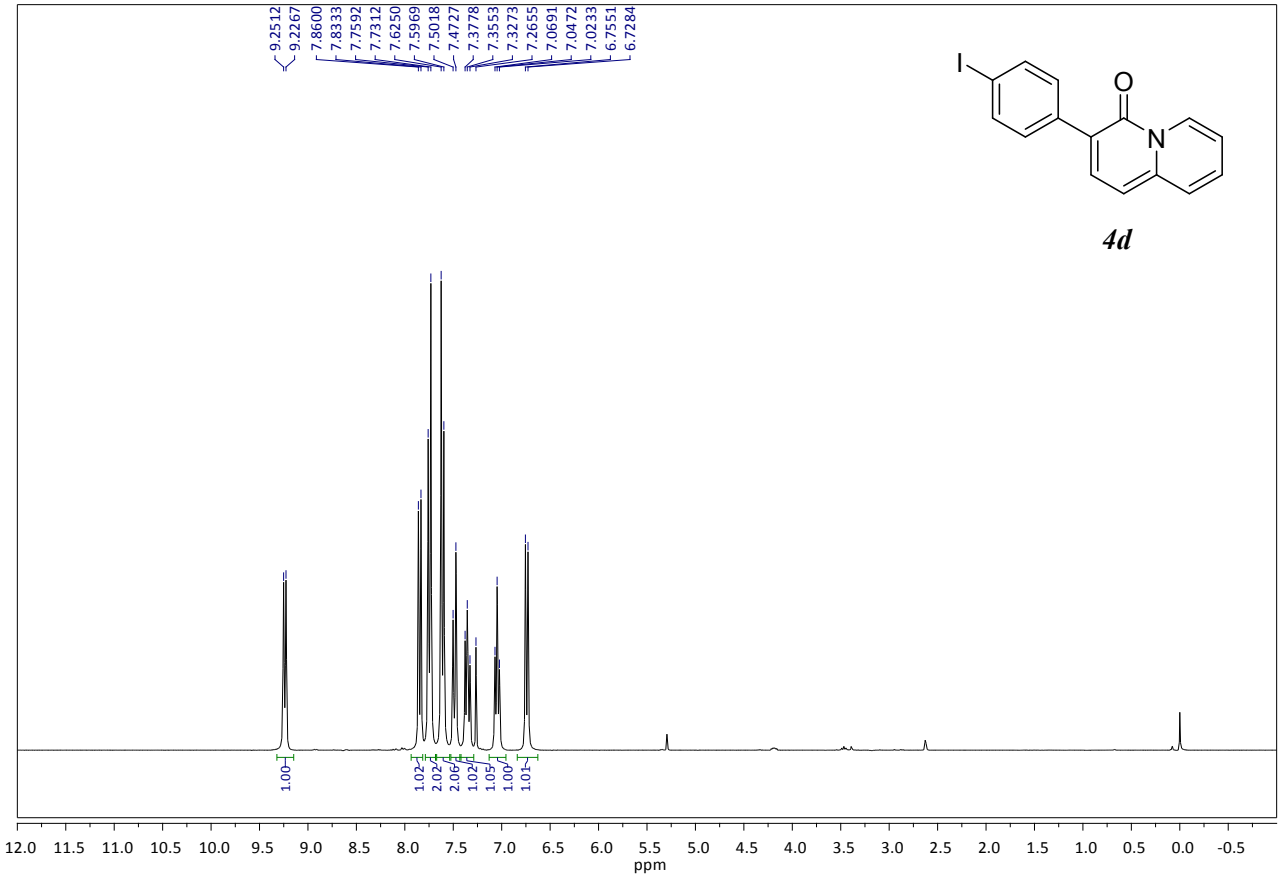
4b


157.22
141.67
136.84
136.57
134.96
129.02
128.88
128.64
127.62
125.37
120.19
115.26
103.35
77.58
77.16
76.74
21.31
ppm

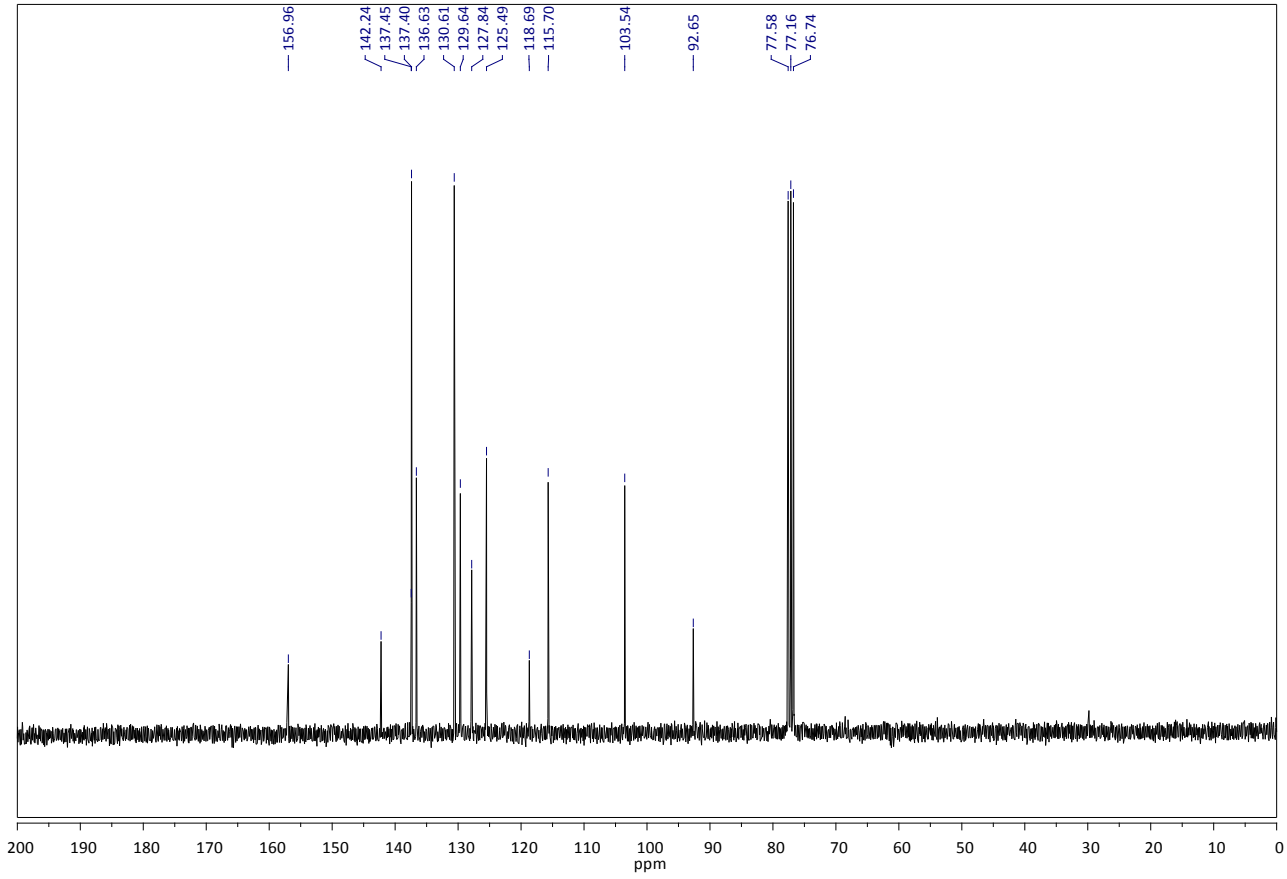

9.2491
9.2246
7.8581
7.8314
7.7567
7.7285
7.5527
7.5245
7.4970
7.4677
7.3727
7.3497
7.3223
7.0629
7.0415
7.0199
6.7511
6.7244
Br
O
N
1.00
1.06
2.02
3.38
1.01
1.07
0.99
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

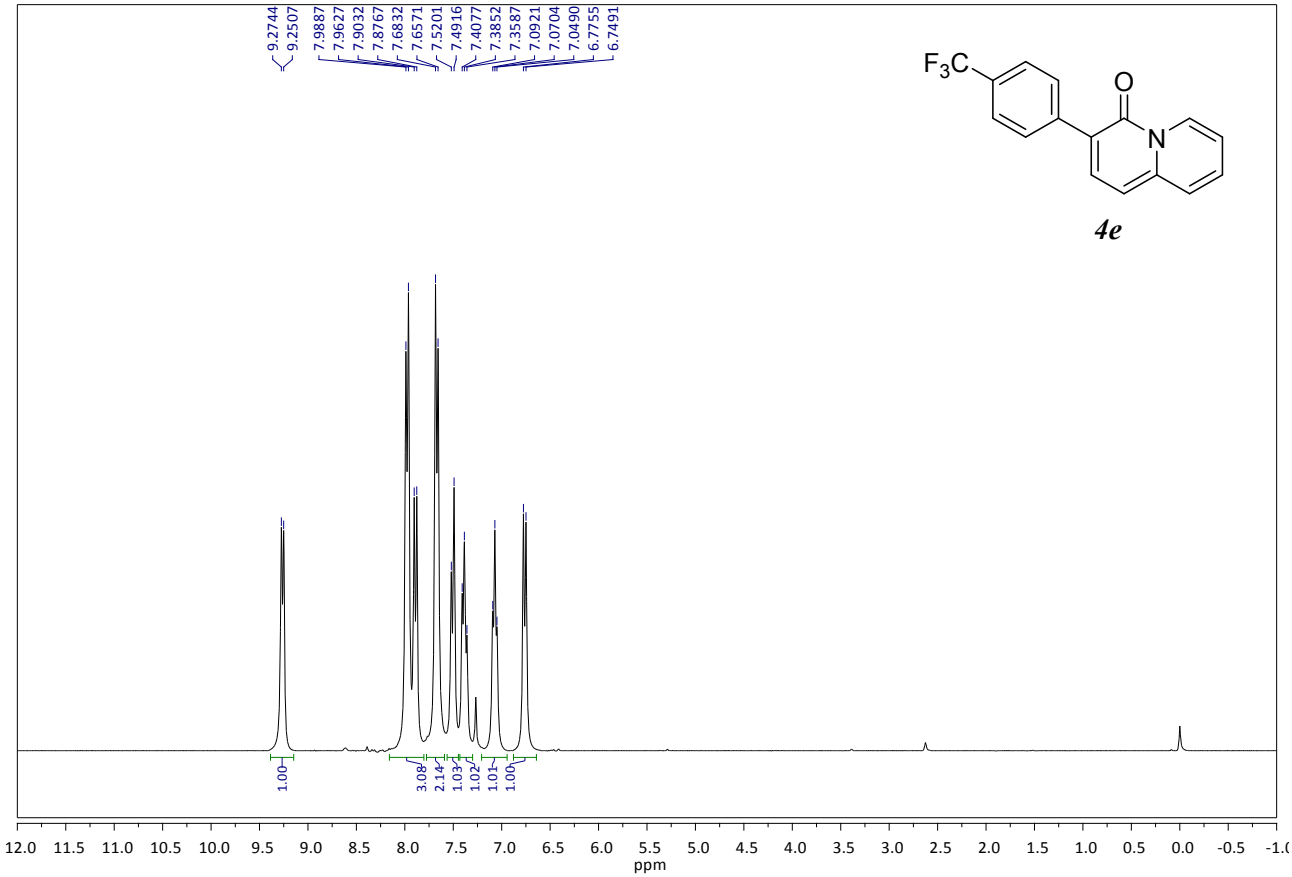
4c


156.97
142.18
136.81
136.62
131.38
130.35
129.59
127.78
125.46
121.03
118.59
115.66
103.49
77.58
77.16
76.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

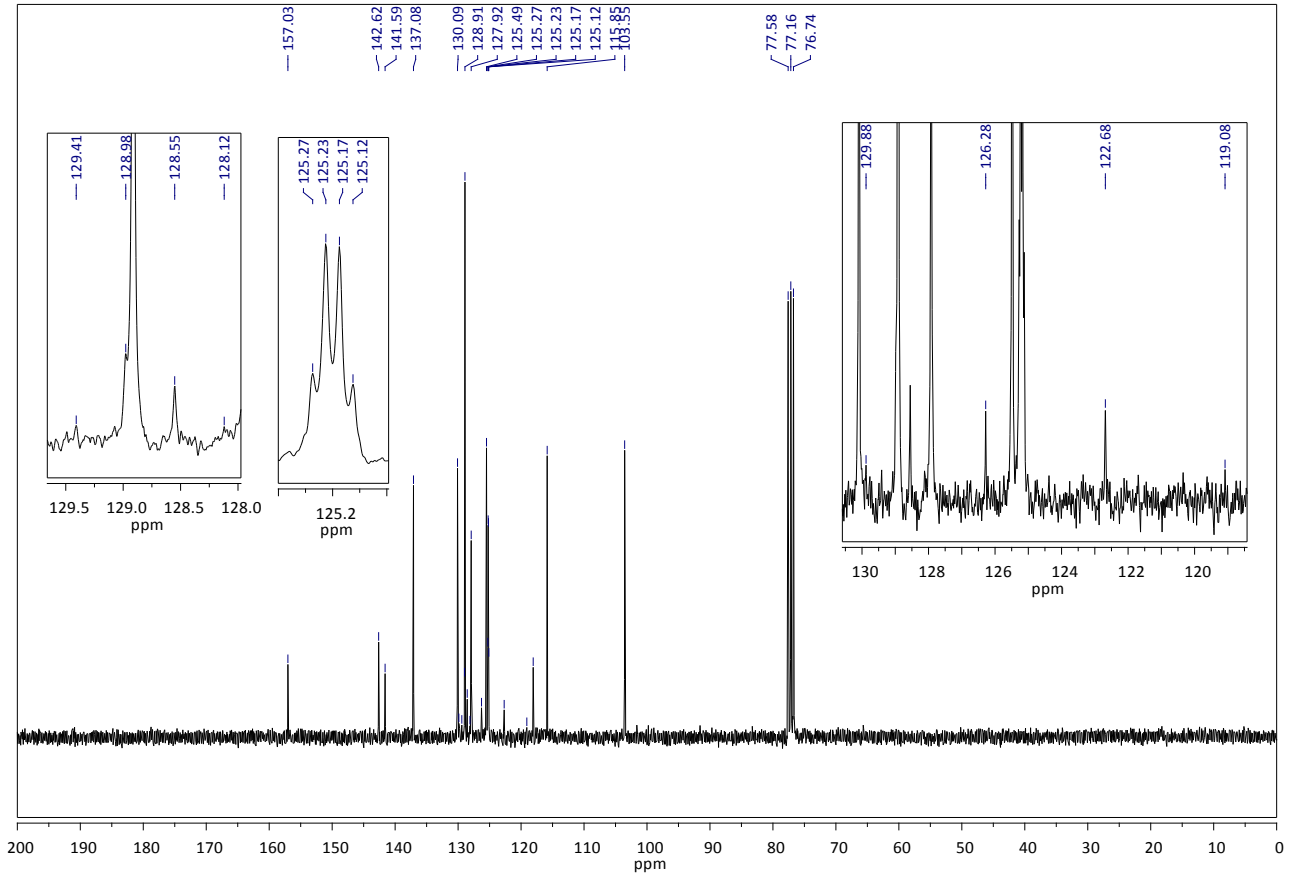

9.2512
9.2267
7.8600
7.8333
7.7592
7.7312
7.6250
7.5969
7.5018
7.4727
7.3778
7.3553
7.3273
7.2655
7.0691
7.0472
7.0233
6.7551
6.7284
I
O
N
1.00
1.02
2.02
2.06
1.02
1.05
1.00
1.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

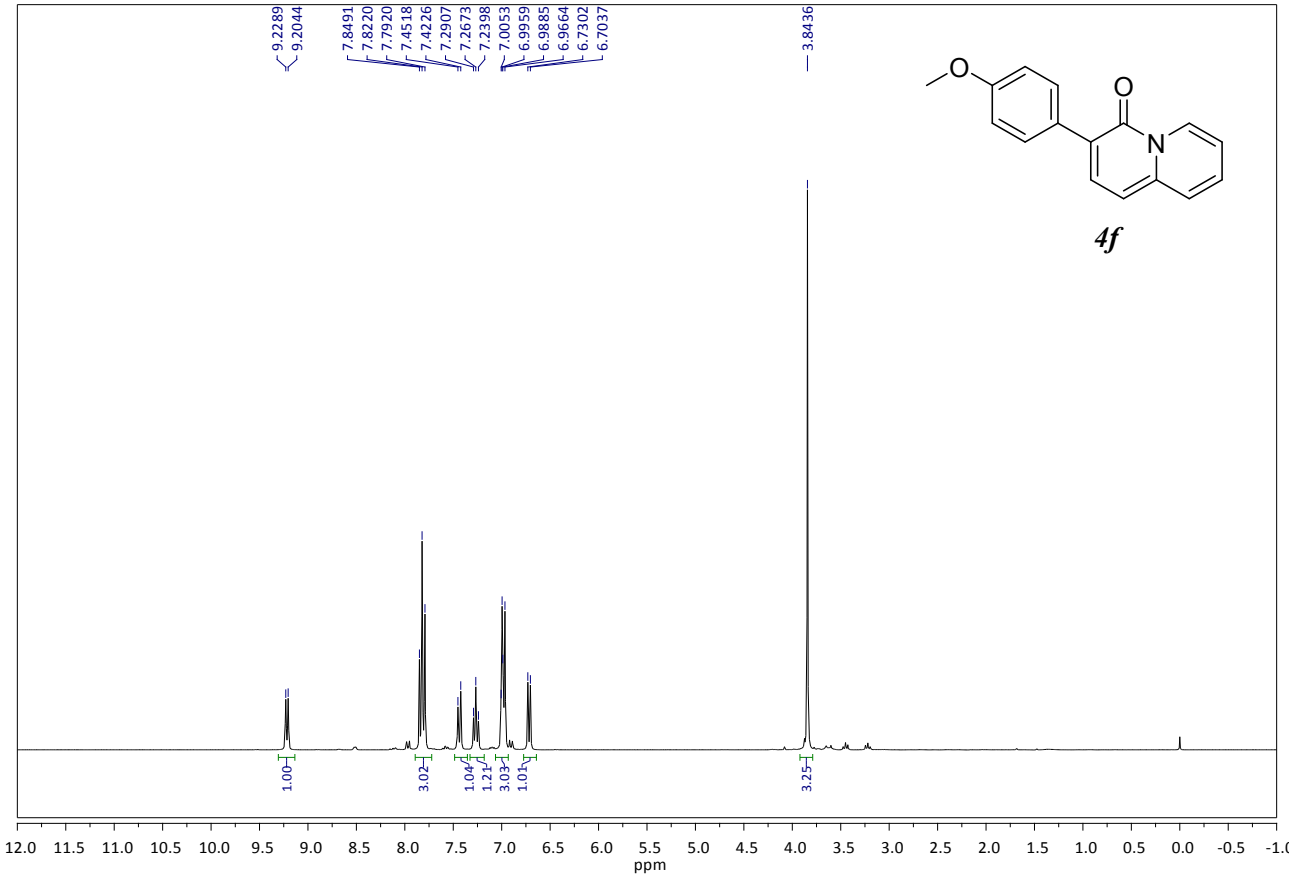
4d


156.96
142.24
137.45
137.40
136.63
130.61
129.64
127.84
125.49
118.69
115.70
103.54
92.65
77.58
77.16
76.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

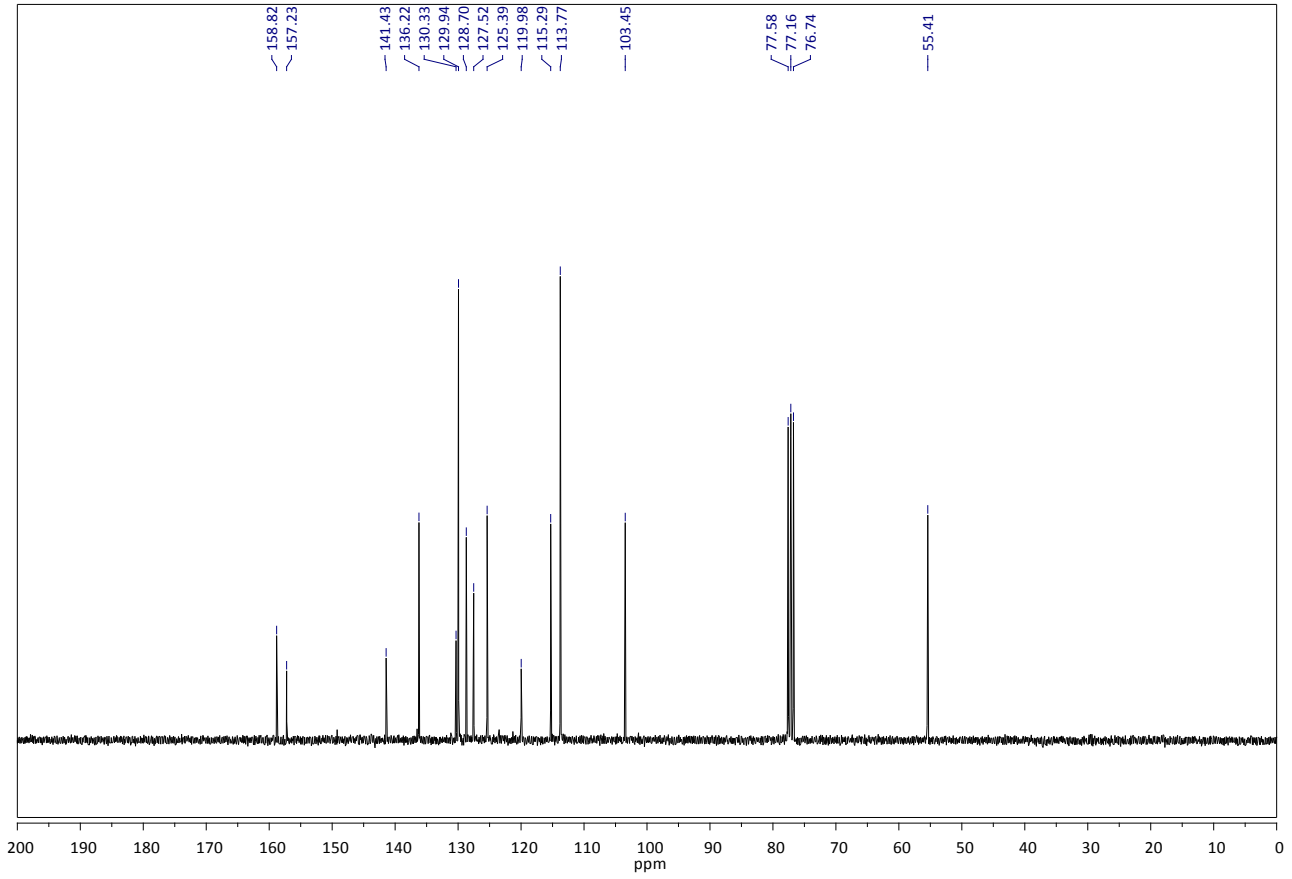

9.2744
9.2507
7.9887
7.9627
7.9032
7.8767
7.6832
7.6571
7.5201
7.4916
7.4077
7.3852
7.3587
7.0921
7.0704
7.0490
6.7755
6.7491
1.00
3.08
2.14
1.03
1.02
1.01
1.00
F3C
O
N
ppm

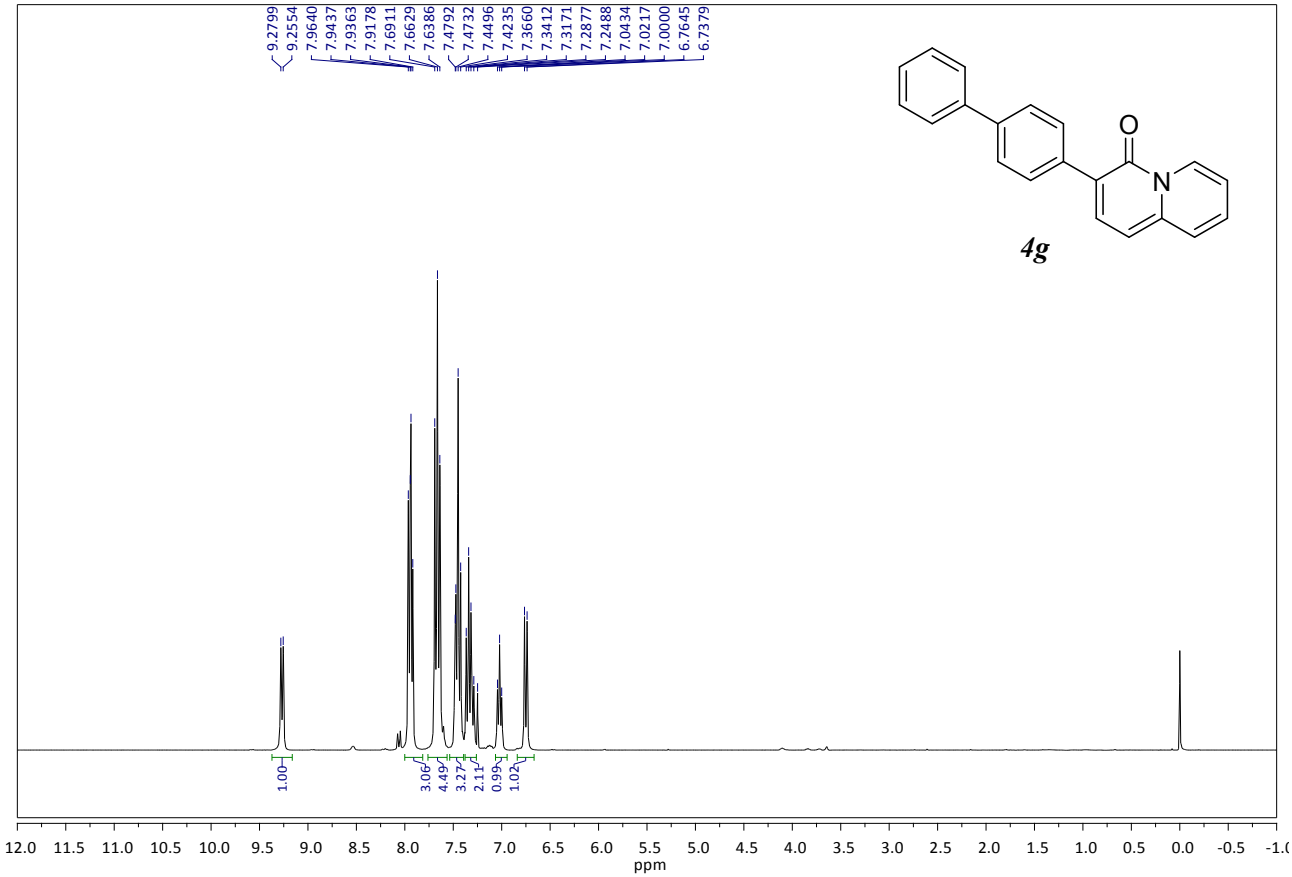
4e


157.03
142.62
141.59
137.08
130.09
128.91
127.92
125.49
125.27
125.23
125.17
125.12
77.58
77.16
76.74
129.41
128.98
128.55
128.12
129.5
129.0
128.5
128.0
ppm
125.27
125.23
125.17
125.12
125.2
ppm
129.88
126.28
122.68
119.08
130
128
126
124
122
120
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

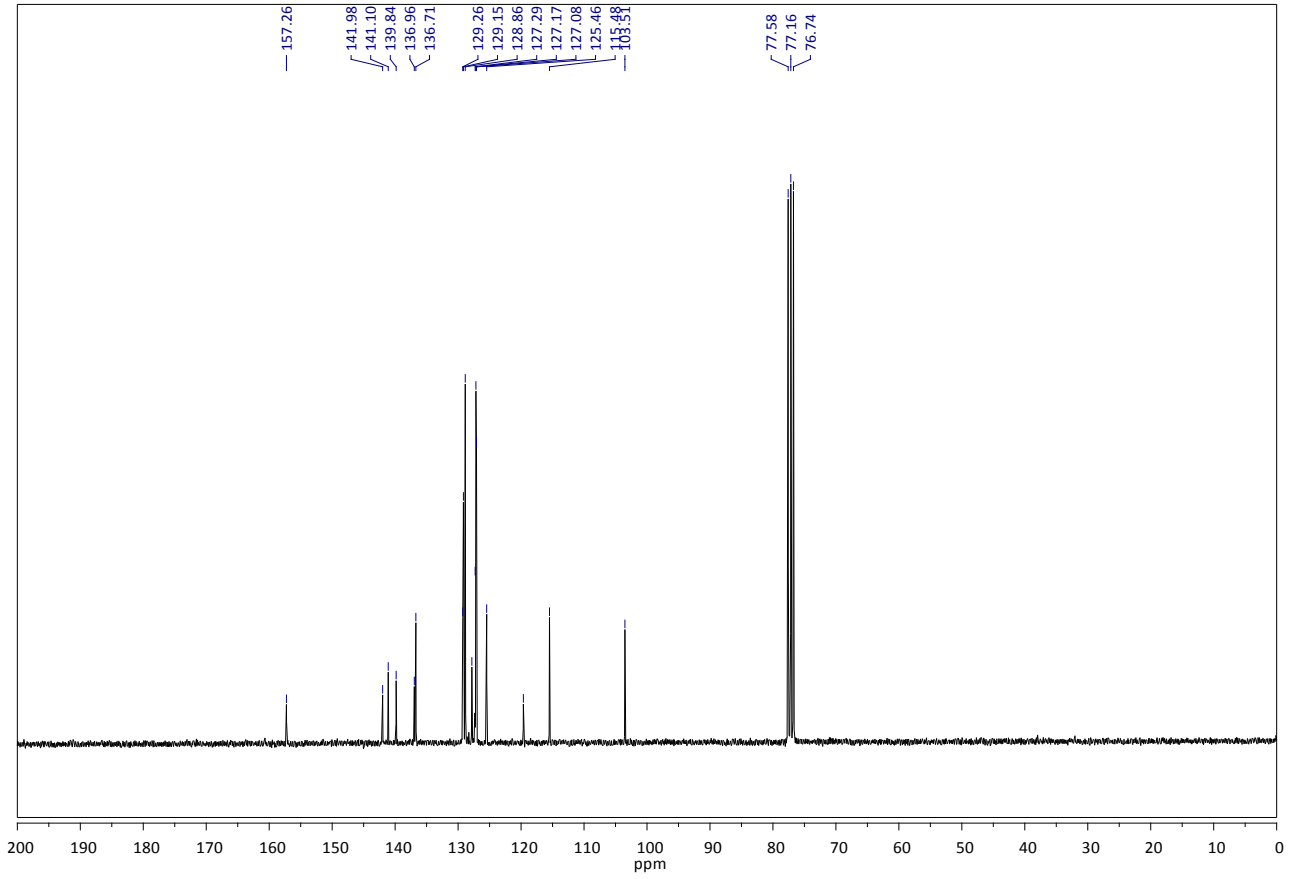

9.2289
9.2044
7.8491
7.8220
7.7920
7.4518
7.4426
7.2907
7.2673
7.2398
7.0053
6.9959
6.9885
6.9664
6.7302
6.7037
3.8436
1.00
3.02
1.04
1.21
3.03
1.01
3.25
ppm

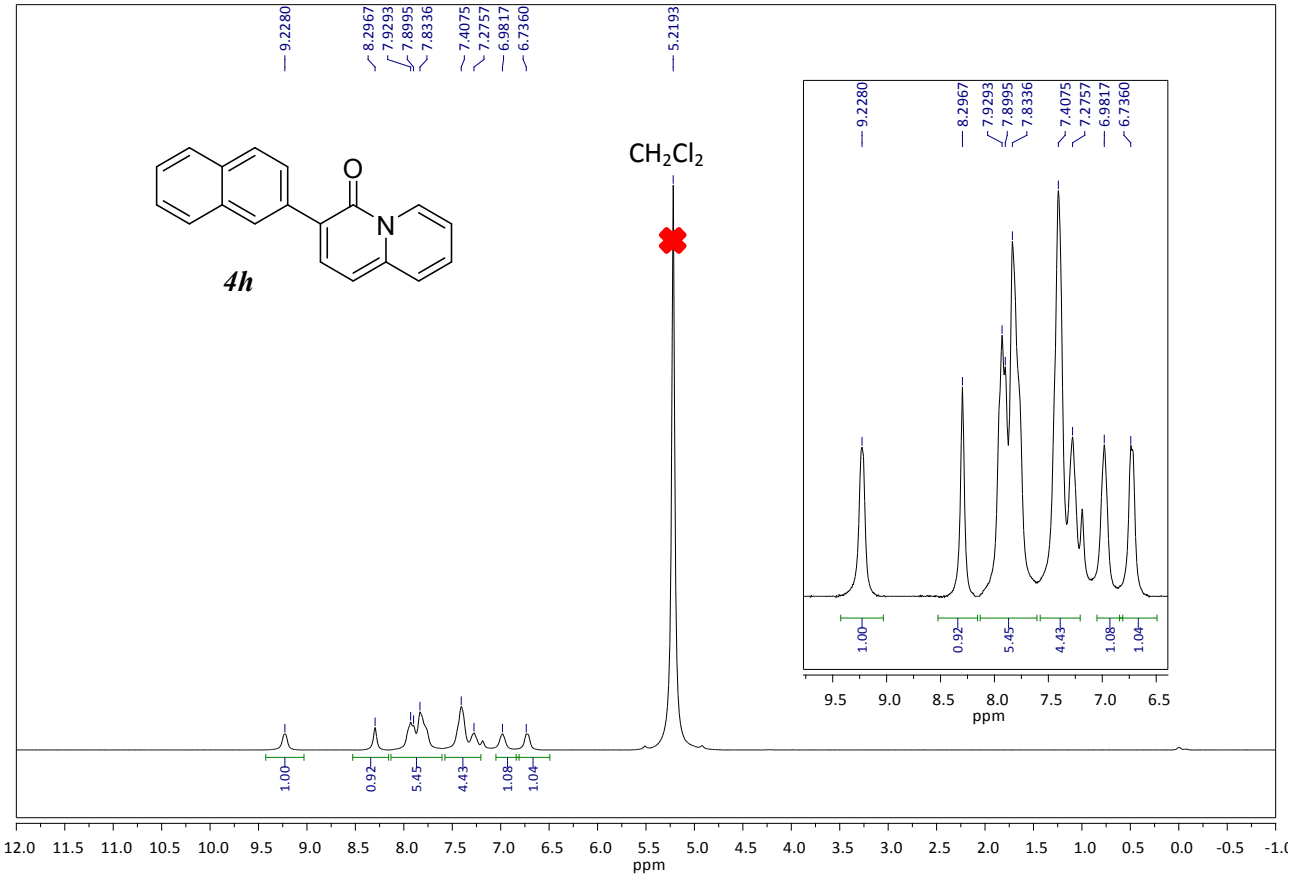
4f

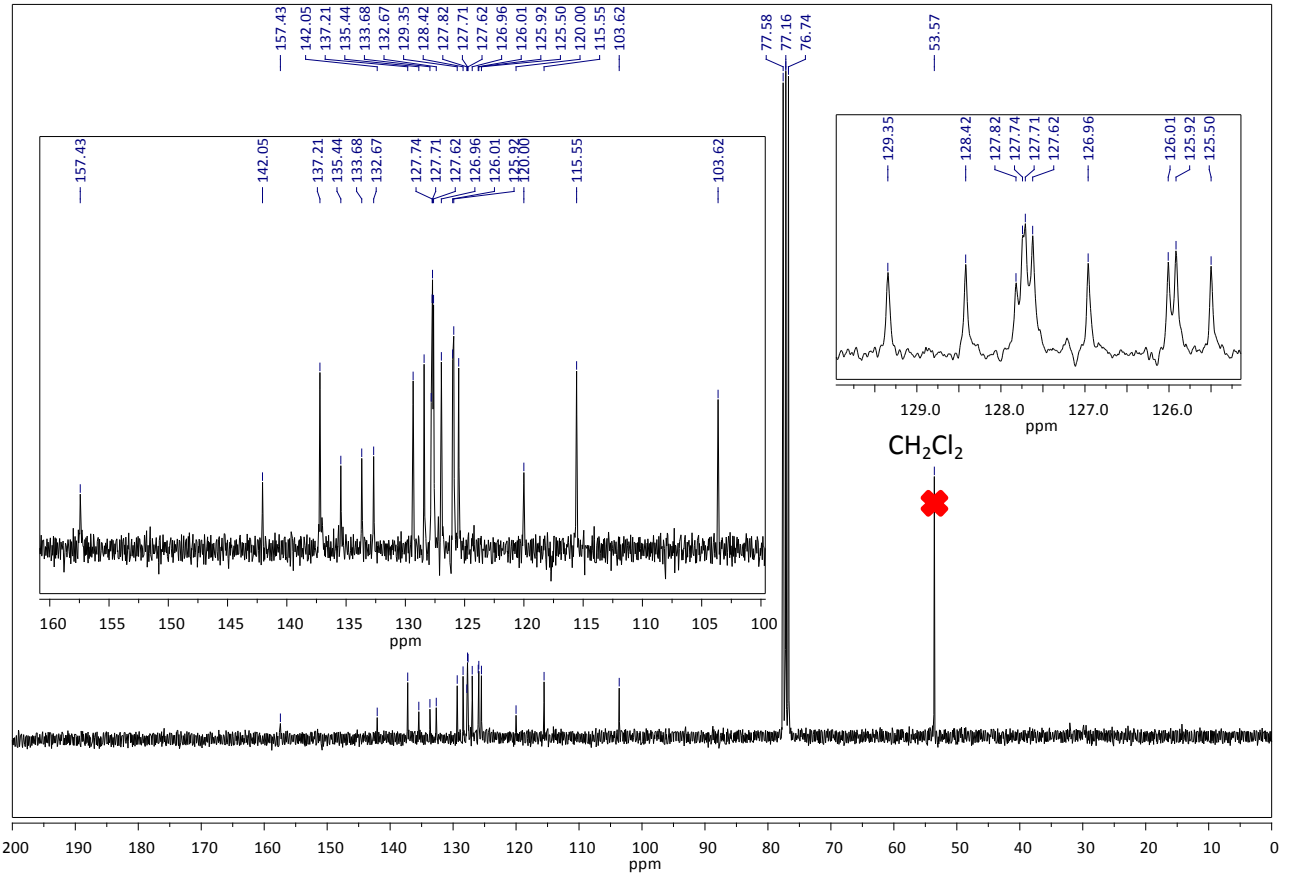

158.82
157.23
141.43
136.22
130.33
129.94
128.70
127.52
125.39
119.98
115.29
113.77
103.45
77.58
77.16
76.74
55.41
ppm

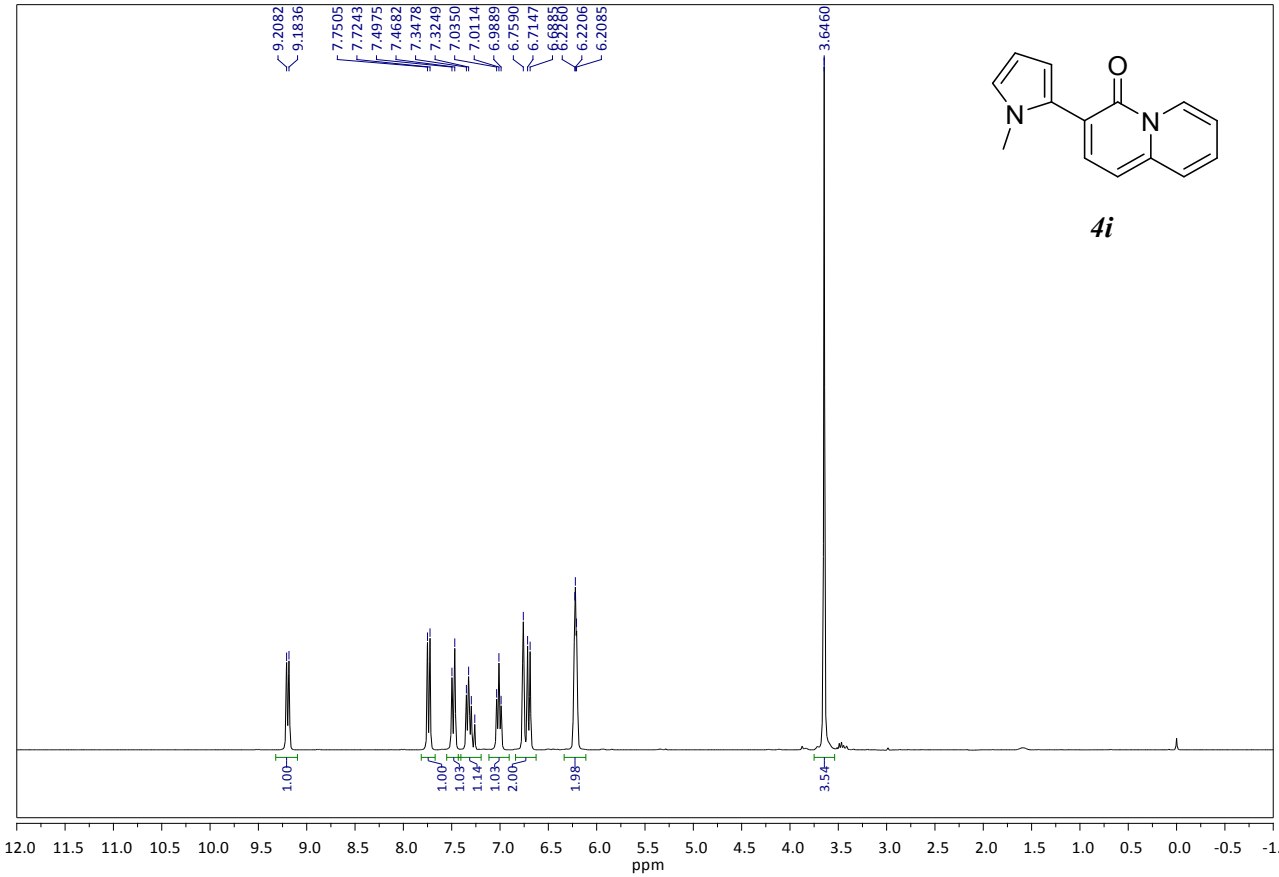

9.2799
9.2554
7.9640
7.9437
7.9363
7.9178
7.6911
7.6629
7.6386
7.4792
7.4732
7.4496
7.4235
7.3660
7.3412
7.3171
7.2877
7.2488
7.0434
7.0217
7.0000
6.7645
6.7379
O
N
1.00
3.06
4.49
3.27
2.11
0.99
1.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

4g


157.26
141.98
141.10
139.84
136.96
136.71
129.26
129.15
128.86
127.29
127.17
127.08
125.46
115.48
103.51
77.58
77.16
76.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

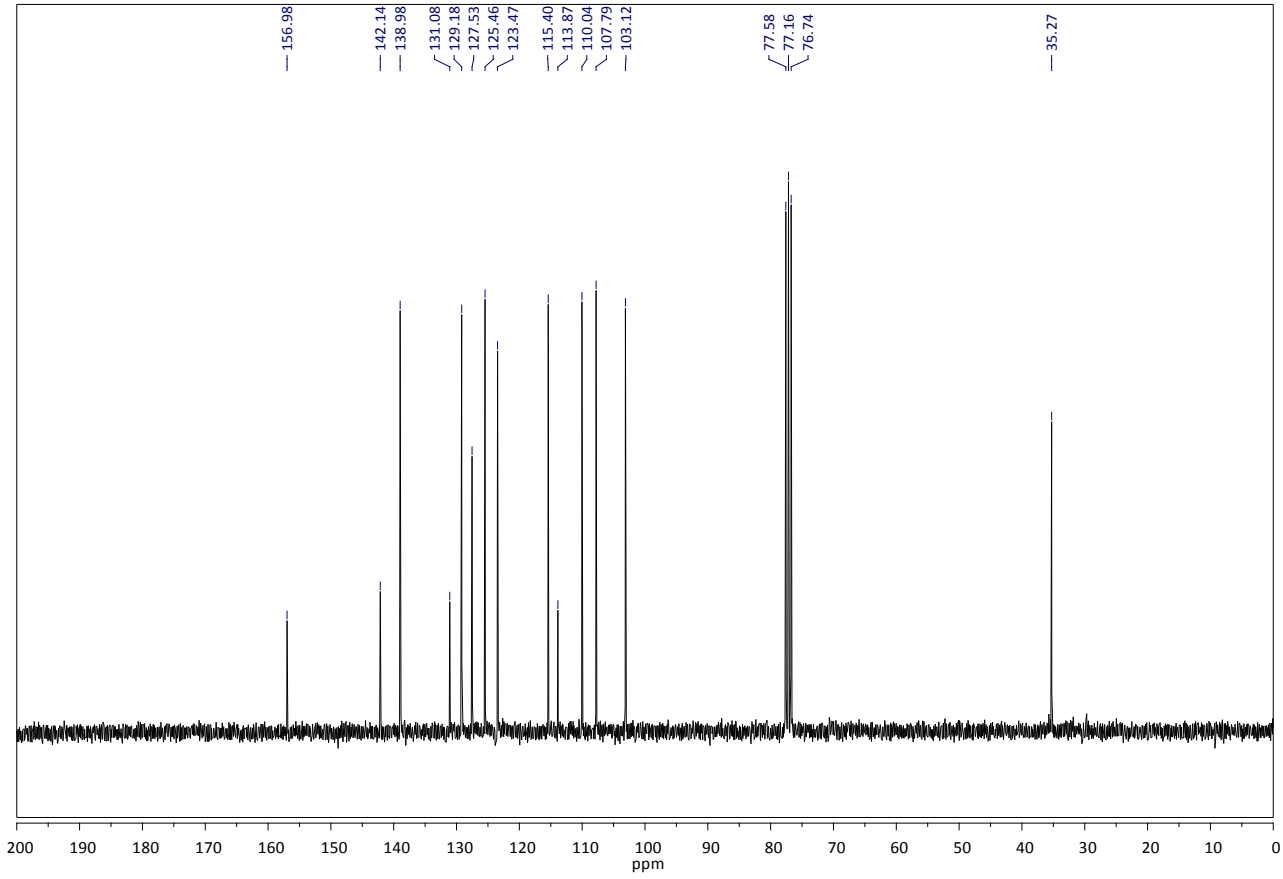

9.2280
8.2967
7.9293
7.8995
7.8336
7.4075
7.2757
6.9817
6.7360
5.2193
CH2Cl2
4h
1.00
0.92
5.45
4.43
1.08
1.04
ppm

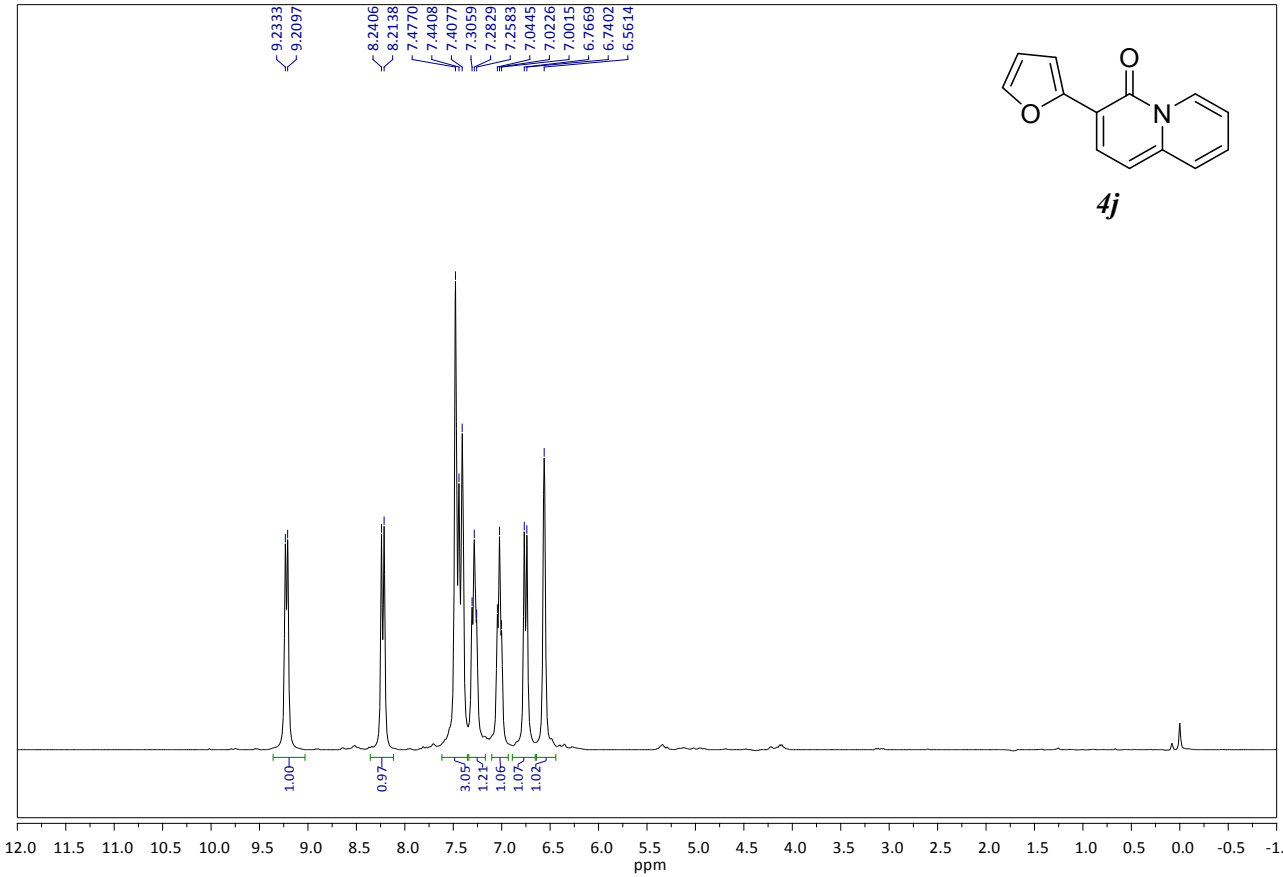

157.43
142.05
137.21
135.44
133.68
132.67
129.35
128.42
127.82
127.71
127.62
126.96
126.01
125.92
125.50
120.00
115.55
103.62
77.58
77.16
76.74
53.57
CH2Cl2
ppm


9.2082
9.1836
7.7505
7.7243
7.4975
7.4682
7.3478
7.3249
7.0350
7.0114
6.9889
6.7590
6.7147
6.6885
6.6660
6.2206
6.2085
3.6460
1.00
1.00
1.03
1.14
1.03
2.00
1.98
3.54
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 -0.5
ppm

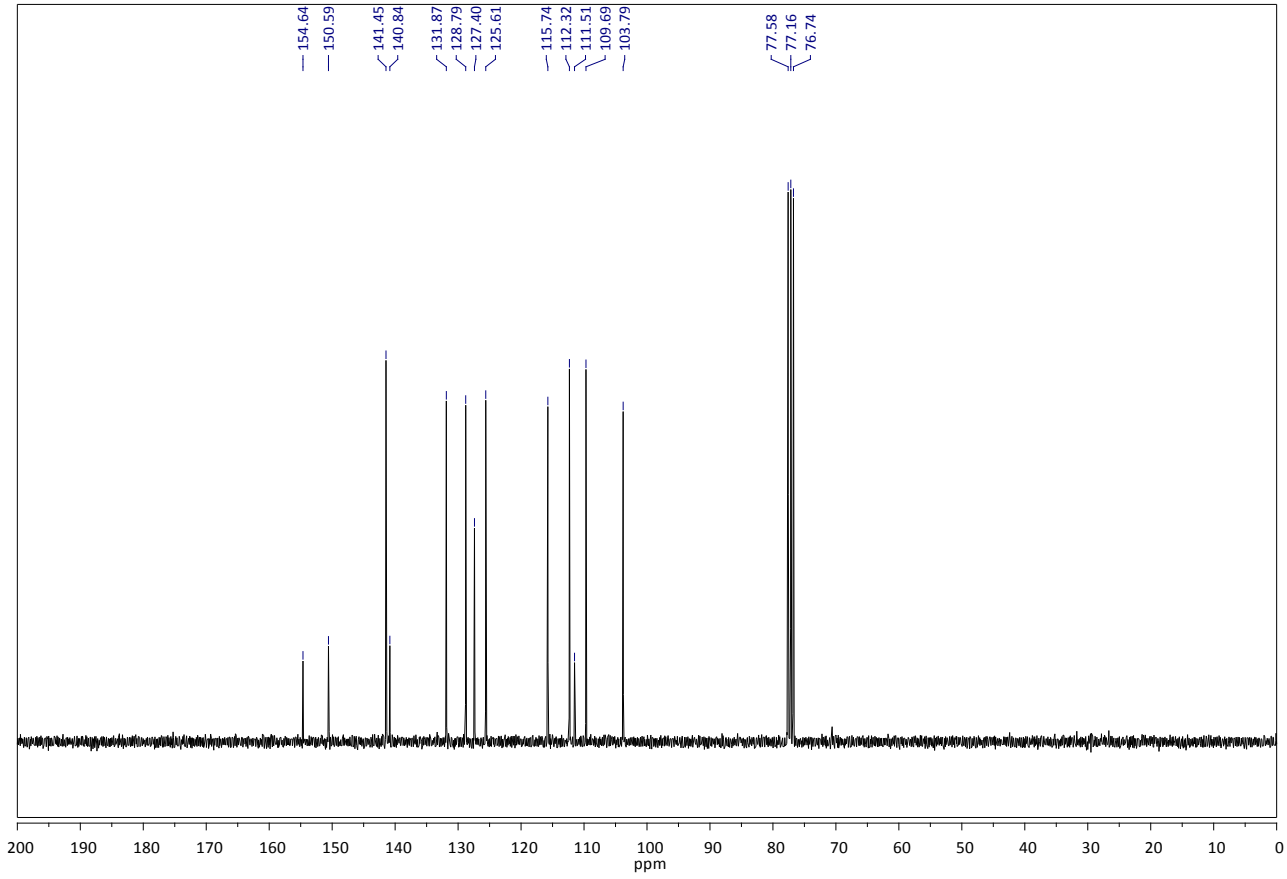
O
N
N

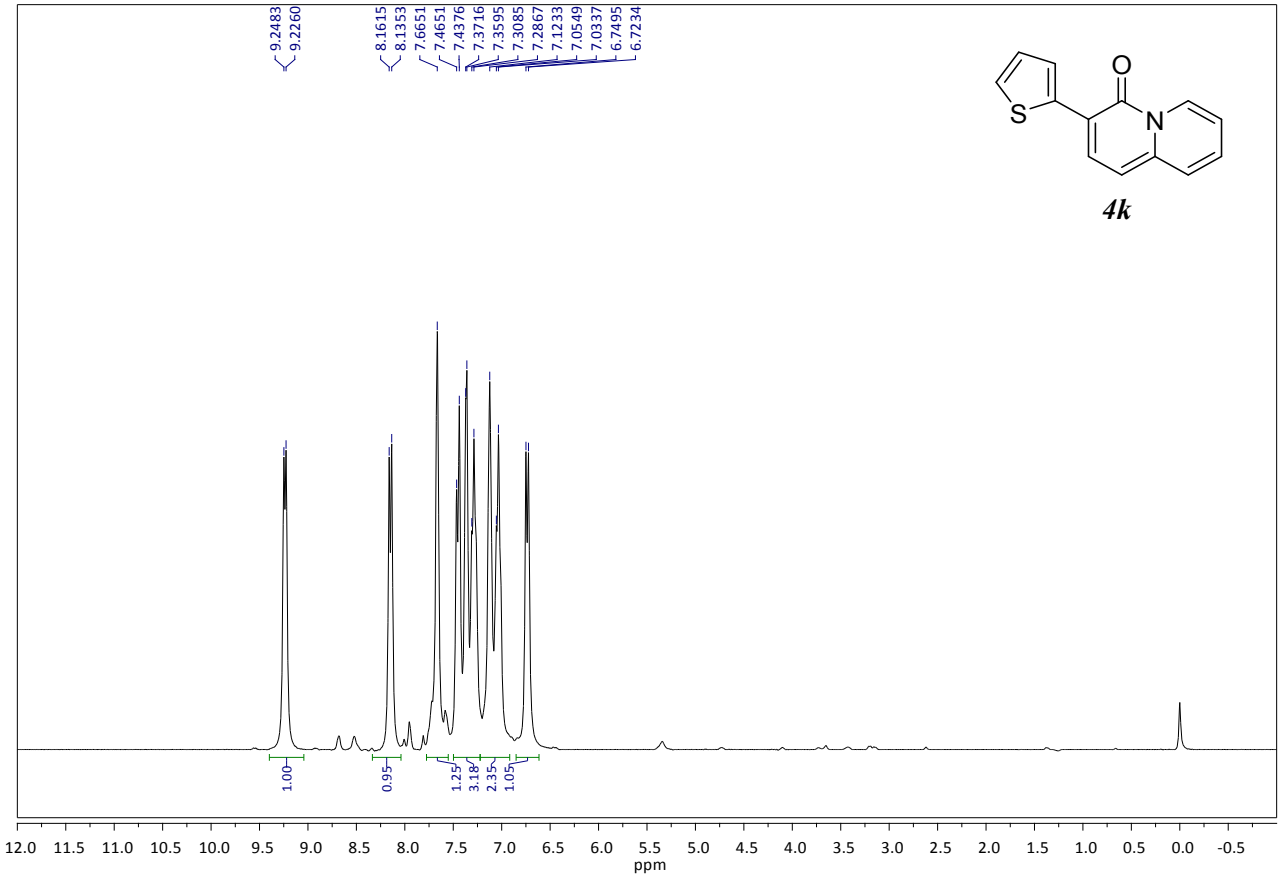
4i


156.98
142.14
138.98
131.08
129.18
127.53
125.46
123.47
115.40
113.87
110.04
107.79
103.12
77.58
77.16
76.74
35.27
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


9.2333
9.2097
8.2406
8.2138
7.4770
7.4408
7.4077
7.3059
7.2829
7.2583
7.0445
7.0226
7.0015
6.7669
6.7402
6.5614
O
O
N
1.00
0.97
3.05
1.21
1.06
1.07
1.02
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 -0.5
ppm

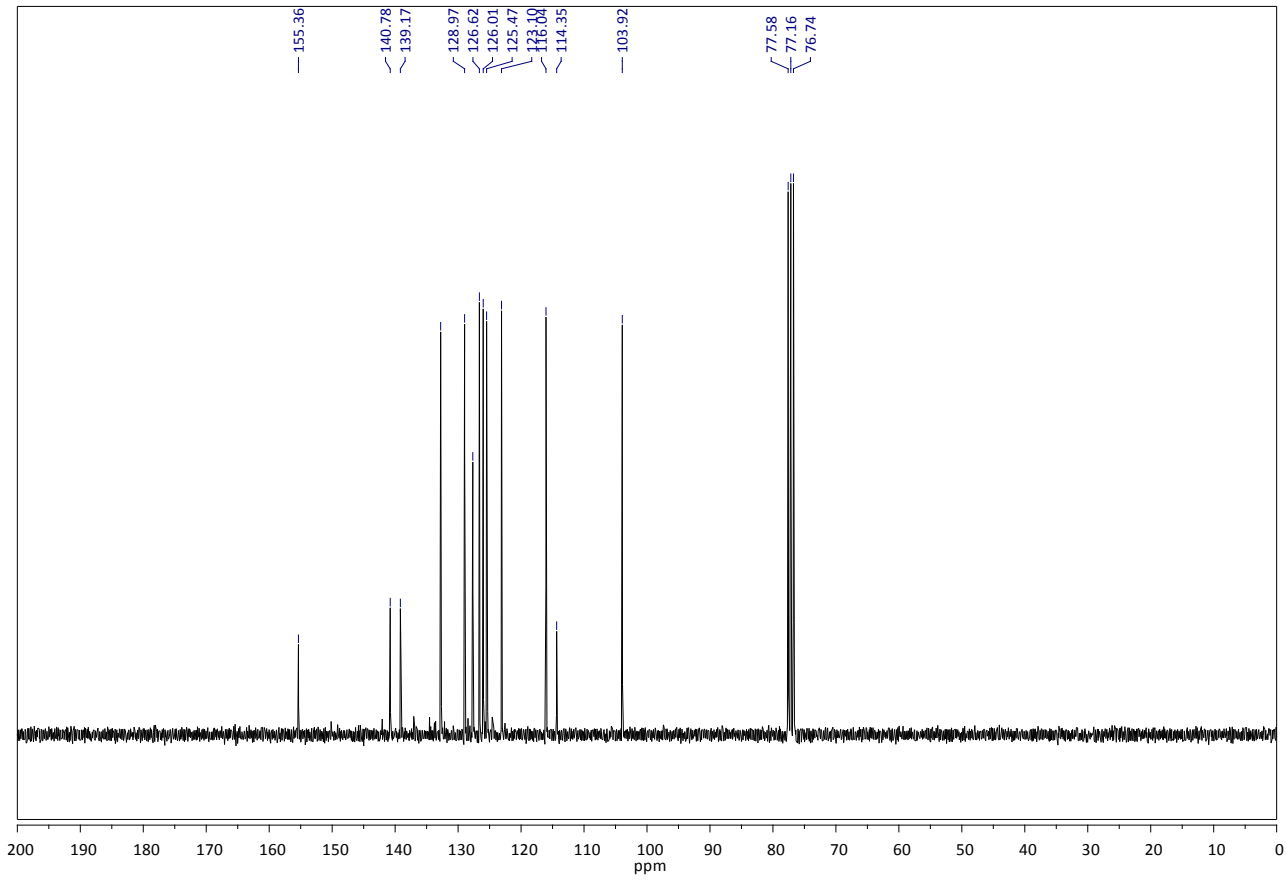
4j

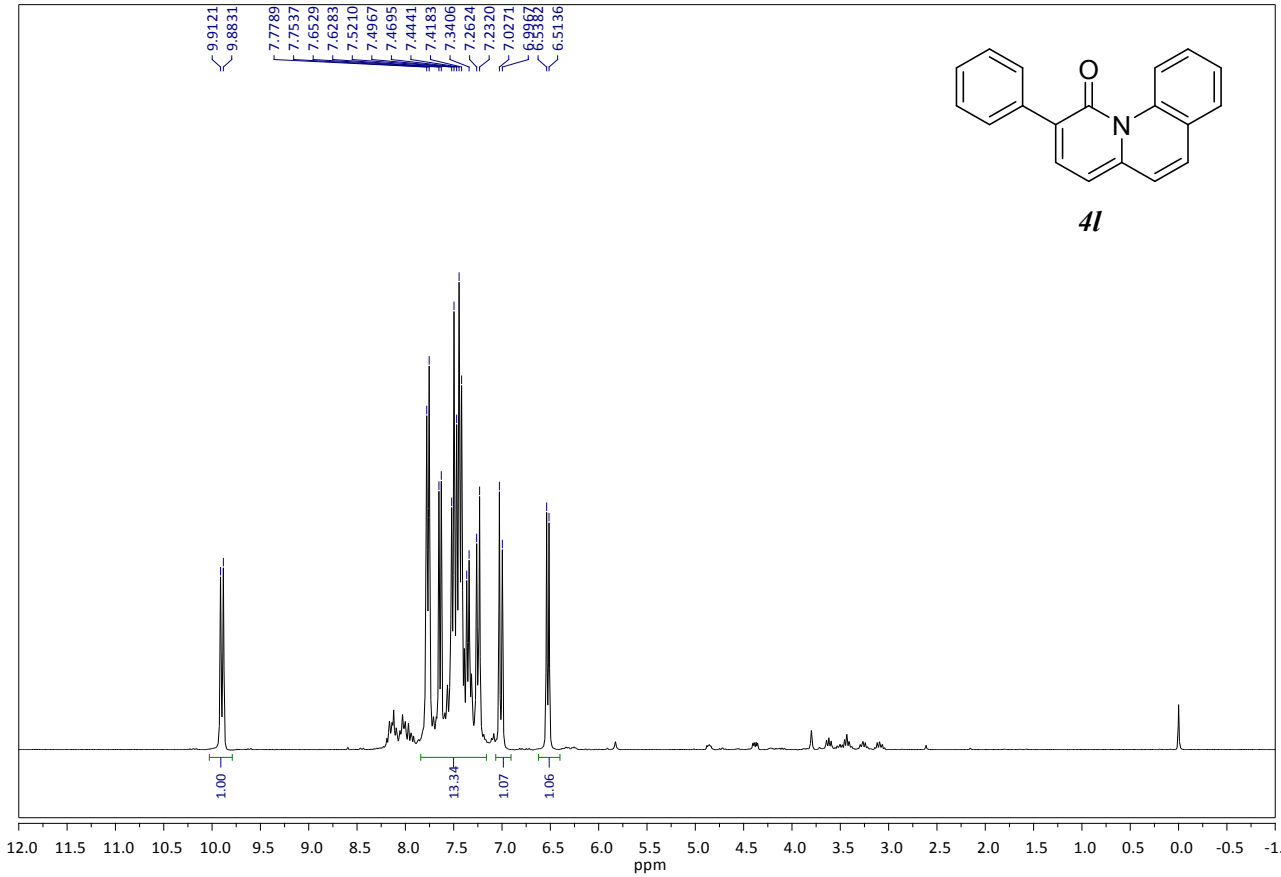

154.64
150.59
141.45
140.84
131.87
128.79
127.40
125.61
115.74
112.32
111.51
109.69
103.79
77.58
77.16
76.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


9.2483
9.2260
8.1615
8.1353
7.6651
7.4651
7.4376
7.3716
7.3595
7.3085
7.2867
7.1233
7.0549
7.0337
6.7495
6.7234
1.00
0.95
1.25
3.18
2.35
1.05
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 -0.5
ppm

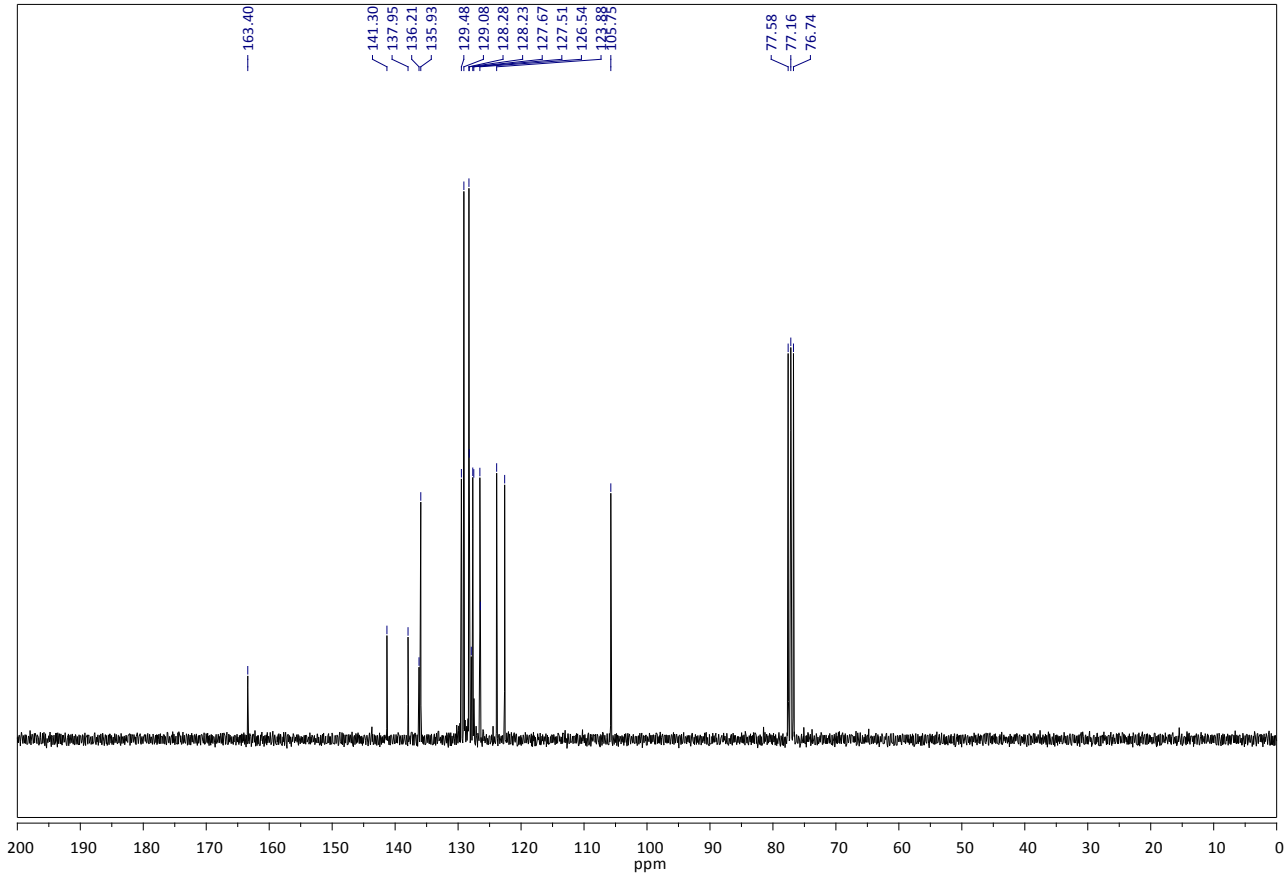
O
S
N

4k


155.36
140.78
139.17
128.97
126.62
126.01
125.47
123.10
115.04
114.35
103.92
77.58
77.16
76.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


9.9121
9.8831
7.7789
7.7537
7.6529
7.6283
7.5210
7.4967
7.4695
7.4441
7.4183
7.3406
7.2624
7.2320
7.0271
6.9967
6.5382
6.5136
O
N
1.00
13.34
1.07
1.06
ppm

4l


163.40
141.30
137.95
136.21
135.93
129.48
129.08
128.28
128.23
127.67
127.51
126.54
77.58
77.16
76.74
ppm

2. Absorption and Emission Spectroscopy of Compounds 4*a-l*

Table S1. Electronic absorption and fluorescence of compounds **4** in $CHCl_3$[a,b]

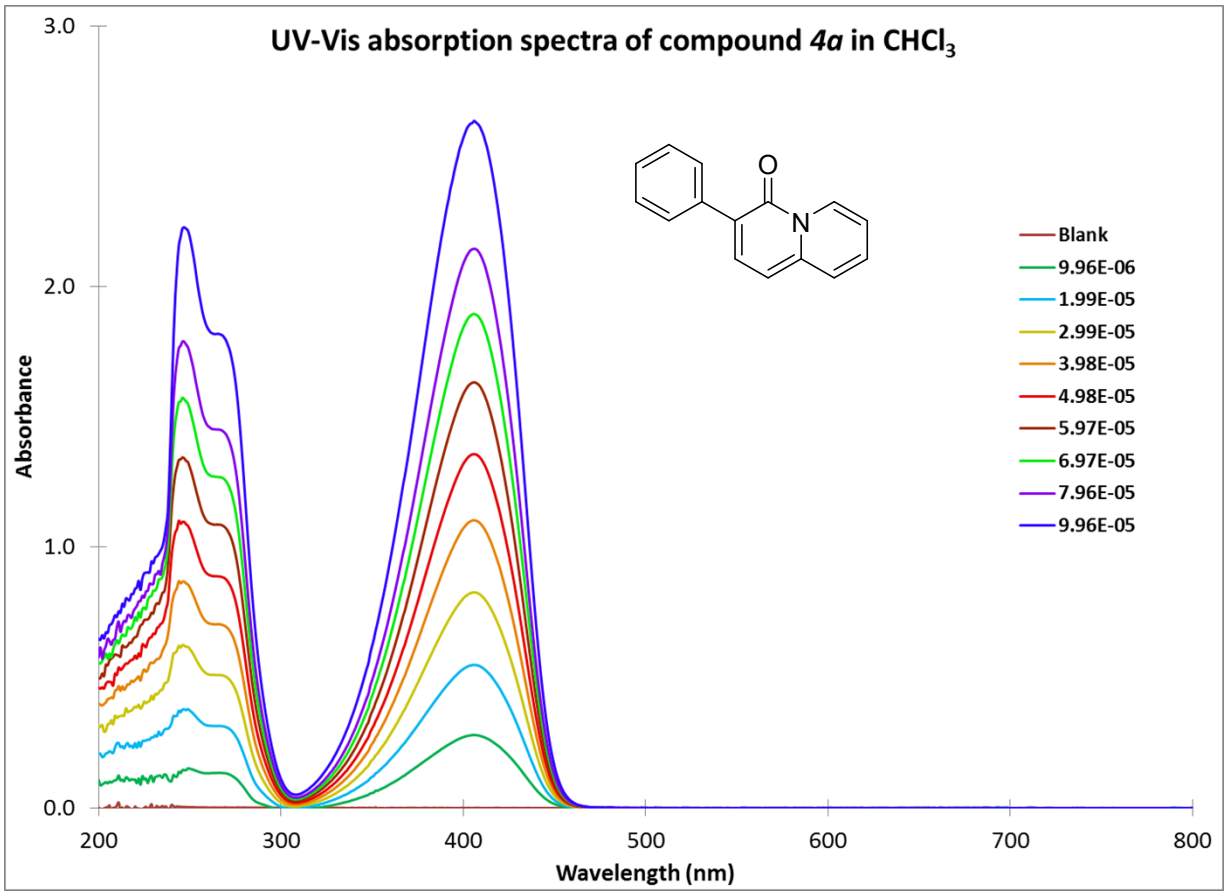
Compound	Absorption maxima			Fluorescence[c]	Quantum yield[d]
	λ_{1abs}, ($\varepsilon_1\times10^4$)	λ_{2abs}, ($\varepsilon_2\times10^4$)	λ_{3abs}, ($\varepsilon_3\times10^4$)	λ_{em}	Φ
4a	246 (2.40)	270 (1.88)	406 (2.72)	483	0.25
4b	245 (1.67)	------	407 (1.66)	486	0.25
4c	245 (1.56)	278 (1.37)	409 (1.92)	485	0.23
4d	245 (1.38)	280 (1.24)	410 (1.68)	485	0.10
4e	246 (1.40)	269 (1.17)	410 (1.79)	483	0.36
4f	250 (2.09)	------	408 (2.52)	491	0.23
4g	249 (1.95)	291 (2.15)	412 (2.41)	491	0.32
4h	259 (2.39)	------	412 (2.05)	494	0.29
4i	------	------	418 (1.06)	495	0.19
4k	258 (1.94)	291 (1.27)	428 (2.67)	498	0.26
4l	243 (1.82)	------	418 (0.99)	525	0.04

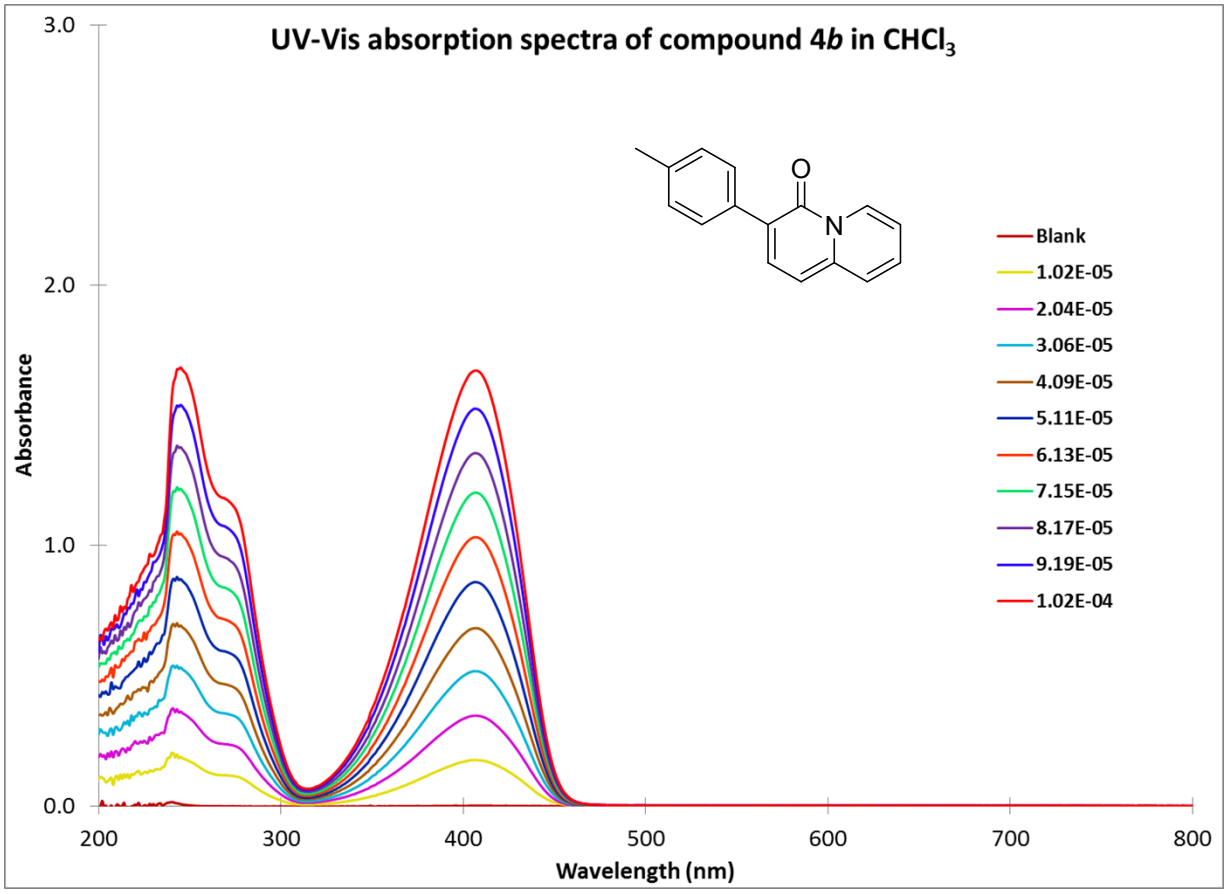
[a] λ in nm; ε in $L\cdot mol^{-1}\cdot cm^{-1}$

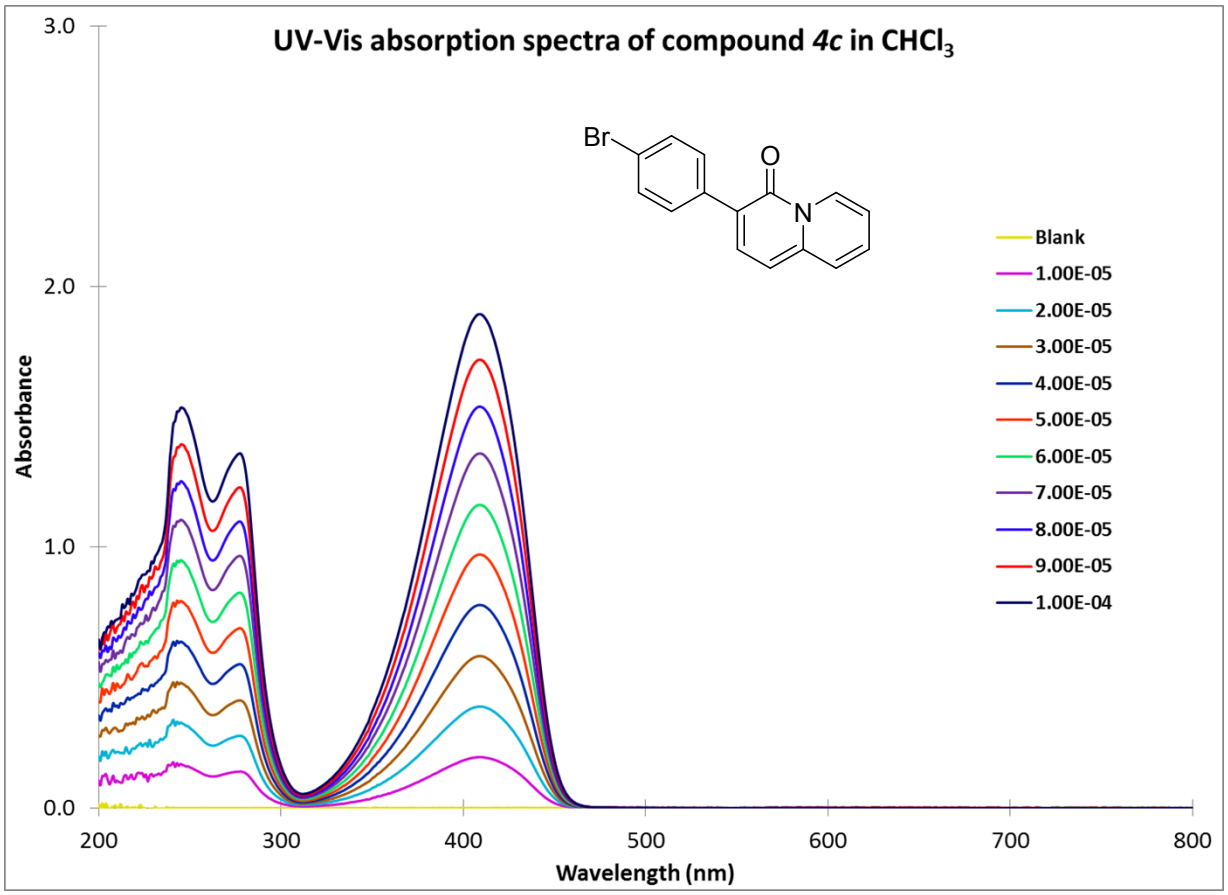
[b] Compounds **4i** and **4j** decompose in solution

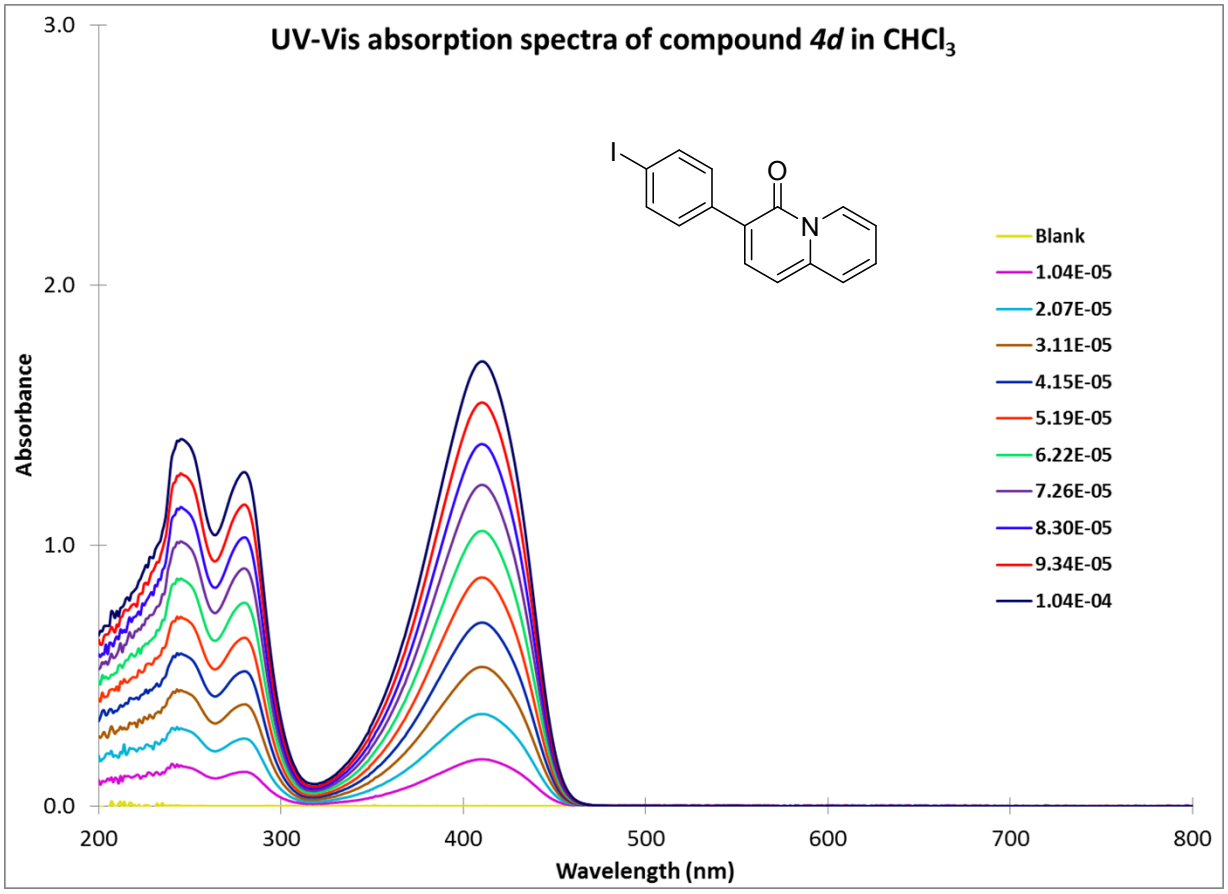
[c] λ_{ex} = 365 nm

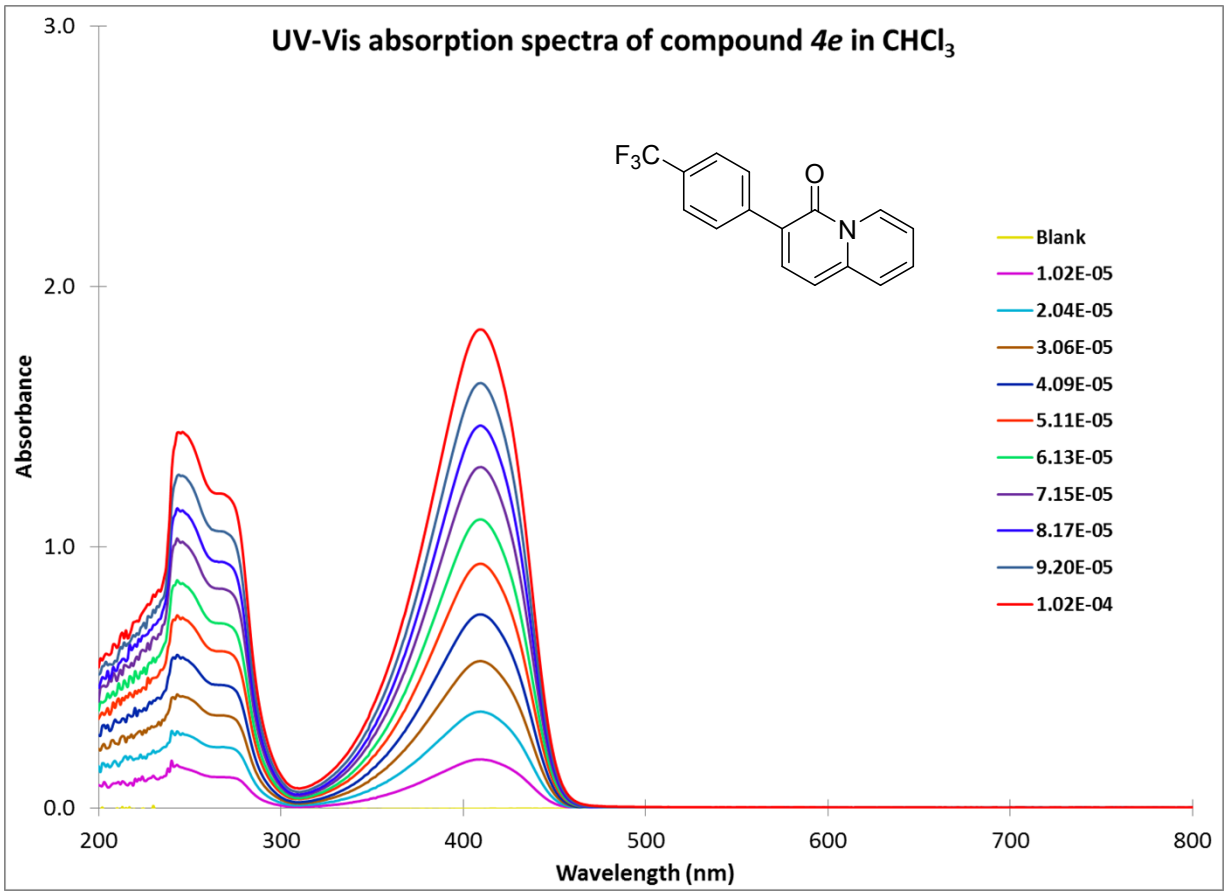
[d] Referred to quinine sulfate in 0.1 M H_2SO_4 (Φ = 0.546)

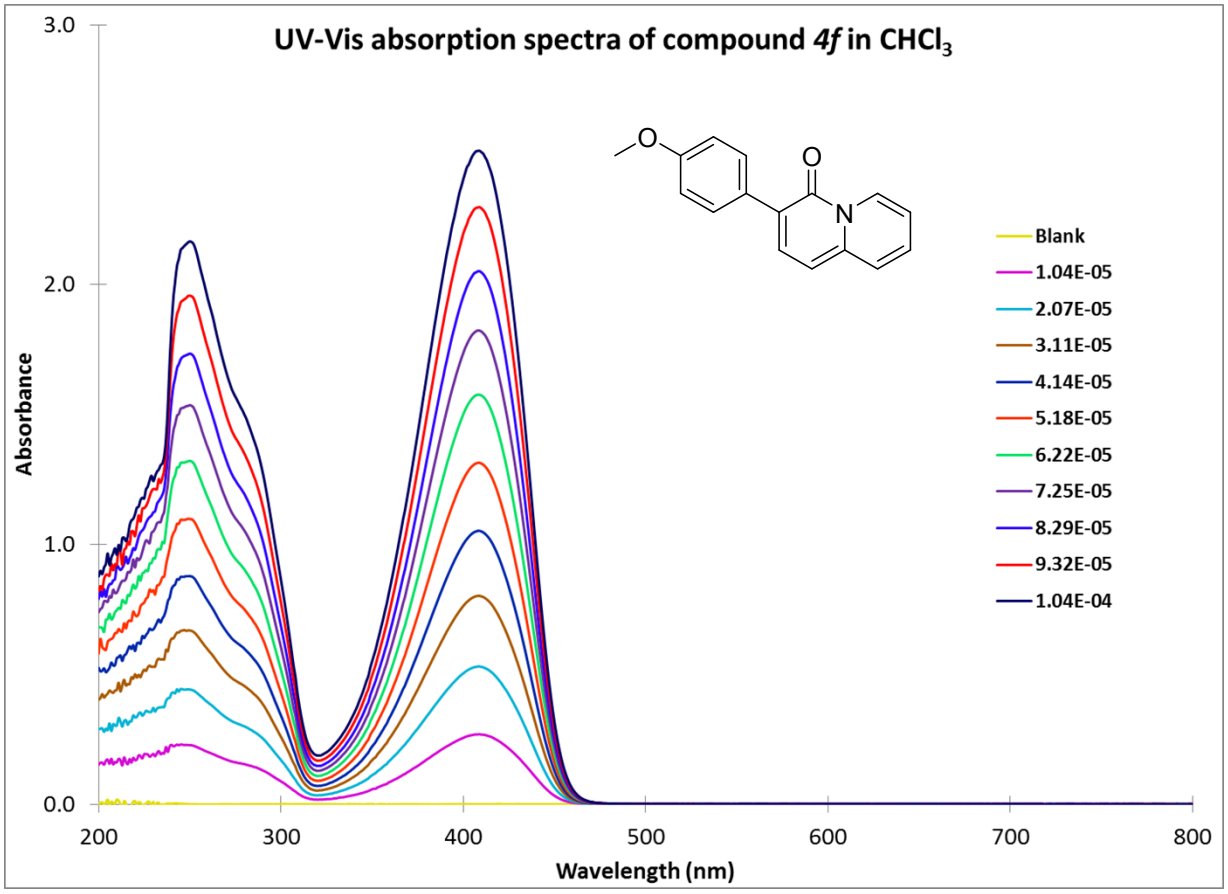

UV-Vis absorption spectra of compound 4a in CHCl3
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
O
N
Blank
9.96E-06
1.99E-05
2.99E-05
3.98E-05
4.98E-05
5.97E-05
6.97E-05
7.96E-05
9.96E-05

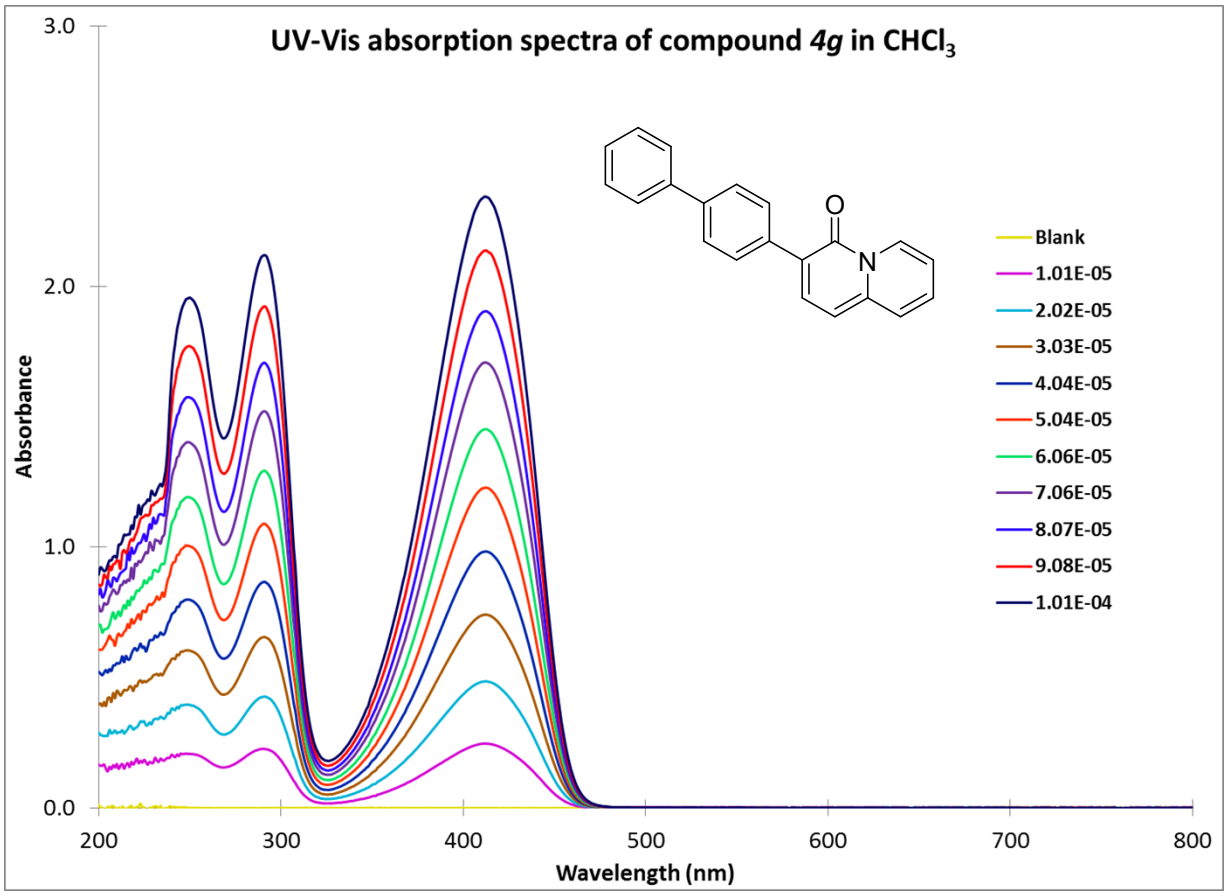

UV-Vis absorption spectra of compound 4b in CHCl3
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
O
N
Blank
1.02E-05
2.04E-05
3.06E-05
4.09E-05
5.11E-05
6.13E-05
7.15E-05
8.17E-05
9.19E-05
1.02E-04

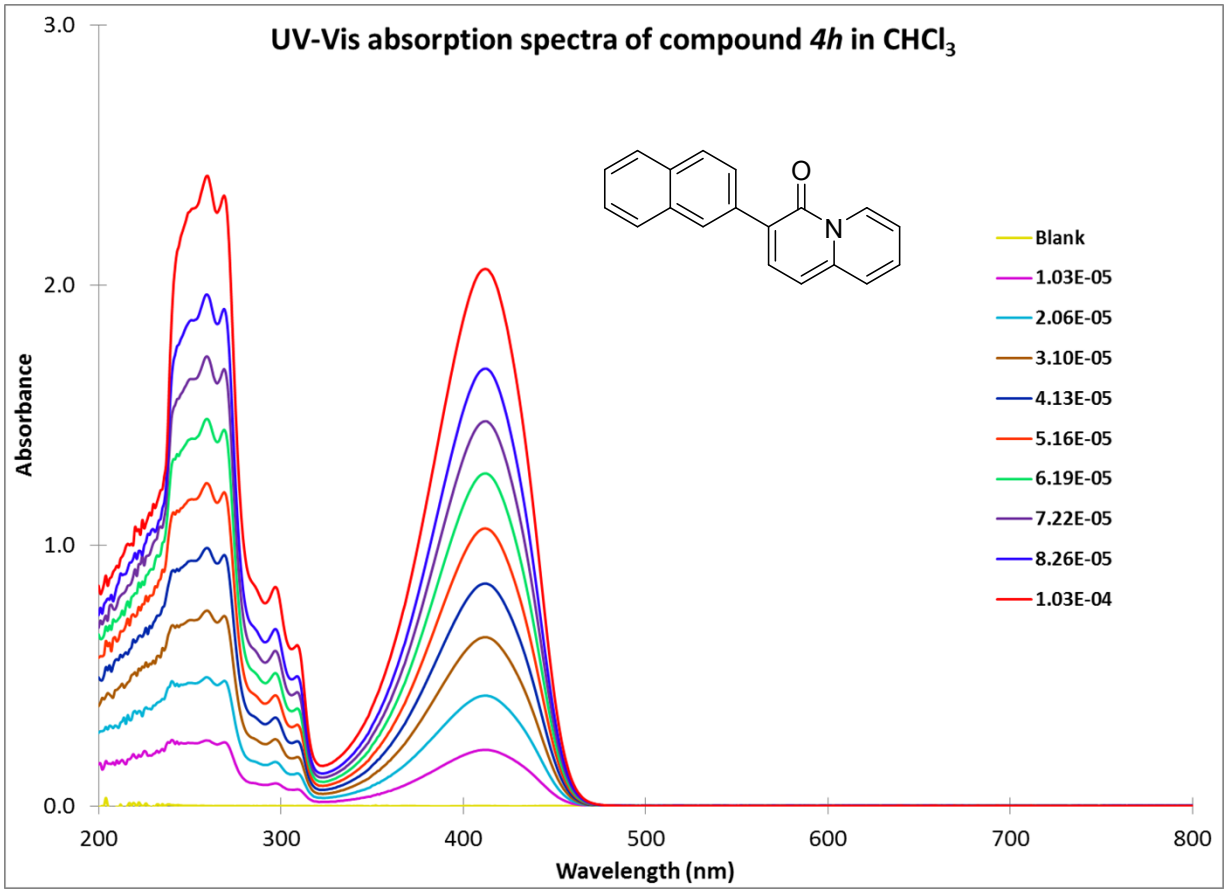

UV-Vis absorption spectra of compound 4c in CHCl3
Br
O
N
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
Blank
1.00E-05
2.00E-05
3.00E-05
4.00E-05
5.00E-05
6.00E-05
7.00E-05
8.00E-05
9.00E-05
1.00E-04

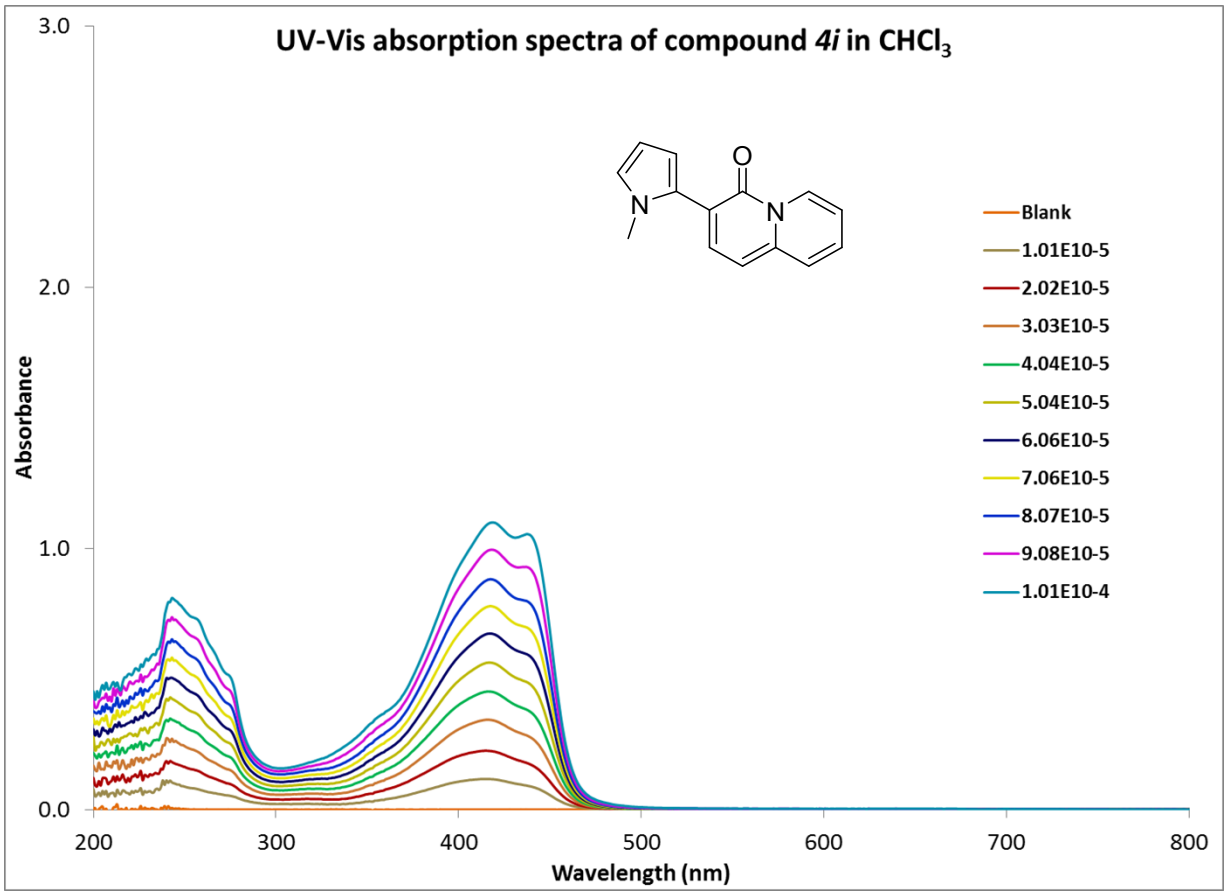

UV-Vis absorption spectra of compound 4d in CHCl3
I
O
N
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
Blank
1.04E-05
2.07E-05
3.11E-05
4.15E-05
5.19E-05
6.22E-05
7.26E-05
8.30E-05
9.34E-05
1.04E-04

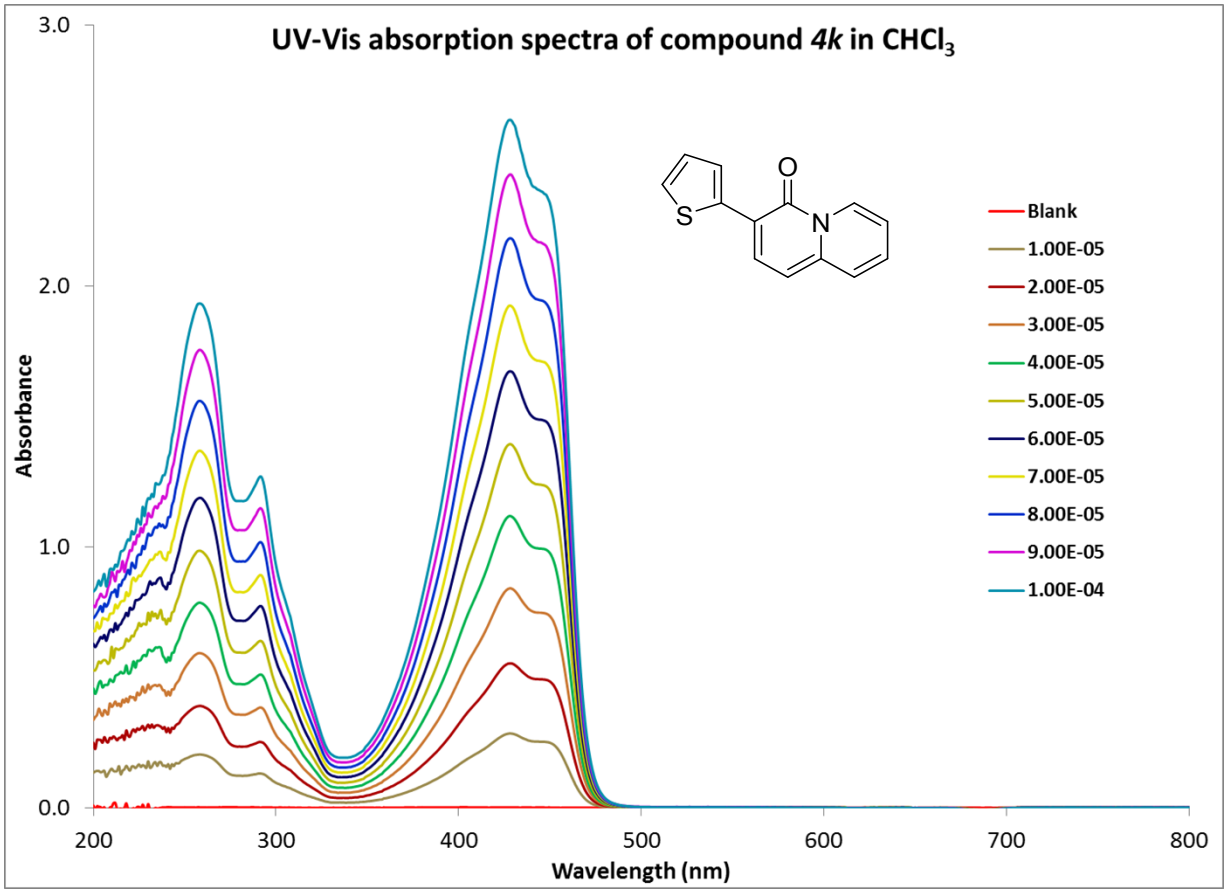

UV-Vis absorption spectra of compound 4e in CHCl3
F3C
O
N
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
Blank
1.02E-05
2.04E-05
3.06E-05
4.09E-05
5.11E-05
6.13E-05
7.15E-05
8.17E-05
9.20E-05
1.02E-04


UV-Vis absorption spectra of compound 4f in CHCl3
O
O
N
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
Blank
1.04E-05
2.07E-05
3.11E-05
4.14E-05
5.18E-05
6.22E-05
7.25E-05
8.29E-05
9.32E-05
1.04E-04


UV-Vis absorption spectra of compound 4g in CHCl3
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
O
N
Blank
1.01E-05
2.02E-05
3.03E-05
4.04E-05
5.04E-05
6.06E-05
7.06E-05
8.07E-05
9.08E-05
1.01E-04


UV-Vis absorption spectra of compound 4h in CHCl3
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
O
N
Blank
1.03E-05
2.06E-05
3.10E-05
4.13E-05
5.16E-05
6.19E-05
7.22E-05
8.26E-05
1.03E-04


UV-Vis absorption spectra of compound 4i in CHCl3
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
O
N
N
Blank
1.01E10-5
2.02E10-5
3.03E10-5
4.04E10-5
5.04E10-5
6.06E10-5
7.06E10-5
8.07E10-5
9.08E10-5
1.01E10-4


UV-Vis absorption spectra of compound 4k in CHCl3
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800
O
S
N
Blank
1.00E-05
2.00E-05
3.00E-05
4.00E-05
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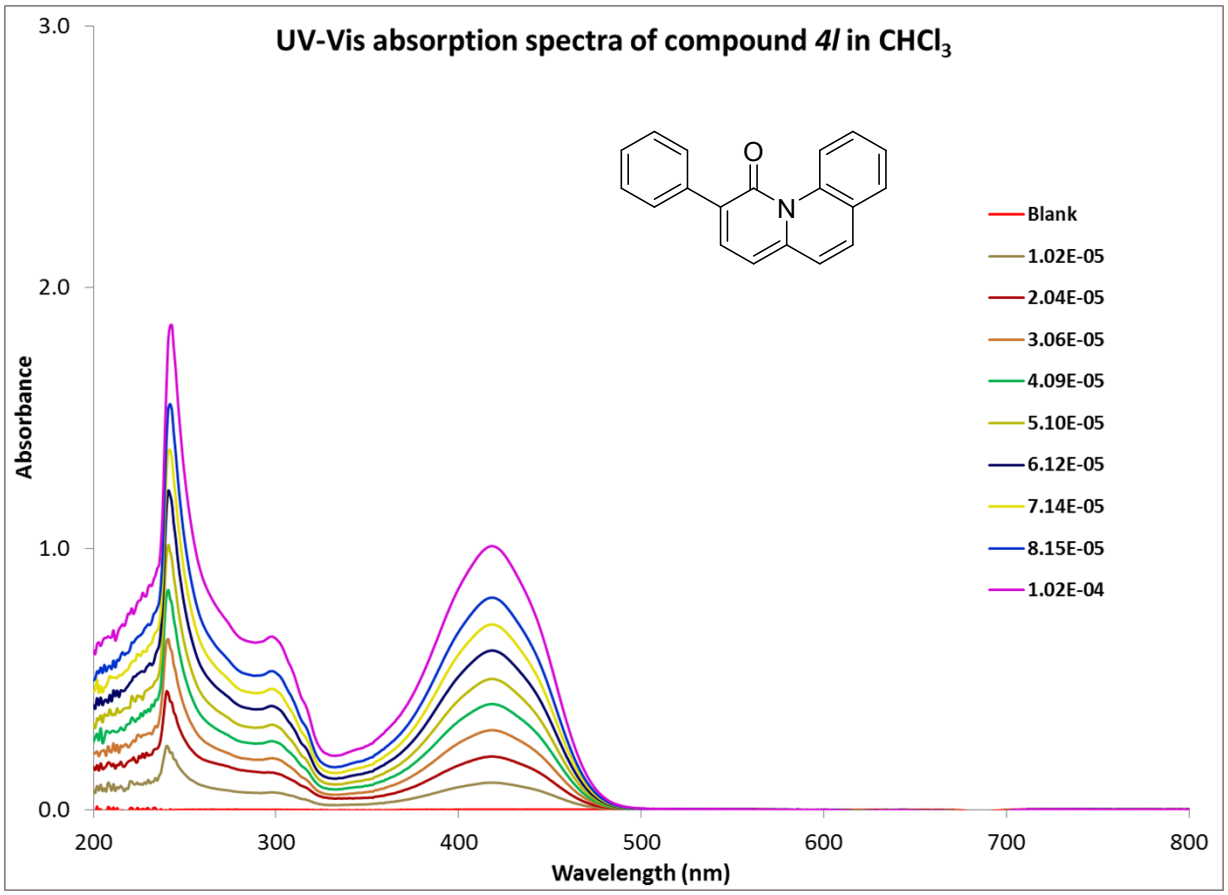
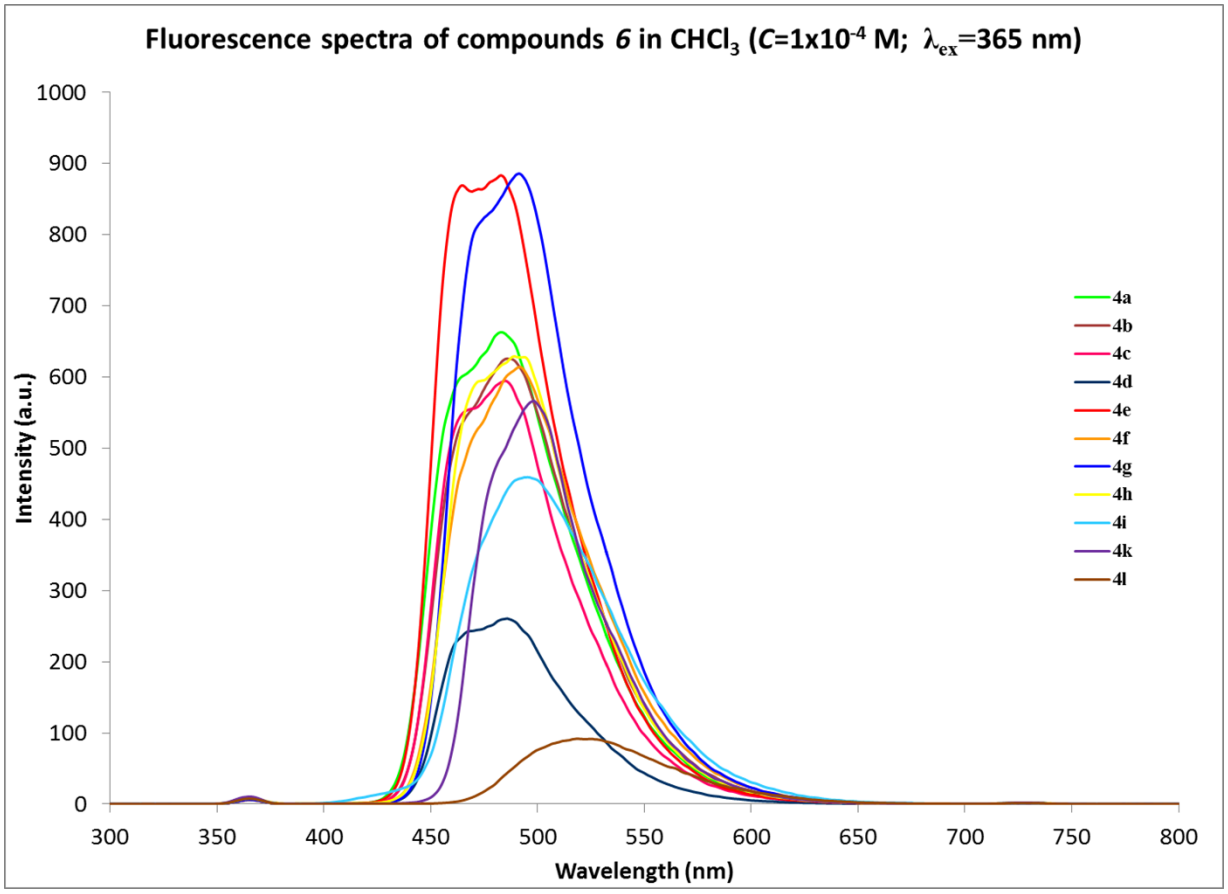
7.00E-05
8.00E-05
9.00E-05
1.00E-04


UV-Vis absorption spectra of compound 4l in CHCl3
O
N
Blank
1.02E-05
2.04E-05
3.06E-05
4.09E-05
5.10E-05
6.12E-05
7.14E-05
8.15E-05
1.02E-04
Absorbance
Wavelength (nm)
3.0
2.0
1.0
0.0
200
300
400
500
600
700
800


Fluorescence spectra of compounds 6 in CHCl3 (C=1x10-4 M; λex=365 nm)
4a
4b
4c
4d
4e
4f
4g
4h
4i
4k
4l
Intensity (a.u.)
Wavelength (nm)
1000
900
800
700
600
500
400
300
200
100
0
300
350
400
450
500
550
600
650
700
750
800

5. X-ray Analysis Data

Table S2. X-ray Data Collection and Structure Refinement Details for Compounds **2a**, **2h**, **3g**, **4a**, **4d** and **4e**.

	2a	**2h**	**3g**	**4a**	**4d**	**4e**
Formula	$C_{18}H_{11}FeNO_5$	$C_{22}H_{13}Fe\ NO_5$	$C_{24}H_{15}FeNO_4$	$C_{15}H_{11}NO$	$C_{15}H_{10}INO$	$C_{16}H_{10}F_3NO$
MW (g^{-1} mol^{-1})	377.13	427.18	437.22	221.25	347.14	289.25
Crystal size (mm^3)	0.312 x 0.296 x 0.282	0.430 x 0.326 x 0.140	0.458 x 0.292 x 0.108	0.442 x 0.403 x 0.156	0.478 x 0.232 x 0.174	0.486 x 0.264 x 0.236
Crystal system	Triclinic	Monoclinic	Triclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1/c$	*P*-1	$Pca2_1$	$P2_1/n$	$P2_1/c$
Cell parameters						
a (Å)	7.136(1)	10.5432(4)	9.1323(6)	15.2083(8)	6.492(4)	13.9430(15)
b (Å)	10.037(1)	15.2269(5)	10.4497(7)	6.5450(3)	21.091(13)	12.7966(14)
c (Å)	12.659(2)	12.0419(4)	11.6044(8)	21.7516(12)	9.629(6)	7.3613(8)
α (°)	92.570(2)	90	87.700(1)	90	90	90
β (°)	104.792(2)	91.721(1)	82.514(1)	90	102.311(10)	98.394(8)
γ (°)	105.483(2)	90	69.343(1)	90	90	90
V ($Å^3$)	838.51(18)	1932.34(12)	1027.36(12)	2165.12(19)	1288.1(14)	1299.4(4)
Z	2	4	2	8	4	4
d_c (Mg m^{-3})	1.494	1.468	1.413	1.357	1.790	1.479
Reflections collected	9209	11033	8848	13809	10484	10269
Independent reflections, *R*(int)	3065, 0.0206	3544, 0.0290	3736, 0.0436	4802, 0.0442	2368, 0.0629	2388, 0.0650
Data / parameters	3065 / 226	3544 / 262	3736 / 271	4802 / 307	2368 / 163	2388 / 247
Final *R*1, *wR*2 [$I>2\sigma(I)$]	0.0308, 0.0800	0.0349, 0.0868	0.0330, 0.0698	0.0563, 0.1249	0.0415, 0.0973	0.0534, 0.1072
*R*1, *wR*2 (all data)	0.0332, 0.0818	0.0448, 0.0934	0.0414, 0.0737	0.0808, 0.1431	0.0548, 0.1033	0.0926, 0.1219
GoF on F^2	1.062	1.016	0.945	1.024	1.063	1.034
CCDC number	1026201	1026202	1026203	1026204	1026205	1026206

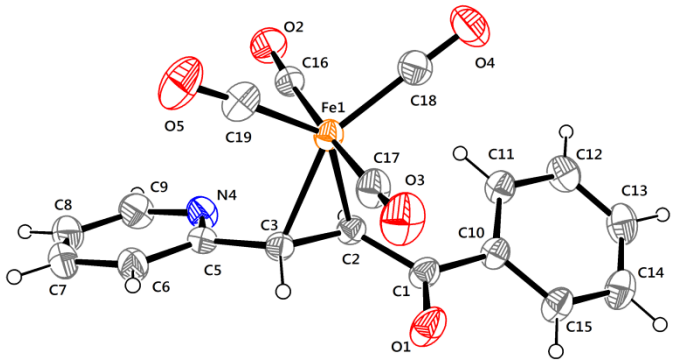


Figure S1. ORTEP view of **2a** with thermal ellipsoids at 30% of probability level.

Table S3. Bond lengths [Å] and angles [°] for compound **2a**

Fe(1)-C(18) 1.804(2)	O(2)-C(16) 1.126(2)	C(3)-C(5) 1.478(2)	C(10)-C(11) 1.385(3)
Fe(1)-C(19) 1.807(2)	O(3)-C(17) 1.125(3)	N(4)-C(9) 1.337(3)	C(10)-C(15) 1.393(3)
Fe(1)-C(16) 1.825(2)	O(4)-C(18) 1.139(2)	N(4)-C(5) 1.338(2)	C(11)-C(12) 1.385(3)
Fe(1)-C(17) 1.829(2)	O(5)-C(19) 1.134(3)	C(5)-C(6) 1.389(3)	C(12)-C(13) 1.377(3)
Fe(1)-C(2) 2.110(2)	C(1)-C(2) 1.478(2)	C(6)-C(7) 1.379(3)	C(13)-C(14) 1.375(3)
Fe(1)-C(3) 2.124(2)	C(1)-C(10) 1.498(2)	C(7)-C(8) 1.369(3)	C(14)-C(15) 1.372(3)
O(1)-C(1) 1.220(2)	C(2)-C(3) 1.412(2)	C(8)-C(9) 1.371(3)	

C(18)-Fe(1)-C(19) 116.34(10)	C(16)-Fe(1)-C(3) 94.37(7)	C(2)-C(3)-C(5) 123.66(16)	C(11)-C(10)-C(1) 122.96(16)
C(18)-Fe(1)-C(16) 87.77(8)	C(17)-Fe(1)-C(3) 88.75(8)	C(2)-C(3)-Fe(1) 69.99(10)	C(15)-C(10)-C(1) 118.23(17)
C(19)-Fe(1)-C(16) 90.18(9)	C(2)-Fe(1)-C(3) 38.97(6)	C(5)-C(3)-Fe(1) 115.19(11)	C(12)-C(11)-C(10) 120.14(19)
C(18)-Fe(1)-C(17) 89.79(9)	O(1)-C(1)-C(2) 121.61(16)	C(9)-N(4)-C(5) 117.25(18)	C(13)-C(12)-C(11) 120.2(2)
C(19)-Fe(1)-C(17) 89.15(9)	O(1)-C(1)-C(10) 119.50(17)	N(4)-C(5)-C(6) 122.13(17)	C(14)-C(13)-C(12) 120.1(2)
C(16)-Fe(1)-C(17) 176.87(8)	C(2)-C(1)-C(10) 118.89(15)	N(4)-C(5)-C(3) 118.39(16)	O(3)-C(17)-Fe(1) 176.0(2)
C(18)-Fe(1)-C(2) 108.18(8)	C(3)-C(2)-C(1) 120.70(15)	C(6)-C(5)-C(3) 119.46(17)	O(4)-C(18)-Fe(1) 178.0(2)
C(19)-Fe(1)-C(2) 135.36(9)	C(15)-C(14)-C(13) 120.0(2)	C(7)-C(6)-C(5) 119.2(2)	O(5)-C(19)-Fe(1) 176.1(2)
C(16)-Fe(1)-C(2) 88.37(7)	C(14)-C(15)-C(10) 120.8(2)	C(8)-C(7)-C(6) 118.8(2)	
C(17)-Fe(1)-C(2) 94.26(8)	O(2)-C(16)-Fe(1) 175.20(17)	C(7)-C(8)-C(9) 118.5(2)	
C(18)-Fe(1)-C(3) 146.79(9)	C(3)-C(2)-Fe(1) 71.04(10)	N(4)-C(9)-C(8) 124.0(2)	
C(19)-Fe(1)-C(3) 96.81(9)	C(1)-C(2)-Fe(1) 111.39(12)	C(11)-C(10)-C(15) 118.79(18)	

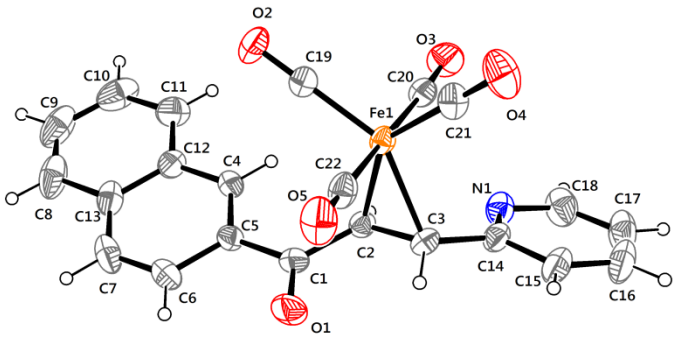


Figure S2. ORTEP view of **2h** with thermal ellipsoids at 30% of probability level.

Table S4. Bond lengths [Å] and angles [°] for compound **2h**

Fe(1)-C(21) 1.786(3)	O(3)-C(20) 1.131(3)	C(3)-C(14) 1.471(3)	C(9)-C(10) 1.403(5)
Fe(1)-C(19) 1.812(2)	O(4)-C(21) 1.141(3)	C(4)-C(5) 1.367(3)	C(10)-C(11) 1.358(4)
Fe(1)-C(20) 1.821(2)	O(5)-C(22) 1.126(3)	C(4)-C(12) 1.415(3)	C(11)-C(12) 1.419(3)
Fe(1)-C(22) 1.835(2)	N(1)-C(14) 1.338(3)	C(5)-C(6) 1.415(3)	C(12)-C(13) 1.414(4)
Fe(1)-C(2) 2.113(2)	N(1)-C(18) 1.339(3)	C(6)-C(7) 1.355(4)	C(14)-C(15) 1.387(3)
Fe(1)-C(3) 2.125(2)	C(1)-C(2) 1.482(3)	C(7)-C(13) 1.405(4)	C(15)-C(16) 1.376(4)
O(1)-C(1) 1.218(3)	C(1)-C(5) 1.498(3)	C(8)-C(9) 1.345(6)	C(16)-C(17) 1.360(5)
O(2)-C(19) 1.134(2)	C(2)-C(3) 1.415(3)	C(8)-C(13) 1.422(4)	C(17)-C(18) 1.377(5)

C(21)-Fe(1)-C(19) 111.18(11)	C(22)-Fe(1)-C(3) 87.15(10)	C(4)-C(5)-C(6) 118.5(2)	C(7)-C(13)-C(8) 123.1(3)
C(21)-Fe(1)-C(20) 88.56(11)	C(2)-Fe(1)-C(3) 39.00(8)	C(4)-C(5)-C(1) 123.6(2)	C(12)-C(13)-C(8) 118.2(3)
C(19)-Fe(1)-C(20) 89.98(10)	C(14)-N(1)-C(18) 116.9(2)	C(6)-C(5)-C(1) 117.9(2)	N(1)-C(14)-C(15) 122.5(2)
C(21)-Fe(1)-C(22) 88.66(11)	O(1)-C(1)-C(2) 121.1(2)	C(7)-C(6)-C(5) 120.9(2)	N(1)-C(14)-C(3) 117.7(2)
C(19)-Fe(1)-C(22) 90.91(10)	O(1)-C(1)-C(5) 119.3(2)	C(6)-C(7)-C(13) 121.4(2)	C(15)-C(14)-C(3) 119.7(2)
C(20)-Fe(1)-C(22) 177.21(10)	C(2)-C(1)-C(5) 119.60(19)	C(9)-C(8)-C(13) 121.3(3)	C(16)-C(15)-C(14) 119.1(3)
C(21)-Fe(1)-C(2) 143.31(10)	C(3)-C(2)-C(1) 120.4(2)	C(8)-C(9)-C(10) 120.5(3)	C(17)-C(16)-C(15) 118.9(3)
C(19)-Fe(1)-C(2) 105.33(9)	C(3)-C(2)-Fe(1) 70.97(12)	C(11)-C(10)-C(9) 120.5(3)	C(16)-C(17)-C(18) 118.9(3)
C(20)-Fe(1)-C(2) 87.92(9)	C(1)-C(2)-Fe(1) 110.32(14)	C(10)-C(11)-C(12) 120.5(3)	N(1)-C(18)-C(17) 123.7(3)
C(22)-Fe(1)-C(2) 94.39(10)	C(2)-C(3)-C(14) 123.8(2)	C(13)-C(12)-C(4) 118.5(2)	O(2)-C(19)-Fe(1) 179.8(2)
C(21)-Fe(1)-C(3) 104.94(10)	C(2)-C(3)-Fe(1) 70.04(12)	C(13)-C(12)-C(11) 119.0(2)	O(3)-C(20)-Fe(1) 174.9(2)
C(19)-Fe(1)-C(3) 143.77(9)	C(14)-C(3)-Fe(1) 114.67(15)	C(4)-C(12)-C(11) 122.5(2)	O(4)-C(21)-Fe(1) 177.4(2)
C(20)-Fe(1)-C(3) 93.68(9)	C(5)-C(4)-C(12) 121.9(2)	C(7)-C(13)-C(12) 118.7(2)	O(5)-C(22)-Fe(1) 176.6(2)

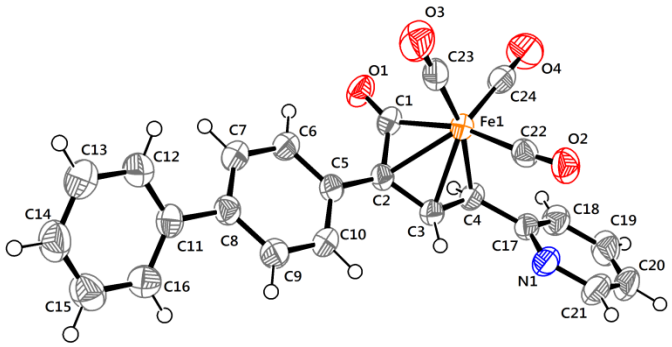


Figure S3. ORTEP view of **3g** with thermal ellipsoids at 50% of probability level.

Table S5. Bond lengths [Å] and angles [°] for compound **3g**

Fe(1)-C(24) 1.792(2)	C(1)-C(2) 1.474(3)	C(8)-C(9) 1.394(3)	C(15)-C(16) 1.381(3)
Fe(1)-C(23) 1.801(2)	C(2)-C(3) 1.412(2)	C(8)-C(11) 1.492(3)	C(15)-H(15) 0.9300
Fe(1)-C(22) 1.858(2)	C(2)-C(5) 1.481(3)	C(9)-C(10) 1.381(3)	C(16)-H(16) 0.9300
Fe(1)-C(1) 1.931(2)	C(3)-C(4) 1.415(3)	C(9)-H(9) 0.9300	C(17)-C(18) 1.387(3)
Fe(1)-C(3) 2.1037(19)	C(3)-H(3) 0.9800	C(10)-H(10) 0.9300	C(18)-C(19) 1.380(3)
Fe(1)-C(2) 2.1522(18)	C(4)-C(17) 1.481(3)	C(11)-C(12) 1.390(3)	C(18)-H(18) 0.9300
Fe(1)-C(4) 2.1612(19)	C(4)-H(4) 0.9800	C(11)-C(16) 1.391(3)	C(19)-C(20) 1.377(3)
O(1)-C(1) 1.194(2)	C(5)-C(6) 1.393(3)	C(12)-C(13) 1.390(3)	C(19)-H(19) 0.9300
O(2)-C(22) 1.135(2)	C(5)-C(10) 1.394(3)	C(12)-H(12) 0.9300	C(20)-C(21) 1.372(3)
O(3)-C(23) 1.139(2)	C(6)-C(7) 1.380(3)	C(13)-C(14) 1.368(3)	C(20)-H(20) 0.9300
O(4)-C(24) 1.141(2)	C(6)-H(6) 0.9300	C(13)-H(13) 0.9300	C(21)-H(21) 0.9300
N(1)-C(21) 1.342(3)	C(7)-C(8) 1.392(3)	C(14)-C(15) 1.380(3)	
N(1)-C(17) 1.349(2)	C(7)-H(7) 0.9300	C(14)-H(14) 0.9300	

C(24)-Fe(1)-C(23) 100.30(10)	C(22)-Fe(1)-C(3) 93.83(8)	C(23)-Fe(1)-C(4) 166.10(8)	C(7)-C(8)-C(9) 116.82(19)
C(24)-Fe(1)-C(22) 98.51(9)	C(1)-Fe(1)-C(3) 72.15(8)	C(22)-Fe(1)-C(4) 93.82(8)	C(7)-C(8)-C(11) 121.10(19)
C(23)-Fe(1)-C(22) 92.28(9)	C(24)-Fe(1)-C(2) 134.92(9)	C(1)-Fe(1)-C(4) 80.45(8)	C(9)-C(8)-C(11) 122.07(18)
C(24)-Fe(1)-C(1) 96.80(9)	C(23)-Fe(1)-C(2) 97.44(8)	C(3)-Fe(1)-C(4) 38.73(7)	C(10)-C(9)-C(8) 121.76(19)
C(23)-Fe(1)-C(1) 90.30(9)	C(22)-Fe(1)-C(2) 121.86(8)	C(2)-Fe(1)-C(4) 68.76(7)	C(10)-C(9)-H(9) 119.1
C(22)-Fe(1)-C(1) 163.75(8)	C(1)-Fe(1)-C(2) 41.89(8)	C(21)-N(1)-C(17) 116.65(19)	C(8)-C(9)-H(9) 119.1
C(24)-Fe(1)-C(3) 129.16(9)	C(3)-Fe(1)-C(2) 38.73(7)	O(1)-C(1)-C(2) 137.09(19)	C(9)-C(10)-C(5) 121.13(19)

C(23)-Fe(1)-C(3) 128.36(8)	C(24)-Fe(1)-C(4) 91.14(9)	O(1)-C(1)-Fe(1) 145.11(17)	C(9)-C(10)-H(10) 119.4
C(2)-C(1)-Fe(1) 77.10(11)	C(5)-C(10)-H(10) 119.4	C(2)-C(3)-Fe(1) 72.49(11)	C(14)-C(13)-H(13) 119.6
C(3)-C(2)-C(1) 111.10(16)	C(12)-C(11)-C(16) 117.40(19)	C(4)-C(3)-Fe(1) 72.83(11)	C(12)-C(13)-H(13) 119.6
C(3)-C(2)-C(5) 126.60(18)	C(12)-C(11)-C(8) 120.75(19)	C(2)-C(3)-H(3) 120.3	C(13)-C(14)-C(15) 118.6(2)
C(1)-C(2)-C(5) 121.62(17)	C(16)-C(11)-C(8) 121.8(2)	C(4)-C(3)-H(3) 120.3	C(13)-C(14)-H(14) 120.7
C(3)-C(2)-Fe(1) 68.78(10)	C(13)-C(12)-C(11) 121.1(2)	Fe(1)-C(3)-H(3) 120.3	C(15)-C(14)-H(14) 120.7
C(1)-C(2)-Fe(1) 61.01(10)	C(13)-C(12)-H(12) 119.5	C(3)-C(4)-C(17) 121.83(17)	C(14)-C(15)-C(16) 121.0(2)
C(5)-C(2)-Fe(1) 130.64(13)	C(11)-C(12)-H(12) 119.5	C(3)-C(4)-Fe(1) 68.44(10)	C(14)-C(15)-H(15) 119.5
C(2)-C(3)-C(4) 118.99(17)	C(14)-C(13)-C(12) 120.8(2)	C(17)-C(4)-Fe(1) 121.35(13)	C(16)-C(15)-H(15) 119.5
C(3)-C(4)-H(4) 112.8	C(15)-C(16)-C(11) 121.0(2)	C(5)-C(6)-H(6) 119.3	C(21)-C(20)-C(19) 118.3(2)
C(17)-C(4)-H(4) 112.8	C(15)-C(16)-H(16) 119.5	C(6)-C(7)-C(8) 121.7(2)	C(21)-C(20)-H(20) 120.8
Fe(1)-C(4)-H(4) 112.8	C(11)-C(16)-H(16) 119.5	C(6)-C(7)-H(7) 119.2	C(19)-C(20)-H(20) 120.8
C(6)-C(5)-C(10) 117.24(18)	N(1)-C(17)-C(18) 122.23(18)	C(8)-C(7)-H(7) 119.2	N(1)-C(21)-C(20) 124.5(2)
C(6)-C(5)-C(2) 120.70(18)	N(1)-C(17)-C(4) 116.95(17)	C(17)-C(18)-H(18) 120.2	C(20)-C(21)-H(21) 117.7
C(10)-C(5)-C(2) 122.02(18)	C(18)-C(17)-C(4) 120.81(19)	C(20)-C(19)-C(18) 118.7(2)	N(1)-C(21)-H(21) 117.7
C(7)-C(6)-C(5) 121.36(19)	C(19)-C(18)-C(17) 119.6(2)	C(20)-C(19)-H(19) 120.6	
C(7)-C(6)-H(6) 119.3	C(19)-C(18)-H(18) 120.2	C(18)-C(19)-H(19) 120.6	
O(4)-C(24)-Fe(1) 176.7(2)	O(3)-C(23)-Fe(1) 177.9(2)	O(2)-C(22)-Fe(1) 175.91(18)	

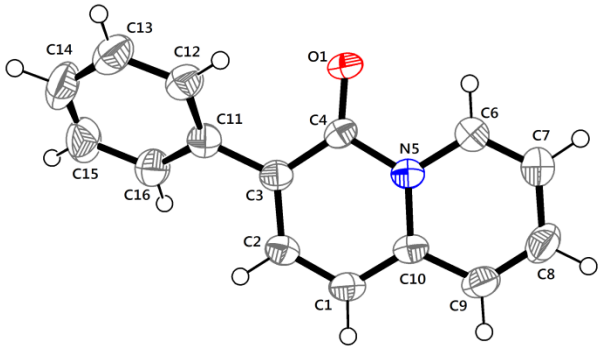


Figure S4. ORTEP view of **4a** with thermal ellipsoids at 50% of probability level.

Table S6. Bond lengths [Å] and angles [°] for compound **4a**

O(1)-C(4) 1.236(5)	N(5)-C(6) 1.384(5)	C(11)-C(16) 1.397(6)
C(1)-C(10) 1.379(6)	N(5)-C(10) 1.393(5)	C(12)-C(13) 1.375(6)
C(1)-C(2) 1.381(7)	C(6)-C(7) 1.336(7)	C(13)-C(14) 1.388(7)
C(2)-C(3) 1.389(6)	C(7)-C(8) 1.405(6)	C(14)-C(15) 1.351(7)
C(3)-C(4) 1.428(5)	C(8)-C(9) 1.347(6)	C(15)-C(16) 1.391(7)
C(3)-C(11) 1.478(6)	C(9)-C(10) 1.425(5)	
C(4)-N(5) 1.439(5)	C(11)-C(12) 1.385(6)	

C(10)-C(1)-C(2) 119.3(4)	C(3)-C(4)-N(5) 115.6(3)	C(8)-C(9)-C(10) 121.8(4)	C(13)-C(12)-C(11) 121.3(5)
C(1)-C(2)-C(3) 123.7(4)	C(6)-N(5)-C(10) 119.5(4)	C(1)-C(10)-N(5) 118.8(4)	C(12)-C(13)-C(14) 119.9(5)
C(2)-C(3)-C(4) 119.1(4)	C(6)-N(5)-C(4) 117.0(3)	C(1)-C(10)-C(9) 123.7(4)	C(15)-C(14)-C(13) 119.8(5)
C(2)-C(3)-C(11) 120.3(4)	C(10)-N(5)-C(4) 123.5(3)	N(5)-C(10)-C(9) 117.5(3)	C(14)-C(15)-C(16) 120.8(5)
C(4)-C(3)-C(11) 120.6(3)	C(7)-C(6)-N(5) 121.8(4)	C(12)-C(11)-C(16) 117.8(4)	C(15)-C(16)-C(11) 120.3(5)
O(1)-C(4)-C(3) 127.5(4)	C(6)-C(7)-C(8) 120.5(4)	C(12)-C(11)-C(3) 122.5(4)	
O(1)-C(4)-N(5) 117.0(3)	C(9)-C(8)-C(7) 118.9(4)	C(16)-C(11)-C(3) 119.5(4)	

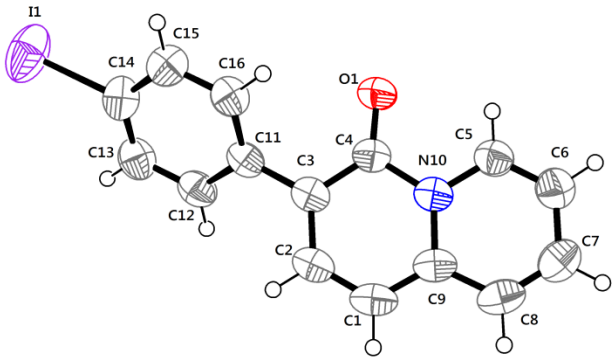


Figure S5. ORTEP view of **4d** with thermal ellipsoids at 50% of probability level.

Table S7. Bond lengths [Å] and angles [°] for compound **4d**

I(1)-C(14) 2.095(4)	C(4)-N(10) 1.438(5)	C(11)-C(16) 1.393(5)
O(1)-C(4) 1.231(4)	C(5)-C(6) 1.331(6)	C(11)-C(12) 1.396(5)
C(1)-C(9) 1.370(5)	C(5)-N(10) 1.382(5)	C(12)-C(13) 1.378(6)
C(1)-C(2) 1.371(6)	C(6)-C(7) 1.409(6)	C(13)-C(14) 1.380(5)
C(2)-C(3) 1.386(5)	C(7)-C(8) 1.333(6)	C(14)-C(15) 1.377(5)
C(3)-C(4) 1.426(5)	C(8)-C(9) 1.426(6)	C(15)-C(16) 1.378(5)
C(3)-C(11) 1.474(5)	C(9)-N(10) 1.393(4)	

C(9)-C(1)-C(2) 120.7(3)	C(6)-C(5)-N(10) 122.4(4)	N(10)-C(9)-C(8) 116.8(3)	C(12)-C(13)-C(14) 120.2(4)
C(1)-C(2)-C(3) 122.7(4)	C(5)-C(6)-C(7) 119.8(4)	C(5)-N(10)-C(9) 119.6(3)	C(15)-C(14)-C(13) 119.9(4)
C(2)-C(3)-C(4) 119.7(3)	C(8)-C(7)-C(6) 119.0(4)	C(5)-N(10)-C(4) 116.8(3)	C(15)-C(14)-I(1) 119.7(3)
C(2)-C(3)-C(11) 121.1(3)	C(7)-C(8)-C(9) 122.5(4)	C(9)-N(10)-C(4) 123.6(3)	C(13)-C(14)-I(1) 120.4(3)
C(4)-C(3)-C(11) 119.2(3)	C(1)-C(9)-N(10) 118.1(3)	C(16)-C(11)-C(12) 117.6(3)	C(14)-C(15)-C(16) 119.8(4)
O(1)-C(4)-C(3) 127.5(3)	C(1)-C(9)-C(8) 125.1(4)	C(16)-C(11)-C(3) 121.8(3)	C(15)-C(16)-C(11) 121.5(3)
O(1)-C(4)-N(10) 117.4(3)	C(6)-C(5)-N(10) 122.4(4)	C(12)-C(11)-C(3) 120.6(3)	
C(3)-C(4)-N(10) 115.2(3)	C(5)-C(6)-C(7) 119.8(4)	C(13)-C(12)-C(11) 120.9(4)	

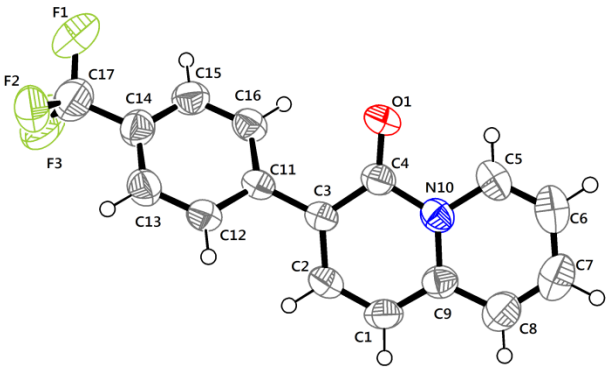


Figure S6. ORTEP view of **4e** with thermal ellipsoids at 50% of probability level.

Table S8. Bond lengths [Å] and angles [°] for compound **4e**

O(1)-C(4) 1.229(2)	C(5)-N(10) 1.388(3)	C(13)-C(14) 1.384(3)
C(1)-C(9) 1.371(3)	C(6)-C(7) 1.405(4)	C(14)-C(15) 1.378(3)
C(1)-C(2) 1.378(3)	C(7)-C(8) 1.343(3)	C(14)-C(17) 1.479(4)
C(2)-C(3) 1.384(3)	C(8)-C(9) 1.412(3)	C(15)-C(16) 1.377(3)
C(3)-C(4) 1.424(3)	C(9)-N(10) 1.389(3)	C(17)-F(1) 1.351(5)
C(3)-C(11) 1.478(3)	C(11)-C(16) 1.395(3)	C(17)-F(2) 1.353(5)
C(4)-N(10) 1.436(3)	C(11)-C(12) 1.395(3)	C(17)-F(3) 1.349(6)
C(5)-C(6) 1.330(3)	C(12)-C(13) 1.370(3)	

C(9)-C(1)-C(2) 120.7(2)	C(5)-C(6)-C(7) 120.2(3)	C(16)-C(11)-C(12) 117.6(2)	C(15)-C(16)-C(11) 120.9(2)
C(1)-C(2)-C(3) 122.3(2)	C(8)-C(7)-C(6) 119.3(2)	C(16)-C(11)-C(3) 122.71(19)	F(1)-C(17)-F(2) 104.7(4)
C(2)-C(3)-C(4) 19.63(19)	C(7)-C(8)-C(9) 121.7(3)	C(12)-C(11)-C(3) 119.64(19)	F(3)-C(17)-F(2) 105.8(5)
C(2)-C(3)-C(11) 120.58(18)	C(1)-C(9)-N(10) 118.10(19)	C(13)-C(12)-C(11) 121.2(2)	F(3)-C(17)-F(1) 105.9(5)
C(4)-C(3)-C(11) 119.78(18)	C(1)-C(9)-C(8) 124.4(2)	C(12)-C(13)-C(14) 120.5(2)	F(1)-C(17)-C(14) 112.2(5)
O(1)-C(4)-C(3) 127.2(2)	N(10)-C(9)-C(8) 117.5(2)	C(15)-C(14)-C(13) 119.2(2)	F(2)-C(17)-C(14) 113.1(5)
O(1)-C(4)-N(10) 117.34(19)	C(5)-N(10)-C(9) 119.80(19)	C(15)-C(14)-C(17) 121.0(2)	F(3)-C(17)-C(14) 114.3(6)
C(3)-C(4)-N(10) 115.48(18)	C(5)-N(10)-C(4) 116.76(18)	C(13)-C(14)-C(17) 119.8(2)	
C(6)-C(5)-N(10) 121.5(2)	C(9)-N(10)-C(4) 123.42(18)	C(16)-C(15)-C(14) 120.5(2)	