Supporting information

Bifunctional N-heterocyclic carbene ligands for Cu-catalyzed direct C-H carboxylation with CO_2

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[b]*Department of Chemistry, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju 61186, Republic of Korea*

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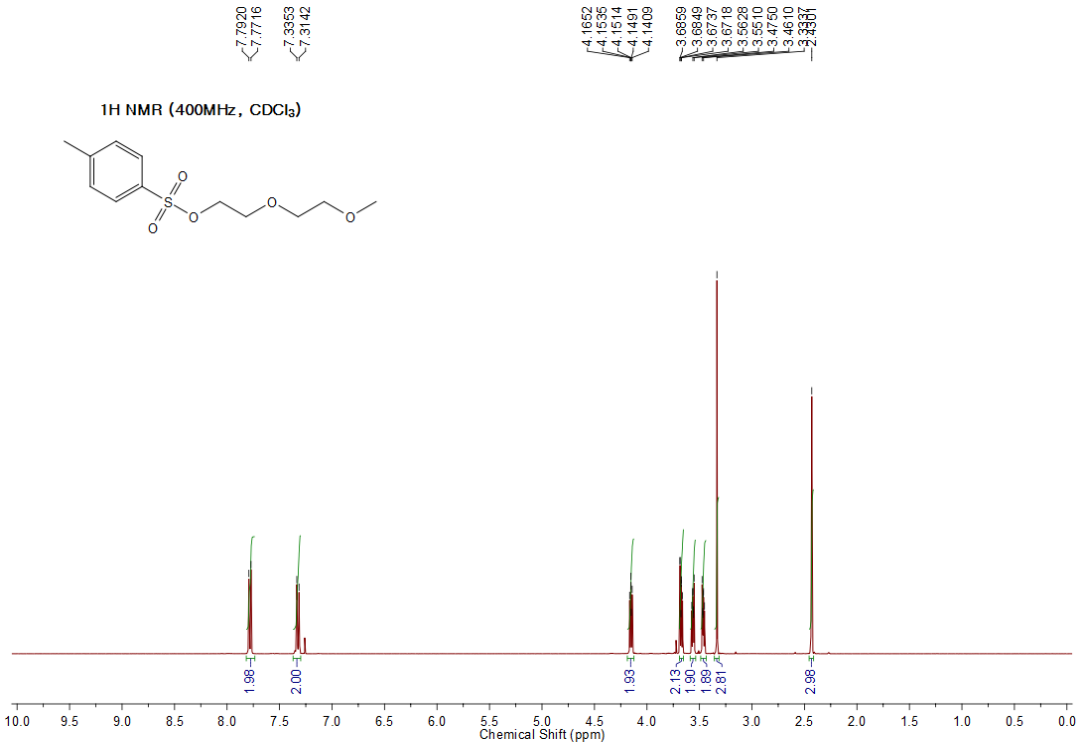
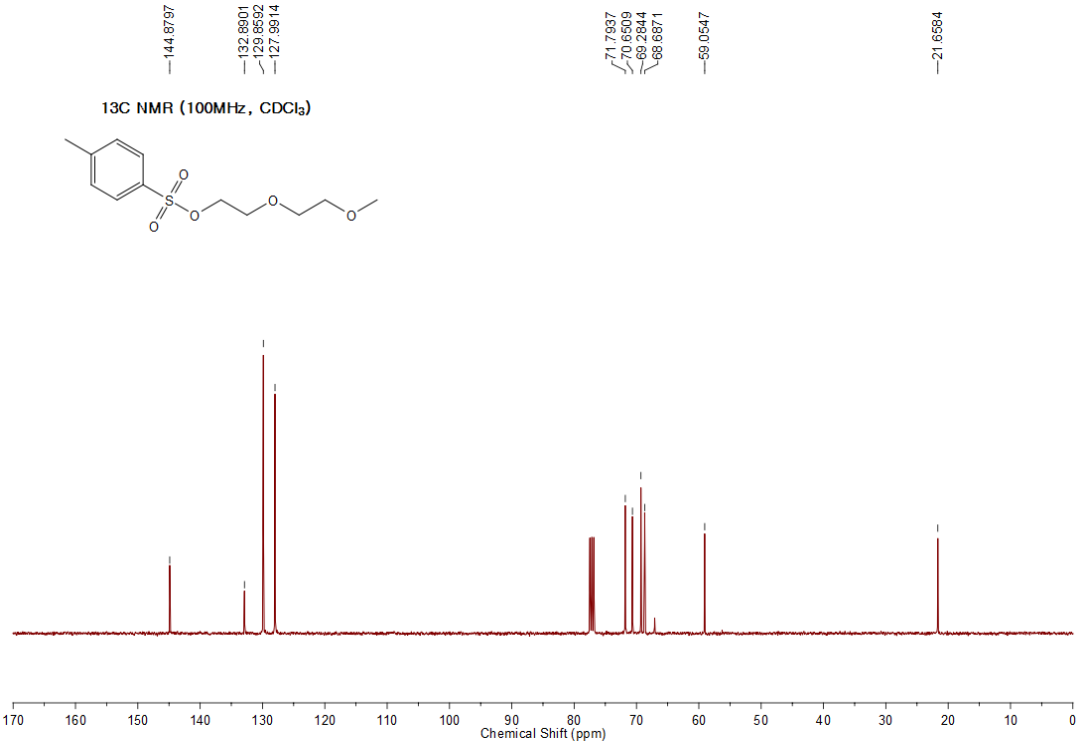
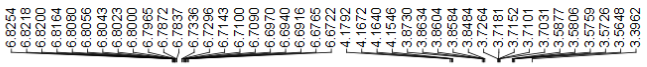
Contents

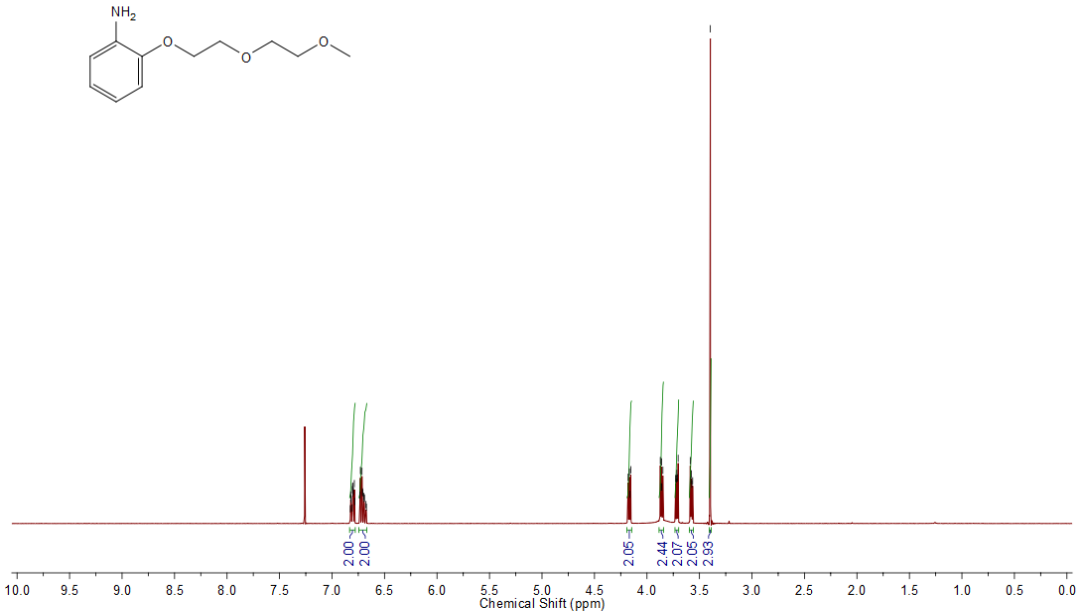
1. ^{1}H and ^{13}C NMR Spectra for Ligands and Catalysts

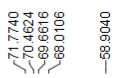




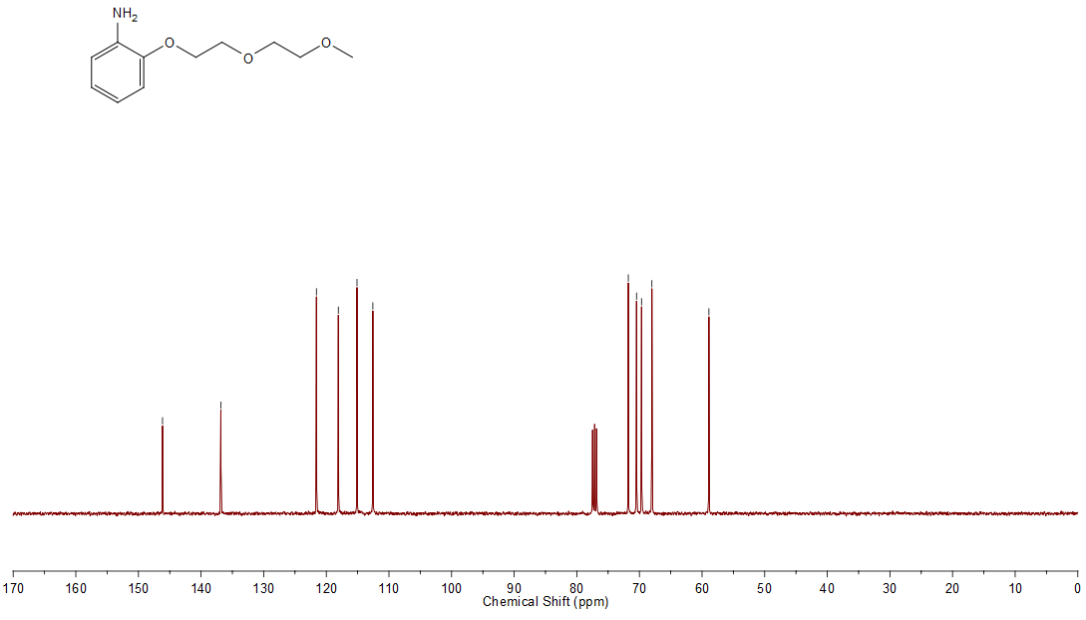


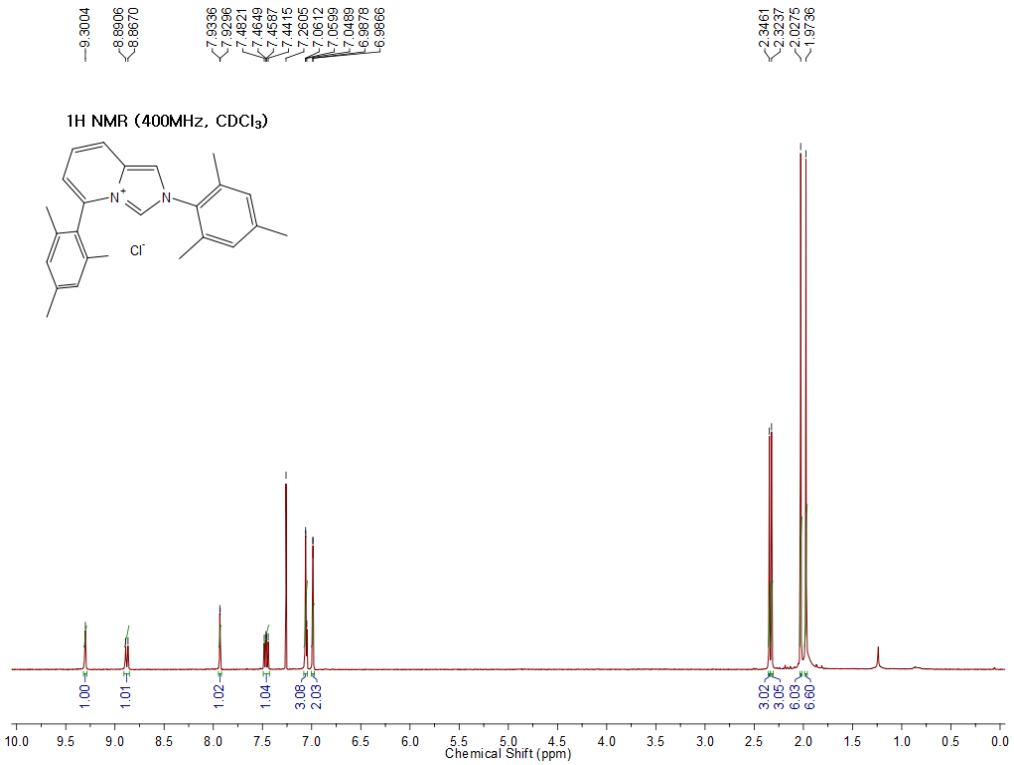
1H NMR (400MHz, $CDCl_3$)





13C NMR (100MHz, $CDCl_3$)

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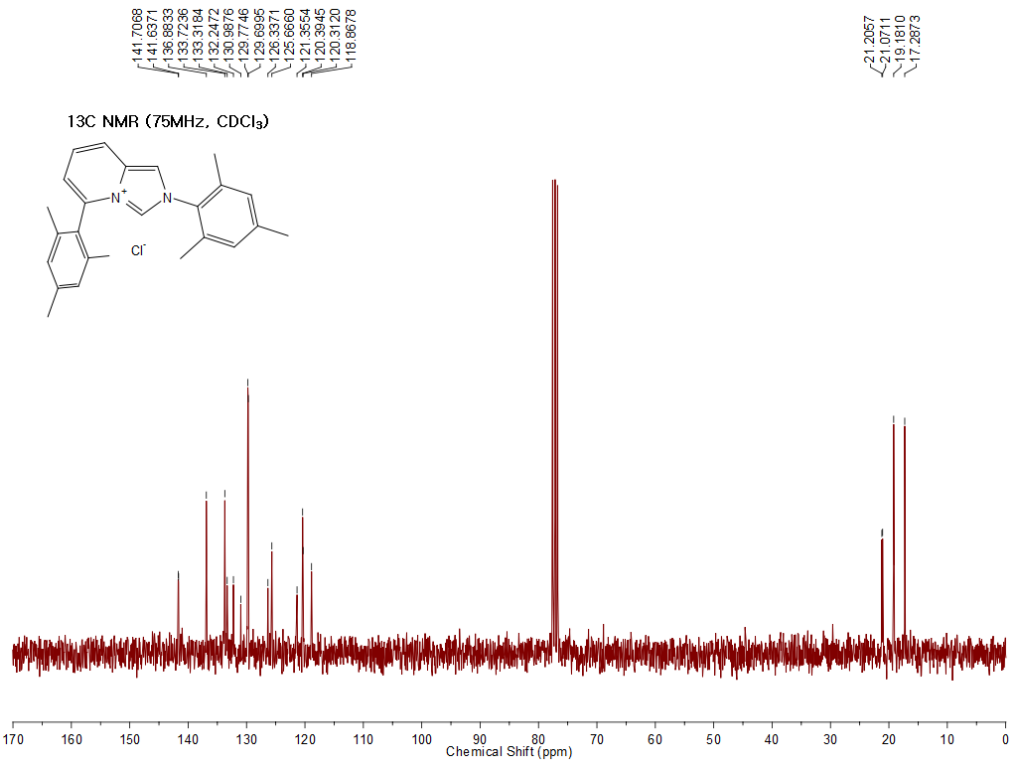
7.0612
7.0599
7.0499
6.9878
6.9866
2.3461
2.3237
2.0275
1.9736
1H NMR (400MHz, CDCl3)
Cl-
1.00
1.01
1.02
1.04
3.08
2.03
3.02
3.05
6.03
6.60
Chemical Shift (ppm)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125.6660
121.3554
120.3945
120.3120
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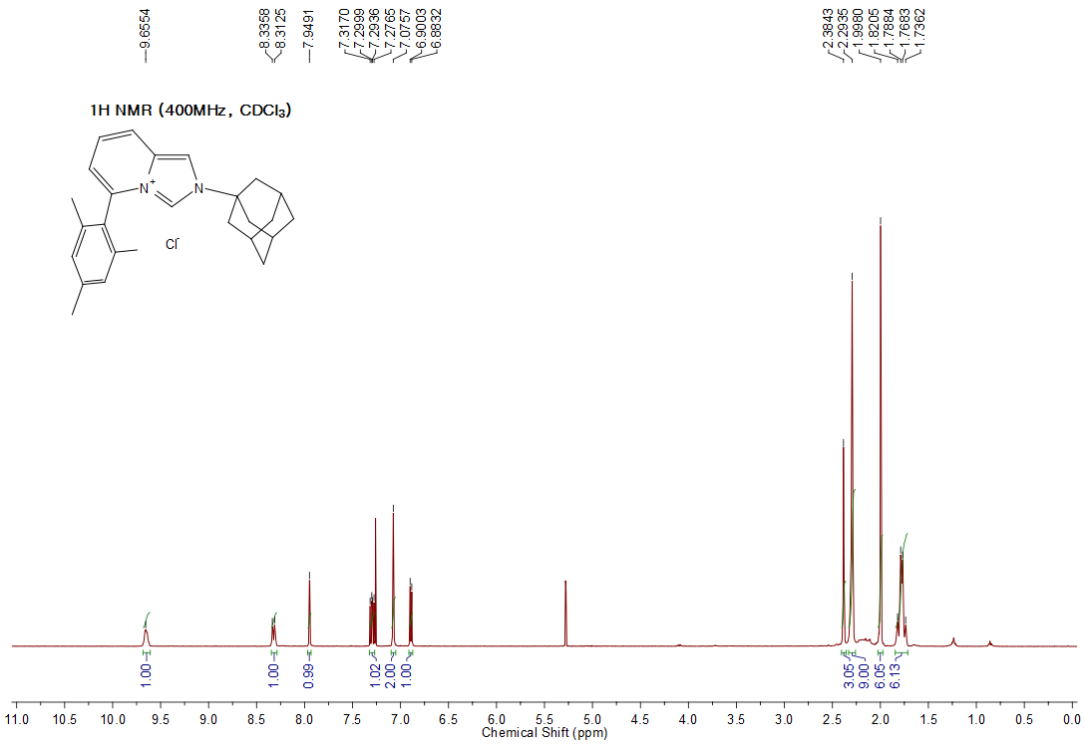
21.2057
21.0711
19.1810
17.2873
13C NMR (75MHz, CDCl3)
Cl-
Chemical Shift (ppm)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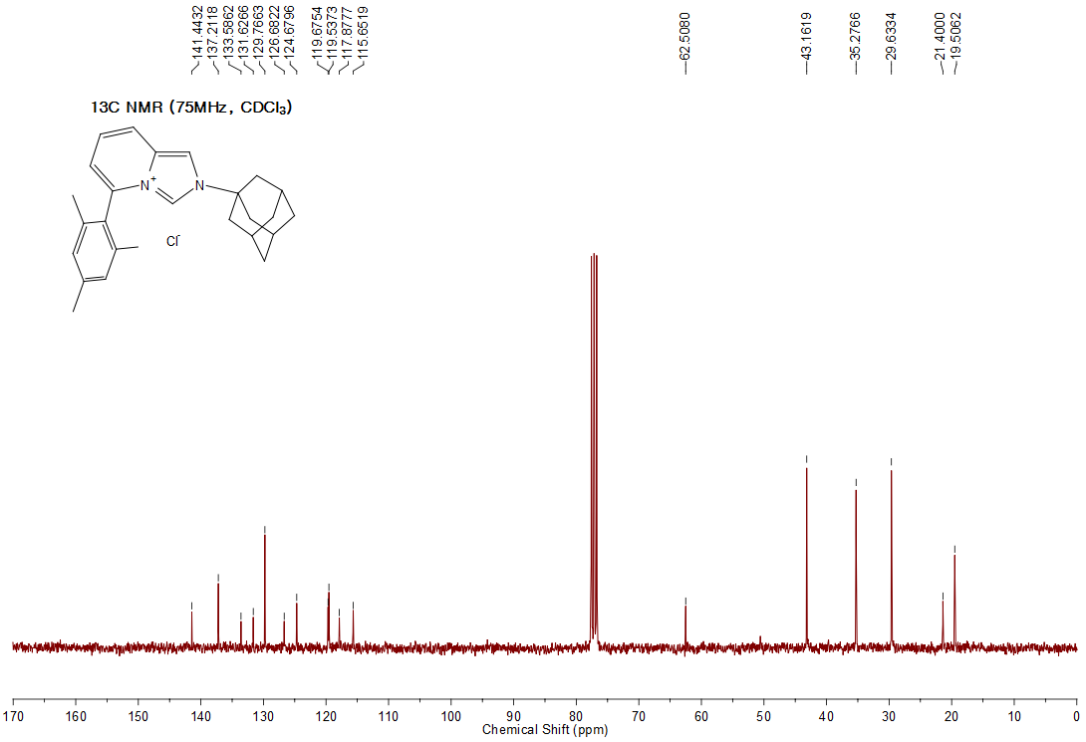
6.8832
2.3843
2.2935
1.9980
1.8205
1.7884
1.7683
1.7362
1H NMR (400MHz, CDCl3)
Cl
1.00
1.00
0.99
1.02
2.00
1.00
3.05
9.00
6.05
6.13
Chemical Shift (ppm)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115.6519
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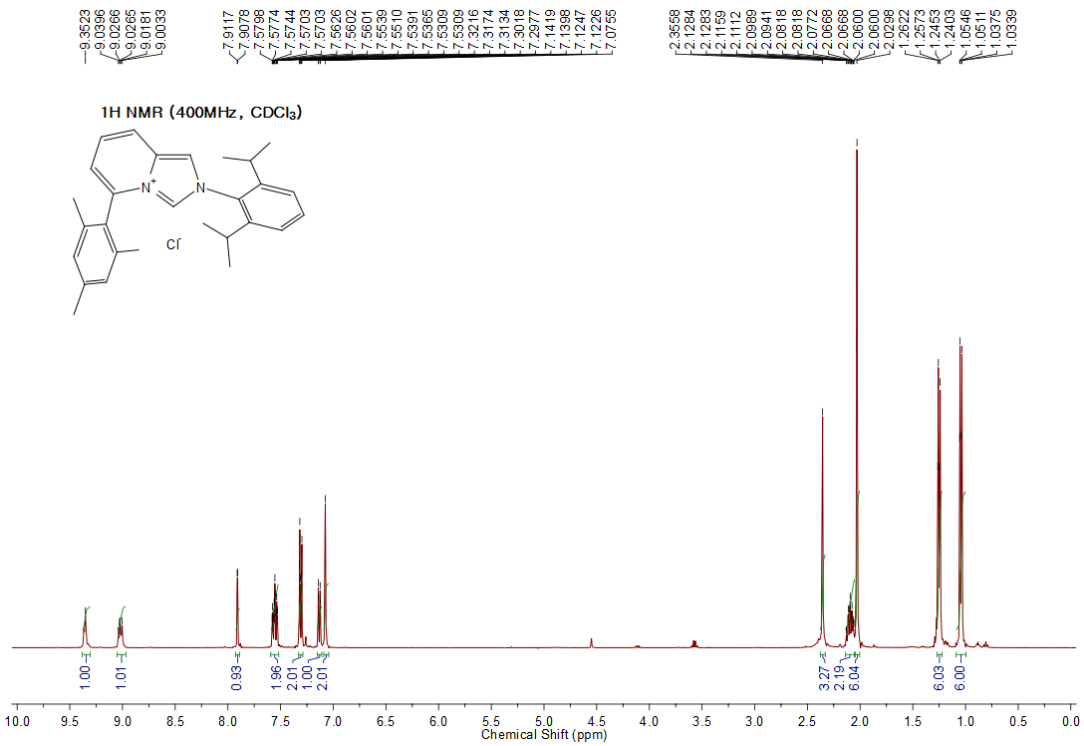
19.5062
13C NMR (75MHz, CDCl3)
Cl
Chemical Shift (ppm)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9.0265
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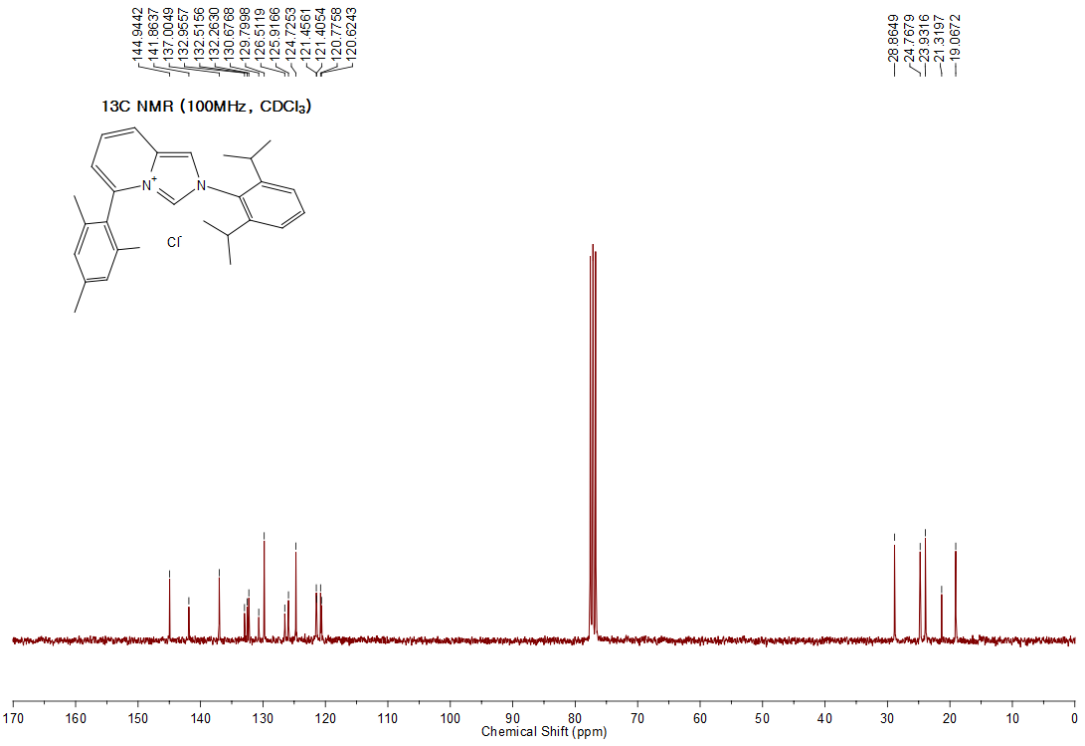
7.5744
7.5703
7.5703
7.5626
7.5602
7.5601
7.5539
7.5510
7.5391
7.5365
7.5309
7.5309
7.3216
7.3174
7.3134
7.3018
7.2977
7.1419
7.1398
7.1247
7.1226
7.0755
2.3558
2.1284
2.1283
2.1159
2.1112
2.0989
2.0941
2.0818
2.0818
2.0772
2.0668
2.0668
2.0600
2.0600
2.0298
1.2622
1.2573
1.2453
1.2403
1.0546
1.0511
1.0375
1.0339
1H NMR (400MHz, CDCl3)
Cl
1.00
1.01
0.93
1.96
2.01
1.00
2.01
3.27
2.19
6.04
6.03
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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124.7253
121.4561
121.4054
120.7758
120.6243
28.8649
24.7679
23.9316
21.3197
19.0672
13C NMR (100MHz, CDCl3)
Cl
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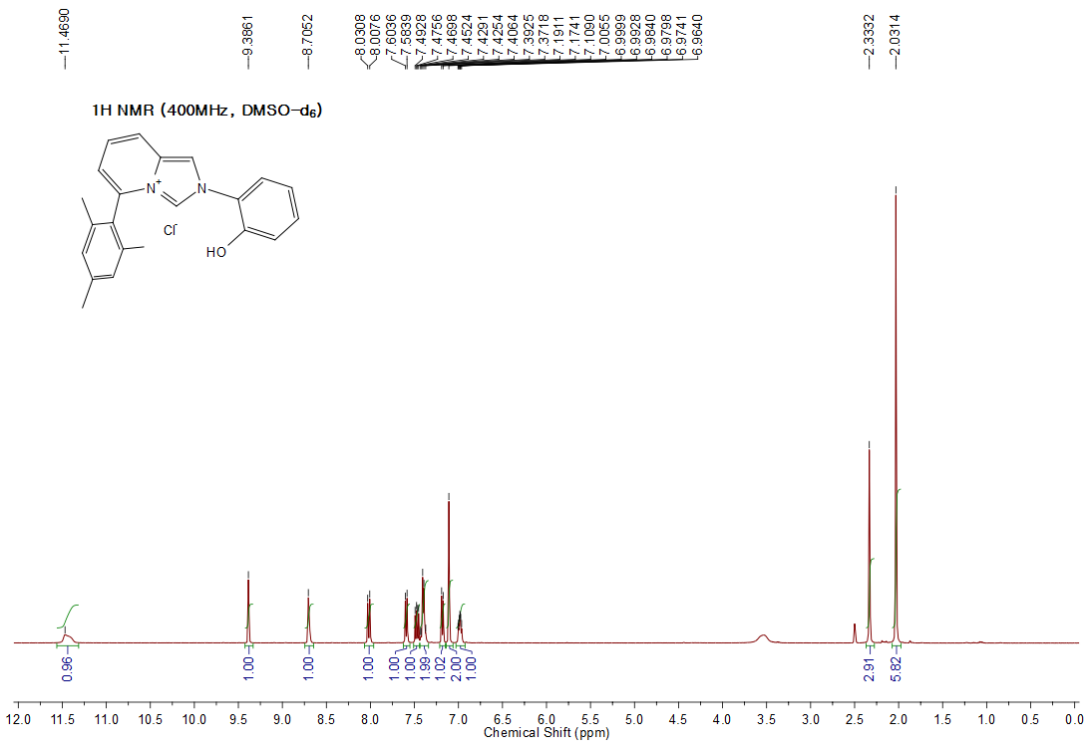
Chemical Shift (ppm)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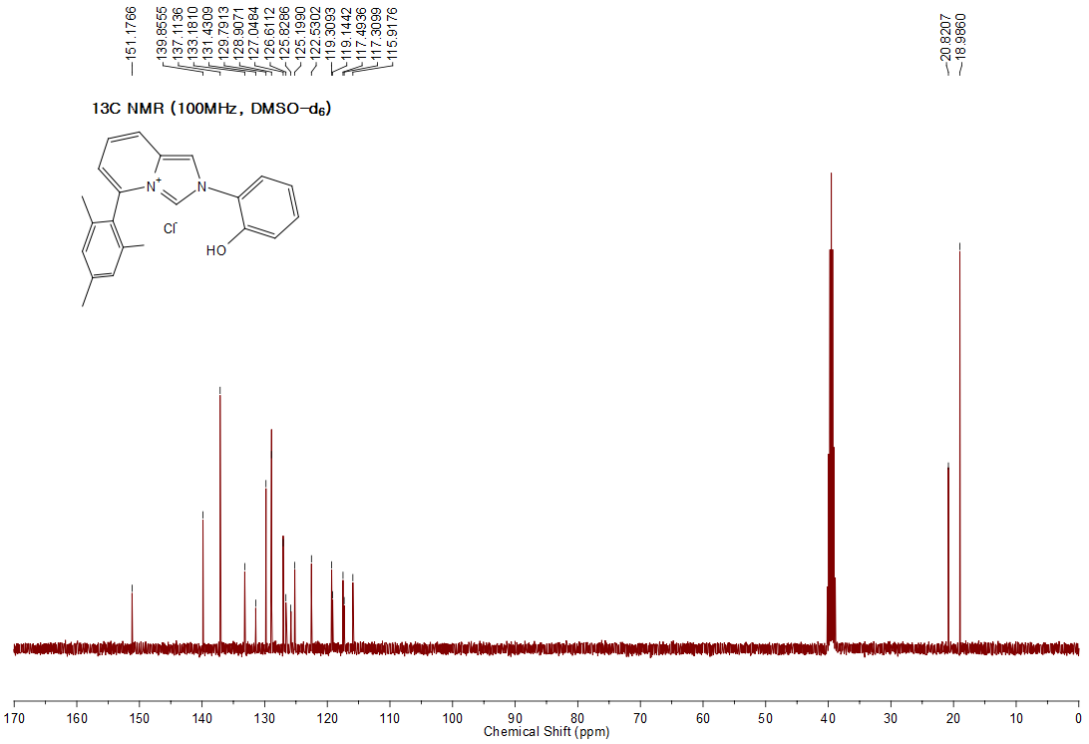
7.4524
7.4291
7.4254
7.4064
7.3925
7.3718
7.1911
7.1741
7.1090
7.0055
6.9999
6.9928
6.9840
6.9798
6.9741
6.9640
2.3332
2.0314
1H NMR (400MHz, DMSO-d6)
Cl
HO
0.96
1.00
1.00
1.00
1.00
1.00
1.99
1.02
2.00
1.00
2.91
5.82
Chemical Shift (ppm)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133.1810
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129.7913
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127.0484
126.6112
125.8286
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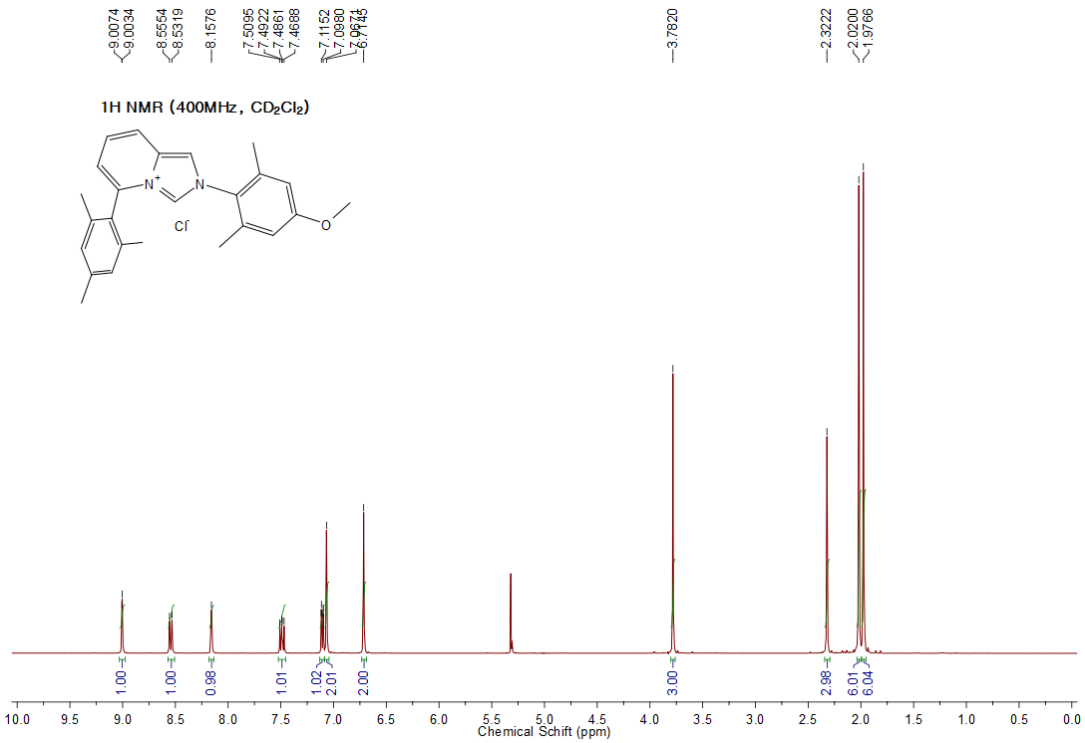
122.5302
119.3093
119.1442
117.4936
117.3099
115.9176
20.8207
18.9860
13C NMR (100MHz, DMSO-d6)
Cl
HO
Chemical Shift (ppm)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7.0980
7.0744
6.7145
3.7820
2.3222
2.0200
1.9766
1H NMR (400MHz, CD2Cl2)
Cl
O
1.00
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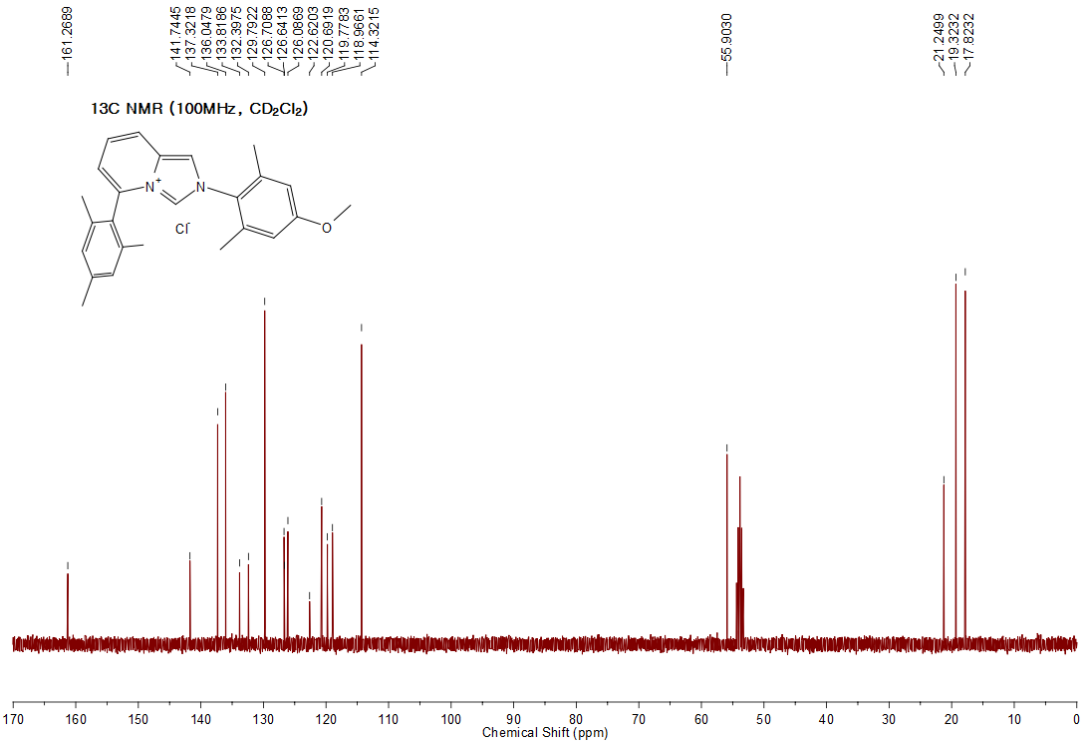
1.02
2.01
2.00
3.00
2.98
6.01
6.04
Chemical Schift (ppm)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122.6203
120.6919
119.7783
118.9661
114.3215
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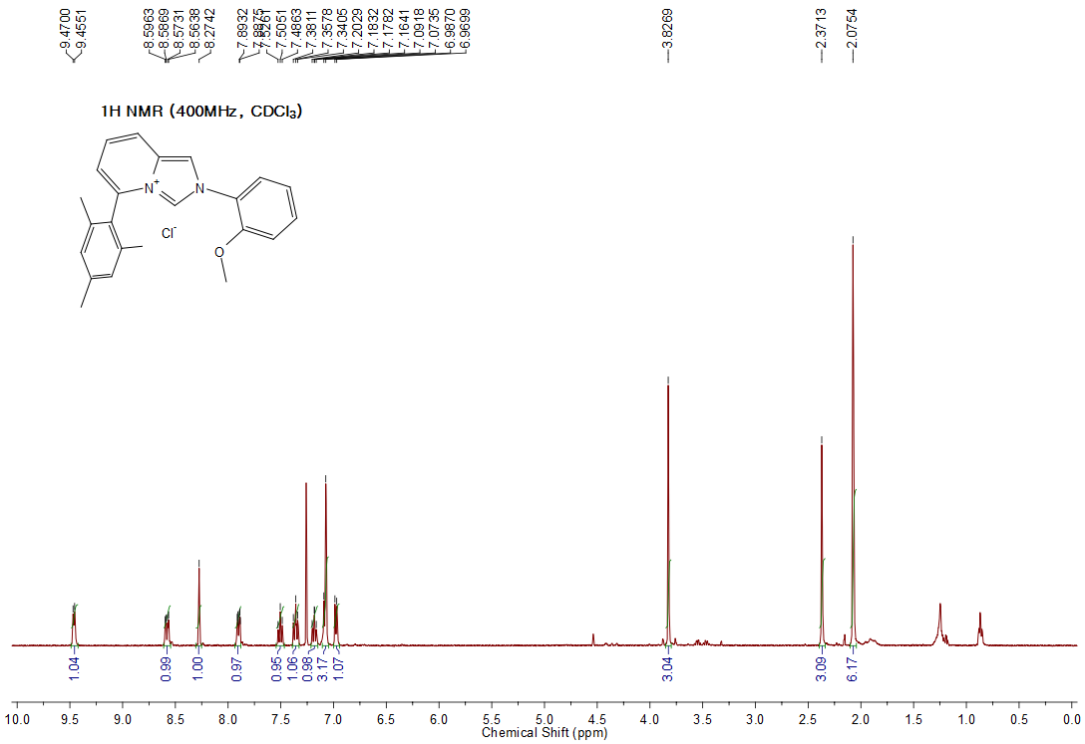
21.2499
19.3232
17.8232
13C NMR (100MHz, CD2Cl2)
Cl
O
Chemical Shift (ppm)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8.5731
8.5638
8.2742
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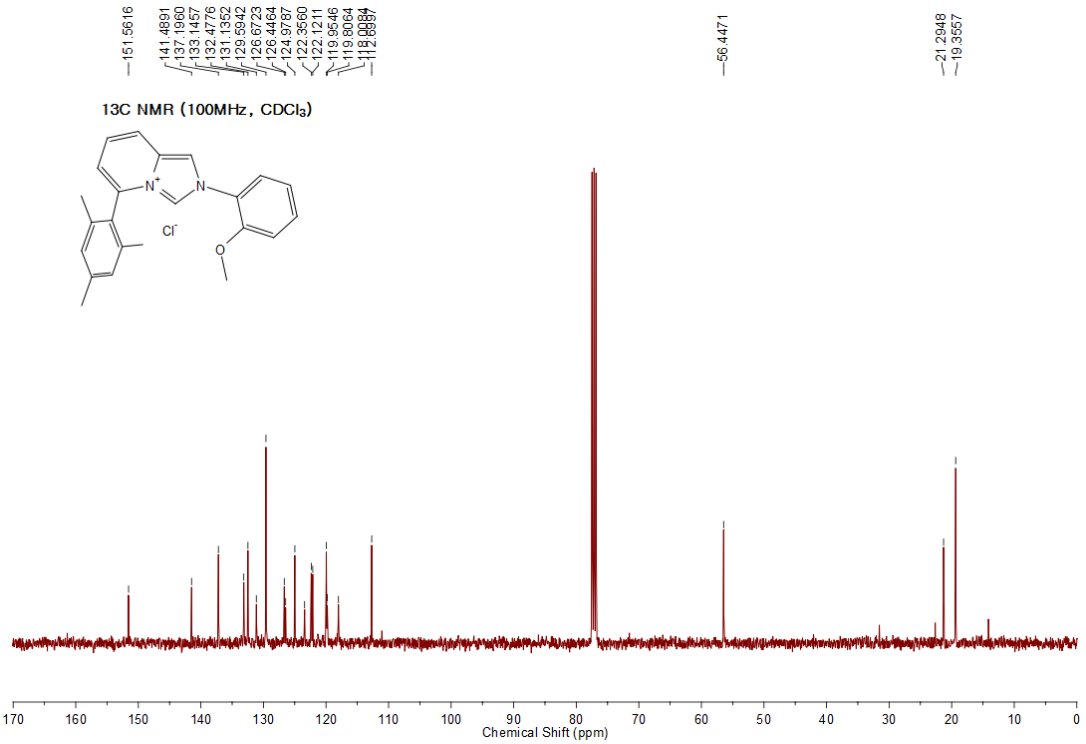
7.5051
7.4863
7.3811
7.3578
7.3405
7.2029
7.1832
7.1782
7.1641
7.0918
7.0735
6.9870
6.9699
3.8269
2.3713
2.0754
1H NMR (400MHz, CDCl3)
Cl-
1.04
0.99
1.00
0.97
0.95
1.06
0.98
3.17
1.07
3.04
3.09
6.17
Chemical Shift (ppm)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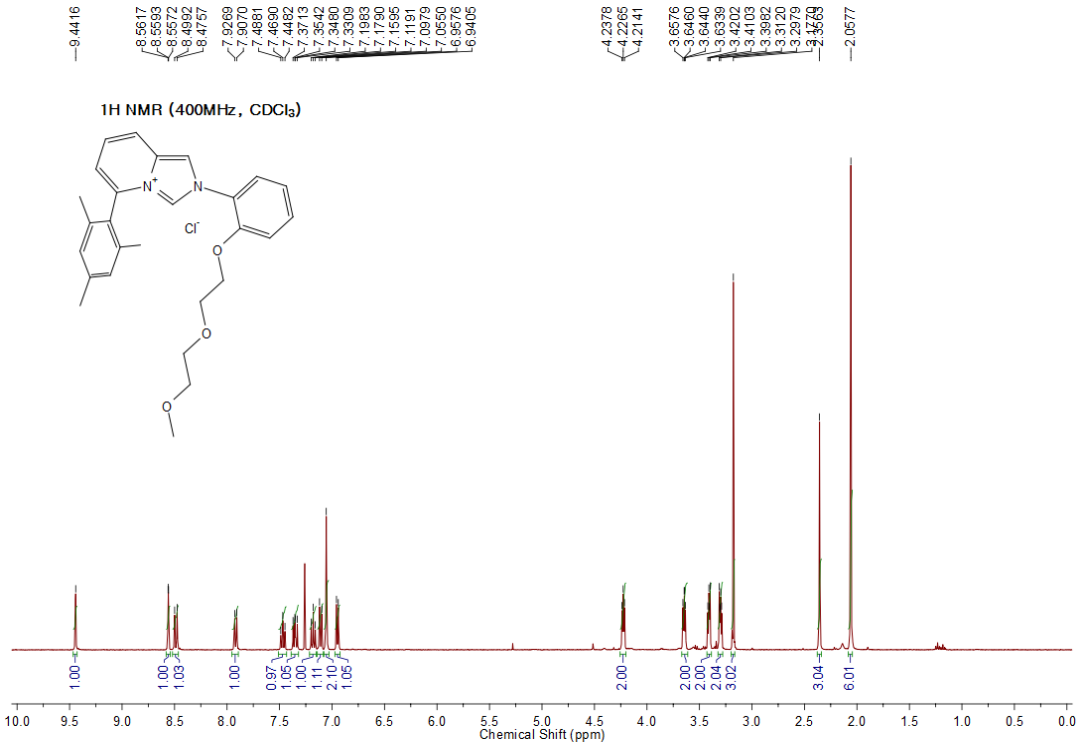
124.9787
122.3560
122.1211
119.9546
119.8064
56.4471
21.2948
19.3557
13C NMR (100MHz, CDCl3)
Cl-
Chemical Shift (ppm)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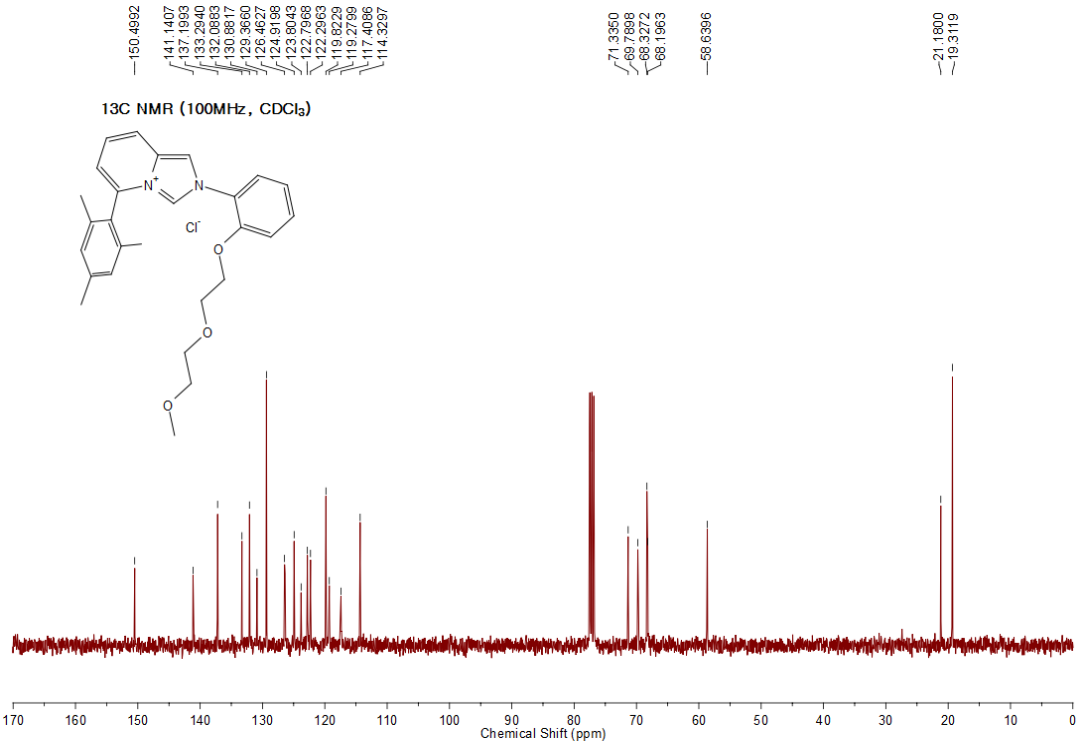
7.9269
7.9070
7.4881
7.4690
7.4482
7.3713
7.3542
7.3480
7.3309
7.1983
7.1790
7.1595
7.1191
7.0979
7.0550
6.9576
6.9405
4.2378
4.2265
4.2141
3.6576
3.6460
3.6440
3.6339
3.4202
3.4103
3.3982
3.3120
3.2979
3.1779
3.1563
2.0577
1H NMR (400MHz, CDCl3)
Cl-
1.00
1.00
1.03
1.00
0.97
1.05
1.00
1.11
2.10
1.05
2.00
2.00
2.00
2.04
3.02
3.04
6.01
Chemical Shift (ppm)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117.4086
114.3297
71.3350
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68.1963
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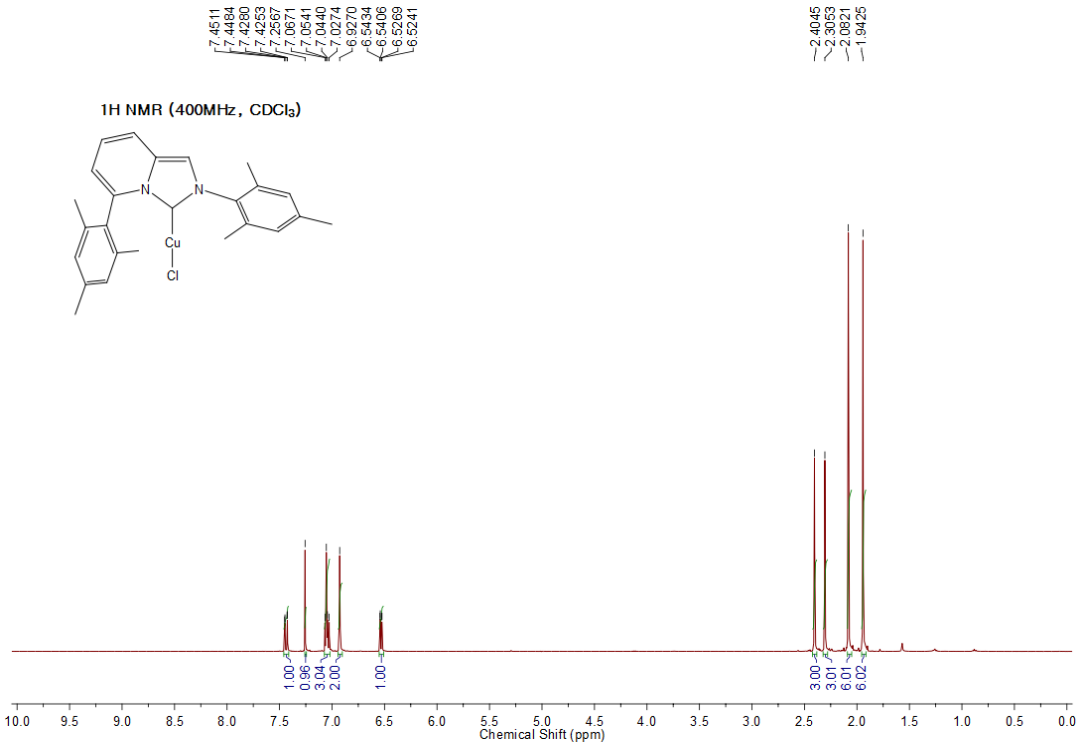
19.3119
13C NMR (100MHz, CDCl3)
Cl-
Chemical Shift (ppm)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7.4253
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7.0541
7.0440
7.0274
6.9270
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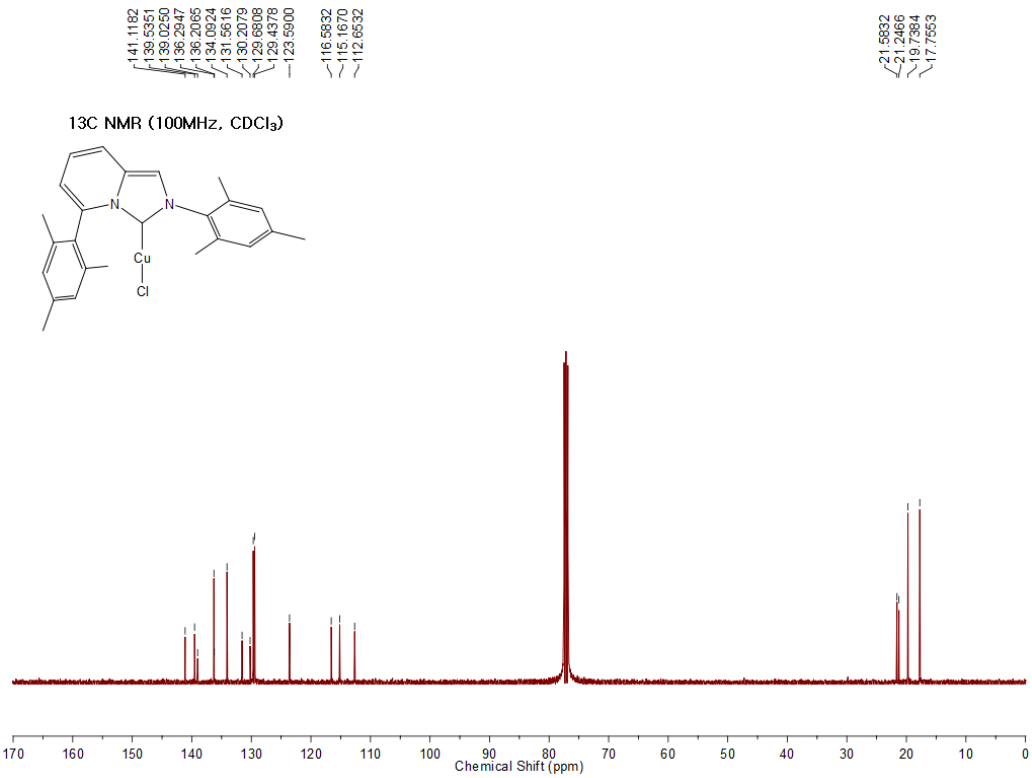
6.5406
6.5269
6.5241
2.4045
2.3053
2.0821
1.9425
1H NMR (400MHz, CDCl3)
Cu
Cl
1.00
0.96
3.04
2.00
1.00
3.00
3.01
6.01
6.02
Chemical Shift (ppm)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116.5832
115.1670
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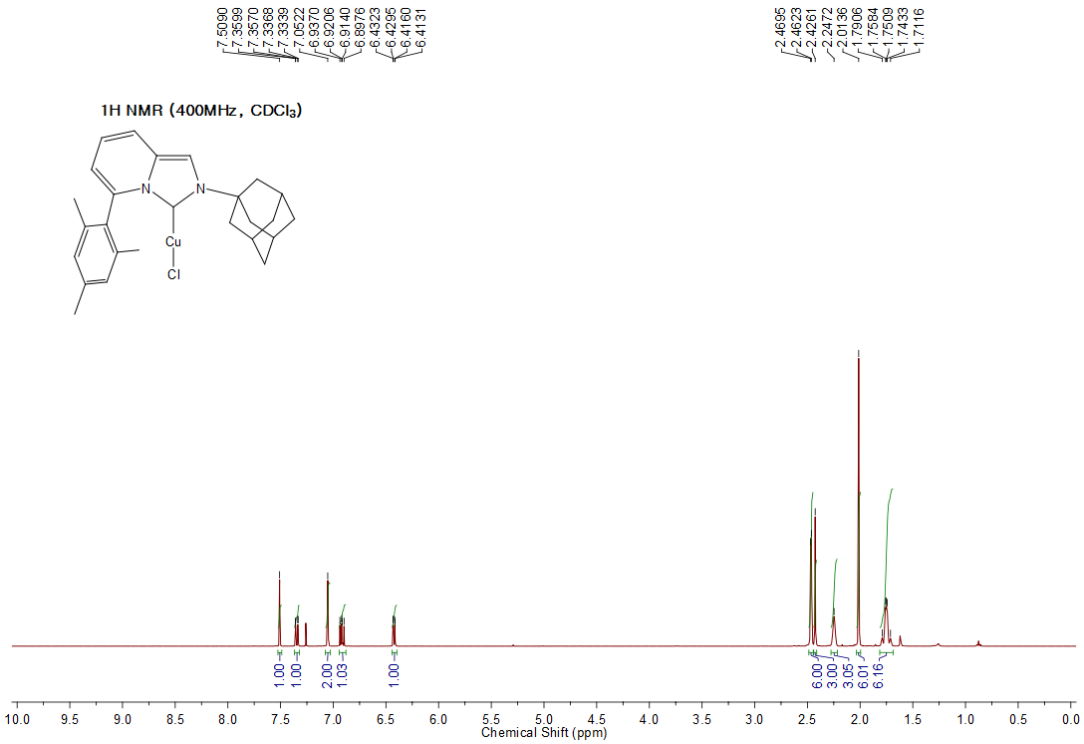
13C NMR (100MHz, CDCl3)
Cu
Cl
Chemical Shift (ppm)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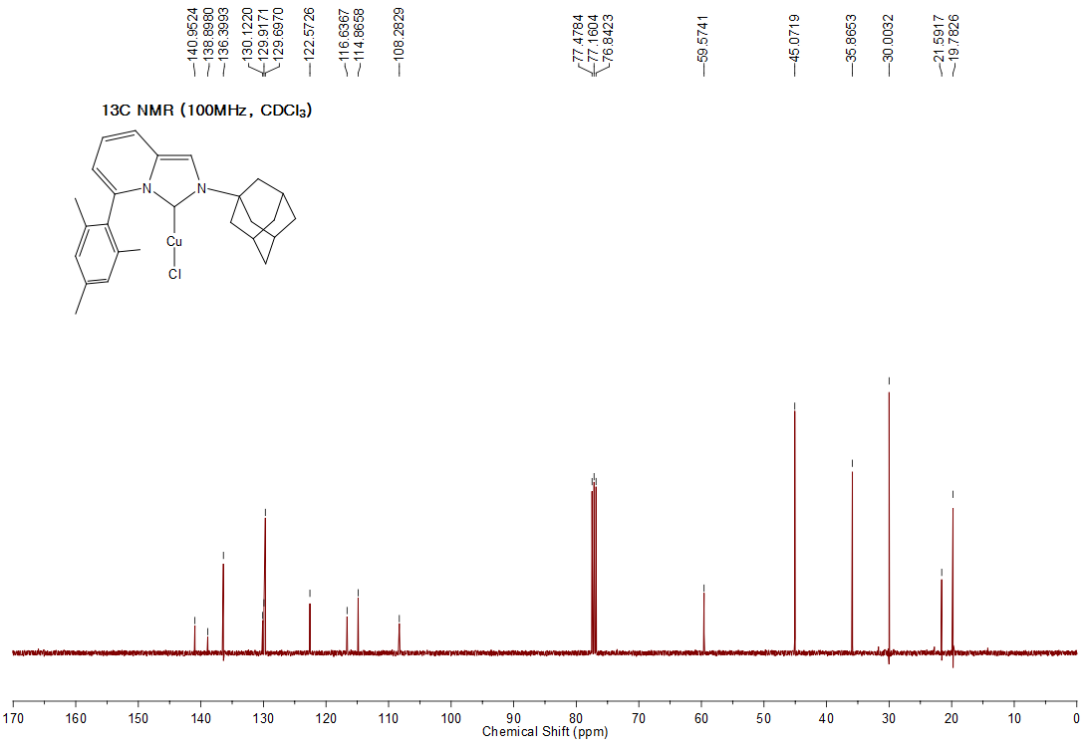
1.7584
1.7509
1.7433
1.7116
1H NMR (400MHz, CDCl3)
N
N
Cu
Cl
1.00
1.00
2.00
1.03
1.00
6.00
3.00
3.05
6.01
6.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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130.1220
129.9171
129.6970
122.5726
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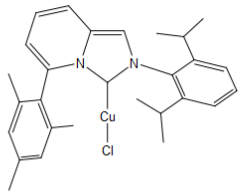
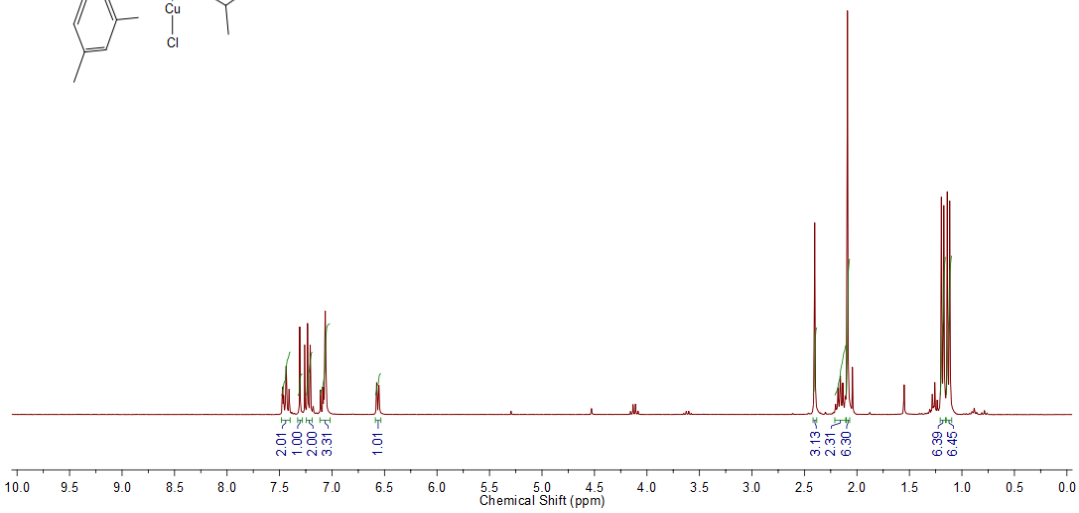
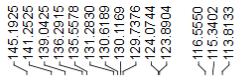
114.8658
108.2829
77.4784
77.1604
76.8423
59.5741
45.0719
35.8653
30.0032
21.5917
19.7626
13C NMR (100MHz, CDCl3)
N
N
Cu
Cl
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

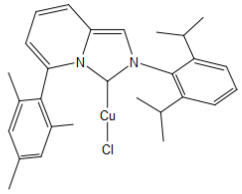
1H NMR (300MHz, $CDCl_3$)

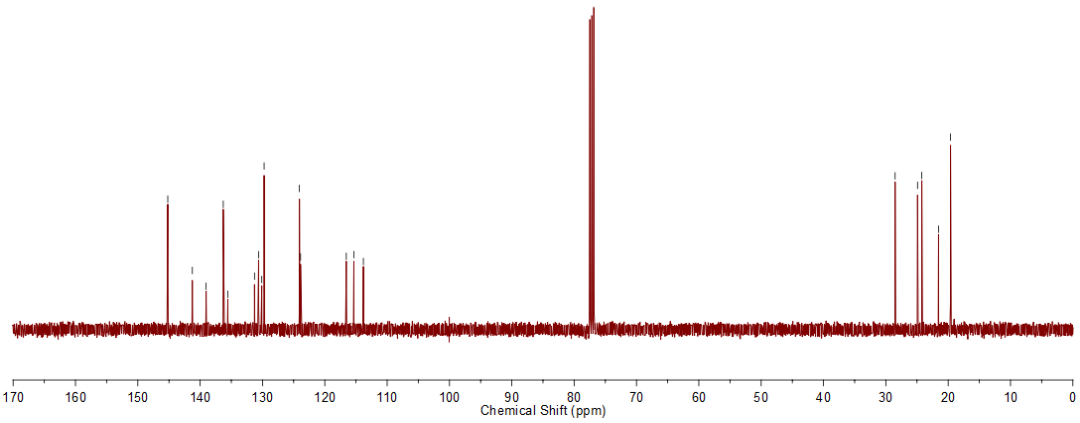


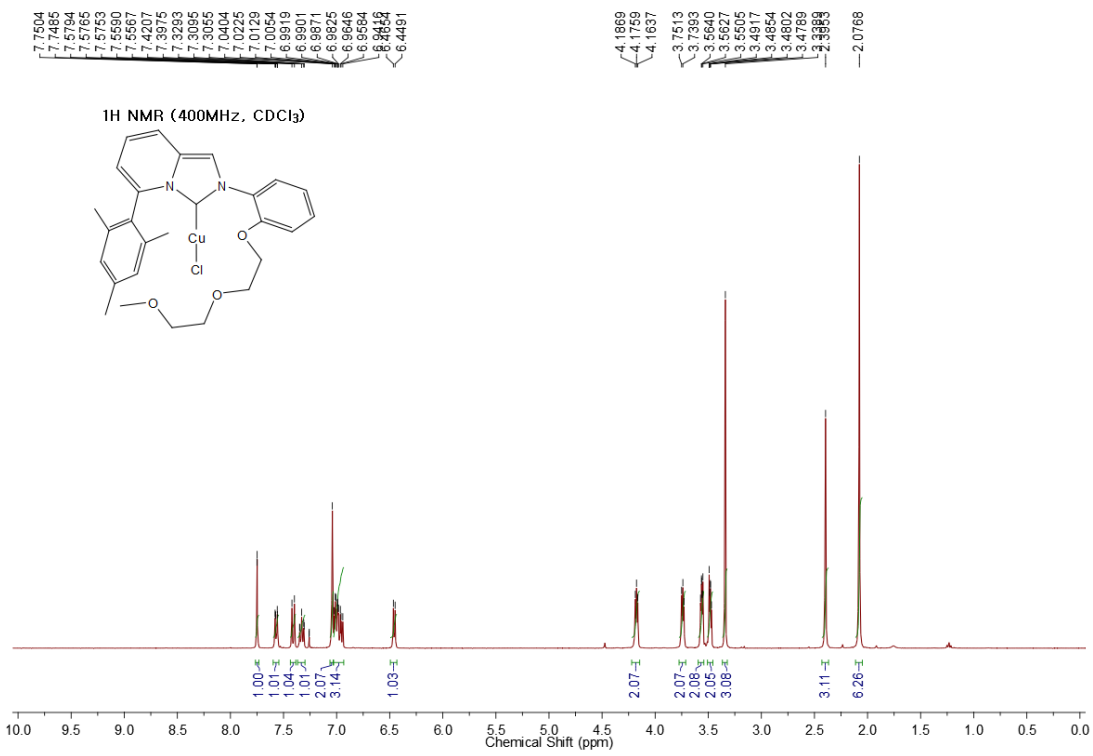


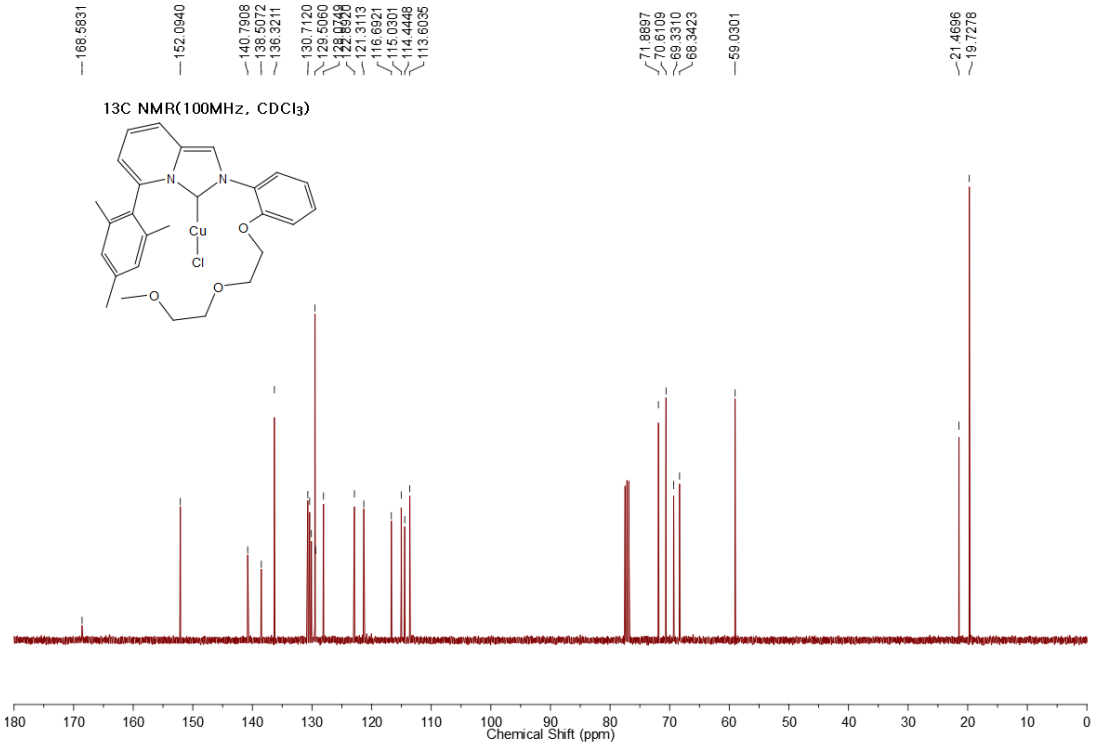


13C NMR (100MHz, $CDCl_3$)

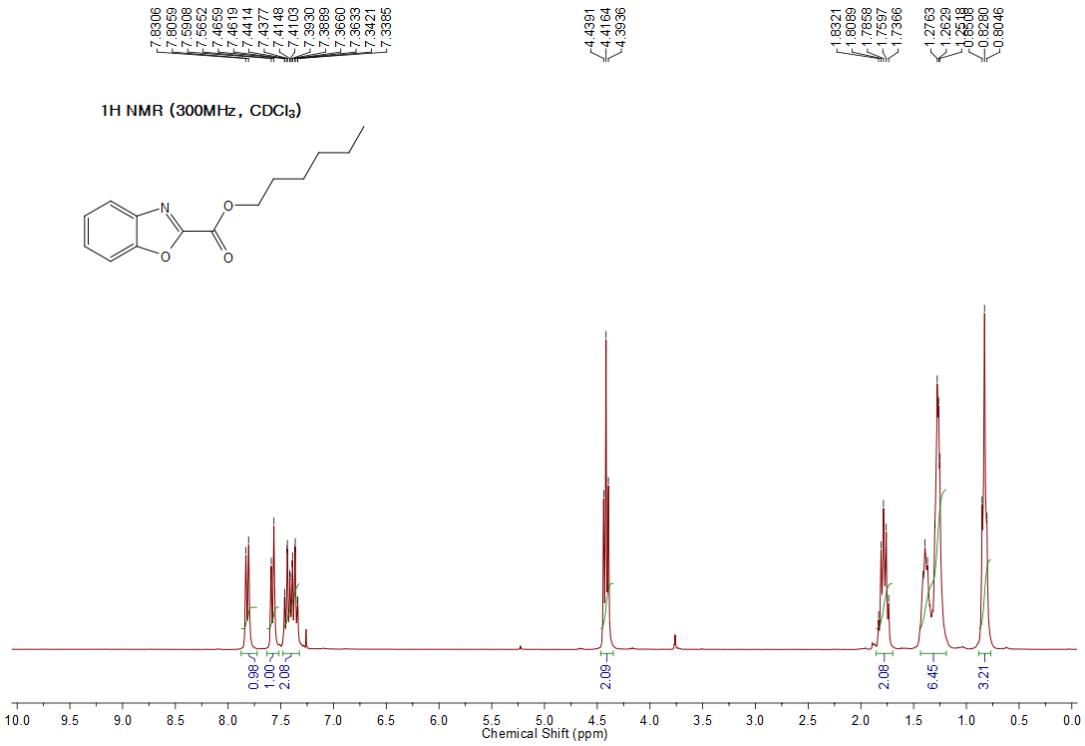


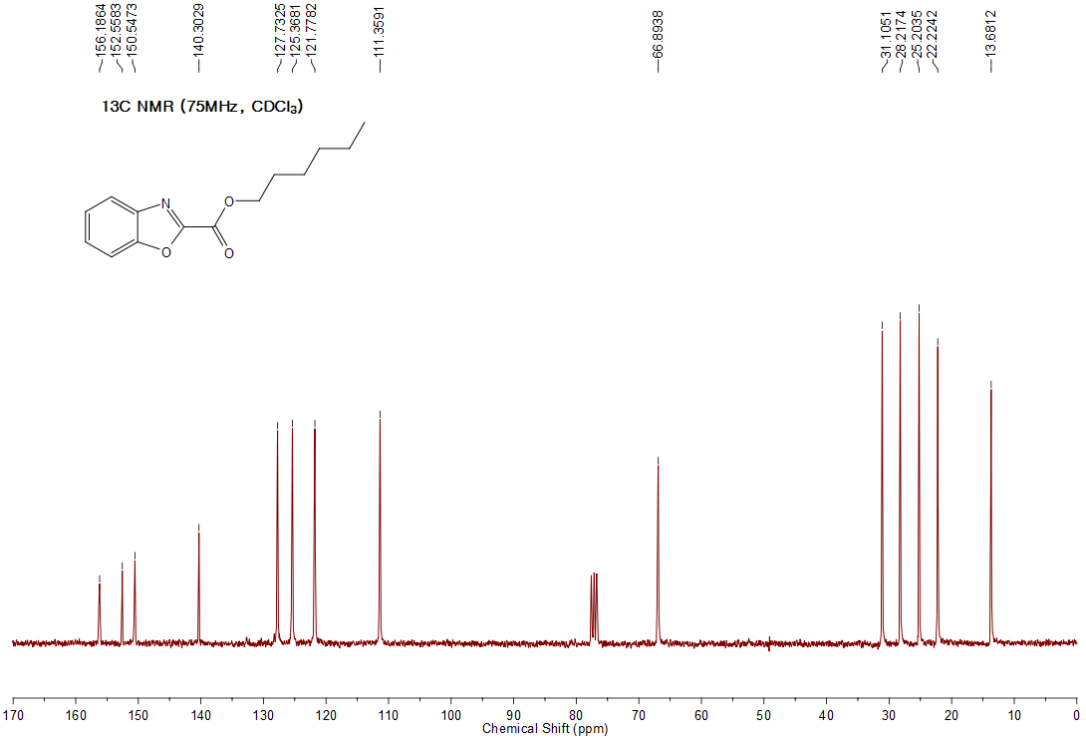


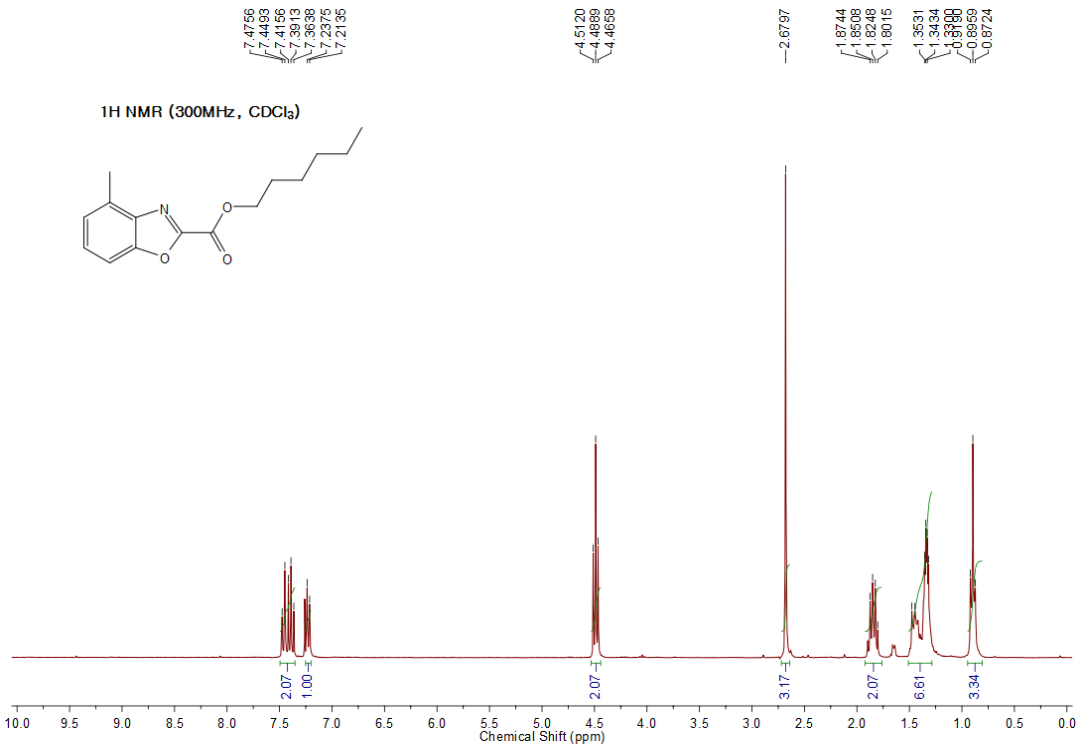

1H NMR (400MHz, CDCl3)
Cu
Cl
Chemical Shift (ppm)

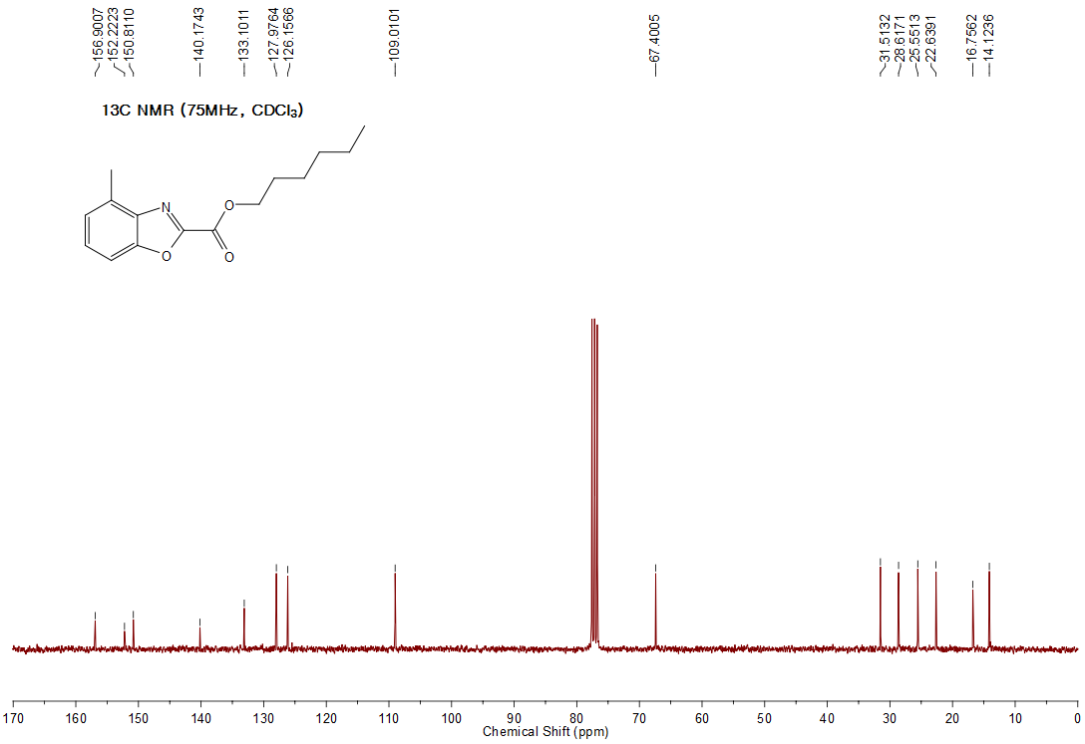

13C NMR(100MHz, CDCl3)
Cu
Cl
Chemical Shift (ppm)

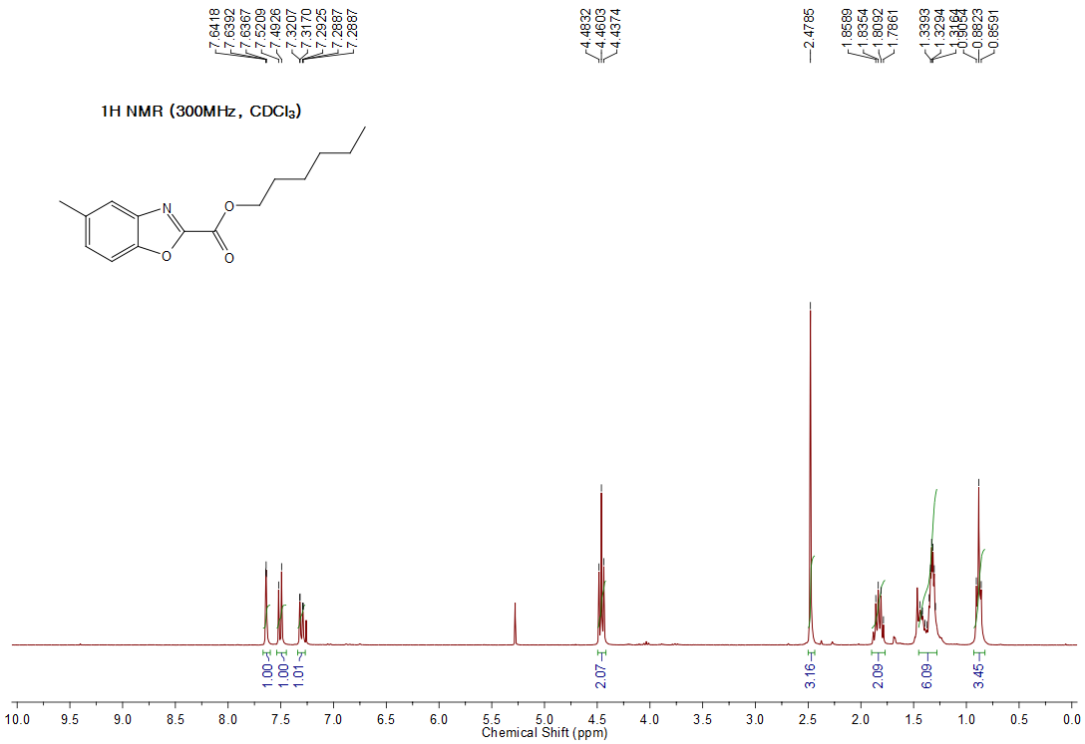
2. ^{1}H and ^{13}C NMR Spectra for Other Compounds

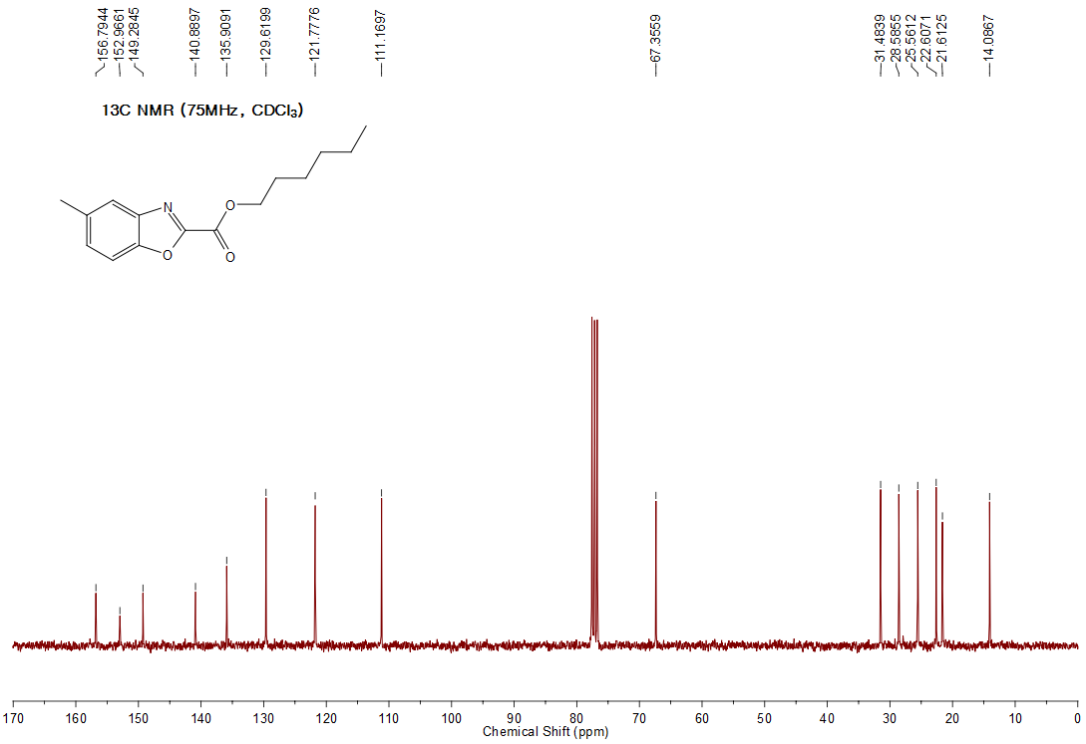


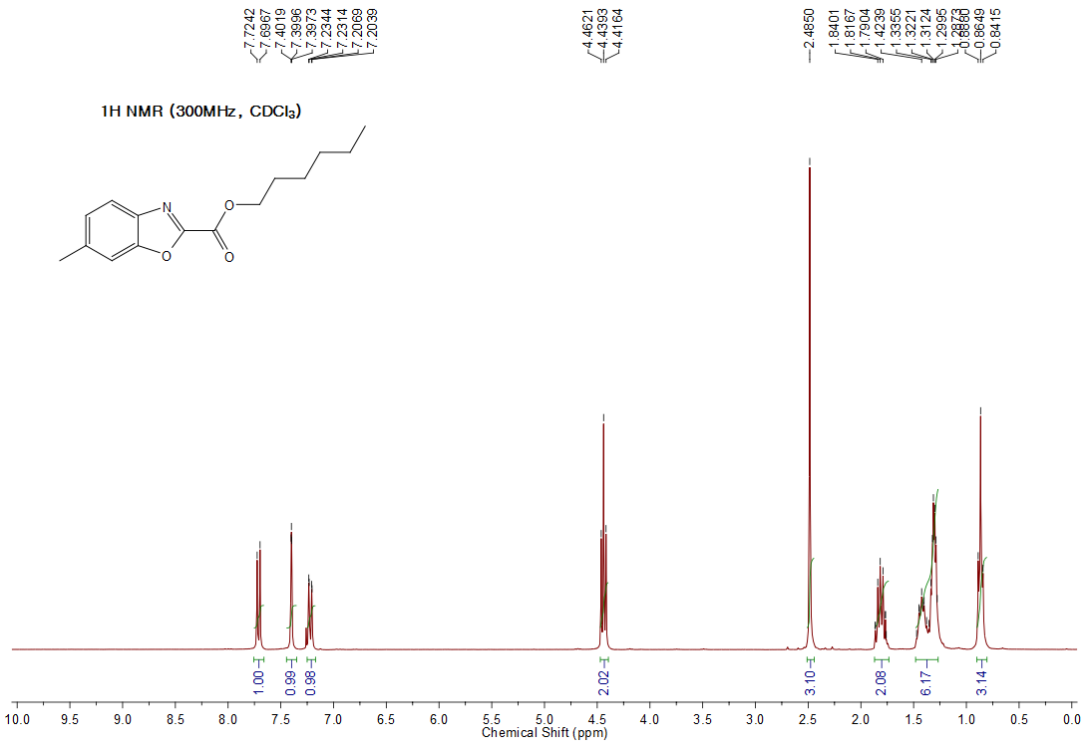


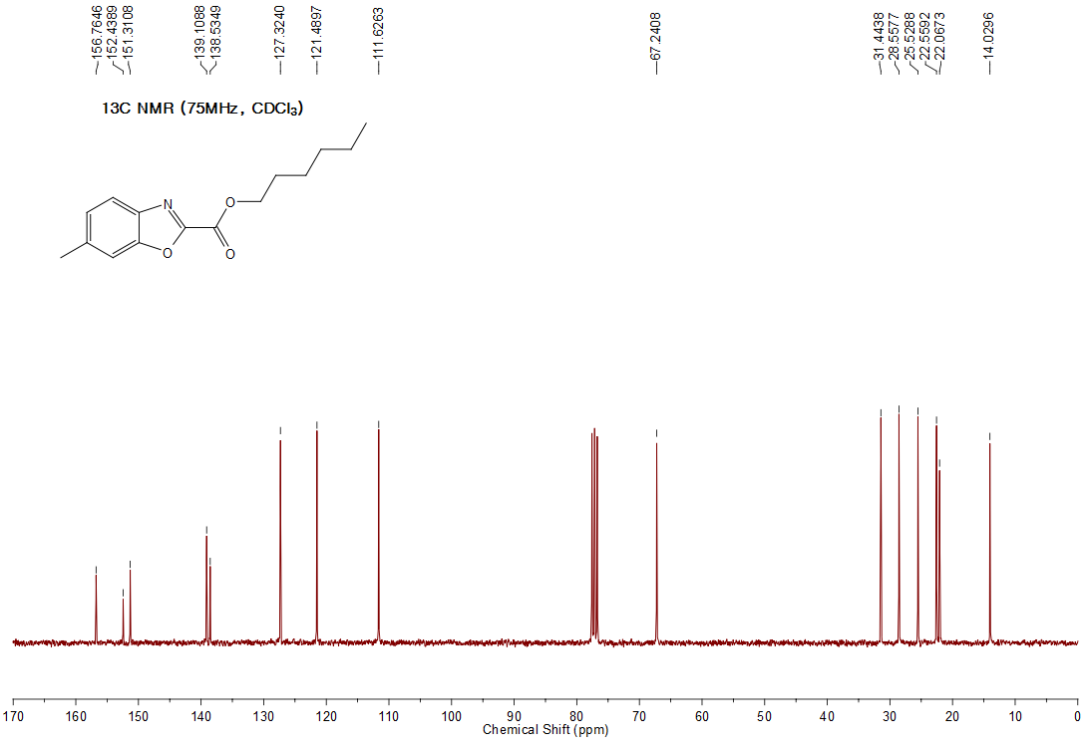

7.4756
7.4493
7.4156
7.3913
7.3638
7.2375
7.2135
4.5120
4.4889
4.4658
2.6797
1.8744
1.8508
1.8248
1.8015
1.3531
1.3434
1.3300
0.9198
0.8959
0.8724
1H NMR (300MHz, CDCl3)
2.07
1.00
2.07
3.17
2.07
6.61
3.34
Chemical Shift (ppm)

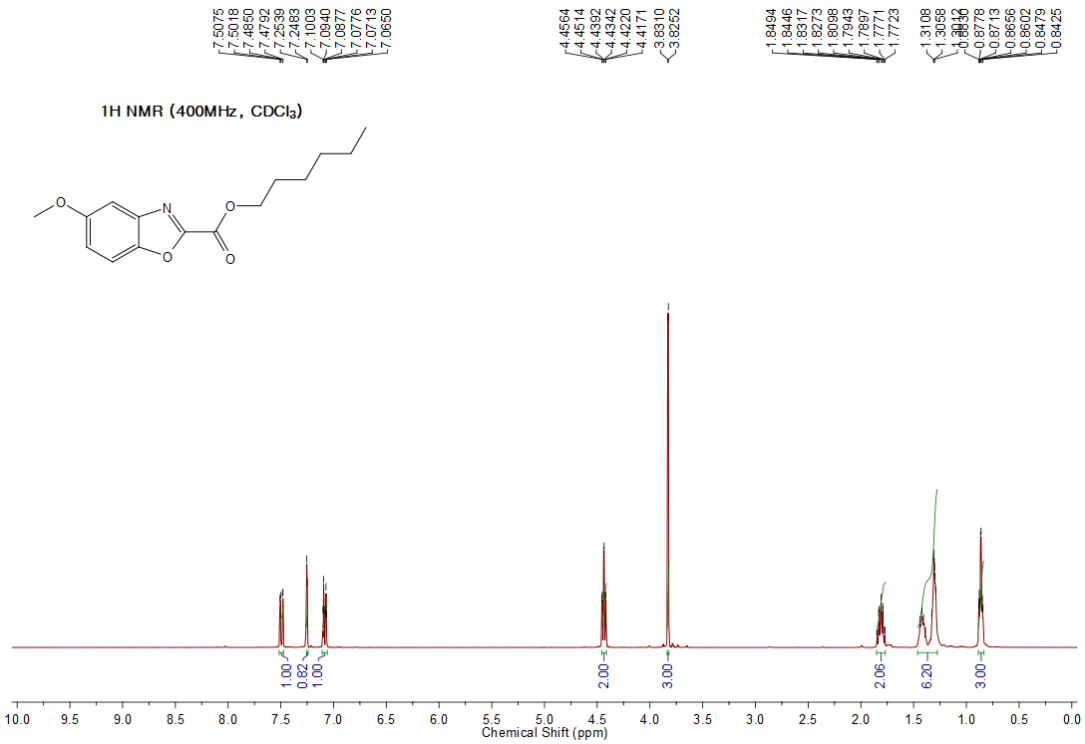

156.9007
152.2223
150.8110
140.1743
133.1011
127.9764
126.1566
109.0101
67.4005
31.5132
28.6171
25.5513
22.6391
16.7562
14.1236
13C NMR (75MHz, CDCl3)
Chemical Shift (ppm)

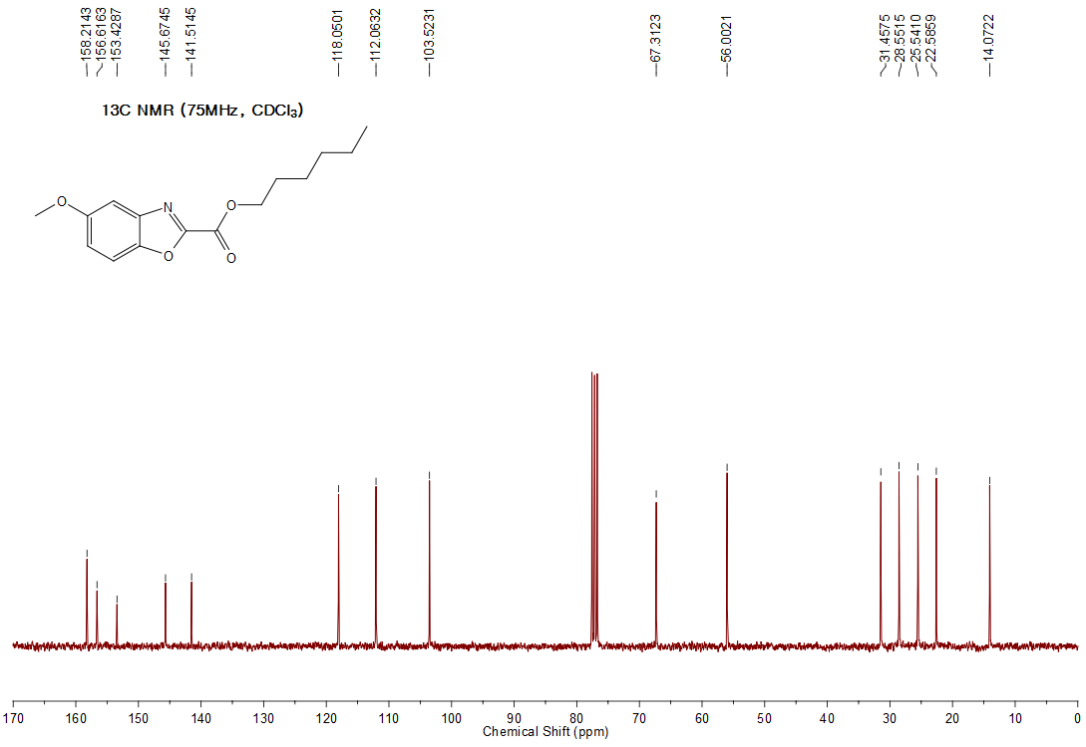

7.6418
7.6392
7.6367
7.5209
7.4926
7.3207
7.3170
7.2925
7.2887
7.2887
4.4832
4.4603
4.4374
2.4785
1.8589
1.8354
1.8092
1.7861
1.3393
1.3294
0.8823
0.8591
1H NMR (300MHz, CDCl3)
N
O
O
O
1.00
1.00
1.01
2.07
3.16
2.09
6.09
3.45
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

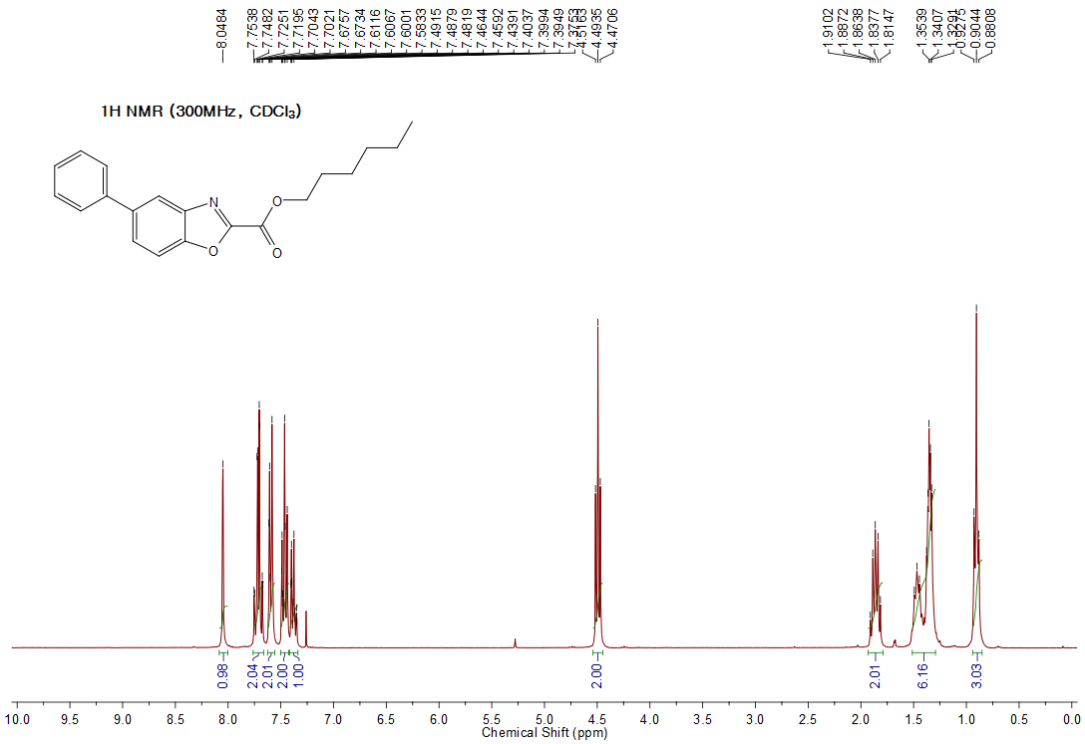

156.7944
152.9661
149.2845
140.8807
135.9091
129.6199
121.7776
111.1697
67.3559
31.4839
28.5855
25.5612
22.6071
21.6125
14.0867
13C NMR (75MHz, CDCl3)
N
O
O
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

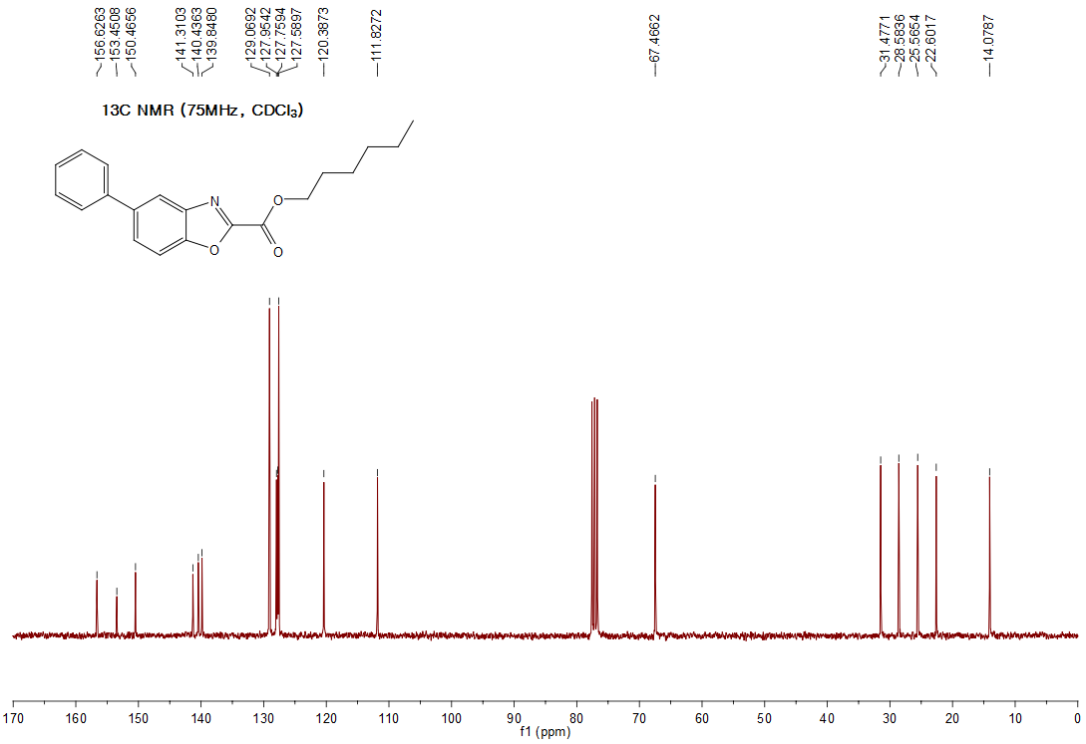

7.7242
7.6967
7.4019
7.3996
7.3973
7.2344
7.2314
7.2069
7.2039
4.4621
4.4393
4.4164
2.4850
1.8401
1.8167
1.7904
1.4239
1.3355
1.3221
1.3124
1.2995
0.8849
0.8415
1H NMR (300MHz, CDCl3)
1.00
0.99
0.98
2.02
3.10
2.08
6.17
3.14
Chemical Shift (ppm)

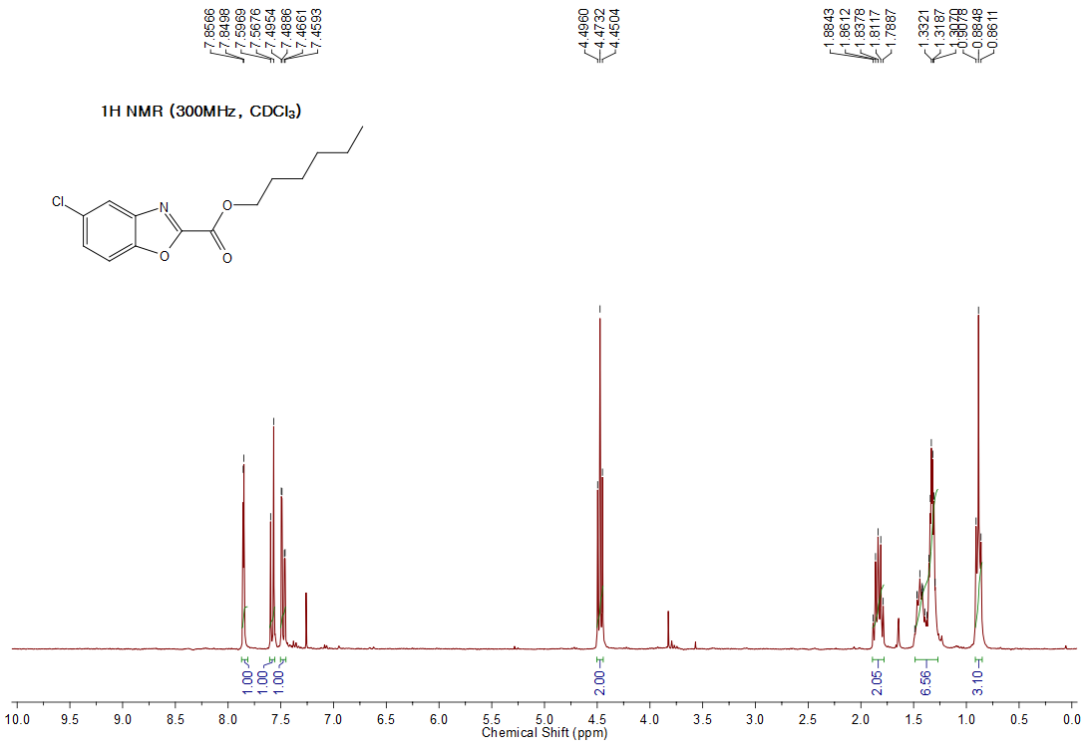

156.7646
152.4389
151.3108
139.1088
138.5349
127.3240
121.4897
111.6263
67.2408
31.4438
28.5577
25.5288
22.5592
22.0673
14.0296
13C NMR (75MHz, CDCl3)
Chemical Shift (ppm)

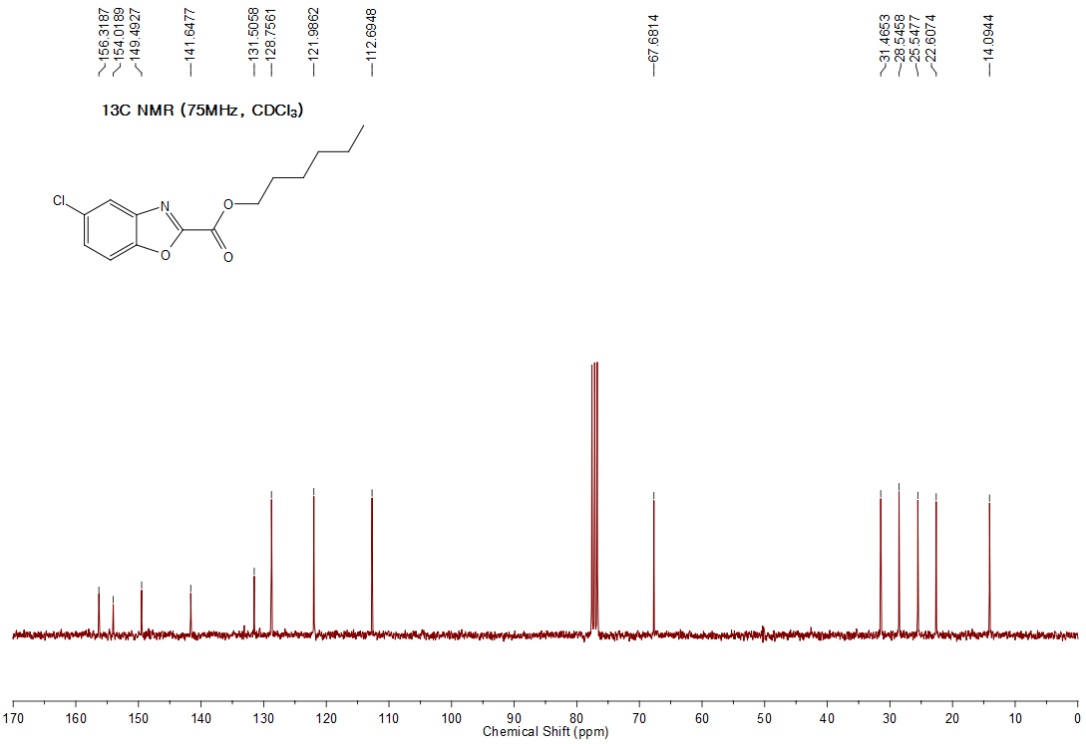

7.5075
7.5018
7.4850
7.4792
7.2539
7.2483
7.1003
7.0940
7.0877
7.0776
7.0713
7.0650
4.4564
4.4514
4.4392
4.4342
4.4220
4.4171
3.8310
3.8252
1.8494
1.8446
1.8317
1.8273
1.8098
1.7943
1.7897
1.7771
1.7723
1.3108
1.3058
0.9778
0.8713
0.8656
0.8602
0.8479
0.8425
1H NMR (400MHz, CDCl3)
O
N
O
O
O
1.00
0.82
1.00
2.00
3.00
2.06
6.20
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

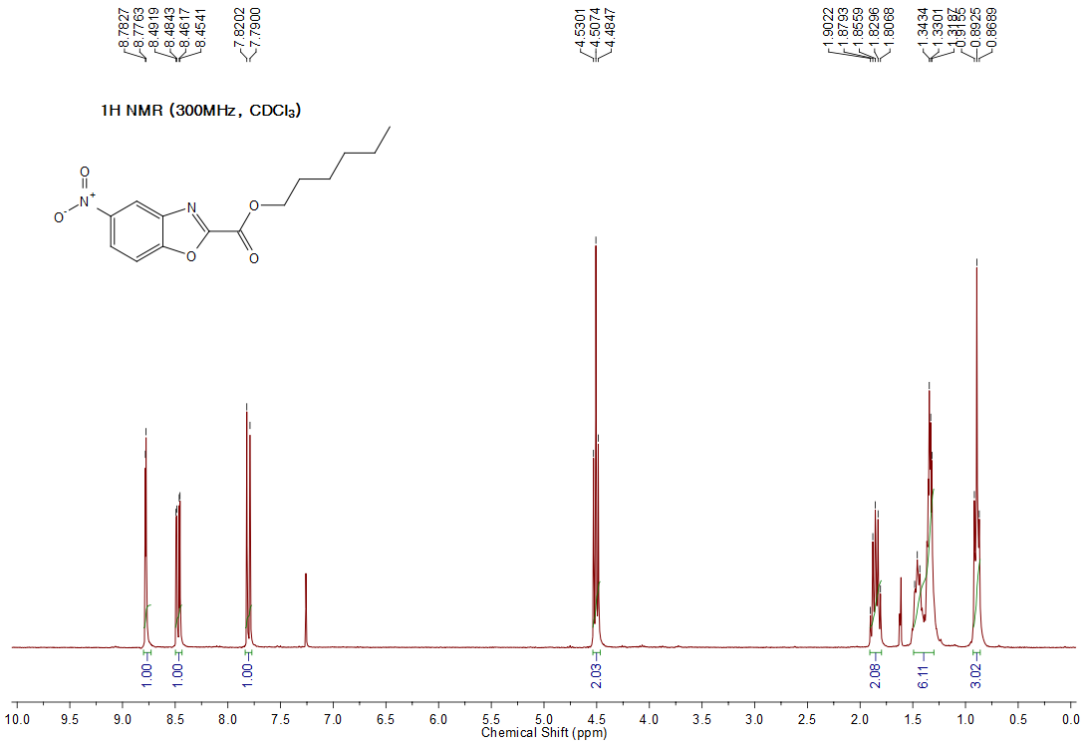

158.2143
156.6163
153.4287
145.6745
141.5145
118.0501
112.0632
103.5231
67.3123
56.0021
31.4575
28.5515
25.5410
22.5859
14.0722
13C NMR (75MHz, CDCl3)
O
N
O
O
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

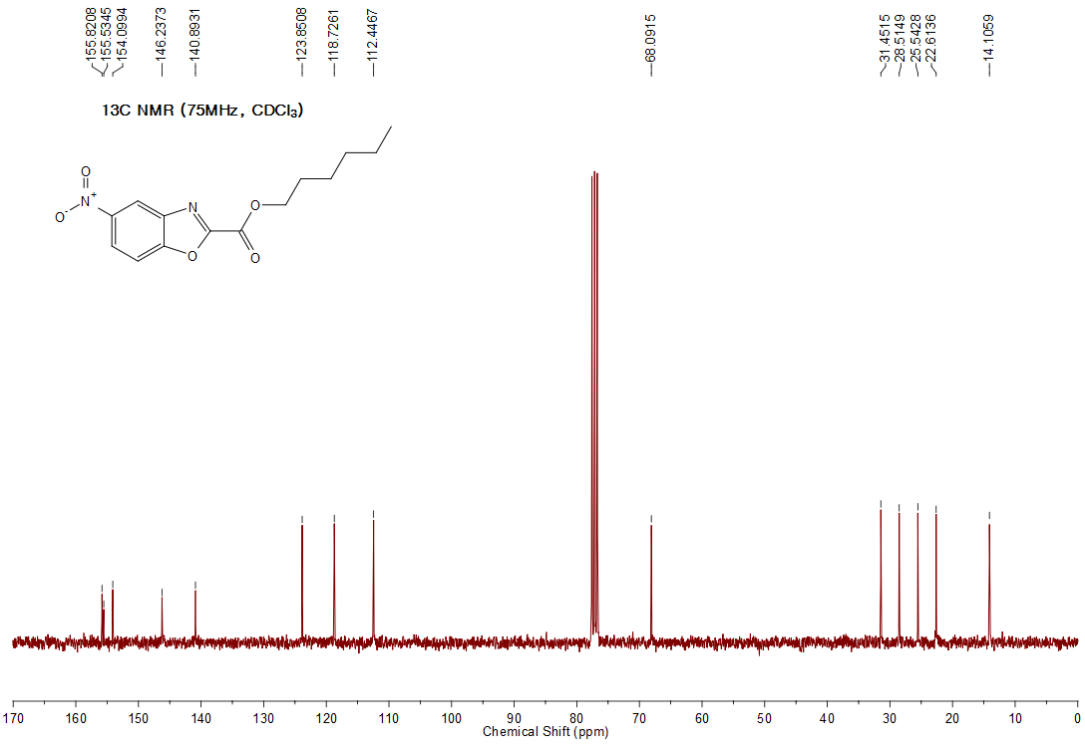

8.0484
7.7538
7.7482
7.7251
7.7195
7.7043
7.7021
7.6757
7.6734
7.6116
7.6067
7.6001
7.5833
7.4915
7.4879
7.4819
7.4644
7.4592
7.4391
7.4037
7.3994
7.3949
4.4935
4.4706
1.9102
1.8872
1.8638
1.8377
1.8147
1.3539
1.3407
0.9044
0.8808
1H NMR (300MHz, CDCl3)
N
O
O
O
0.98
2.04
2.01
2.00
1.00
2.00
2.01
6.16
3.03
Chemical Shift (ppm)

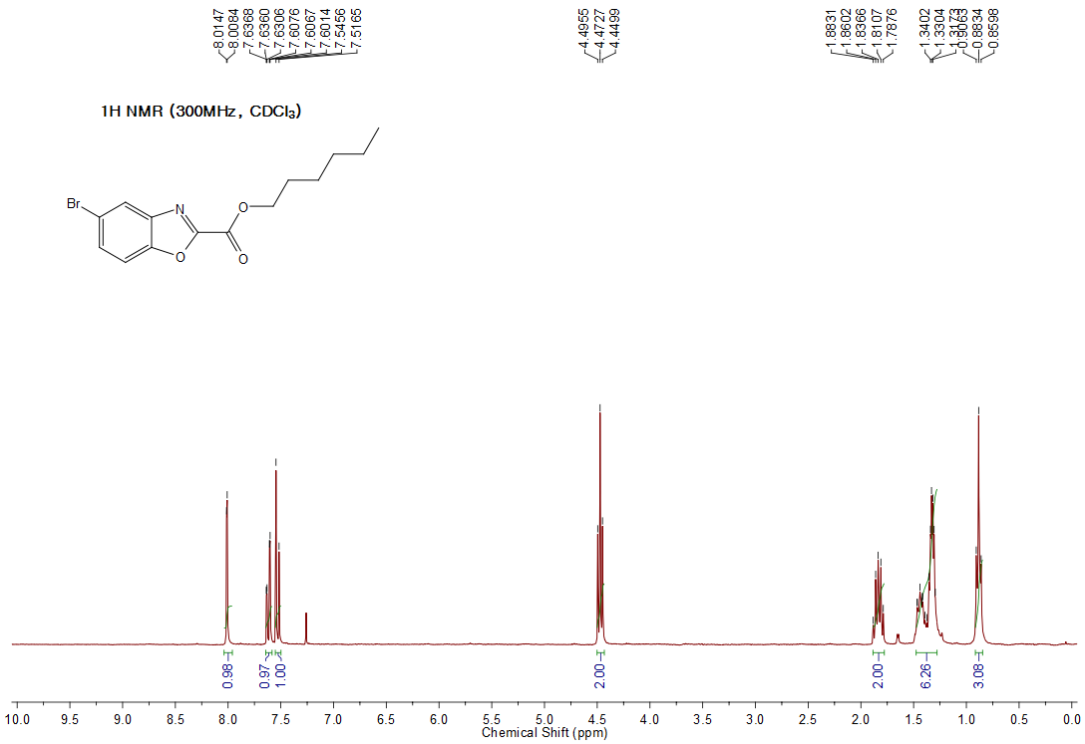

156.6263
153.4508
150.4656
141.3103
140.4363
139.8480
129.0692
127.9542
127.7594
127.5897
120.3873
111.8272
67.4662
31.4771
28.5836
25.5654
22.6017
14.0787
13C NMR (75MHz, CDCl3)
N
O
O
O
f1 (ppm)

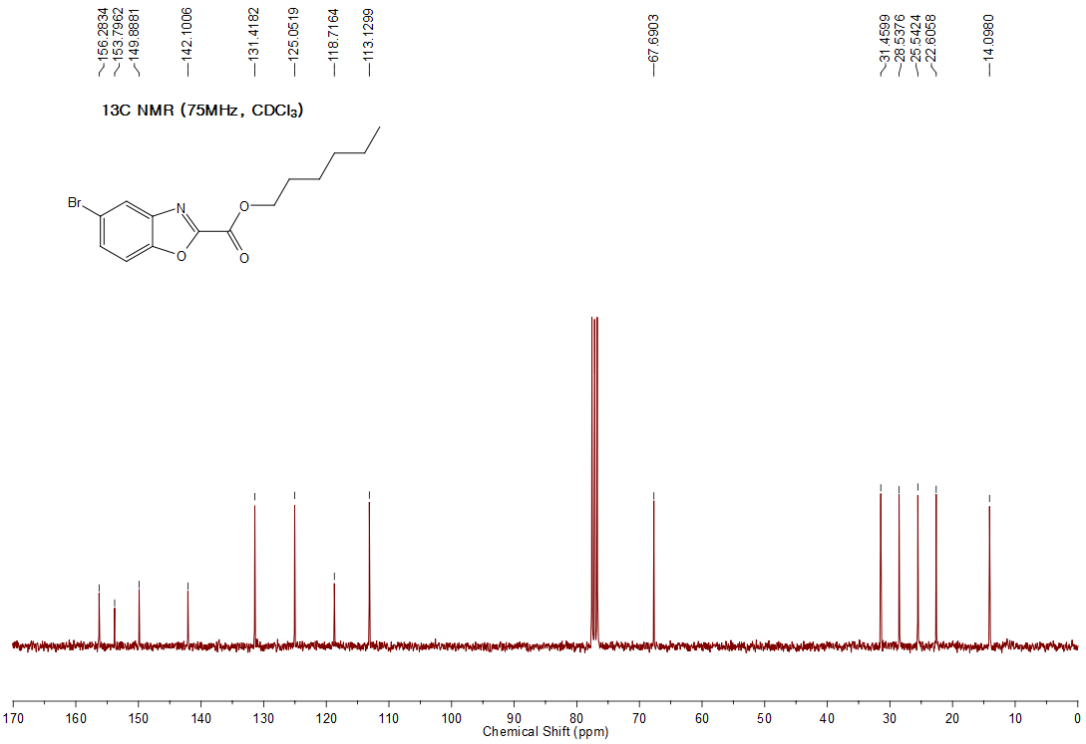

7.8566
7.8498
7.5969
7.5676
7.4954
7.4886
7.4661
7.4593
4.4960
4.4732
4.4504
1.8843
1.8612
1.8378
1.8117
1.7887
1.3321
1.3187
0.8848
0.8611
1H NMR (300MHz, CDCl3)
Cl
N
O
O
O
1.00
1.00
1.00
2.00
2.05
6.56
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

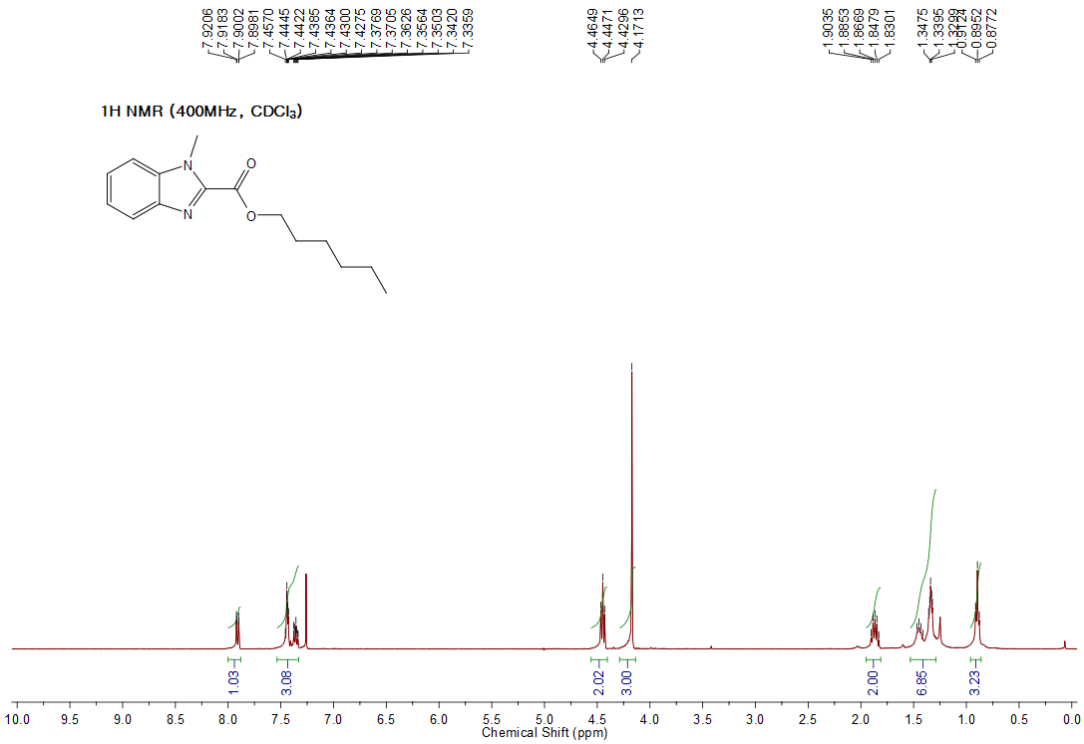

156.3187
154.0189
149.4927
141.6477
131.5058
128.7561
121.9862
112.6948
67.6814
31.4653
28.5458
25.5477
22.6074
14.0944
13C NMR (75MHz, CDCl3)
Cl
N
O
O
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

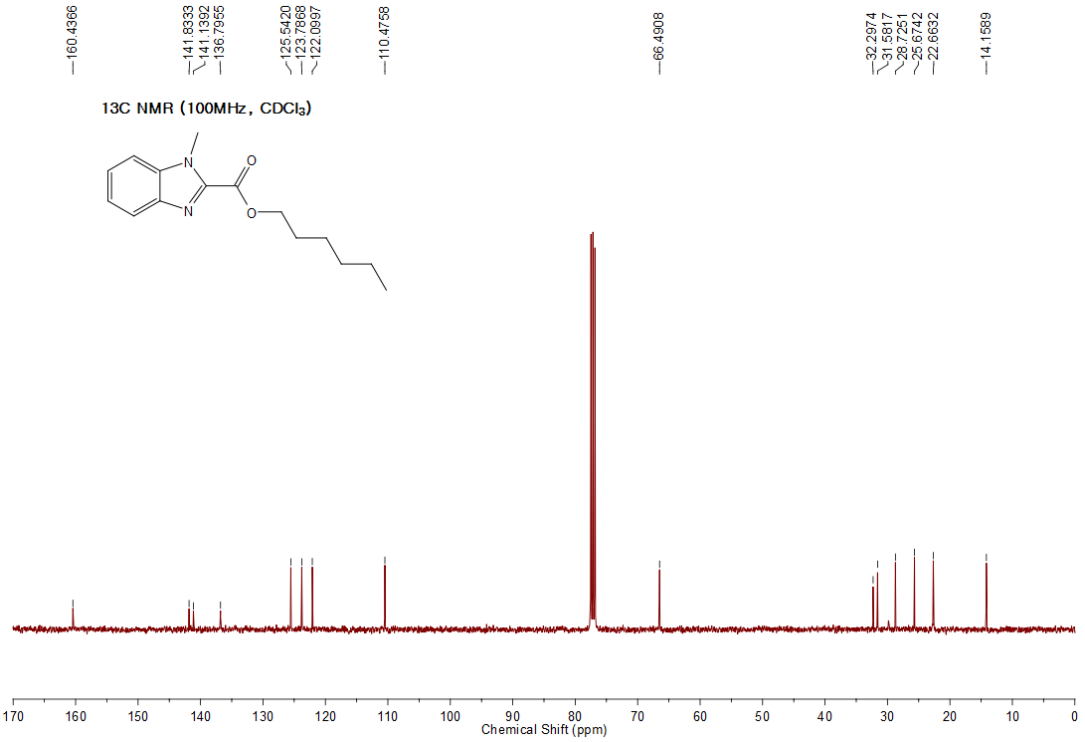

8.7827
8.7763
8.4919
8.4843
8.4617
8.4541
7.8202
7.7900
4.5301
4.5074
4.4847
1.9022
1.8793
1.8559
1.8296
1.8068
1.3434
1.3301
0.8925
0.8689
1H NMR (300MHz, CDCl3)
1.00
1.00
1.00
2.03
2.08
6.11
3.02
Chemical Shift (ppm)

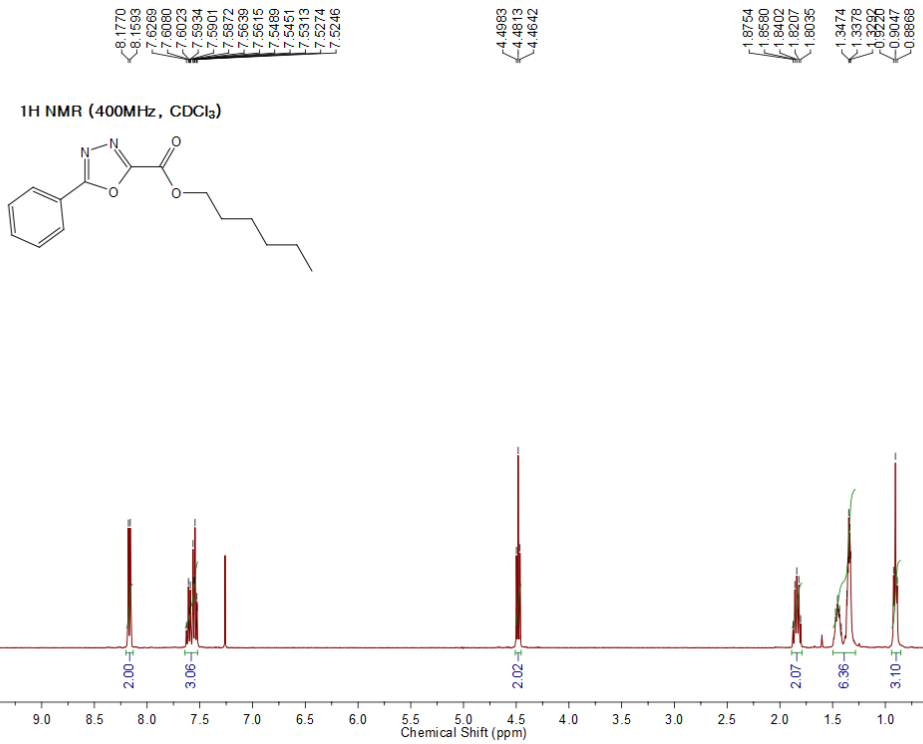

155.8208
155.5345
154.0994
146.2373
140.8931
123.8508
118.7261
112.4467
68.0915
31.4515
28.5149
25.5428
22.6136
14.1059
13C NMR (75MHz, CDCl3)
Chemical Shift (ppm)

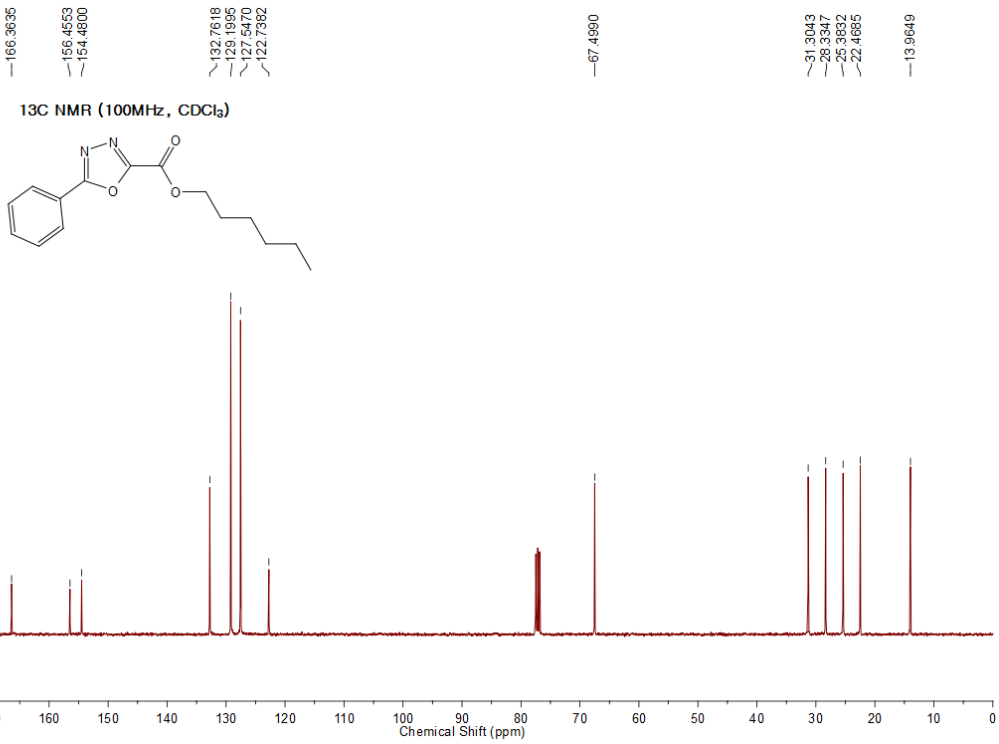

8.0147
8.0084
7.6368
7.6360
7.6306
7.6076
7.6067
7.6014
7.5456
7.5165
4.4955
4.4727
4.4499
1.8831
1.8602
1.8366
1.8107
1.7876
1.3402
1.3304
0.8834
0.8598
1H NMR (300MHz, CDCl3)
Br
N
O
O
O
0.98
0.97
1.00
2.00
2.00
6.26
3.08
Chemical Shift (ppm)


156.2834
153.7962
149.8881
142.1006
131.4182
125.0519
118.7164
113.1299
67.6903
31.4599
28.5376
25.5424
22.6058
14.0980
13C NMR (75MHz, CDCl3)
Br
N
O
O
O
Chemical Shift (ppm)


7.9206
7.9183
7.9002
7.8981
7.4570
7.4445
7.4422
7.4385
7.4364
7.4300
7.4275
7.3769
7.3705
7.3626
7.3564
7.3503
7.3420
7.3359
4.4649
4.4471
4.4296
4.1713
1.9035
1.8853
1.8669
1.8479
1.8301
1.3475
1.3395
0.8952
0.8772
1H NMR (400MHz, CDCl3)
1.03
3.08
2.02
3.00
2.00
6.85
3.23
Chemical Shift (ppm)


160.4366
141.8333
141.1392
136.7955
125.5420
123.7868
122.0997
110.4758
66.4908
32.2974
31.5817
28.7251
25.6742
22.6632
14.1589
13C NMR (100MHz, CDCl3)
Chemical Shift (ppm)


8.1770
8.1593
7.6269
7.6080
7.6023
7.5934
7.5901
7.5872
7.5639
7.5615
7.5489
7.5451
7.5313
7.5274
7.5246
4.4983
4.4813
4.4642
1.8754
1.8580
1.8402
1.8207
1.8035
1.3474
1.3378
0.9047
0.8868
1H NMR (400MHz, CDCl3)
2.00
3.06
2.02
2.07
6.36
3.10
Chemical Shift (ppm)


166.3635
156.4553
154.4800
132.7618
129.1995
127.5470
122.7382
67.4990
31.3043
28.3347
25.3832
22.4685
13.9649
13C NMR (100MHz, CDCl3)
Chemical Shift (ppm)

3. X-ray Crystallography data for 5a and 5g

Reflection data for **5a** and **5g** were collected on a Bruker APEX-II CCD-based diffractometer with graphite-monochromated MoKα radiation (λ = 0.7107 Å). The hemisphere of reflection data were collected as ω scan frames with 0.5°/frame and an exposure time of 10s/frame. Cell parameters were determined and refined by the SMART program. Data reduction was performed using SAINT software. The data were corrected for Lorentz and polarization effects. An empirical absorption correction was applied using the SADABS program. The structures of the compounds were solved by direct methods and refined by full matrix least-squares methods using the SHELXTL program package with anisotropic thermal parameters for all non-hydrogen atoms.

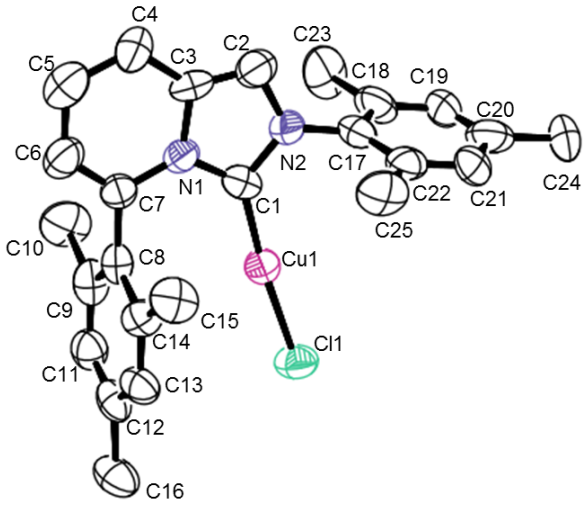


Table S2. Crystallographic data and parameters for **5a**

Identification code	**5a**
CCDC number	1576746
Empirical formula	$C_{25}H_{26}ClCuN_2$
Formula weight	453.47
Temperature	293(2) *T* (K)
Wavelength	0.71073
Crystal system	Triclinic

Space group	*P-1*	
Unit cell dimensions	a = 9.9670(8) Å	α = 89.092(6)°
	b = 18.1432(16) Å	β = 82.857(4)°
	c = 20.1268(16) Å	γ = 74.117(4)°
Volume	3472.8(5) $Å^3$	
Z	6	
Density (calculated)	1.301 g cm^{-3}	
Absorption coefficient	1.071	
F(000)	1416	
θ range for data collection	1.167 to 25.636°	
Index ranges	-12 ≤ h ≤ 12, -21 ≤ k ≤21, -24 ≤ l ≤ 24	
Reflections collected	17569	
Independent reflections	4739 [R(int) =0.0279]	
Completeness to θ = 25.636°	95.2%	
Data / restraints / parameters	12486/6/1604	
Goodness-of-fit on F2	1.068	
Final R indices [I > 2σ((I)]	R1 = 0.0636, wR2 = 0.0872[3521]	
R indices (all data)	R1 = 0.1252, wR2 = 0.1021	
Largest diff. peak and hole	0.260 and -0.297 e·$Å^{-3}$	

Table S3. Bond Lengths [A°] and Angle [°] for **5a**

Cu1-Cl1	2.122(1)
Cu1-C1	1.886(4)
N1-C1	1.359(5)
N1-C3	1.411(6)
N1-C7	1.397(5)
N2 C1	1.371(5)
N2-C2	1.384(6)
N2-C17	1.439(5)
C2-C3	1.346(6)
C3-C4	1.428(7)
C4-C5	1.343(8)
C5-C6	1.426(7)
C6-C7	1.344(7)
C7-C8	1.486(7)
C8-C9	1.408(5)
C8-C13	1.412(6)
C9-C10	1.389(7)
C9-C14	1.501(5)
C10-C11	1.385(6)
C11-C12	1.370(6)
C11-C15	1.512(8)
C12-C13	1.383(7)
C13-C16	1.520(5)
C17-C18	1.384(5)
C17-C22	1.391(6)
C18-C19	1.377(7)
C19-C20	1.379(6)
C20-C21	1.380(5)
C21-C22	1.384(7)
C22-O1	1.364(4)
C23-C24	1.499(6)

C23-O1	1.441(5)
C24-O2	1.414(7)
C25-C26	1.50(2)
C25-O2	1.415(6)
C26-O3	1.39(2)
O3-C27	1.36(1)

Cu1-C1-N2	125.9(8)
N1-C1-N2	102.4(8)
C1-N2-C2	112.7(9)
C1-N2-C17	122.8(9)
C2-N2-C17	124.5(9)
N2-C2-C3	106(1)
N2-C17-C22	119(1)
N2-C17-C18	121(1)
C22-C17-C18	120(1)
C17-C22-C21	119(1)
C17-C22-C25	122(1)
C21-C22-C25	120(1)
C22-C21-C20	118(1)
N1-C7-C8	117.7(9)
N1-C7-C6	118(1)
C8-C7-C6	124(1)
C11-C9-C8	122(1)
C11-C9-C10	120(1)
C8-C9-C10	118(1)
C9-C11-C12	119(1)
C11-C12-C13	120(1)
C11-C12-C16	121(1)
C13-C12-C16	119(1)
C12-C13-C14	122(1)
C13-C14-C8	119(1)

C13-C14-C15	121(1)
C8-C14-C15	120(1)
C7-C8-C9	124(1)
C7-C8-C14	118(1)
C9-C8-C14	118(1)
C17-C18-C19	120(1)
C17-C18-C23	118(1)
C19-C18-C23	122(1)
C18-C19-C20	119(1)
N1-C3-C2	108(1)
N1-C3-C4	118(1)
C2-C3-C4	134(2)
C7-C6-C5	123(1)
C6-C5-C4	117(2)
C3-C4-C5	120(2)
C21-C20-C19	123(1)
C21-C20-C24	115(1)
C19-C20-C24	121(1)

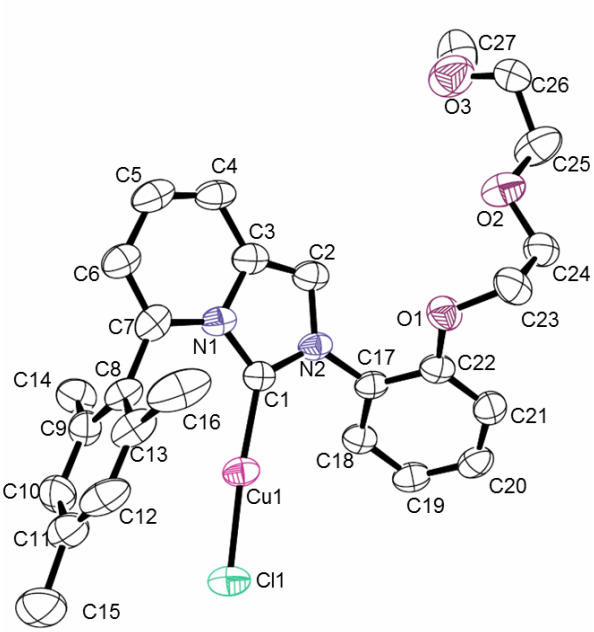


Table S4. Crystallographic data and parameters for **5g**

Identification code	**5g**	
CCDC number	1576622	
Empirical formula	$C_{27.50}H_{32}ClCuN_2O_{3.50}$	
Formula weight	545.54	
Temperature	296(2) *T* (K)	
Wavelength	0.71073	
Crystal system	Triclinic	
Space group	*P-1*	
Unit cell dimensions	a = 10.6797(2) Å	α = 99.8551(8)°
	b = 11.1444(2) Å	β = 103.2083(8)°
	c = 13.1053(2) Å	γ = 116.2178(7)°
Volume	1294.49(4) $Å^3$	
Z	2	

Density (calculated)	1.400 g cm^{-3}
Absorption coefficient	0.981
F(000)	570
θ range for data collection	2.144 to 25.376°.
Index ranges	-12 ≤ h ≤ 12, -13 ≤ k ≤13, -15 ≤ l ≤ 15
Reflections collected	17569
Independent reflections	4739 [R(int) =0.0279]
Completeness to θ = 25.376°	99.9%
Data / restraints / parameters	4739/4/359
Goodness-of-fit on F2	0.997
Final R indices [I > 2σ((I)]	R1 = 0.0481, wR2 = 0.1226[3521]
R indices (all data)	R1 = 0.0689, wR2 = 0.1329
Largest diff. peak and hole	0.836 and -0.422 e·$Å^{-3}$

Table S5. Bond Lengths [A°] and Angle [°] for **5g**

Cu1-Cl1	2.135(5)
Cu1-C1	1.83(1)
N1-C1	1.38(1)
N1-C7	1.39(1)
N1-C3	1.43(2)
C1-N2	1.39(1)
N2-C2	1.40(2)
N2-C17	1.42(1)
C2-C3	1.31(2)
C17-C22	1.39(2)

C17-C18	1.40(1)
C22-C21	1.40(2)
C22-C25	1.52(2)
C21-C20	1.37(2)
C7-C8	1.47(1)
C7-C6	1.35(2)
C9-C11	1.39(2)
C9-C8	1.38(2)
C9-C10	1.60(2)
C11-C12	1.38(2)
C12-C13	1.38(2)
C12-C16	1.56(2)
C13-C14	1.38(2)
C14-C8	1.44(1)
C14-C15	1.53(2)
C18-C19	1.34(2)
C18-C23	1.55(2)
C19-C20	1.38(2)
C3-C4	1.41(3)
C6-C5	1.45(3)
C5-C4	1.46(4)
C20-C24	1.57(2)

Cl1-Cu1-C1	173.5(1)
C1-N1-C3	111.2(3)
C1-N1-C7	126.8(3)
C3-N1-C7	122.1(3)
C1-N2-C2	112.1(3)
C1-N2-C17	122.7(3)
C2-N2-C17	125.1(3)
Cu1-C1-N1	129.4(3)
Cu1-C1-N2	127.0(3)

N1-C1-N2	103.5(3)
N2-C2-C3	106.6(4)
N1-C3-C2	106.6(3)
N1-C3-C4	118.3(3)
C2-C3-C4	135.1
C3-C4-C5	118.9(4)
C4-C5-C6	121.2(4)
C5-C6-C7	121.9(4)
N1-C7-C6	117.7(4)
N1-C7-C8	116.7(3)
C6-C7-C8	125.7(4)
C7-C8-C9	120.0(4)
C7-C8-C13	120.7(4)
C9-C8-C13	119.3(4)
C8-C9-C10	118.6(4)
C8-C9-C14	121.1(4)
C10-C9-C14	120.3(4)
C9-C10-C11	122.3(4)
C10-C11-C12	118.3(4)
C10-C11-C15	121.1(4)
C12-C11-C15	120.6(5)
C11-C12-C13	122.1(5)
C8-C13-C12	119.3(4)
C8-C13-C16	119.4(4)
C12-C13-C16	121.2(4)
N2-C17-C18	119.8(3)
N2-C17-C22	119.3(3)
C18-C17-C22	120.8(4)
C17-C18-C19	119.9(4)
C18-C19-C20	119.4(4)
C19-C20-C21	121.2(4)
C20-C21-C22	119.7(4)

C17-C22-C21	119.0(4)
C17-C22-O1	115.9(3)
C21-C22-O1	125.1(4)
C24-C23-O1	112.8(3)
C23-C24-O2	108.3(3)
C26-C25-O2	109.7(6)
C25-C26-O3	105.7(9)
C26-O3-C27	112(1)
C22-O1-C23	119.5(3)
C24-O2-C25	110.7(4)