SUPPORTING INFORMATION

Microwave-assisted annulation for the construction of pyrido-fused heterocycles and their application as photoluminescent chemosensors

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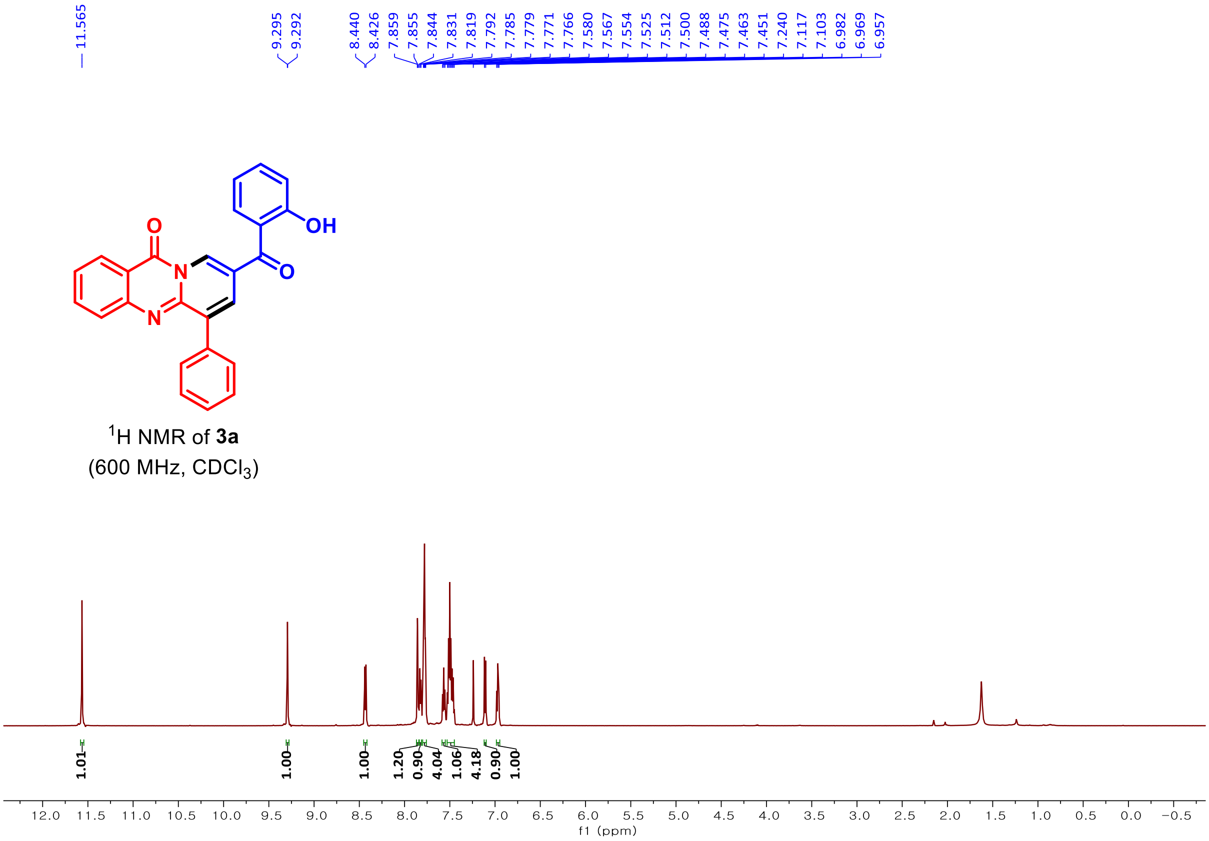
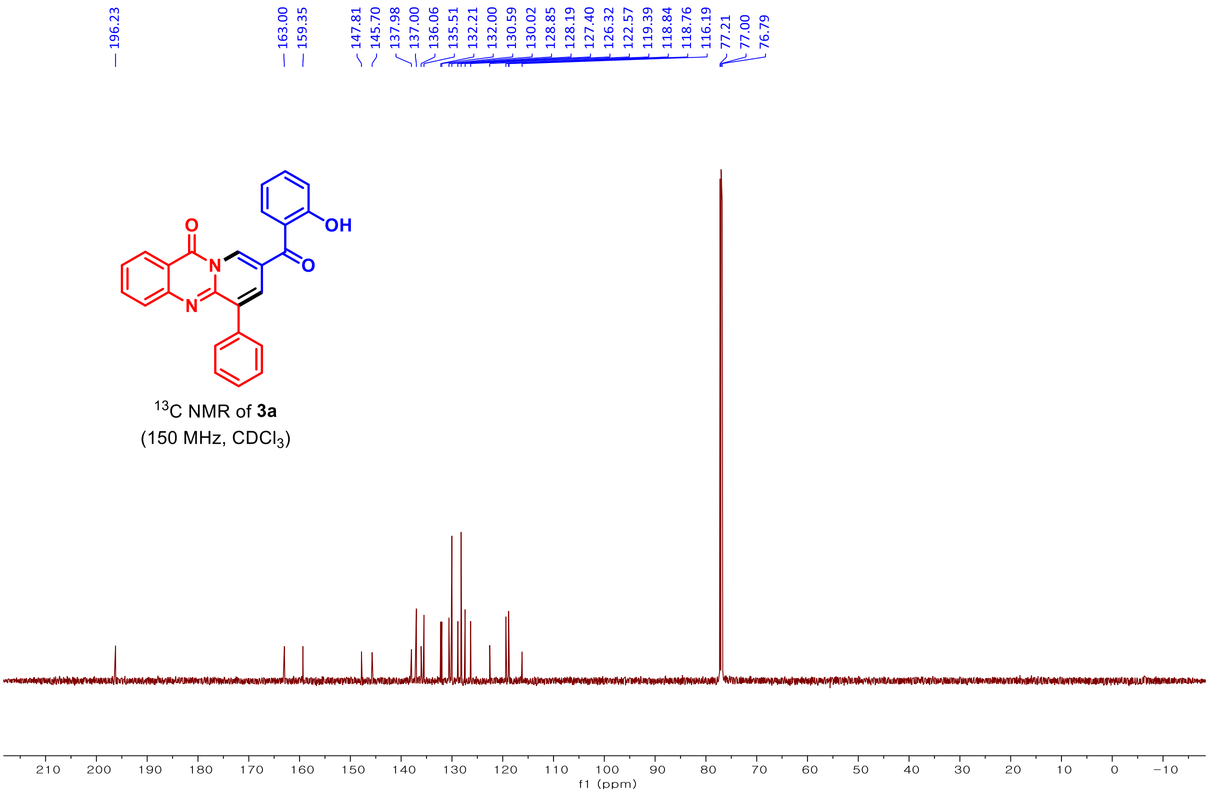
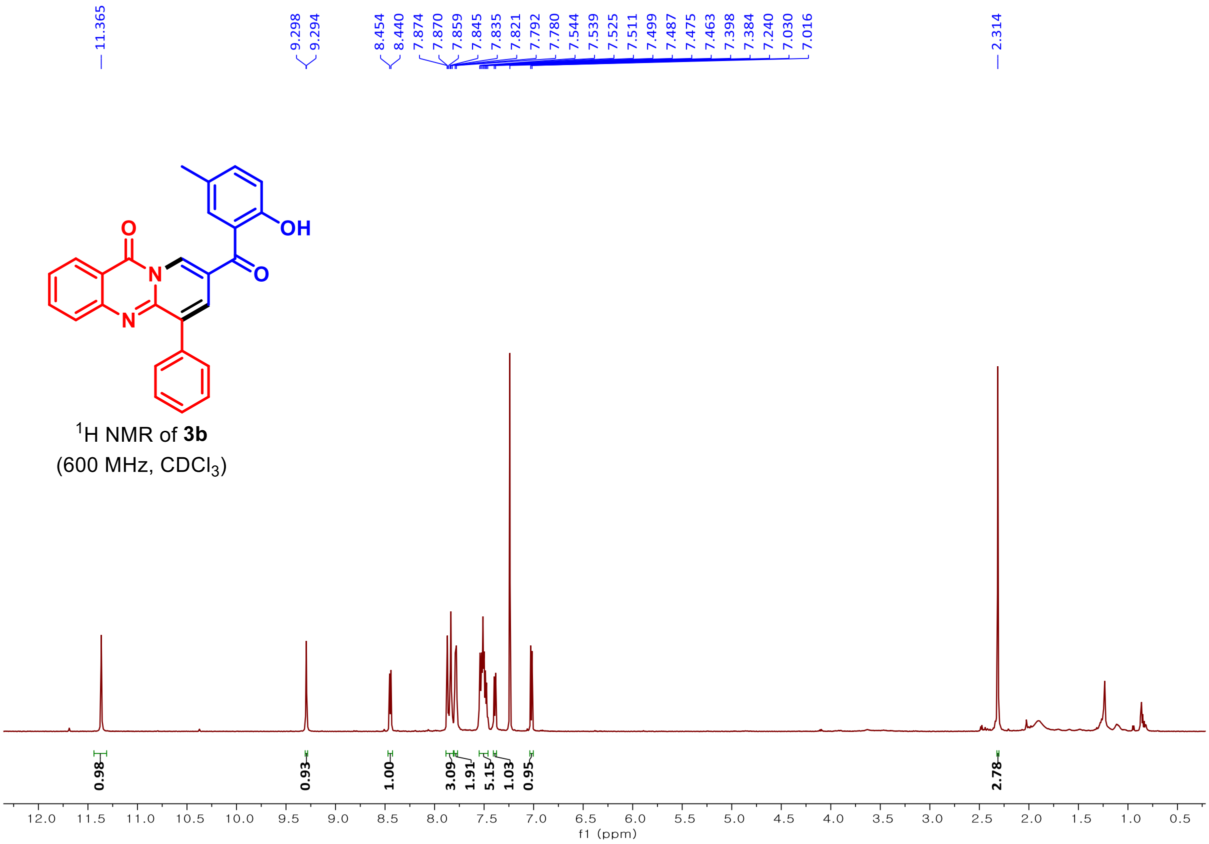
^{1}H NMR and ^{13}C NMR spectra of the synthesized compounds



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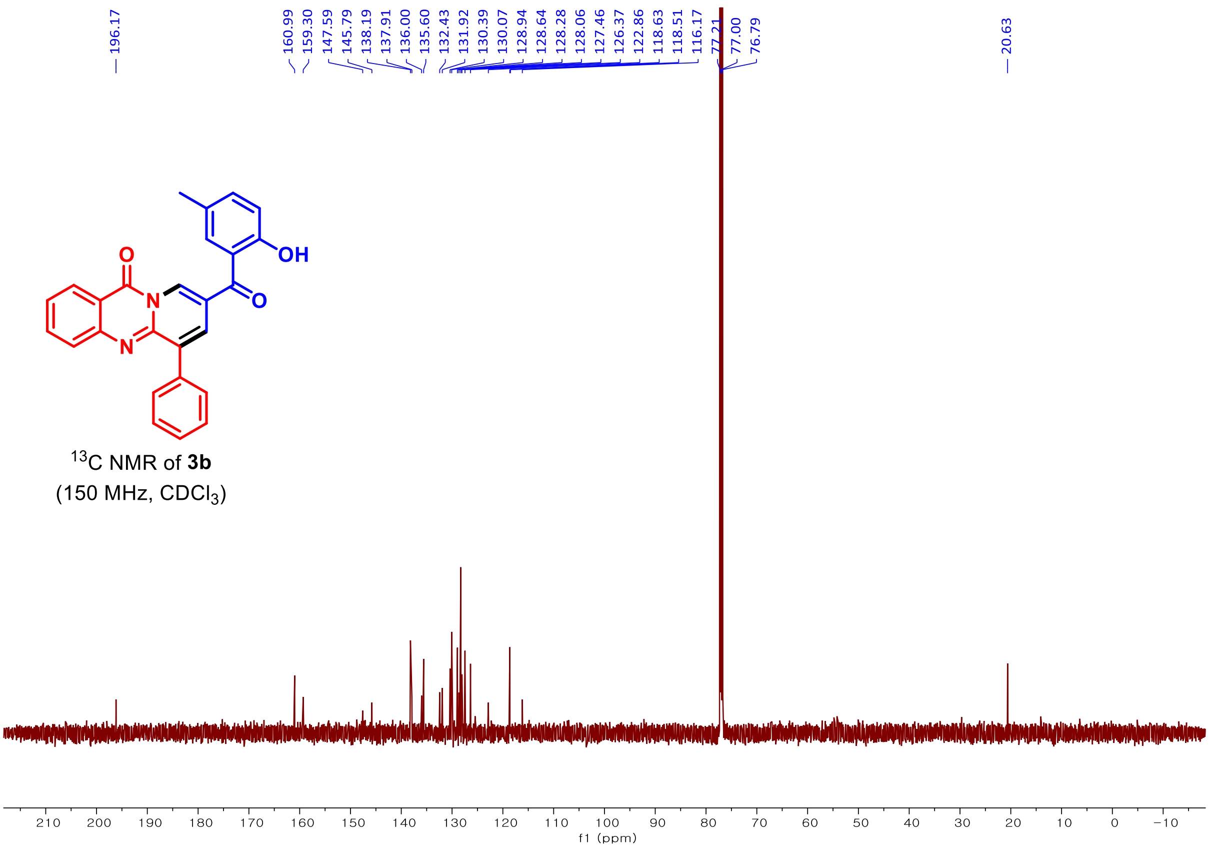
7.792
7.780
7.544
7.539
7.525
7.511
7.499
7.487
7.475
7.463
7.398
7.384
7.240
7.030
7.016
2.314
OH
O
N
N
O
^{1}H NMR of **3b**
(600 MHz, $CDCl_3$)
0.98
0.93
1.00
3.09
1.91
5.15
1.03
0.95
2.78
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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159.30
147.59
145.79
138.19
137.91
136.00
135.60
132.43
131.92
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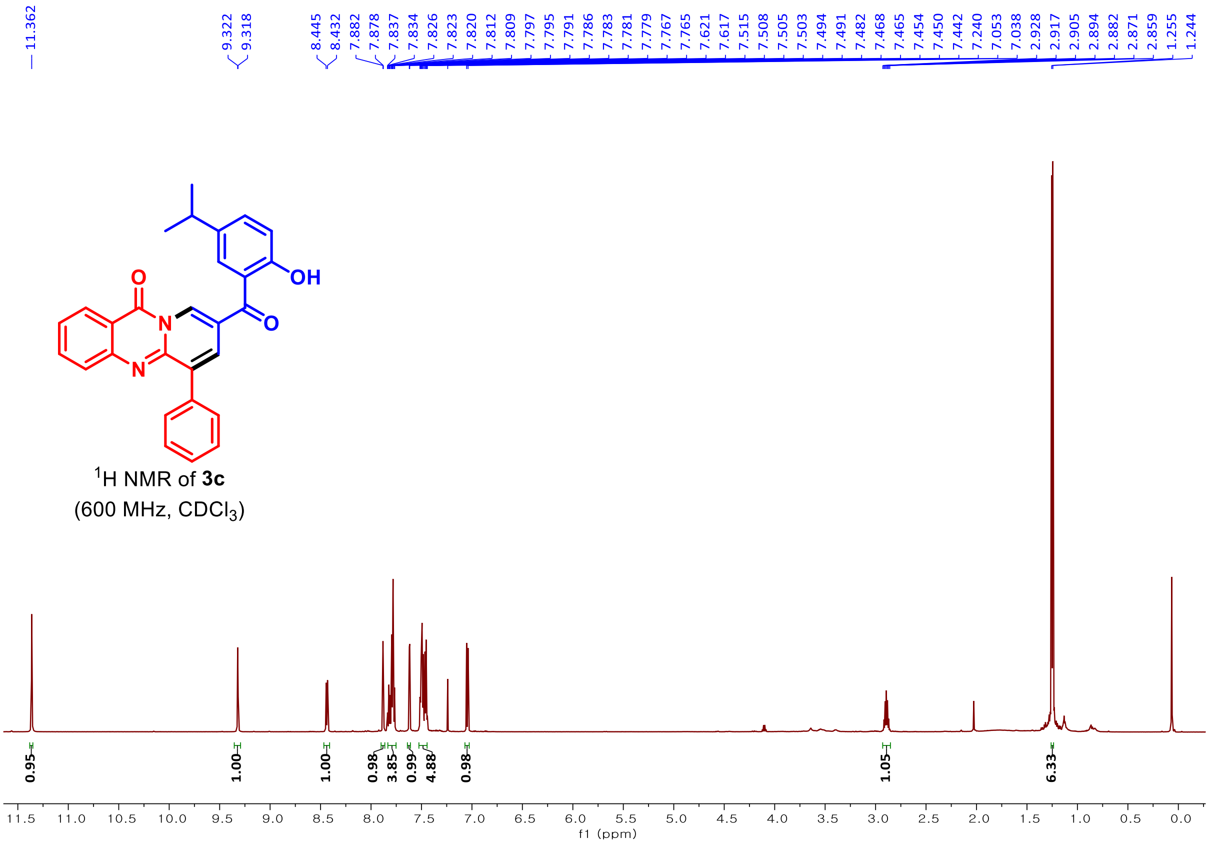
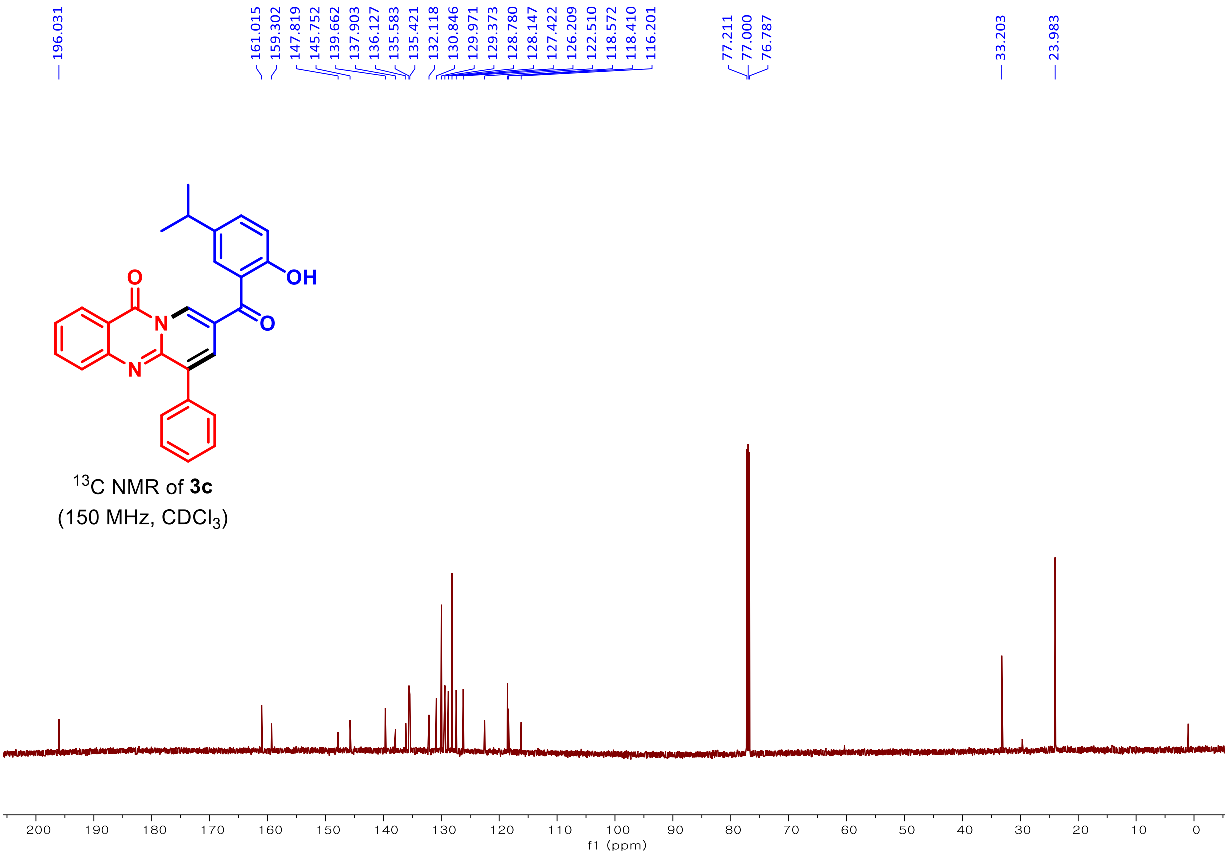
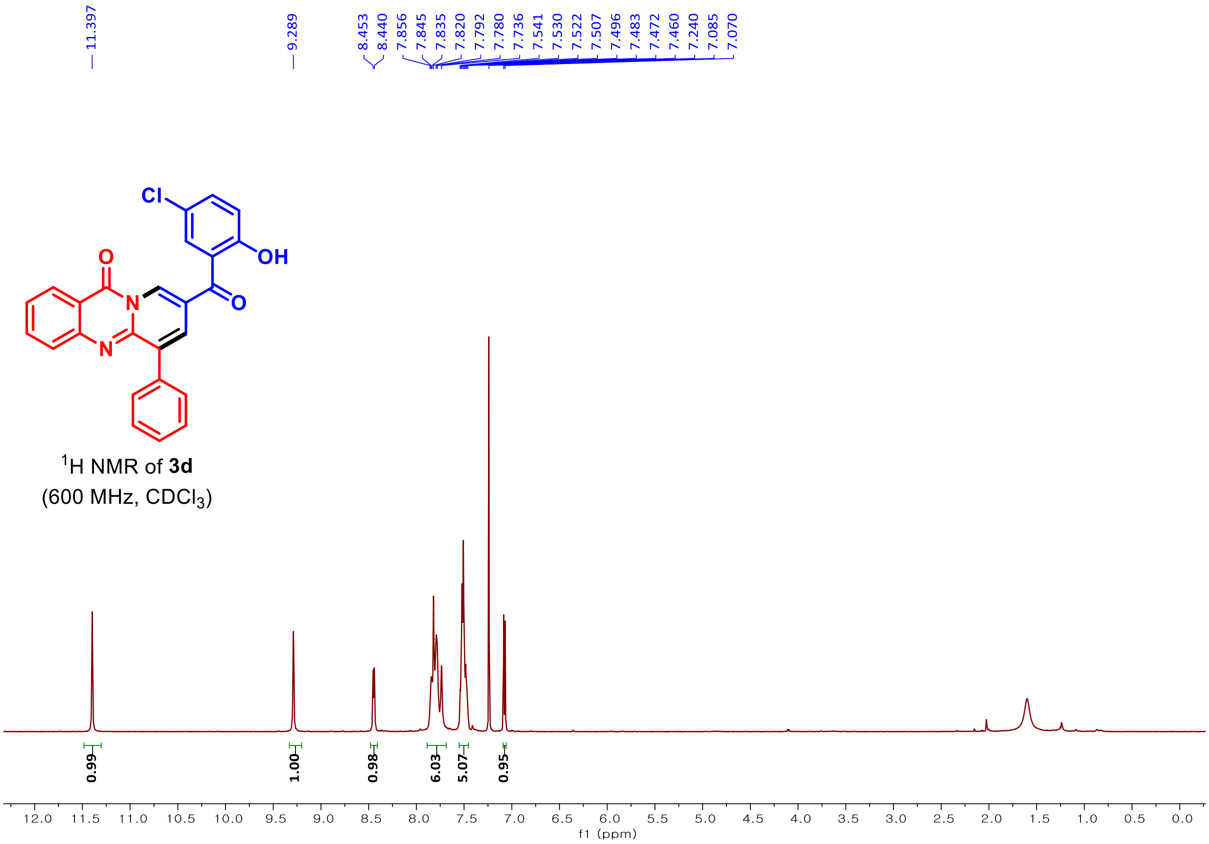
130.07
128.94
128.64
128.28
128.06
127.46
126.37
122.86
118.63
118.51
116.17
77.21
77.00
76.79
20.63
OH
O
N
N
O
^{13}C NMR of **3b**
(150 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



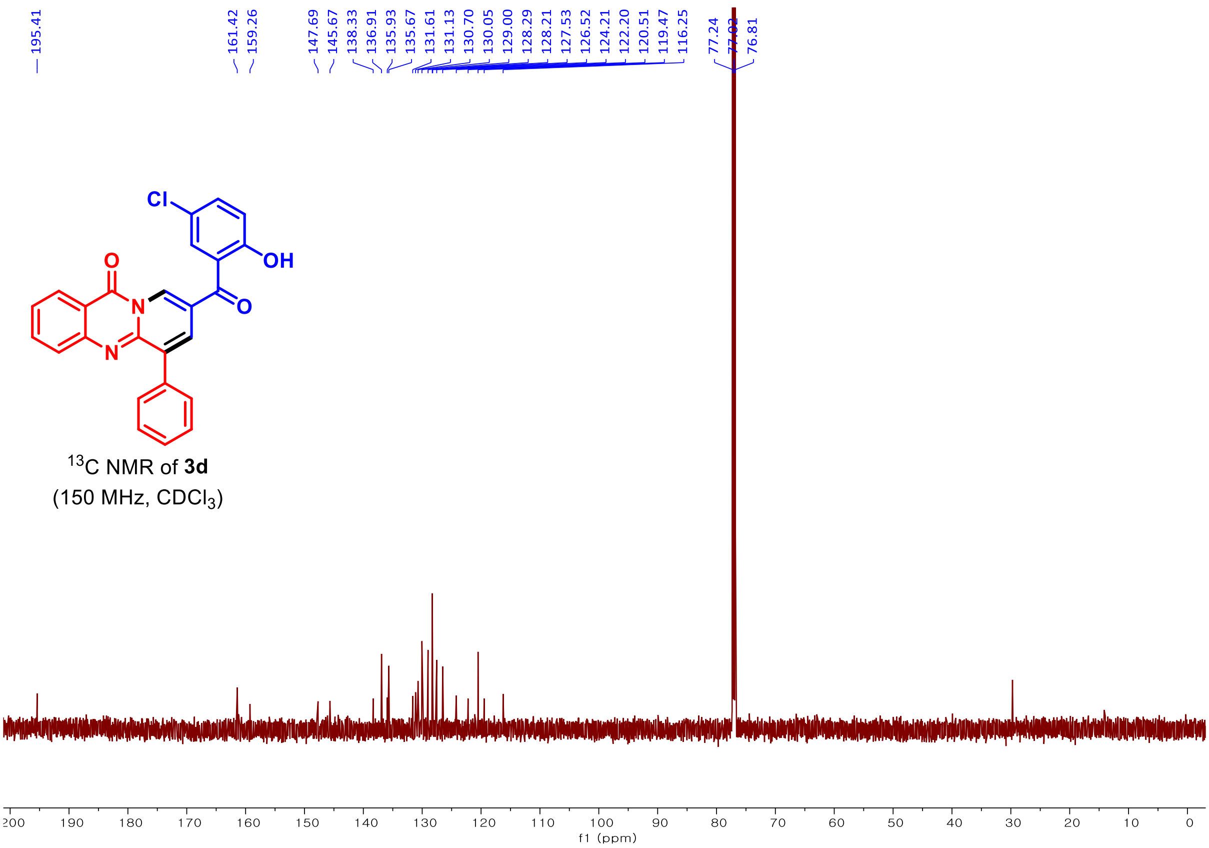
^{1}H NMR of **3c**
(600 MHz, $CDCl_3$)



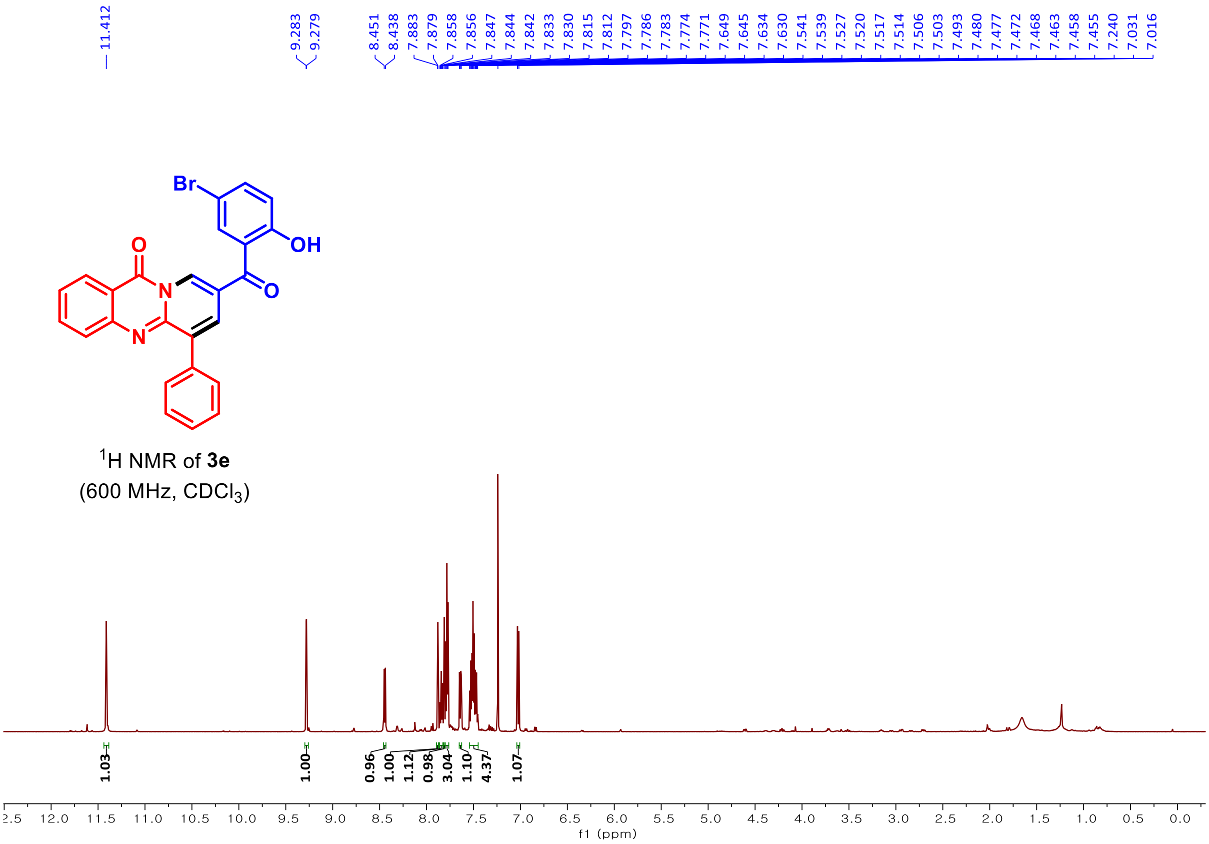
^{13}C NMR of **3c**
(150 MHz, $CDCl_3$)



^{1}H NMR of **3d**
(600 MHz, $CDCl_3$)



^{13}C NMR of **3d**
(150 MHz, $CDCl_3$)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9.279
8.451
8.438
7.883
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7.858
7.856
7.847
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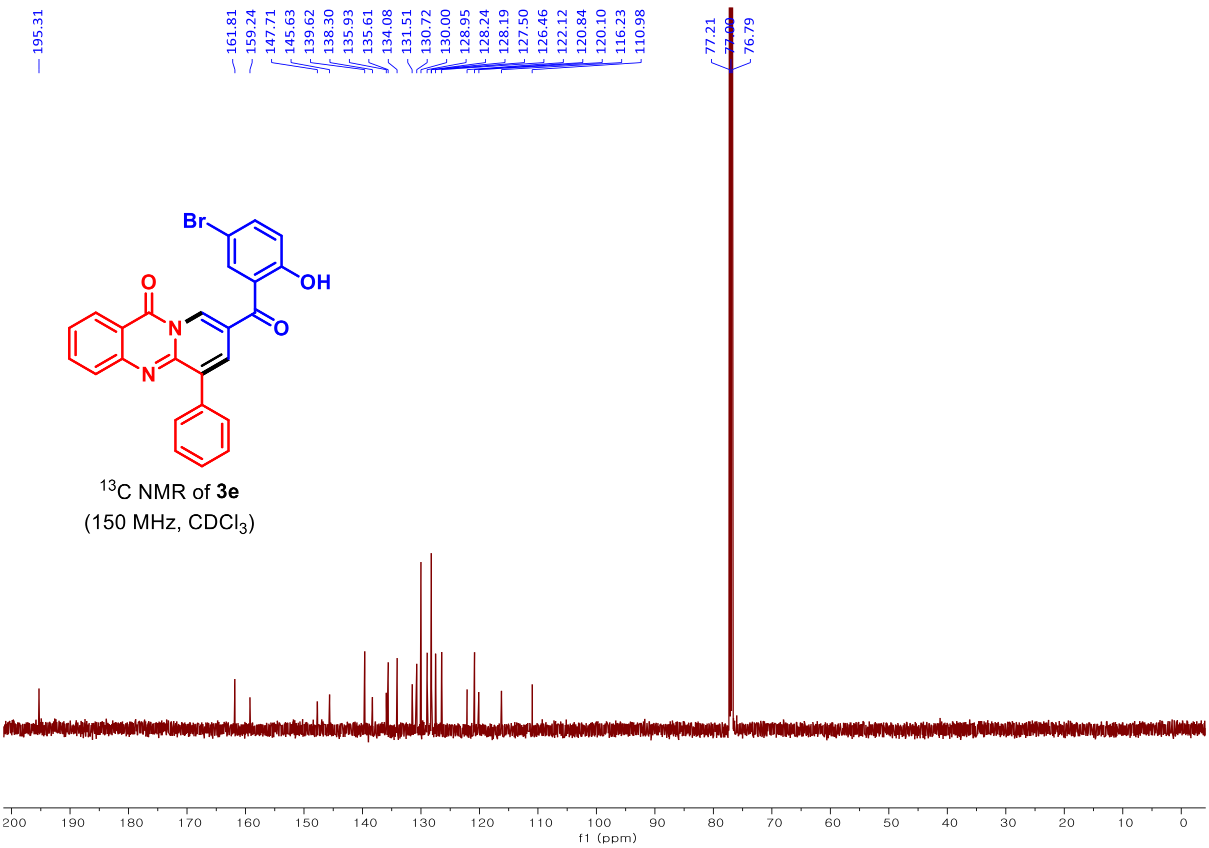
7.842
7.833
7.830
7.815
7.812
7.797
7.786
7.783
7.774
7.771
7.649
7.645
7.634
7.630
7.541
7.539
7.527
7.520
7.517
7.514
7.506
7.503
7.493
7.480
7.477
7.472
7.468
7.463
7.458
7.455
7.240
7.031
7.016
Br
OH
O
N
N
O
^{1}H NMR of **3e**
(600 MHz, $CDCl_3$)
1.03
1.00
0.96
1.00
1.12
0.98
3.04
1.10
4.37
1.07
f1 (ppm)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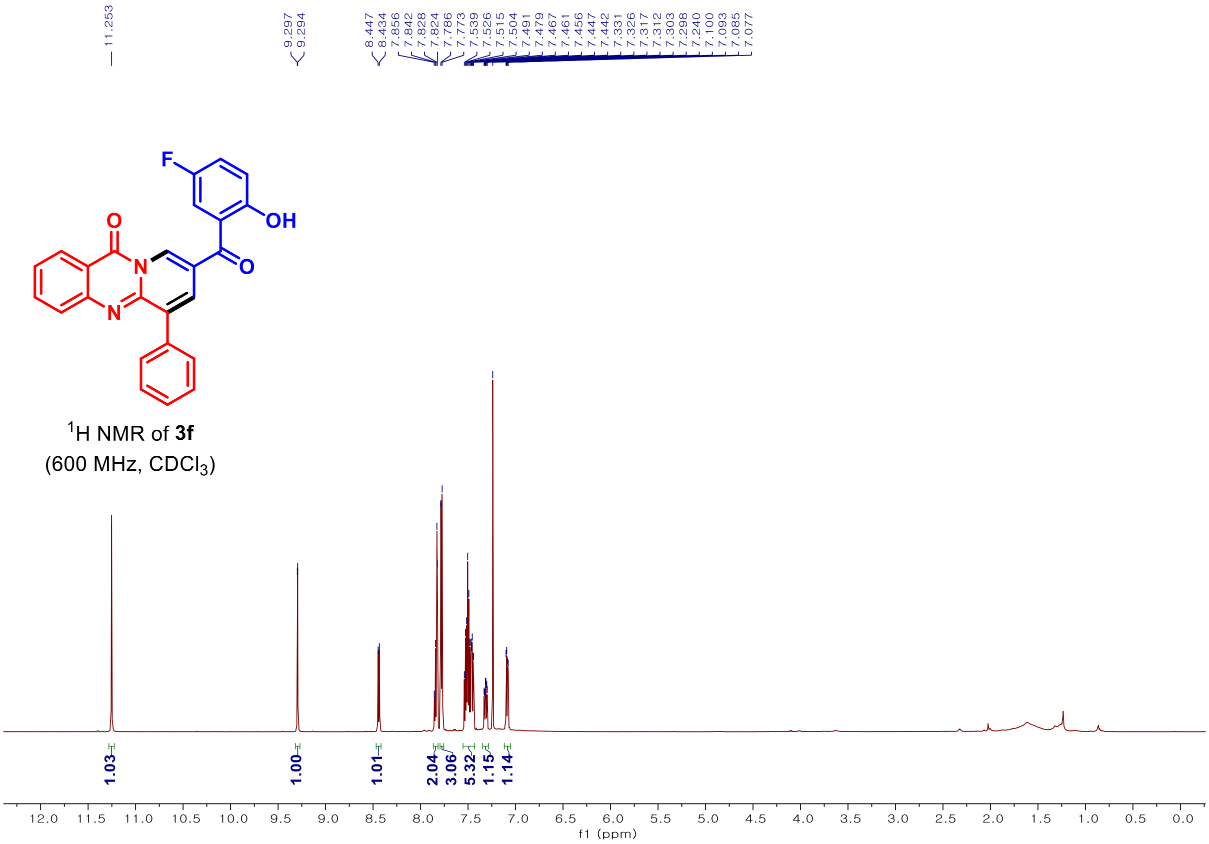
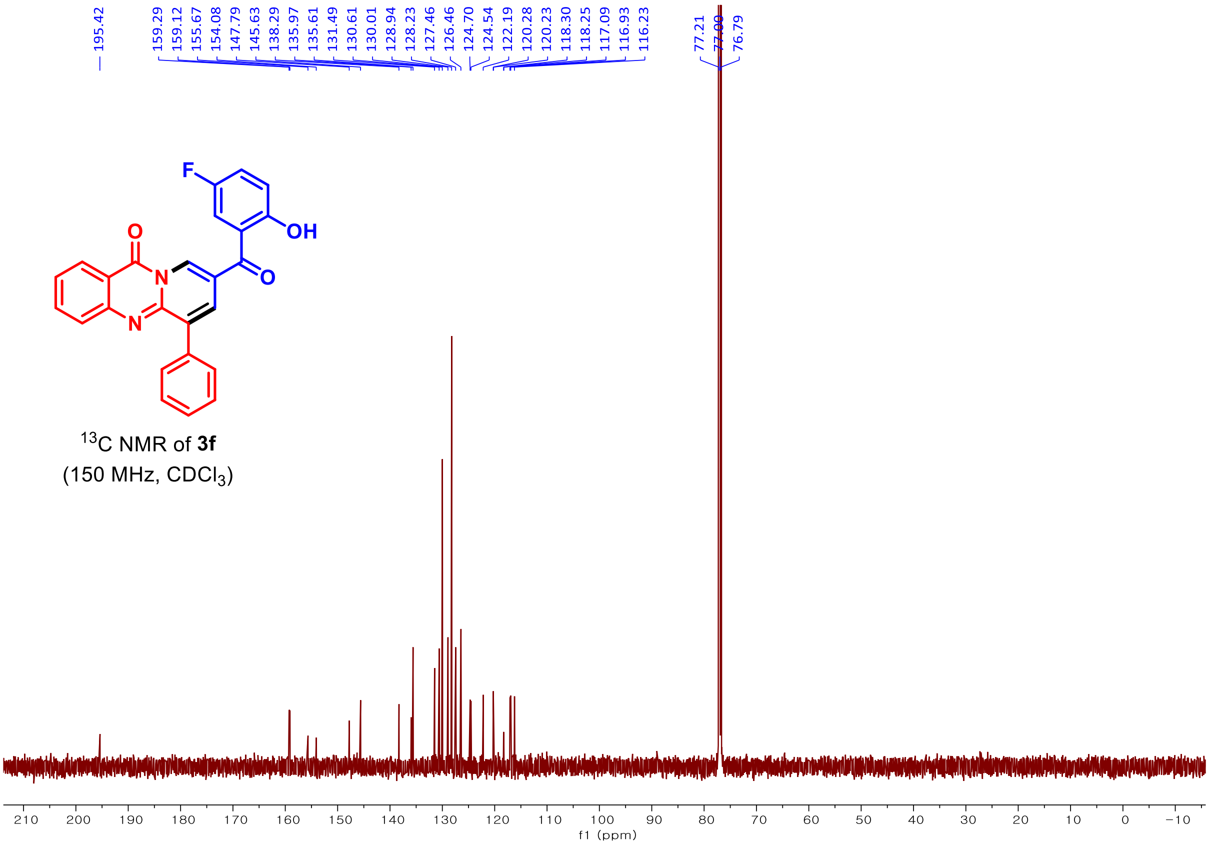
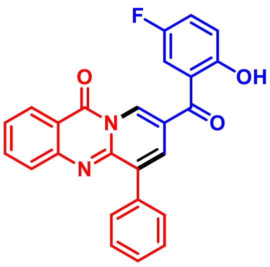
161.81
159.24
147.71
145.63
139.62
138.30
135.93
135.61
134.08
131.51
130.72
130.00
128.95
128.24
128.19
127.50
126.46
122.12
120.84
120.10
116.23
110.98
77.21
77.00
76.79
Br
OH
O
N
N
O
^{13}C NMR of **3e**
(150 MHz, $CDCl_3$)
f1 (ppm)



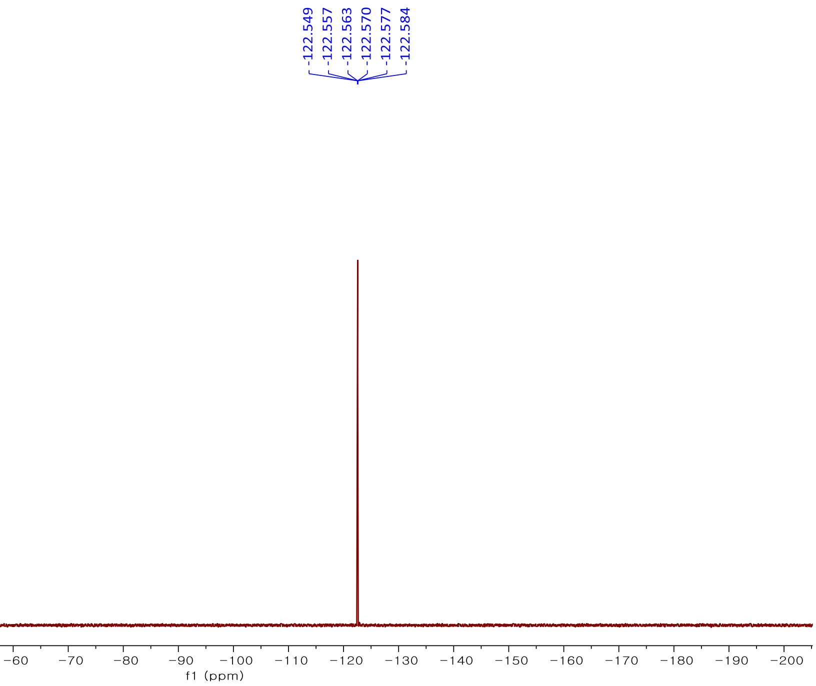
^{1}H NMR of **3f**
(600 MHz, $CDCl_3$)

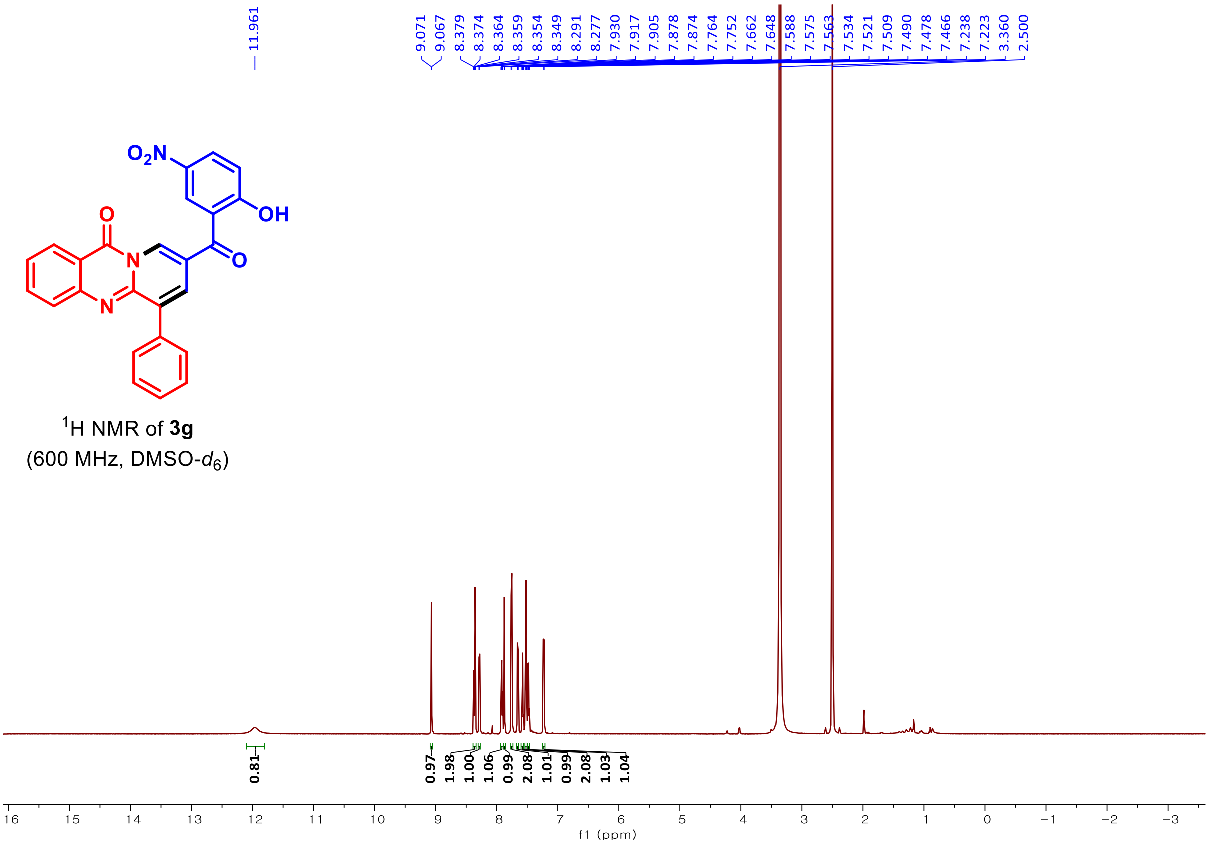


^{13}C NMR of **3f**
(150 MHz, $CDCl_3$)

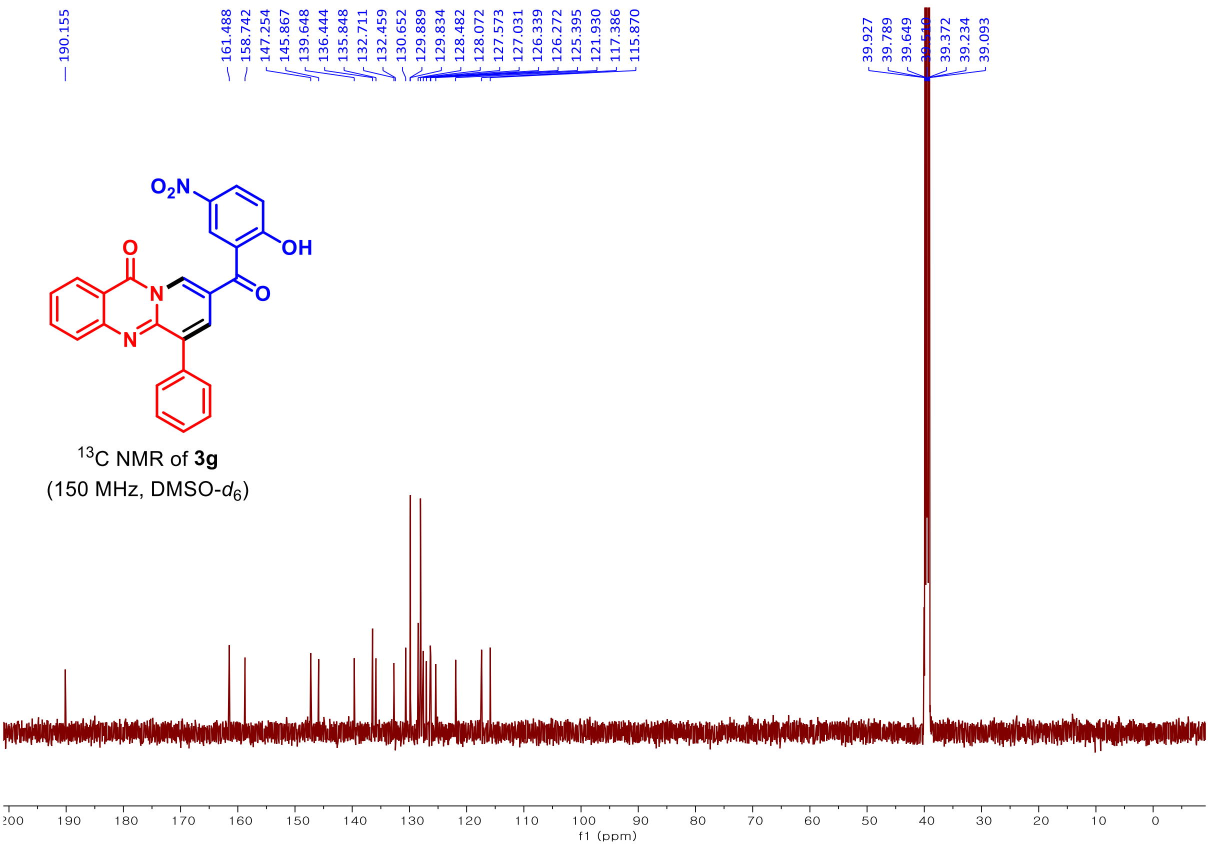


^{19}F NMR of **3f**
(564 MHz, $CDCl_3$)

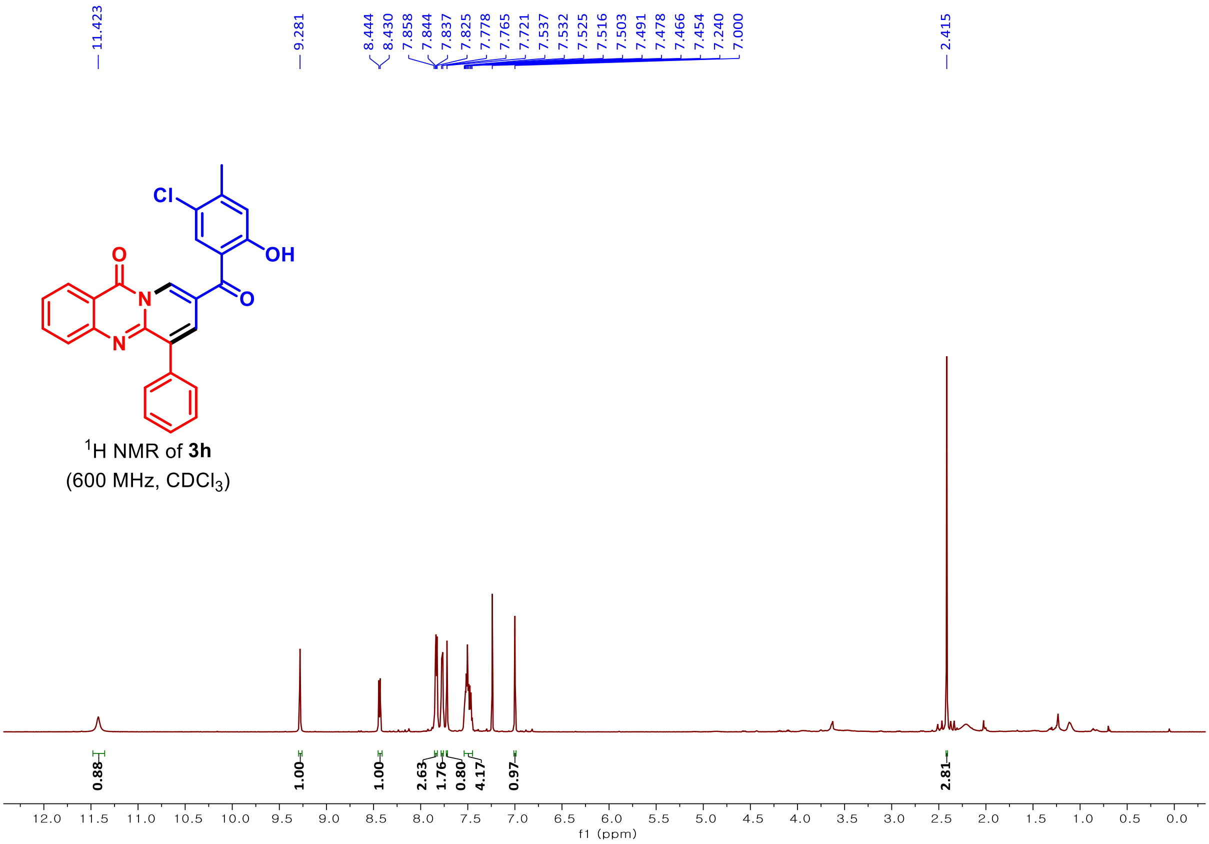


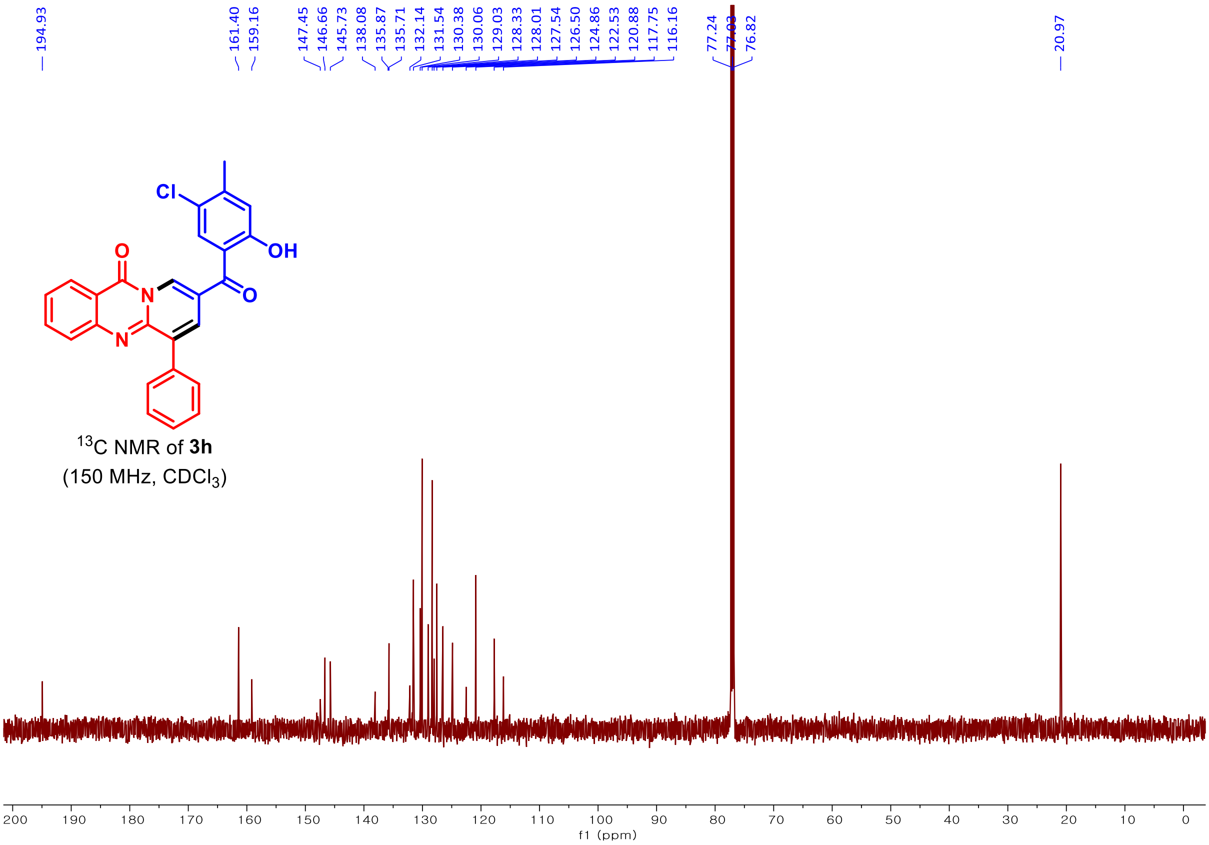


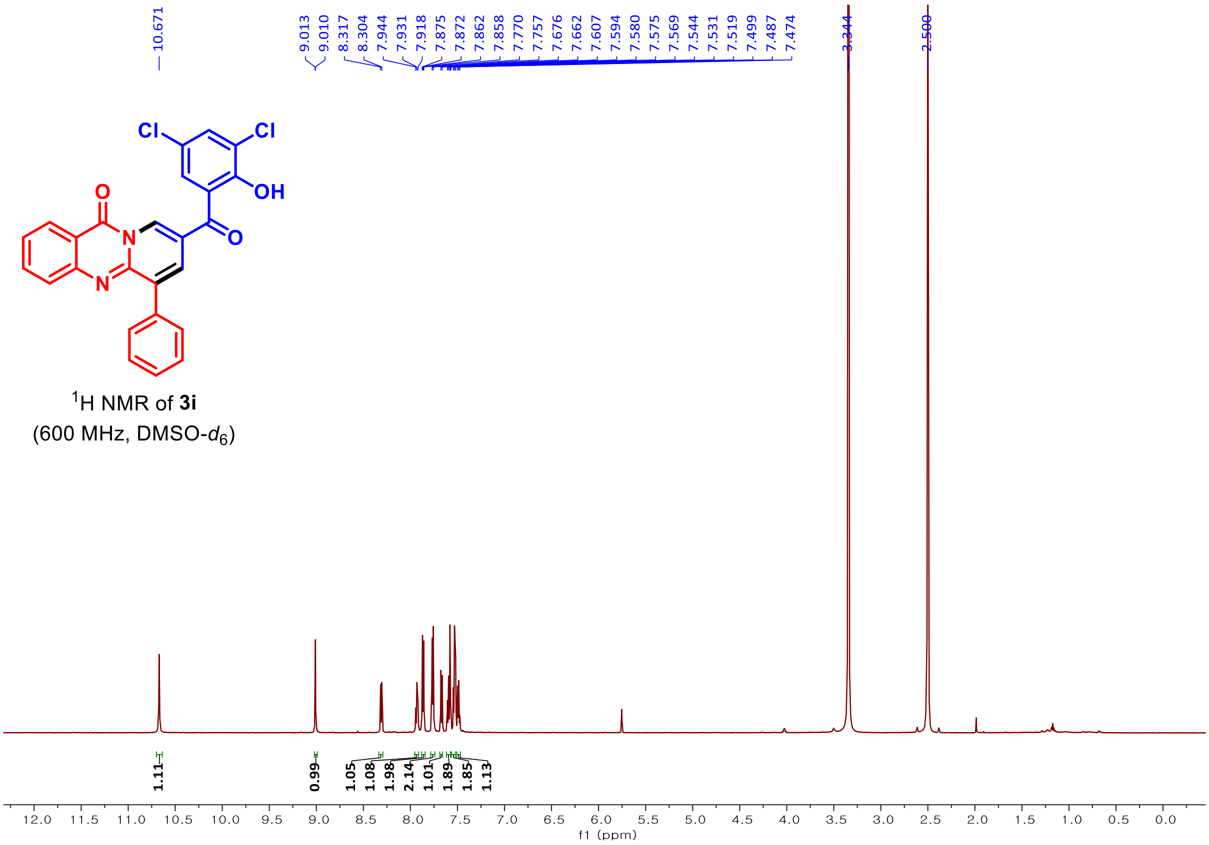
^{1}H NMR of **3g**
(600 MHz, DMSO-d_6)



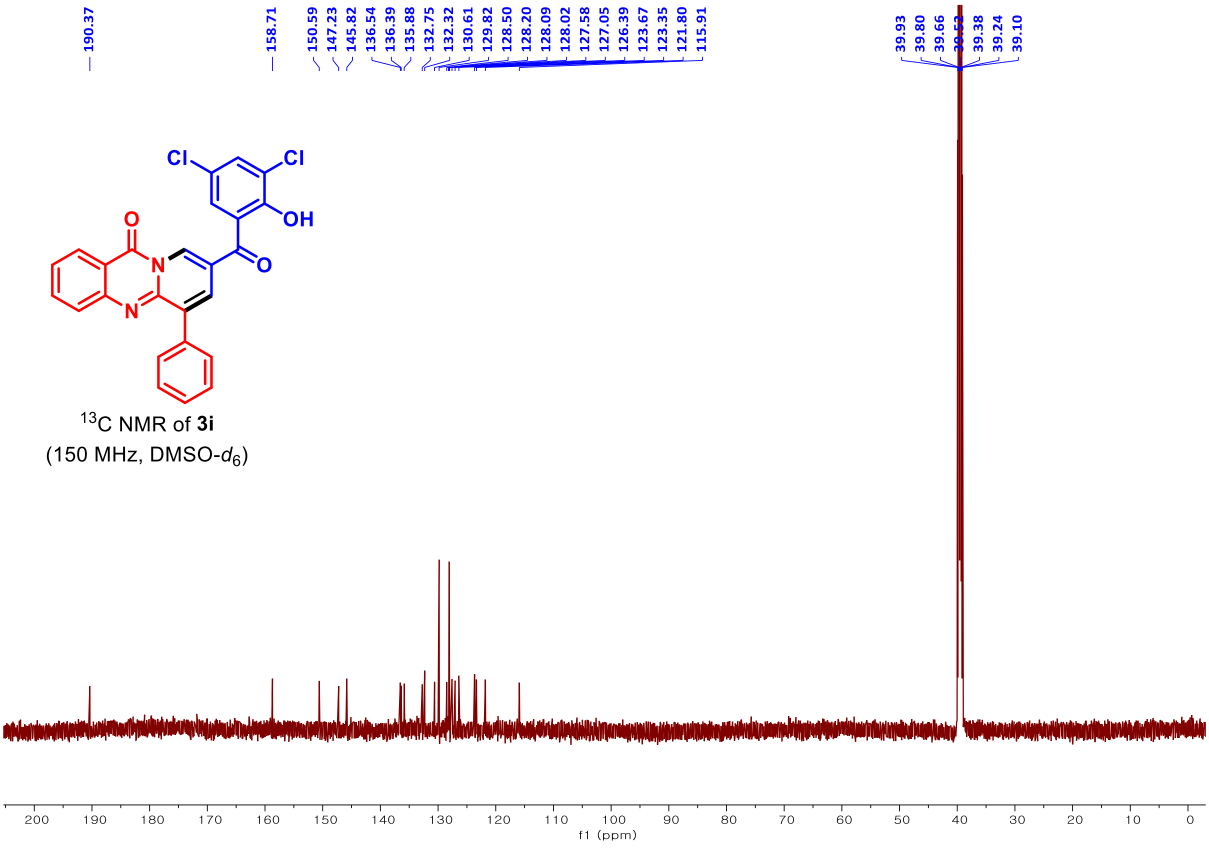
^{13}C NMR of **3g**
(150 MHz, DMSO-d_6)


11.423
9.281
8.444
8.430
7.858
7.844
7.837
7.825
7.778
7.765
7.721
7.537
7.532
7.525
7.516
7.503
7.491
7.478
7.466
7.454
7.240
7.000
2.415
Cl
OH
O
O
N
N
1H NMR of 3h
(600 MHz, CDCl3)
0.88
1.00
1.00
2.63
1.76
0.80
4.17
0.97
2.81
f1 (ppm)

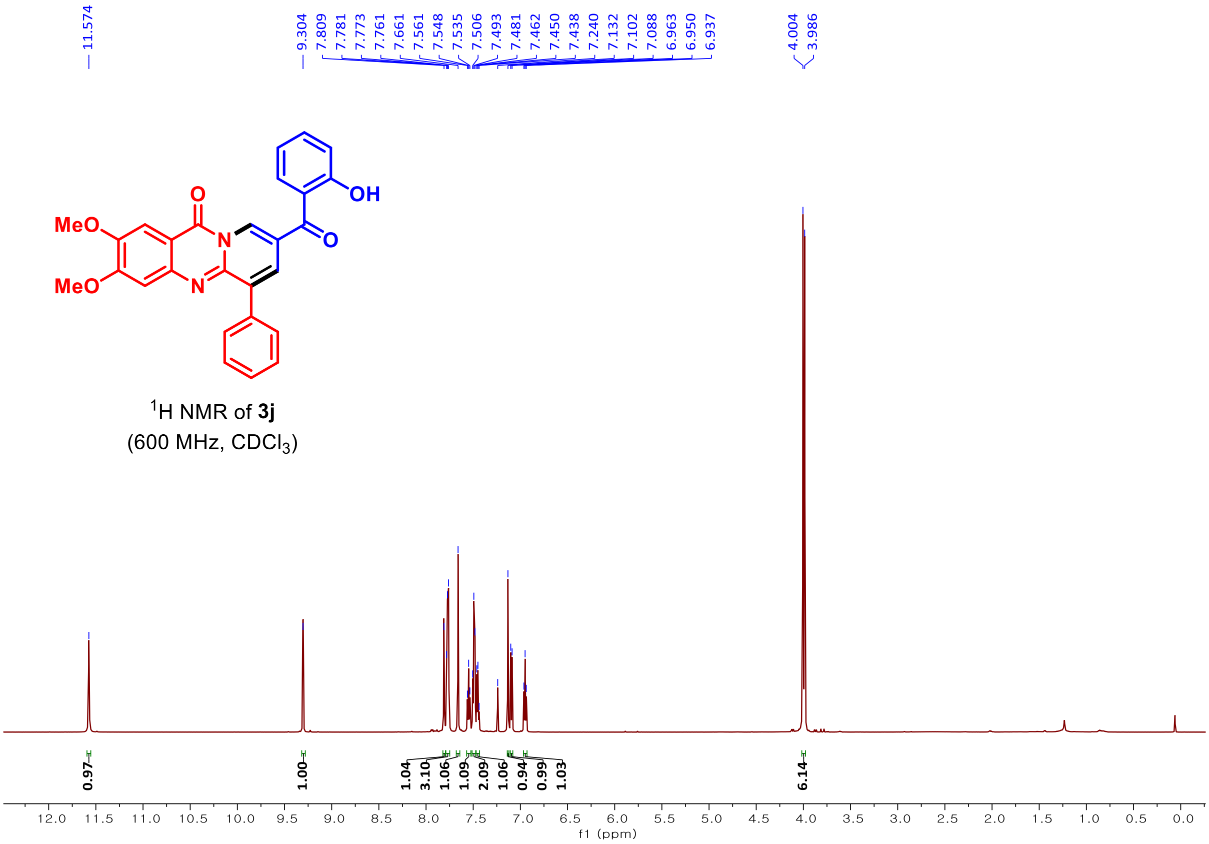

194.93
161.40
159.16
147.45
146.66
145.73
138.08
135.87
135.71
132.14
131.54
130.38
130.06
129.03
128.33
128.01
127.54
126.50
124.86
122.53
120.88
117.75
116.16
77.24
77.03
76.82
20.97
Cl
OH
O
O
N
N
13C NMR of 3h
(150 MHz, CDCl3)
f1 (ppm)



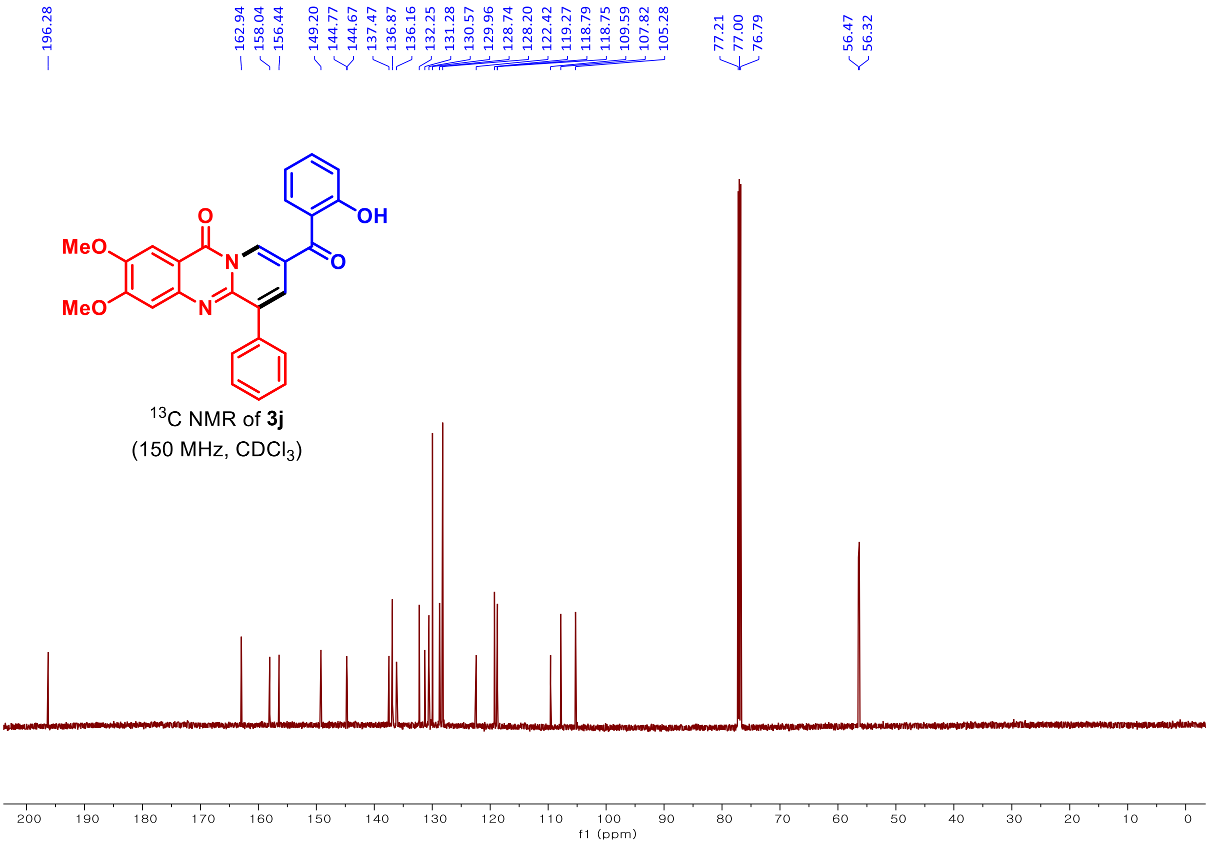
^{1}H NMR of **3i**
(600 MHz, DMSO-d_6)



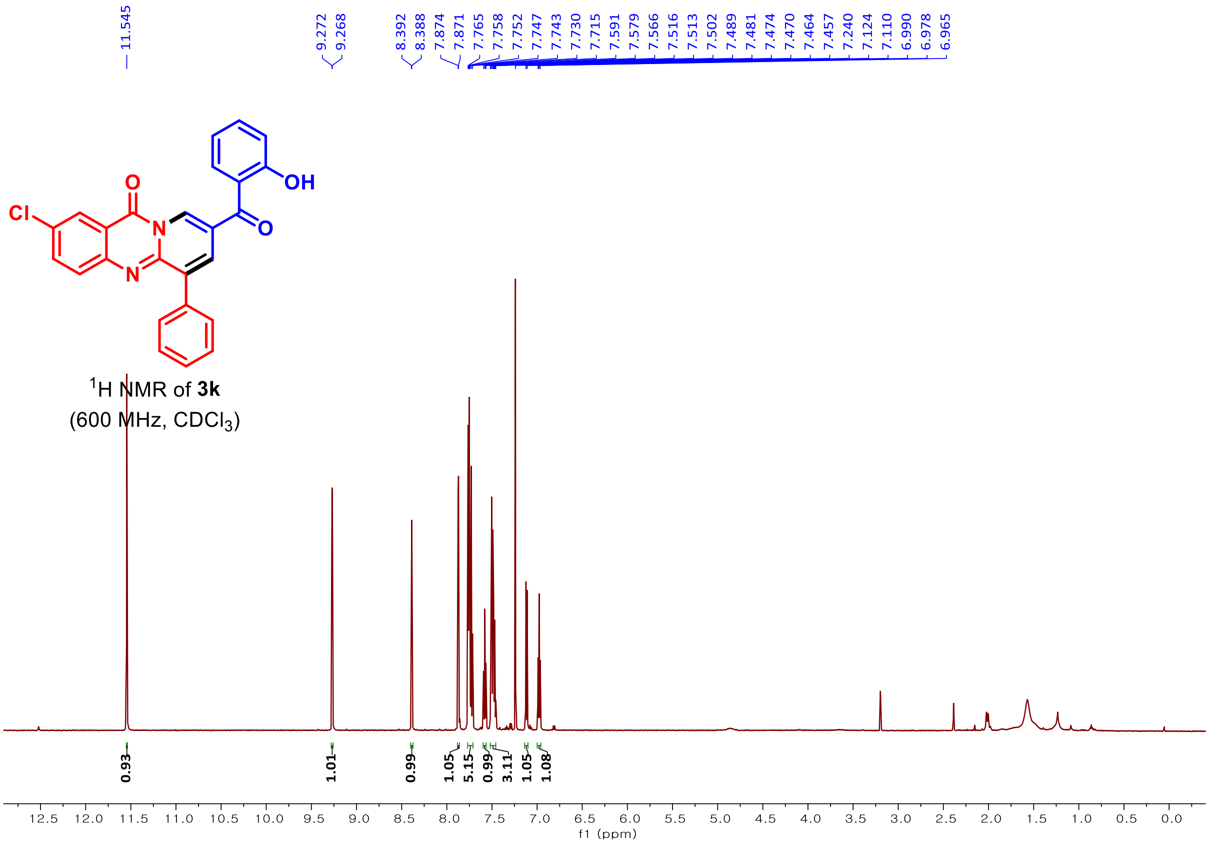
^{13}C NMR of **3i**
(150 MHz, DMSO-d_6)

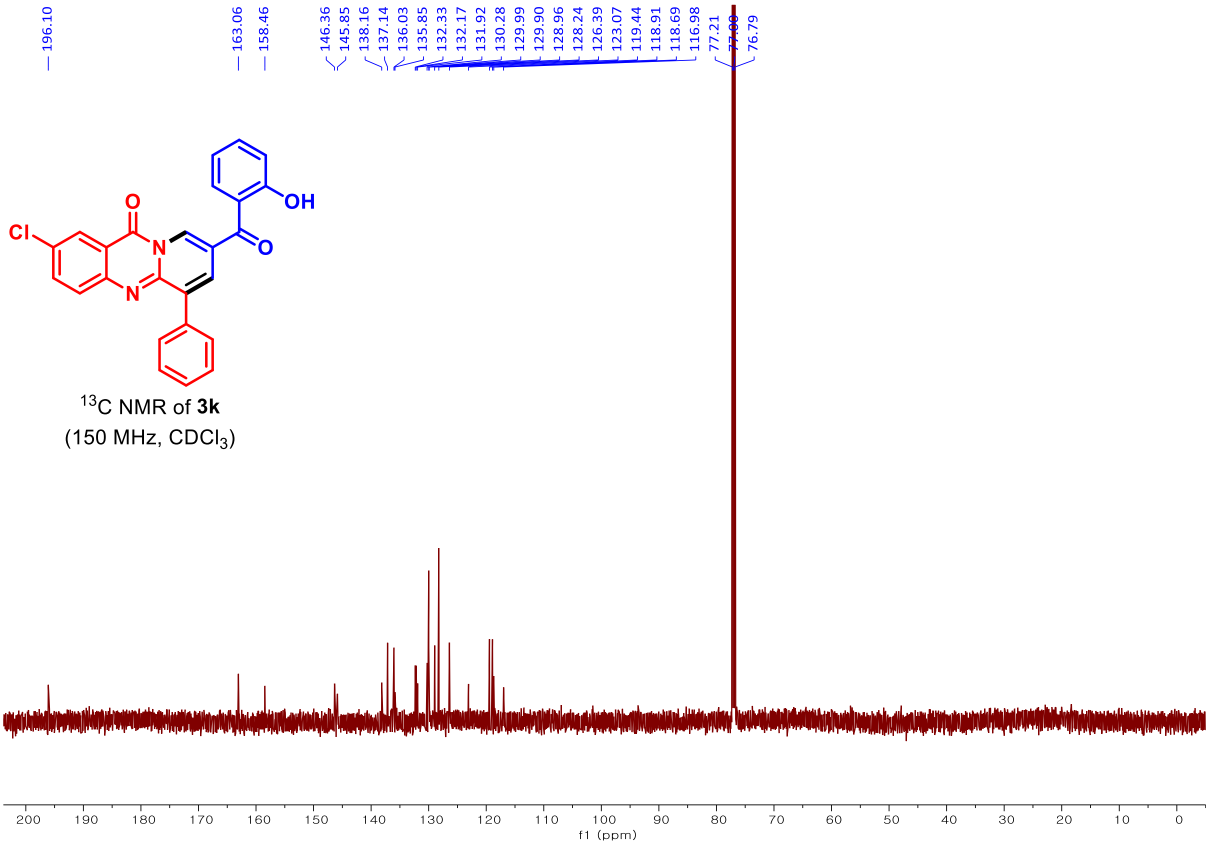


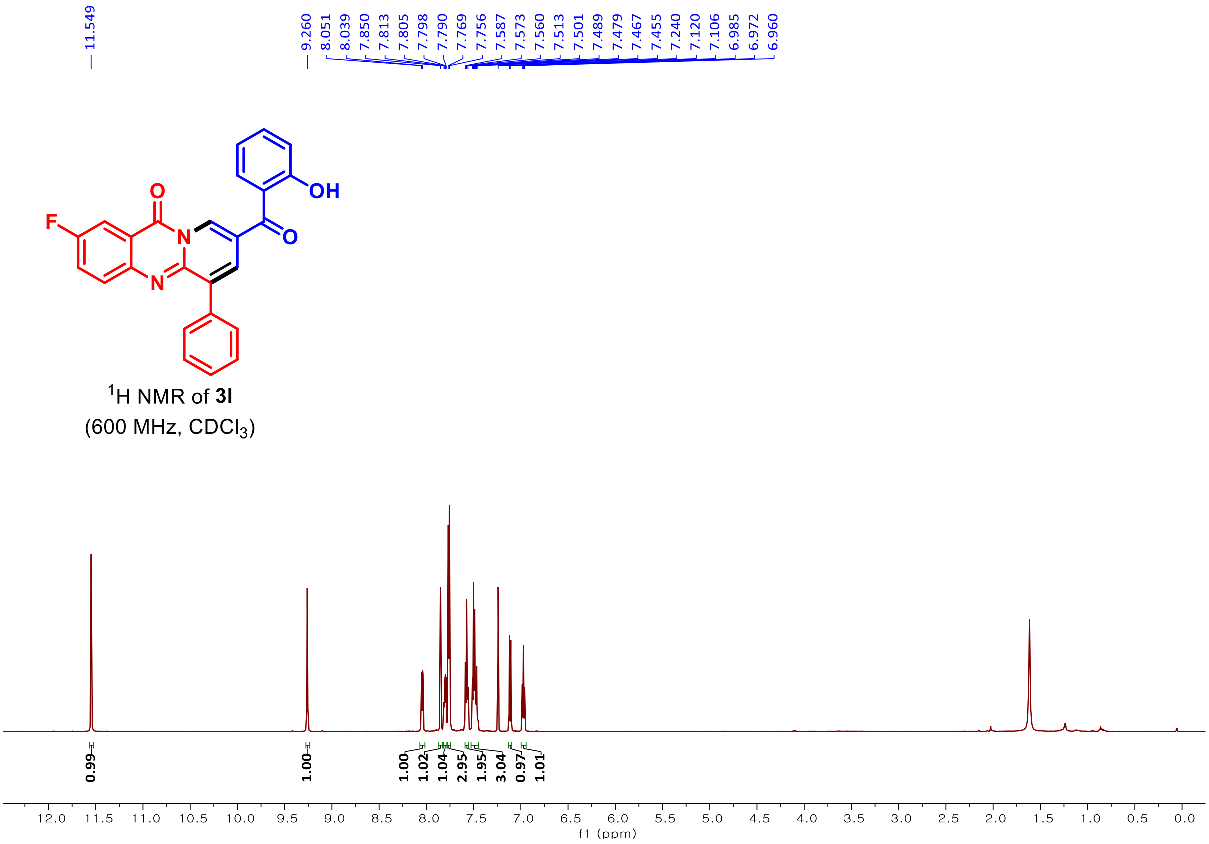
[1]H NMR of **3j**
(600 MHz, $CDCl_3$)



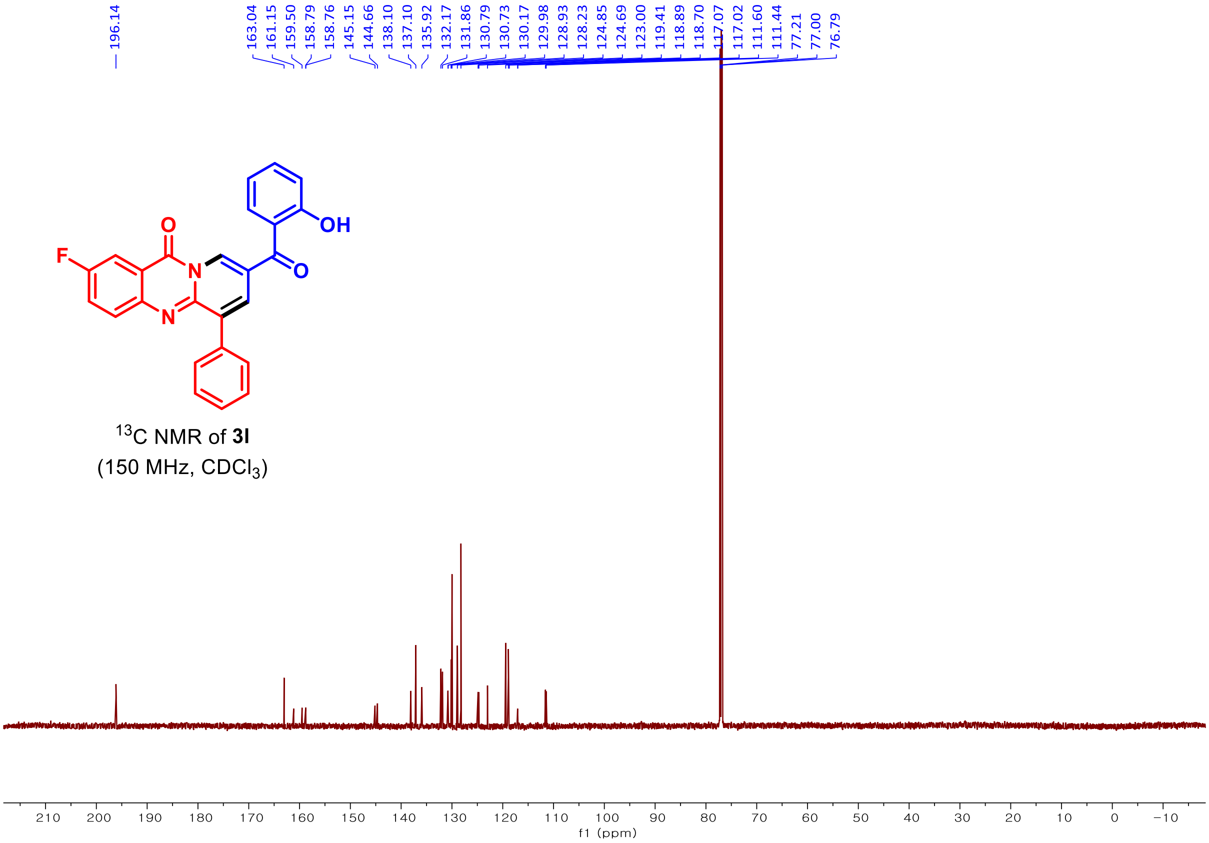
[13]C NMR of **3j**
(150 MHz, $CDCl_3$)


11.545
9.272
9.268
8.392
8.388
7.874
7.871
7.765
7.758
7.752
7.747
7.743
7.730
7.715
7.591
7.579
7.566
7.516
7.513
7.502
7.489
7.481
7.474
7.470
7.464
7.457
7.240
7.124
7.110
6.990
6.978
6.965
Cl
O
N
N
OH
O
^{1}H NMR of **3k**
(600 MHz, $CDCl_3$)
0.93
1.01
0.99
1.05
5.15
0.99
3.11
1.05
1.08
f1 (ppm)

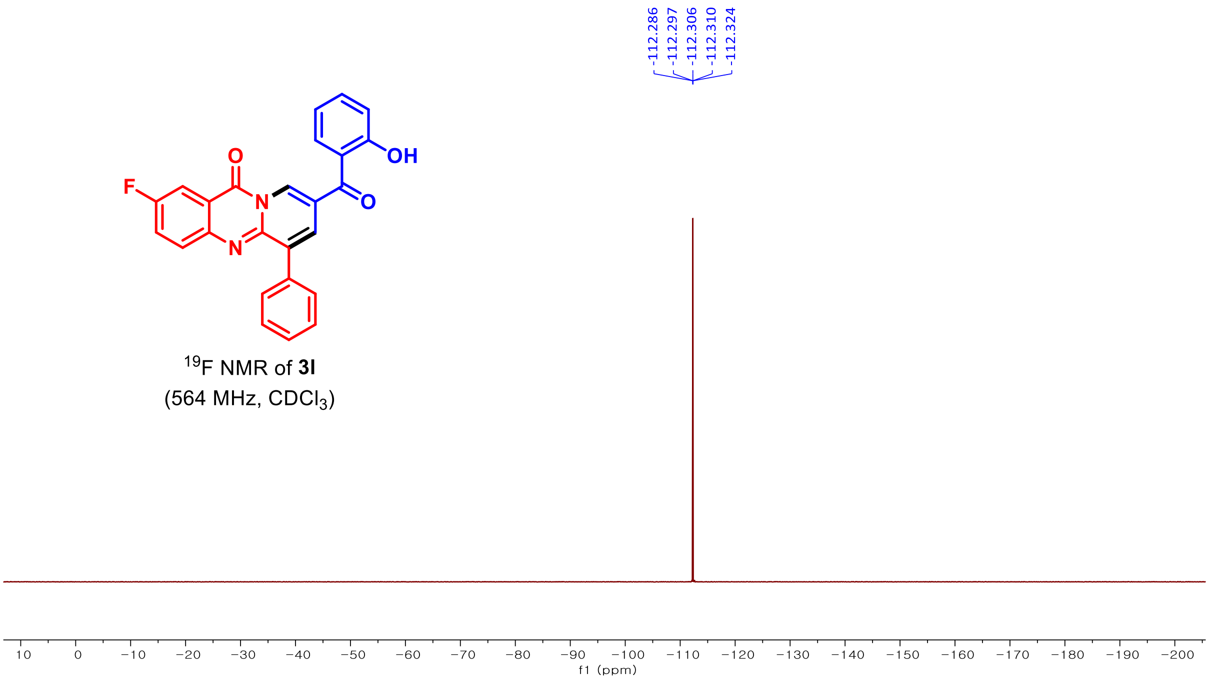

196.10
163.06
158.46
146.36
145.85
138.16
137.14
136.03
135.85
132.33
132.17
131.92
130.28
129.99
129.90
128.96
128.24
126.39
123.07
119.44
118.91
118.69
116.98
77.21
77.00
76.79
Cl
O
N
N
OH
O
^{13}C NMR of **3k**
(150 MHz, $CDCl_3$)
f1 (ppm)



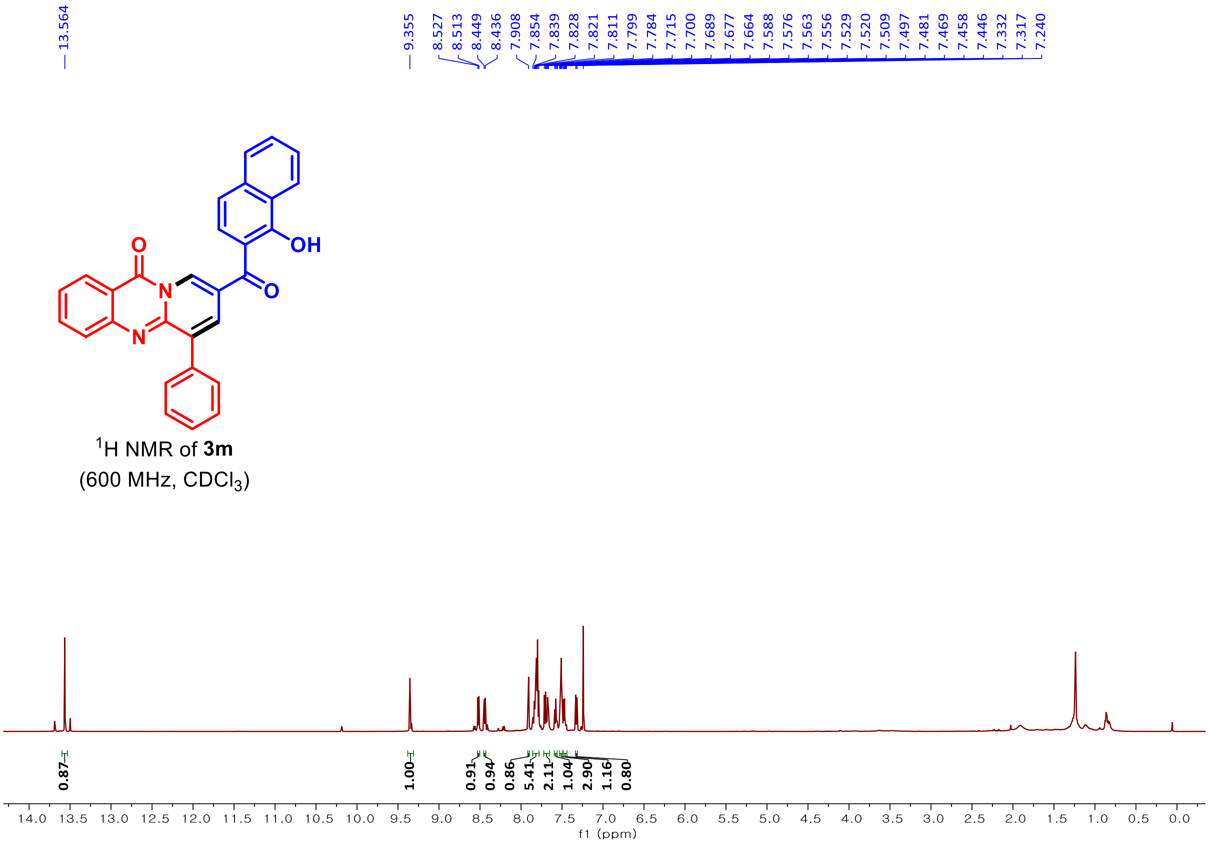
^{1}H NMR of **3l**
(600 MHz, $CDCl_3$)



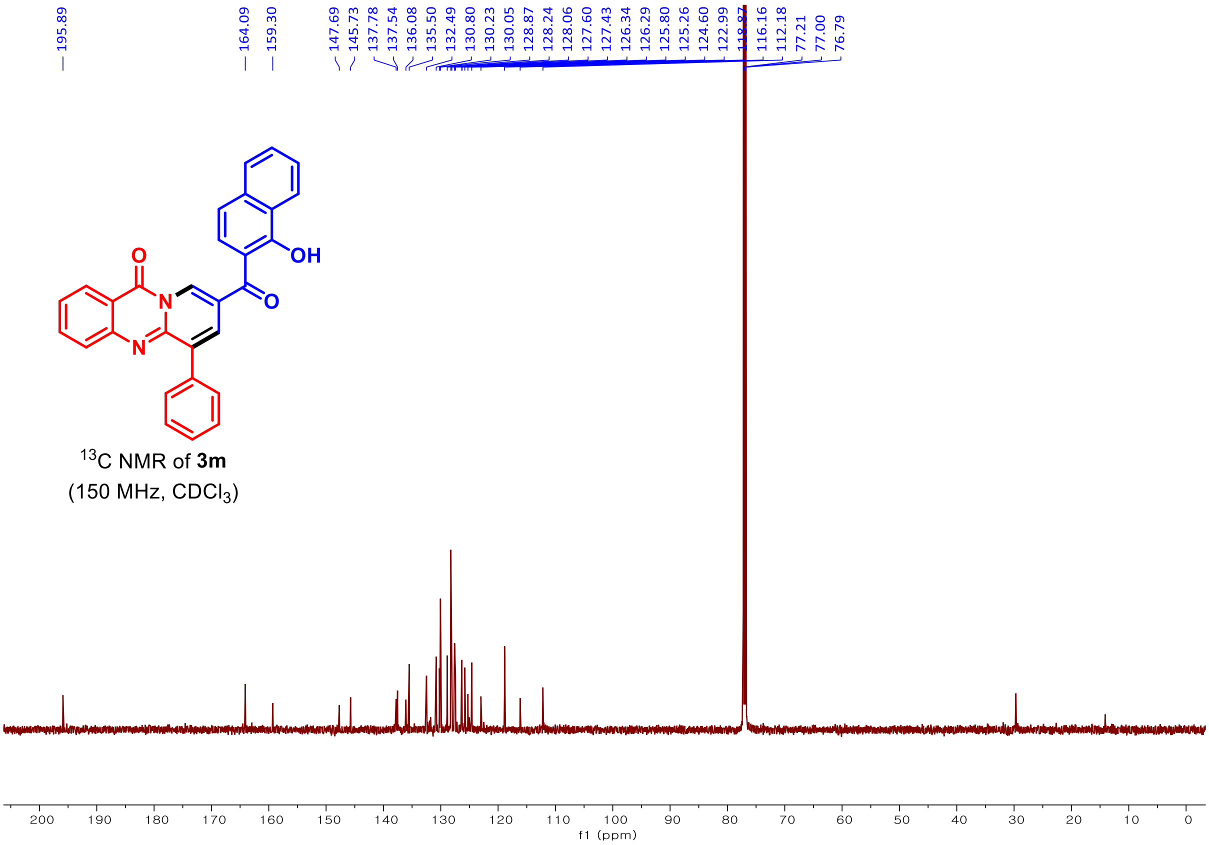
^{13}C NMR of **3l**
(150 MHz, $CDCl_3$)



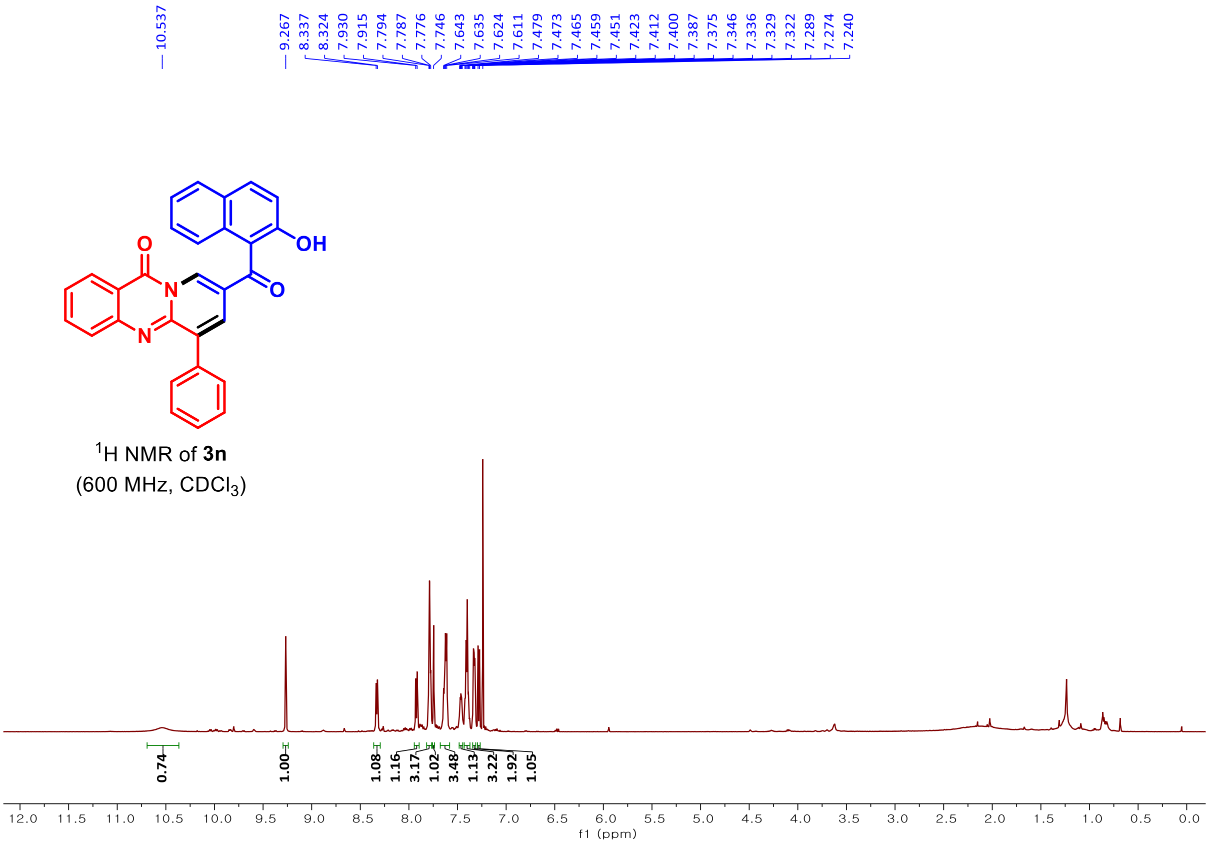
^{19}F NMR of **3l**
(564 MHz, $CDCl_3$)



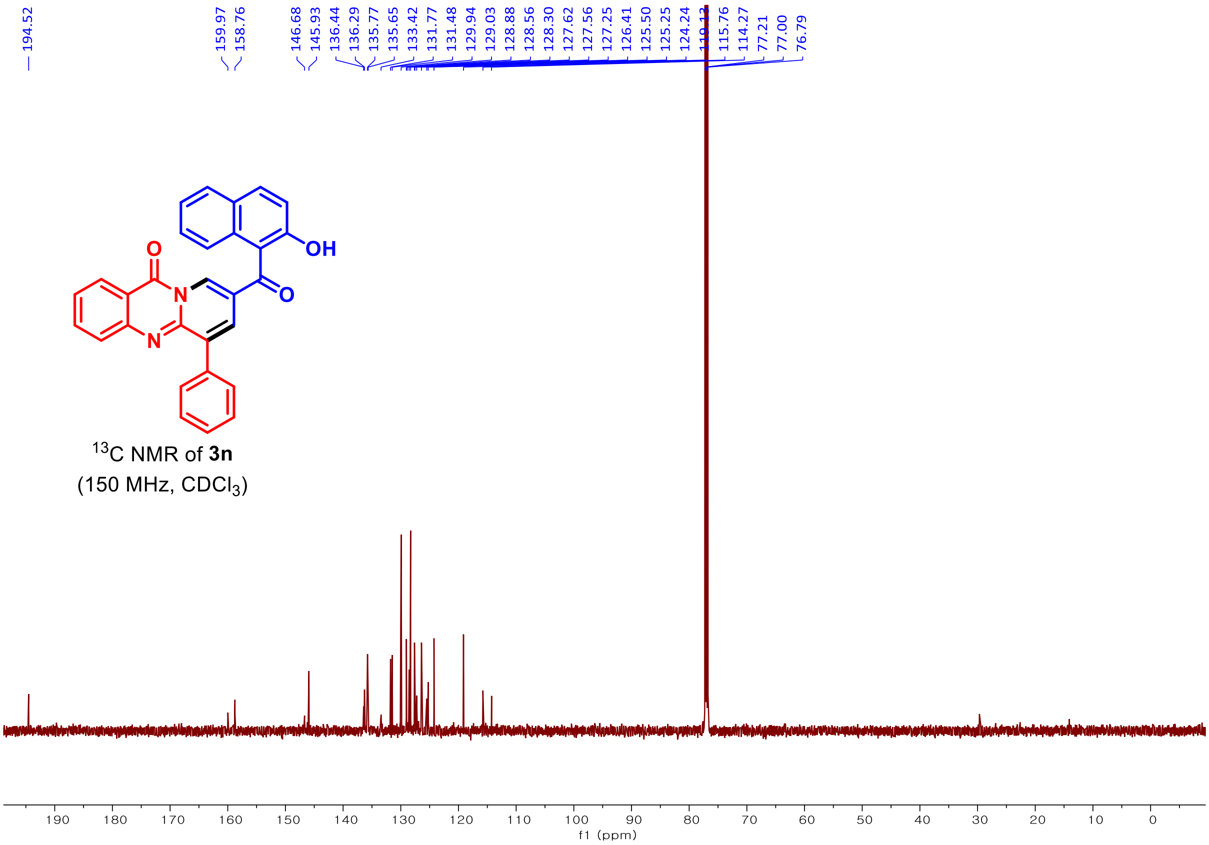
^{1}H NMR of **3m**
(600 MHz, $CDCl_3$)



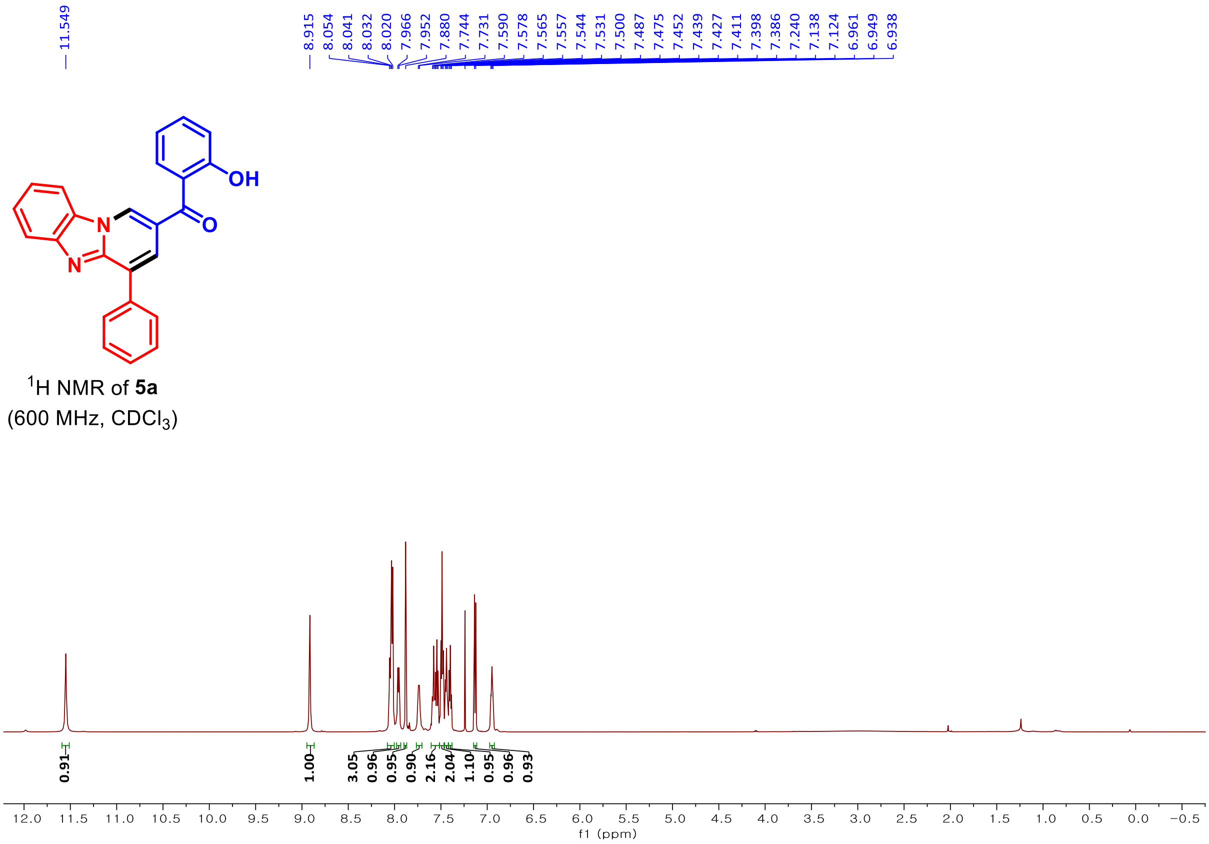
^{13}C NMR of **3m**
(150 MHz, $CDCl_3$)

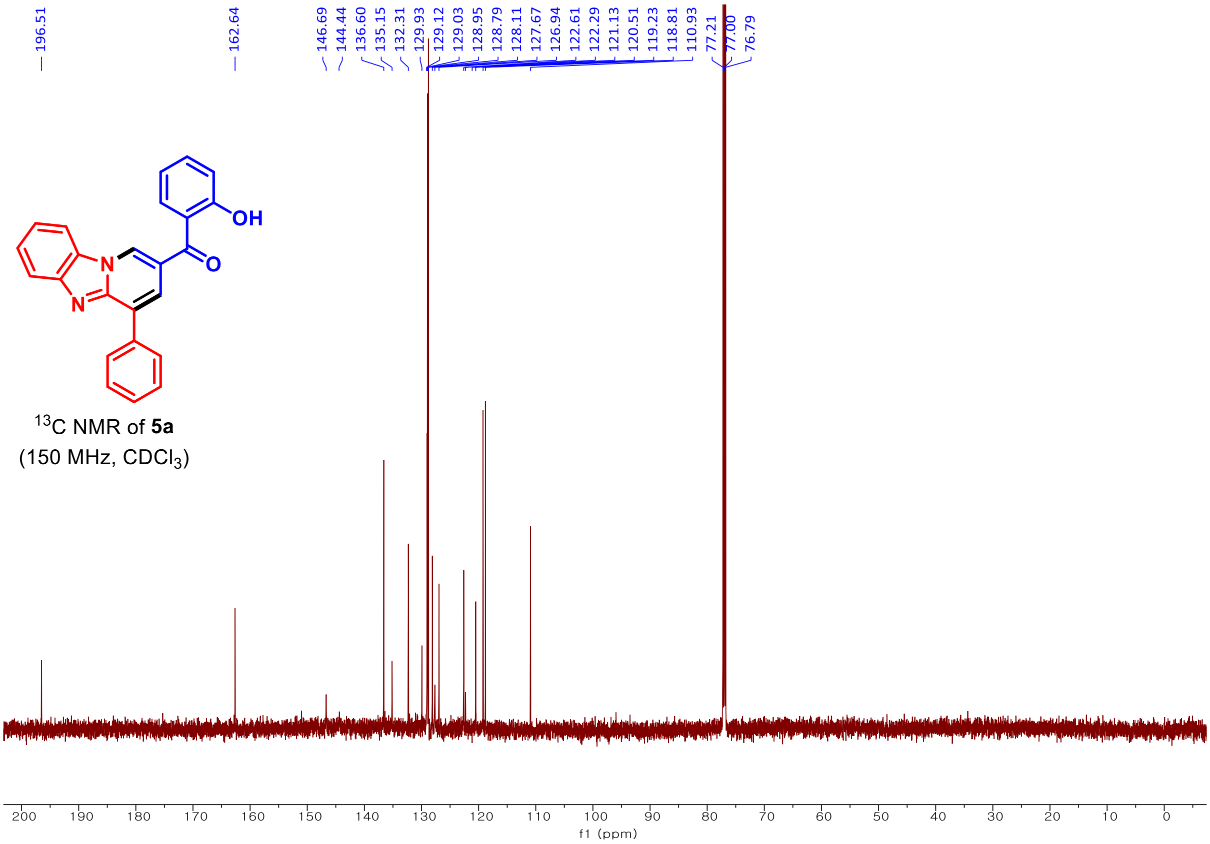


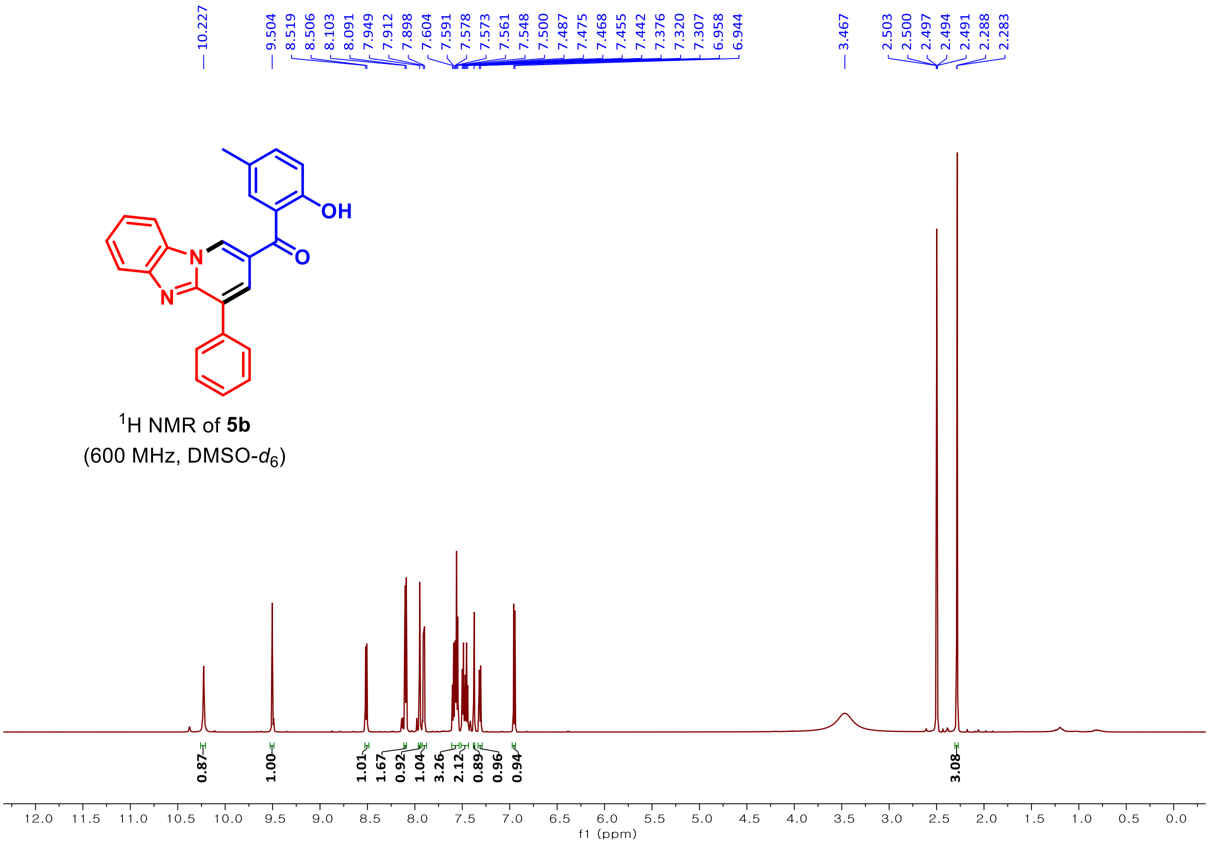
^{1}H NMR of **3n**
(600 MHz, $CDCl_3$)



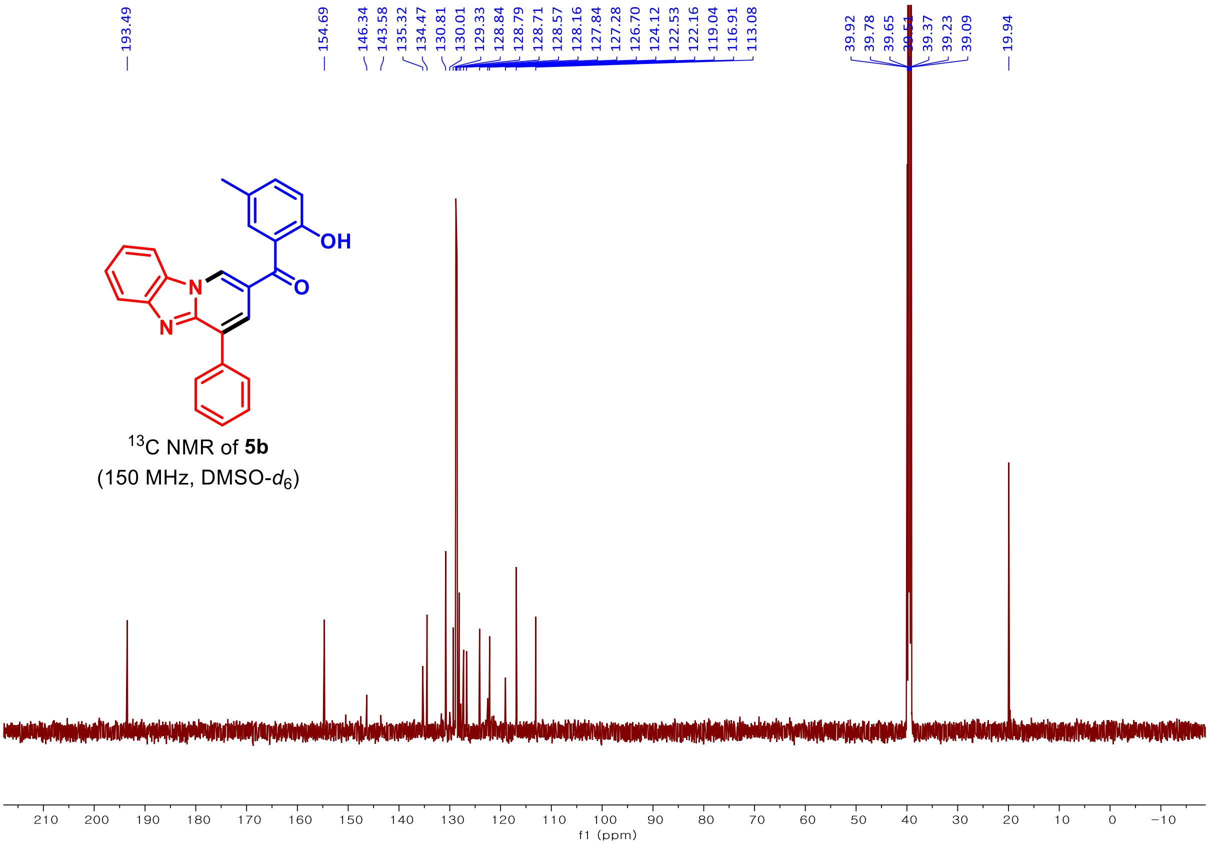
^{13}C NMR of **3n**
(150 MHz, $CDCl_3$)


11.549
8.915
8.054
8.041
8.032
8.020
7.966
7.952
7.880
7.744
7.731
7.590
7.578
7.565
7.557
7.544
7.531
7.500
7.487
7.475
7.452
7.439
7.427
7.411
7.398
7.386
7.240
7.138
7.124
6.961
6.949
6.938
OH
O
N
N
^{1}H NMR of 5a
(600 MHz, $CDCl_3$)
0.91
1.00
3.05
0.96
0.95
0.90
2.16
2.04
1.10
0.95
0.96
0.93
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
f1 (ppm)

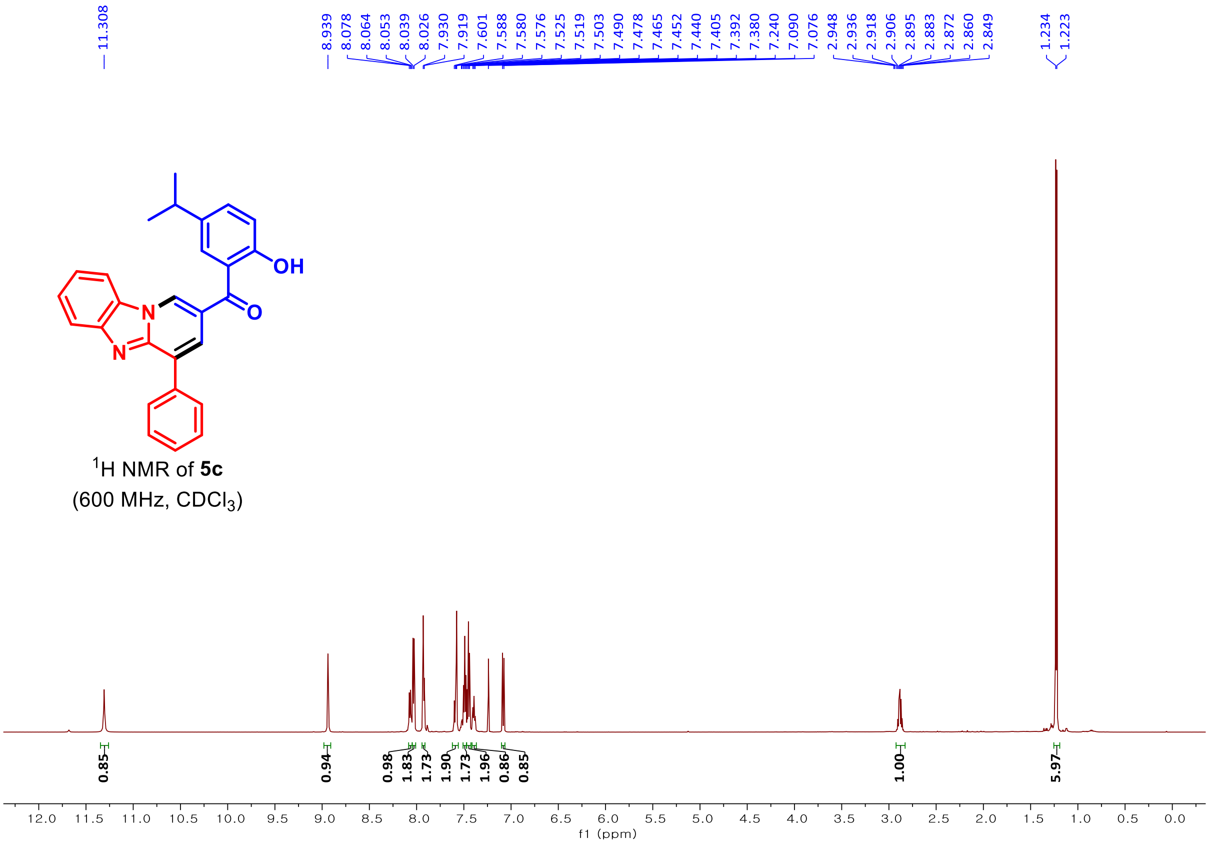

196.51
162.64
146.69
144.44
136.60
135.15
132.31
129.93
129.12
129.03
128.95
128.79
128.11
127.67
126.94
122.61
122.29
121.13
120.51
119.23
118.81
110.93
77.21
77.00
76.79
OH
O
N
N
^{13}C NMR of 5a
(150 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



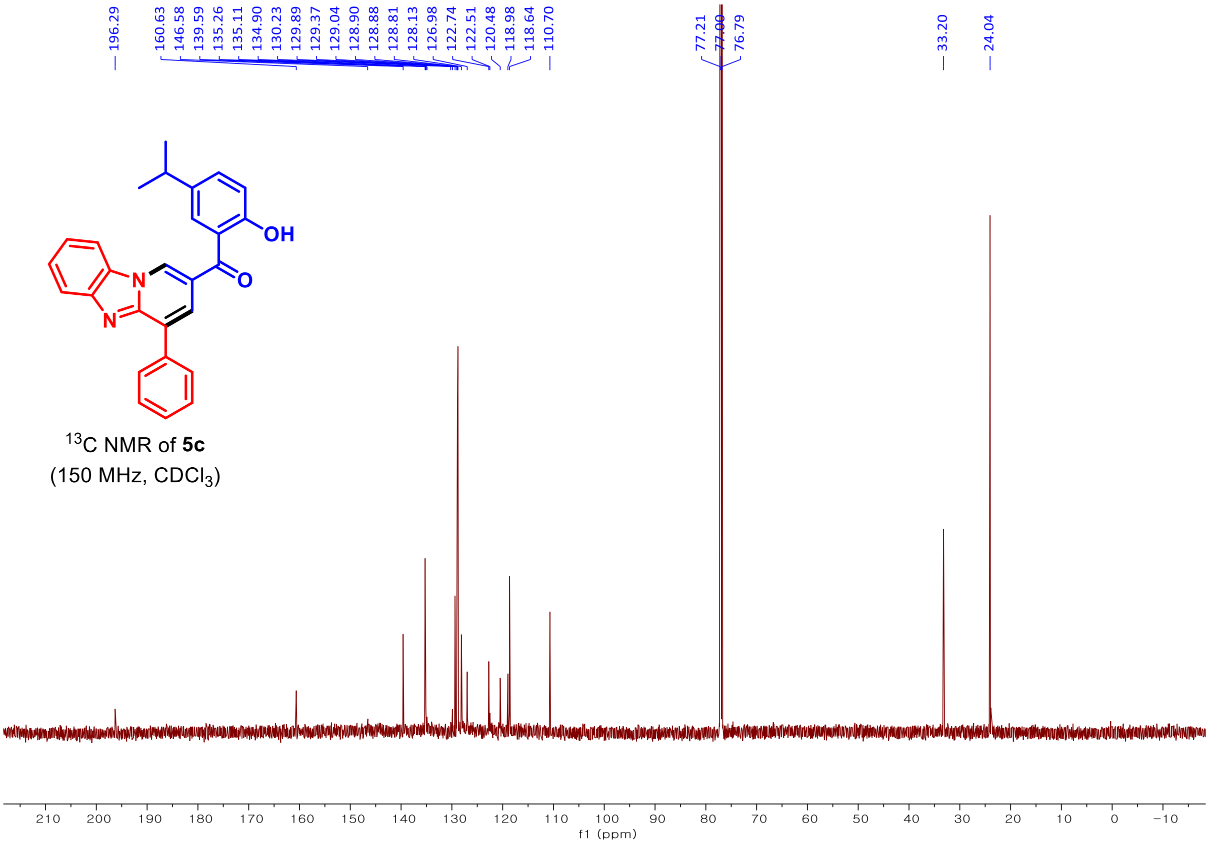
^{1}H NMR of **5b**
(600 MHz, DMSO-d_6)



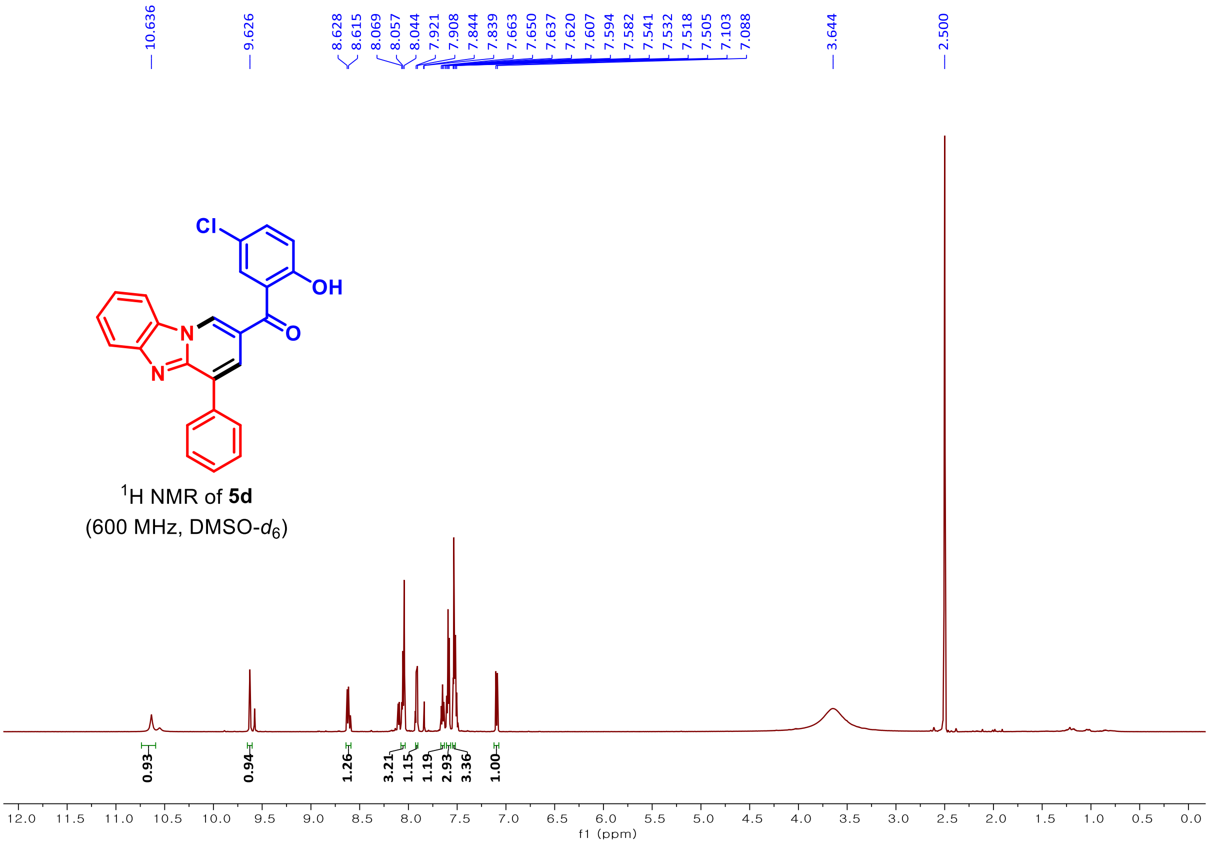
^{13}C NMR of **5b**
(150 MHz, DMSO-d_6)

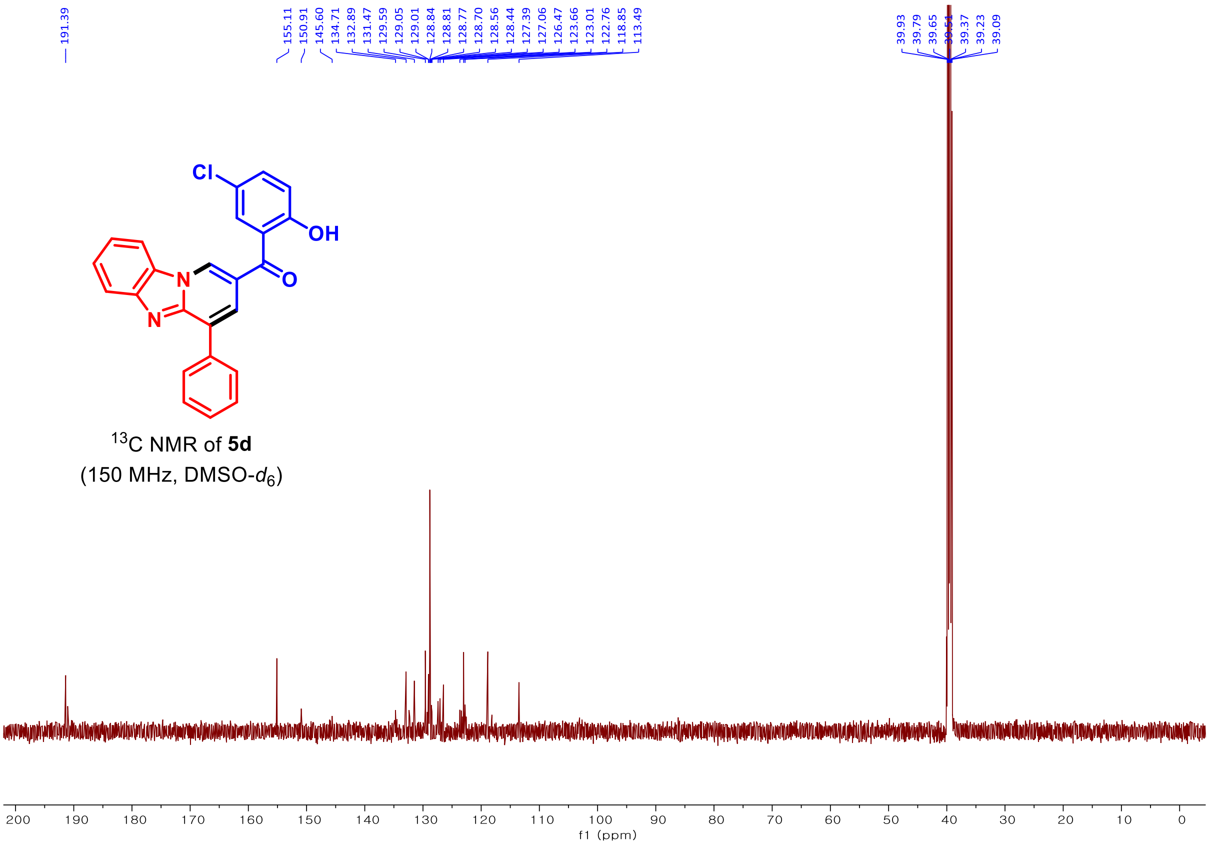


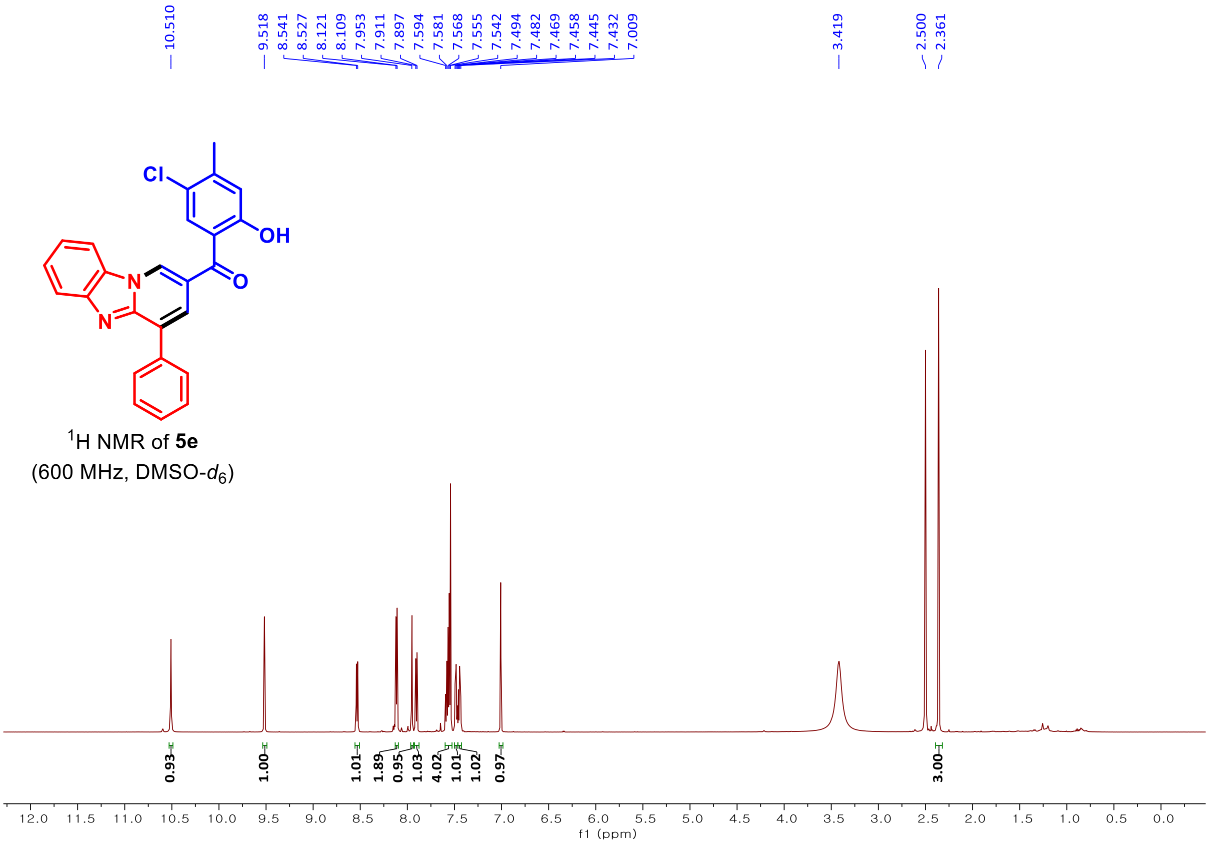
^{1}H NMR of **5c**
(600 MHz, $CDCl_3$)



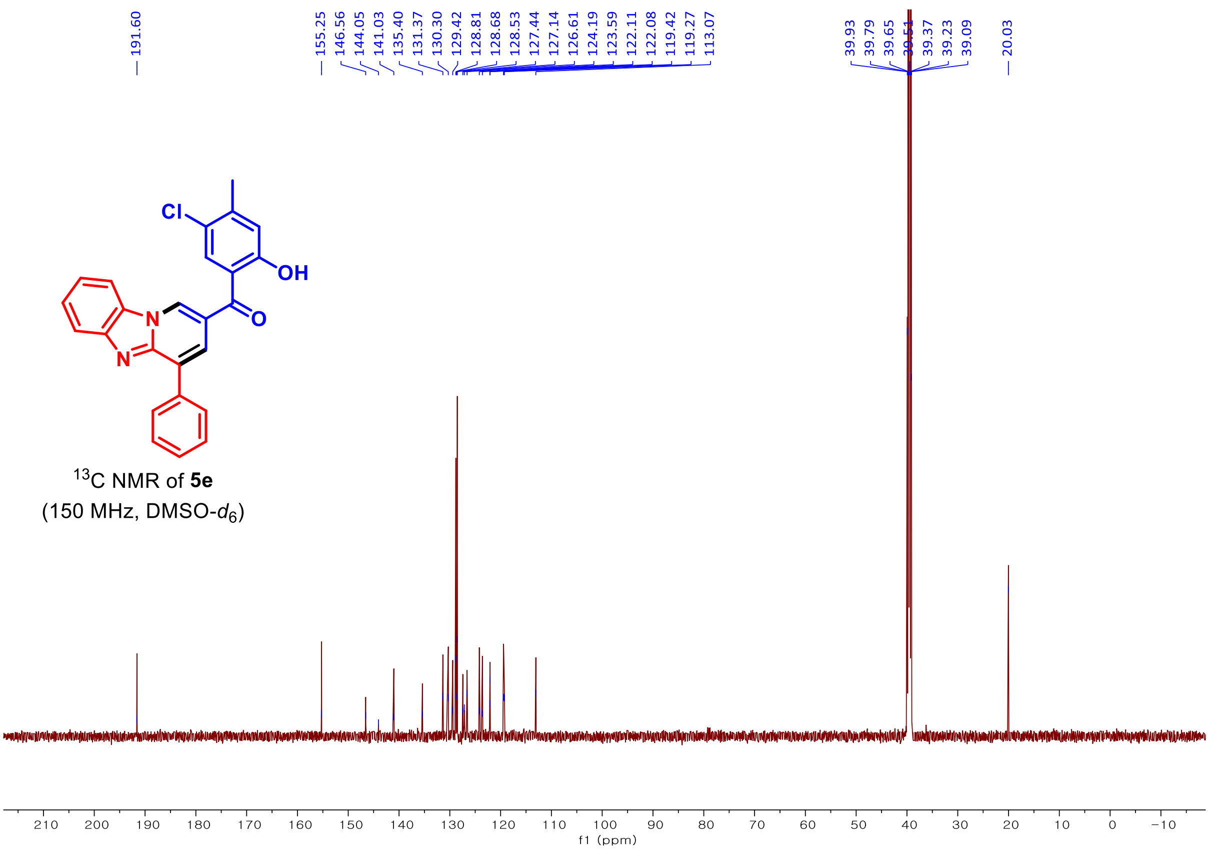
^{13}C NMR of **5c**
(150 MHz, $CDCl_3$)


10.636
9.626
8.628
8.615
8.069
8.057
8.044
7.921
7.908
7.844
7.839
7.663
7.650
7.637
7.620
7.607
7.594
7.582
7.541
7.532
7.518
7.505
7.103
7.088
3.644
2.500
Cl
OH
N
O
N
^{1}H NMR of **5d**
(600 MHz, DMSO-d_6)
0.93
0.94
1.26
3.21
1.15
1.19
2.93
3.36
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
f1 (ppm)

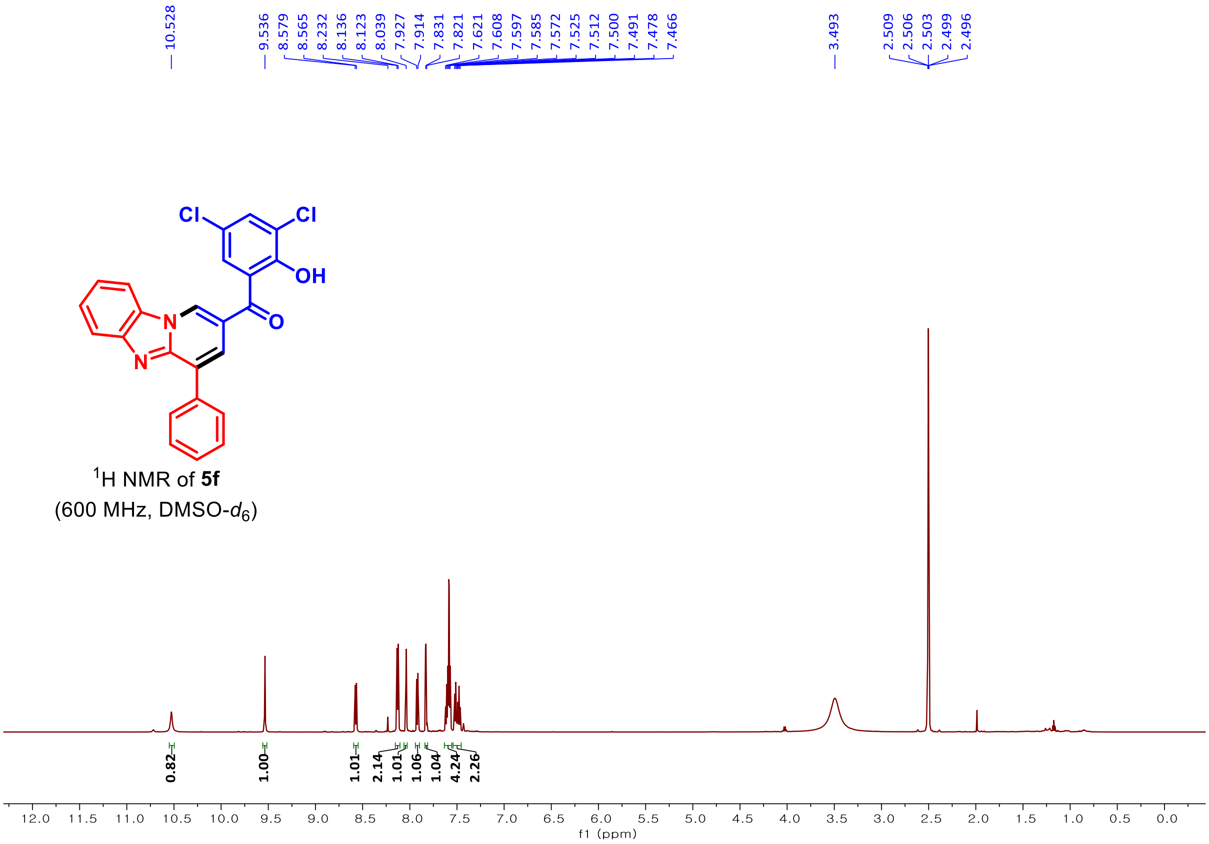

191.39
155.11
150.91
145.60
134.71
132.89
131.47
129.59
129.05
129.01
128.84
128.81
128.77
128.70
128.56
128.44
127.39
127.06
126.47
123.66
123.01
122.76
118.85
113.49
39.93
39.79
39.65
39.51
39.37
39.23
39.09
Cl
OH
N
O
N
^{13}C NMR of **5d**
(150 MHz, DMSO-d_6)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



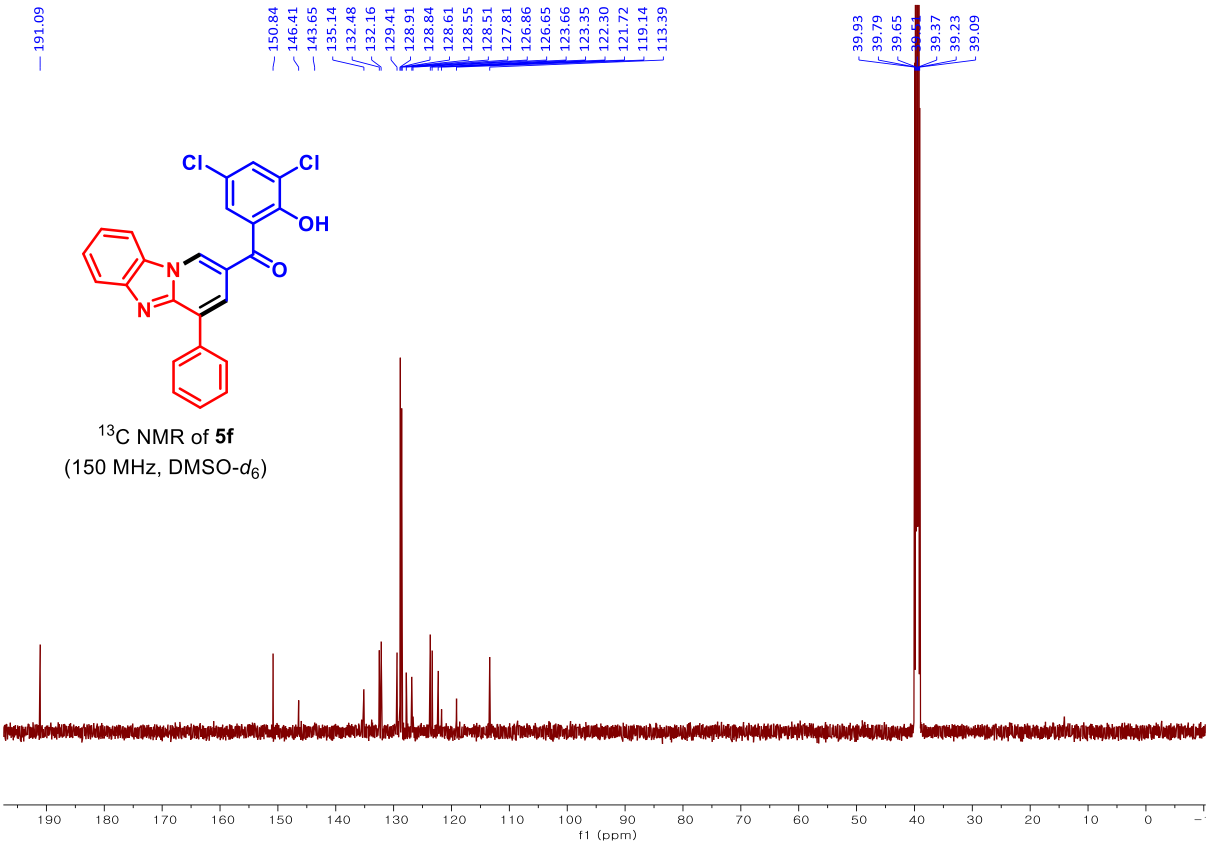
^{1}H NMR of **5e**
(600 MHz, DMSO-d_6)



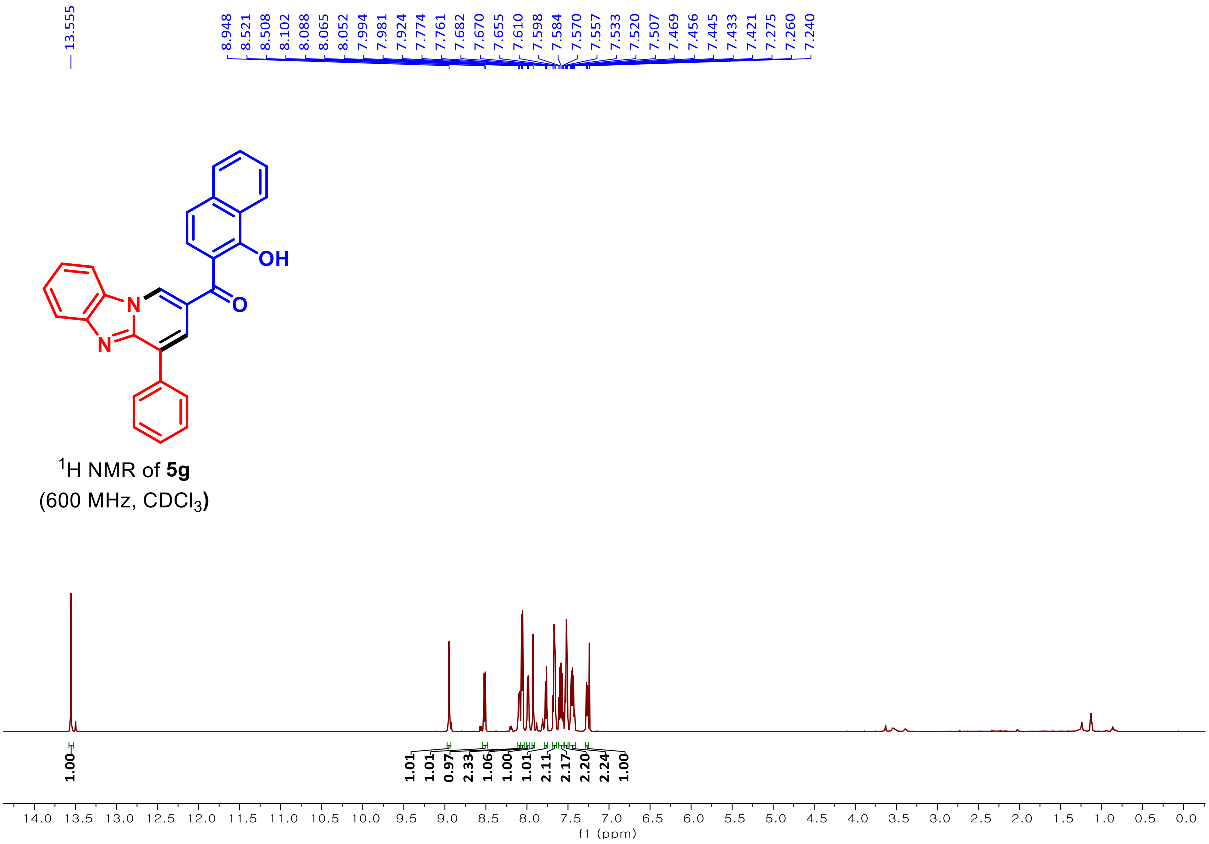
^{13}C NMR of **5e**
(150 MHz, DMSO-d_6)

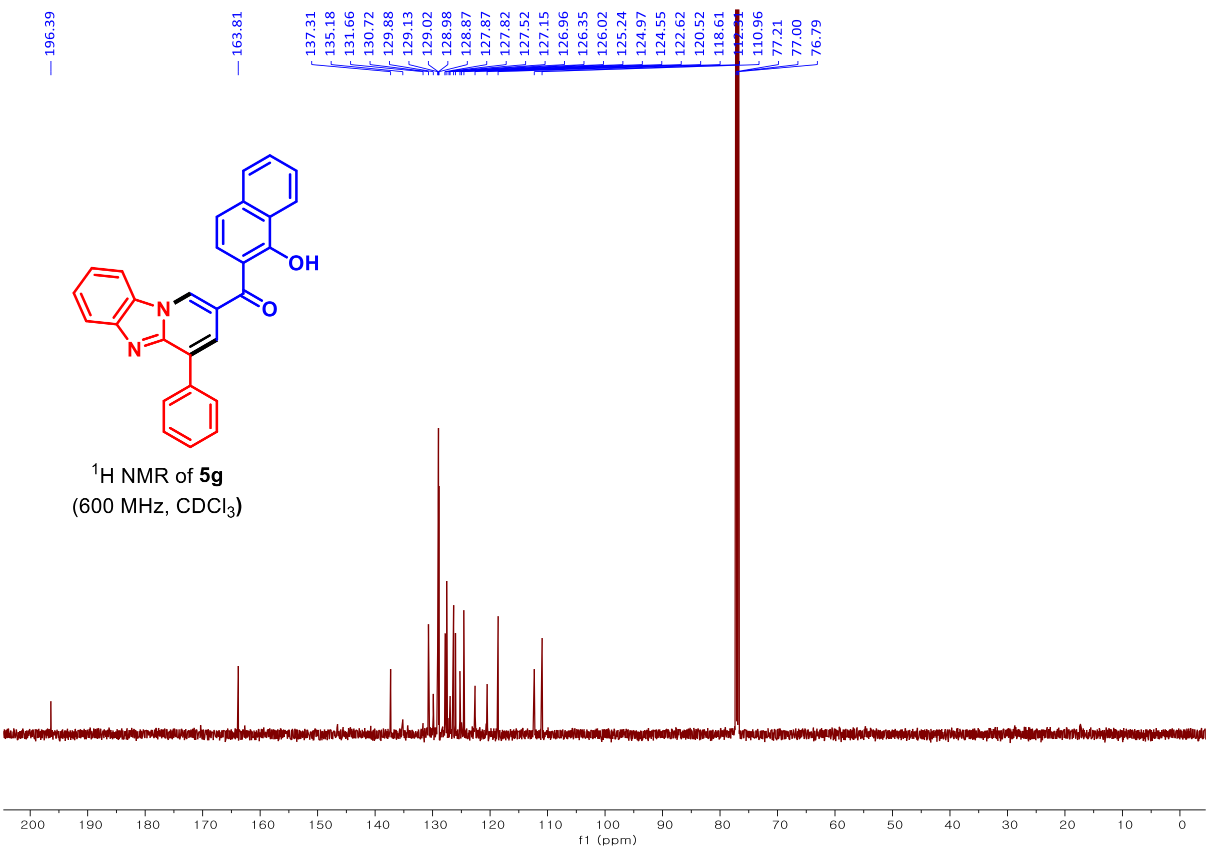


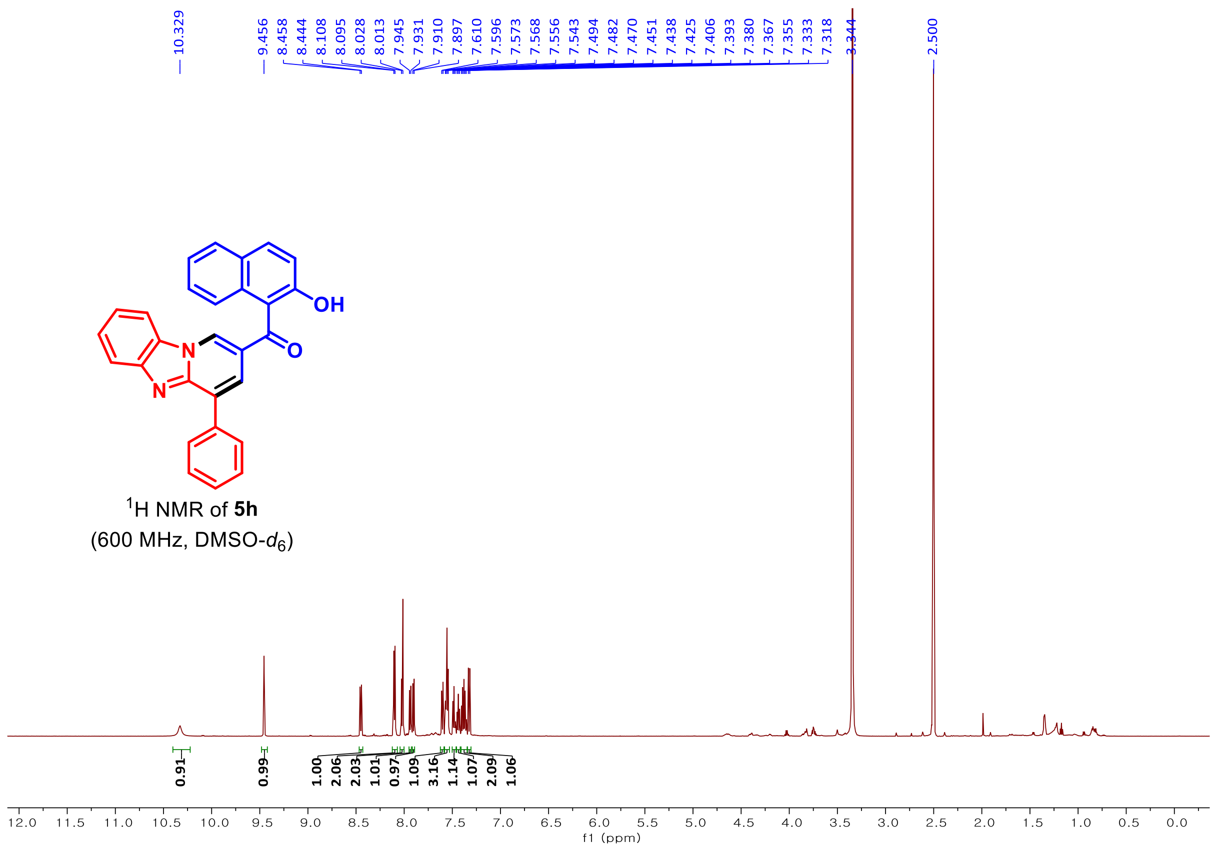
^{1}H NMR of **5f**
(600 MHz, DMSO-d_6)



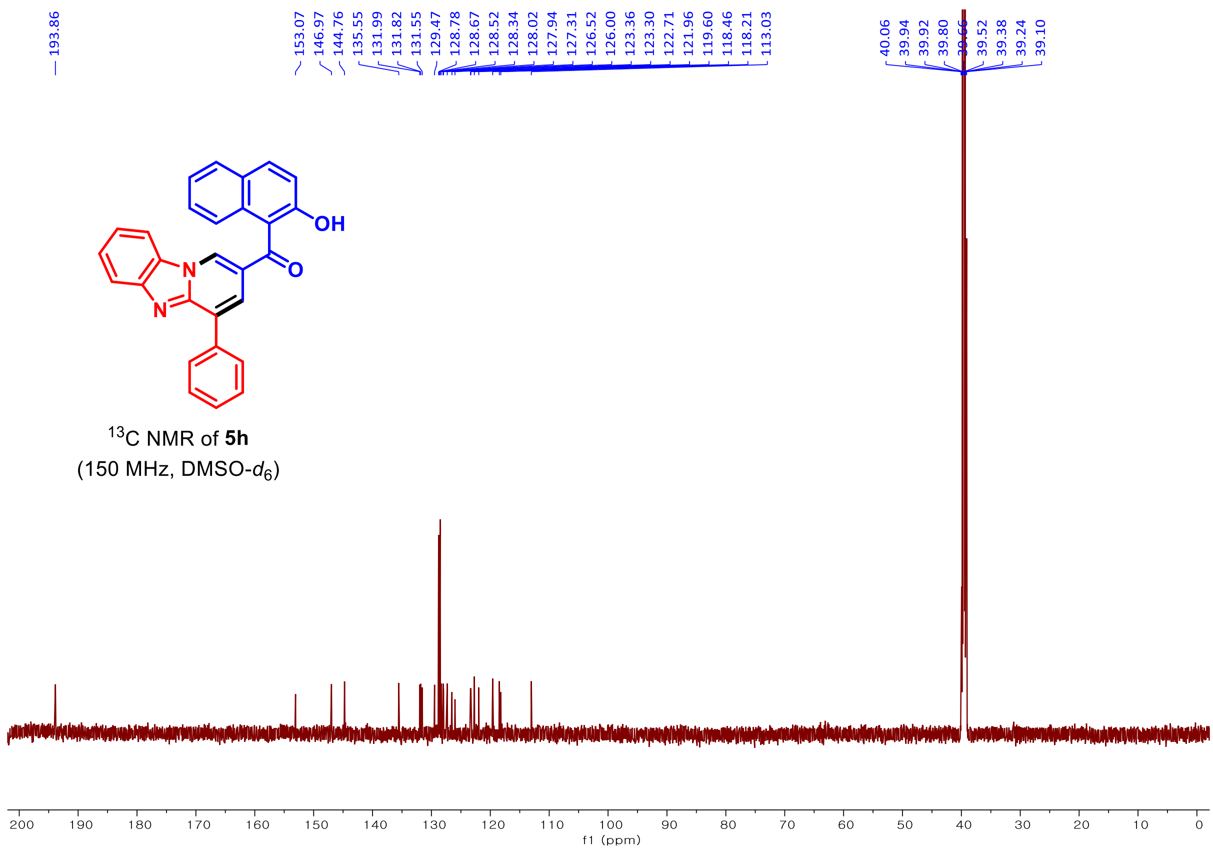
^{13}C NMR of **5f**
(150 MHz, DMSO-d_6)


13.555
8.948
8.521
8.508
8.102
8.088
8.065
8.052
7.994
7.981
7.924
7.774
7.761
7.682
7.670
7.655
7.610
7.598
7.584
7.570
7.557
7.533
7.520
7.507
7.469
7.456
7.445
7.433
7.421
7.275
7.260
7.240
OH
O
N
N
^{1}H NMR of **5g**
(600 MHz, $CDCl_3$)
1.00
1.01
1.01
0.97
2.33
1.06
1.00
1.01
2.11
2.17
2.20
2.24
1.00
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

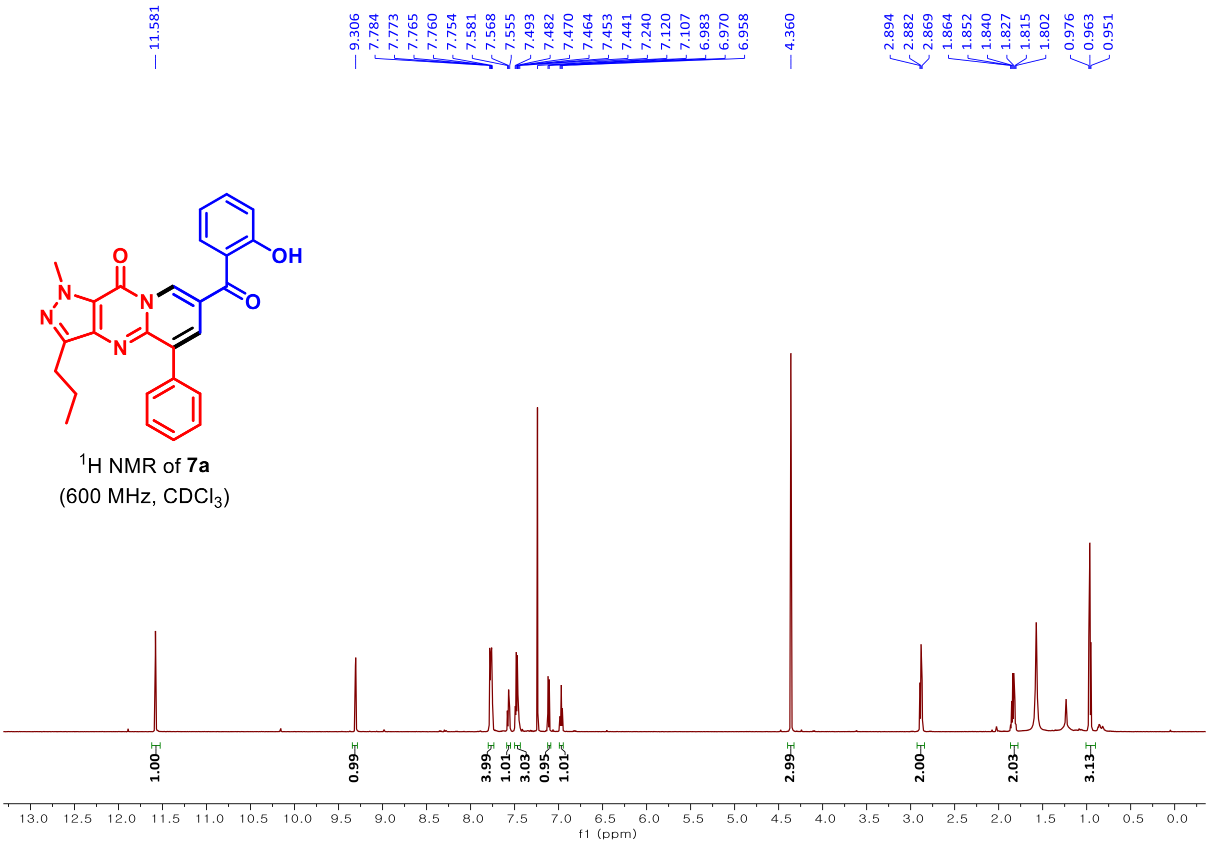

196.39
163.81
137.31
135.18
131.66
130.72
129.88
129.13
129.02
128.98
128.87
127.87
127.82
127.52
127.15
126.96
126.35
126.02
125.24
124.97
124.55
122.62
120.52
118.61
110.96
77.21
77.00
76.79
OH
O
N
N
^{1}H NMR of **5g**
(600 MHz, $CDCl_3$)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



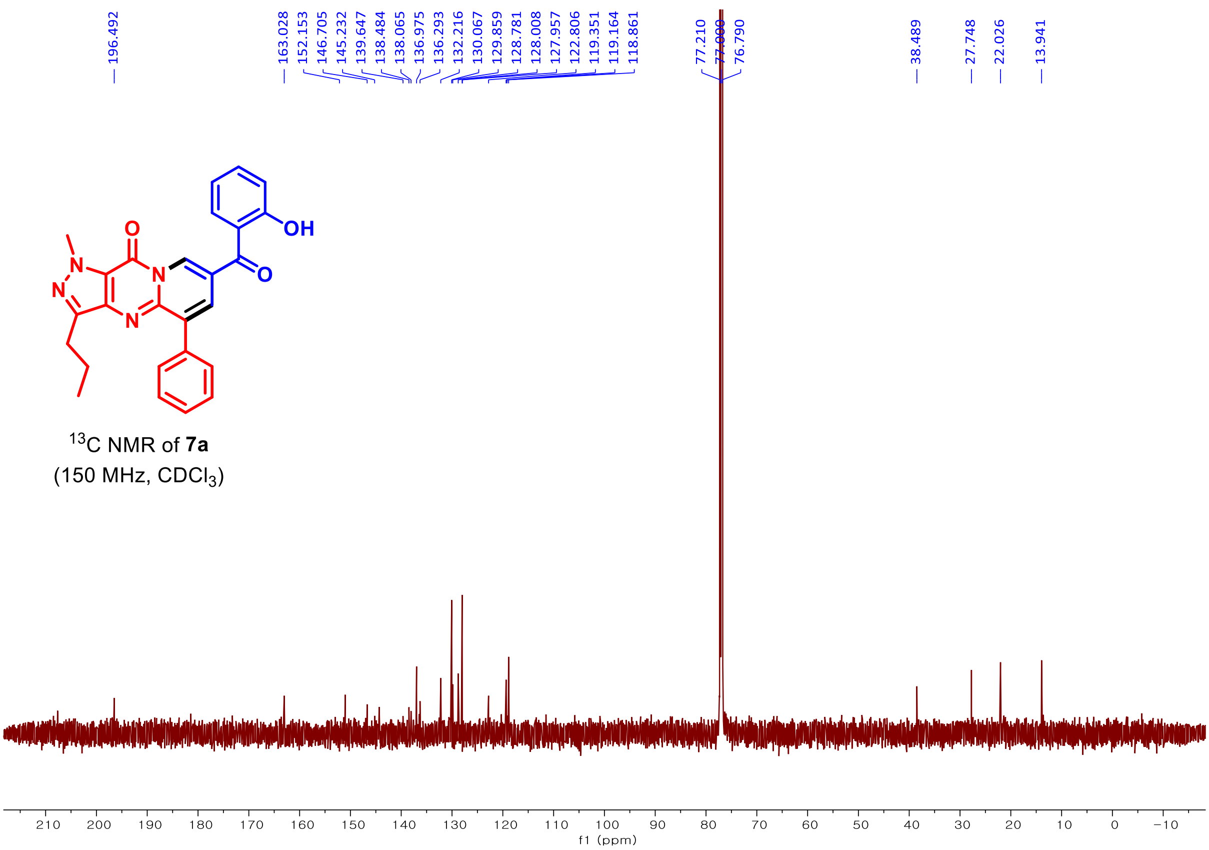
^{1}H NMR of **5h**
(600 MHz, DMSO-d_6)



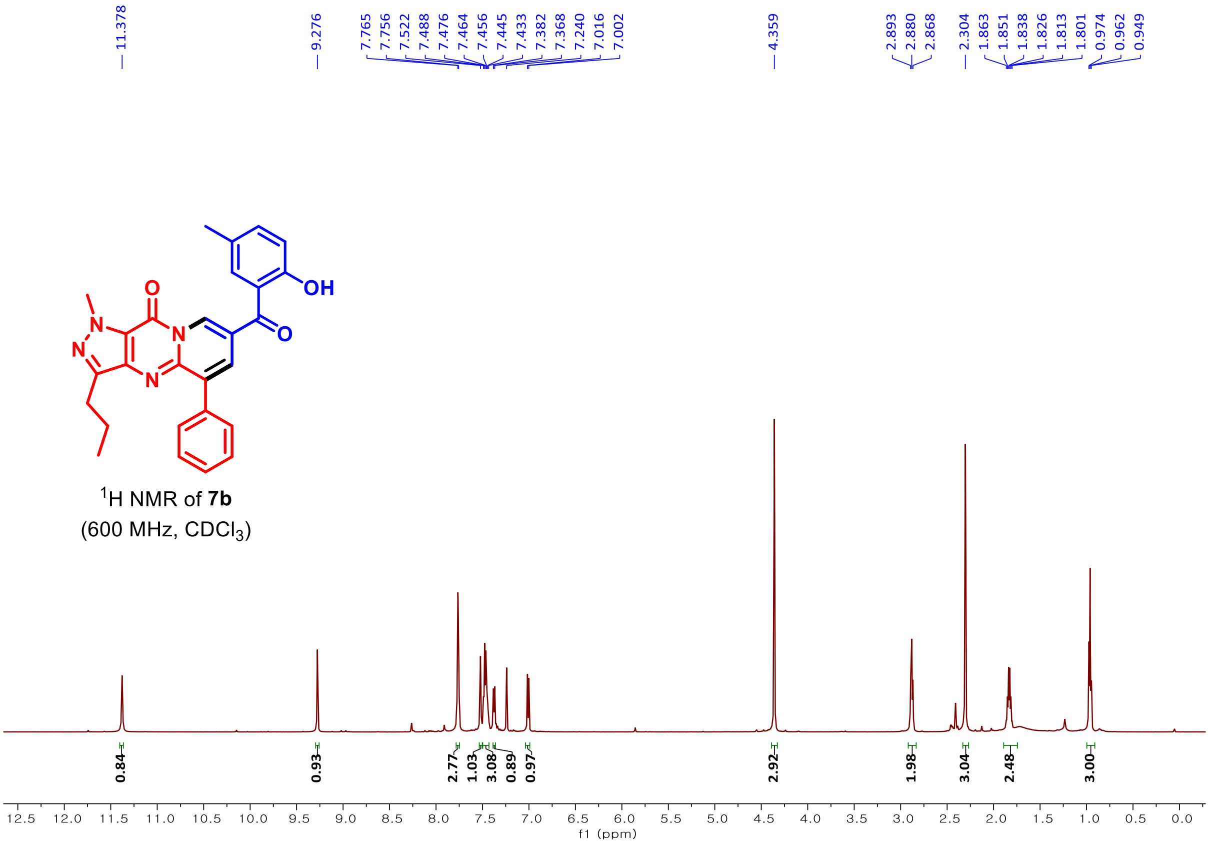
^{13}C NMR of **5h**
(150 MHz, DMSO-d_6)



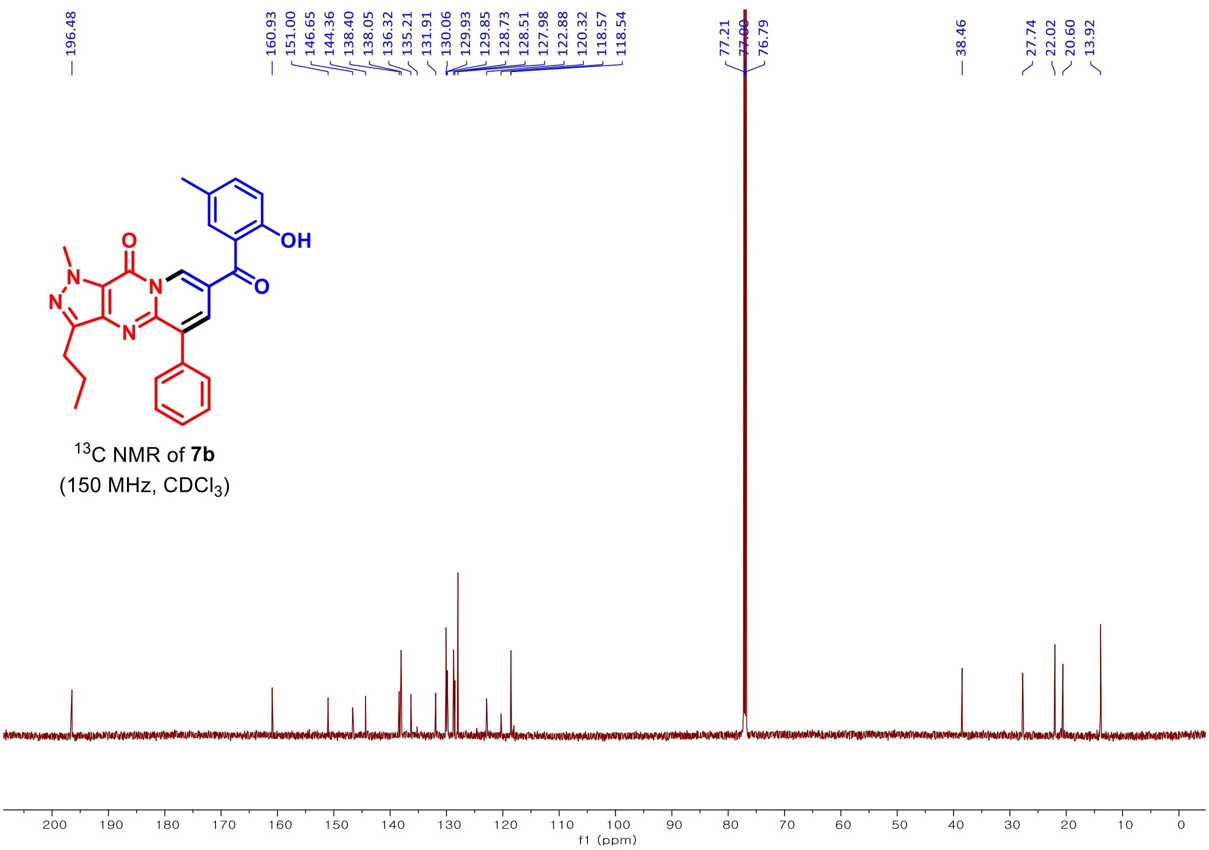
^1H NMR of **7a**
(600 MHz, $CDCl_3$)



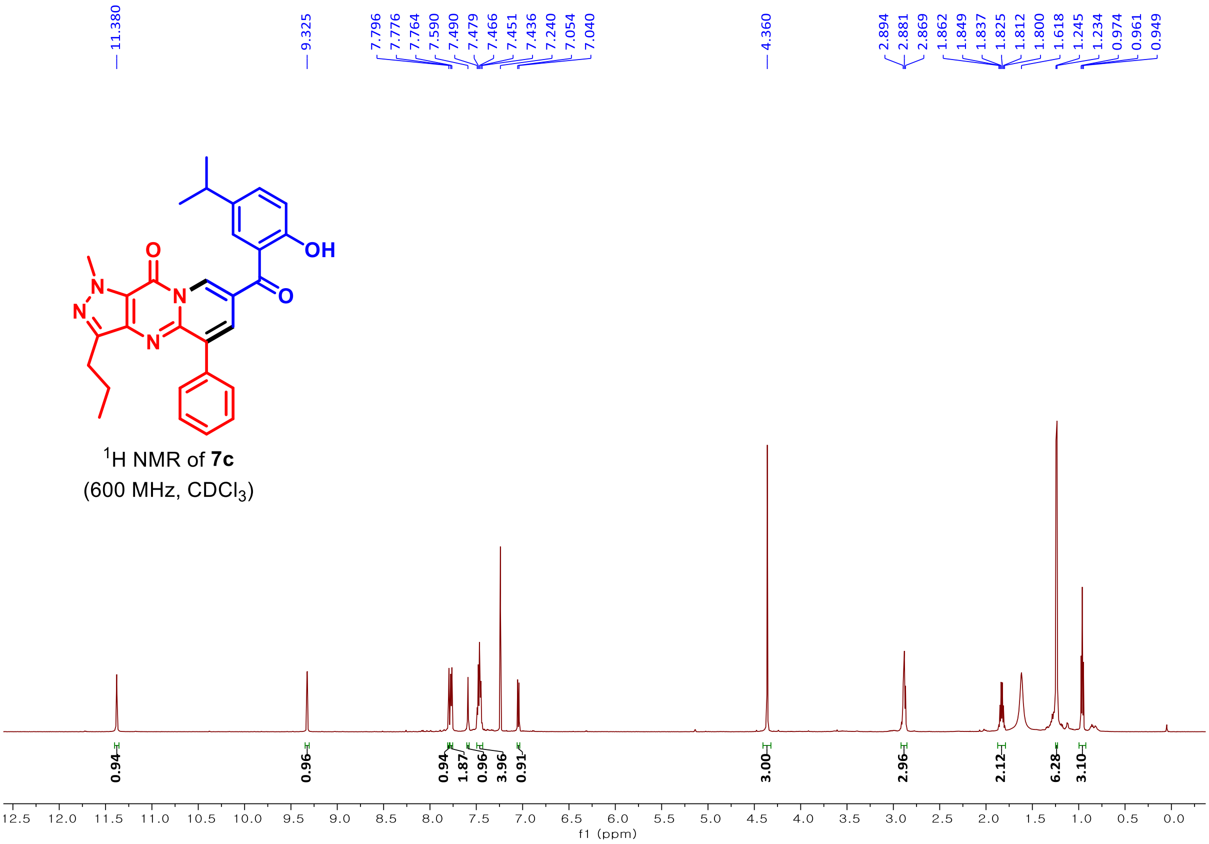
^{13}C NMR of **7a**
(150 MHz, $CDCl_3$)

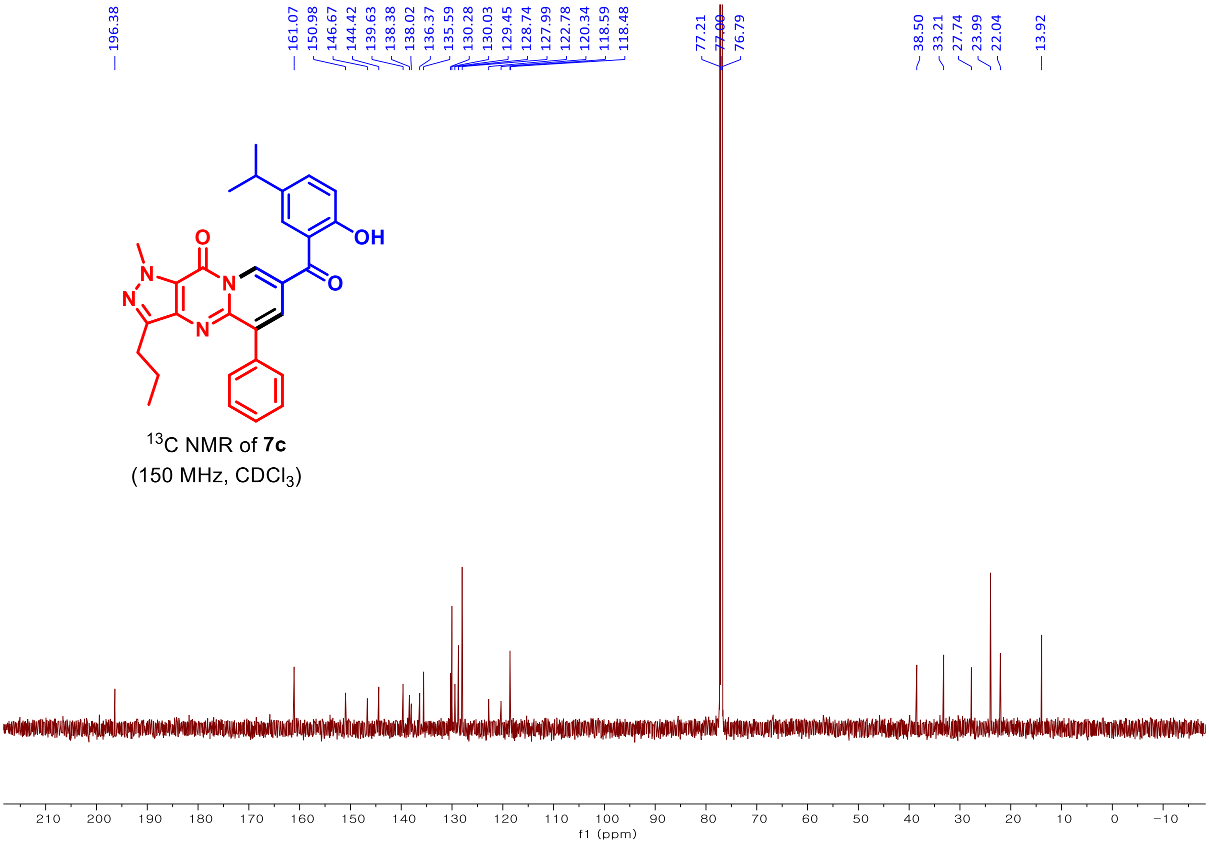


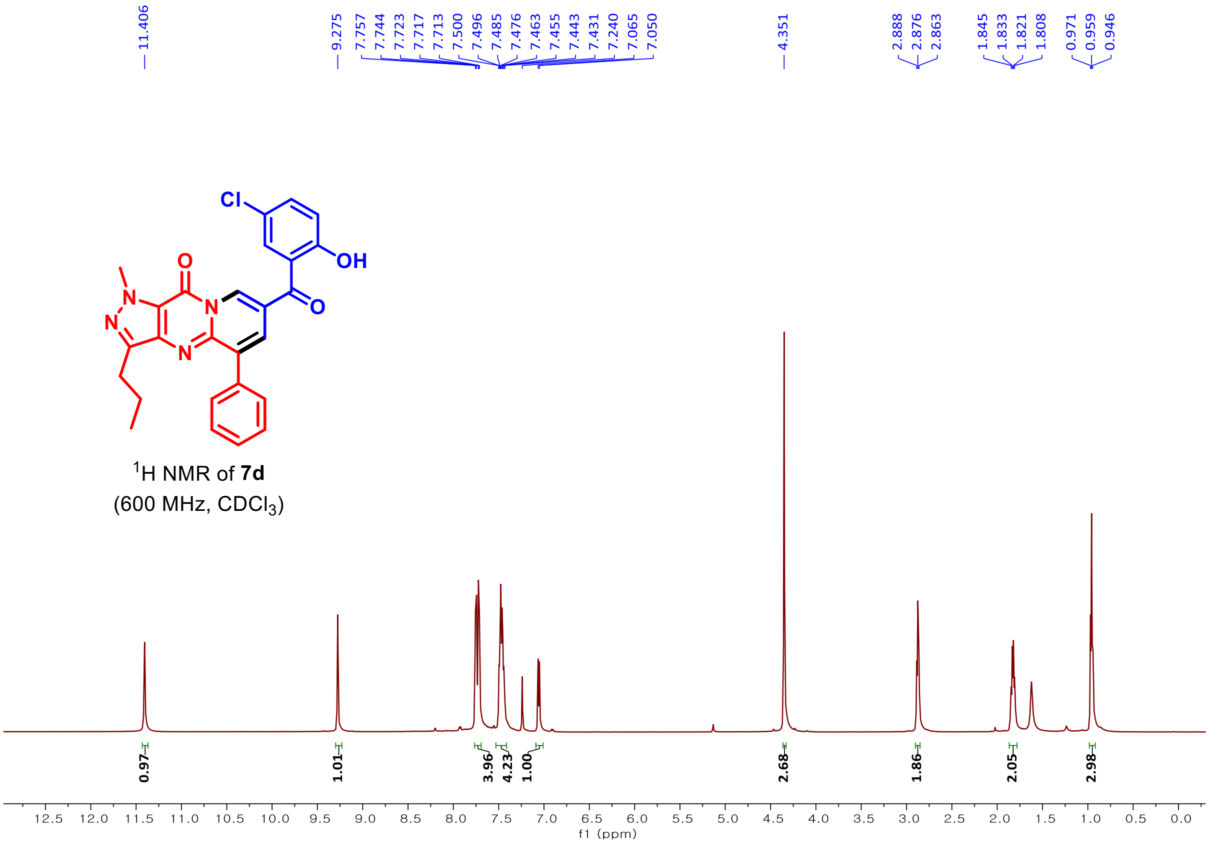
^{1}H NMR of **7b**
(600 MHz, $CDCl_3$)



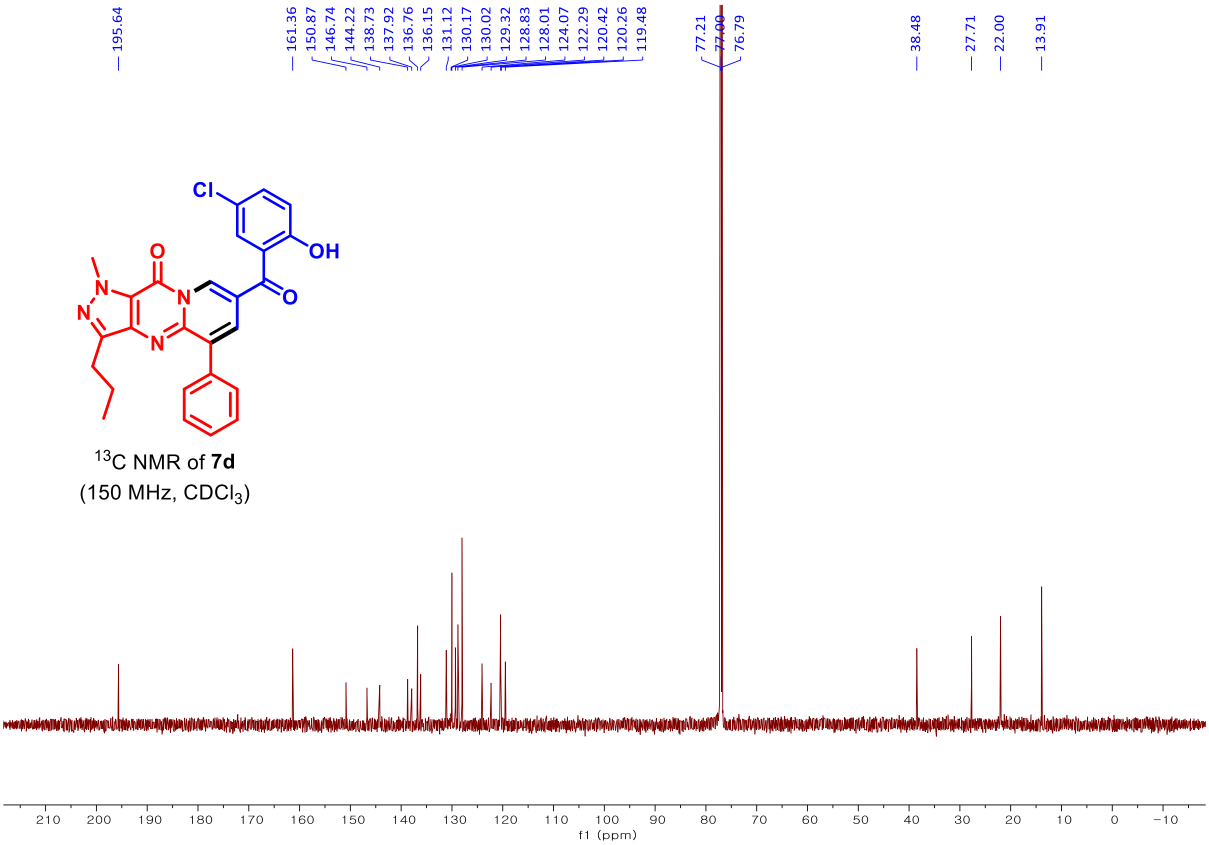
^{13}C NMR of **7b**
(150 MHz, $CDCl_3$)


11.380
9.325
7.796 7.776 7.764 7.590 7.490 7.479 7.466 7.451 7.436 7.240 7.054 7.040
4.360
2.894 2.881 2.869 1.862 1.849 1.837 1.825 1.812 1.800 1.618 1.245 1.234 0.974 0.961 0.949
OH
O
N
N
N
N
O
^{1}H NMR of **7c**
(600 MHz, $CDCl_3$)
0.94 0.96 0.94 1.87 0.96 3.96 0.91 3.00 2.96 2.12 6.28 3.10
f1 (ppm)

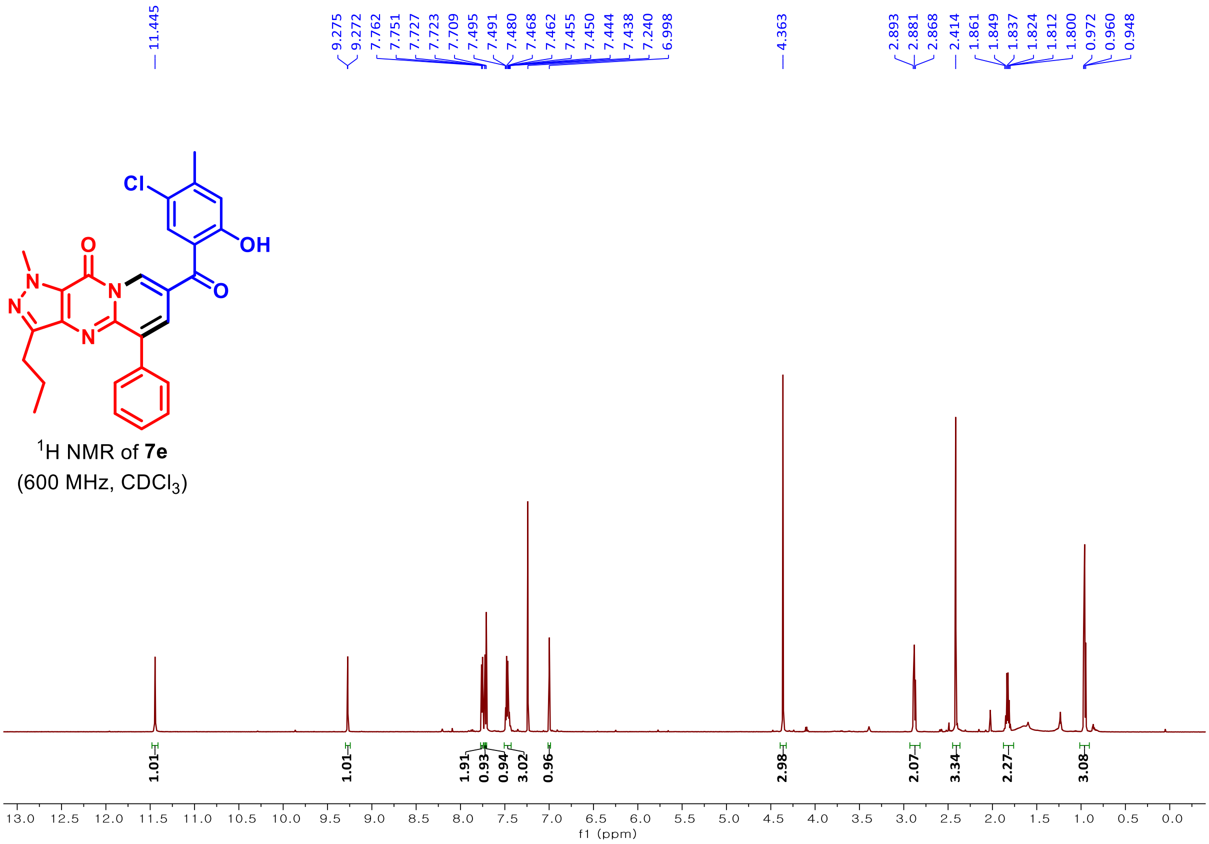

196.38
161.07 150.98 146.67 144.42 139.63 138.38 138.02 136.37 135.59 130.28 130.03 129.45 128.74 127.99 122.78 120.34 118.59 118.48
77.21 77.00 76.79
38.50 33.21 27.74 23.99 22.04
13.92
OH
O
N
N
N
N
O
^{13}C NMR of **7c**
(150 MHz, $CDCl_3$)
f1 (ppm)



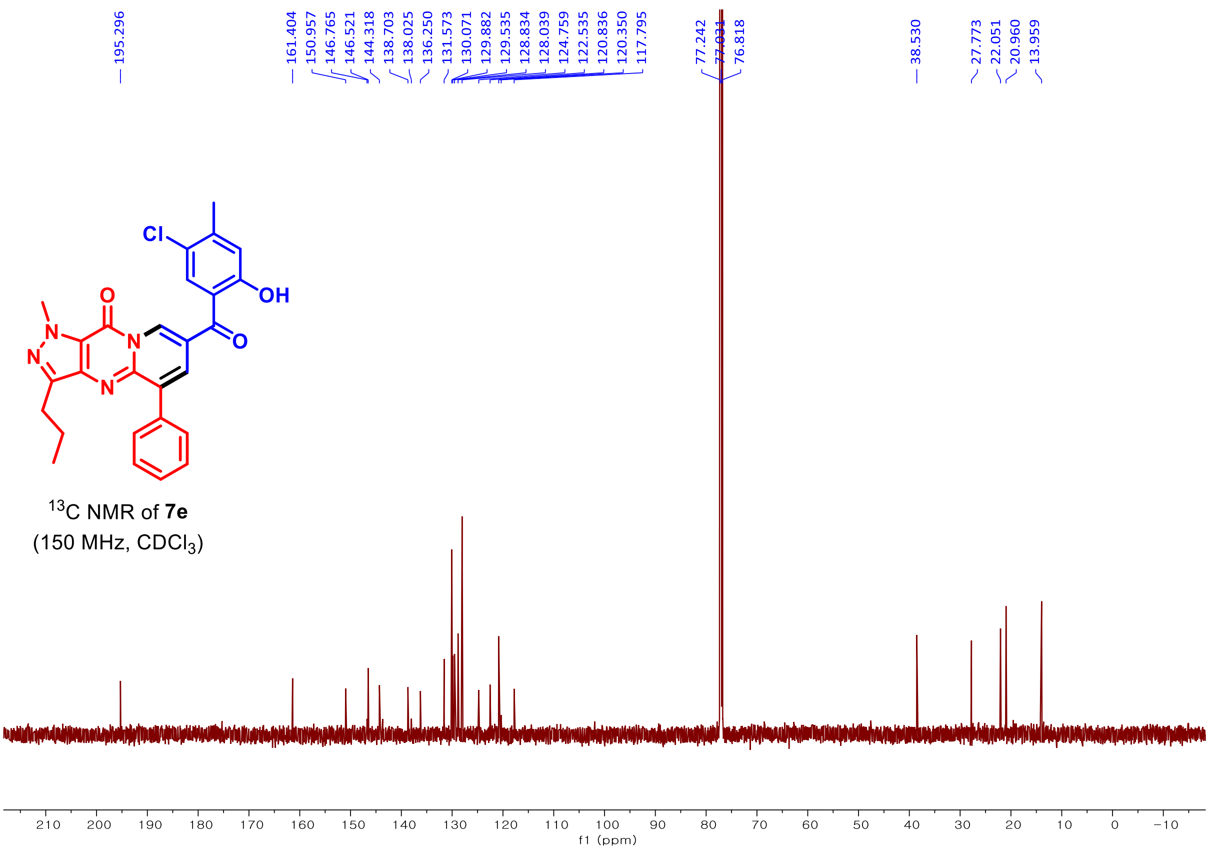
^{1}H NMR of **7d**
(600 MHz, $CDCl_3$)



^{13}C NMR of **7d**
(150 MHz, $CDCl_3$)



[1]H NMR of **7e**
(600 MHz, $CDCl_3$)



[13]C NMR of **7e**
(150 MHz, $CDCl_3$)

X-ray structure and data for compound 3f

Empirical Formula $C_{25}H_{16}FN_2O_3$, M = 410.39, Monoclinic, Space group *P-1*, a = 7.147(6) Å, b = 11.942(10) Å, *c* = 12.279(13) Å, *V* = 889.9(14) Å^3, *Z* = 2, T = 223(2) K, ρ_{calcd} = 1.532 Mg/m^3, $2\Theta_{max.}$ = 25.242°, Refinement of 281 parameters on 4538 independent reflections out of 21859 collected reflections (R_{int} = 0.1677) led to R1 = 0.0580 [I >2σ(I)], wR_2 = 0.1696 (all data) and S = 1.032 with the largest difference peak and hole of 0.313 and -0.188 e.Å^{-3} respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2142456). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

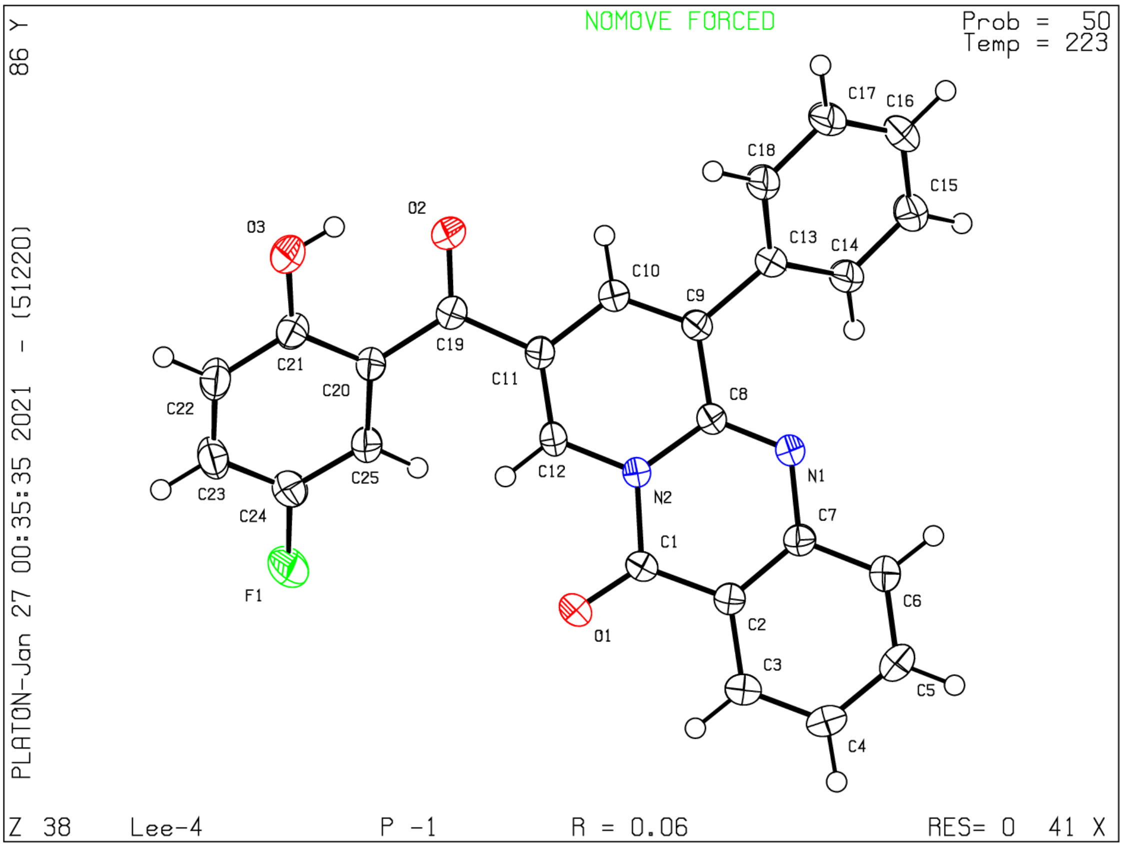


Figure S1. X-ray crystal structure of compound **3f**.

Table 1. Crystal data and structure refinement for **3f**.

Identification code	**3f**	
Empirical formula	C25 H15 F N2 O3	
Formula weight	410.39	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.147(6) Å	α= 61.56(3)°.
	b = 11.942(10) Å	β= 87.07(3)°.
	c = 12.279(13) Å	γ = 75.58(3)°.
Volume	889.8(14) Å^3	
Z	2	
Density (calculated)	1.532 Mg/m^3	
Absorption coefficient	0.109 mm^{-1}	
F(000)	424	
Crystal size	0.220 x 0.180 x 0.060 mm^3	
Theta range for data collection	1.892 to 28.754°.	
Index ranges	-9<=h<=9, -16<=k<=16, -16<=l<=16	
Reflections collected	21859	
Independent reflections	4538 [R(int) = 0.1677]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7453 and 0.5901	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4538 / 0 / 281	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0580, wR2 = 0.1509	
R indices (all data)	R1 = 0.0793, wR2 = 0.1696	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.268 and -0.378 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3f**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3306(2)	4280(1)	3399(1)	40(1)
C(1)	2897(2)	5033(2)	3829(1)	27(1)
C(2)	2477(2)	6438(2)	3145(1)	26(1)
C(3)	2444(3)	7049(2)	1846(2)	34(1)
C(4)	2034(3)	8386(2)	1188(2)	38(1)
C(5)	1720(3)	9127(2)	1815(2)	36(1)
C(6)	1770(3)	8543(2)	3086(2)	32(1)
C(7)	2115(2)	7170(2)	3779(1)	26(1)
N(1)	2023(2)	6626(1)	5048(1)	28(1)
C(8)	2292(2)	5362(2)	5692(1)	25(1)
C(9)	2127(2)	4730(2)	7027(1)	26(1)
C(10)	2392(2)	3413(2)	7652(1)	28(1)
C(11)	2917(2)	2609(2)	7059(1)	27(1)
C(12)	3132(2)	3189(2)	5831(2)	27(1)
N(2)	2767(2)	4534(1)	5146(1)	25(1)
C(13)	1696(2)	5501(2)	7713(1)	27(1)
C(14)	312(2)	6686(2)	7283(2)	32(1)
C(15)	-101(3)	7319(2)	7997(2)	36(1)
C(16)	846(3)	6788(2)	9147(2)	40(1)
C(17)	2229(3)	5617(2)	9581(2)	41(1)
C(18)	2660(3)	4981(2)	8871(2)	35(1)
C(19)	3372(2)	1160(2)	7850(2)	28(1)
O(2)	3640(2)	740(1)	8974(1)	40(1)
C(20)	3563(2)	250(2)	7339(1)	27(1)
C(21)	4670(2)	-1052(2)	8029(2)	31(1)
C(22)	4868(3)	-1928(2)	7556(2)	37(1)
C(23)	3962(3)	-1557(2)	6436(2)	39(1)
C(24)	2864(3)	-287(2)	5779(2)	35(1)
C(25)	2636(2)	602(2)	6201(2)	31(1)
O(3)	5611(2)	-1513(1)	9141(1)	42(1)
F(1)	1968(2)	85(1)	4670(1)	52(1)

Table 3. Bond lengths [Å] and angles [°] for **3f**.

O(1)-C(1)	1.216(2)
C(1)-C(2)	1.430(2)
C(1)-N(2)	1.439(2)
C(2)-C(7)	1.397(2)
C(2)-C(3)	1.401(3)
C(3)-C(4)	1.360(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.399(3)
C(4)-H(4)	0.9400
C(5)-C(6)	1.372(3)
C(5)-H(5)	0.9400
C(6)-C(7)	1.402(2)
C(6)-H(6)	0.9400
C(7)-N(1)	1.379(2)
N(1)-C(8)	1.294(2)
C(8)-N(2)	1.409(2)
C(8)-C(9)	1.455(3)
C(9)-C(10)	1.347(2)
C(9)-C(13)	1.491(2)
C(10)-C(11)	1.432(2)
C(10)-H(10)	0.9400
C(11)-C(12)	1.347(3)
C(11)-C(19)	1.481(2)
C(12)-N(2)	1.371(2)
C(12)-H(12)	0.9400
C(13)-C(14)	1.380(2)
C(13)-C(18)	1.389(3)
C(14)-C(15)	1.386(3)
C(14)-H(14)	0.9400
C(15)-C(16)	1.373(3)
C(15)-H(15)	0.9400

C(16)-C(17)	1.368(3)
C(16)-H(16)	0.9400
C(17)-C(18)	1.385(3)
C(17)-H(17)	0.9400
C(18)-H(18)	0.9400
C(19)-O(2)	1.229(2)
C(19)-C(20)	1.471(2)
C(20)-C(21)	1.401(2)
C(20)-C(25)	1.402(3)
C(21)-O(3)	1.346(2)
C(21)-C(22)	1.396(3)
C(22)-C(23)	1.369(3)
C(22)-H(22)	0.9400
C(23)-C(24)	1.368(3)
C(23)-H(23)	0.9400
C(24)-F(1)	1.354(2)
C(24)-C(25)	1.360(3)
C(25)-H(25)	0.9400
O(3)-H(3A)	0.8300
O(1)-C(1)-C(2)	126.32(16)
O(1)-C(1)-N(2)	120.31(15)
C(2)-C(1)-N(2)	113.37(14)
C(7)-C(2)-C(3)	121.54(16)
C(7)-C(2)-C(1)	119.62(15)
C(3)-C(2)-C(1)	118.84(15)
C(4)-C(3)-C(2)	119.18(16)
C(4)-C(3)-H(3)	120.4
C(2)-C(3)-H(3)	120.4
C(3)-C(4)-C(5)	119.78(17)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(6)-C(5)-C(4)	121.74(17)
C(6)-C(5)-H(5)	119.1
C(4)-C(5)-H(5)	119.1
C(5)-C(6)-C(7)	119.36(16)

C(5)-C(6)-H(6)	120.3
C(7)-C(6)-H(6)	120.3
N(1)-C(7)-C(2)	123.96(15)
N(1)-C(7)-C(6)	117.68(15)
C(2)-C(7)-C(6)	118.34(16)
C(8)-N(1)-C(7)	118.06(14)
N(1)-C(8)-N(2)	122.21(15)
N(1)-C(8)-C(9)	120.94(14)
N(2)-C(8)-C(9)	116.85(14)
C(10)-C(9)-C(8)	118.69(15)
C(10)-C(9)-C(13)	119.65(15)
C(8)-C(9)-C(13)	121.65(15)
C(9)-C(10)-C(11)	122.34(16)
C(9)-C(10)-H(10)	118.8
C(11)-C(10)-H(10)	118.8
C(12)-C(11)-C(10)	118.97(15)
C(12)-C(11)-C(19)	122.68(15)
C(10)-C(11)-C(19)	118.12(15)
C(11)-C(12)-N(2)	120.58(15)
C(11)-C(12)-H(12)	119.7
N(2)-C(12)-H(12)	119.7
C(12)-N(2)-C(8)	122.40(15)
C(12)-N(2)-C(1)	114.99(13)
C(8)-N(2)-C(1)	122.60(13)
C(14)-C(13)-C(18)	117.71(16)
C(14)-C(13)-C(9)	123.28(15)
C(18)-C(13)-C(9)	118.94(15)
C(13)-C(14)-C(15)	120.55(16)
C(13)-C(14)-H(14)	119.7
C(15)-C(14)-H(14)	119.7
C(16)-C(15)-C(14)	121.24(17)
C(16)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
C(17)-C(16)-C(15)	118.77(17)
C(17)-C(16)-H(16)	120.6
C(15)-C(16)-H(16)	120.6

C(16)-C(17)-C(18)	120.43(17)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-C(13)	121.29(17)
C(17)-C(18)-H(18)	119.4
C(13)-C(18)-H(18)	119.4
O(2)-C(19)-C(20)	120.72(15)
O(2)-C(19)-C(11)	116.45(15)
C(20)-C(19)-C(11)	122.80(15)
C(21)-C(20)-C(25)	117.39(16)
C(21)-C(20)-C(19)	119.22(16)
C(25)-C(20)-C(19)	123.35(15)
O(3)-C(21)-C(22)	117.04(16)
O(3)-C(21)-C(20)	123.00(16)
C(22)-C(21)-C(20)	119.95(17)
C(23)-C(22)-C(21)	121.53(17)
C(23)-C(22)-H(22)	119.2
C(21)-C(22)-H(22)	119.2
C(24)-C(23)-C(22)	117.88(17)
C(24)-C(23)-H(23)	121.1
C(22)-C(23)-H(23)	121.1
F(1)-C(24)-C(25)	119.26(16)
F(1)-C(24)-C(23)	118.09(16)
C(25)-C(24)-C(23)	122.64(18)
C(24)-C(25)-C(20)	120.58(16)
C(24)-C(25)-H(25)	119.7
C(20)-C(25)-H(25)	119.7
C(21)-O(3)-H(3A)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for **3f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$[h^2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	65(1)	29(1)	28(1)	-18(1)	5(1)	-8(1)
C(1)	34(1)	26(1)	23(1)	-14(1)	2(1)	-7(1)
C(2)	30(1)	24(1)	24(1)	-11(1)	1(1)	-6(1)
C(3)	45(1)	32(1)	24(1)	-14(1)	3(1)	-9(1)
C(4)	51(1)	35(1)	22(1)	-8(1)	3(1)	-11(1)
C(5)	44(1)	25(1)	30(1)	-6(1)	2(1)	-9(1)
C(6)	41(1)	24(1)	31(1)	-14(1)	4(1)	-10(1)
C(7)	28(1)	25(1)	24(1)	-11(1)	1(1)	-6(1)
N(1)	40(1)	22(1)	24(1)	-12(1)	2(1)	-7(1)
C(8)	30(1)	23(1)	24(1)	-12(1)	1(1)	-6(1)
C(9)	31(1)	24(1)	23(1)	-13(1)	0(1)	-4(1)
C(10)	36(1)	24(1)	24(1)	-12(1)	2(1)	-7(1)
C(11)	33(1)	21(1)	26(1)	-11(1)	-1(1)	-5(1)
C(12)	33(1)	20(1)	29(1)	-14(1)	1(1)	-5(1)
N(2)	33(1)	19(1)	22(1)	-10(1)	2(1)	-5(1)
C(13)	34(1)	25(1)	23(1)	-13(1)	3(1)	-7(1)
C(14)	38(1)	29(1)	26(1)	-14(1)	-2(1)	-3(1)
C(15)	42(1)	31(1)	35(1)	-18(1)	2(1)	-2(1)
C(16)	56(1)	37(1)	35(1)	-25(1)	3(1)	-8(1)
C(17)	58(1)	36(1)	28(1)	-18(1)	-8(1)	-3(1)
C(18)	47(1)	27(1)	29(1)	-14(1)	-6(1)	-2(1)
C(19)	35(1)	22(1)	26(1)	-10(1)	1(1)	-7(1)
O(2)	65(1)	26(1)	24(1)	-9(1)	-4(1)	-7(1)
C(20)	34(1)	22(1)	27(1)	-12(1)	4(1)	-8(1)
C(21)	36(1)	24(1)	30(1)	-10(1)	3(1)	-7(1)
C(22)	44(1)	23(1)	42(1)	-15(1)	6(1)	-6(1)
C(23)	50(1)	30(1)	45(1)	-24(1)	11(1)	-13(1)
C(24)	45(1)	33(1)	33(1)	-19(1)	3(1)	-14(1)
C(25)	38(1)	24(1)	31(1)	-14(1)	0(1)	-8(1)
O(3)	57(1)	26(1)	32(1)	-10(1)	-7(1)	1(1)
F(1)	76(1)	45(1)	42(1)	-27(1)	-11(1)	-13(1)

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

	x	y	z	U(eq)
H(3)	2701	6541	1435	41
H(4)	1963	8811	315	46
H(5)	1467	10049	1352	43
H(6)	1576	9059	3489	38
H(10)	2226	3008	8508	33
H(12)	3537	2668	5439	32
H(14)	-356	7068	6498	38
H(15)	-1046	8126	7688	43
H(16)	549	7221	9627	48
H(17)	2891	5242	10366	49
H(18)	3625	4183	9179	42
H(22)	5641	-2793	8018	45
H(23)	4091	-2155	6127	46
H(25)	1849	1459	5725	37
H(3A)	5248	-969	9395	63

Table 6. Torsion angles [°] for **3f**.

O(1)-C(1)-C(2)-C(7)	-177.14(16)
N(2)-C(1)-C(2)-C(7)	3.8(2)
O(1)-C(1)-C(2)-C(3)	2.7(3)
N(2)-C(1)-C(2)-C(3)	-176.30(14)
C(7)-C(2)-C(3)-C(4)	-0.5(3)
C(1)-C(2)-C(3)-C(4)	179.61(16)
C(2)-C(3)-C(4)-C(5)	2.2(3)
C(3)-C(4)-C(5)-C(6)	-1.4(3)
C(4)-C(5)-C(6)-C(7)	-1.1(3)
C(3)-C(2)-C(7)-N(1)	176.25(15)
C(1)-C(2)-C(7)-N(1)	-3.9(2)
C(3)-C(2)-C(7)-C(6)	-1.9(2)
C(1)-C(2)-C(7)-C(6)	177.94(14)
C(5)-C(6)-C(7)-N(1)	-175.63(15)
C(5)-C(6)-C(7)-C(2)	2.7(2)
C(2)-C(7)-N(1)-C(8)	0.1(2)
C(6)-C(7)-N(1)-C(8)	178.35(14)
C(7)-N(1)-C(8)-N(2)	3.3(2)
C(7)-N(1)-C(8)-C(9)	-177.14(14)
N(1)-C(8)-C(9)-C(10)	179.02(15)
N(2)-C(8)-C(9)-C(10)	-1.4(2)
N(1)-C(8)-C(9)-C(13)	-1.7(2)
N(2)-C(8)-C(9)-C(13)	177.96(14)
C(8)-C(9)-C(10)-C(11)	2.9(2)
C(13)-C(9)-C(10)-C(11)	-176.39(14)
C(9)-C(10)-C(11)-C(12)	-0.8(2)
C(9)-C(10)-C(11)-C(19)	173.78(15)
C(10)-C(11)-C(12)-N(2)	-3.0(2)
C(19)-C(11)-C(12)-N(2)	-177.34(14)
C(11)-C(12)-N(2)-C(8)	4.7(2)
C(11)-C(12)-N(2)-C(1)	-175.11(14)
N(1)-C(8)-N(2)-C(12)	177.22(14)
C(9)-C(8)-N(2)-C(12)	-2.4(2)
N(1)-C(8)-N(2)-C(1)	-3.0(2)

C(9)-C(8)-N(2)-C(1)	177.36(13)
O(1)-C(1)-N(2)-C(12)	0.0(2)
C(2)-C(1)-N(2)-C(12)	179.09(13)
O(1)-C(1)-N(2)-C(8)	-179.80(15)
C(2)-C(1)-N(2)-C(8)	-0.7(2)
C(10)-C(9)-C(13)-C(14)	-137.19(18)
C(8)-C(9)-C(13)-C(14)	43.5(2)
C(10)-C(9)-C(13)-C(18)	39.7(2)
C(8)-C(9)-C(13)-C(18)	-139.64(17)
C(18)-C(13)-C(14)-C(15)	-0.7(3)
C(9)-C(13)-C(14)-C(15)	176.24(16)
C(13)-C(14)-C(15)-C(16)	-0.1(3)
C(14)-C(15)-C(16)-C(17)	0.5(3)
C(15)-C(16)-C(17)-C(18)	-0.1(3)
C(16)-C(17)-C(18)-C(13)	-0.7(3)
C(14)-C(13)-C(18)-C(17)	1.1(3)
C(9)-C(13)-C(18)-C(17)	-175.96(17)
C(12)-C(11)-C(19)-O(2)	160.47(17)
C(10)-C(11)-C(19)-O(2)	-13.9(2)
C(12)-C(11)-C(19)-C(20)	-17.6(3)
C(10)-C(11)-C(19)-C(20)	168.00(15)
O(2)-C(19)-C(20)-C(21)	-22.0(2)
C(11)-C(19)-C(20)-C(21)	156.03(16)
O(2)-C(19)-C(20)-C(25)	155.81(17)
C(11)-C(19)-C(20)-C(25)	-26.2(3)
C(25)-C(20)-C(21)-O(3)	-179.22(16)
C(19)-C(20)-C(21)-O(3)	-1.3(3)
C(25)-C(20)-C(21)-C(22)	2.1(2)
C(19)-C(20)-C(21)-C(22)	-179.92(15)
O(3)-C(21)-C(22)-C(23)	179.68(17)
C(20)-C(21)-C(22)-C(23)	-1.6(3)
C(21)-C(22)-C(23)-C(24)	0.7(3)
C(22)-C(23)-C(24)-F(1)	179.91(16)
C(22)-C(23)-C(24)-C(25)	-0.5(3)
F(1)-C(24)-C(25)-C(20)	-179.27(16)
C(23)-C(24)-C(25)-C(20)	1.1(3)

C(21)-C(20)-C(25)-C(24)	-1.9(3)
C(19)-C(20)-C(25)-C(24)	-179.76(16)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **3f** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3A)...O(2)#1	0.83	2.35	2.985(3)	134.1
O(3)-H(3A)...O(2)	0.83	1.91	2.623(3)	143.7

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+2

Procedure for optical properties

UV–Vis and photoluminescence spectra were recorded using a UV 3220 spectrometer (Optizen) and spectrofluorometer (HITACHI) F-2700 equipped with a Xe arc lamp, respectively. A stock solution of **3a**, **3f**, **3j**, **3k**, and **7a** compounds (1 μM) was prepared in ethanol:water (8:2). Stock solutions of various cations (100 μM; Ag^{+}, Al^{3+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Ce^{3+}, Co^{2+}, Cr^{3+}, Cu^{2+}, Fe^{3+}, Hg^{2+}, Ir^{3+}, Mg^{2+}, Mn^{2+}, Na^{+}, Ni^{2+}, Pb^{2+}, Sn^{2+}, Sr^{2+}, and Zn^{2+}) and common anions (100 μM; Br^{-}, Cl^{-}, CO_3^{2-}, I^{-}, NO_3^{2-}, PO_4^{3-}, SO_4^{2-}, and S^{2-}) were prepared in deionized water. Before the spectroscopic measurements, test solutions were prepared in 1990 μL of ethanol:water mixed with 5 μL stock solutions of **3a** (1 μM) and 5 μL of each metal ions (100 μM) stock into cuvettes with the final volume of 2.0 mL, respectively. Fe^{3+} and Ag^{+} metal ions (0 – 100 μM) were detected by adding a different aliquot of stock solution with **3a** (1 μM). For Fe^{3+} and Ag^{+} competitive experimental procedures, above conditions were followed. 5 μL of cations or anions solution (100 μM) with 5 μL of **3a** (1 μM) was taken and added into in 1990 μL of ethanol:water (8:2) solution. For PL interference studies, 5 μL of the cations and anions solutions (100 μM) were individually added to the above solution. All UV–Vis spectra were recorded at room temperature after the addition of samples for a few seconds. All the photoluminescence measurements were carried out after 2 min of incubation at 366 nm (λ_{ex}) emission wavelength range from 380 – 700 nm with 5 nm of slit width, 250 V of photomultiplier tube voltage, and a scan speed of 240 nm/min.

Calculation of the photoluminescence quantum yield

The solution was diluted to keep the absorption intensity below 0.1 and the excitation wavelength set to 366 nm. After that, solutions for absorption and emission measurements were carried out in a 1 × 1 cm quartz cuvette. Quantum yield (QY) was measured using a fluorescence spectrophotometer F-7000 (Hitachi). Photoluminescence QY can be calculated using the following equation:

$$QY = \frac{\int L_{emission}}{\int E_{solvent} - \int E_{sample}}$$

Here, QY was the quantum yield and $L_{emission}$ was the photoluminescence emission spectrum of the sample. E_{sample} was the spectrum of light used to excite the sample and $E_{solvent}$ was the spectrum of light used to excite only the solvent of the sphere, collected using a sphere.

Interference effect

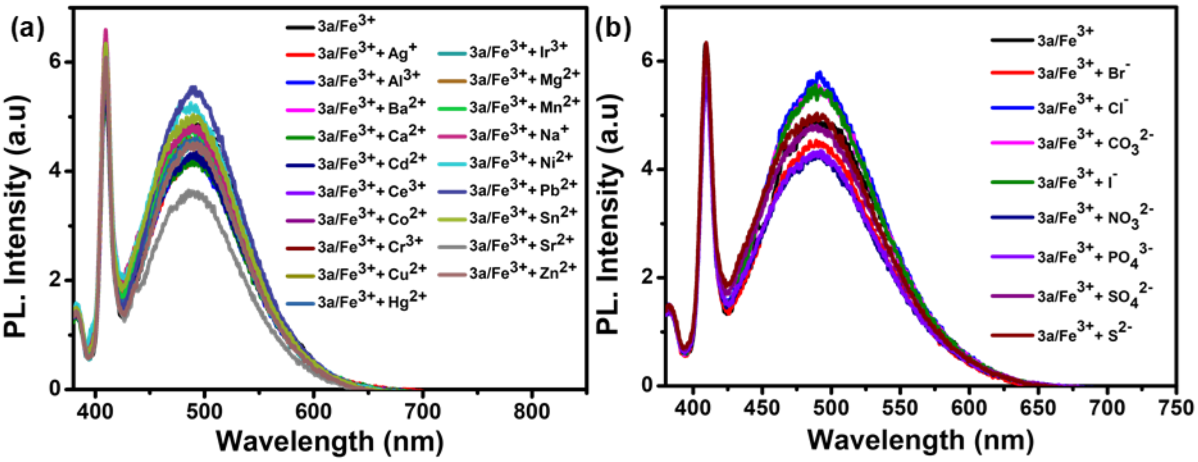


Figure S2. PL spectra of **3a**/Fe^{3+} (**3a**; 1 µM and Fe^{3+};100 µM) with the addition of (a) various cations (Ag^{+}, Al^{3+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Ce^{3+}, Co^{2+}, Cr^{3+}, Cu^{2+}, Hg^{2+}, Ir^{3+}, Mg^{2+}, Mn^{2+}, Na^{+}, Ni^{2+}, Pb^{2+}, Sn^{2+}, Sr^{2+}, and Zn^{2+}; 100 µM) and (b) various anions (Br^{-}, Cl^{-}, CO_3^{2-}, I^{-}, NO_3^{2-}, PO_4^{3-}, SO_4^{2-}, and S^{2-}; 100 µM) in ethanol:water (8:2) solution (λ_{ex} = 366 nm; λ_{em} = 490 nm).

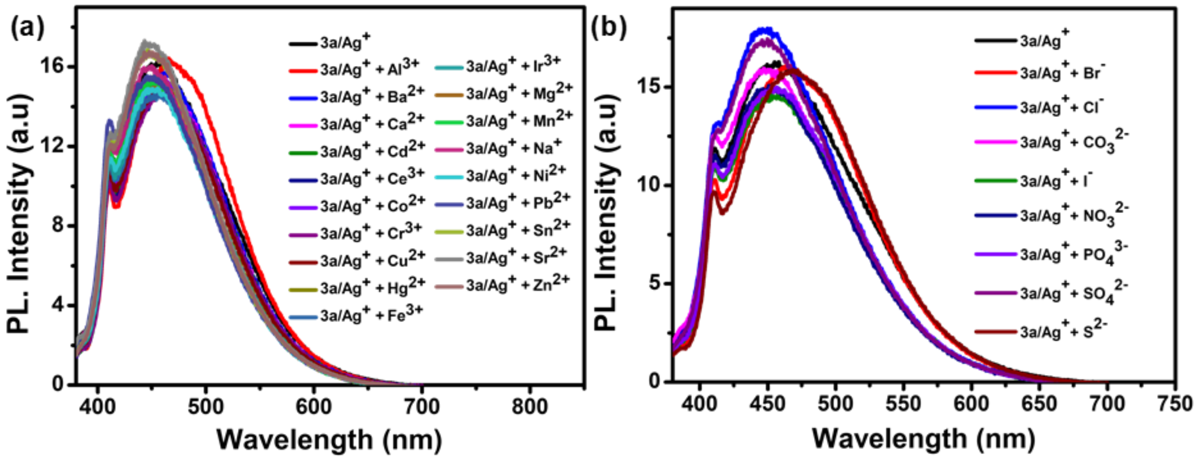


Figure S3. PL spectra of **3a**/Ag^+ (**3a**;1 μM and Ag^+;100 μM) with the addition of (a) various cations (Al^{3+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Ce^{3+}, Co^{2+}, Cr^{3+}, Cu^{2+}, Hg^{2+}, Fe^{3+}, Ir^{3+}, Mg^{2+}, Mn^{2+}, Na^+, Ni^{2+}, Pb^{2+}, Sn^{2+}, Sr^{2+}, and Zn^{2+}; 100 μM) and (b) various anions ($Br^–$, $Cl^–$, $CO_3^{2–}$, $I^–$, $NO_3^{2–}$, $PO_4^{3–}$, SO_4^{2-}, and S^{2-}; 100 μM) in ethanol:water (8:2) solution (λ_{ex} = 366 nm; λ_{em} = 490 nm).