Electronic Supplementary Information

Regioselective Double Dehydrative Cyclization Route to Polyheterocyclic Skeletons Consisting of 2,3-Dihydroquinazolin-4(1*H*)-ones and 1,2-Dihydropyrrolo[1,2-*a*]pyrazines

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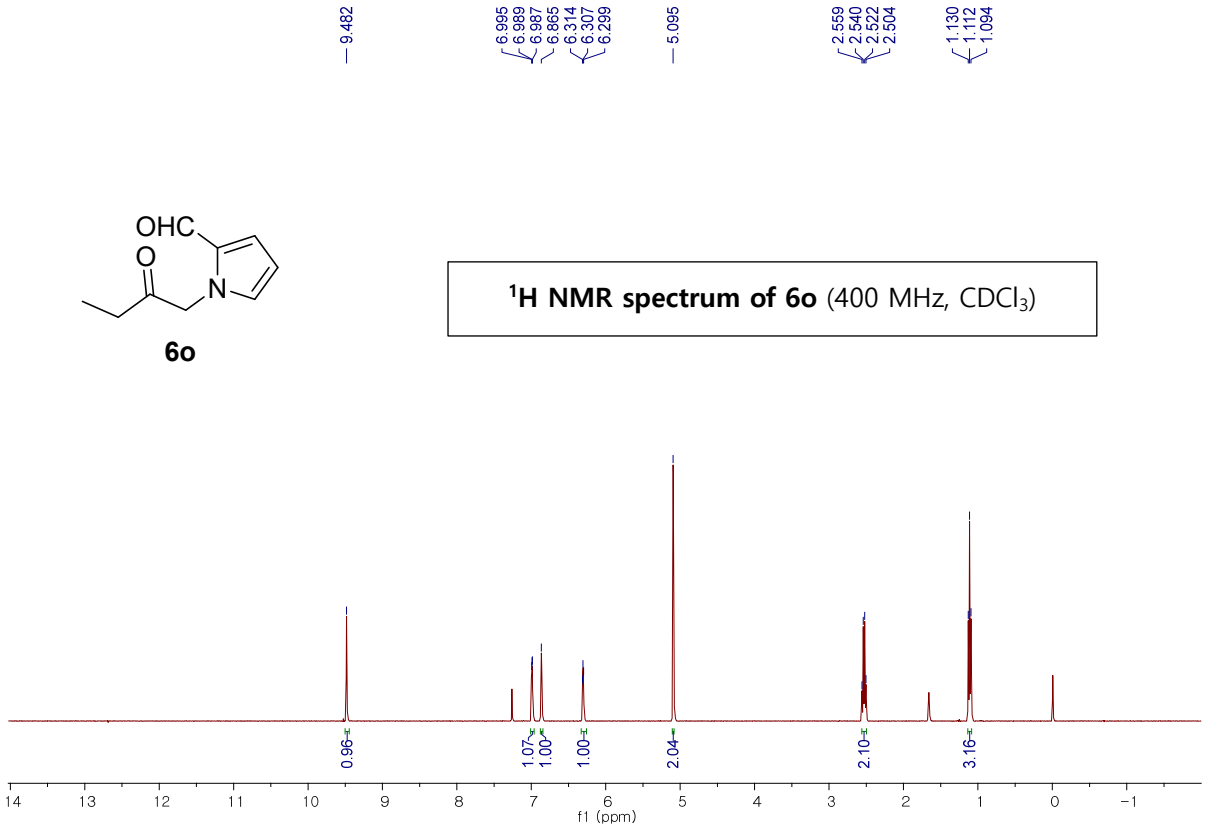
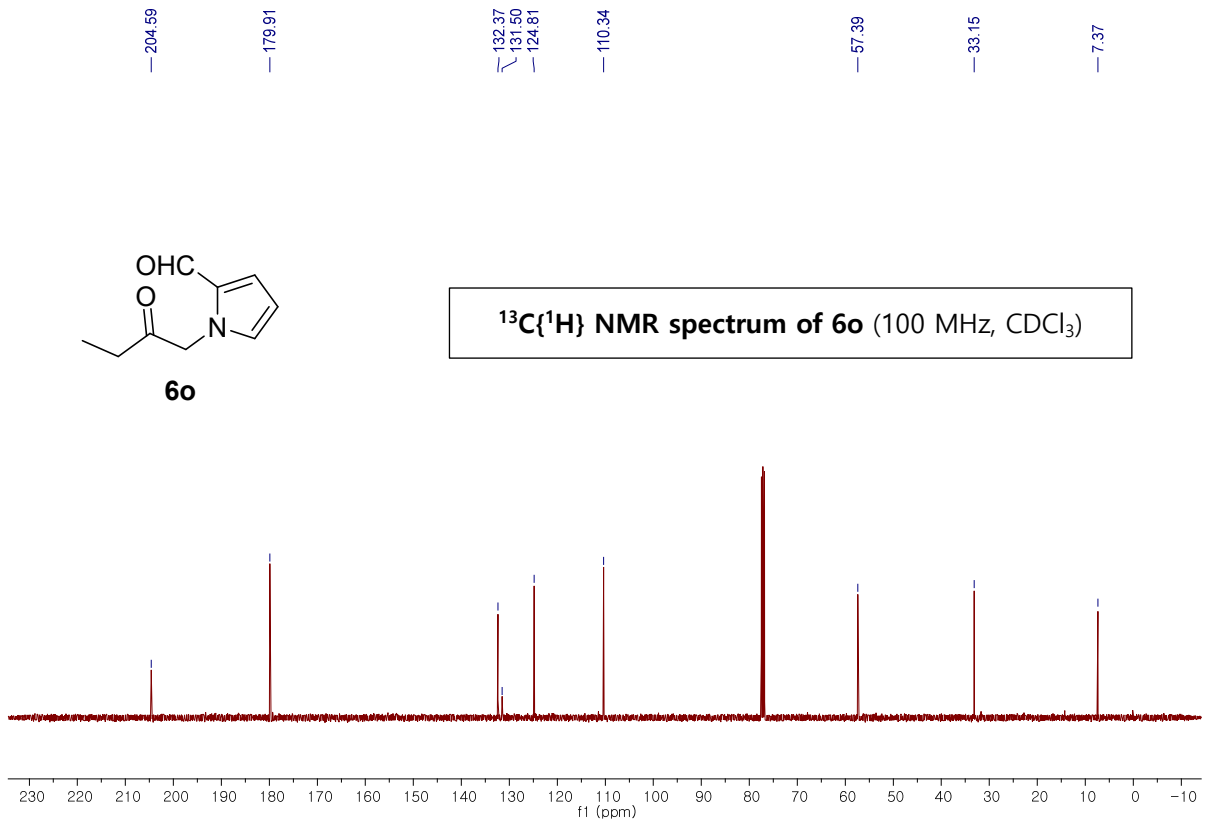
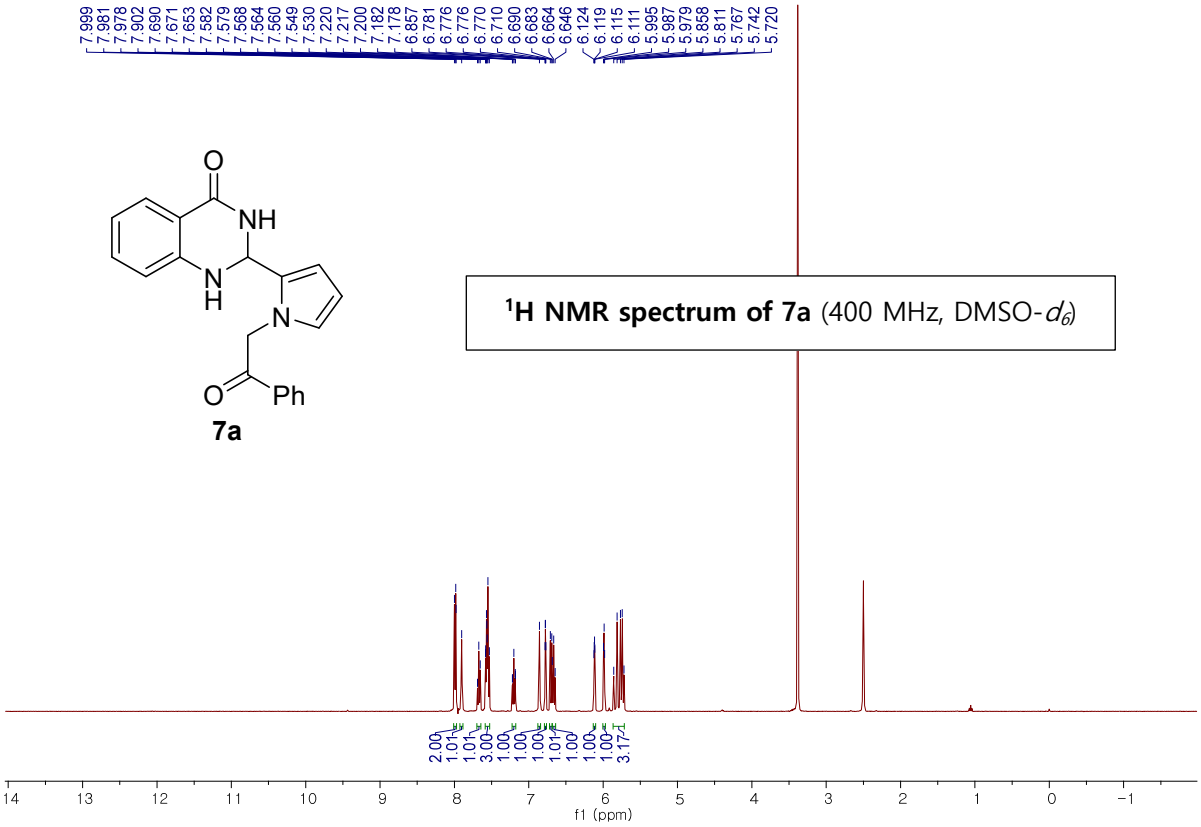


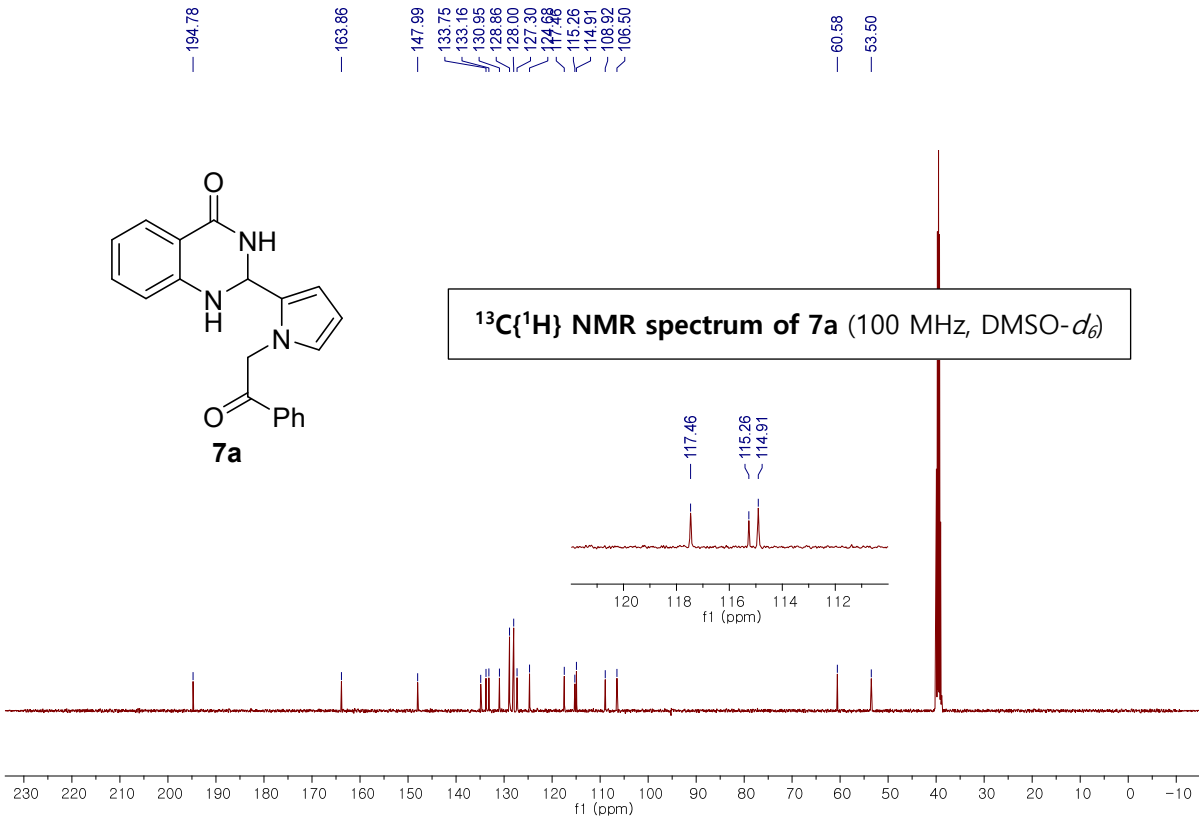
^{1}H NMR spectrum of 6o (400 MHz, $CDCl_3$)



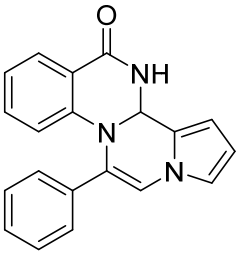
^{13}C{^{1}H} NMR spectrum of 6o (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of 7a (400 MHz, DMSO-d_6)

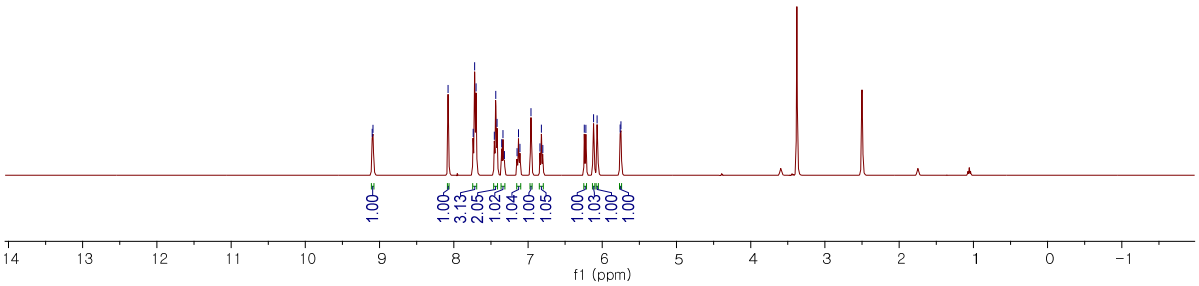


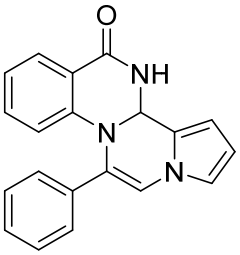
^{13}C{^{1}H} NMR spectrum of 7a (100 MHz, DMSO-d_6)



8a

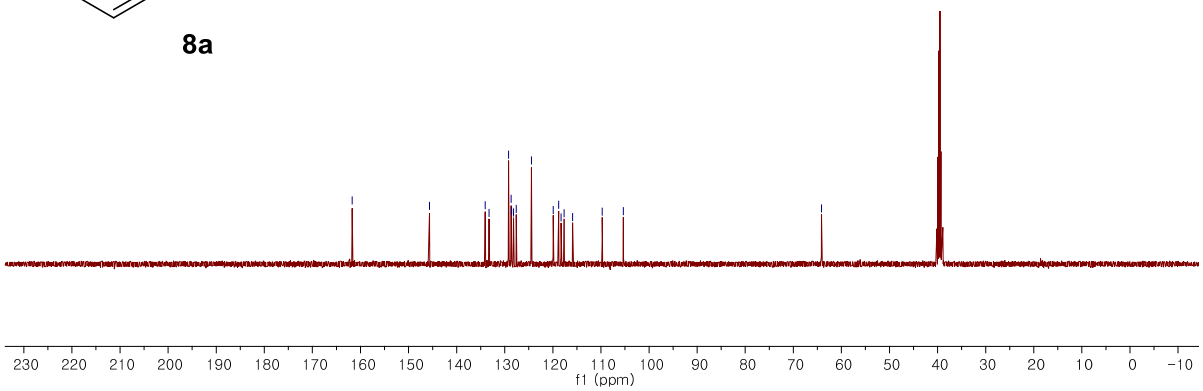
^{1}H NMR spectrum of 8a (400 MHz, DMSO-d_6)

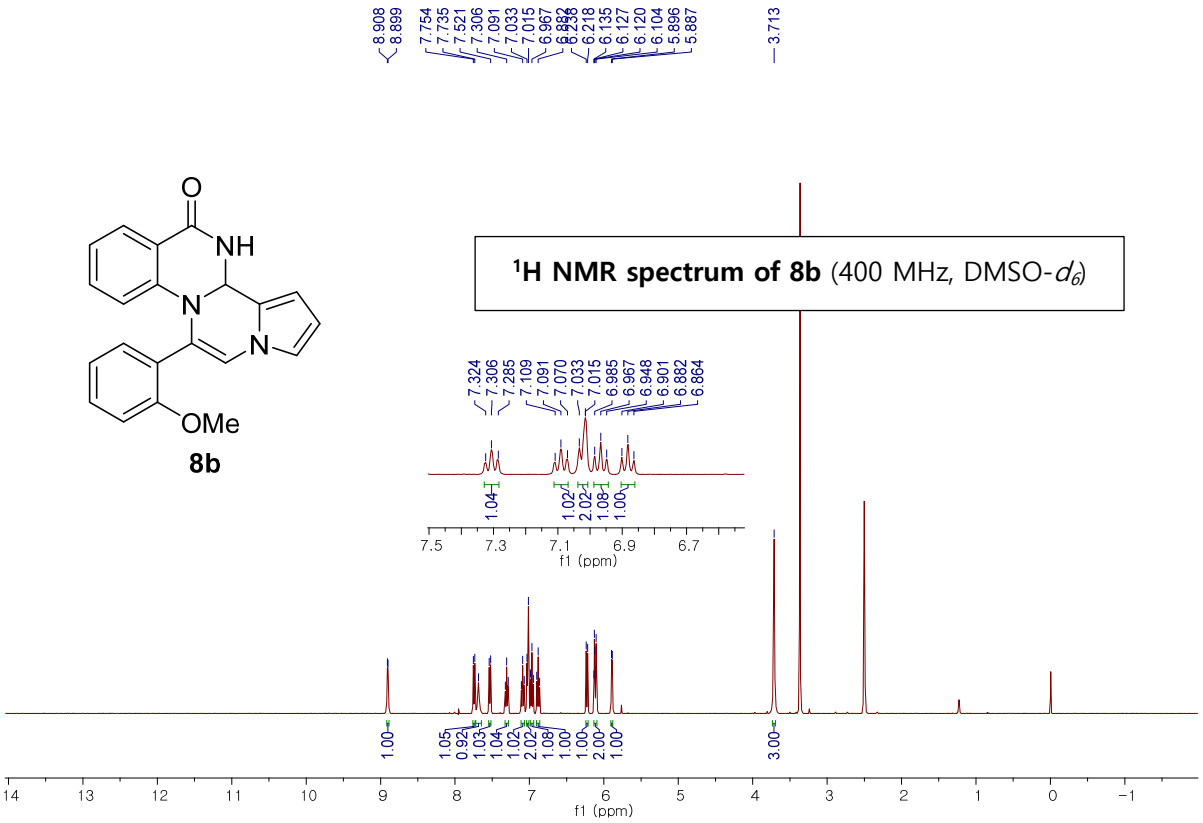




8a

^{13}C{^{1}H} NMR spectrum of 8a (100 MHz, DMSO-d_6)

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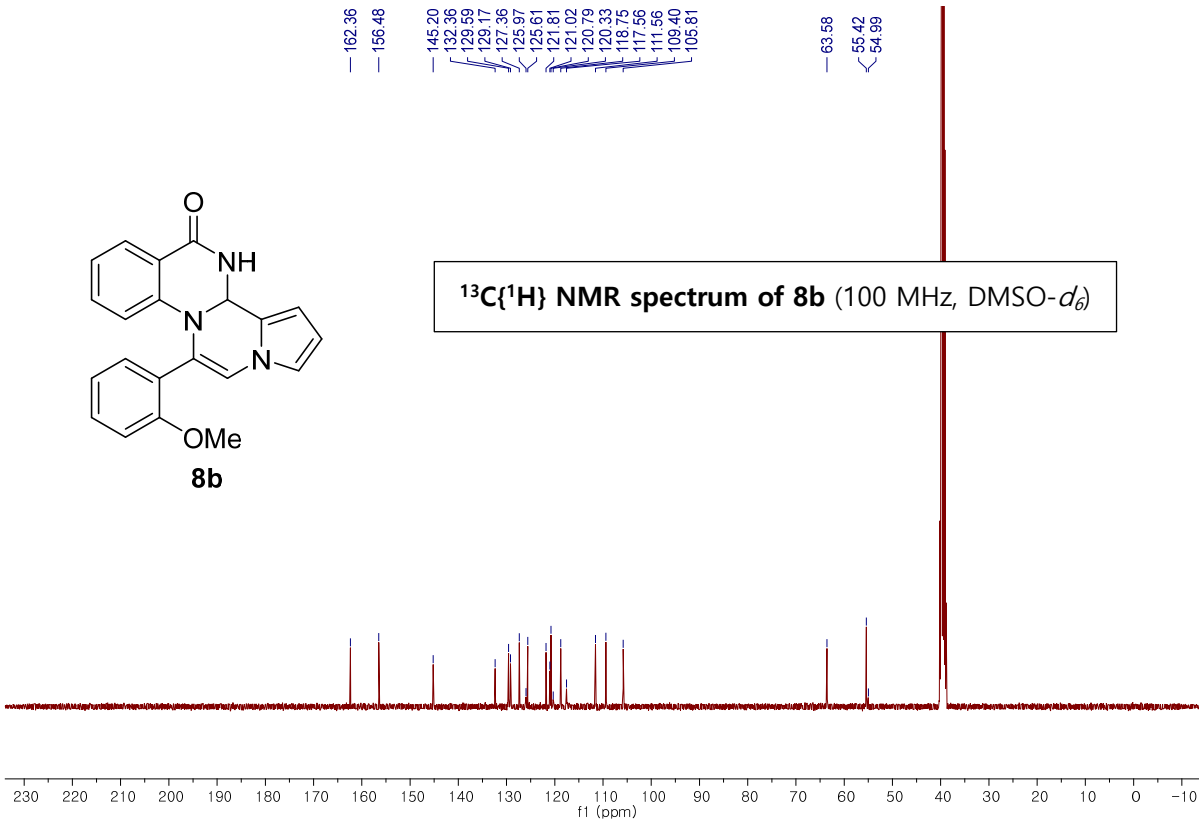
7.754
7.735
7.521
7.306
7.091
7.033
7.015
6.967
6.218
6.135
6.127
6.120
6.104
5.896
5.887
3.713
O
NH
N
N
OMe
8b
¹H NMR spectrum of 8b (400 MHz, DMSO-d6)
7.324
7.306
7.285
7.109
7.091
7.070
7.033
7.015
6.985
6.967
6.948
6.901
6.882
6.864
1.04
1.02
2.02
1.08
1.00
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
1.00
1.05
0.92
1.03
1.04
1.02
2.02
1.08
1.00
1.00
2.00
1.00
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)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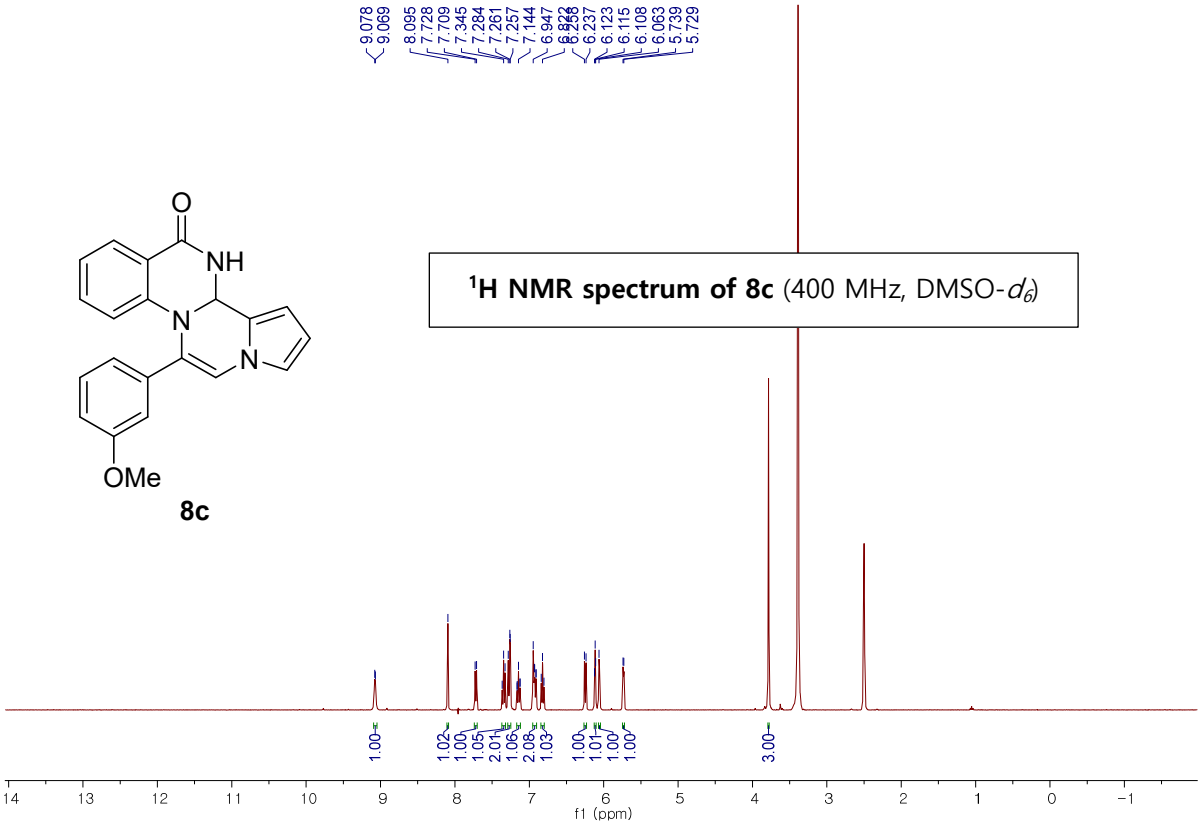
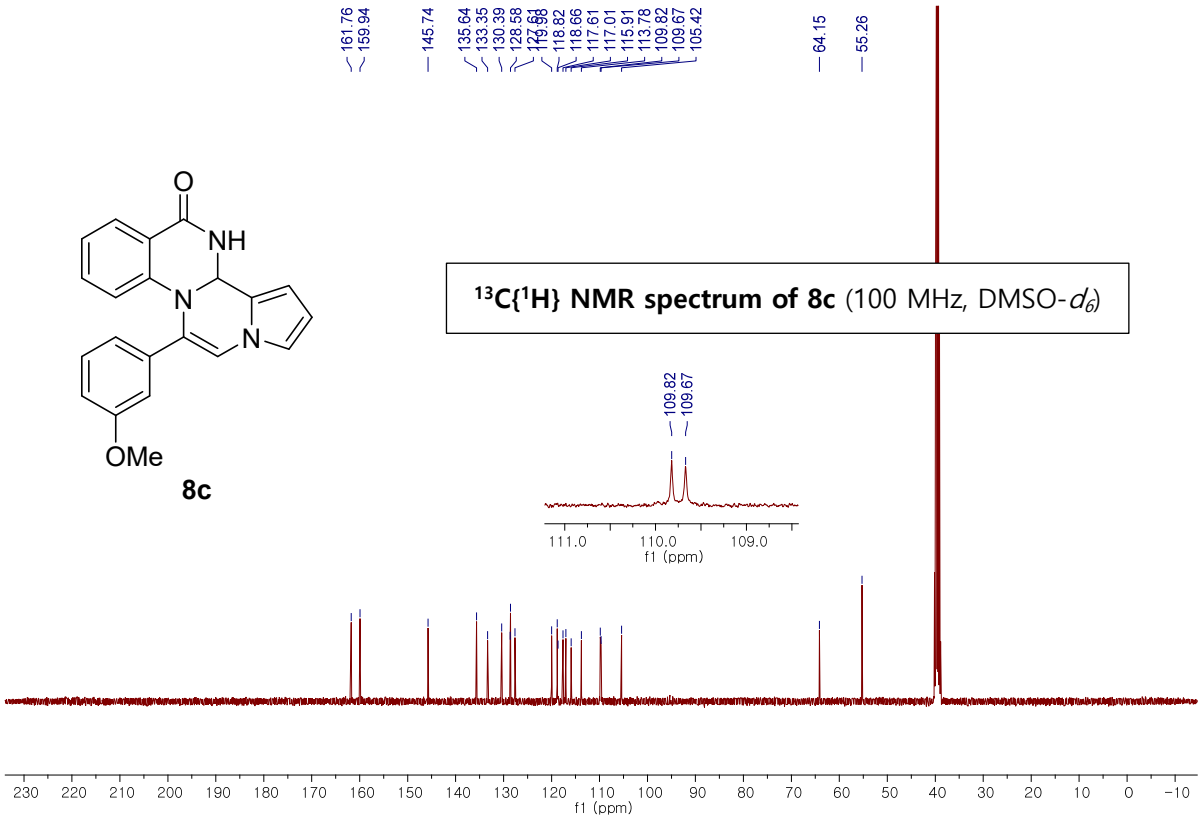
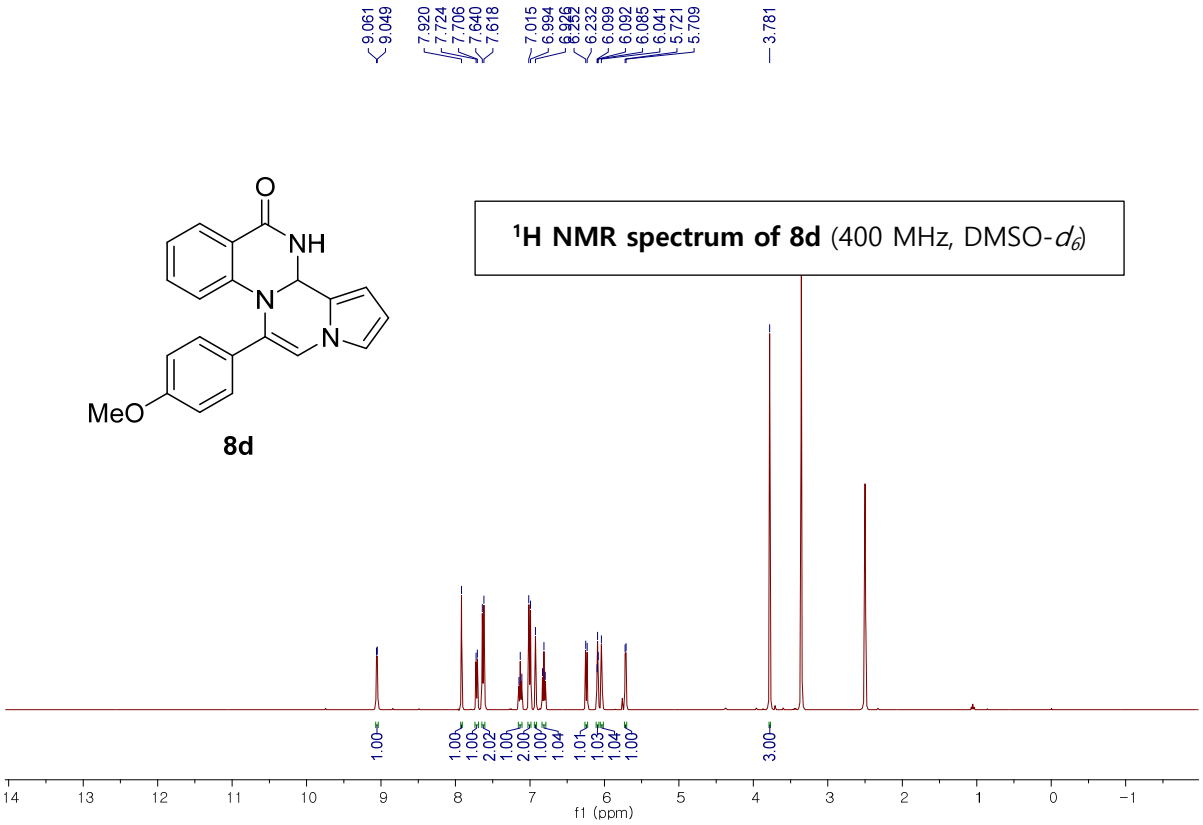
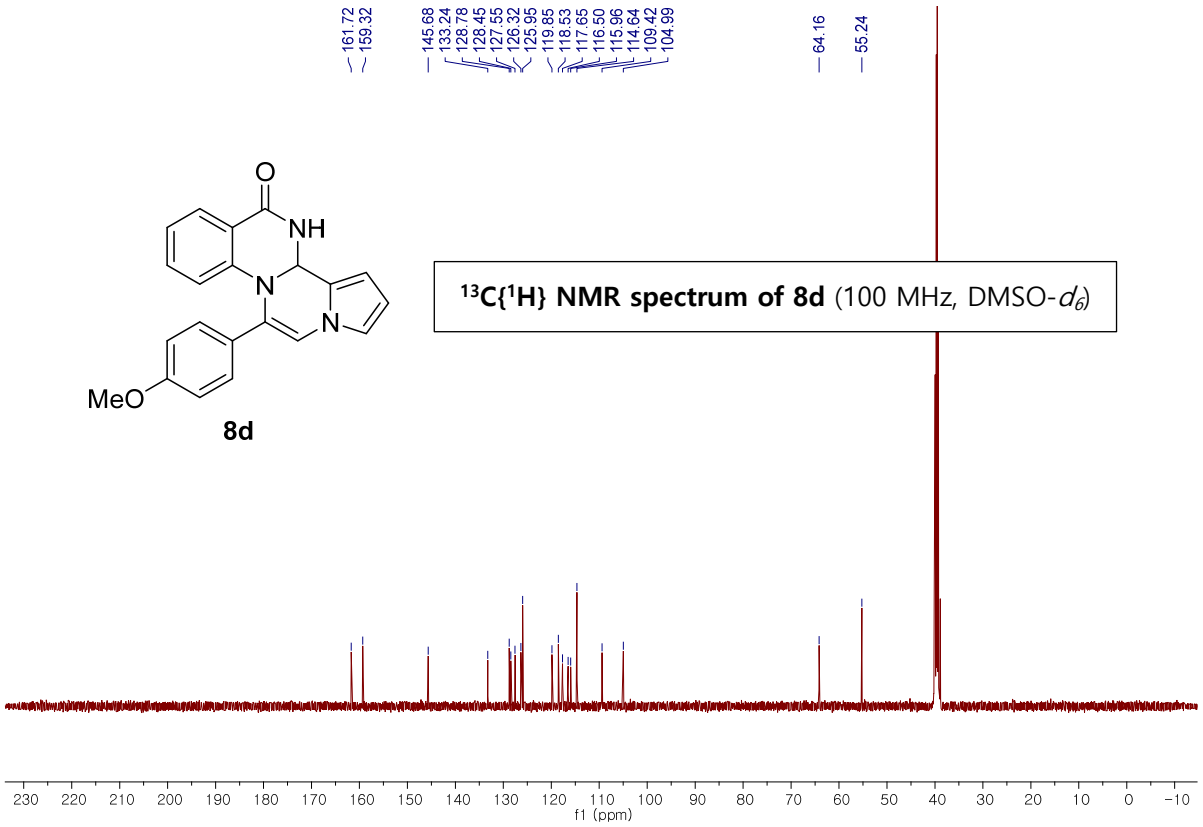
156.48
145.20
132.36
129.59
129.17
127.36
125.97
125.61
121.81
121.02
120.79
120.33
118.75
117.56
111.56
109.40
105.81
63.58
55.42
54.99
O
NH
N
N
OMe
8b
¹³C{¹H} NMR spectrum of 8b (100 MHz, DMSO-d6)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


9.078
9.069
8.095
7.728
7.709
7.345
7.284
7.261
7.257
7.144
6.947
6.237
6.123
6.115
6.108
6.063
5.739
5.729
O
NH
N
N
OMe
8c
1H NMR spectrum of 8c (400 MHz, DMSO-d6)
1.00
1.02
1.00
1.05
2.01
1.06
2.08
1.03
1.00
1.01
1.00
1.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)


161.76
159.94
145.74
135.64
133.35
130.39
128.58
118.82
118.66
117.61
117.01
115.91
113.78
109.82
109.67
105.42
64.15
55.26
O
NH
N
N
OMe
8c
13C{1H} NMR spectrum of 8c (100 MHz, DMSO-d6)
109.82
109.67
111.0
110.0
109.0
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



^{1}H NMR spectrum of 8d (400 MHz, DMSO-d_6)



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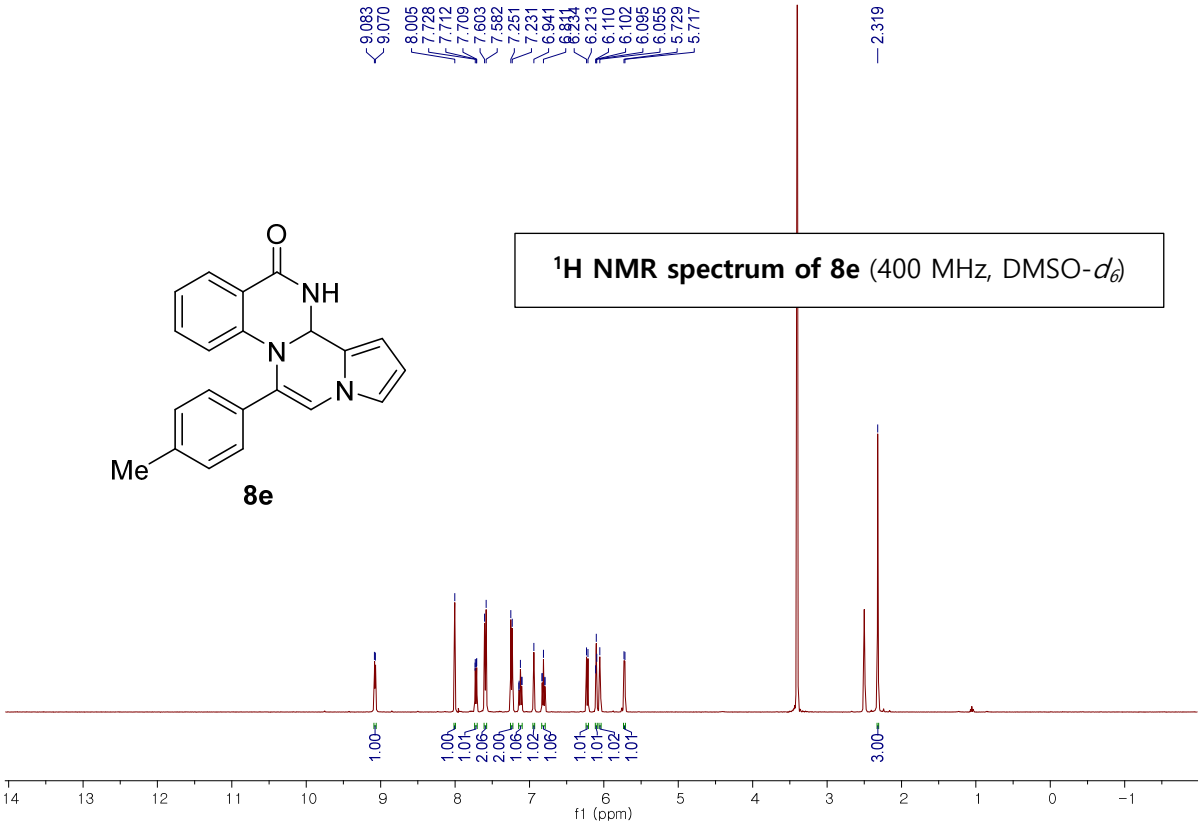
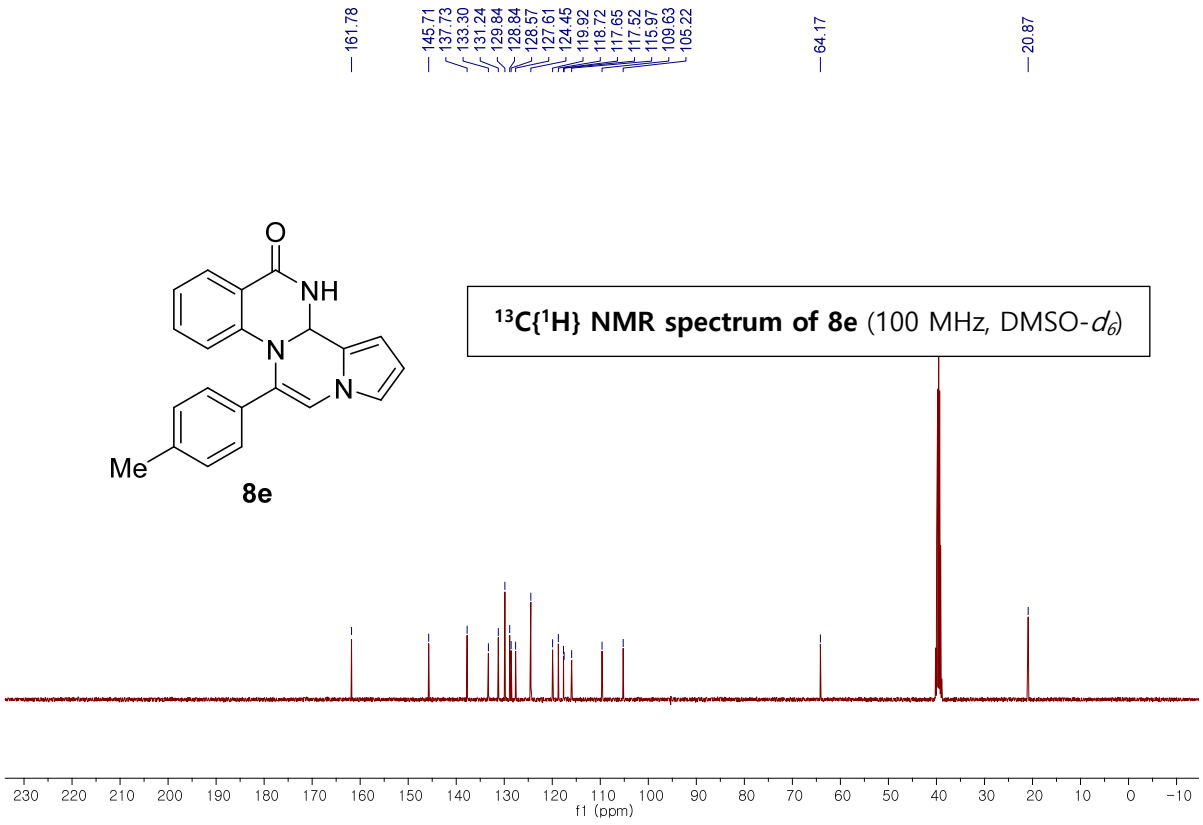


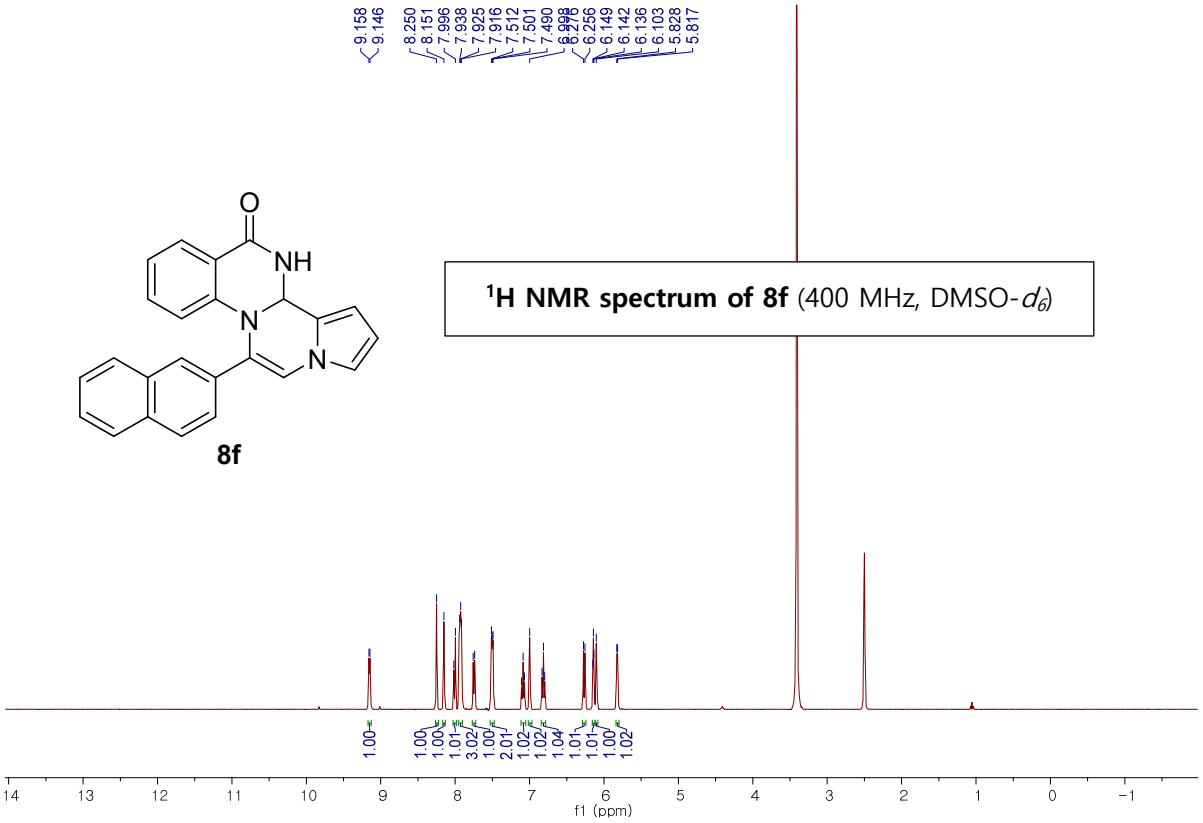
^{1}H NMR spectrum of 8e (400 MHz, DMSO-d_6)

8e

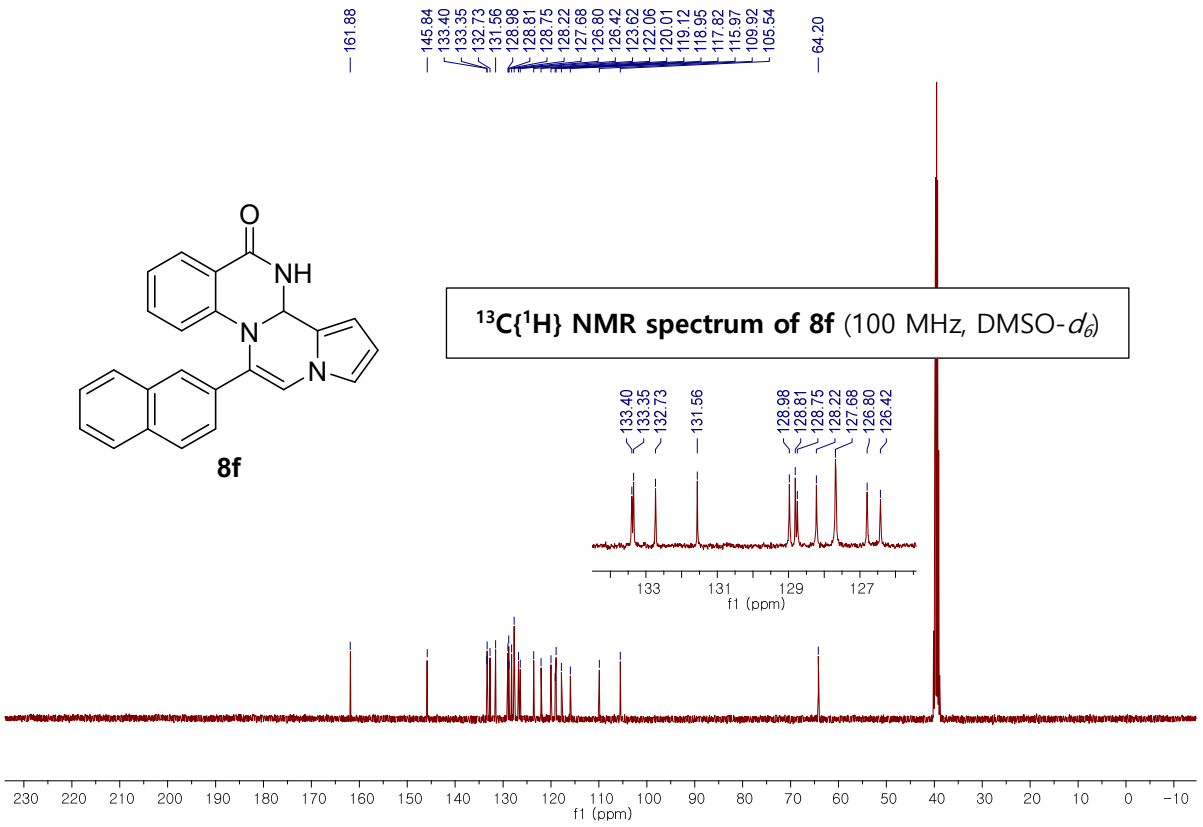


^{13}C{^{1}H} NMR spectrum of 8e (100 MHz, DMSO-d_6)

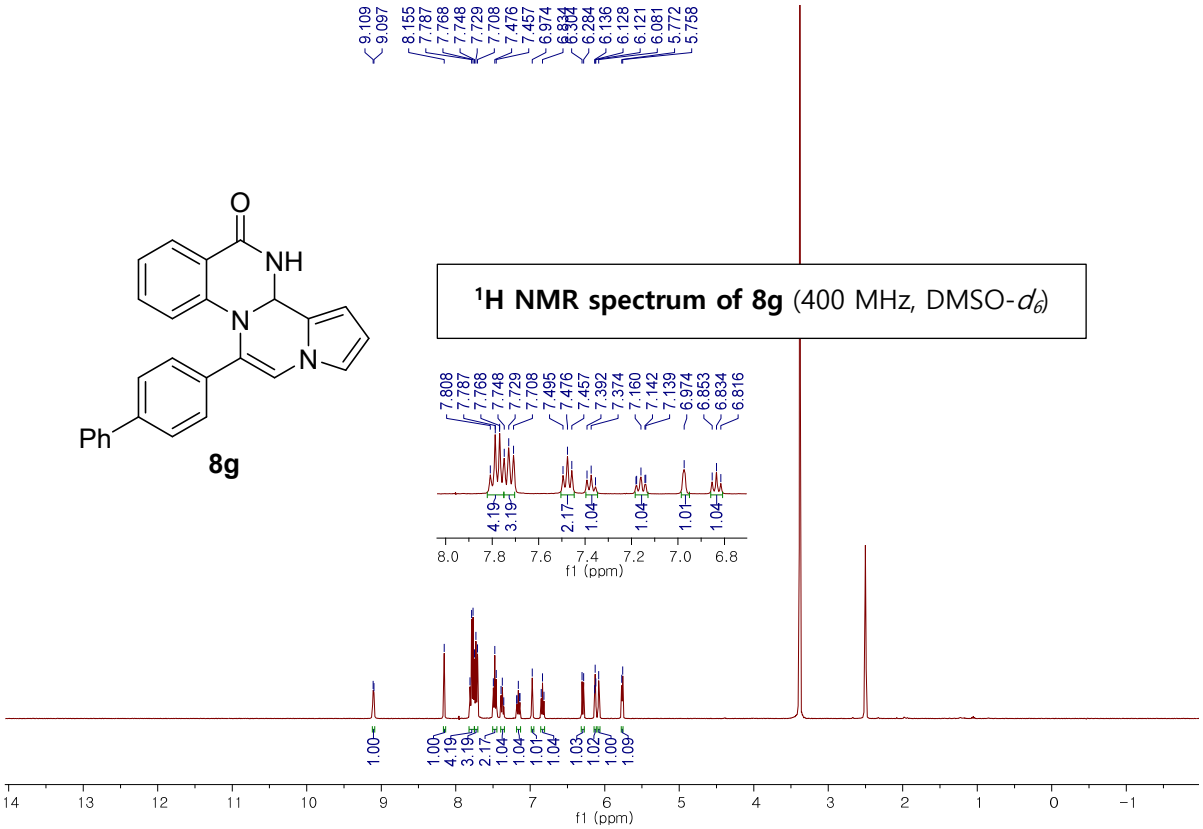
8e



^{1}H NMR spectrum of 8f (400 MHz, DMSO-d_6)



^{13}C{^{1}H} NMR spectrum of 8f (100 MHz, DMSO-d_6)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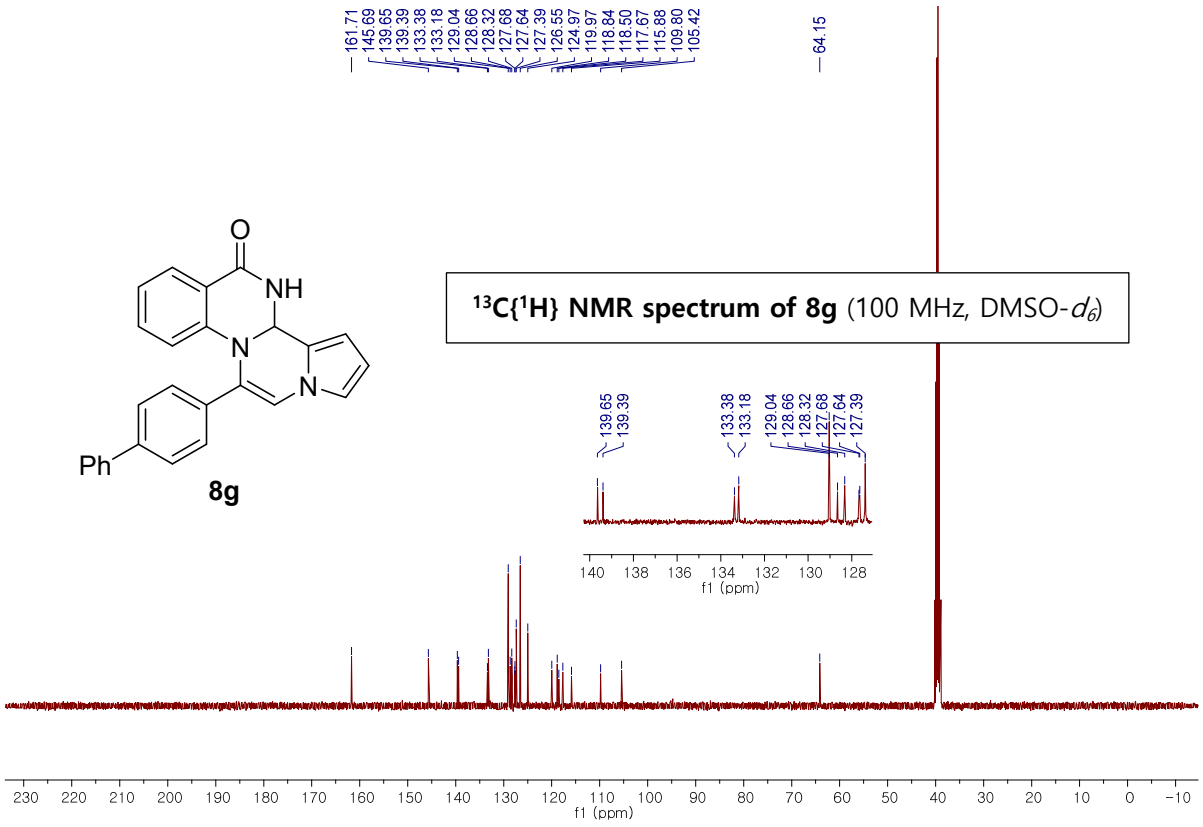
9.097
8.155
7.787
7.768
7.748
7.729
7.708
7.476
7.457
6.974
6.284
6.136
6.128
6.121
6.081
5.772
5.758
O
NH
N
N
Ph
8g
1H NMR spectrum of 8g (400 MHz, DMSO-d6)
7.808
7.787
7.768
7.748
7.729
7.708
7.495
7.476
7.457
7.392
7.374
7.160
7.142
7.139
6.974
6.853
6.834
6.816
4.19
3.19
2.17
1.04
1.04
1.01
1.04
8.0
7.8
7.6
7.4
7.2
7.0
6.8
f1 (ppm)
1.00
1.00
4.19
3.19
2.17
1.04
1.04
1.01
1.04
1.03
1.02
1.00
1.09
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)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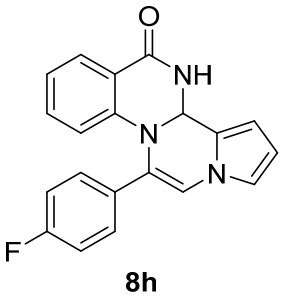
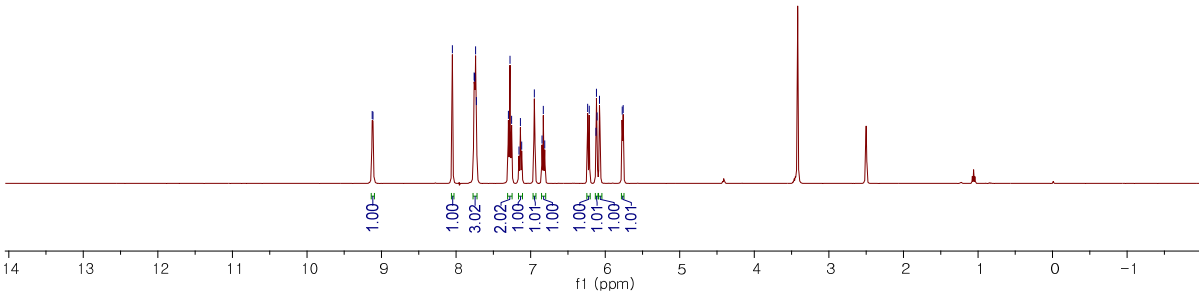
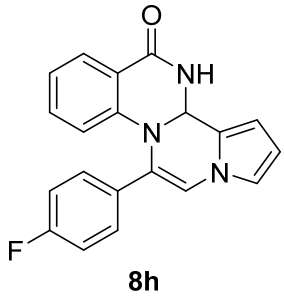
145.69
139.65
139.39
133.38
133.18
129.04
128.66
128.32
127.68
127.64
127.39
126.55
124.97
119.97
118.84
118.50
117.67
115.88
109.80
105.42
64.15
O
NH
N
N
Ph
8g
13C{1H} NMR spectrum of 8g (100 MHz, DMSO-d6)
139.65
139.39
133.38
133.18
129.04
128.66
128.32
127.68
127.64
127.39
140
138
136
134
132
130
128
f1 (ppm)
230
220
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)



8h

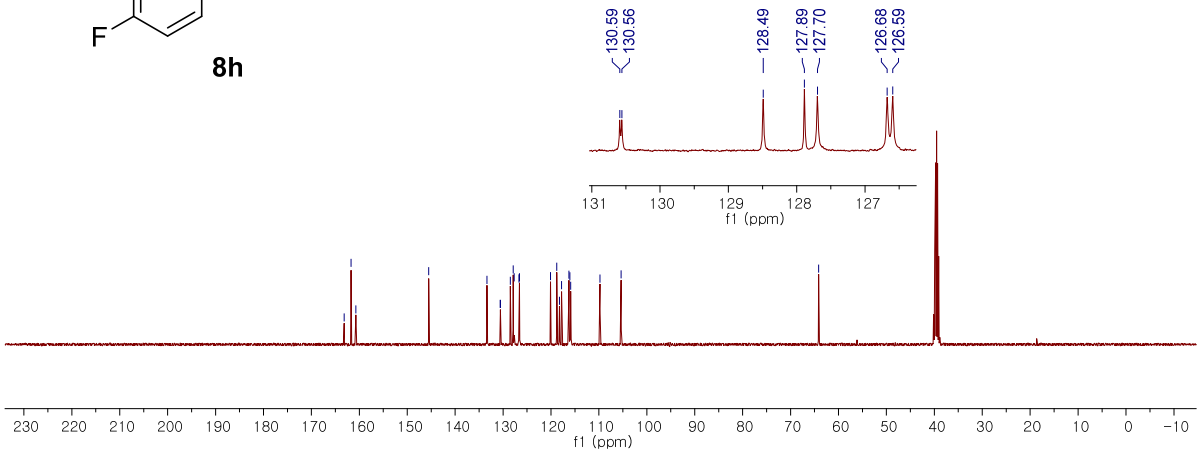
^{1}H NMR spectrum of 8h (400 MHz, DMSO-d_6)

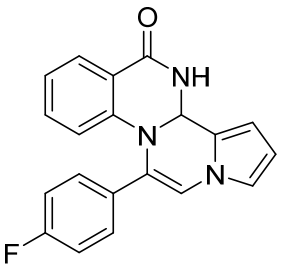




8h

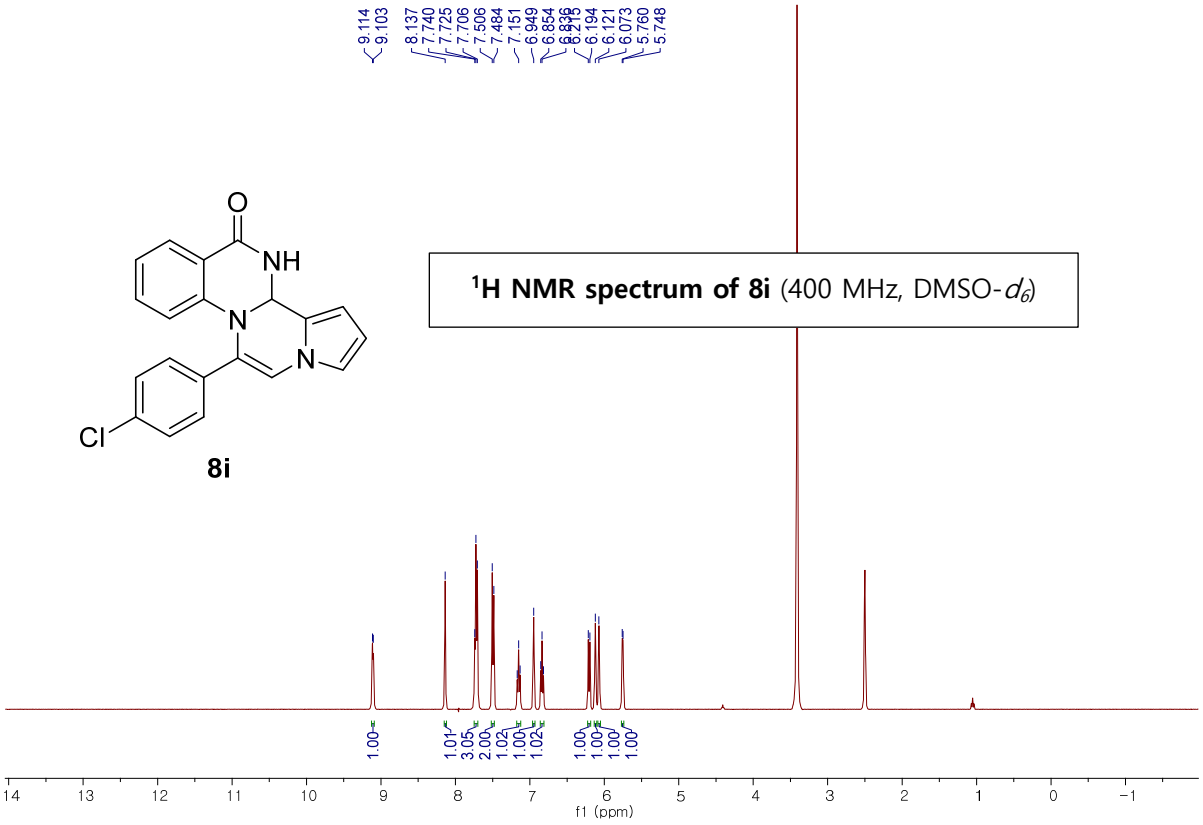
^{13}C{^{1}H} NMR spectrum of 8h (100 MHz, DMSO-d_6)



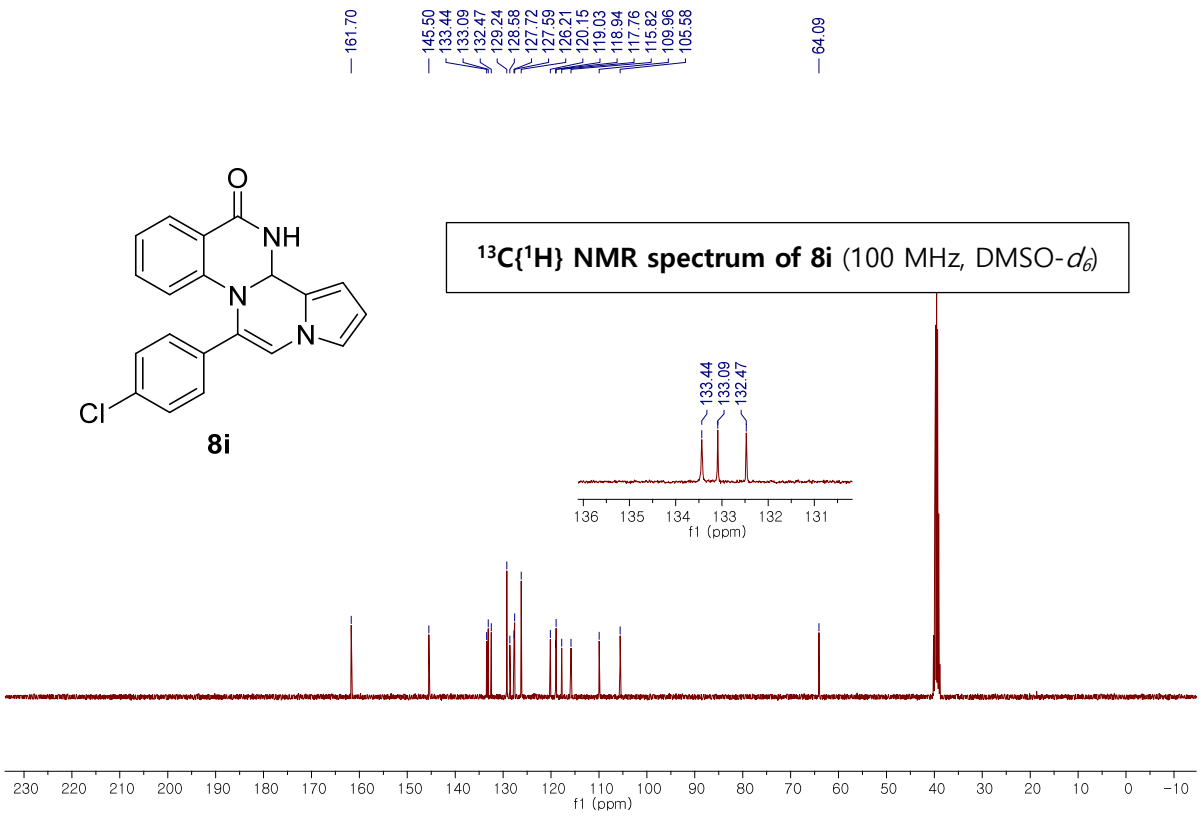


8h

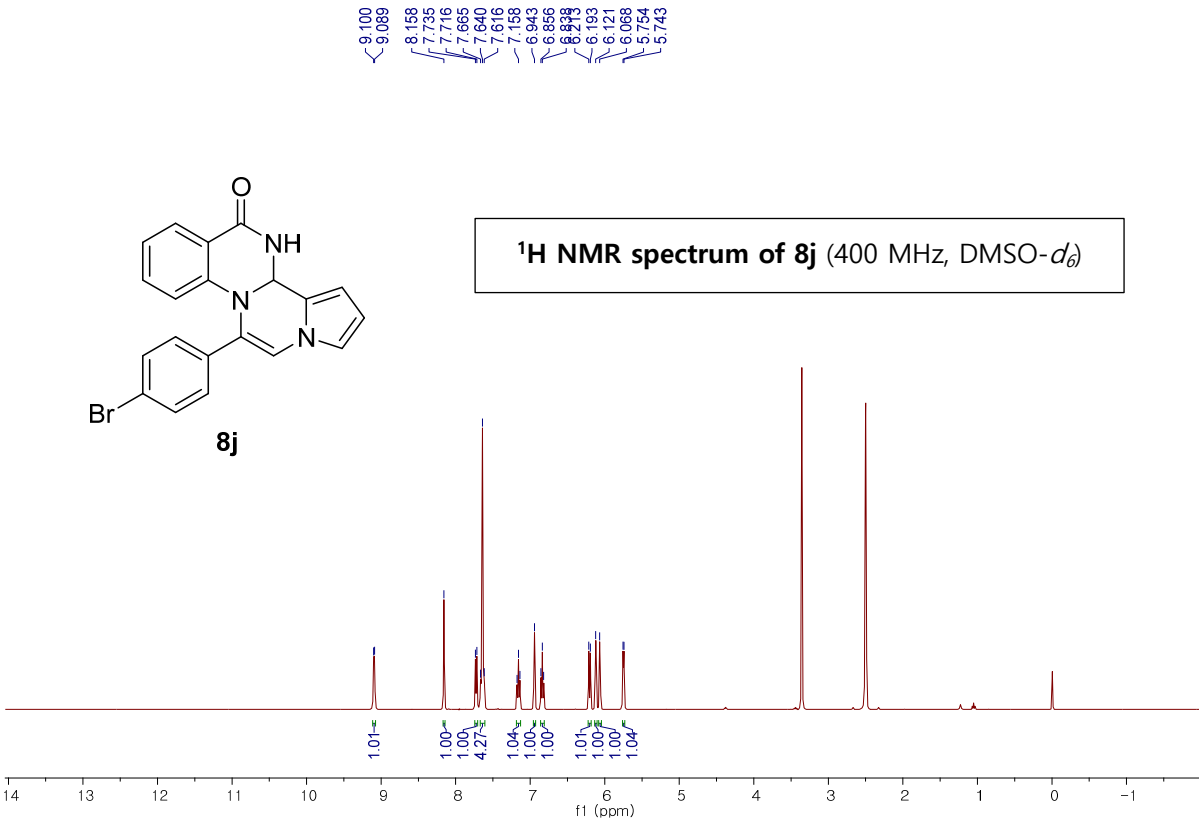
^{19}F NMR spectrum of 8h (376 MHz, DMSO-d_6)



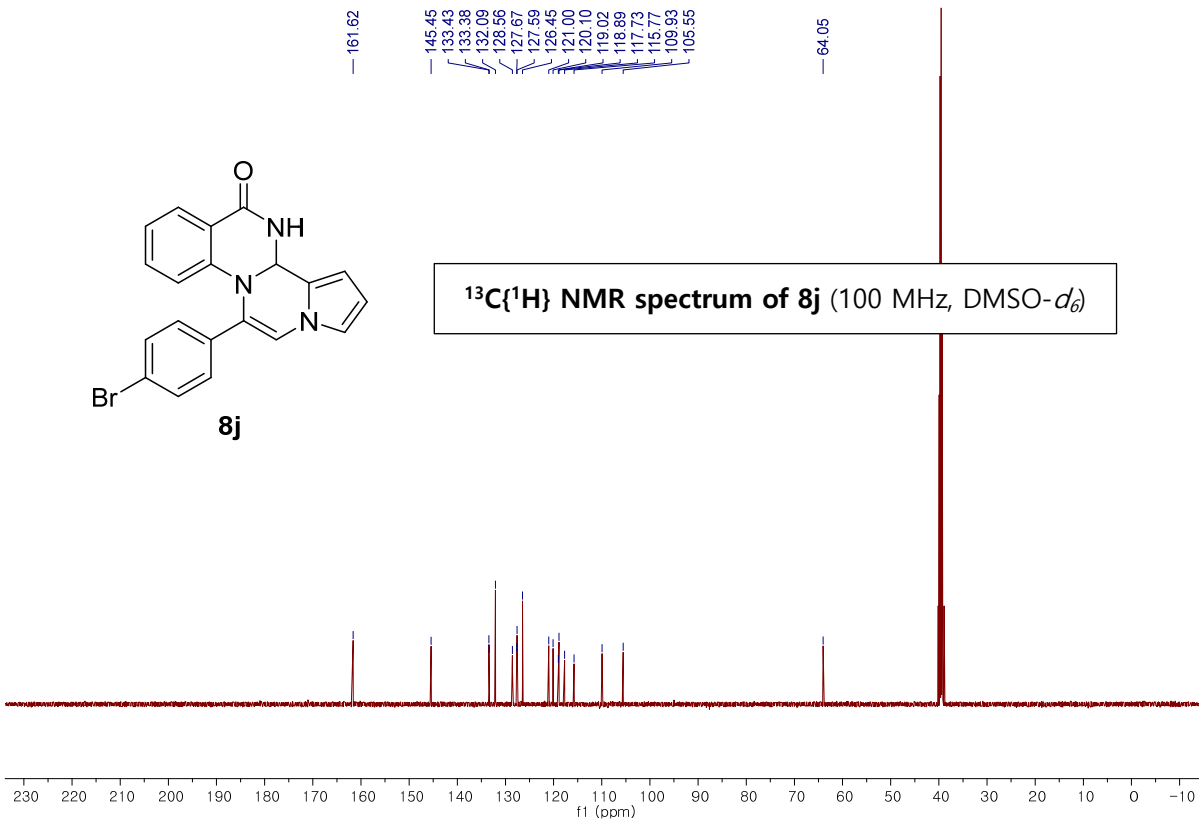
^{1}H NMR spectrum of 8i (400 MHz, DMSO-d_6)



^{13}C{^{1}H} NMR spectrum of 8i (100 MHz, DMSO-d_6)



^{1}H NMR spectrum of 8j (400 MHz, DMSO-d_6)



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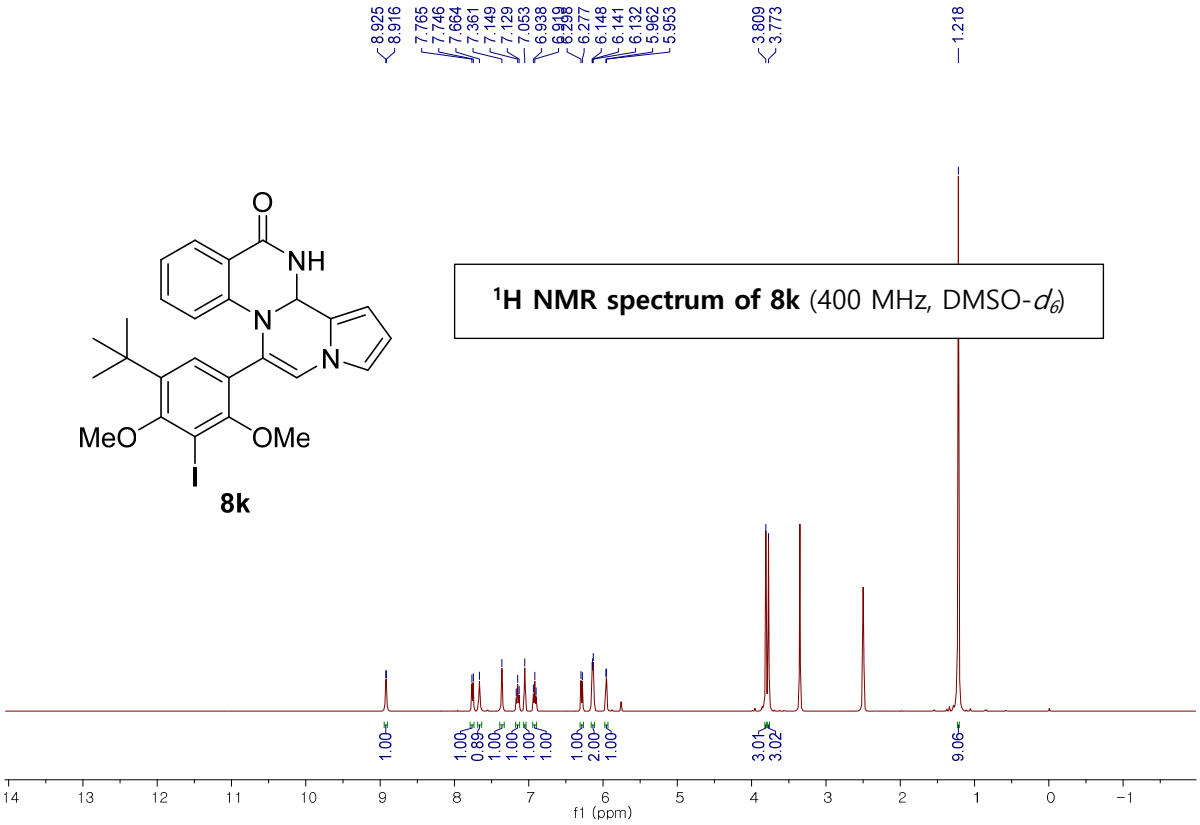
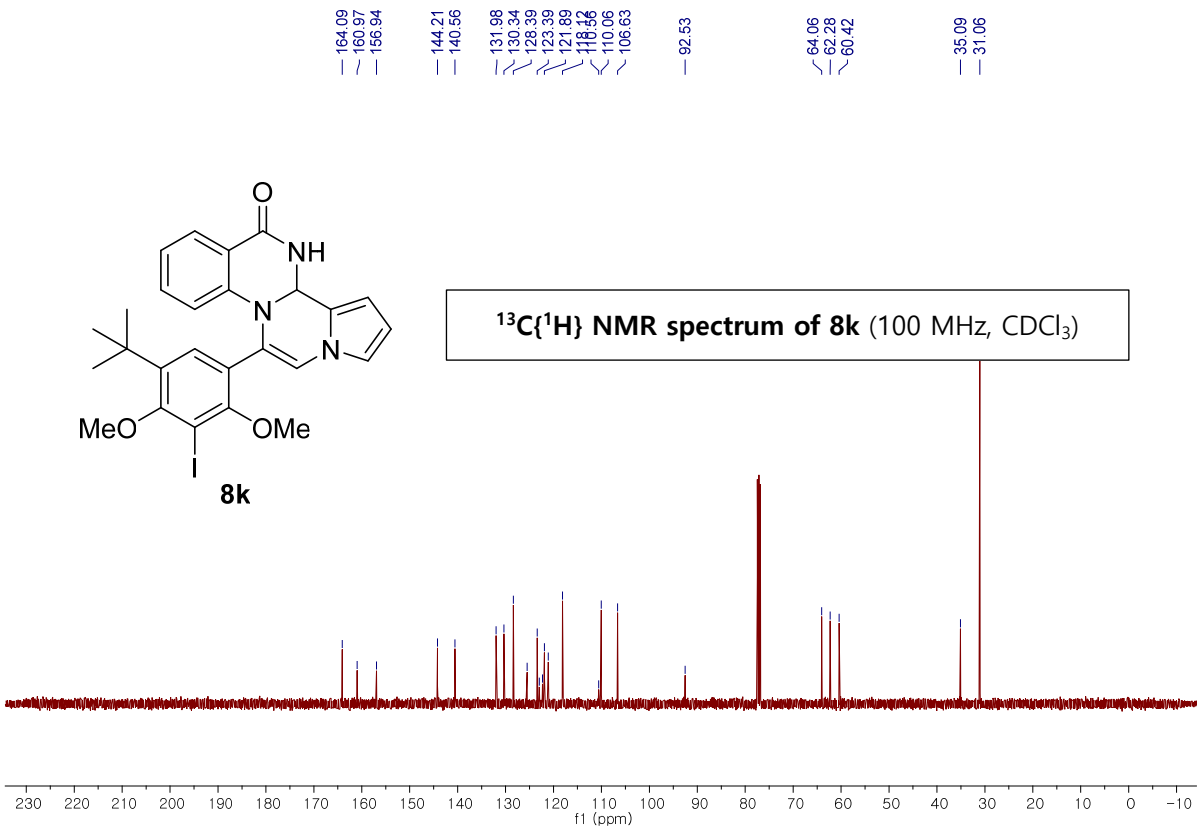
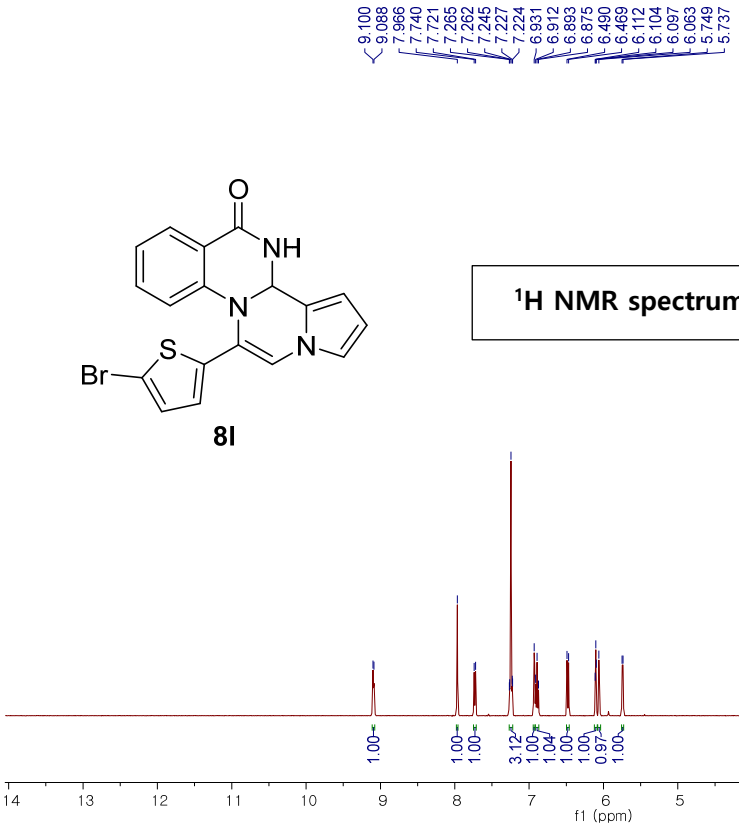


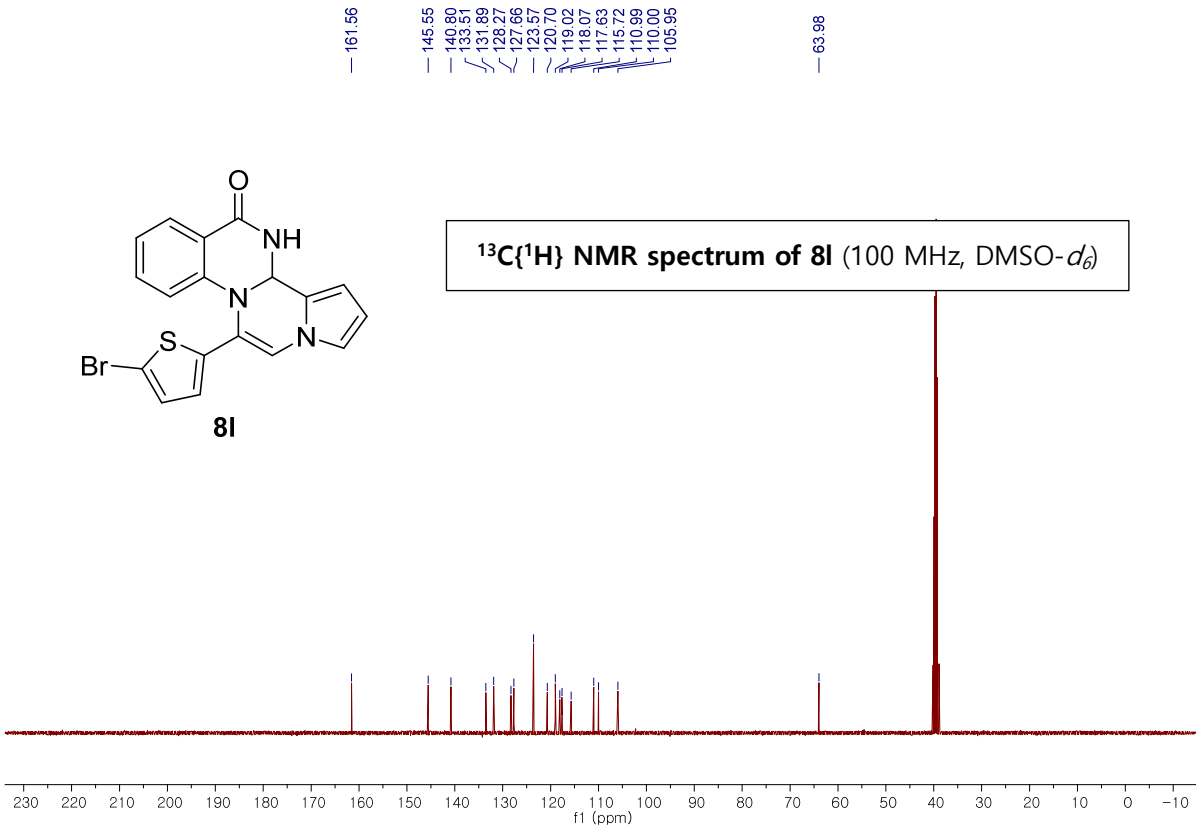
^{1}H NMR spectrum of 8k (400 MHz, DMSO-d_6)



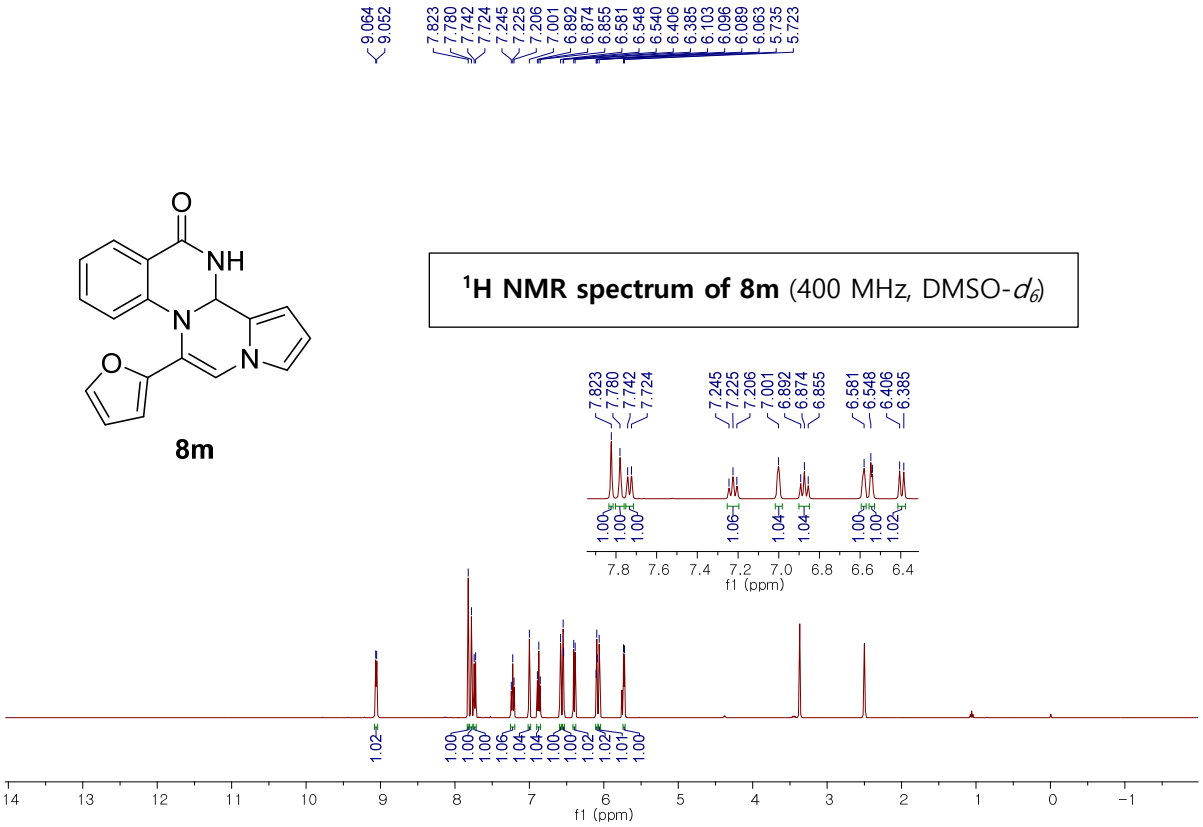
^{13}C{^{1}H} NMR spectrum of 8k (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of 8l (400 MHz, DMSO-d_6)



^{13}C{^{1}H} NMR spectrum of 8l (100 MHz, DMSO-d_6)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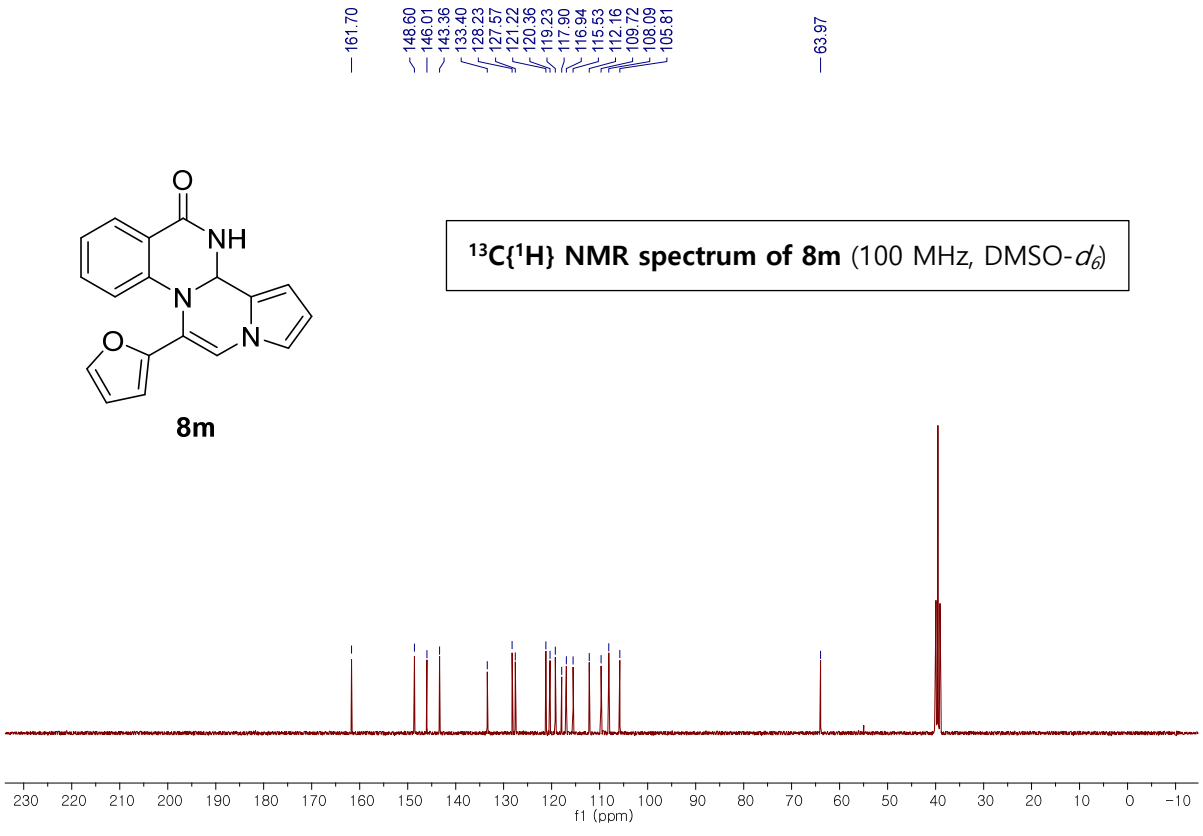
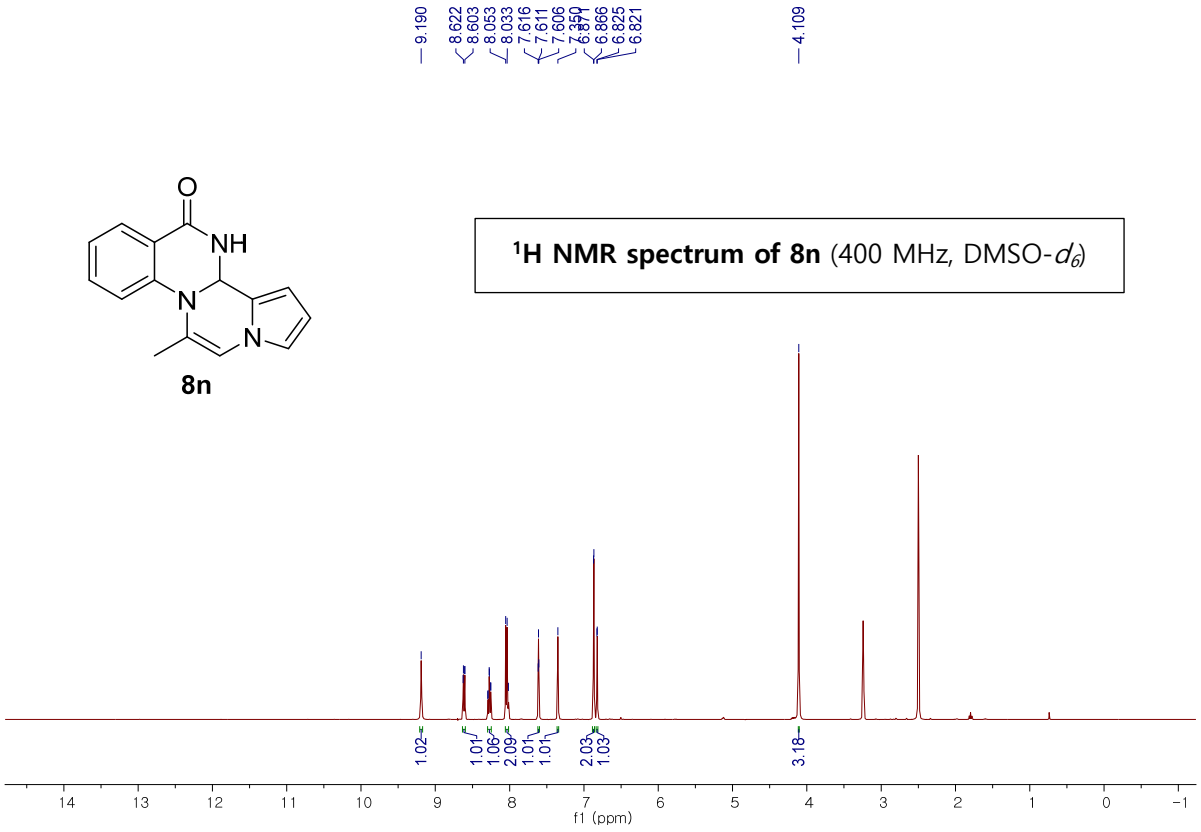
9.052
7.823
7.780
7.742
7.724
7.245
7.225
7.206
7.001
6.892
6.874
6.855
6.581
6.548
6.540
6.406
6.385
6.103
6.096
6.089
6.063
5.735
5.723
O
NH
N
O
N
8m
1H NMR spectrum of 8m (400 MHz, DMSO-d6)
f1 (ppm)


161.70
148.60
146.01
143.36
133.40
128.23
127.57
121.22
120.36
119.23
117.90
116.94
115.53
112.16
109.72
108.09
105.81
63.97
O
NH
N
O
N
8m
13C{1H} NMR spectrum of 8m (100 MHz, DMSO-d6)
f1 (ppm)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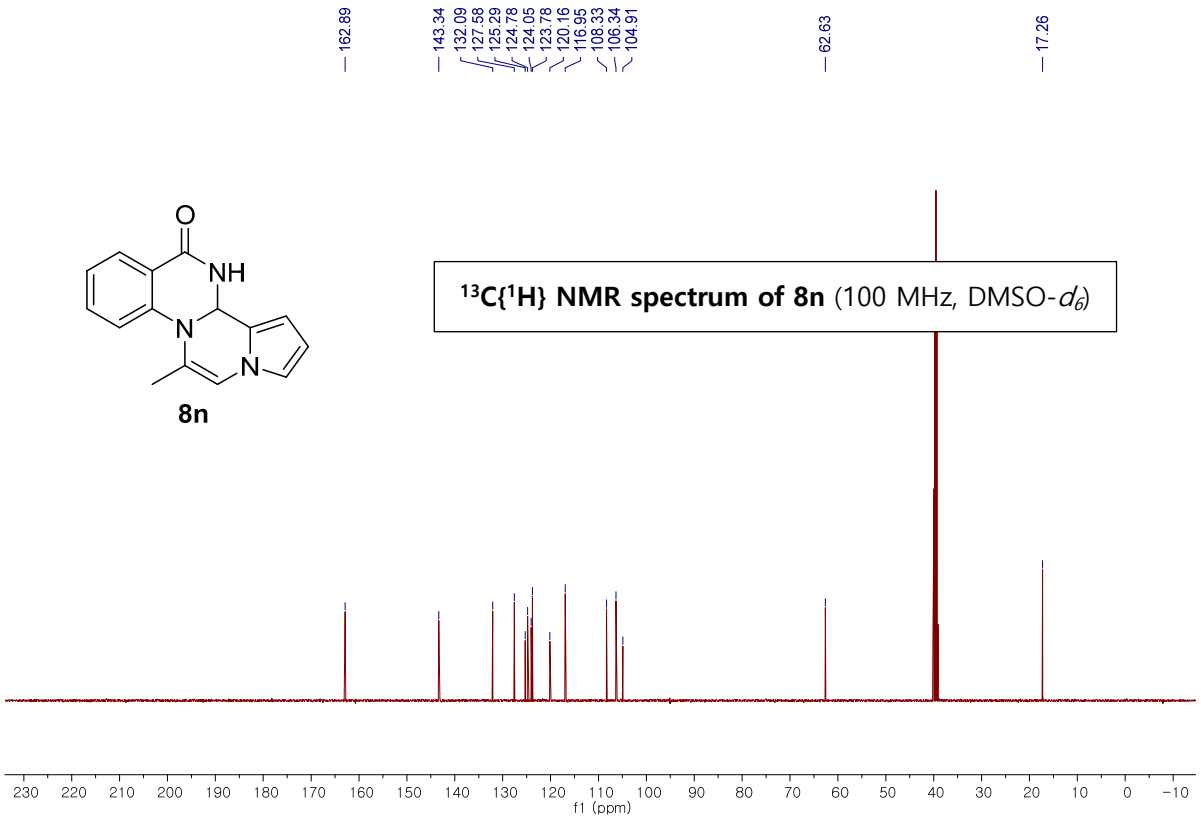
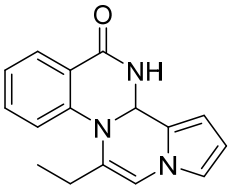
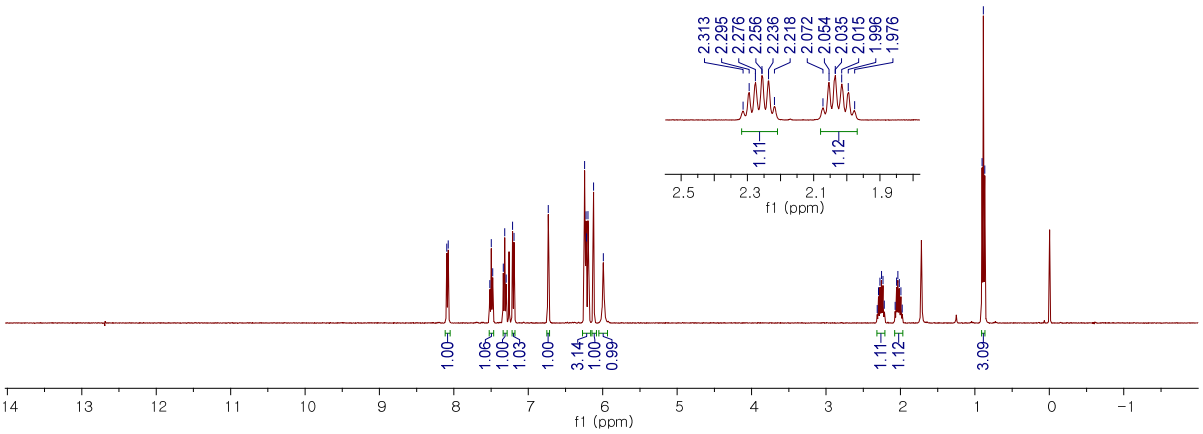
8.603
8.053
8.033
7.616
7.611
7.606
7.350
6.886
6.825
6.821
4.109
O
NH
N
N
8n
1H NMR spectrum of 8n (400 MHz, DMSO-d6)
1.02
1.01
1.06
2.09
1.01
1.01
2.03
1.03
3.18
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)

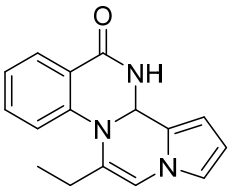

162.89
143.34
132.09
127.58
125.29
124.78
124.05
123.78
120.16
116.95
108.33
106.34
104.91
62.63
17.26
O
NH
N
N
8n
13C{1H} NMR spectrum of 8n (100 MHz, DMSO-d6)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



8o

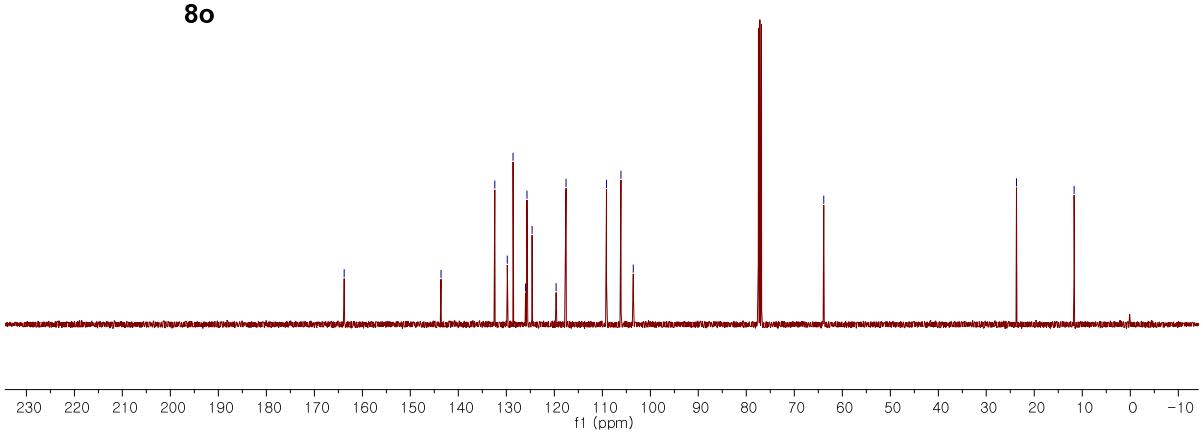
^{1}H NMR spectrum of 8o (400 MHz, $CDCl_3$)

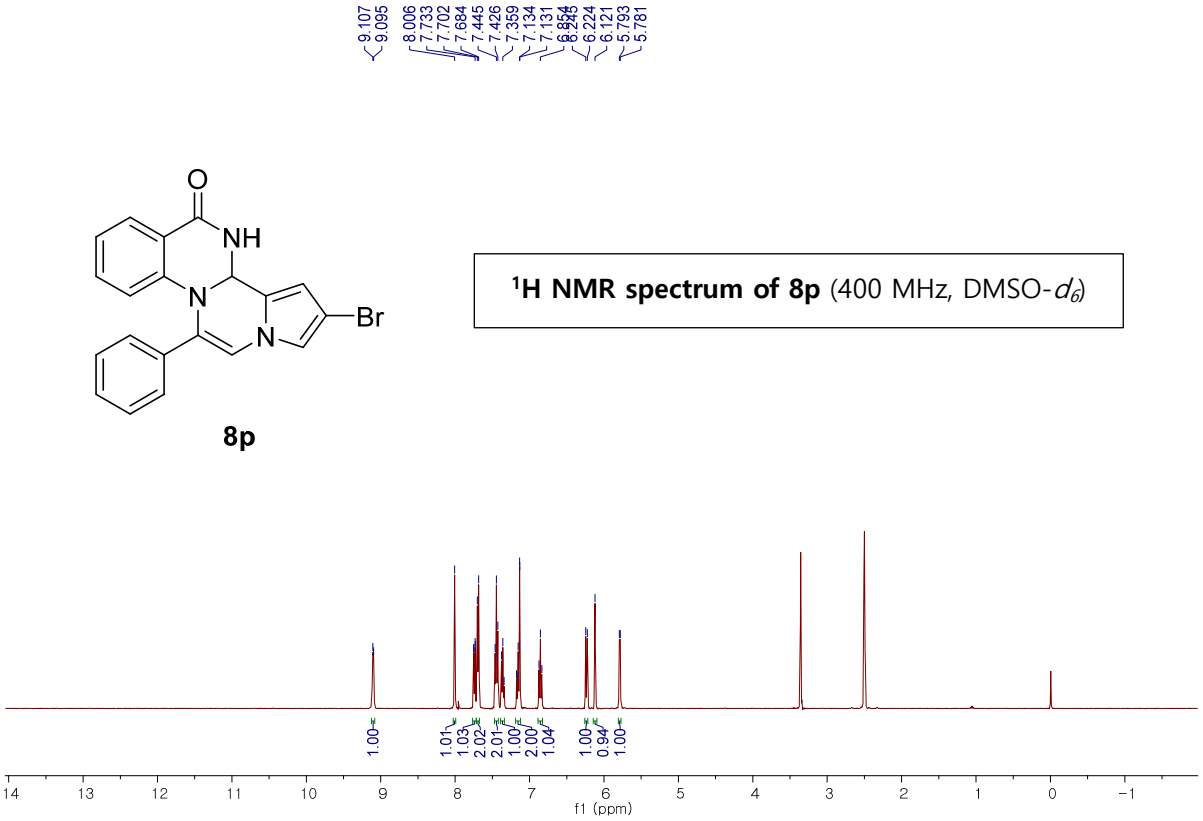




8o

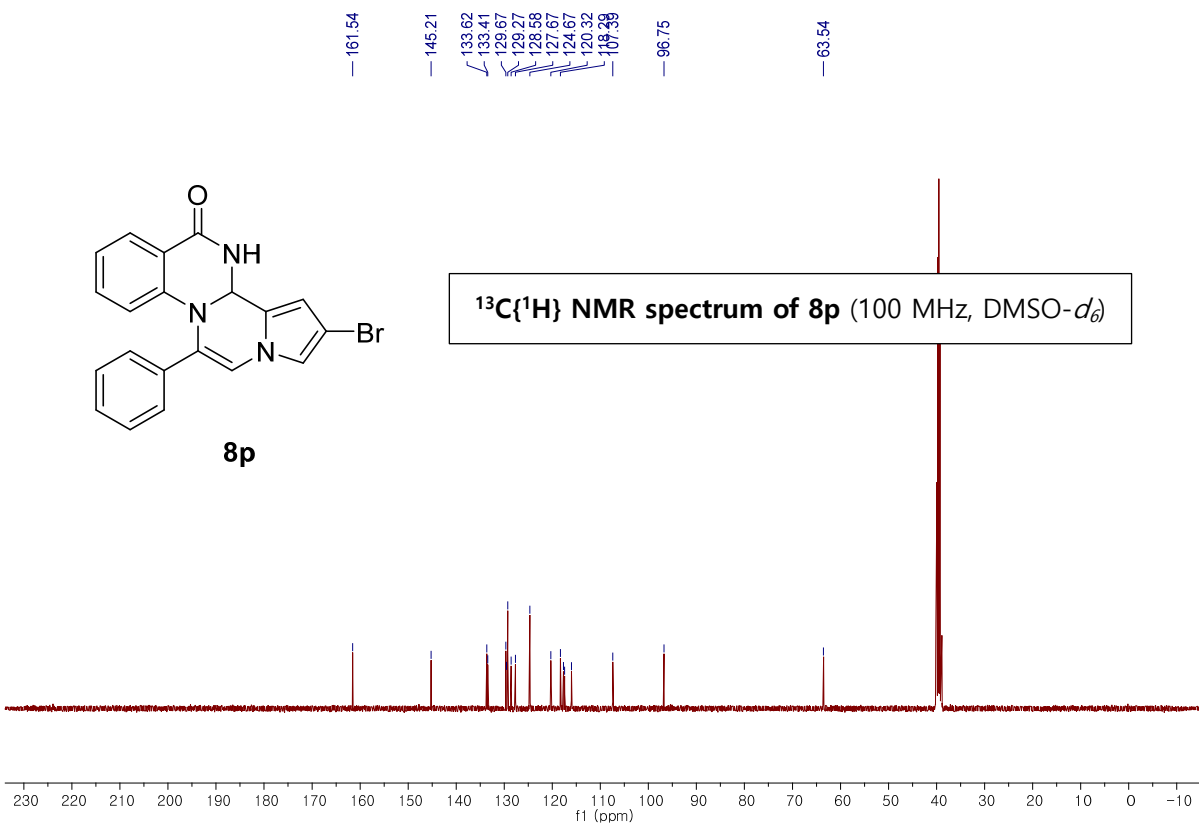
^{13}C{^{1}H} NMR spectrum of 8o (100 MHz, $CDCl_3$)





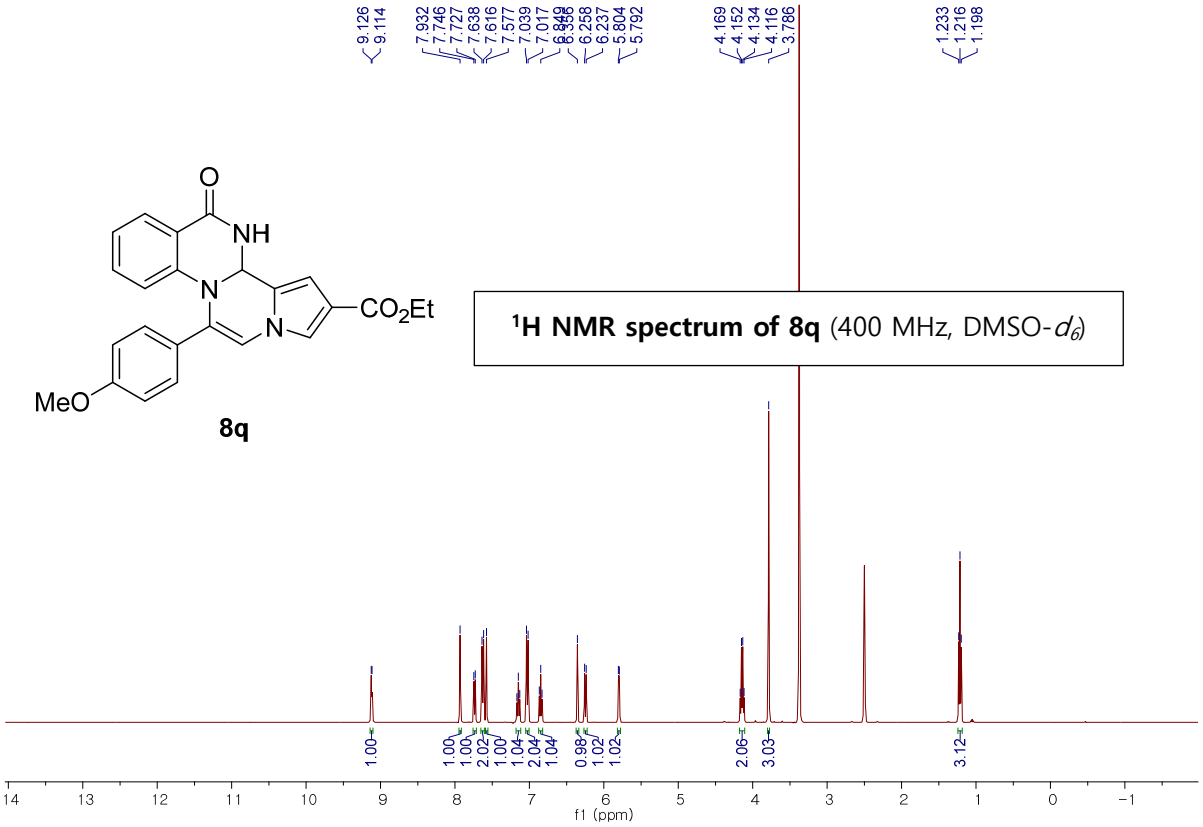
8p

^{1}H NMR spectrum of 8p (400 MHz, DMSO-d_6)



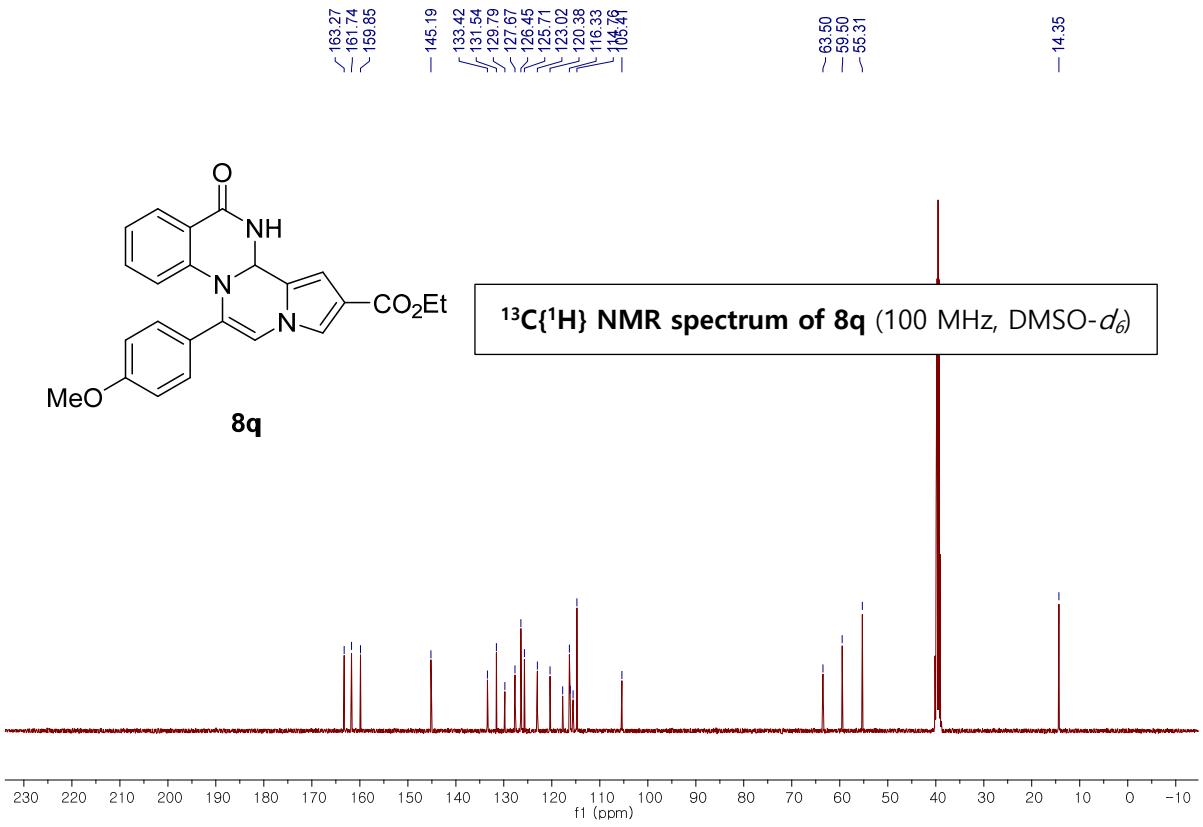
8p

^{13}C{^{1}H} NMR spectrum of 8p (100 MHz, DMSO-d_6)



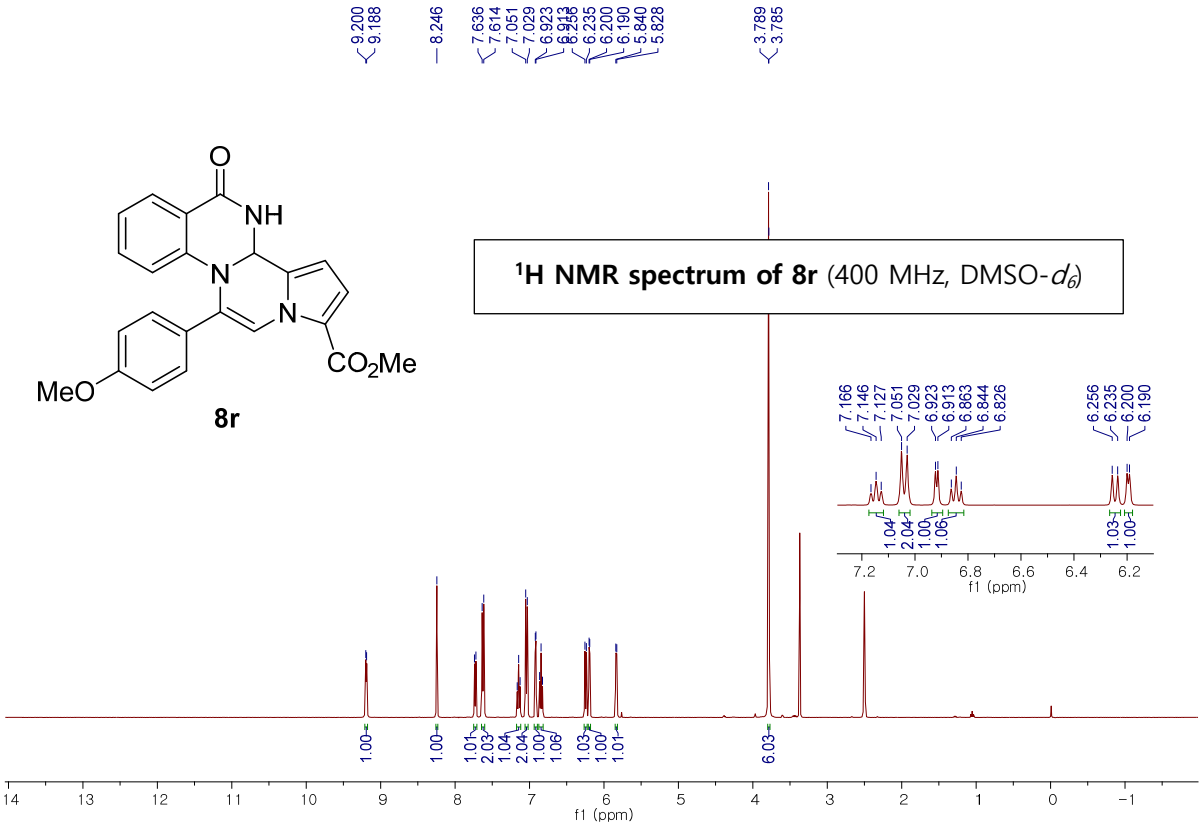
8q

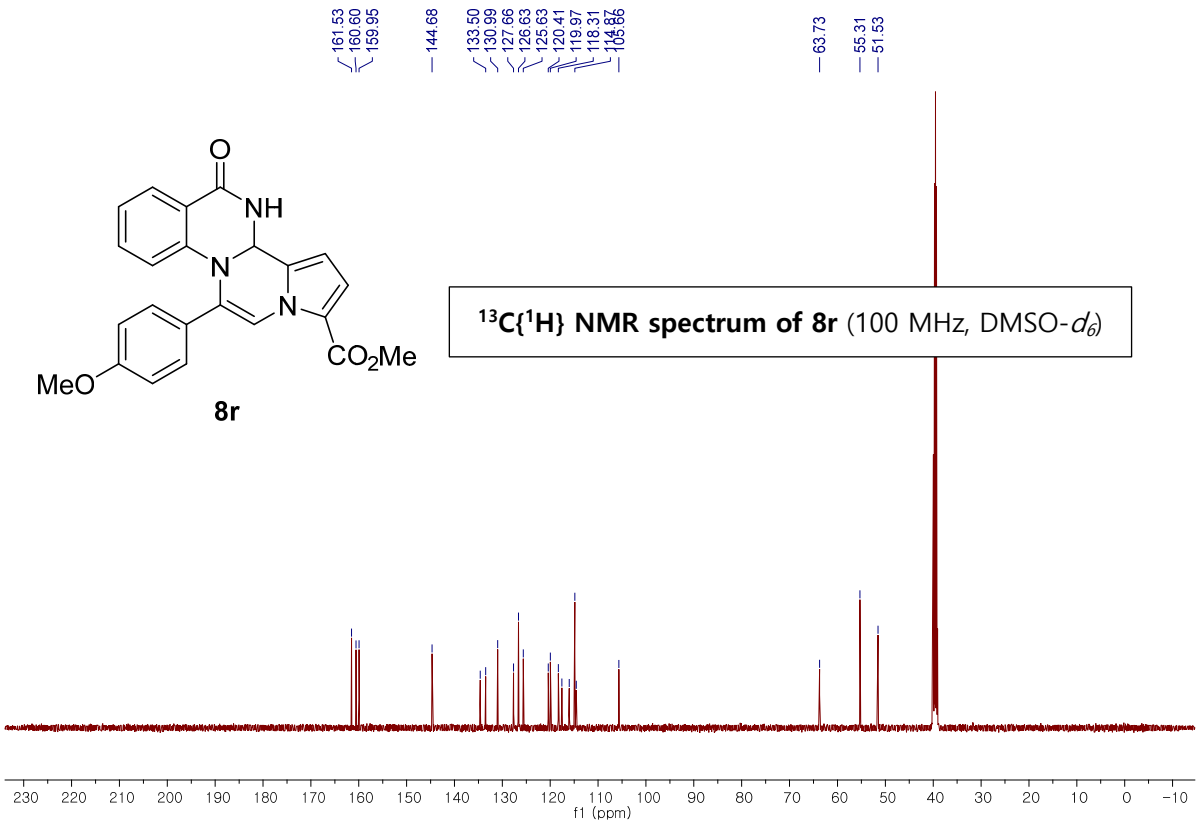
^{1}H NMR spectrum of 8q (400 MHz, DMSO-d_6)

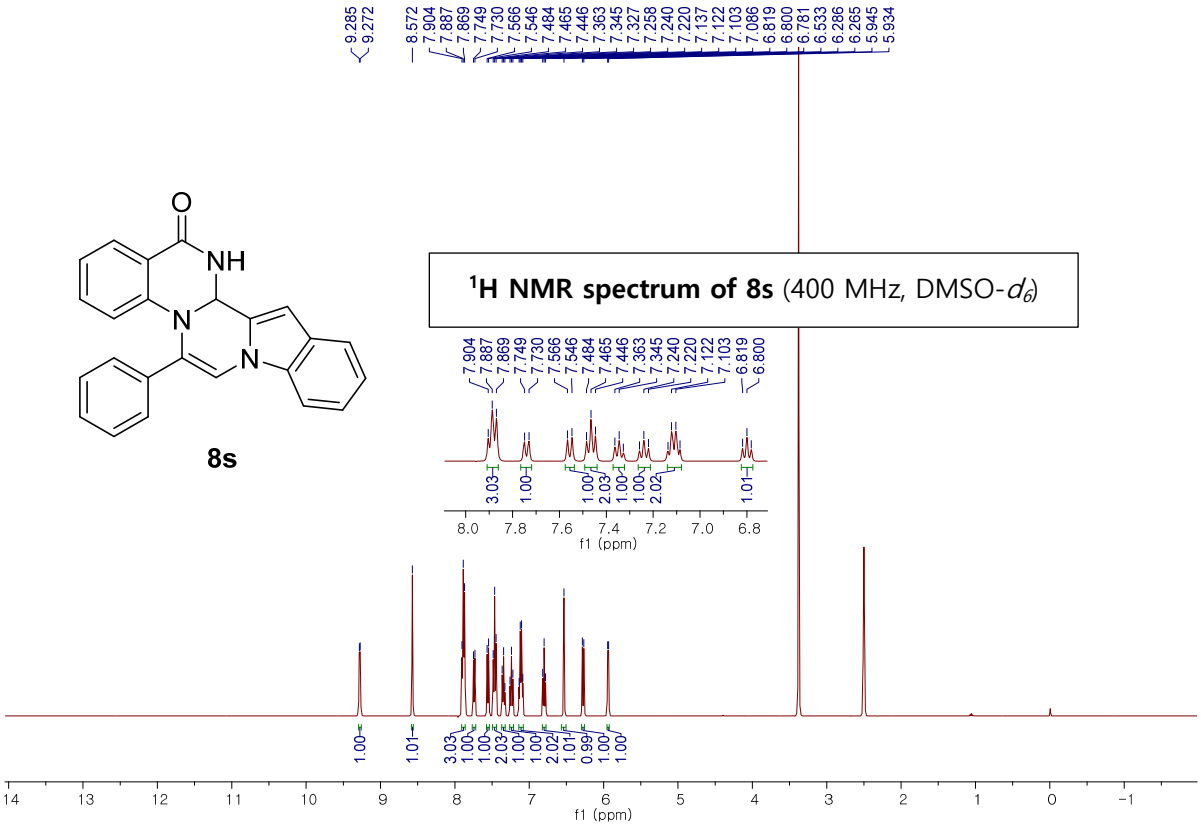


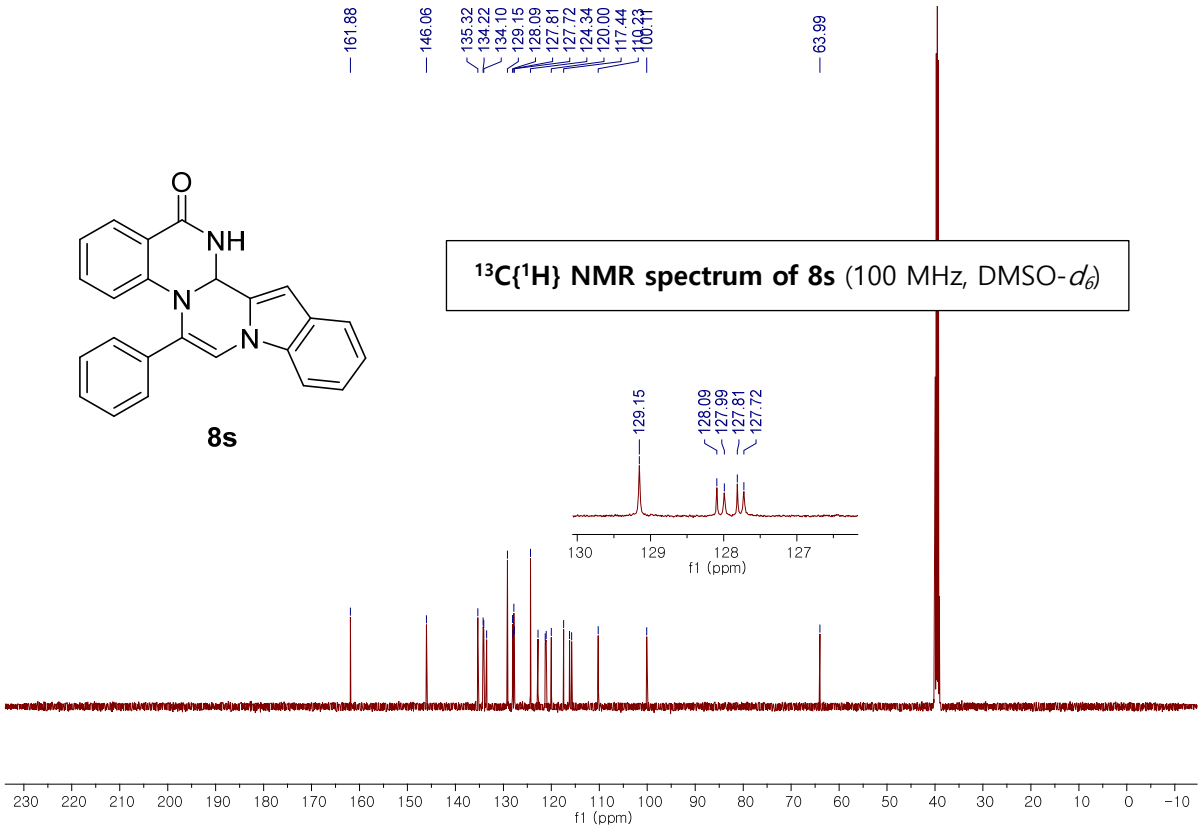
8q

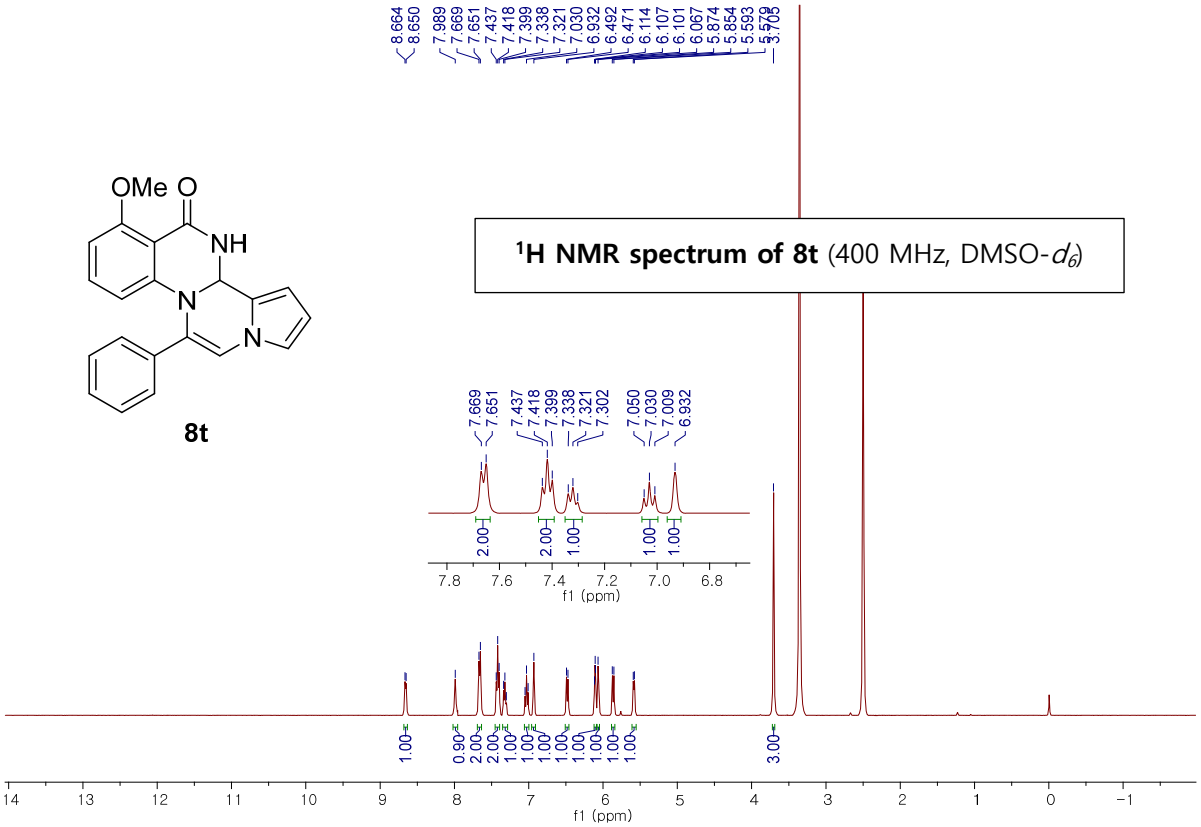
^{13}C{^{1}H} NMR spectrum of 8q (100 MHz, DMSO-d_6)

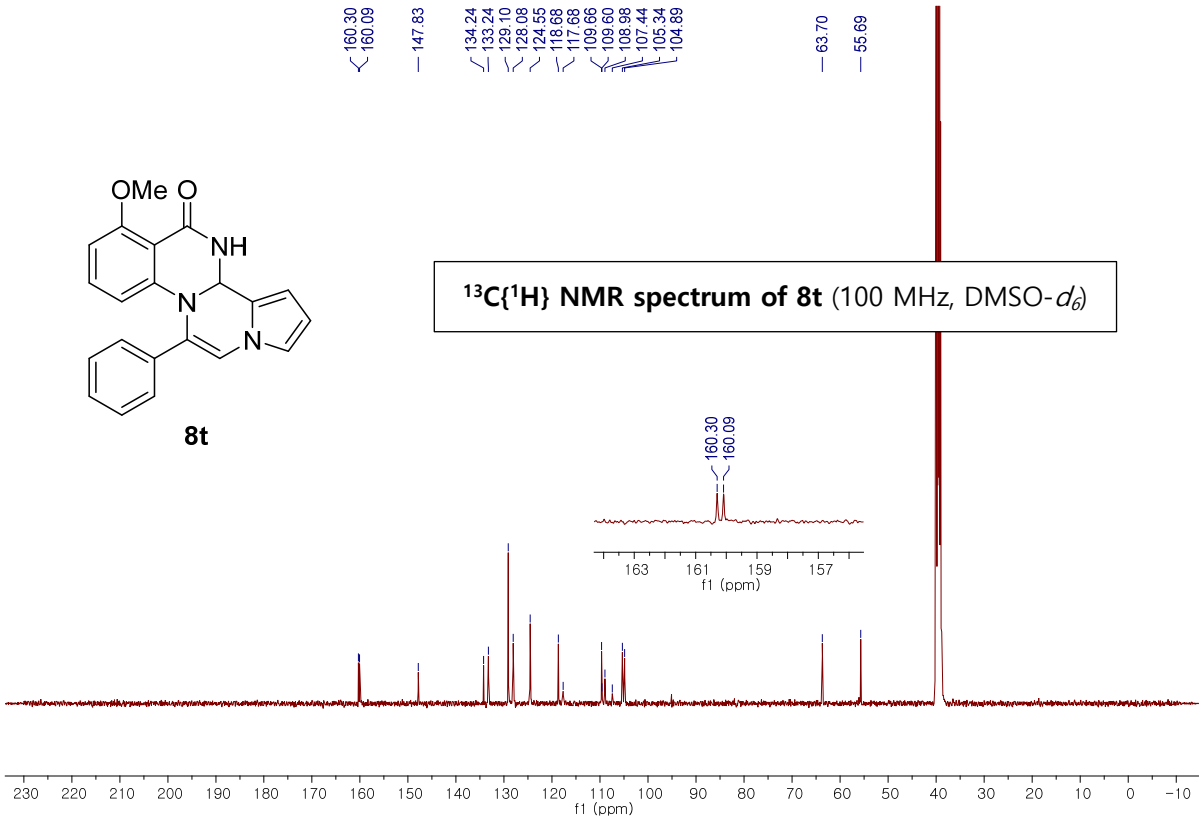

9.200
9.188
8.246
7.636
7.614
7.051
7.029
6.923
6.913
6.235
6.200
6.190
5.840
5.828
3.789
3.785
O
NH
N
N
CO2Me
MeO
8r
1H NMR spectrum of 8r (400 MHz, DMSO-d6)
7.166
7.146
7.127
7.051
7.029
6.923
6.913
6.863
6.844
6.826
6.256
6.235
6.200
6.190
1.04
2.04
1.00
1.06
1.03
1.00
7.2
7.0
6.8
6.6
6.4
6.2
f1 (ppm)
1.00
1.00
1.01
2.03
1.04
2.04
1.00
1.06
1.03
1.00
1.01
6.03
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)

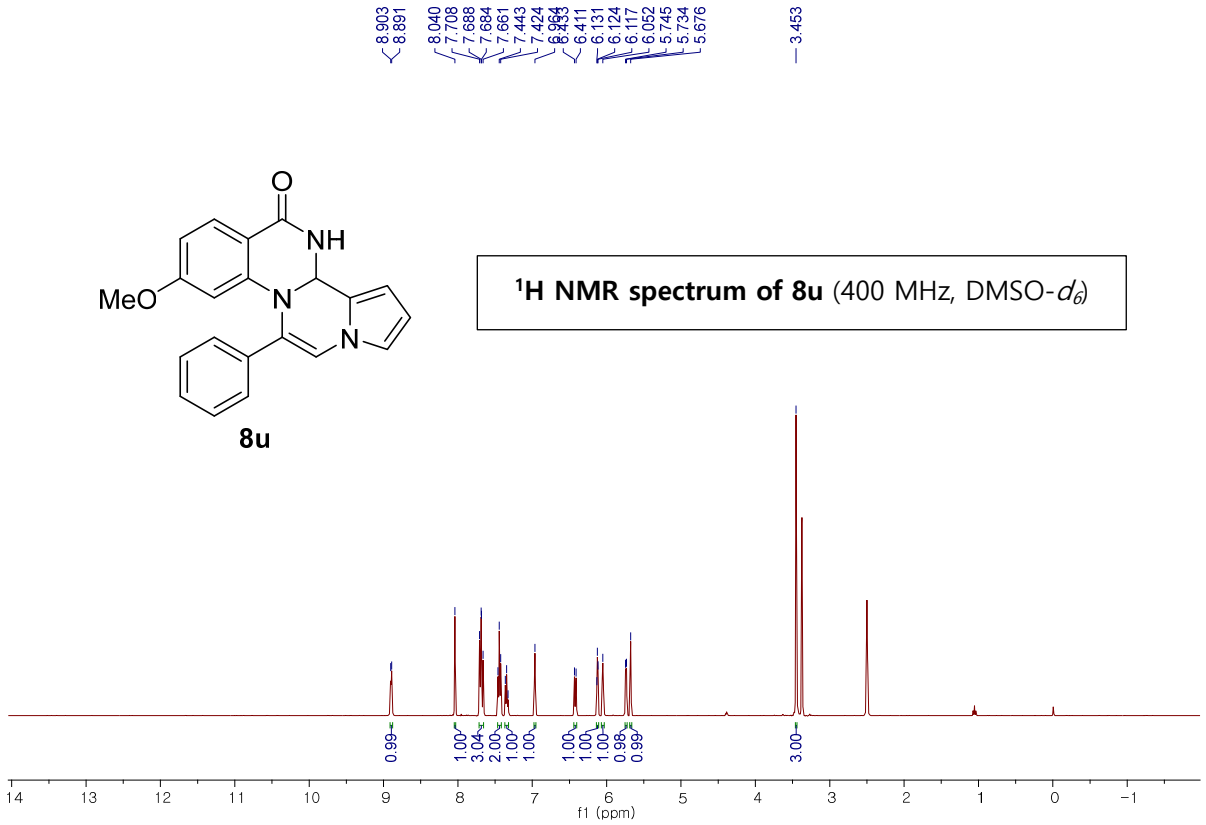

161.53
160.60
159.95
144.68
133.50
130.99
127.66
126.63
125.63
120.41
119.97
118.31
114.87
105.66
63.73
55.31
51.53
O
NH
N
N
CO2Me
MeO
8r
13C{1H} NMR spectrum of 8r (100 MHz, DMSO-d6)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


9.285
9.272
8.572
7.904
7.887
7.869
7.749
7.730
7.566
7.546
7.484
7.465
7.446
7.363
7.345
7.327
7.258
7.240
7.220
7.137
7.122
7.103
7.086
6.819
6.800
6.781
6.533
6.286
6.265
5.945
5.934
O
NH
N
N
8s
1H NMR spectrum of 8s (400 MHz, DMSO-d6)
f1 (ppm)

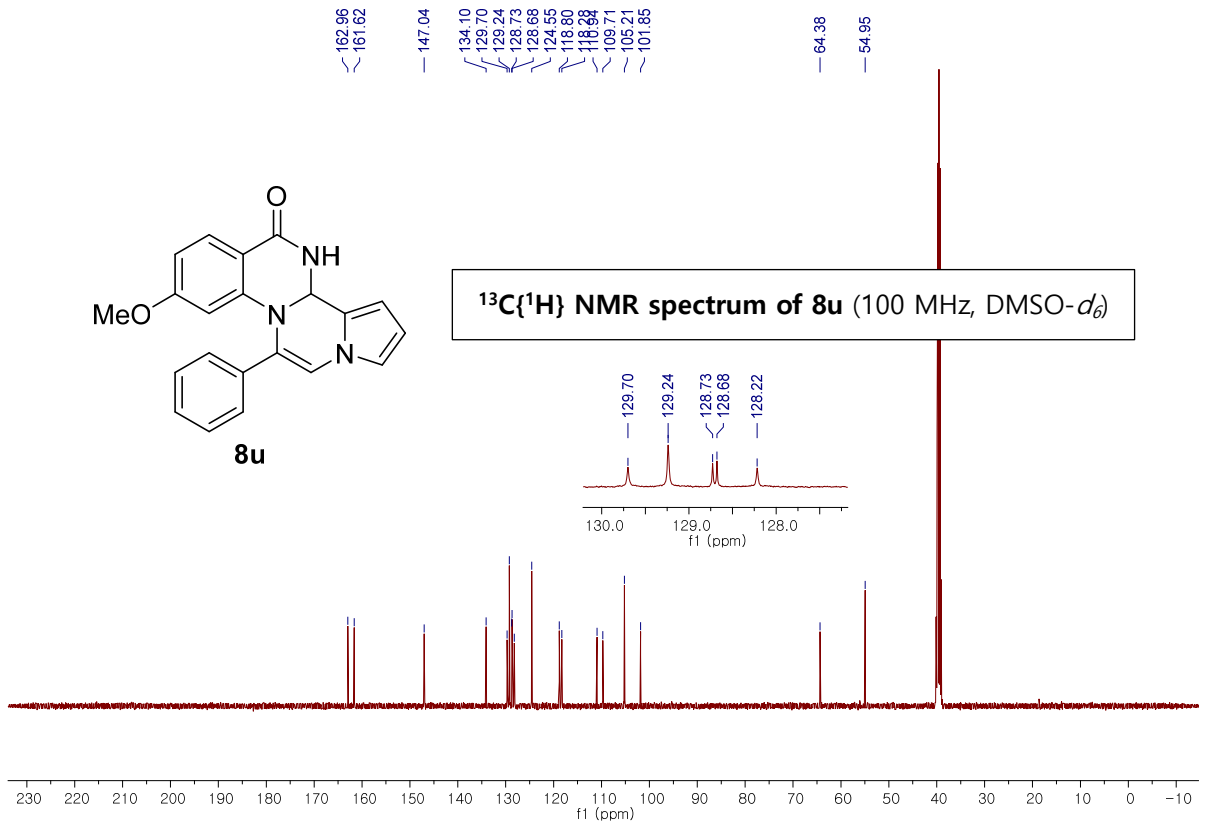

161.88
146.06
135.32
134.22
134.10
129.15
128.09
127.81
127.72
124.34
120.00
117.44
63.99
O
NH
N
N
8s
13C{1H} NMR spectrum of 8s (100 MHz, DMSO-d6)
f1 (ppm)


OMe O
NH
N
N
8t
¹H NMR spectrum of 8t (400 MHz, DMSO-d6)
f1 (ppm)

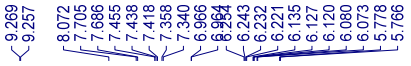

OMe O
NH
N
N
8t
¹³C{¹H} NMR spectrum of 8t (100 MHz, DMSO-d6)
f1 (ppm)

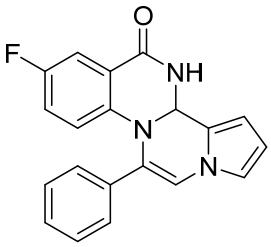


^{1}H NMR spectrum of 8u (400 MHz, DMSO-d_6)



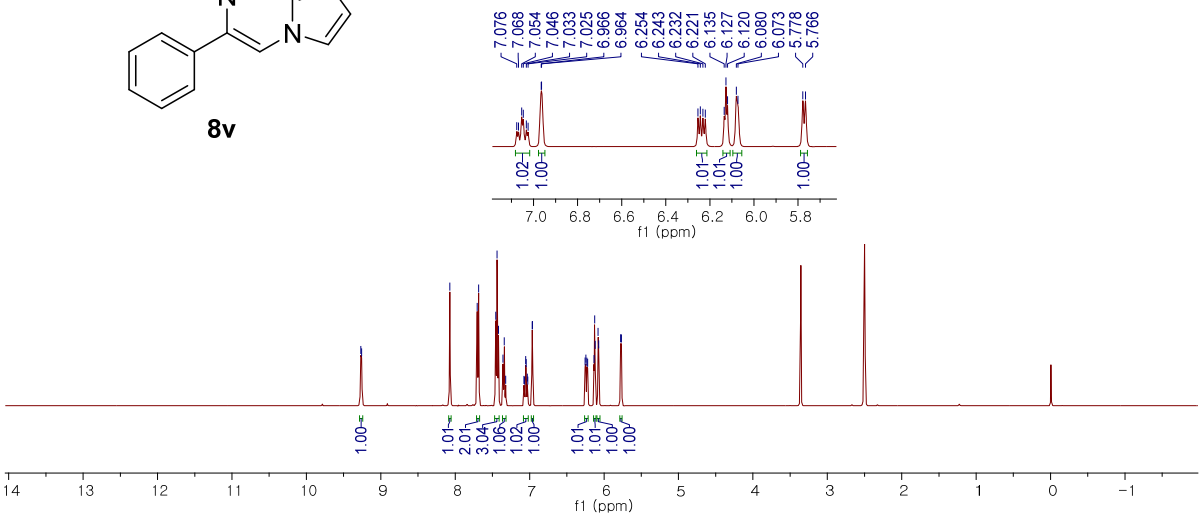
^{13}C{^{1}H} NMR spectrum of 8u (100 MHz, DMSO-d_6)

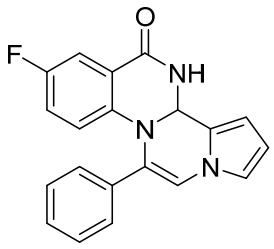




8v

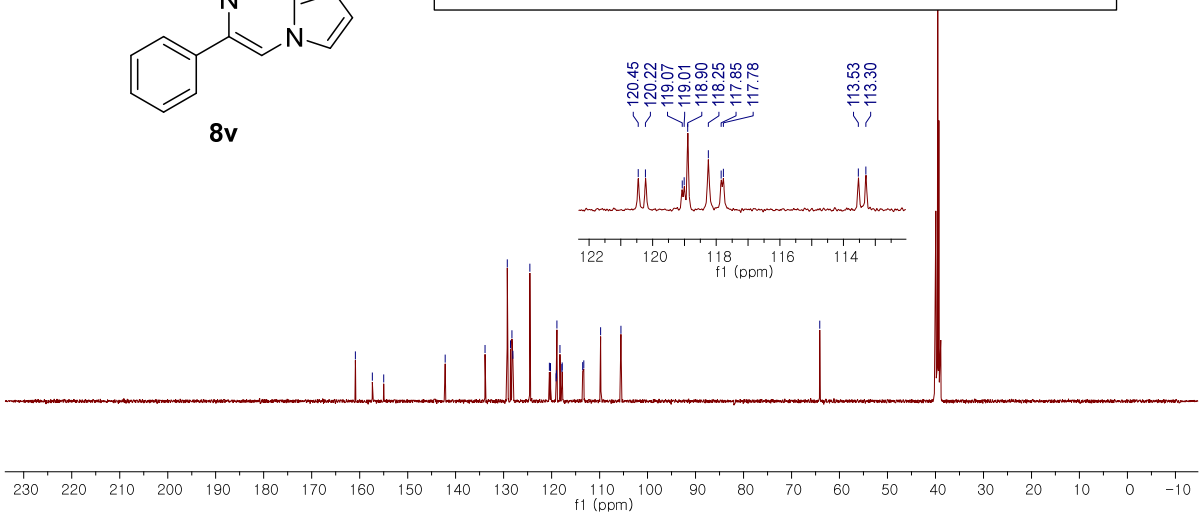
^{1}H NMR spectrum of 8v (400 MHz, DMSO-d_6)

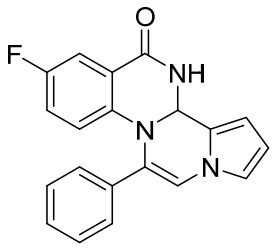




8v

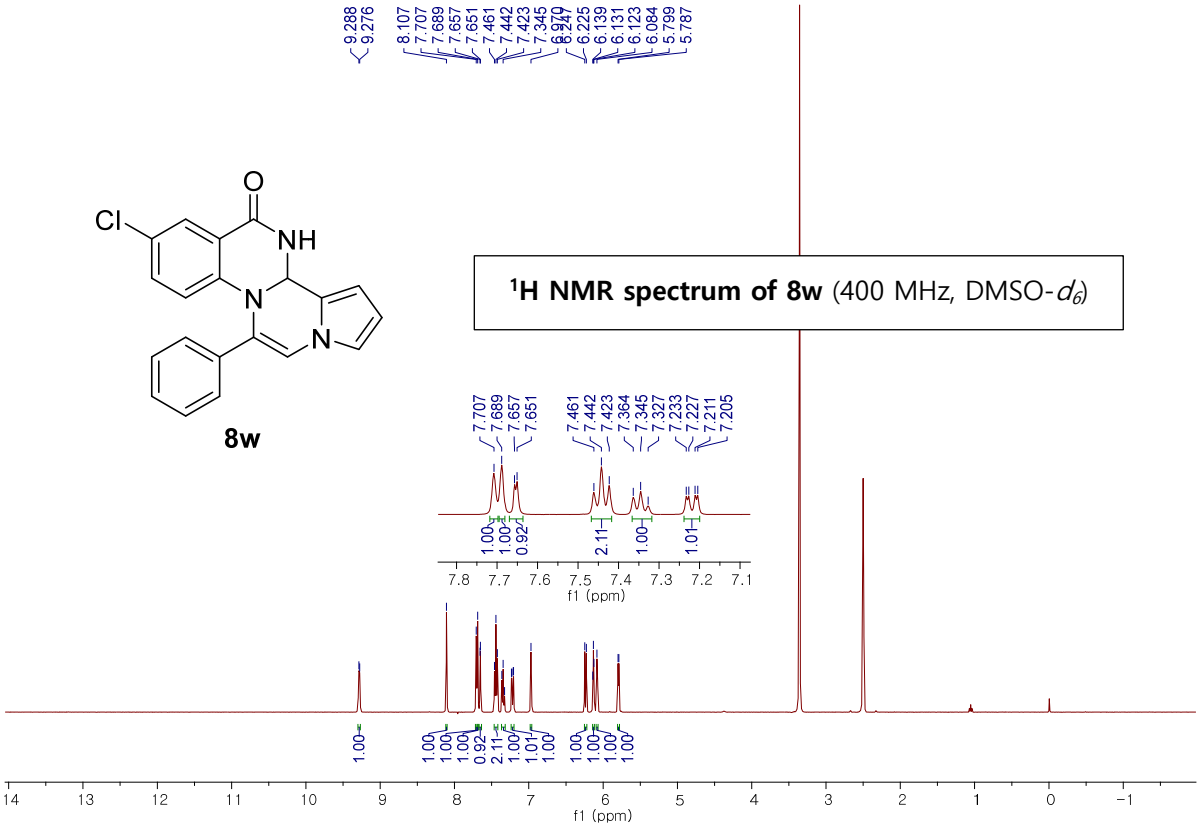
^{13}C{^{1}H} NMR spectrum of 8v (100 MHz, DMSO-d_6)

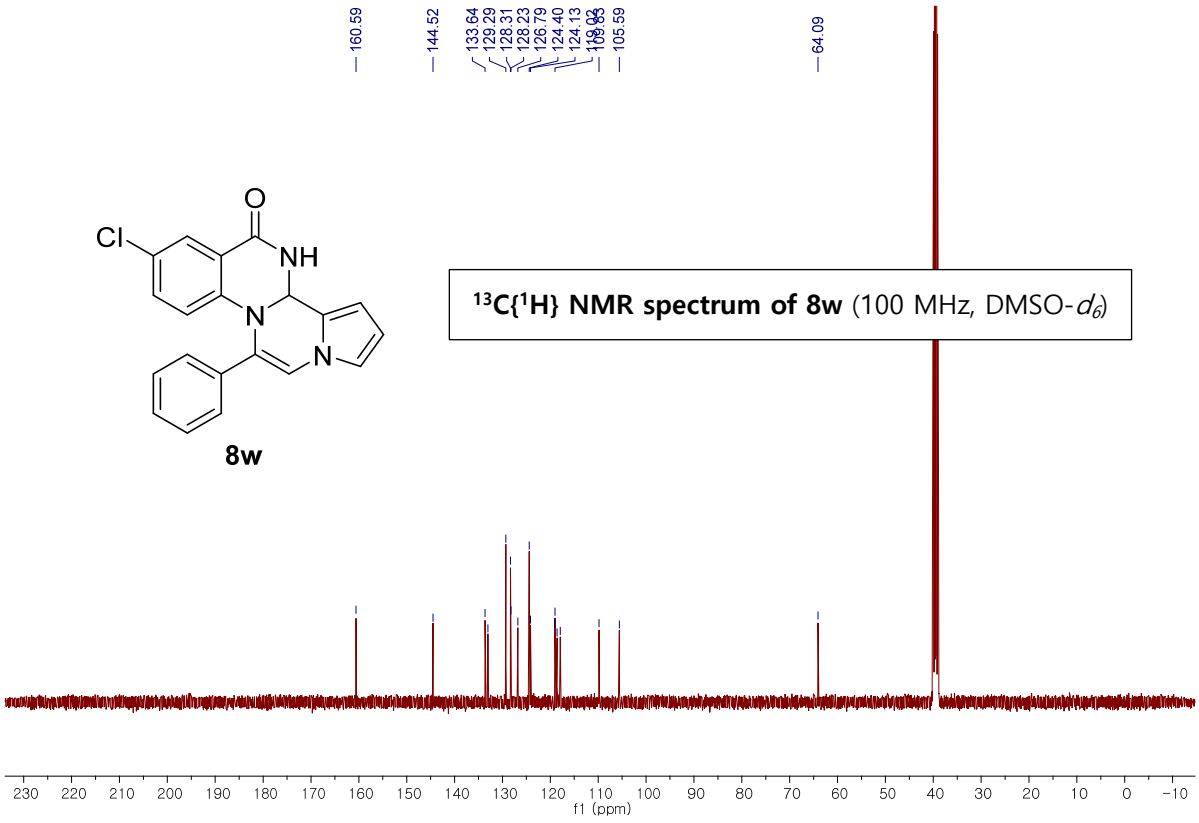


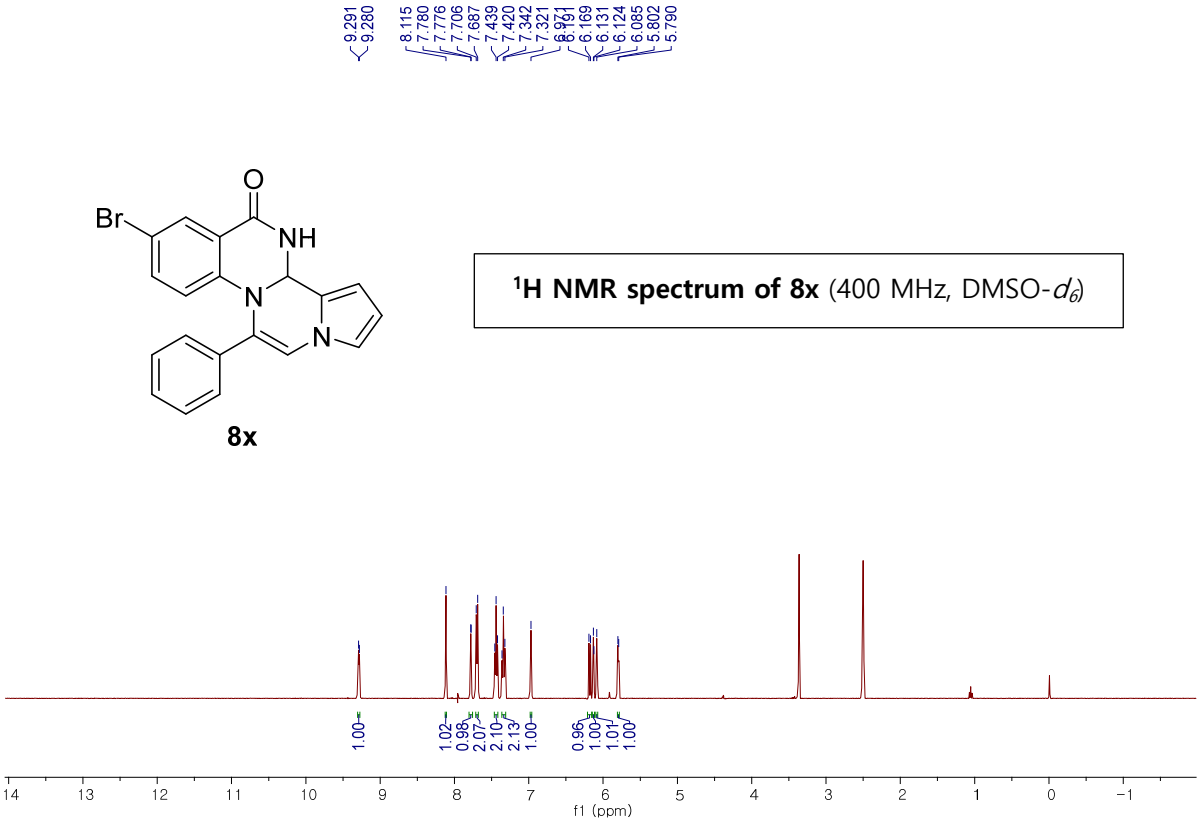


8v

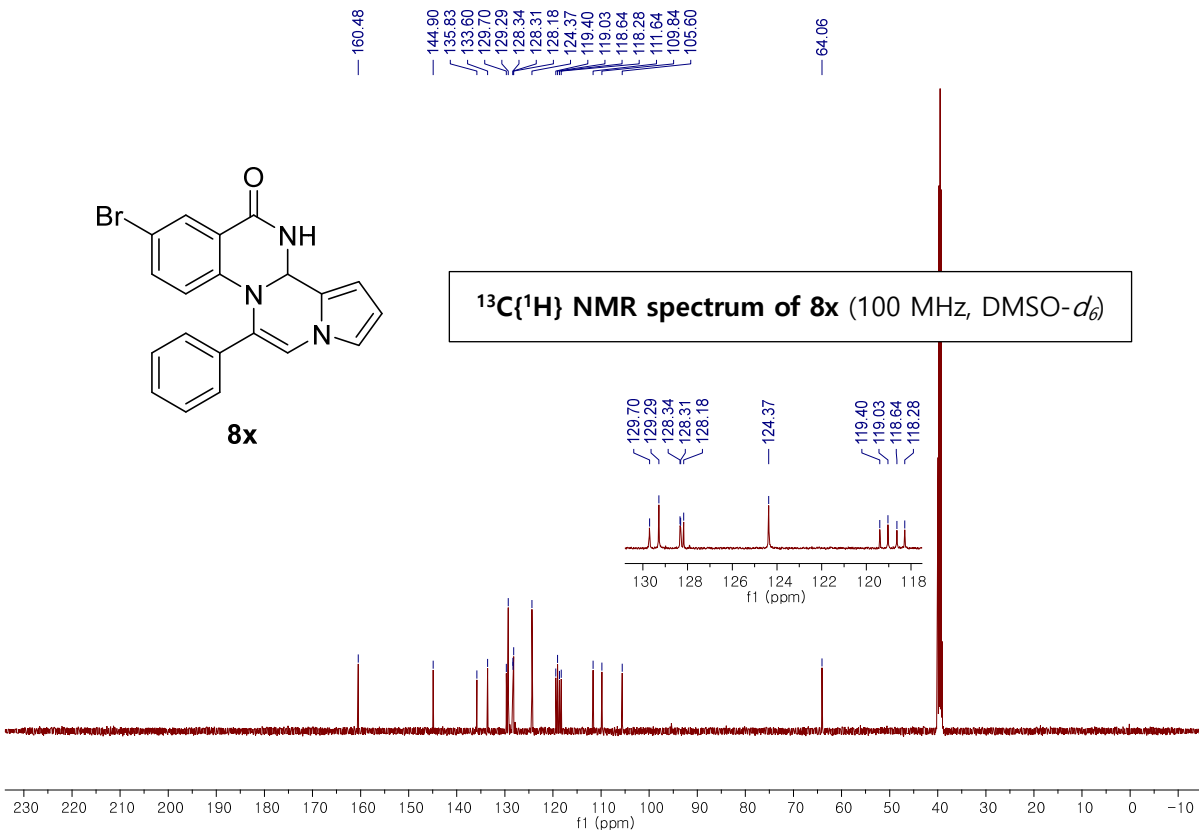
^{19}F NMR spectrum of 8v (376 MHz, DMSO-d_6)


9.288
9.276
8.107
7.707
7.689
7.657
7.651
7.461
7.442
7.423
7.345
6.225
6.139
6.131
6.123
6.084
5.799
5.787
Cl
O
NH
N
N
8w
¹H NMR spectrum of 8w (400 MHz, DMSO-d6)
7.707
7.689
7.657
7.651
7.461
7.442
7.423
7.364
7.345
7.327
7.233
7.227
7.211
7.205
1.00
1.00
0.92
2.11
1.00
1.01
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
1.00
1.00
1.00
0.92
2.11
1.00
1.01
1.00
1.00
1.00
1.00
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)

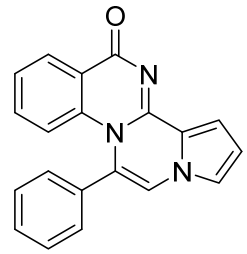

160.59
144.52
133.64
129.29
128.31
128.23
126.79
124.40
124.13
105.59
64.09
Cl
O
NH
N
N
8w
¹³C{¹H} NMR spectrum of 8w (100 MHz, DMSO-d6)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



^{1}H NMR spectrum of 8x (400 MHz, DMSO-d_6)

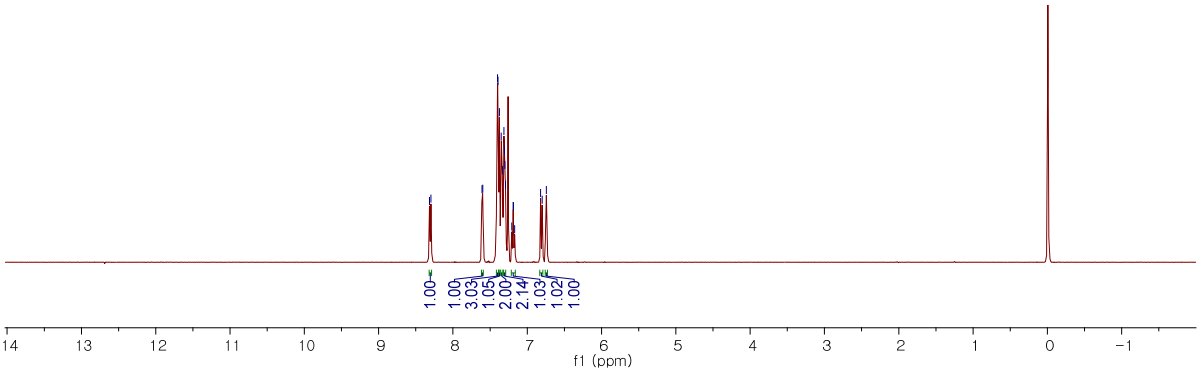


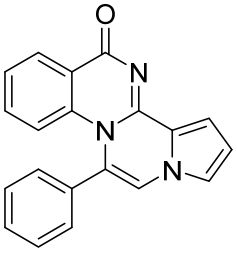
^{13}C{^{1}H} NMR spectrum of 8x (100 MHz, DMSO-d_6)



10a

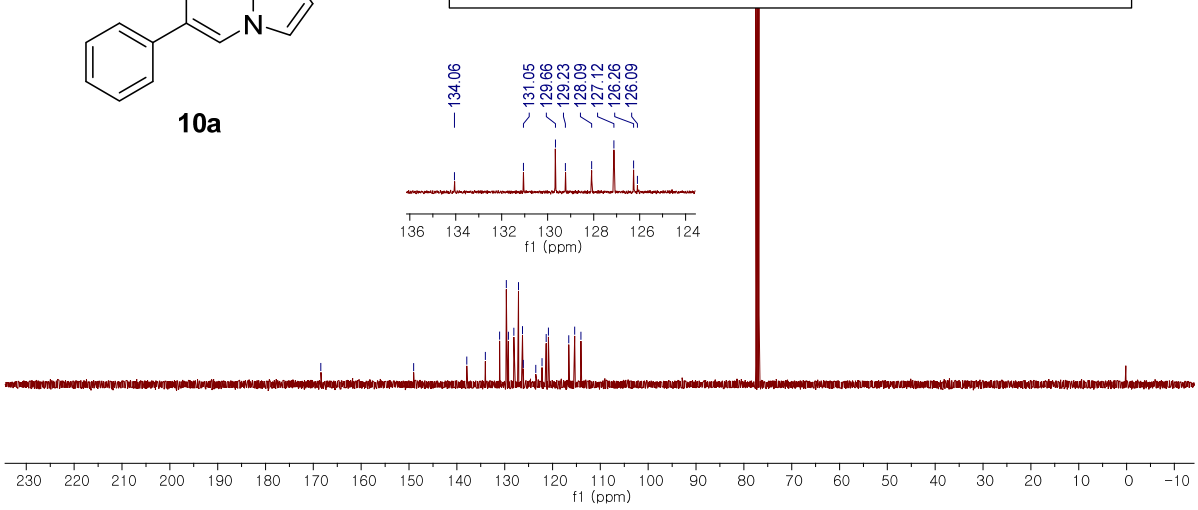
^{1}H NMR spectrum of 10 (400 MHz, $CDCl_3$)

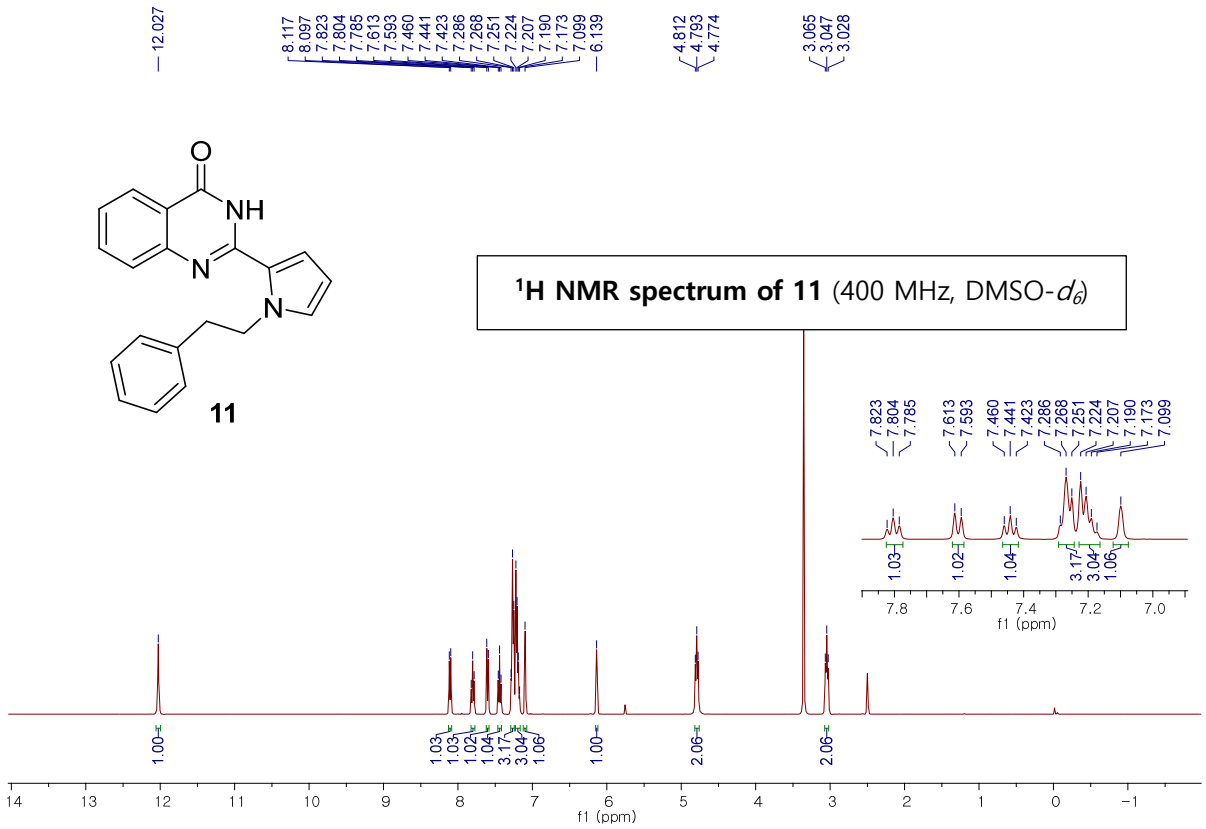


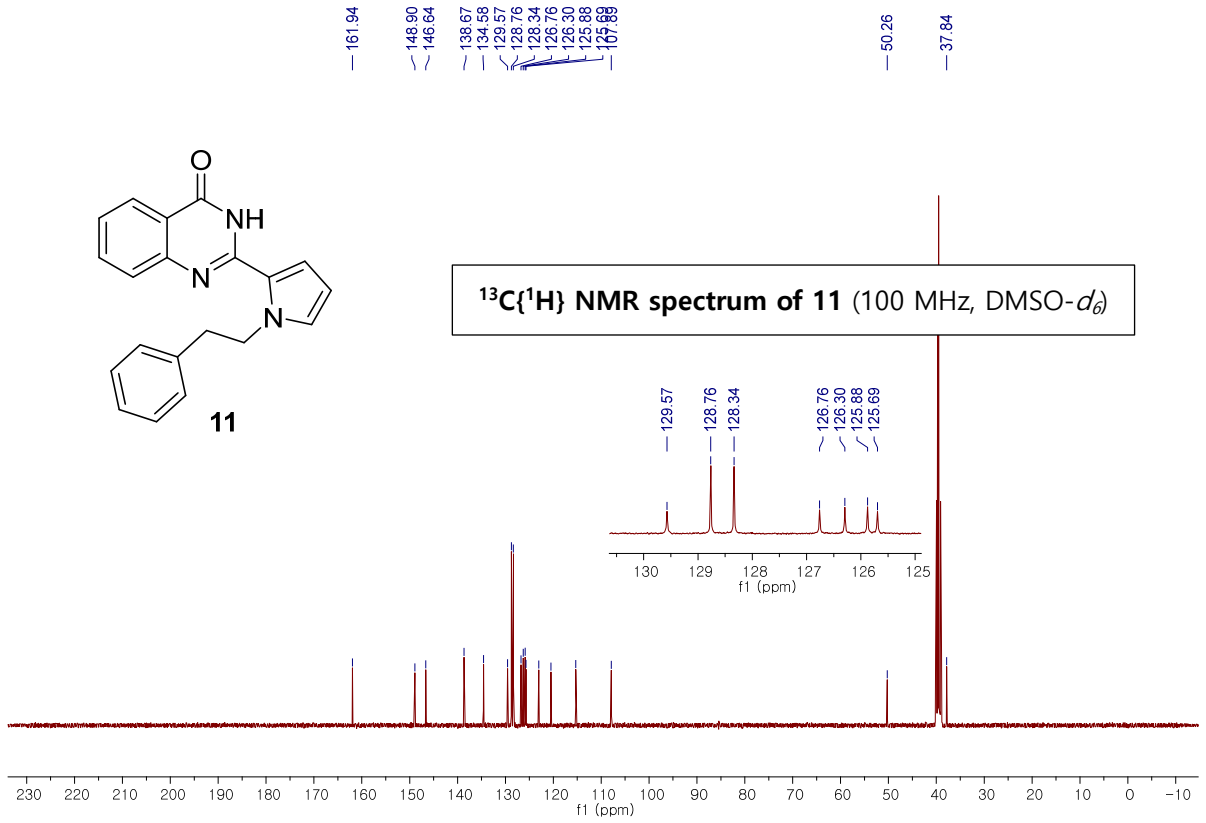


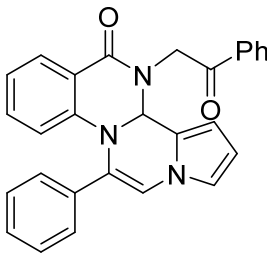
10a

^{13}C{^{1}H} NMR spectrum of 10 (100 MHz, $CDCl_3$)



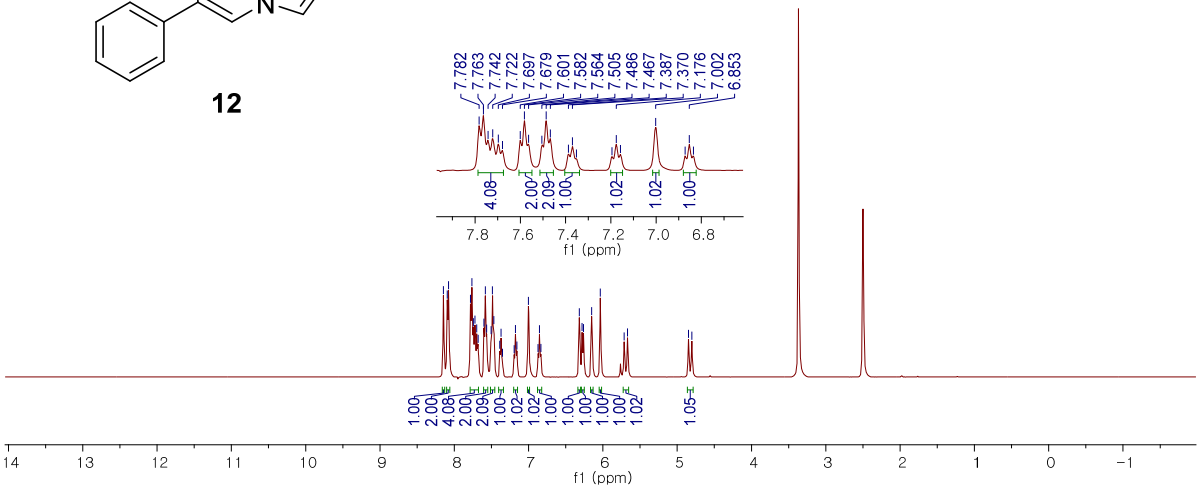

12.027
8.117
8.097
7.823
7.804
7.785
7.613
7.593
7.460
7.441
7.423
7.286
7.268
7.251
7.224
7.207
7.190
7.173
7.099
6.139
4.812
4.793
4.774
3.065
3.047
3.028
O
NH
N
N
11
1H NMR spectrum of 11 (400 MHz, DMSO-d6)
f1 (ppm)

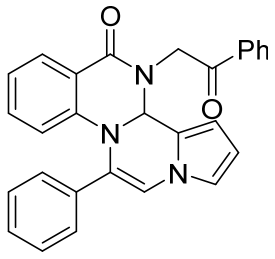

161.94
148.90
146.64
138.67
134.58
129.57
128.76
128.34
126.76
126.30
125.88
125.69
50.26
37.84
O
NH
N
N
11
13C{1H} NMR spectrum of 11 (100 MHz, DMSO-d6)
f1 (ppm)



12

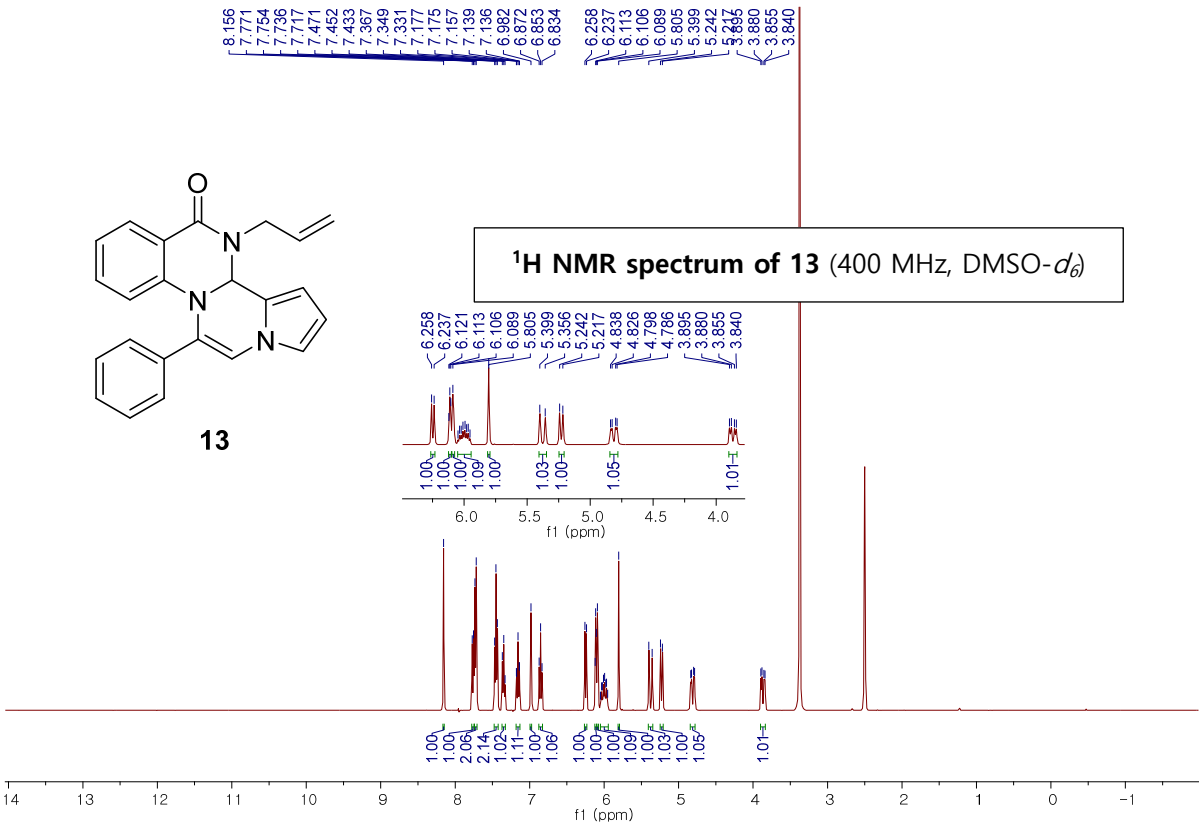
^{1}H NMR spectrum of 12 (400 MHz, DMSO-d_6)

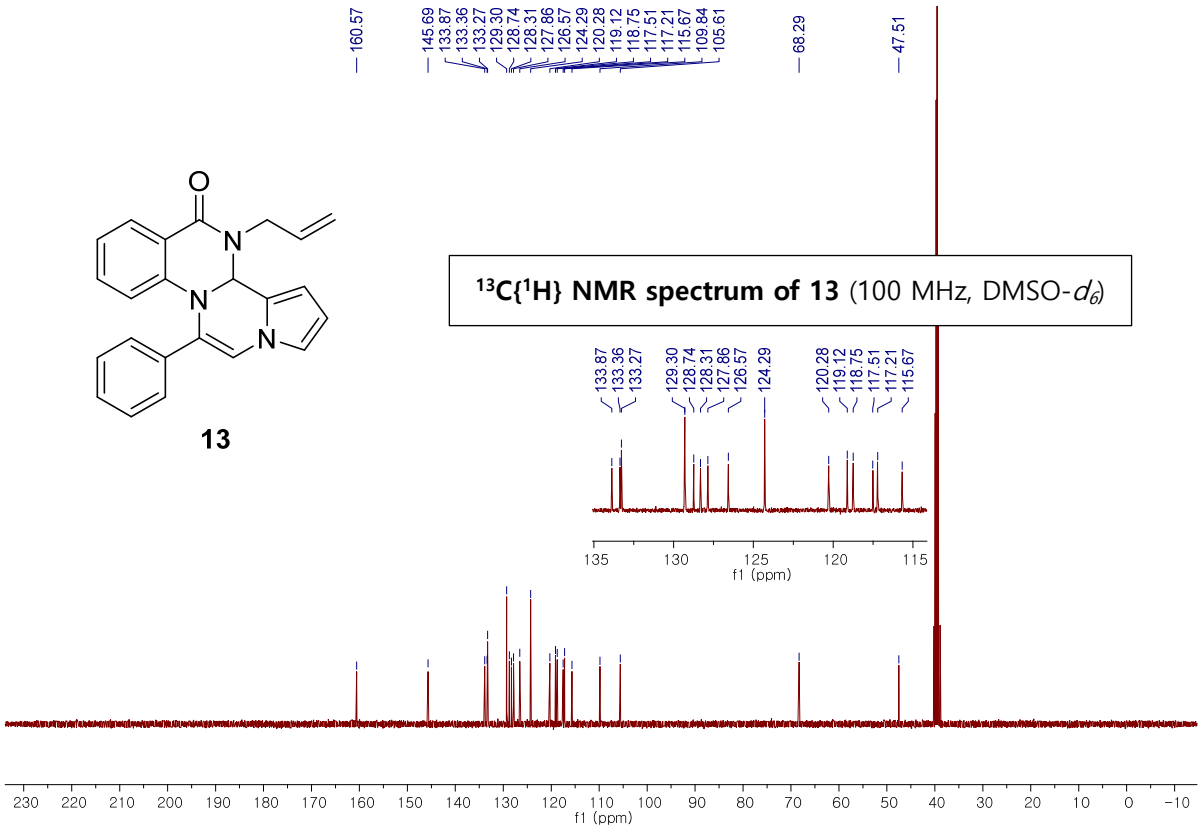


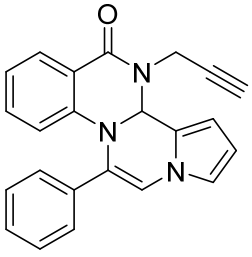


12

^{13}C{^{1}H} NMR spectrum of 12 (100 MHz, DMSO-d_6)

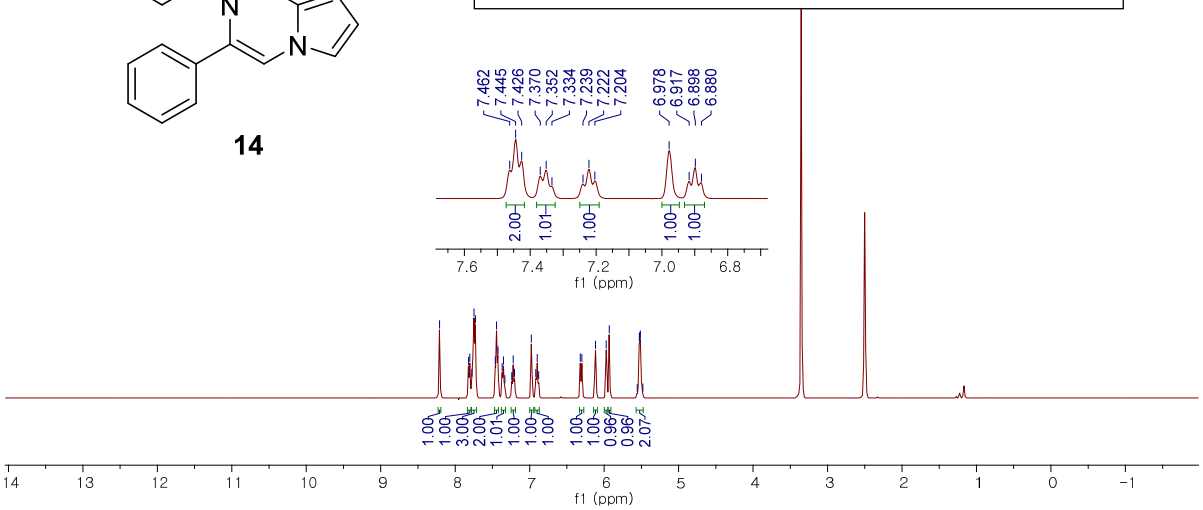

13
^{1}H NMR spectrum of 13 (400 MHz, DMSO-d_6)
f1 (ppm)

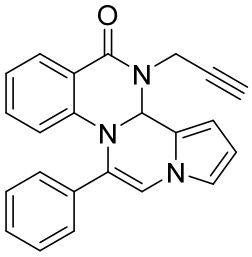

13
^{13}C{^{1}H} NMR spectrum of 13 (100 MHz, DMSO-d_6)
f1 (ppm)



14

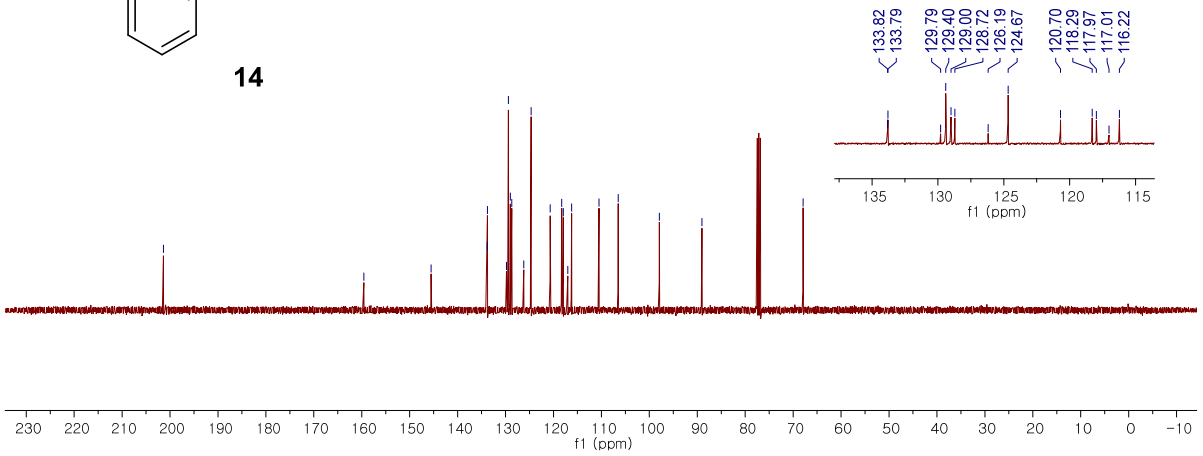
^{1}H NMR spectrum of 14 (400 MHz, DMSO-d_6)

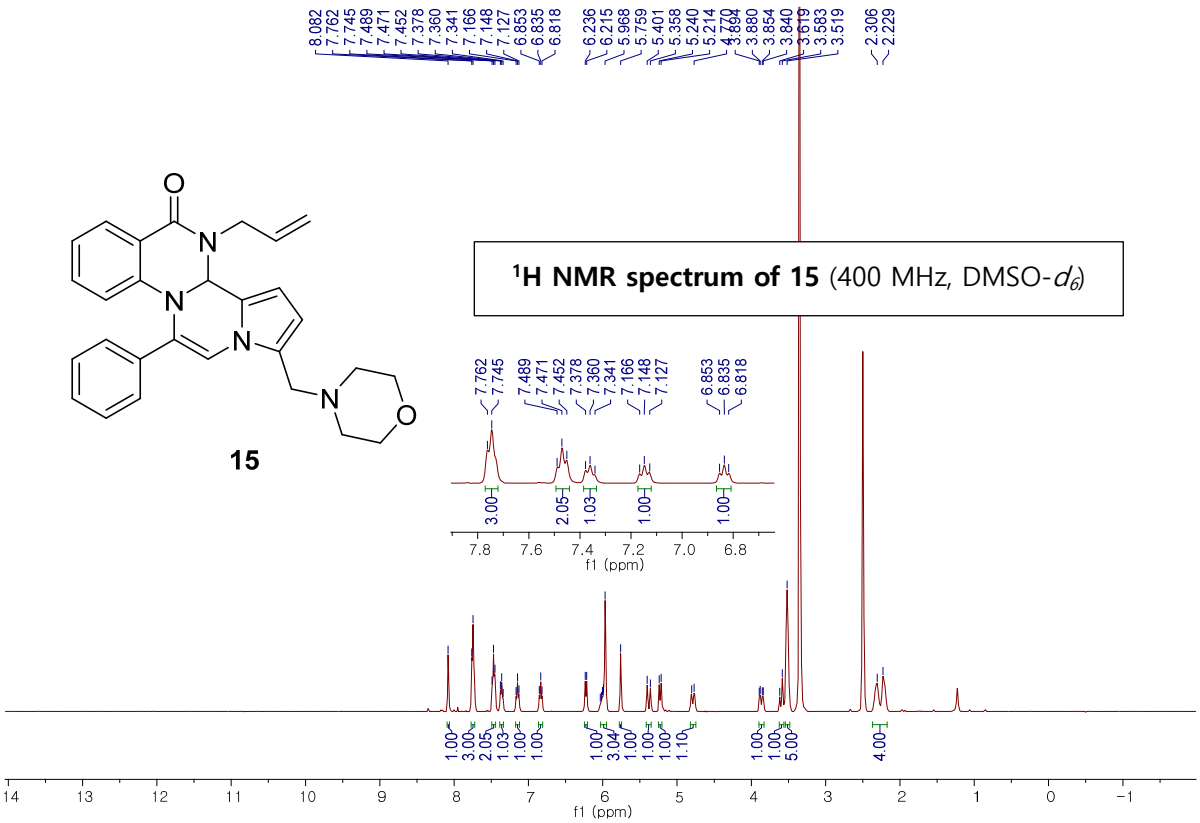


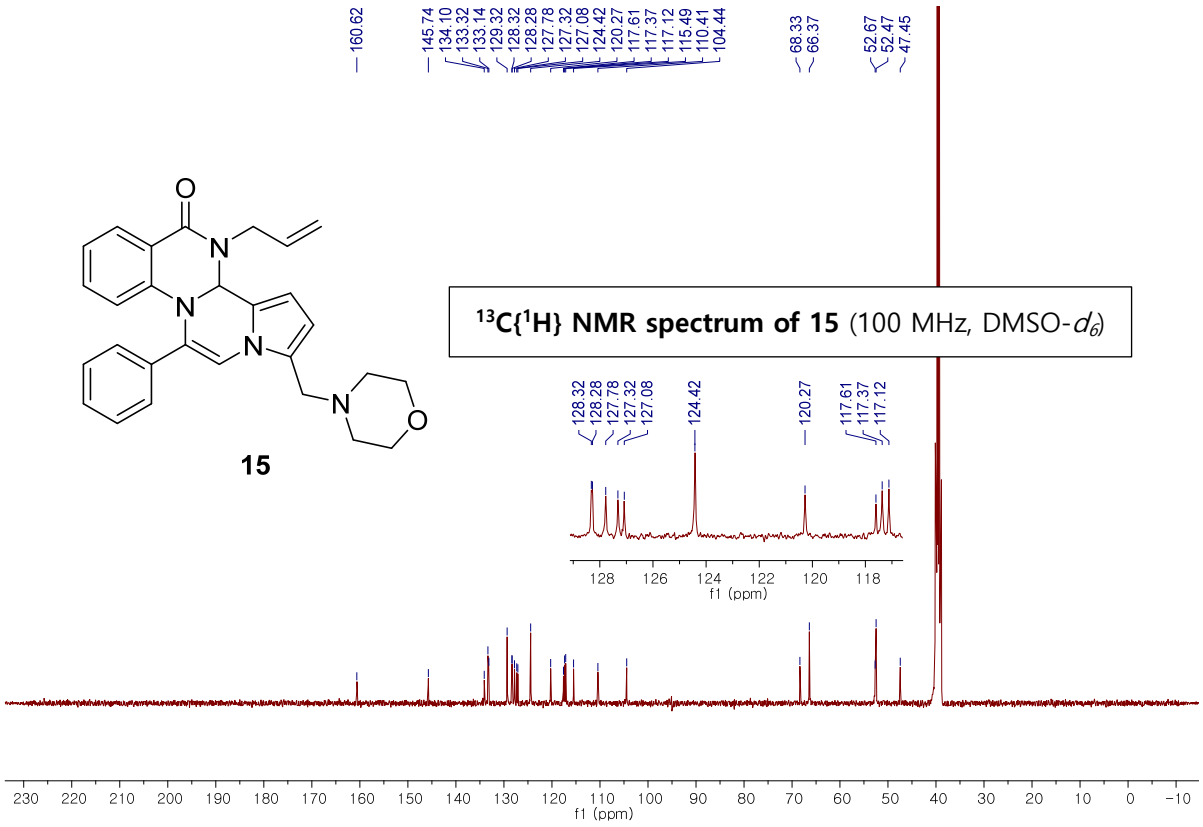


14

^{13}C{^{1}H} NMR spectrum of 14 (100 MHz, $CDCl_3$)




15
1H NMR spectrum of 15 (400 MHz, DMSO-d6)
f1 (ppm)


15
13C{1H} NMR spectrum of 15 (100 MHz, DMSO-d6)
f1 (ppm)

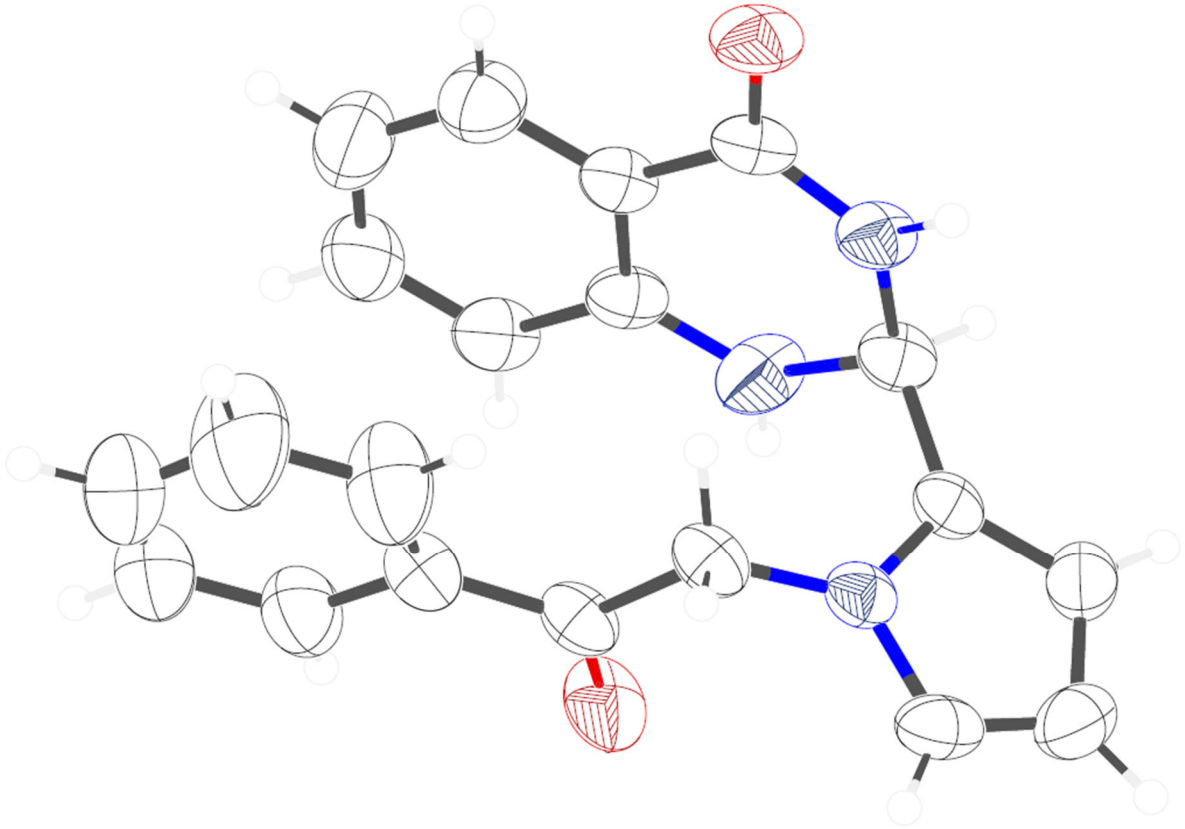


Figure S1. Thermal ellipsoid plot for **7a** with 50 % probability

The crystal **7a** for X-ray crystallographic analysis was obtained via dissolution of the compound in a mixed solvent (THF/EtOH, 1:1) and slow evaporation of the solvent at room temperature.

Table S1. Crystal data for 2-(1-(2-Oxo-2-phenylethyl)-1*H*-pyrrol-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one 7a.

Identification code	2-(1-(2-Oxo-2-phenylethyl)-1*H*-pyrrol-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one 7a	
Chemical formula	$C_{20}H_{17}N_3O_2$	
Formula weight	331.36 g/mol	
Temperature/K	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.200 × 0.500 × 0.800 mm	
Crystal habit	Clear white Block	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.809(3) Å	α = 99.417(4)°
	b = 9.962(4) Å	β = 109.569(4)°
	c = 11.501(4) Å	γ = 95.765(4)°
Volume	820.0(5) $Å^3$	
Z	2	
Density (calculated)	1.342 g/cm^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	348	

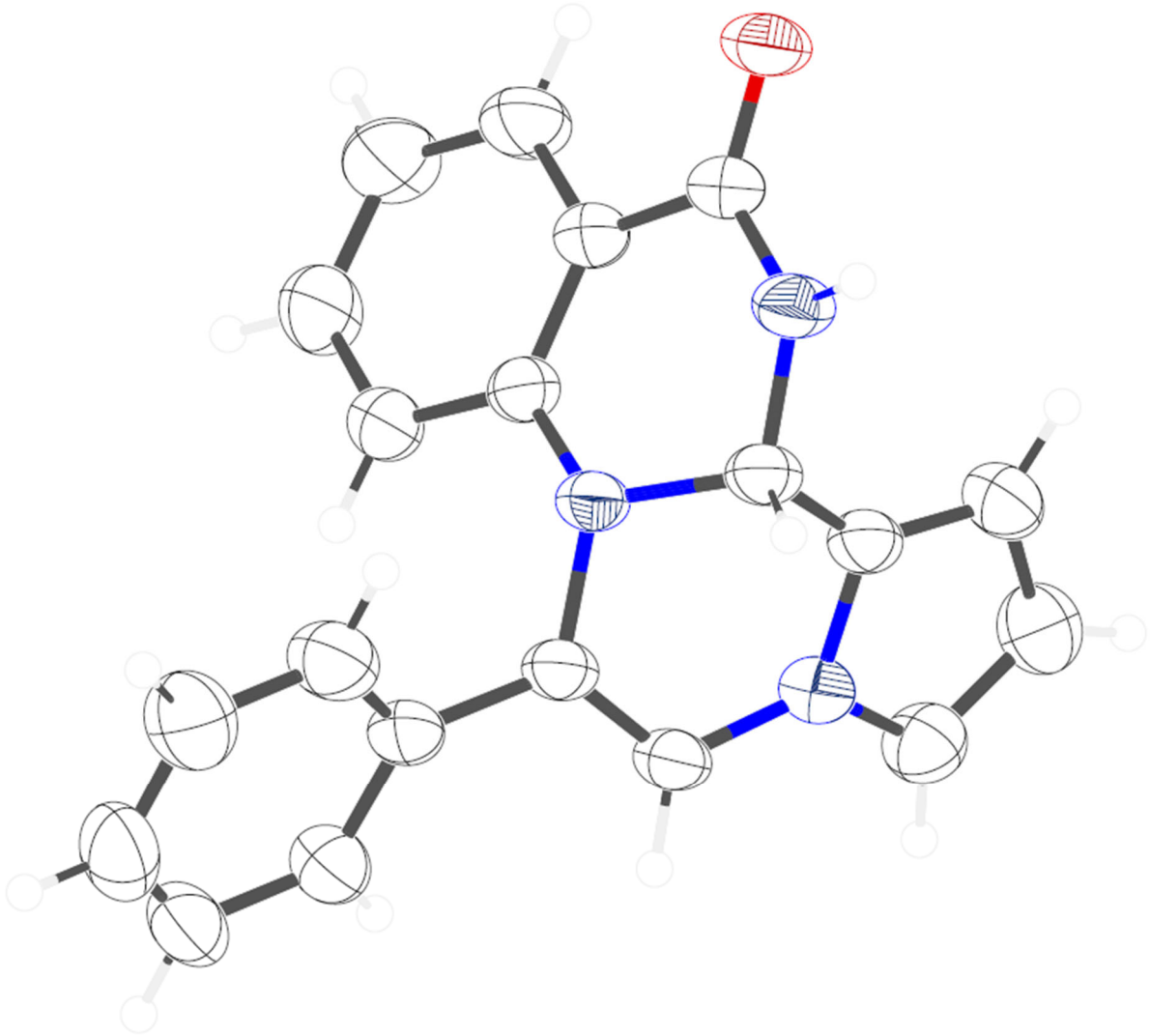


Figure S2. Thermal ellipsoid plot for **8a** with 50 % probability

The crystal **8a** for X-ray crystallographic analysis was obtained via dissolution of the compound in a mixed solvent (acetone/EtOH, 1:1) and slow evaporation of the solvent at room temperature.

Table S2. Crystal data for 11-Phenyl-3b,4-dihydro-5*H*-pyrrolo[2',1':3,4]pyrazino[1,2-*a*]quinazolin-5-one 8a.

Identification code	11-Phenyl-3b,4-dihydro-5*H*-pyrrolo[2',1':3,4]pyrazino[1,2-*a*]quinazolin-5-one 8a	
Chemical formula	$C_{20}H_{15}N_3O$	
Formula weight	313.35 g/mol	
Temperature/K	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.220 × 0.300 × 0.380 mm	
Crystal habit	Clear yellow Block	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.3010(5) Å	α = 68.139(2)°
	b = 9.0115(5) Å	β = 81.424(2)°
	c = 11.8908(6) Å	γ = 86.433(2)°
Volume	816.27(8) $Å^3$	
Z	2	
Density (calculated)	1.275 g/cm^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	328	