Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Pd(TFA)$_2$-catalyzed direct arylation of quinoxalinones with arenes

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General experimental information

All the reactions were carried out under nitrogen atmosphere in a 25 mL two-necked round-bottom flask with magnetic stirring. Quinoxalin-2(*H*)-one derivatives were synthesized according to literature procedure.[1] Merck precoated silica gel plates (Art. 5554) with a fluorescent indicator were used for analytical thin layer chromatography (TLC). Visualization was done under a UV lamp (254 nm). Melting points were determined with micro-cover glasses on a Fisher-Johns apparatus and are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian VNS or DPX (600 or 300 MHz and 150 or 75 MHz, respectively) spectrometers in $CDCl_3$. Chemical shifts for protons were reported as parts per million in δ scale using solvent residual peak ($CHCl_3$: 7.24 ppm or DMSO-d_6: 2.50 ppm) as internal standard. Chemical shifts of ^{13}C NMR spectra were reported in ppm from the central peak of $CDCl_3$ (77.00 ppm) or DMSO-d_6 (39.50 ppm) on the δ scale. Data are represented as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, dd = double of doublet, t = triplet, q = quartet, td = triplet of doublet, sept = septet, m = multiplet or overlap of non-equivalent resonances), and coupling constant (*J* in Hz). IR spectra were recorded on a PerkinElmer Spectrum Two™ IR spectrometer with frequencies expressed in cm^{-1}. High-resolution mass spectrometry (HRMS) were obtained with a JEOL JMS-700 spectrometer at the Korea Basic Science Institute. X-ray diffraction (XRD) was performed using powdered samples on a PANalytical X'PertPRO MPD (operating at 40 kV and 30 mA with Cu Kα as the X-ray source (λ=1.5406Å) over the 2θ angle range, 20° to 80°, and a scanning rate of 1.2°/min.

General procedure for the 3-arylation of quinoxalin-2(*H*)-ones

A mixture of quinoxalin-2(*H*)-one (1.0 mmol), $Pd(TFA)_2$ (33 mg, 10 mol %) and Ag_2O (346 mg, 1.5 mmol) in arene (3.0 mL), taken in a 25mL two-necked round-bottom flask was sealed and stirred at 110 ^{o}C for 20 h under nitrogen atmosphere. After completion of the reaction, as monitored by TLC, solvent was evaporated in vacuum, and the residue was subjected to column chromatography using ethyl acetate in hexanes as the eluent to afford pure 3-aryl-quinoxalin-2(*H*)-one derivatives (**3**, **4**, **5** and **7**).

Spectroscopic data of synthesized compounds

1-Methyl-3-phenylquinoxalin-2(1*H*)-one (3a): The compound was prepared according to the general procedure. Yield: 75% (177 mg); Appearance: Light yellow crystalline solid; Mp: 133-135 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.31-8.29 (2H, m), 7.91 (1H, dd, J = 7.8, 1.2 Hz), 7.51 (1H, td, J = 7.2, 1.2 Hz), 7.47-7.45 (3H, m), 7.32 (1H, td, J = 7.8, 1.2 Hz), 7.27 (1H, dd, J = 8.4, 1.2 Hz), 3.71 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.6, 153.9, 135.9, 133.2, 132.9, 130.3, 130.2, 130.1, 129.5, 127.9, 123.6, 113.5, 29.2; IR: 1644, 1573, 1492, 1463, 1297, 1236, 1059, 948 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{15}H_{12}N_2O$: 236.0950, Found: 236.0952.

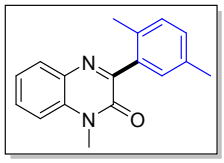
1-Methyl-3-(*p*-tolyl)quinoxalin-2(1*H*)-one and 1-Methyl-3-(*o*-tolyl)quinoxalin-2(1*H*)-one (3b): The compound was prepared according to the general procedure. The product was obtained as a regioisomeric mixture. The isomeric ratio was found to be 5:1 (*p*:*o*) as per NMR. Combined yield: 78% (195 mg); Appearance: Light yellow crystalline solid; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.23 (2H, d, J = 8.1 Hz), 7.92 (1H, d, J = 8.1 Hz), 7.55 (1H, t, J = 7.2 Hz), 7.38-7.25 (4H, m), 3.76 (3H, s), 2.41 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.8, 154.0, 140.6, 133.3, 133.3, 133.1, 130.3, 130.0, 129.5, 128.8, 123.6, 113.5, 29.3, 21.5; IR: 1629, 1590, 1462, 1290, 1230, 1180, 953 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{16}H_{14}N_2O$: 250.1106, Found: 250.1103.

3-(4-Isopropylphenyl)-1-methylquinoxalin-2(1*H*)-one (3c): The compound was prepared according to the general procedure. Yield: 75% (208 mg); Appearance: Yellow liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.22 (2H, d, J = 8.4 Hz), 7.91 (1H, d, J = 7.8 Hz), 7.53 (1H, t, J = 7.8 Hz), 7.53-7.29 (4H, m), 3.74 (3H, s), 2.96 (1H, sept, J = 6.6 Hz), 1.27 (6H, d, J = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.7, 154.1, 151.4, 133.6, 133.2, 133.1, 130.3, 130.0, 129.5, 126.2, 123.6, 113.4, 34.1, 29.2, 23.8; IR: 1639, 1578, 1462, 1292, 1232, 841, 755 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{18}H_{18}N_2O$: 278.1419, Found: 278.1422

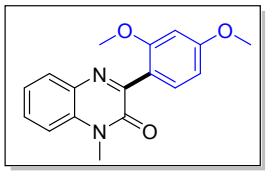
3-(4-Methoxyphenyl)-1-methylquinoxalin-2(1*H*)-one (3d): The compound was prepared according to the general procedure. Yield: 80% (213 mg); Appearance: Light yellow crystalline solid; Mp: 128-130 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.38 (2H, d, J = 7.8 Hz), 7.91 (1H, d, J = 7.8 Hz), 7.52 (1H, t, J = 7.8 Hz), 7.34 (1H, t, J = 7.2 Hz), 7.30 (1H, d, J = 8.4 Hz), 6.98 (2H, d, J = 7.8 Hz), 3.86 (3H, s), 3.75 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.5, 154.8,

153.2, 133.1, 133.0, 131.4, 130.1, 129.8, 128.6, 123.7, 113.5, 55.4, 29.3; IR: 1630, 1604, 1571, 1504, 1461, 1244, 1171, 1033 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{16}H_{14}N_2O_2$: 266.1055, Found: 266.1053.

3-(2,5-Dimethylphenyl)-1-methylquinoxalin-2(1*H*)-one (3e): The compound was prepared according to the general procedure. Yield: 67% (177 mg); Appearance: Light yellow crystalline solid; Mp: 135-137 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 7.91 (1H, dd, J = 8.4, 1.2 Hz), 7.58 (1H, t, J = 8.4 Hz), 7.37-7.34 (2H, m), 7.24 (1H, s), 7.17-7.13 (2H, m), 3.74 (3H, s), 2.33 (3H, s), 2.27 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.6, 154.4, 135.9, 134.9, 133.5, 133.4, 132.8, 130.3, 130.3, 130.0, 129.4, 123.6, 113.6, 29.2, 20.8, 19.3; IR: 1646, 1599, 1462, 1305, 809, 759 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{17}H_{16}N_2O$: 264.1263, Found: 264.1260.

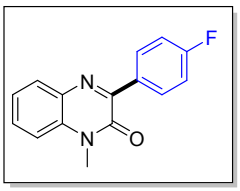


3-(2,4-Dimethoxyphenyl)-1-methylquinoxalin-2(1*H*)-one (3f): The compound was prepared according to the general procedure. Yield: 83% (246 mg); Appearance: Yellow crystalline solid; Mp: 175-177 °C; ^1H NMR (300 MHz, $CDCl_3$): δ 7.91 (1H, d, J = 7.8 Hz), 7.54 (1H, td, J = 9.0, 1.5 Hz), 7.39-7.31 (3H, m), 6.60-6.55 (2H, m), 3.84 (3H, s), 3.79 (3H, s), 3.73 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.2, 159.2, 156.8, 154.5, 133.6, 132.9, 130.9, 130.2, 130.1, 123.4, 119.3, 113.6, 104.9, 99.1, 55.9, 55.5, 29.3; IR: 1661, 1609, 1576, 1507, 1309, 1255, 1026, 822 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{17}H_{16}N_2O_3$: 296.1161, Found: 296.1159.



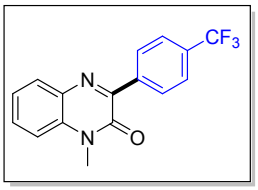
3-(4-Chlorophenyl)-1-methylquinoxalin-2(1*H*)-one (3g): The compound was prepared according to the general procedure. Yield: 58% (156 mg); Appearance: Yellow crystalline solid; Mp: 180-182 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 8.31 (2H, d, J = 8.4 Hz), 7.88 (1H, d, J = 8.4 Hz), 7.53 (1H, t, J = 7.2 Hz), 7.40 (2H, d, J = 8.4 Hz), 7.34 (1H, t, J = 6.6 Hz), 7.28 (1H, d, J = 8.4 Hz), 3.71 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.4, 152.4, 136.4, 134.3, 133.2, 132.8, 130.9, 130.4, 130.3, 128.1, 123.7, 113.5, 29.2; IR: 1628, 1598, 1582, 1460, 1284, 1225, 1093, 1012 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{15}H_{11}ClN_2O$: 270.0560, Found: 270.0562.

3-(4-Fluorophenyl)-1-methylquinoxalin-2(1*H*)-one (3h): The compound was prepared



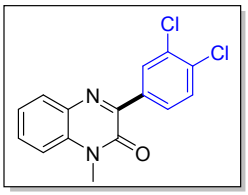
according to the general procedure. Yield: 52% (132 mg); Appearance: yellow crystalline solid; Mp: 176-178 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.31 (2H, d, J = 8.4 Hz), 7.88 (1H, d, J = 8.4 Hz), 7.53 (1H, t, J = 7.2 Hz), 7.40 (2H, d, J = 8.4 Hz), 7.34 (1H, t, J = 6.6 Hz), 7.28 (1H, d, J = 8.4 Hz), 3.71 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2 (d, J = 249.0 Hz), 154.6, 152.7, 133.3, 132.9, 132.1 (d, J = 1.5 Hz), 131.8 (d, J = 9.0 Hz), 130.4, 130.3, 123.8, 115.0 (d, J = 21.0 Hz), 113.5, 29.3; IR: 1629, 1596, 1501, 1294, 1226, 1159, 842 cm^{-1}; HRMS (EI) *m/z* calcd for $C_{15}H_{11}FN_2O$: 254.0855, Found: 254.0853.

1-Methyl-3-(4-(trifluoromethyl)phenyl)quinoxalin-2(1*H*)-one (3i): The compound was



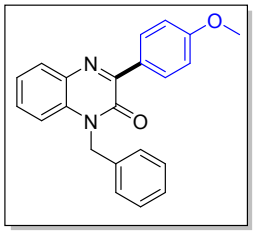
prepared according to the general procedure. Yield: 50% (152 mg); Appearance: Yellow crystalline solid; Mp: 168-170 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.44 (2H, d, J = 7.8 Hz), 7.94 (1H, d, J = 7.8 Hz), 7.71 (2H, d, J = 7.8 Hz), 7.59 (1H, t, J = 7.2 Hz), 7.38 (1H, t, J = 7.2 Hz), 7.34 (1H, d, J = 8.4 Hz), 3.76 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.5, 152.5, 139.2, 133.5, 132.9, 131.7 (q, J = 32.7 Hz), 131.0, 130.7, 129.8, 124.9 (q, J = 4.5 Hz), 124.3 (q, J = 378.5 Hz), 123.9, 113.6, 29.3; IR: 1651, 1635, 1599, 1320, 1293, 1163, 1100, 1070 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{16}H_{11}F_3N_2O$: 304.0823, Found: 304.0820.

3-(3,4-Dichlorophenyl)-1-methylquinoxalin-2(1*H*)-one (3j): The compound was prepared

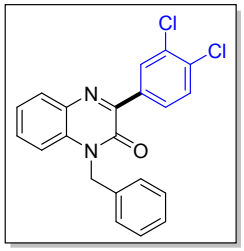


according to the general procedure. Yield: 58% (177 mg); Appearance: Yellow crystalline solid; Mp: 190-192 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.55 (1H, d, J = 2.1 Hz), 8.30 (1H, dd, J = 8.4, 2.1 Hz), 7.93 (1H, dd, J = 8.1, 1.2 Hz), 7.59 (1H, td, J = 8.4, 1.2 Hz), 7.52 (1H, d, J = 8.7 Hz), 7.41-7.32 (2H, m), 3.76 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.4, 151.1, 135.7, 134.5, 133.4, 132.8, 132.3, 131.4, 130.9, 130.6, 129.9, 128.8, 124.0, 113.7, 29.3; IR: 1655, 1583, 1478, 1383, 1300, 1140, 1025, 823, 749 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{15}H_{10}Cl_2N_2O$: 304.0170, Found: 304.0168.

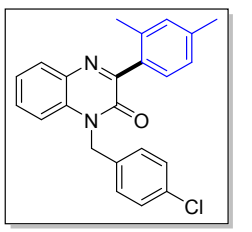
1-Benzyl-3-(4-methoxyphenyl)quinoxalin-2(1*H*)-one (3l): The compound was prepared according to the general procedure. Yield: 70% (239 mg); Appearance: Light yellow crystalline solid; Mp: 169-171 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.38 (2H, d, J = 9.0 Hz), 7.83 (1H, dd, J = 7.8, 1.2 Hz), 7.31 (1H, td, J = 9.0, 1.8 Hz), 7.23-7.15 (7H, m), 6.92 (2H, d, J = 9.0 Hz), 5.47 (2H, s), 3.78 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.5, 154.8, 153.1, 135.4, 133.3, 132.4, 131.4, 130.2, 129.7, 128.8, 128.6, 127.6, 126.9, 123.6, 114.2, 113.4, 55.3, 46.0; IR: 1643, 1598, 1499, 1456, 1303, 1239, 1170, 1035, 843, 748 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_{18}N_2O_2$: 342.1368, Found: 342.1369.



1-Benzyl-3-(3,4-dichlorophenyl)quinoxalin-2(1*H*)-one (3m): The compound was prepared according to the general procedure. Yield: 48% (183 mg); Appearance: Off white crystalline solid; Mp: 148-150 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.60 (1H, s), 8.34 (1H, d, J = 8.7 Hz), 7.92 (1H, d, J = 7.8 Hz), 7.52 (1H, d, J = 8.4 Hz), 7.48-7.43 (1H, m), 7.35-7.26 (7H, m), 5.54 (2H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.5, 151.1, 135.7, 135.0, 134.6, 133.1, 132.8, 132.3, 131.5, 130.9, 130.7, 130.0, 128.9, 128.9, 127.8, 126.8, 124.0, 114.4, 46.1; IR: 1647, 1457, 1381, 1293, 1235, 945, 756 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{14}Cl_2N_2O$: 380.0483, Found: 380.0484.



1-(4-Chlorobenzyl)-3-(2,4-dimethylphenyl)quinoxalin-2(1*H*)-one (3n): The compound was prepared according to the general procedure. Yield: 60% (225 mg); Appearance: White crystalline solid; Mp: 145-147 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.93 (1H, d, J = 8.4 Hz), 7.47-7.43 (2H, m), 7.33 (1H, t, J = 7.8 Hz), 7.29-7.28 (2H, m), 7.26-7.24 (3H, m), 7.12-7.10 (2H, m), 5.49 (2H, s), 2.37 (3H, s), 2.35 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.3, 154.5, 139.4, 136.7, 133.9, 133.6, 133.1, 132.9, 132.5, 131.4, 130.5, 130.3, 129.3, 129.0, 128.5, 126.3, 123.8, 114.1, 45.5, 21.3, 19.9; IR: 1658, 1600, 1492, 1434, 1300, 1255, 1059, 1011, 752 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{23}H_{19}ClN_2O$: 374.1186, Found: 374.1185.



(*E*)-1-(3,7-Dimethylocta-2,6-dien-1-yl)-3-phenylquinoxalin-2(1*H*)-one (3o): The compound was prepared according to the general procedure. Yield: 62% (222 mg); Appearance: Yellow liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.31-8.29 (2H, m), 7.93 (1H, dd, J = 7.8, 1.2 Hz), 7.51 (1H, td, J = 8.4, 1.2 Hz), 7.47-7.45 (3H, m), 7.33 (1H, td, J = 8.4, 1.2 Hz), 7.27 (1H, d, J = 7.8 Hz), 5.19 (1H, t, J = 6.0 Hz), 5.01 (1H, t, J = 6.6 Hz), 4.96

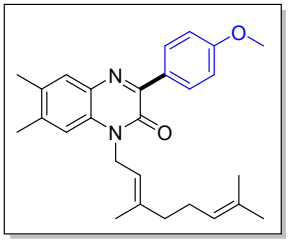
(2H, d, J = 6.0 Hz), 2.08-2.01 (4H, m), 1.90 (3H, s), 1.60 (3H, s), 1.54 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.2, 154.1, 140.5, 136.1, 133.3, 132.6, 131.7, 130.5, 130.2, 130.1, 129.5, 127.9, 123.6, 123.5, 117.9, 114.0, 40.9, 39.4, 26.2, 25.6, 17.6, 16.8; IR: 1650, 1602, 1465, 1292, 1177, 1027, 749 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{24}H_{26}N_2O$: 358.2045, Found: 358.2046.

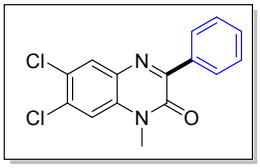
1,6,7-Trimethyl-3-(*p*-tolyl)quinoxalin-2(1*H*)-one and 1,6,7-Trimethyl-3-(*o*-tolyl)quinoxalin-2(1*H*)-one (4a): The compound was prepared according to the general procedure. The product was obtained as an isomeric mixture of regioisomers. The isomeric ratio was found to be 1:1 (*p:o*) as per NMR. Combined yield: 80% (222 mg); Appearance: Light yellow crystalline solid; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.21 (2H, d, J = 8.4 Hz), 8.06 (2H, s), 7.68 (2H, d, J = 3.6 Hz), 7.35 (1H, m), 7.26 (3H, d, J = 8.1 Hz), 7.07 (2H, d, J = 3.0 Hz), 3.72 (3H, s), 3.71 (3H, s), 2.42 (3H, s), 2.41 (6H, s), 2.40 (3H, s), 2.35 (6H, s).^{13}C NMR (75 MHz, $CDCl_3$): δ 154.8, 153.2, 152.8, 140.2, 139.9, 137.5, 136.2, 133.5, 132.6, 132.6, 131.5, 131.5, 131.3, 131.3, 130.8, 130.4, 130.3, 129.8, 129.4, 128.7, 127.9, 126.6, 125.5, 114.1, 114.1, 29.1, 21.5, 21.5, 20.6, 19.2; IR: 1649, 1616, 1570, 1462, 1298, 1242, 1007 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{18}H_{18}N_2O$: 278.1419, Found: 278.1423.

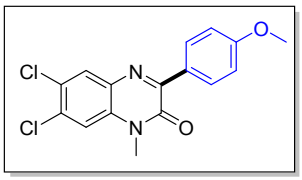
3-(4-Methoxyphenyl)-1,6,7-trimethylquinoxalin-2(1*H*)-one (4b): The compound was prepared according to the general procedure. Yield: 50% (147 mg); Appearance: Light orange crystalline solid; Mp: 214-216 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.36 (2H, d, J = 7.8 Hz), 7.71 (1H, s), 7.06 (1H, s), 6.96 (2H, d, J = 7.8 Hz), 3.85 (3H, s), 3.72 (3H, s), 2.41 (3H, s), 2.34 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.4, 151.9, 139.8, 132.6, 131.4, 131.2, 129.9, 128.6, 114.1, 113.4, 55.3, 29.3, 20.6, 19.2; IR: 1618, 1459, 1177, 1243, 1026, 845 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{18}H_{18}N_2O_2$: 294.1368, Found: 294.1365.

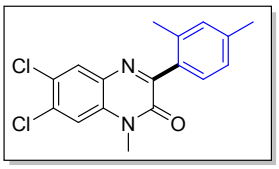
3-(3,4-dichlorophenyl)-1,6,7-trimethylquinoxalin-2(1*H*)-one (4c): The compound was prepared according to the general procedure. Yield: 48% (159 mg); Appearance: Light yellow crystalline solid; Mp: 178-180 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.52 (1H, d, J = 2.1 Hz), 8.28 (1H, dd, J = 8.7, 2.1 Hz), 7.64 (1H, s), 7.49 (1H, d, J = 8.4 Hz), 7.06 (1H, s), 3.71 (3H, s), 2.42 (3H, s), 2.35 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.4, 149.6, 141.2, 136.0, 134.0, 133.0, 132.2, 131.4, 131.3, 131.2, 130.5, 129.8, 128.7, 114.2, 29.2, 20.7, 19.2; IR: 1643, 1616, 1571, 1461, 1380, 1292, 1229, 1021 cm^{-1}; HRMS *m/z* (M^+) calcd for

$C_{17}H_{14}Cl_2N_2O$: 332.0483, Found: 332.0486.

(*E*)-1-(3,7-Dimethylocta-2,6-dien-1-yl)-3-(4-methoxyphenyl)-6,7-dimethylquinoxalin-2(1*H*)-one (4d):  The compound was prepared according to the general procedure. Yield: 70% (291 mg); Appearance: Light yellow crystalline solid; Mp: 125-127 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.36 (2H, d, J = 8.4 Hz), 7.67 (1H, s), 7.02 (1H, s), 6.96 (2H, d, J = 8.4 Hz), 5.17 (1H, t, J = 5.4 Hz), 5.01 (1H, t, J = 6.6 Hz), 4.92 (2H, d, J = 6.0 Hz), 3.85 (3H, s), 2.39 (3H, s), 2.34 (3H, s), 2.07-2.00 (4H, m), 1.90 (3H, s), 1.59 (3H, s), 1.53 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.2, 154.5, 152.1, 140.2, 139.4, 132.4, 131.8, 131.3, 130.5, 130.1, 128.9, 123.6, 118.3, 114.5, 113.4, 55.3, 40.7, 39.4, 26.3, 25.6, 20.7, 19.2, 17.7, 16.8; IR: 1606, 1567, 1505, 1451, 1243, 1172, 1027 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{27}H_{32}N_2O_2$: 416.2464, Found: 416.2464.

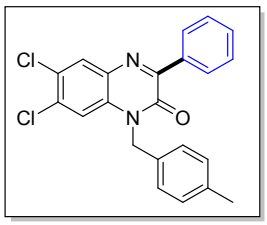
6,7-Dichloro-1-methyl-3-phenylquinoxalin-2(1*H*)-one (4e):  The compound was prepared according to the general procedure. Yield: 73% (222 mg); Appearance: Light yellow crystalline solid; Mp: 168-170 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.26 (2H, dd, J = 6.0, 1.8 Hz), 7.94 (1H, s), 7.50-7.42 (3H, m), 7.34 (1H, s), 3.64 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.9, 153.9, 135.2, 134.1, 132.5, 131.9, 130.9, 130.8, 129.5, 128.2, 128.1, 127.8, 127.3, 114.9, 29.5; IR: 1638, 1590, 1442, 1237, 882, 670, cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{15}H_{10}Cl_2N_2O$: 304.0170, Found: 304.0167.

6,7-Dichloro-3-(4-methoxyphenyl)-1-methylquinoxalin-2(1*H*)-one (4f):  The compound was prepared according to the general procedure. Yield: 75% (251 mg); Appearance: Yellow crystalline solid; Mp: 228-230 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.37 (2H, d, J = 8.4 Hz), 7.94 (1H, s), 7.36 (1H, s), 6.96 (2H, d, J = 9.0 Hz), 3.86 (3H, s), 3.68 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.9, 154.2, 154.0, 133.5, 132.4, 132.2, 131.5, 130.7, 128.0, 127.3, 114.9, 113.5, 55.3, 29.4; IR: 1658, 1601, 1506, 1255, 1241, 1173, 898, 831cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{16}H_{12}Cl_2N_2O_2$: 334.0276, Found: 334.0279.

6,7-Dichloro-3-(2,4-dimethylphenyl)-1-methylquinoxalin-2(1*H*)-one (4g):  The compound was prepared according to the general procedure. Yield: 64% (212 mg); Appearance: Yellow crystalline solid; Mp: 200-202 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97 (1H, s), 7.86 (2H, s), 7.36 (1H, s), 7.12 (1H, s), 3.67 (3H, s), 2.37 (6H, s); ^{13}C NMR (150 MHz,

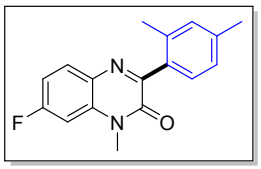
$CDCl_3$): δ 155.5, 154.1, 137.6, 135.2, 134.0, 132.6, 132.6, 132.1, 130.9, 127.3, 127.3, 114.9, 29.4, 21.3; IR: 1661, 1597, 1564, 1458, 1302, 1195, 1114, 859 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{17}H_{14}Cl_2N_2O$: 332.0483, Found: 332.0486.

6,7-Dichloro-1-(4-methylbenzyl)-3-phenylquinoxalin-2(1*H*)-one (4h): The compound was



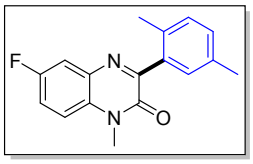
prepared according to the general procedure. Yield: 70% (276 mg); Appearance: Yellow crystalline solid; Mp: 215-217 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 8.35 (2H, dd, *J* = 7.8, 1.8 Hz), 7.99 (1H, s), 7.52-7.46 (3H, m), 7.38 (1H, s), 7.16 (2H, d, *J* = 8.4 Hz), 7.13 (2H, d, *J* = 7.8 Hz), 5.43 (2H, s), 2.31 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 155.1, 154.2, 137.8, 135.3, 134.2, 132.4, 132.0, 131.5, 131.1, 130.9, 129.8, 129.7, 128.1, 127.5, 126.9, 115.7, 46.2, 21.1; IR: 1660, 1572, 1449, 1408, 1246, 1123, 1057, 886 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{22}H_{16}Cl_2N_2O$: 394.0640, Found: 394.0638.

3-(2,4-Dimethylphenyl)-7-fluoro-1-methylquinoxalin-2(1*H*)-one (4i): The compound was



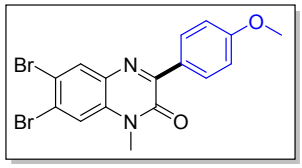
prepared according to the general procedure. Yield: 58% (163 mg); Appearance: White crystalline solid; Mp: 108-110 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 7.88 (1H, dd, *J* = 9.0, 6.0 Hz), 7.34 (1H, d, *J* = 7.2 Hz), 7.10- 7.05 (3H, m), 7.03 (1H, dd, *J* = 10.2, 2.4 Hz), 3.71 (3H, s), 2.36 (3H, s), 2.30 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.5 (d, *J* = 249.8 Hz), 157.2, 154.5, 139.4, 136.7, 134.9 (d, *J* = 12.0 Hz), 132.9, 132.2 (d, *J* = 10.5 Hz), 131.4, 129.2, 127.1 (d, *J* = 27.8 Hz), 126.3, 111.5 (d, *J* = 23.3 Hz), 100.6 (d, *J* = 27.8 Hz), 29.6, 21.2, 19.8; IR: 1656, 1611, 1583, 1453, 1304, 1238, 1185, 982 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{17}H_{15}FN_2O$: 282.1168, Found: 282.1170.

3-(2,5-Dimethylphenyl)-6-fluoro-1-methylquinoxalin-2(1*H*)-one (4j): The compound was



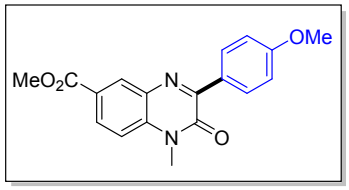
prepared according to the general procedure. Yield: 54% (152 mg); Appearance: White Crystalline Solid; Mp: 105-107 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 7.61 (1H, dd, *J* = 8.4, 2.4 Hz), 7.35-7.29 (2H, m), 7.24 (1H, s), 7.17-7.14 (2H, m), 3.74 (3H, s), 2.34 (3H, s), 2.27 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 160.0, 158.7 (d, *J* = 242.3 Hz), 154.2, 135.6, 135.0, 133.6, 133.3 (d, *J* = 11.3 Hz), 130.5, 130.3, 130.2, 129.5, 118.2 (d, *J* = 24.0 Hz), 115.7 (d, *J* = 22.5 Hz), 114.7 (d, *J* = 8.3 Hz), 29.6, 20.9, 19.4; IR: 1651, 1593, 1497, 1266, 1054, 813 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{17}H_{15}FN_2O$: 282.1168, Found: 282.1168.

6,7-Dibromo-3-(4-methoxyphenyl)-1-methylquinoxalin-2(1*H*)-one (4k): The compound



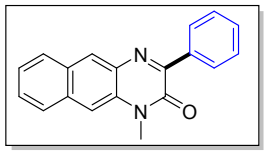
was prepared according to the general procedure. Yield: 53% (223 mg); Appearance: Yellow crystalline solid; Mp: 231-233 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.38 (2H, d, J = 8.4 Hz), 8.12 (1H, s), 7.55 (1H, s), 6.96 (2H, d, J = 9.0 Hz), 3.86 (3H, s), 3.68 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.0, 154.1, 133.8, 132.9, 132.9, 131.6, 128.0, 125.7, 118.7, 118.0, 113.5, 110.0, 55.4, 29.4; IR: 1649, 1598, 1448, 1241, 1171, 1111, 1022, 896 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{16}H_{12}Br_2N_2O_2$: 421.9266, Found: 421.9267.

Methyl 3-(4-methoxyphenyl)-1-methyl-2-oxo-1,2-dihydroquinoxaline-6-carboxylate (4l):



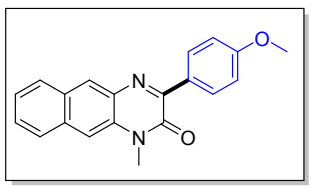
The compound was prepared according to the general procedure. Yield: 68% (220 mg); Appearance: Yellow solid; Mp: 165-167 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.57 (1H, s), 8.40 (2H, d, J = 8.4 Hz), 8.16 (1H, d, J = 8.4 Hz), 7.32 (1H, d, J = 8.4 Hz), 6.98 (2H, d, J = 8.4 Hz), 3.95 (3H, s), 3.86 (3H, s), 3.76 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.1, 161.8, 154.7, 153.7, 136.3, 132.4, 131.8, 131.5, 130.4, 128.1, 125.5, 113.5, 113.5, 55.3, 52.3, 29.5; IR: 1658, 1714, 1605, 1513, 1426, 1284, 1243, 1212, 1098 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{18}H_{16}N_2O_4$: 324.1110, Found: 324.1112.

1-Methyl-3-phenylbenzo[*g*]quinoxalin-2(1*H*)-one (5a): The compound was prepared



according to the general procedure. Yield: 75% (214 mg); Appearance: Yellow crystalline solid; Mp: 162-164 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.41 (1H, s), 8.33-8.31 (2H, m), 7.94 (1H, d, J = 7.8 Hz), 7.88 (1H, d, J = 8.4 Hz), 7.55-7.53 (2H, m), 7.50-7.48 (3H, m), 7.47-7.44 (1H, m), 3.77 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.7, 154.5, 135.9, 133.7, 132.3, 131.8, 130.5, 129.8, 129.7, 129.5, 128.5, 128.1, 127.8, 127.1, 125.2, 109.7, 29.2; IR: 1645, 1622, 1595, 1463, 1255, 888, 748 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{19}H_{14}N_2O$: 286.1106, Found: 286.1109.

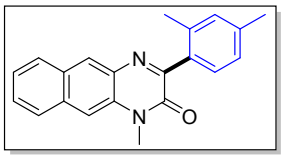
3-(4-Methoxyphenyl)-1-methylbenzo[*g*]quinoxalin-2(1*H*)-one (5b): The compound was



prepared according to the general procedure. Yield: 54% (170 mg); Appearance: Orange crystalline solid; Mp: 169-171 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.41 (2H, d, J = 5.4 Hz), 8.39 (1H, s), 7.95 (1H, d, J = 8.4 Hz), 7.88 (1H, d, J = 8.4 Hz), 7.57 (1H, s), 7.53 (1H, t, J = 7.2 Hz), 7.45 (1H, t, J = 7.2 Hz), 6.99 (2H, d, J = 8.4 Hz), 3.87 (3H, s), 3.80 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.7, 154.7, 153.6, 133.5, 132.3, 131.7, 131.6,

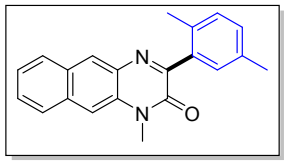
129.9, 128.9, 128.4, 127.6, 127.1, 125.2, 113.5, 109.7, 55.3, 29.2; IR: 1597, 1506, 1458, 1244, 1172, 1024, 832 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{20}H_{16}N_2O_2$: 316.1212, Found: 316.1208.

3-(2,4-Dimethylphenyl)-1-methylbenzo[*g*]quinoxalin-2(1*H*)-one (5c): The compound was



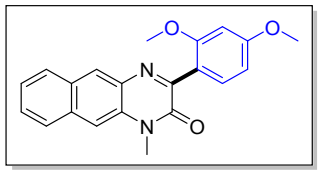
prepared according to the general procedure. Yield: 61% (191 mg); Appearance: Yellow crystalline solid; Mp: 178-180 °C; ^1H NMR (300 MHz, $CDCl_3$): δ 8.41 (1H, s), 7.98-7.91 (2H, m), 7.64 (1H, s), 7.57 (1H, t, J = 7.2 Hz), 7.45 (1H, t, J = 7.8 Hz), 7.41 (1H, d, J = 7.5 Hz), 7.12-7.09 (2H, m), 3.81 (3H, s), 2.37 (3H, s), 2.35 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.8, 154.5, 139.4, 136.8, 133.7, 133.0, 132.1, 131.9, 131.4, 129.7, 129.5, 129.3, 128.5, 127.9, 127.2, 126.3, 125.3, 109.9, 29.4, 21.3, 20.0; IR: 1656, 1603, 1585, 1505, 1421, 1252, 1172, 1023, 819 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{18}N_2O$: 314.1419, Found: 314.1420.

3-(2,5-Dimethylphenyl)-1-methylbenzo[*g*]quinoxalin-2(1*H*)-one (5d): The compound was



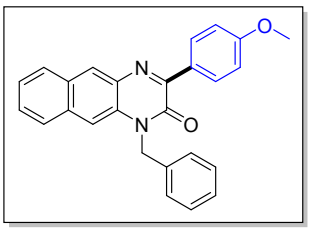
prepared according to the general procedure. Yield: 63% (198 mg); Appearance: Yellow crystalline solid; Mp: 155-157 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 8.42 (1H, s), 7.96 (1H, d, J = 7.8 Hz), 7.91 (1H, d, J = 8.4 Hz), 7.62 (1H, s), 7.57 (1H, t, J = 7.2 Hz), 7.48 (1H, t, J = 7.8 Hz), 7.31 (1H, s), 7.19-7.16 (2H, m), 3.80 (3H, s), 2.36 (3H, s), 2.32 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 159.1, 154.4, 135.8, 134.9, 133.8, 133.7, 132.1, 131.9, 130.5, 130.2, 129.7, 129.6, 129.5, 128.5, 127.9, 127.1, 125.3, 109.9, 29.3, 20.9, 19.5; IR: 1661, 1627, 1601, 1462, 1256, 1049, 831 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{18}N_2O$: 314.1419, Found: 314.1418.

3-(2,4-Dimethoxyphenyl)-1-methylbenzo[*g*]quinoxalin-2(1*H*)-one (5e): The compound

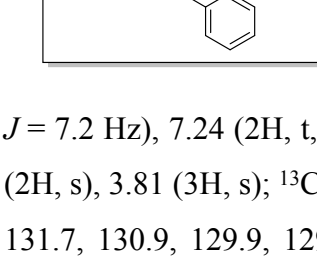


was prepared according to the general procedure. Yield: 80% (277 mg); Appearance: Yellow crystalline solid; Mp: 163-165 °C; ^1H NMR (300 MHz, $CDCl_3$): δ 8.39 (1H, s), 7.94 (1H, d, J = 8.4 Hz), 7.88 (1H, d, J = 8.4 Hz), 7.57-7.41 (4H, m), 6.62-6.56 (2H, m), 3.85 (3H, s), 3.81 (3H, s), 3.77 (3H, s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.3, 159.3, 157.4, 154.4, 133.6, 132.3, 132.1, 131.0, 129.65, 129.3, 128.5, 127.7, 127.1, 125.1, 119.3, 109.8, 104.9, 99.1, 55.9, 55.5, 29.3; IR: 1659, 1585, 1455, 1276, 1202, 1107, 1024, 822 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{21}H_{18}N_2O_3$: 346.1317, Found: 346.1320.

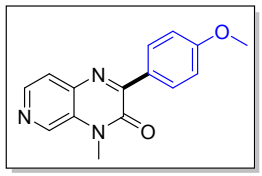
1-Benzyl-3-(4-methoxyphenyl)benzo[*g*]quinoxalin-2(1*H*)-one (5f): The compound was prepared according to the general procedure. Yield: 75% (294 mg); Appearance: Yellow crystalline solid; Mp: 205-207 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.40 (2H, d, J = 9.0 Hz), 8.35 (1H, s), 7.86 (1H, d, J = 8.4 Hz), 7.69 (1H, d, J = 8.4 Hz), 7.47 (1H, s), 7.40 (1H, t, J = 7.2 Hz), 7.35 (1H, t, J = 7.8 Hz), 7.27 (2H, d, J = 7.2 Hz), 7.24 (2H, t, J = 7.2 Hz), 7.17 (1H, t, J = 7.8 Hz), 6.94 (2H, d, J = 9.0 Hz), 5.54 (2H, s), 3.81 (3H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.8, 154.8, 153.6, 135.4, 133.4, 132.7, 131.7, 130.9, 129.9, 129.2, 128.9, 128.5, 128.3, 127.6, 127.5, 127.3, 126.9, 125.2, 113.5, 110.6, 55.4, 46.1; IR: 1658, 1599, 1496, 1309, 1253, 1170, 1028, 847 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{26}H_{20}N_2O_2$: 392.1525, Found: 392.1523.



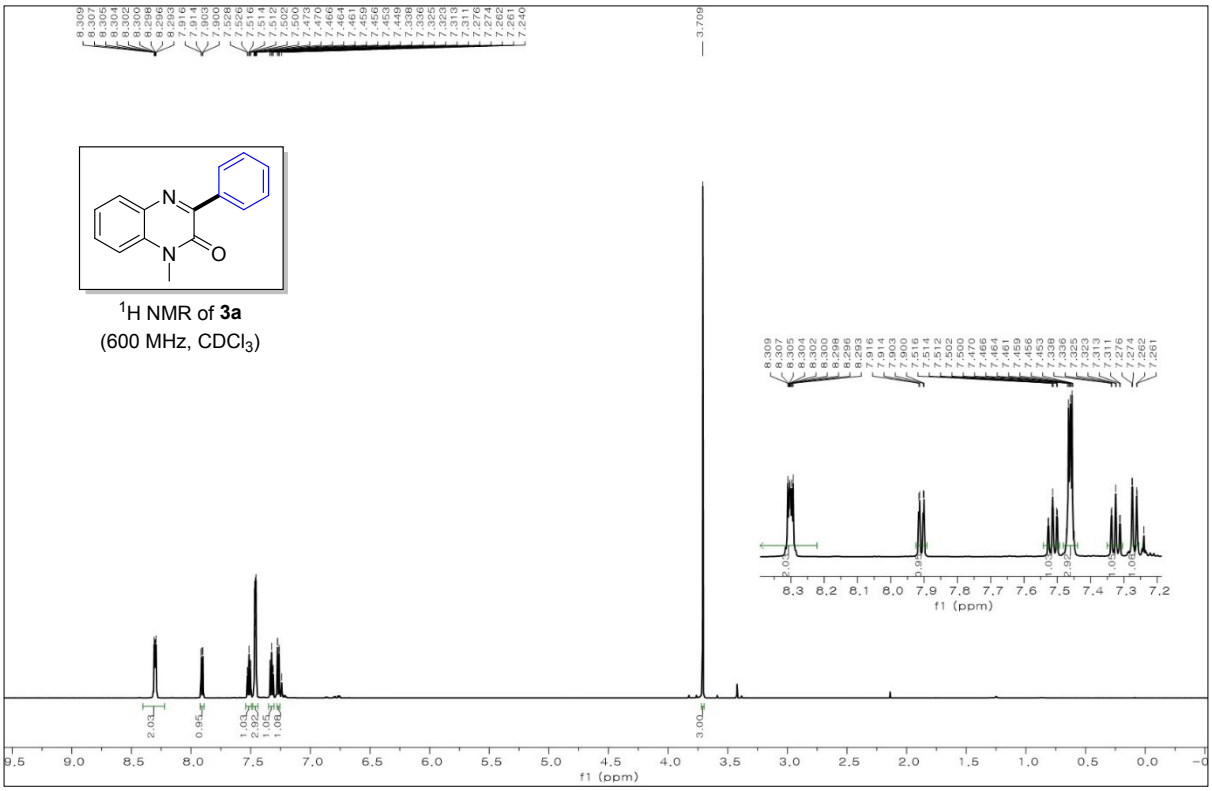
1-Benzyl-3-(4-chlorophenyl)benzo[*g*]quinoxalin-2(1*H*)-one (5g): The compound was prepared according to the general procedure. Yield: 52% (206 mg); Appearance: Yellow crystalline solid; Mp: 203-205 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.10 (1H, s), 8.05 (2H, dd, J = 9.0, 2.4 Hz), 7.60 (1H, d, J = 8.4 Hz), 7.43 (1H, d, J = 8.4 Hz), 7.16 (1H, t, J = 7.2 Hz), 7.14-7.09 (3H, m), 7.00-6.95 (4H, m), 6.91-6.89 (2H, m), 5.27 (2H, s); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.6, 153.2, 136.8, 135.2, 134.3, 133.8, 132.5, 131.2, 131.0, 129.9, 128.9, 128.4, 128.3, 127.9, 127.7, 127.3, 126.9, 125.4, 110.8, 46.2; IR: 1651, 1593, 1453, 1396, 1259, 1171, 1088, 834 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{25}H_{17}ClN_2O$: 396.1029, Found: 396.1031.



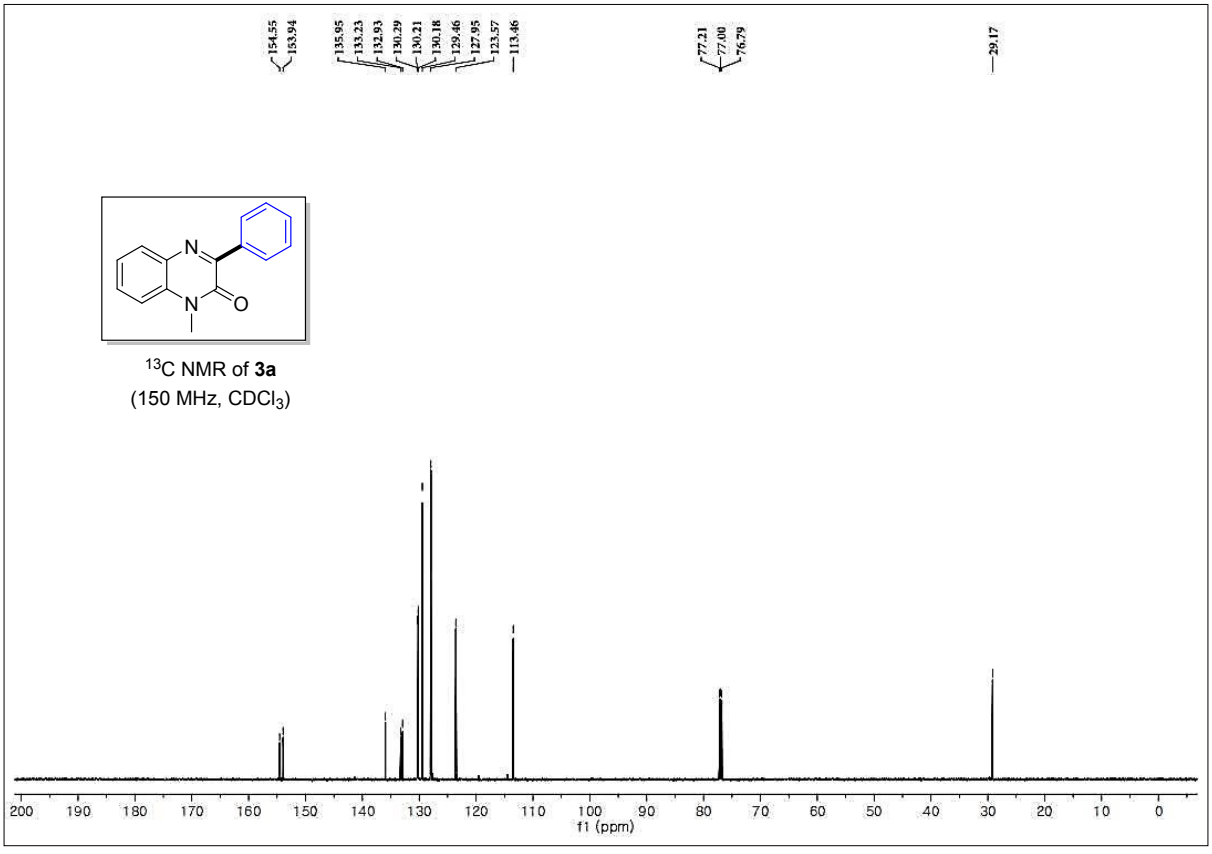
2-(4-Methoxyphenyl)-4-methylpyrido[3,4-*b*]pyrazin-3(4*H*)-one (7): The compound was prepared according to the general procedure. Yield: 52% (139 mg); Appearance: White Crystalline Solid; Mp: 170-172 °C; ^{1}H NMR (600 MHz, DMSO-d_6): δ 9.05 (1H, s), 8.62 (1H, d, J = 2.4 Hz), 8.32 (2H, d, J = 9.0 Hz), 7.63 (1H, d, J = 5.4 Hz), 7.07 (2H, d, J = 9.0 Hz), 3.84 (3H, s), 3.63 (3H, s); ^{13}C NMR (150 MHz, DMSO-d_6): δ 161.9, 154.8, 154.7, 149.2, 147.2, 139.9, 131.7, 128.0, 113.9, 109.9, 55.8, 29.7; IR: 1652, 1603, 1587, 1505, 1421, 1251, 1173, 1023 cm^{-1}; HRMS *m/z* (M^+) calcd for $C_{15}H_{13}N_3O_2$: 267.1008, Found: 267.1004.



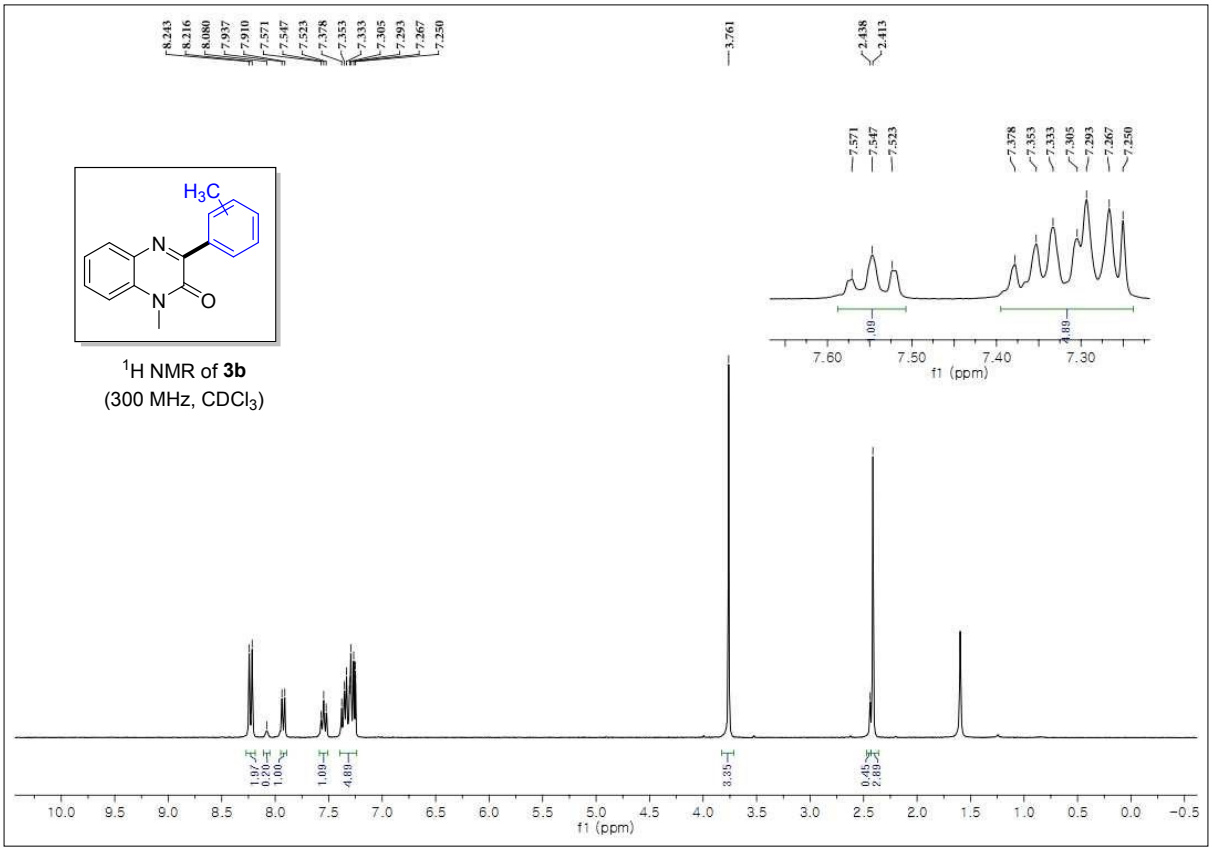
^{1}H NMR and ^{13}C NMR spectra of synthesized compounds



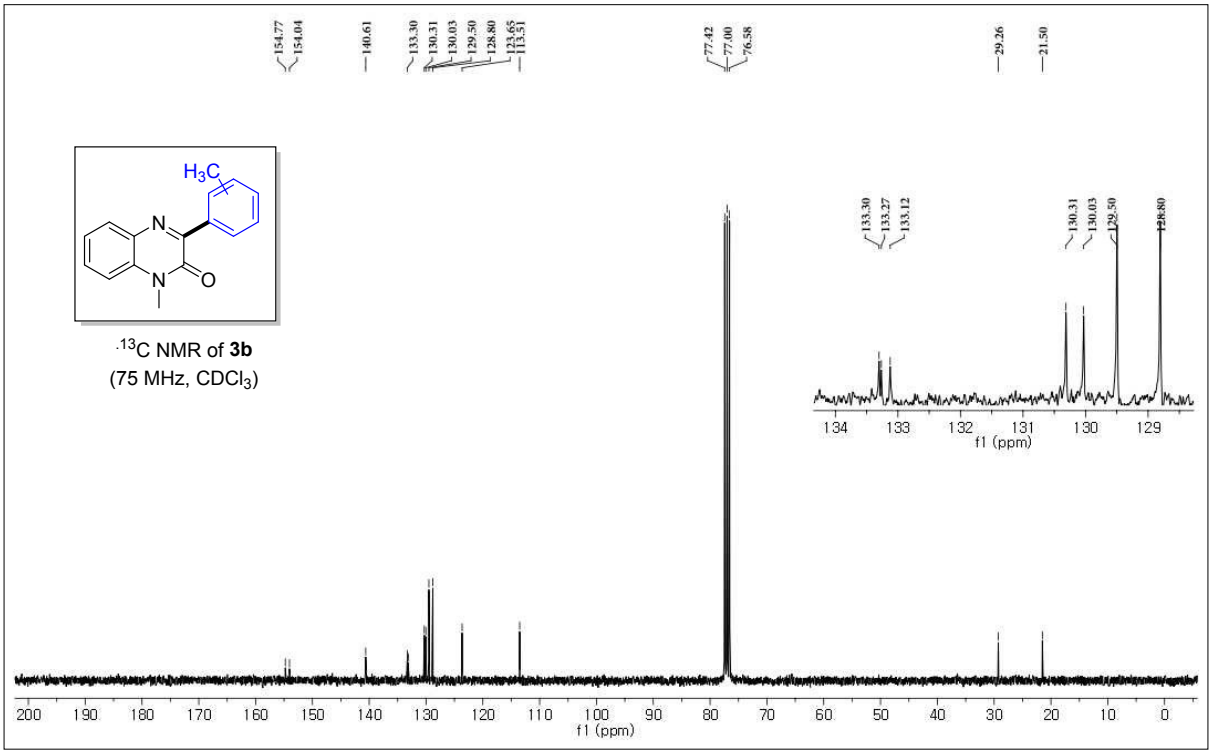
^{1}H NMR of **3a**
(600 MHz, $CDCl_3$)



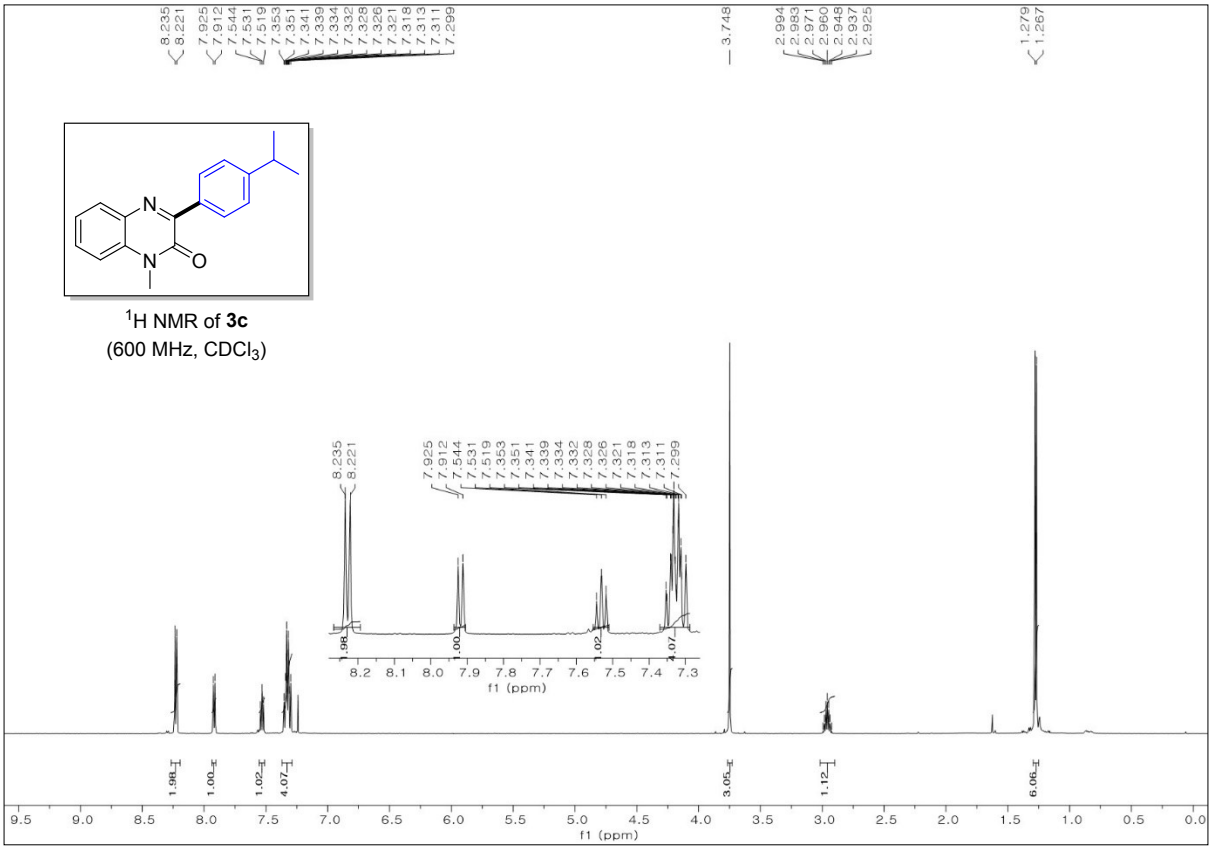
^{13}C NMR of **3a**
(150 MHz, $CDCl_3$)



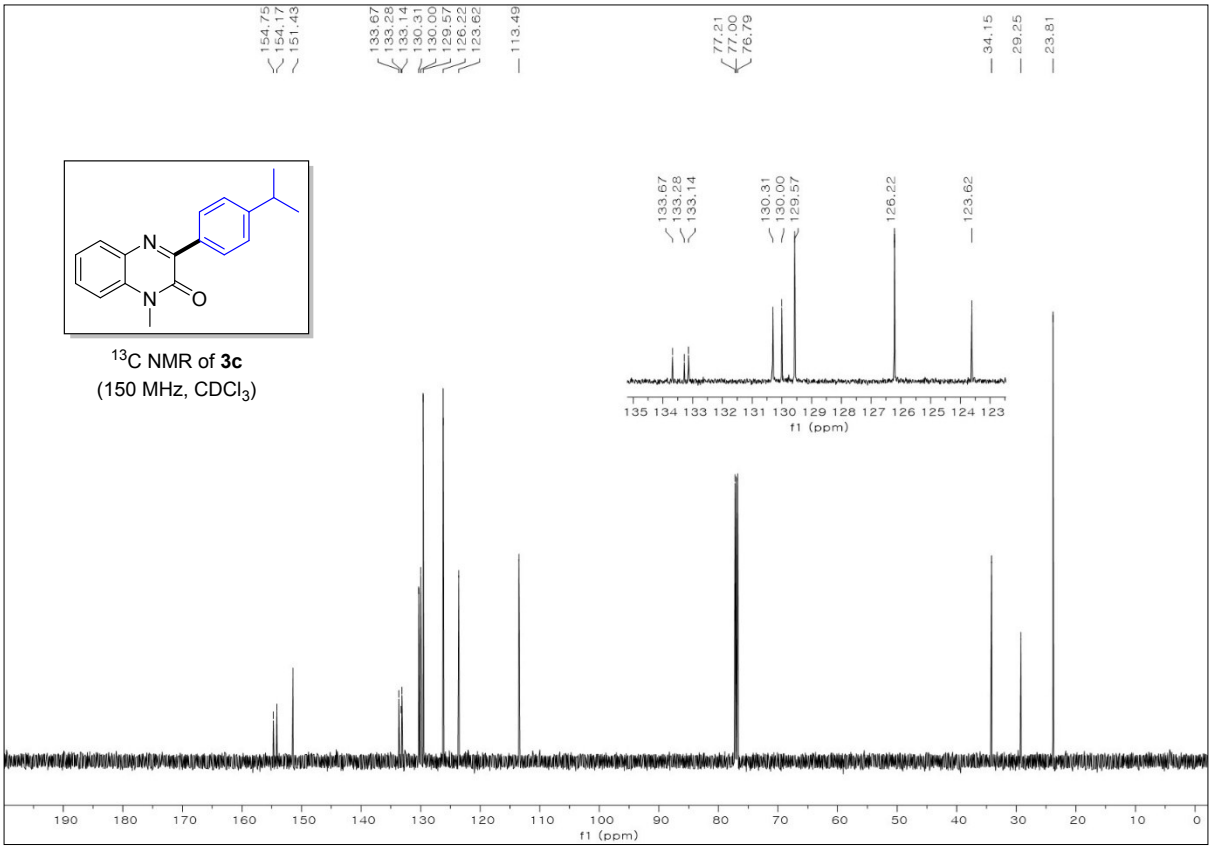
^{1}H NMR of **3b**
(300 MHz, $CDCl_3$)



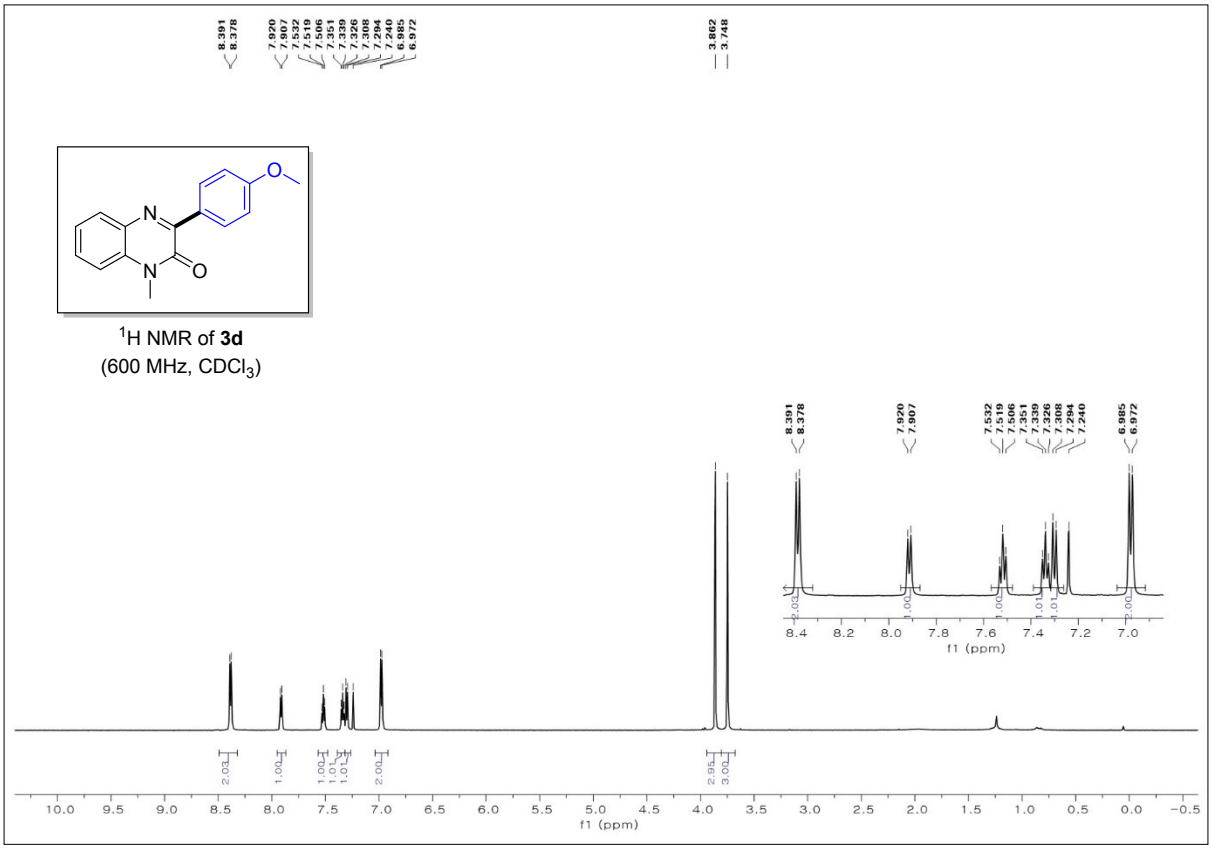
^{13}C NMR of **3b**
(75 MHz, $CDCl_3$)



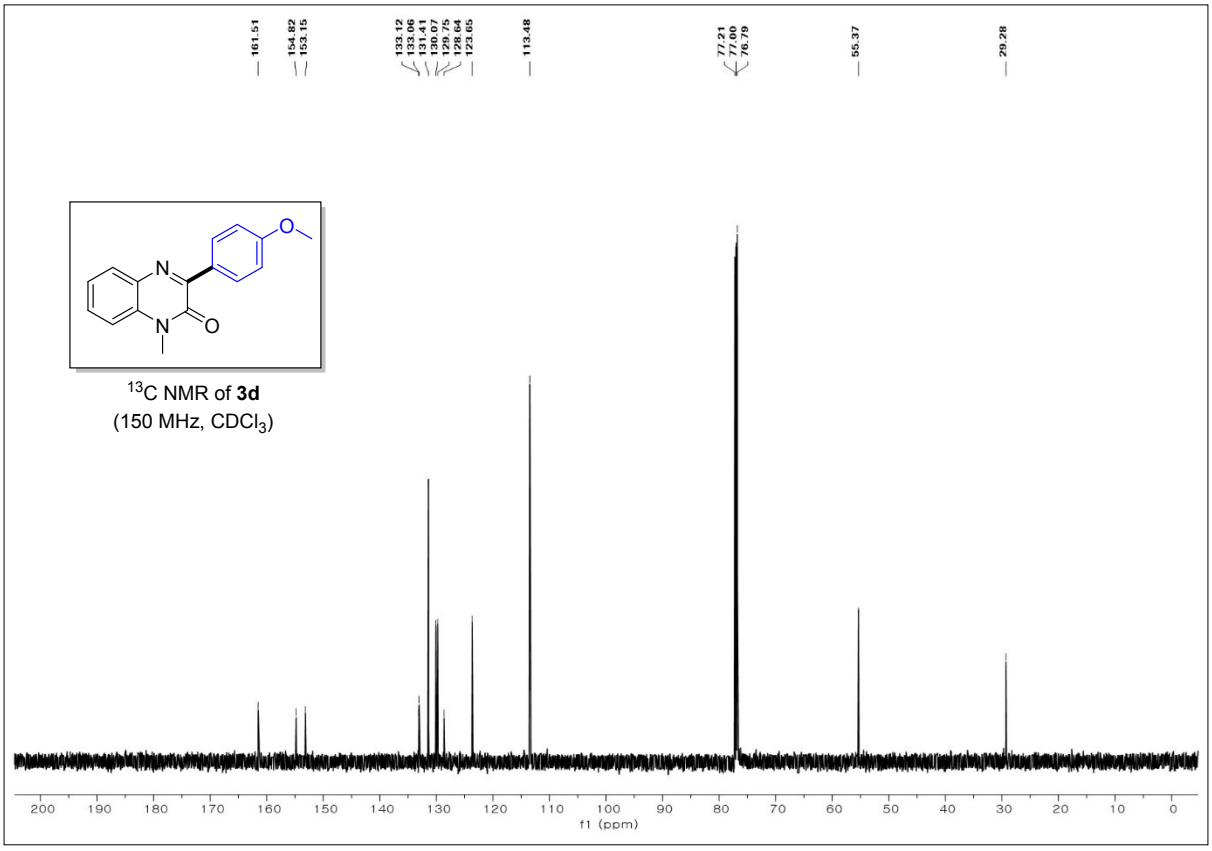
^{1}H NMR of **3c**
(600 MHz, $CDCl_3$)



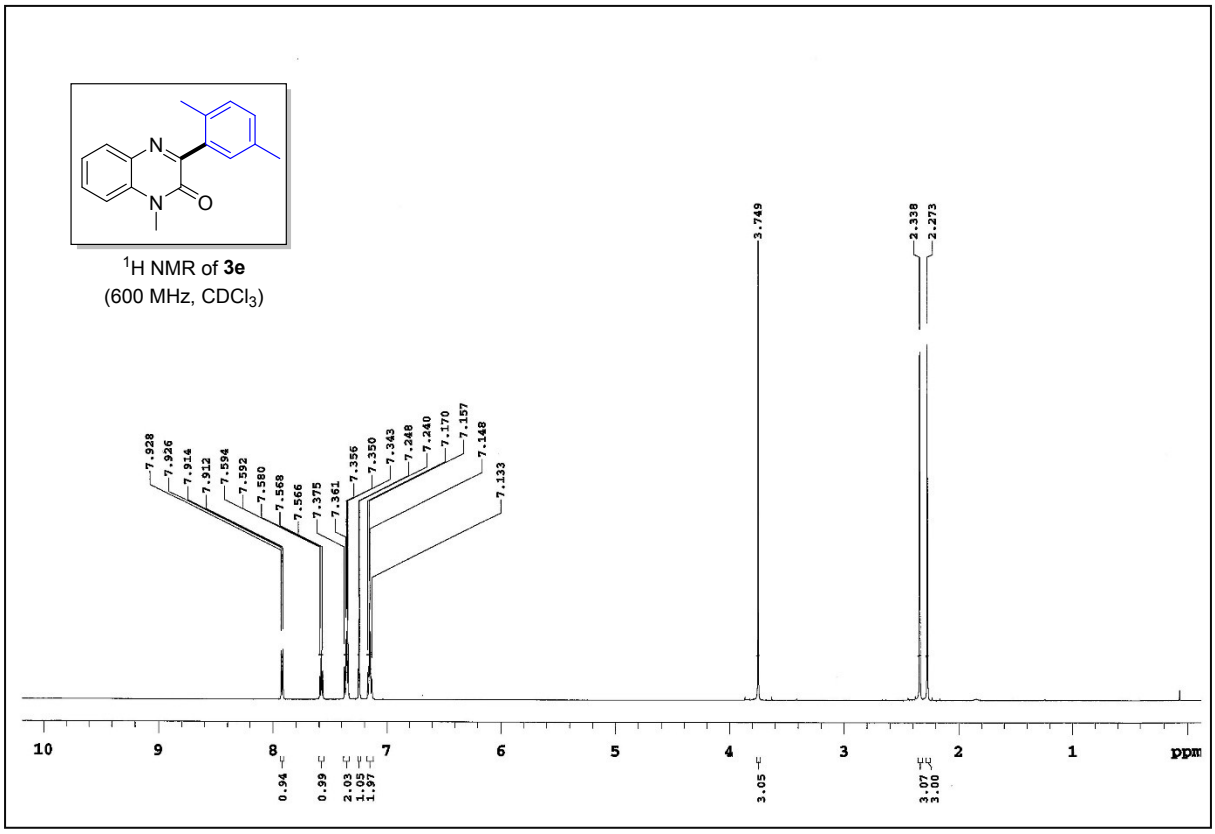
^{13}C NMR of **3c**
(150 MHz, $CDCl_3$)

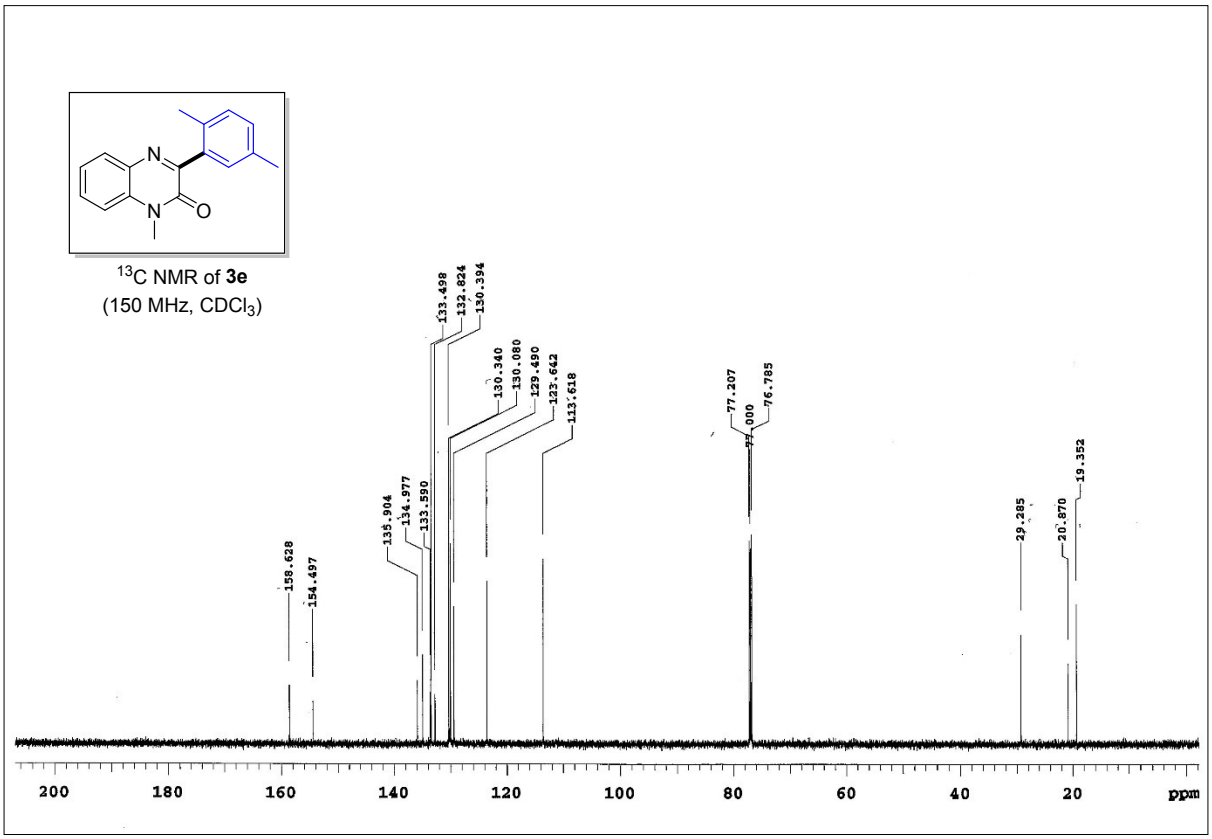


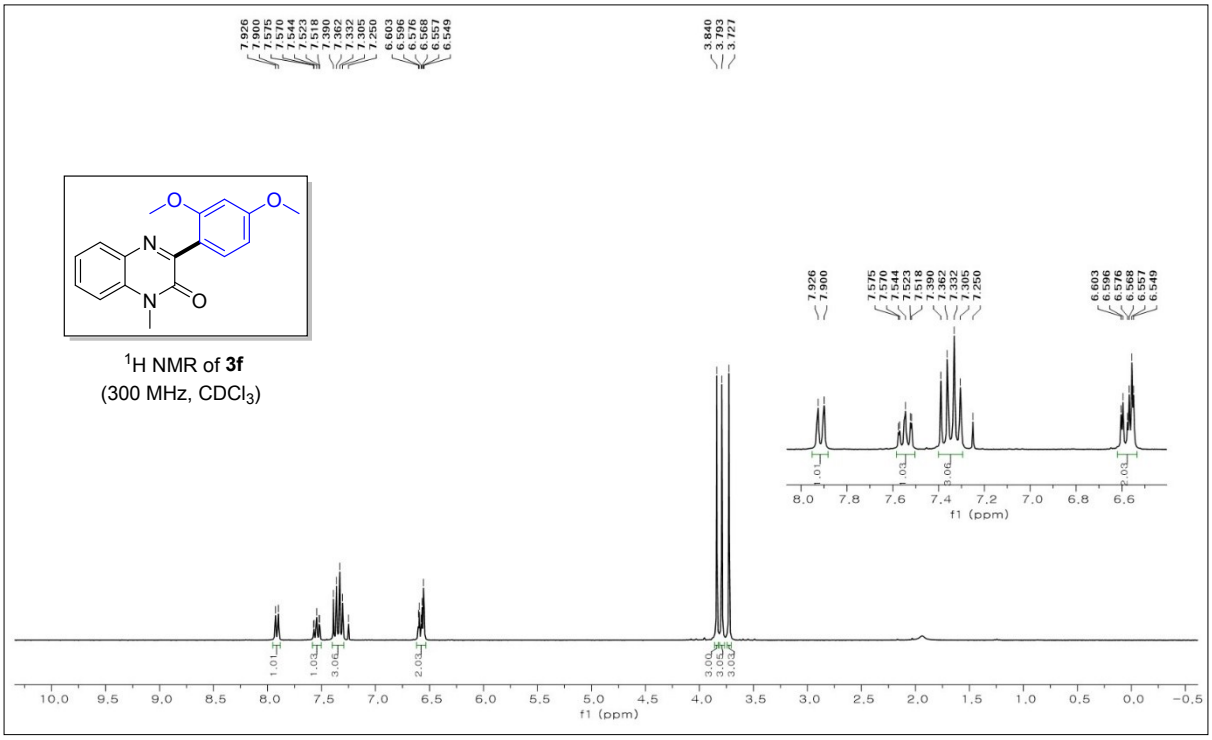
^{1}H NMR of **3d**
(600 MHz, $CDCl_3$)



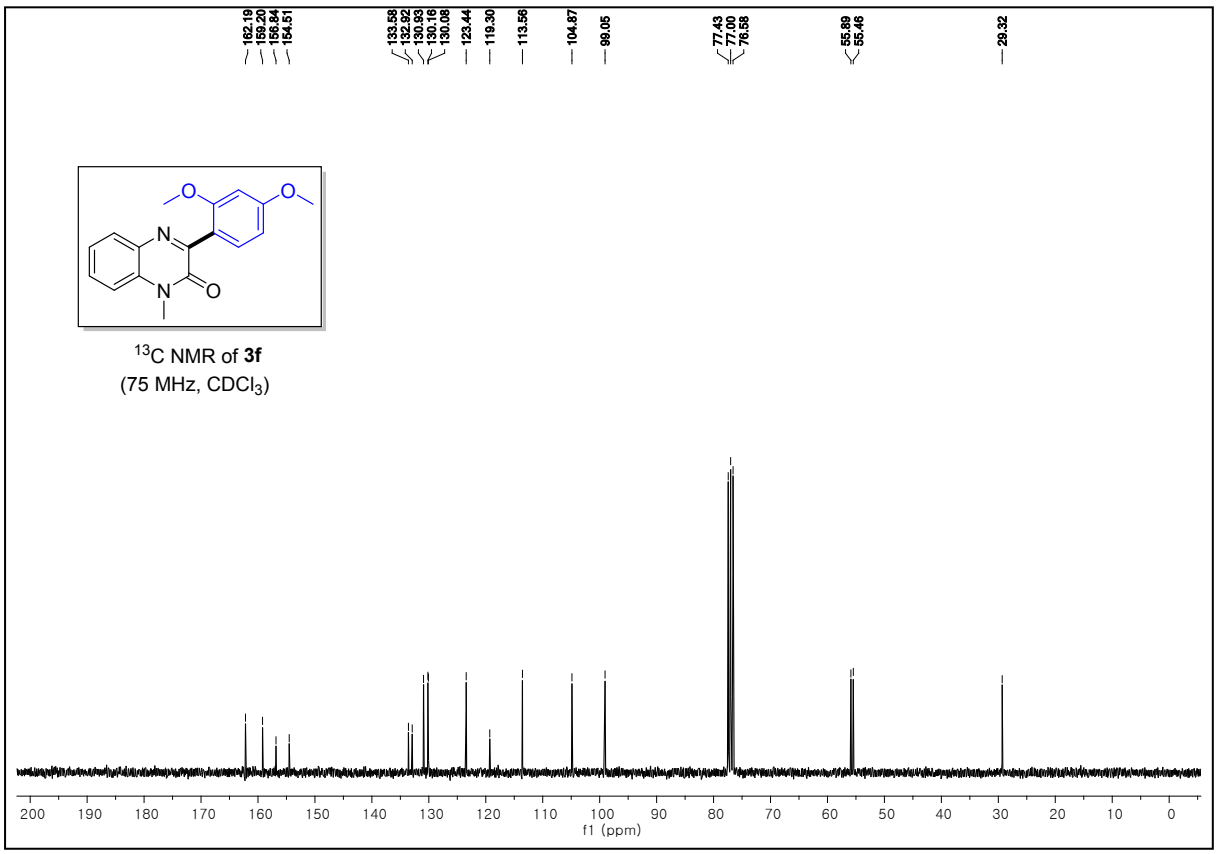
^{13}C NMR of **3d**
(150 MHz, $CDCl_3$)


^{1}H NMR of **3e**
(600 MHz, $CDCl_3$)
7.928
7.926
7.914
7.912
7.594
7.592
7.580
7.568
7.566
7.375
7.361
7.356
7.350
7.343
7.248
7.240
7.170
7.157
7.148
7.133
3.749
2.338
2.273
10
9
8
7
6
5
4
3
2
1
ppm
0.94
0.99
2.03
1.05
1.97
3.05
3.07
3.00

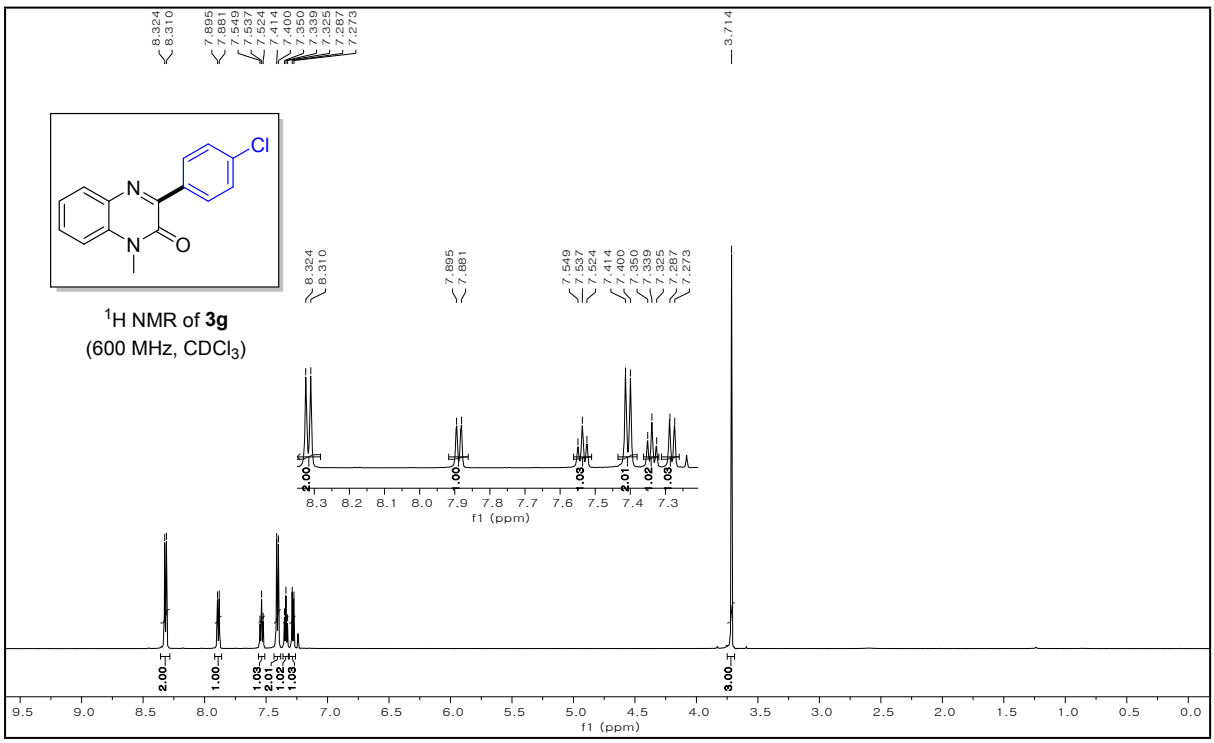

^{13}C NMR of **3e**
(150 MHz, $CDCl_3$)
158.628
154.497
135.904
134.977
133.590
133.498
132.824
130.394
130.340
130.080
129.490
123.642
113.618
77.207
77.000
76.785
29.285
20.870
19.352
200
180
160
140
120
100
80
60
40
20
ppm



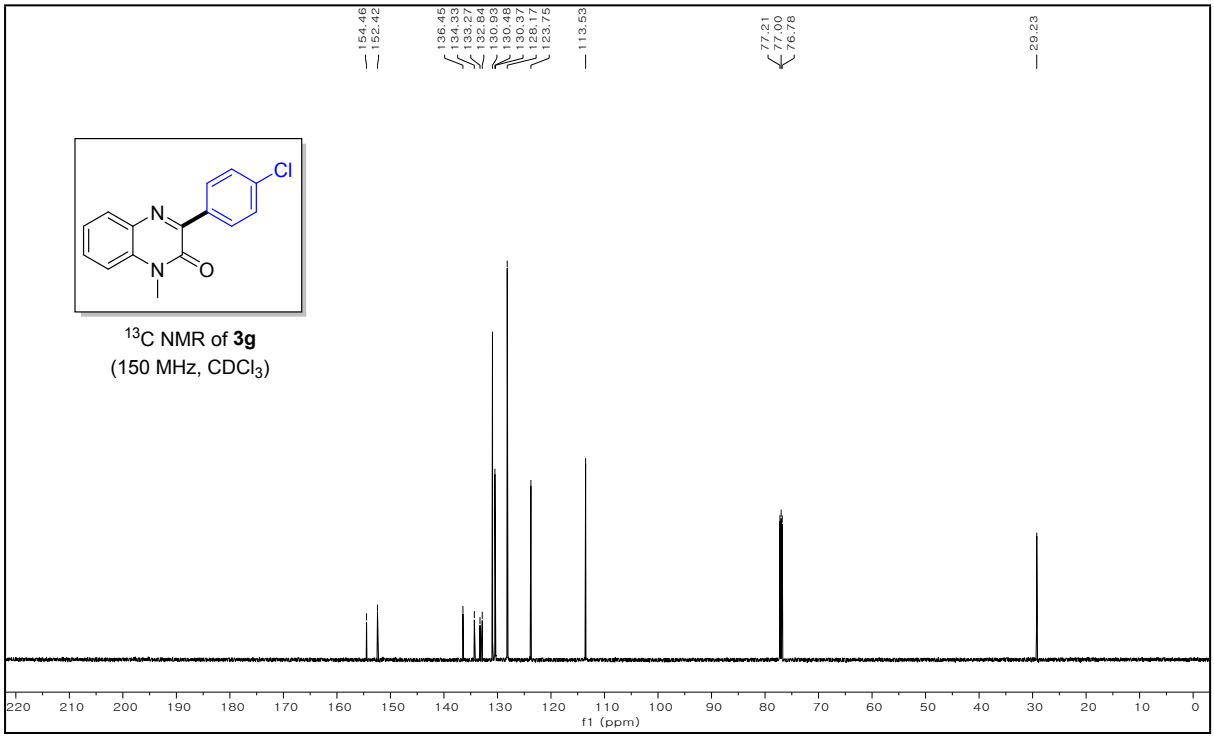
^{1}H NMR of **3f**
(300 MHz, $CDCl_3$)



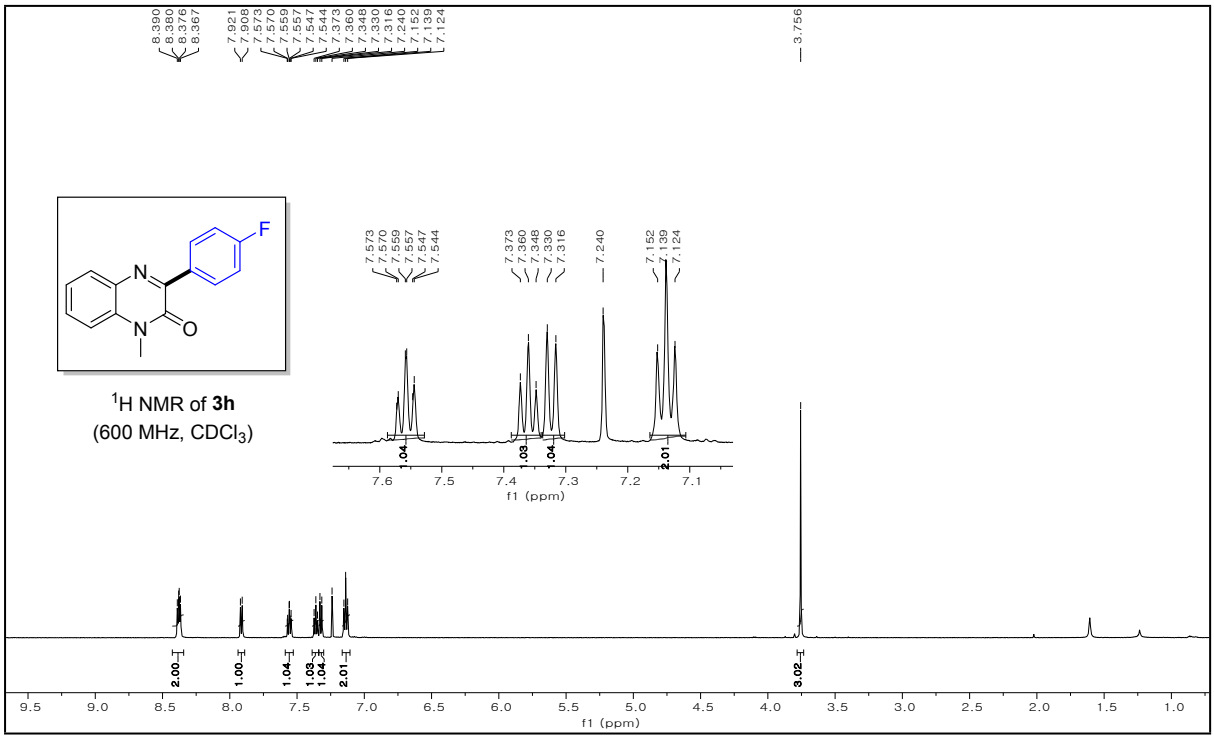
^{13}C NMR of **3f**
(75 MHz, $CDCl_3$)



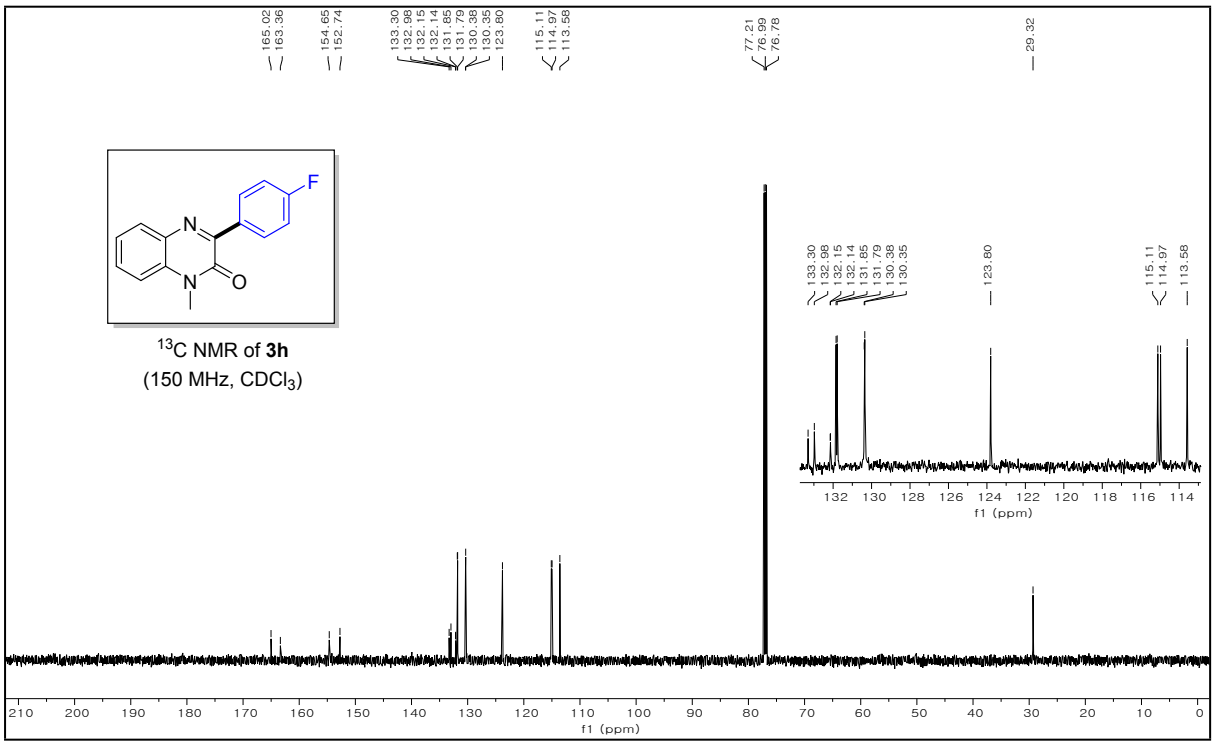
^{1}H NMR of **3g**
(600 MHz, $CDCl_3$)



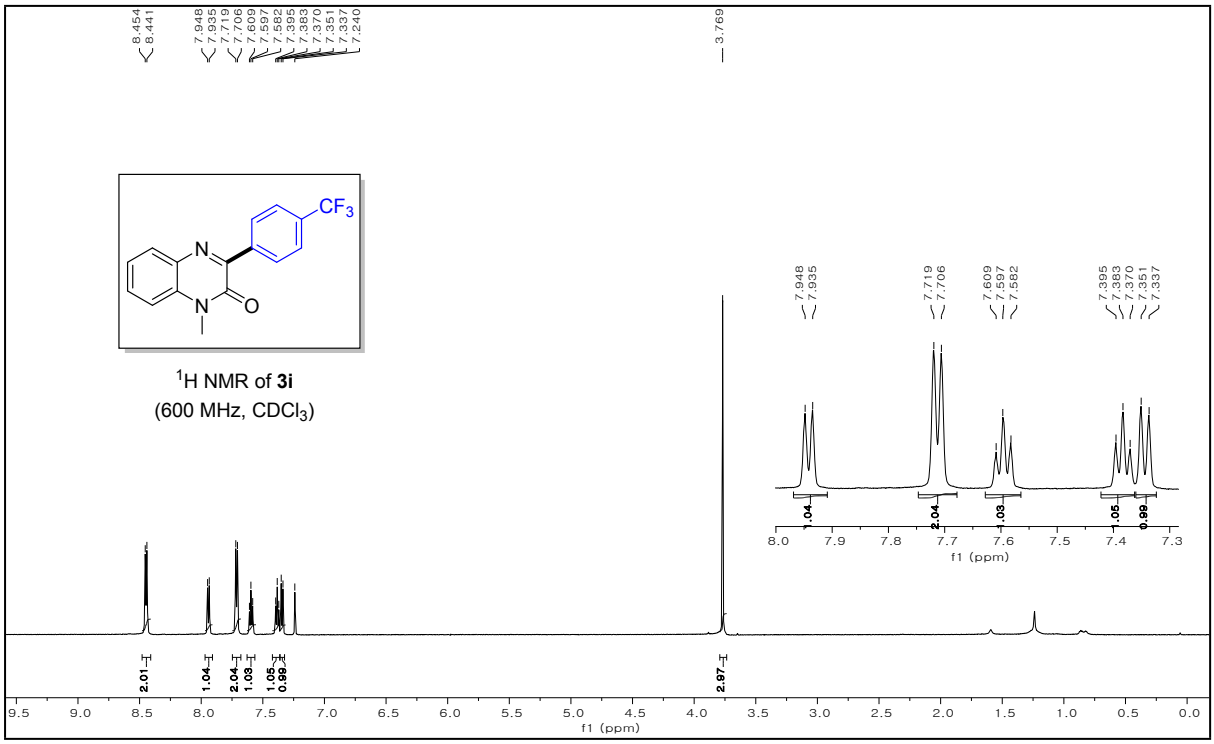
^{13}C NMR of **3g**
(150 MHz, $CDCl_3$)



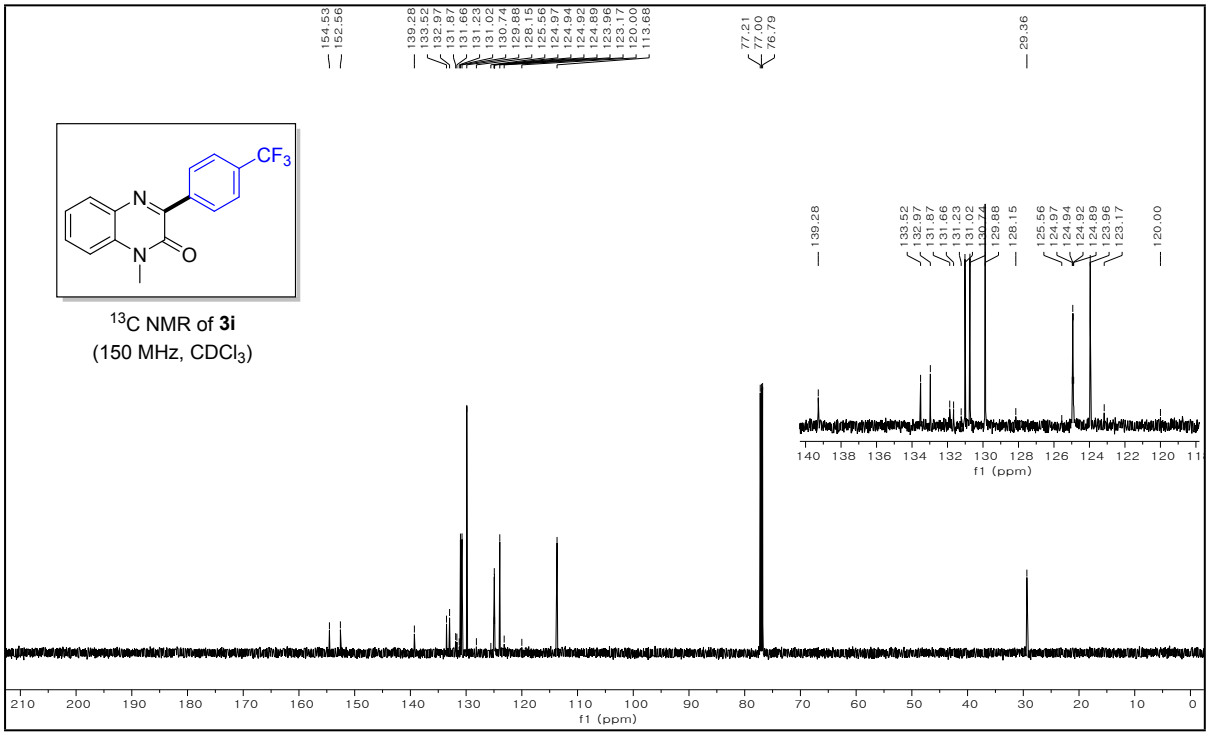
^{1}H NMR of **3h**
(600 MHz, $CDCl_3$)



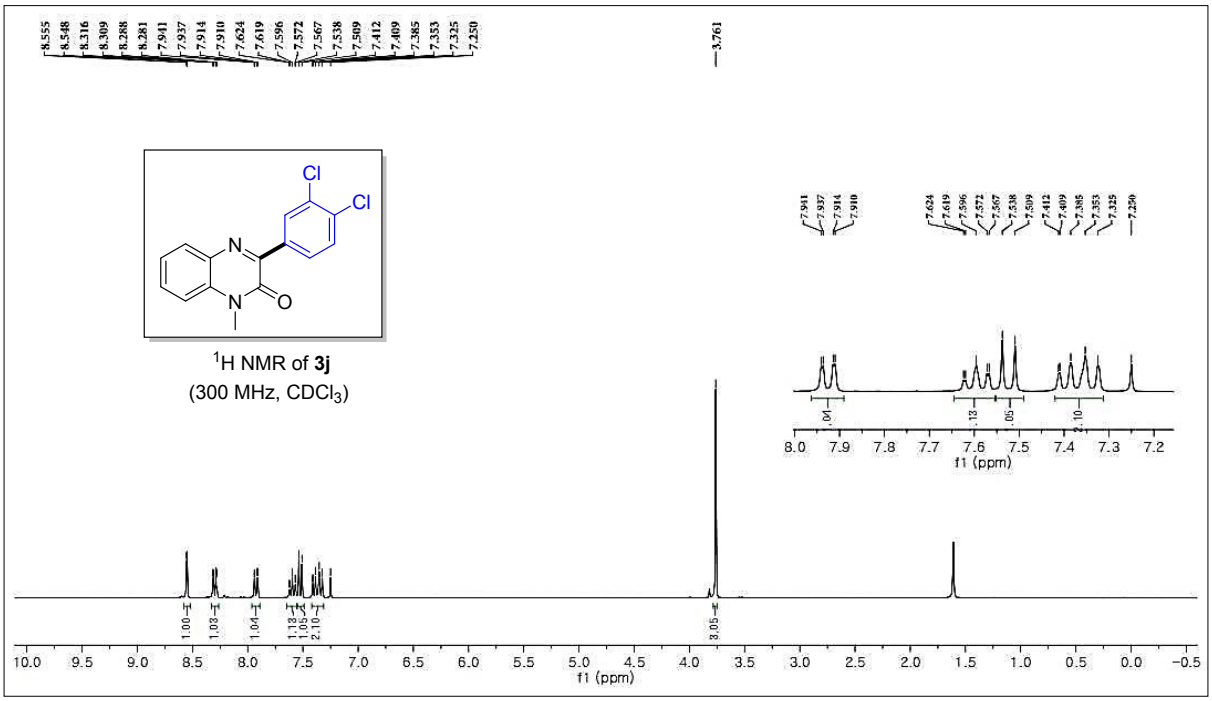
^{13}C NMR of **3h**
(150 MHz, $CDCl_3$)



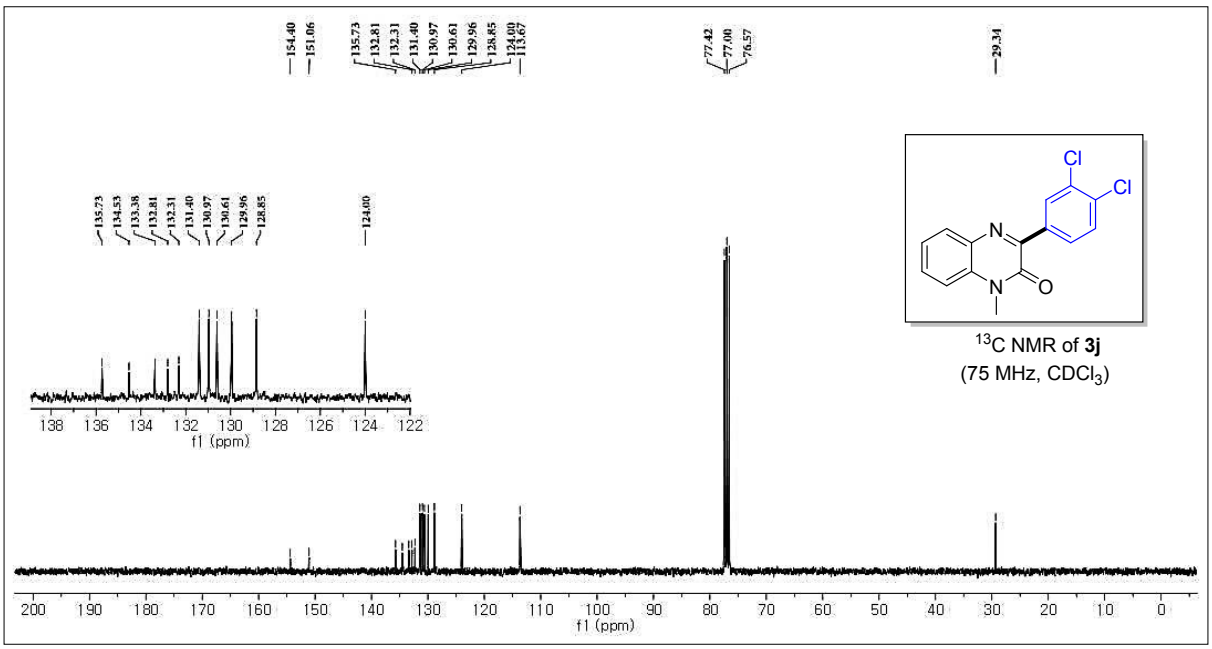
^{1}H NMR of **3i**
(600 MHz, $CDCl_3$)



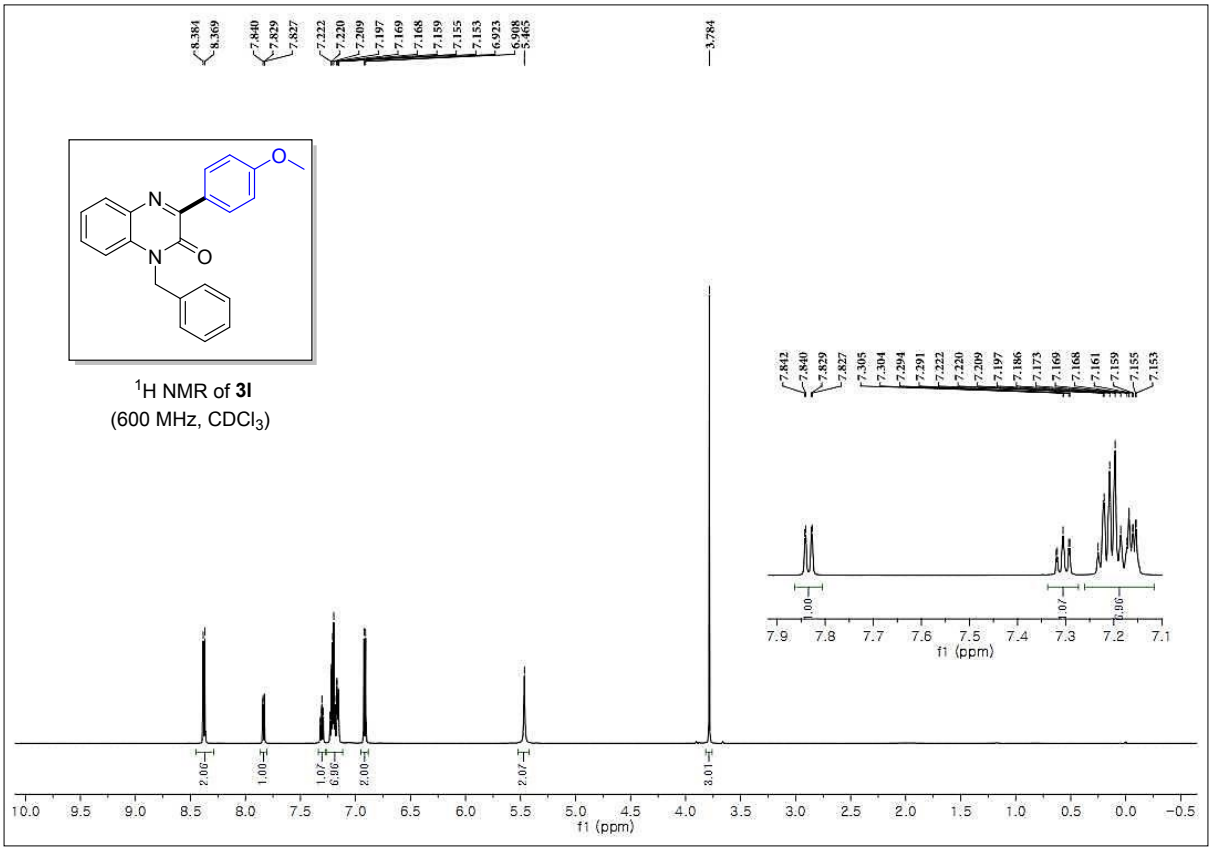
^{13}C NMR of **3i**
(150 MHz, $CDCl_3$)

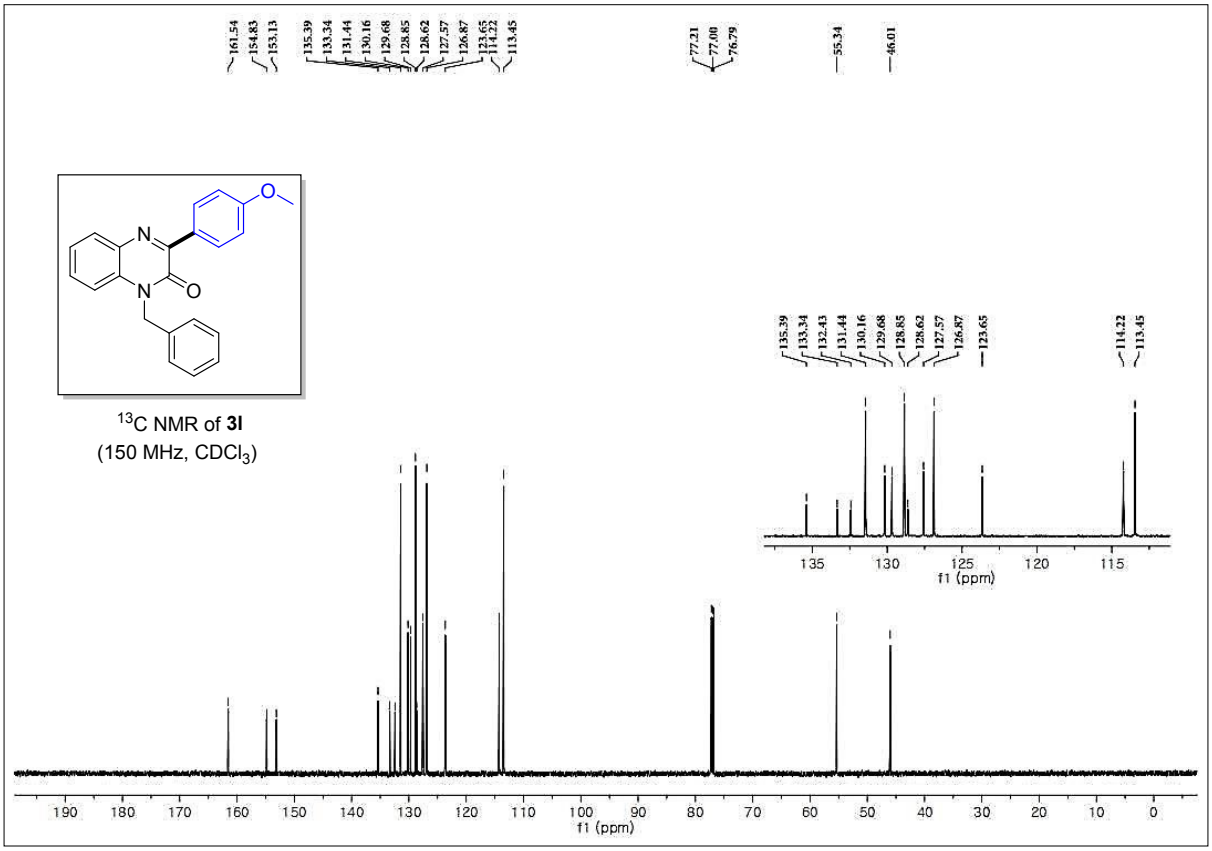


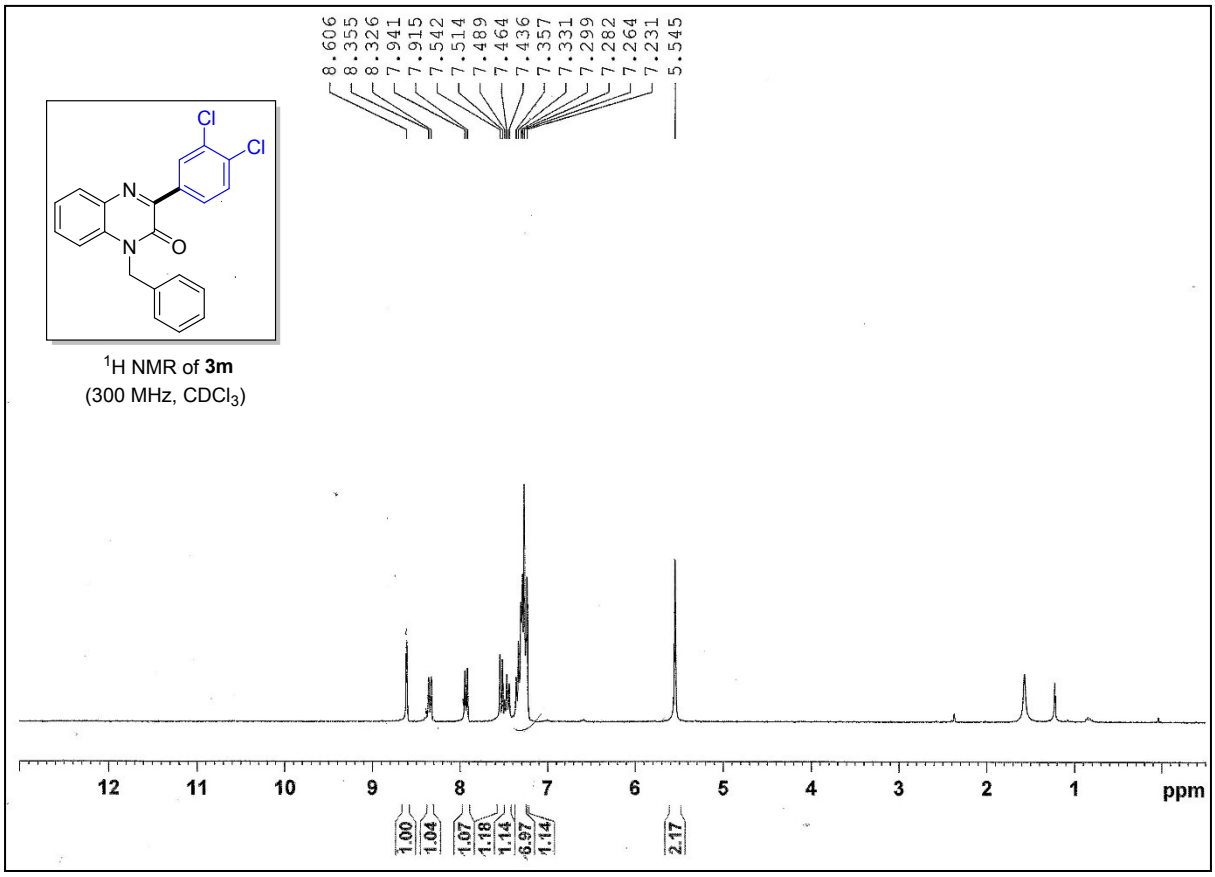
^{1}H NMR of **3j**
(300 MHz, $CDCl_3$)



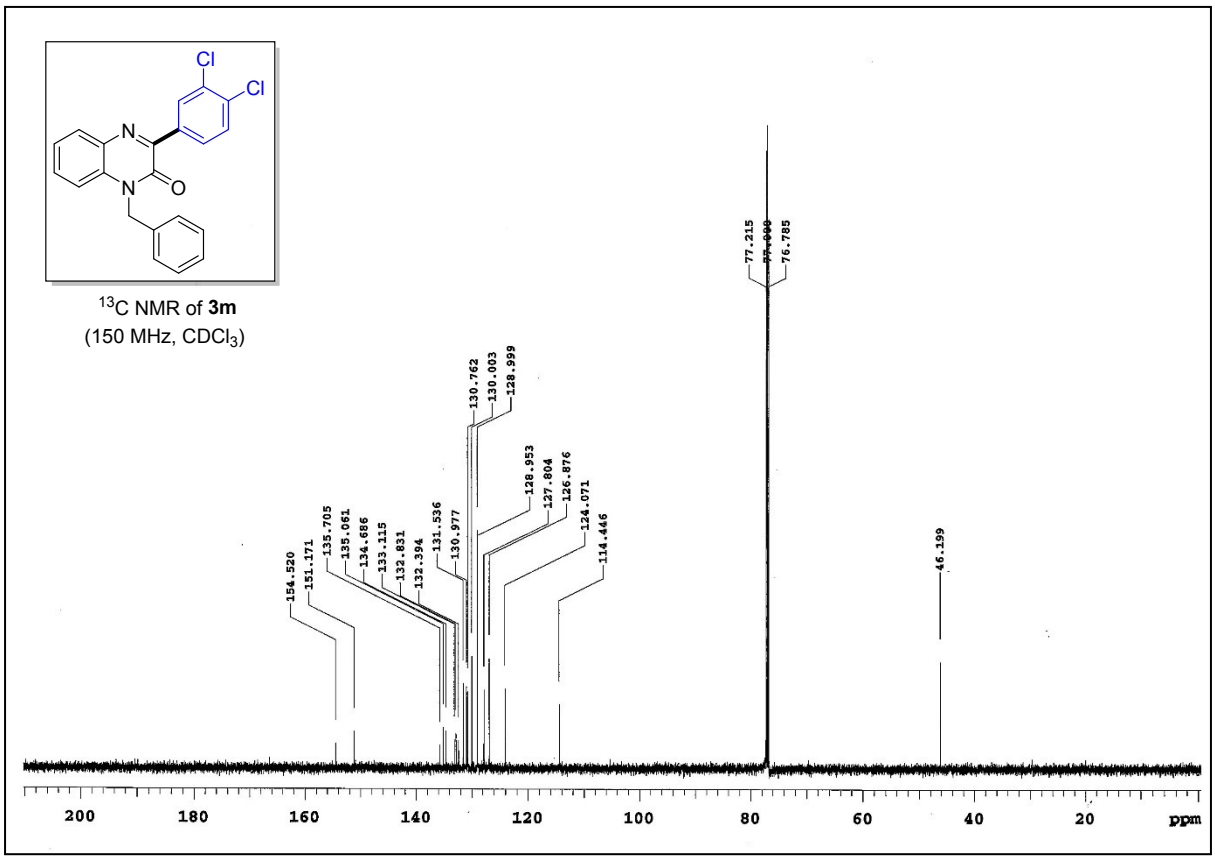
^{13}C NMR of **3j**
(75 MHz, $CDCl_3$)


8.384
8.369
7.840
7.829
7.827
7.222
7.220
7.209
7.197
7.169
7.168
7.159
7.155
7.153
6.923
6.908
5.465
3.784
O
N
N
O
^{1}H NMR of **3l**
(600 MHz, $CDCl_3$)
7.842
7.840
7.829
7.827
7.305
7.304
7.294
7.291
7.222
7.220
7.209
7.197
7.186
7.173
7.169
7.168
7.161
7.159
7.155
7.153
1.00
1.07
0.90
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
2.00
1.00
1.07
0.90
2.00
2.07
3.01
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)

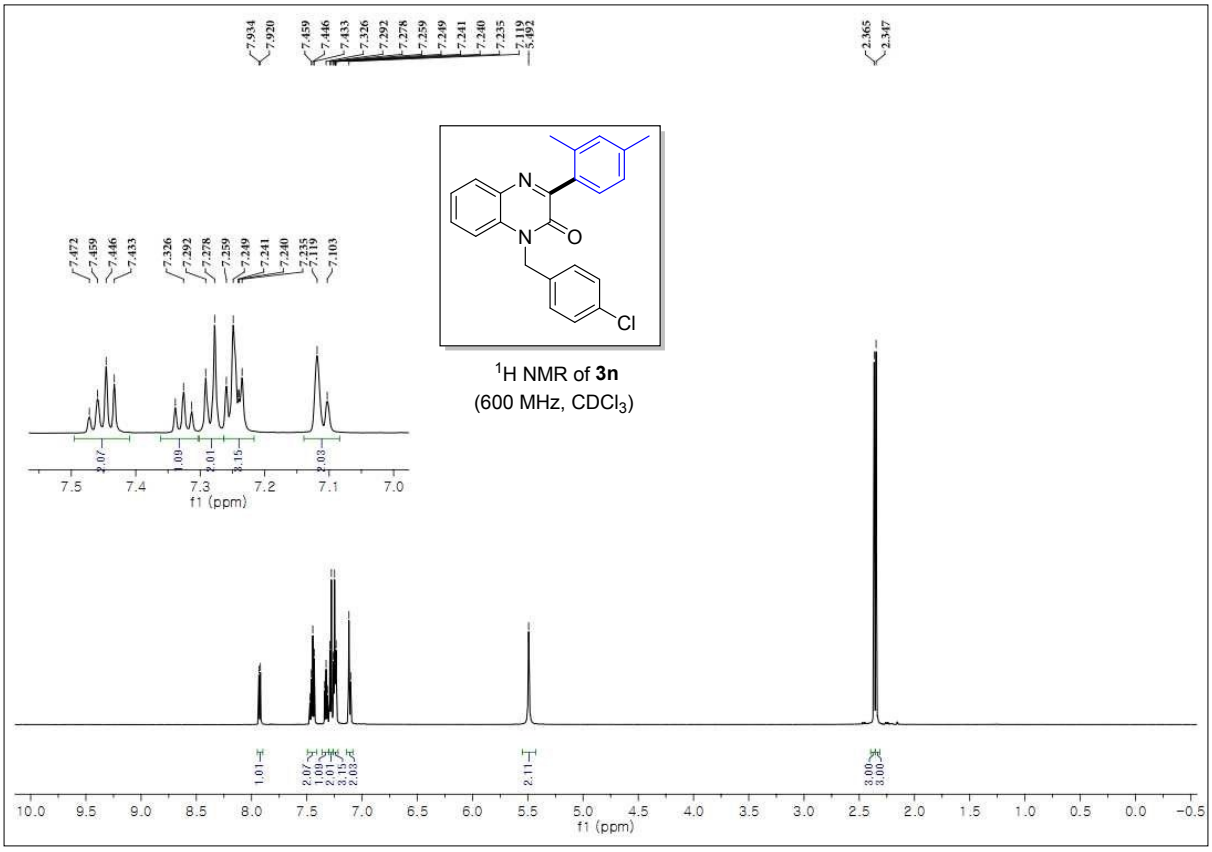

161.54
154.83
153.13
135.39
133.34
131.44
130.16
129.68
128.85
128.62
127.57
126.87
123.65
114.22
113.45
77.21
77.00
76.79
55.34
46.01
O
N
N
O
^{13}C NMR of **3l**
(150 MHz, $CDCl_3$)
135.39
133.34
132.43
131.44
130.16
129.68
128.85
128.62
127.57
126.87
123.65
114.22
113.45
135 130 125 120 115
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



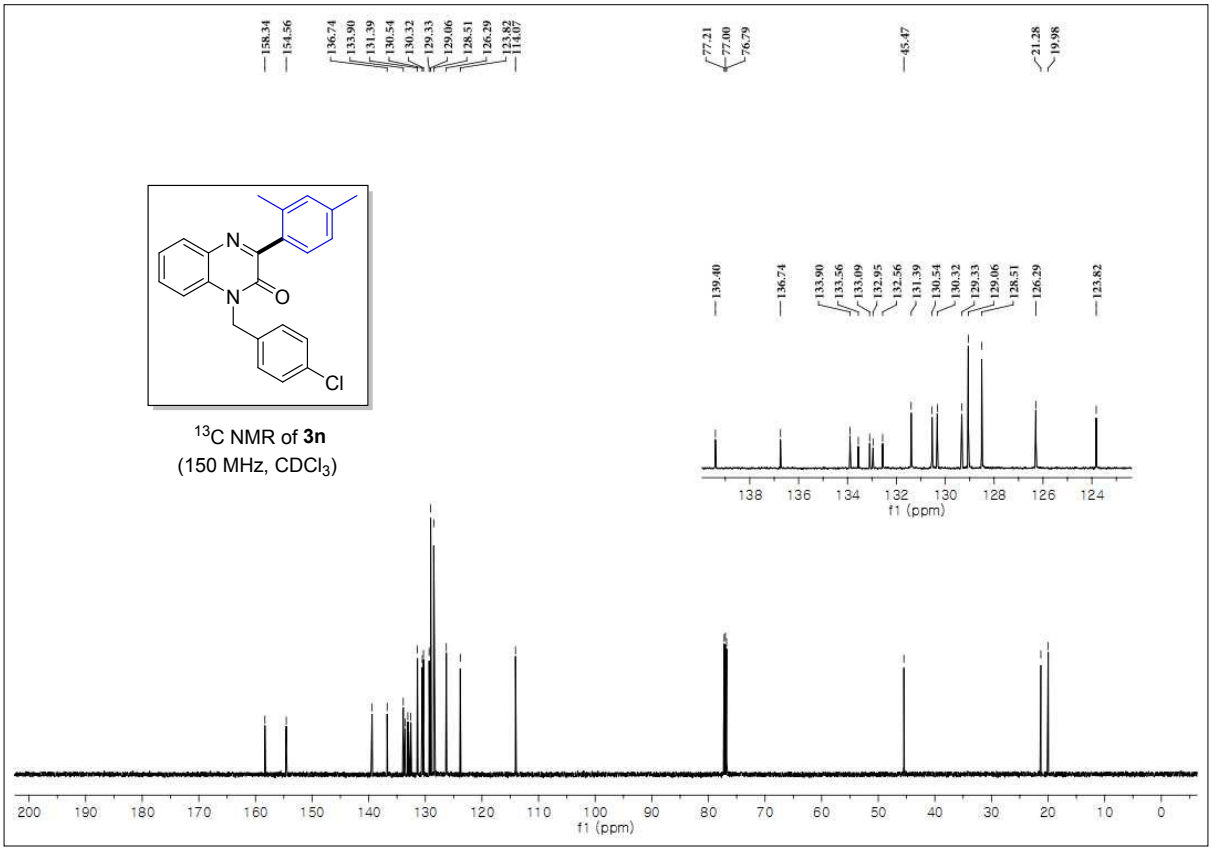
^{1}H NMR of **3m**
(300 MHz, $CDCl_3$)



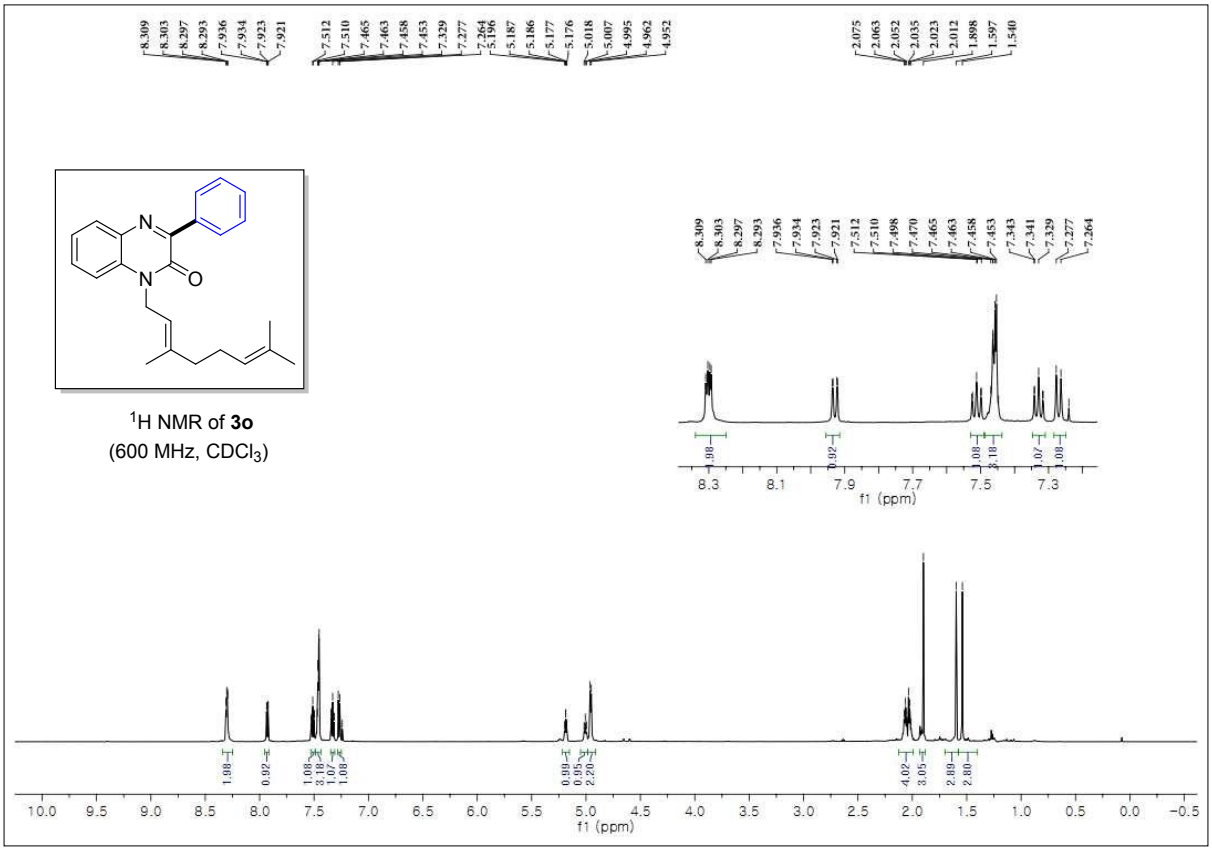
^{13}C NMR of **3m**
(150 MHz, $CDCl_3$)



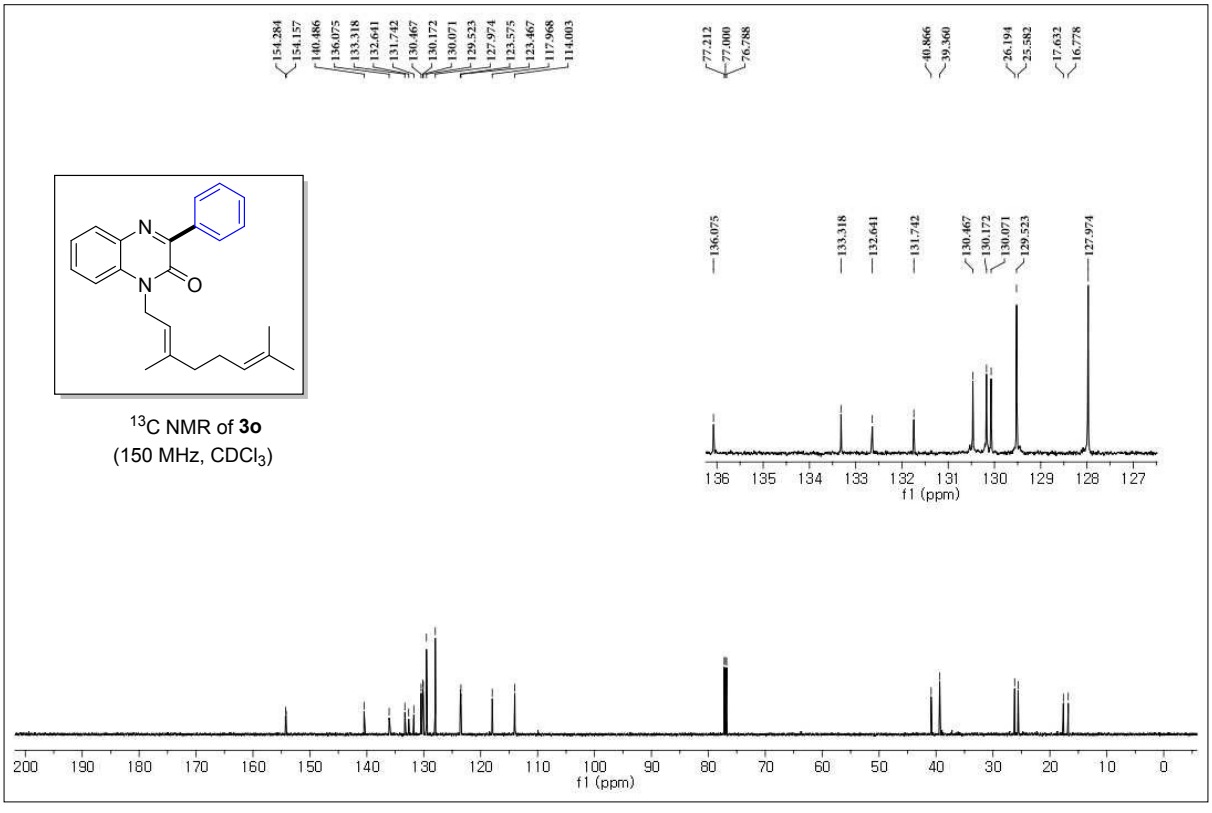
^{1}H NMR of **3n**
(600 MHz, $CDCl_3$)



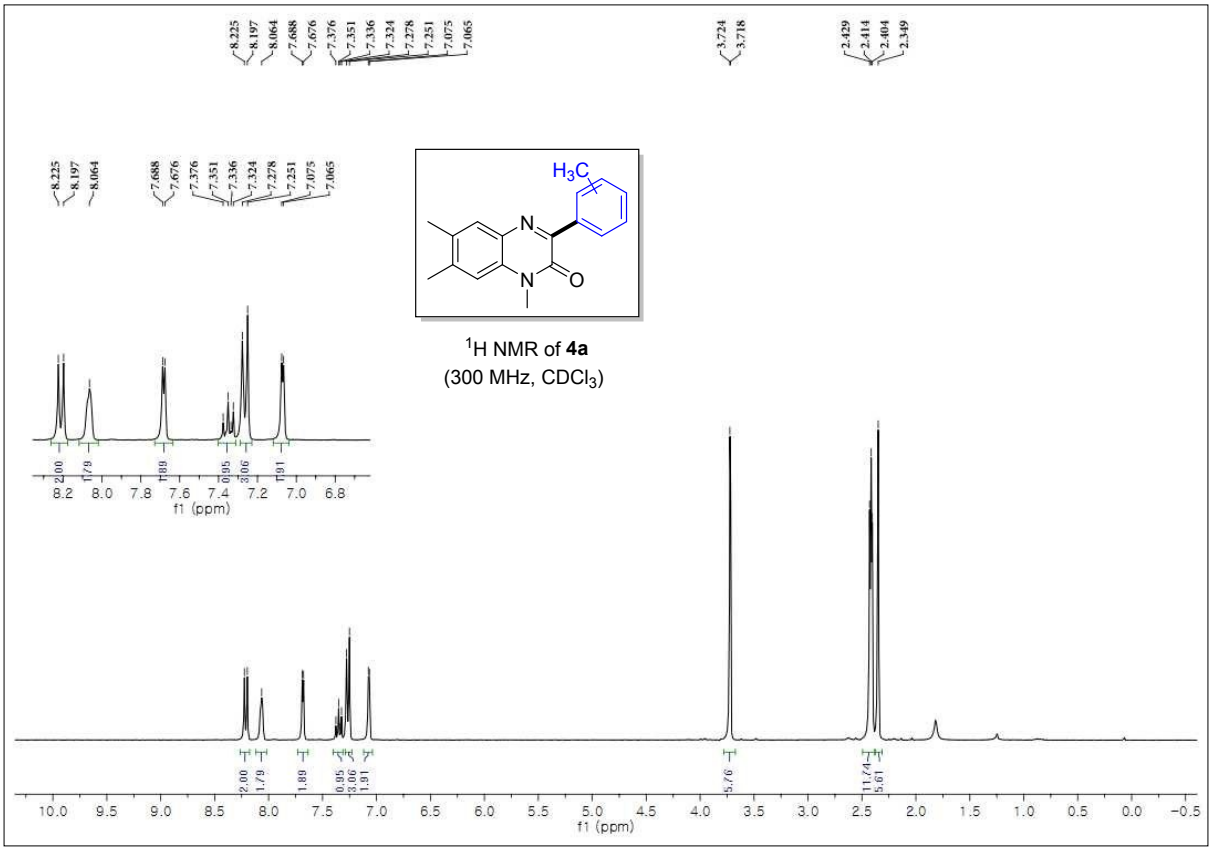
^{13}C NMR of **3n**
(150 MHz, $CDCl_3$)



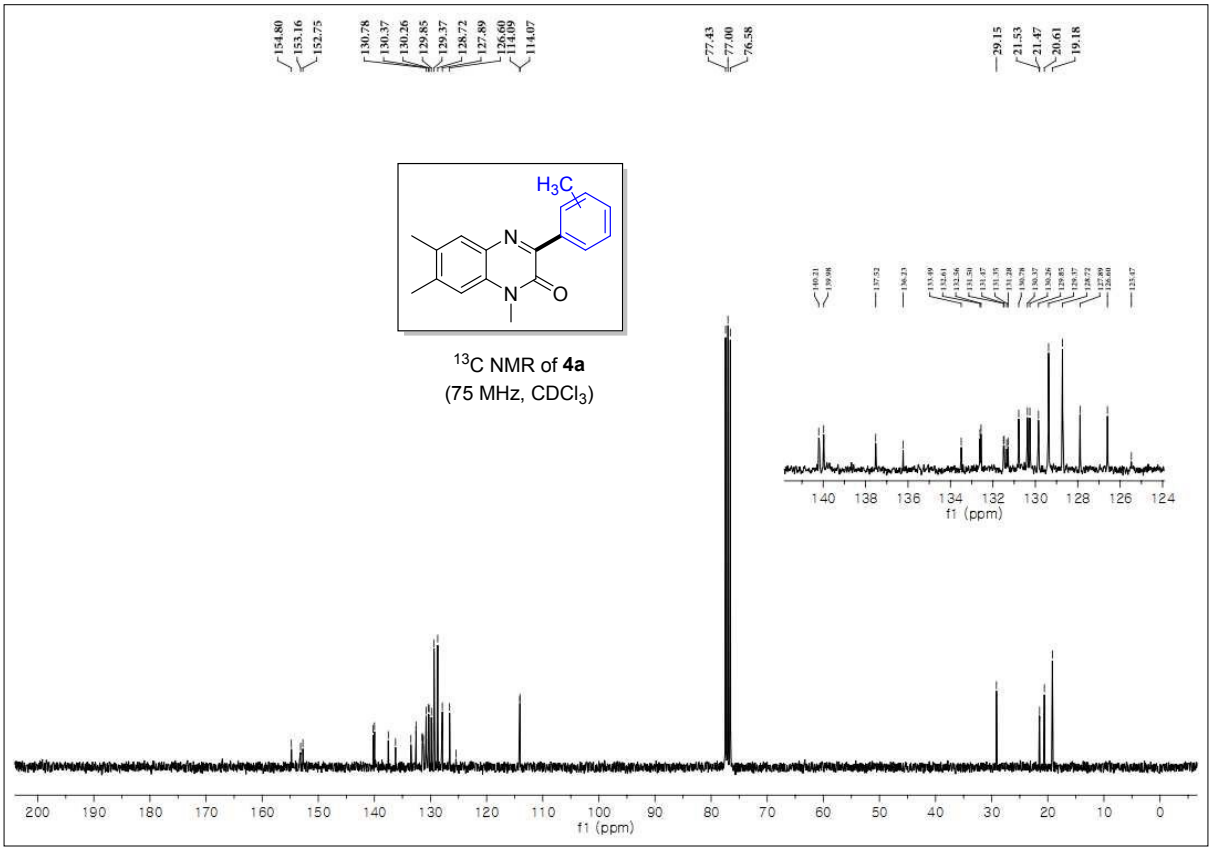
^{1}H NMR of **3o**
(600 MHz, $CDCl_3$)



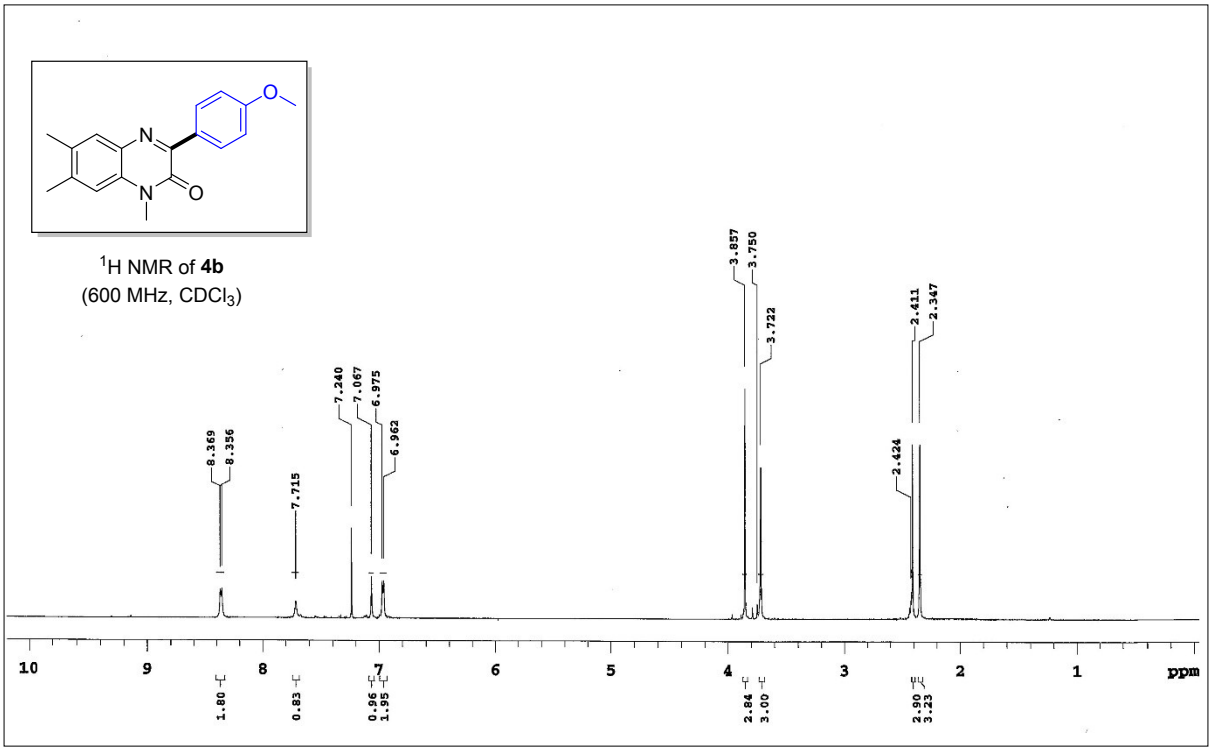
^{13}C NMR of **3o**
(150 MHz, $CDCl_3$)

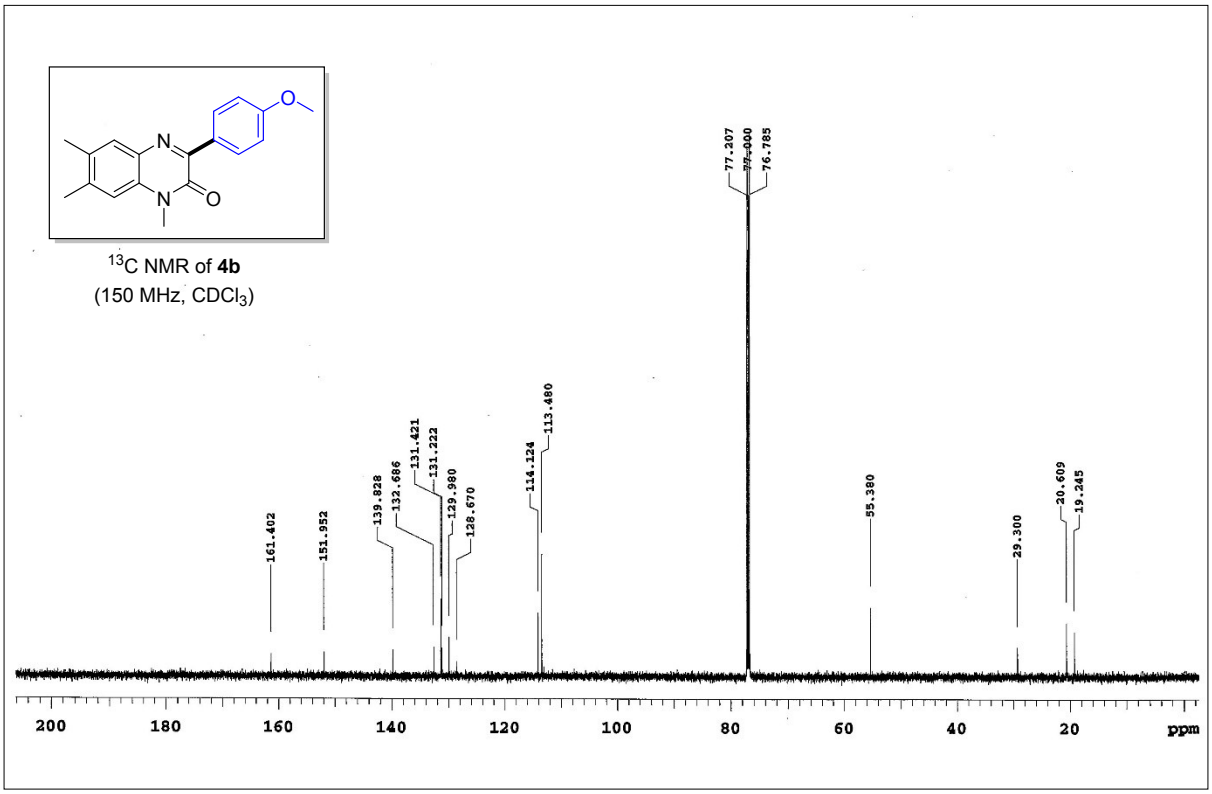


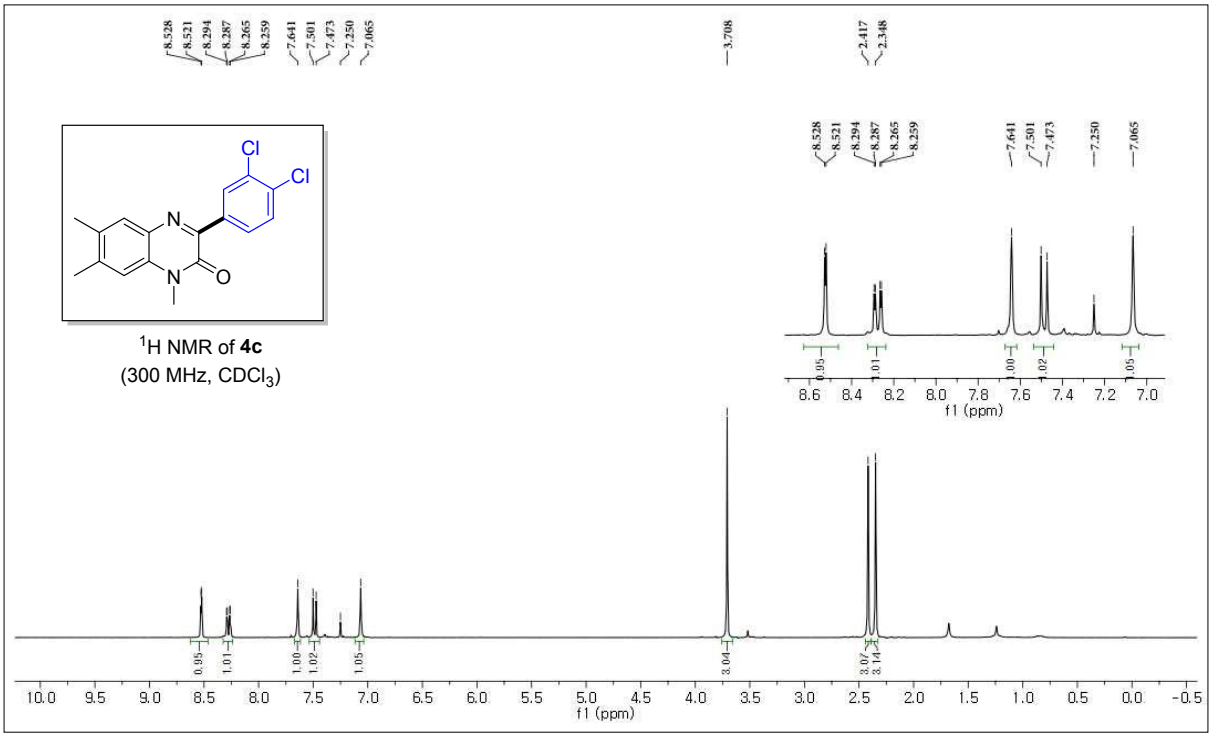
^{1}H NMR of **4a**
(300 MHz, $CDCl_3$)



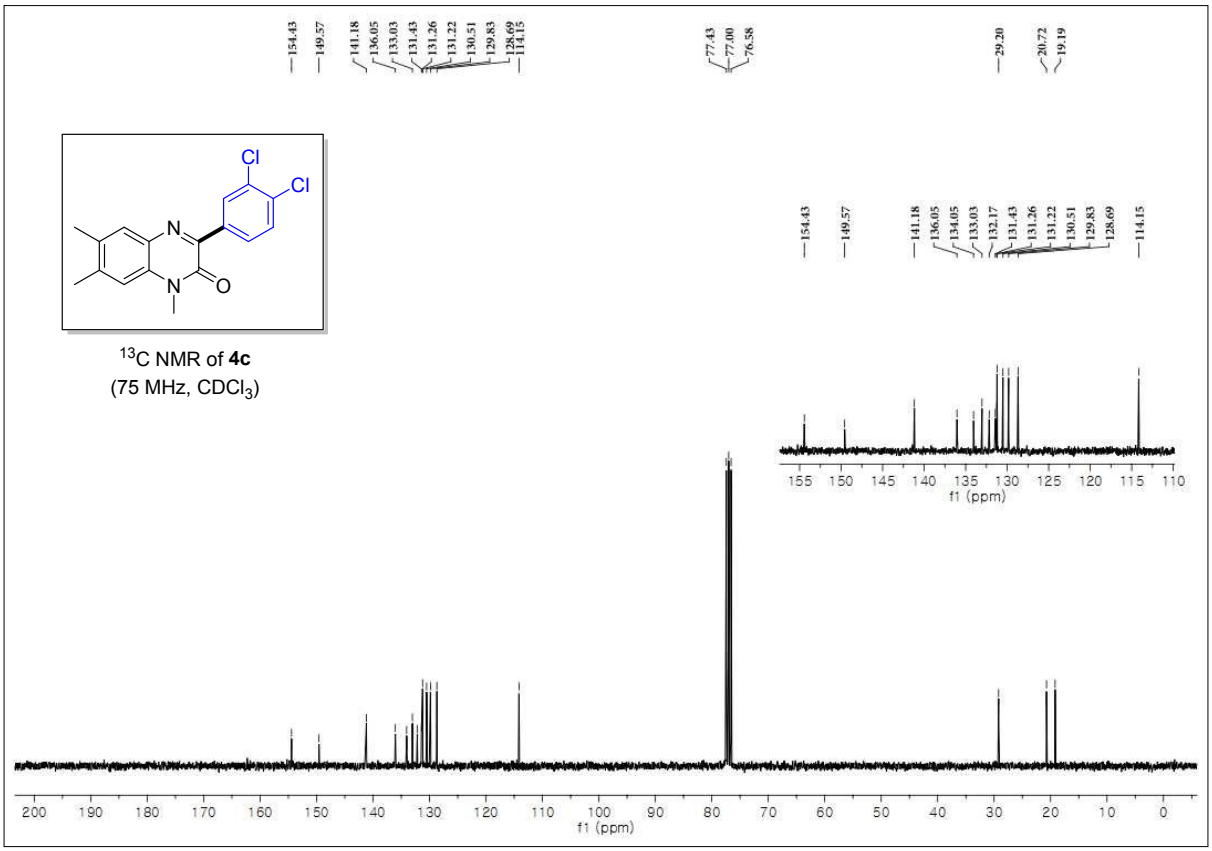
^{13}C NMR of **4a**
(75 MHz, $CDCl_3$)


^{1}H NMR of **4b**
(600 MHz, $CDCl_3$)
8.369
8.356
7.715
7.240
7.067
6.975
6.962
3.857
3.750
3.722
2.424
2.411
2.347
10
9
8
7
6
5
4
3
2
1
ppm
1.80
0.83
0.96
1.95
2.84
3.00
2.90
3.23

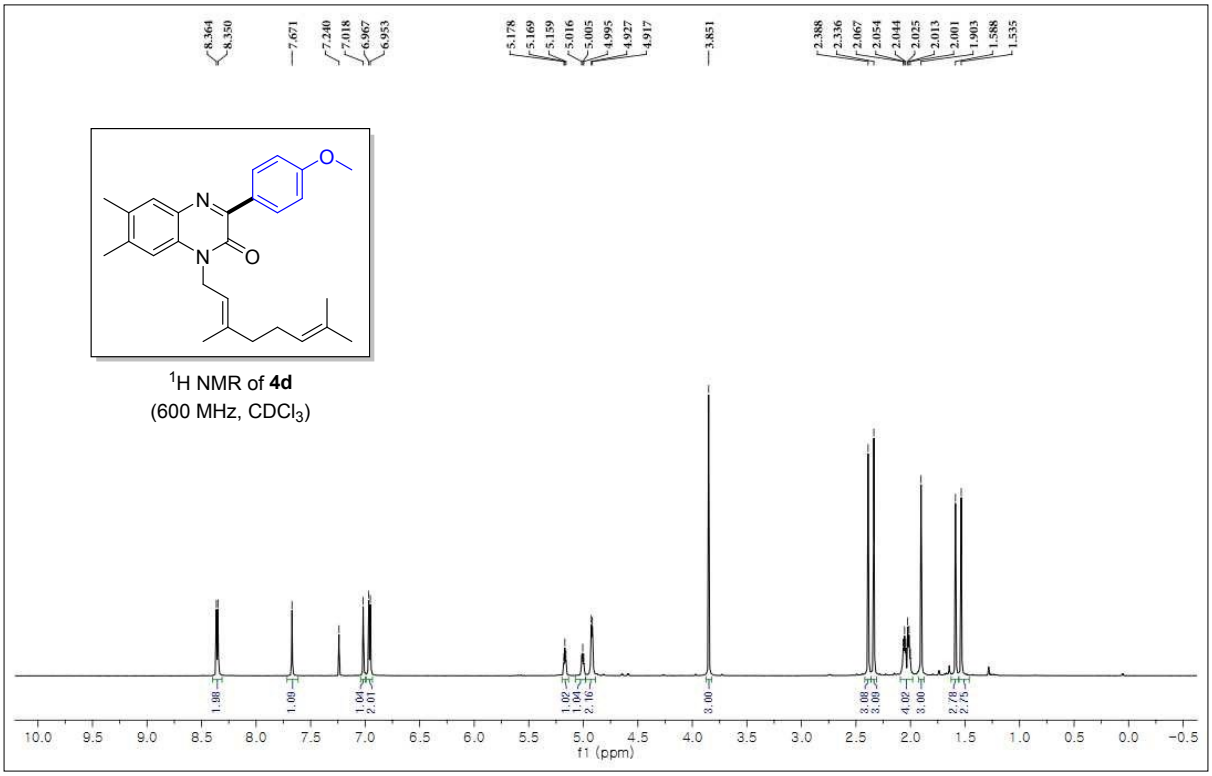

^{13}C NMR of **4b**
(150 MHz, $CDCl_3$)
161.402
151.952
139.828
132.686
131.421
131.222
129.980
128.670
114.124
113.480
77.207
77.000
76.785
55.380
29.300
20.609
19.245
200
180
160
140
120
100
80
60
40
20
ppm



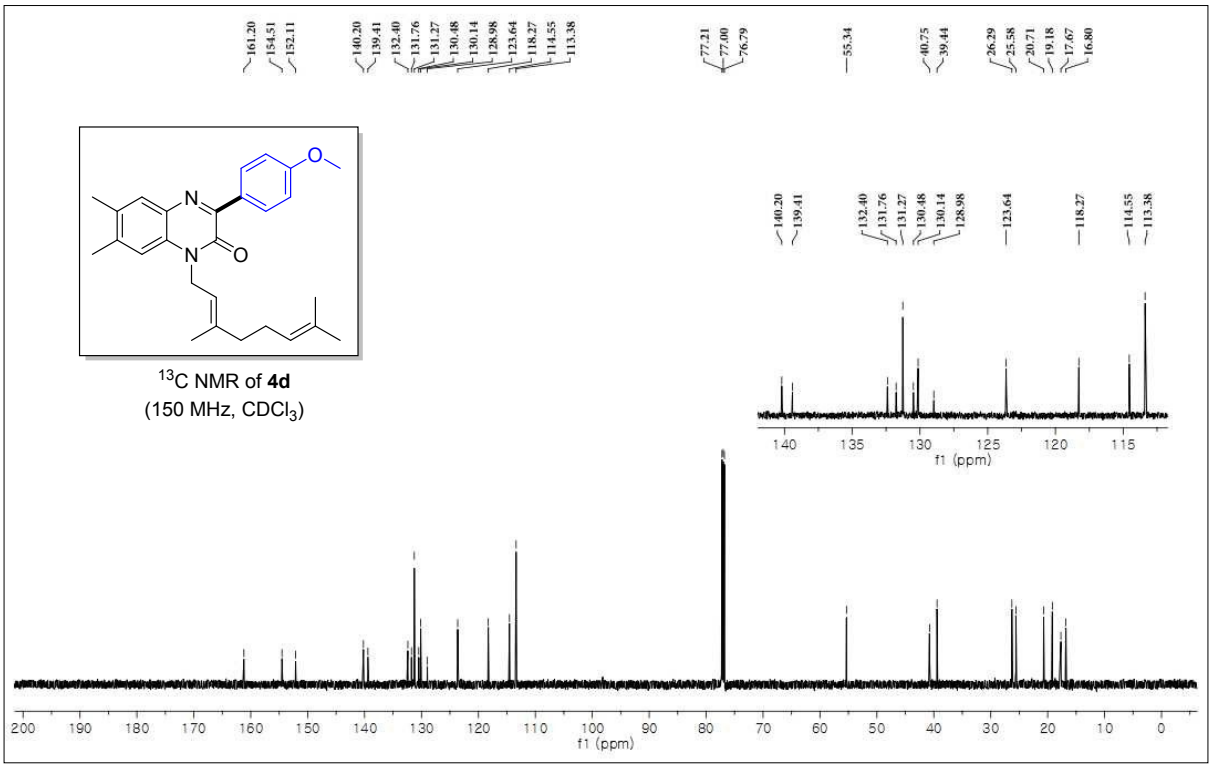
^{1}H NMR of **4c**
(300 MHz, $CDCl_3$)



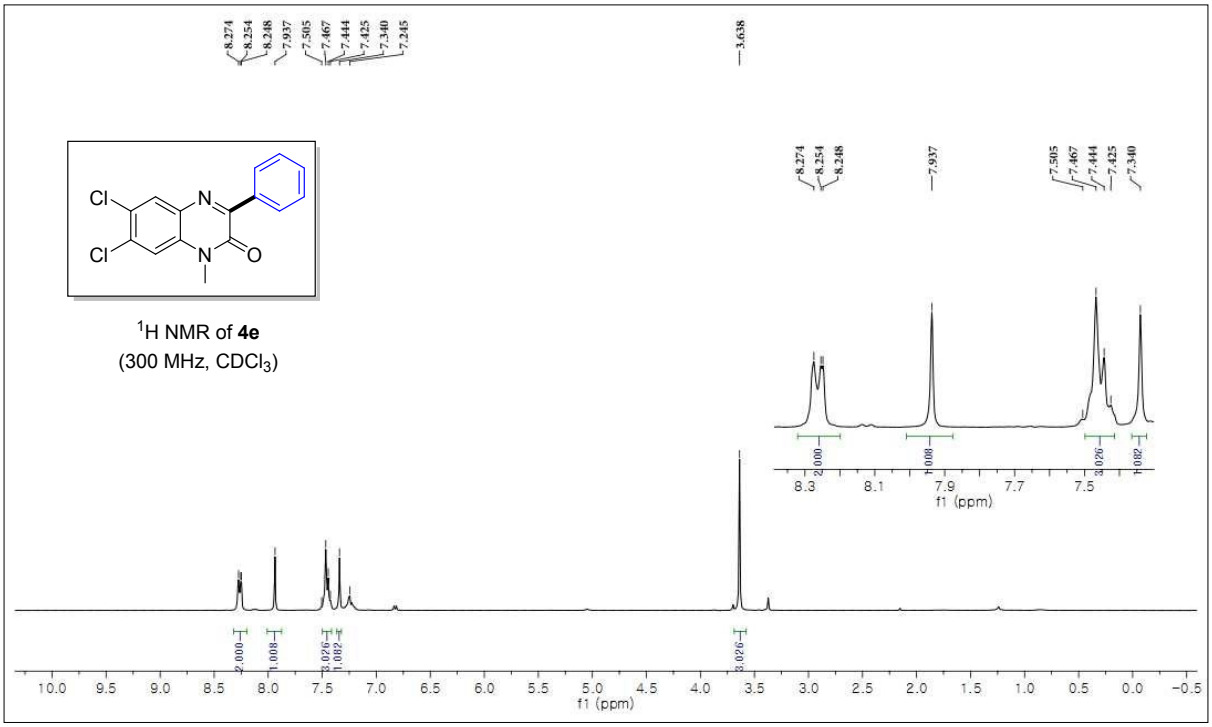
^{13}C NMR of **4c**
(75 MHz, $CDCl_3$)



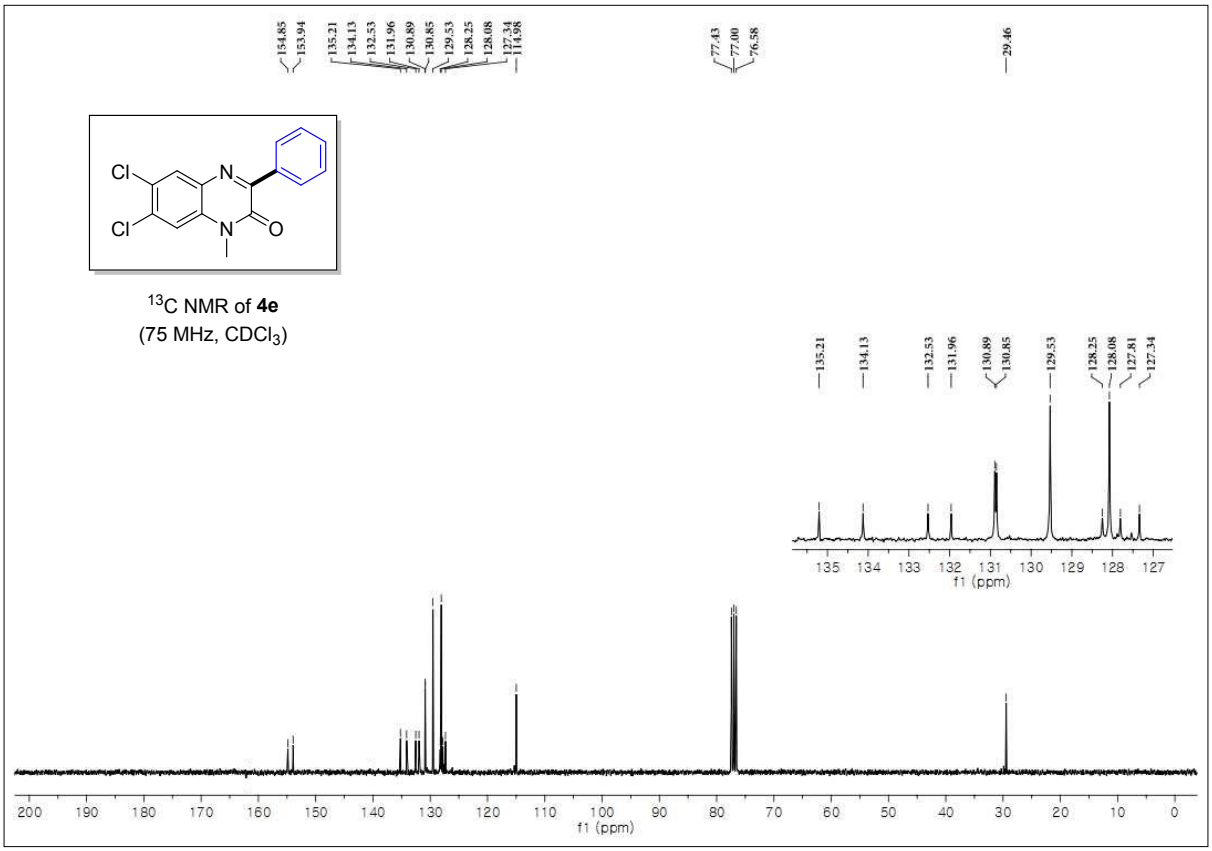
^{1}H NMR of **4d**
(600 MHz, $CDCl_3$)



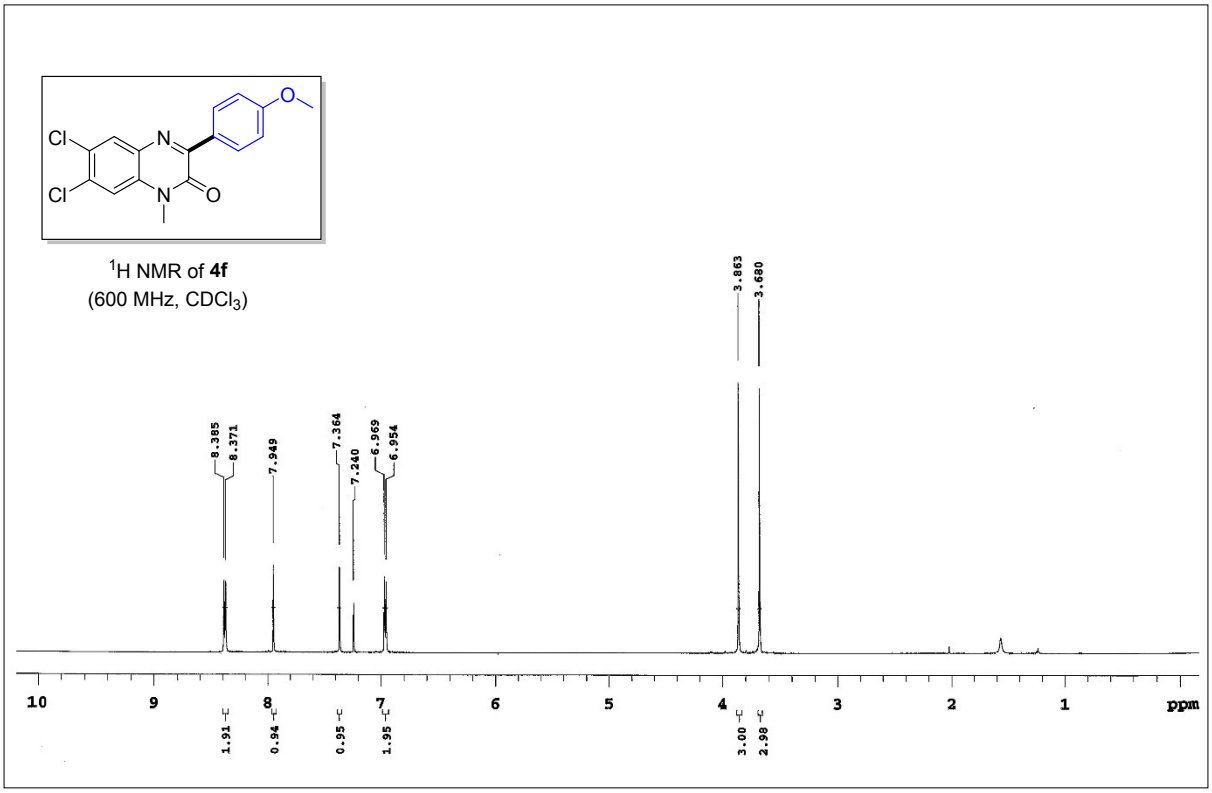
^{13}C NMR of **4d**
(150 MHz, $CDCl_3$)

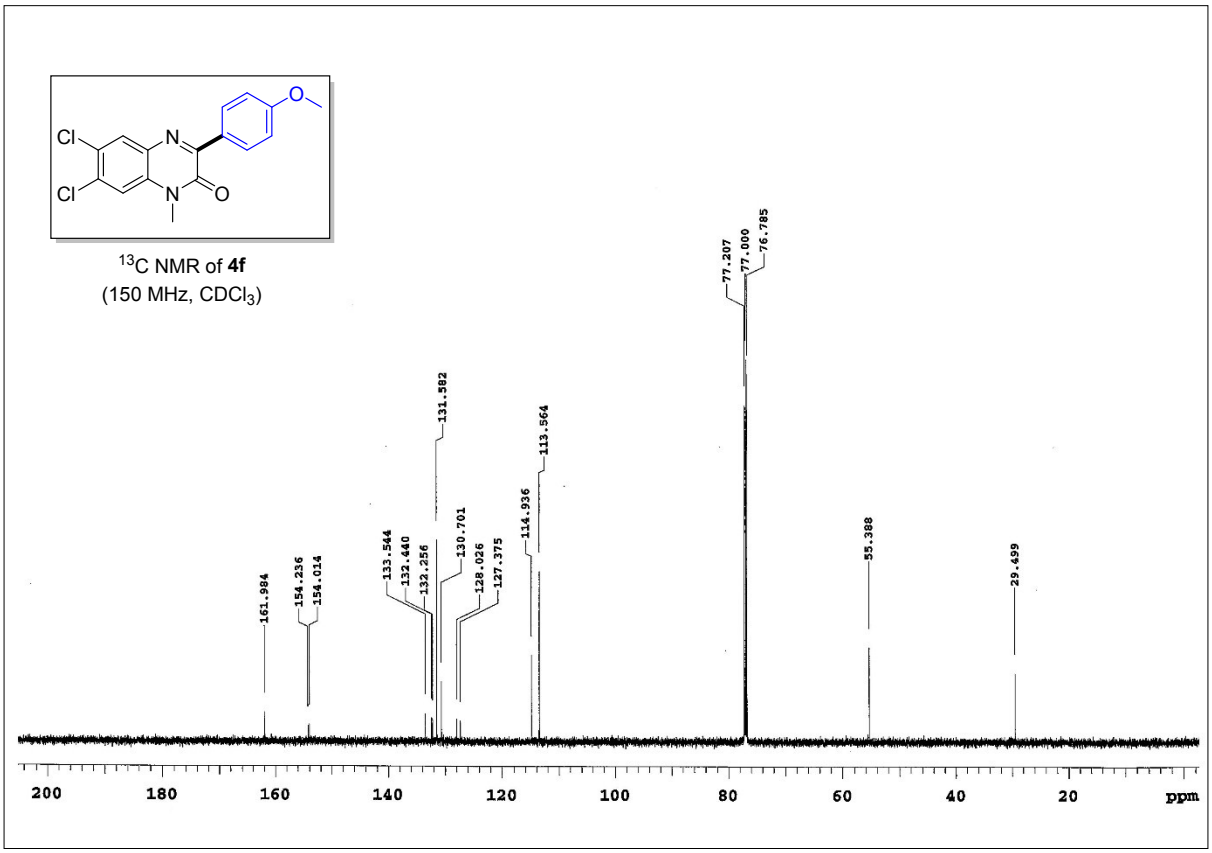


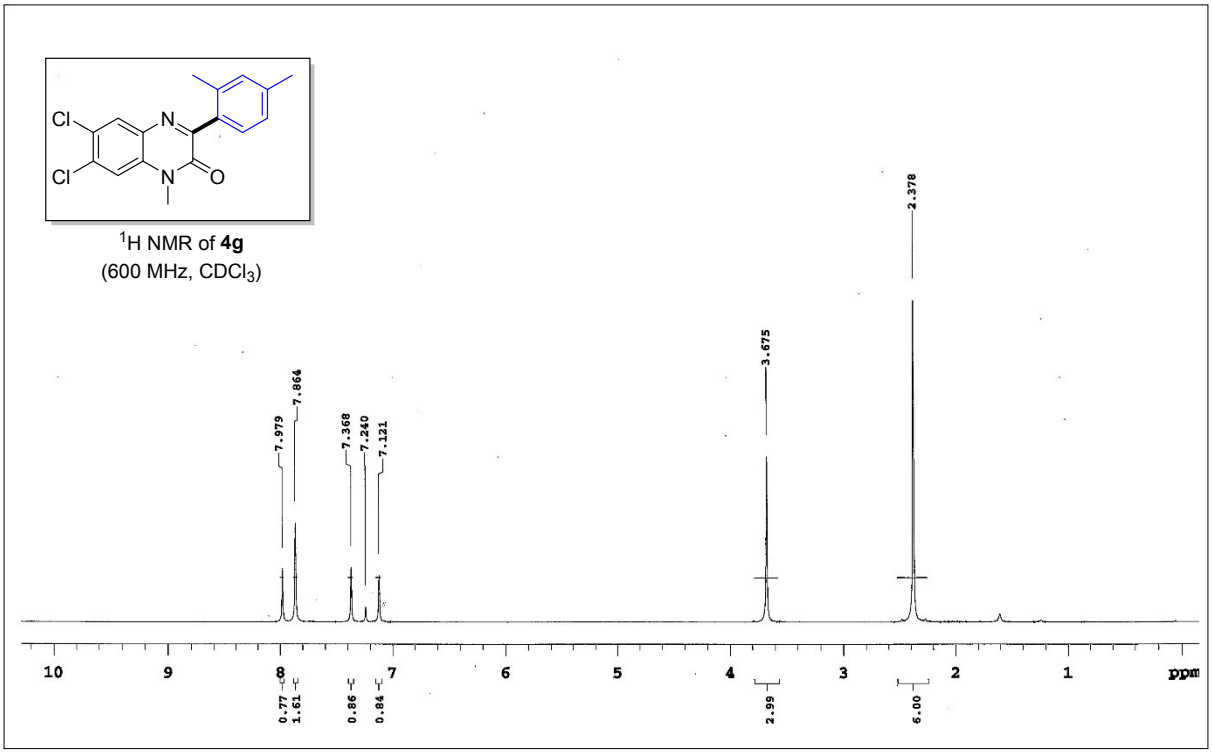
^{1}H NMR of **4e**
(300 MHz, $CDCl_3$)



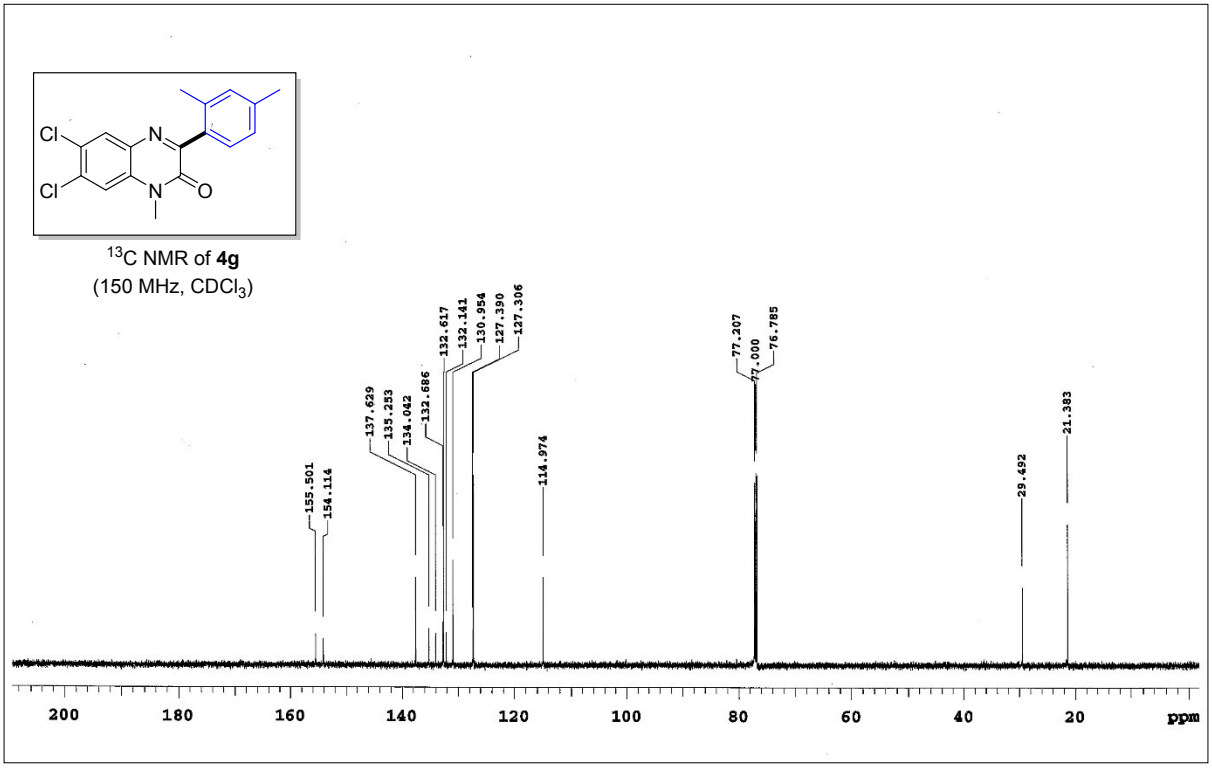
^{13}C NMR of **4e**
(75 MHz, $CDCl_3$)


Cl
Cl
N
N
O
O
^{1}H NMR of **4f**
(600 MHz, $CDCl_3$)
8.385
8.371
7.949
7.364
7.240
6.969
6.954
3.863
3.680
10
9
8
7
6
5
4
3
2
1
ppm
1.91
0.94
0.95
1.95
3.00
2.98

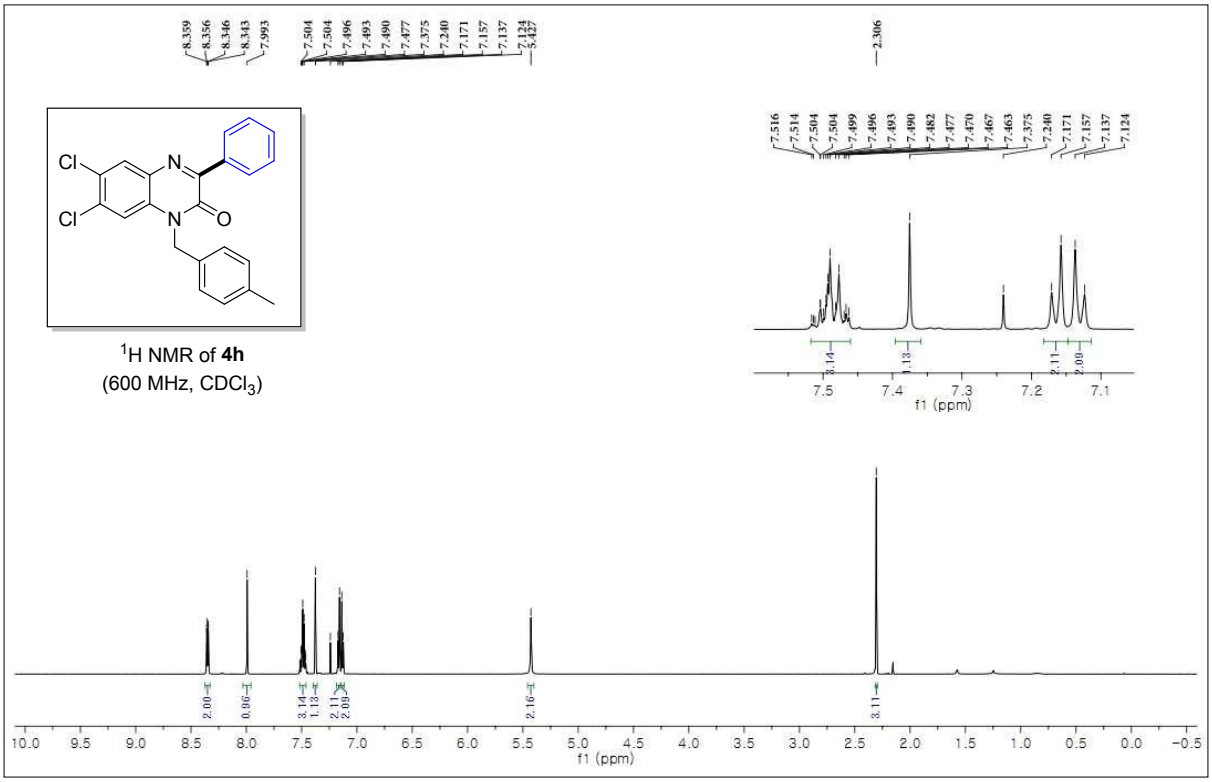

Cl
Cl
N
N
O
O
^{13}C NMR of **4f**
(150 MHz, $CDCl_3$)
161.984
154.236
154.014
133.544
132.440
132.256
131.382
130.701
128.026
127.375
114.936
113.564
77.207
77.000
76.785
55.388
29.499
200
180
160
140
120
100
80
60
40
20
ppm



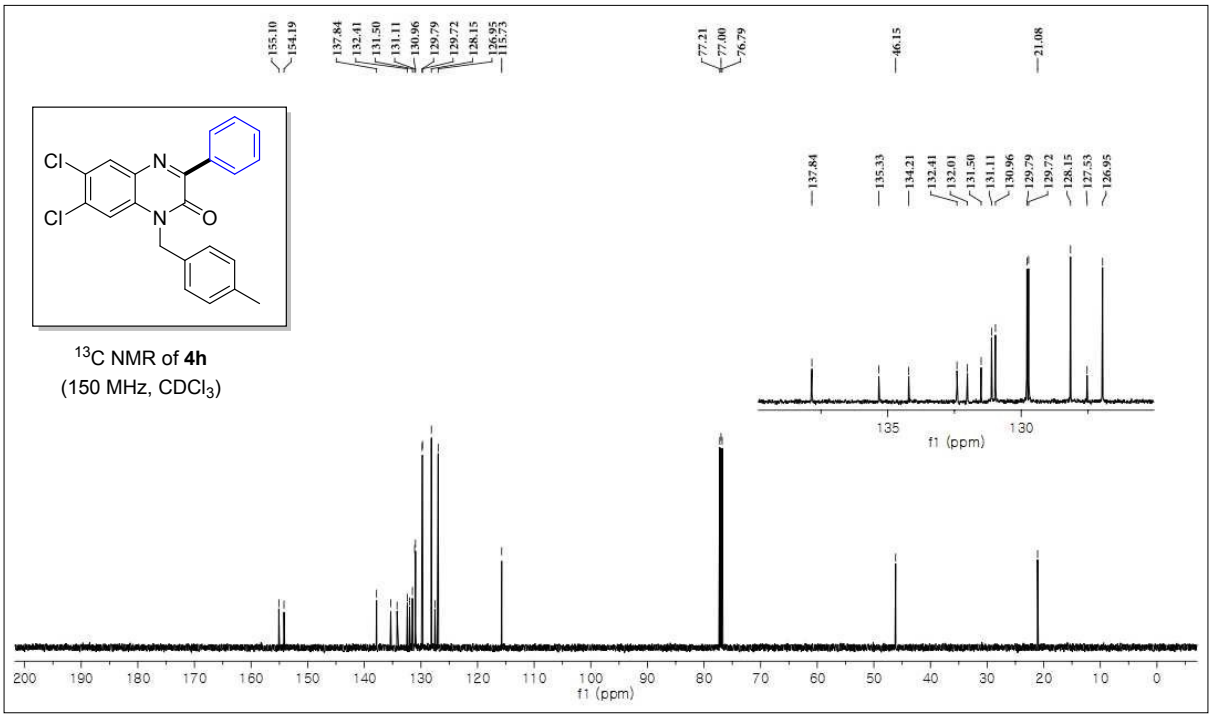
^{1}H NMR of **4g**
(600 MHz, $CDCl_3$)



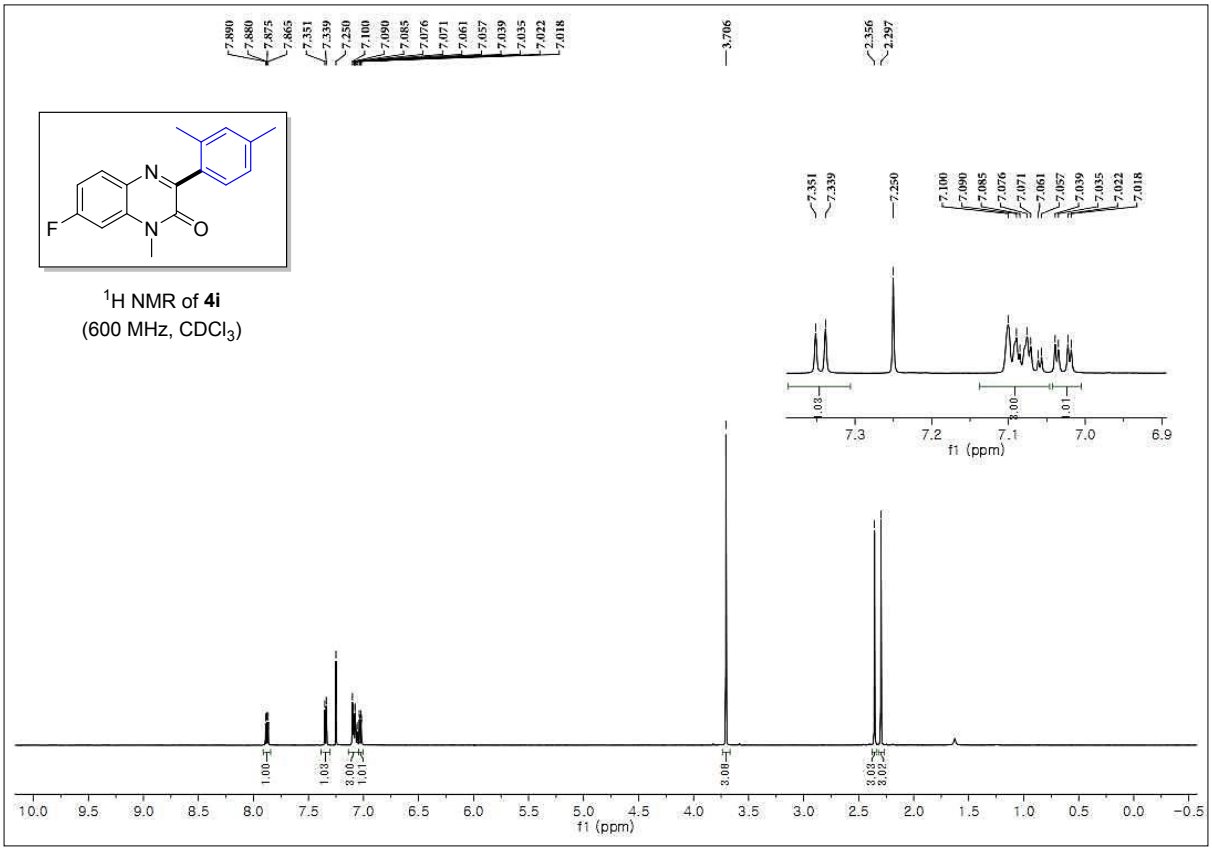
^{13}C NMR of **4g**
(150 MHz, $CDCl_3$)



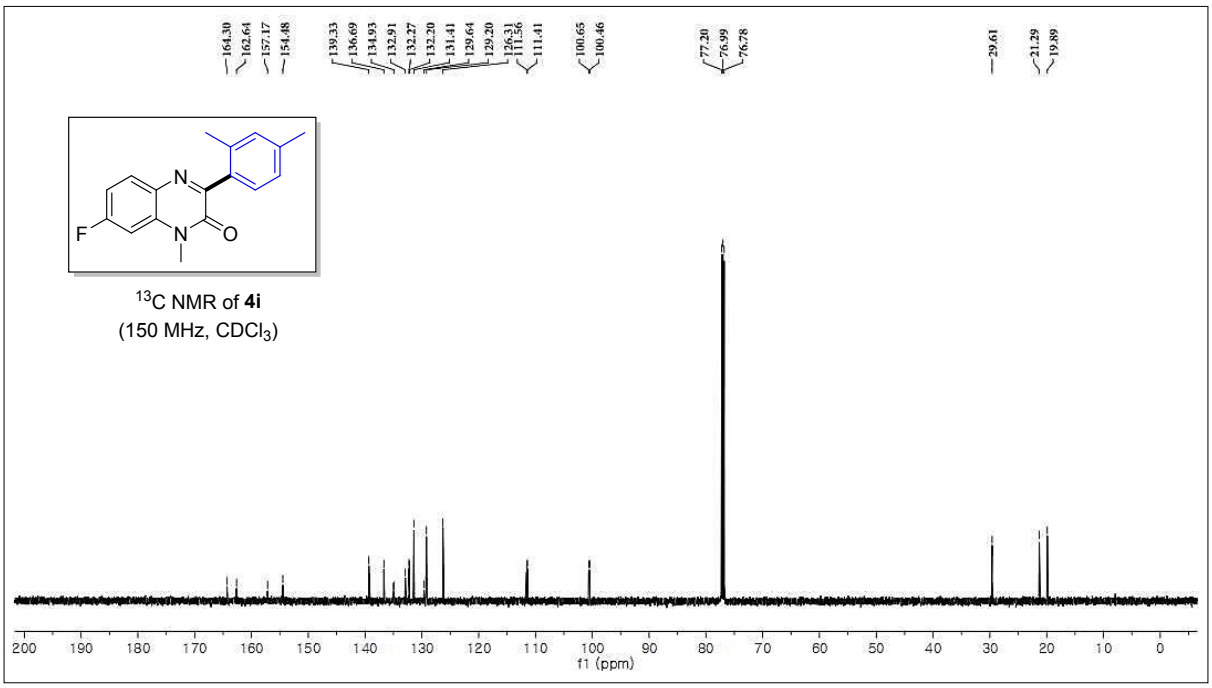
^{1}H NMR of **4h**
(600 MHz, $CDCl_3$)



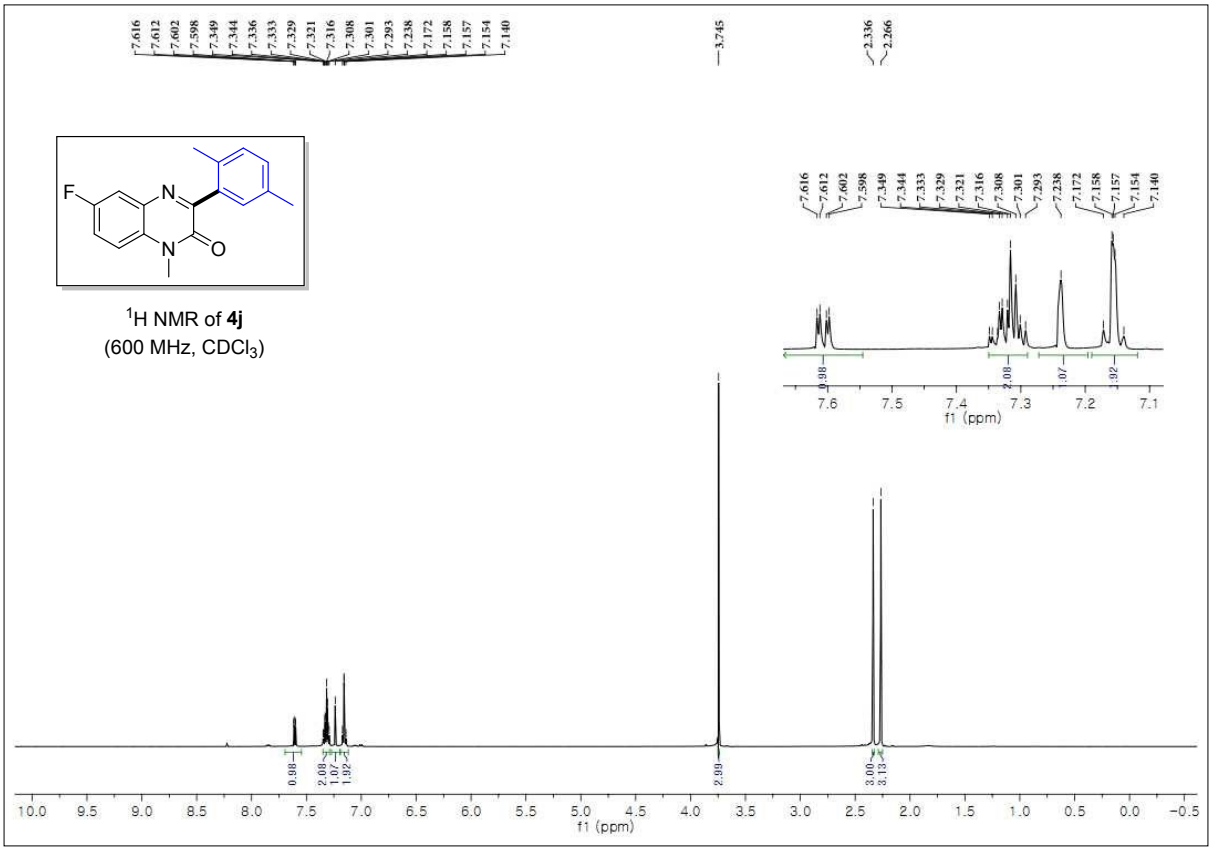
^{13}C NMR of **4h**
(150 MHz, $CDCl_3$)



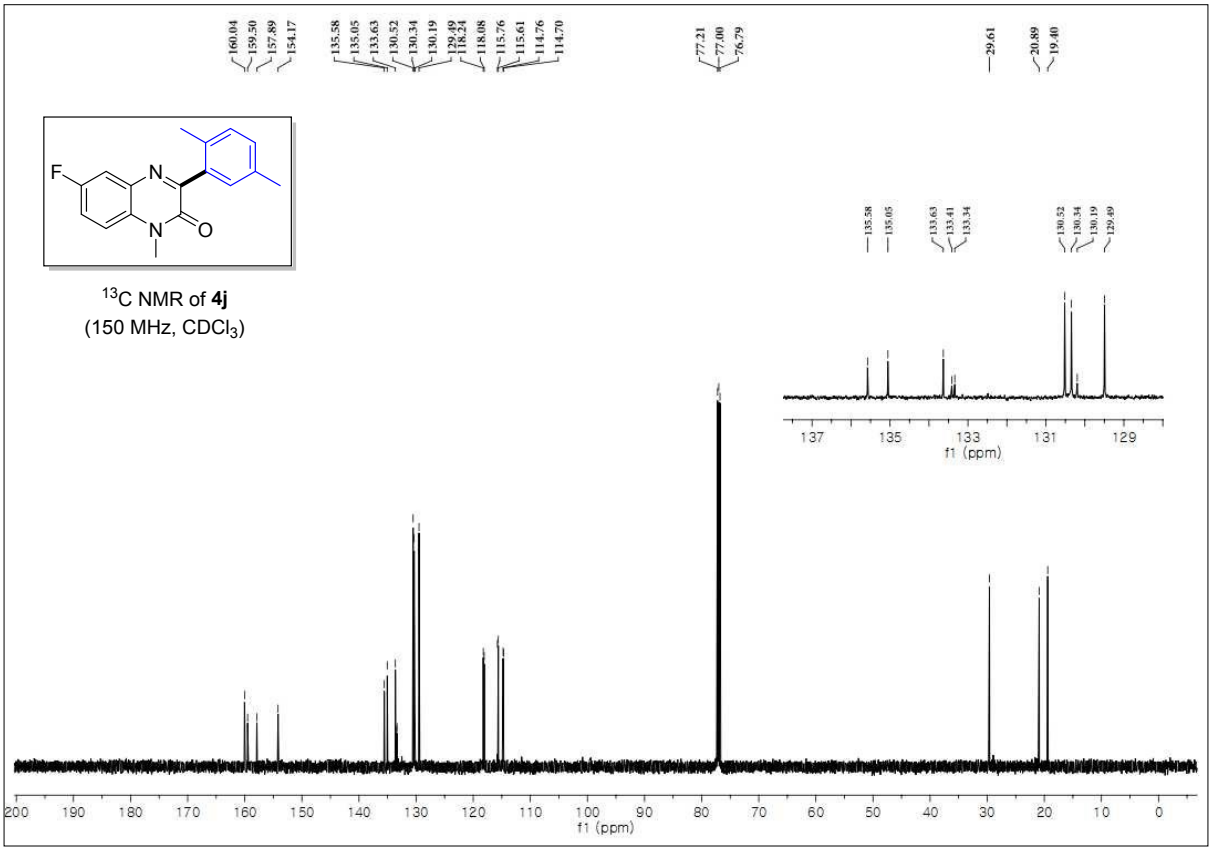
^{1}H NMR of **4i**
(600 MHz, $CDCl_3$)



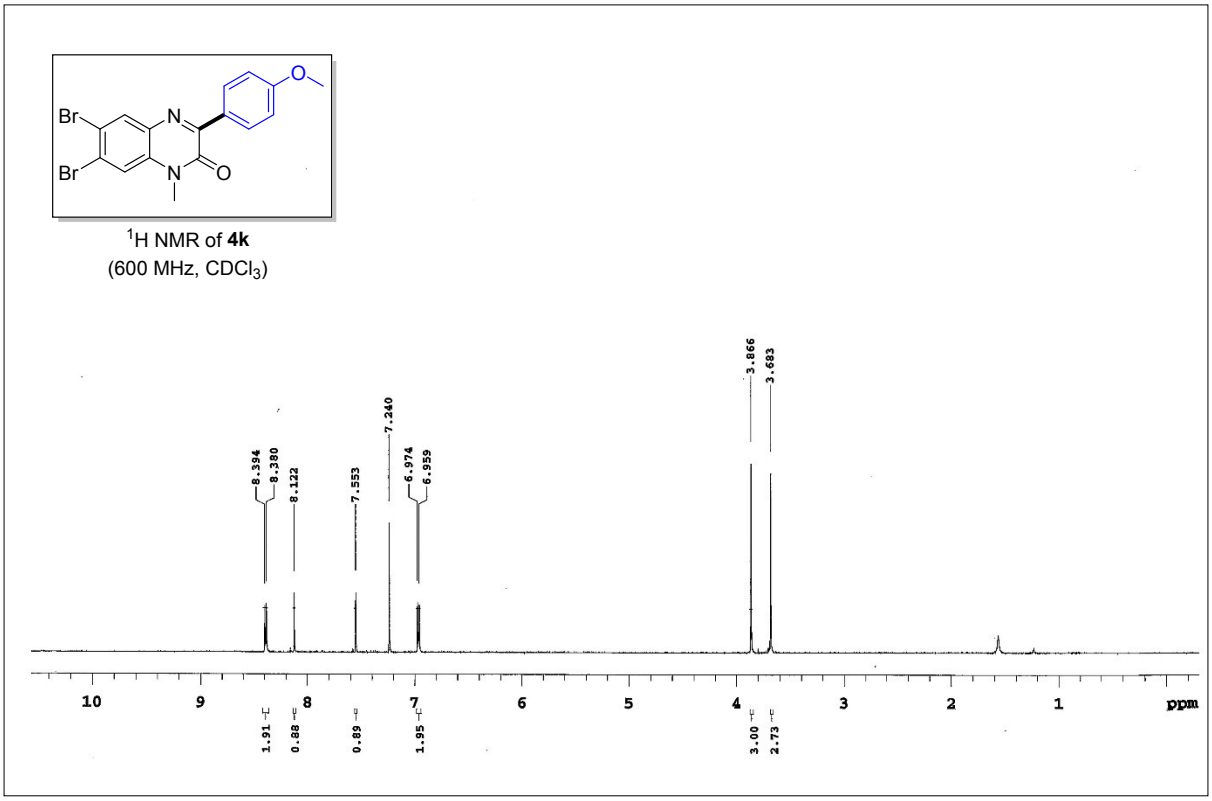
^{13}C NMR of **4i**
(150 MHz, $CDCl_3$)



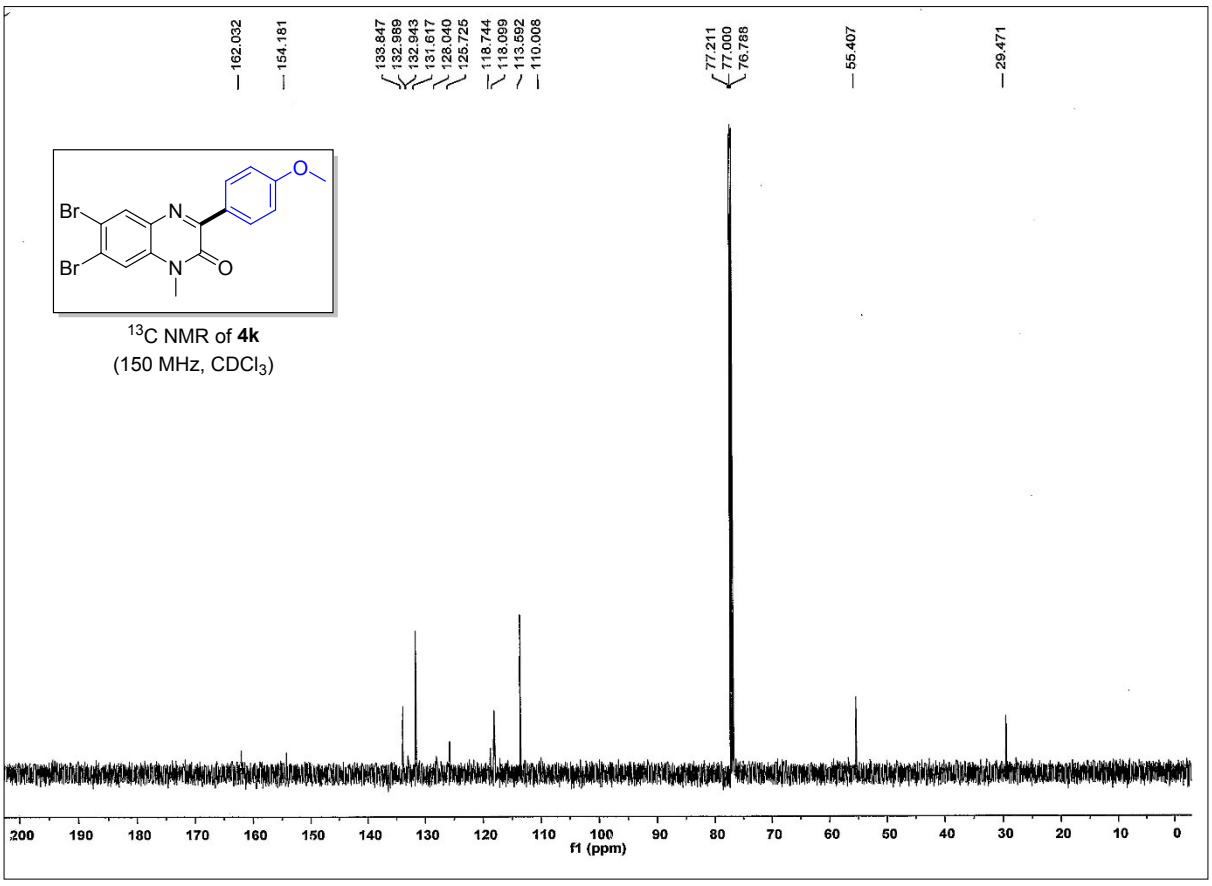
^{1}H NMR of **4j**
(600 MHz, $CDCl_3$)



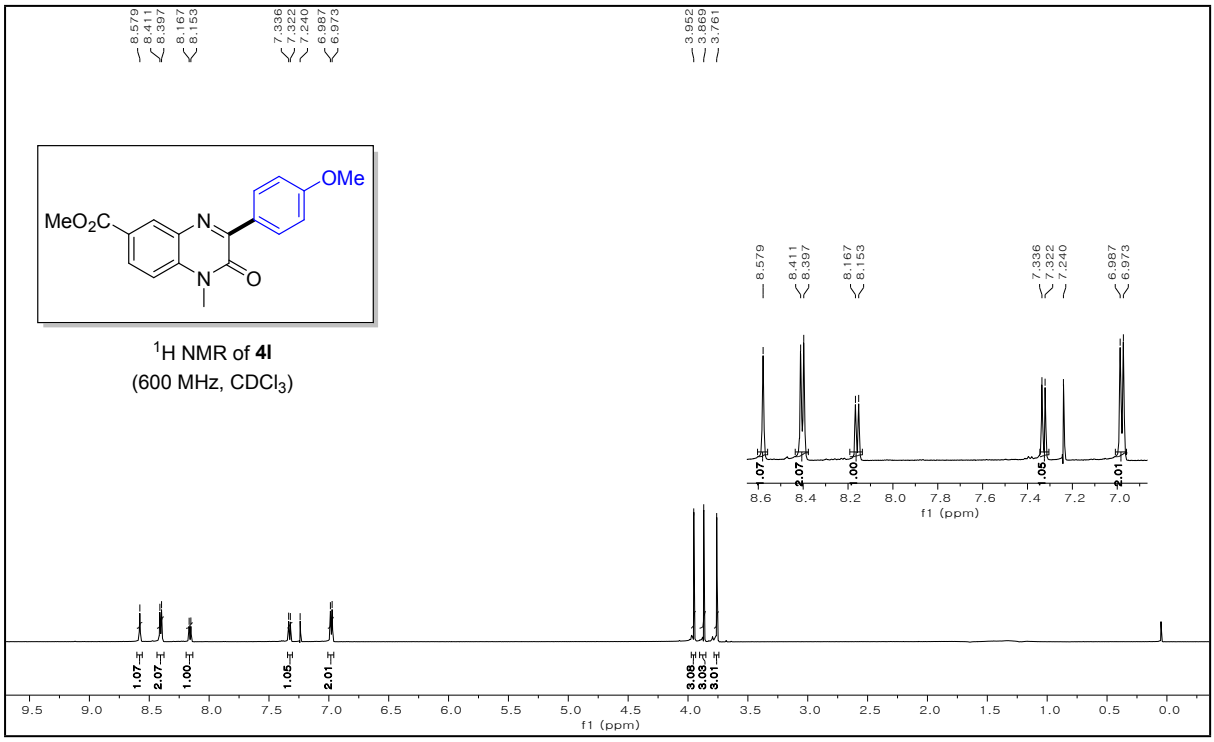
^{13}C NMR of **4j**
(150 MHz, $CDCl_3$)

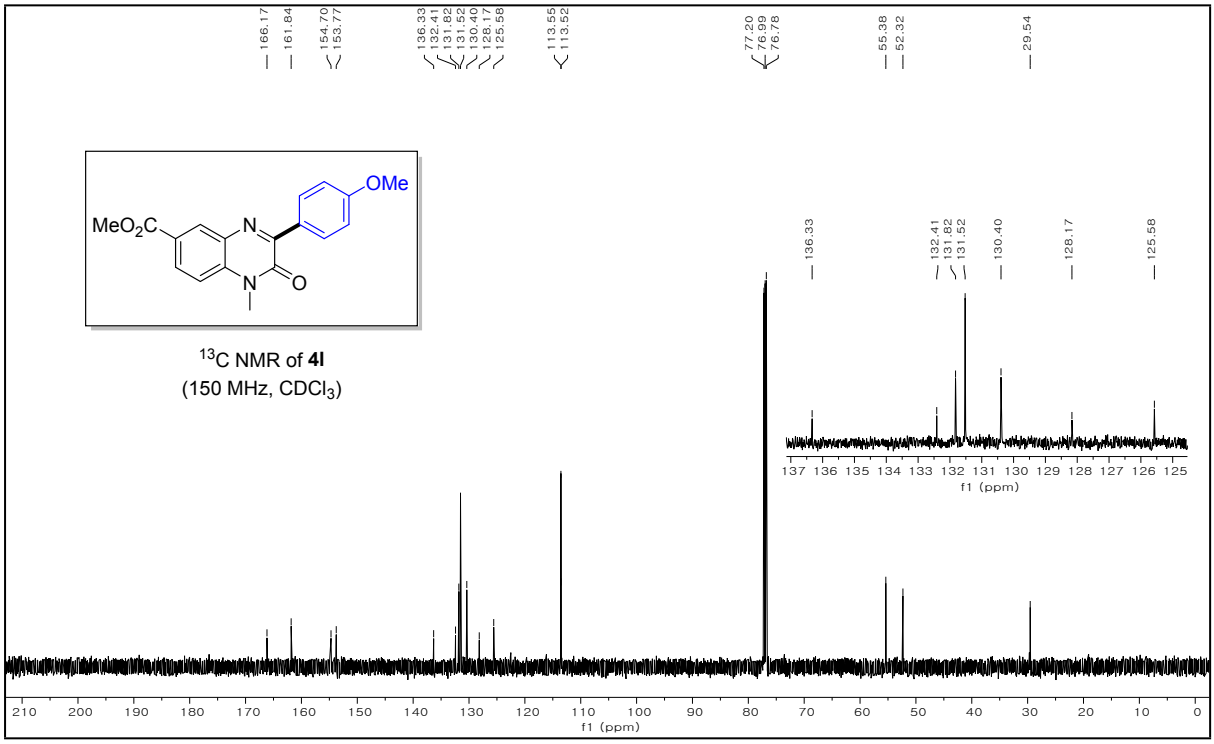


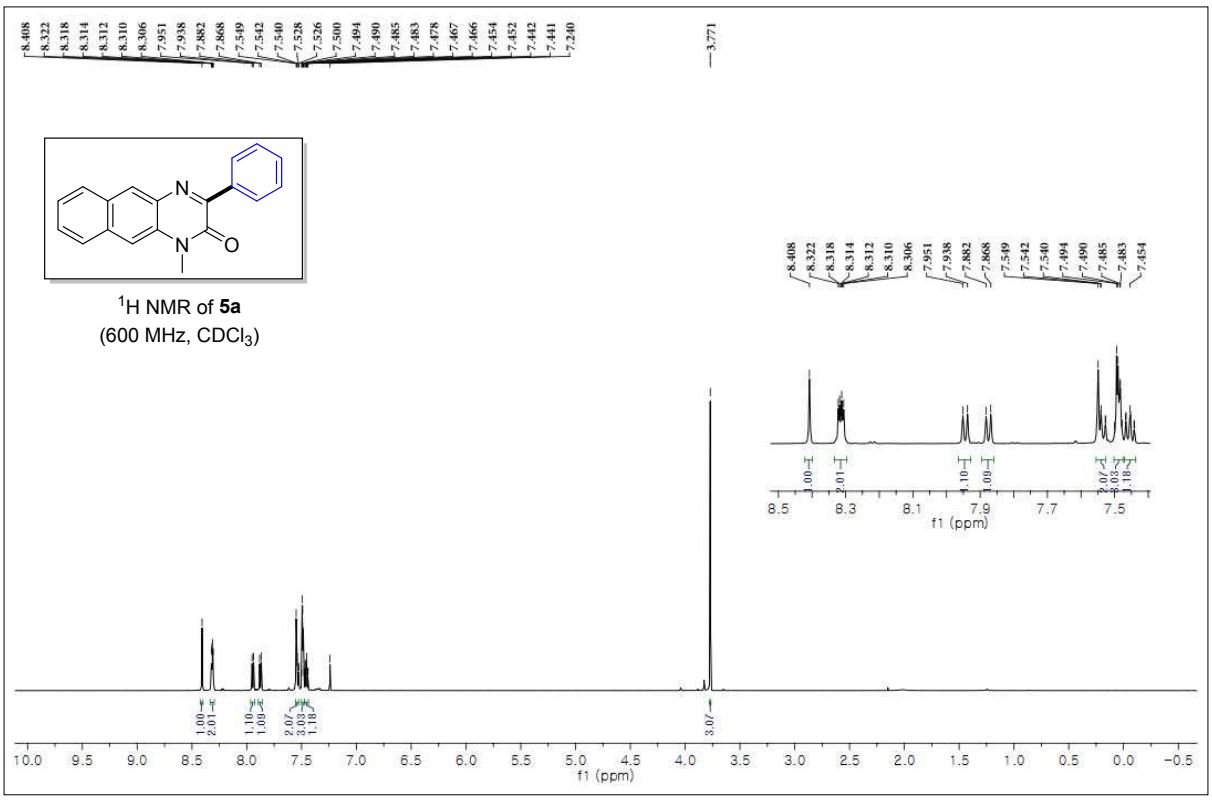
^{1}H NMR of **4k**
(600 MHz, $CDCl_3$)



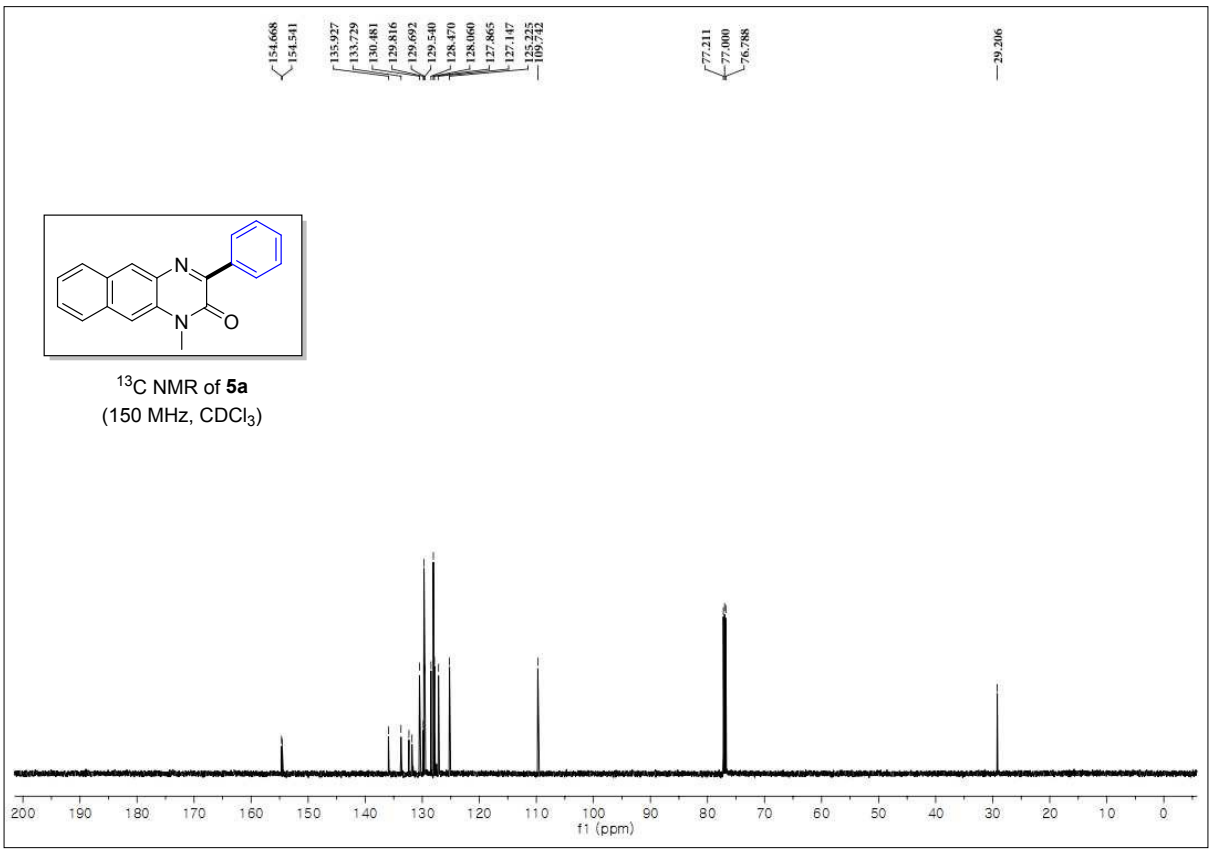
^{13}C NMR of **4k**
(150 MHz, $CDCl_3$)


8.579
8.411
8.397
8.167
8.153
7.336
7.322
7.240
6.987
6.973
3.952
3.869
3.761
OMe
MeO2C
N
N
O
1H NMR of 4l
(600 MHz, CDCl3)
1.07
2.07
1.00
1.05
2.01
3.08
3.03
3.01
f1 (ppm)

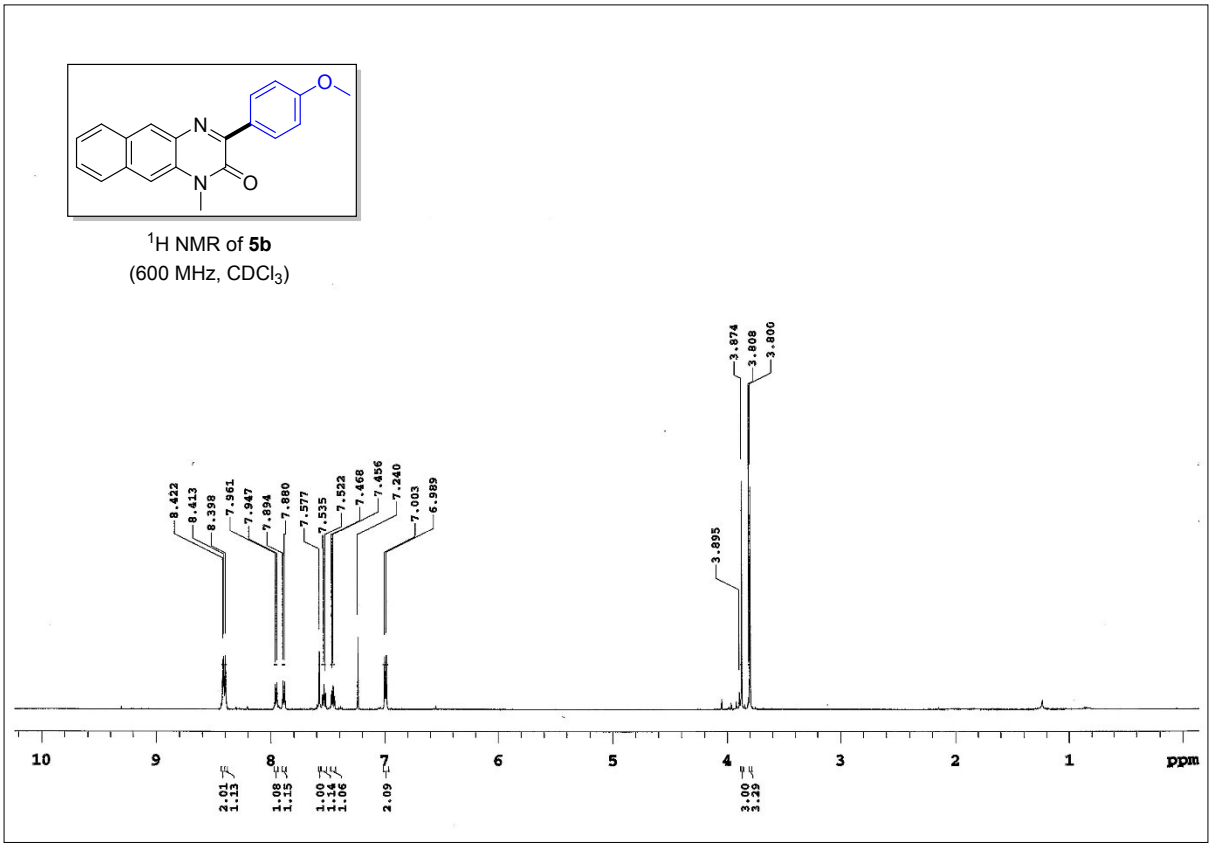

166.17
161.84
154.70
153.77
136.33
132.41
131.82
131.52
130.40
128.17
125.58
113.55
113.52
77.20
76.99
76.78
55.38
52.32
29.54
OMe
MeO2C
N
N
O
13C NMR of 4l
(150 MHz, CDCl3)
f1 (ppm)



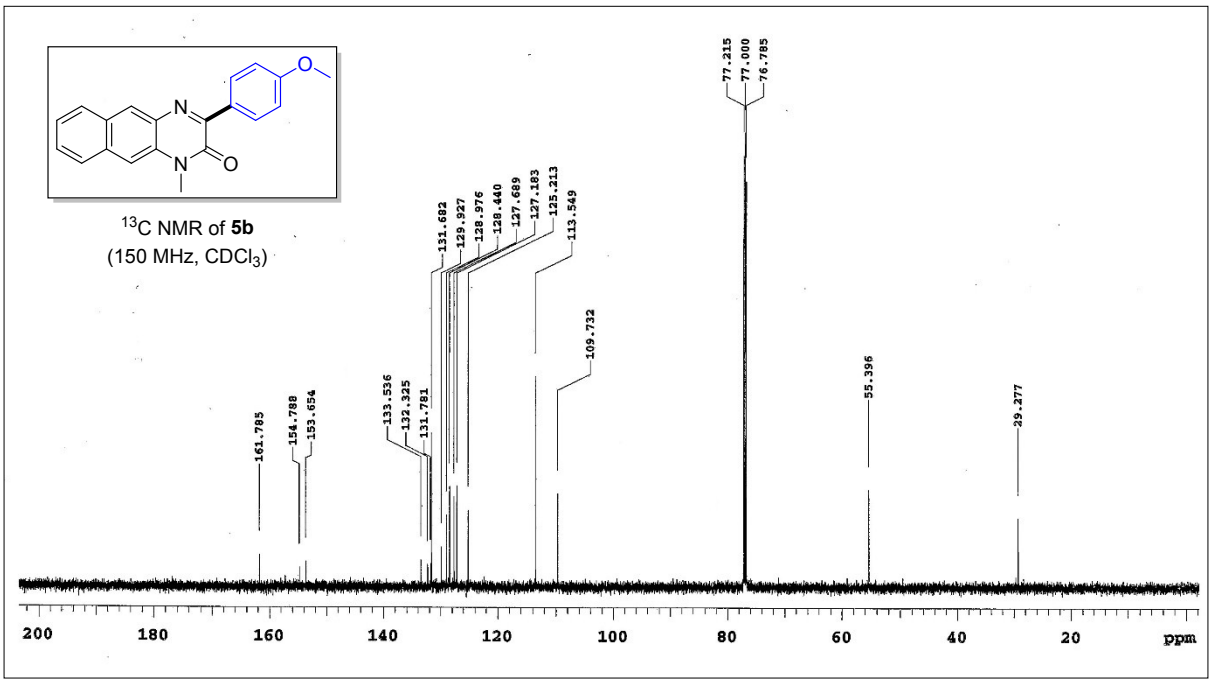
^{1}H NMR of **5a**
(600 MHz, $CDCl_3$)



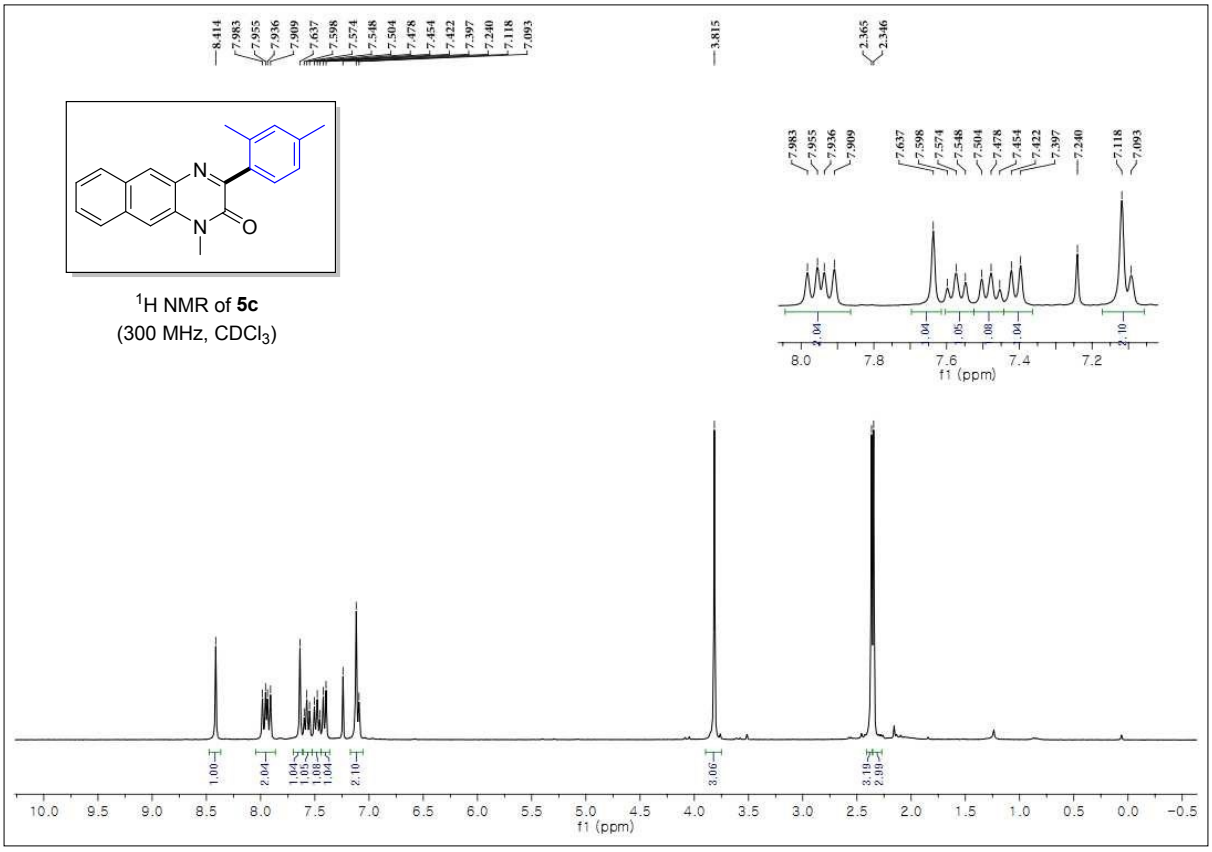
^{13}C NMR of **5a**
(150 MHz, $CDCl_3$)



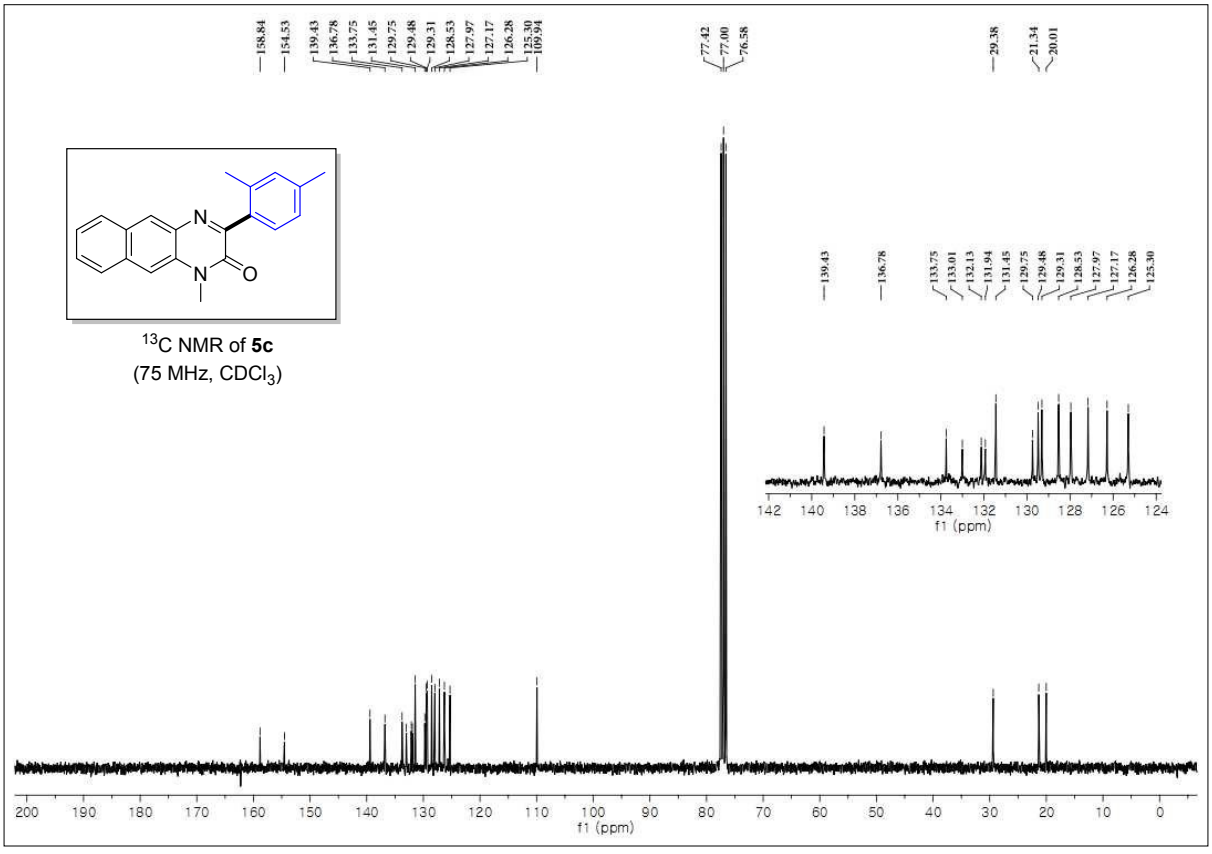
^{1}H NMR of **5b**
(600 MHz, $CDCl_3$)



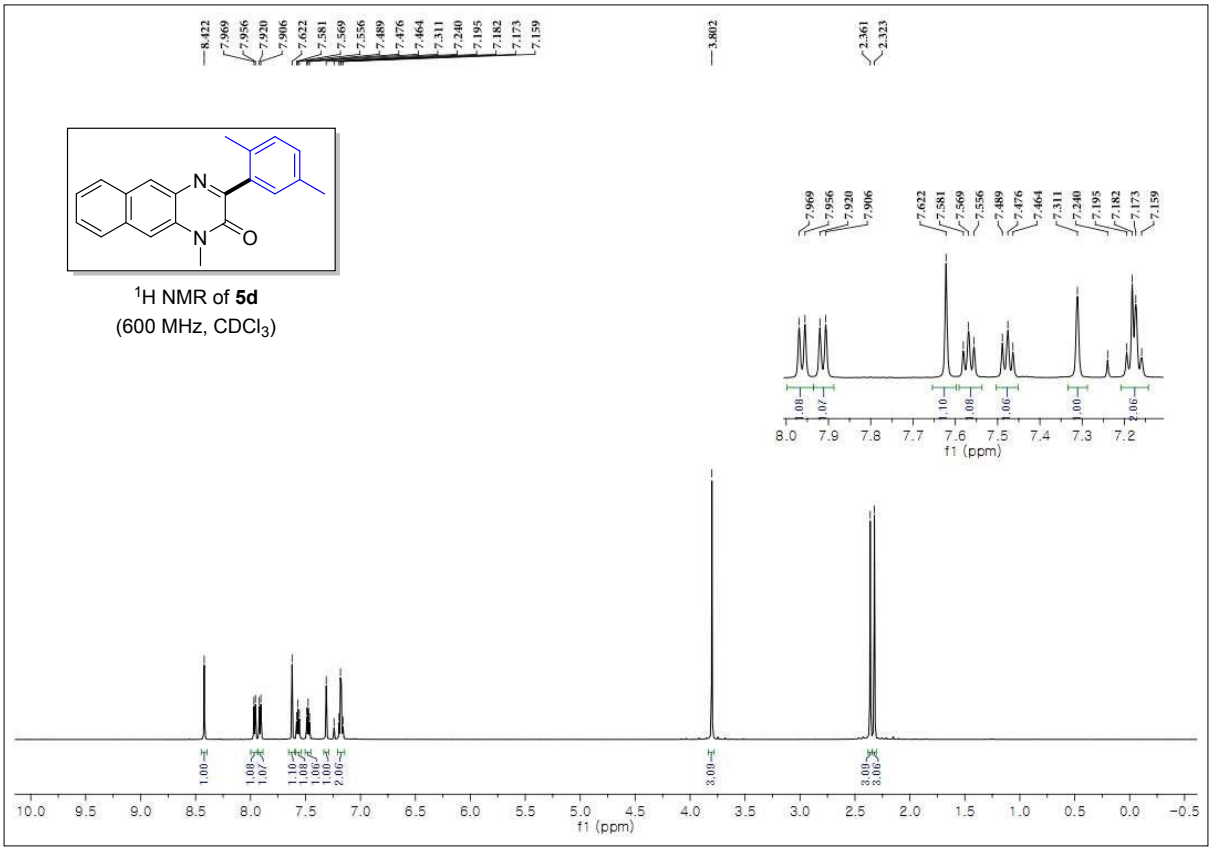
^{13}C NMR of **5b**
(150 MHz, $CDCl_3$)



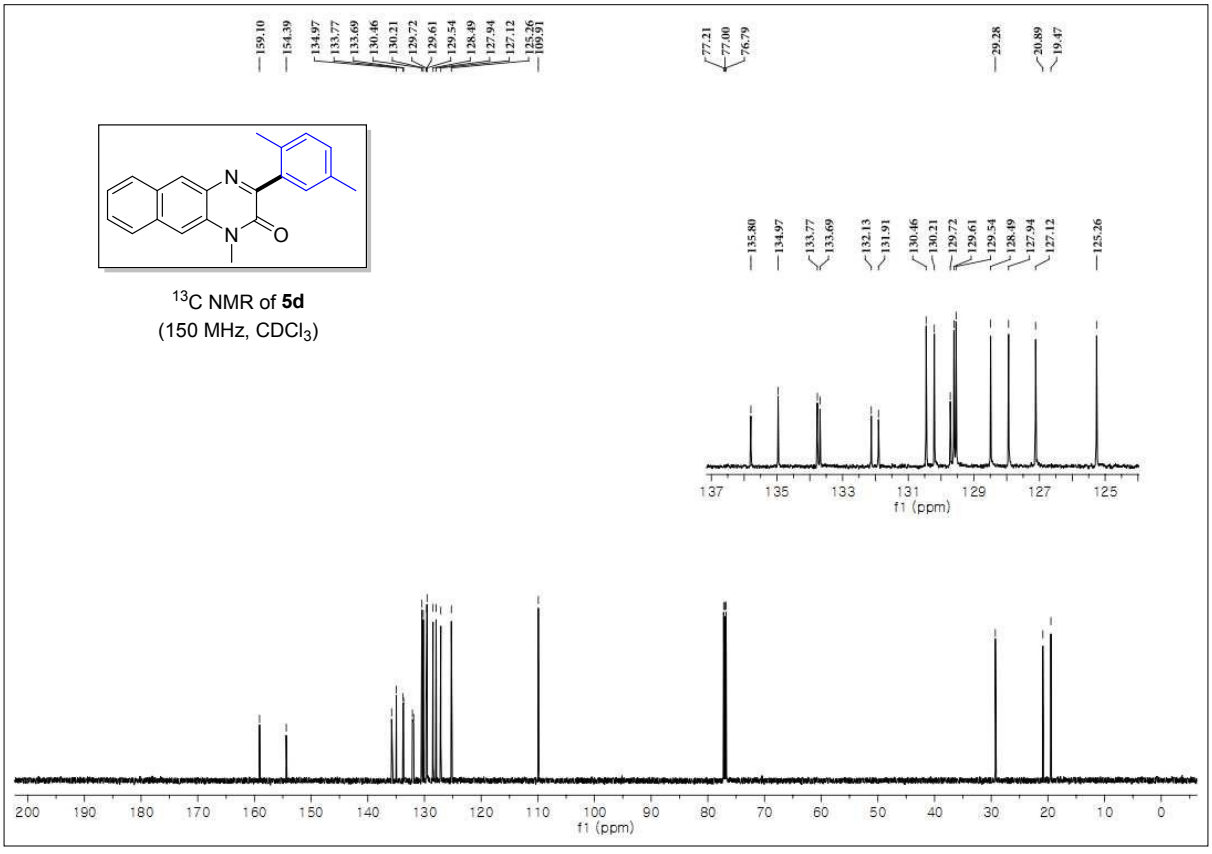
^{1}H NMR of **5c**
(300 MHz, $CDCl_3$)



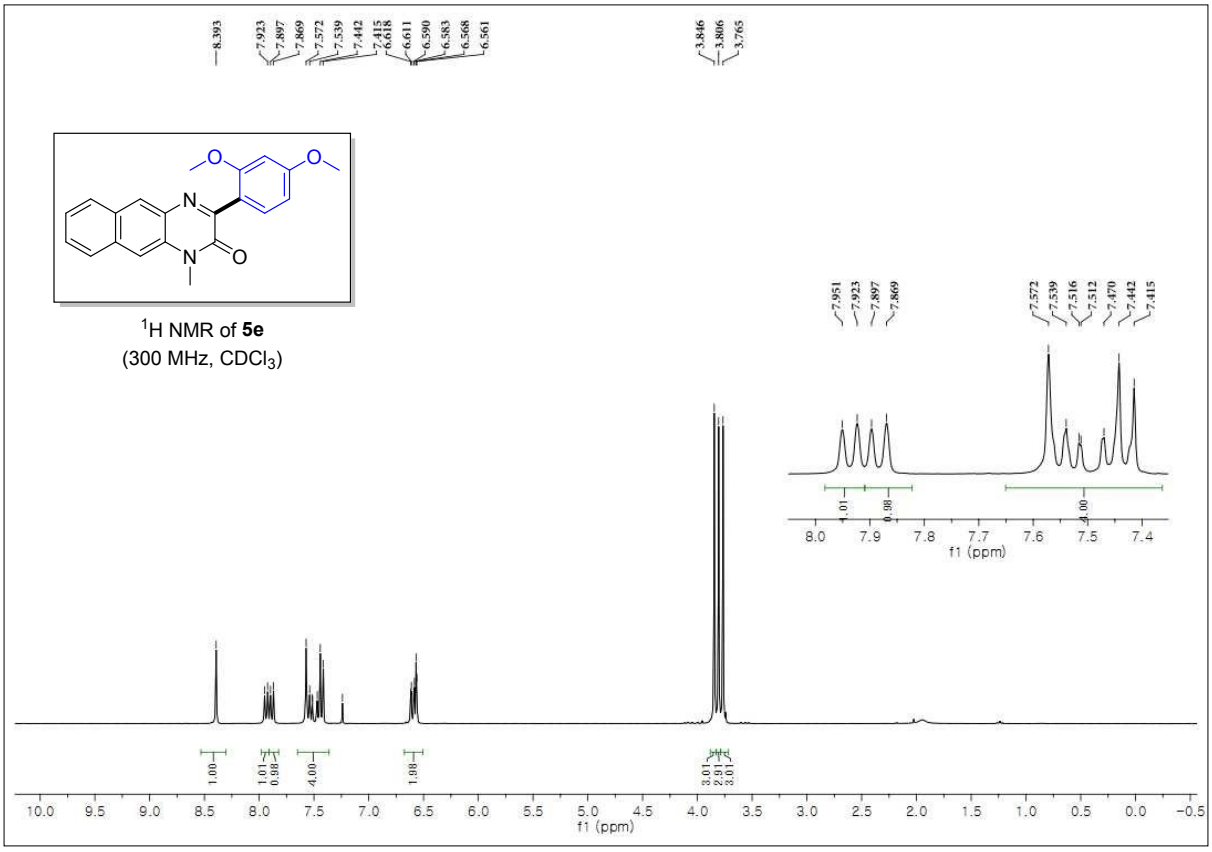
^{13}C NMR of **5c**
(75 MHz, $CDCl_3$)



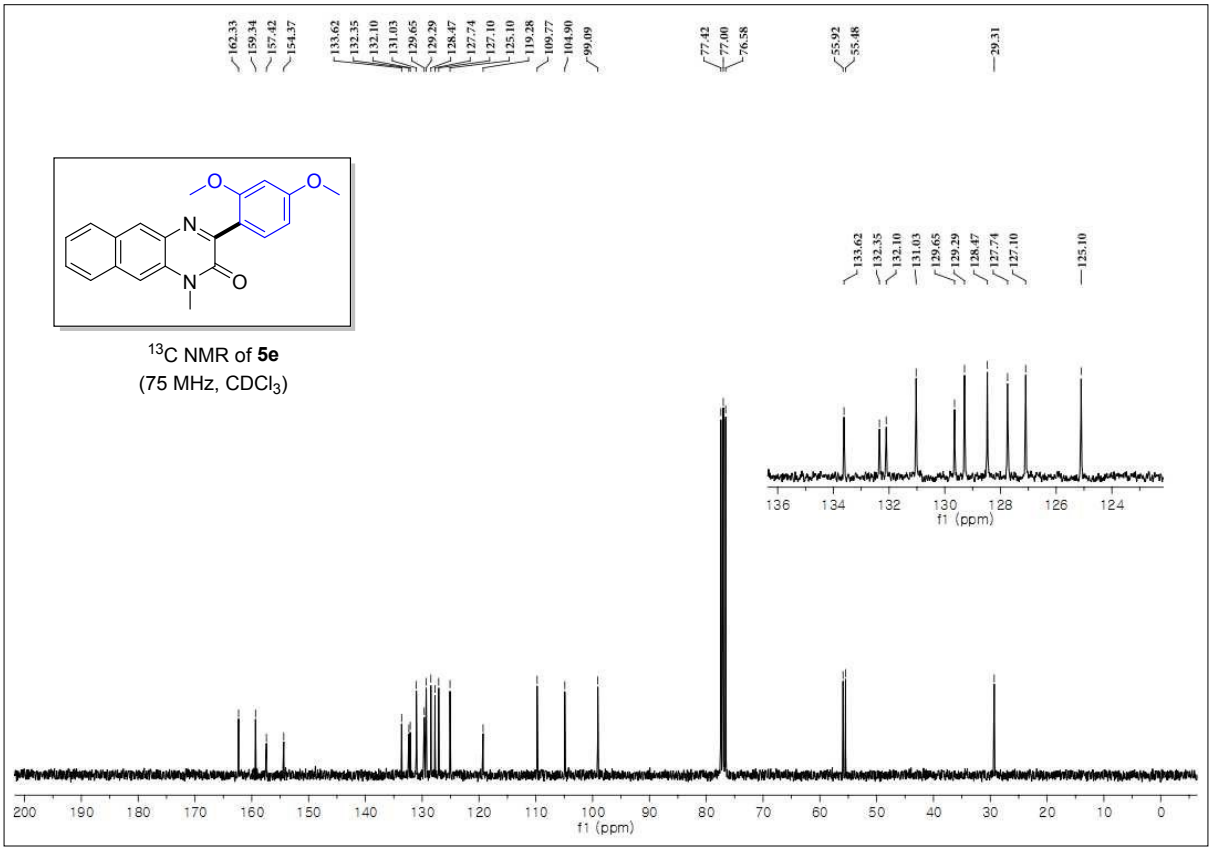
^{1}H NMR of **5d**
(600 MHz, $CDCl_3$)



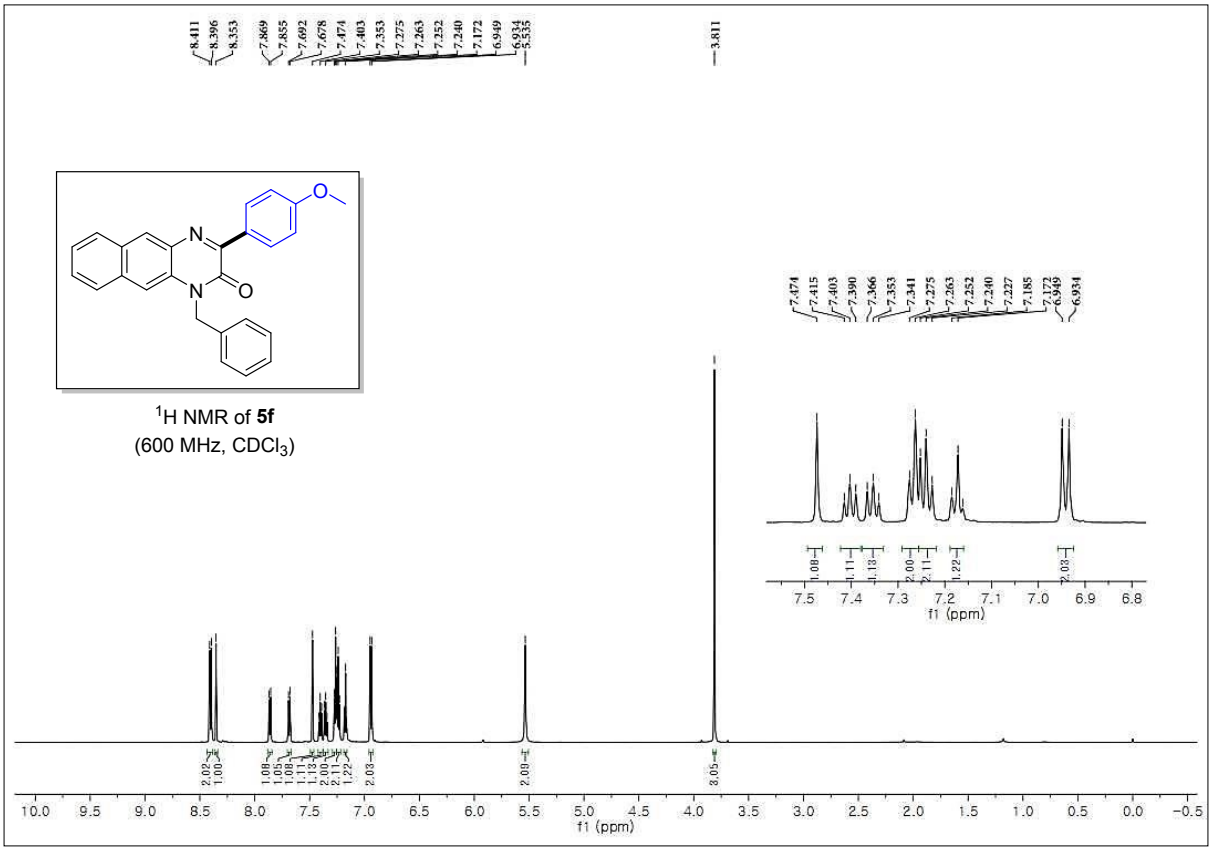
^{13}C NMR of **5d**
(150 MHz, $CDCl_3$)



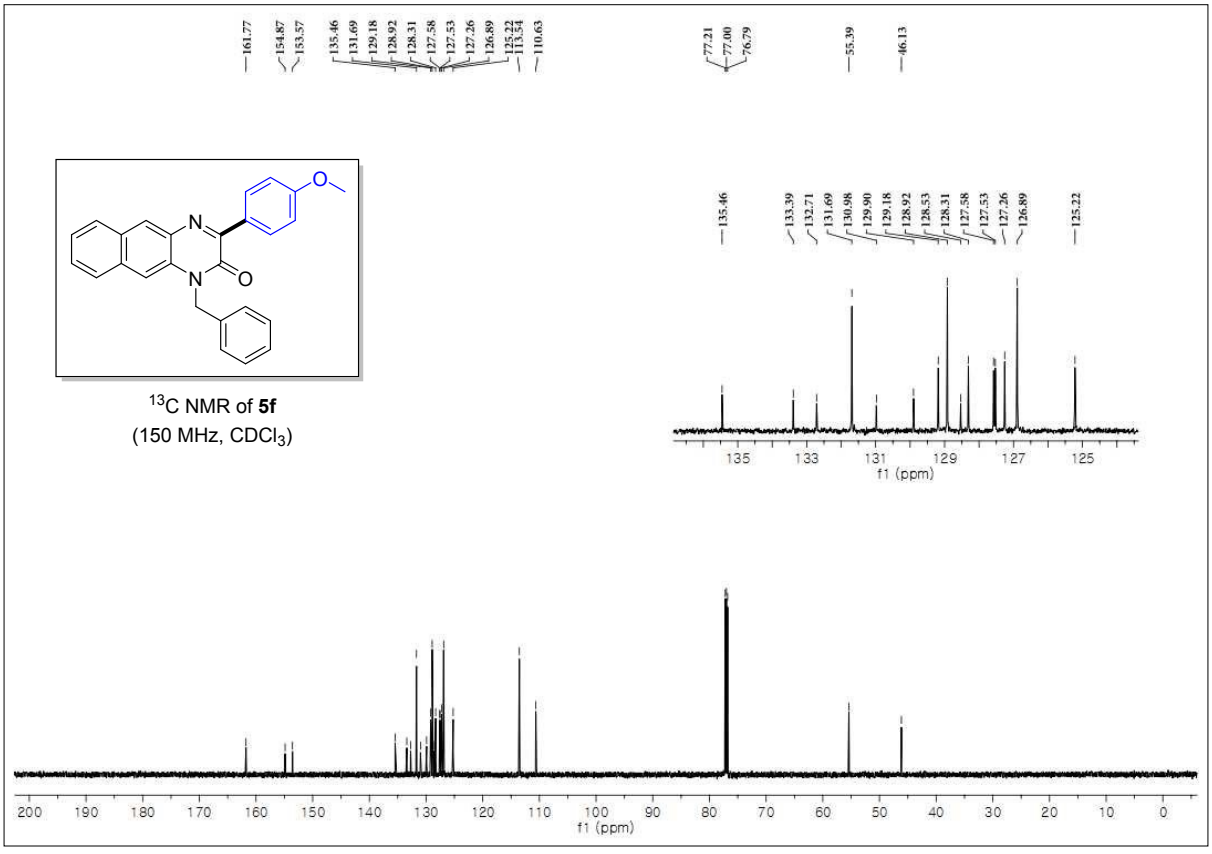
^{1}H NMR of **5e**
(300 MHz, $CDCl_3$)



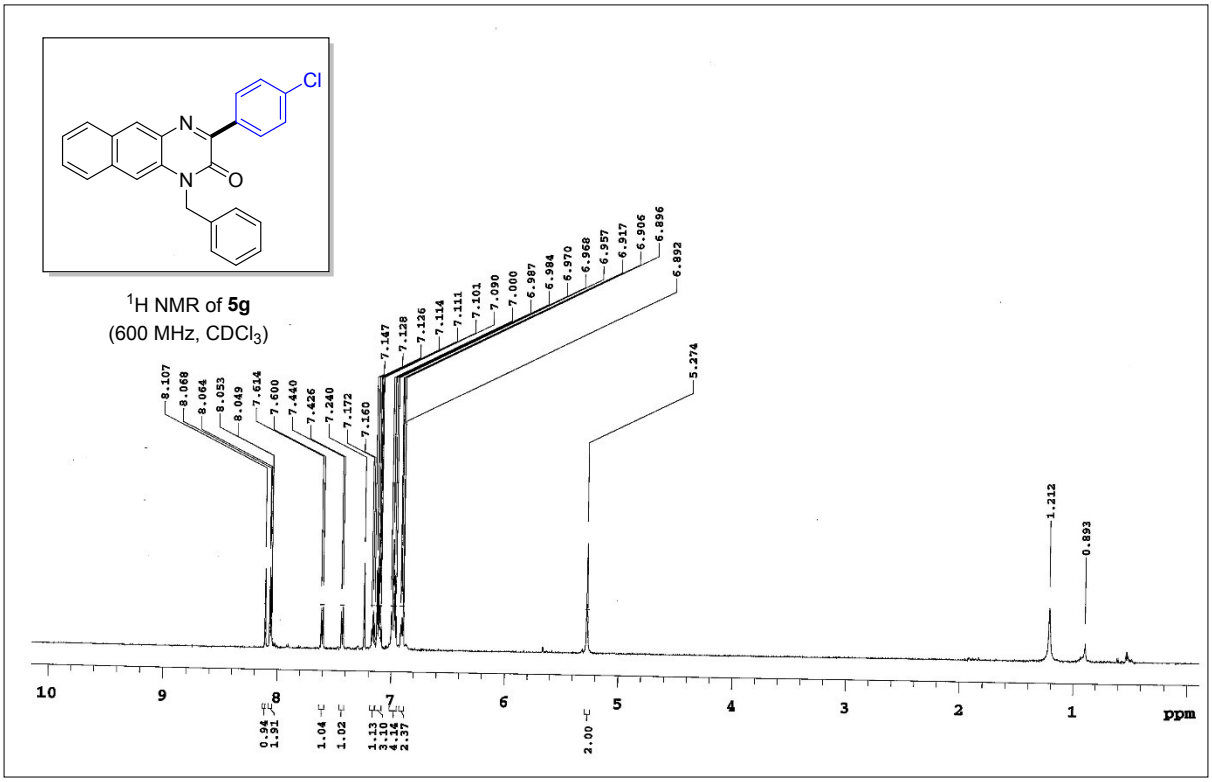
^{13}C NMR of **5e**
(75 MHz, $CDCl_3$)



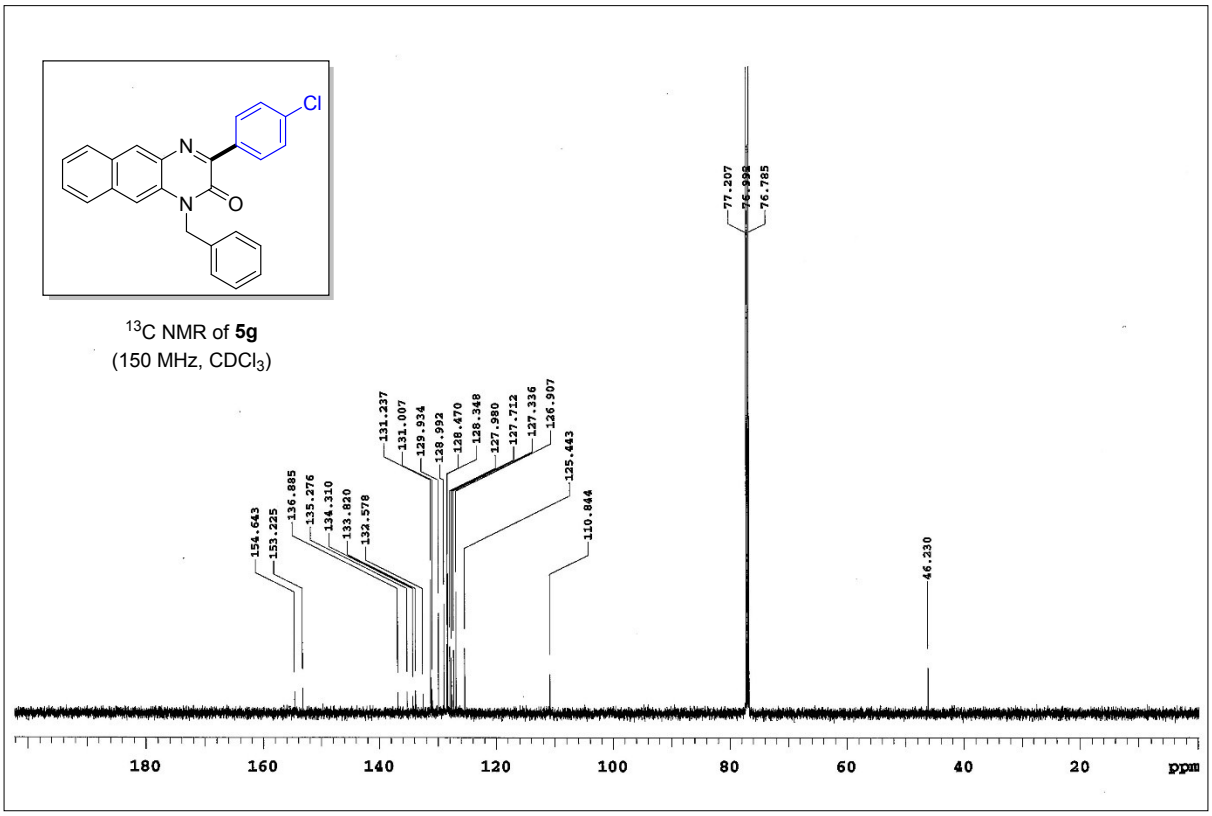
^{1}H NMR of **5f**
(600 MHz, $CDCl_3$)



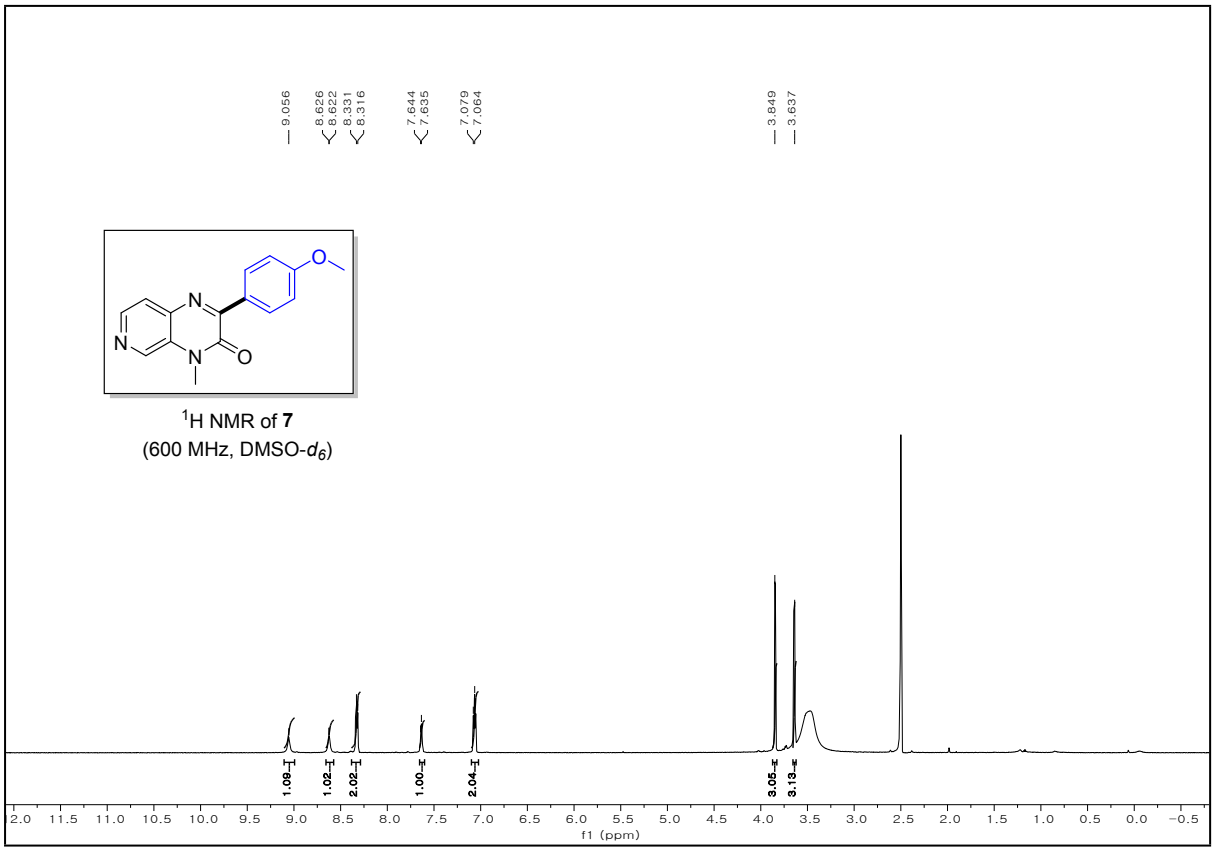
^{13}C NMR of **5f**
(150 MHz, $CDCl_3$)



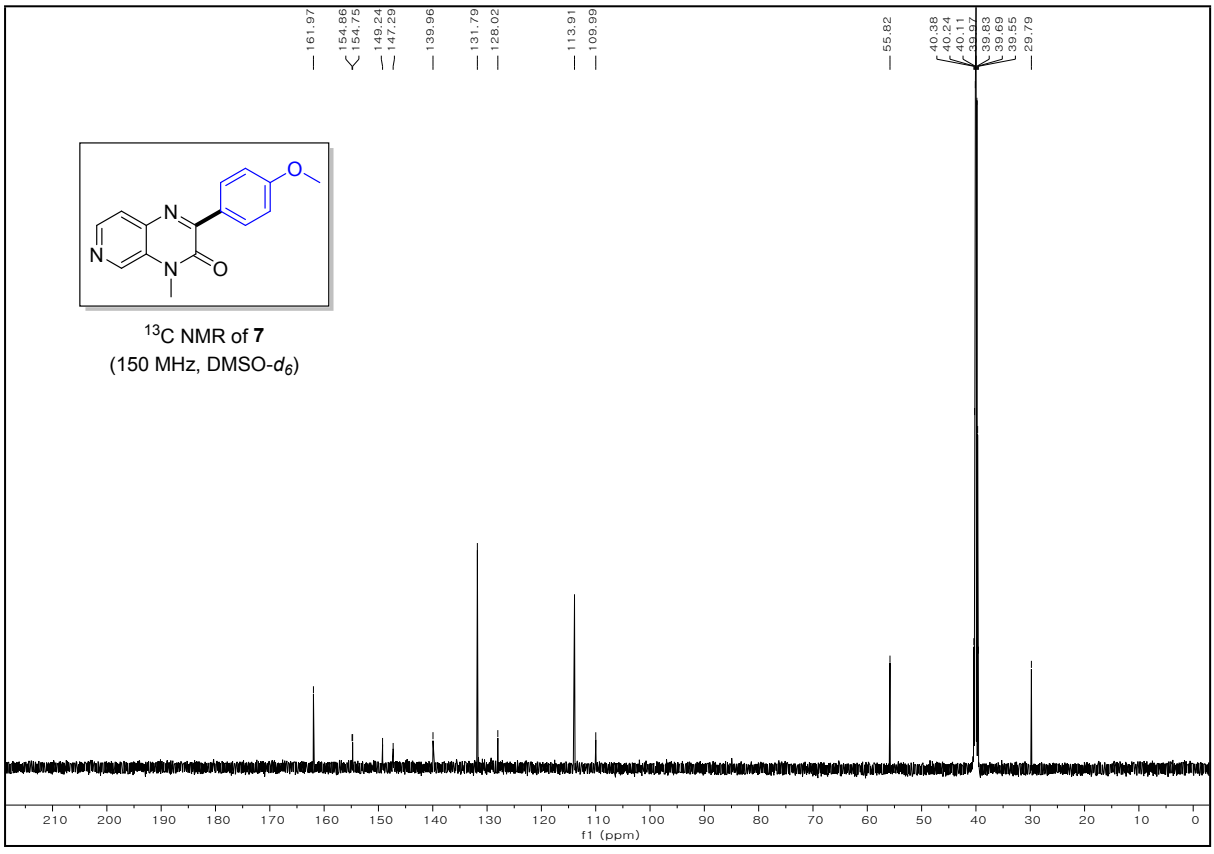
^{1}H NMR of **5g**
(600 MHz, $CDCl_3$)



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



^{1}H NMR of **7**
(600 MHz, DMSO-d_6)



^{13}C NMR of **7**
(150 MHz, DMSO-d_6)

X-Ray diffraction (XRD)

After the completion of the reaction between **1a** and **2h**, the leftover mixture of the catalyst and the oxidant was filtered off, washed several times with ethanol, and dried in vacuo. The X-Ray diffraction (XRD) of the dried powder was taken and compared with the XRD pattern of the mixture of catalyst and oxidant before the reaction. The powder XRD patterns of silver before and after reaction showed well resolved peaks (Figure S1). The XRD peaks of silver after reaction at 38.2, 44.5, 64.6, and 77.4 2θ were indexed to the (111), (200), (220), and (311) crystalline planes, respectively, corresponding to the face centered cubic (fcc) arrangement of Ag^0 state.[2] The corresponding XRD peaks of Ag^+ before the reaction was observed to be changed after the reaction, which confirms the generation of Ag^0.

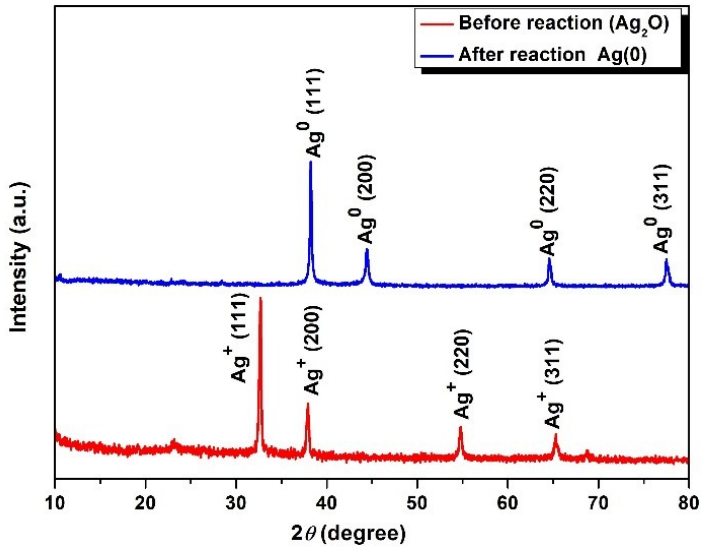


Fig. S1. XRD patterns of the Ag^+ (before the reaction) and Ag^0 (after the reaction).

References

1. A. Carrër, J.-D. Brion, S. Messaoudi and M. Alami, *Org. Lett.* 2013, **15**, 5606.
2. K. Mishra, N. Basavegowda and Y. R. Lee, *Appl. Catal., A* 2015, **506**, 180.