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SUPPORTING INFORMATION

Transition Metal-Catalyzed Regioselective Functionalization of Carbazoles and Indolines with Maleimides

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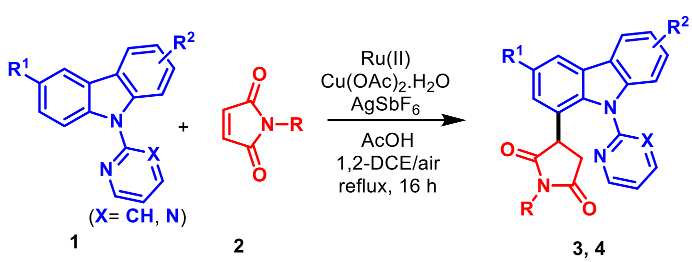
1. General remarks

All experiments were carried out under an open atmosphere. All the reactions were performed in oven-dried glassware with magnetic stirring. Unless otherwise noted, solvents and reagents were purchased from Sigma Aldrich and TCI chemicals and used without further purification. Merck, pre-coated silica gel plates (Art. 5554) with a fluorescent indicator were used for analytical TLC and were visualized with a UV lamp. Flash column chromatography was performed using silica gel 9385 (Merck). ^{1}H NMR spectra were recorded on Varian VNS (600 and 150 MHz) spectrometer at the core research center for natural products and medical materials of Yeungnam University. The chemical shifts were described in parts per million (δ) relative to TMS (0 ppm) as an internal standard or relative to the resonance of the residual protonated solvent (^{1}H : $CDCl_3$, δ = 7.24 ppm). ^{13}C NMR spectra were referenced to the internal solvent signals (^{13}C: $CDCl_3$, δ = 77.0 ppm). IR spectra were recorded on a PerkinElmer Spectrum Two ™IR spectrometer. Melting points were measured with a Fisher Johns melting point apparatus and uncorrected. The high-resolution mass spectra (HRMS) were measured using a JEOL JMS-600 mass spectrometer (positive ion EI mode) at the core research center for natural products and medical materials of Yeungnam University.

2. General procedures:

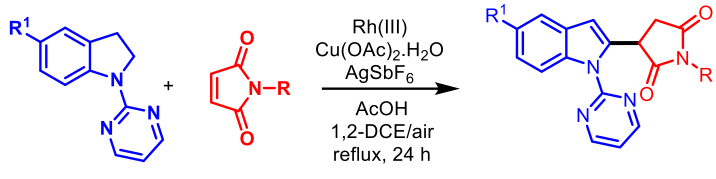
2.1. General procedure for the synthesis of compounds 3 and 4



A mixture of carbazole derivatives **1** (0.4 mmol), maleimides **2** (0.48 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol%), $AgSbF_6$ (20 mol%), $Cu(OAc)_2.H_2O$ (2 equiv.) and AcOH (2 equiv.) was stirred in 1,2-DCE (5 mL) at reflux for the described time. When the reaction was complete as indicated by

TLC, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired products **3** and **4**.

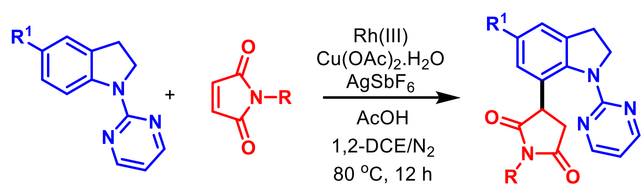
2.2 General procedure for the synthesis of compounds 6



5 **2** **6**

A mixture of indolines **5** (0.4 mmol), maleimides **2** (0.48 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), $Cu(OAc)_2.H_2O$ (1 equiv.) and AcOH (2 equiv.) was stirred in 1,2-DCE (5 mL) at reflux for the described time. When the reaction was complete as indicated by TLC, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired products **6**.

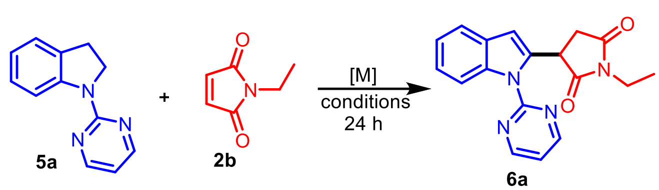
2.3 General procedure for the synthesis of compounds 7



5 **2** **7**

A mixture of indolines **5** (0.4 mmol), maleimides **2** (0.48 mmol), $[Cp^*RhCl_2]_2$ (2 mol%), $AgSbF_6$ (10 mol%), $Cu(OAc)_2.H_2O$ (1 equiv.) and AcOH (2 equiv.) was stirred in 1,2-DCE (5 mL) at 80 °C for the described time under nitrogen atmosphere. When the reaction was complete as indicated by TLC, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired products **7**.

3. Table S1. Reaction optimization for the synthesis of 6a[a]



5a **2b** **6a**

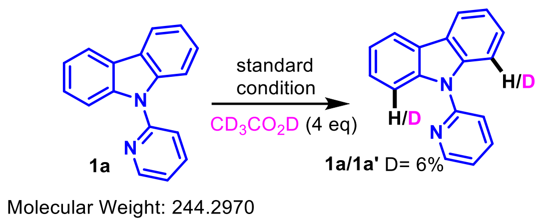
Entry	Catalyst (mol%)	Co-catalyst (mol%)	Oxidant (equiv.)	Additive (equiv.)	Solvent	Temp (°C)	Yield (%)[b]
1	$[Ru(p\text{-cymene})Cl_2]_2$ (5)	$AgSbF_6$ (20)	$Cu(OAc)_2.H_2O$ (2)	AcOH (2)	1,2-1,2-DCE	reflux	0
2	**$[RhCp^*Cl_2]_2$ (5)**	**$AgSbF_6$ (20)**	**$Cu(OAc)_2.H_2O$ (2)**	**AcOH (2)**	**1,2-1,2-DCE**	**reflux**	**76**
3	$[IrCp^*Cl_2]_2$ (2)	$AgSbF_6$ (20)	$Cu(OAc)_2.H_2O$ (2)	AcOH (2)	1,2-1,2-DCE	reflux	0

[a]Conditions: 1-(pyrimidin-2-yl)indoline (**5a**, 0.4 mmol), 1-ethyl-1H-pyrrole-2,5-dione (**2b**, 0.48 mmol), metal catalyst, oxidant and acid additives in solvent (5.0 mL) for 24 h. [b]Isolated yields.

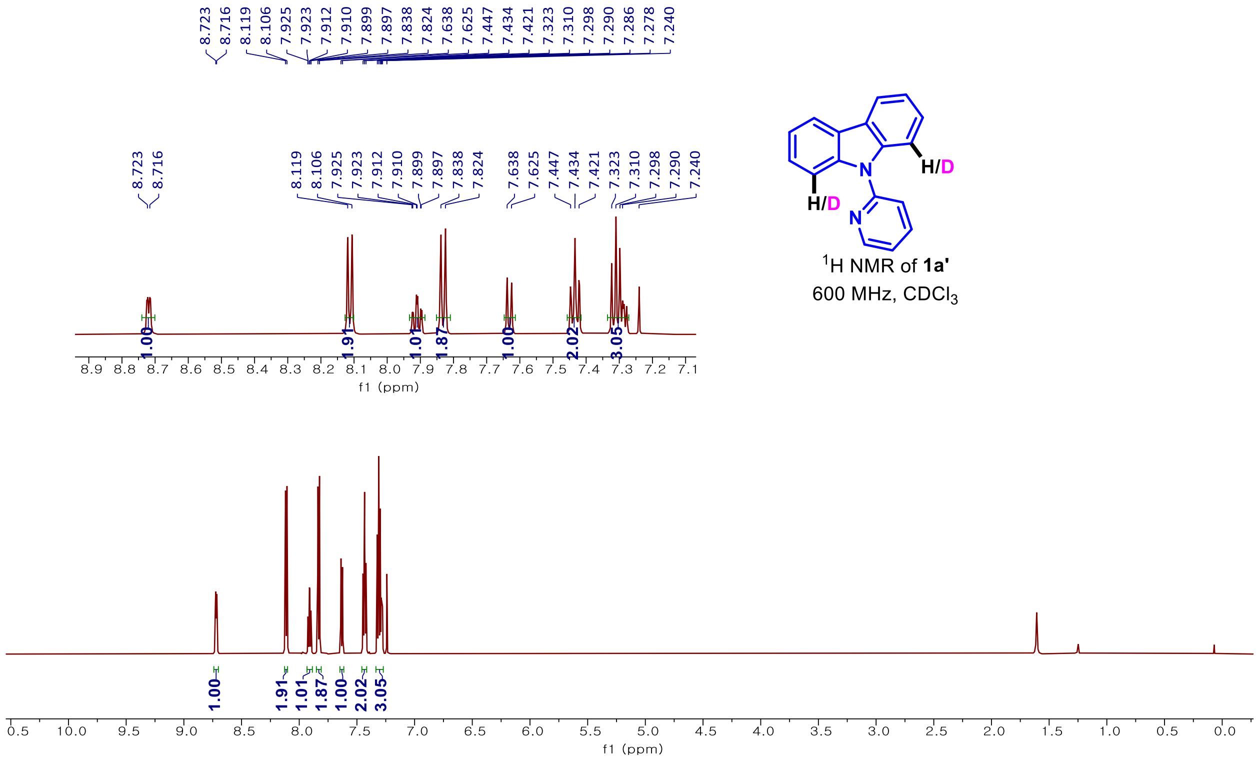
4. Control experiments:

4.1 Deuterium exchange:

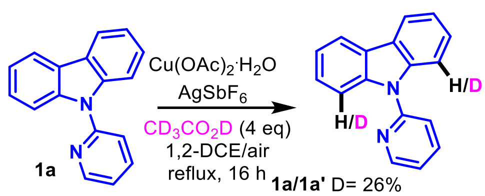
(i) Standard Reaction conditions



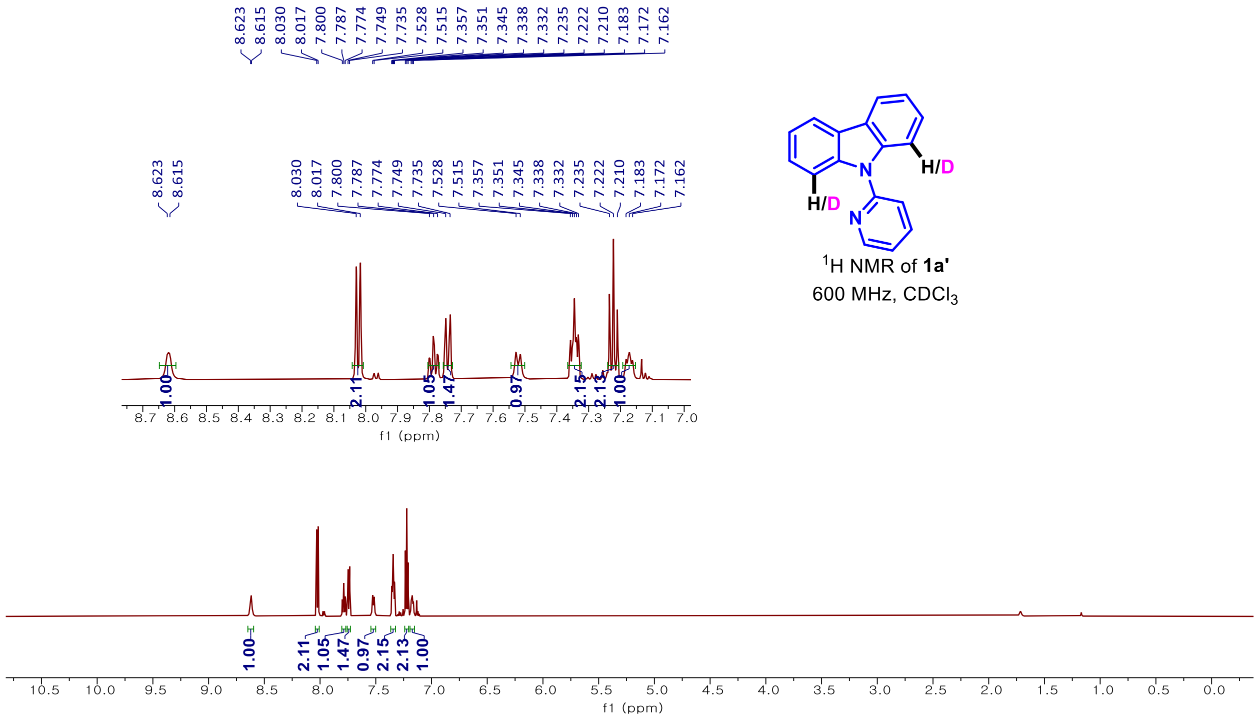
A mixture of **1a** (0.4 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), $Cu(OAc)_2.H_2O$ (2 equiv.) and CD_3CO_2D (4 equiv.) were stirred in 1,2-DCE (5 mL) at reflux for the described time. Next, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired products **1a′**.



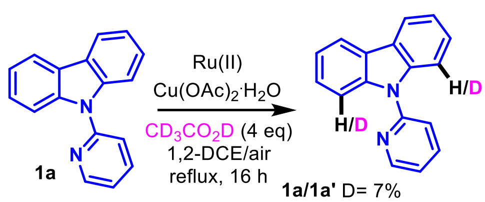
(ii) Without [Ru(*p*-cymene)Cl_2]$_2$



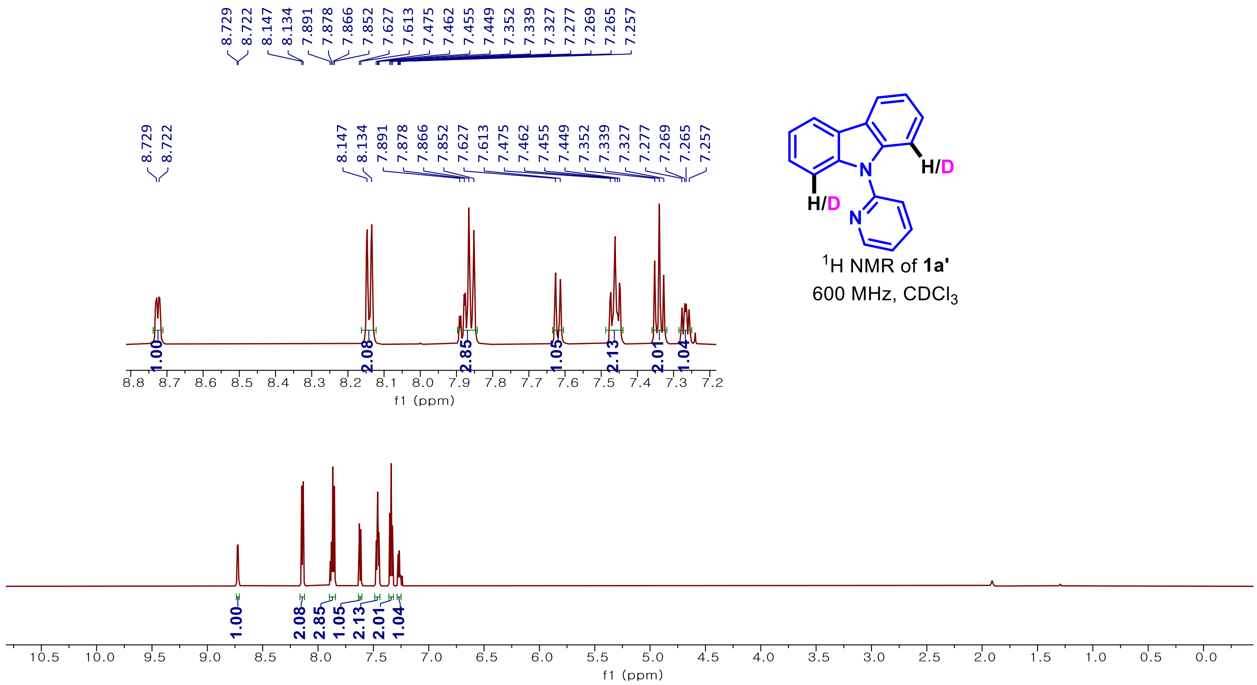
A mixture of **1a** (0.4 mmol), $AgSbF_6$ (20 mol%), $Cu(OAc)_2.H_2O$ (2 equiv.) and CD_3CO_2D (4 equiv.) were stirred in 1,2-DCE (5 mL) at reflux for the described time. Next, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired products **1a′**.



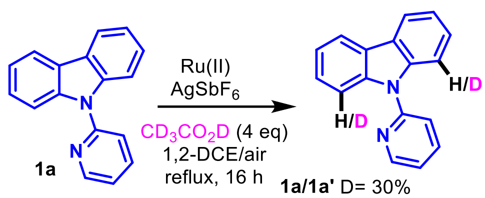
(iii) Without $AgSbF_6$



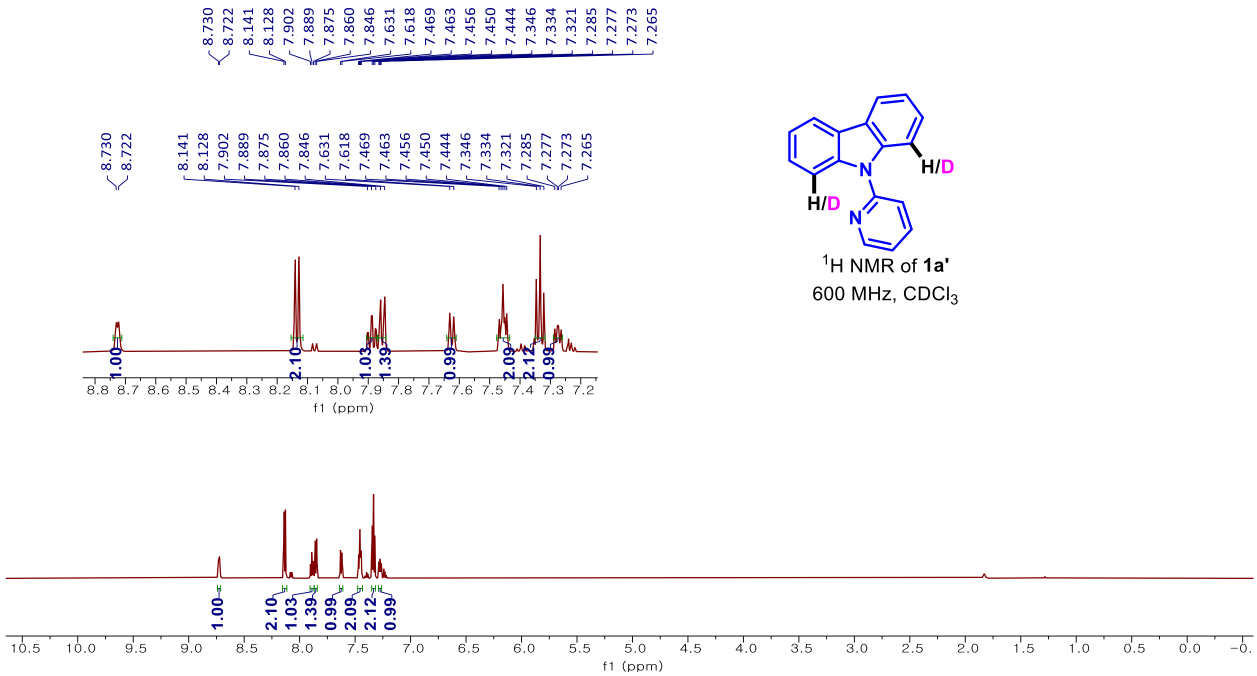
A mixture of **1a** (0.4 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol%), $Cu(OAc)_2.H_2O$ (2 equiv.) and CD_3CO_2D (4 equiv.) were stirred in 1,2-DCE (5 mL) at reflux for the described time. Next, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired products **1a′**.



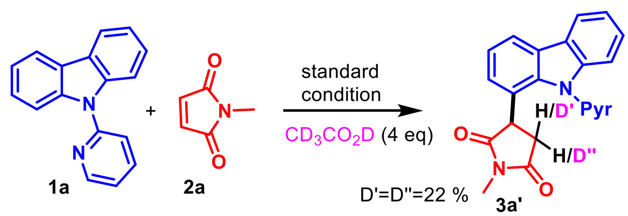
(iv) Without $Cu(OAc)_2.H_2O$



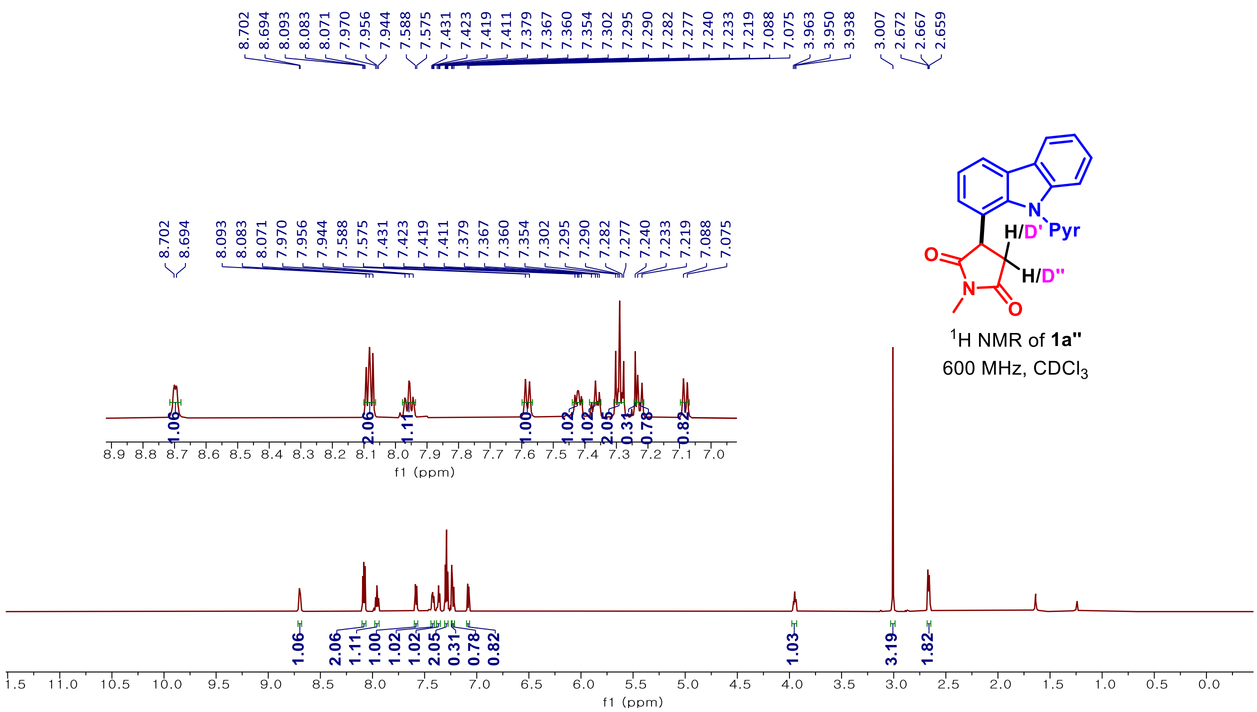
A mixture of **1a** (0.4 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol%), $AgSbF_6$ (20 mol%), and CD_3CO_2D (4 equiv.) were stirred in 1,2-DCE (5 mL) at reflux for the described time. Next, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired products **1a′**.



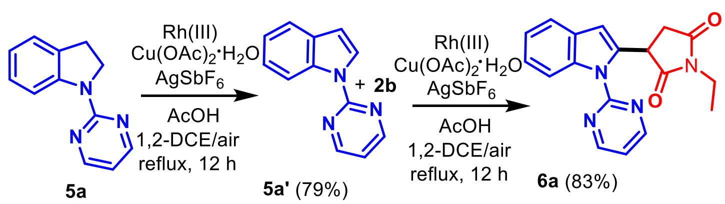
4.2 KIE experiment:



A mixture of **1a** (0.4 mmol) with **2a** (0.48 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), $Cu(OAc)_2.H_2O$ (2 equiv.) and CD_3CO_2D (4 equiv.) were stirred in 1,2-DCE (5 mL) at reflux for the described time. When the reaction was complete as indicated by TLC, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the desired product **3a′**.



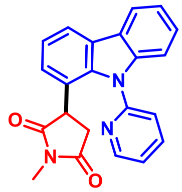
4.3 Confirmation experiment for the formation of 5a′ and 6a from 5a:



A mixture of indoline **5a** (0.4 mmol), [Cp*RhCl$_2$]$_2$ (5 mol%), AgSbF$_6$ (20 mol%), Cu(OAc)$_2$.H$_2$O (2 equiv.) and AcOH (2 equiv.) was stirred in 1,2-1,2-1,2-DCE (5 mL) at reflux for the 12 hours. After the specified time, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the products **5a′** in 79% yield. Next, to a mixture of indole **5a′** (0.4 mmol), maleimides **2b** (0.48 mmol), [Cp*RhCl$_2$]$_2$ (5 mol%), AgSbF$_6$ (20 mol%), Cu(OAc)$_2$.H$_2$O (2 equiv.) and AcOH (2 equiv.) was stirred in 1,2-DCE (5 mL) at reflux for the 12 hours. After the specified time, the volatiles were removed in vacuo and the residue was purified by silica gel column chromatography (EtOAc/*n*-Hexane) to obtain the products **6a** in 83% yield.

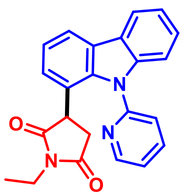
5. Characterization data of synthesized compounds

1-Methyl-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3a)



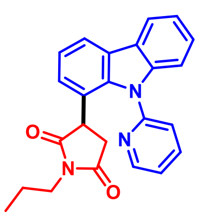
Yield 76% (108 mg) as a yellow solid: mp 124-126 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.68 (1H, d, J = 7.2 Hz), 8.07 (2H, t, J = 6.6 Hz), 7.95 – 7.94 (1H, m), 7.57 (1H, d, J = 7.8 Hz), 7.41 – 7.39 (1H, m), 7.36 (1H, d, J = 7.8 Hz), 7.28 (2H, t, J = 7.8 Hz), 7.21 (1H, t, J = 6.0 Hz), 7.07 (1H, d, J = 7.8 Hz), 3.93 (1H, t, J = 7.8 Hz), 2.99 (3H, s), 2.65 (2H, d, J = 6.0 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.8, 176.2, 152.7, 150.0, 142.2, 138.9, 138.7, 126.6, 126.2, 124.7, 123.8, 123.5, 123.1, 122.3, 121.5, 121.2, 120.2, 120.0, 110.2, 42.2, 38.3, 25.1. IR (ATR): 1695, 1468, 1435, 1281, 1381, 1119 cm^{-1}. HRMS *m/z* (MH^+): calcd for $C_{22}H_{18}N_3O_2$: 356.1394; found: 356.1392.

1-Ethyl-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3b)



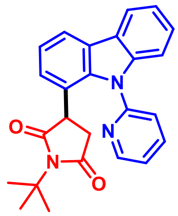
Yield 74% (109 mg) as a yellow solid: mp 122-124 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.70 (1H, d, J = 4.2 Hz), 8.07 (2H, t, J = 7.2 Hz), 7.98 – 7.95 (1H, m), 7.59 (1H, d, J = 7.8 Hz), 7.43 (1H, dd, J = 7.2, 4.8 Hz), 7.38 – 7.35 (1H, m), 7.29 (2H, t, J = 7.2 Hz), 7.23 (1H, d, J = 7.8 Hz), 7.05 (1H, d, J = 7.8), 3.90 (1H, t, J = 7.8 Hz), 3.57 (2H, q, J = 6.0 Hz), 2.64 – 2.62 (2H, m), 1.18 (3H , t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.5, 176.0, 152.6, 149.9, 142.1, 139.0, 138.7, 126.6, 126.2, 124.4, 123.7, 123.4, 123.1, 122.6, 121.5, 121.1, 120.2, 119.9, 110.1, 41.9, 38.4, 34.0, 13.0. IR (ATR): 1693, 1467, 1453, 1435, 1402, 1335, 1311, 1219, 1122, 750 cm^{-1}. HRMS *m/z* (MH^+): calcd for $C_{23}H_{20}N_3O_2$: 370.1550; found: 370.1547.

1-Propyl-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3c)



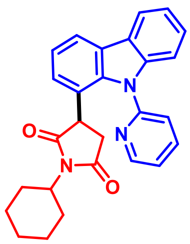
Yield 78% (119 mg) as a brown solid: mp 160-162 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.71 (1H, d, J = 4.2 Hz), 8.08 (2H, t, J = 7.2 Hz), 7.96 (1H, t, J = 7.8 Hz), 7.59 (1H, d, J = 7.8 Hz), 7.44 – 7.41 (1H, m), 7.37 (1H, t, J = 7.8 Hz), 7.29 (2H, t, J = 7.2 Hz), 7.22 (1H, d, J = 7.8k Hz), 7.06 (1H, d, J = 7.8 Hz), 3.92 – 3.90 (1H, m), 3.48 (2H, t, J = 7.2 Hz), 2.64 – 2.62 (2H, m), 1.63 – 1.59 (2H, m), 0.90 (3H, t, J = 7.8 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.7, 176.2, 152.6, 150.0, 142.1, 138.9, 138.7, 126.6, 126.2, 124.4, 123.7, 123.4, 123.1, 122.6, 121.5, 121.1, 120.1, 119.9, 110.1, 41.9, 40.6, 38.3, 21.0, 11.3. IR (ATR): 1693, 1468, 1454, 1338, 1310, 1131 cm^{-1}. HRMS *m/z* (MH^+): calcd for $C_{24}H_{22}N_3O_2$: 384.1707; found: 384.1703.

1-(*tert*-Butyl)-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3d)



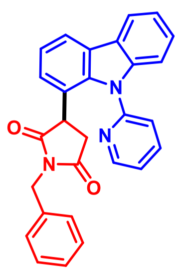
Yield 68% (108 mg) as a yellow solid: mp 99-101 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.68 (1H, d, J = 3.0 Hz), 8.03 (2H, t, J = 8.4 Hz), 7.94 (1H, t, J = 7.8 Hz), 7.56 (1H, d, J = 7.8 Hz), 7.41 – 7.39 (1H, m), 7.33 (1H, t, J = 7.8 Hz), 7.28 – 7.25 (2H, m), 7.21 (1H, d, J = 8.4 Hz), 7.04 (1H, d, J = 7.8 Hz), 3.72 – 3.70 (1H, m), 2.50 (2H, t, J = 6.0 Hz), 1.54 (9H, s). ^{13}C NMR (150 MHz, $CDCl_3$): δ 178.7, 177.1, 152.6, 149.7, 142.1, 139.0, 138.8, 126.5, 126.2, 124.0, 123.8, 123.6, 123.4, 123.1, 121.5, 121.1, 120.1, 119.7, 110.2, 58.7, 41.8, 38.6, 28.3. IR (ATR): 1695, 1467, 1405, 1310, 1213, 1132 cm^{-1}. HRMS m/z (MH^+): calcd for $C_{25}H_{24}N_3O_2$: 398.1863; found: 398.1859.

1-Cyclohexyl-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3e)



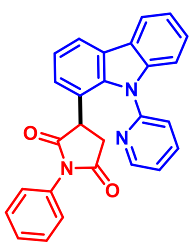
Yield 66% (112 mg) as a yellow solid: mp 125-127 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.66 (1H, d, J = 4.8 Hz), 8.03 (2H, t, J = 9.0 Hz), 7.91 (1H, t, J = 7.8 Hz), 7.54 (1H, d, J = 7.8 Hz), 7.37 (1H, t, J = 7.2 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.24 (2H, t, J = 7.8 Hz), 7.19 (1H, d, J = 7.8 Hz), 7.00 (1H, d, J = 7.2 Hz), 3.98 – 3.94 (1H, m), 3.79 (1H, t, J = 7.8 Hz), 2.53 (2H, d, J = 6.0 Hz), 2.16 – 2.08 (2H, m), 1.77 (2H, d, J = 13.2 Hz), 1.60 – 1.55 (3H, m), 1.28 – 1.14 (3H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.8, 176.3, 142.1, 138.7, 126.6, 126.2, 124.1, 123.8, 123.2, 121.8, 121.6, 121.2, 120.2, 120.0, 119.8, 111.3, 110.2, 52.0, 41.5, 38.3, 28.9, 28.6, 25.8, 25.7, 24.9. IR (ATR): 1695, 1438, 1415, 1373, 1284, 1189 cm^{-1}. HRMS m/z (MH^+): calcd for $C_{27}H_{26}N_3O_2$: 424.2020; found: 424.2016.

1-Benzyl-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3f)



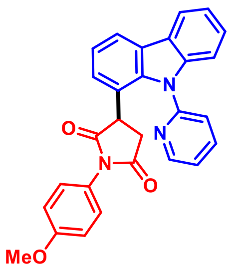
Yield 79% (136 mg) as a yellow solid: mp 139-141 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.71 (1H, d, J = 4.8), 8.10 – 8.07 (2H, m), 7.96 (1H, t, J = 7.8), 7.60 (1H, d, J = 7.8 Hz), 7.44 – 7.37 (4H, m), 7.35 – 7.29 (4H, m), 7.26 – 7.24 (2H, m), 6.98 (1H d, J = 7.8 Hz), 4.72 – 4.66 (2H, m), 3.96 (1H, t, J = 7.2 Hz), 2.69 – 2.67 (2H, m).^{13}C NMR (150 MHz, $CDCl_3$): δ 177.3, 175.7, 152.5, 149.8, 142.1, 139.0, 138.6, 135.7, 128.8, 128.6, 128.0, 126.6, 126.2, 124.5, 123.4, 123.0, 122.5, 121.5, 121.1, 120.1, 119.9, 110.1, 42.6, 42.0, 38.3. IR (ATR): 1707, 1470, 1432, 1380, 1217, 1182 cm^{-1}. HRMS m/z (MH+): calcd for $C_{28}H_{22}N_3O_2$: 432.1707; found: 432.1703.

1-Phenyl-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3g)



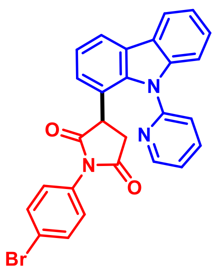
Yield 76% (127 mg) as a white solid: mp 202-204 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.68 (1H, s), 8.04 (2H, d, J = 8.4 Hz), 7.92 (1H, t, J = 7.8 Hz), 7.56 (1H, d, J = 7.8 Hz), 7.39 (3H, t, J = 7.8 Hz), 7.33 – 7.30 (2H, m), 7.27(1H, t, J = 7.8 Hz), 7.25 – 7.22 (3H, m), 7.20 – 7.16 (2H, m), 4.07 (1H, t, J = 7.2 Hz), 2.78 (2H, d, J = 6.6 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.7, 175.1, 152.6, 149.9, 142.1, 139.1, 138.6, 131.8, 129.1, 128.7, 126.6, 126.4, 126.3, 124.4, 123.7, 123.5, 123.2, 122.5, 121.5, 121.2, 120.2, 120.1, 110.1, 42.0, 38.4. IR (ATR): 1705, 1438, 1415, 1373, 1284, 1189 cm^{-1}. HRMS m/z (MH^+): calcd for $C_{27}H_{20}N_3O_2$: 418.1550; found: 418.1546.

1-(4-Methoxyphenyl)-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3h)



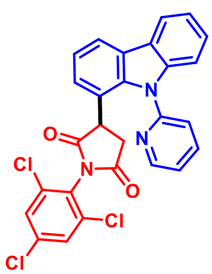
Yield 78% (139 mg) as a yellow solid: mp 214-216 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.77 (1H, d, J = 4.8 Hz,), 8.15 (2H, d, J = 7.8 Hz), 8.01 (1H, t, J = 7.8 Hz), 7.65 (1H, d, J = 7.8 Hz), 7.49 – 7.47 (1H, m), 7.42 (1H, t, J = 7.2 Hz), 7.39 – 7.33 (2H, m), 7.30 – 7.27 (2H, m), 7.26 – 7.24 (2H, m), 7.00 (2H, d, J = 8.4 Hz), 4.16 (1H, t, J = 7.2 Hz), 3.84 (3H, s), 2.86 – 2.84 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.9, 175.3, 159.5, 152.5, 150.0, 142.1, 138.9, 138.6, 127.5, 126.6, 126.2, 124.4, 124.3, 123.6, 123.4, 123.1, 122.5, 121.4, 121.1, 120.1, 120.0, 114.4, 110.1, 55.4, 42.0, 38.3. IR (ATR): 1707, 1435, 1387, 1217, 1242 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{28}H_{22}N_3O_3$: 448.1656; found: 448.1654.

1-(4-Bromophenyl)-3-(9-(pyridin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (3i)



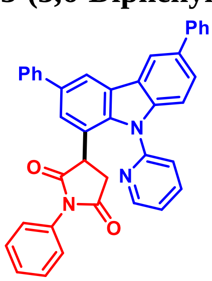
Yield 72% (143 mg) as a white solid: mp 222-224 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.74 (1H, d, J = 4.8 Hz), 8.11 (2H, dd, J = 7.8, 3.6 Hz), 7.99 (1H, t, J = 7.8 Hz), 7.62 (1H, d, J = 7.8 Hz), 7.58 (2H, d, J = 9.0 Hz), 7.47 – 7.45 (1H, m), 7.38 (1H, t, J = 7.2 Hz), 7.34 – 7.29 (2H, m), 7.25 (2H, d, J = 8.4 Hz), 7.21 – 7.18 (3H, m), 4.13 (1H, t, J = 8.4, Hz), 2.84 – 2.83 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.4, 174.8, 152.6, 150.1, 142.2, 139.0, 138.6, 132.3, 130.8, 127.9, 126.7, 126.4, 124.3, 123.7, 123.5, 123.1, 122.5, 122.3, 121.5, 121.3, 120.2, 120.2, 110.2, 42.1, 38.4. IR (ATR): 1706, 1470, 1432, 1380, 1337, 1183 cm^{-1}. HRMS *m/z* (MH^+): calcd for $C_{27}H_{19}BrN_3O_2$: 496.0655; found: 496.0656.

3-(9-(Pyridin-2-yl)-9*H*-carbazol-1-yl)-1-(2,4,6-trichlorophenyl)pyrrolidine-2,5-dione (3j)



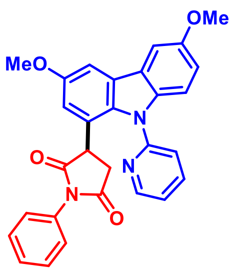
Yield 81% (168mg) as a white solid: mp 126-128 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.64 (1H d, J = 4.8 Hz), 8.01 (2H, t, J = 7.8 Hz), 7.87 (1H, t, J = 7.8 Hz), 7.52 (1H, d, J = 7.8 Hz), 7.37 – 7.33 (3H, m), 7.30 – 7.25 (3H, m), 7.21 (1H, t, J = 7.2 Hz), 7.17 – 7.13 (1H, m), 4.14 (1H, t, J = 7.2 Hz), 2.86 (2H, d, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 174.7, 173.0, 152.5, 149.9, 142.1, 139.1, 138.7, 136.5, 135.0, 134.8, 128.8, 128.7, 127.1, 126.6, 126.2, 124.9, 123.6, 123.5, 123.1, 121.5, 121.2, 120.2, 120.1, 110.1, 42.3, 38.6. IR (ATR): 1707, 1469, 1453, 1380, 1217, 1182 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{27}H_{17}Cl_3N_3O_2$: 520.0381; found: 520.0381.

3-(3,6-Diphenyl-9-(pyridin-2-yl)-9*H*-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4a)



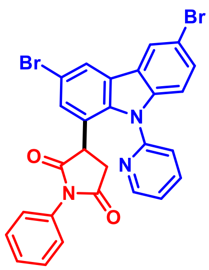
Yield 73% (166 mg) as a yellow solid: mp 152-154 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.78 (1H, d, J = 4.8), 8.35 (2H, d, J = 2.4), 8.04 – 8.01 (1H, m), 7.70 – 7.64 (6H, m), 7.51 – 7.44 (8H, m), 7.39 – 7.33 (4H, m), 7.32 – 7.27 (2H, d, J = 7.2 Hz), 4.24 – 4.22 (1H, m), 2.92 – 2.90 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.5, 175.0, 152.4, 149.9, 142.1, 141.4, 141.0, 139.2, 138.6, 135.3, 134.9, 131.7, 129.2, 128.9, 128.8, 128.7, 127.3, 127.3, 127.0, 126.8, 126.4, 126.3, 124.4, 124.1, 123.6, 123.0, 122.8, 118.7, 118.7, 110.6, 42.1, 38.4. IR (ATR): 1707, 1588, 1454, 1433, 1378, 1182 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{39}H_{28}N_3O_2$: 570.2170; found: 570.2172.

3-(3,6-Dimethoxy-9-(pyridin-2-yl)-9H-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4b)



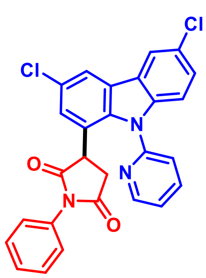
Yield 66% (126 mg) as a brown solid: mp 205-207 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.70 (1H, d, *J* = 3.9 Hz), 7.96 (1H, td, *J* = 7.7, 1.5 Hz), 7.58 (1H, d, *J* = 7.9 Hz), 7.49 – 7.48 (2H, m), 7.45 (2H, t, *J* = 7.8 Hz), 7.41 – 7.39 (1H, m), 7.37 (1H, t, *J* = 7.4 Hz), 7.28 – 7.26 (3H, m), 7.00 (1H, dd, *J* = 8.9, 2.4 Hz), 6.86 (d, *J* = 2.3 Hz, 1H), 4.14 (dd, *J* = 8.4, 6.0 Hz, 1H), 3.92 (3H s), 3.91 (3H s), 2.85 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.3, 175.0, 155.0, 155.0, 152.9, 149.3, 139.3, 137.7, 134.3, 131.7, 129.1, 128.7, 127.4, 126.4, 124.6, 124.2, 122.9, 122.4, 115.8, 113.7, 111.5, 102.7, 102.4, 55.9, 55.9, 42.0, 38.3. IR (ATR): 2935, 1708, 1581, 1455, 1385, 1190, 847 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{29}H_{24}N_3O_4$: 478.1761; found: 478.1758.

3-(3,6-Dibromo-9-(pyridin-2-yl)-9*H*-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4c)



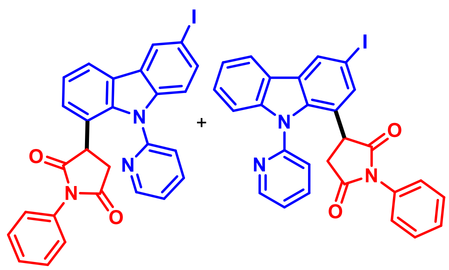
Yield 72% (165 mg) as a white solid: mp 213-215°C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.74 (1H, d, *J* = 6.6 Hz), 8.17 (2H, s), 8.03 – 8.00 (1H, m), 7.60 (1H, d, *J* = 7.8 Hz,), 7.52 – 7.49 (1H, m), 7.48 – 7.45 (3H, m), 7.39 (1H, t, *J* = 7.2 Hz), 7.33 (1H, d, *J* = 1.8 Hz), 7.28 – 7.27 (2H, d, *J* = 7.8 Hz), 7.10 (1H, d, *J* = 9.0 Hz), 4.06 (1H, t, *J* = 7.2 Hz), 2.83 (2H, d, *J* = 7.8 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 175.8, 174.4, 152.2, 151.7, 150.2, 141.1, 139.3, 137.8, 131.5, 130.2, 129.2, 128.8, 127.8, 126.8, 126.3, 124.3, 124.2, 124.1, 123.1, 123.1, 123.0, 114.4, 111.9, 41.6, 38.0. IR (ATR): 1705, 1588, 1469, 1379, 1335, 1182 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{27}H_{18}N_3O_2Br_2$: 573.9760; found: 573.9762.

3-(3,6-Dichloro-9-(pyridin-2-yl)-9H-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4d)



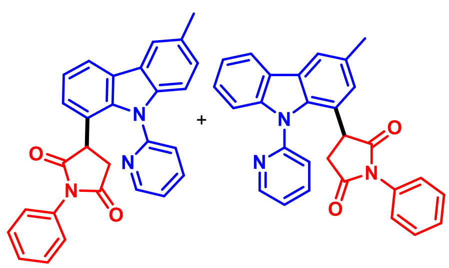
Yield 81% (157 mg) as a white solid: mp 215-217 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.72 (1H, d, *J* = 4.6 Hz), 8.00 – 7.97 (3H, m), 7.57 (1H, d, *J* = 7.9 Hz), 7.49 – 7.44 (3H, m), 7.38 (1H, t, *J* = 7.5 Hz), 7.33 (1H, dd, *J* = 8.7, 2.1 Hz), 7.28 (2H, m) 7.21 (1H, d, *J* = 1.9 Hz), 7.13 (1H, d, *J* = 8.7 Hz), 4.07 (1H, t, *J* = 7.4 Hz), 2.81 (2H, d, *J* = 7.4 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 175.8, 174.4, 151.7, 150.2, 140.9, 139.2, 137.5, 131.5, 129.2, 128.8, 127.4, 127.0, 127.0, 126.3, 126.3, 125.2, 124.0, 123.9, 123.8, 122.9, 120.0, 120.0, 111.4, 41.6, 37.9. IR (ATR): 2928, 1704, 1589, 1435, 1383, 1182, 861 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{27}H_{18}Cl_2N_3O_2$: 486.0770; found: 486.0768.

3-(6-Iodo-9-(pyridin-2-yl)-9H-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4e) and 3-(3-Iodo-9-(pyridin-2-yl)-9H-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4e′)



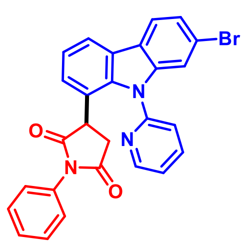
4e and **4e′** were obtained as an inseparable 50:50 mixture in 69% (150 mg) yield. A brown solid: mp 163-165 °C; ^{1}H NMR (600 MHz, CDCl$_3$): δ 8.73 (2H, t, J = 4.3 Hz), 8.40 (2H, s), 8.03 (2H, d, J = 7.7 Hz), 7.99 – 7.97 (2H, m), 7.63 – 7.56 (3H, m), 7.47 – 7.43 (7H, m), 7.41 – 7.36 (3H, m), 7.35 – 7.27 (6H, m), 7.25 (1H, d, J = 7.5 Hz), 7.21 (1H, d, J = 8.2 Hz), 7.01 (1H, d, J = 8.6 Hz), 4.08 (2H, q, J = 7.5 Hz), 2.82 (4H, dd, J = 11.5, 7.3 Hz). ^{13}C NMR (150 MHz, CDCl$_3$): δ 176.5, 176.0, 174.9, 174.6, 152.0, 152.0, 150.0, 150.0, 142.1, 141.3, 139.2, 139.2, 138.6, 138.1, 134.9, 132.5, 131.7, 131.6, 129.2, 129.1, 129.0, 129.0, 128.7, 128.7, 128.5, 127.3, 126.3, 126.1, 125.1, 124.8, 124.5, 123.8, 123.8, 123.1, 123.0, 122.6, 122.3, 121.9, 121.6, 120.3, 120.2, 112.2, 110.2, 84.0, 84.0, 41.8, 41.6, 38.3, 38.1 IR (ATR): 3062, 1707, 1587, 1436, 1376, 1179, 855 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{27}H_{19}IN_3O_2$: 543.0517; found: 543.0515.

3-(6-Methyl-9-(pyridin-2-yl)-9H-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4f) and 3-(3-Methyl-9-(pyridin-2-yl)-9H-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4f′)



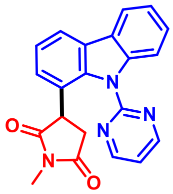
4f and **4f′** were obtained as an inseparable 50:50 mixture in 83% (143 mg) yield. A brown solid: mp 174-176 °C; ^{1}H NMR (600 MHz, CDCl$_3$): δ 8.72 – 8.71 (2H, m), 8.06 (2H, d, J = 7.7 Hz), 7.96 (2H, t, J = 7.7 Hz), 7.89 (2H, s), 7.59 (2H, d, J = 7.8 Hz), 7.48 – 7.42 (6H, m), 7.40 – 7.35 (3H, m), 7.32 – 7.26 (7H, m), 7.22 – 7.15 (3H, m), 7.03 (1H, s), 4.16 – 4.11 (2H, m), 2.84 – 2.82 (4H, m), 2.52 (6H, s). ^{13}C NMR (150 MHz, CDCl$_3$): δ 176.8, 176.8, 175.2, 175.2, 152.9, 150.0, 150.0, 142.5, 140.5, 138.9, 137.1, 131.9, 131.1, 130.7, 129.2, 128.7, 128.0, 126.6, 126.5, 126.4, 126.4, 126.3, 125.6, 124.2, 123.9, 123.8, 123.3, 123.3, 122.9, 122.9, 122.6, 122.2, 121.4, 121.1, 120.2, 120.2, 120.1, 120.0, 42.1, 42.0, 38.5, 38.5, 21.3. IR (ATR): 2974, 1709, 1588, 1434, 1377, 1182 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{28}H_{22}N_3O_2$: 432.1706; found: 432.1704.

3-(7-Bromo-9-(pyridin-2-yl)-9*H*-carbazol-1-yl)-1-phenylpyrrolidine-2,5-dione (4g)



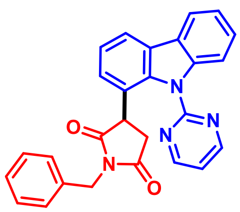
Yield 75% (148 mg) as a brown solid: mp 229-231 °C; ^{1}H NMR (600 MHz, CDCl$_3$): δ 8.75 (1H, d, J = 4.8 Hz), 8.06 (1H, d, J = 7.8 Hz), 8.01 (1H, t, J = 7.2 Hz), 7.94 (1H, d, J = 8.4 Hz), 7.61 (1H, d, J = 7.8 Hz,), 7.50 – 7.47 (1H, m), 7.45 (2H, t, J = 7.8 Hz), 7.42 – 7.31 (4H, m), 7.27 (2H, d, J = 7.8 Hz), 7.23 (1H, s), 4.05 (1H, t, J = 7.2 Hz), 2.83 (2H, d, J = 7.2 Hz). ^{13}C NMR (150 MHz, CDCl$_3$): δ 176.5, 175.0, 152.0, 150.2, 142.8, 139.3, 138.8, 131.7, 129.2, 128.7, 126.3, 125.6, 124.8, 124.4, 124.0, 123.1, 122.6, 122.0, 121.4, 120.2, 120.1, 113.3, 41.8, 38.4. IR (ATR): 1705, 1587, 1453, 1377, 1336, 1182 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{27}H_{19}BrN_3O_2$: 496.0655; found: 496.0655.

1-Methyl-3-(9-(pyrimidin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (4h)



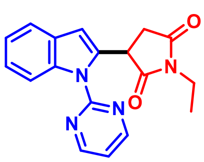
Yield 78% (111 mg) as a brown solid: mp 240-242 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.83 (2H, d, J = 4.8 Hz), 8.25 (1H, d, J = 8.4 Hz), 8.02 (2H, dd, J = 7.2, 3.0 Hz), 7.43 (1H, t, J = 8.4 Hz), 7.37 – 7.33 (2H, m), 7.22 – 7.19 (2H, m), 4.22 – 4.19 (1H, m), 3.03 (3H, s), 2.90 – 2.88 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.8, 176.5, 159.1, 158.4, 141.4, 138.1, 128.0, 127.1, 125.5, 125.3, 125.2, 123.2, 122.7, 119.9, 119.6, 118.0, 113.5, 43.8, 37.9, 25.1. IR (ATR): 1707, 1469, 1453, 1412, 1397, 1336 cm^{-1}. HRMS *m/z* (M+): calcd for $C_{21}H_{16}N_4O_2$: 356.1273; found: 356.1272.

1-Benzyl-3-(9-(pyrimidin-2-yl)-9*H*-carbazol-1-yl)pyrrolidine-2,5-dione (4i)



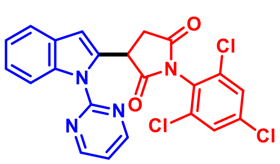
Yield 68% (118 mg) as a yellow solid: mp 86-88 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.82 (2H, d, J = 4.8 Hz), 8.25 (1H, d, J = 8.4 Hz), 8.02 – 7.99 (2H, m), 7.42 – 7.39 (3H, m) 7.35 – 7.28 (5H, m), 7.21 (1H, t, J = 4.8 Hz), 7.08 (1H, d, J = 7.8 Hz), 4.72 – 4.65 (2H, m), 4.17 (1H, t, J = 8.4 Hz), 2.89 – 2.87 (2H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.4, 176.0, 159.1, 158.4, 141.4, 138.0, 135.7, 129.0, 128.7, 128.0, 127.9, 127.07, 125.4, 125.4, 125.0, 123.2, 122.6, 119.8, 119.5, 117.9 113.4, 43.6, 42.6, 37.9. IR (ATR): 1706, 1469, 1453, 1433, 1412, 1179 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{27}H_{21}N_4O_2$: 433.1659; found: 433.1655.

1-Ethyl-3-(1-(pyrimidin-2-yl)-1H-indol-2-yl)pyrrolidine-2,5-dione (6a)



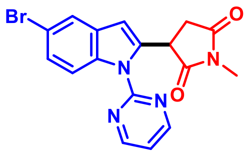
Yield 76% (97 mg) as a yellow solid: mp 173-175 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.63 (2H, d, J = 4.2 Hz), 8.59 (1H, d, J = 7.8 Hz), 7.54 (1H, d, J = 7.8 Hz), 7.30 (1H, t, J = 8.4 Hz), 7.21 (1H, t, J = 8.4 Hz), 7.08 (1H, t, J = 4.8 Hz), 6.67 (1H, s), 4.79 (1H, t, J = 8.4 Hz), 3.66 – 3.59 (2H, m), 3.11 (1H, dd, J = 18.0, 9.6 Hz), 2.90 (1H, dd, J = 18.0, 6.0 Hz), 1.22 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.6, 176.1, 157.8, 157.8, 137.3, k133.8, 128.7, 125.5, 124.1, 122.5, 120.3, 116.8, 115.7, 42.3, 39.5, 36.6, 33.9, 13.2. IR (ATR): 1706, 1468, 1454, 1413, 1384, 1179 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{18}H_{17}N_4O_2$: 321.1346; found: 321.1344.

3-(1-(Pyrimidin-2-yl)-1H-indol-2-yl)-1-(2,4,6-trichlorophenyl)pyrrolidine-2,5-dione (6b)



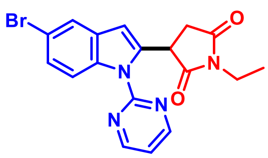
Yield 72% (135 mg) as a yellow solid: mp 202-204 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.79 (2H, d, J = 4.8 Hz), 8.50 (1H, d, J = 8.4 Hz), 7.59 (1H, d, J = 7.8 Hz), 7.49 – 7.47 (2H, m), 7.33 – 7.30 (1H, m), 7.25 – 7.22 (1H, m), 7.16 (1H, t, J = 4.8 Hz), 6.76 (1H, s), 5.56 (1H, dd, J = 9.6, 6.0 Hz), 3.52 (1H, dd, J = 18.6, 9.6 Hz), 3.16 (1H, dd, J = 18.6, 5.4 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 173.8, 173.0, 158.2, 157.9, 137.1, 136.5, 135.1, 134.9, 128.8, 128.5, 127.3, 124.1, 122.5, 120.6, 117.1, 115.1, 107.8, 42.0, 37.8. IR (ATR): 1688, 1565, 1424, 1355, 1187, 1145 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{22}H_{14}Cl_3N_4O_2$: 471.0177; found: 471.0178.

3-(5-Bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)-1-methylpyrrolidine-2,5-dione (6c)



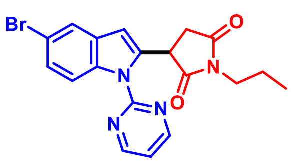
Yield 70% (108 mg) as a white solid: mp 252-254 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.63 (2H, d, J = 4.8 Hz), 8.59 (1H, d, J = 8.4 Hz), 7.65 (1H, s), 7.37 (1H, d, J = 9.0 Hz), 7.09 (1H, t, J = 5.4 Hz), 6.67 (1H, s), 4.75 (1H, t, J = 7.2 Hz), 3.13 (1H, dd, J = 18.6, 9.6 Hz), 3.06 (1H, s), 2.89 (1H, dd, J = 18.0, 6.0 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.6, 176.1, 157.8, 157.3, 135.9, 134.9, 130.3, 126.9, 122.8, 117.5, 117.1, 115.7, 110.4, 42.2, 36.4, 25.0. IR (ATR): 1687, 1565, 1452, 1424, 1380, 1145 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{17}H_{14}BrN_4O_2$: 385.0295; found: 385.0296.

3-(5-Bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)-1-ethylpyrrolidine-2,5-dione (6d)



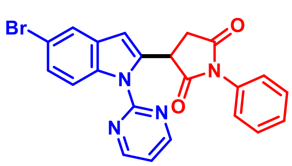
Yield 77% (123 mg) as a white solid: mp 194-196 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.63 (2H, d, J = 4.8 Hz), 8.49 (1H, d, J = 9.0 Hz), 7.66 (1H, d, J = 2.4 Hz), 7.37 (1H, dd, J = 9.0, 2.4 Hz), 7.11 (1H, t, J = 4.8 Hz), 6.60 (1H, s), 4.75 (1H, t, J = 8.4 Hz), 3.66 – 3.59 (2H, m), 3.11 (1H, dd, J = 18.0, 9.6 Hz), 2.89 (1H, dd, J = 18.0, 6.0 Hz), 1.22 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.4, 175.9, 157.9, 157.5, 136.0, 132.0, 130.4, 126.9, 122.8, 117.4, 117.2, 115.8, 100.3, 42.3, 36.5, 33.9, 13.2. IR (ATR): 1685, 1564, 1422, 1377, 1313, 1219 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{18}H_{16}BrN_4O_2$: 399.0451; found: 399.0452.

3-(5-Bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)-1-propylpyrrolidine-2,5-dione (6e)



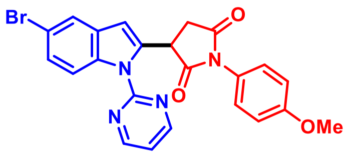
Yield 81% (133 mg) as a yellow solid: mp 200-202 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.61 (2H, d, J = 4.8 Hz), 8.46 (1H, d, J = 9.0 Hz), 7.65 (1H, d, J = 1.8 Hz), 7.36 (1H, dd, J = 9.0, 2.4 Hz), 7.09 (1H, t, J = 4.8 Hz), 6.58 (1H, s), 4.80 (1H, t, J = 7.8 Hz), 3.57 – 3.44 (2H, m), 3.12 (1H, dd, J = 18.0, 9.6 Hz), 2.87 (1H dd, J = 18.0, 6.0 Hz), 1.66 – 1.59 (2H, m), 0.92 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.5, 176.1, 157.9, 157.4, 136.0, 135.3, 130.4, 126.8, 122.8, 117.4, 117.2, 115.7, 109.8, 42.1, 40.6, 36.5, 21.2, 11.4. IR (ATR): 1688, 1566, 1420, 1376, 1355, 1203 cm^{-1}. HRMS *m/z* (MNa^+): calcd for $C_{19}H_{17}BrN_4O_2Na$: 435.0427; found: 435.0423.

3-(5-Bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)-1-phenylpyrrolidine-2,5-dione (6f)



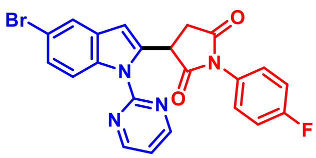
Yield 80% (142 mg) as a white solid: mp 241-243 °C; ^{1}H NMR (600 MHz, $CDCl_3$); δ 8.64 (2H, d, J = 4.8 Hz), 8.58 (1H, d, J = 9.0 Hz), 7.69 (1H, d, J = 1.8 Hz), 7.47 (2H, t, J = 7.8 Hz), 7.41 – 7.36 (4H, m), 7.09 (1H, t, J = 4.8 Hz), 6.71 (1H, s), 4.85 (1H, t, J = 7.8 Hz), 3.27 (1H, dd, J = 18.0, 9.6 Hz), 3.05 (1H, dd, J = 18.0, 6.0 Hz). ^{13}C NMR (150 MHz, $CDCl_{3:}$) δ 175.3, 175.0, 157.9, 157.4, 136.1, 134.5, 132.2, 130.4, 129.1, 128.3, 127.1, 125.8, 122.8, 117.8, 117.1, 115.9, 42.6, 36.2. IR (ATR): 1699, 1568, 1417, 1393, 1316, 1167 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{22}H_{16}BrN_4O_2$: 447.0451; found: 447.0450.

3-(5-Bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)-1-(4-methoxyphenyl)pyrrolidine-2,5-dione (6g)



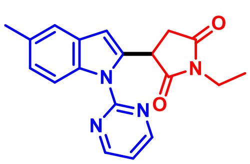
Yield 70% (133 mg) as a white solid: mp 223-225 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.64 (2H, d, J = 4.8 Hz), 8.56 (1H, d, J = 9.0 Hz), 7.69 (1H, d, J = 2.4 Hz), 7.40 (1H, dd, J = 9.0, 2.4 Hz), 7.27 – 7.26 (2H, m), 7.09 (1H, t, J = 4.8 Hz), 6.98 – 6.95 (2H, m), 6.69 (1H, s), 4.85 (1H, s), 3.81 (3H, s), 3.26 (1H, dd, J = 18.0, 9.6 Hz), 3.03 (1H, dd, J = 18.0, 6.0 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 175.5, 175.3, 159.3, 158.0, 157.4, 136.1, 130.4, 127.1, 127.0, 124.8, 122.9, 117.7, 117.1, 115.9, 114.5, 55.5, 42.6, 36.2. IR (ATR): 1689, 1562, 1453, 1423, 1384, 1274 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{23}H_{18}BrN_4O_3$: 477.0556; found: 477.0555.

3-(5-Bromo-1-(pyrimidin-2-yl)-1H-indol-2-yl)-1-(4-fluorophenyl)pyrrolidine-2,5-dione (6h)



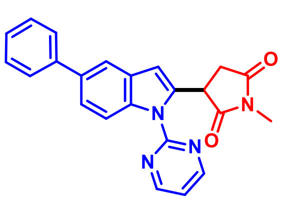
Yield 66% (122 mg) as a yellow solid: mp 244-246 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.63 (2H, d, J = 4.8 Hz), 8.58 (1H, d, J = 9.0 Hz), 7.69 (1H, d, J = 1.8 Hz), 7.41 (1H, dd, J = 9.0, 2.4 Hz), 7.37 – 7.35 (2H, m), 7.17 – 7.14 (2H, m), 7.10 (1H, t, J = 4.8 Hz), 6.70 (1H, s), 4.86 (1H, s), 3.28 (1H, dd, J = 18.0, 9.6 Hz), 3.05 (1H, dd, J = 18.0, 6.0 Hz). ^{13}C NMR (150 MHz, DMSO-d_6): δ 175.7, 175.0, 161.3, 158.7 (d, $^{1}J_{C\text{-}F}$ = 243.7 Hz), 156.5, 135.8, 135.3, 130.2, 128.8 (d, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 128.7, 128.7, 126.1, 122.6, 118.3, 117.3, 115.9, (d, $^{2}J_{C\text{-}F}$ = 22.6 Hz), 114.7, 41.6, 35.9. IR (ATR): 1699, 1568, 1419, 1395, 1317, 1175 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{22}H_{15}BrFN_4O_2$: 465.0357; found: 465.0354.

1-Ethyl-3-(5-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)pyrrolidine-2,5-dione (6i)



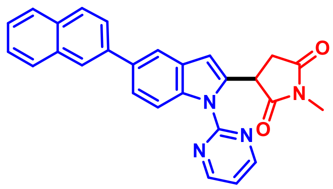
Yield 73% (97 mg) as a white solid: mp 199-201 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.59 (2H, d, J = 4.8 Hz), 8.48 (1H, d, J = 8.6 Hz), 7.32 (1H, s), 7.11 (1H, d, J = 8.6 Hz), 7.04 (1H, t, J = 4.8 Hz), 6.59 (1H, s), 4.74 (1H, s), 3.69 – 3.58 (2H, m), 3.09 (1H, dd, J = 18.0, 9.4 Hz), 2.88 (1H, dd, J = 18.0, 5.9 Hz), 2.43 (3H, s), 1.23 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.7, 176.1, 157.7, 135.5, 133.7, 131.9, 128.9, 125.5, 120.1, 116.5, 115.6, 111.9, 42.4, 36.6, 33.8, 21.2, 13.2. IR (ATR) 2944, 1740, 1686, 1563, 1423, 1348, 1216, 1125, 803 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{19}H_{19}N_4O_2$: 335.1502; found: 335.1501.

1-Methyl-3-(5-phenyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)pyrrolidine-2,5-dione (6j)



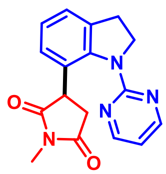
Yield 74% (113 mg) as a yellow solid: mp 223-225 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.68 (1H, d, J = 8.4 Hz), 8.61 (2H, d, J = 4.8 Hz), 7.75 (1H, d, J = 1.8 Hz), 7.65 – 7.63 (2H, m,), 7.56 (1H, dd, J = 8.4, 1.8 Hz), 7.44 (2H, t, J = 7.8 Hz), 7.32 (1H, t, J = 7.8 Hz), 7.08 (1H, t, J = 4.8 Hz), 6.74 (1H, s), 4.78 (1H, s), 3.15 (1H, dd, J = 18.0, 9.6 Hz), 3.08 (3H, s), 2.93 (1H dd, J = 18.0, 6.0 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.0, 176.4, 157.8, 157.6, 141.6, 136.8, 135.9, 134.3, 129.2, 128.7, 127.3, 126.8, 123.7, 118.7, 116.9, 116.2, 42.5, 36.6, 25.1. IR (ATR): 1689, 1562, 1453, 1423, 1384, 1274 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{23}H_{19}N_4O_2$: 383.1503; found: 383.1504.

1-methyl-3-(5-(naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indol-2-yl)pyrrolidine-2,5-dione (6k)



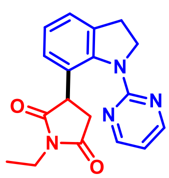
Yield 68% (118 mg) as a yellow solid: mp 221-223 °C; ^{1}H NMR (600 MHz, DMSO-d_6): δ 8.80 (2H, d, J = 4.8 Hz), 8.61 (1H, d, J = 9.0 Hz), 8.26 (1H, dd, J = 9.0, 1.8 Hz), 8.05 (1H, d, J = 1.8 Hz), 8.02 – 8.00 (2H, m), 7.95 – 7.91 (2H, m), 7.77 (1H, dd, J = 8.4, 1.8 Hz), 7.56 – 7.48 (2H, m), 7.39 (1H, t, J = 4.8 Hz), 6.93 (1H, s), 4.97 – 4.95 (1H, m), 3.14 (1H, dd, J = 18.0, 9.6 Hz), 2.93 (3H, s), 2.89 (1H, dd, J = 18.0, 6.0 Hz). ^{13}C NMR (151 MHz, DMSO-d_6) δ 177.0, 176.3, 158.5, 156.7, 138.0, 136.1, 135.5, 134.2, 133.4, 132.0, 129.0, 128.4, 128.1, 127.5, 126.3, 125.8, 125.4, 124.9, 122.8, 118.5, 117.9, 115.8, 111.0, 41.4, 35.9, 24.6. IR (ATR): 1691, 1572, 1414, 1381, 1276, 1119 cm^{-1}. HRMS m/z (MH+): calcd for $C_{27}H_{21}N_4O_2$: 433.1659; found: 433.1660.

1-Methyl-3-(1-(pyrimidin-2-yl)indolin-7-yl)pyrrolidine-2,5-dione (7a)



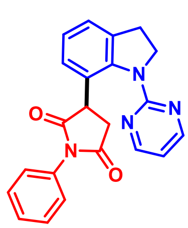
Yield 73% (90 mg) as a brown solid: mp 130-132 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.41 (2H, d, J = 4.9 Hz), 7.19 (1H, d, J = 7.3 Hz), 7.08 (1H, t, J = 7.6 Hz), 6.92 (1H, d, J = 7.9 Hz), 6.75 (1H, t, J = 4.7 Hz), 4.68 – 4.64 (1H, m), 4.36 – 4.31 (1H, m), 4.17 (dd, J = 9.4, 5.2 Hz, 1H), 3.22 (dd, J = 18.7, 9.4 Hz, 1H), 3.17 – 3.11 (1H, m), 3.02 (3H, s), 3.00 – 2.95 (1H, m), 2.92 – 2.87 (1H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 178.3, 177.1, 160.2, 157.5, 142.5, 135.9, 128.8, 125.7, 125.5, 124.1, 112.6, 52.9, 44.3, 37.6, 29.7, 25.0. IR (ATR): 2970, 1738, 1694, 1576, 1421, 1375, 1216, 1122, 807 cm^{-1}. HRMS m/z (MH+): calcd for $C_{17}H_{17}N_4O_2$: 309.1346; found: 309.1346.

1-Ethyl-3-(1-(pyrimidin-2-yl)indolin-7-yl)pyrrolidine-2,5-dione (7b)



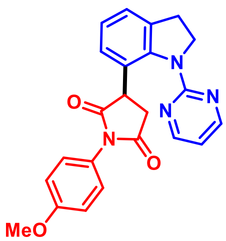
Yield 71% (92 mg) as a yellow solid: mp 159-161 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.41 (2H, d, J = 4.8 Hz), 7.18 (1H, d, J = 7.2 Hz), 7.07 (1H, t, J = 7.6 Hz), 6.90 (1H, d, J = 7.8 Hz), 6.74 (1H, t, J = 4.8 Hz), 4.68 – 4.64 (1H, m), 4.34 – 4.29 (1H, m), 4.13 (1H, dd, J = 9.4, 5.1 Hz), 3.59 (2H, q, J = 7.2 Hz), 3.21 (1H, dd, J = 18.7, 9.4 Hz), 3.17 – 3.11 (1H, m), 2.99 – 2.95 (1H, m), 2.87 (1H, dd, J = 18.7, 5.1 Hz), 1.17 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 178.0, 176.9, 160.3, 157.5, 142.5, 135.8, 129.1, 125.5, 125.3, 124.1, 112.6, 52.8, 44.1, 37.7, 33.8, 29.7, 13.0. IR (ATR): 2946, 1693, 1575, 1423, 1223, 1127, 996, 807 cm^{-1}. HRMS m/z (MH+): calcd for $C_{18}H_{19}N_4O_2$: 323.1502; found: 323.1504.

1-Phenyl-3-(1-(pyrimidin-2-yl)indolin-7-yl)pyrrolidine-2,5-dione (7c)



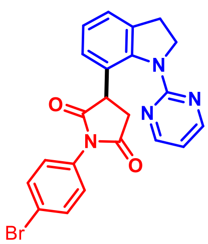
Yield 74% (110 mg) as a white solid: mp 111-113 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.40 (2H, d, J = 4.8 Hz), 7.45 (2H, t, J = 7.6 Hz), 7.37 (1H, t, J = 7.4 Hz), 7.29 (2H, d, J = 7.8 Hz), 7.21 (1H, d, J = 6.8 Hz), 7.11 – 7.07 (2H, m), 6.72 (1H, t, J = 4.8 Hz), 4.68 – 4.64 (1H, m), 4.38 (1H, dd, J = 9.6, 5.4 Hz), 4.34 – 4.29 (1H, m), 3.40 (1H, dd, J = 18.8, 9.6 Hz), 3.17 – 3.09 (2H, m), 3.00 – 2.95 (1H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.1, 176.1, 161.2, 157.7, 142.9, 136.1, 132.0, 129.1, 128.7, 128.5, 126.3, 125.6, 125.2, 124.1, 112.7, 52.5, 44.5, 37.6, 29.6. IR (ATR): 2970, 1707, 1575, 1456, 1431, 1375, 1217, 1169, 897 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{22}H_{19}N_4O_2$: 371.1502; found: 371.1505.

1-(4-methoxyphenyl)-3-(1-(pyrimidin-2-yl)indolin-7-yl)pyrrolidine-2,5-dione (7d)



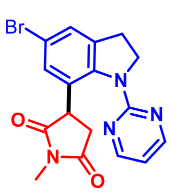
Yield 63% (101 mg) as a yellow solid: mp 122-124 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.40 (2H, d, J = 4.7 Hz), 7.20 – 7.18 (3H, m), 7.11 – 7.06 (2H, m), 6.96 (2H, d, J = 9.0 Hz), 6.72 (1H, t, J = 4.7 Hz), 4.67 – 4.63 (1H, m), 4.36 – 4.28 (2H, m), 3.80 (3H, s), 3.38 (1H, dd, J = 18.9, 9.6 Hz), 3.15 (1H, dd, J = 15.5, 8.9 Hz), 3.09 (1H, dd, J = 18.9, 5.5 Hz), 2.99 – 2.95 (1H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.4, 176.4, 161.2, 159.4, 157.7, 142.9, 136.0, 128.8, 127.6, 125.6, 125.2, 124.6, 124.1, 114.4, 112.7, 55.4, 52.5, 44.4, 37.6, 29.6. IR (ATR): 2970, 1738, 1698, 1584, 1515, 1453, 1378, 1229, 1217, 1023, 900, 831 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{23}H_{21}N_4O_3$: 401.1608; found: 401.1610.

1-(4-bromophenyl)-3-(1-(pyrimidin-2-yl)indolin-7-yl)pyrrolidine-2,5-dione (7e)



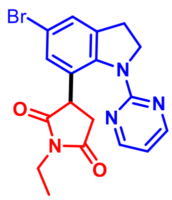
Yield 67% (120 mg) as a yellow solid: mp 172-174 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.44 (2H, d, J = 4.6 Hz), 7.57 (2H, d, J = 8.4 Hz), 7.23 (1H, d, J = 7.2 Hz), 7.20 (2H, d, J = 8.4 Hz), 7.13 (1H, t, J = 7.6 Hz), 7.06 (1H, d, J = 7.8 Hz), 6.79 (1H, t, J = 4.6 Hz), 4.71 – 4.67 (1H, m), 4.39 – 4.33 (2H, m), 3.39 (1H, dd, J = 18.9, 9.4 Hz), 3.19 – 3.11 (1H, m), 3.10 (1H, dd, J = 18.8, 5.1 Hz), 3.03 - 2.98 (1H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 176.6, 175.5, 142.3, 136.1, 132.3, 132.3, 130.9, 128.6, 127.8, 125.0, 124.4, 122.3, 112.7, 53.0, 44.4, 37.5, 29.7. IR (ATR): 2928, 1703, 1579, 1548, 1489, 1427, 1376, 1166, 1070, 897 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{22}H_{18}BrN_4O_2$: 449.0607; found: 449.0609.

3-(5-Bromo-1-(pyrimidin-2-yl)indolin-7-yl)-1-methylpyrrolidine-2,5-dione (7f)



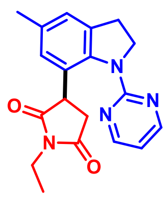
Yield 69% (106 mg) as a yellow solid: mp 205-207 °C; ^{1}H NMR (600 MHz, DMSO-d_6): δ 8.49 (2H, d, J = 4.8 Hz), 7.39 (1H, s), 7.29 (1H, d, J = 1.7 Hz), 6.92 (1H, t, J = 4.8 Hz), 4.61 – 4.57 (1H, m), 4.12 (1H, q, J = 10.1, 9.7 Hz), 4.04 (1H, dd, J = 9.2, 5.8 Hz3.17 – 3.09 (2H, m), 2.96 – 2.92 (1H, m), 2.81 (3H, s), 2.81 – 2.77 (1H, m). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.7, 176.6, 161.0, 157.7, 142.3, 138.2, 130.2, 128.5, 127.2, 117.5, 113.1, 52.6, 44.1, 37.2, 29.4, 25.1. IR (ATR): 2973, 1737, 1694, 1573, 1552, 1440, 1381, 1280, 1123, 996, 807 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{17}H_{16}BrN_4O_2$: 387.0451; found: 387.0452.

3-(5-Bromo-1-(pyrimidin-2-yl)indolin-7-yl)-1-ethylpyrrolidine-2,5-dione (7g)



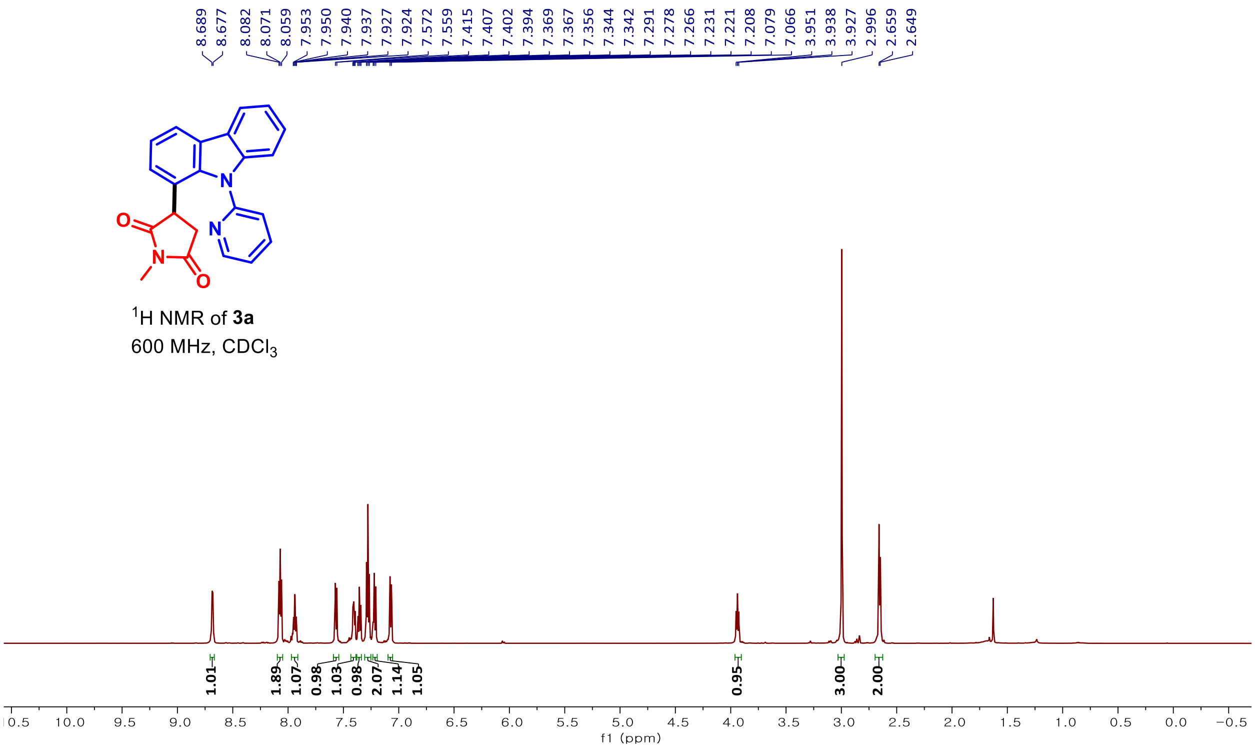
Yield 72% (115 mg) as a yellow solid: mp 204-206 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.38 (2H, d, J = 4.7 Hz), 7.28 (1H, s), 7.02 (1H, s), 6.74 (1H, t, J = 4.8 Hz), 4.64 – 4.60 (1H, m), 4.31 – 4.27 (1H, m), 4.13 (1H, dd, J = 9.5, 5.3 Hz), 3.59 (2H, q, J = 7.2 Hz), 3.20 – 3.07 (2H, m), 2.97 – 2.92 (1H, m), 2.84 (1H, dd, J = 18.6, 5.3 Hz), 1.17 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 177.4, 176.5, 161.0, 157.7, 142.3, 138.2, 128.2, 127.1, 117.5, 113.1, 113.0, 52.6, 43.9, 37.4, 33.9, 29.4, 13.0. IR (ATR): 2958, 1767, 1687, 1574, 1555, 1434, 1402, 1228, 1125, 866 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{18}H_{18}BrN_4O_2$: 401.0607; found: 401.0612.

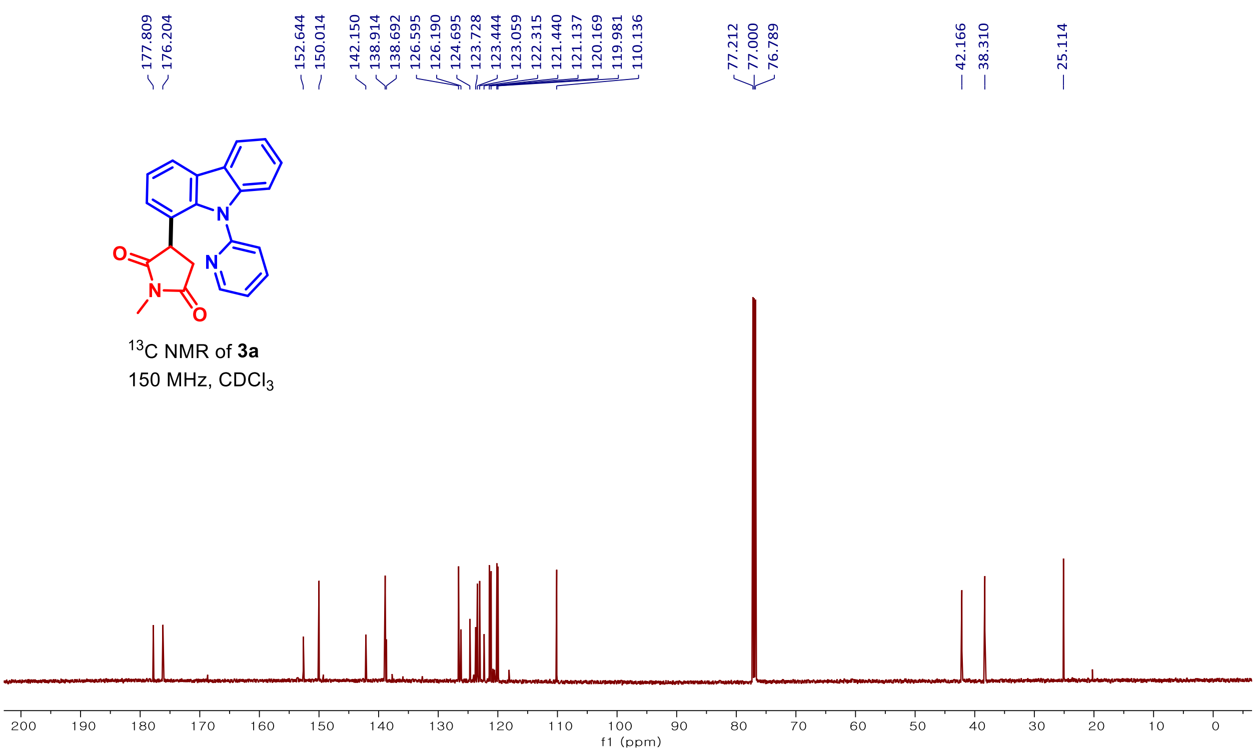
1-Ethyl-3-(5-methyl-1-(pyrimidin-2-yl)indolin-7-yl)pyrrolidine-2,5-dione (7h)

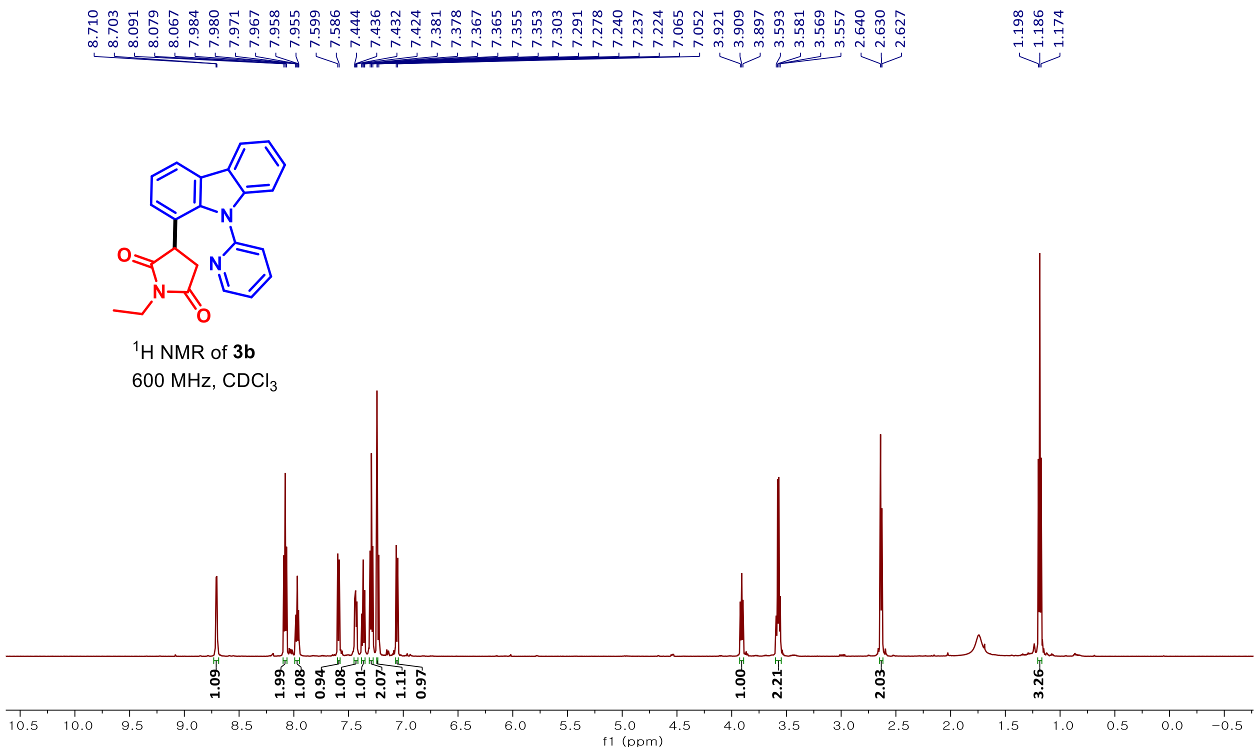


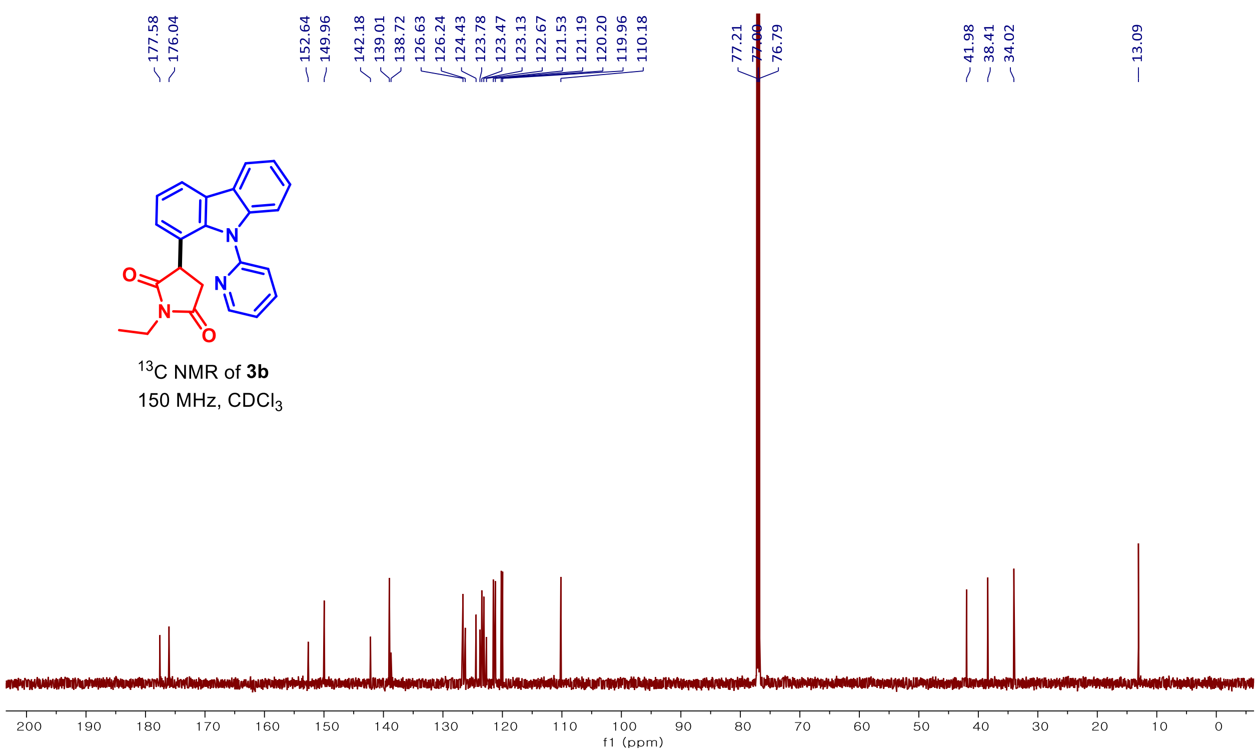
Yield 76% (102 mg) as a white solid: mp 166-168 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.36 (2H, d, J = 4.8 Hz), 6.99 (1H, s), 6.69 – 6.67 (2H, m), 4.65 – 4.61 (1H, m), 4.27 – 4.23 (1H, m), 4.12 (1H, dd, J = 9.4, 5.0 Hz), 3.59 (2H, q, J = 7.1 Hz), 3.21 (1H, dd, J = 18.7, 9.4 Hz), 3.11 – 3.05 (1H, m), 2.91 – 2.84 (2H, m), 2.27 (3H, s), 1.18 (3H, t, J = 7.2 Hz). ^{13}C NMR (150 MHz, $CDCl_3$): δ 178.2, 177.1, 161.3, 157.6, 140.5, 136.0, 135.0, 128.6, 125.6, 124.9, 112.4, 52.6, 44.0, 37.7, 33.8, 29.6, 21.0, 13.0. IR (ATR): 2959, 1738, 1692, 1574, 1400, 1223, 1125, 804 cm^{-1}. HRMS *m/z* (MH+): calcd for $C_{19}H_{21}N_4O_2$: 337.1659; found: 337.1655.

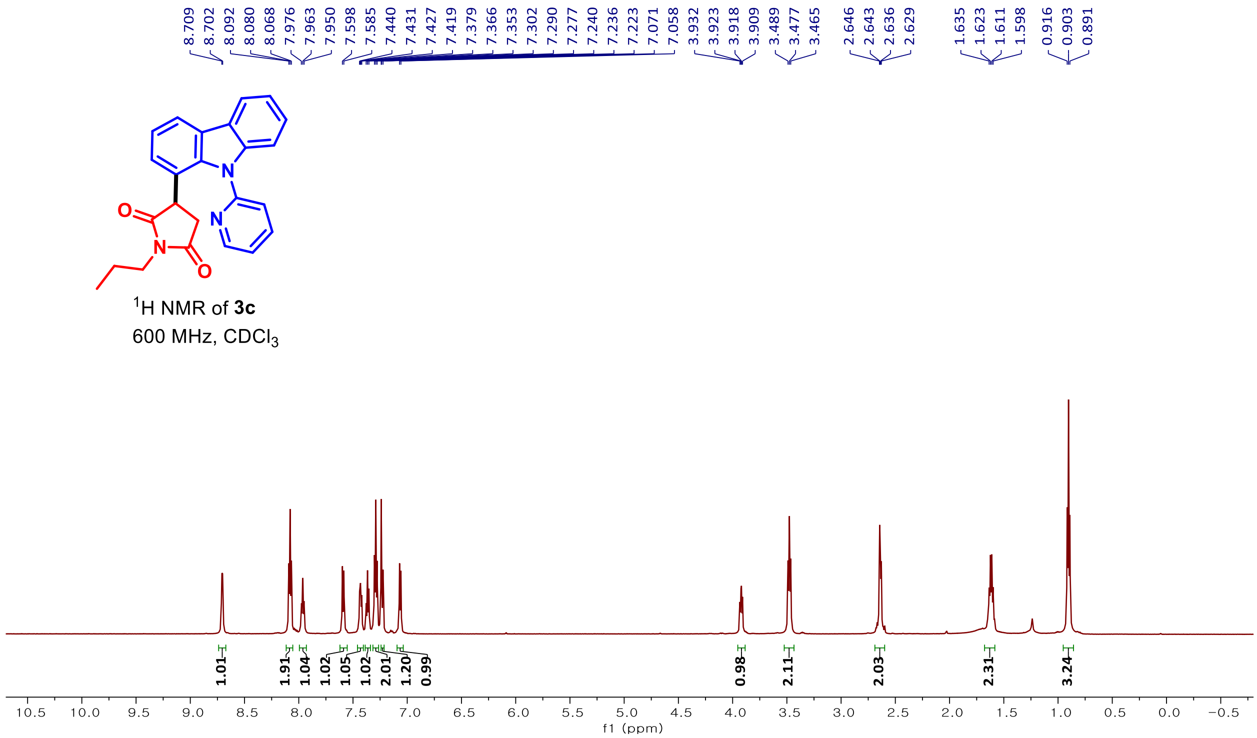
4. NMR Spectra's of synthesized compounds





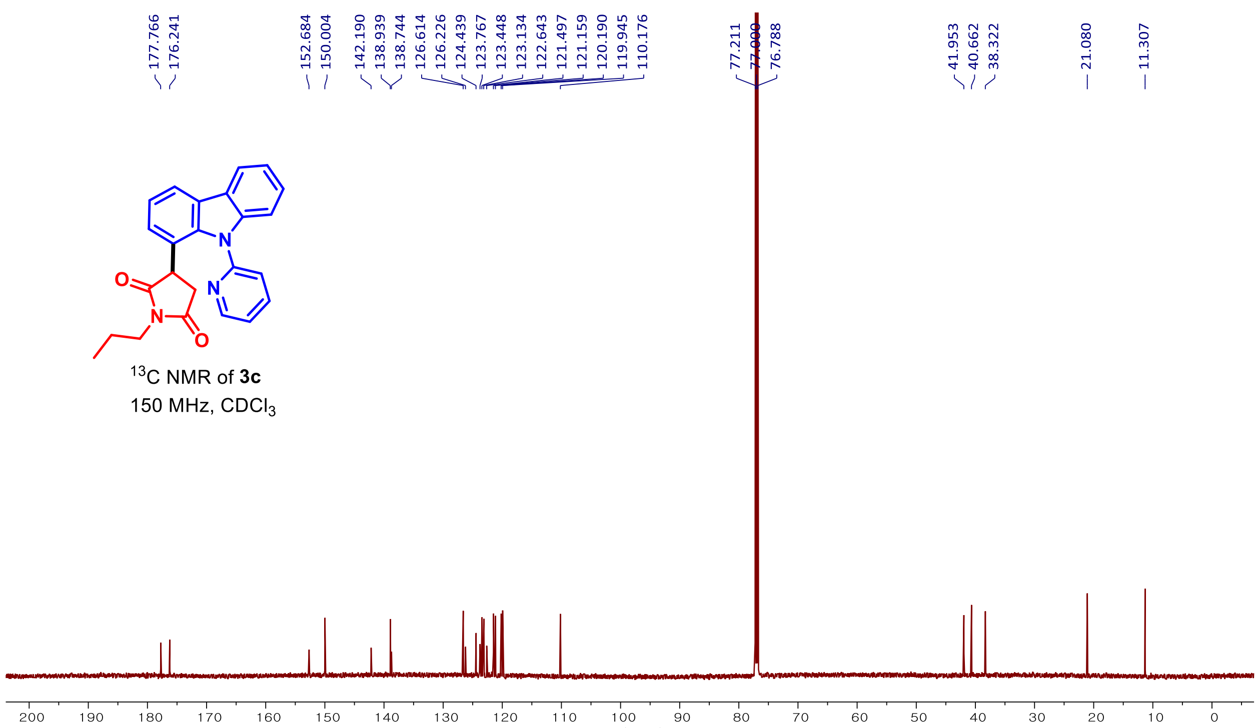

8.710
8.703
8.091
8.079
8.067
7.984
7.980
7.971
7.967
7.958
7.955
7.599
7.586
7.444
7.436
7.432
7.424
7.381
7.378
7.367
7.365
7.355
7.353
7.303
7.291
7.278
7.240
7.237
7.224
7.065
7.052
3.921
3.909
3.897
3.593
3.581
3.569
3.557
2.640
2.630
2.627
1.198
1.186
1.174
N
O
N
N
O
[1]H NMR of 3b
600 MHz, CDCl3
1.09
1.99
1.08
0.94
1.08
1.01
2.07
1.11
0.97
1.00
2.21
2.03
3.26
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)


177.58
176.04
152.64
149.96
142.18
139.01
138.72
126.63
126.24
124.43
123.78
123.47
123.13
122.67
121.53
121.19
120.20
119.96
110.18
77.21
77.00
76.79
41.98
38.41
34.02
13.09
N
O
N
N
O
[13]C NMR of 3b
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



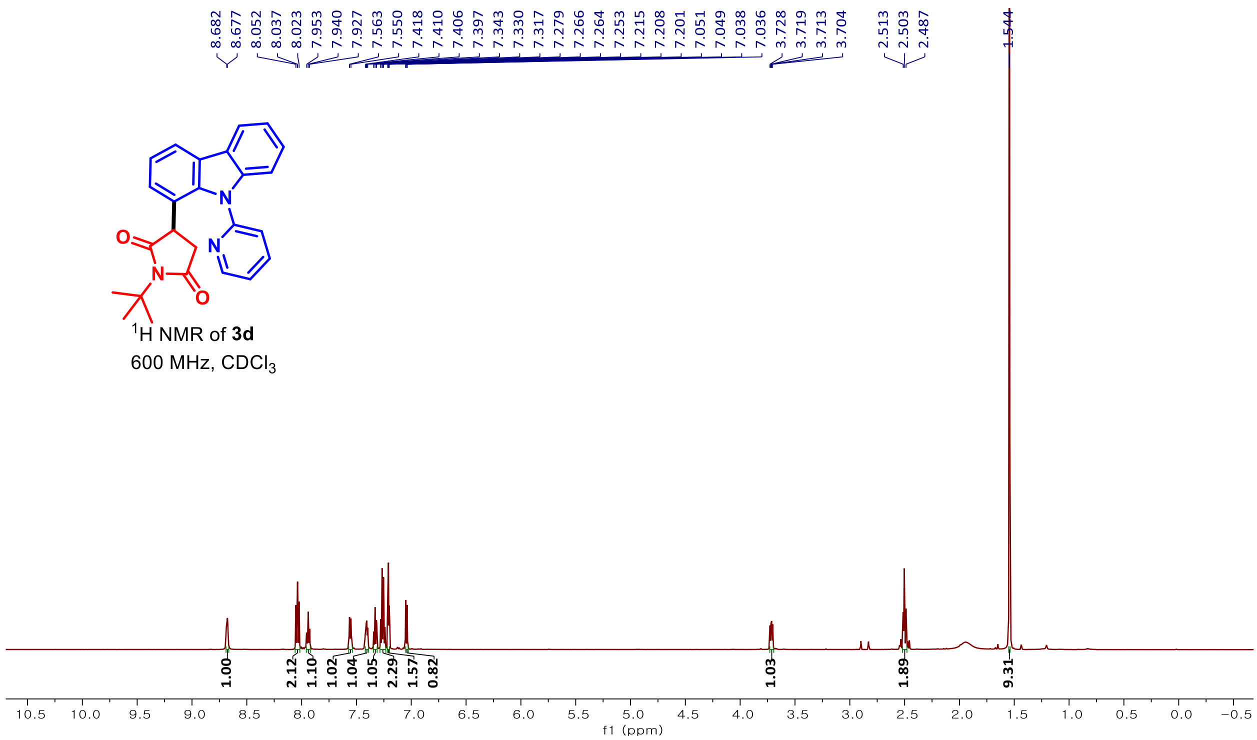
^{1}H NMR of **3c**

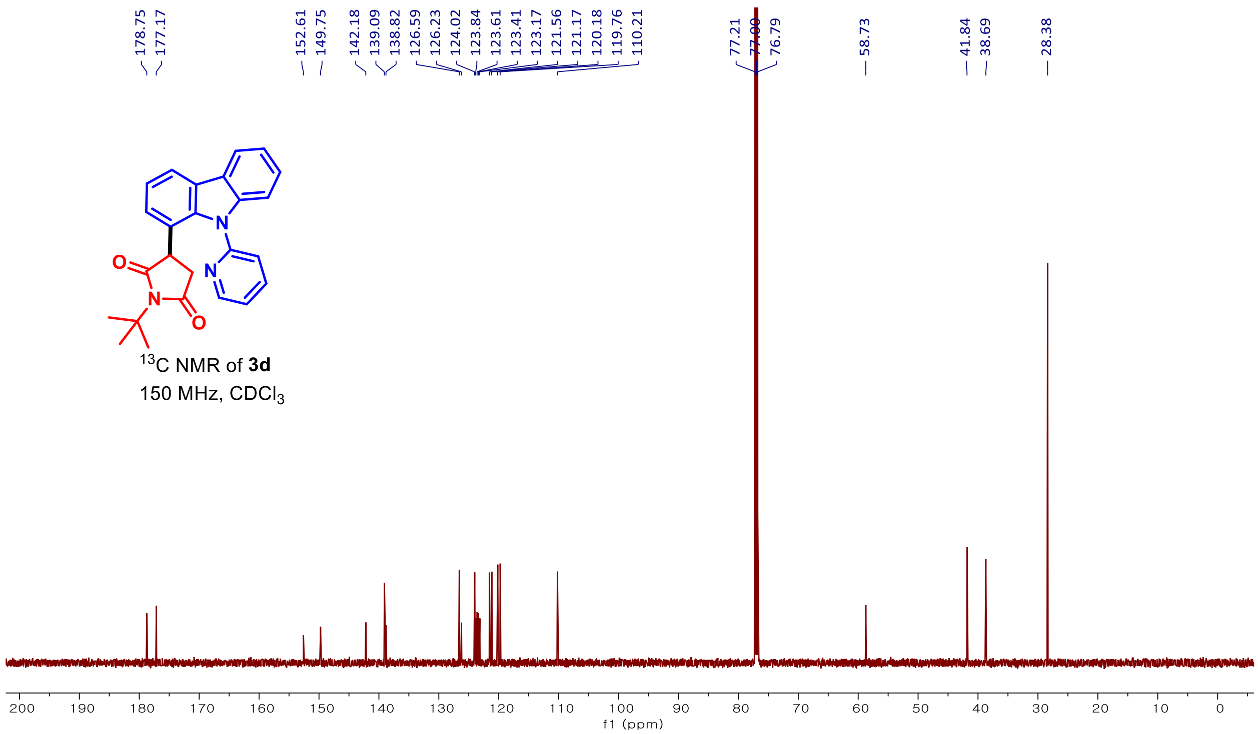
600 MHz, $CDCl_3$

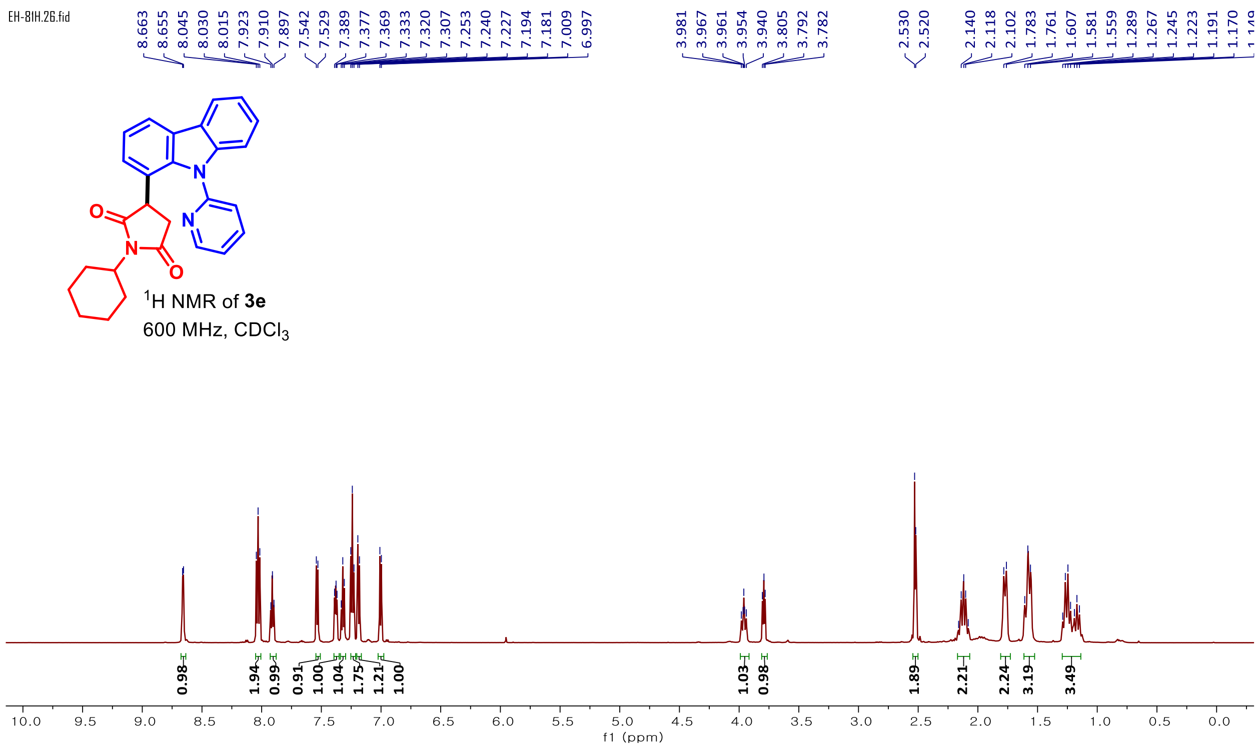


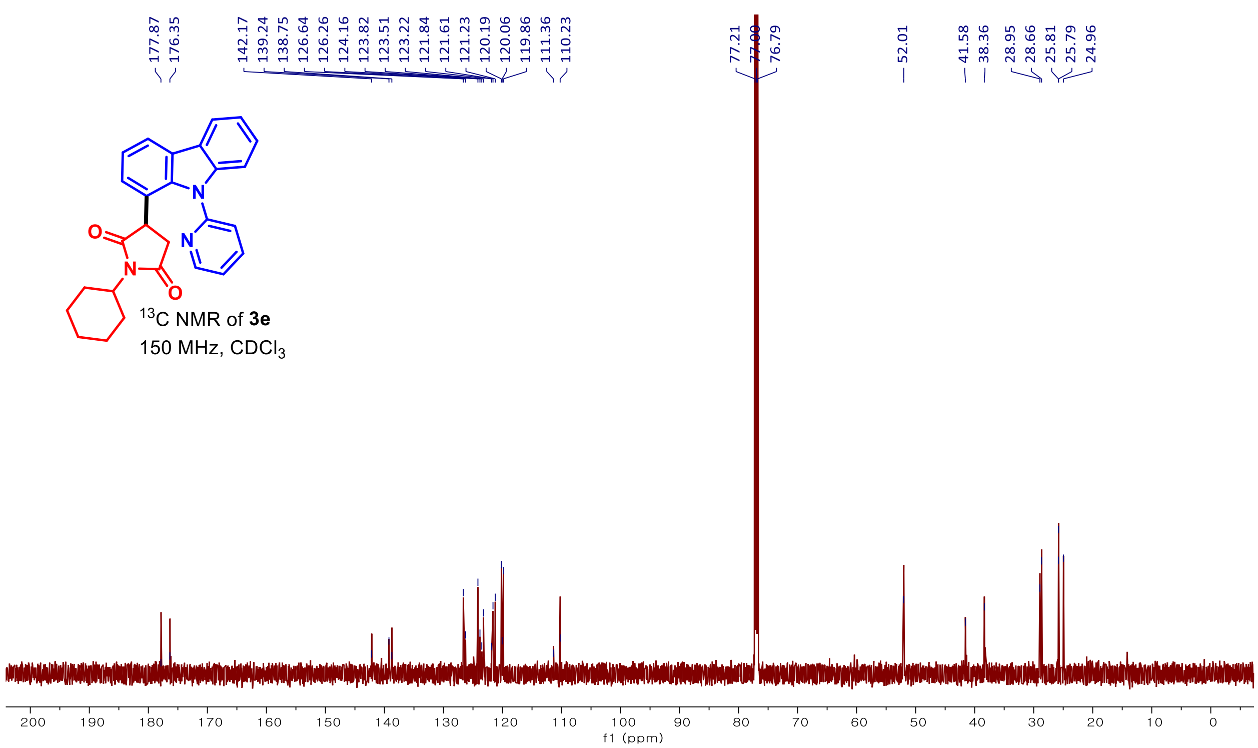
^{13}C NMR of **3c**

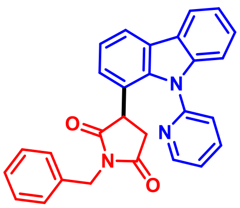
150 MHz, $CDCl_3$


8.682
8.677
8.052
8.037
8.023
7.953
7.940
7.927
7.563
7.550
7.418
7.410
7.406
7.397
7.343
7.330
7.317
7.279
7.266
7.264
7.253
7.215
7.208
7.201
7.051
7.049
7.038
7.036
3.728
3.719
3.713
3.704
2.513
2.503
2.487
1.544
¹H NMR of 3d
600 MHz, CDCl3
f1 (ppm)

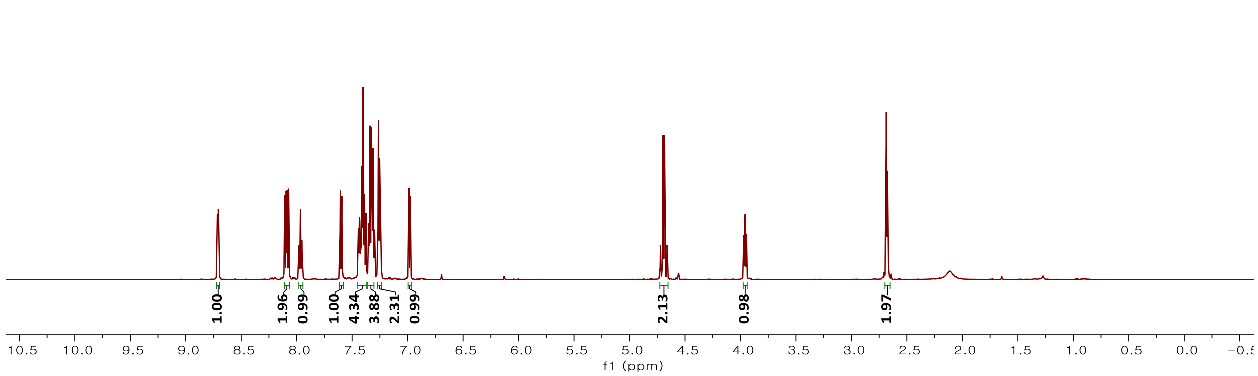

178.75
177.17
152.61
149.75
142.18
139.09
138.82
126.59
126.23
124.02
123.84
123.61
123.41
123.17
121.56
121.17
120.18
119.76
110.21
77.21
77.00
76.79
58.73
41.84
38.69
28.38
¹³C NMR of 3d
150 MHz, CDCl3
f1 (ppm)

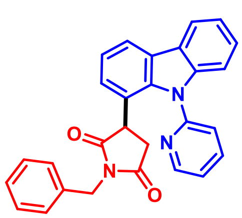

EH-81H.26.fid
8.663 8.655 8.045 8.030 8.015 7.923 7.910 7.897 7.542 7.529 7.389 7.377 7.369 7.333 7.320 7.307 7.253 7.240 7.227 7.194 7.181 7.009 6.997
3.981 3.967 3.961 3.954 3.940 3.805 3.792 3.782
2.530 2.520
2.140 2.118 2.102 1.783 1.761 1.607 1.581 1.559 1.289 1.267 1.245 1.223 1.191 1.170
O
N
O
N
N
^{1}H NMR of **3e**
600 MHz, $CDCl_3$
0.98 1.94 0.99 0.91 1.00 1.04 1.75 1.21 1.00 1.03 0.98 1.89 2.21 2.24 3.19 3.49
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)


177.87 176.35
142.17 139.24 138.75 126.64 126.26 124.16 123.82 123.51 123.22 121.84 121.61 121.23 120.19 120.06 119.86 111.36 110.23
77.21 77.00 76.79
52.01
41.58 38.36 28.95 28.66 25.81 25.79 24.96
O
N
O
N
N
^{13}C NMR of **3e**
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)

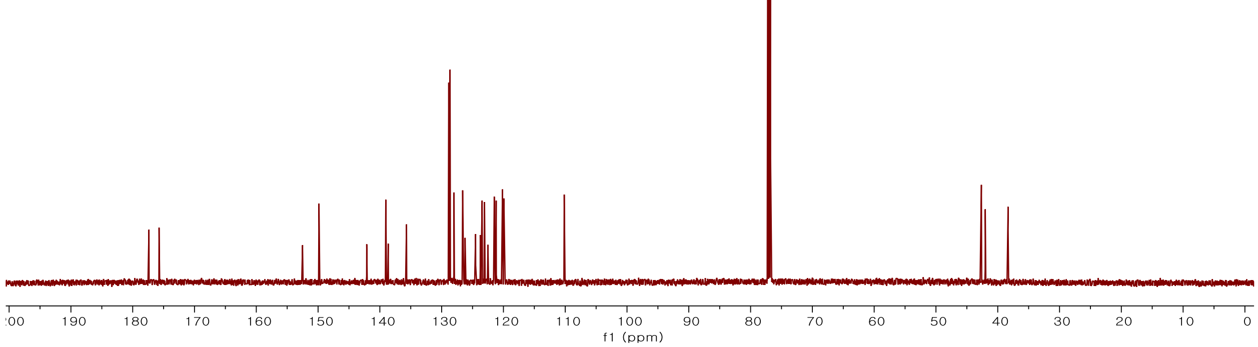


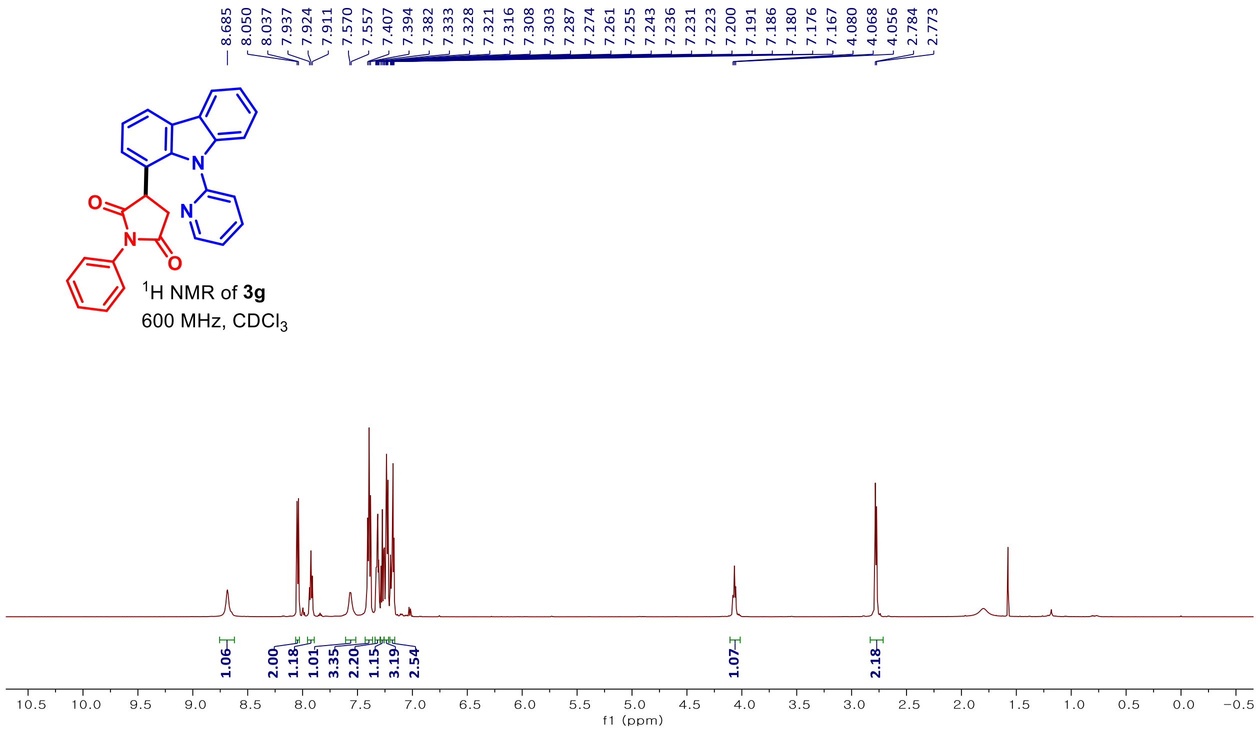
^{1}H NMR of **3f**
600 MHz, $CDCl_3$

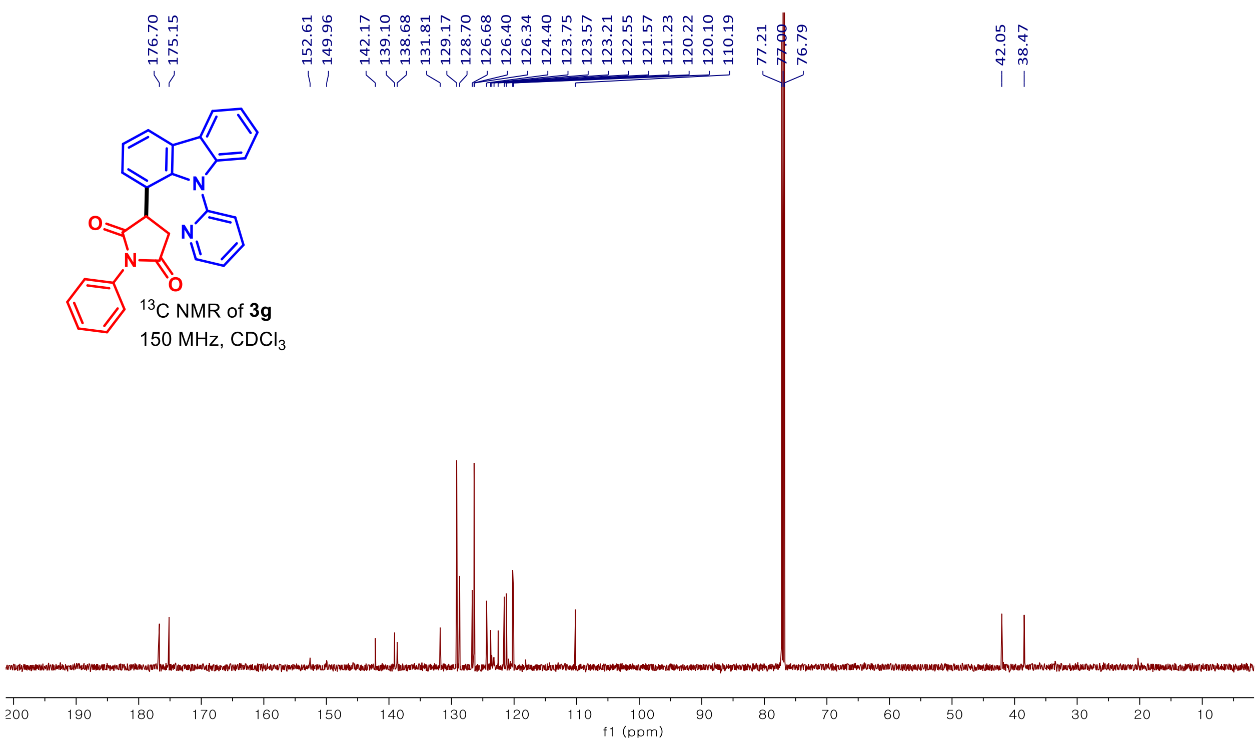


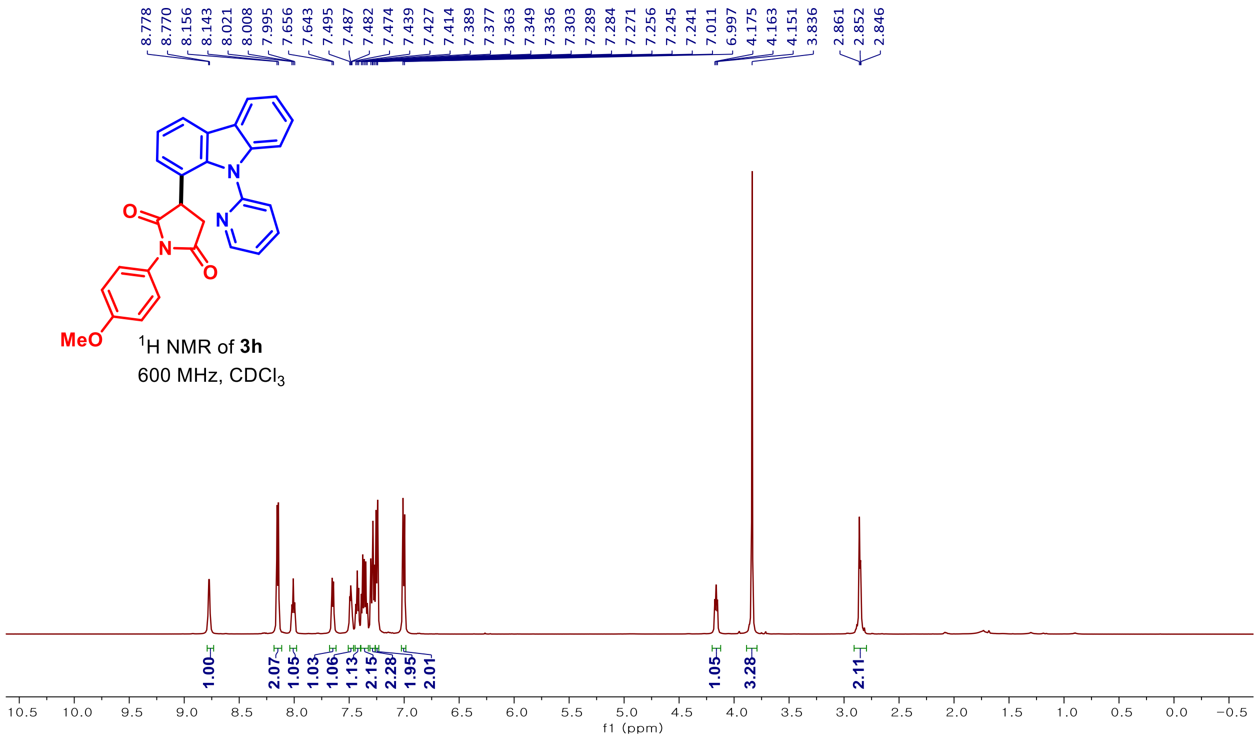


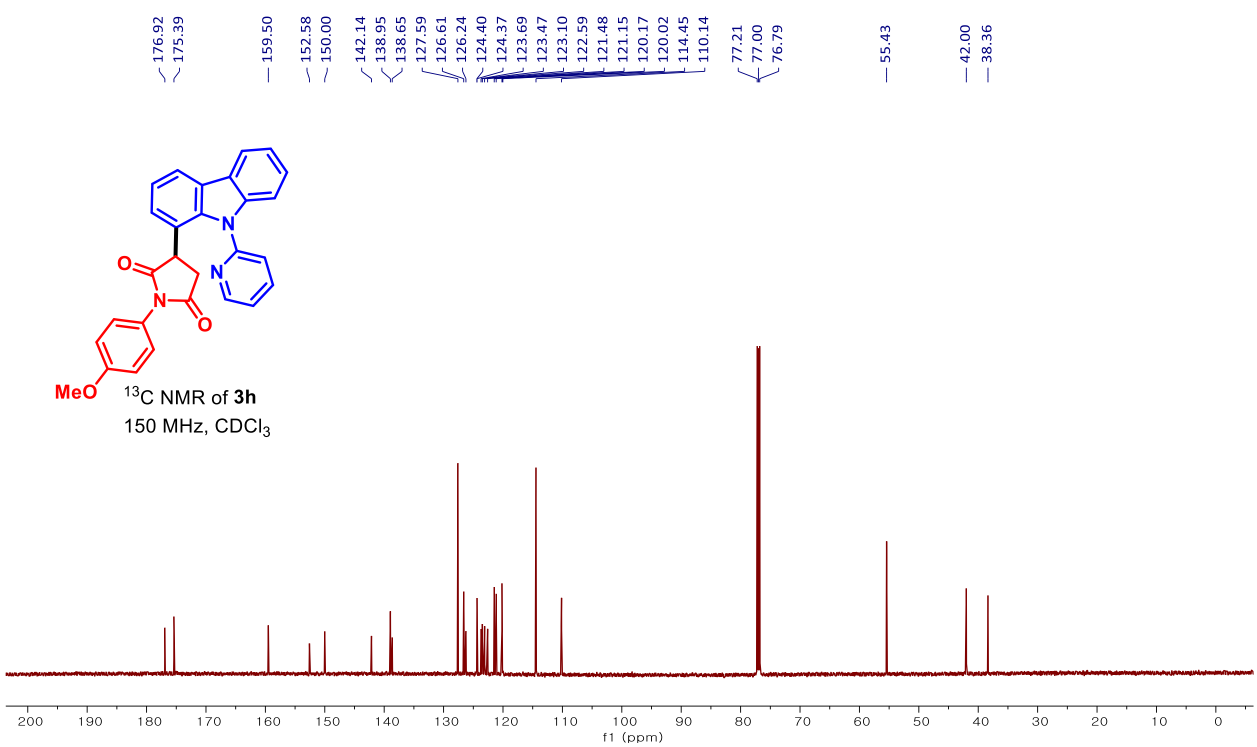
^{13}C NMR of **3f**
150 MHz, $CDCl_3$

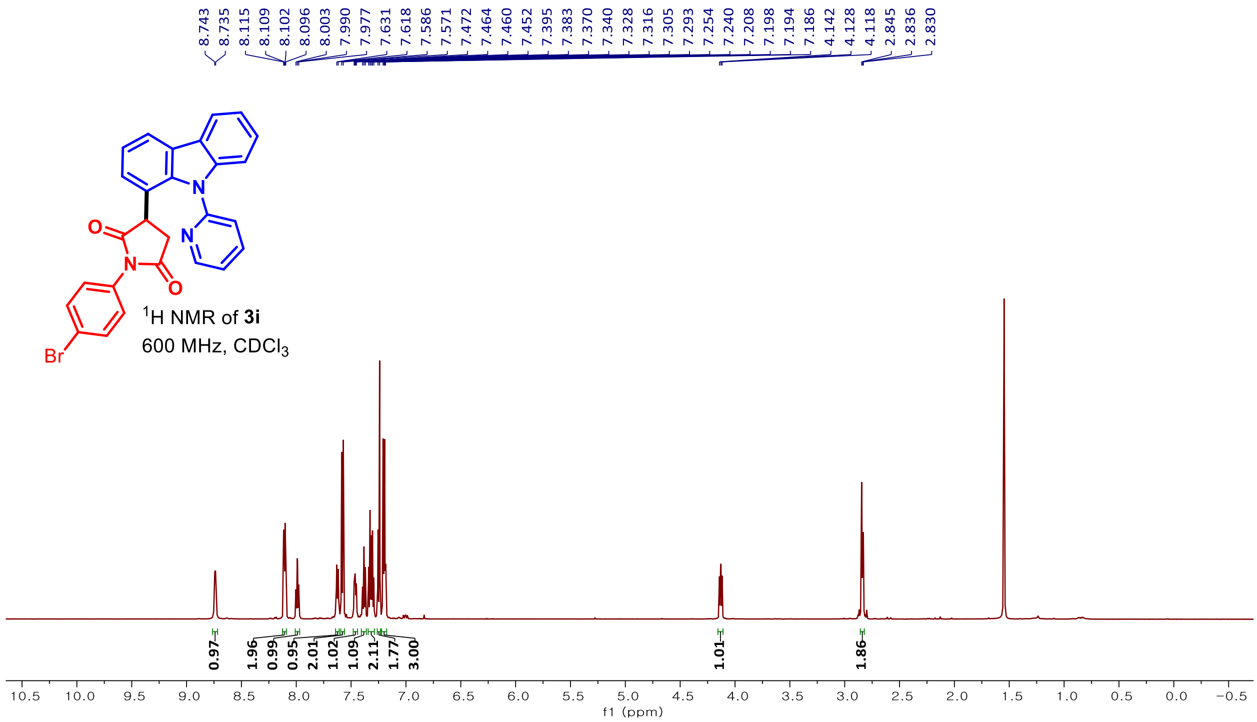


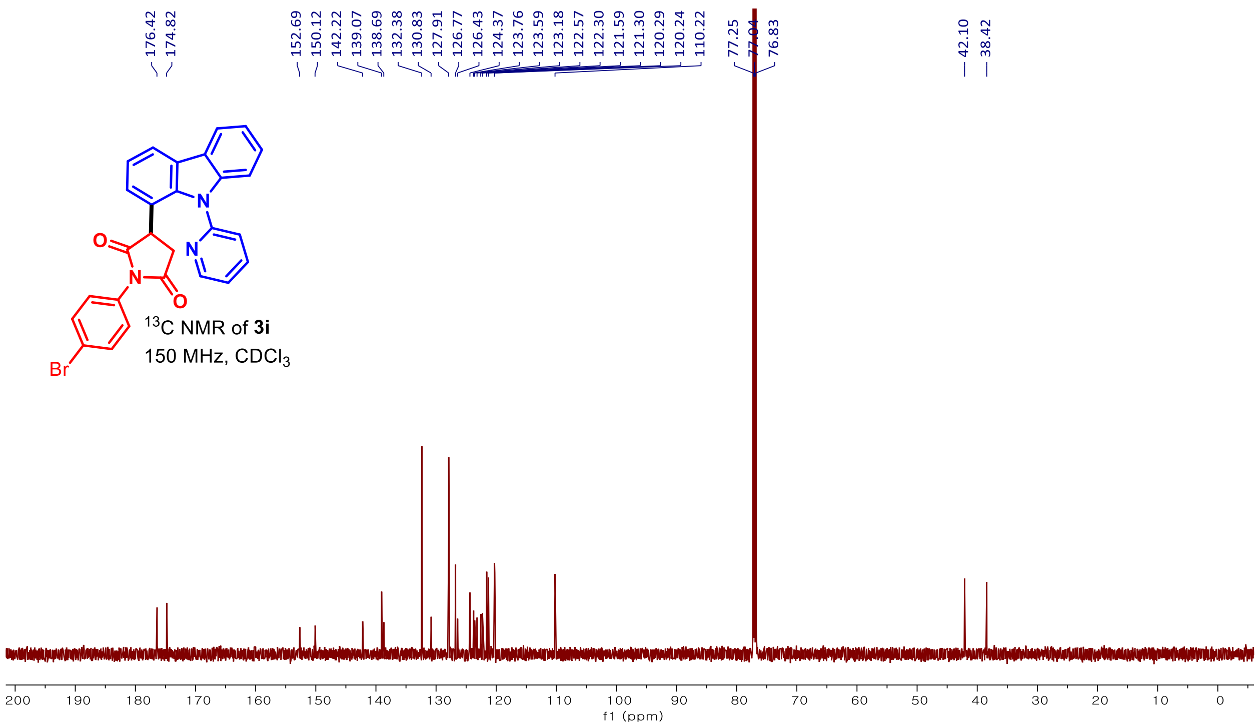

1H NMR of 3g
600 MHz, CDCl3
f1 (ppm)

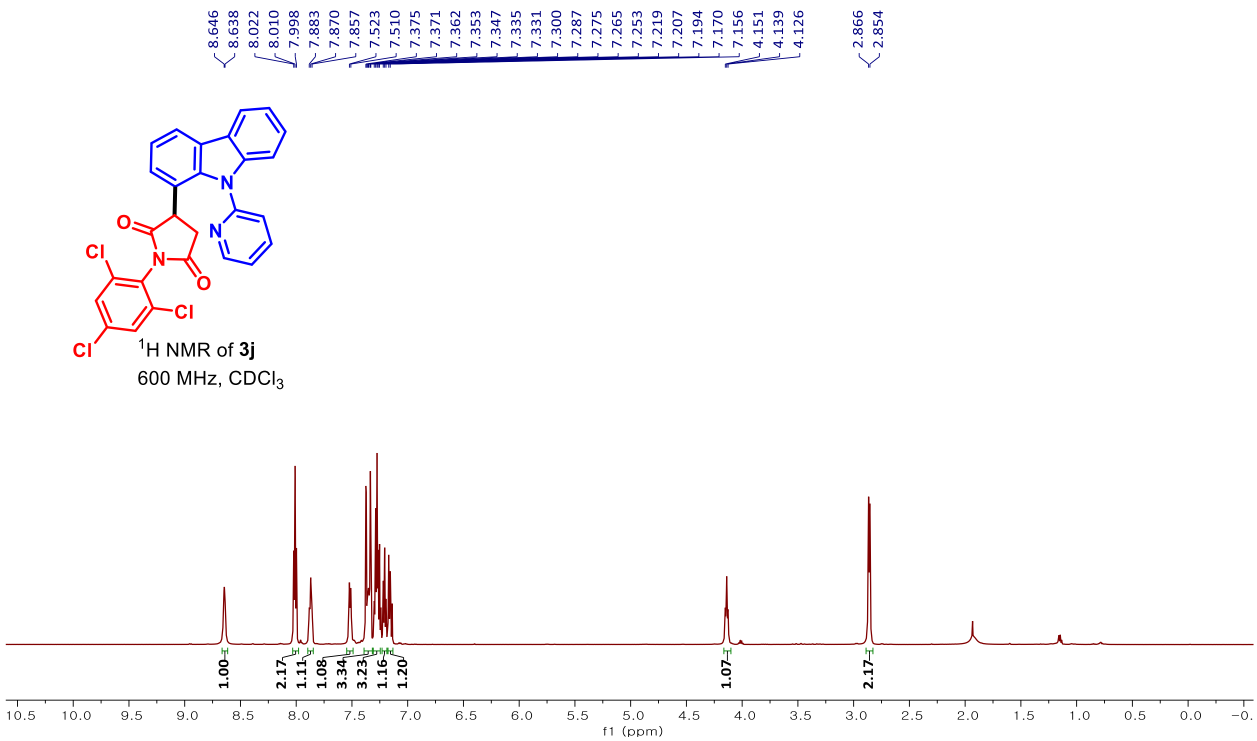

13C NMR of 3g
150 MHz, CDCl3
f1 (ppm)


MeO
N
O
O
N
N
1H NMR of 3h
600 MHz, CDCl3
f1 (ppm)

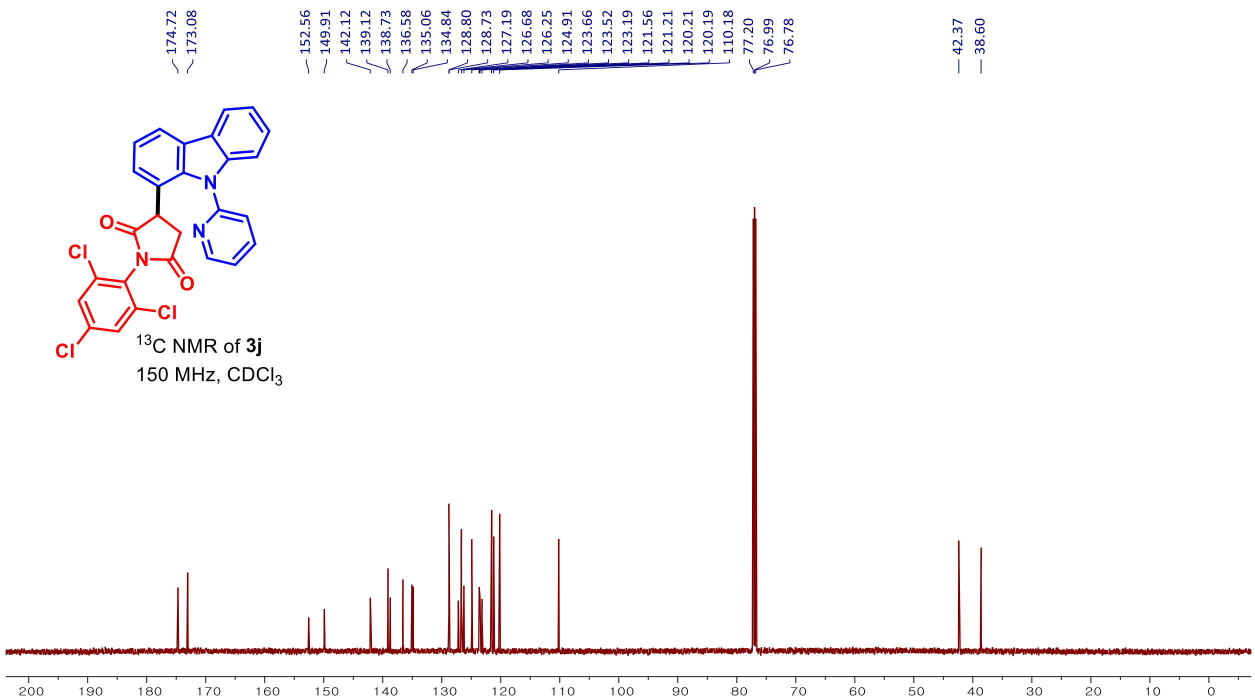

MeO
N
O
O
N
N
13C NMR of 3h
150 MHz, CDCl3
f1 (ppm)


8.743
8.735
8.115
8.109
8.102
8.096
8.003
7.990
7.977
7.631
7.618
7.586
7.571
7.472
7.464
7.460
7.452
7.395
7.383
7.370
7.340
7.328
7.316
7.305
7.293
7.254
7.240
7.208
7.198
7.194
7.186
4.142
4.128
4.118
2.845
2.836
2.830
O
N
O
N
N
Br
^{1}H NMR of **3i**
600 MHz, $CDCl_3$
0.97
1.96
0.99
0.95
2.01
1.02
1.09
2.11
1.77
3.00
1.01
1.86
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)

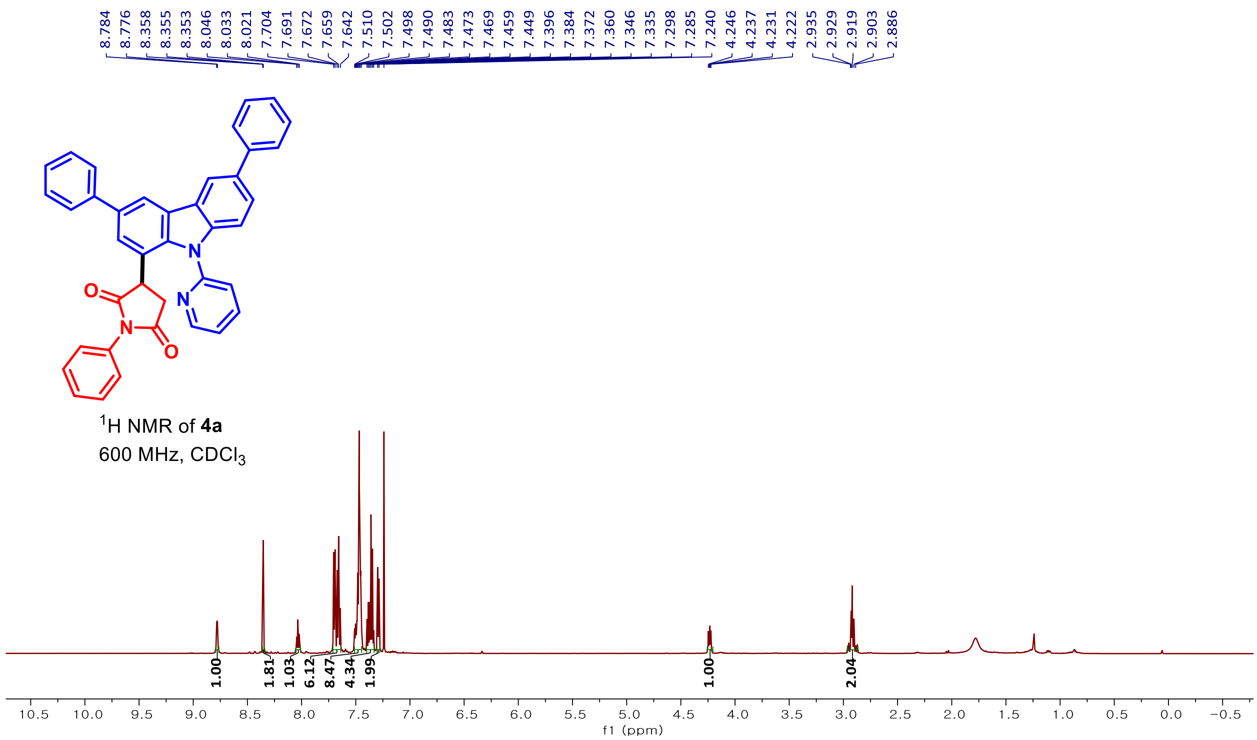

176.42
174.82
152.69
150.12
142.22
139.07
138.69
132.38
130.83
127.91
126.77
126.43
124.37
123.76
123.59
123.18
122.57
122.30
121.59
121.30
120.29
120.24
110.22
77.25
77.04
76.83
42.10
38.42
O
N
O
N
N
Br
^{13}C NMR of **3i**
150 MHz, $CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



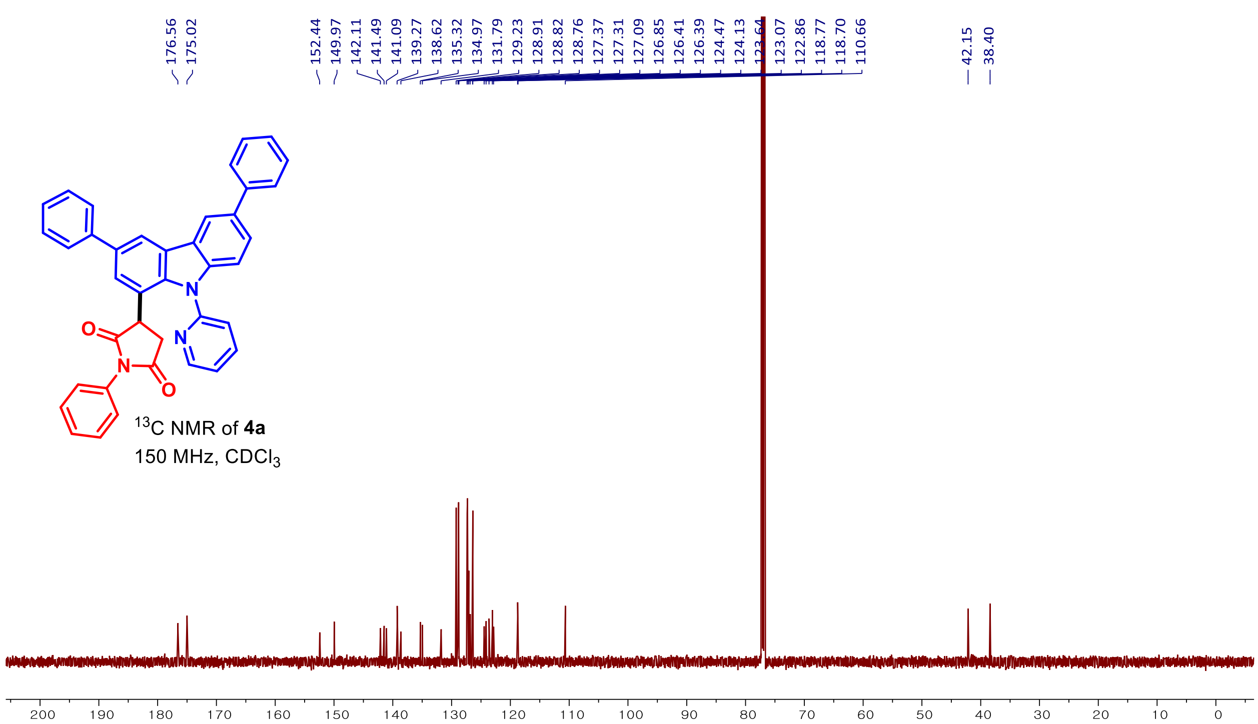
[1]H NMR of **3j**
600 MHz, $CDCl_3$



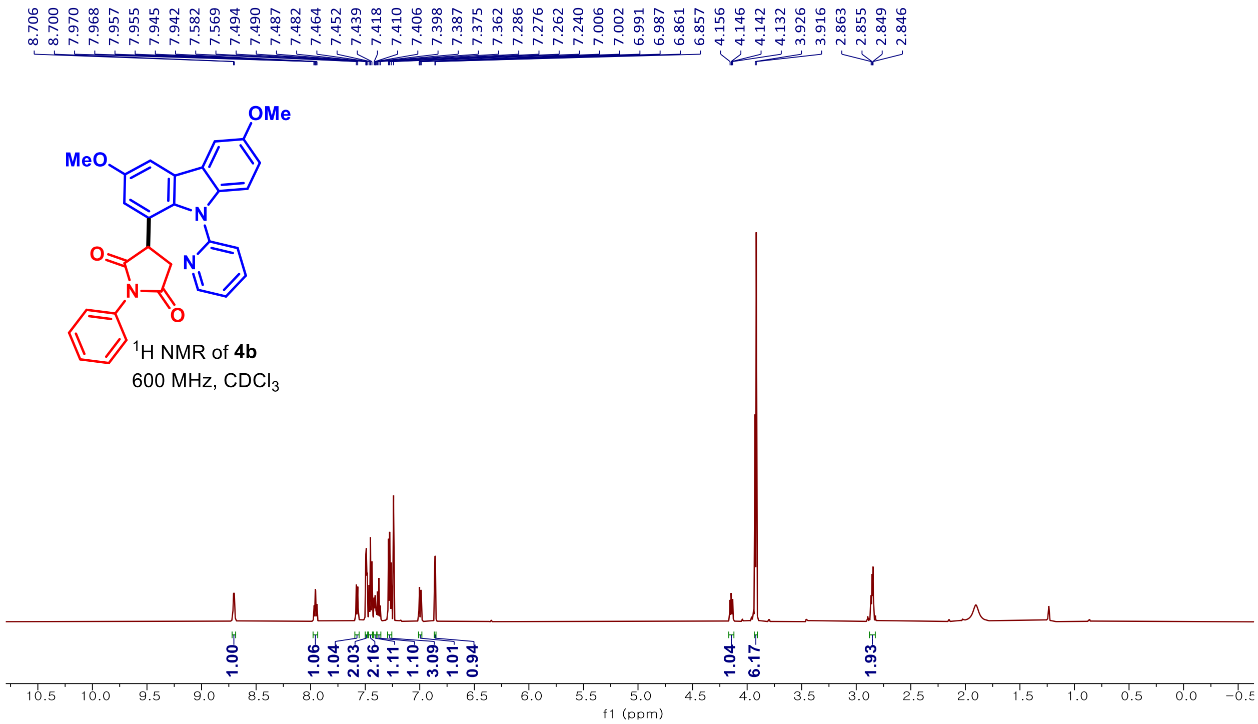
[13]C NMR of **3j**
150 MHz, $CDCl_3$

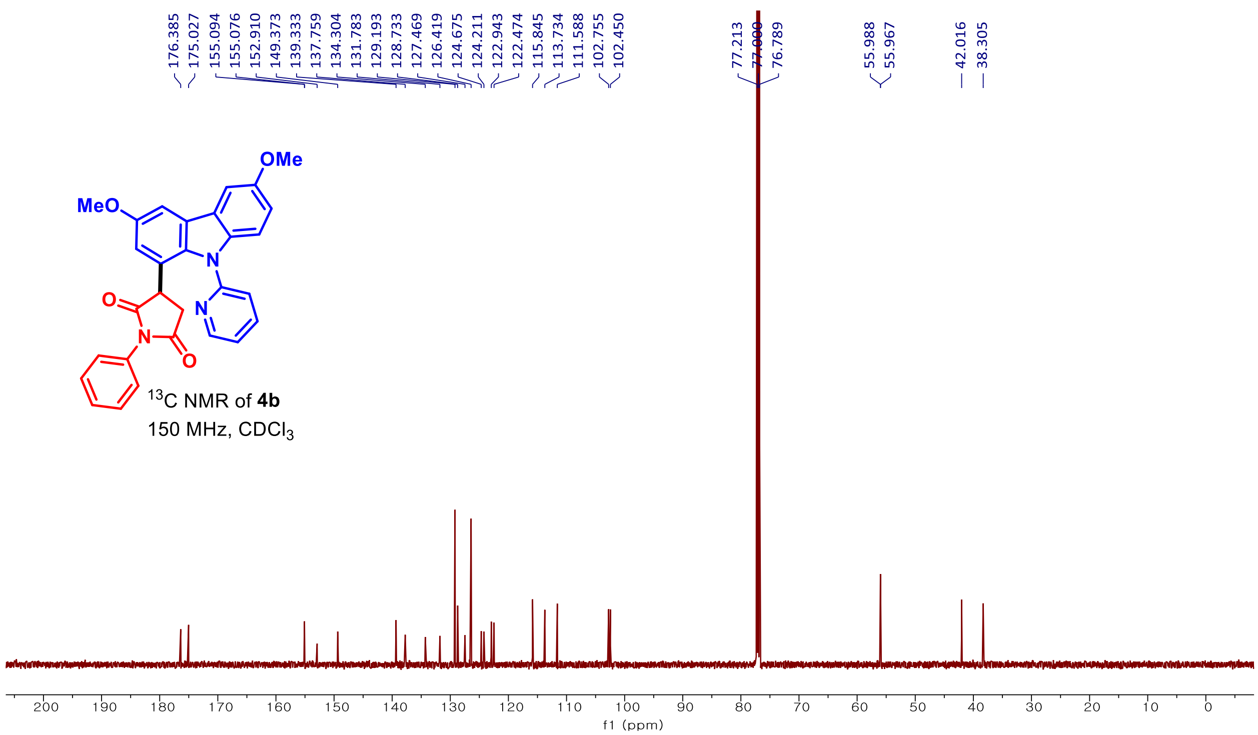


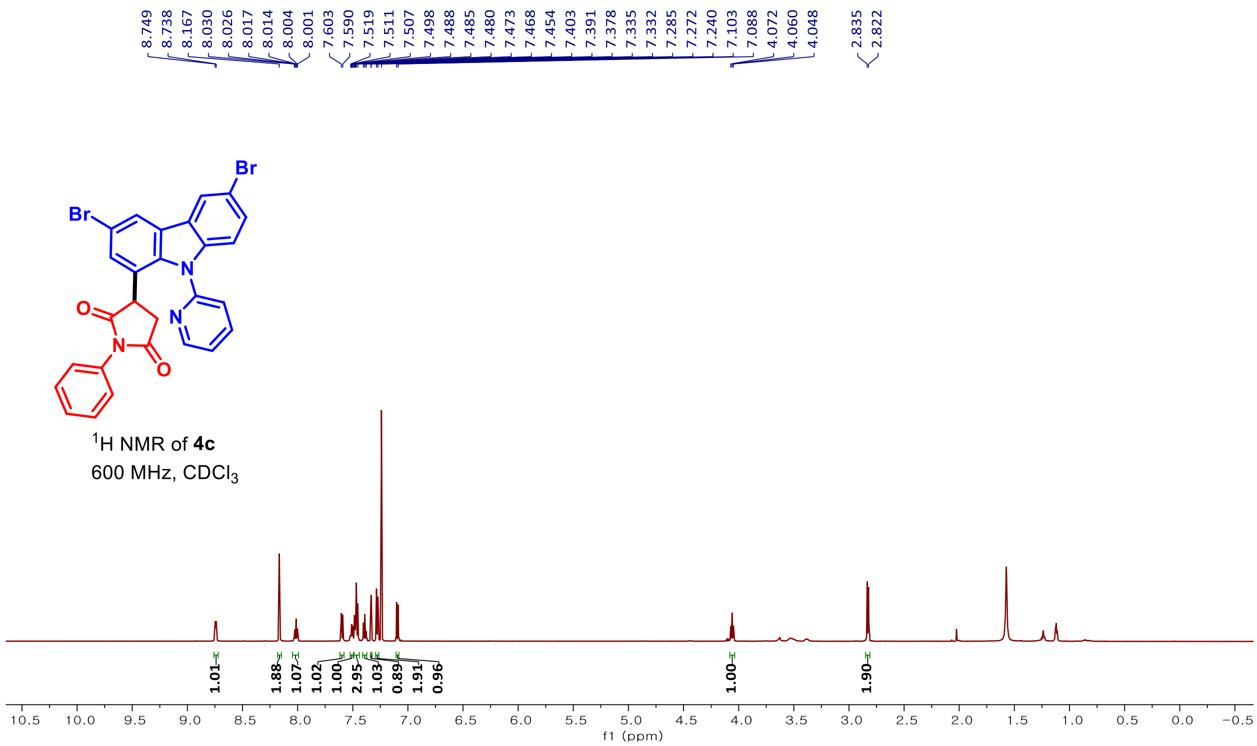
8.784 8.776 8.358 8.355 8.353 8.046 8.033 8.021 7.704 7.691 7.672 7.659 7.642 7.510 7.502 7.498 7.490 7.483 7.473 7.469 7.459 7.449 7.396 7.384 7.372 7.360 7.346 7.335 7.298 7.285 7.240 4.246 4.237 4.231 4.222 2.935 2.929 2.919 2.903 2.886
O
N
O
N
N
^{1}H NMR of **4a**
600 MHz, $CDCl_3$
1.00 1.81 1.03 6.12 8.47 4.34 1.99 1.00 2.04
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)

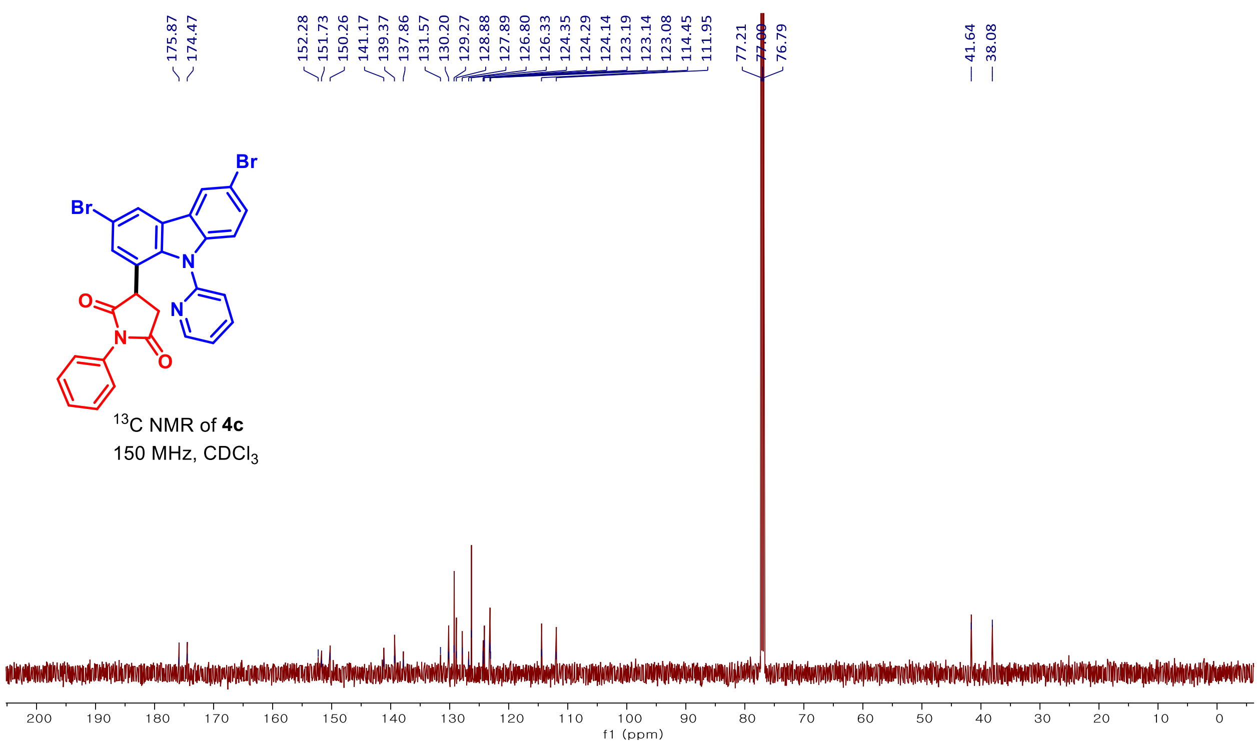


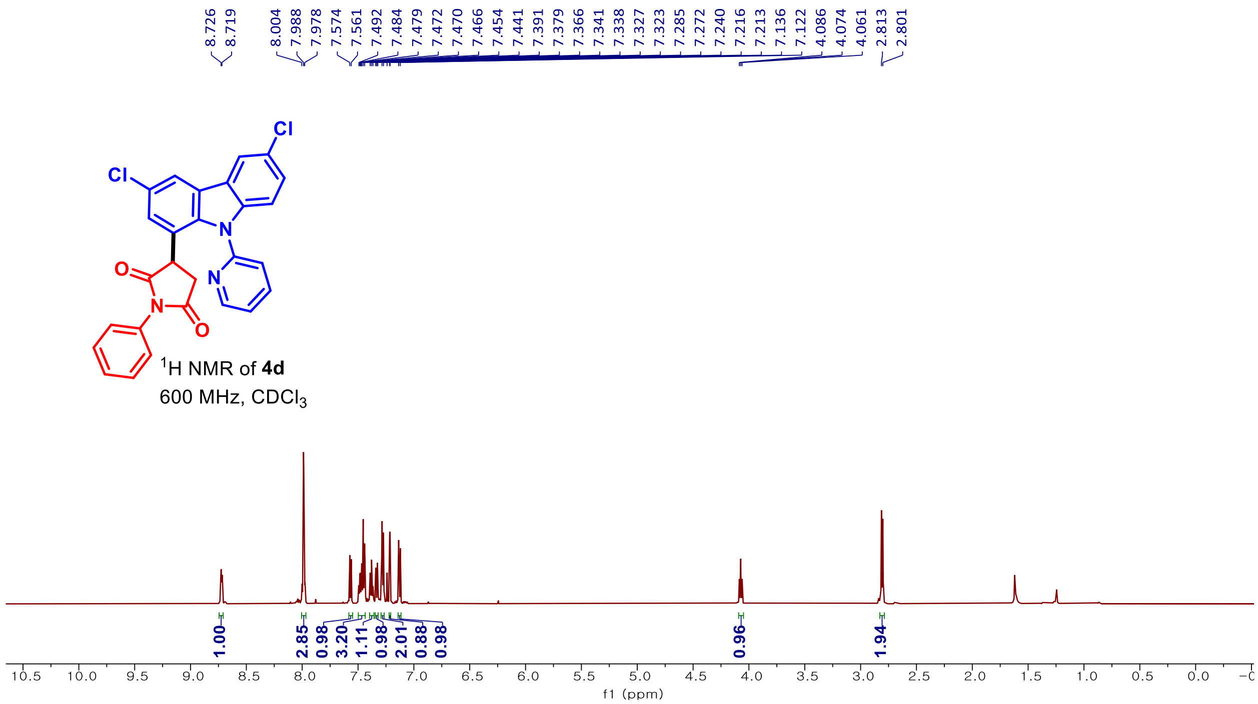
176.56 175.02 152.44 149.97 142.11 141.49 141.09 139.27 138.62 135.32 134.97 131.79 129.23 128.91 128.82 128.76 127.37 127.31 127.09 126.85 126.41 126.39 124.47 124.13 123.64 123.07 122.86 118.77 118.70 110.66 42.15 38.40
O
N
O
N
N
^{13}C NMR of **4a**
150 MHz, $CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

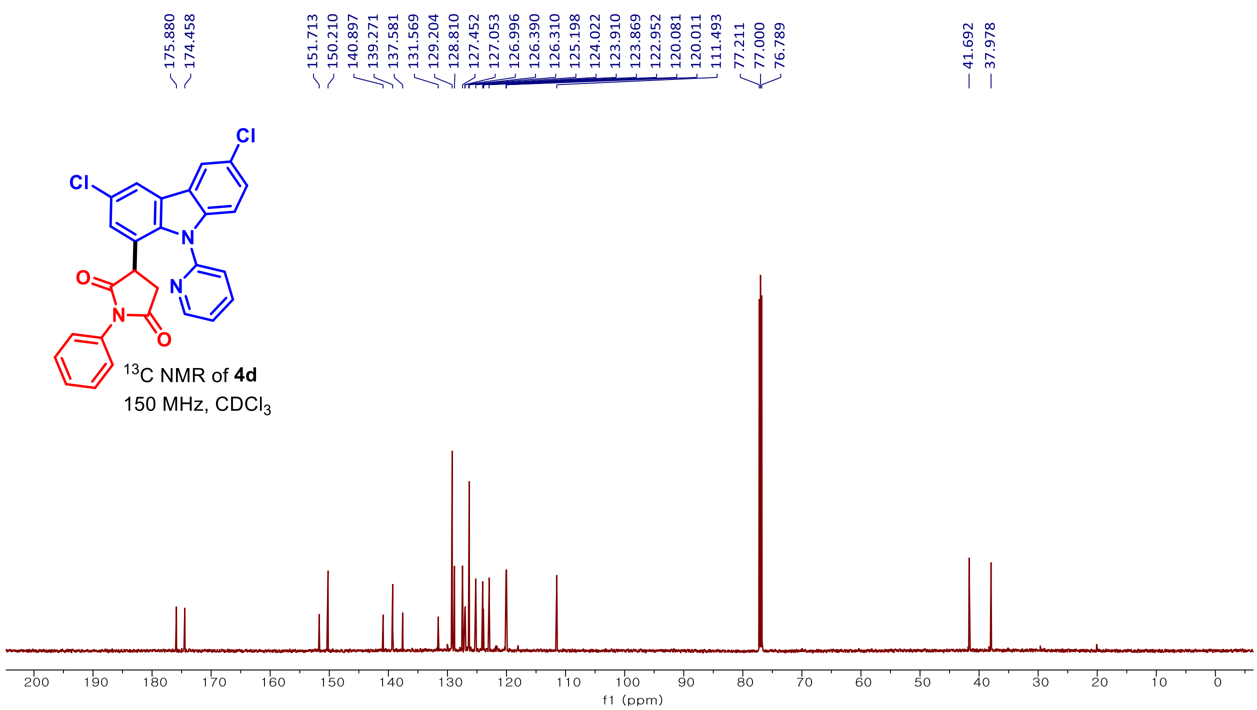

8.706 8.700 7.970 7.968 7.957 7.955 7.945 7.942 7.582 7.569 7.494 7.490 7.487 7.482 7.464 7.452 7.439 7.418 7.410 7.406 7.398 7.387 7.375 7.362 7.286 7.276 7.262 7.240 7.006 7.002 6.991 6.987 6.861 6.857 4.156 4.146 4.142 4.132 3.926 3.916 2.863 2.855 2.849 2.846
OMe
MeO
N
O
N
O
N
^{1}H NMR of **4b**
600 MHz, $CDCl_3$
1.00 1.06 1.04 2.03 2.16 1.11 1.10 3.09 1.01 0.94 1.04 6.17 1.93
f1 (ppm)

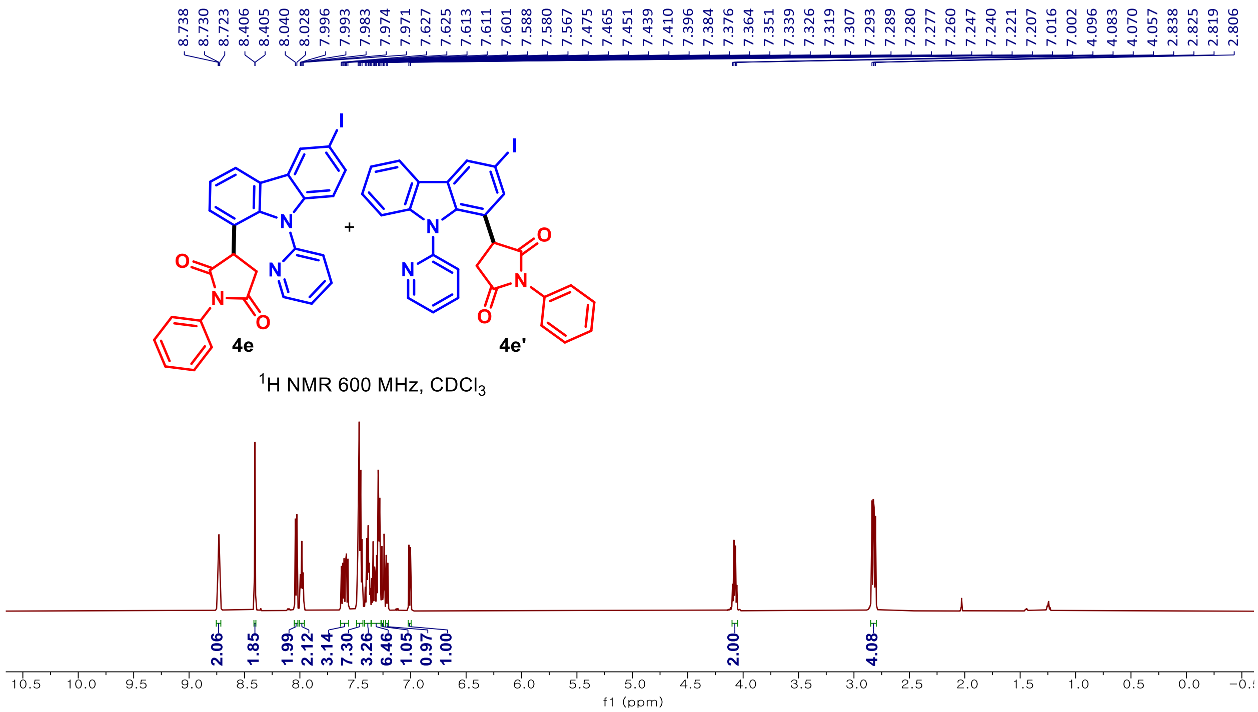

176.385 175.027 155.094 155.076 152.910 149.373 139.333 137.759 134.304 131.783 129.193 128.733 127.469 126.419 124.675 124.211 122.943 122.474 115.845 113.734 111.588 102.755 102.450 77.213 77.000 76.789 55.988 55.967 42.016 38.305
OMe
MeO
N
O
N
O
N
^{13}C NMR of **4b**
150 MHz, $CDCl_3$
f1 (ppm)

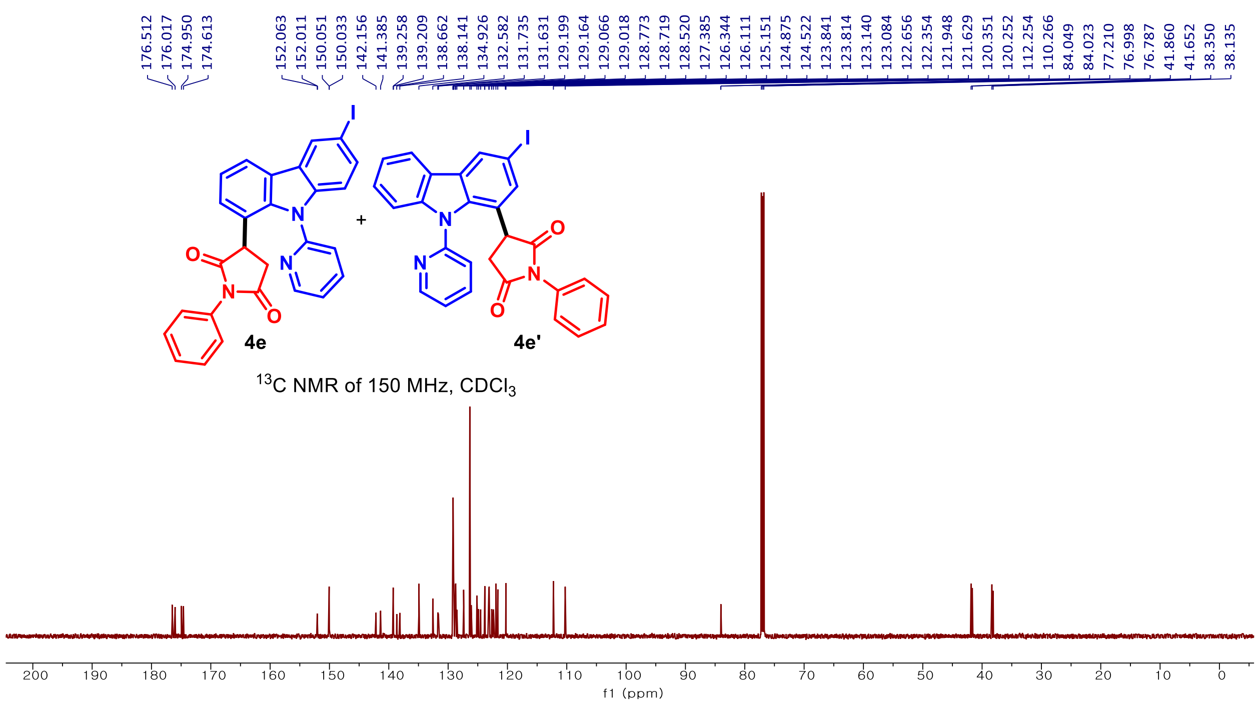

8.749 8.738 8.167 8.030 8.026 8.017 8.014 8.004 8.001 7.603 7.590 7.519 7.511 7.507 7.498 7.488 7.485 7.480 7.473 7.468 7.454 7.403 7.391 7.378 7.335 7.332 7.285 7.272 7.240 7.103 7.088 4.072 4.060 4.048 2.835 2.822
Br
Br
N
N
O
N
O
^{1}H NMR of **4c**
600 MHz, $CDCl_3$
1.01 1.88 1.07 1.02 1.00 2.95 1.03 0.89 1.91 0.96 1.00 1.90
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)

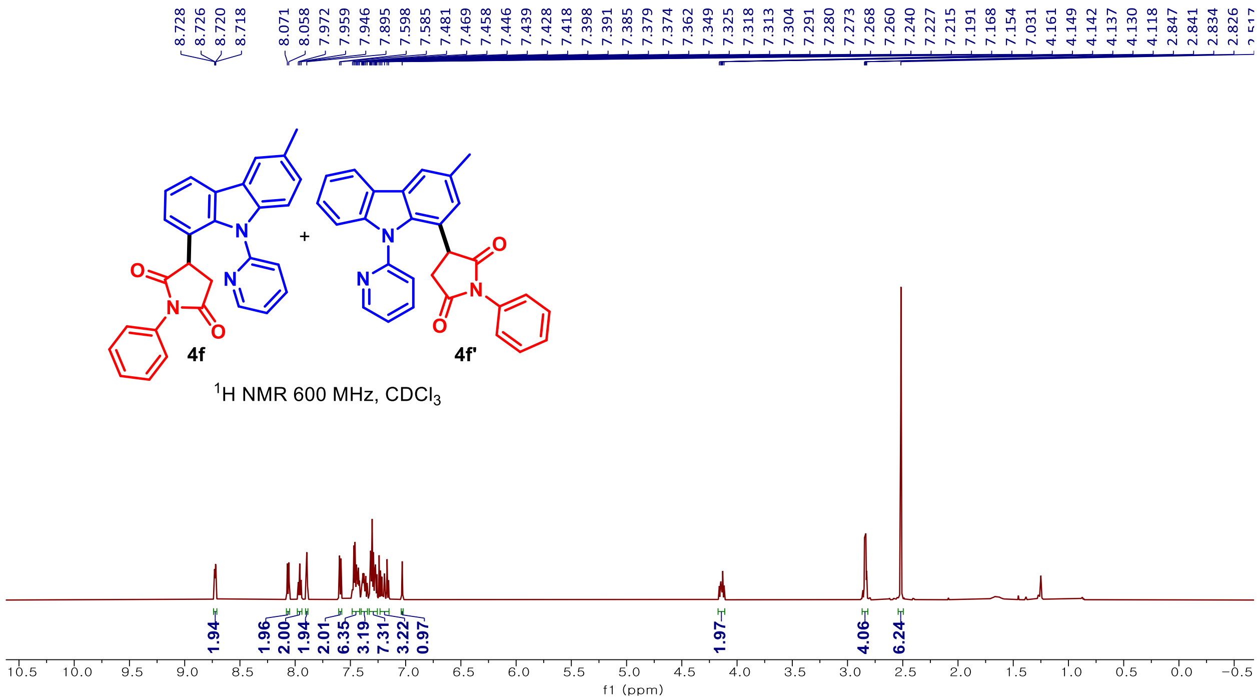

175.87 174.47 152.28 151.73 150.26 141.17 139.37 137.86 131.57 130.20 129.27 128.88 127.89 126.80 126.33 124.35 124.29 124.14 123.19 123.14 123.08 114.45 111.95 77.21 77.00 76.79 41.64 38.08
Br
Br
N
N
O
N
O
^{13}C NMR of **4c**
150 MHz, $CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

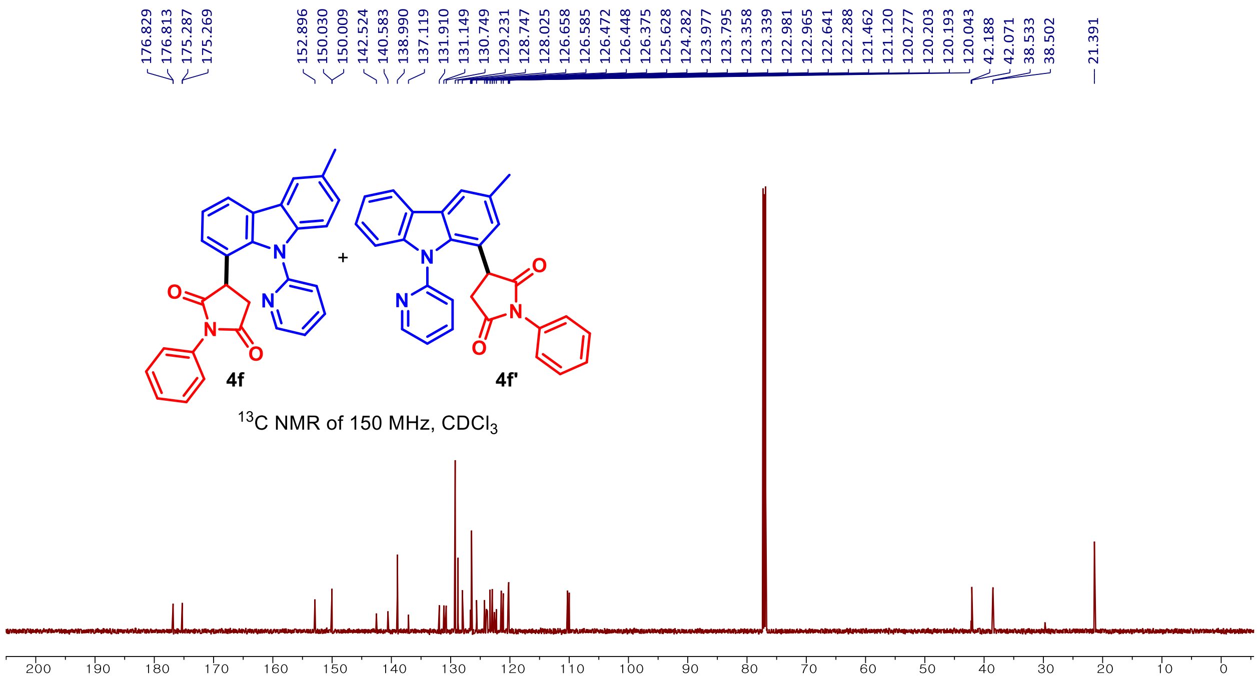

8.726
8.719
8.004
7.988
7.978
7.574
7.561
7.492
7.484
7.479
7.472
7.470
7.466
7.454
7.441
7.391
7.379
7.366
7.341
7.338
7.327
7.323
7.285
7.272
7.240
7.216
7.213
7.136
7.122
4.086
4.074
4.061
2.813
2.801
Cl
Cl
N
N
O
N
O
^{1}H NMR of **4d**
600 MHz, $CDCl_3$
1.00
2.85
0.98
3.20
1.11
0.98
2.01
0.88
0.98
0.96
1.94
f1 (ppm)

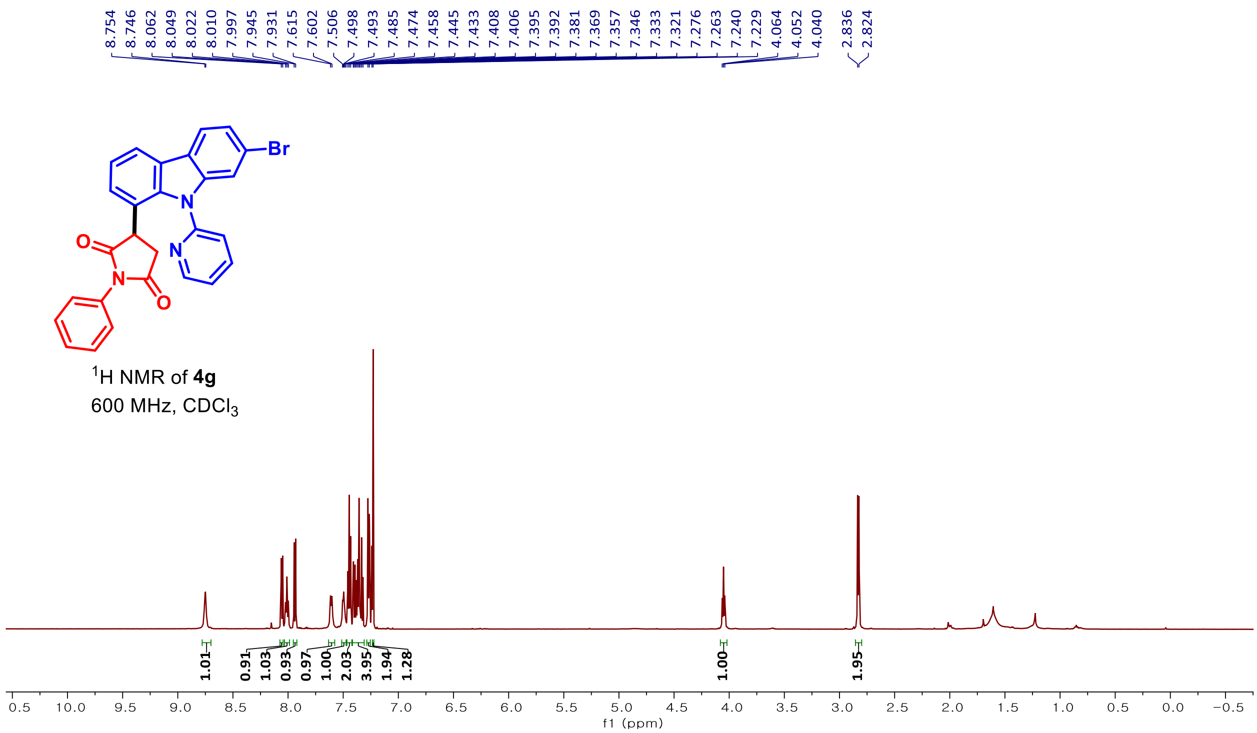

175.880
174.458
151.713
150.210
140.897
139.271
137.581
131.569
129.204
128.810
127.452
127.053
126.996
126.390
126.310
125.198
124.022
123.910
123.869
122.952
120.081
120.011
111.493
77.211
77.000
76.789
41.692
37.978
Cl
Cl
N
N
O
N
O
^{13}C NMR of **4d**
150 MHz, $CDCl_3$
f1 (ppm)

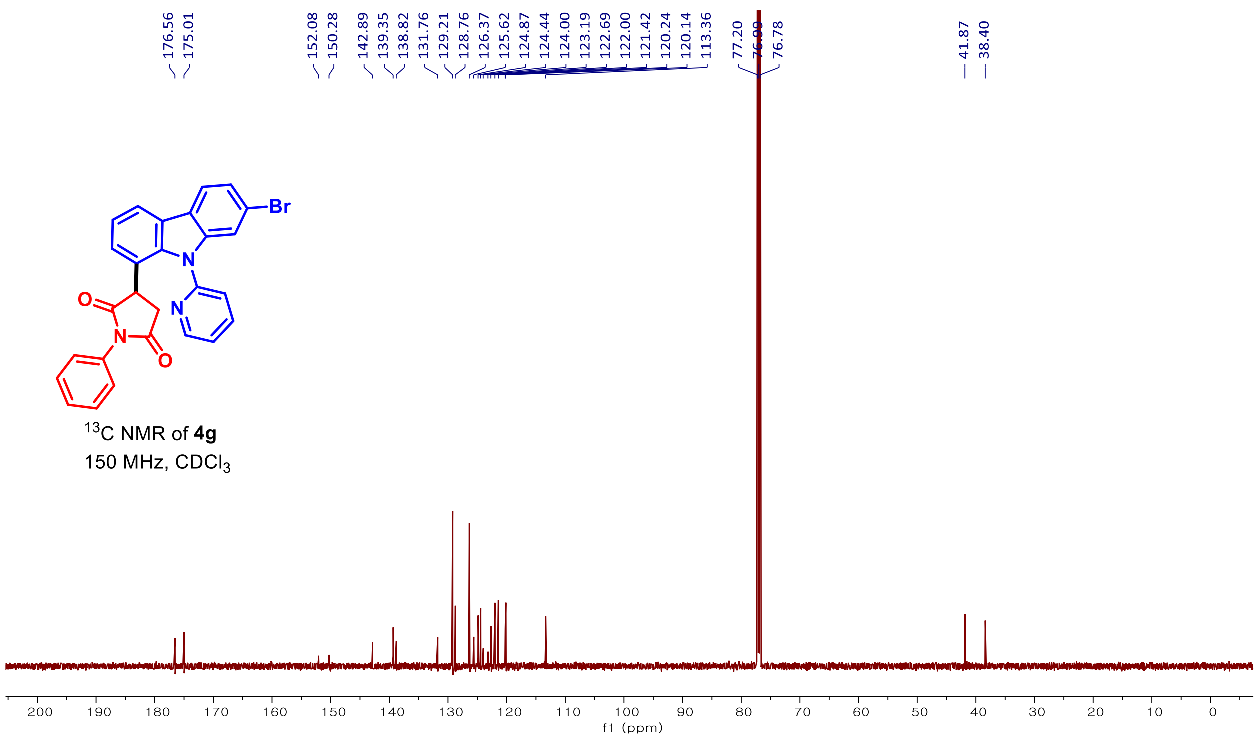


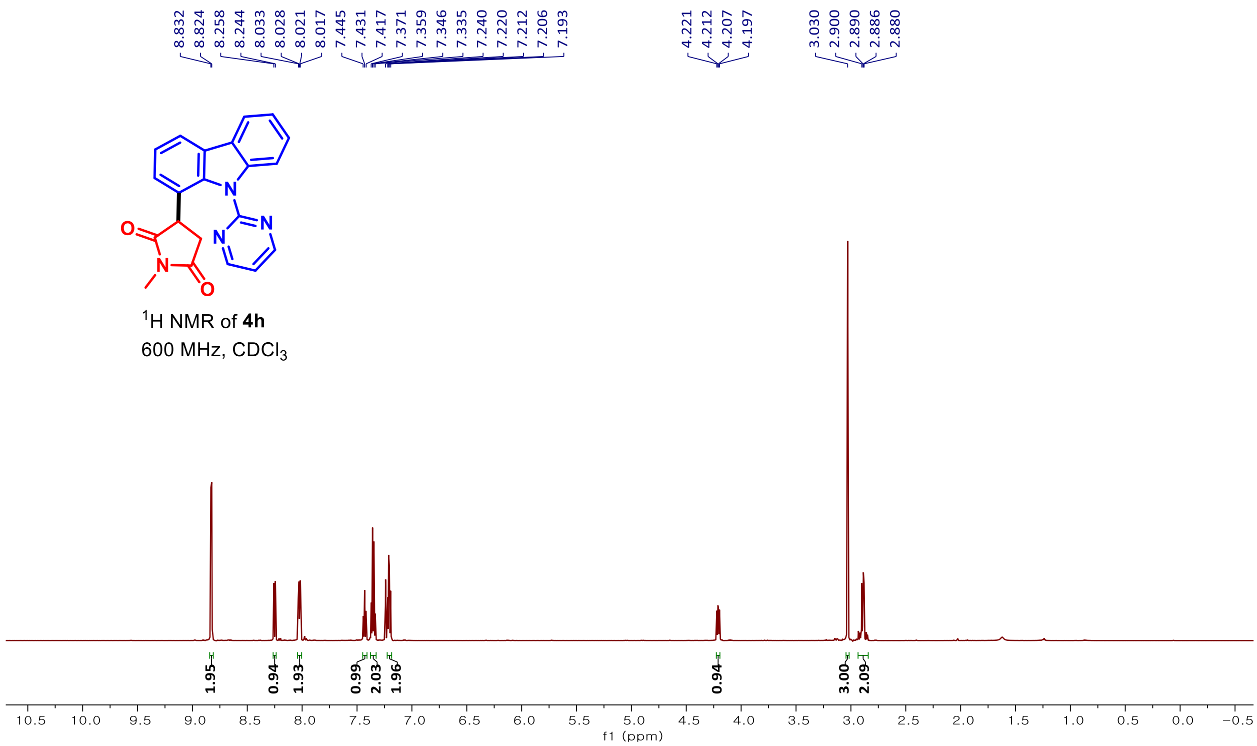



8.728
8.726
8.720
8.718
8.071
8.058
7.972
7.959
7.946
7.895
7.598
7.585
7.481
7.469
7.458
7.446
7.439
7.428
7.418
7.398
7.391
7.385
7.379
7.374
7.362
7.349
7.325
7.318
7.313
7.304
7.291
7.280
7.273
7.268
7.260
7.240
7.227
7.215
7.191
7.168
7.154
7.031
4.161
4.149
4.142
4.137
4.130
4.118
2.847
2.841
2.834
2.826
N
O
+
4f
4f'
^{1}H NMR 600 MHz, $CDCl_3$
1.94
1.96
2.00
1.94
2.01
6.35
3.19
7.31
3.22
0.97
1.97
4.06
6.24
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)

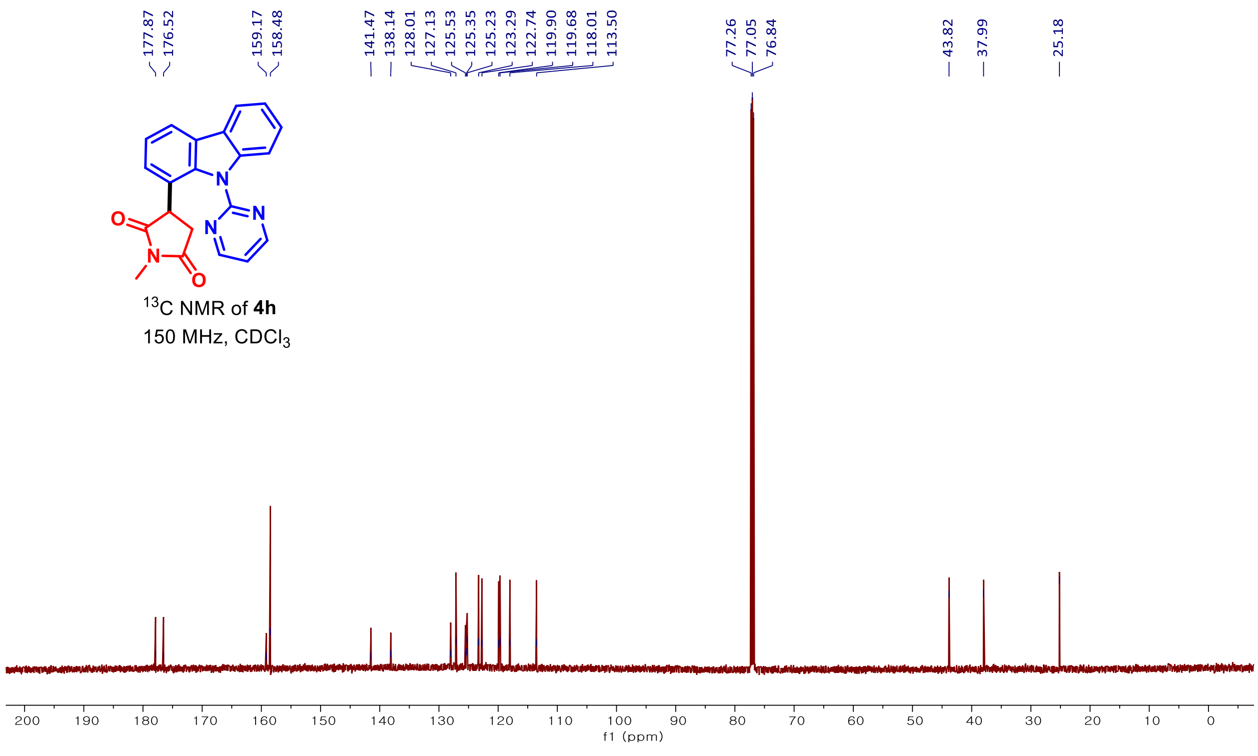

176.829
176.813
175.287
175.269
152.896
150.030
150.009
142.524
140.583
138.990
137.119
131.910
131.149
130.749
129.231
128.747
128.025
126.658
126.585
126.472
126.448
126.375
125.628
124.282
123.977
123.795
123.358
123.339
122.981
122.965
122.641
122.288
121.462
121.120
120.277
120.203
120.193
120.043
42.188
42.071
38.533
38.502
21.391
N
O
+
4f
4f'
^{13}C NMR of 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)


8.754
8.746
8.062
8.049
8.022
8.010
7.997
7.945
7.931
7.615
7.602
7.506
7.498
7.493
7.485
7.474
7.458
7.445
7.433
7.408
7.406
7.395
7.392
7.381
7.369
7.357
7.346
7.333
7.321
7.276
7.263
7.240
7.229
4.064
4.052
4.040
2.836
2.824
Br
N
N
O
N
O
^{1}H NMR of **4g**
600 MHz, $CDCl_3$
1.01
0.91
1.03
0.93
0.97
1.00
2.03
3.95
1.94
1.28
1.00
1.95
f1 (ppm)

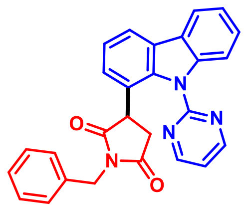

176.56
175.01
152.08
150.28
142.89
139.35
138.82
131.76
129.21
128.76
126.37
125.62
124.87
124.44
124.00
123.19
122.69
122.00
121.42
120.24
120.14
113.36
77.20
76.99
76.78
41.87
38.40
Br
N
N
O
N
O
^{13}C NMR of **4g**
150 MHz, $CDCl_3$
f1 (ppm)



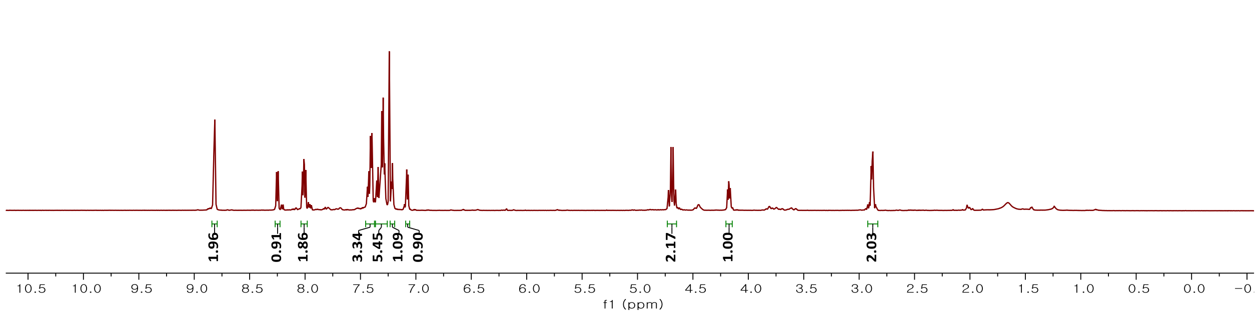
^{1}H NMR of **4h**
600 MHz, $CDCl_3$

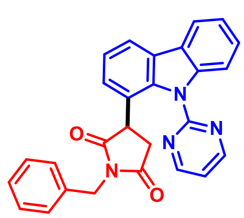


^{13}C NMR of **4h**
150 MHz, $CDCl_3$

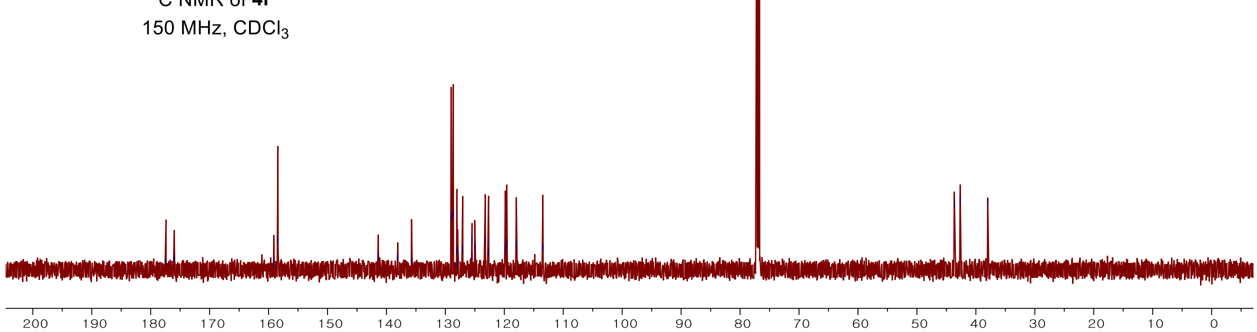


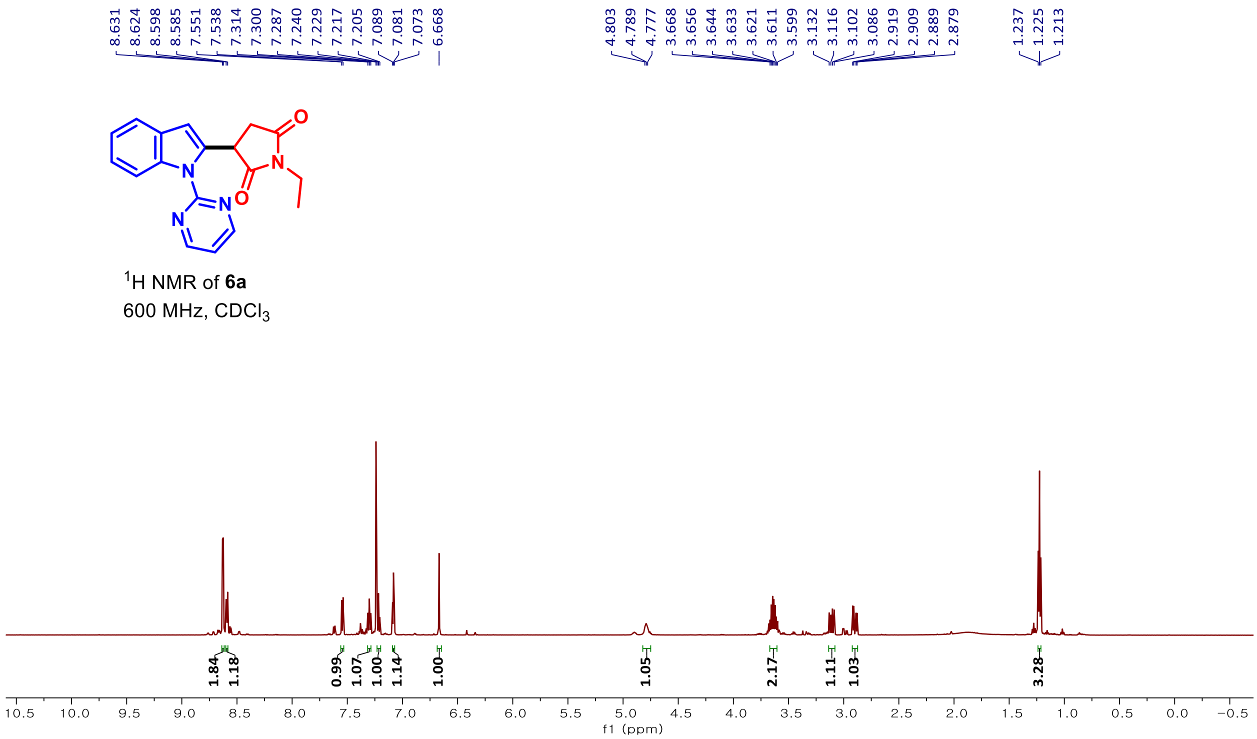
^{1}H NMR of **4i**
600 MHz, $CDCl_3$

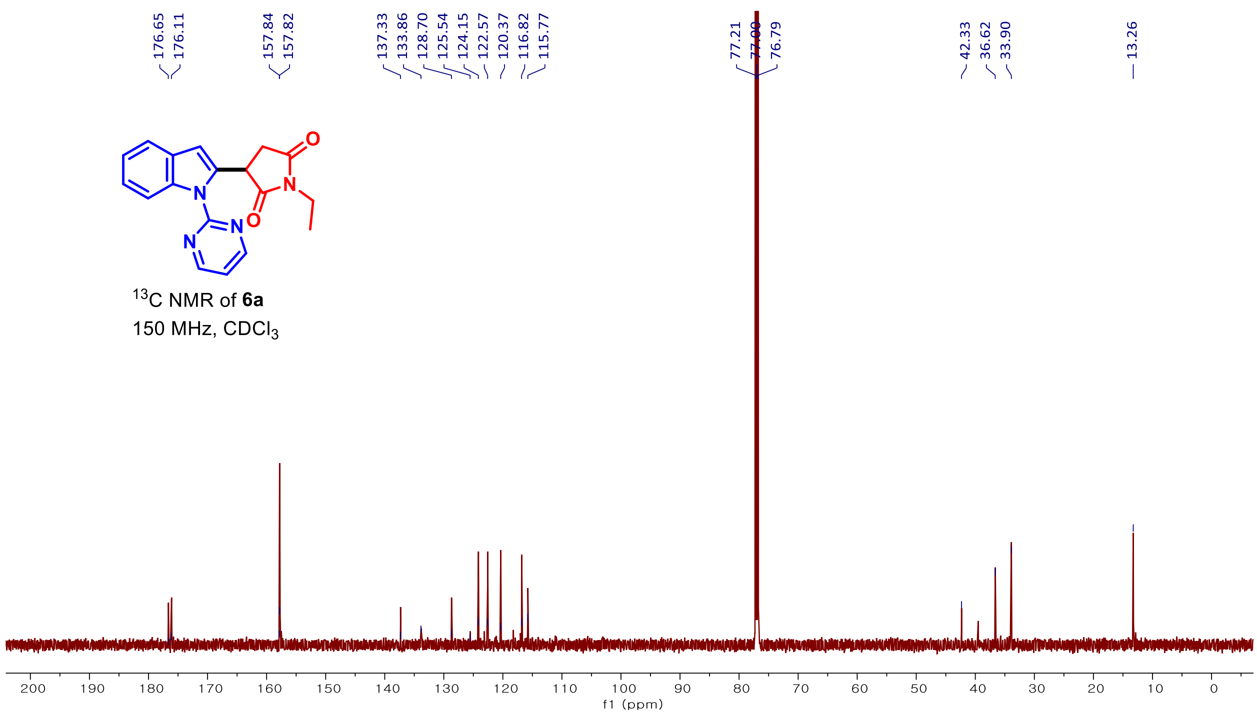


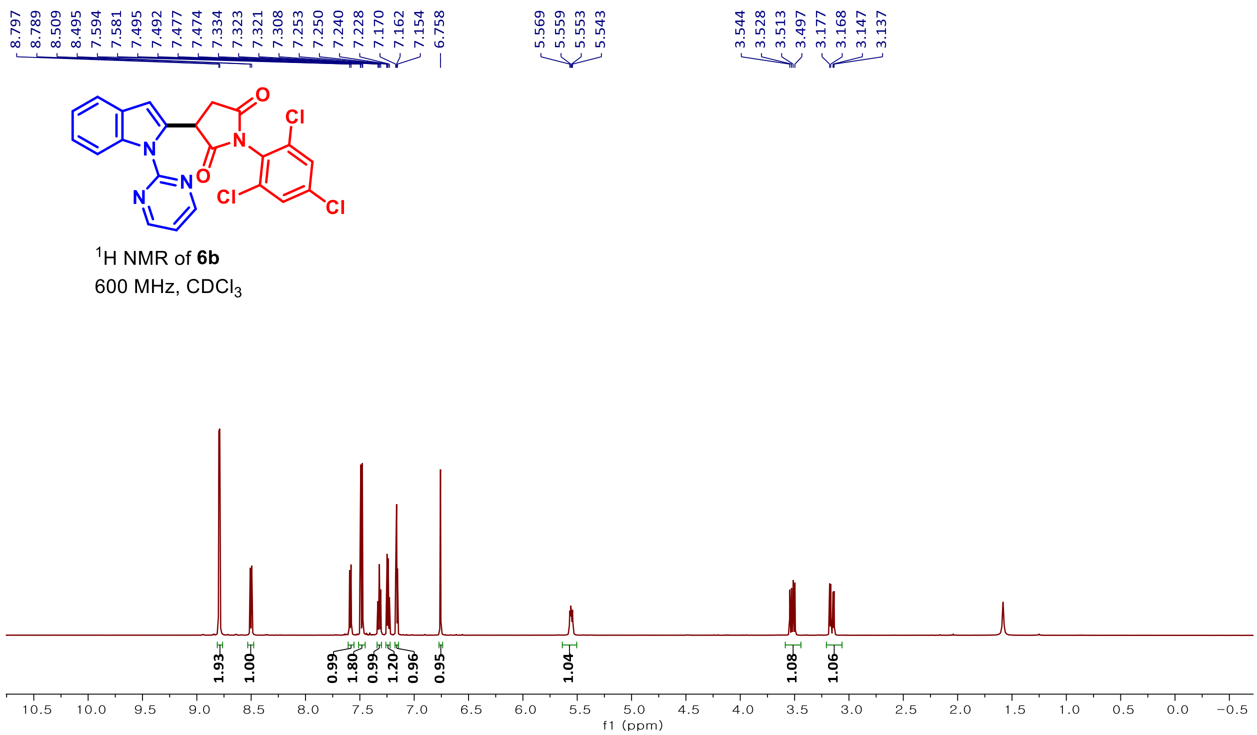


^{13}C NMR of **4i**
150 MHz, $CDCl_3$



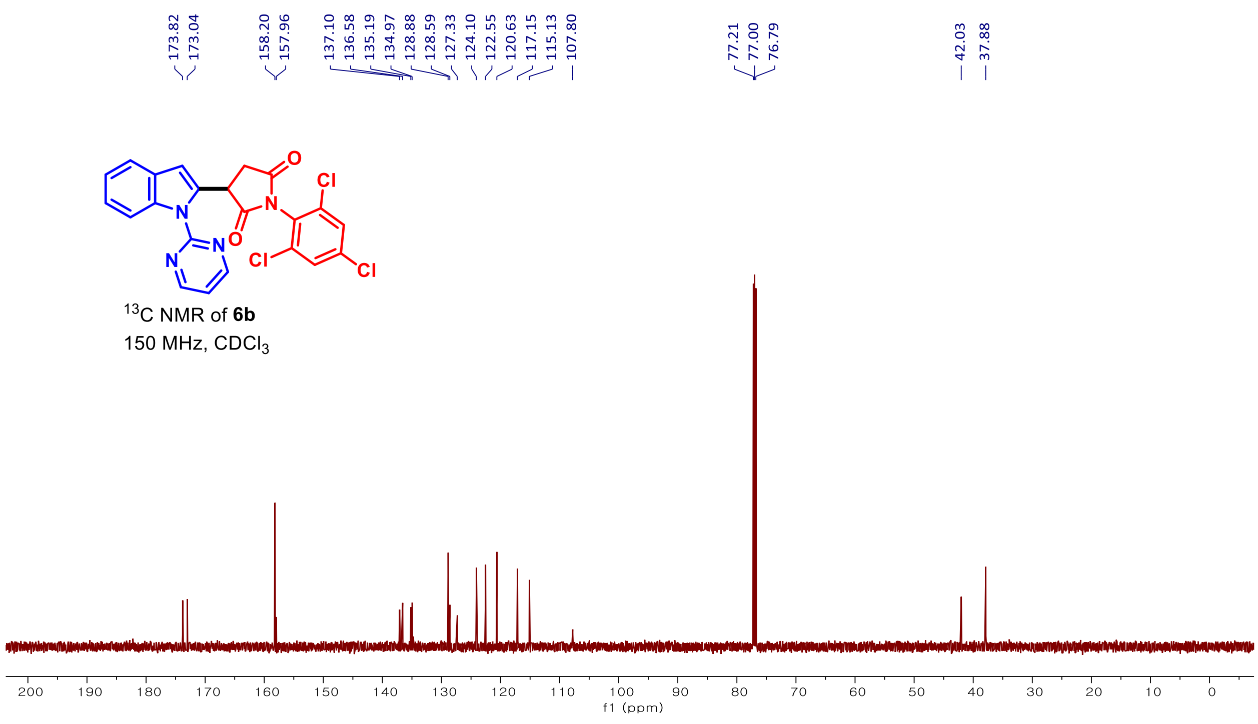

8.631
8.624
8.598
8.585
7.551
7.538
7.314
7.300
7.287
7.240
7.229
7.217
7.205
7.089
7.081
7.073
6.668
4.803
4.789
4.777
3.668
3.656
3.644
3.633
3.621
3.611
3.599
3.132
3.116
3.102
3.086
2.919
2.909
2.889
2.879
1.237
1.225
1.213
^{1}H NMR of **6a**
600 MHz, $CDCl_3$
1.84
1.18
0.99
1.07
1.00
1.14
1.00
1.05
2.17
1.11
1.03
3.28
f1 (ppm)


176.65
176.11
157.84
157.82
137.33
133.86
128.70
125.54
124.15
122.57
120.37
116.82
115.77
77.21
77.00
76.79
42.33
36.62
33.90
13.26
^{13}C NMR of **6a**
150 MHz, $CDCl_3$
f1 (ppm)



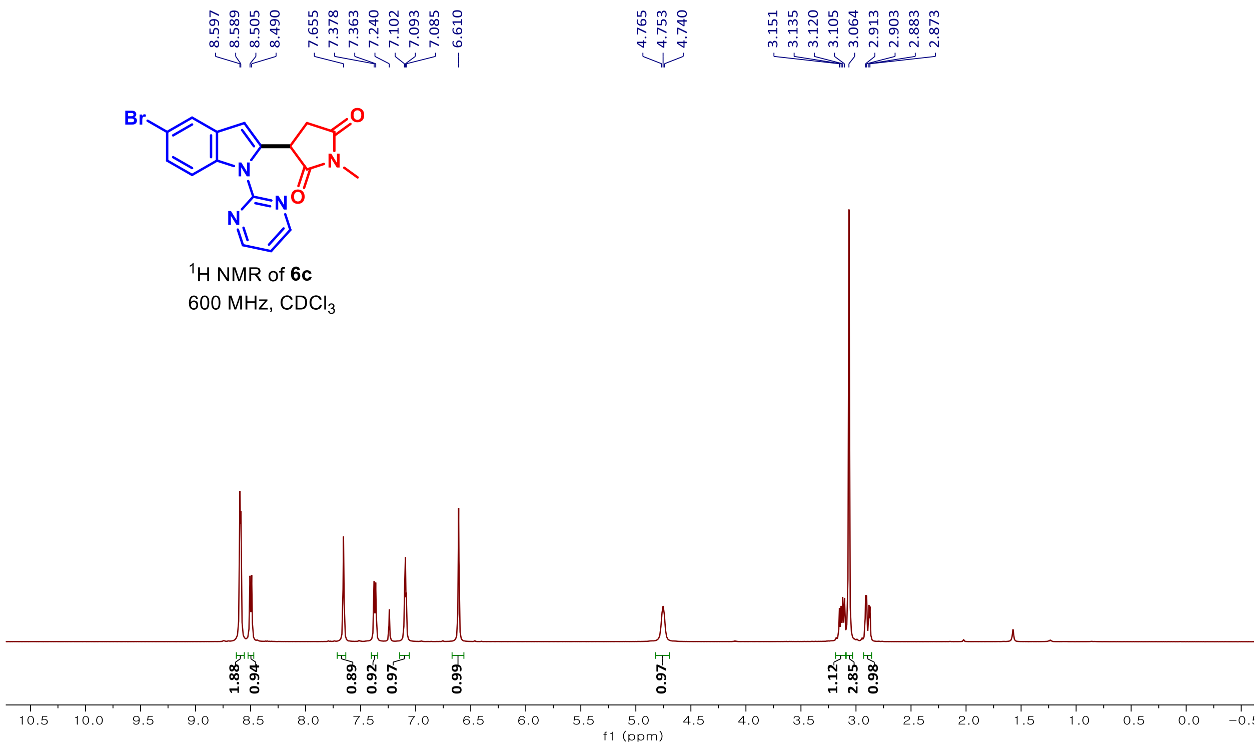
[1]H NMR of **6b**

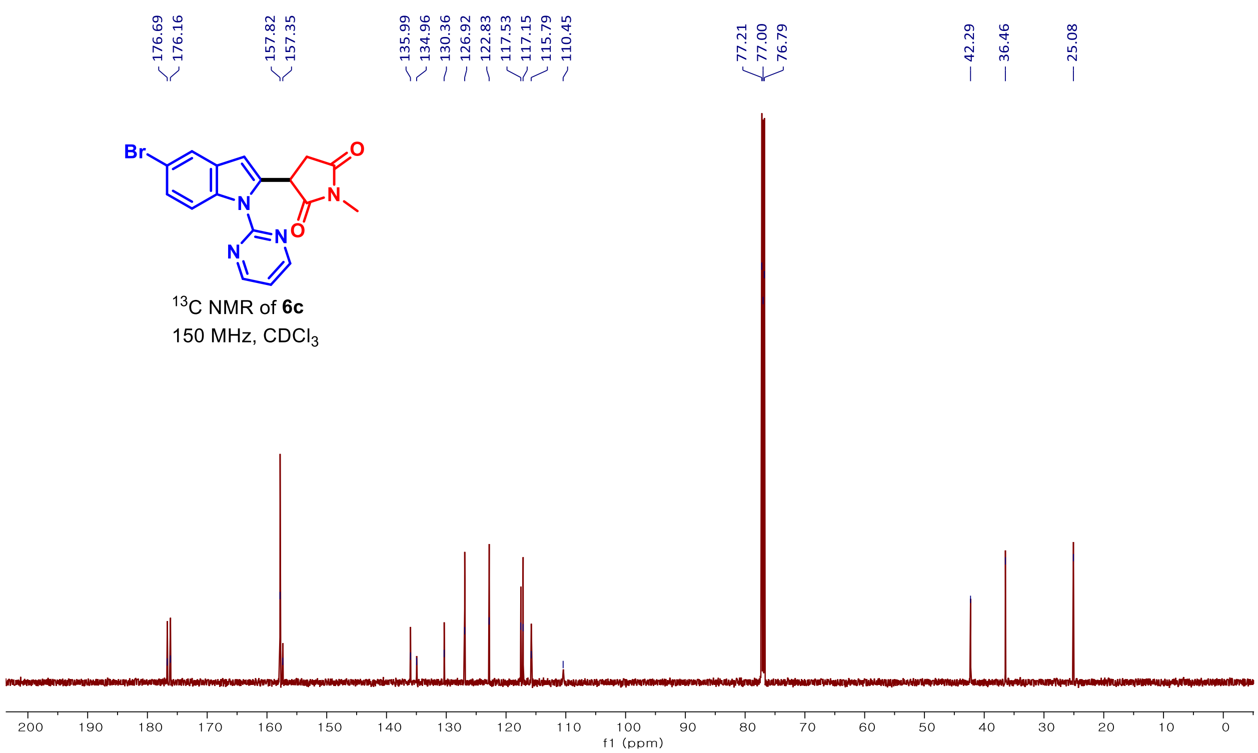
600 MHz, $CDCl_3$

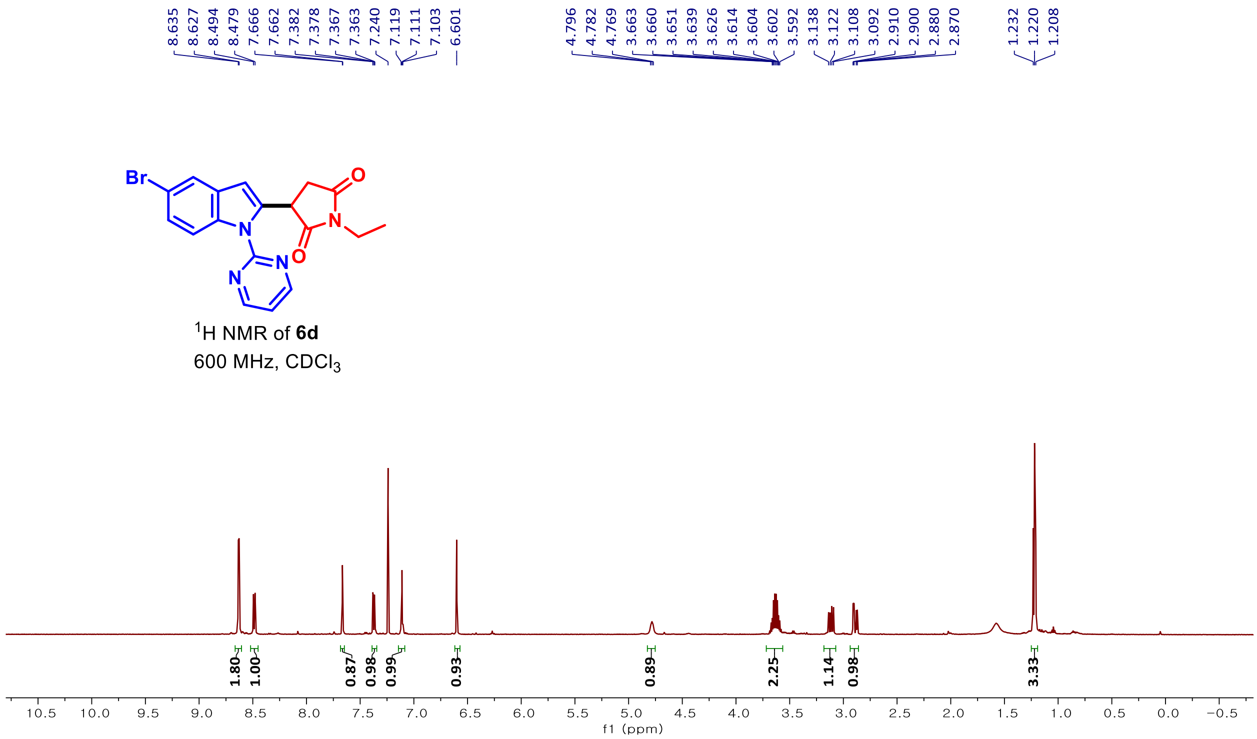


[13]C NMR of **6b**

150 MHz, $CDCl_3$

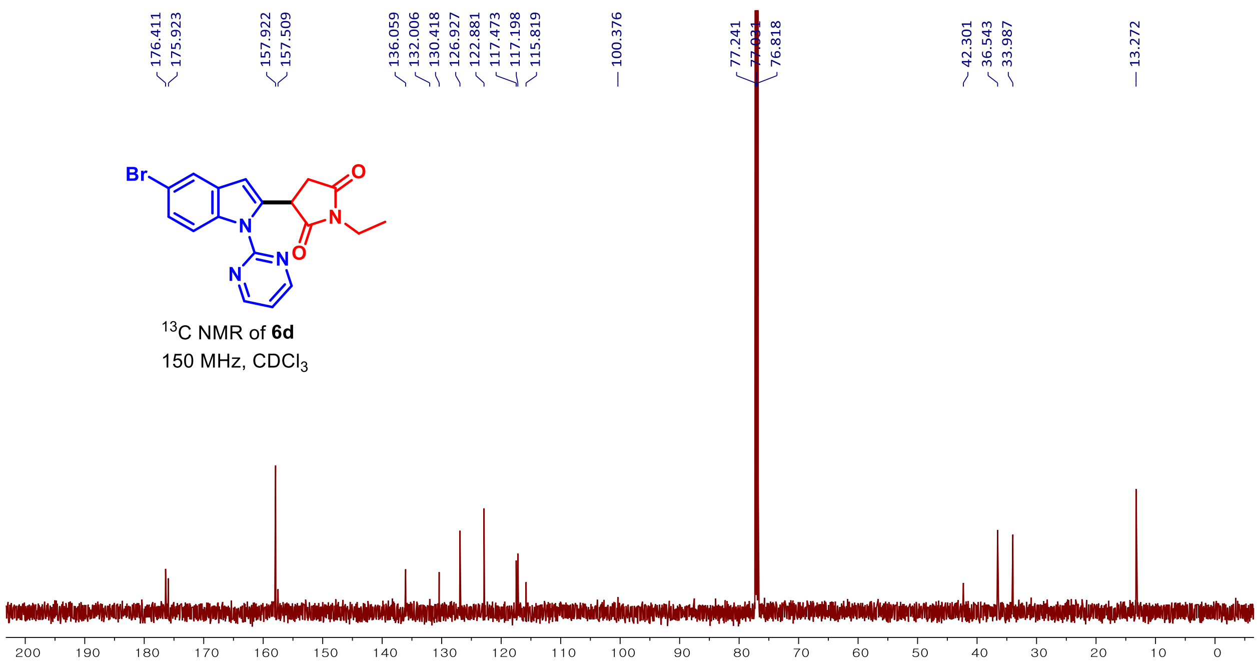

8.597
8.589
8.505
8.490
7.655
7.378
7.363
7.240
7.102
7.093
7.085
6.610
4.765
4.753
4.740
3.151
3.135
3.120
3.105
3.064
2.913
2.903
2.883
2.873
Br
O
N
N
O
N
N
1H NMR of 6c
600 MHz, CDCl3
1.88
0.94
0.89
0.92
0.97
0.99
0.97
1.12
2.85
0.98
f1 (ppm)


176.69
176.16
157.82
157.35
135.99
134.96
130.36
126.92
122.83
117.53
117.15
115.79
110.45
77.21
77.00
76.79
42.29
36.46
25.08
Br
O
N
N
O
N
N
13C NMR of 6c
150 MHz, CDCl3
f1 (ppm)



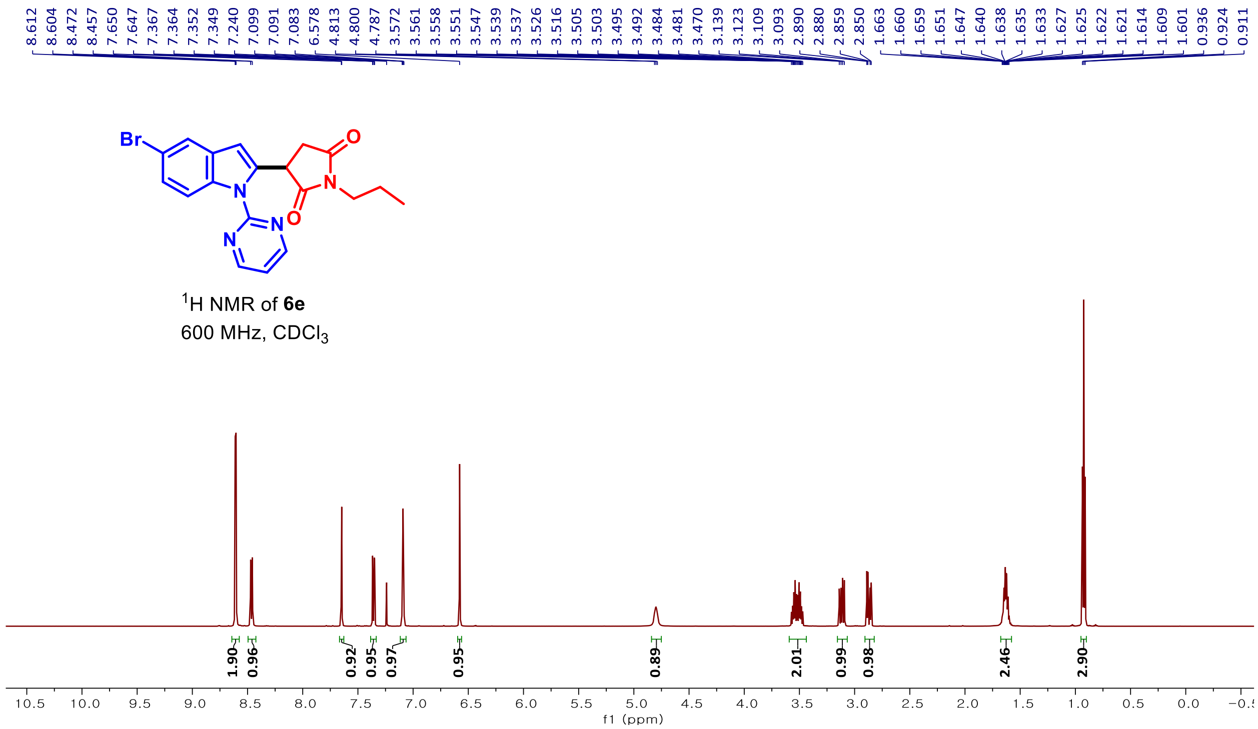
^{1}H NMR of **6d**

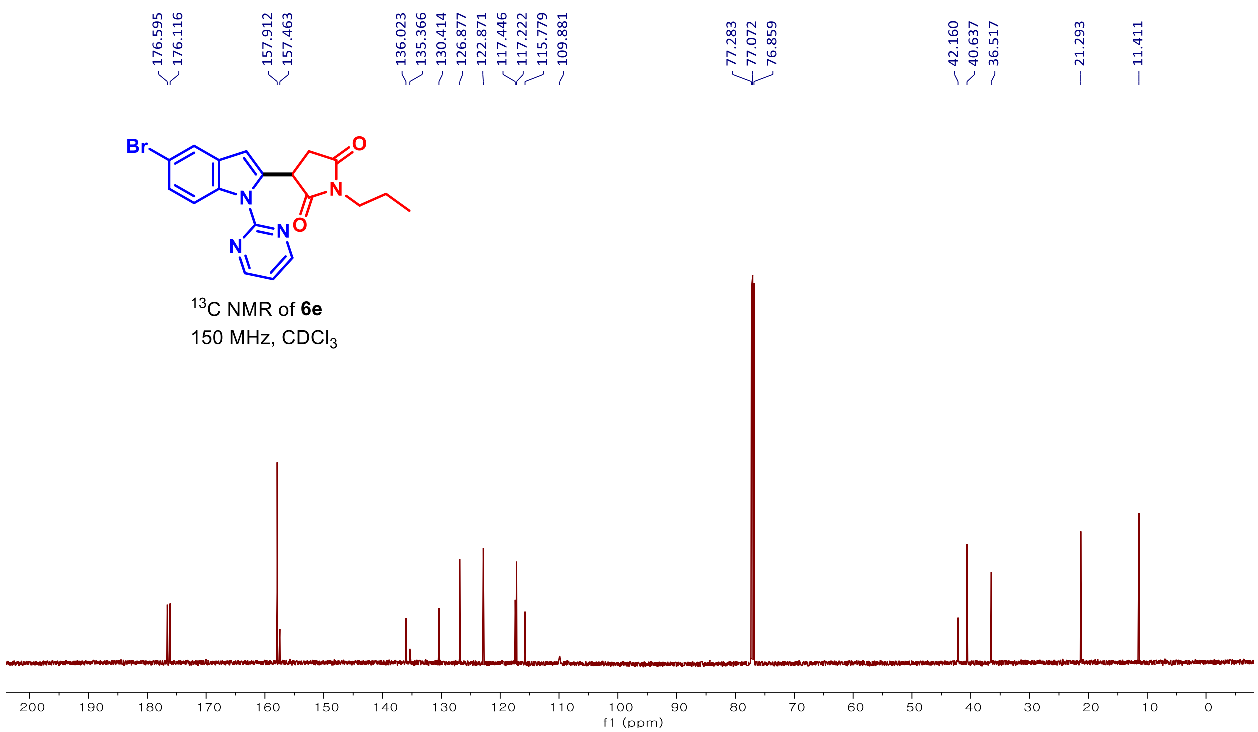
600 MHz, $CDCl_3$

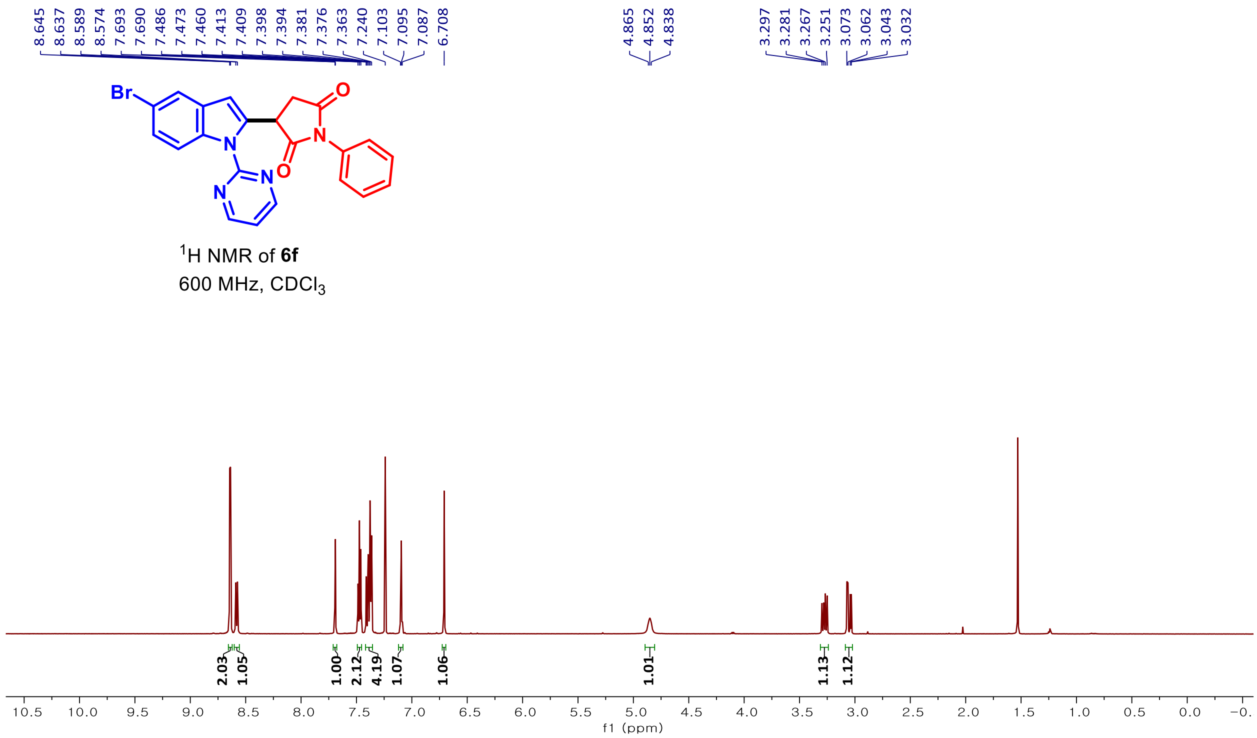


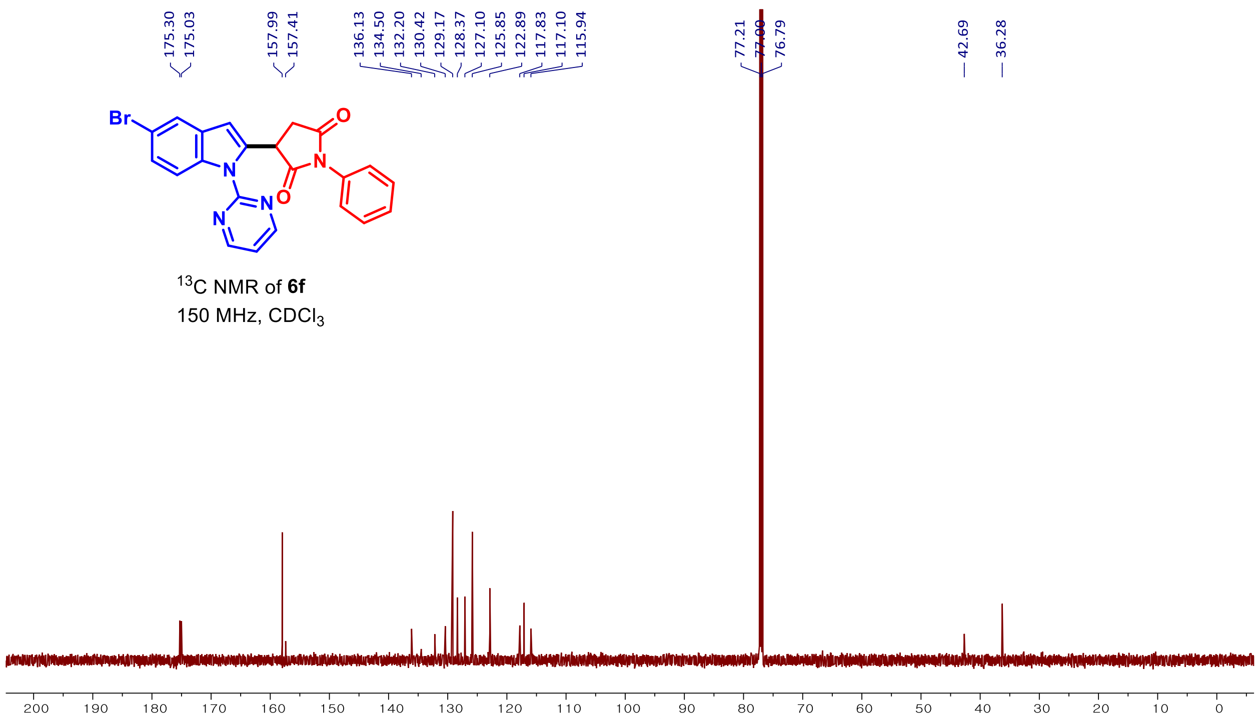
^{13}C NMR of **6d**

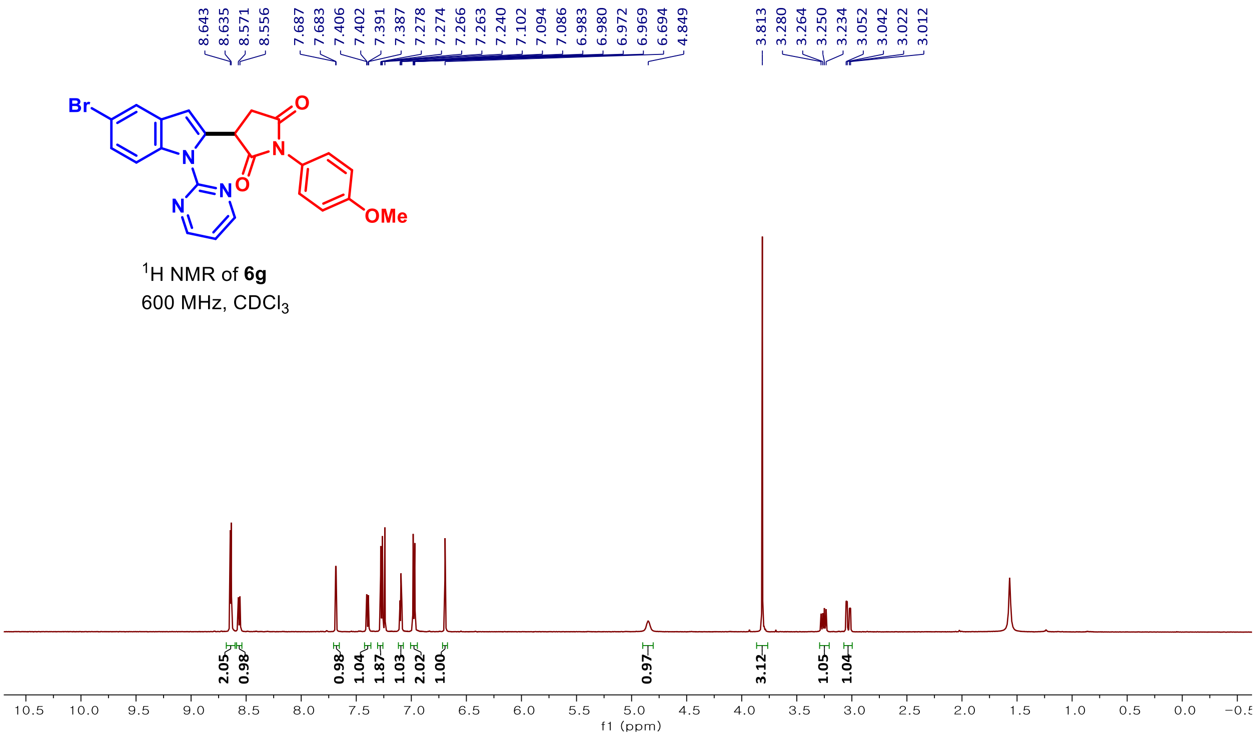
150 MHz, $CDCl_3$

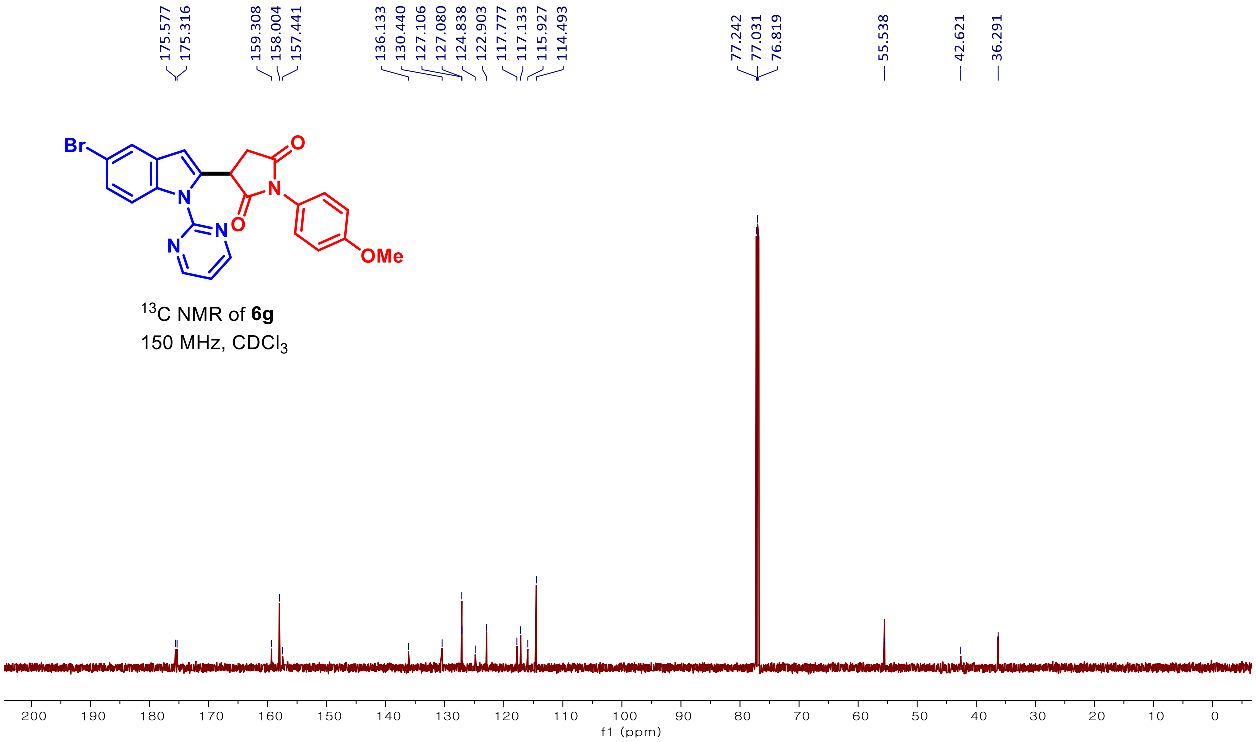

8.612 8.604 8.472 8.457 7.650 7.647 7.367 7.364 7.352 7.349 7.240 7.099 7.091 7.083 6.578 4.813 4.800 4.787 3.572 3.561 3.558 3.551 3.547 3.539 3.537 3.526 3.516 3.505 3.503 3.495 3.492 3.484 3.481 3.470 3.139 3.123 3.109 3.093 2.890 2.880 2.859 2.850 1.663 1.660 1.659 1.651 1.647 1.640 1.638 1.635 1.633 1.627 1.625 1.622 1.621 1.614 1.609 1.601 0.936 0.924 0.911
Br
N
O
N
N
N
O
^{1}H NMR of **6e**
600 MHz, $CDCl_3$
1.90 0.96 0.92 0.95 0.97 0.95 0.89 2.01 0.99 0.98 2.46 2.90
f1 (ppm)

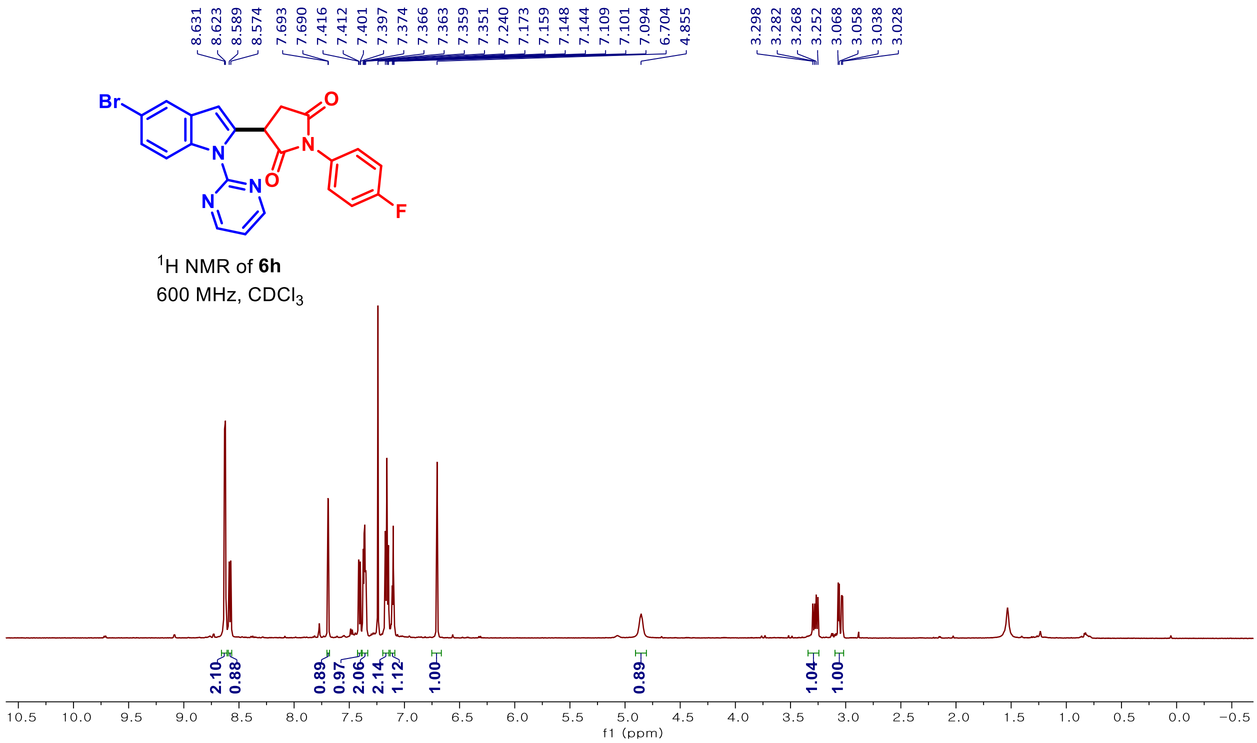

176.595 176.116 157.912 157.463 136.023 135.366 130.414 126.877 122.871 117.446 117.222 115.779 109.881 77.283 77.072 76.859 42.160 40.637 36.517 21.293 11.411
Br
N
O
N
N
N
O
^{13}C NMR of **6e**
150 MHz, $CDCl_3$
f1 (ppm)


8.645
8.637
8.589
8.574
7.693
7.690
7.486
7.473
7.460
7.413
7.409
7.398
7.394
7.381
7.376
7.363
7.240
7.103
7.095
7.087
6.708
4.865
4.852
4.838
3.297
3.281
3.267
3.251
3.073
3.062
3.043
3.032
Br
N
N
N
O
N
O
^{1}H NMR of **6f**
600 MHz, $CDCl_3$
2.03
1.05
1.00
2.12
4.19
1.07
1.06
1.01
1.13
1.12
f1 (ppm)

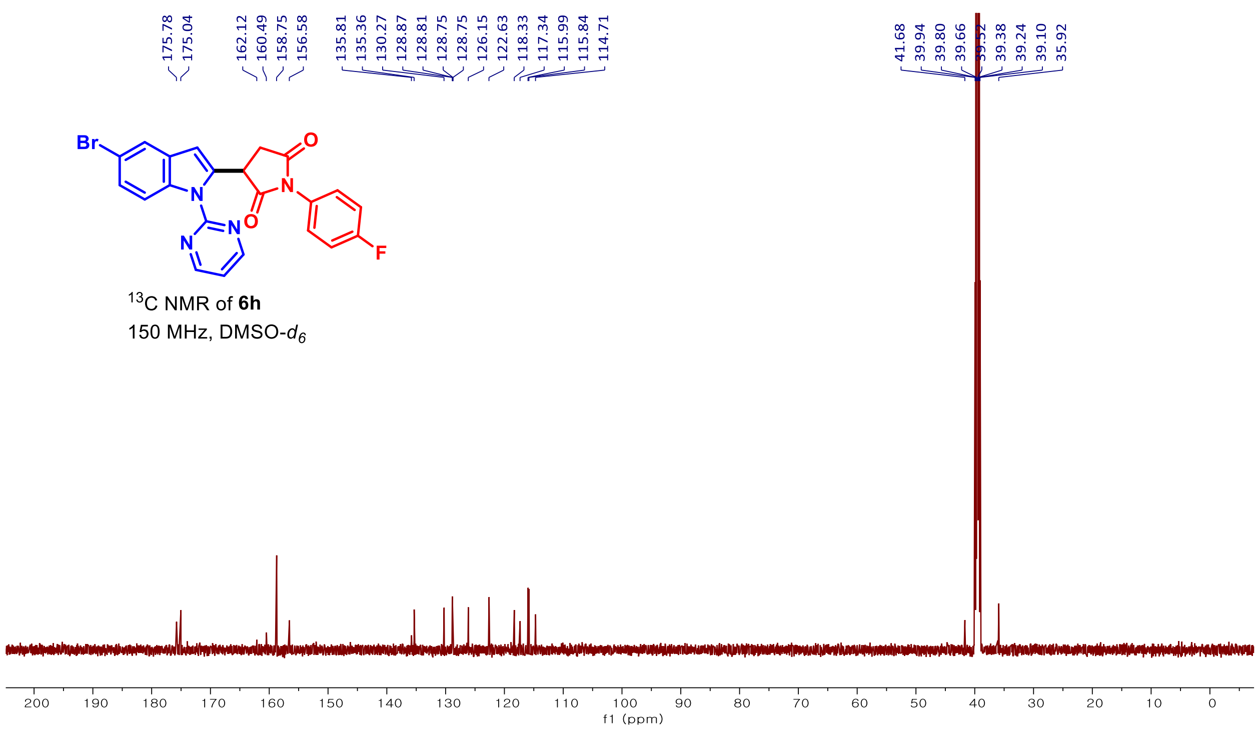

175.30
175.03
157.99
157.41
136.13
134.50
132.20
130.42
129.17
128.37
127.10
125.85
122.89
117.83
117.10
115.94
77.21
77.00
76.79
42.69
36.28
Br
N
N
N
O
N
O
^{13}C NMR of **6f**
150 MHz, $CDCl_3$
f1 (ppm)


8.643
8.635
8.571
8.556
7.687
7.683
7.406
7.402
7.391
7.387
7.278
7.274
7.266
7.263
7.240
7.102
7.094
7.086
6.983
6.980
6.972
6.969
6.694
4.849
3.813
3.280
3.264
3.250
3.234
3.052
3.042
3.022
3.012
Br
N
N
N
O
O
N
OMe
^{1}H NMR of **6g**
600 MHz, $CDCl_3$
2.05
0.98
0.98
1.04
1.87
1.03
2.02
1.00
0.97
3.12
1.05
1.04
f1 (ppm)

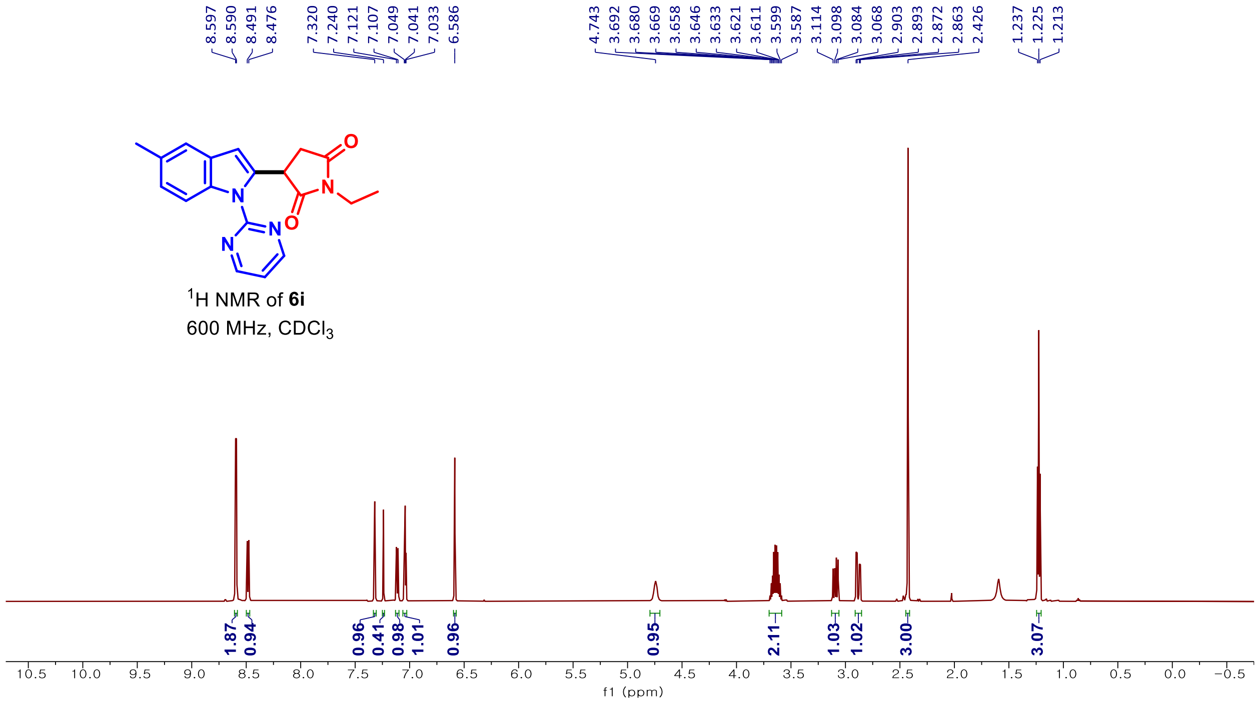

175.577
175.316
159.308
158.004
157.441
136.133
130.440
127.106
127.080
124.838
122.903
117.777
117.133
115.927
114.493
77.242
77.031
76.819
55.538
42.621
36.291
Br
N
N
N
O
O
N
OMe
^{13}C NMR of **6g**
150 MHz, $CDCl_3$
f1 (ppm)

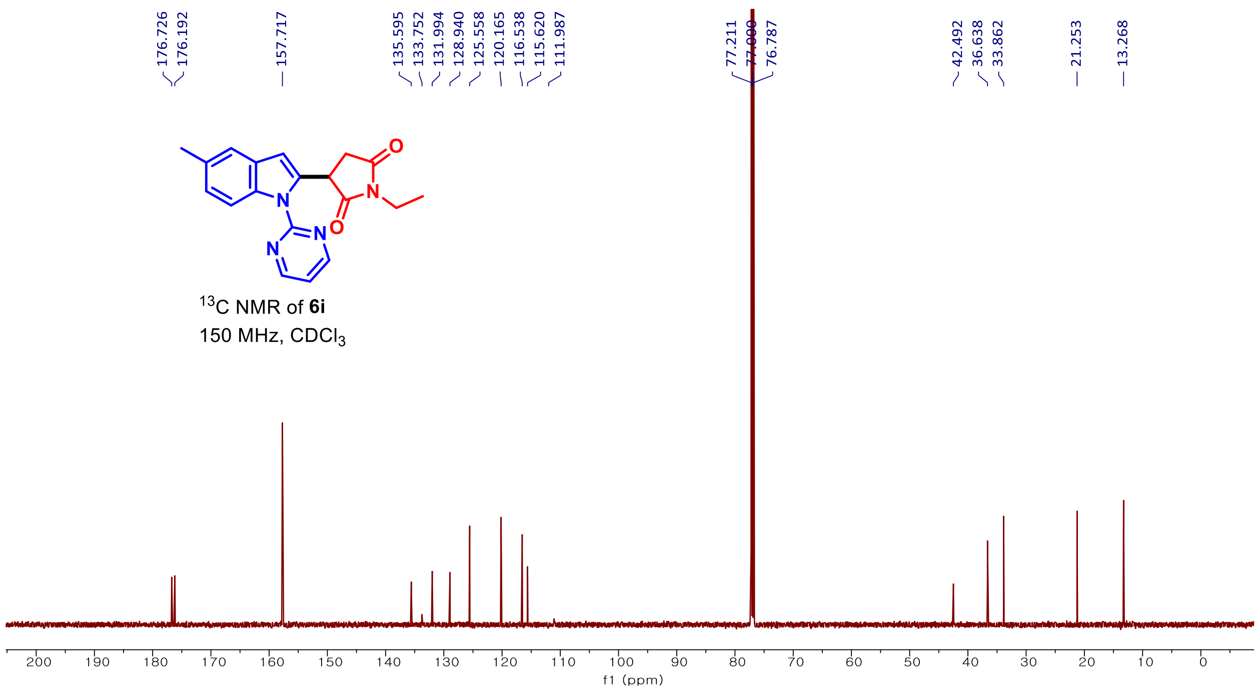


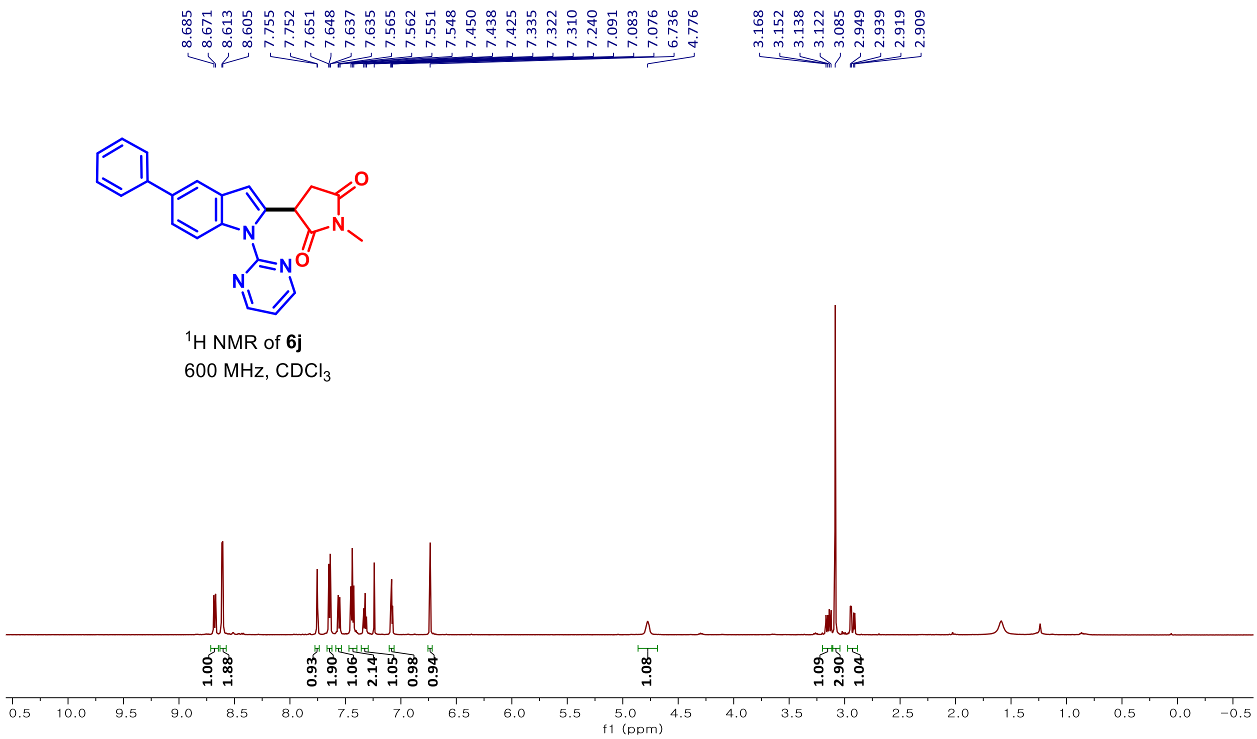
^{1}H NMR of **6h**
600 MHz, $CDCl_3$

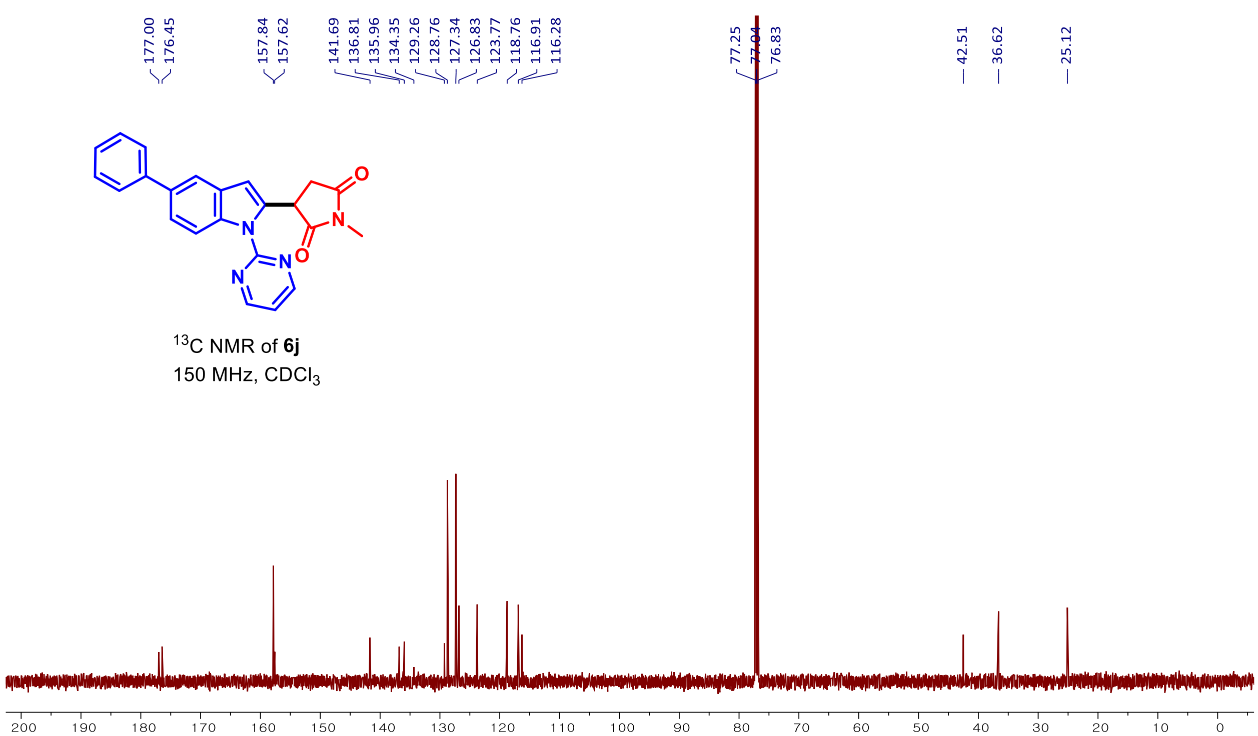


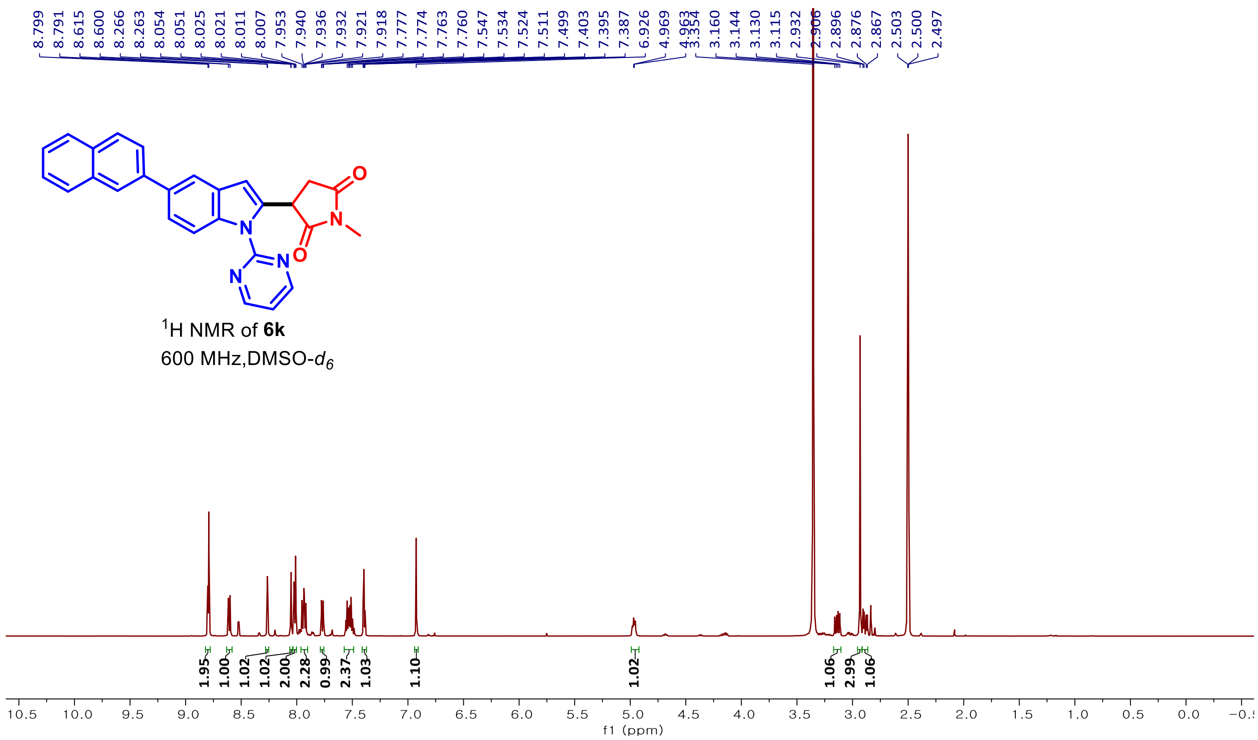
^{13}C NMR of **6h**
150 MHz, DMSO-d_6

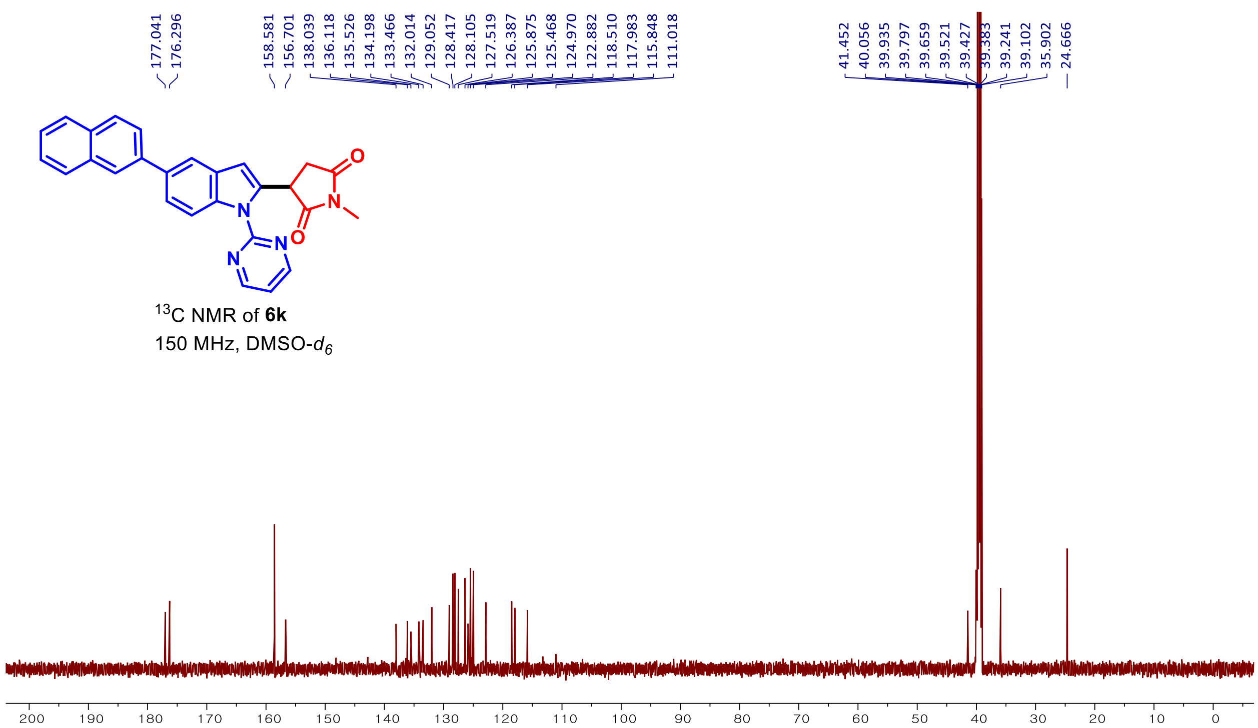

8.597
8.590
8.491
8.476
7.320
7.240
7.121
7.107
7.049
7.041
7.033
6.586
4.743
3.692
3.680
3.669
3.658
3.646
3.633
3.621
3.611
3.599
3.587
3.114
3.098
3.084
3.068
2.903
2.893
2.872
2.863
2.426
1.237
1.225
1.213
O
N
N
N
N
O
1H NMR of 6i
600 MHz, CDCl3
1.87
0.94
0.96
0.41
0.98
1.01
0.96
0.95
2.11
1.03
1.02
3.00
3.07
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)

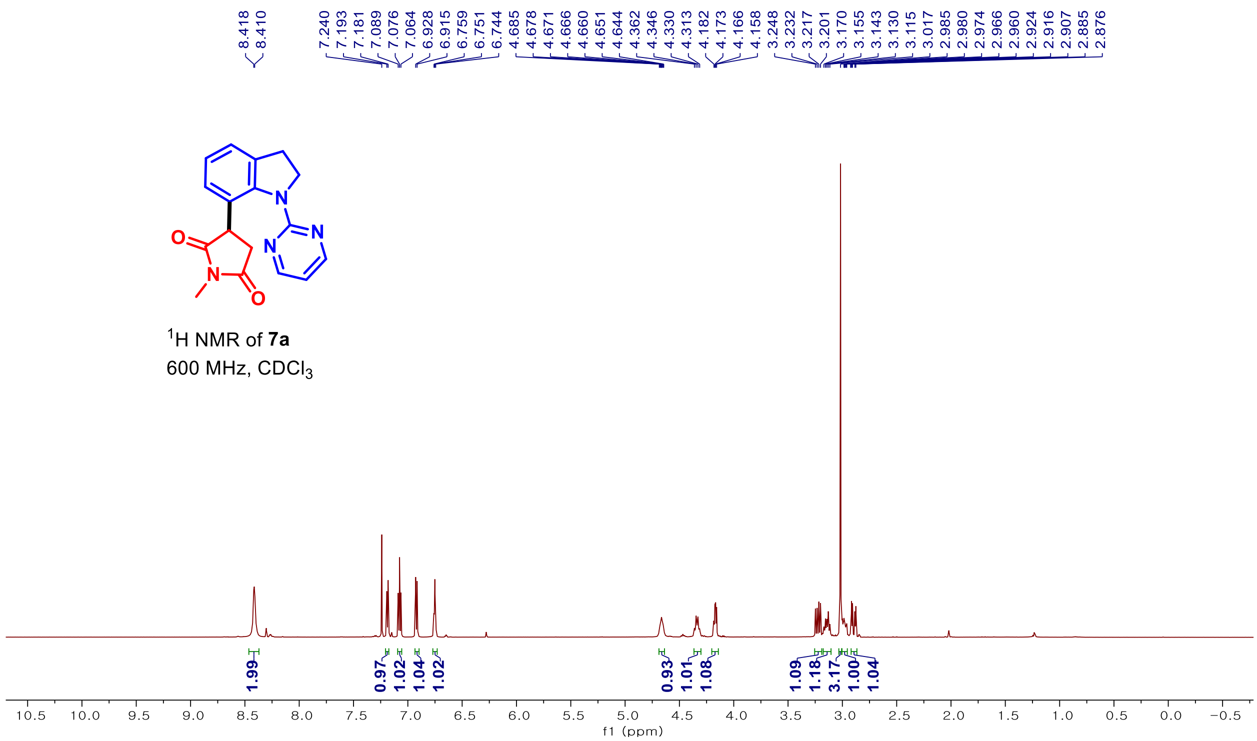

176.726
176.192
157.717
135.595
133.752
131.994
128.940
125.558
120.165
116.538
115.620
111.987
77.211
77.000
76.787
42.492
36.638
33.862
21.253
13.268
O
N
N
N
N
O
13C NMR of 6i
150 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

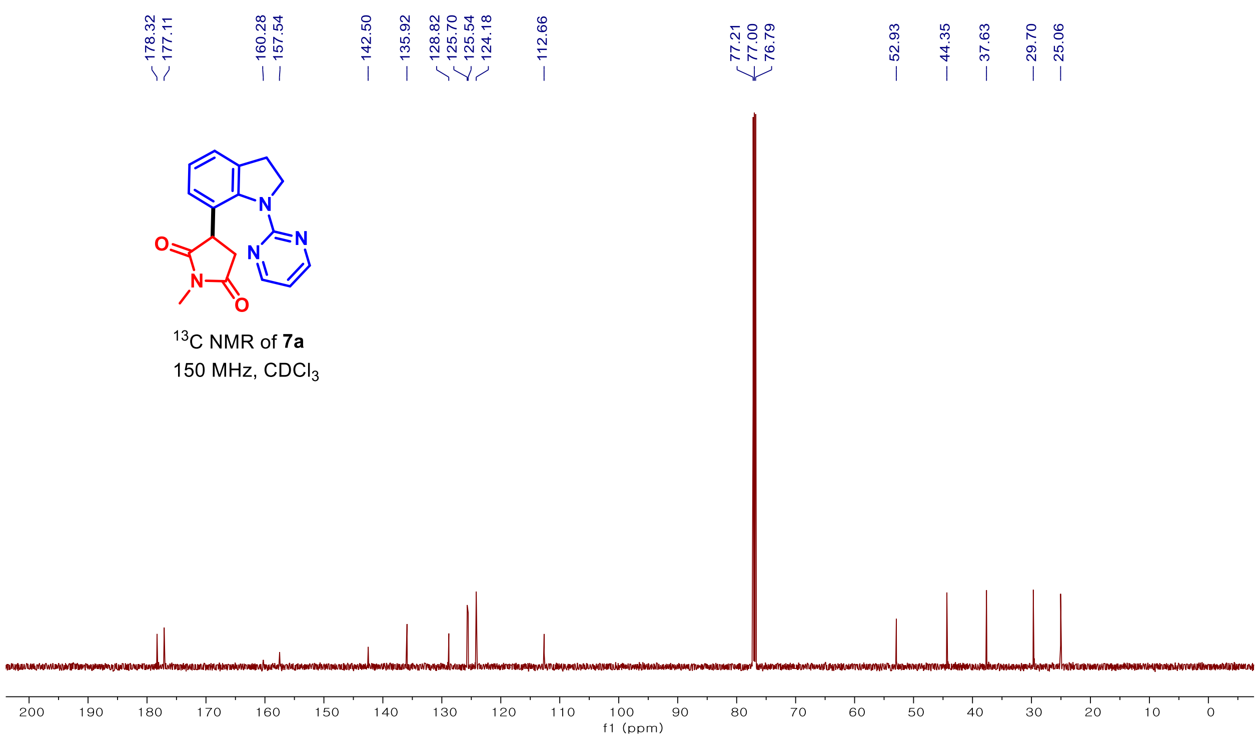

8.685 8.671 8.613 8.605 7.755 7.752 7.651 7.648 7.637 7.635 7.565 7.562 7.551 7.548 7.450 7.438 7.425 7.335 7.322 7.310 7.240 7.091 7.083 7.076 6.736 4.776
3.168 3.152 3.138 3.122 3.085 2.949 2.939 2.919 2.909
N
N
N
O
O
N
^{1}H NMR of **6j**
600 MHz, $CDCl_3$
1.00 1.88 0.93 1.90 1.06 2.14 1.05 0.98 0.94 1.08 1.09 2.90 1.04
0.5 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)

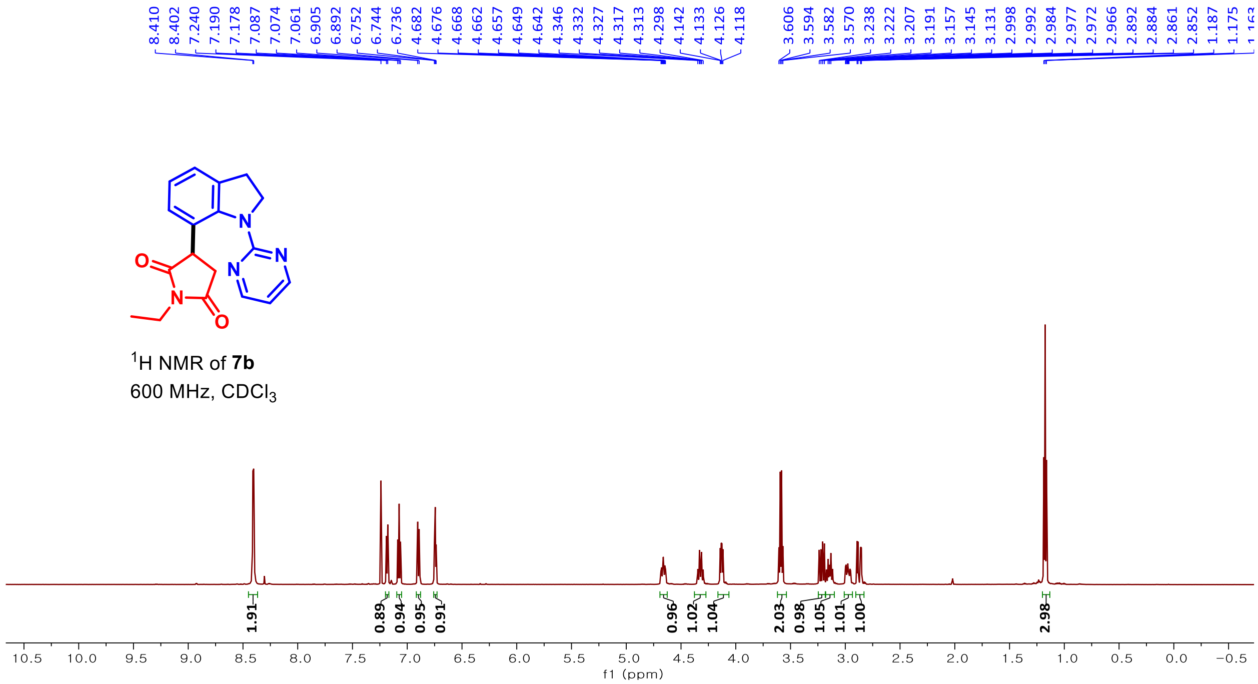

177.00 176.45 157.84 157.62 141.69 136.81 135.96 134.35 129.26 128.76 127.34 126.83 123.77 118.76 116.91 116.28 77.25 77.04 76.83 42.51 36.62 25.12
N
N
N
O
O
N
^{13}C NMR of **6j**
150 MHz, $CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

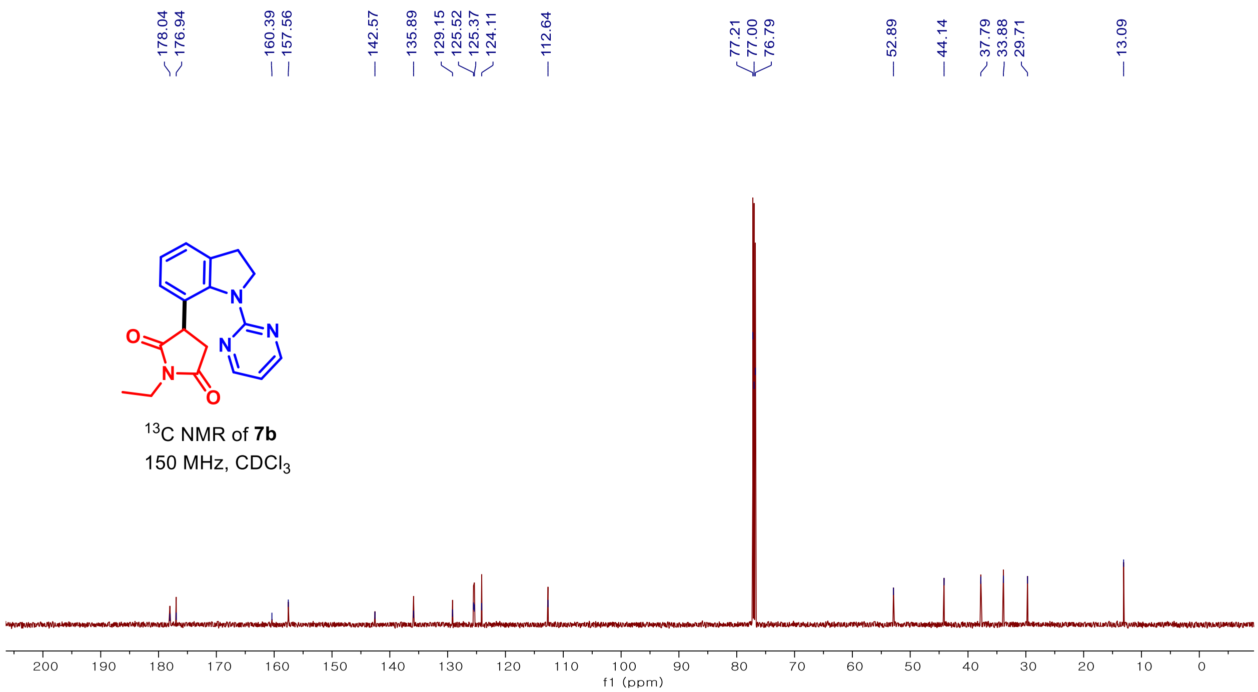

8.799
8.791
8.615
8.600
8.266
8.263
8.054
8.051
8.025
8.021
8.011
8.007
7.953
7.940
7.936
7.932
7.921
7.918
7.777
7.774
7.763
7.760
7.547
7.534
7.524
7.511
7.499
7.403
7.395
7.387
6.926
4.969
4.963
3.354
3.160
3.144
3.130
3.115
2.932
2.906
2.896
2.876
2.867
2.503
2.500
2.497
N
N
N
O
O
N
[1]H NMR of 6k
600 MHz,DMSO-d6
1.95
1.00
1.02
1.02
2.00
2.28
0.99
2.37
1.03
1.10
1.02
1.06
2.99
1.06
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)

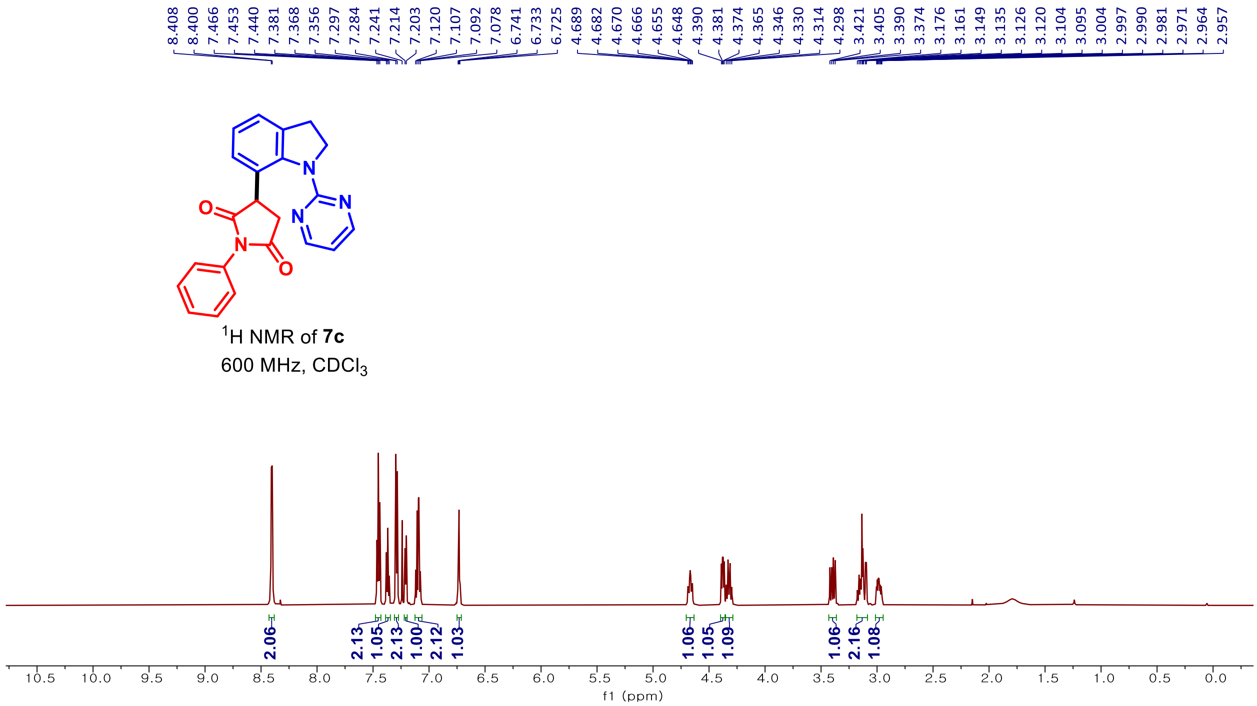

177.041
176.296
158.581
156.701
138.039
136.118
135.526
134.198
133.466
132.014
129.052
128.417
128.105
127.519
126.387
125.875
125.468
124.970
122.882
118.510
117.983
115.848
111.018
41.452
40.056
39.935
39.797
39.659
39.521
39.427
39.383
39.241
39.102
35.902
24.666
N
N
N
O
O
N
[13]C NMR of 6k
150 MHz, DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.418
8.410
7.240
7.193
7.181
7.089
7.076
7.064
6.928
6.915
6.759
6.751
6.744
4.685
4.678
4.671
4.666
4.660
4.651
4.644
4.362
4.346
4.330
4.313
4.182
4.173
4.166
4.158
3.248
3.232
3.217
3.201
3.170
3.155
3.143
3.130
3.115
3.017
2.985
2.980
2.974
2.966
2.960
2.924
2.916
2.907
2.885
2.876
N
N
N
O
N
O
1H NMR of 7a
600 MHz, CDCl3
1.99
0.97
1.02
1.04
1.02
0.93
1.01
1.08
1.09
1.18
3.17
1.00
1.04
f1 (ppm)

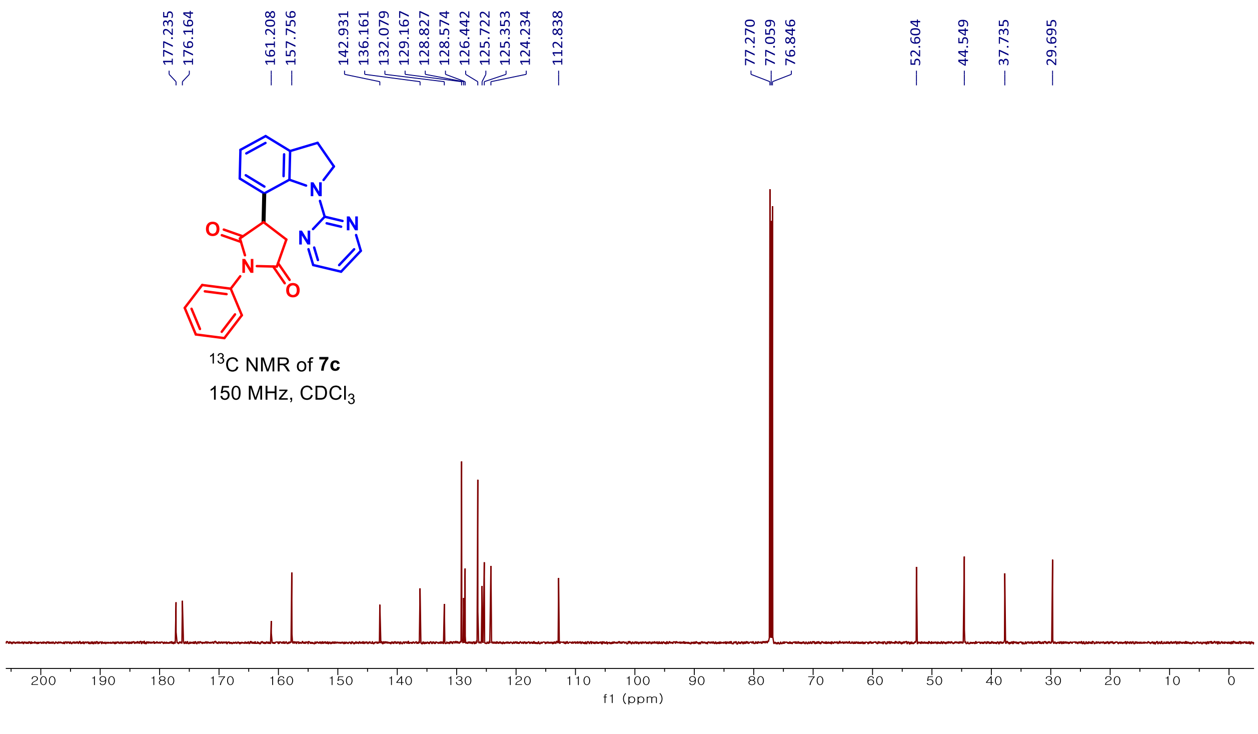

178.32
177.11
160.28
157.54
142.50
135.92
128.82
125.70
125.54
124.18
112.66
77.21
77.00
76.79
52.93
44.35
37.63
29.70
25.06
N
N
N
O
N
O
13C NMR of 7a
150 MHz, CDCl3
f1 (ppm)


8.410
8.402
7.240
7.190
7.178
7.087
7.074
7.061
6.905
6.892
6.752
6.744
6.736
4.682
4.676
4.668
4.662
4.657
4.649
4.642
4.346
4.332
4.327
4.317
4.313
4.298
4.142
4.133
4.126
4.118
3.606
3.594
3.582
3.570
3.238
3.222
3.207
3.191
3.157
3.145
3.131
2.998
2.992
2.984
2.977
2.972
2.966
2.892
2.884
2.861
2.852
1.187
1.175
N
O
N
O
N
N
^{1}H NMR of **7b**
600 MHz, $CDCl_3$
1.91
0.89
0.94
0.95
0.91
0.96
1.02
1.04
2.03
0.98
1.05
1.01
1.00
2.98
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)

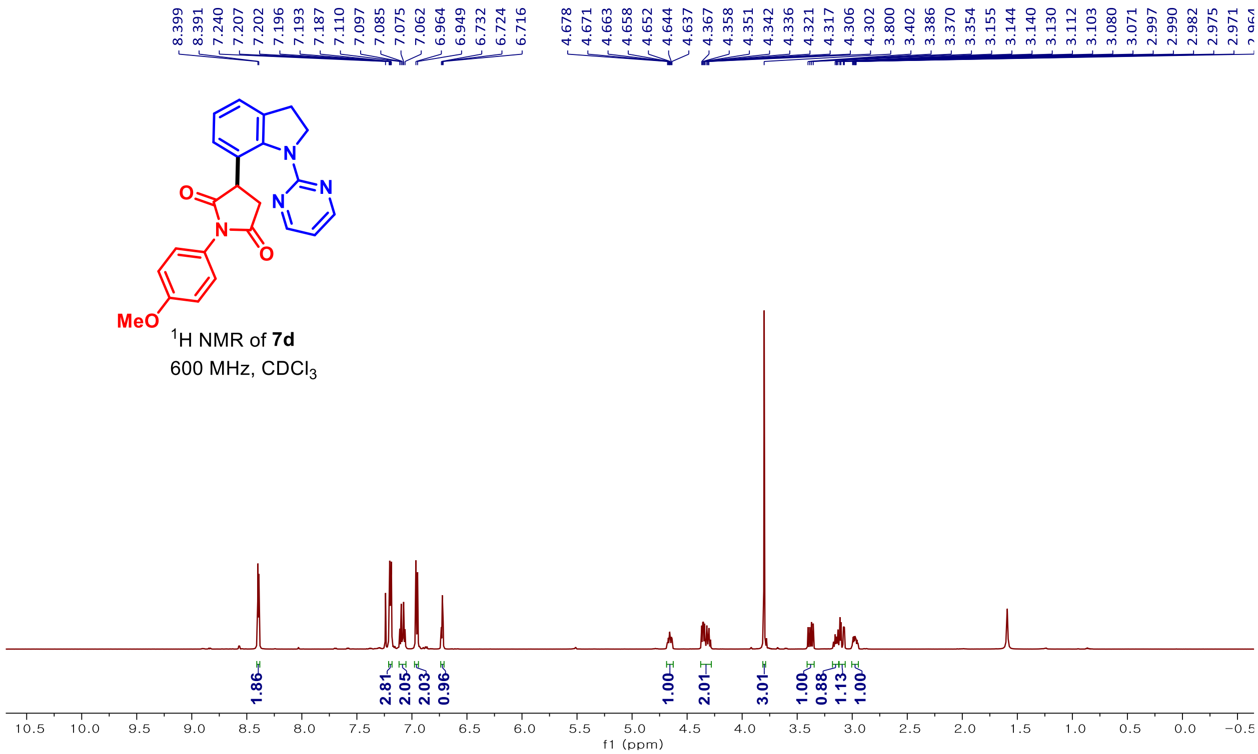

178.04
176.94
160.39
157.56
142.57
135.89
129.15
125.52
125.37
124.11
112.64
77.21
77.00
76.79
52.89
44.14
37.79
33.88
29.71
13.09
N
O
N
O
N
N
^{13}C NMR of **7b**
150 MHz, $CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

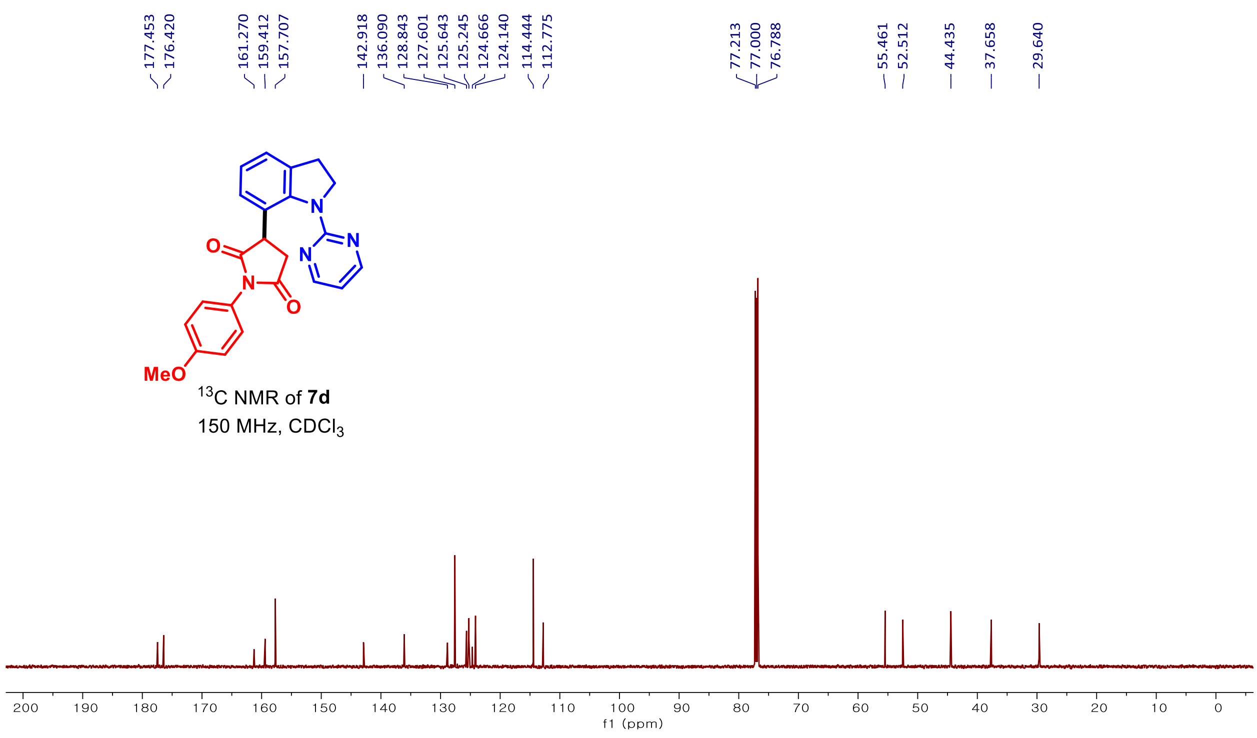


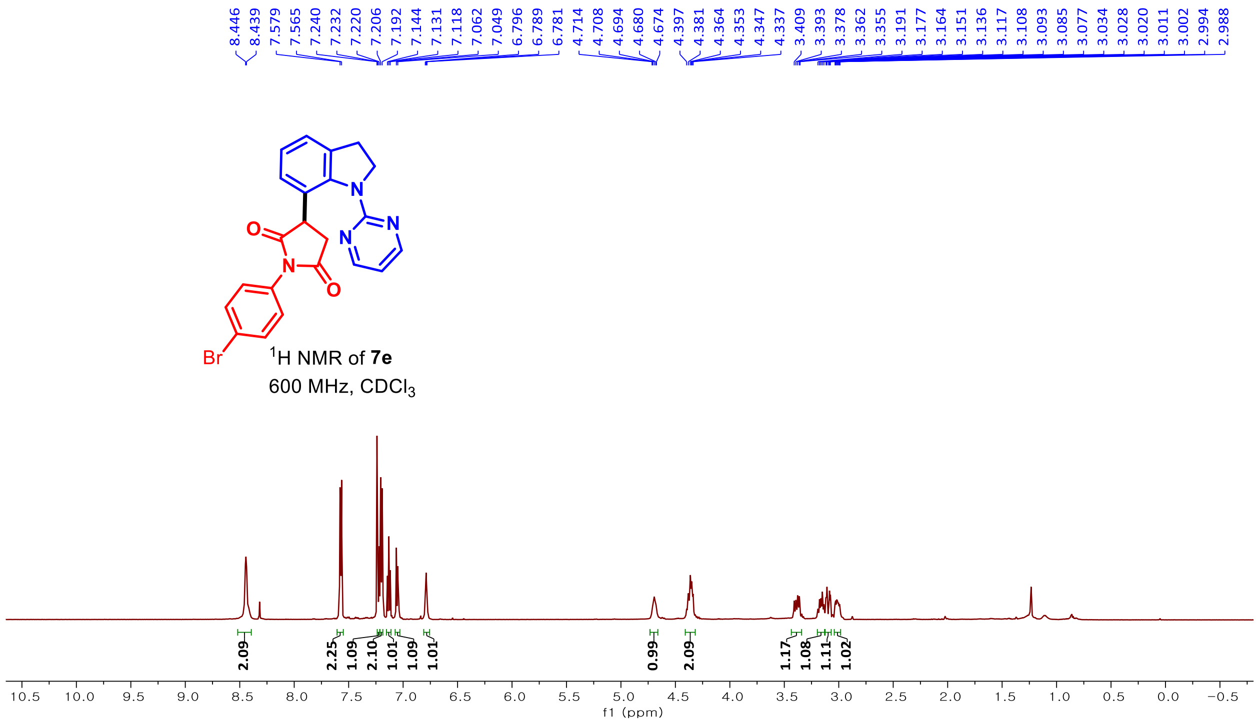
^{1}H NMR of **7c**
600 MHz, $CDCl_3$

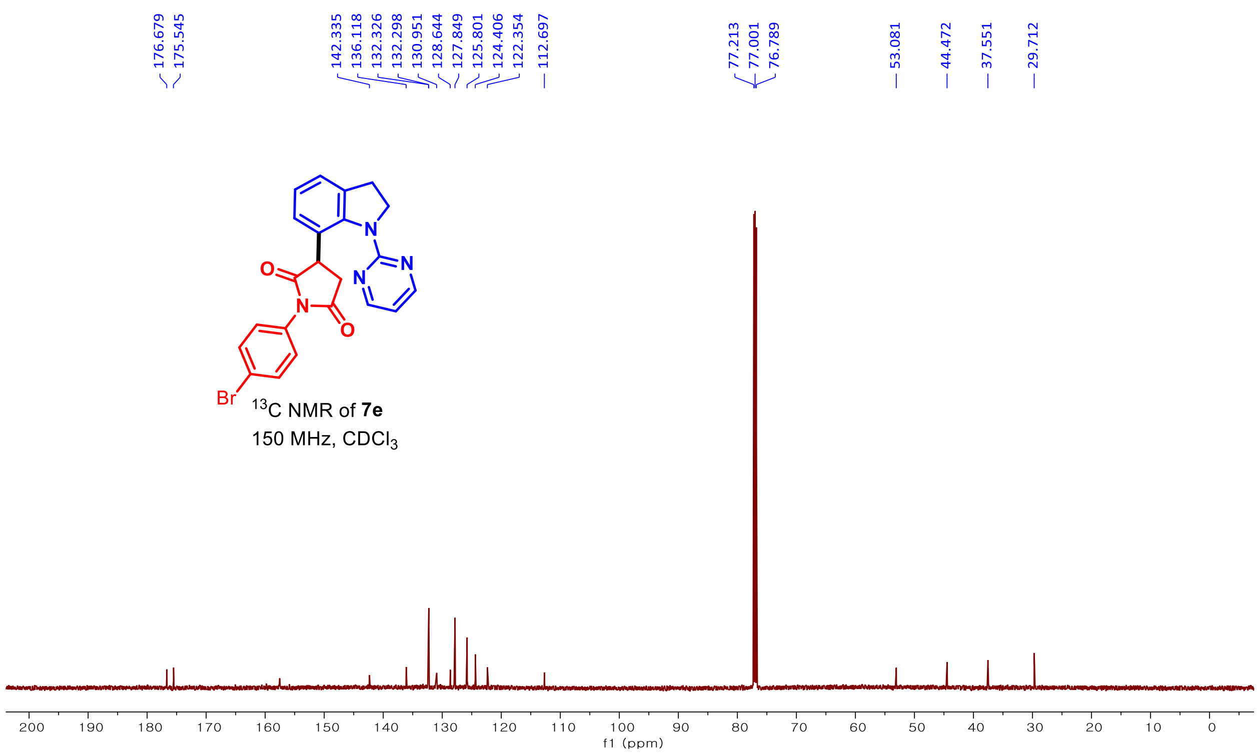


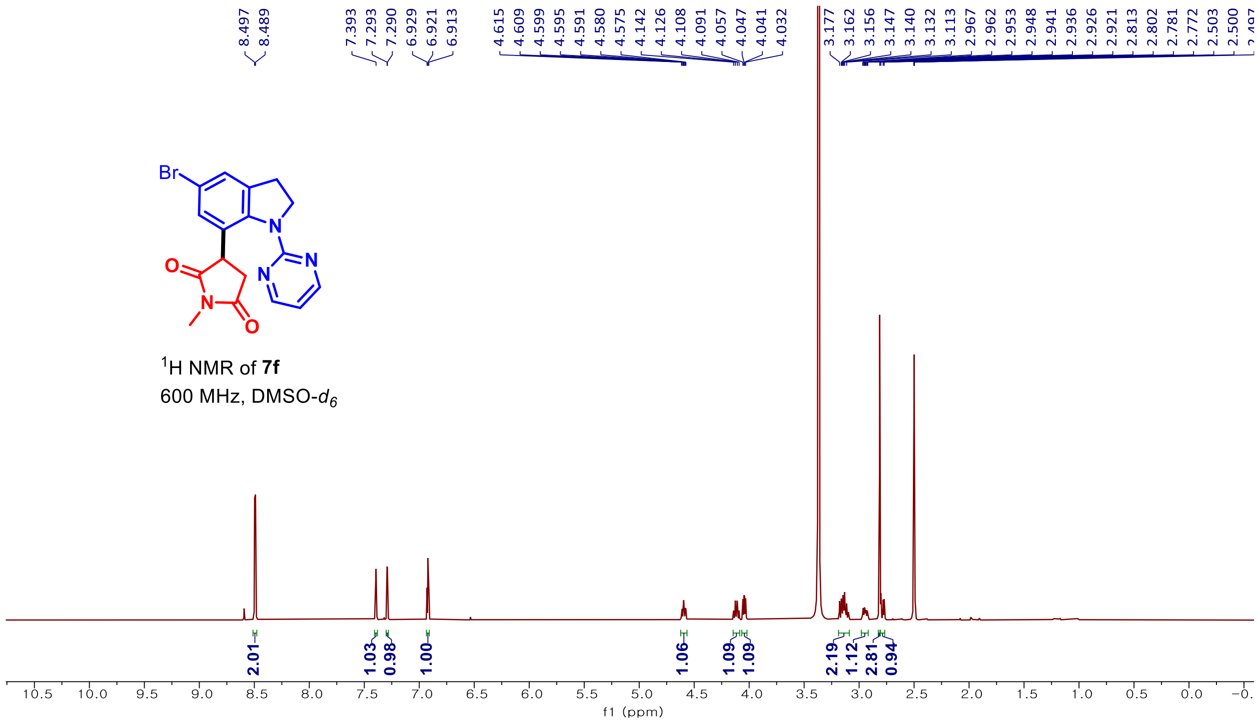
^{13}C NMR of **7c**
150 MHz, $CDCl_3$

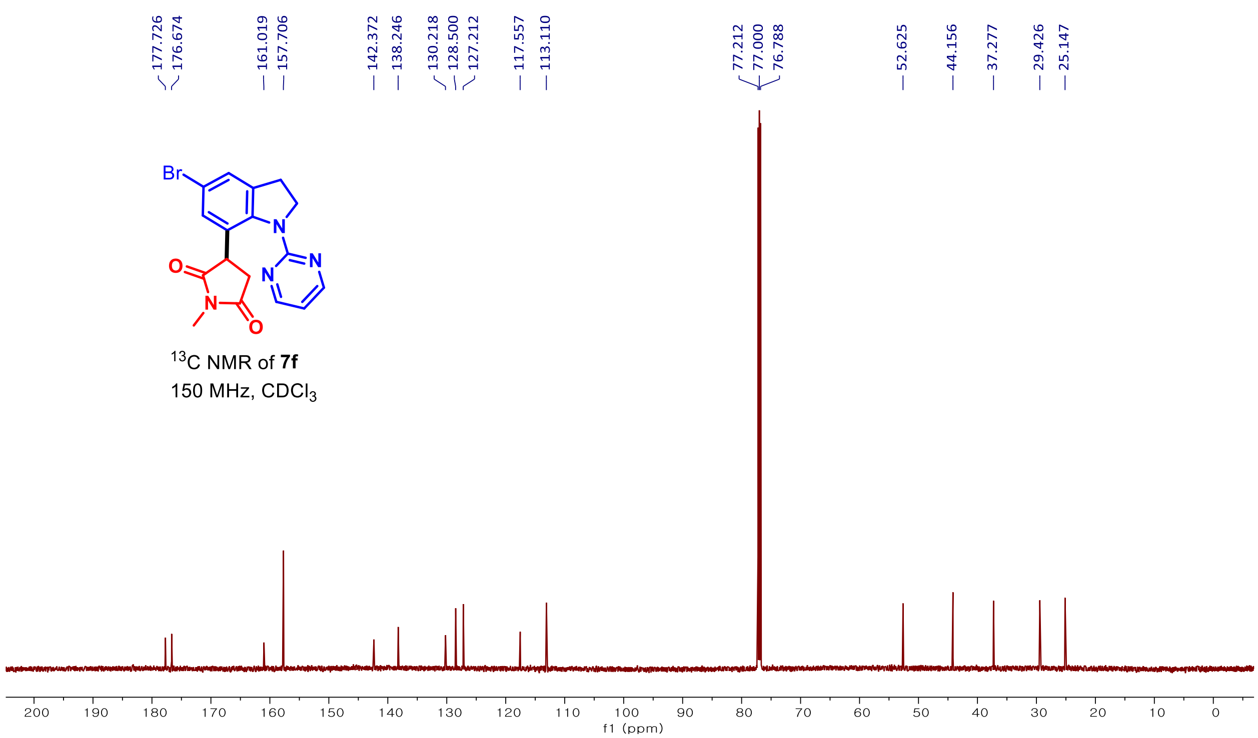

8.399
8.391
7.240
7.207
7.202
7.196
7.193
7.187
7.110
7.097
7.085
7.075
7.062
6.964
6.949
6.732
6.724
6.716
4.678
4.671
4.663
4.658
4.652
4.644
4.637
4.367
4.358
4.351
4.342
4.336
4.321
4.317
4.306
4.302
3.800
3.402
3.386
3.370
3.354
3.155
3.144
3.140
3.130
3.112
3.103
3.080
3.071
2.997
2.990
2.982
2.975
2.971
MeO
N
O
^{1}H NMR of **7d**
600 MHz, $CDCl_3$
1.86
2.81
2.05
2.03
0.96
1.00
2.01
3.01
1.00
0.88
1.13
1.00
f1 (ppm)

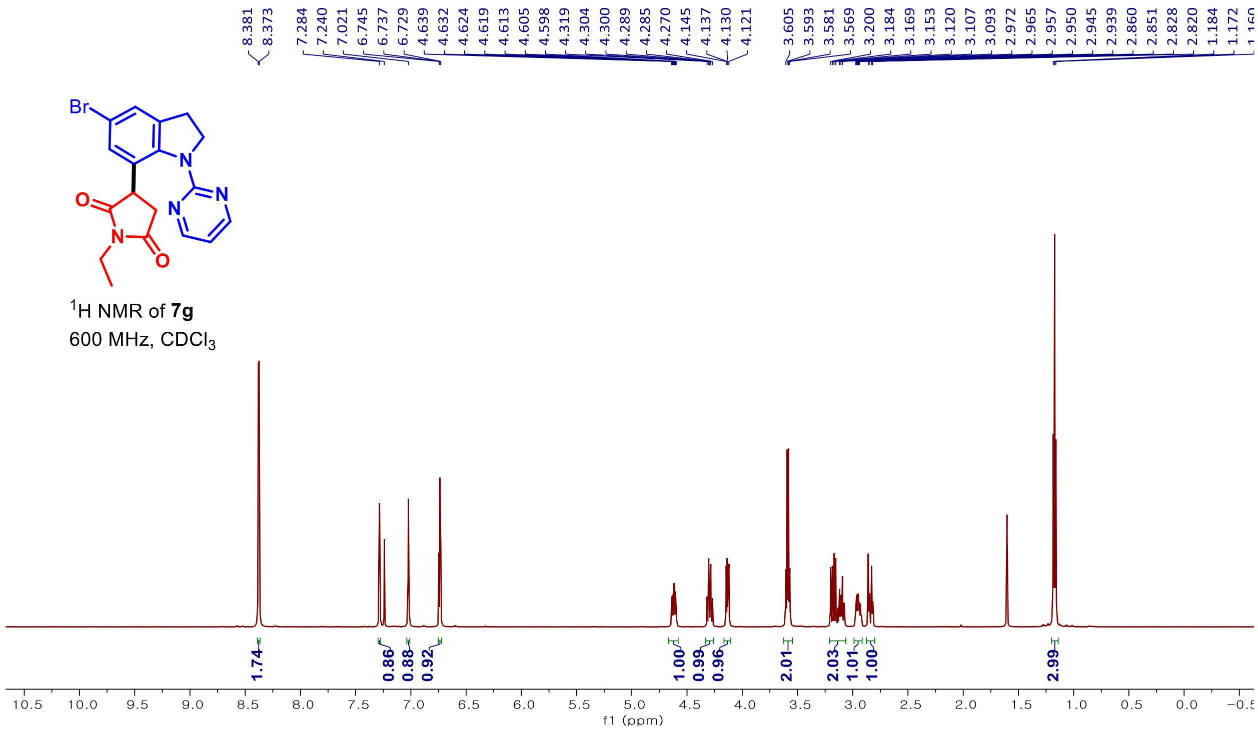

177.453
176.420
161.270
159.412
157.707
142.918
136.090
128.843
127.601
125.643
125.245
124.666
124.140
114.444
112.775
77.213
77.000
76.788
55.461
52.512
44.435
37.658
29.640
MeO
N
O
^{13}C NMR of **7d**
150 MHz, $CDCl_3$
f1 (ppm)


8.446
8.439
7.579
7.565
7.240
7.232
7.220
7.206
7.192
7.144
7.131
7.118
7.062
7.049
6.796
6.789
6.781
4.714
4.708
4.694
4.680
4.674
4.397
4.381
4.364
4.353
4.347
4.337
3.409
3.393
3.378
3.362
3.355
3.191
3.177
3.164
3.151
3.136
3.117
3.108
3.093
3.085
3.077
3.034
3.028
3.020
3.011
3.002
2.994
2.988
O
N
O
N
N
N
Br
^{1}H NMR of **7e**
600 MHz, $CDCl_3$
2.09
2.25
1.09
2.10
1.01
1.09
1.01
0.99
2.09
1.17
1.08
1.11
1.02
f1 (ppm)

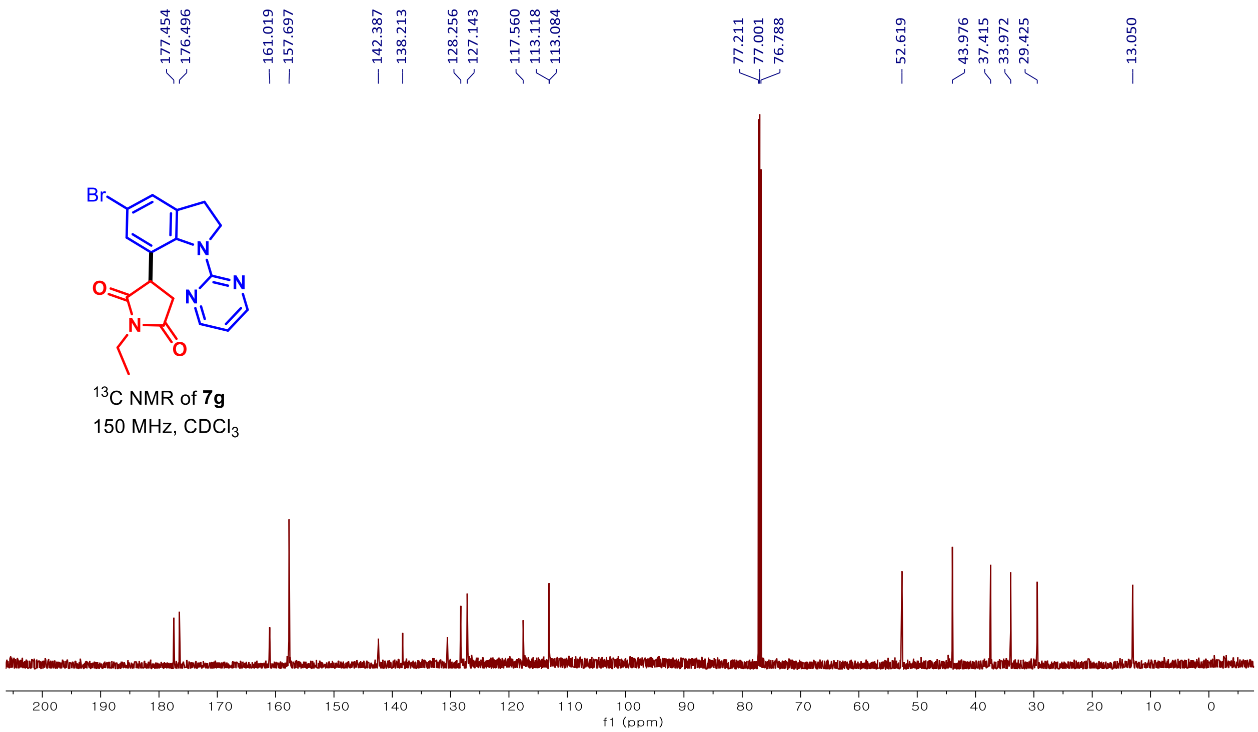

176.679
175.545
142.335
136.118
132.326
132.298
130.951
128.644
127.849
125.801
124.406
122.354
112.697
77.213
77.001
76.789
53.081
44.472
37.551
29.712
O
N
O
N
N
N
Br
^{13}C NMR of **7e**
150 MHz, $CDCl_3$
f1 (ppm)


1H NMR of 7f
600 MHz, DMSO-d6
f1 (ppm)

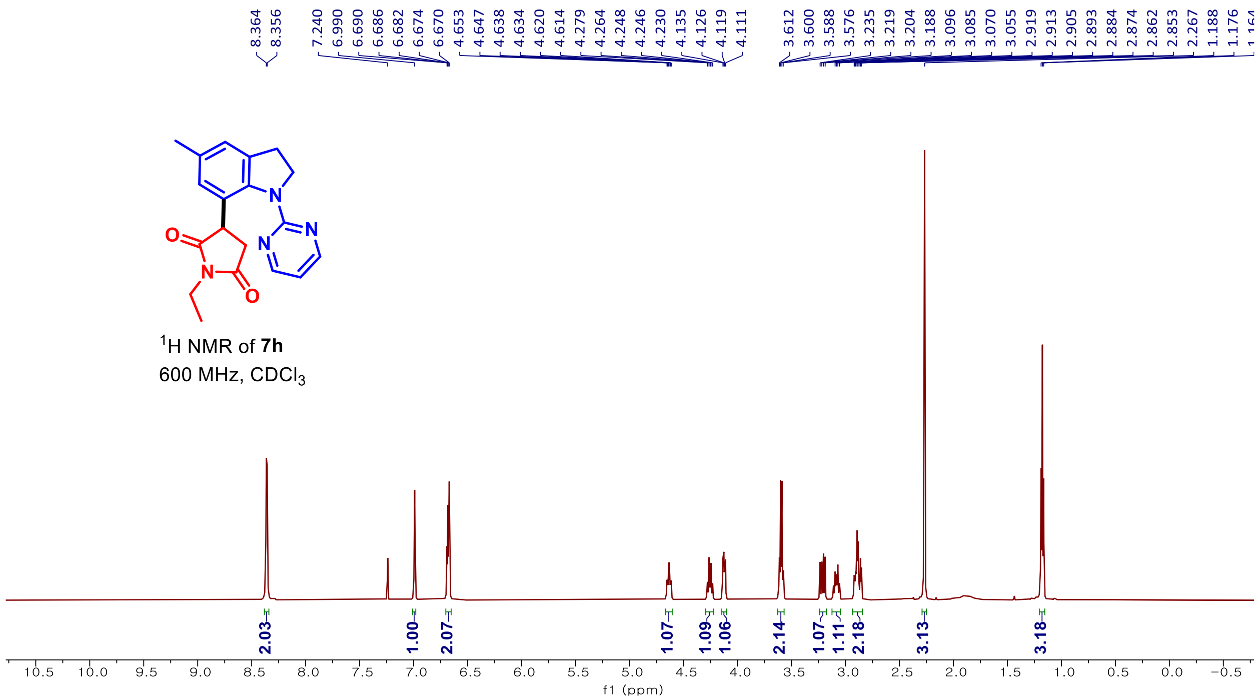

13C NMR of 7f
150 MHz, CDCl3
f1 (ppm)

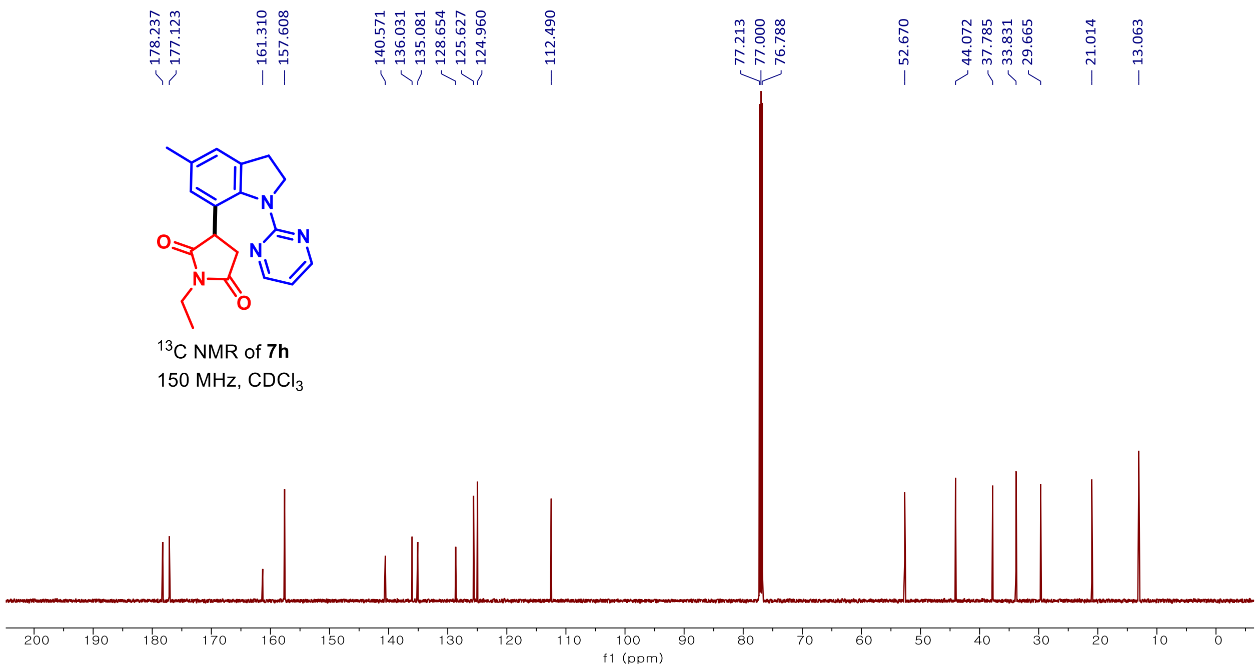


[1]H NMR of **7g**
600 MHz, $CDCl_3$



[13]C NMR of **7g**
150 MHz, $CDCl_3$


8.364
8.356
7.240
6.990
6.690
6.686
6.682
6.674
6.670
4.653
4.647
4.638
4.634
4.620
4.614
4.279
4.264
4.248
4.246
4.230
4.135
4.126
4.119
4.111
3.612
3.600
3.588
3.576
3.235
3.219
3.204
3.188
3.096
3.085
3.070
3.055
2.919
2.913
2.905
2.893
2.884
2.874
2.862
2.853
2.267
1.188
1.176
^{1}H NMR of **7h**
600 MHz, $CDCl_3$
2.03
1.00
2.07
1.07
1.09
1.06
2.14
1.07
1.11
2.18
3.13
3.18
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)


178.237
177.123
161.310
157.608
140.571
136.031
135.081
128.654
125.627
124.960
112.490
77.213
77.000
76.788
52.670
44.072
37.785
33.831
29.665
21.014
13.063
^{13}C NMR of **7h**
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)

X-ray structure and data for compound 3j

Empirical Formula $2(C_{27}H_{16}Cl_3N_3O_2)$, C_3H_6O, M = 1099.63, Monoclinic, Space group C2/c, a = 31.146(18) Å, b = 11.338(7) Å, *c* = 15.115(9) Å, *V* = 5317(5) Å^3, *Z* = 4, T = 223(2) K, ρ_{calcd} = 1.374 Mg/m^3, $2\Theta_{max.}$ = 25.242°, Refinement of 335 parameters on 6666 independent reflections out of 48713 collected reflections (R_{int} = 0.0883) led to R1 = 0.0814 [I >2σ(I)], wR_2 = 0.2937 (all data) and S = 1.043 with the largest difference peak and hole of 2.182 and -0.620 e.Å^{-3} respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2177685). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

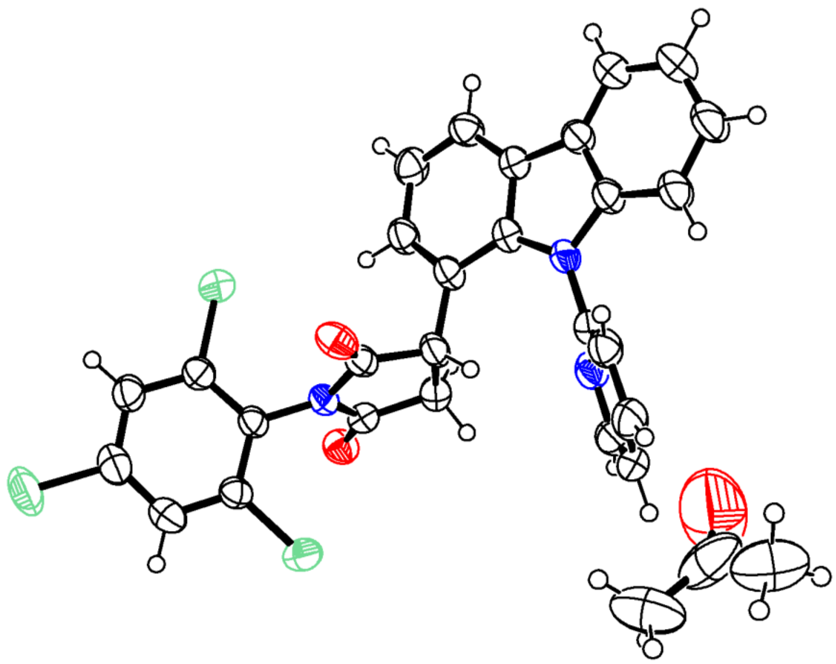


Figure S1. X-ray crystal structure of compound **3j** and acetone.

Table S2. Crystal data and structure refinement for **3j**.

Identification code	**3j**	
Empirical formula	C57 H38 Cl6 N6 O5	
Formula weight	1099.63	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 31.146(18) Å	a= 90°.
	b = 11.338(7) Å	b= 95.043(19)°.
	c = 15.115(9) Å	g = 90°.
Volume	5317(5) $Å^3$	
Z	4	
Density (calculated)	1.374 Mg/m^3	
Absorption coefficient	0.378 mm^{-1}	
F(000)	2256	
Crystal size	0.220 x 0.110 x 0.042 mm^3	
Theta range for data collection	1.912 to 28.522°.	
Index ranges	-41<=h<=41, -15<=k<=15, -15<=l<=20	
Reflections collected	48713	
Independent reflections	6666 [R(int) = 0.0883]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6814	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6666 / 12 / 335	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0814, wR2 = 0.2405	
R indices (all data)	R1 = 0.1378, wR2 = 0.2937	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.182 and -0.620 e.$Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3j**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	2241(1)	3228(1)	3572(1)	54(1)
Cl(2)	2632(1)	6191(1)	6328(1)	55(1)
Cl(3)	1464(1)	2760(2)	6581(1)	79(1)
O(1)	3319(1)	4536(3)	5401(2)	52(1)
O(2)	2278(1)	6078(3)	3426(2)	49(1)
O(3)	5000	811(9)	2500	183(4)
N(1)	2731(1)	5201(3)	4518(2)	38(1)
N(2)	4426(1)	6224(3)	4075(2)	40(1)
N(3)	4072(1)	5613(4)	2733(2)	50(1)
C(1)	2411(1)	4650(3)	4996(2)	37(1)
C(2)	2159(1)	3725(4)	4629(3)	40(1)
C(3)	1858(1)	3166(4)	5086(3)	50(1)
C(4)	1815(1)	3524(4)	5953(3)	51(1)
C(5)	2049(1)	4449(4)	6347(3)	49(1)
C(6)	2343(1)	5014(4)	5853(3)	41(1)
C(7)	3172(1)	5091(3)	4762(3)	39(1)
C(8)	3414(1)	5742(4)	4086(3)	42(1)
C(9)	3061(1)	6130(4)	3367(3)	52(1)
C(10)	2638(1)	5835(4)	3727(3)	40(1)
C(11)	3676(1)	6753(3)	4519(3)	40(1)
C(12)	3466(1)	7598(4)	4996(3)	47(1)
C(13)	3679(1)	8549(4)	5433(3)	51(1)
C(14)	4119(1)	8670(4)	5412(3)	45(1)
C(15)	4341(1)	7848(3)	4943(3)	38(1)
C(16)	4123(1)	6913(3)	4486(3)	38(1)
C(17)	4833(1)	6727(4)	4282(3)	43(1)
C(18)	4796(1)	7727(4)	4821(3)	43(1)
C(19)	5159(1)	8390(4)	5100(3)	51(1)
C(20)	5550(2)	8040(5)	4837(4)	62(1)
C(21)	5591(2)	7063(5)	4293(4)	63(1)
C(22)	5231(1)	6382(4)	4003(3)	56(1)

C(23)	4350(1)	5343(3)	3415(3)	39(1)
C(24)	3996(2)	4776(5)	2105(3)	64(1)
C(25)	4197(2)	3705(5)	2138(4)	70(2)
C(26)	4485(2)	3449(5)	2847(4)	63(1)
C(27)	4561(1)	4279(4)	3509(3)	48(1)
C(28)	5000	-262(8)	2500	99(4)
C(29)	4638(3)	-831(6)	2604(5)	101(2)

Table S4. Bond lengths [Å] and angles [°] for **3j**.

Cl(1)-C(2)	1.734(4)
Cl(2)-C(6)	1.731(4)
Cl(3)-C(4)	1.741(4)
O(1)-C(7)	1.209(5)
O(2)-C(10)	1.205(5)
O(3)-C(28)	1.217(12)
N(1)-C(7)	1.394(5)
N(1)-C(10)	1.403(5)
N(1)-C(1)	1.427(5)
N(2)-C(17)	1.400(5)
N(2)-C(16)	1.412(5)
N(2)-C(23)	1.417(5)
N(3)-C(23)	1.322(5)
N(3)-C(24)	1.348(6)
C(1)-C(6)	1.393(6)
C(1)-C(2)	1.395(5)
C(2)-C(3)	1.367(6)
C(3)-C(4)	1.390(7)
C(3)-H(3)	0.9400
C(4)-C(5)	1.381(6)
C(5)-C(6)	1.387(6)
C(5)-H(5)	0.9400
C(7)-C(8)	1.514(6)
C(8)-C(11)	1.521(6)
C(8)-C(9)	1.540(6)
C(8)-H(8)	0.9900
C(9)-C(10)	1.506(6)
C(9)-H(9A)	0.9800
C(9)-H(9AB)	0.9800
C(11)-C(12)	1.396(6)
C(11)-C(16)	1.409(5)
C(12)-C(13)	1.400(6)
C(12)-H(12)	0.9400
C(13)-C(14)	1.380(6)

C(13)-H(13)	0.9400
C(14)-C(15)	1.391(6)
C(14)-H(14)	0.9400
C(15)-C(16)	1.407(5)
C(15)-C(18)	1.453(6)
C(17)-C(22)	1.399(6)
C(17)-C(18)	1.407(6)
C(18)-C(19)	1.391(6)
C(19)-C(20)	1.373(7)
C(19)-H(19)	0.9400
C(20)-C(21)	1.392(7)
C(20)-H(20)	0.9400
C(21)-C(22)	1.400(6)
C(21)-H(21)	0.9400
C(22)-H(22)	0.9400
C(23)-C(27)	1.376(6)
C(24)-C(25)	1.365(8)
C(24)-H(24)	0.9400
C(25)-C(26)	1.367(8)
C(25)-H(25)	0.9400
C(26)-C(27)	1.379(7)
C(26)-H(26)	0.9400
C(27)-H(27)	0.9400
C(28)-C(29)	1.321(8)
C(28)-C(29)#1	1.321(8)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(29)-H(29C)	0.9700

C(7)-N(1)-C(10)	113.3(3)
C(7)-N(1)-C(1)	122.9(3)
C(10)-N(1)-C(1)	123.7(3)
C(17)-N(2)-C(16)	107.7(3)
C(17)-N(2)-C(23)	122.5(3)
C(16)-N(2)-C(23)	128.4(3)
C(23)-N(3)-C(24)	116.6(4)

C(6)-C(1)-C(2)	117.8(4)
C(6)-C(1)-N(1)	120.8(3)
C(2)-C(1)-N(1)	121.4(3)
C(3)-C(2)-C(1)	122.2(4)
C(3)-C(2)-Cl(1)	118.6(3)
C(1)-C(2)-Cl(1)	119.2(3)
C(2)-C(3)-C(4)	118.0(4)
C(2)-C(3)-H(3)	121.0
C(4)-C(3)-H(3)	121.0
C(5)-C(4)-C(3)	122.5(4)
C(5)-C(4)-Cl(3)	118.4(4)
C(3)-C(4)-Cl(3)	119.0(4)
C(4)-C(5)-C(6)	117.8(4)
C(4)-C(5)-H(5)	121.1
C(6)-C(5)-H(5)	121.1
C(5)-C(6)-C(1)	121.7(4)
C(5)-C(6)-Cl(2)	118.5(3)
C(1)-C(6)-Cl(2)	119.8(3)
O(1)-C(7)-N(1)	123.6(4)
O(1)-C(7)-C(8)	128.0(4)
N(1)-C(7)-C(8)	108.4(3)
C(7)-C(8)-C(11)	110.9(3)
C(7)-C(8)-C(9)	104.4(3)
C(11)-C(8)-C(9)	114.2(4)
C(7)-C(8)-H(8)	109.0
C(11)-C(8)-H(8)	109.0
C(9)-C(8)-H(8)	109.0
C(10)-C(9)-C(8)	105.8(3)
C(10)-C(9)-H(9A)	110.6
C(8)-C(9)-H(9A)	110.6
C(10)-C(9)-H(9AB)	110.6
C(8)-C(9)-H(9AB)	110.6
H(9A)-C(9)-H(9AB)	108.7
O(2)-C(10)-N(1)	123.7(4)
O(2)-C(10)-C(9)	128.8(4)
N(1)-C(10)-C(9)	107.5(3)

C(12)-C(11)-C(16)	116.0(4)
C(12)-C(11)-C(8)	118.8(3)
C(16)-C(11)-C(8)	125.2(4)
C(11)-C(12)-C(13)	123.2(4)
C(11)-C(12)-H(12)	118.4
C(13)-C(12)-H(12)	118.4
C(14)-C(13)-C(12)	119.8(4)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(13)-C(14)-C(15)	118.8(4)
C(13)-C(14)-H(14)	120.6
C(15)-C(14)-H(14)	120.6
C(14)-C(15)-C(16)	121.0(4)
C(14)-C(15)-C(18)	131.4(4)
C(16)-C(15)-C(18)	107.5(3)
C(15)-C(16)-C(11)	121.0(3)
C(15)-C(16)-N(2)	108.6(3)
C(11)-C(16)-N(2)	130.3(4)
C(22)-C(17)-N(2)	128.8(4)
C(22)-C(17)-C(18)	121.3(4)
N(2)-C(17)-C(18)	109.8(3)
C(19)-C(18)-C(17)	120.3(4)
C(19)-C(18)-C(15)	133.4(4)
C(17)-C(18)-C(15)	106.2(3)
C(20)-C(19)-C(18)	118.3(4)
C(20)-C(19)-H(19)	120.9
C(18)-C(19)-H(19)	120.9
C(19)-C(20)-C(21)	122.1(4)
C(19)-C(20)-H(20)	119.0
C(21)-C(20)-H(20)	119.0
C(20)-C(21)-C(22)	120.7(4)
C(20)-C(21)-H(21)	119.6
C(22)-C(21)-H(21)	119.6
C(17)-C(22)-C(21)	117.3(4)
C(17)-C(22)-H(22)	121.4
C(21)-C(22)-H(22)	121.4

N(3)-C(23)-C(27)	123.9(4)
N(3)-C(23)-N(2)	116.4(4)
C(27)-C(23)-N(2)	119.7(4)
N(3)-C(24)-C(25)	123.3(5)
N(3)-C(24)-H(24)	118.3
C(25)-C(24)-H(24)	118.3
C(24)-C(25)-C(26)	119.0(5)
C(24)-C(25)-H(25)	120.5
C(26)-C(25)-H(25)	120.5
C(25)-C(26)-C(27)	118.9(5)
C(25)-C(26)-H(26)	120.6
C(27)-C(26)-H(26)	120.6
C(23)-C(27)-C(26)	118.2(5)
C(23)-C(27)-H(27)	120.9
C(26)-C(27)-H(27)	120.9
O(3)-C(28)-C(29)	119.2(5)
O(3)-C(28)-C(29)#1	119.2(5)
C(29)-C(28)-C(29)#1	121.5(10)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Table S5. Anisotropic displacement parameters ($Å^2$x 10^3) for **3j**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	56(1)	56(1)	48(1)	-12(1)	1(1)	-5(1)
Cl(2)	61(1)	56(1)	49(1)	-13(1)	10(1)	-13(1)
Cl(3)	62(1)	102(1)	74(1)	20(1)	16(1)	-33(1)
O(1)	40(2)	50(2)	63(2)	6(2)	-9(1)	-3(1)
O(2)	40(2)	55(2)	50(2)	3(1)	-3(1)	0(1)
O(3)	186(8)	117(6)	260(9)	0	96(7)	0
N(1)	30(2)	43(2)	40(2)	-1(1)	3(1)	-4(1)
N(2)	29(2)	45(2)	48(2)	-6(2)	7(1)	-1(1)
N(3)	43(2)	66(2)	41(2)	7(2)	3(2)	-5(2)
C(1)	28(2)	42(2)	39(2)	0(2)	3(2)	-2(2)
C(2)	34(2)	45(2)	41(2)	0(2)	-1(2)	-3(2)
C(3)	42(2)	49(2)	57(3)	3(2)	-1(2)	-9(2)
C(4)	41(2)	60(3)	52(2)	14(2)	4(2)	-5(2)
C(5)	38(2)	66(3)	43(2)	1(2)	6(2)	-4(2)
C(6)	37(2)	45(2)	43(2)	0(2)	3(2)	-1(2)
C(7)	32(2)	39(2)	47(2)	-3(2)	3(2)	-1(2)
C(8)	32(2)	45(2)	52(2)	-2(2)	10(2)	-5(2)
C(9)	45(2)	71(3)	43(2)	-4(2)	9(2)	-11(2)
C(10)	41(2)	42(2)	38(2)	-5(2)	5(2)	-2(2)
C(11)	31(2)	41(2)	49(2)	1(2)	6(2)	-2(2)
C(12)	37(2)	46(2)	59(3)	-3(2)	13(2)	-1(2)
C(13)	48(2)	47(2)	59(3)	-4(2)	14(2)	8(2)
C(14)	44(2)	39(2)	52(2)	-4(2)	4(2)	-2(2)
C(15)	35(2)	39(2)	41(2)	1(2)	5(2)	0(2)
C(16)	32(2)	39(2)	44(2)	4(2)	7(2)	1(2)
C(17)	30(2)	50(2)	49(2)	0(2)	4(2)	-2(2)
C(18)	37(2)	44(2)	47(2)	0(2)	4(2)	-4(2)
C(19)	41(2)	54(3)	56(3)	0(2)	2(2)	-4(2)
C(20)	40(2)	68(3)	76(3)	-1(3)	1(2)	-13(2)
C(21)	31(2)	73(3)	87(4)	-12(3)	9(2)	-4(2)
C(22)	34(2)	63(3)	71(3)	-12(2)	11(2)	-2(2)

C(23)	34(2)	46(2)	37(2)	-1(2)	10(2)	-4(2)
C(24)	61(3)	94(4)	38(2)	-3(2)	5(2)	-28(3)
C(25)	72(3)	86(4)	55(3)	-32(3)	32(3)	-38(3)
C(26)	59(3)	52(3)	82(4)	-18(3)	31(3)	-6(2)
C(27)	39(2)	48(2)	58(3)	-3(2)	12(2)	2(2)
C(28)	193(13)	61(5)	49(4)	0	30(6)	0
C(29)	123(5)	64(3)	108(5)	11(3)	-37(4)	-25(4)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **3j**.

	x	y	z	U(eq)
H(3)	1686	2558	4823	59
H(5)	2010	4688	6930	59
H(8)	3611	5185	3821	51
H(9A)	3081	6978	3254	63
H(9AB)	3090	5705	2810	63
H(12)	3167	7526	5026	56
H(13)	3523	9102	5739	61
H(14)	4266	9298	5710	54
H(19)	5137	9060	5460	61
H(20)	5798	8474	5030	74
H(21)	5864	6859	4118	76
H(22)	5256	5721	3637	67
H(24)	3794	4938	1621	77
H(25)	4138	3152	1680	83
H(26)	4629	2720	2882	75
H(27)	4752	4122	4012	58
H(29A)	4689	-1675	2589	152
H(29B)	4536	-619	3171	152
H(29C)	4422	-619	2128	152

X-ray structure and data for compound 6f

Empirical Formula $C_{22}H_{15}BrN_4O_2$, M = 447.29, Monoclinic, Space group $P2_1/n$, a = 17.315(11) Å, b = 7.025(5) Å, c = 17.444(11) Å, V = 2093(2) Å^3, Z = 4, T = 223(2) K, ρ_{calcd} = 1.419 Mg/m^3, $2\Theta_{max.}$ = 25.242°, Refinement of 262 parameters on 5224 independent reflections out of 41083 collected reflections (R_{int} = 0.0500) led to R1 = 0.0475 [I >2σ(I)], wR_2 = 0.1173 (all data) and S = 1.033 with the largest difference peak and hole of 0.627 and -0.755 e.Å^{-3} respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2177686). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

Since the lattice solvent molecules in compound **6f** are highly disordered, the contribution of solvent electron density was removed by the SQUEEZE routine in PLATON.[1]

1. L. Spek, *PLATON*, *A Multipurpose Crystallographic Tool*, University of Ultrecht, Ultrecht, The Netherlands, 2003.

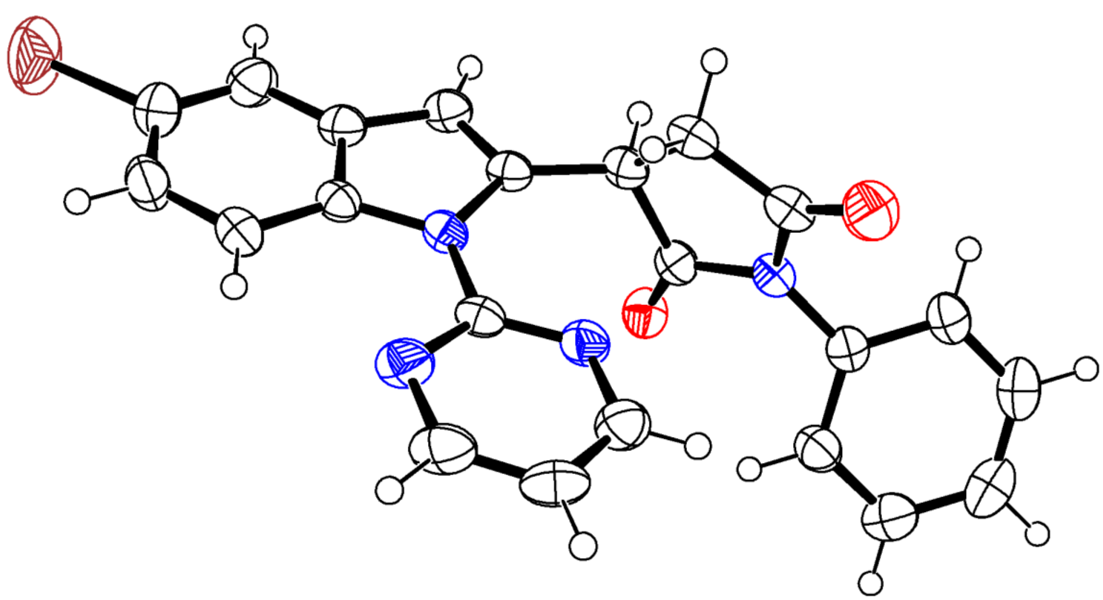


Figure S2. X-ray crystal structure of compound **6f**.

Table S7. Crystal data and structure refinement for **6f**.

Identification code	**6f**	
Empirical formula	$C_{22} H_{15} Br N_4 O_2$	
Formula weight	447.29	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 17.315(11) Å	a= 90°.
	b = 7.025(5) Å	b= 99.42(3)°.
	c = 17.444(11) Å	g = 90°.
Volume	2093(2) $Å^3$	
Z	4	
Density (calculated)	1.419 Mg/m^3	
Absorption coefficient	1.988 mm^{-1}	
F(000)	904	
Crystal size	0.246 x 0.185 x 0.140 mm^3	
Theta range for data collection	2.367 to 28.362°.	
Index ranges	-23<=h<=23, -9<=k<=9, -23<=l<=23	
Reflections collected	41083	
Independent reflections	5224 [R(int) = 0.0500]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6719	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5224 / 0 / 262	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1042	
R indices (all data)	R1 = 0.0754, wR2 = 0.1173	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.627 and -0.755 e.$Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6f**. U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	3150(1)	6048(1)	7958(1)	86(1)
O(1)	3141(1)	5491(2)	2965(1)	39(1)
O(2)	3864(1)	11259(2)	2132(1)	52(1)
N(1)	4072(1)	7677(2)	4837(1)	29(1)
N(2)	5432(1)	7558(3)	5041(1)	44(1)
N(3)	4707(1)	7822(3)	3768(1)	37(1)
N(4)	3458(1)	8226(3)	2351(1)	31(1)
C(1)	3482(2)	6622(4)	6999(2)	48(1)
C(2)	4279(2)	6672(4)	6971(2)	46(1)
C(3)	4547(2)	6983(3)	6279(1)	36(1)
C(4)	3997(1)	7284(3)	5613(1)	30(1)
C(5)	3192(1)	7263(3)	5650(1)	35(1)
C(6)	2933(2)	6908(4)	6350(2)	45(1)
C(7)	2786(1)	7685(3)	4890(1)	35(1)
C(8)	3309(1)	7949(3)	4408(1)	30(1)
C(9)	4773(1)	7680(3)	4534(1)	30(1)
C(10)	6087(2)	7609(4)	4729(2)	49(1)
C(11)	6095(2)	7802(4)	3956(2)	45(1)
C(12)	5377(2)	7896(4)	3488(2)	44(1)
C(13)	3094(1)	8588(3)	3583(1)	31(1)
C(14)	3244(1)	7191(3)	2966(1)	31(1)
C(15)	3610(1)	10130(3)	2546(1)	36(1)
C(16)	3424(1)	10475(3)	3343(1)	35(1)
C(17)	3567(1)	7424(3)	1626(1)	31(1)
C(18)	4000(2)	5775(4)	1607(2)	41(1)
C(19)	4116(2)	5051(4)	900(2)	51(1)
C(20)	3799(2)	5962(4)	215(2)	52(1)
C(21)	3355(2)	7572(4)	238(2)	48(1)
C(22)	3232(1)	8311(4)	940(1)	39(1)

Table S9. Bond lengths [Å] and angles [°] for **6f**.

Br(1)-C(1)	1.901(3)
O(1)-C(14)	1.208(3)
O(2)-C(15)	1.204(3)
N(1)-C(9)	1.400(3)
N(1)-C(4)	1.408(3)
N(1)-C(8)	1.421(3)
N(2)-C(9)	1.327(3)
N(2)-C(10)	1.335(3)
N(3)-C(9)	1.325(3)
N(3)-C(12)	1.332(3)
N(4)-C(14)	1.395(3)
N(4)-C(15)	1.395(3)
N(4)-C(17)	1.425(3)
C(1)-C(6)	1.368(4)
C(1)-C(2)	1.388(4)
C(2)-C(3)	1.379(4)
C(2)-H(2)	0.9400
C(3)-C(4)	1.393(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.405(3)
C(5)-C(6)	1.392(3)
C(5)-C(7)	1.426(3)
C(6)-H(6)	0.9400
C(7)-C(8)	1.345(3)
C(7)-H(7)	0.9400
C(8)-C(13)	1.496(3)
C(10)-C(11)	1.358(4)
C(10)-H(10)	0.9400
C(11)-C(12)	1.373(4)
C(11)-H(11)	0.9400
C(12)-H(12)	0.9400
C(13)-C(14)	1.509(3)
C(13)-C(16)	1.528(3)
C(13)-H(13)	0.9900

C(15)-C(16)	1.497(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(17)-C(18)	1.383(3)
C(17)-C(22)	1.389(3)
C(18)-C(19)	1.379(4)
C(18)-H(18)	0.9400
C(19)-C(20)	1.386(4)
C(19)-H(19)	0.9400
C(20)-C(21)	1.373(4)
C(20)-H(20)	0.9400
C(21)-C(22)	1.379(4)
C(21)-H(21)	0.9400
C(22)-H(22)	0.9400
C(9)-N(1)-C(4)	125.83(18)
C(9)-N(1)-C(8)	126.10(19)
C(4)-N(1)-C(8)	107.96(18)
C(9)-N(2)-C(10)	115.0(2)
C(9)-N(3)-C(12)	115.9(2)
C(14)-N(4)-C(15)	112.05(19)
C(14)-N(4)-C(17)	124.55(19)
C(15)-N(4)-C(17)	123.25(19)
C(6)-C(1)-C(2)	121.8(2)
C(6)-C(1)-Br(1)	119.3(2)
C(2)-C(1)-Br(1)	118.8(2)
C(3)-C(2)-C(1)	120.9(2)
C(3)-C(2)-H(2)	119.6
C(1)-C(2)-H(2)	119.6
C(2)-C(3)-C(4)	118.2(2)
C(2)-C(3)-H(3)	120.9
C(4)-C(3)-H(3)	120.9
C(3)-C(4)-C(5)	120.5(2)
C(3)-C(4)-N(1)	132.3(2)
C(5)-C(4)-N(1)	107.09(19)
C(6)-C(5)-C(4)	120.4(2)

C(6)-C(5)-C(7)	132.3(2)
C(4)-C(5)-C(7)	107.3(2)
C(1)-C(6)-C(5)	118.2(2)
C(1)-C(6)-H(6)	120.9
C(5)-C(6)-H(6)	120.9
C(8)-C(7)-C(5)	109.3(2)
C(8)-C(7)-H(7)	125.4
C(5)-C(7)-H(7)	125.4
C(7)-C(8)-N(1)	108.4(2)
C(7)-C(8)-C(13)	123.8(2)
N(1)-C(8)-C(13)	127.7(2)
N(3)-C(9)-N(2)	126.8(2)
N(3)-C(9)-N(1)	116.34(19)
N(2)-C(9)-N(1)	116.9(2)
N(2)-C(10)-C(11)	123.7(2)
N(2)-C(10)-H(10)	118.2
C(11)-C(10)-H(10)	118.2
C(10)-C(11)-C(12)	116.1(2)
C(10)-C(11)-H(11)	121.9
C(12)-C(11)-H(11)	121.9
N(3)-C(12)-C(11)	122.5(3)
N(3)-C(12)-H(12)	118.7
C(11)-C(12)-H(12)	118.7
C(8)-C(13)-C(14)	116.46(19)
C(8)-C(13)-C(16)	118.58(19)
C(14)-C(13)-C(16)	104.67(19)
C(8)-C(13)-H(13)	105.3
C(14)-C(13)-H(13)	105.3
C(16)-C(13)-H(13)	105.3
O(1)-C(14)-N(4)	124.9(2)
O(1)-C(14)-C(13)	127.0(2)
N(4)-C(14)-C(13)	107.90(19)
O(2)-C(15)-N(4)	124.0(2)
O(2)-C(15)-C(16)	127.3(2)
N(4)-C(15)-C(16)	108.7(2)
C(15)-C(16)-C(13)	105.11(19)

C(15)-C(16)-H(16A)	110.7
C(13)-C(16)-H(16A)	110.7
C(15)-C(16)-H(16B)	110.7
C(13)-C(16)-H(16B)	110.7
H(16A)-C(16)-H(16B)	108.8
C(18)-C(17)-C(22)	120.4(2)
C(18)-C(17)-N(4)	120.3(2)
C(22)-C(17)-N(4)	119.3(2)
C(19)-C(18)-C(17)	119.3(2)
C(19)-C(18)-H(18)	120.3
C(17)-C(18)-H(18)	120.3
C(18)-C(19)-C(20)	120.4(3)
C(18)-C(19)-H(19)	119.8
C(20)-C(19)-H(19)	119.8
C(21)-C(20)-C(19)	120.0(3)
C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(20)-C(21)-C(22)	120.4(3)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(21)-C(22)-C(17)	119.5(2)
C(21)-C(22)-H(22)	120.2
C(17)-C(22)-H(22)	120.2

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2$x 10^3) for **6f**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	93(1)	121(1)	50(1)	30(1)	26(1)	7(1)
O(1)	46(1)	32(1)	38(1)	0(1)	6(1)	-8(1)
O(2)	65(1)	35(1)	59(1)	7(1)	20(1)	-6(1)
N(1)	24(1)	29(1)	33(1)	0(1)	0(1)	-1(1)
N(2)	26(1)	59(1)	44(1)	-12(1)	-2(1)	4(1)
N(3)	29(1)	42(1)	40(1)	4(1)	6(1)	4(1)
N(4)	29(1)	29(1)	33(1)	2(1)	2(1)	0(1)
C(1)	55(2)	51(2)	38(1)	7(1)	12(1)	2(1)
C(2)	54(2)	44(1)	36(1)	7(1)	-3(1)	7(1)
C(3)	36(1)	33(1)	39(1)	3(1)	0(1)	2(1)
C(4)	31(1)	24(1)	34(1)	-2(1)	1(1)	0(1)
C(5)	34(1)	32(1)	39(1)	-4(1)	5(1)	2(1)
C(6)	43(2)	48(2)	45(1)	2(1)	15(1)	1(1)
C(7)	27(1)	39(1)	40(1)	-6(1)	3(1)	0(1)
C(8)	24(1)	30(1)	35(1)	-4(1)	0(1)	0(1)
C(9)	26(1)	24(1)	39(1)	-3(1)	2(1)	0(1)
C(10)	26(1)	61(2)	57(2)	-17(1)	-2(1)	4(1)
C(11)	30(1)	41(1)	66(2)	-11(1)	14(1)	-1(1)
C(12)	40(1)	46(1)	48(2)	2(1)	13(1)	2(1)
C(13)	24(1)	33(1)	35(1)	-2(1)	-3(1)	1(1)
C(14)	25(1)	34(1)	32(1)	-1(1)	-2(1)	-2(1)
C(15)	31(1)	30(1)	44(1)	3(1)	2(1)	2(1)
C(16)	31(1)	30(1)	42(1)	0(1)	0(1)	4(1)
C(17)	27(1)	34(1)	33(1)	2(1)	3(1)	-4(1)
C(18)	38(1)	41(1)	42(1)	4(1)	4(1)	5(1)
C(19)	49(2)	52(2)	53(2)	-6(1)	13(1)	5(1)
C(20)	60(2)	58(2)	41(1)	-6(1)	18(1)	-17(2)
C(21)	52(2)	54(2)	37(1)	9(1)	3(1)	-14(1)
C(22)	37(1)	39(1)	39(1)	8(1)	3(1)	-3(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6f**.

	x	y	z	U(eq)
H(2)	4640	6491	7429	55
H(3)	5086	6991	6258	44
H(6)	2396	6866	6377	53
H(7)	2240	7766	4749	42
H(10)	6569	7505	5064	59
H(11)	6565	7867	3753	54
H(12)	5357	8018	2948	52
H(13)	2519	8764	3500	38
H(16A)	3036	11495	3334	42
H(16B)	3896	10828	3704	42
H(18)	4212	5153	2071	49
H(19)	4412	3935	882	61
H(20)	3889	5477	-265	63
H(21)	3133	8174	-227	58
H(22)	2924	9408	955	46