Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Preparation of Pyridopyrazines Through Tandem Pd-Catalyzed CN/C-C Coupling Reactions of Ugi Adducts

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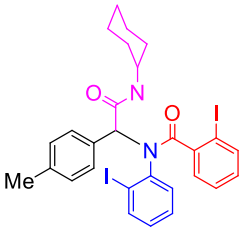
EXPERIMENTAL SECTION

General Considerations. All materials were purchased from Merck, Aldrich, and Fluka, and used as received. Melting points were measured by an Electrothermal 9100 apparatus and are uncorrected. The ^{1}HNMR (600 MHz) and ^{13}CNMR (151 MHz) spectra were run on Bruker spectrometer using CDCl3 and DMSO-d_6 as solvent and Me_4Si (TMS) as internal standard at 298 K. The chemical shifts (δ) are reported in parts per million (ppm) and coupling constants (*J*) are given in Hz. High-resolution mass spectra (HRMS) were obtained on an Agilent HRMS-ESI/QTOF instrument. Single crystals of **6h, 6j** were mounted on a MiTeGen loop with grease and examined on a Bruker D8 Venture APEX diffractometer equipped with Photon 100 CCD area detector at 296 (2) K using graphite-monochromated Mo-Kα radiation (λ = 0.71073Å). The structures of **6h** and **6j** have been deposited with the CCDC (CCDC deposition number for **6j** is 5565884 and for **6h** is 2259069).

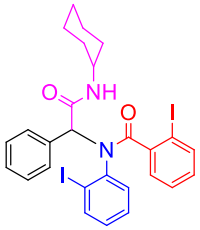
General procedure for the synthesis of Ugi products (5a-s). The mixture of aldehyde (**1a-g,** 1 mmol) and amine (**2a-b**, 1 mmol) was stirred in MeOH (5 mL) at 25 °C for 1 hour. Afterward, acid (**3**a**-e,** 1 mmol) and then isocyanide (**4a-b**, 1mmol) was added, and the resulting mixture was stirred for 24 h at ambient temperature. The progress of the reaction was monitored by thin-layer chromatography (TLC) (n-hexane/ EtOAc 5:1). White precipitate was filtered and washed with cold methanol. Yields (47-89%).

N-(2-(cyclohexylamino)-2-oxo-1-(p-tolyl)ethyl)-2-iodo-N-(2-iodophenyl)benzamide (***5a***):



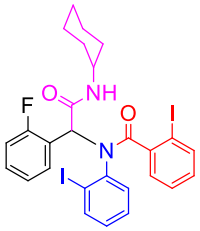
White solid, mp: 223-225 °C; Yield 69% (467 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.72–7.66 (m, 1H), 7.44 (dt, *J* = 7.9, 2.0 Hz, 2H), 7.25–7.21 (m, 2H), 7.14–7.08 (m, 1H), 7.01 (td, *J* = 7.6, 1.1 Hz, 1H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.80 (td, *J* = 7.7, 1.7 Hz, 1H), 6.69 (td, *J* = 7.6, 1.6 Hz, 1H), 5.87–5.79 (m, 2H), 3.84–3.75 (m, 1H), 2.22 (s, 3H), 2.04–1.98 (m, 1H), 1.88–1.82 (m, 1H), 1.70–1.47 (m, 3H), 1.38–1.24 (m, 2H), 1.23–0.98 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.1, 168.4, 141.9, 141.7, 139.8, 139.4, 138.5, 133.5, 133.2, 131.2, 130.1, 129.4, 128.9, 128.6, 128.2, 126.7, 102.7, 94.4, 66.4, 48.9, 32.8, 32.6, 25.5, 24.8124.7, 21.1; HRMS (ESI) m/z: Calcd for $C_{28}H_{28}I_2N_2O_2$ $[M + H]^+$ 679.0318, Found 679.0321; FT-IR *δ* 3343, 2922, 2853, 1675, 1631, 1369, 1013, 627 cm^{-1}.

N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-2-iodo-N-(2-iodophenyl)benzamide (5b):



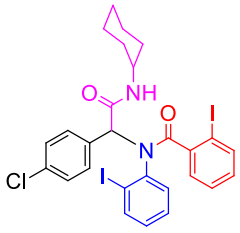
White solid, mp: 194-196 ℃; Yield 73% (484 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (dd, J = 7.9, 1.6 Hz, 1H), 7.69 (dd, J = 7.9, 1.1 Hz, 1H), 7.44 (dd, J = 7.9, 1.5 Hz, 2H), 7.36 (dd, J = 7.0, 1.5 Hz, 2H), 7.22–7.16 (m, 1H), 7.16 – 7.08 (m, 3H), 7.02 (td, J = 7.5, 1.1 Hz, 1H), 6.80 (td, J = 7.7, 1.7 Hz, 1H), 6.69 (td, J = 7.6, 1.6 Hz, 1H), 5.88–5.83 (m, 2H), 3.86–3.77 (m, 1H), 2.06–2.00 (m, 1H), 1.88–1.83 (m, 1H), 1.71–1.52 (m, 5H), 1.39–1.24 (m, 1H), 1.23–1.05 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.2, 168.2, 141.9, 139.90, 139.5, 133.5, 132.9, 131.4, 130.2, 129.5, 129.0, 128.7, 128.3, 128.1, 127.9, 126.8, 102.7, 94.5, 66.7, 48.9, 32.9, 32.7, 25.5, 24.8, 24.7; HRMS (ESI) m/z: Calcd for $C_{27}H_{26}I_2N_2O_2$ $[M + H]^+$ 665.0161, Found 665.0168; FT-IR δ 3350, 3041, 2970, 1687, 1632, 1016, 726 cm^{-1}.

N-(2-(cyclohexylamino)-1-(2-fluorophenyl)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5c):



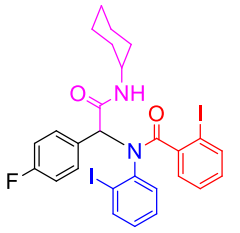
White solid, mp: 202-204 ℃; Yield 77% (525 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (dd, J = 8.0, 1.6 Hz, 1H), 7.66 (d, J = 7.9 Hz, 1H), 7.55–7.38 (m, 2H), 7.29–7.24 (m, 1H), 7.25–7.17 (m, 1H), 7.13 (td, J = 7.7, 1.5 Hz, 1H), 7.04 (td, J = 7.6, 1.2 Hz, 1H), 6.95 (ddd, J = 9.8, 8.2, 1.2 Hz, 1H), 6.86–6.78 (m, 2H), 6.73 (td, J = 7.7, 1.7 Hz, 1H), 6.30 (s, 1H), 6.05 (d, J = 7.9 Hz, 1H), 3.86–3.75 (m, 1H), 2.08–2.02 (m, 1H), 1.87–1.80 (m, 1H), 1.73–1.51 (m, 3H), 1.42–1.21 (m, 3H), 1.20–0.96 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.5, 167.5, 161.2 (d, J = 248.1 Hz), 141.6, 139.7, 139.4, 133.5, 132.6, 130.5 (d, J = 8.4 Hz), 130.4, 130.2, 129.7, 128.5, 127.6, 126.9, 123.5 (d, J = 3.5 Hz), 120.4 (d, J = 13.0 Hz), 115.2 (d, J = 23.0 Hz), 102.6, 94.2, 57.3, 49.0, 32.9, 32.6, 25.5, 24.7, 24.7; HRMS (ESI) m/z: Calcd for $C_{27}H_{25}FI_2NO_2$ $[M + H]^+$ 683.0067, Found 683.0061; FT-IR δ 3335, 2927, 2852, 1677, 1639, 1370, 1014, 637 cm^{-1}.

N-(1-(4-chlorophenyl)-2-(cyclohexylamino)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5d):



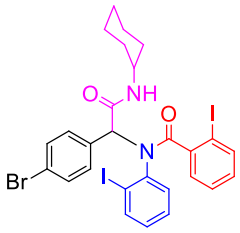
White solid, mp: 204-206 °C; Yield 79% (551 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.71–7.66 (m, 1H), 7.48 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.45–7.41 (m, 1H), 7.31 (d, *J* = 8.5 Hz, 2H), 7.14 (td, *J* = 7.8, 1.4 Hz, 1H), 7.10 (d, *J* = 8.5 Hz, 2H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.82 (td, *J* = 7.7, 1.7 Hz, 1H), 6.73 (td, *J* = 7.6, 1.6 Hz, 1H), 6.05 (d, *J* = 8.0 Hz, 1H), 5.81 (s, 1H), 3.87–3.75 (m, 1H), 2.07–1.99 (m, 1H), 1.88–1.78 (m, 1H), 1.73–1.66 (m, 1H), 1.6–1.51 (m, 2H), 1.37–1.19 (m, 3H), 1.19–1.03 (m, 2H); ^{13}C NMR (151 MHz, CDCl3) δ 170.3, 167.9, 141.6, 139.9, 139.6, 134.8, 133.5, 132.8, 131.3, 130.9, 130.3, 129.8, 129.4, 128.5, 128.1, 126.9, 102.7, 94.3, 65.9, 49.1, 32.9, 32.7, 25.5, 24.8, 24.7; HRMS (ESI) m/z: Calcd for $C_{27}H_{25}ClI_2N_2O_2$ $[M + H]^+$ 698.9772, Found 698.9776; FT-IR *δ* 3334, 2930, 2853, 1630, 1260, 1014, 749 cm^{-1}.

N-(2-(cyclohexylamino)-1-(4-fluorophenyl)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5e):



Yellow crystalline solid, mp: 130-133 °C; Yield 81% (552 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.68 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.50–7.40 (m, 2H), 7.37–7.30 (m, 2H), 7.13 (td, *J* = 7.7, 1.5 Hz, 1H), 7.03 (td, *J* = 7.6, 1.1 Hz, 1H), 6.83–6.78 (m, 3H), 6.72 (td, *J* = 7.6, 1.6 Hz, 1H), 5.99 (d, *J* = 8.0 Hz, 1H), 5.83 (s, 1H), 3.86–3.75 (m, 1H), 2.08–2.00 (m, 1H), 1.88–1.81 (m, 1H), 1.73–1.52 (m, 3H), 1.43–1.26 (m, 3H), 1.25–1.00 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) *δ* 170.2, 168.0, 162.8 (d, *J* = 248.6 Hz), 141.6, 139.8, 139.5, 133.5, 133.3 (d, *J* = 8.3 Hz), 131.2, 130.2, 129.7, 128.6 (d, *J* = 3.3 Hz), 128.4, 128.0, 126.8, 114.8 (d, *J* = 21.5 Hz), 102.9, 94.3, 65.6, 49.0, 32.9, 32.6, 25.5, 24.7, 24.7; HRMS (ESI) m/z: Calcd for $C_{27}H_{25}FI_2N_2O_2$ $[M + H]^+$ 683.0067, Found 683.0062; FT-IR *δ* 3337, 2926, 2854, 1676, 1634, 1246, 1013, 730 cm^{-1}.

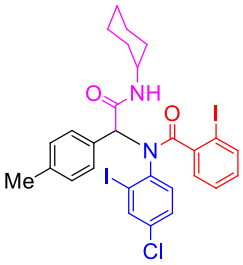
N-(1-(4-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5f):



White solid, mp: 170-173 °C; Yield 78% (578 mg); ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 7.92 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.50–7.46 (m, 2H), 7.46–7.42 (m, 1H), 7.26 (d, *J* = 2.3 Hz, 3H), 7.13 (td, *J* = 7.7, 1.5 Hz, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.82 (td, *J* = 7.7, 1.7 Hz, 1H), 6.73 (td, *J* = 7.7, 1.6 Hz, 1H), 6.06 (s, 1H), 5.79 (s, 1H), 3.86–3.75 (m, 1H), 2.10–2.00 (m,

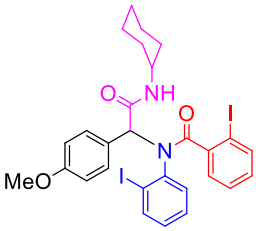
1H), 1.90–1.81 (m, 1H), 1.73–1.66 (m, 1H), 1.66–1.52 (m, 2H), 1.44–1.28 (m, 2H), 1.27–0.99 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.3, 167.7, 141.6, 139.8, 139.6, 133.4, 133.1, 131.8, 131.3, 131.0, 130.7, 130.3, 129.8, 128.5, 126.9, 123.1, 102.7, 94.3, 65.9, 49.1, 32.9, 32.6, 25.5, 24.8, 24.7; HRMS (ESI) m/z: Calcd for $C_{27}H_{25}BrI_2N_2O_2$ $[M + H]^+$ 742.9267, Found 742.9271; FT-IR δ 3336, 2926, 2855, 1677, 1632, 1012, 730 cm^{-1}.

N-(4-chloro-2-iodophenyl)-N-(2-(cyclohexylamino)-2-oxo-1-(p-tolyl)ethyl)-2-iodobenzamide (5g):



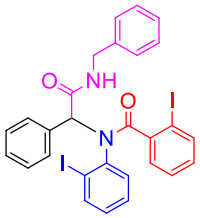
White solid, mp: 185-187 °C; Yield 69% (491 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, J = 8.6 Hz, 1H), 7.70 (dd, J = 8.0, 1.1 Hz, 1H), 7.41 (d, J = 2.5 Hz, 2H), 7.20 (d, J = 8.1 Hz, 2H), 7.14–7.09 (m, 1H), 7.05 (td, J = 7.6, 1.2 Hz, 1H), 6.95 (d, J = 7.9 Hz, 2H), 6.84 (td, J = 7.7, 1.7 Hz, 1H), 5.86 (s, 1H), 5.67 (d, J = 8.0 Hz, 1H), 3.83–3.74 (m, 1H), 2.24 (s, 3H), 2.03–1.98 (m, 1H), 1.87–1.81 (m, 1H), 1.65–1.53 (m, 3H), 1.38–1.24 (m, 2H), 1.20–0.98 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.9, 168.3, 140.6, 140.0, 138.8, 138.6, 134.1, 134.1, 131.2, 130.3, 129.4, 129.0, 128.8, 128.4, 126.9, 103.3, 66.0, 49.0, 32.8, 32.6, 25.5, 24.8, 24.7, 21.1; HRMS (ESI) m/z: Calcd for $C_{28}H_{27}ClI_2N_2O_2$ $[M + H]^+$ 712.9928, Found 712.9934; FT-IR δ 3337, 2910, 2852, 1675, 1643, 1015, 736 cm^{-1}.

N-(2-(cyclohexylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5h):



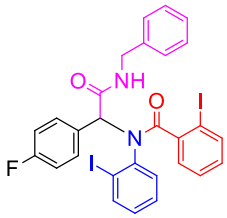
White solid, mp: 151-154 °C; Yield 54% (374 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (dd, J = 8.0, 1.6 Hz, 1H), 7.69–7.65 (m, 1H), 7.43 (dt, J = 8.1, 2.1 Hz, 2H), 7.28–7.23 (m, 2H), 7.13–7.09 (m, 1H), 7.01 (td, J = 7.6, 1.1 Hz, 1H), 6.79 (dt, J = 7.6, 2.9 Hz, 1H), 6.70–6.67 (m, 1H), 6.64–6.61 (m, 2H), 5.88 (d, J = 8.0 Hz, 1H), 5.80 (s, 1H), 3.81–3.76 (m, 1H), 3.69 (s, 3H), 2.05–1.98 (m, 1H), 1.87–1.81 (m, 1H), 1.70–1.63 (m, 1H), 1.59–1.53 (m, 2H), 1.34–1.27 (m, 2H), 1.20–1.02 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.1, 168.5, 159.7, 141.8, 139.8, 139.4, 133.5, 132.7, 130.9, 130.1, 129.5, 128.8, 128.3, 126.7, 124.8, 113.2, 102.9, 94.3, 65.9, 55.1, 48.9, 32.9, 32.7, 25.5, 24.8, 24.7; HRMS (ESI) m/z: Calcd for $C_{28}H_{28}I_2N_2O_3$ $[M + H]^+$ 695.0267, Found 695.0251; FT-IR δ 3335, 2933, 2843, 1676, 1631, 1249, 1012, 756 cm^{-1}.

N-(2-(benzylamino)-2-oxo-1-phenylethyl)-2-iodo-N-(2-iodophenyl)benzamide (5i):



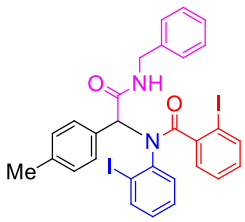
White solid, mp: 197-199 °C; Yield 84% (564 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (dd, J = 8.0, 1.6 Hz, 1H), 7.75–7.71 (m, 1H), 7.50 (ddd, J = 20.9, 7.8, 1.5 Hz, 2H), 7.42–7.36 (m, 3H), 7.36–7.30 (m, 3H), 7.27–7.22 (m, 2H), 7.20–7.14 (m, 3H), 7.08 (td, J = 7.6, 1.1 Hz, 1H), 6.86 (qd, J = 6.9, 1.6 Hz, 1H), 6.75 (td, J = 7.6, 1.6 Hz, 1H), 6.40 (t, J = 5.8 Hz, 1H), 6.01 (s, 1H), 4.61 (dd, J = 15.0, 5.8 Hz, 1H), 4.50 (dd, J = 15.0, 5.6 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.3, 169.1, 141.6, 139.8, 139.4, 138.0, 133.6, 132.4, 131.6, 130.2, 129.6, 129.3, 128.8, 128.6, 128.4, 128.2, 127.9, 127.7, 127.3, 126.8, 103.0, 94.2, 66.4, 43.9; HRMS (ESI) m/z: Calcd for $C_{28}H_{22}I_2N_2O_2$ $[M + H]^+$ 672.9848, Found 672.9834. FT-IR δ 3313, 3062, 2924, 1684, 1629, 1230, 1016, 726 cm^{-1}.

N-(2-(benzylamino)-1-(4-fluorophenyl)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5j):



White solid, mp: 92-95 °C; Yield 89% (614 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (dd, J = 8.0, 1.6 Hz, 1H), 7.72–7.64 (m, 1H), 7.46 (dd, J = 8.0, 1.5 Hz, 2H), 7.35–7.29 (m, 3H), 7.28 (d, J = 2.4 Hz, 2H), 7.25–7.20 (m, 2H), 7.15 (td, J = 7.7, 1.4 Hz, 1H), 7.04 (td, J = 7.6, 1.1 Hz, 1H), 6.84–6.79 (m, 3H), 6.74 (td, J = 7.6, 1.6 Hz, 1H), 6.45 (t, J = 5.8 Hz, 1H), 5.96 (s, 1H), 4.57 (dd, J = 14.9, 5.8 Hz, 1H), 4.46 (dd, J = 14.9, 5.7 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.4, 169.0, 162.9 (d, J = 248.7 Hz), 141.3, 140.4, 139.8, 139.5, 137.8, 133.5 (d, J = 8.3 Hz), 133.4, 130.3, 129.8, 128.6, 128.6, 128.2, 128.1 (d, J = 3.4 Hz), 127.7, 127.4, 126.9, 114.8 (d, J = 21.5 Hz), 103.1, 94.1, 65.2, 43.9; HRMS (ESI) m/z: Calcd for $C_{28}H_{21}FI_2N_2O_2$ $[M + H]^+$ 690.9754, Found 690.9759; FT-IR δ 3353, 3012, 2904, 1683, 1640, 1223, 1018, 721 cm^{-1}.

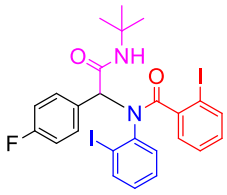
N-(2-(benzylamino)-2-oxo-1-(p-tolyl)ethyl)-2-iodo-N-(2-iodophenyl)benzamide (5k):



White solid, mp: 92-95 °C; Yield 76% (521 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (dd, J = 8.0, 1.6 Hz, 1H), 7.68 (dt, J = 8.3, 1.9 Hz, 1H), 7.52–7.46 (m, 2H), 7.37–7.26 (m, 3H), 7.24–7.19 (m, 3H), 7.15–7.01 (m, 3H), 6.92 (d, J = 7.9 Hz, 2H), 6.84–6.78 (m, 1H), 6.71 (td, J = 7.7, 1.6 Hz, 1H), 6.27 (t, J = 5.8 Hz, 1H), 5.91 (s, 1H), 4.57 (dd, J = 15.0, 5.9 Hz, 1H), 4.44 (dd, J = 15.0, 5.6 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.3, 169.3, 141.8, 139.8, 139.4, 138.7,

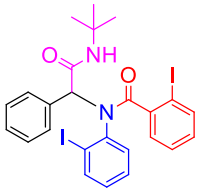
138.0, 133.5, 131.4, 130.2, 129.5, 129.3, 128.9, 128.7, 128.6, 128.4, 128.2, 127.7, 127.3, 126.8, 102.9, 94.2, 66.2, 43.8, 21.1; HRMS (ESI) m/z: Calcd for $C_{29}H_{24}I_2N_2O_2$ $[M + H]^+$ 687.0005, Found 687.0012; FT-IR δ 3353, 3012, 2983, 1683, 1640, 1231, 1017, 721 cm^{-1}.

N-(2-(tert-butylamino)-1-(4-fluorophenyl)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5l):



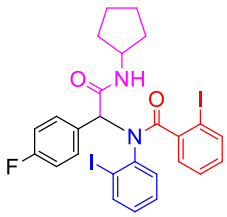
White solid, mp: 96-98 ℃; Yield 57% (373 mg); ^{1}H NMR (600 MHz,) δ 7.95 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.72–7.67 (m, 1H), 7.45 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.40 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.36–7.30 (m, 2H), 7.13 (td, *J* = 7.7, 1.5 Hz, 1H), 7.04–7.00 (m, 1H), 6.83–6.78 (m, 3H), 6.72–6.70 (m, 1H), 5.95 (s, 1H), 5.76 (s, 1H), 1.37 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.1, 168.2, 162.8 (d, *J* = 248.4 Hz), 141.6, 140.0, 139.4, 133.7, 133.3 (d, *J* = 8.3 Hz), 130.7, 130.2, 129.6, 128.6 (d, *J* = 3.3 Hz), 128.4, 128.2, 126.8, 114.7 (d, *J* = 21.4 Hz), 102.9, 94.4, 66.0, 51.8, 28.7; HRMS (ESI) m/z: Calcd for $C_{25}H_{23}FI_2N_2O_2$ $[M + H]^+$ 656.9911, Found 656.9902; FT-IR δ 3354, 3056, 2964, 1684, 1635, 1015, 728 cm^{-1}.

N-(2-(tert-butylamino)-2-oxo-1-phenylethyl)-2-iodo-N-(2-iodophenyl)benzamide (5m):



White solid, mp: 181-183 ℃; Yield 47% (300 mg); ^{1}H NMR (600 MHz,) δ 8.03 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.75 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.46 (td, *J* = 7.8, 1.5 Hz, 2H), 7.42–7.39 (m, 2H), 7.23–7.20 (m, 1H), 7.16 (ddd, *J* = 8.6, 6.6, 1.5 Hz, 3H), 7.05 (td, *J* = 7.6, 1.2 Hz, 1H), 6.85 (td, *J* = 7.7, 1.7 Hz, 1H), 6.73–6.70 (m, 1H), 5.90 (s, 1H), 5.84 (s, 1H), 1.40 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.0, 168.3, 141.8, 140.0, 139.3, 133.7, 132.8, 131.4, 130.2, 129.4, 129.0, 128.6, 128.2, 128.1, 127.8, 126.7, 102.9, 94.6, 67.0, 51.7, 28.7; HRMS (ESI) m/z: Calcd for $C_{25}H_{24}I_2N_2O_2$ $[M + H]^+$ 639.0005, Found 639.0011; FT-IR δ 3349, 3058, 2966, 1679, 1635, 1014, 730 cm^{-1}.

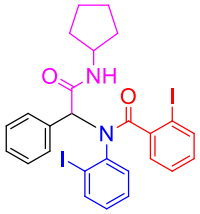
N-(2-(cyclopentylamino)-1-(4-fluorophenyl)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5n):



White solid, mp: 124-127 ℃; Yield 83% (554 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.67 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.47–7.43 (m, 2H), 7.36–7.32 (m, 2H), 7.14 (td, *J* = 7.7, 1.5 Hz, 1H), 7.03 (td, *J* = 7.6, 1.1 Hz, 1H), 6.82–6.77 (m, 3H), 6.72 (td, *J* = 7.6, 1.6 Hz, 1H), 6.23 (d, *J* = 7.1 Hz, 1H), 5.87 (s, 1H), 4.28–4.17 (m, 1H), 2.06–1.96 (m, 1H), 1.95–1.87 (m, 1H), 1.70–1.63

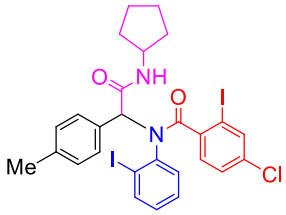
(m, 1H), 1.61–1.50 (m, 4H), 1.41–1.26 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.3, 168.6, 162.8 (d, *J* = 248.1 Hz), 141.5, 139.8, 139.5, 133.5 (d, *J* = 9.9 Hz), 133.4, 133.0, 130.2, 129.7, 128.5, 128.4 (d, *J* = 3.3 Hz), 127.9, 126.8, 114.7 (d, *J* = 21.5 Hz), 103.0, 94.2, 65.4, 51.9, 33.0, 32.8, 23.8, 23.7; HRMS (ESI) m/z: Calcd for $C_{26}H_{23}FI_2N_2O_2$ $[M + H]^+$ 668.9911, Found 668.9905; FT-IR *δ* 3336, 3012, 2954, 1681, 1633, 1014, 728 cm^{-1}.

N-(2-(cyclopentylamino)-2-oxo-1-phenylethyl)-2-iodo-N-(2-iodophenyl)benzamide (5o):



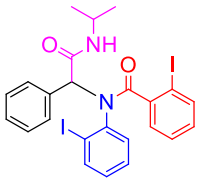
White solid, mp: 221-223 °C; Yield 72% (468 mg); ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 8.00 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.70–7.66 (m, 1H), 7.43 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.38–7.33 (m, 2H), 7.32–7.24 (m, 1H), 7.21–7.15 (m, 1H), 7.12 (td, *J* = 7.6, 1.5 Hz, 3H), 7.04–6.99 (m, 1H), 6.83–6.77 (m, 1H), 6.71–6.66 (m, 1H), 6.08 (d, *J* = 7.2 Hz, 1H), 5.88 (s, 1H), 4.28–4.18 (m, 1H), 2.03–1.96 (m, 1H), 1.95–1.86 (m, 1H), 1.66–1.61 (m, 1H), 1.58–1.50 (m, 4H), 1.37–1.30 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) *δ* 170.1, 168.7, 141.8, 140.2, 139.9, 139.4, 133.6, 132.7, 131.5, 130.2, 129.5, 128.7, 128.3, 128.1, 127.8, 126.7, 102.9, 94.4, 66.5, 51.9, 33.0, 32.8, 23.8, 23.7; HRMS (ESI) m/z: Calcd for $C_{26}H_{24}I_2N_2O_2$ $[M + H]^+$ 651.0005, Found 651.0011; FT-IR *δ* 3341, 2998, 2937, 1668, 1628, 1011, 724 cm^{-1}.

4-chloro-N-(2-(cyclopentylamino)-2-oxo-1-(p-tolyl)ethyl)-2-iodo-N-(2-iodophenyl)benzamide (5p):



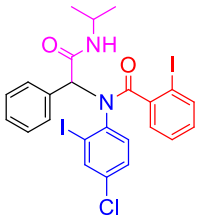
White solid, mp: 208-210 °C; Yield 74% (516 mg); ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 8.04 (d, *J* = 8.6 Hz, 1H), 7.69 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.45–7.38 (m, 2H), 7.22–7.18 (m, 2H), 7.10 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.06–7.03 (m, 1H), 6.93 (d, *J* = 7.9 Hz, 2H), 6.86–6.80 (m, 1H), 5.96–5.83 (m, 2H), 4.23–4.16 (m, 1H), 2.23 (s, 3H), 2.01–1.95 (m, 1H), 1.92–1.85 (m, 1H), 1.64–1.59 (m, 1H), 1.56–1.47 (m, 4H), 1.32–1.26 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) *δ* 169.9, 168.9, 140.6, 140.0, 138.8, 138.5, 134.1, 134.1, 131.3, 130.3, 129.4, 129.3, 129.0, 128.7, 128.4, 126.9, 103.5, 94.3, 65.8, 51.9, 33.0, 32.7, 23.8, 23.7, 21.2; HRMS (ESI) m/z: Calcd for $C_{27}H_{25}ClI_2N_2O_2$ $[M + H]^+$ 698.9772, Found 698.9763; FT-IR *δ* 3339, 3016, 2947, 1676, 1630, 1015, 728 cm^{-1}.

2-iodo-N-(2-iodophenyl)-N-(2-(isopropylamino)-2-oxo-1-phenylethyl)benzamide (5q):



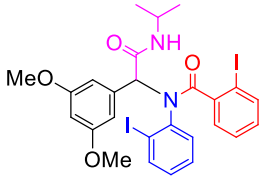
White solid, mp: 194-196 °C; Yield 52% (324 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (dd, J = 7.9, 1.6 Hz, 1H), 7.69 (dd, J = 8.0, 1.1 Hz, 1H), 7.44 (td, J = 7.6, 1.6 Hz, 2H), 7.37–7.34 (m, 2H), 7.21–7.16 (m, 1H), 7.12 (ddd, J = 8.5, 6.3, 1.5 Hz, 3H), 7.02 (td, J = 7.6, 1.2 Hz, 1H), 6.80 (td, J = 7.7, 1.7 Hz, 1H), 6.68 (td, J = 7.6, 1.7 Hz, 1H), 5.86 (s, 1H), 5.83 (d, J = 7.8 Hz, 1H), 4.16–4.05 (m, 1H), 1.21 (d, J = 6.6 Hz, 3H), 1.08 (d, J = 6.5 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.1, 168.3, 141.8, 139.9, 139.4, 133.6, 132.7, 131.4, 130.2, 129.5, 129.0, 128.7, 128.3, 128.1, 127.8, 126.7, 102.8, 94.4, 66.6, 42.1, 22.7, 22.4; HRMS (ESI) m/z: Calcd for $C_{24}H_{22}I_2N_2O_2$ $[M + H]^+$ 624.9848, Found 624.9854; FT-IR δ 3351, 3048, 2975, 1681, 1638, 1017, 736 cm^{-1}.

N-(4-chloro-2-iodophenyl)-2-iodo-N-(2-(isopropylamino)-2-oxo-1-phenylethyl)benzamide (5r):



White solid, mp: 204-206 °C; Yield 56% (368 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (dd, J = 8.0, 1.6 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.47 (dd, J = 7.9, 1.4 Hz, 1H), 7.43 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 8.3 Hz, 2H), 7.18 – 7.08 (m, 3H), 7.04 (t, J = 7.6 Hz, 1H), 6.82 (td, J = 7.7, 1.6 Hz, 1H), 6.73 (td, J = 7.7, 1.6 Hz, 1H), 5.93 (d, J = 7.7 Hz, 1H), 5.80 (s, 1H), 4.14-4.06 (m, 1H), 1.24 (d, J = 6.6 Hz, 3H), 1.10 (d, J = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.3, 167.9, 141.5, 139.9, 139.6, 134.8, 133.5, 132.8, 131.1, 130.5, 130.3, 129.8, 128.5, 128.3, 128.0, 126.8, 102.8, 94.2, 65.7, 42.2, 22.7, 22.4; HRMS (ESI) m/z: Calcd for $C_{24}H_{21}ClI_2N_2O_2$ $[M + H]^+$ 658.9459, Found 658.9478; FT-IR δ 3353, 3049, 2945, 1661, 1618, 1015, 726 cm^{-1}.

N-(1-(3,5-dimethoxyphenyl)-2-(isopropylamino)-2-oxoethyl)-2-iodo-N-(2-iodophenyl)benzamide (5s):



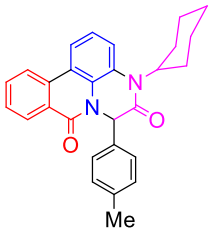
White solid, mp: 201-203 °C; Yield 64% (437 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (dd, J = 8.0, 1.6 Hz, 1H), 7.64 – 7.53 (m, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.34 (dd, J = 7.9, 1.5 Hz, 1H), 7.05 (td, J = 7.6, 1.5 Hz, 1H), 6.95 – 6.86 (m, 1H), 6.68 (td, J = 7.6, 1.6 Hz, 1H), 6.58 (td, J = 7.6, 1.6 Hz, 1H), 6.49 (d, J = 2.3 Hz, 2H), 6.34 (d, J = 7.7 Hz, 1H), 6.16 (t, J = 2.3 Hz, 1H), 5.89 (s, 1H), 4.02 – 3.98 (m, 1H), 3.50 (s, 6H), 1.12 (d, J = 6.6 Hz, 3H), 0.99 (d, J = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.8, 168.3, 159.8, 141.9, 139.9, 139.3, 134.6, 133.6, 130.1, 129.4, 128.1, 126.6, 109.6, 107.3, 103.2, 101.1, 100.3, 94.5, 66.2, 55.3, 42.0, 22.5, 22.3; HRMS (ESI) m/z: Calcd for

$C_{26}H_{26}I_2N_2O_4$ $[M + H]^+$ 685.0060, Found 685.0031; FT-IR δ 3334, 3014, 2957, 1686, 1635, 1015, 718 cm^{-1}.

General procedure of the synthesis of 4-(alkyl)-6-(aryl)-6-hydro-4*H*,8*H*-pyrazino[3,2,1-de]phenanthridine-5,8-diones (6a-q).

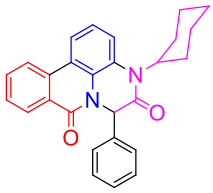
Ugi product **5** (0.50 mmol) was added to a solution containing potassium carbonate (1.15 mmol, 159 mg), $Pd(OAc)_2$ (0.10 mmol, 11.20 mg) in DMF (2.5 mL) at 110 °C for 12 h. The progress of the reaction was monitored employing thin-layer chromatography (TLC) (n-hexane/ EtOAc 4:1). Upon completion, the reaction mixture was cooled to room temperature, H_2O (20 mL) was added, the reaction mixture was extracted by DCM (3*20 mL). Combined organic layers were washed with brine, dried with sodium sulfate, filtered, and concentrated under the vacuum. The obtained mixture was purified by employing column chromatography on silica gel using (n-hexane/EtOAc 4:1) as the eluent to afford desired product 4-(alkyl)-6-(aryl)-6-hydro-4*H*,8*H*-pyrazino[3,2,1-de]phenanthridine-5,8-diones as the desired products. Yields (52-93%).

4-cyclohexyl-6-(p-tolyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6a):



White solid, mp: 194-196 °C; Yield 85% (179 mg);^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 7.96 (dd, 1H), 7.78–7.73 (m, 1H), 7.59–7.54 (m, 1H), 7.36–7.28 (m, 2H), 7.05–7.01 (m, 2H), 6.97–6.93 (m, 2H), 6.72 (s, 1H), 4.36 (s, 1H), 2.57–2.47 (m, 1H), 2.40–2.31 (m, 1H), 2.17 (s, 3H), 1.90–1.85 (m, 2H), 1.81 (d, *J* = 12.8 Hz, 1H), 1.74–1.66 (m, 3H), 1.45–1.34 (m, 2H); ^{13}C NMR (151 MHz, CDCl3) δ ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.9, 160.6, 138.0, 133.8, 133.3, 133.0, 129.4, 129.3, 128.9, 128.4, 126.3, 125.6, 125.3, 122.9, 122.2, 119.5, 117.6, 115.5, 58.9, 29.9, 28.5, 26.6, 26.3, 25.3, 21.0; HRMS (ESI) m/z: Calcd for $C_{28}H_{26}N_2O_2$ $[M + H]^+$ 423.2072, Found 423.2063; FT-IR δ 2931, 2854, 1675, 1630, 1260, 1012, 749 cm^{-1}.

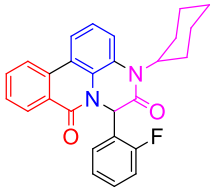
4-cyclohexyl-6-phenylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6b):



White solid, mp: 208-210 °C; Yield 80% (163 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, J = 6.7 Hz, 1H), 8.24 (d, J = 8.2 Hz, 1H), 7.95 (d, J = 7.9 Hz, 1H), 7.75 (t, J = 7.6 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.35–7.28 (m, 2H), 7.14 (s, 5H), 6.76 (s, 1H), 4.36 (s, 1H), 2.58–2.46 (m, 1H), 2.40–2.29 (m, 1H), 1.87–

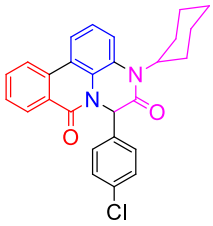
1.80 (m, 2H), 1.72–1.65 (m, 2H), 1.37–1.25 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.7, 160.5, 136.7, 133.3, 133.0, 128.8, 128.8, 128.5, 128.2, 126.4, 125.5, 125.3, 123.0, 122.2, 119.5, 117.6, 115.6, 59.1, 29.9, 28.5, 26.6, 26.3, 25.3; HRMS (ESI) m/z: Calcd for $C_{27}H_{24}N_2O_2$ $[M + H]^+$ 409.1916, Found 409.1923; FT-IR δ 2930, 2856, 1671, 1601, 1258, 1011, 751 cm^{-1}.

4-cyclohexyl-6-(2-fluorophenyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione ***(6c)***:



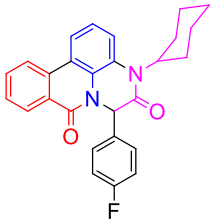
White solid, mp: 121-123 °C; Yield 81% (172 mg); ^{1}H NMR (600 MHz, $CDCl_3$) *δ* ^{1}H NMR (600 MHz,) *δ* 8.40 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 7.98 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.75 (ddd, *J* = 8.3, 7.1, 1.5 Hz, 1H), 7.54 (ddd, *J* = 8.1, 7.1, 1.0 Hz, 1H), 7.40–7.31 (m, 2H), 7.23–7.13 (m, 2H), 6.97–6.90 (m, 2H), 6.80 (s, 1H), 4.33 (s, 1H), 2.66–2.51 (m, 1H), 2.43–2.28 (m, 1H), 1.92–1.66 (m, 6H), 1.50–1.25 (m, 2H); ^{13}C NMR (151 MHz, DMSO) δ 163.1, 159.6 (d, *J* = 247.9 Hz), 159.1, 133.5, 133.1, 130.4 (d, *J* = 8.2 Hz), 128.7, 128.6, 128.0, 127.7, 125.8, 125.7, 124.6, 124.3, 123.5, 123.1, 118.4, 118.1, 115.7 (d, *J* = 22.0 Hz), 54.0, 28.9, 27.98, 25.9, 25.5, 25.0; ^{19}F NMR (565 MHz, $CDCl_3$) δ -112.55; HRMS (ESI) m/z: Calcd for $C_{27}H_{23}FN_2O_2$ $[M + H]^+$ 427.1821, Found 427.1829; FT-IR *δ* 2925, 2852, 1655, 1592, 1260, 1012, 750 cm^{-1}.

6-(4-chlorophenyl)-4-cyclohexylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione ***(6d)***:



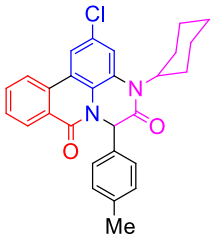
White solid, mp: 191-193 °C; Yield 87% (192 mg); ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 8.44 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.97 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.80–7.74 (m, 1H), 7.60–7.55 (m, 1H), 7.36–7.29 (m, 2H), 7.14–7.09 (m, 2H), 7.09–7.05 (m, 2H), 6.70 (s, 1H), 4.34 (s, 1H), 2.55–2.46 (m, 1H), 2.38–2.29 (m, 1H), 1.89–1.84 (m, 2H), 1.82–1.76 (m, 1H), 1.71–1.66 (m, 3H), 1.43–1.31 (m, 2H); ^{13}C NMR (151 MHz, CDCl3) *δ* 164.3, 160.5, 135.3, 134.3, 133.3, 133.2, 130.3, 129.0, 128.9, 128.6, 127.8, 125.3, 125.2, 123.2, 122.3, 119.6, 117.8, 115.7, 58.6, 29.9, 28.6, 26.7, 26.3, 25.3; HRMS (ESI) m/z: Calcd for $C_{27}H_{23}ClN_2O_2$ $[M + H]^+$ 443.1526, Found 443.1521; FT-IR *δ* 2929, 2850, 1651, 1596, 1261, 1012, 748 cm^{-1}.

4-cyclohexyl-6-(4-fluorophenyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione ***(6e)***:



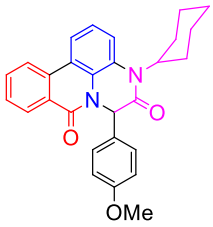
White solid, mp: 131-133 ℃; Yield 84% (178 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.97 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.80–7.75 (m, 1H), 7.60–7.56 (m, 1H), 7.37–7.30 (m, 2H), 7.15–7.10 (m, 2H), 6.86–6.80 (m, 2H), 6.72 (s, 1H), 4.35 (s, 1H), 2.56–2.47 (m, 1H), 2.39–2.30 (m, 1H), 1.88–1.86 (m, 2H), 1.82–1.76 (m, 1H), 1.72–1.66 (m, 2H), 1.42–1.32 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.6, 162.6 (d, J = 247.1 Hz), 160.6, 133.3, 133.2, 132.7 (d, J = 3.3 Hz), 128.9, 128.6, 128.3 (d, J = 8.3 Hz), 125.3, 125.3, 123.2, 122.3, 119.6, 117.8, 115.8 (d, J = 21.6 Hz), 58.5, 29.9, 28.6, 26.7, 26.3, 25.3; ^{19}F NMR (565 MHz, $CDCl_3$) δ -113.20; HRMS (ESI) m/z: Calcd for $C_{27}H_{21}FN_2O_2$ [M + H]+ 427.1821, Found 427.1813; FT-IR δ 2934, 2861, 1669, 1595, 1260, 1012, 749 cm^{-1}.

2-chloro-4-cyclohexyl-6-(p-tolyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione ***(6f)***:



White solid, mp: 197-199 ℃; Yield 72% (164 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.17 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 2.0 Hz, 1H), 7.80–7.75 (m, 1H), 7.62–7.58 (m, 1H), 7.27 (d, *J* = 2.0 Hz, 1H), 7.03–6.94 (m, 4H), 6.68 (s, 1H), 4.27 (s, 1H), 2.53–2.45 (m, 1H), 2.38–2.29 (m, 1H), 2.19 (s, 3H), 1.91–1.85 (m, 3H), 1.78 (d, *J* = 12.9 Hz, 1H), 1.69 (s, 2H), 1.46–1.29 (m, 2H); ^{13}C NMR (151 MHz, CDCl3) δ 164.8, 160.3, 138.3, 133.5, 133.3, 132.3, 129.6, 129.1, 129.0, 128.7, 126.3, 125.5, 124.3, 122.3, 120.5, 117.1, 115.5, 58.8, 29.8, 28.4, 26.6, 26.3, 25.3, 21.0. HRMS (ESI) m/z: Calcd for $C_{28}H_{25}ClN_2O_2$ $[M + H]^+$ 457.1683, Found 457.1674; FT-IR δ 2928, 2854, 1681, 1656, 1566, 1313, 773 cm^{-1}.

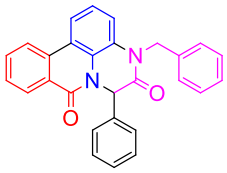
4-cyclohexyl-6-(4-methoxyphenyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione ***(6g)***:



White solid, mp: 187-189 ℃; Yield 63% (138 mg); ^{1}H NMR (600 MHz, CDCl3) δ 8.45 (d, *J* = 7.9 Hz, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 7.9 Hz, 1H), 7.75 (t, *J* = 7.3 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.37–7.28 (m, 2H), 7.07 (d, *J* = 8.5 Hz, 2H), 6.71–6.64 (m, 3H), 4.36 (s, 1H), 3.64 (s, 3H), 2.57–2.47 (m, 1H), 2.41–2.30 (m, 1H), 1.90–1.83 (m, 2H), 1.83–1.77 (m, 1H), 1.72–1.66 (m, 2H), 1.44–1.29 (m, 3H); ^{13}C NMR (151 MHz, CDCl3) δ 165.0, 160.6, 159.5, 133.3, 133.0, 129.0, 128.9, 128.5, 127.8, 125.5, 125.4, 122.9, 122.2, 119.6, 117.6, 115.6, 114.4, 114.2, 58.6, 55.2, 29.9, 28.6, 26.7,

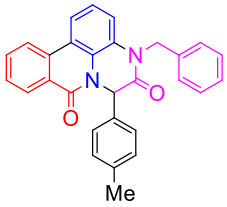
26.3, 25.4; HRMS (ESI) m/z: Calcd for $C_{28}H_{26}N_2O_3$ $[M + H]^+$ 439.2021, Found 439.2029; FT-IR δ 2925, 2853, 1656, 1592, 1509, 1259, 750 cm^{-1}.

4-benzyl-6-phenylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6h):



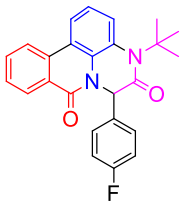
White solid, mp:174-176 ℃; Yield 90% (187 mg); ^{1}H NMR (600 MHz,) δ 8.56 (d, *J* = 8.3 Hz, 1H), 8.28 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.22 (d, *J* = 8.1 Hz, 1H), 7.92–7.86 (m, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.32–7.26 (m, 4H), 7.21 (td, *J* = 12.8, 7.6 Hz, 4H), 7.17–7.10 (m, 4H), 6.65 (s, 1H), 5.40 (d, *J* = 16.6 Hz, 1H), 5.14 (d, *J* = 16.5 Hz, 1H); ^{13}C NMR (151 MHz, DMSO) δ 163.4, 159.3, 137.3, 136.0, 133.6, 133.0, 128.9, 128.9, 128.6, 128.4, 127.8, 127.2, 127.0, 126.4, 126.1, 124.5, 124.1, 123.5, 123.2, 118.4, 118.3, 115.9, 58.5, 44.6; HRMS (ESI) m/z: Calcd for $C_{28}H_{20}N_2O_2$ $[M + H]^+$ 417.1603, Found 417.1611; FT-IR δ 2931, 2858, 1665, 1607, 1519, 1260, 765 cm^{-1}.

4-benzyl-6-(p-tolyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6i):



White solid, mp: 224-226 ℃; Yield 93% (200 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.26 (d, *J* = 8.2 Hz, 1H), 7.97–7.94 (m, 1H), 7.79–7.75 (m, 1H), 7.60–7.56 (m, 1H), 7.23–7.17 (m, 4H), 7.15–7.09 (m, 4H), 7.07–7.04 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.87 (s, 1H), 5.60 (d, *J* = 16.3 Hz, 1H), 4.93 (d, *J* = 16.3 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (151 MHz, CDCl3) δ 164.4, 160.4, 138.4, 135.8, 134.0, 133.3, 133.1, 131.5, 129.6, 129.0, 128.9, 128.6, 127.5, 126.4, 126.3, 125.4, 124.8, 123.3, 122.7, 119.1, 117.9, 115.4, 58.7, 46.0, 21.1. HRMS (ESI) m/z: Calcd for $C_{29}H_{22}N_2O_2$ $[M + H]^+$ 431.1760, Found 431.1764; FT-IR δ 2923, 2859, 1671, 1651, 1599, 1509, 1259, 750 cm^{-1}.

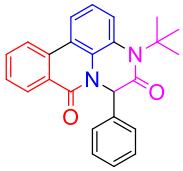
4-(tert-butyl)-6-(4-fluorophenyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6j):



White solid, mp: 118-120 ℃; Yield 58% (116 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.22 (d, *J* = 8.1 Hz, 1H), 7.94 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.79–7.74 (m, 1H), 7.58–7.55 (m, 1H), 7.34–7.32 (m, 1H), 7.28 (t, *J* = 8.0 Hz, 1H), 7.03–6.98 (m, 2H), 6.82–6.76 (m, 2H), 6.63 (s, 1H), 1.64 (s, 9H); ^{13}C NMR (151 MHz, CDCl3) δ 169.1, 162.5 (d, *J* = 246.8 Hz), 161.1, 133.3, 133.2, 132.6 (d, *J* = 3.3 Hz), 129.6 (d, *J* = 7.9 Hz), 128.9, 128.6, 128.5, 128.3, 128.1, 125.5, 122.1, 120.8, 119.5, 117.9, 115.6 (d, *J* = 21.8 Hz), 61.2, 60.8, 30.2; ^{19}F NMR (565 MHz, $CDCl_3$) δ -115.69; HRMS (ESI) m/z:

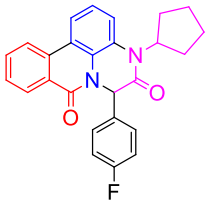
Calcd for $C_{25}H_{21}FN_2O_2$ $[M + H]^+$ 401.1665, Found 401.1673; FT-IR δ 2926, 2850, 1659, 1590, 1502, 1269, 760 cm^{-1}.

4-(tert-butyl)-6-phenylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6k):



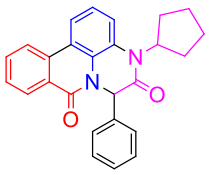
White solid, mp: 158-160 °C; Yield 52% (99 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.78 (s, 1H), 8.54 (dd, J = 8.0, 1.5 Hz, 1H), 8.20 (d, J = 8.1 Hz, 1H), 8.11 (d, J = 8.0 Hz, 1H), 7.84–7.79 (m, 1H), 7.77–7.73 (m, 2H), 7.67–7.63 (m, 1H), 7.54–7.49 (m, 1H), 7.40 (t, J = 7.7 Hz, 2H), 7.14 (dd, J = 7.6, 1.2 Hz, 1H), 7.01 (t, J = 7.9 Hz, 1H), 1.62 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.7, 160.8, 134.2, 133.2, 132.9, 131.4, 129.2, 128.7, 128.7, 126.9, 125.9, 124.2, 123.0, 123.0, 122.2, 121.7, 119.9, 116.3, 60.7, 28.3; HRMS (ESI) m/z: Calcd for $C_{25}H_{22}N_2O_2$ $[M + H]^+$ 383.1759, Found 383.1768; FT-IR δ 2932, 2857, 1663, 1594, 1505, 1266, 757 cm^{-1}.

4-cyclopentyl-6-(4-fluorophenyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6l):



White solid, mp: 147-149 °C; Yield 85% (175 mg); ^{1}H NMR (600 MHz, DMSO) δ 8.55 (d, J = 8.2 Hz, 1H), 8.29–8.22 (m, 2H), 8.06 (s, 1H), 7.92–7.86 (m, 1H), 7.71–7.64 (m, 1H), 7.56 (d, J = 8.1 Hz, 1H), 7.41 (t, J = 8.1 Hz, 1H), 7.12–7.02 (m, 3H), 6.48 (s, 1H), 4.97–4.88 (m, 1H), 2.24–2.16 (m, 1H), 1.95–1.77 (m, 5H), 1.61–1.53 (m, 2H); ^{13}C NMR (151 MHz, DMSO) δ 163.1, 161.8 (d, J = 245.0 Hz), 159.5, 133.6, 133.1 (d, J = 3.2 Hz), 133.0, 129.5, 128.9, 128.2, 128.1 (d, J = 8.4 Hz), 127.9, 124.4, 123.7, 123.2, 118.7, 118.3, 116.2, 115.8 (d, J = 21.9 Hz), 58.0, 56.7, 28.3, 27.7, 25.4, 25.2; ^{19}F NMR (565 MHz, CDCl3) δ -114.87; HRMS (ESI) m/z: Calcd for $C_{26}H_{21}FN_2O_2$ $[M + H]$+ 413.1665, Found 413.1672; FT-IR δ 2937, 2863, 1666, 1599, 1262, 1014, 750 cm^{-1}.

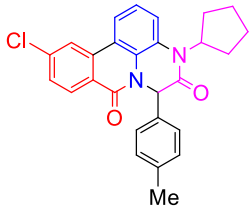
4-cyclopentyl-6-phenylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6m):



White solid, mp: 221-223 °C; Yield 66% (130 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (dd, J = 8.0, 1.4 Hz, 1H), 8.25 (d, J = 8.2 Hz, 1H), 7.97 (dd, J = 8.0, 1.2 Hz, 1H), 7.79–7.74 (m, 1H), 7.60–7.54 (m, 1H), 7.34–7.25 (m, 2H), 7.15 (s, 5H), 6.77 (s, 1H), 5.07–4.98 (m, 1H), 2.34–2.25 (m, 1H), 2.11–1.87 (m, 5H), 1.70–1.61 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.4, 160.5, 136.7, 133.3, 133.0, 128.9, 128.8, 128.6, 128.5, 128.3, 126.5, 125.5, 125.3, 122.9, 122.2, 119.5, 117.6, 115.6, 59.1, 56.9, 28.7, 27.8,

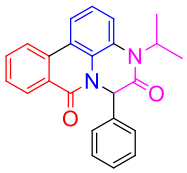
25.8, 25.4; HRMS (ESI) m/z: Calcd for $C_{26}H_{22}N_2O_2$ $[M + H]^+$ 395.1759, Found 395.1751; FT-IR δ 2934, 2853, 1677, 1600, 1253, 1012, 756 cm^{-1}.

10-chloro-4-cyclopentyl-6-(p-tolyl)pyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6n):



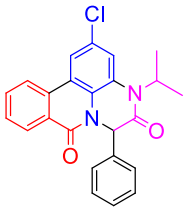
White solid, mp: 201-203 ℃; Yield 74% (163 mg); ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 8.43 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.14 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 2.0 Hz, 1H), 7.80–7.73 (m, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.23 (s, 1H), 7.02 (d, *J* = 8.1 Hz, 2H), 6.97 (d, *J* = 8.1 Hz, 2H), 6.69 (s, 1H), 4.99–4.90 (m, 1H), 2.31–2.23 (m, 1H), 2.18 (s, 3H), 2.09–1.88 (m, 5H), 1.71–1.62 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) *δ* 164.4, 160.1, 138.3, 133.5, 133.2, 132.2, 129.8, 129.6, 129.1, 128.9, 128.6, 126.3, 125.5, 124.1, 122.2, 120.4, 117.0, 115.6, 58.8, 57.1, 28.8, 27.8, 25.8, 25.5, 21.0; HRMS (ESI) m/z: Calcd for $C_{27}H_{23}ClN_2O_2$ $[M + H]^+$ 443.1526, Found 443.1531; FT-IR δ 2939, 2850, 1672, 1590, 1258, 1013, 754 cm^{-1}.

4-isopropyl-6-phenylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6o):



White solid, mp: 165-167 ℃; Yield 81% (149 mg); ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 8.45 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.97 (dd, *J* = 6.5, 2.7 Hz, 1H), 7.78–7.73 (m, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 6.6 Hz, 2H), 7.15 (s, 5H), 6.76 (s, 1H), 5.01–4.90 (m, 1H), 1.59 (d, *J* = 7.0 Hz, 3H), 1.49 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) *δ* 164.4, 160.5, 136.7, 133.3, 133.0, 128.9, 128.8, 128.5, 128.3, 128.2, 126.4, 125.5, 125.3, 123.0, 122.2, 119.5, 117.6, 115.5, 59.0, 20.5, 19.0; HRMS (ESI) m/z: Calcd for $C_{24}H_{20}N_2O_2$ $[M + H]^+$ 369.1603, Found 369.1609; FT-IR *δ* 2937, 2849, 1657, 1584, 1500, 1261, 753 cm^{-1}.

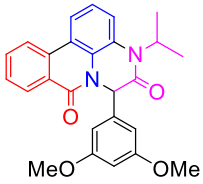
2-chloro-4-isopropyl-6-phenylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6p):



White solid, mp: 171-173 ℃; Yield 76% (152 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.27 (d, *J* = 8.2 Hz, 1H), 7.99 (dd, *J* = 5.2, 4.0 Hz, 1H), 7.79 (ddd, *J* = 8.4, 7.1, 1.5 Hz, 1H), 7.59 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 7.35 – 7.31 (m, 2H), 7.16 – 7.11 (m, 2H), 7.11 – 7.05 (m, 2H), 6.71 (s, 1H), 4.98 – 4.89 (m, 1H), 1.59 (d, *J* = 7.0 Hz, 3H), 1.50 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.1, 160.5, 135.2, 134.3, 133.3, 133.2, 129.0, 128.9, 128.6, 127.8, 125.2, 125.2, 123.1, 122.3,

119.6, 117.8, 115.6, 58.5, 20.5, 19.0; HRMS (ESI) m/z: Calcd for $C_{24}H_{19}ClN_2O_2$ $[M + H]^+$ 403.1213, Found 403.1234; FT-IR δ 2947, 2841, 1667, 1580, 1507, 1249, 751 cm^{-1}.

6-(3,5-dimethoxyphenyl)-4-isopropylpyrazino[3,2,1-de]phenanthridine-5,8(4H,6H)-dione (6q):



White solid, mp: 153-155 °C; Yield 81% (173 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.97 (dd, *J* = 6.4, 2.9 Hz, 1H), 7.77 (ddd, *J* = 8.4, 7.2, 1.5 Hz, 1H), 7.58 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H), 7.34 – 7.30 (m, 2H), 6.68 (s, 1H), 6.30 (d, *J* = 2.3 Hz, 2H), 6.25 (t, *J* = 2.3 Hz, 1H), 5.01 – 4.87 (m, 1H), 3.61 (s, 6H), 1.59 (d, *J* = 6.9 Hz, 3H), 1.50 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.2, 160.8, 138.9, 133.3, 133.0, 128.9, 128.5, 128.1, 125.5, 125.2, 123.0, 122.2, 119.5, 117.7, 115.5, 104.6, 100.2, 59.1, 55.2, 20.5, 19.0; HRMS (ESI) m/z: Calcd for $C_{26}H_{24}N_2O_4$ $[M + H]^+$ 429.1814, Found 429.1792; FT-IR δ 2936, 2859, 1655, 1564, 1511, 1267, 761 cm^{-1}.

Crystal Data

X-ray Crystallography

Crystal data are summarized in Table 1. Single crystal of **6j** and **6h** were mounted on a MiTeGen loop with grease and examined on a Bruker D8 Venture APEX diffractometer equipped with Photon 100 CCD area detector at 296 (2) K using graphite mono-chromatized Mo-K_α radiation (λ = 0.71073Å). Data were collected using the APEX 3 software,[1] integrated using SAINT [2] and corrected for absorption using a multi-scan approach (SADABS).[3] Final cell constants were determined from full least squares refinement of all observed reflections. The structure was solved using intrinsic phasing (SHELXT).[4] All non-H atoms were located in subsequent difference maps and refined anisotropically. H-atoms were added at calculated positions and refined with a riding model.

Table 1: Crystal data for **6h** and **6j**.

Compounds	**6j**	**6h**
Chemical formula	$C_{25}H_{21}FN_2O_2$	$C_{28}H_{20}N_2O_2$
Mr	400.456	416.46
Crystal system, space group	Monoclinic, Cc	Triclinic, P-1

Temperature (K)	296	296
a (Å)	13.9745(6)	9.0733(17)
b (Å)	20.9846(8)	11.2285(18)
c (Å)	7.8209(4)	21.135(4)
α (°)	90	85.568(7)
β (°)	119.645(1)	87.255(8)
γ (°)	90	81.710(7)
V ($Å^3$)	1993.27(15)	2122.9(7)
Z	4	4
Radiation type	MoK_α	MoK_α
μ (mm^{-1})	0.092	0.083
Absorption correction	Multi-scan, SADABS	Multi-scan, SADABS
T_{min}, T_{max}	0.7059, 07454	0.6797, 0.7454
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11556, 4066, 3499	63534, 8660, 6331
R_{int}	0.0302	0.0578
$(\sin\theta/\lambda)_{max}$ ($Å^{-1}$)	0.625	0.625
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0351, 0.0893, 1.0922	0.0752, 0.2705, 1.093
No. of reflections	4066	8660
No. of parameters	163275	579
$\Delta\rho_{max}$, $\Delta\rho_{min}$ ($eÅ^{-3}$)	0.15, -0.14	0.360, -0.289
CCDC	2259069	2265884

References

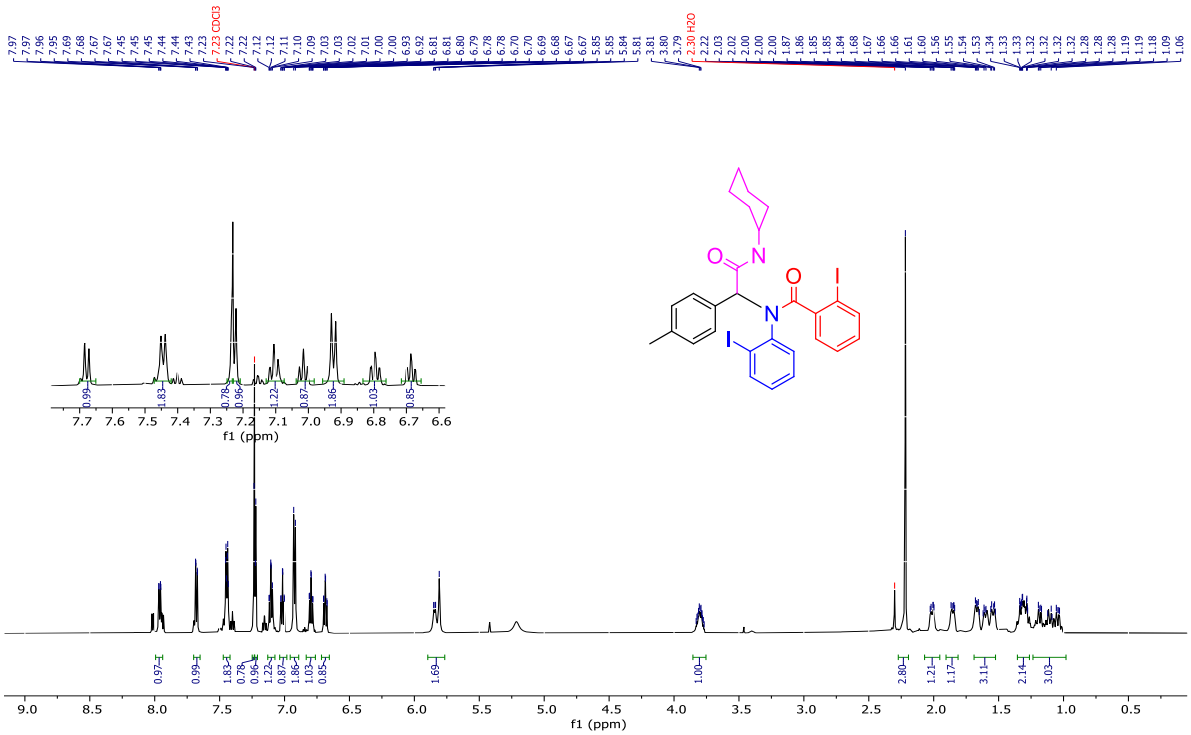
1. APEX 4, v 2022. 1-1, Bruker AXS, Madison, Wisconsin, USA.

2. SAINT V8.40B, Bruker AXS, Madison, Wisconsin, USA.

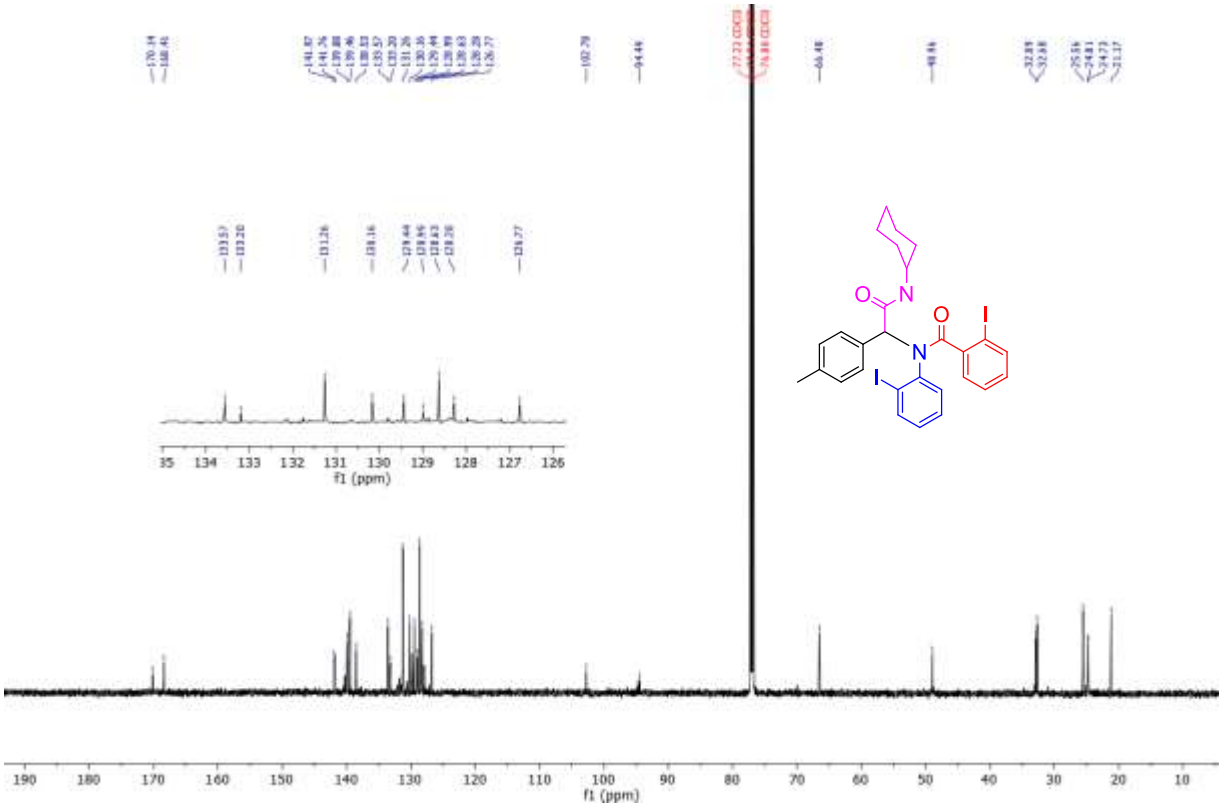
3. SADABS-2016/2, Bruker AXS, Madison, Wisconsin, USA.

4. G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Crystallogr.* **1990**, *46*, 467–473.

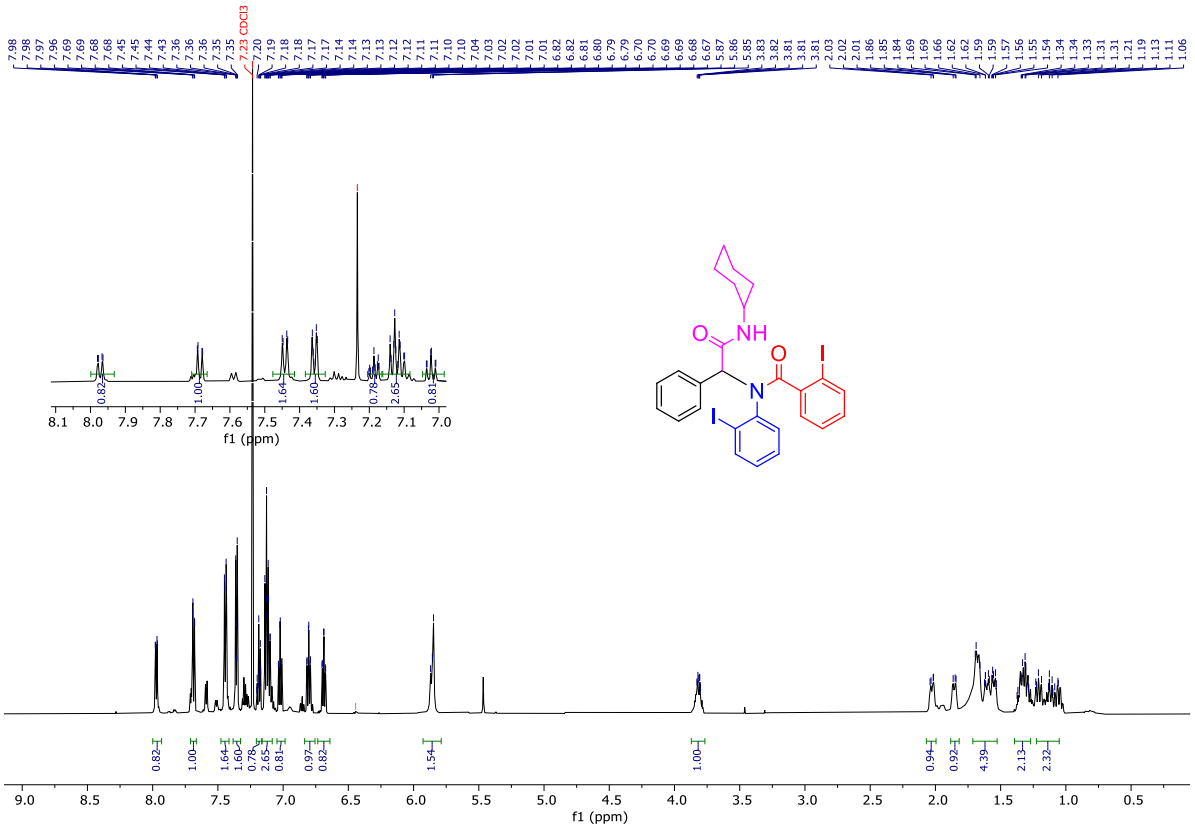
Copy of spectra



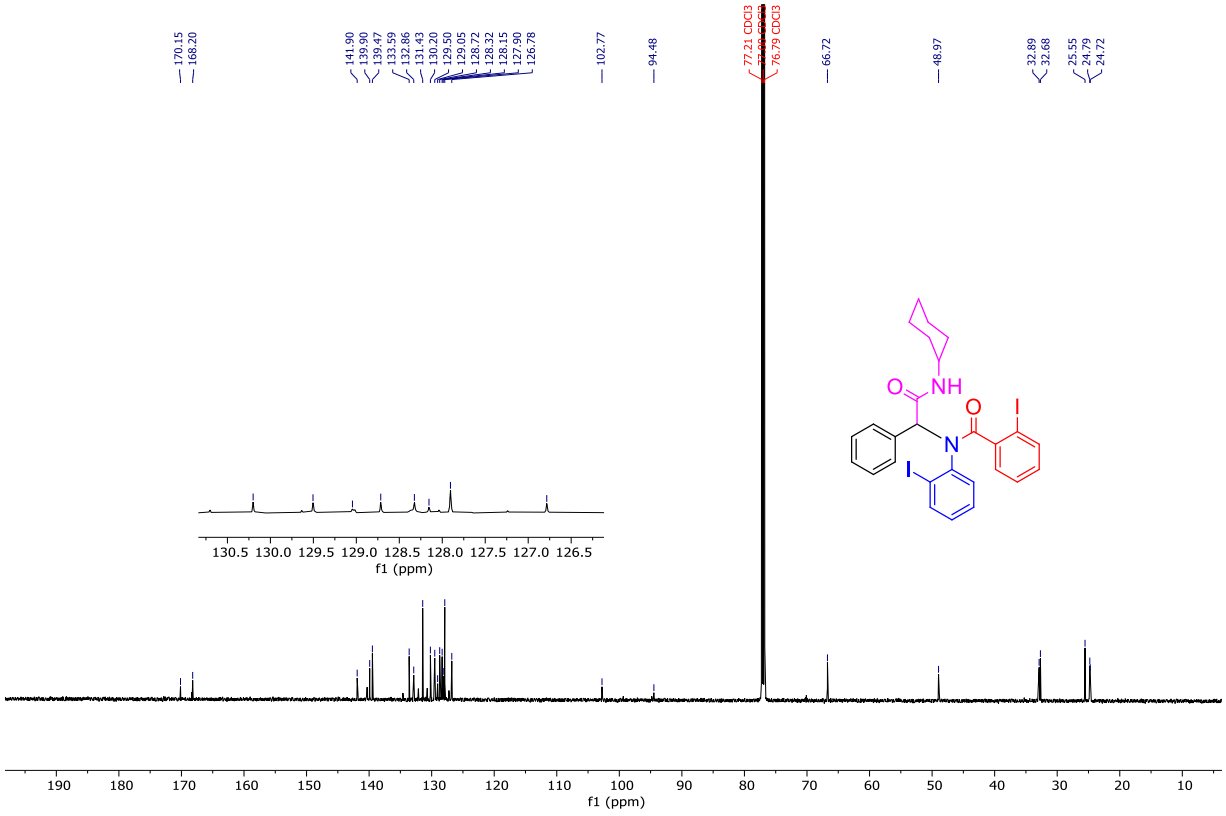
^{1}H-NMR of compound 5a (600MHz, $CDCl_3$)



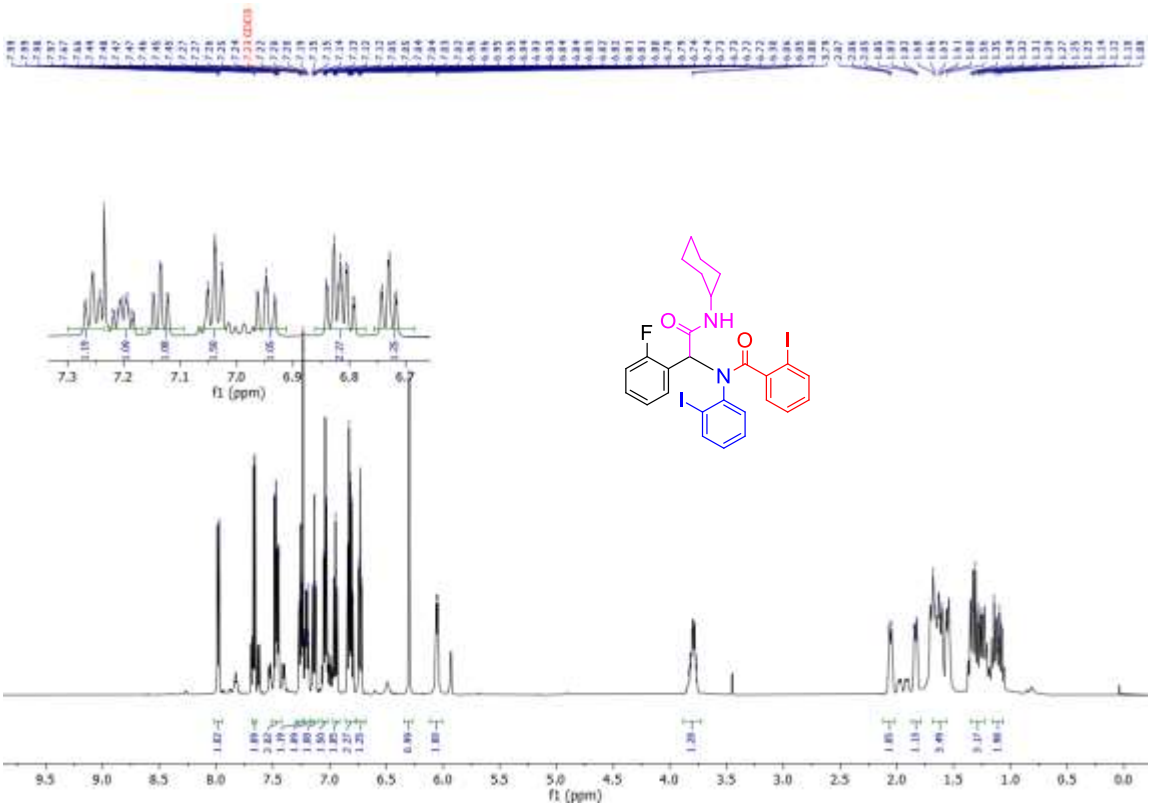
^{13}C-NMR of compound **5a** (151MHz, $CDCl_3$)



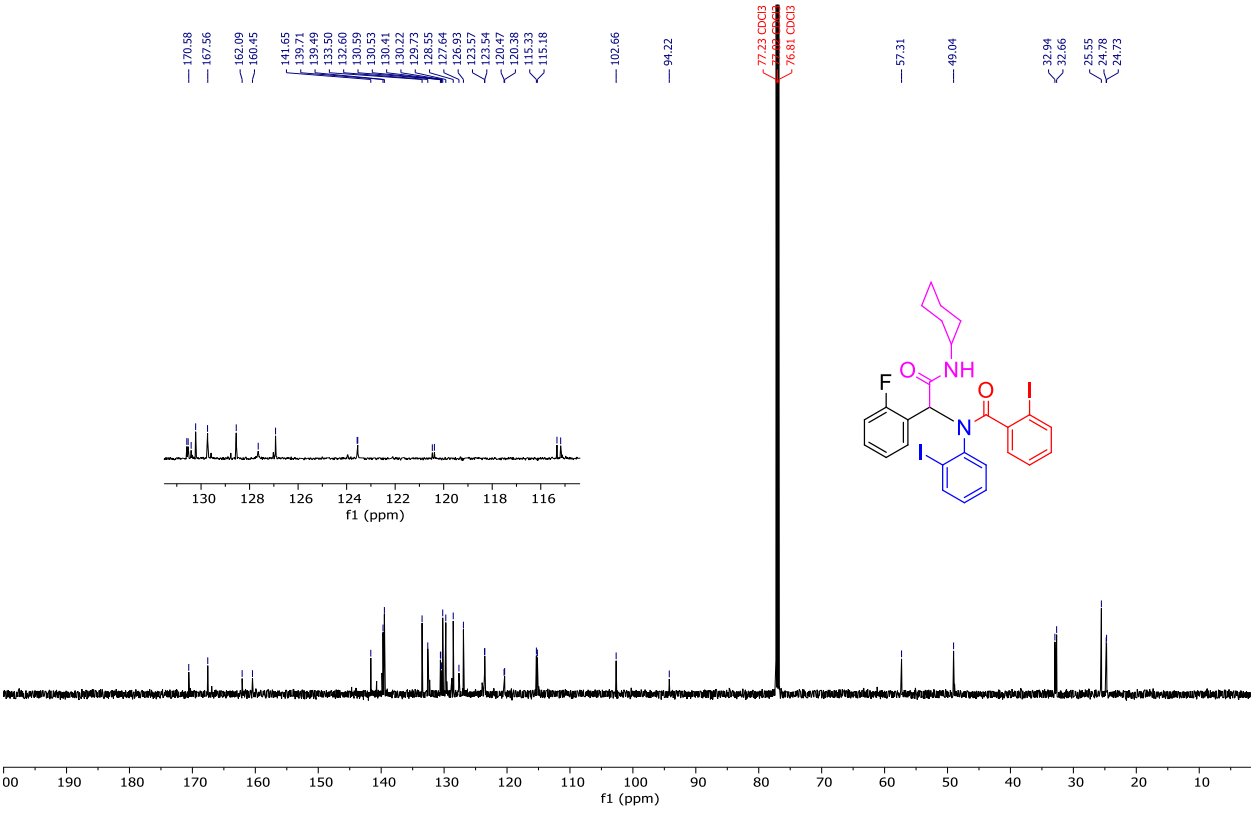
^{1}H-NMR of compound **5b** (600MHz, $CDCl_3$)



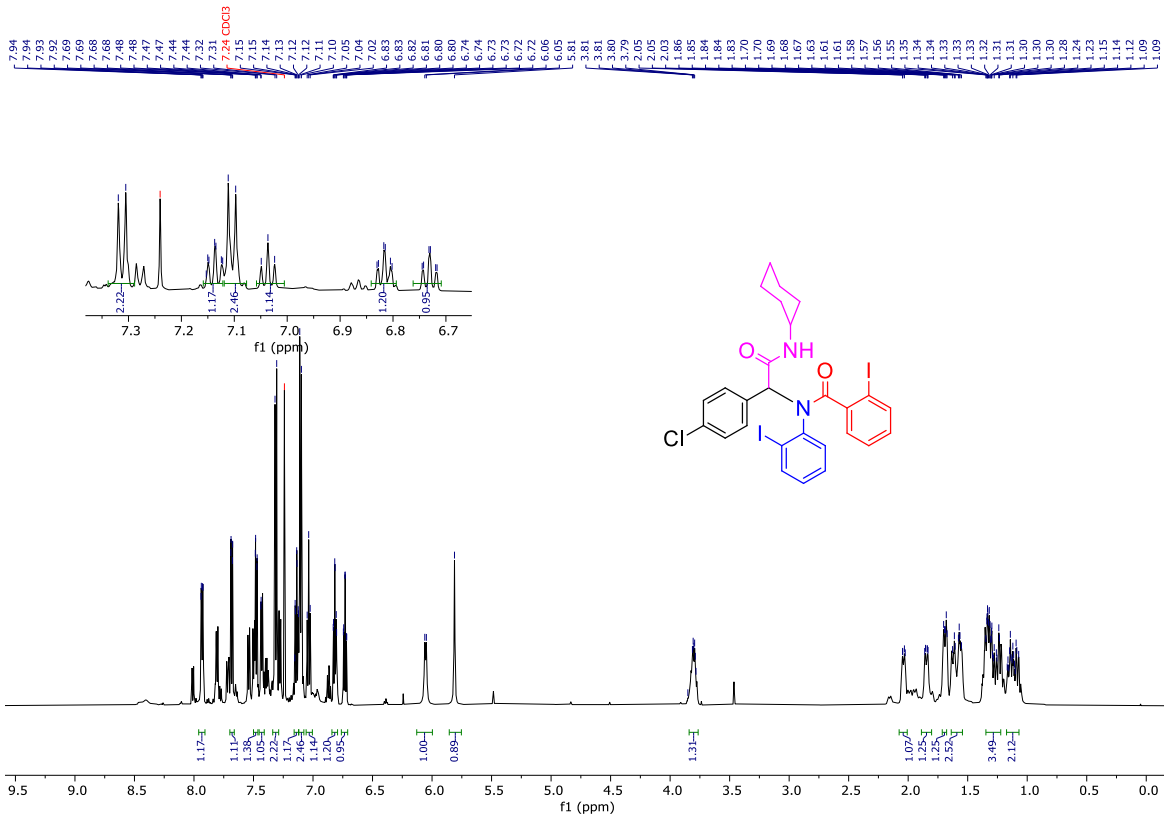
^{13}C-NMR of compound **5b** (151MHz, $CDCl_3$)



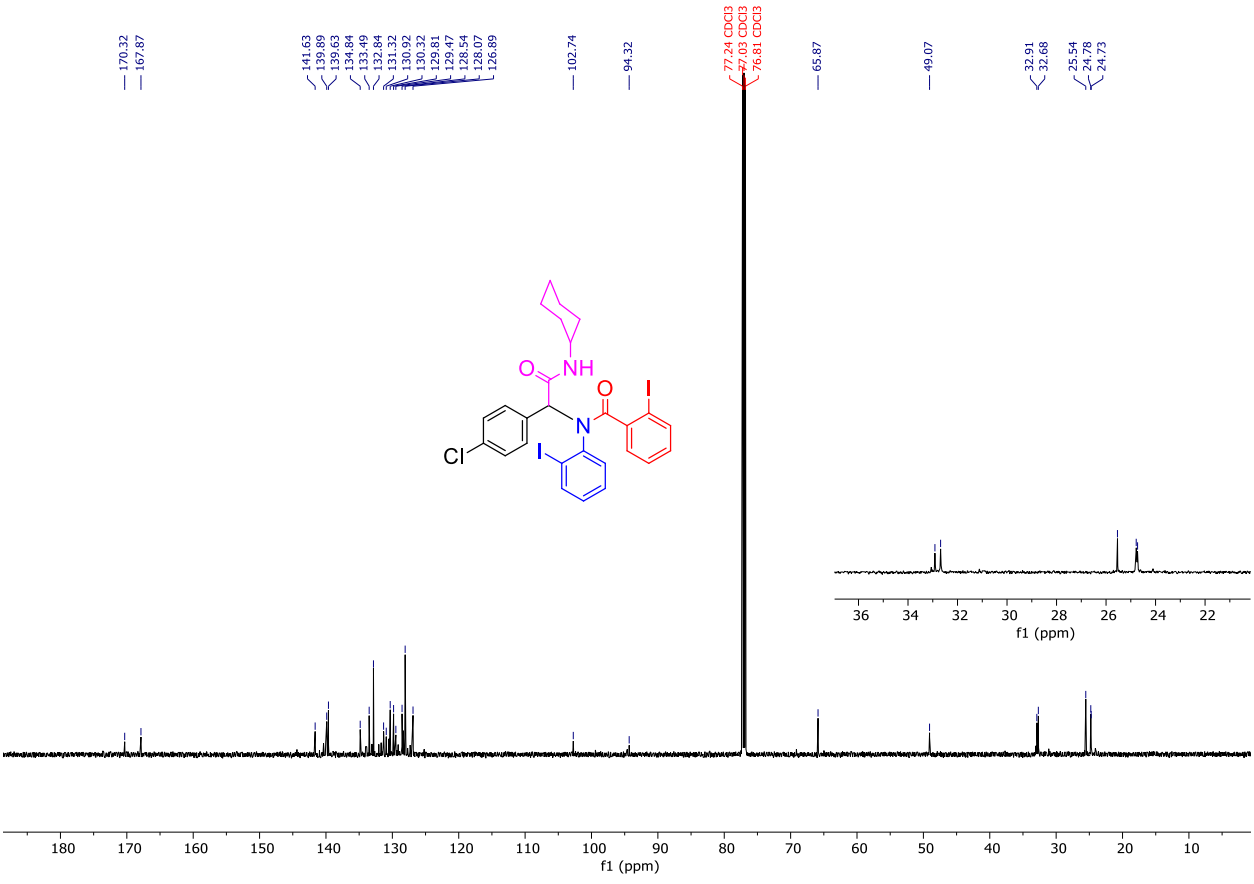
^{1}H-NMR of compound **5c** (600MHz, $CDCl_3$)



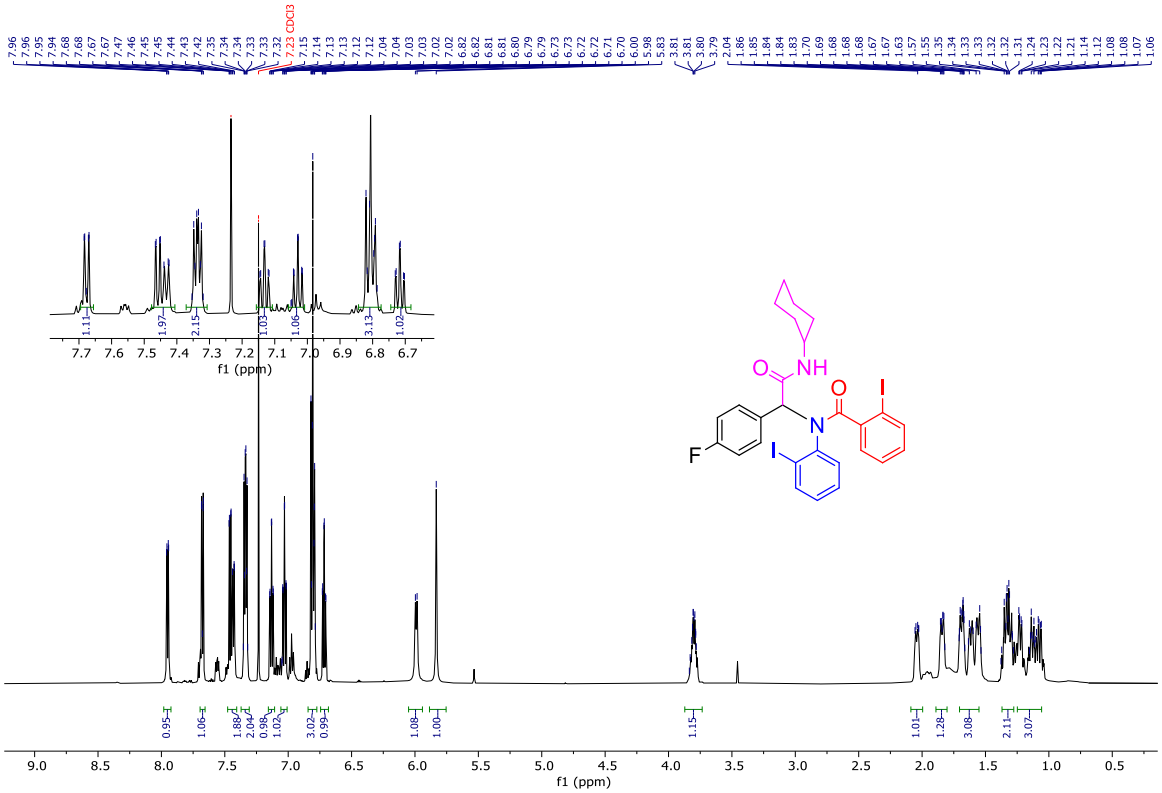
^{13}C-NMR of compound **5c** (151MHz, $CDCl_3$)



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



^{13}C-NMR of compound **5d** (151MHz, $CDCl_3$)



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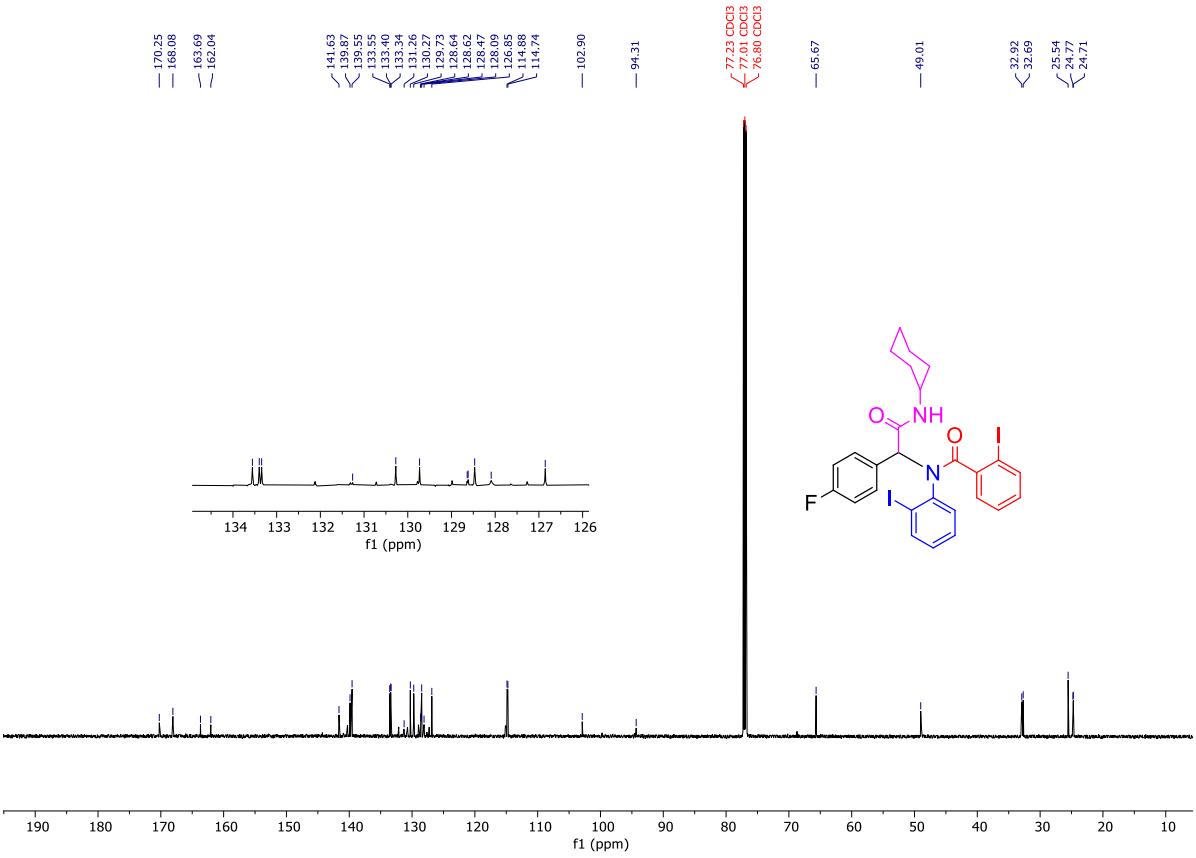

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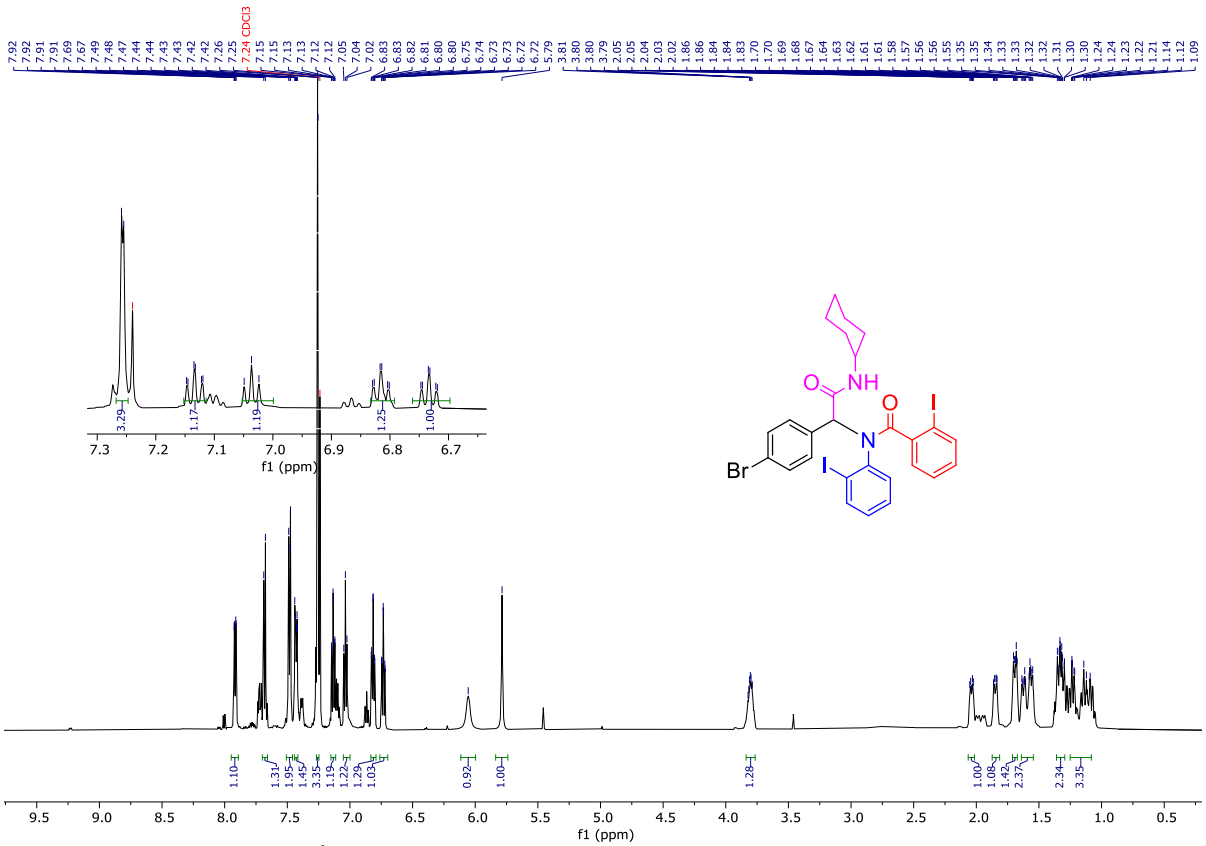
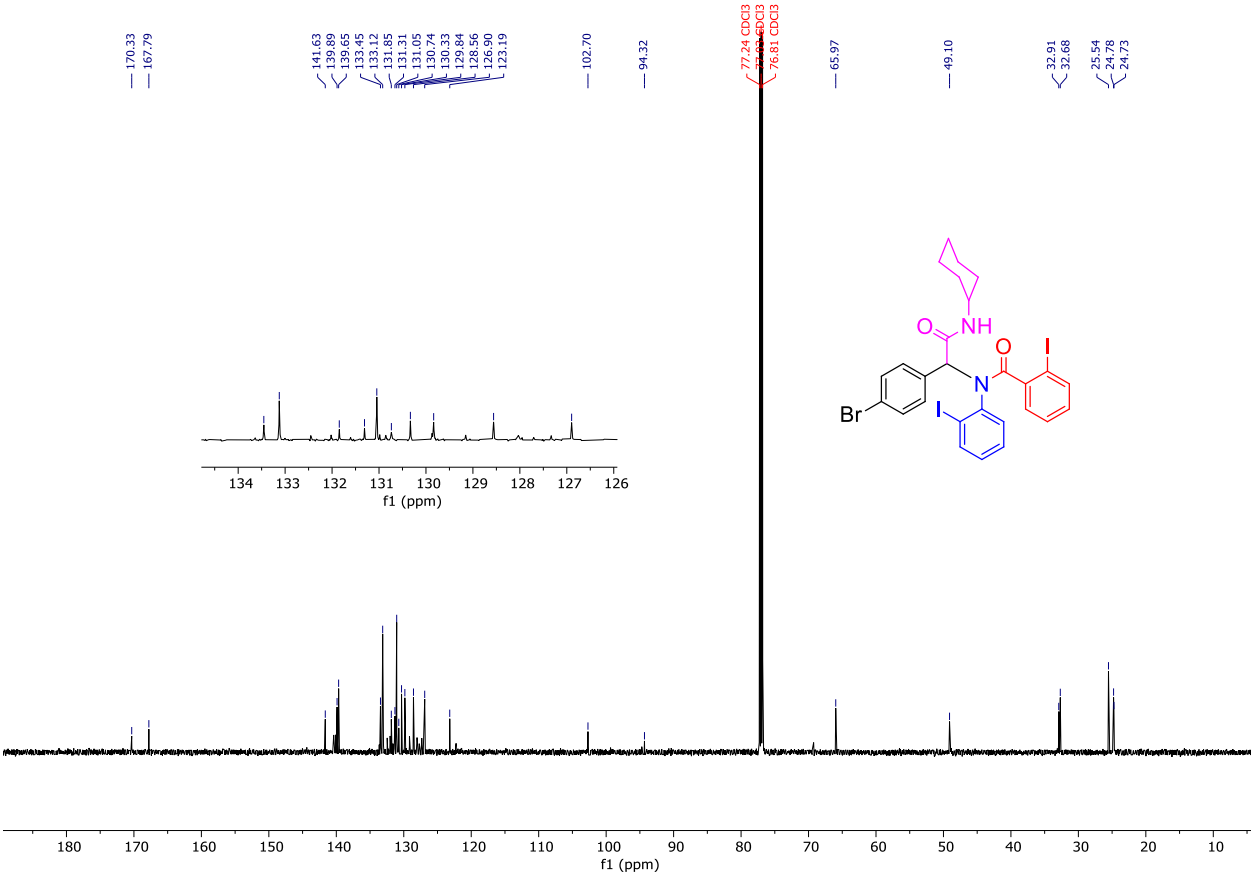


^{1}H-NMR of compound **5f** (600MHz, $CDCl_3$)



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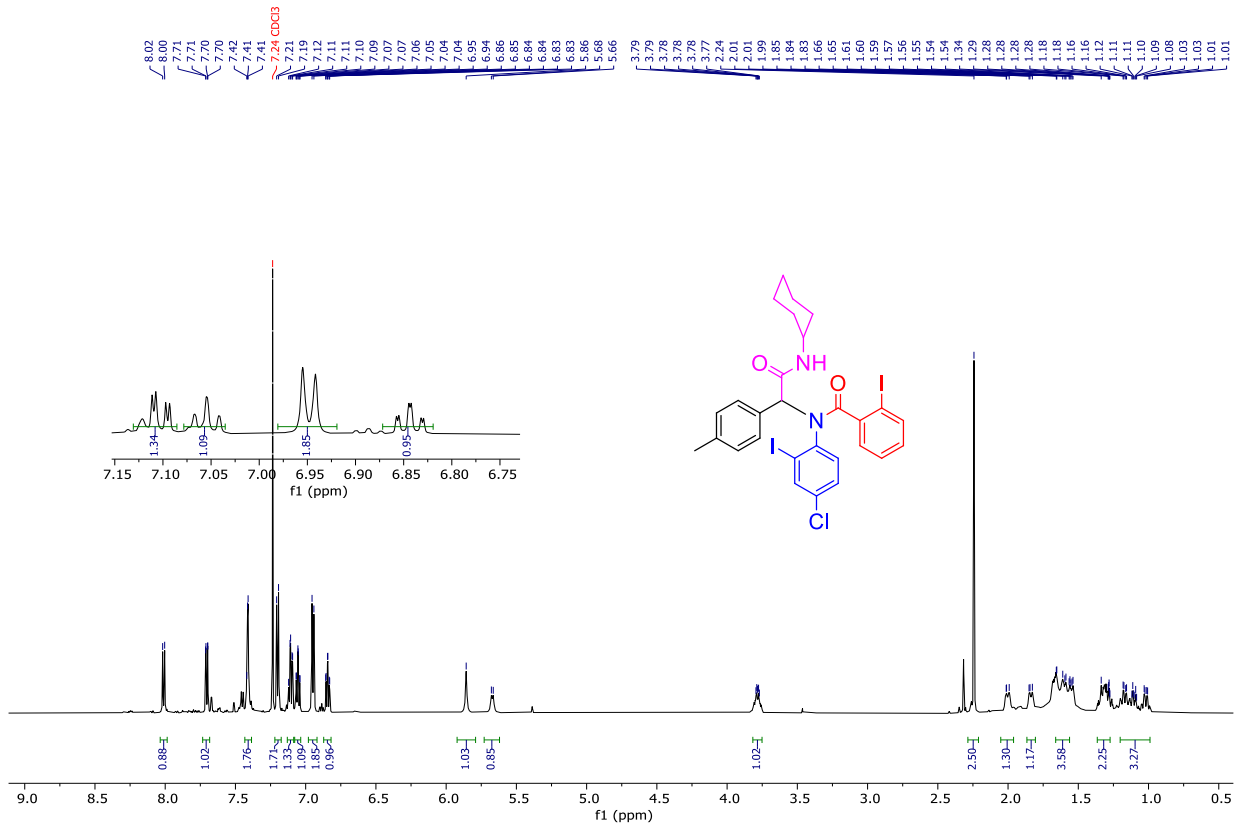
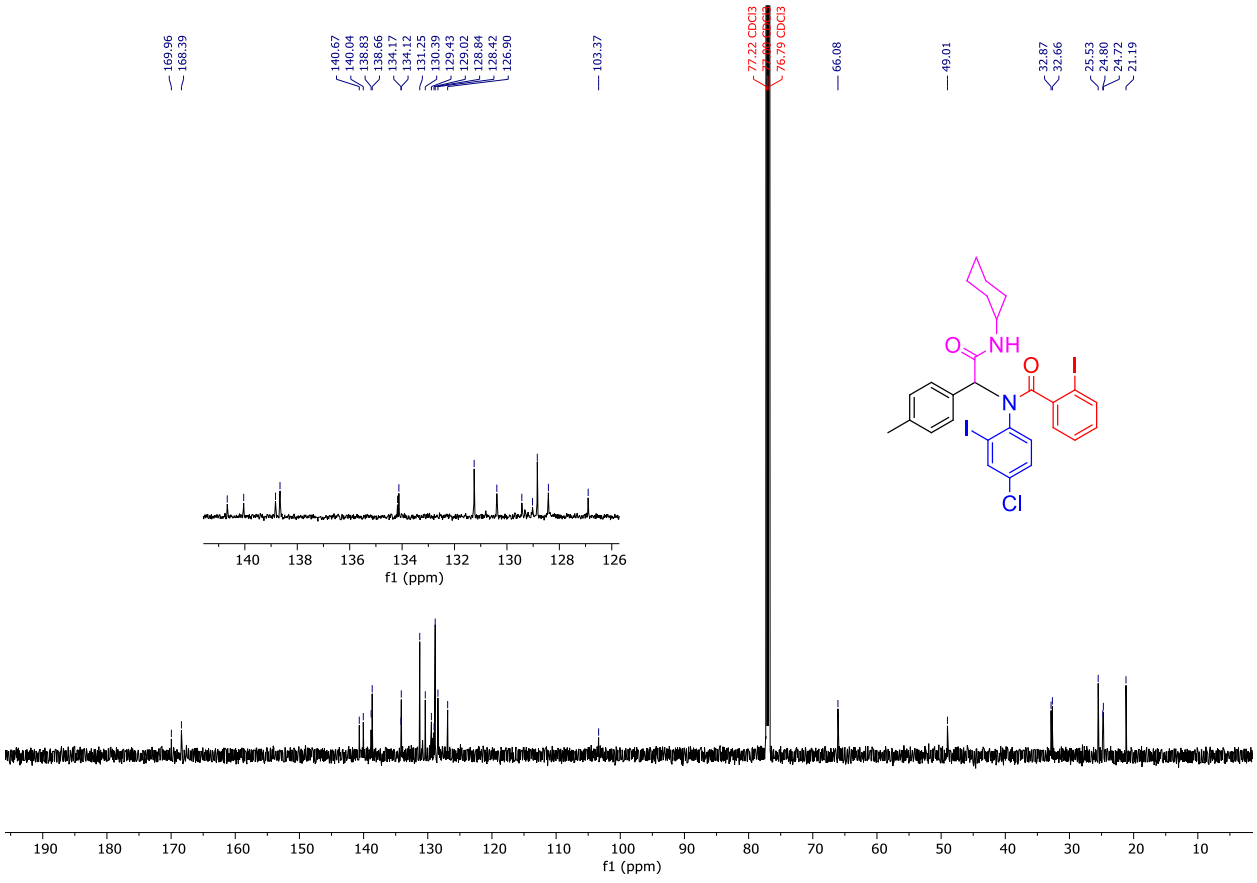
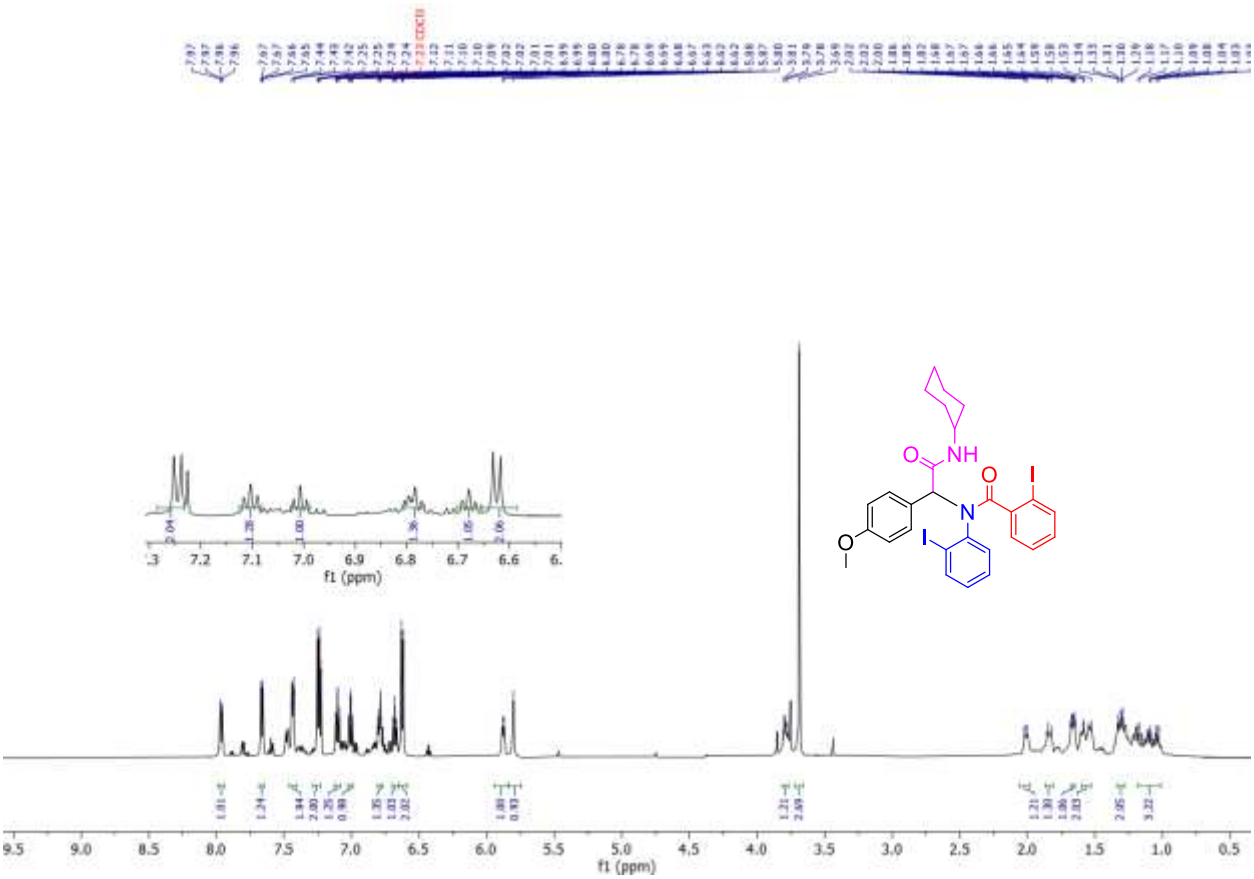


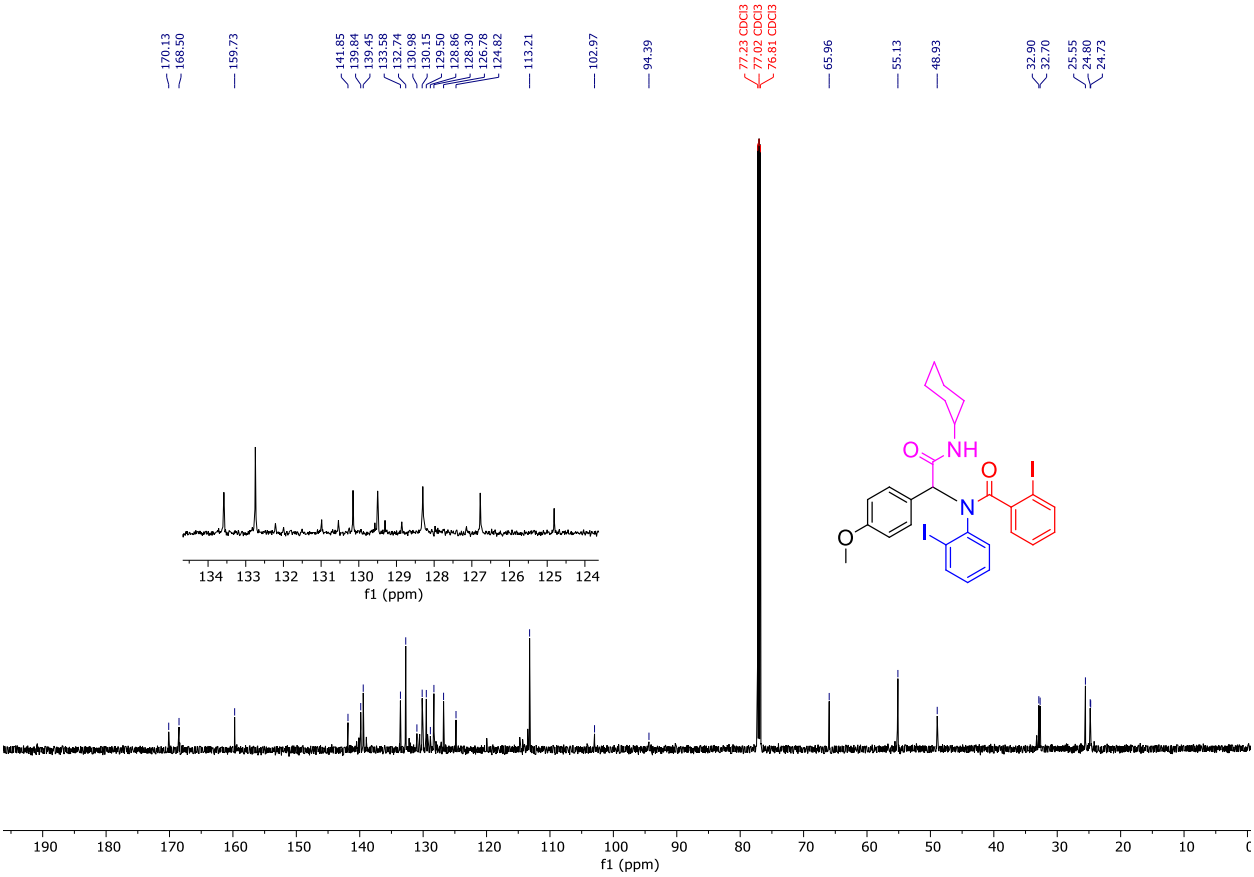
^{1}H-NMR of compound **5g** (600MHz, $CDCl_3$)



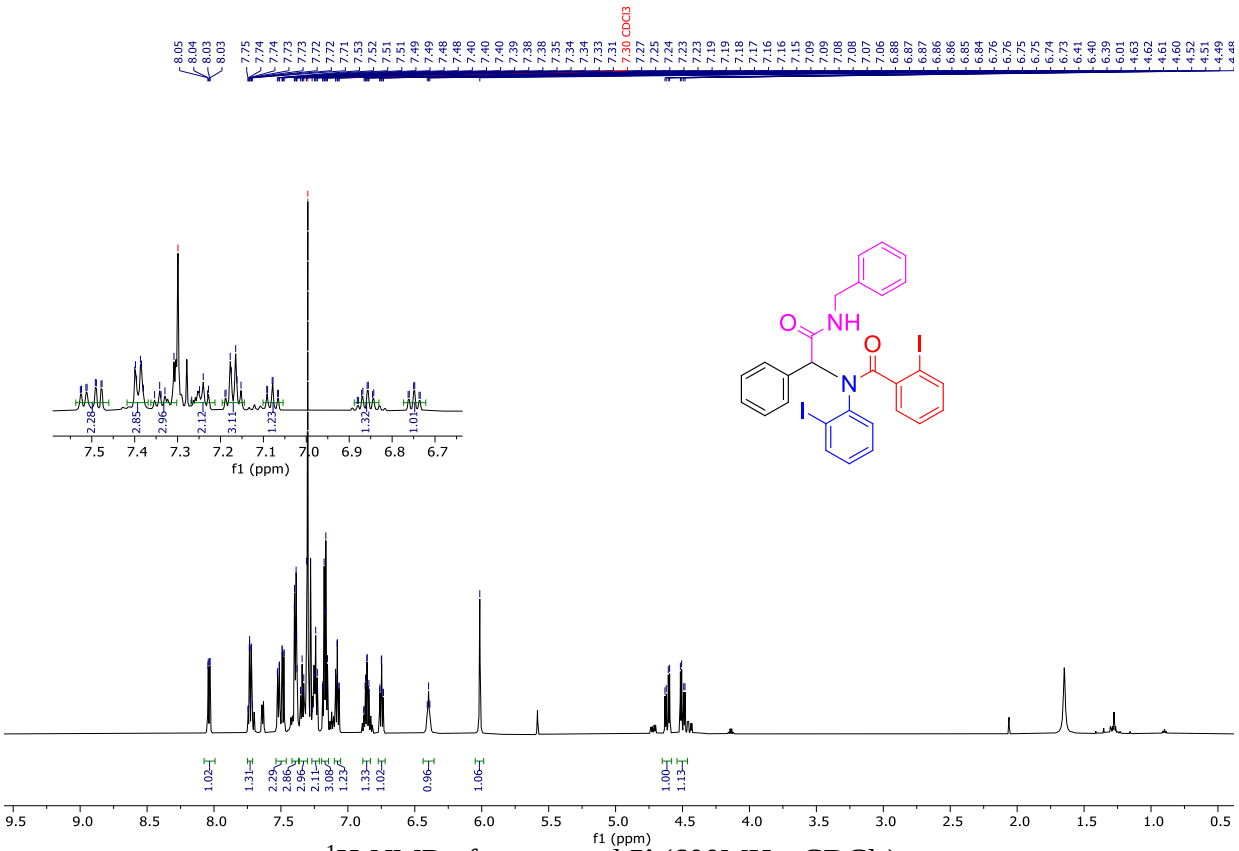
^{13}C-NMR of compound **5g** (151MHz, $CDCl_3$)



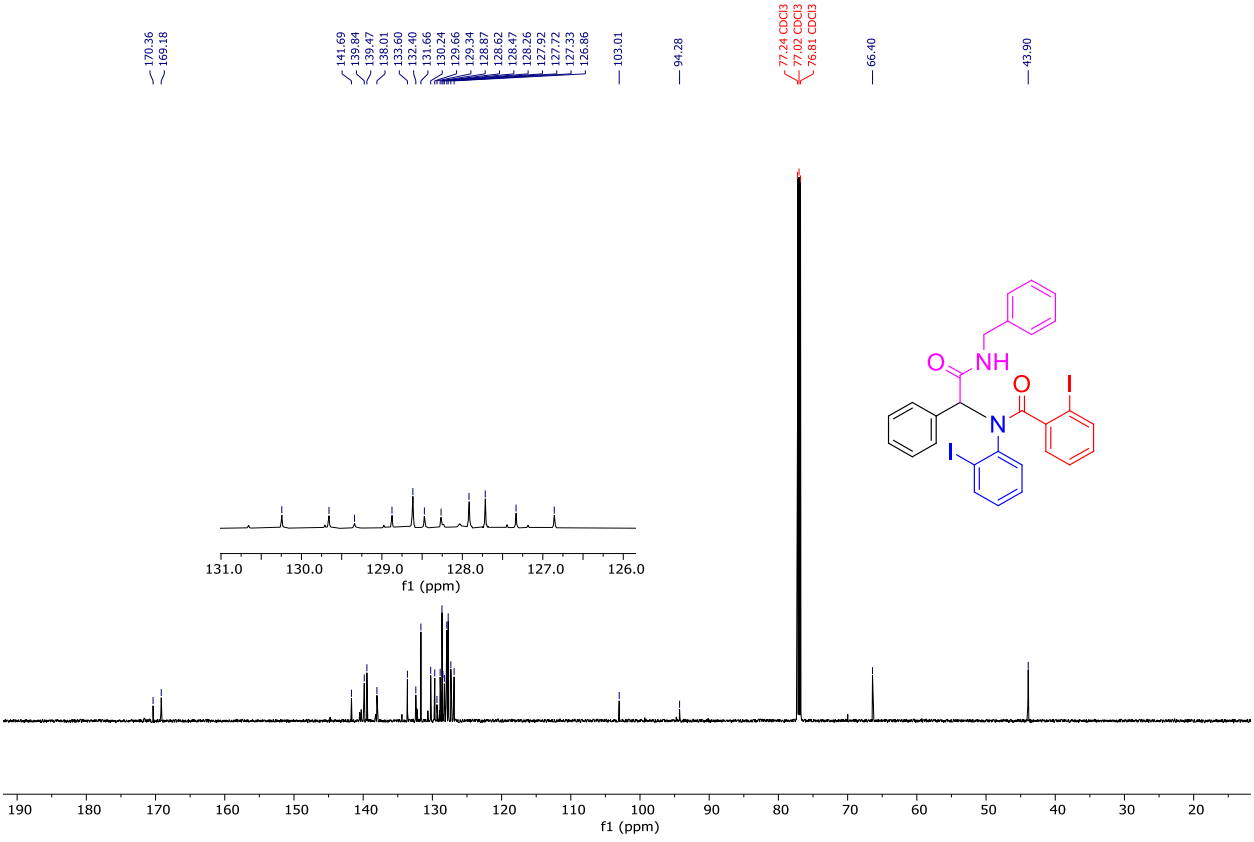
^{1}H-NMR of compound **5h** (600MHz, $CDCl_3$)



^{13}C-NMR of compound **5h** (151MHz, $CDCl_3$)



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



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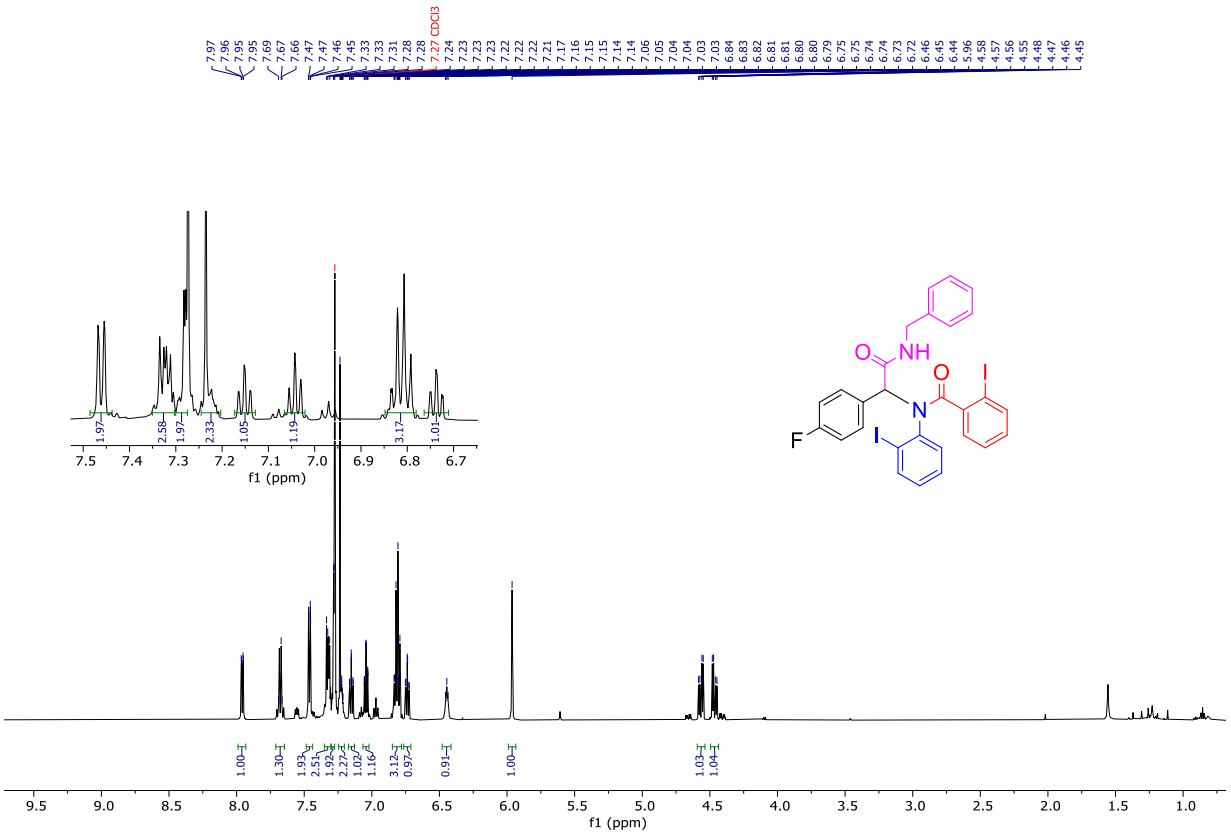

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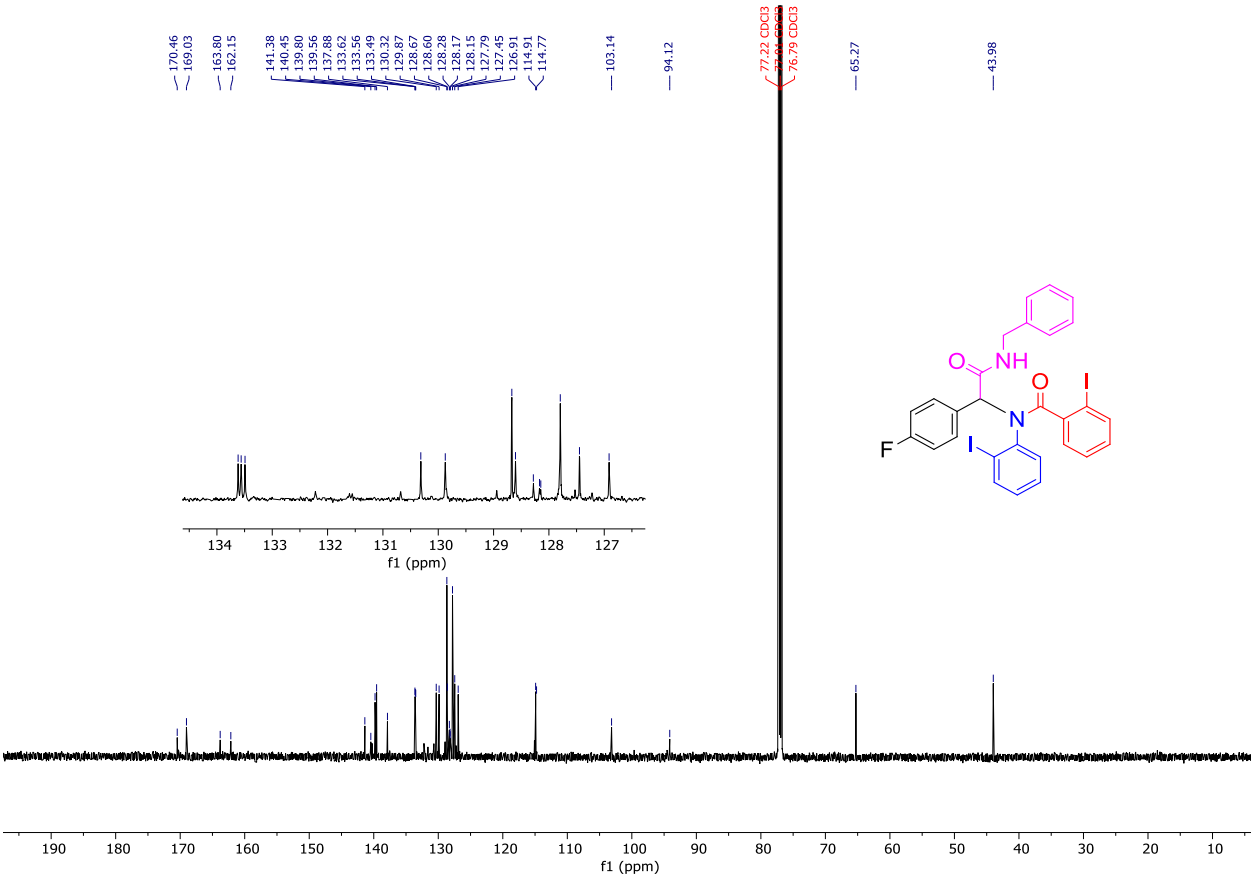

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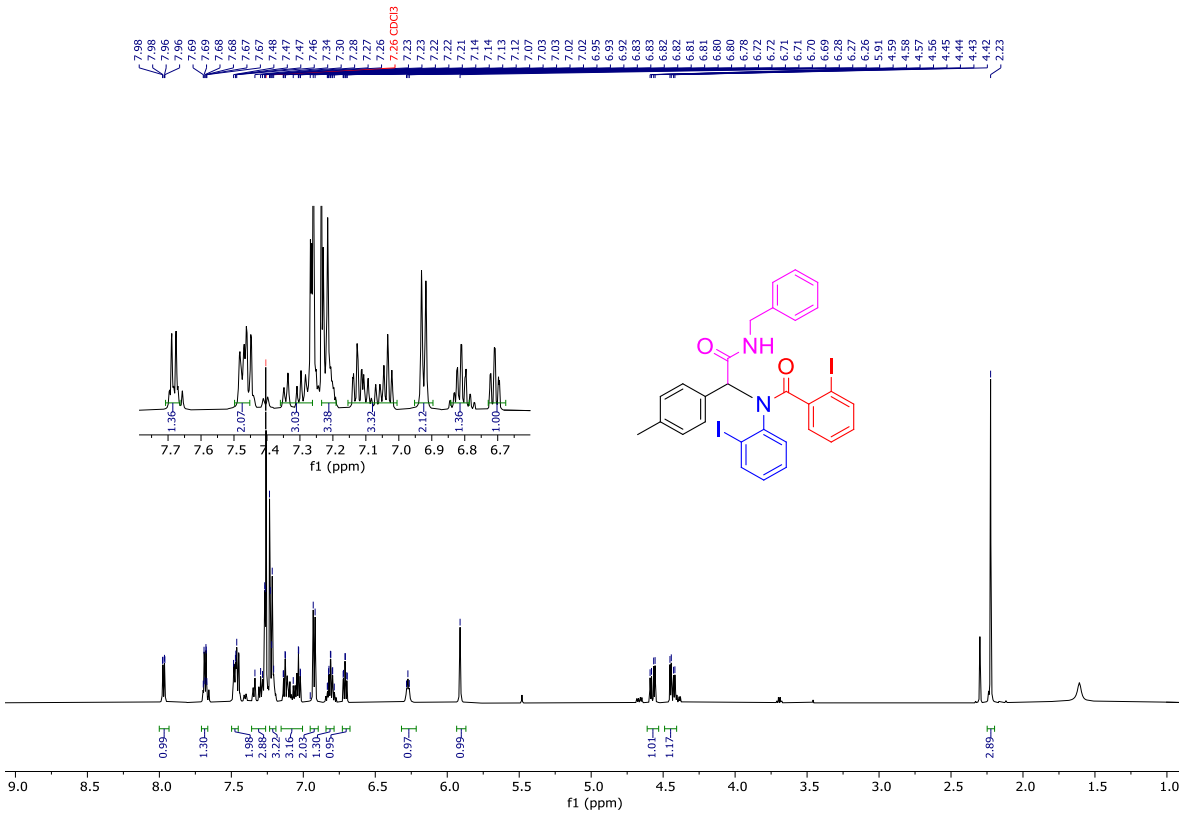
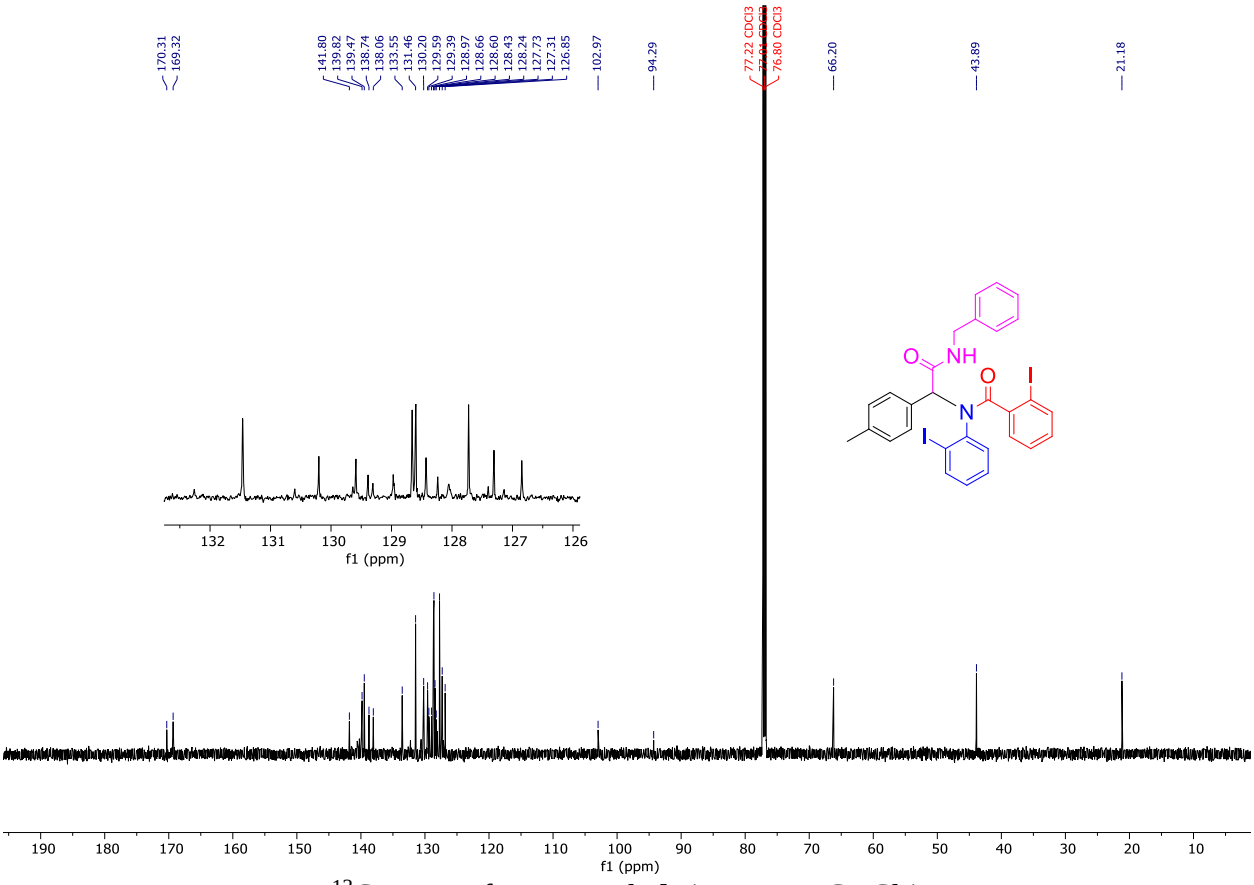


^{1}H-NMR of compound **5k** (600MHz, $CDCl_3$)



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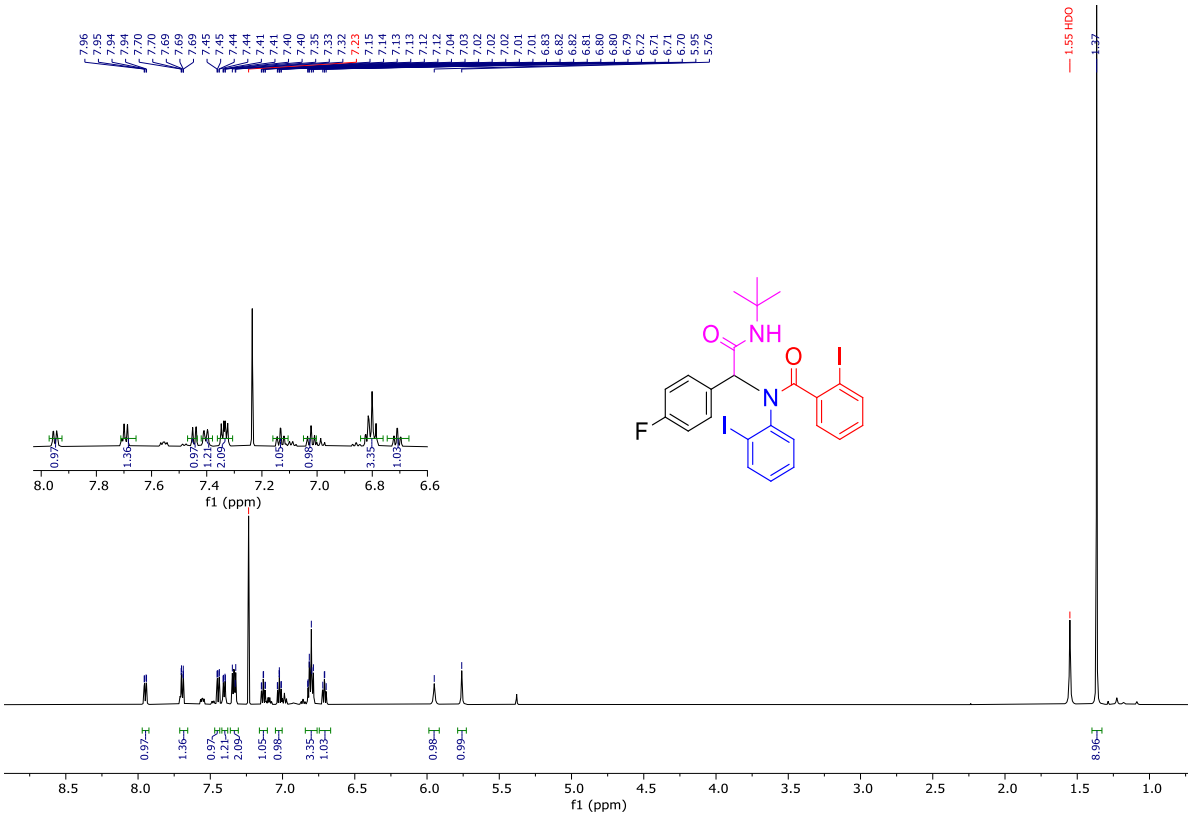
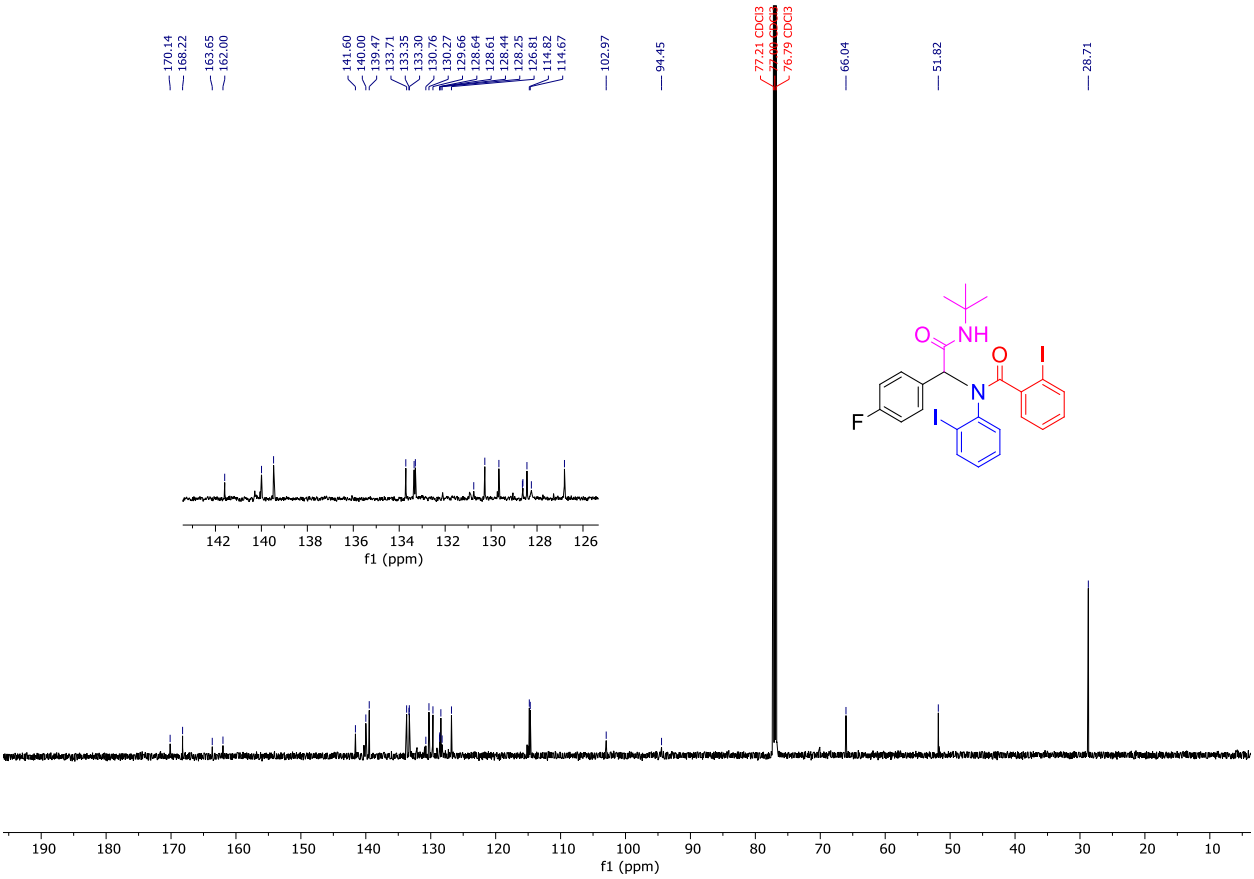


^{1}H-NMR of compound **5l** (600MHz, $CDCl_3$)



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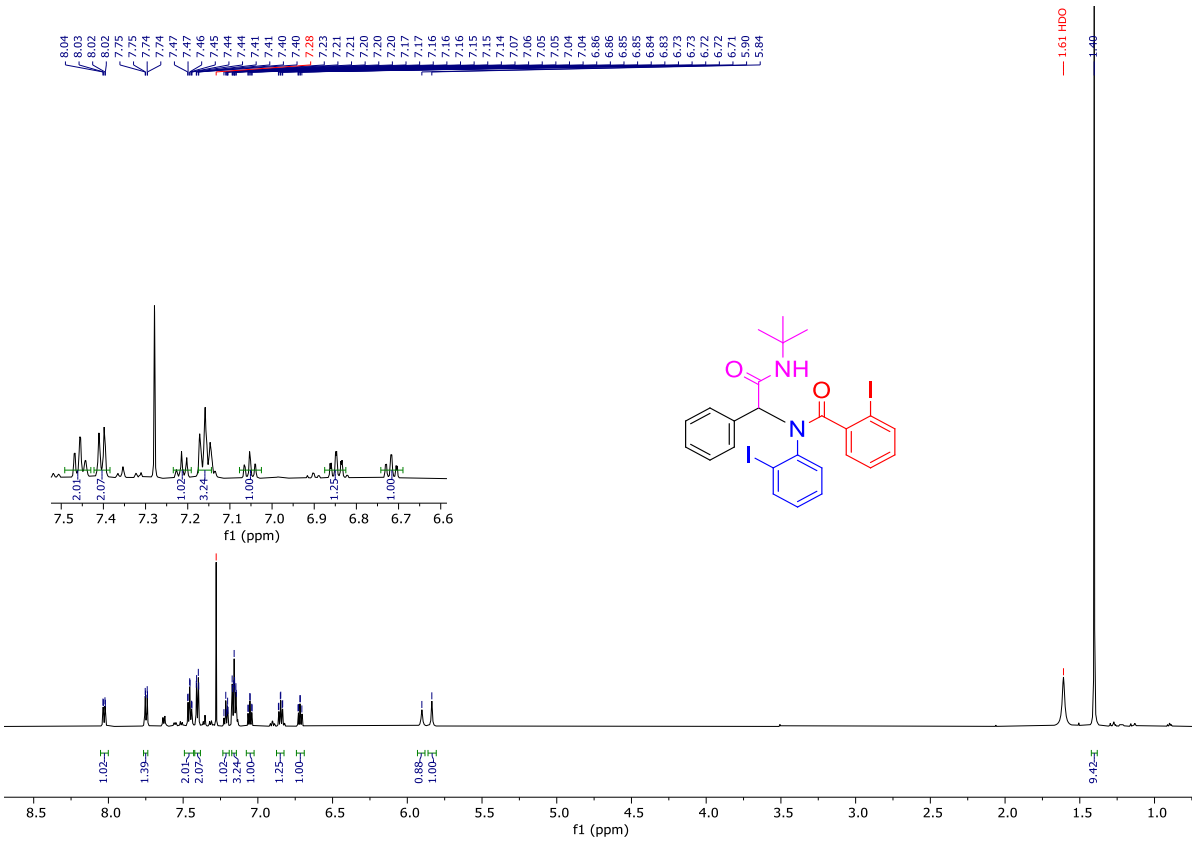
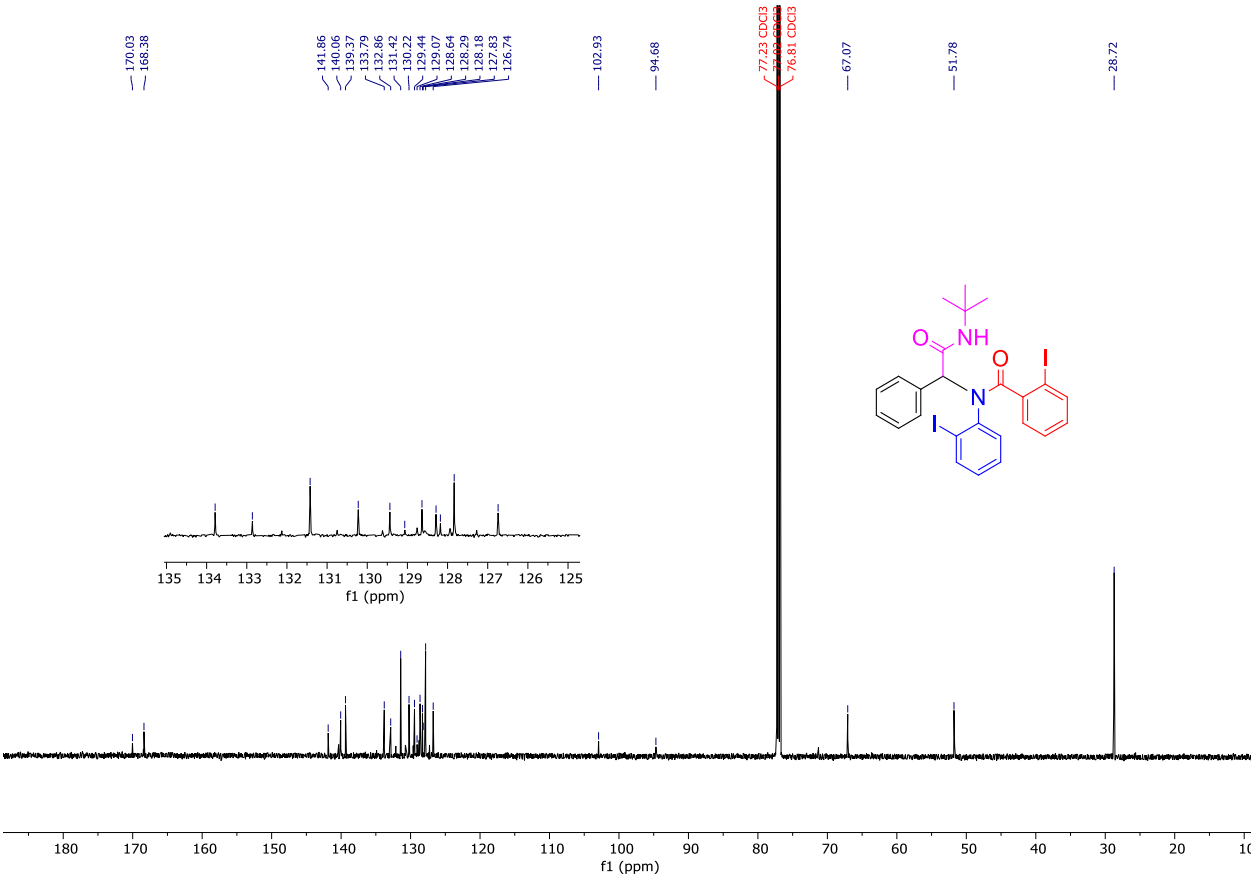
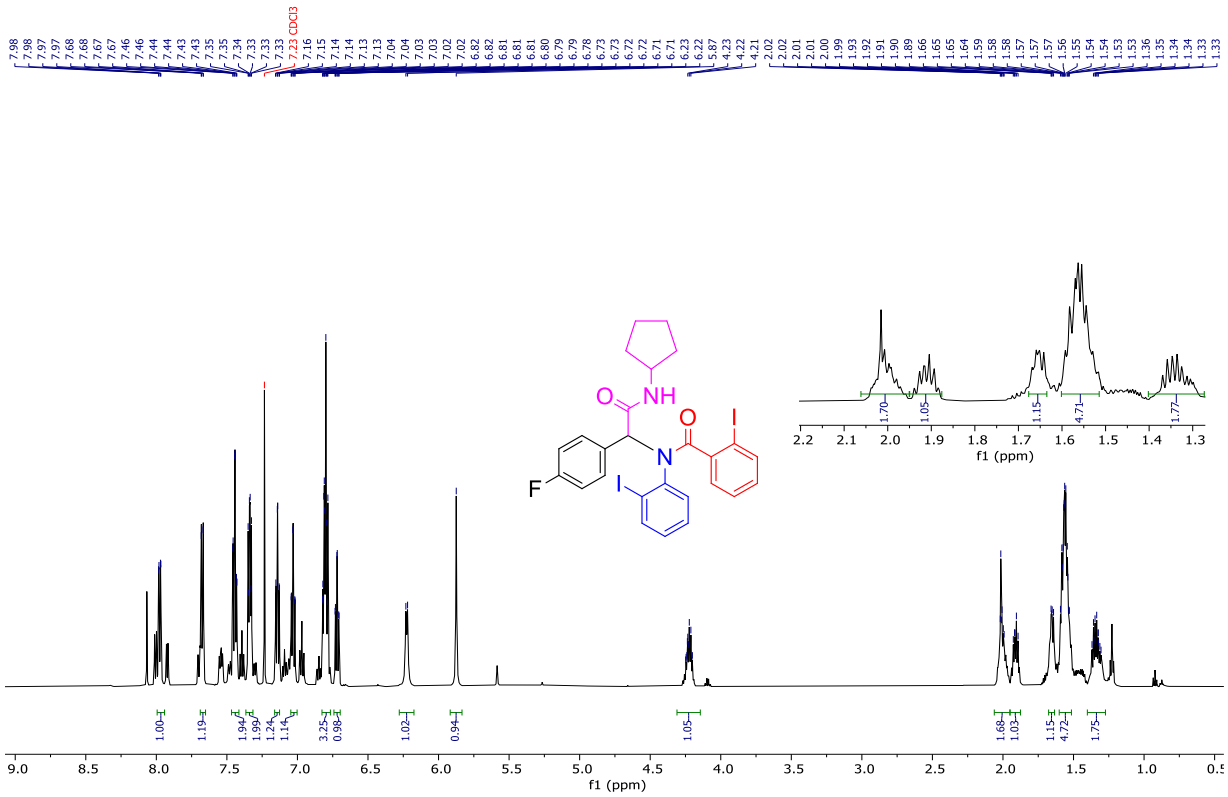


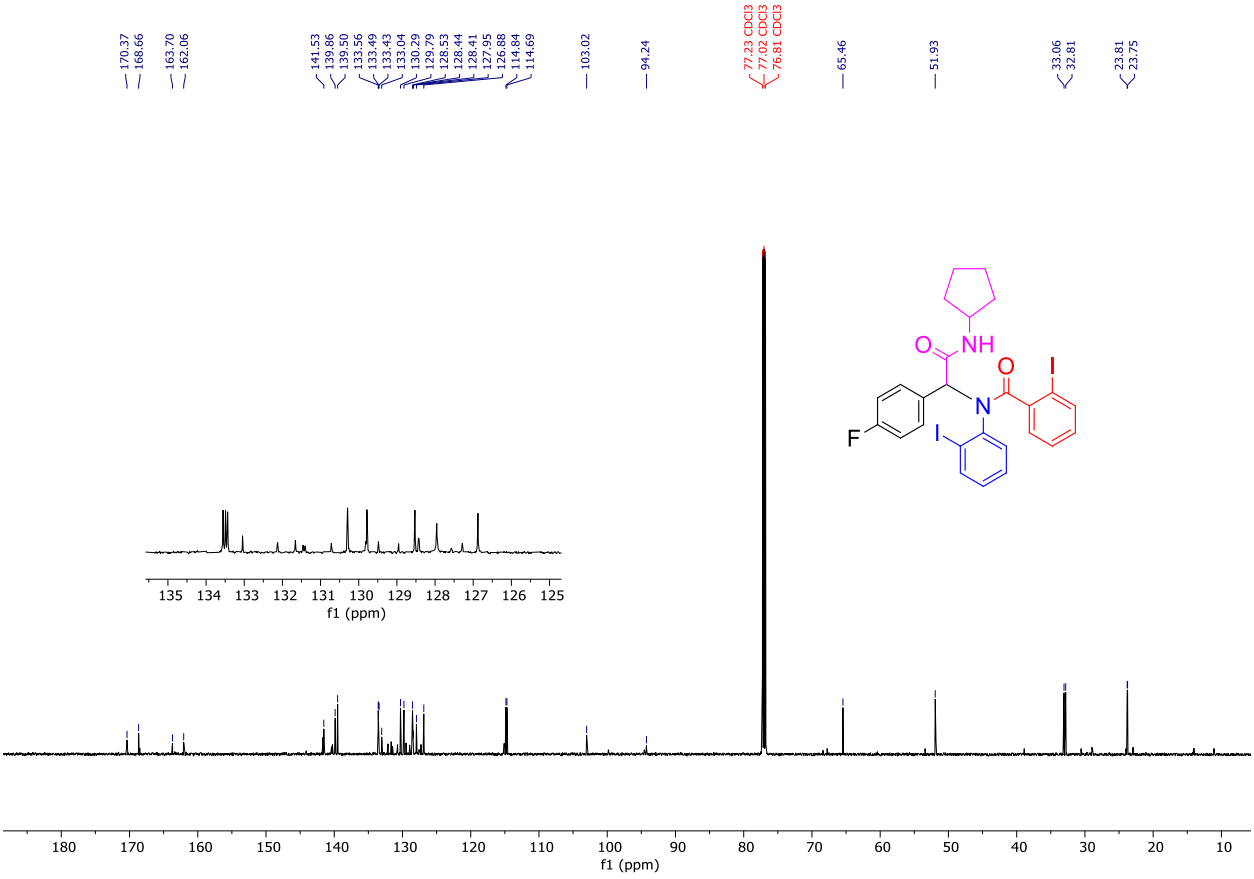
^{1}H-NMR of compound **5m** (600MHz, $CDCl_3$)



^{13}C-NMR of compound **5m** (151MHz, $CDCl_3$)



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



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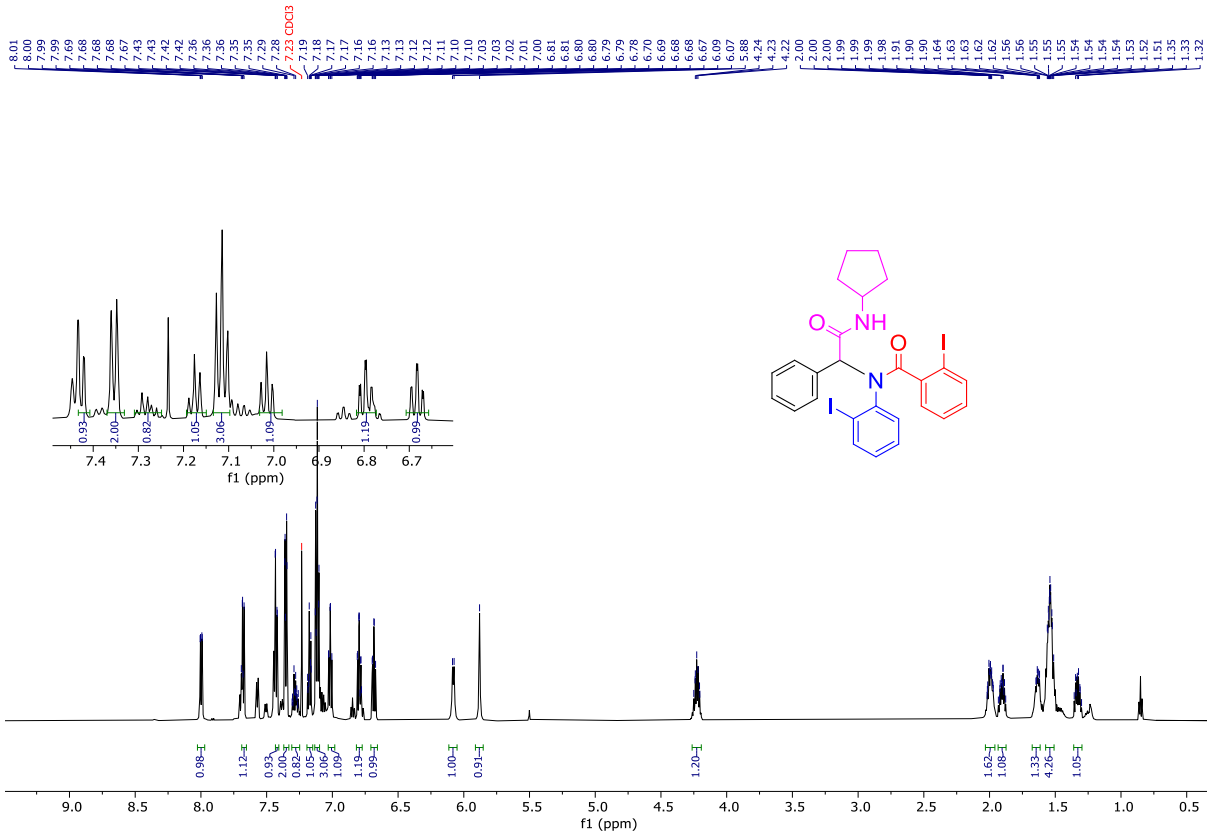
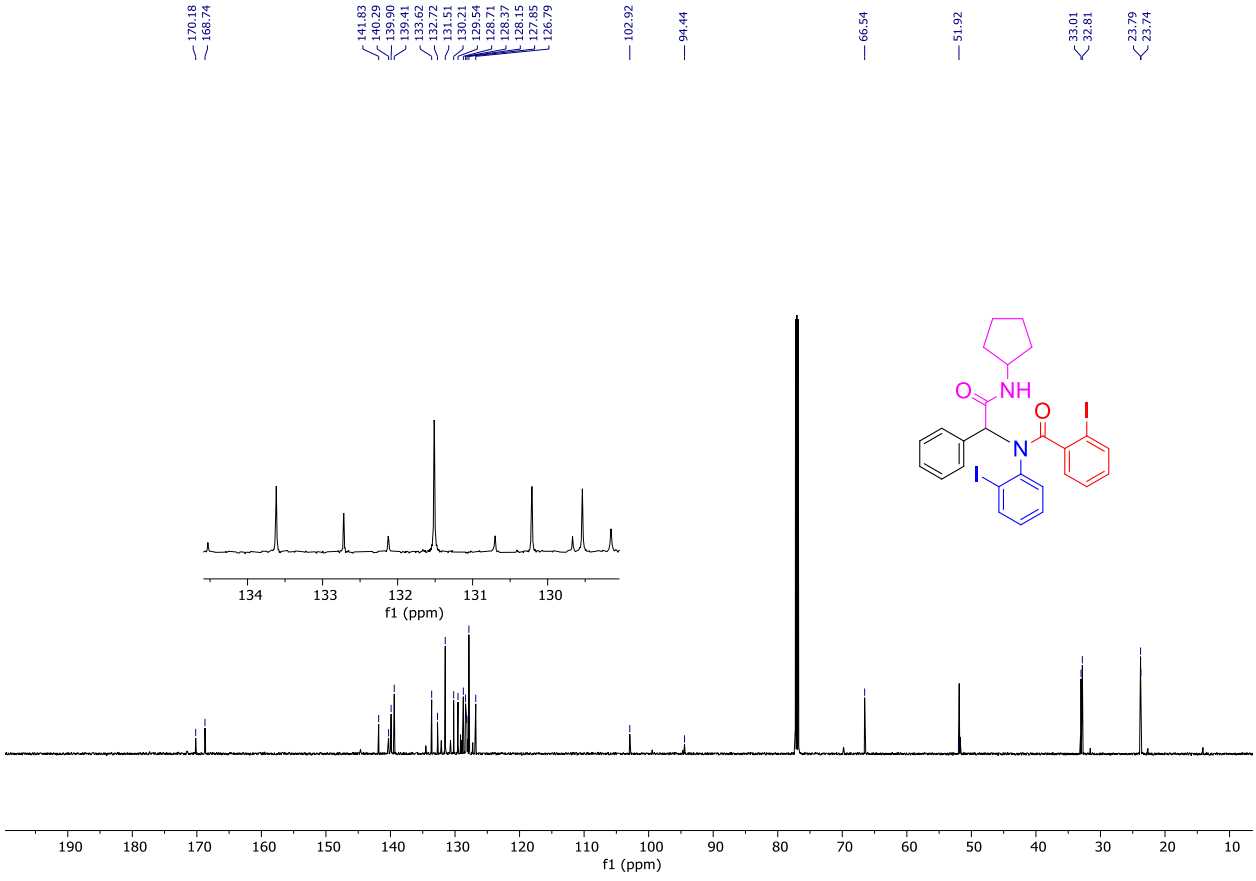


^{1}H-NMR of compound **5o** (600MHz, $CDCl_3$)



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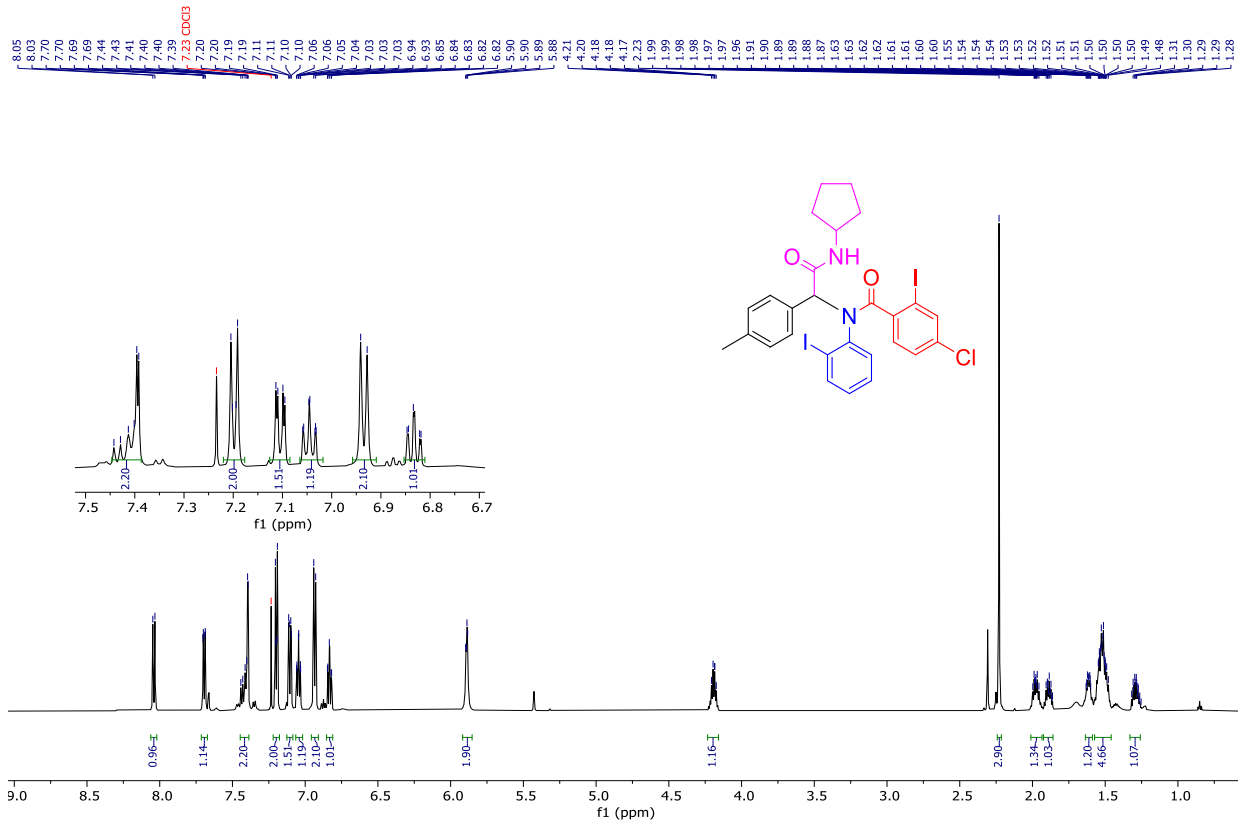
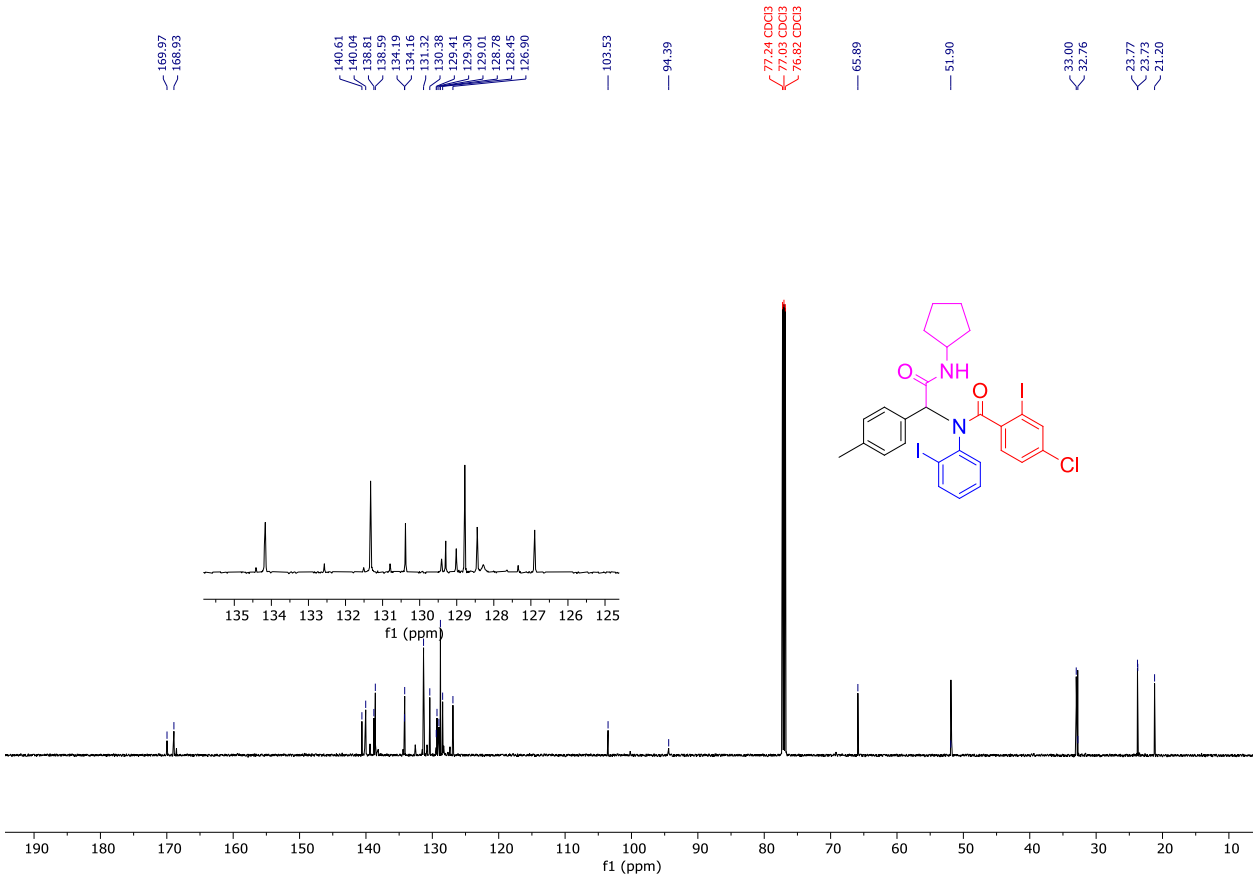


^{1}H-NMR of compound **5p** (600MHz, $CDCl_3$)



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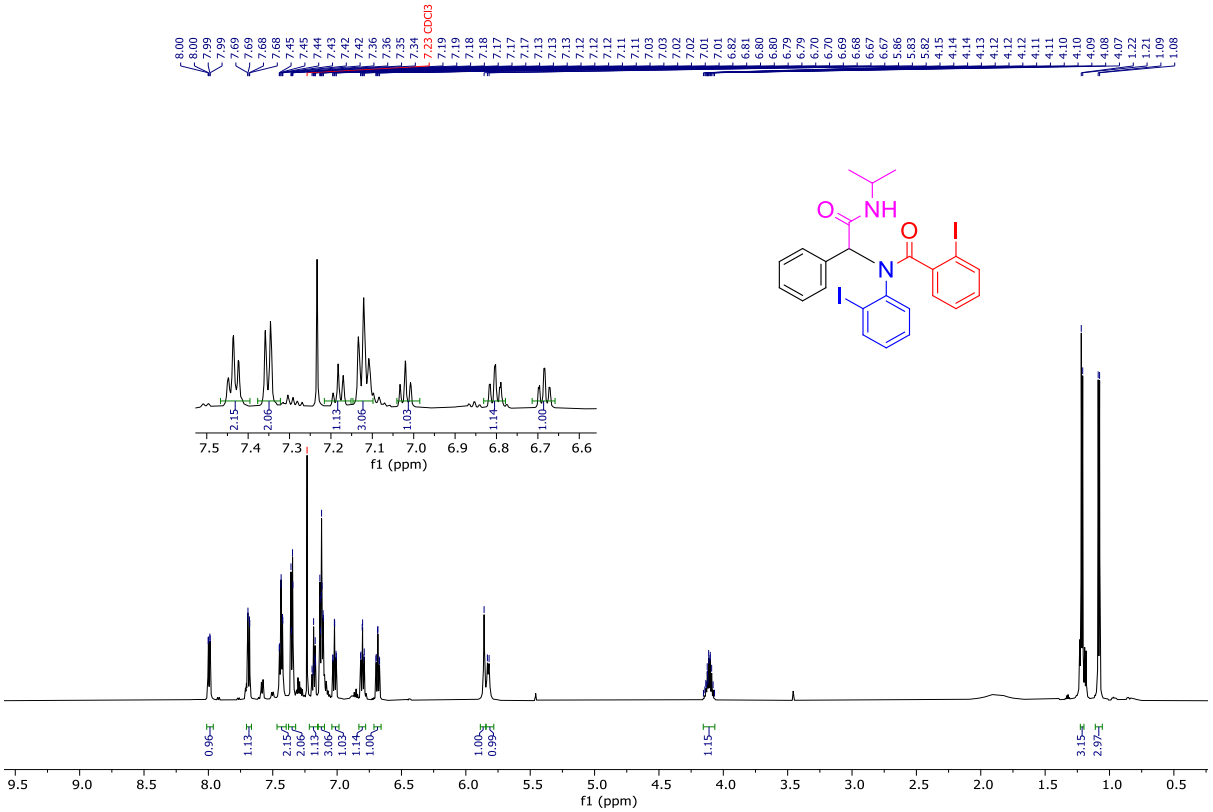
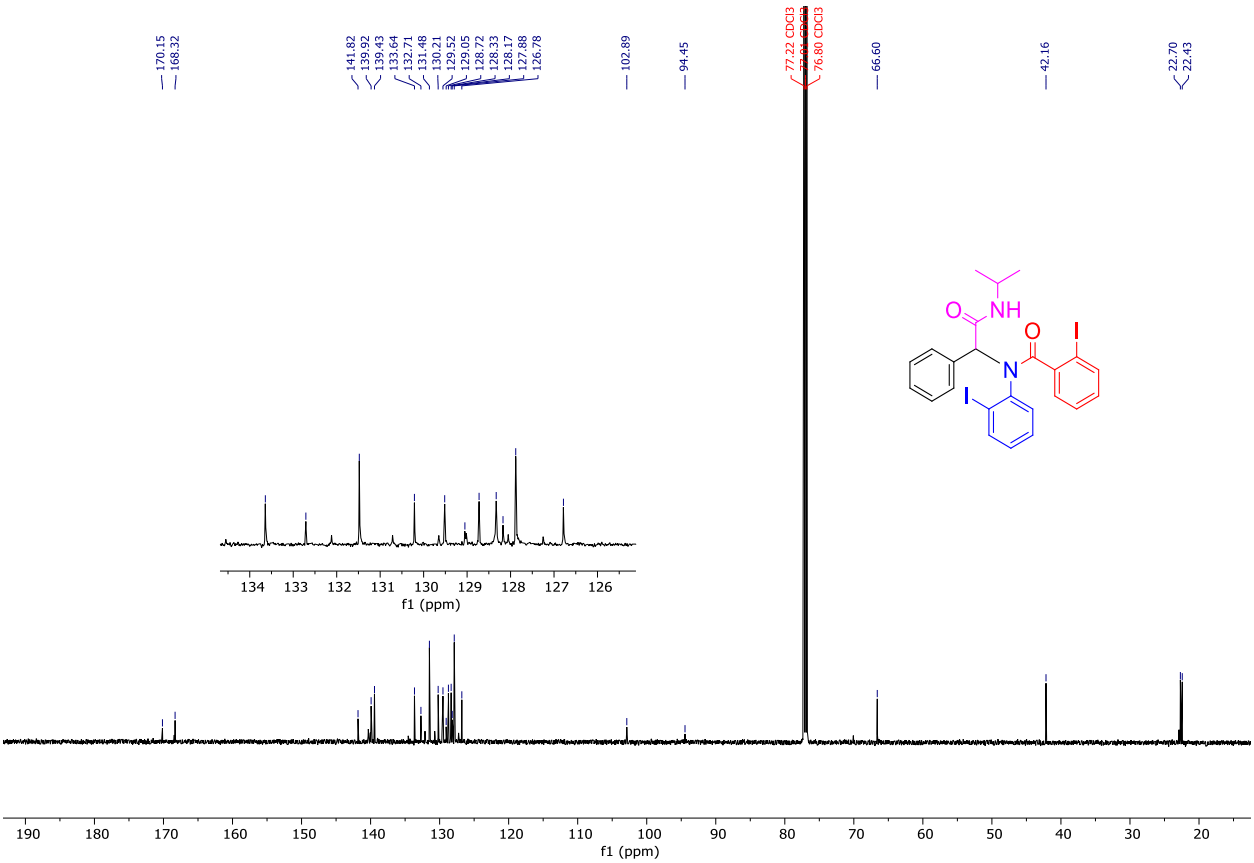


^{1}H-NMR of compound **5q** (600MHz, $CDCl_3$)



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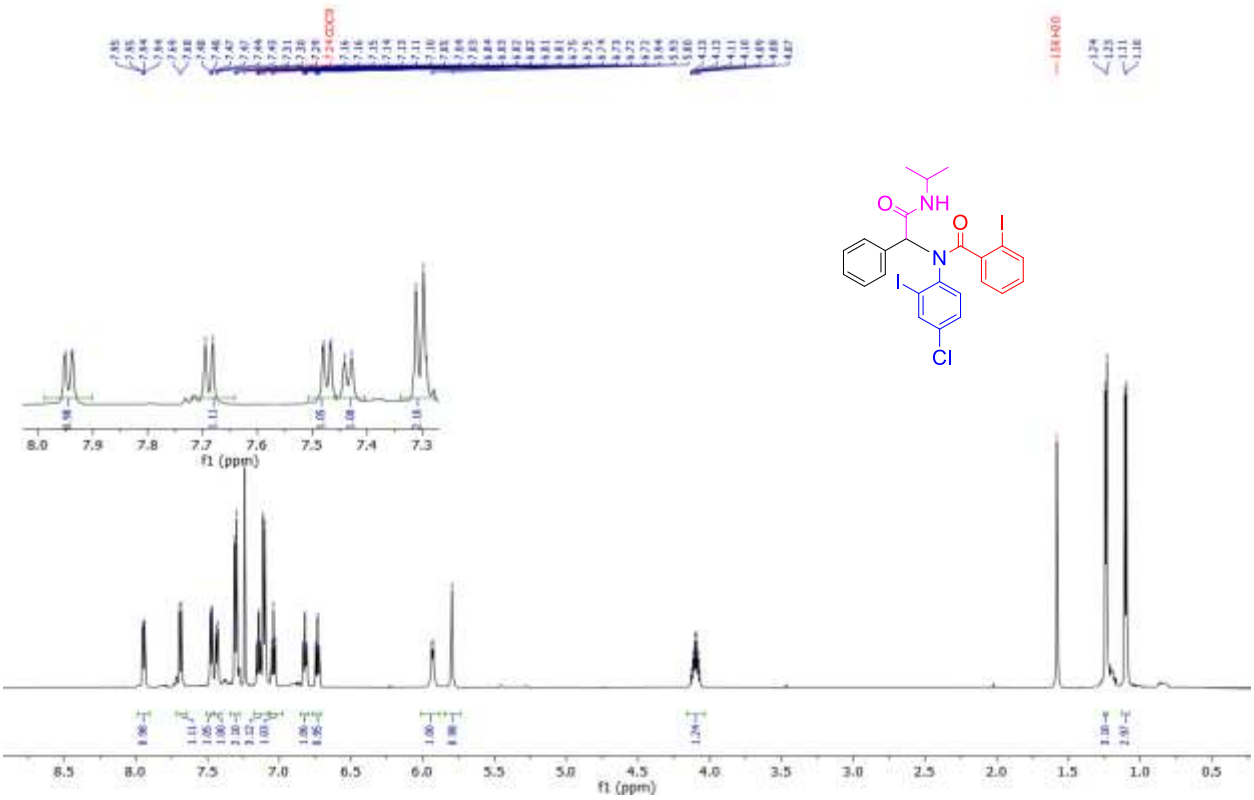
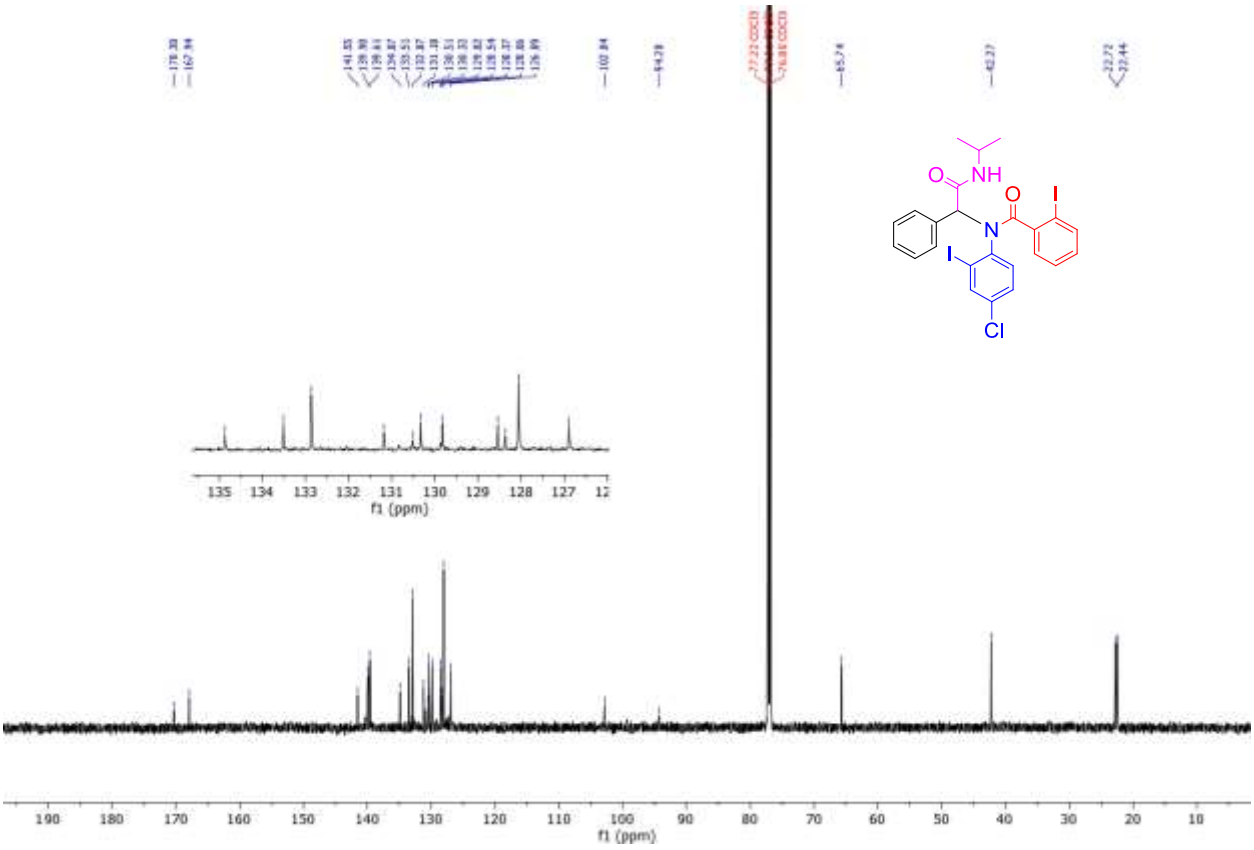


^{1}H-NMR of compound **5r** (600MHz, $CDCl_3$)



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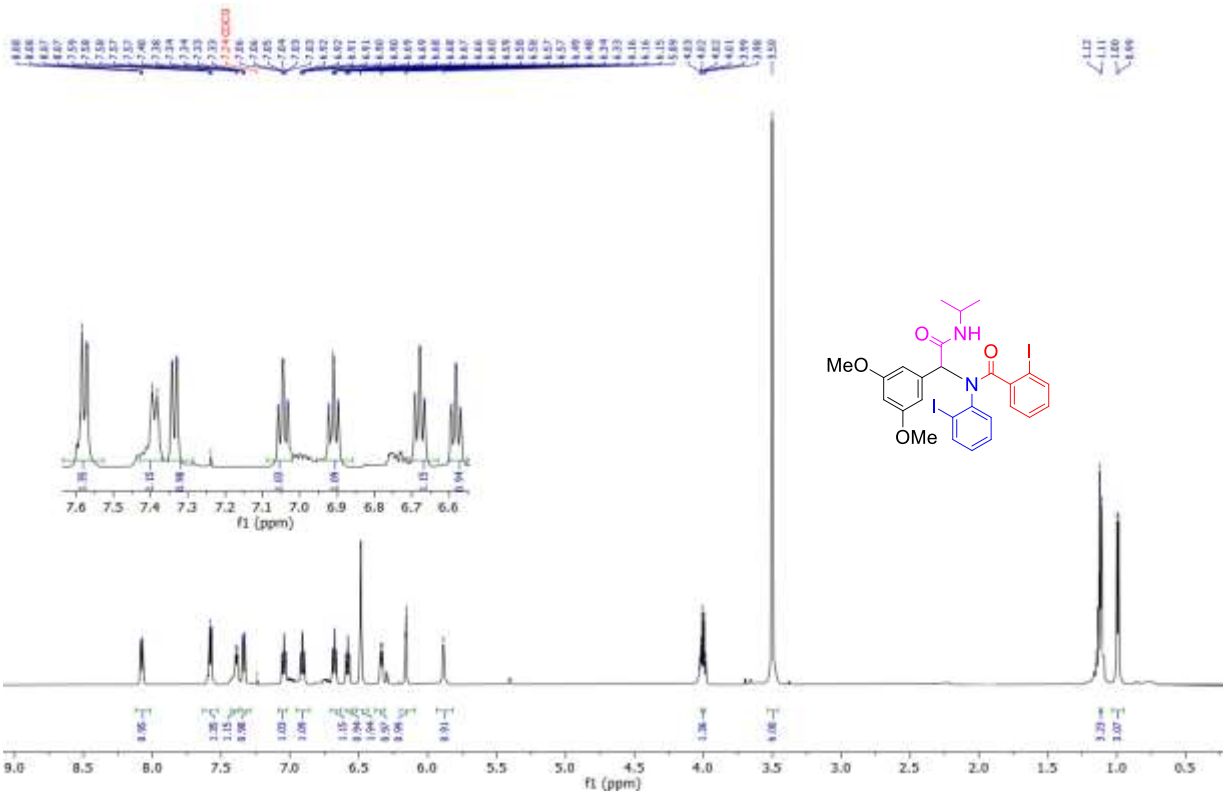
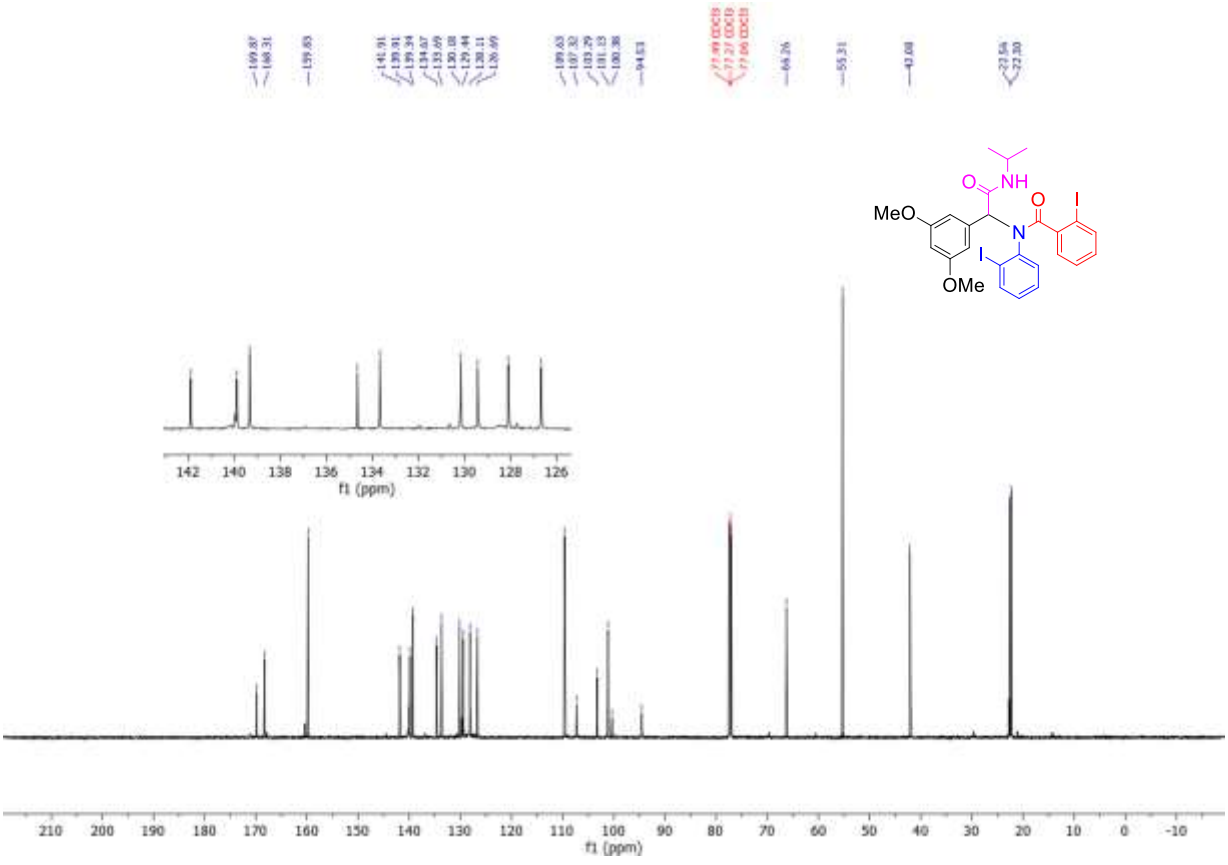


^{1}H-NMR of compound **5s** (600MHz, $CDCl_3$)



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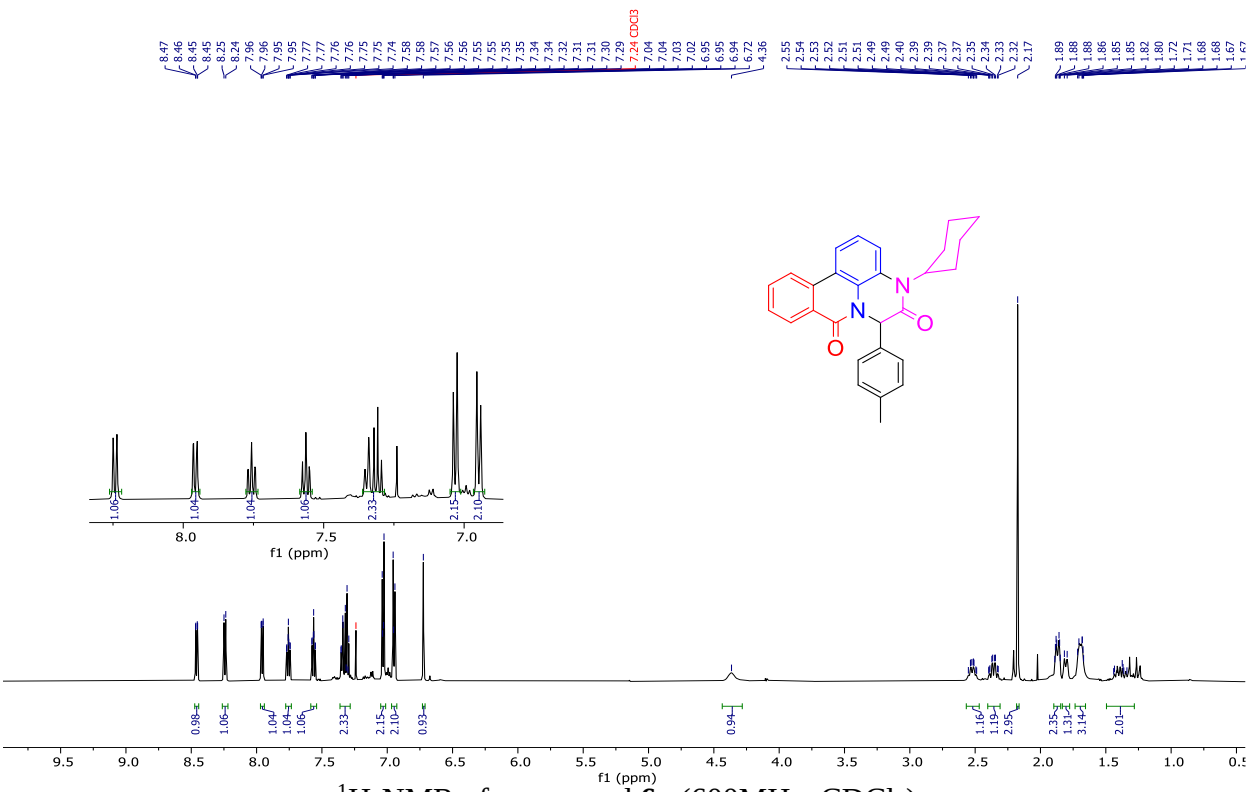
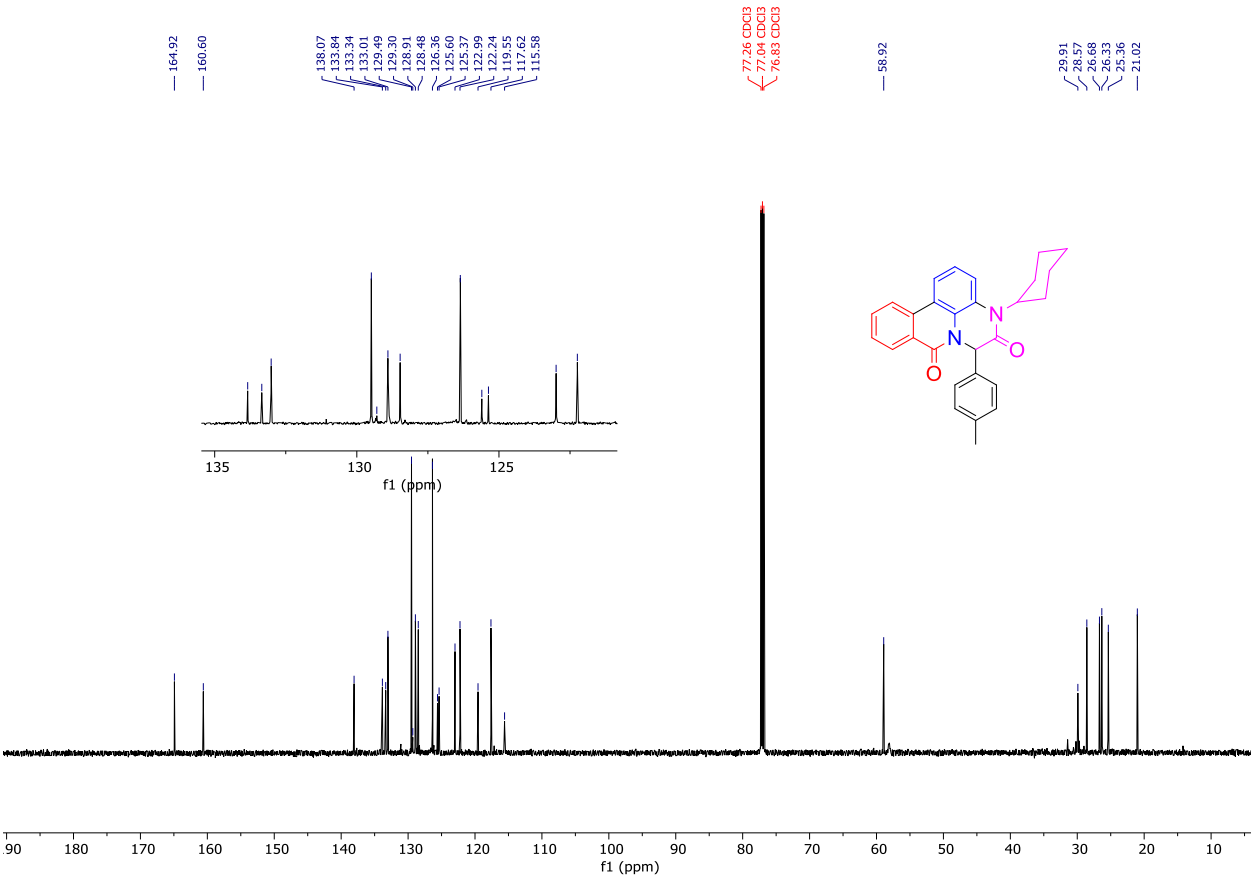


^{1}H-NMR of compound **6a** (600MHz, $CDCl_3$)



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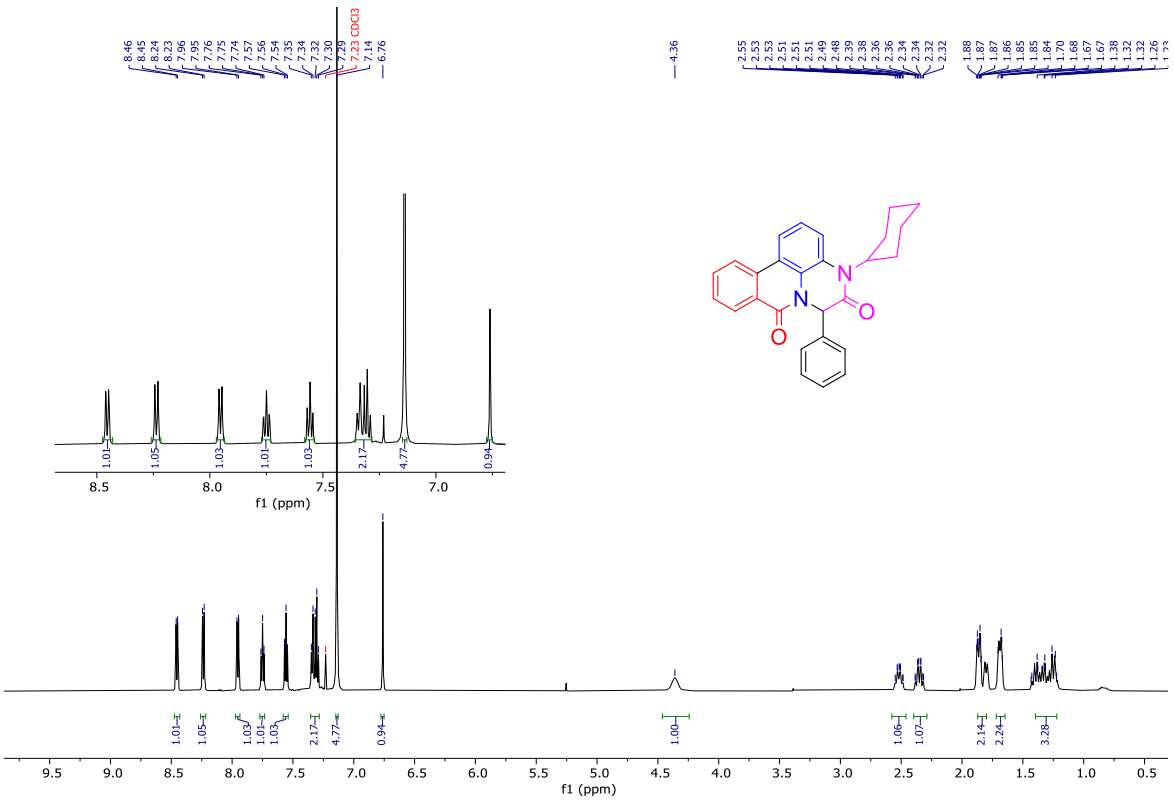
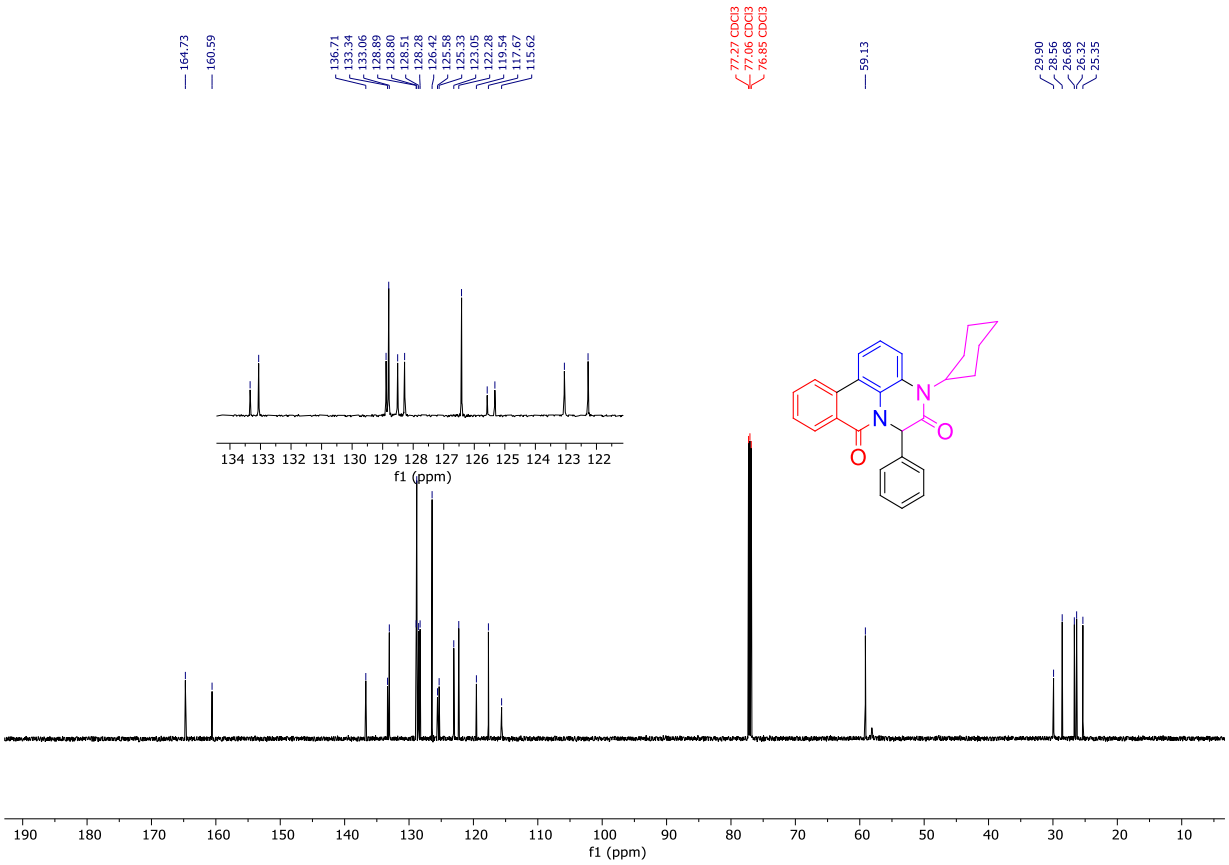
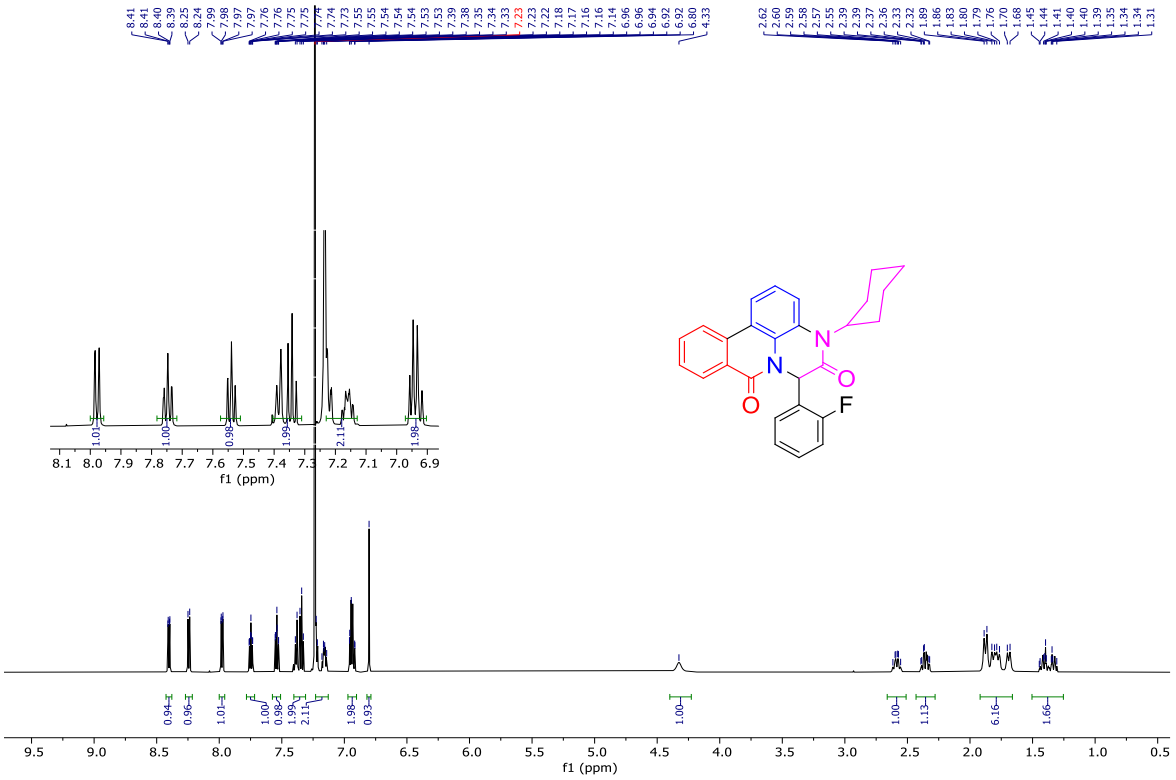


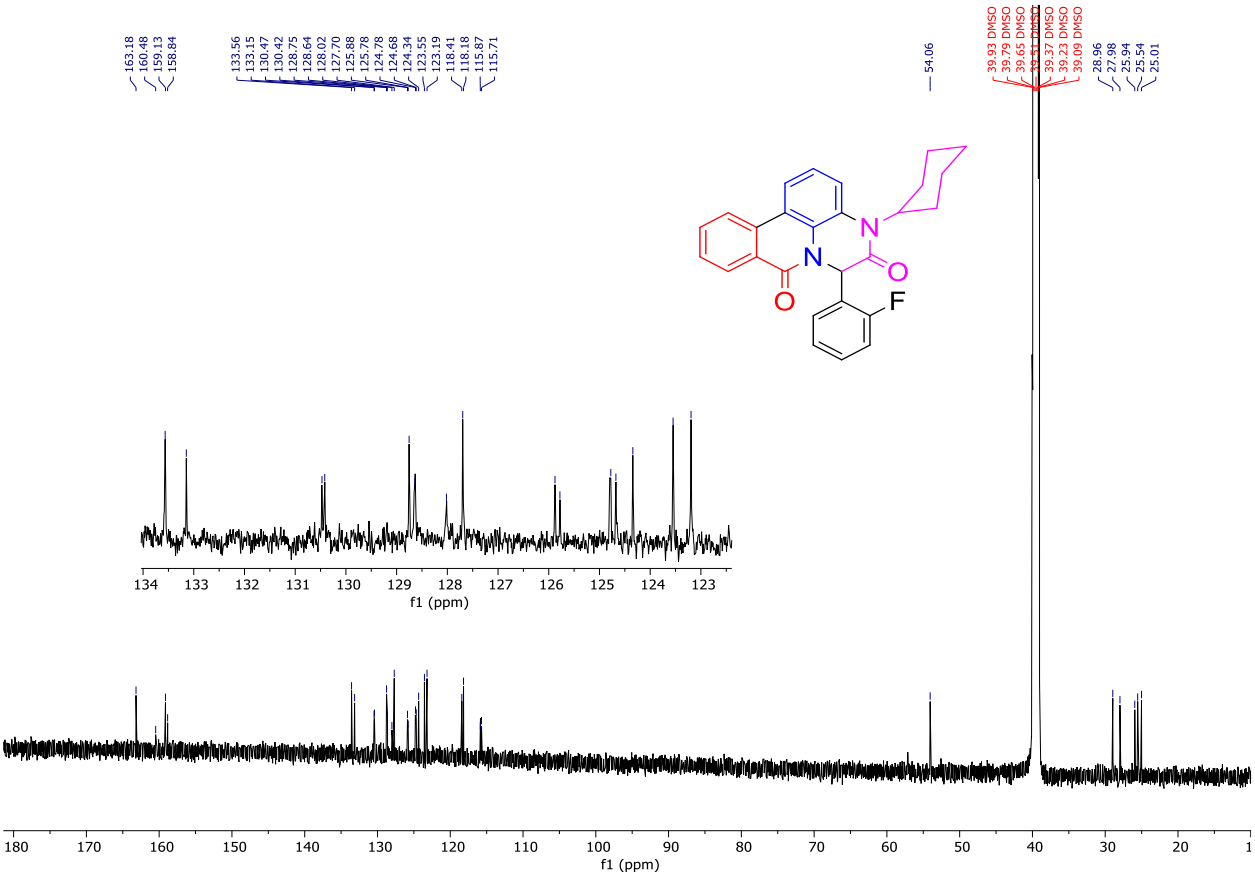
^{1}H-NMR of compound **6b** (600MHz, $CDCl_3$)



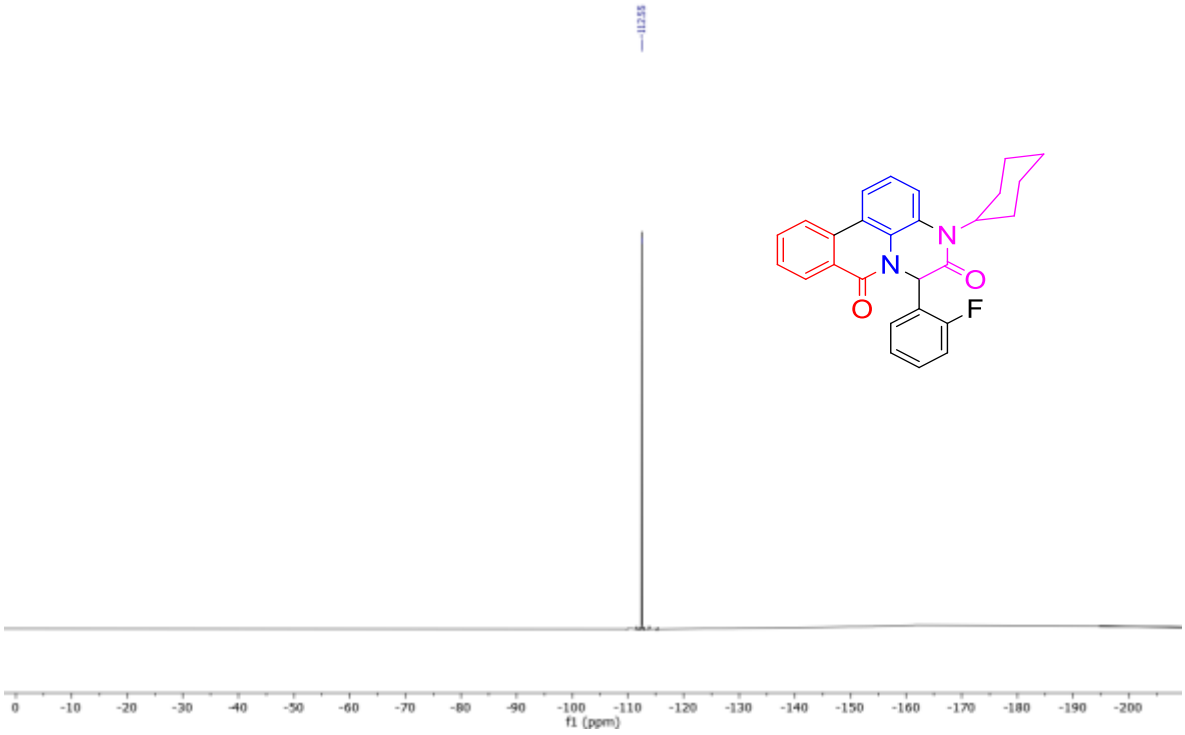
^{13}C-NMR of compound **6b** (151MHz, $CDCl_3$)



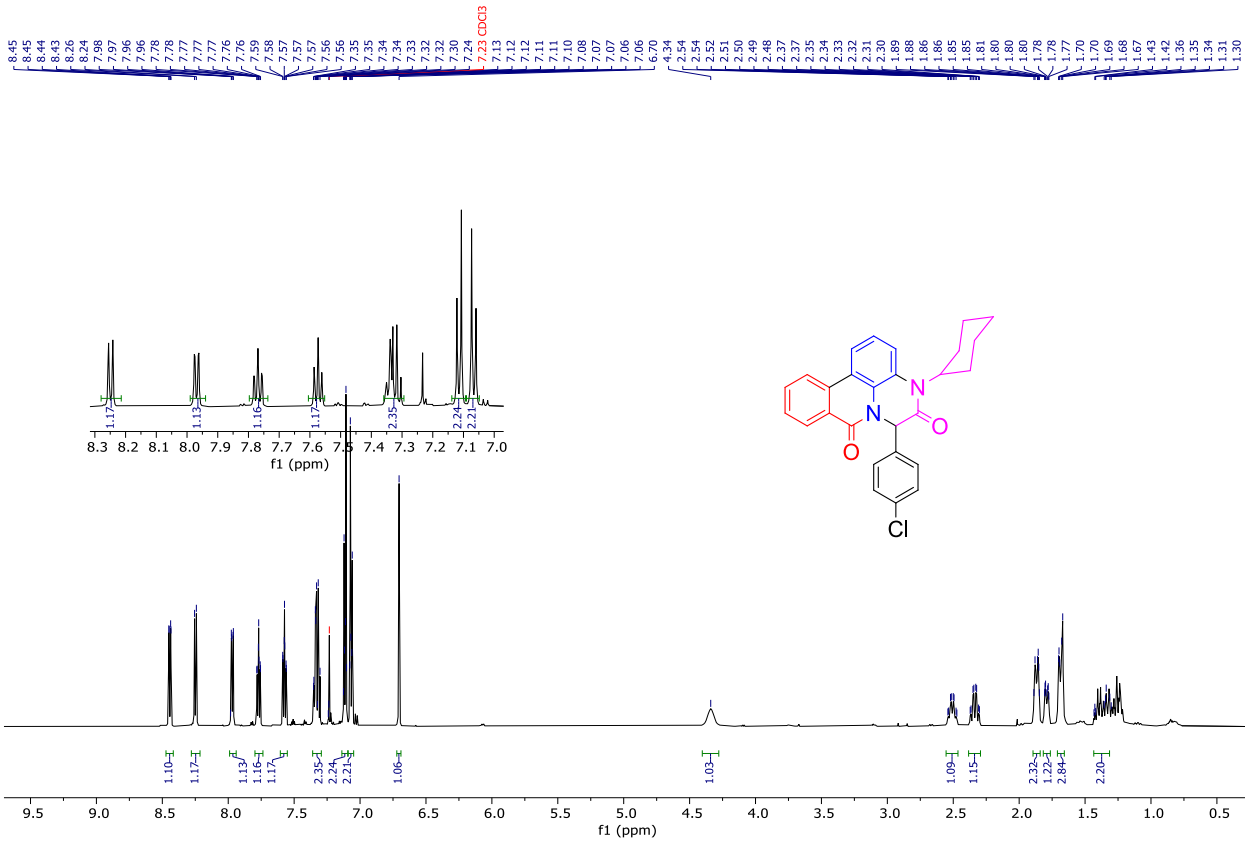
^{1}H-NMR of compound **6c** (600 MHz, $CDCl_3$)



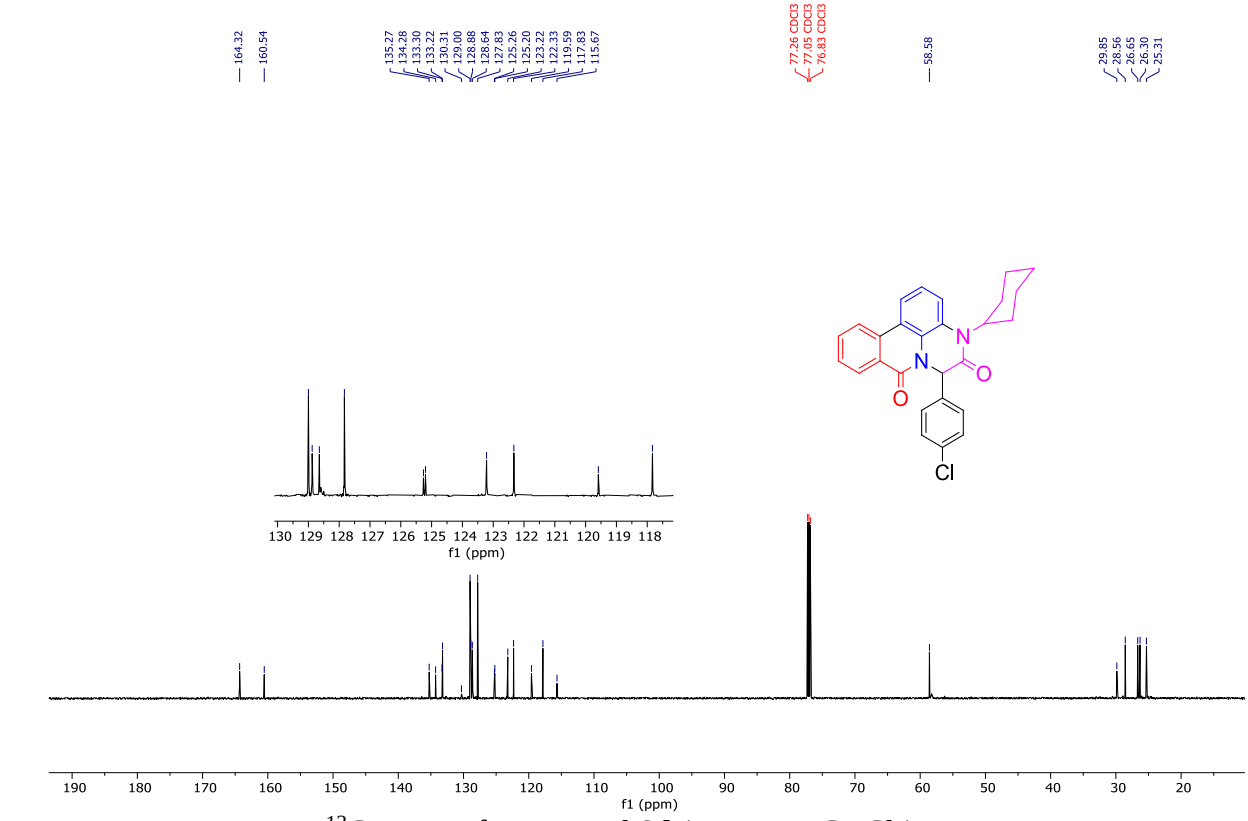
^{13}C-NMR of compound **6c** (151 MHz, DMSO-d6)



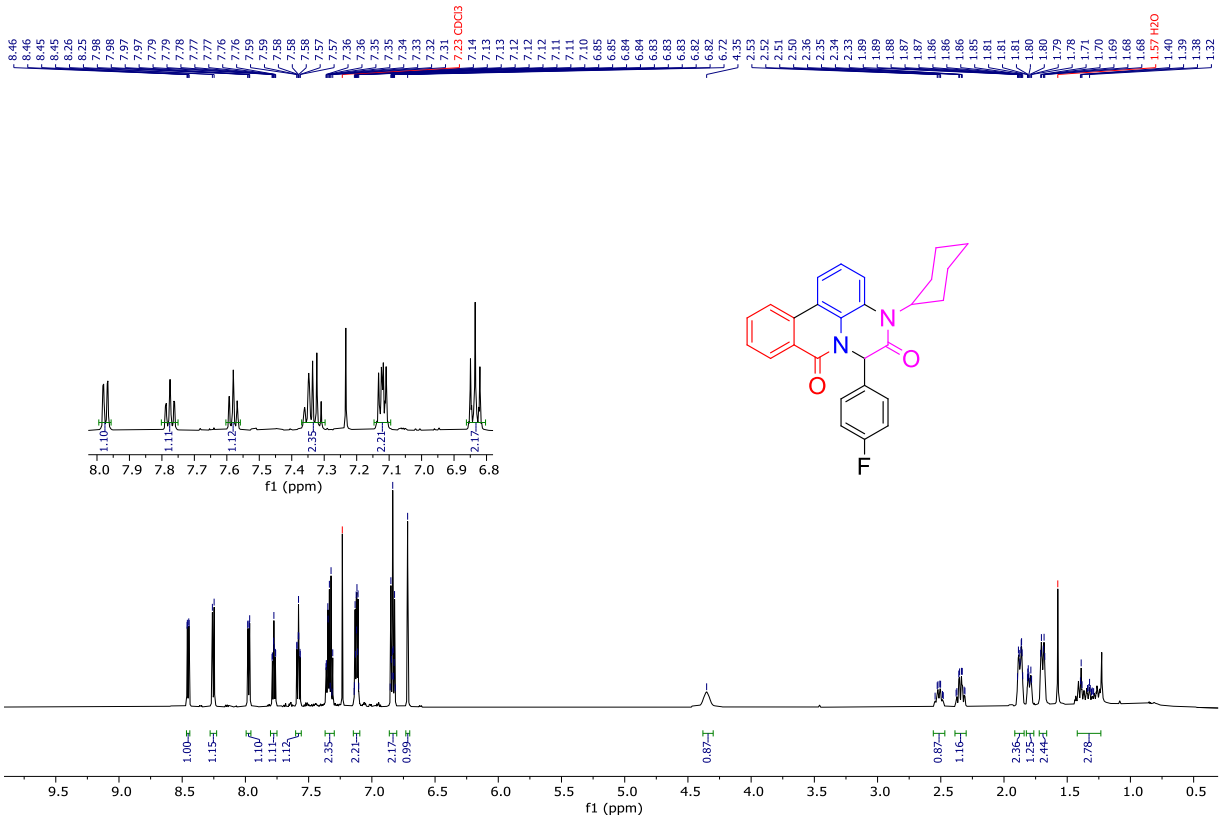
^{19}F NMR of compound **6c** (565 MHz, $CDCl_3$)



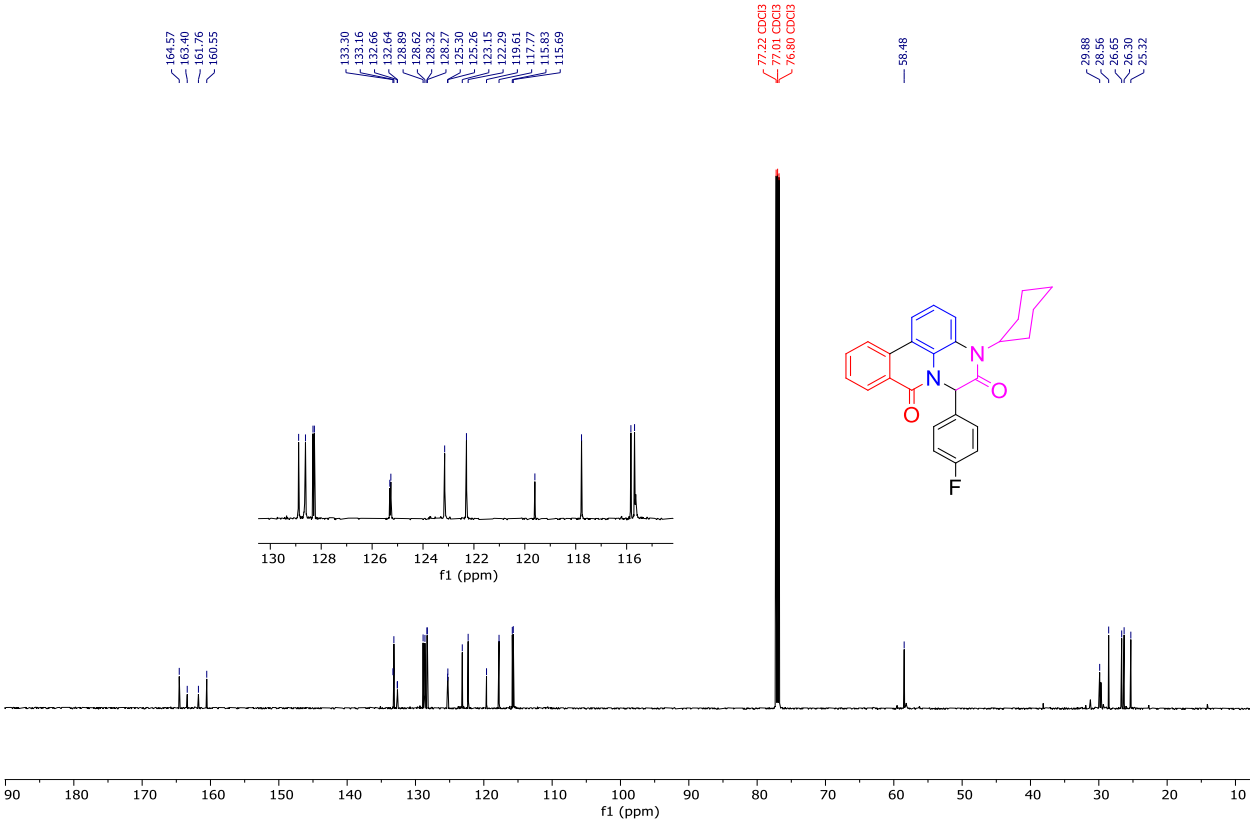
^{1}H-NMR of compound **6d** (600MHz, $CDCl_3$)



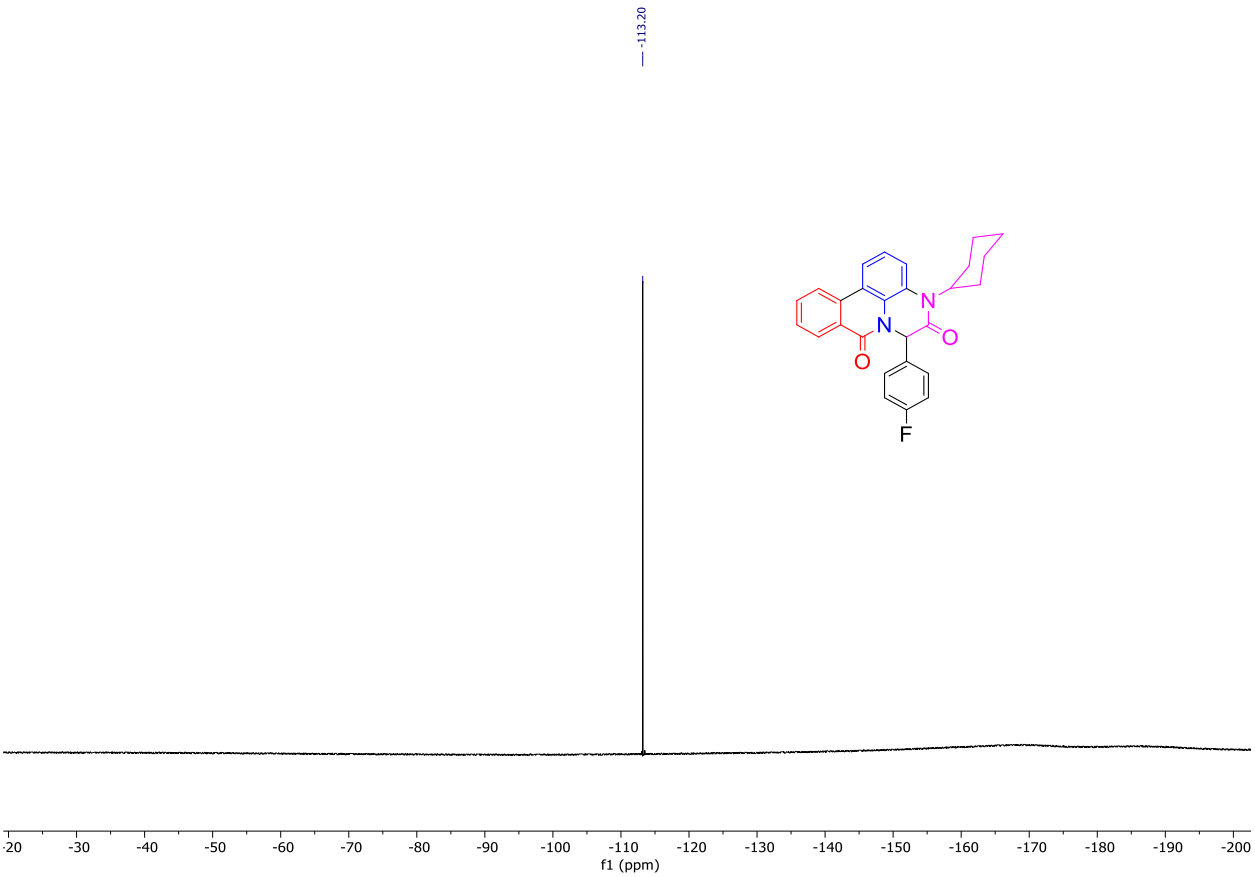
^{13}C-NMR of compound **6d** (151MHz, $CDCl_3$)



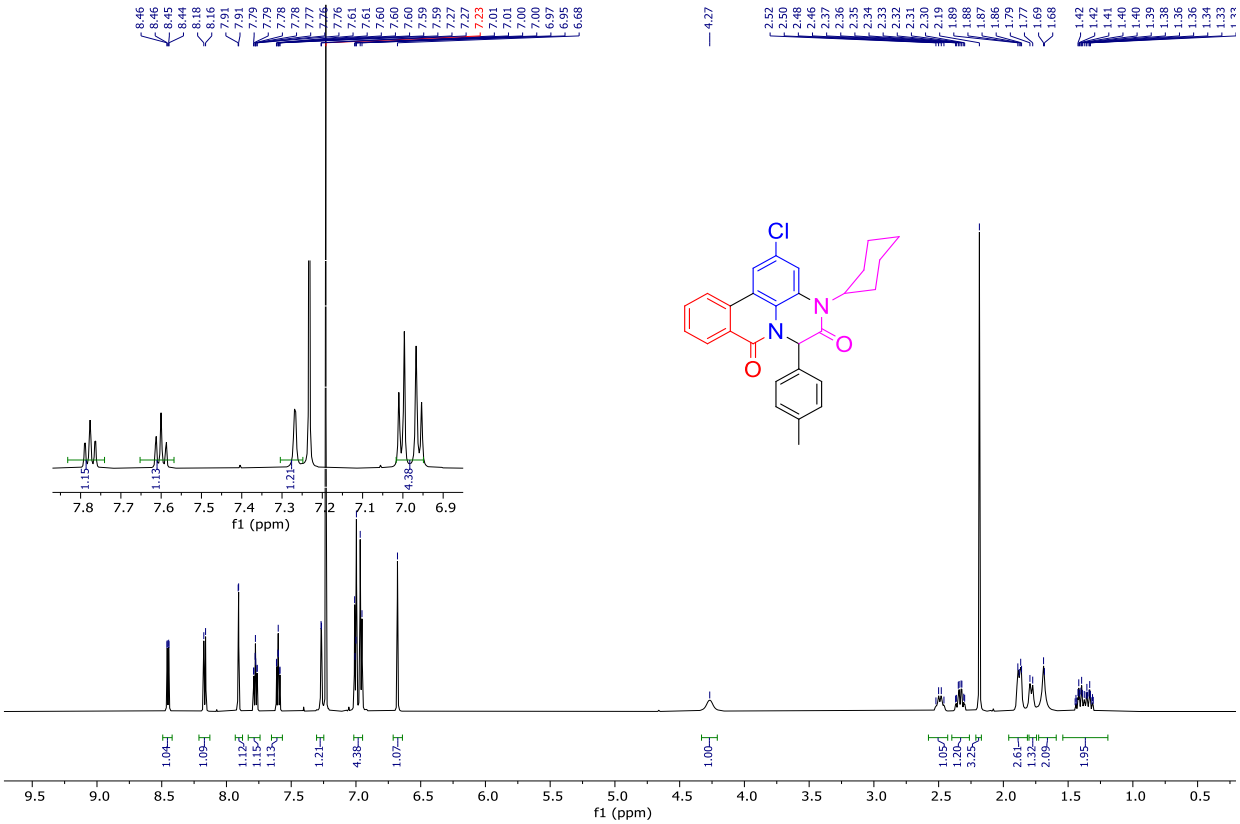
^{1}H-NMR of compound **6e** (600MHz, $CDCl_3$)



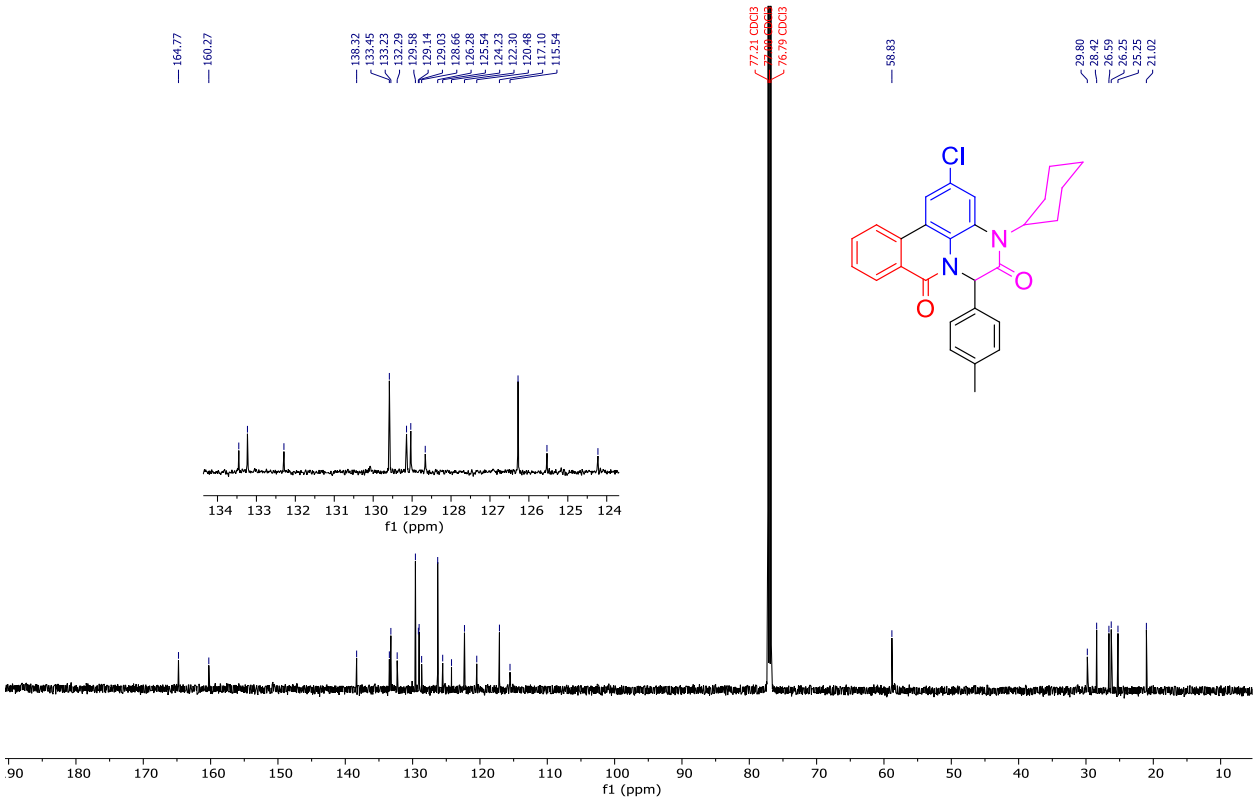
^{13}C-NMR of compound **6e** (151MHz, $CDCl_3$)



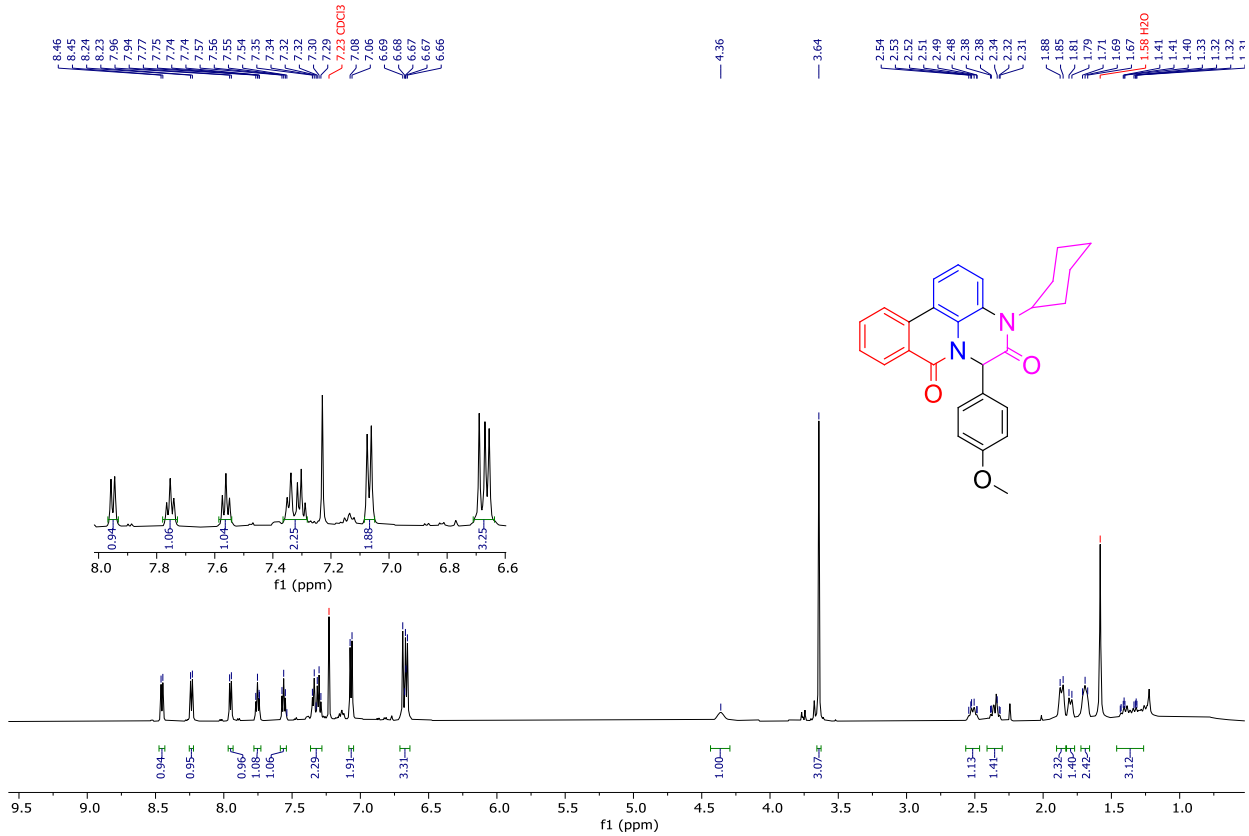
^{19}F NMR of compound **6e** (565 MHz, $CDCl_3$)



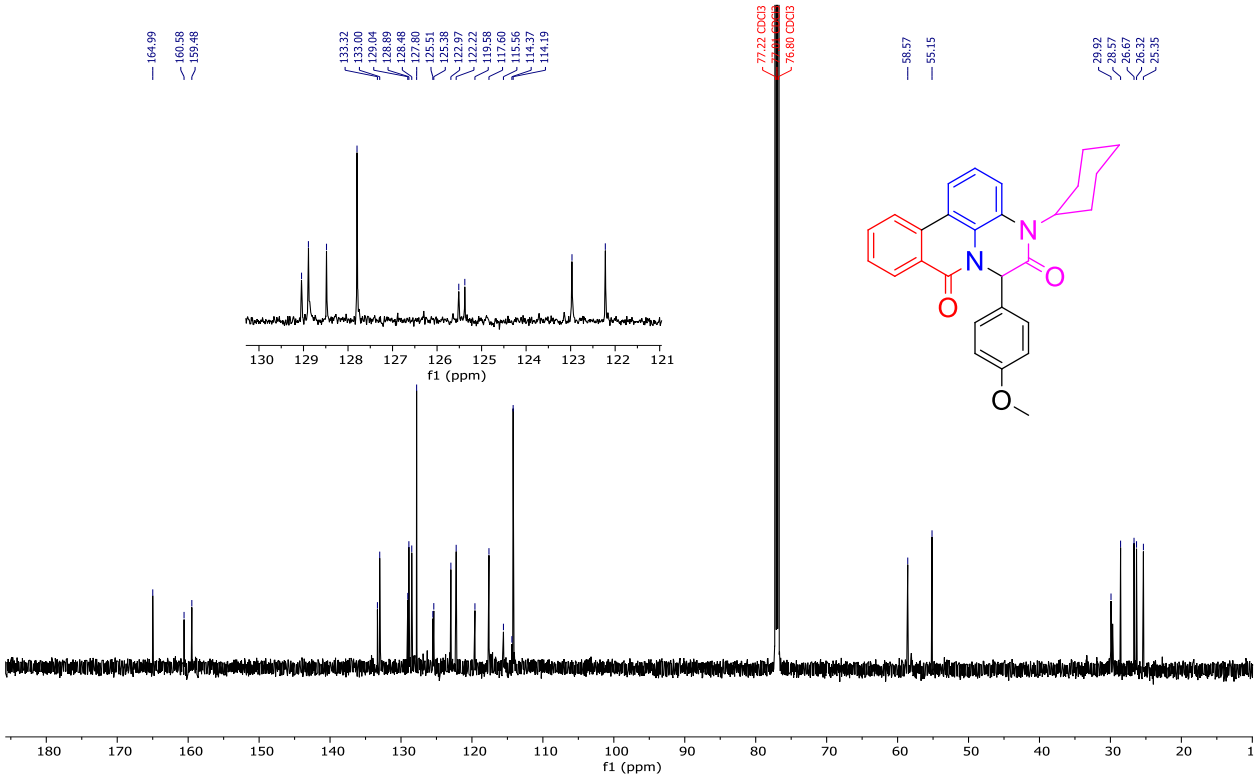
^{1}H-NMR of compound **6f** (600MHz, $CDCl_3$)



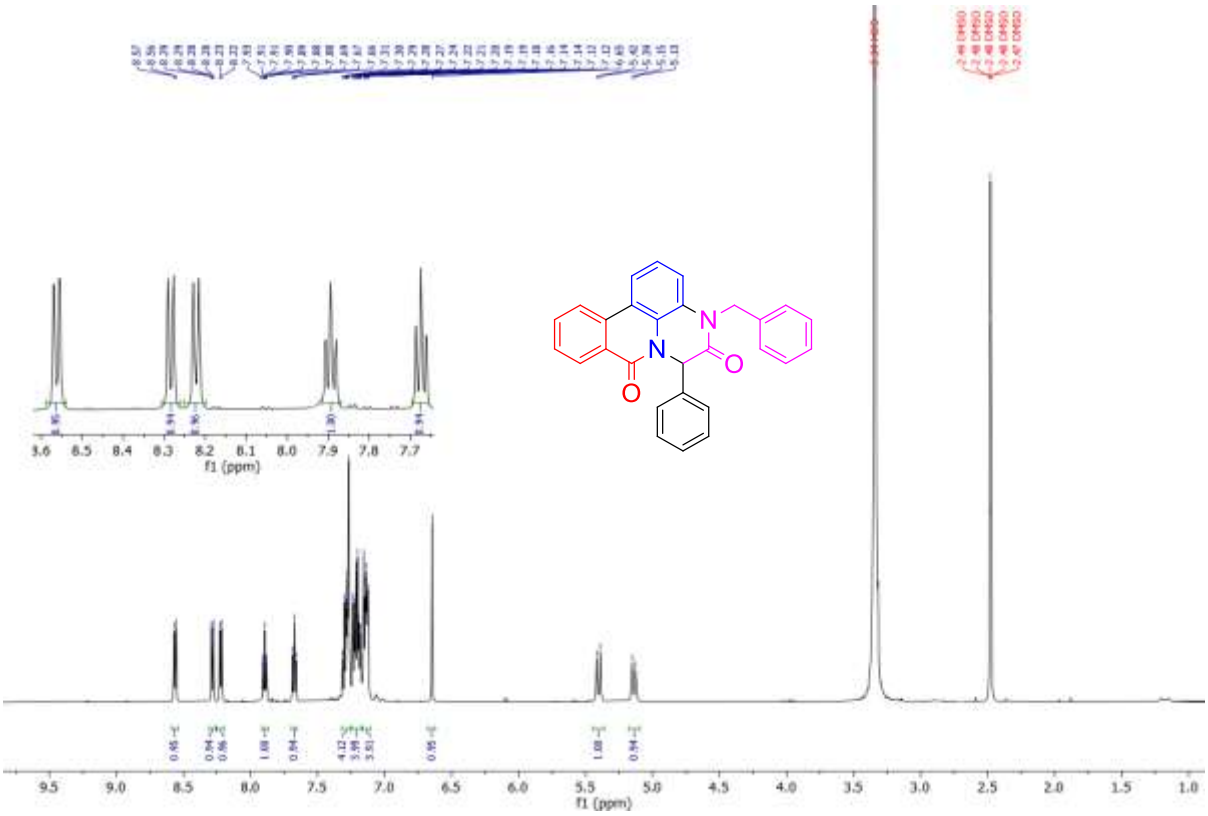
^{13}C-NMR of compound **6f** (151MHz, $CDCl_3$)



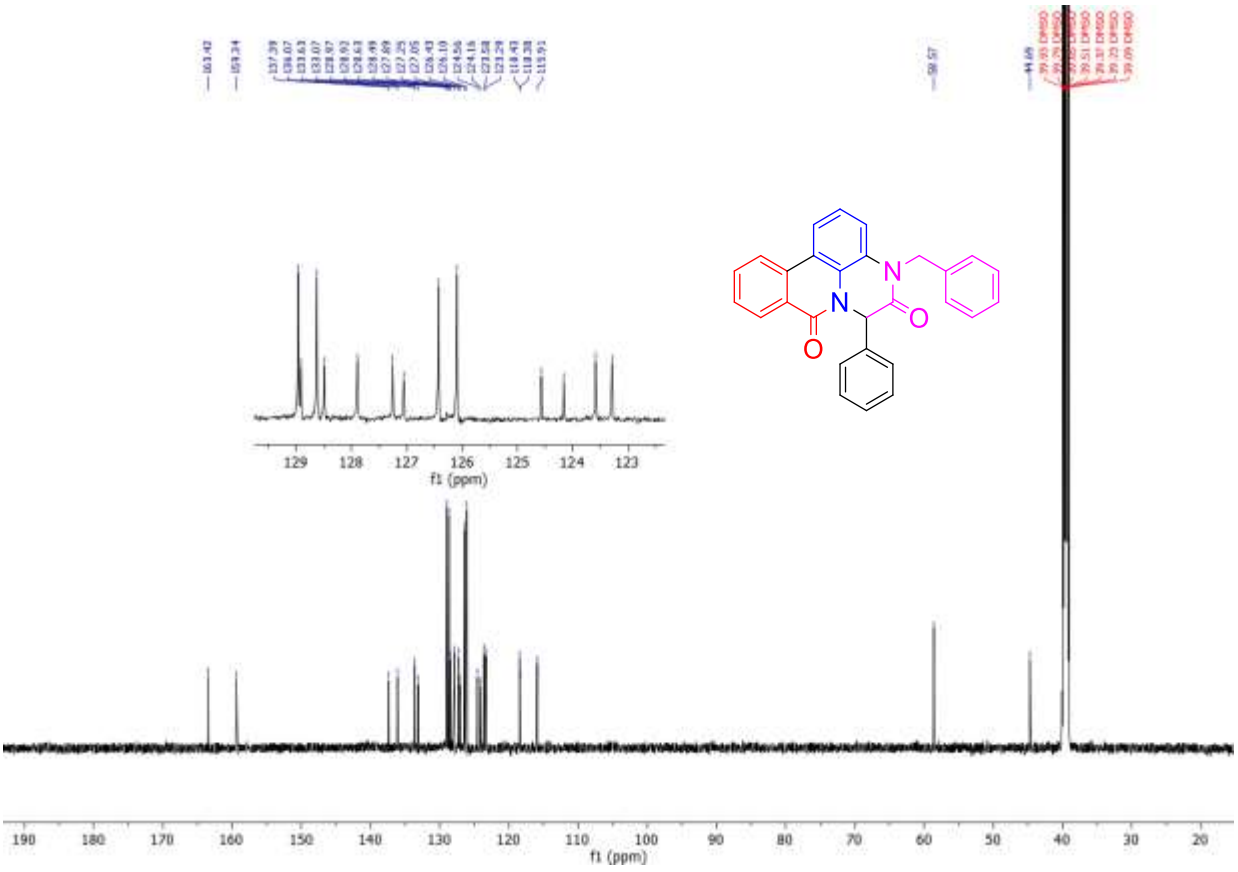
^{1}H-NMR of compound **6g** (600MHz, $CDCl_3$)



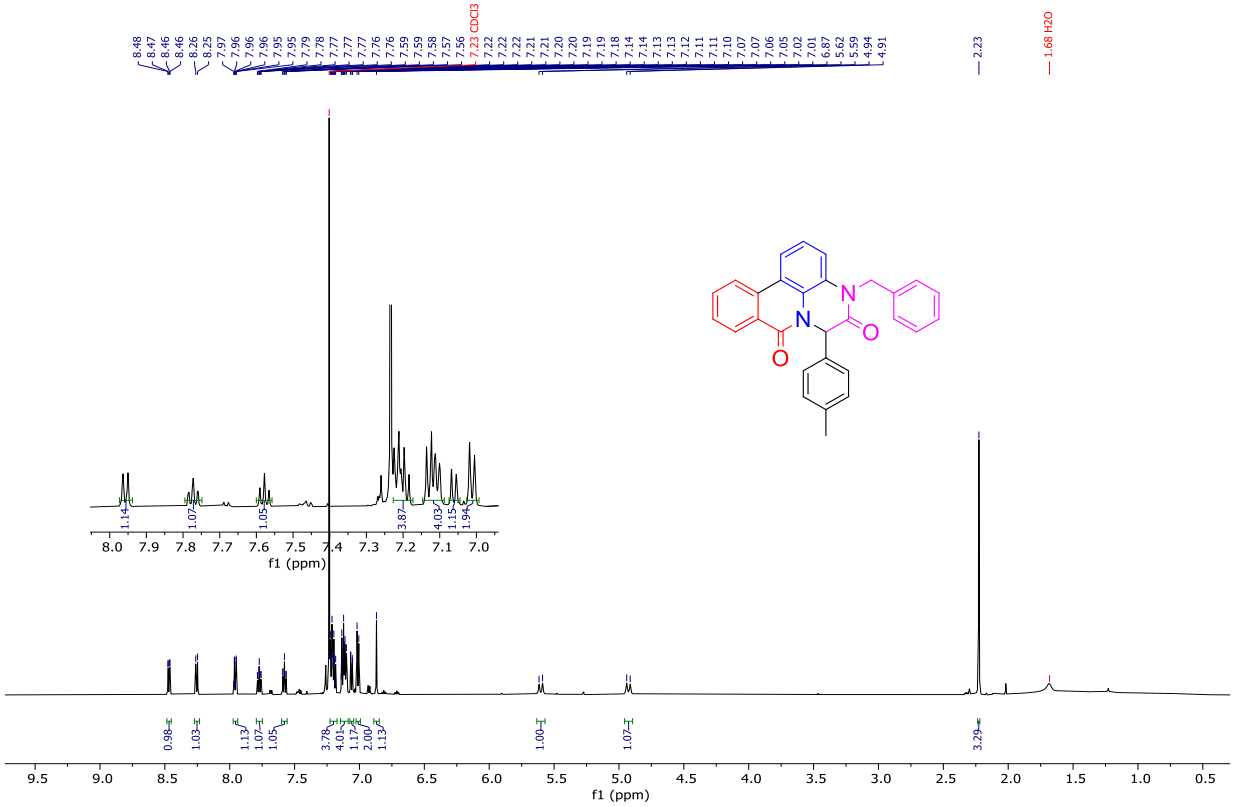
^{13}C-NMR of compound **6g** (151MHz, $CDCl_3$)



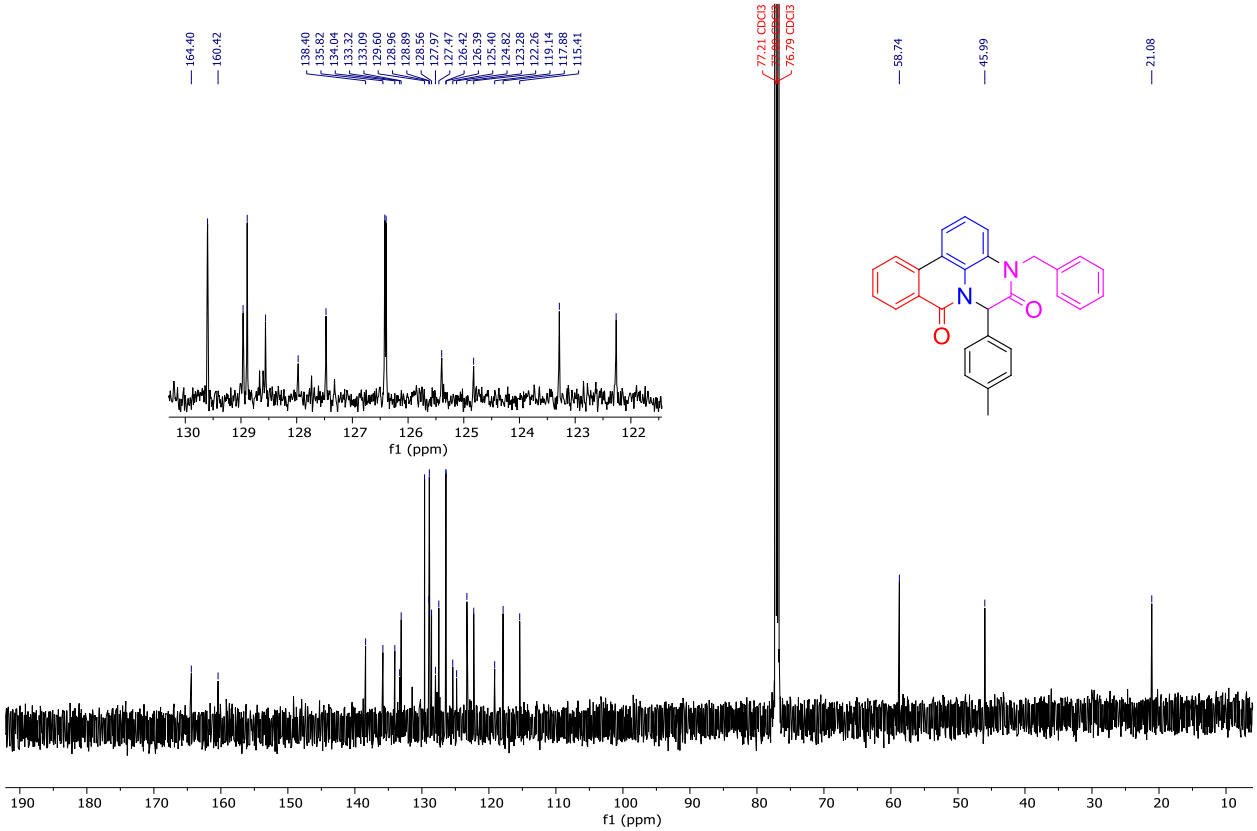
^{1}H-NMR of compound **6h** (600MHz, DMSO-d6)



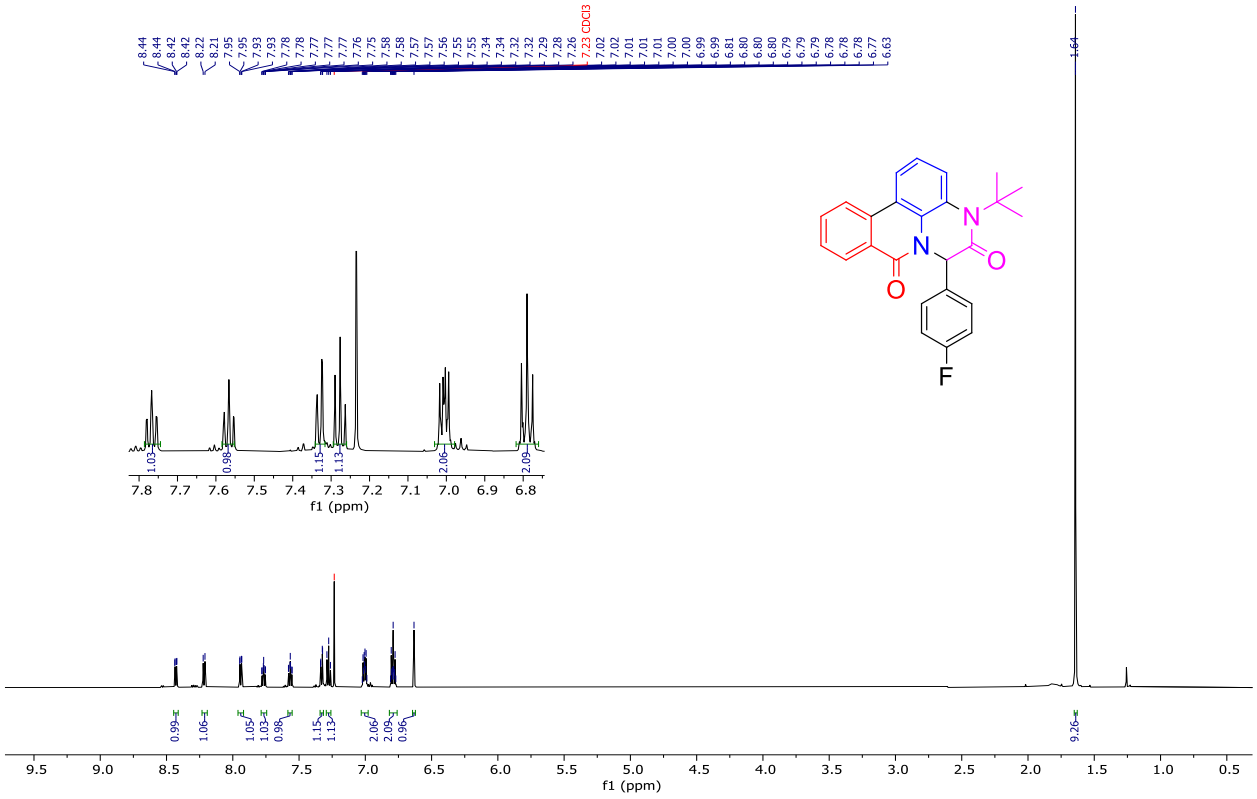
^{13}C-NMR of compound **6h** (151 MHz, DMSO-d6)



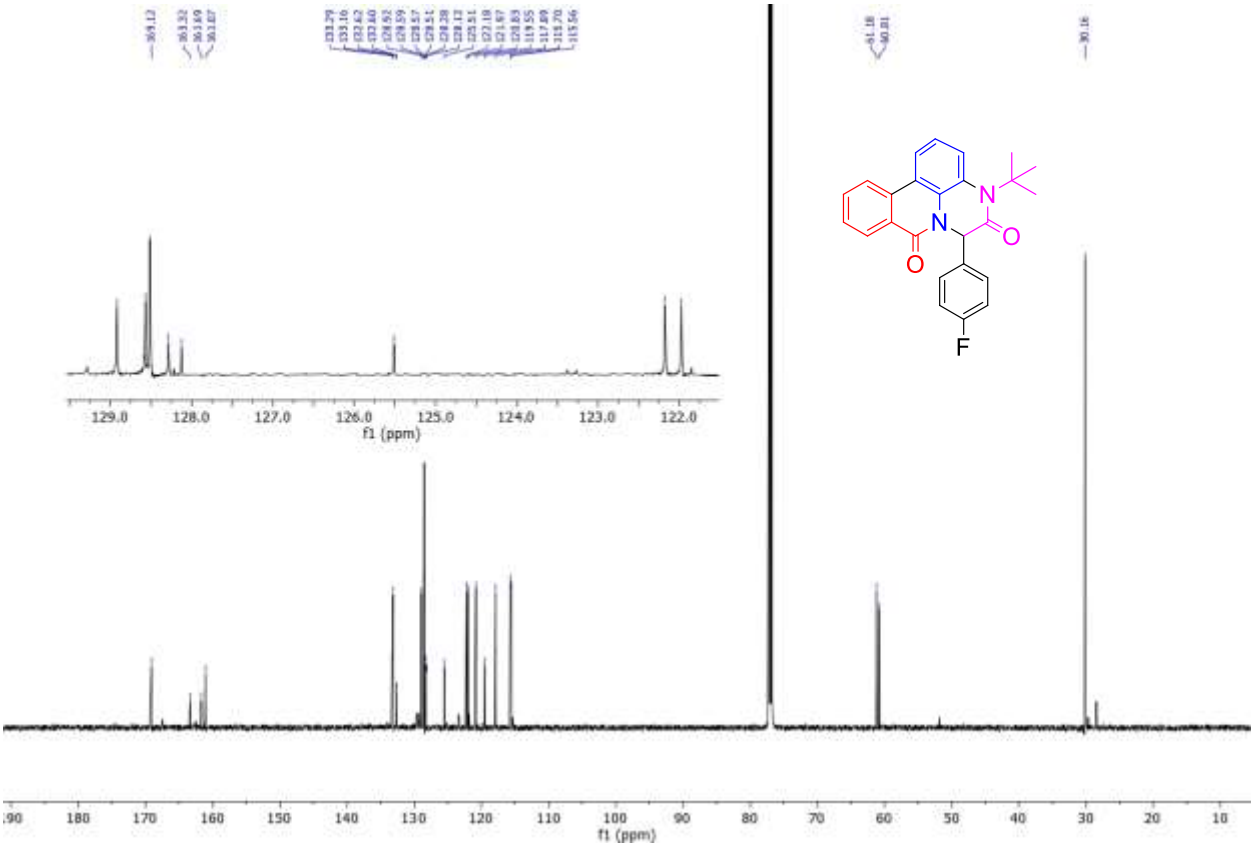
^{1}H-NMR of compound **6i** (600MHz, $CDCl_3$)



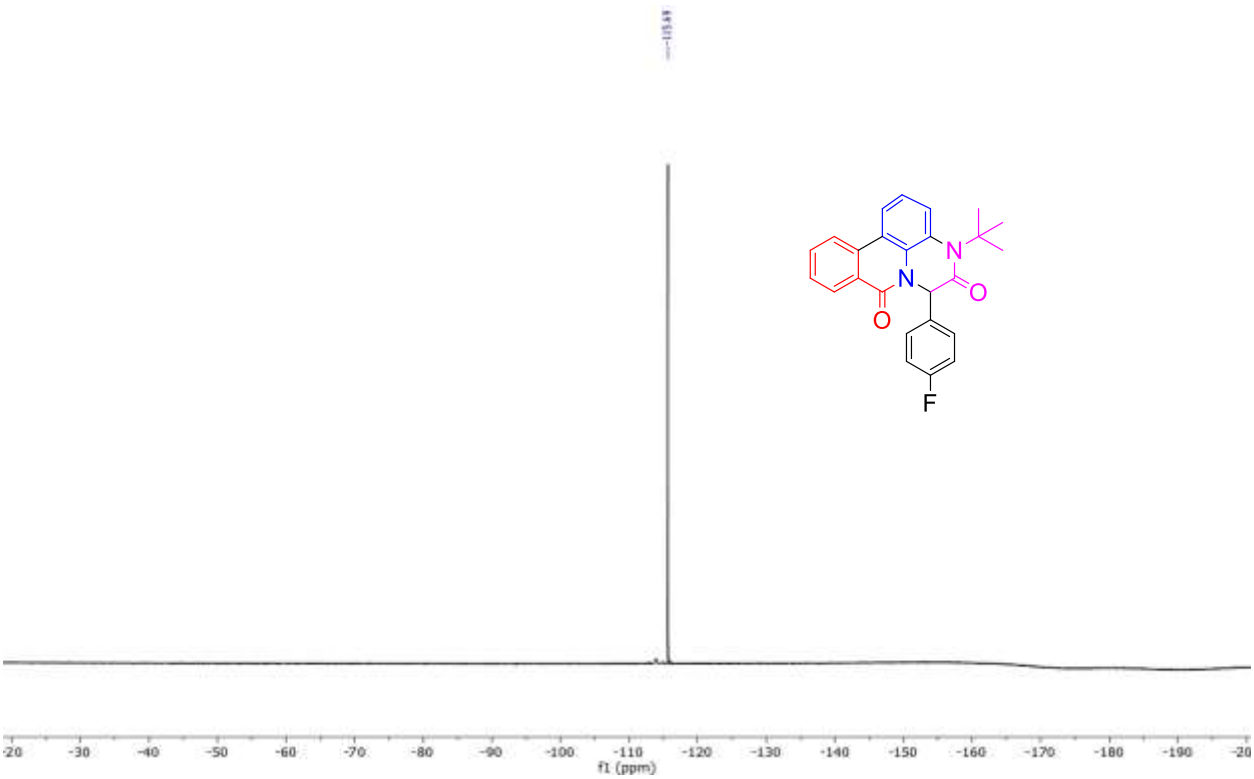
^{13}C-NMR of compound **6i** (151MHz, $CDCl_3$)



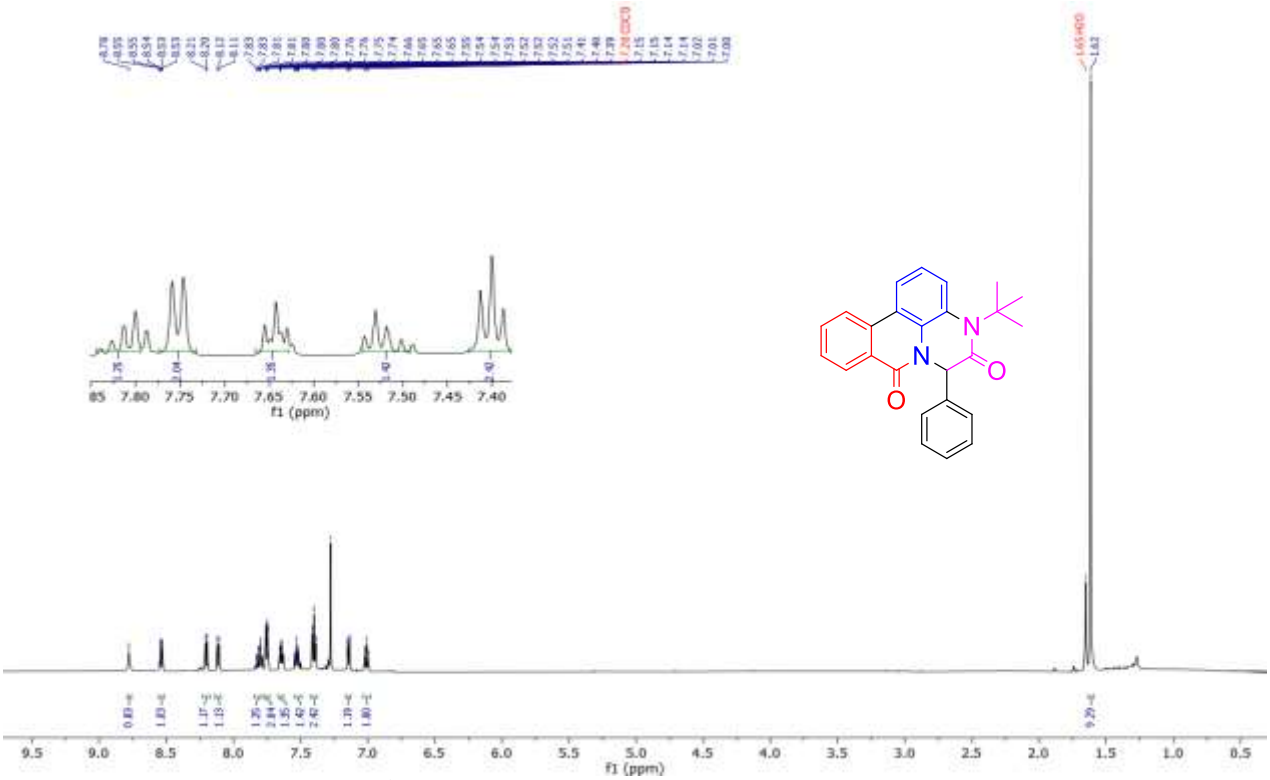
^{1}H-NMR of compound **6j** (600MHz, $CDCl_3$)



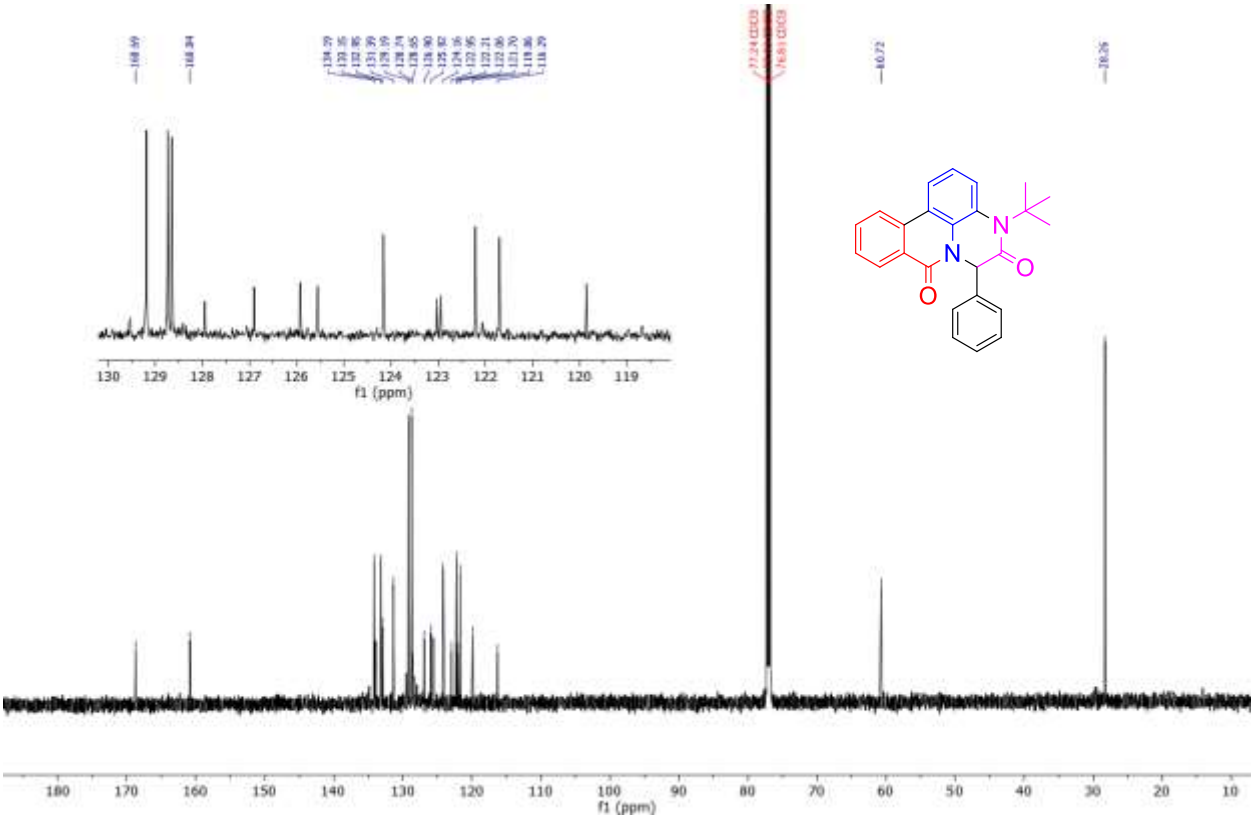
^{13}C-NMR of compound **6j** (151MHz, $CDCl_3$)



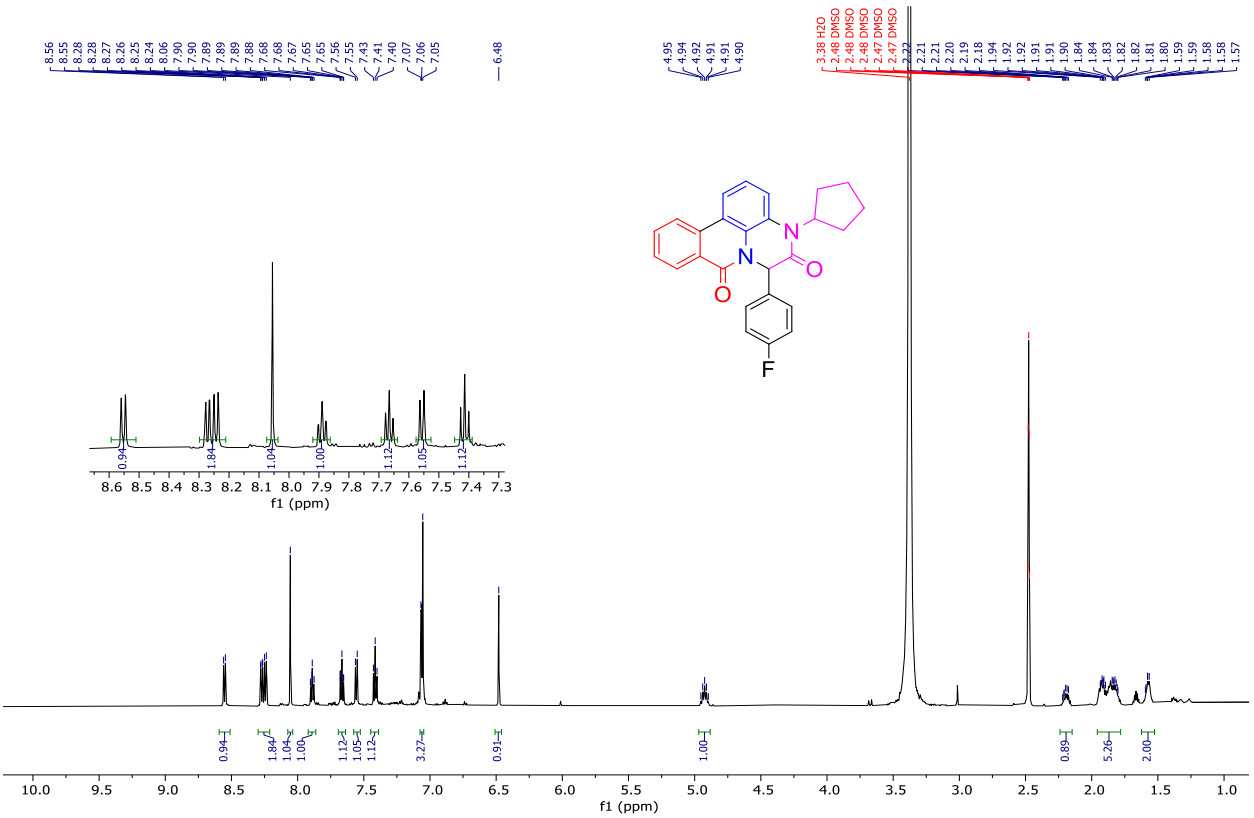
^{19}F NMR of compound **6j** (565 MHz, $CDCl_3$)



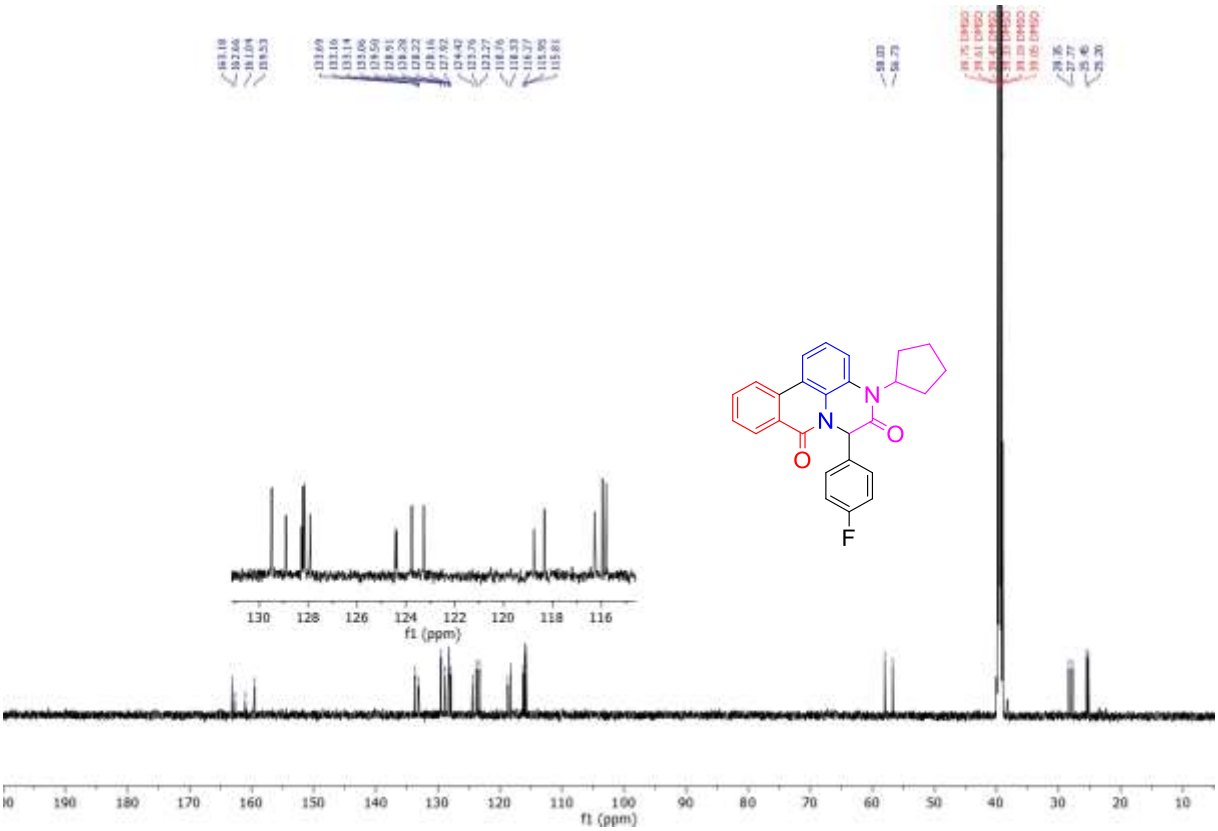
^{1}H-NMR of compound **6k** (600MHz, $CDCl_3$)



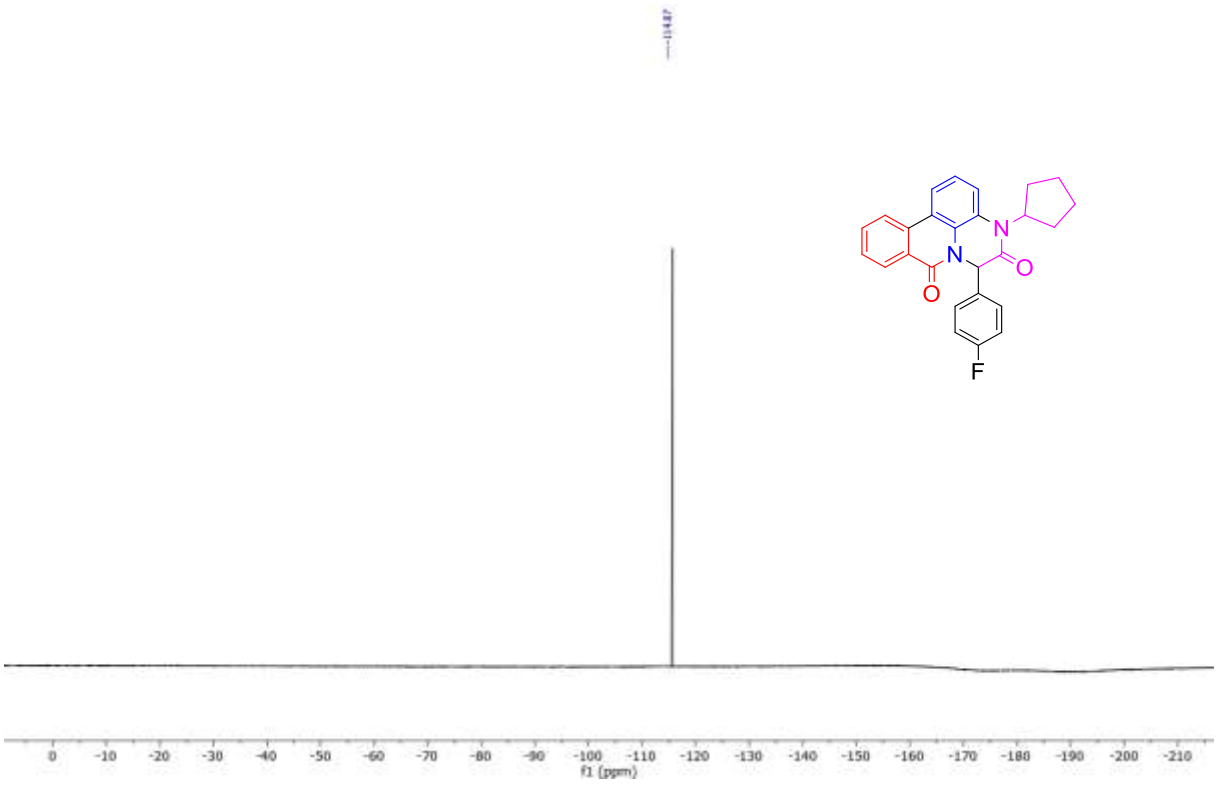
^{13}C-NMR of compound **6k** (151MHz, $CDCl_3$)



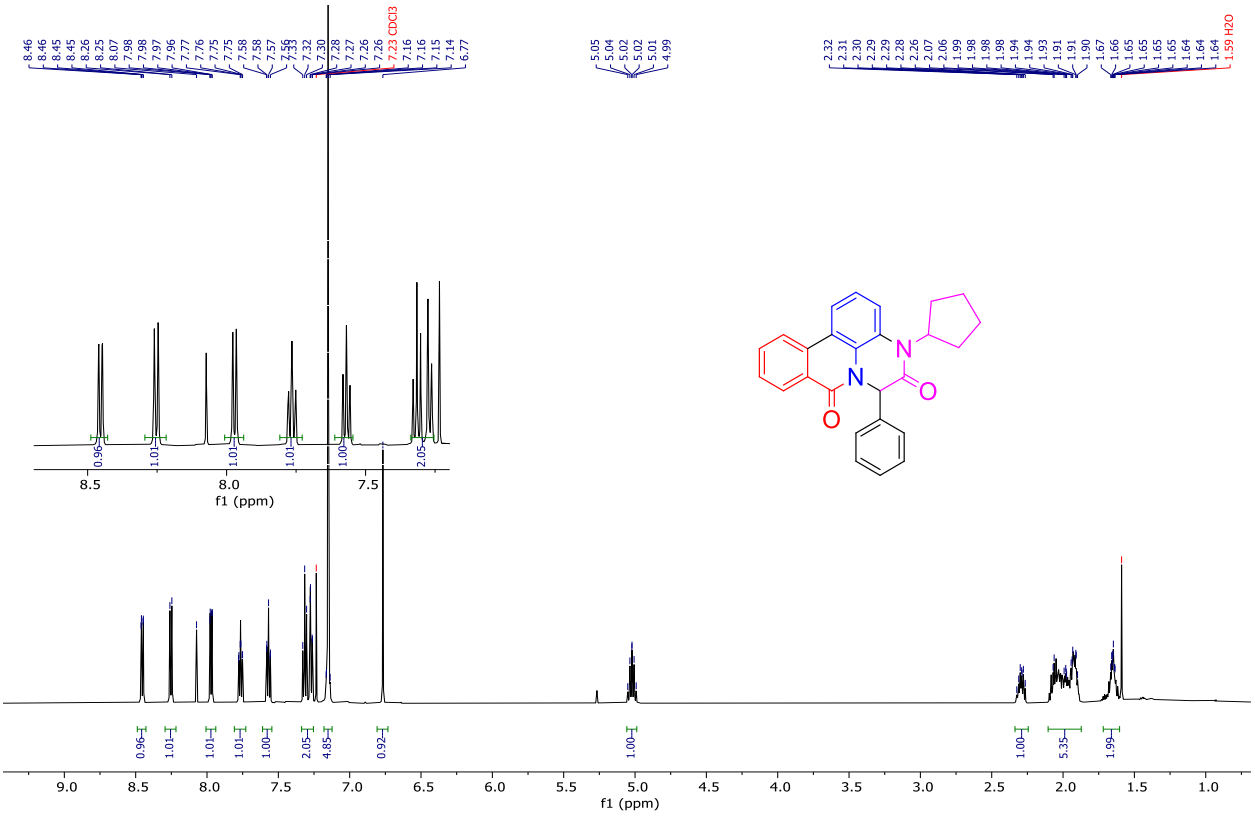
^{1}H-NMR of compound **6l** (600MHz, $CDCl_3$)



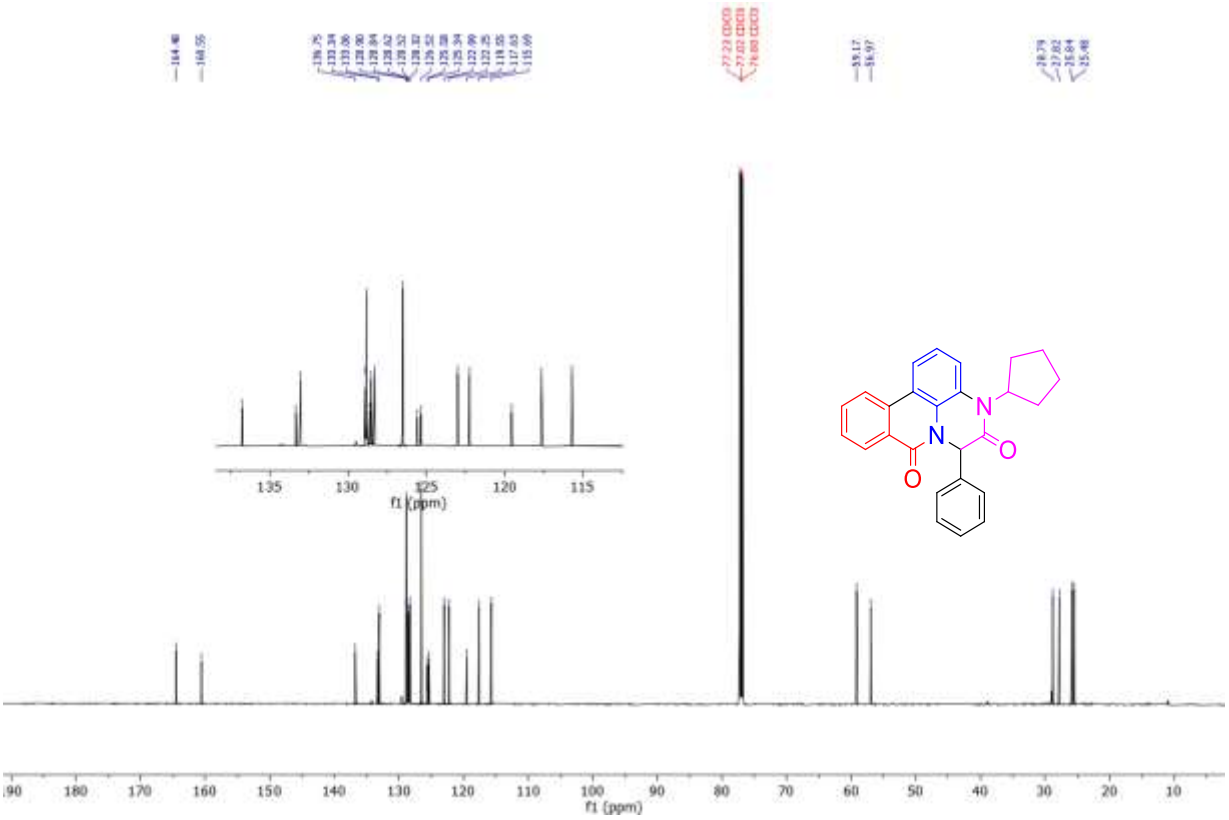
^{13}C-NMR of compound **6l** (151MHz, DMSO-d6)



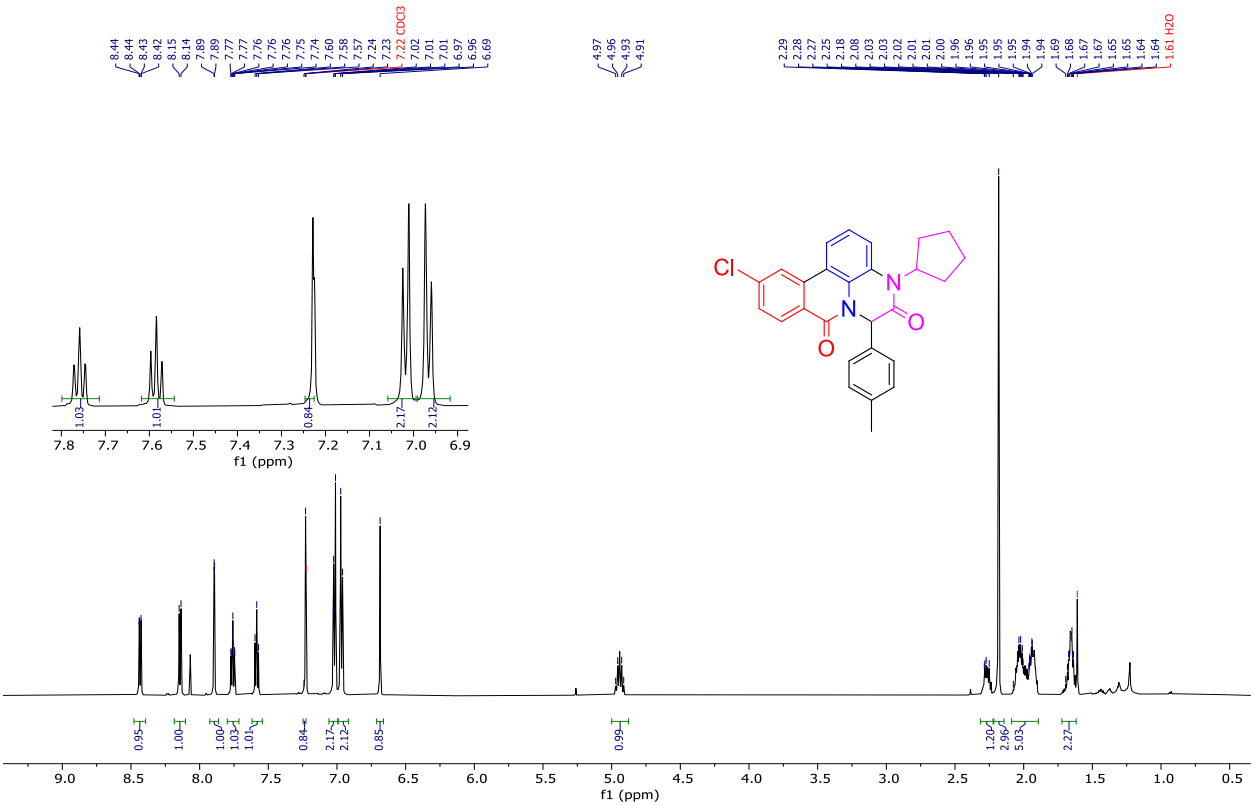
^{19}F NMR of compound **6l** (565 MHz, $CDCl_3$)



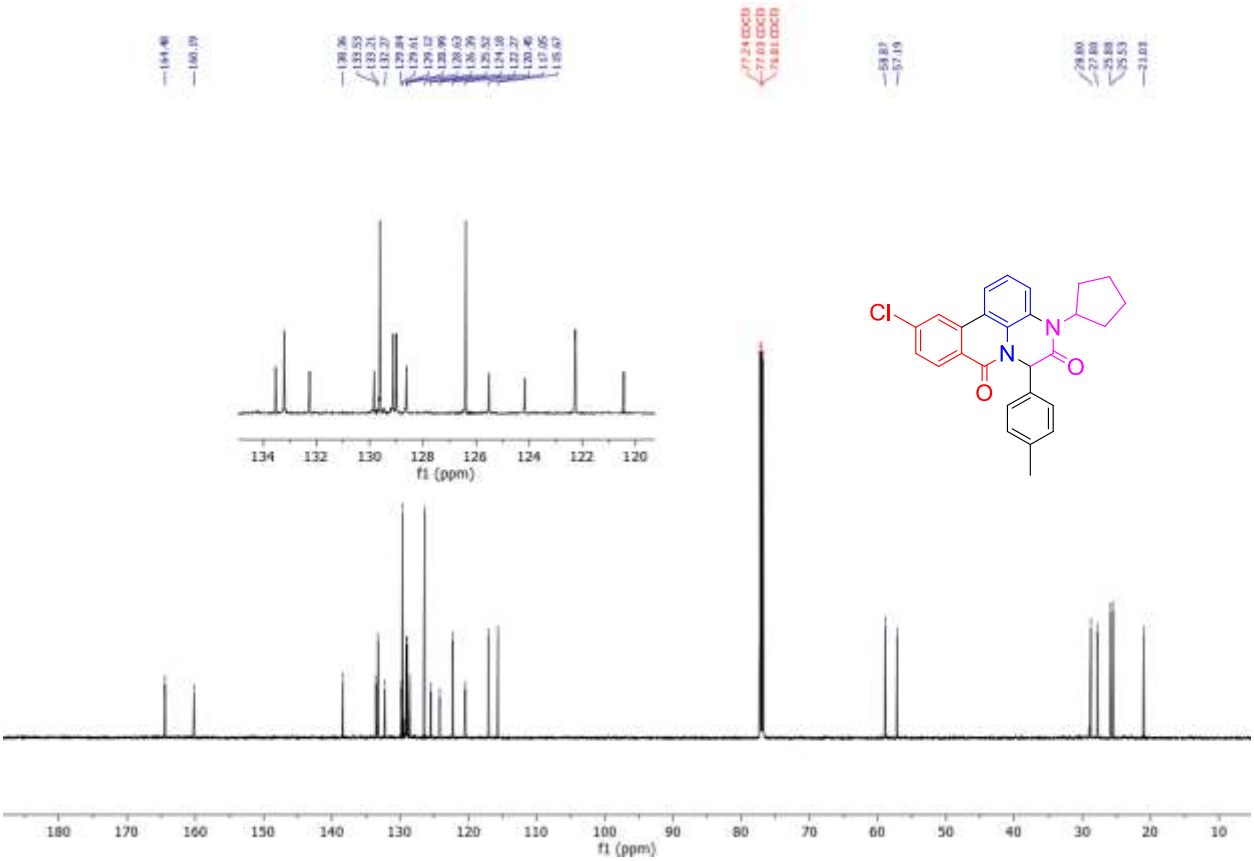
^{1}H-NMR of compound **6m** (600MHz, $CDCl_3$)



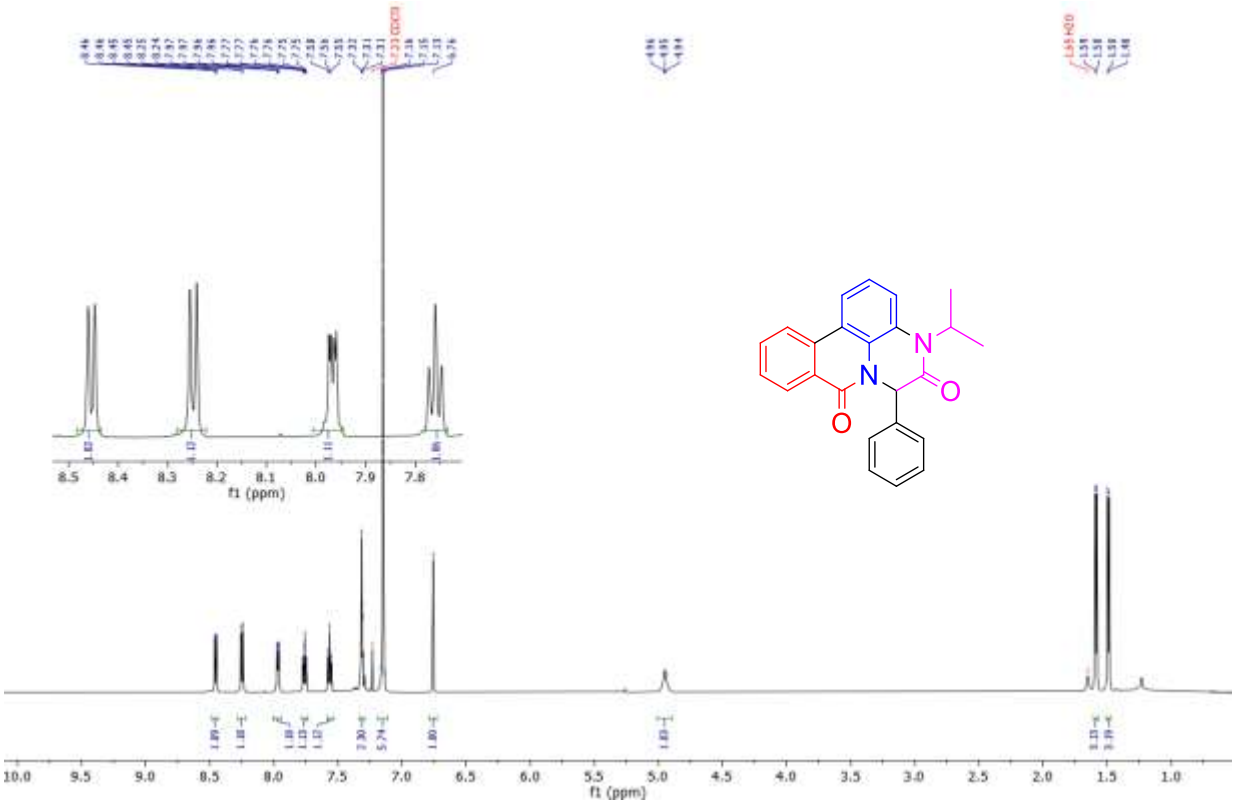
^{13}C-NMR of compound **6m** (151MHz, $CDCl_3$)



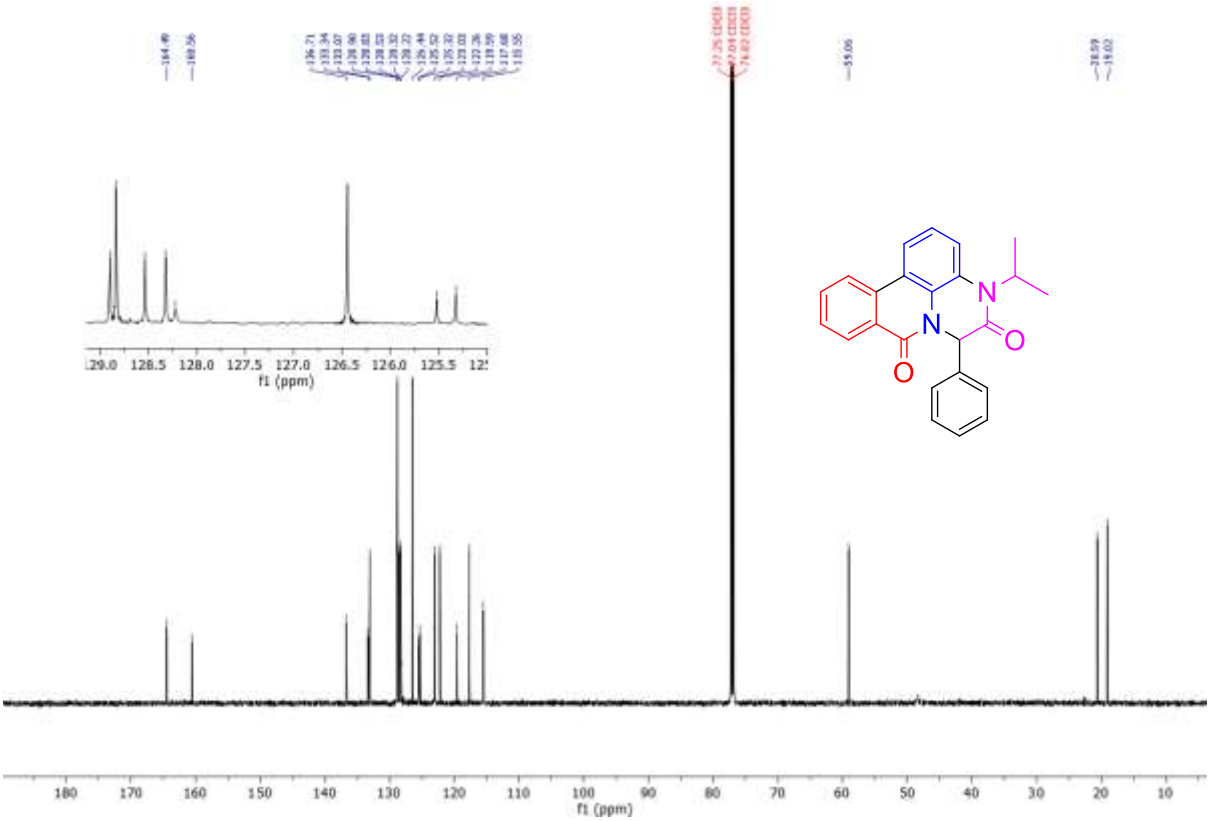
^{1}H-NMR of compound **6n** (600MHz, $CDCl_3$)



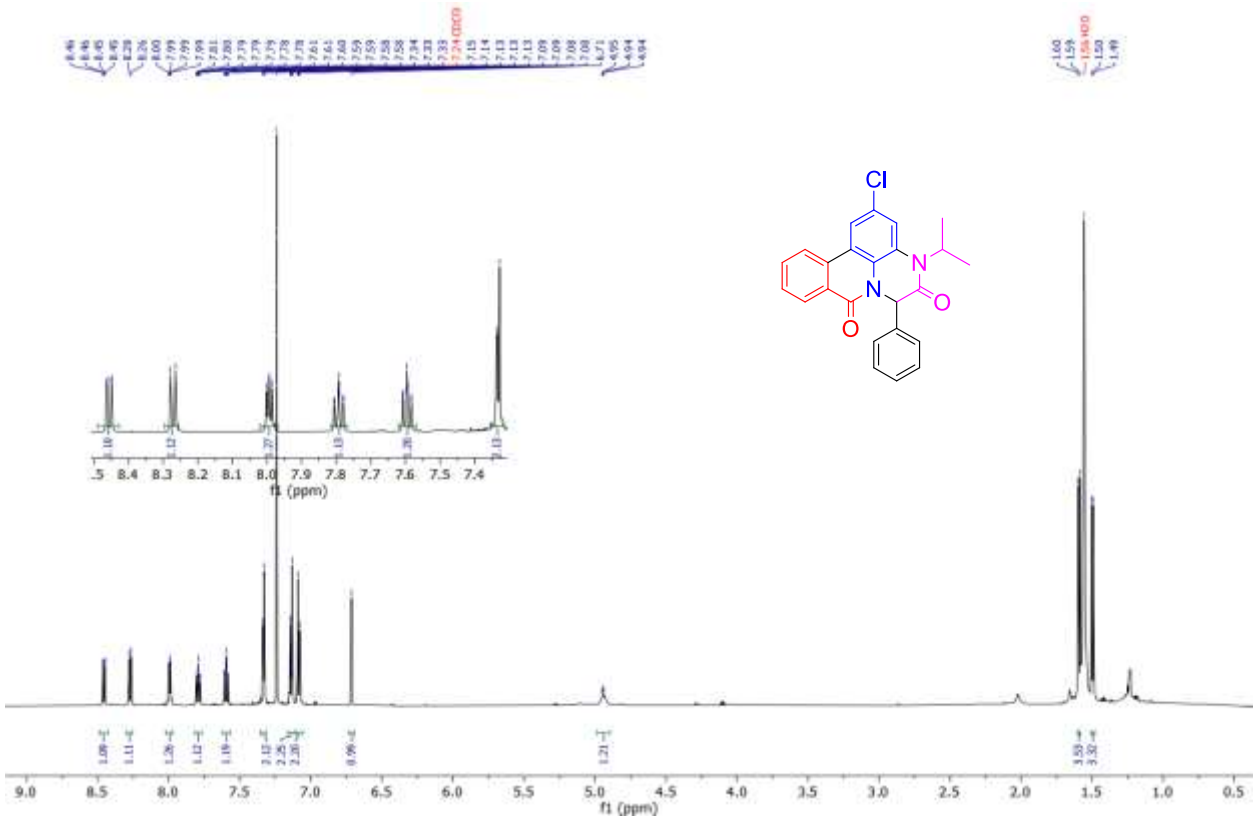
^{13}C-NMR of compound **6n** (151MHz, $CDCl_3$)



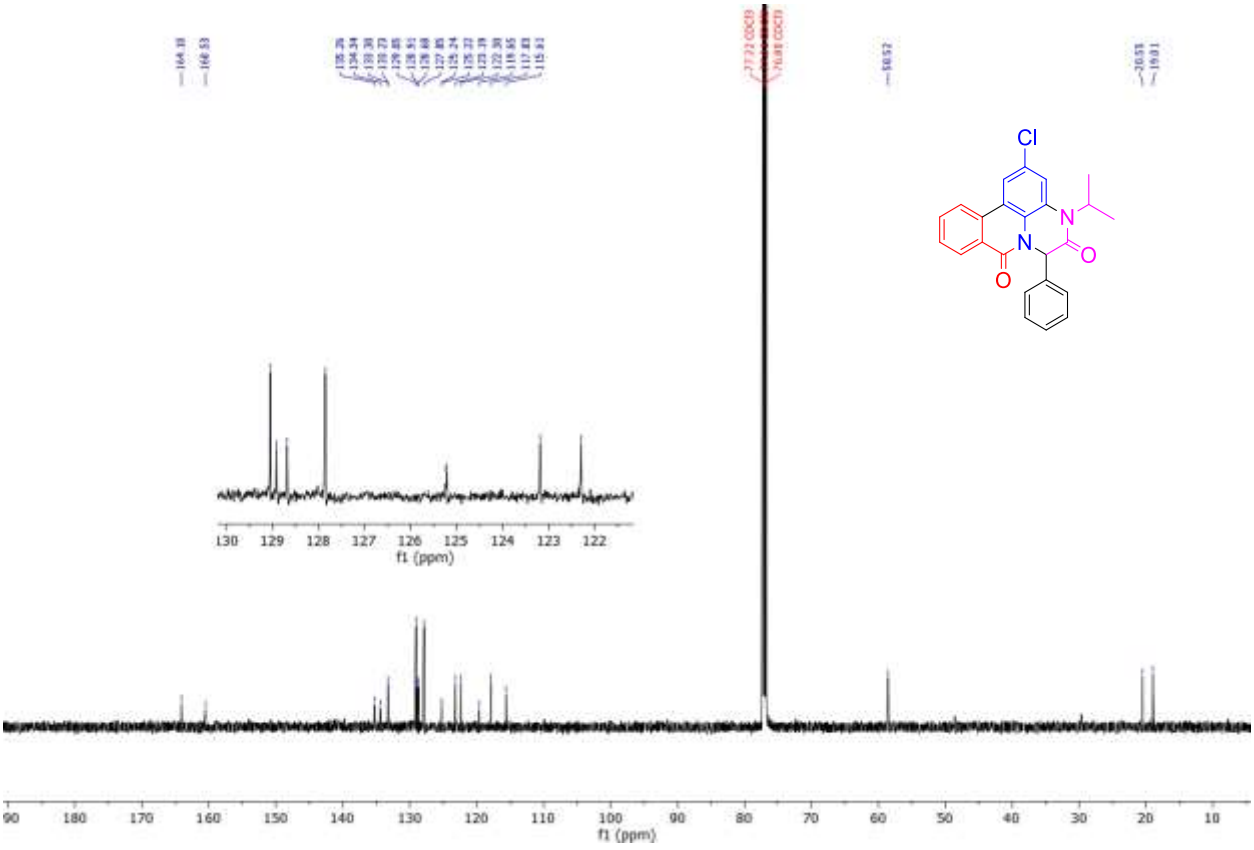
^{1}H-NMR of compound **6o** (600MHz, $CDCl_3$)



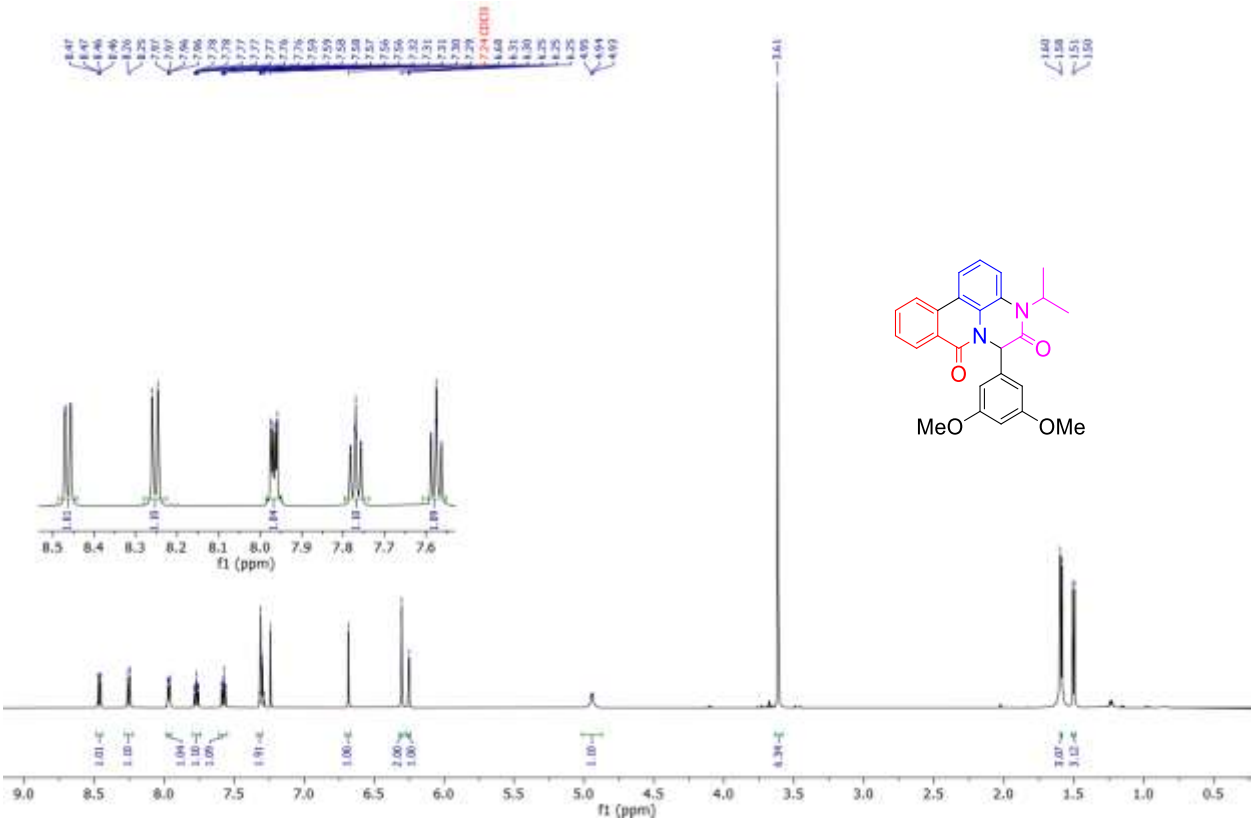
^{13}C-NMR of compound **6o** (151MHz, $CDCl_3$)



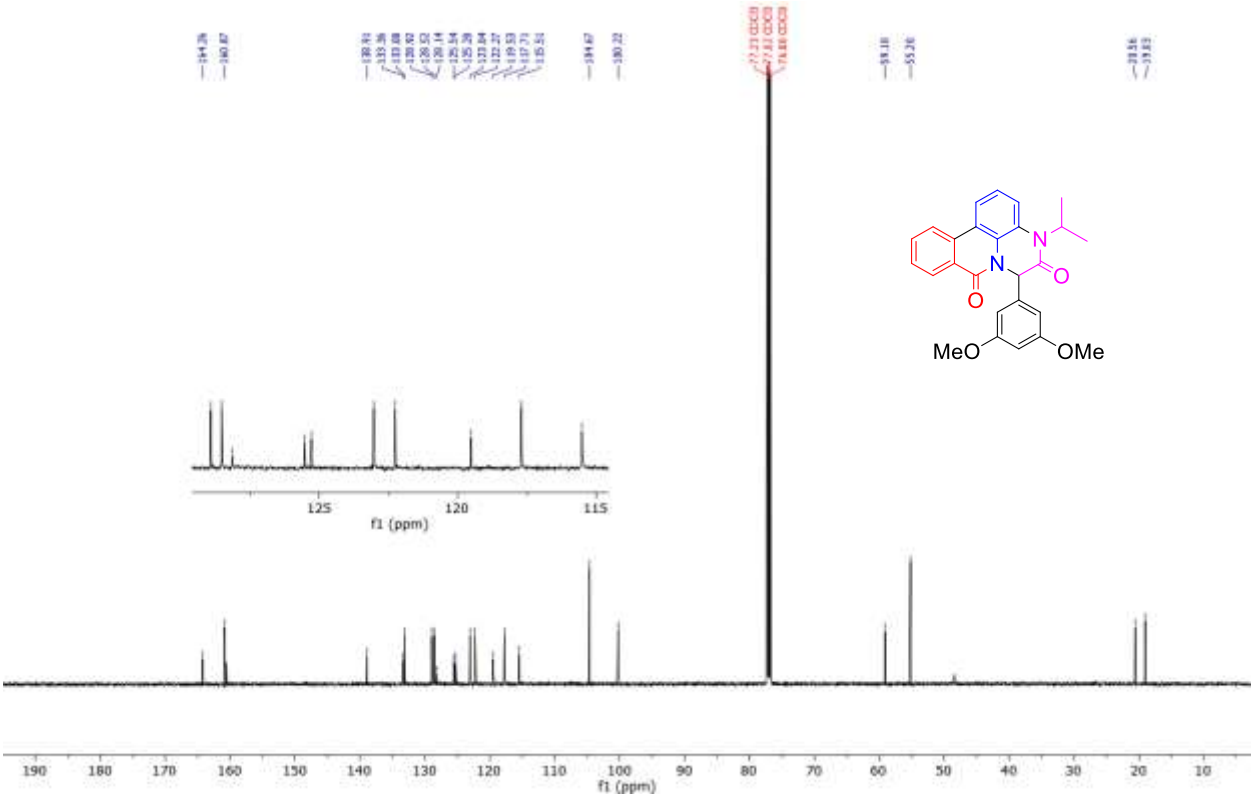
^{1}H-NMR of compound **6p** (600MHz, $CDCl_3$)



^{13}C-NMR of compound **6p** (151MHz, $CDCl_3$)



^{1}H-NMR of compound **6q** (600MHz, $CDCl_3$)



^{13}C-NMR of compound **6q** (151MHz, $CDCl_3$)