Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Supporting Information

for

Cytotoxic activity, cell imaging and DNA Photocleavage induced by a Pt(II) cyclophane bearing 1, 2 diamino ethane as a terminal ligand

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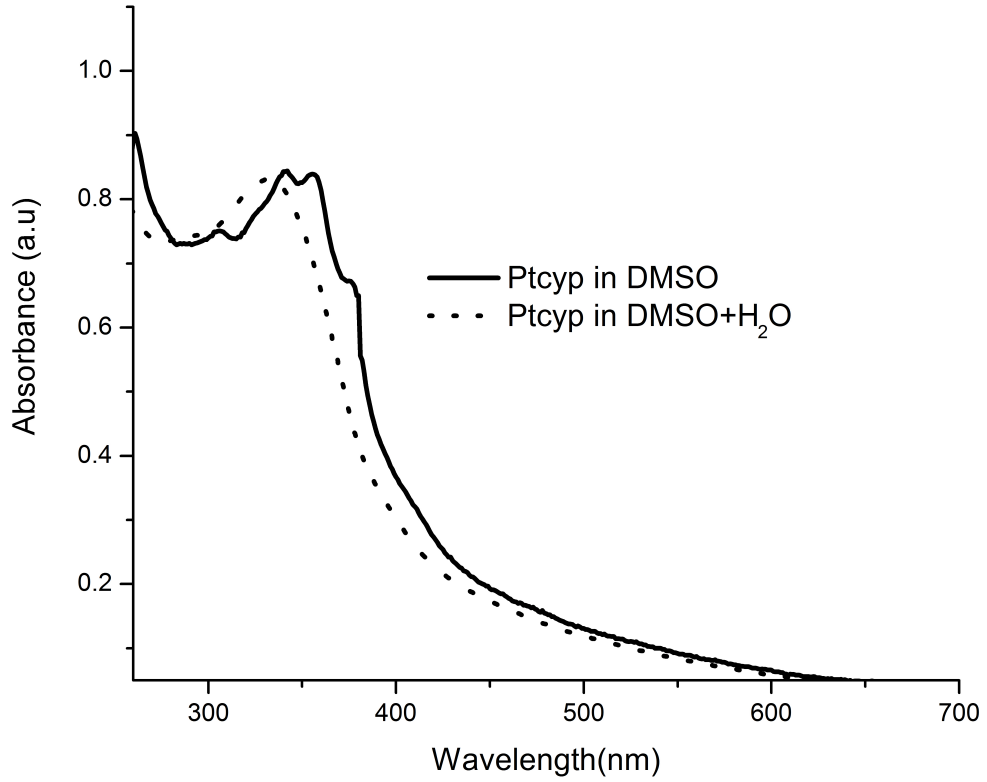
S1: **Synthetic procedure of Pt^{II} complex Ptcyp [$C_{44}H_{48}O_4N_8P_4F_{24}Pt_2$]**

Materials and methods. K_2PtCl_4, purchased from Sigma-Aldrich, was converted into $Pt(en)Cl_2$ using a reported procedure. All the solvent used in the spectroscopic measurement were of spectroscopic grade. Elemental analysis and mass measurements are carried out on Carbo-Erba 1108 elemental analyzer and JEOL SX-102 mass spectrometer respectively. IR spectra were recorded as KBr pellets on a Varian 3100 FTIR spectrometer, whereas ^{1}H NMR spectra are recorded on a JEOL AL 300 MHz spectrometer using DMSO-d_6 as solvent & TMS as internal reference.

Synthesis of complex (Ptcyp). Complex **Ptcyp** was prepared and characterized by a reported procedure in which a solution of $Pt(en)Cl_2$ (0.672 g, 2.0 mmol) in DMF (10 mL) was added to *N,N′*-bis(salicylidene)-*p*-phenylenediamine (LH_2) (0.630 g, 2.0 mmol) in DMF followed by addition of Et_3N (~5.0 mmol) while stirring. The resultant mixture was stirred while heating on water bath for 5 h. Solid product was obtained after addition of aqueous solution of NH_4PF_6. It was then filtered, washed with distilled water, methanol and diethyl ether and was recrystallized with DMSO/MeOH mixture. It was finally dried in *vacuo* as $[Pt(en)LH_2]_2 \cdot 4PF_6$ **(Ptcyp)**. Yield: 35%. m.p.: >230 °C d. Elemental analysis calcd (%) for $C_{44}H_{48}N_8O_4P_4F_{24}Pt_2$: C, 30.66; H, 2.98; N, 6.50. Found: C, 30.78; H, 3.14; N, 6.72. IR (KBr pellet, cm^{-1}): 1633 υ(HC=N), 1264 δ(O-H; phenolic), 2924 υ(C-H; phenyl), 846 $\upsilon(PF_6^-)$. ^{1}H NMR (DMSO-d_6, δ ppm): 13.1 (s, 4H; OH), 9.0 (s, 4H; HC=N), 7.5 (m, 20H; phenyl), 7.0 (m, 8H; NH_2), 6.5 (m, 4H, phenyl), 3.6 (s, 4H; N-CH_2), 3.5 (s, 4H; N-CH_2), ^{1}H NMR (D_2O exchange, δ ppm): 9.0 (s, 4H; HC=N), 7.5 (m, 20H; phenyl), 6.5 (m, 4H, phenyl), 3.6 (s, 4H; N-CH_2), 3.5 (s, 4H; N-CH_2), FAB-MS: *m/z:* 1722 $[M]^+$, 1577 [M - PF_6], 1142 [M - $4PF_6$]. UV-vis (DMSO, 10^{-4} M): λ_{max} (nm) (ε_{max} M^{-1} cm^{-1}) 339

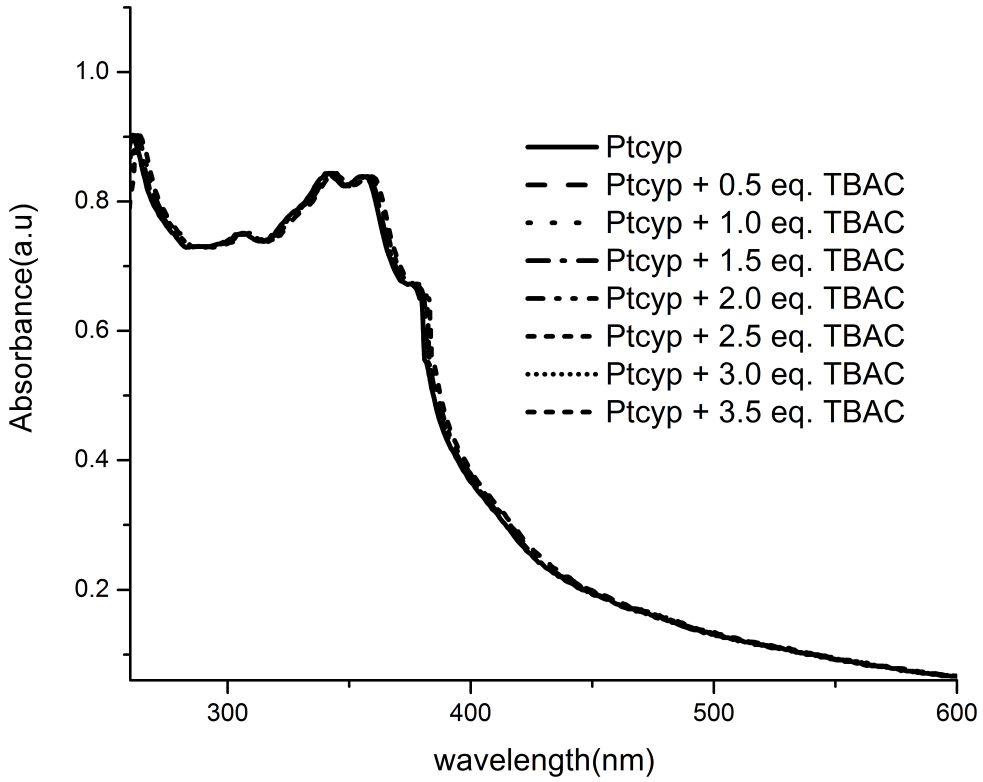
(16900), 354 (16800), 439 (4300); Emission at λ_{ex} 340 nm (DMSO, 10^{-4} M): λ_{max} (nm) (intensity in a. u) 493 (459). Conductivity: Λ_m (DMSO, 10^{-4} M) 360 Ω^{-1} cm^2 mol^{-1}



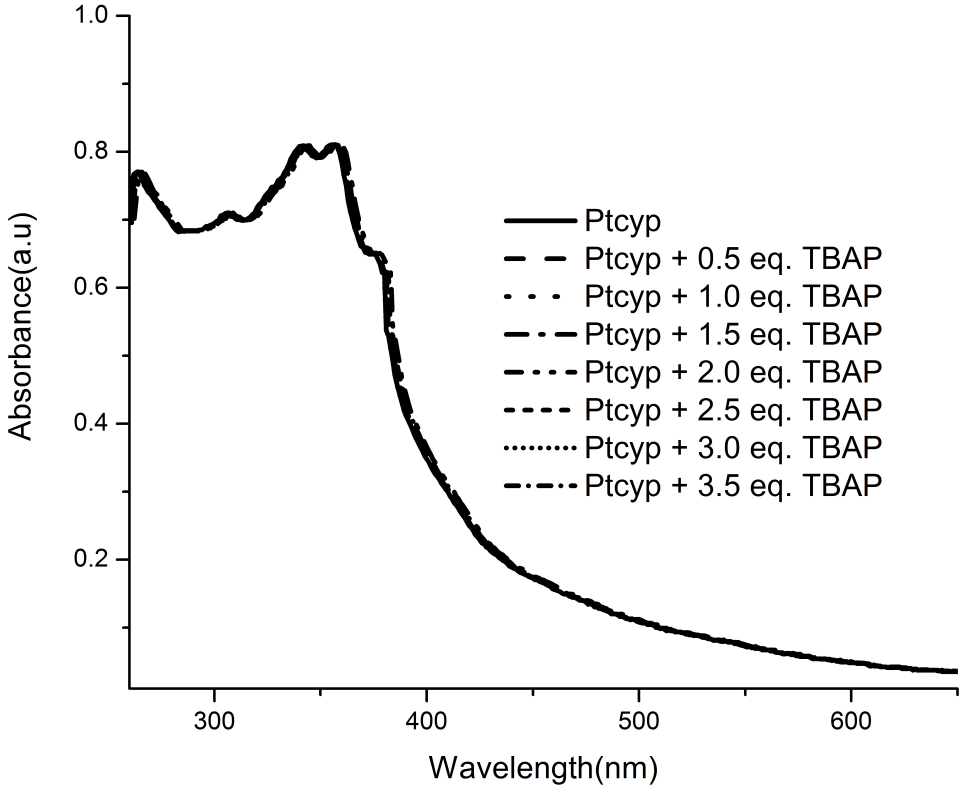
S2: UV-vis spectrum of Ptcyp in DMSO and in presence of Water

Absorption titration

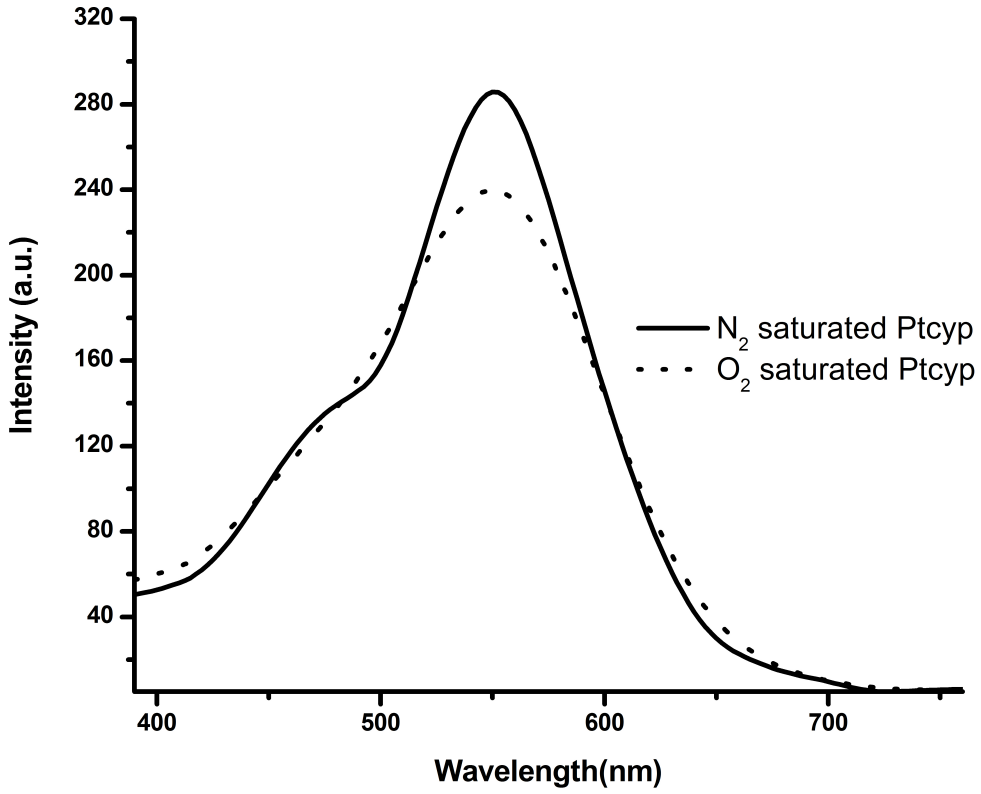
UV-vis spectra were recorded on a JASCO V-630 spectrometer. The absorption titrations of **Ptcyp** with tetrabutyl ammonium chloride and tetrabutyl ammonium phosphate are performed by monitoring the changes in absorption spectrum of **Ptcyp** (10 μM) in DMSO. The concentration of Ptcyp is kept constant at 10 μM while the concentrations of tetrabutyl ammonium chloride and tetrabutyl ammonium phosphate are varied from 0–35 μM.



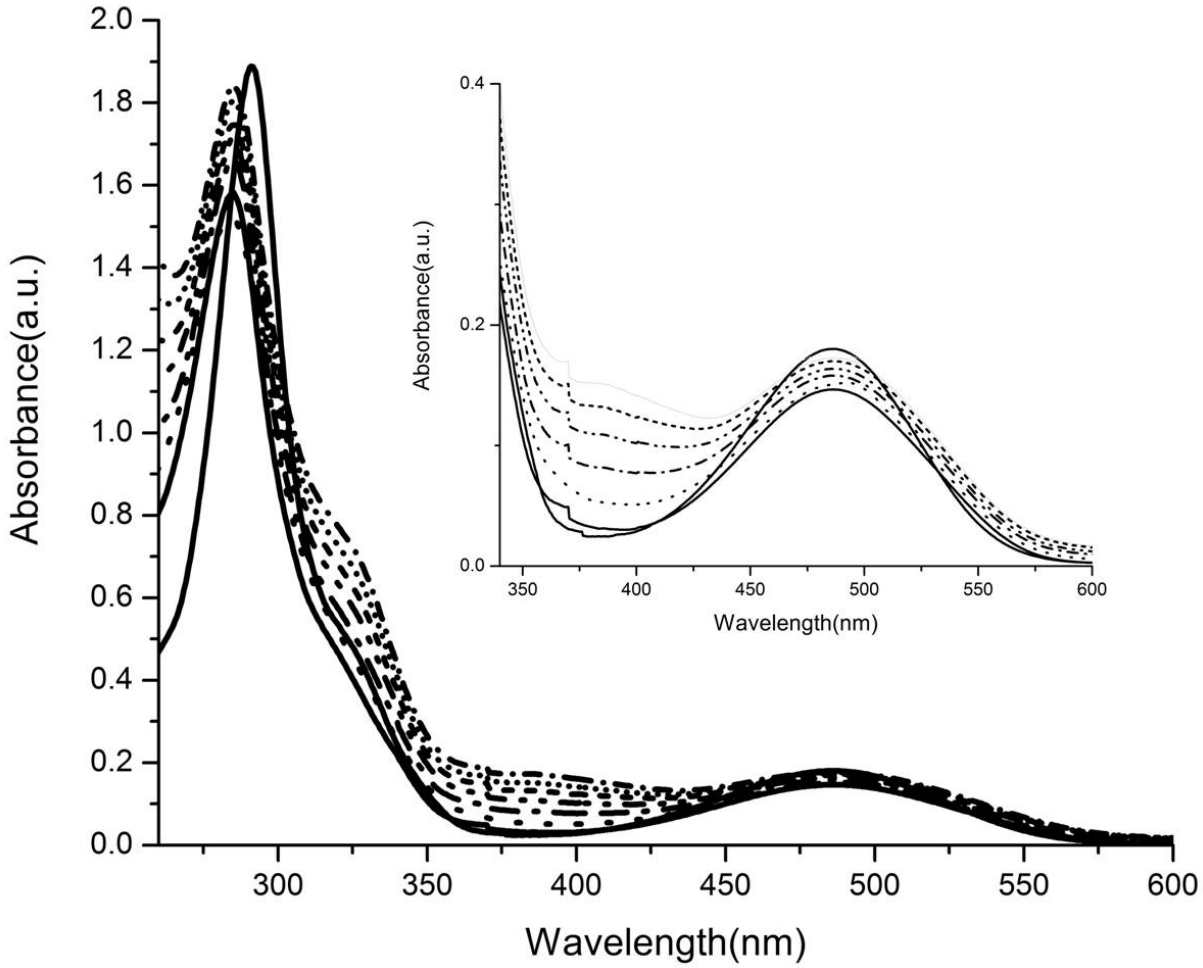
S3: Absorption spectra of Ptcyp = 10 μM in absence and presence of increasing amounts of TBAC =0-35



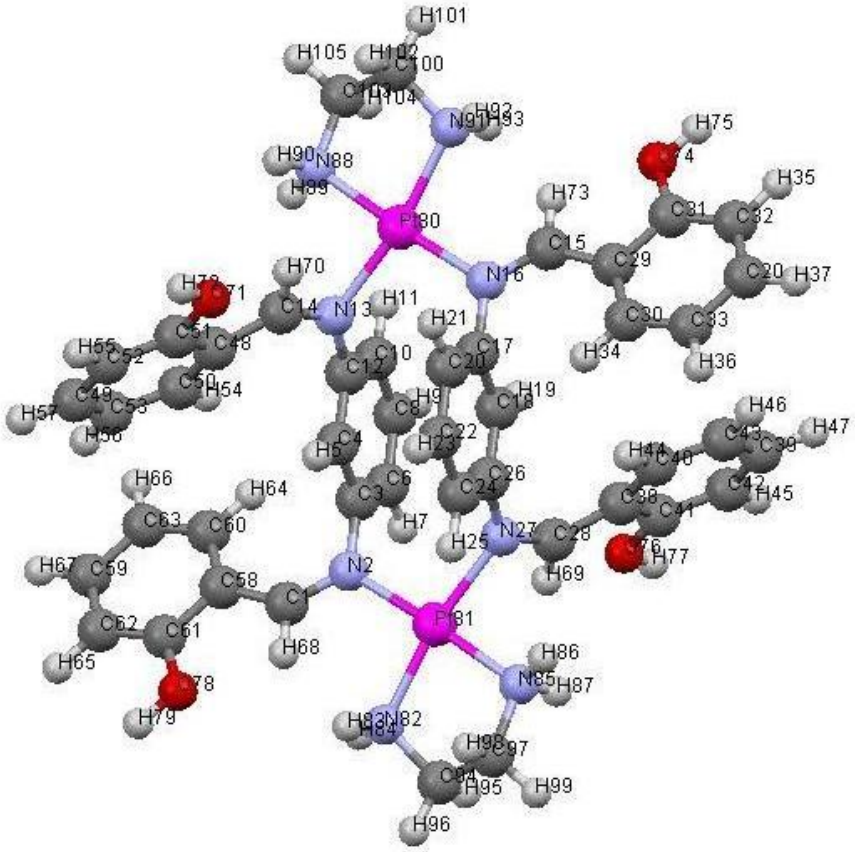
S4: Absorption spectra of Ptcyp = 10 μM in the absence and presence of increasing amounts of TBAP =0-35μM



S5: Emission spectrum of Ptcyp in presence and absence of O_2



S6: Absorption pattern of ethidium bromide bound to DNA by Pt^{II} complex. [DNA] = 10 μM, [**Ptcyp**] = 0 – 0.75μM



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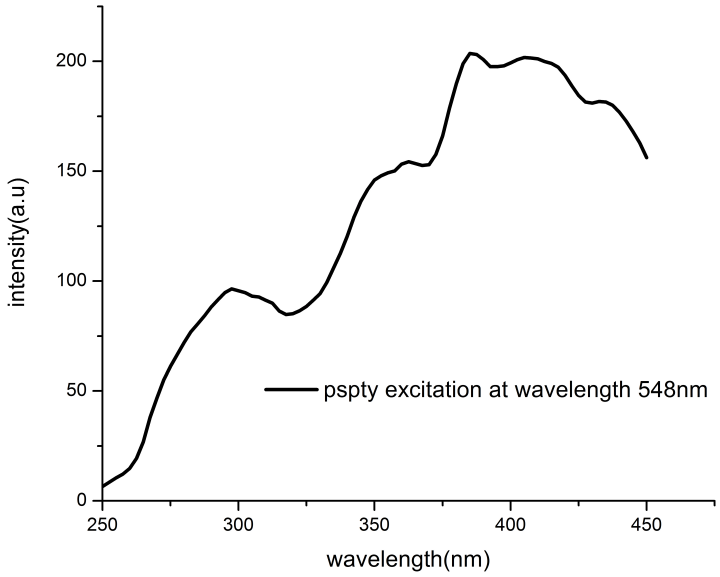
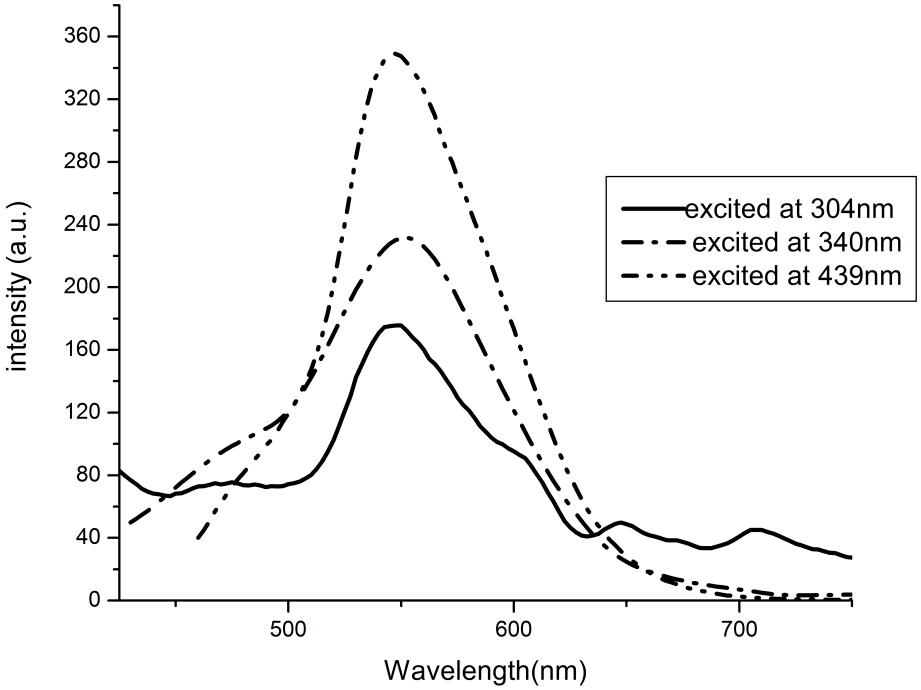
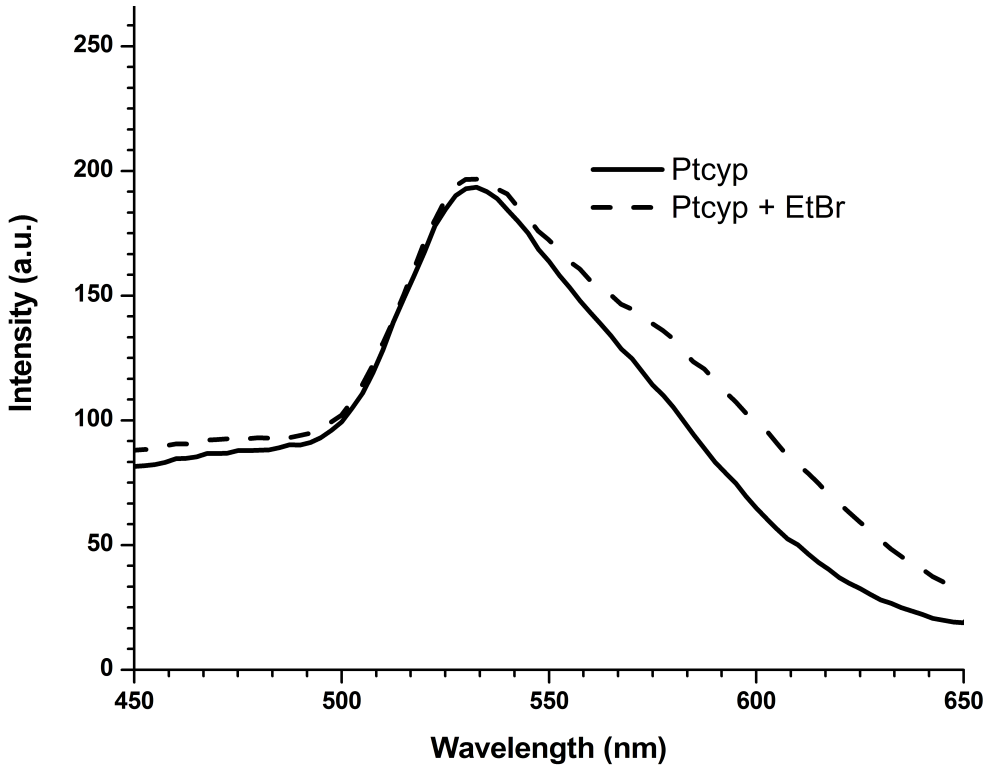
S7: Optimized structure of Pt^{II} complex **Ptcyp**



S8: Excitation spectrum of **Ptcyp**



S9: Emission spectrum for **Ptcyp**



S10: Emission spectrum of **Ptcyp (**0.75μM) in absence and presence of EtBr (10 μM)