materials

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Electronic Supplementary Information (ESI)

Pentafluorophenyl Platinum(II) Complexes of PTA and its N-Allyl and N-Benzyl Derivatives: Synthesis, Characterization and Biological Activity

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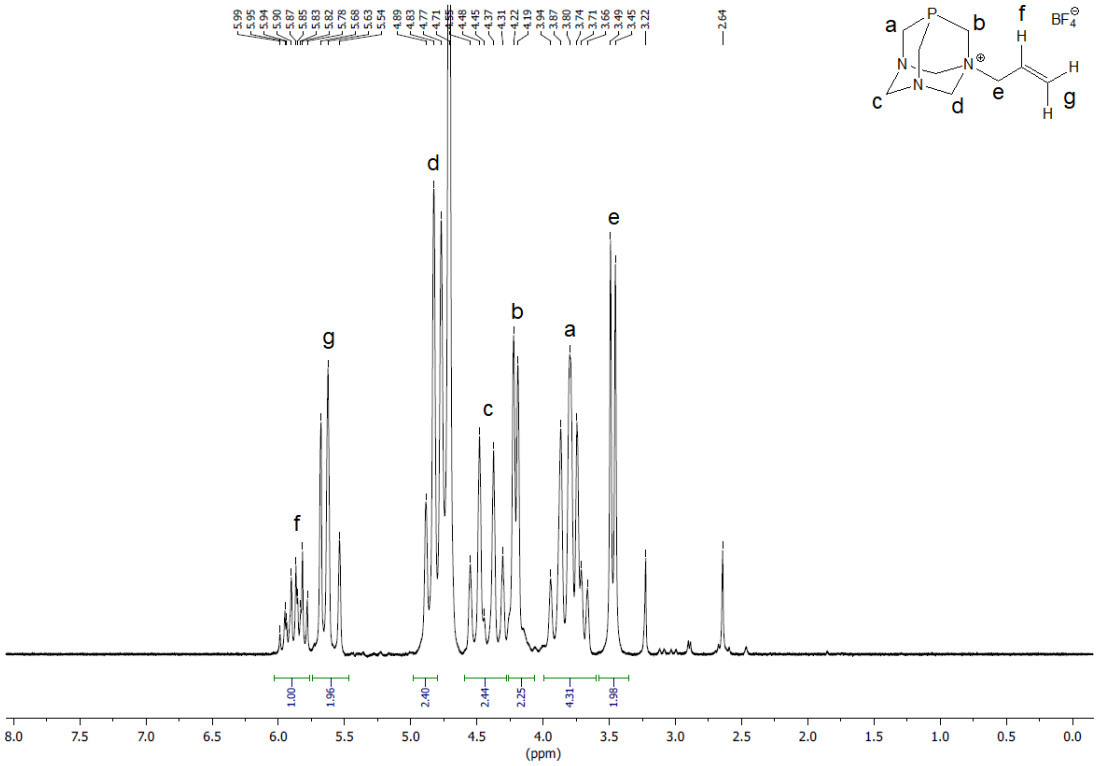

Figure S1. [1]H NMR spectrum of ligand **1b**.

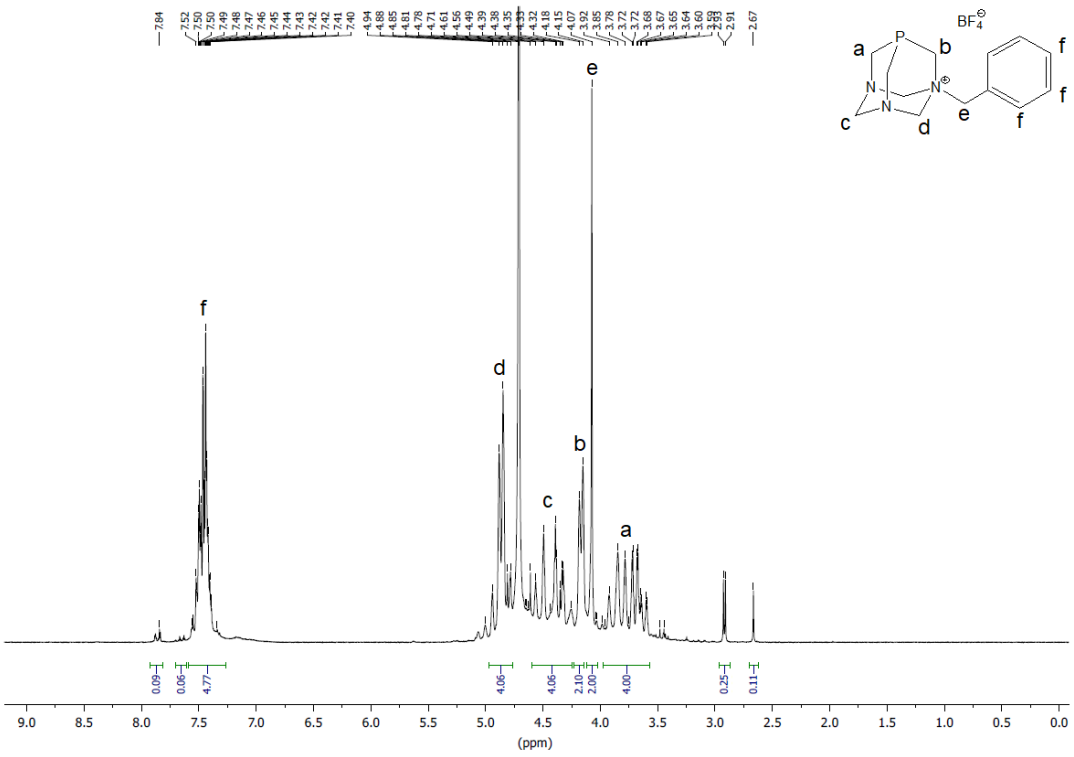

Figure S2. [1]H NMR spectrum of ligand **1c**.

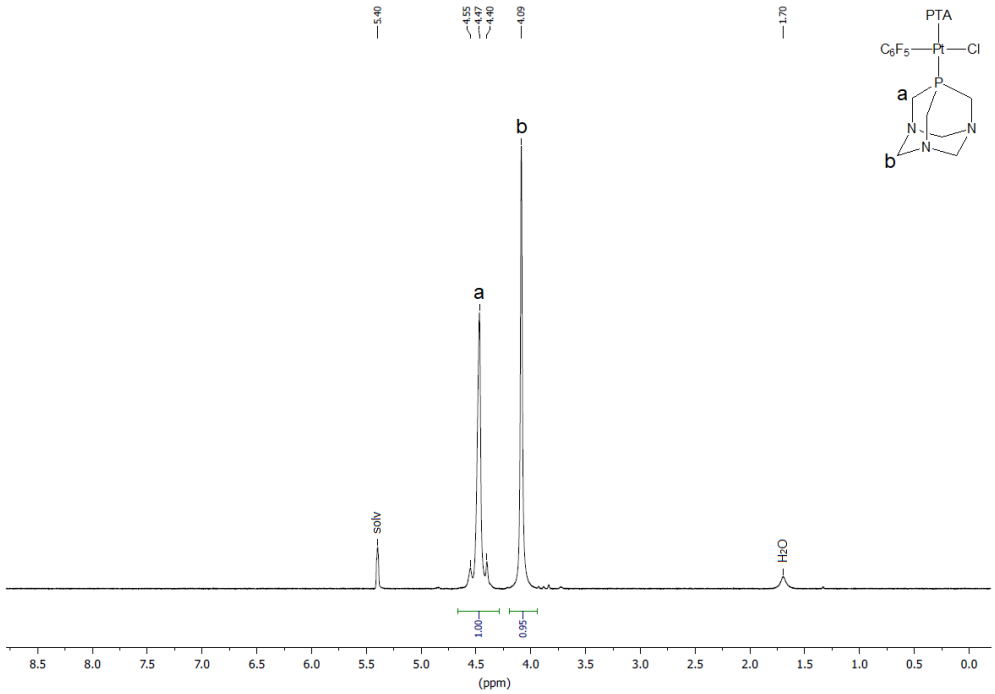

Figure S3. ^{1}H NMR spectrum of complex **2a**.

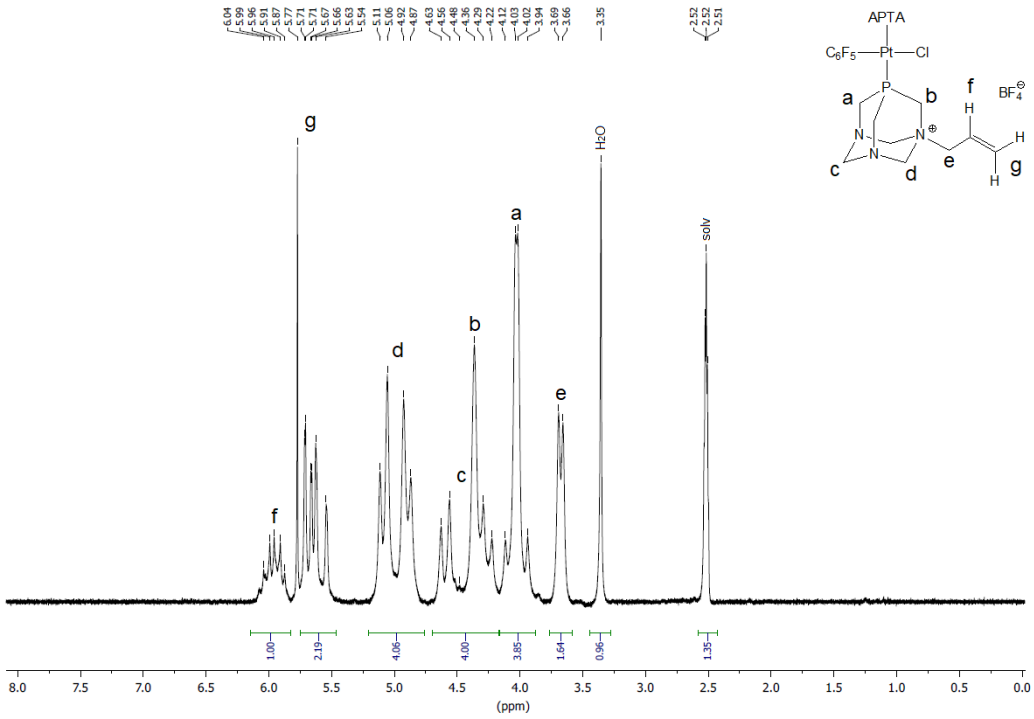

Figure S4. ^{1}H NMR spectrum of complex **2b**.

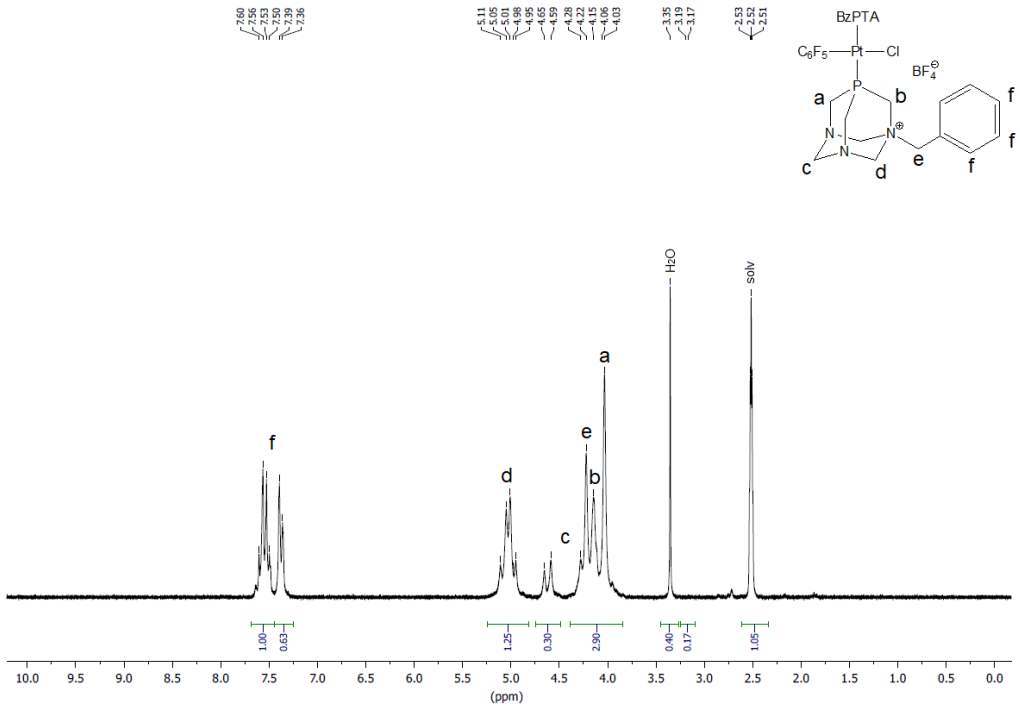

Figure S5. ^{1}H NMR spectrum of complex **2c**.

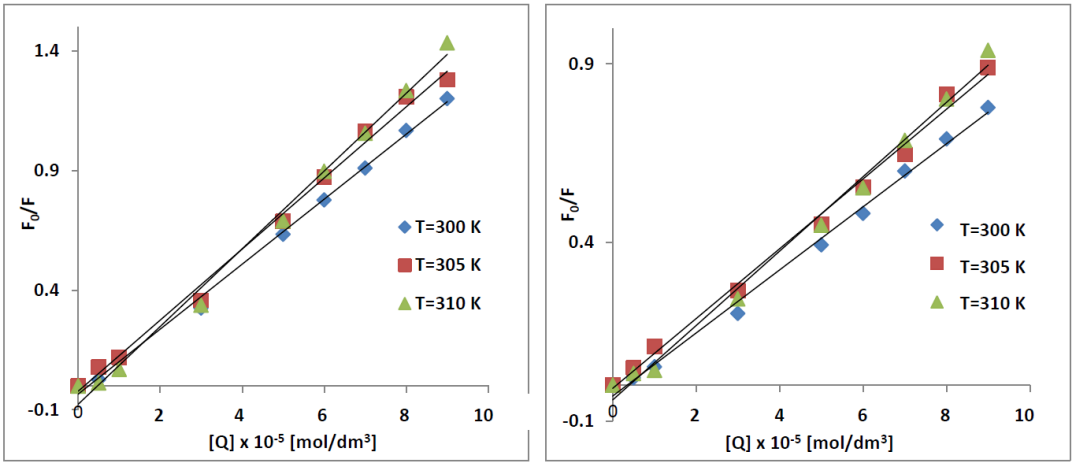

Figure S6. Stern-Volmer plots for quenching of HSA fluorescence by **2b** (left) and **2c** (right) at different concentrations and temperatures (300 K, 305 K, 310 K). [HSA] = 10 μM, [complex] = 5, 10, 30, 50, 60, 70, 80 and 90 μM; pH = 7.40, 0.05 M phosphate buffer, incubation at 37 °C during 24 h, λ_{ex} = 295 nm.

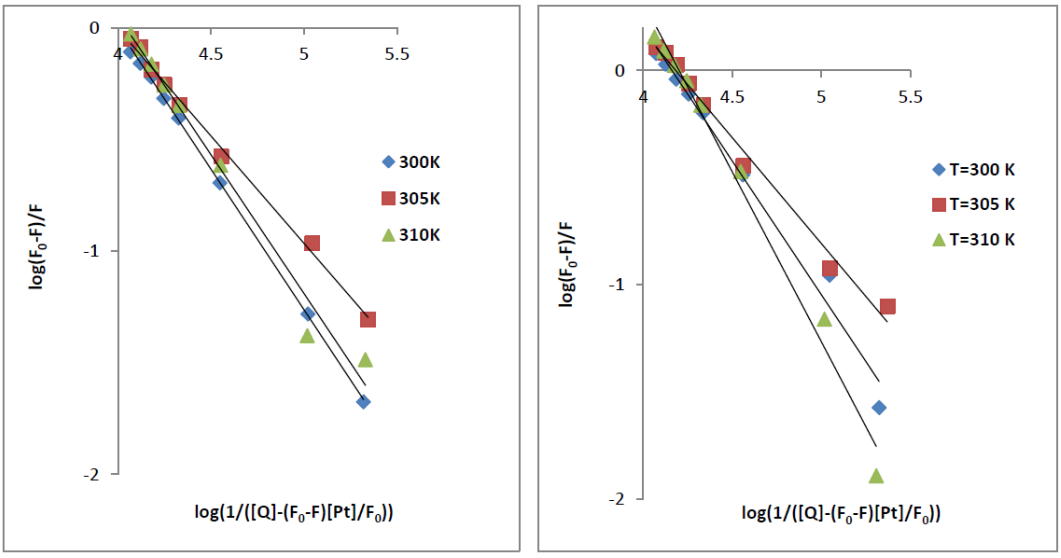

Figure S7. Plots of log(F_0-F)/F versus log(1/([Q] − (F_0-F)[P_t]/F_0)) at different temperatures for HSA (10 μM, Ph = 7.40) in the presence of complexes **2b** (left) and **2c** (right).

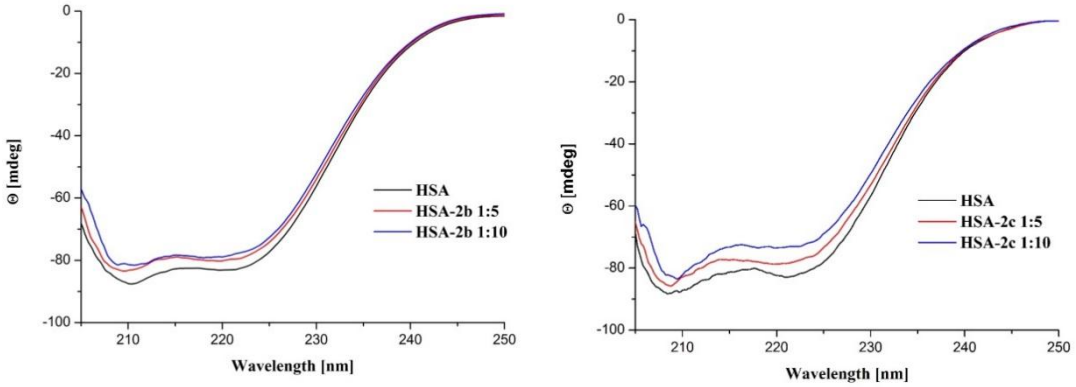

Figure S8. Circular dichroism spectra of HSA in the absence and presence of platinum complexes **2b** (left) and **2c** (right). [HSA] = 8 μM, pH = 7.40, 0.05M phosphate buffer, incubation at 37 °C during 24 h.

$$\frac{F_0}{F} = 1 + K_{SV}[Q] = 1 + K_q\tau_0[Q] \frac{F_0}{F} = 1 + K_{SV}[Q] = 1 + K_q\tau_0[Q] \quad \text{(S1)}$$

$$K_q = \frac{K_{SV}}{\tau_0} \quad \text{(S2)}$$

F_0 and F—fluorescence intensity in the absence and presence of a quencher, respectively;
K_{SV}—the Stern-Volmer constant;
[Q]—the concentration of quencher;
Kq—the quenching rate constant of protein;
τ_0—the lifetime of protein without the quencher (for HSA~5 ns).

$$\log\frac{F_0 - F}{F} = n\log K_A - n\log\left(\frac{1}{[Q_t] - (F_0 - F)[P_t]/F_0}\right) \quad \text{(S3)}$$

F_0 and F—fluorescence intensities in the absence and in the presence of the platinum complex, respectively;
$[Q_t]$ and $[P_t]$ are the total concentrations of the platinum complexes and HSA, respectively.

$$\ln K_q = -\frac{\Delta H^0}{RT} + \frac{\Delta S^0}{R} \quad \text{(S4)}$$

Kq—the bimolecular binding constant at the corresponding temperature (T);
R—the gas constant;
ΔH^0 and ΔS^0 are enthalpy and entropy change, respectively.

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \quad \text{(S5)}$$

ΔH^0—enthalpy change;
ΔS^0—entropy change;
ΔG^0—free energy change.