

Mononuclear Copper (I) Complexes of Triphenylphosphine and *N, N'*-Disubstituted Thioureas as Potential DNA Binding Chemotherapeutics

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Supplemental Data

Table S1. FTIR Vibration of Thiourea Ligands [38] and Complexes (1-9)

FTIR Vibrations	Wavenumbers/cm⁻¹
Ligands	
$\nu(\text{N-H})_{\text{str}}$	3120-3382 cm ⁻¹
$\nu(\text{C-H})_{\text{aromatic str}}$	2950-3100cm ⁻¹
$\nu(\text{C-S})_{\text{str}}$	1150-1190 cm ⁻¹
$\nu(\text{C-N})_{\text{str}}$	1550-1630 cm ⁻¹
$\nu(\text{C=S})_{\text{str}}$	1250-1275 cm ⁻¹
Complexes	
$\nu(\text{N-H})_{\text{str}}$	3150-3350 cm ⁻¹
$\nu(\text{C-H})_{\text{aromatic str}}$	2910-3050cm ⁻¹
$\nu(\text{C=O})_{\text{str}}$	1660-1685 cm ⁻¹
$\nu(\text{C=C})_{\text{str}}$	1475-1600 cm ⁻¹
$\nu(\text{C-P})_{\text{str}}$	1433-1477 cm ⁻¹
$\nu(\text{C-F})_{\text{str}}$	1320-1327 cm ⁻¹
$\nu(\text{C-O})_{\text{str}}$	1146 cm ⁻¹
$\nu(\text{C-N})_{\text{str}}$	1035-1090 cm ⁻¹
$\nu(\text{C-Cl})_{\text{str}}$	690-695 cm ⁻¹
$\nu(\text{Cu-S})_{\text{str}}$	320-337 cm ⁻¹
$\nu(\text{Cu-X})_{\text{str}}$	263-297 cm ⁻¹
$\nu(\text{C=S})_{\text{str}}$	1220-1270 cm ⁻¹

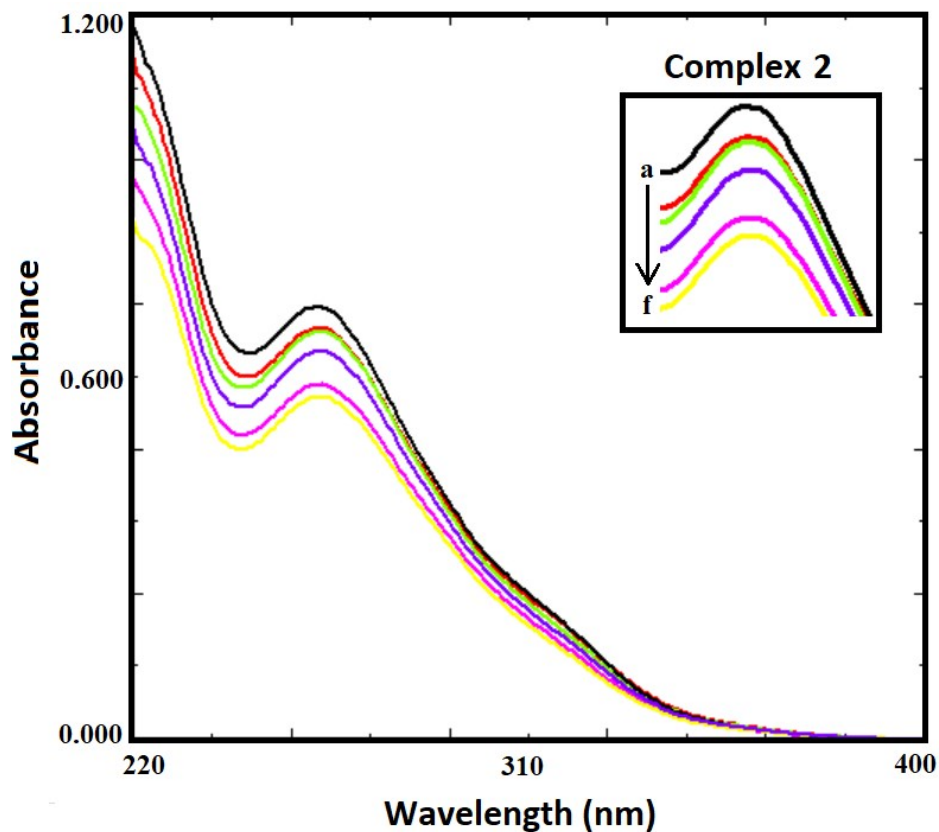


Figure S1 (a). UV-Vis Absorption Spectra of Complex 2; in absence of DNA (a) and presence of increasing concentration of DNA (b-f) [10-50 μ M from b-f respectively]

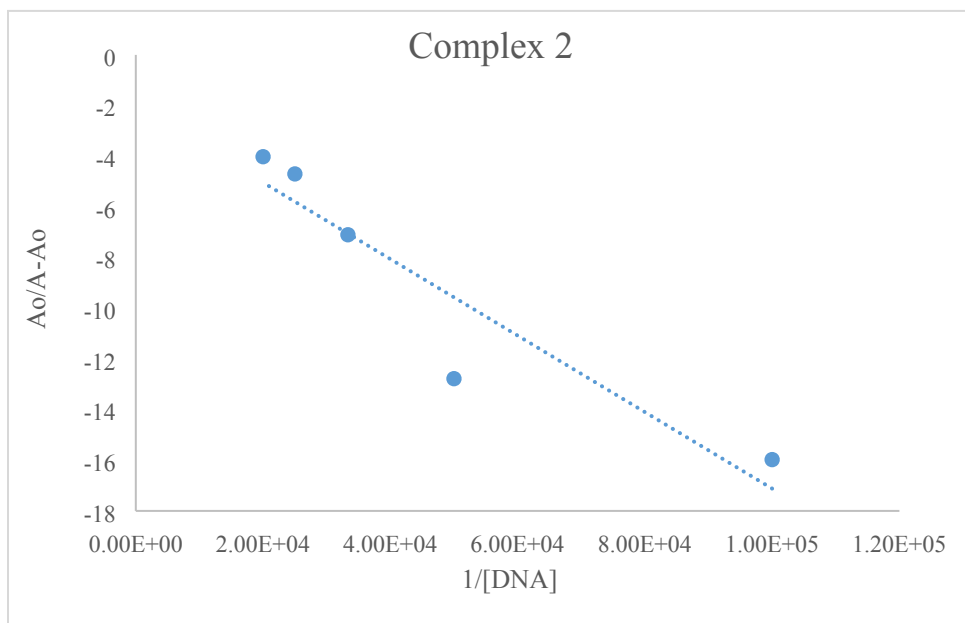


Figure S1 (b). Straight line Graph to Determine Binding Constant (K)

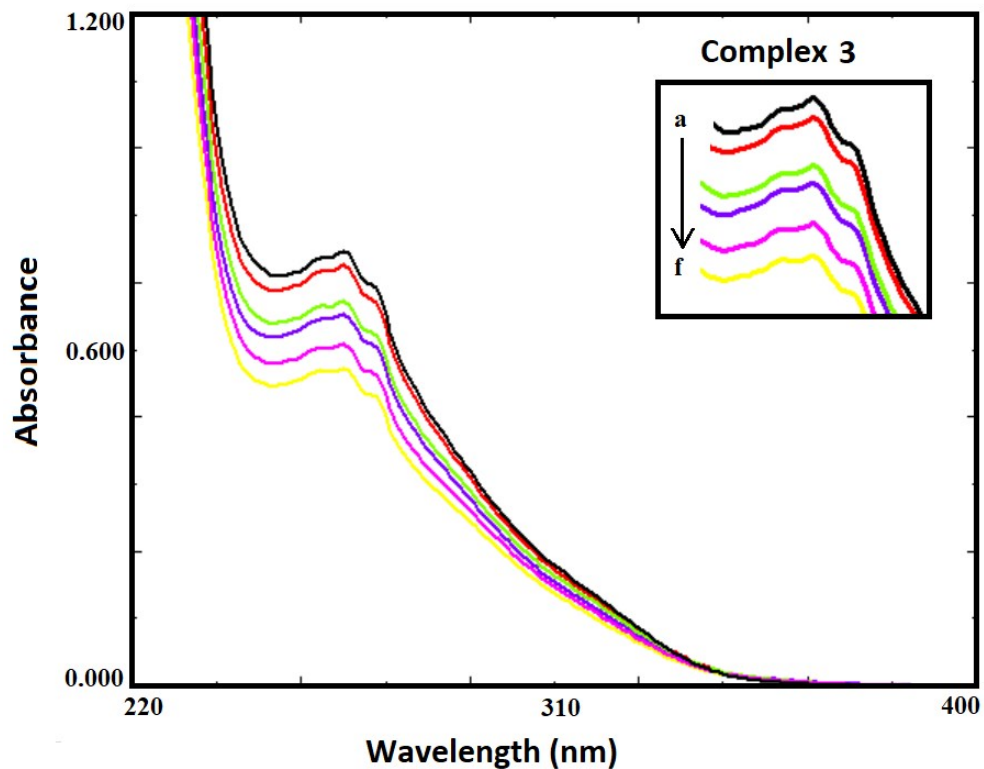


Figure S2 (a). UV-Vis Absorption Spectra of Complex 3; in absence of DNA (a) and presence of increasing concentration of DNA (b-f) [10-50 μ M from b-f respectively]

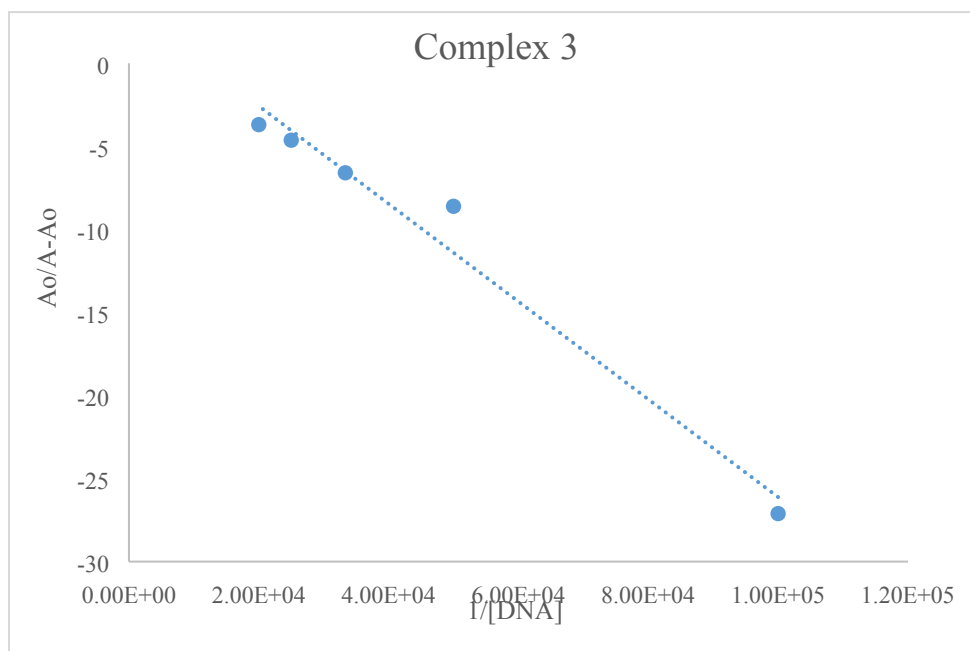


Figure S2 (b). Straight line Graph to Determine Binding Constant (K)

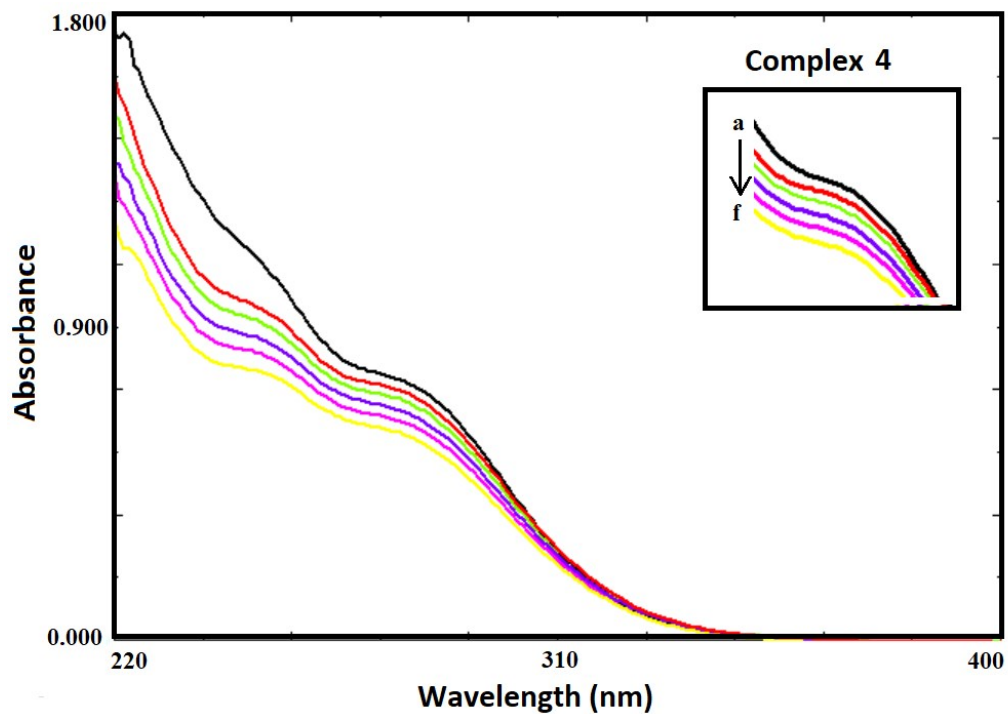


Figure S3 (a). UV-Vis Absorption Spectra of Complex 4; in absence of DNA (a) and presence of increasing concentration of DNA (b-f) [10-50 μ M from b-f respectively]

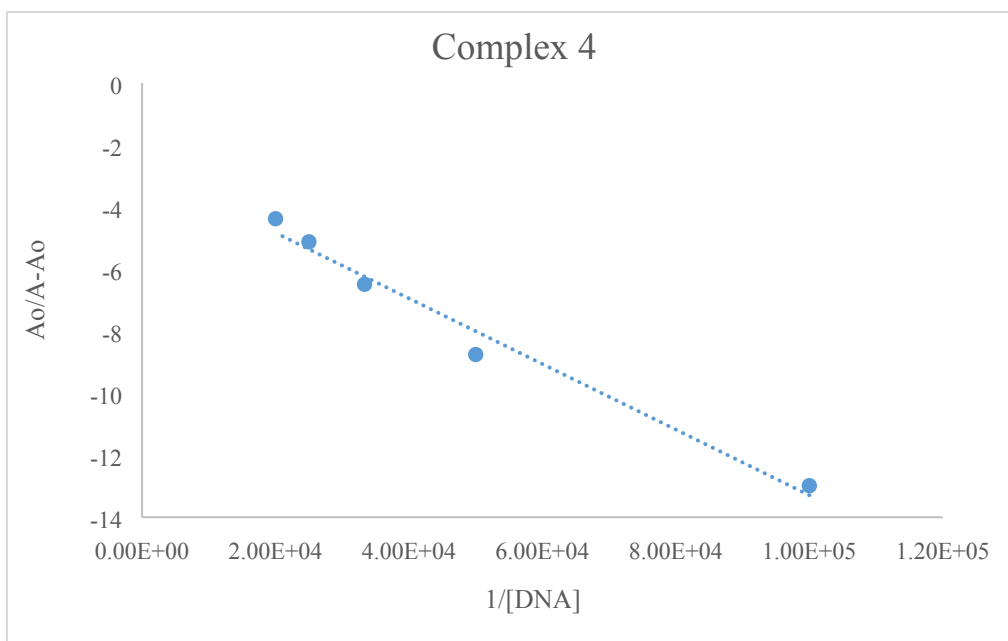


Figure S3 (b). Straight line Graph to Determine Binding Constant (K)

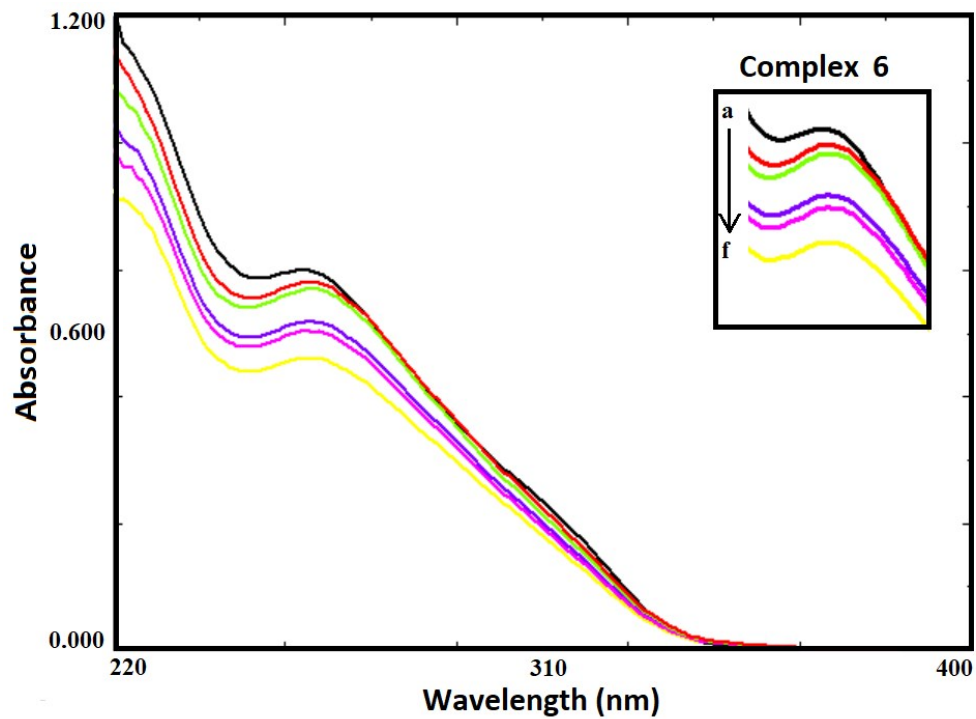


Figure S4 (a). UV-Vis Absorption Spectra of Complex 2; in absence of DNA (a) and presence of increasing concentration of DNA (b-f) [10-50 μ M from b-f respectively]

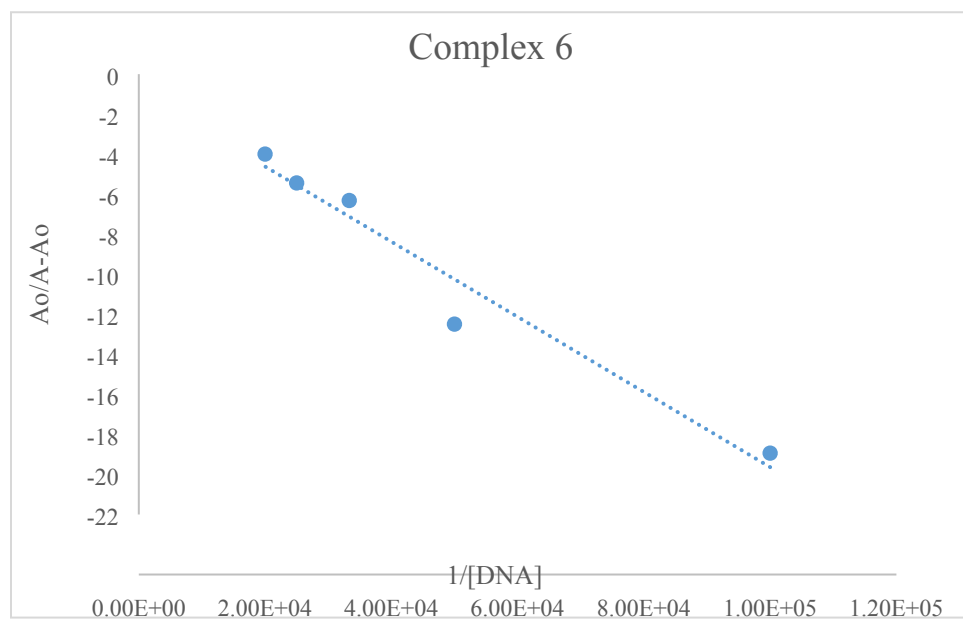


Figure S4 (b). Straight line Graph to Determine Binding Constant (K)

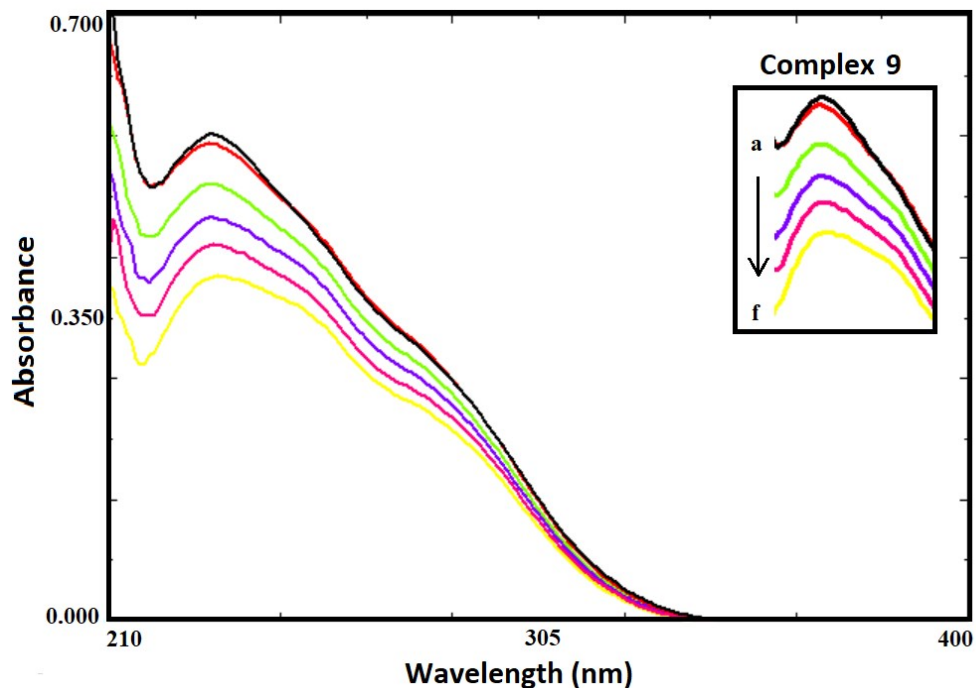


Figure S5 (a). UV-Vis Absorption Spectra of Complex 2; in absence of DNA (a) and presence of increasing concentration of DNA (b-f) [10-50 μ M from b-f respectively]

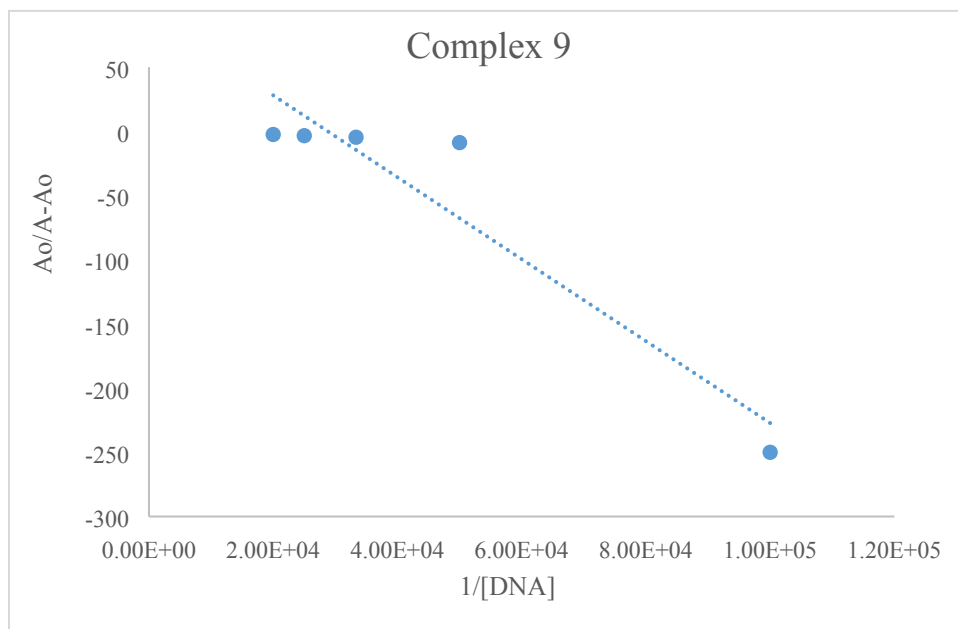


Figure S5 (b). Straight line Graph to Determine Binding Constant (K)

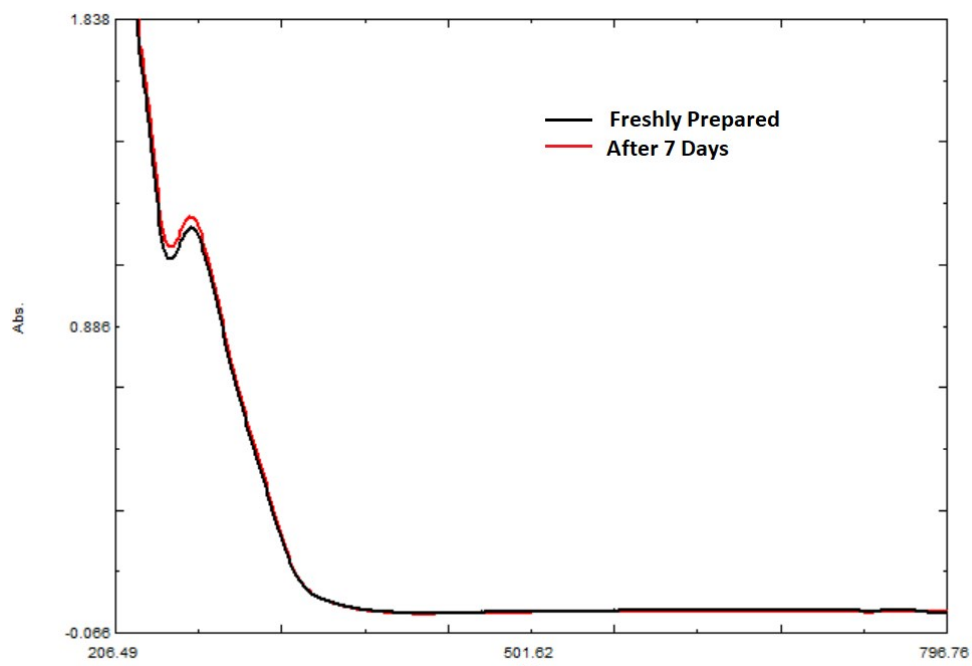


Figure S6. UV Spectrum of Complex 1 just after solution preparation and after keeping 7 days