Electronic Supplementary Material (ESI) for Dalton Transactions.

Tuning the Coordination Properties of Phenothiazine by Regioselective Introduction of Diphenylphosphanyl Groups

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Table S1 TD-DFT-derived UV-vis spectra for **1**, **3** and **4** showing the main contributors to each band

Wavelength (nm)	Oscillator strength	Excitation	Contribution (%)
1			
242	0.057	102 → 107 (HOMO-2→ LUMO+2)	57.9
		104 → 113 (HOMO-1 → LUMO+5)	21.9
292	0.107	103 → 105 (HOMO-1 → LUMO)	74.8
3			
255	0.202	106 → 109 (HOMO-2 → LUMO)	30.4
		107 → 113 (HOMO-1 → LUMO+4)	28.9
		108 → 117 (HOMO → LUMO+8)	16.8
282	0.083	107 → 109 (HOMO-1 → LUMO)	42.2
		108 → 113 (HOMO → LUMO+4)	22.7
		107 → 110 (HOMO-1 → LUMO+1)	15.1
289	0.090	108 → 113 (HOMO → LUMO+4)	56.7
		107 → 109 (HOMO-1 → LUMO)	24.4
4			
242	0.1226	106 → 111 (HOMO-2 → LUMO+2)	55.6
		108 → 117 (HOMO → LUMO+8)	24.6
296	0.0996	107 → 109 (HOMO-1 → LUMO)	86.6

Fig. S1 Frontier orbitals involved in the main UV transitions in the ~250-300 nm region for **1**, **3** and **4**.

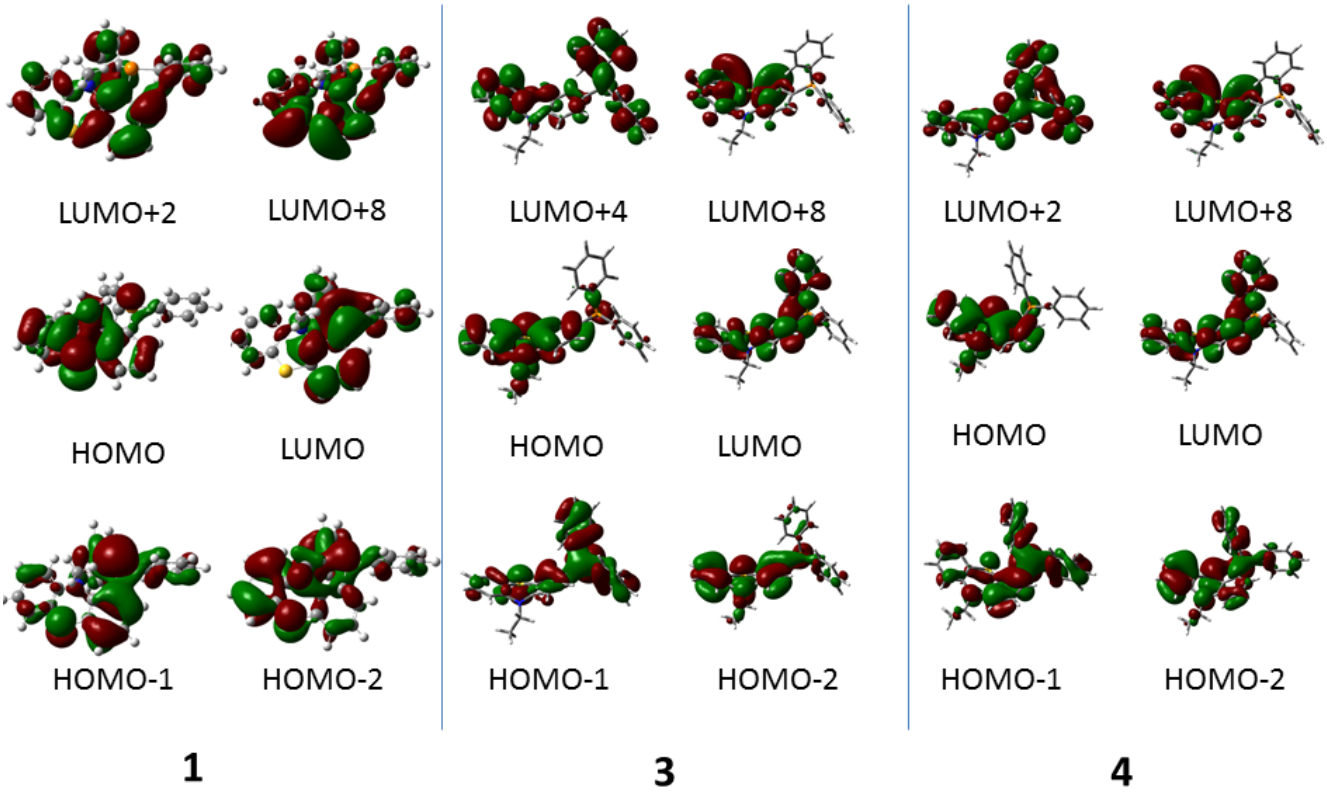

Fig. S2 Cyclic voltammograms of compounds **1**, **3** and **4**

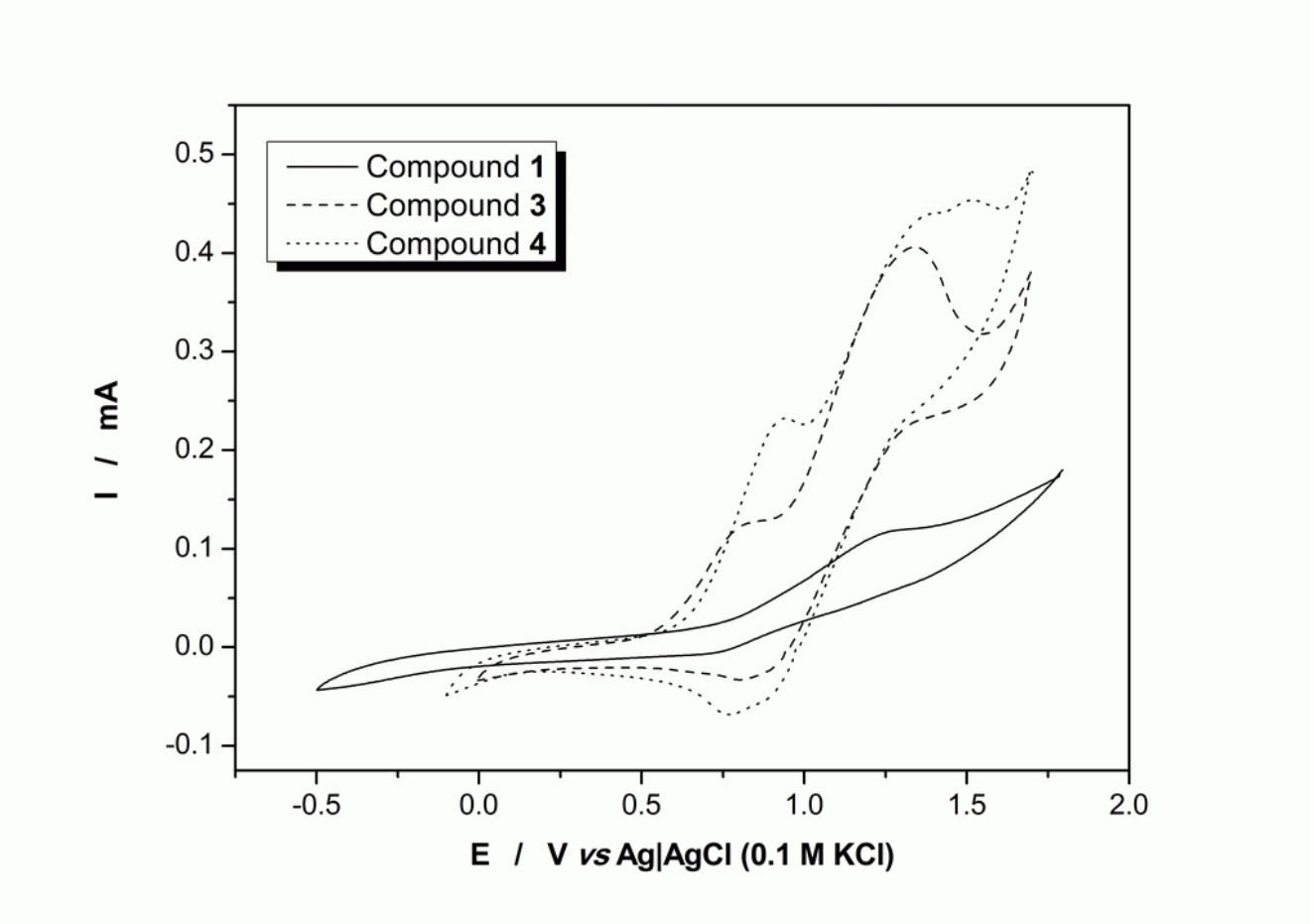

Fig S3 Interaction of **1** (a), **3, 4** (b), **14** and **15** (c) with plasmid DNA (pTZ57R). (a) Lane 1: GeneRuler 100bp Plus DNA ladder (Thermo Scientific); lane 2: closed circular plasmid DNA without complex to be tested; lanes 3-7: plasmid DNA with 0.5, 1, 2, 4 and 8 µl of **1** ($c = 10^{-3}$ M). (b) Lanes 1 and 8: closed circular plasmid DNA without complex to be tested; lanes 2-6: plasmid DNA with 0.5, 1, 2, 4 and 8 µl of **3** ($c = 10^{-3}$ M) respectively; lanes 9-13: plasmid DNA with 0.5, 1, 2, 4 and 8 µl of **4** ($c = 5 \cdot 10^{-4}$ M); lane 7: GeneRuler 1 kb DNA ladder (Thermo Scientific). (c) Lanes 1 and 8: closed circular plasmid DNA without complex to be tested; lanes 2-6: plasmid DNA with 0.5, 1, 2, 4 and 8 µl of **14** ($c = 2 \cdot 10^{-4}$ M) respectively; lanes 9-13: plasmid DNA with 0.5, 1, 2, 4 and 8 µl of **15** ($c = 4 \cdot 10^{-4}$ M); lane 7: GeneRuler 1 kb DNA ladder (Thermo Scientific).

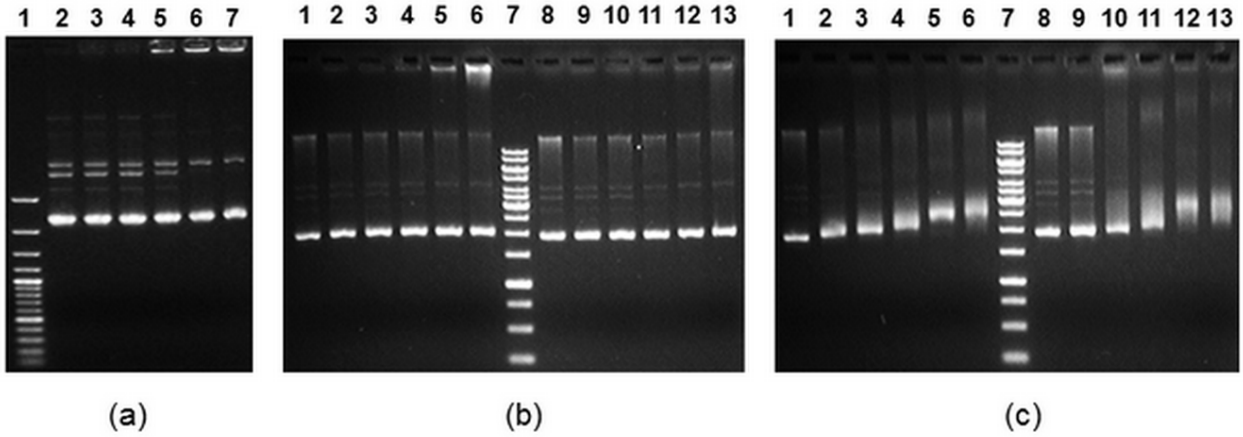

Fig S4 Electronic absorption spectral titration of complexes **14** and **15**

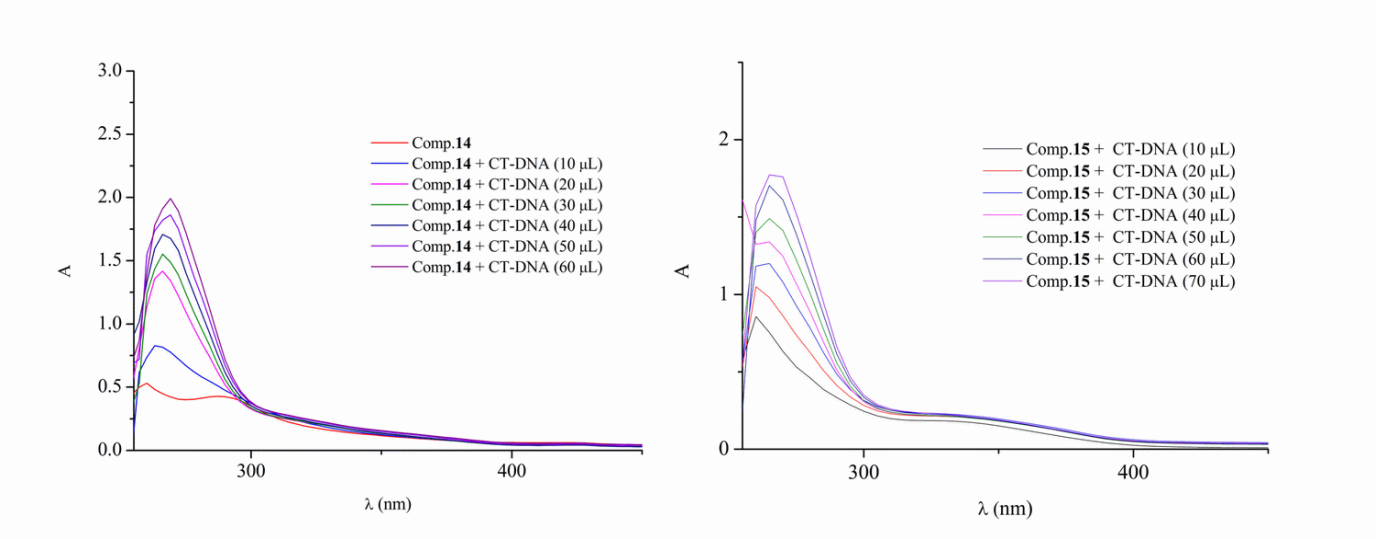

Fig. S5 Emission spectra of free ethidium bromide ($0.25 \cdot 10^{-5}$ M) and ethidium bromide bound to DNA in the absence and the presence of complex **15** (stock solution $0.38 \cdot 10^{-5}$ M) at increasing concentrations of **15**.

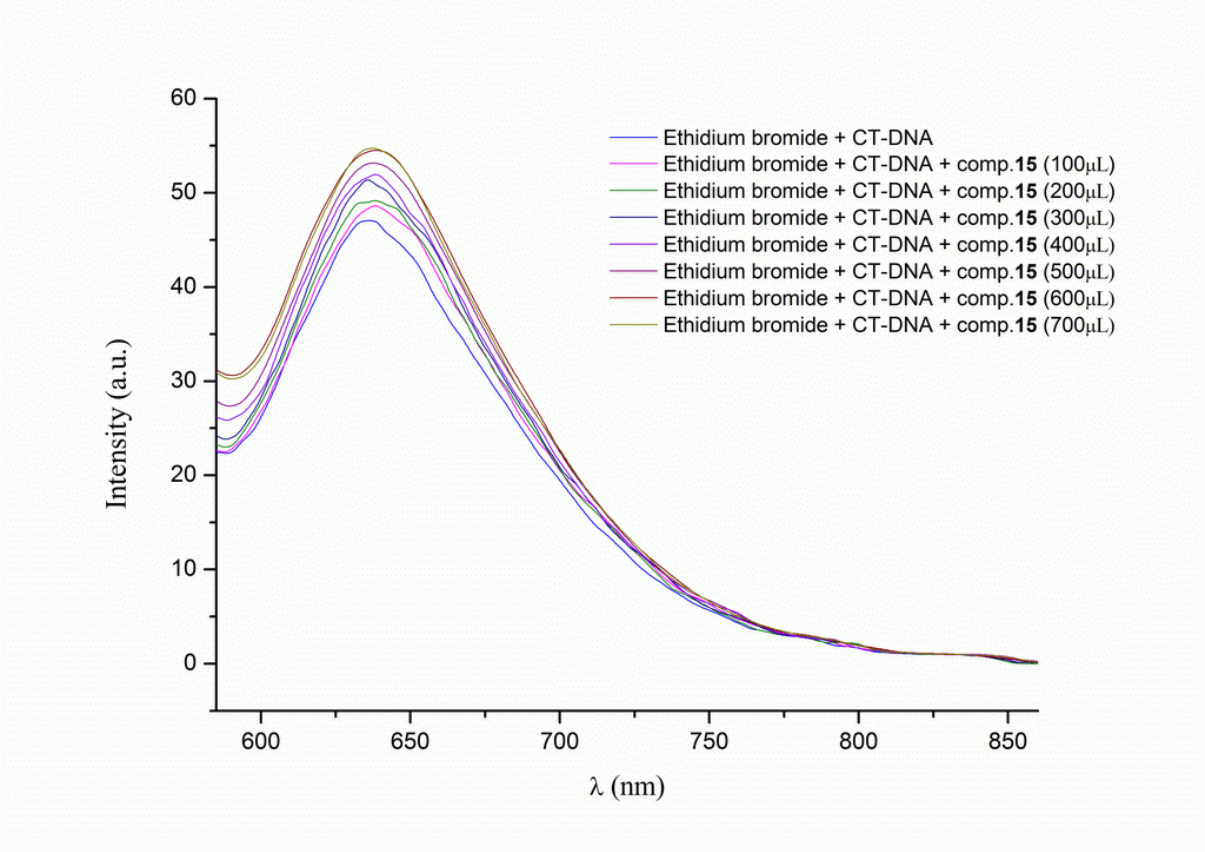

Fig. S6 Thermal denaturation of CT-DNA in the absence and presence of complexes **14** and **15**. Complexes **14** (20 μM), 15 (20 μM) and CT-DNA (30 μM).

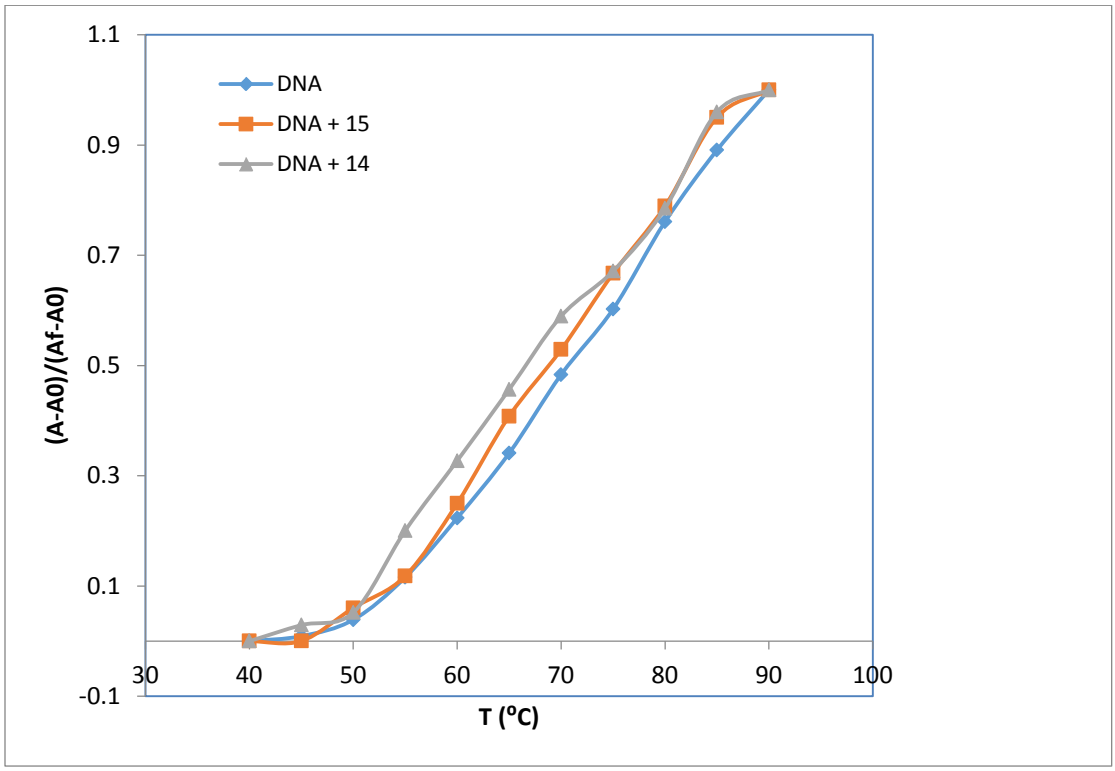

Fig. S7 The effect of complexes **11**, **15**, cisplatin and oxaliplatin (IC_{50} values) on breast carcinoma (MCF7), hepatocarcinoma (HepG2) and colorectal carcinoma (DLD1) cell lines