

Electronic Supporting Information

for

Ruthenium Complexes Containing 2,6-bis(benzimidazolyl)pyridine Derivatives Induce Cancer Cell Apoptosis by Triggering DNA Damage-mediated P53 Phosphorylation

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Experimental Section.

Determination of the lipophilicity of Ru complexes: The lipophilicity of phen was determined by using the shake-flask method of octanol/water phase partition. Octanol-saturated water (OSW) and Water-saturated octanol (WSO) were prepared using analytical grade octanol (Sigma) and double distilled water. 100 µg/ml phen in ethanol was diluted to 0, 2, 4, 6, 8, 10 µg/ml and their absorbance at 261 nm were determined and used to draw the standard curve of phen. 0.5 mg/ml phen in WSO was added to equal volume of OSW and shaken in an IKA Vibrax VXC basic shaker for 48 h at 500 g/min after partition. The octanol layer was separated by centrifugation at 4000 g for 30 min. The sample solution was determined by its absorbance at 261 nm and used to calculate log *P*. Partition coefficients of phen were calculated using the equation $\log P_{\text{oct}} = \log ([\text{phen}]_{\text{oct}} / [\text{phen}]_{\text{aq}})$.

Reverse titration experiment: Absorption spectral titration experiments were carried out by titrating a fixed concentration of DNA with increasing concentrations of RuBmP. Due correction was made for the absorbance of RuBmP itself by adding RuBmP in the reference cuvette. Each spectrum was recorded after equilibration of the sample for 5 min.

Light-switch effect of the complexes on DNA: Emission intensity measurements were carried out using 970 CRT spectrofluorometer. A 5 mM Tris-HCl/50 mM NaCl buffer solution was used as the blank to make preliminary adjustment. The excitation wavelength was fixed and the emission range was adjusted before measurements. DNA was added to a fixed concentration of complex and then Cu²⁺ was added. Their effect on the emission intensity was measured.

Results

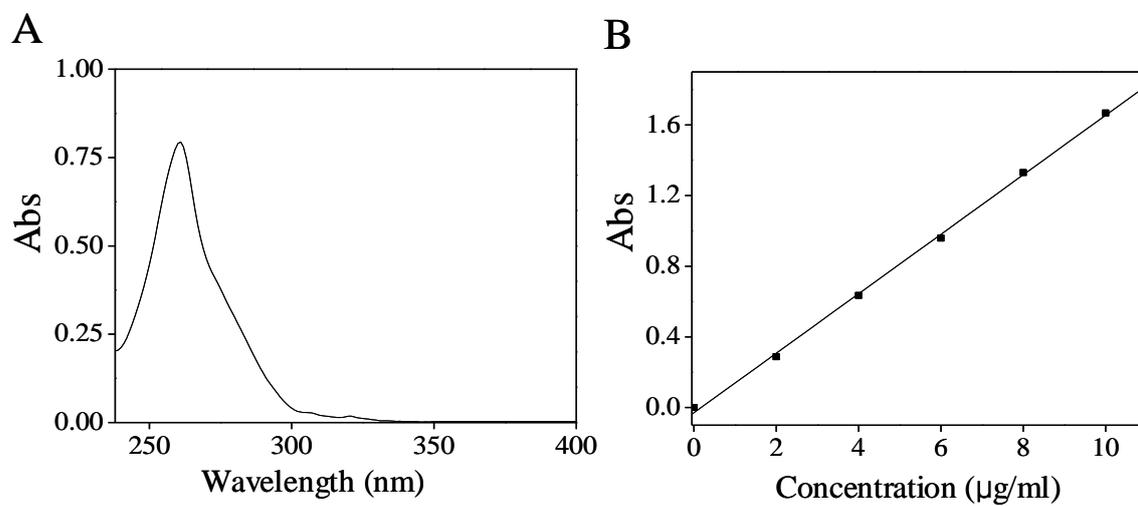


Fig. S1. Spectroscopic determination of the lipophilicity of the ligand. (A) The absorption spectra of the ligand phen; (B) The standard curve of phen ($P < 0.0001$).

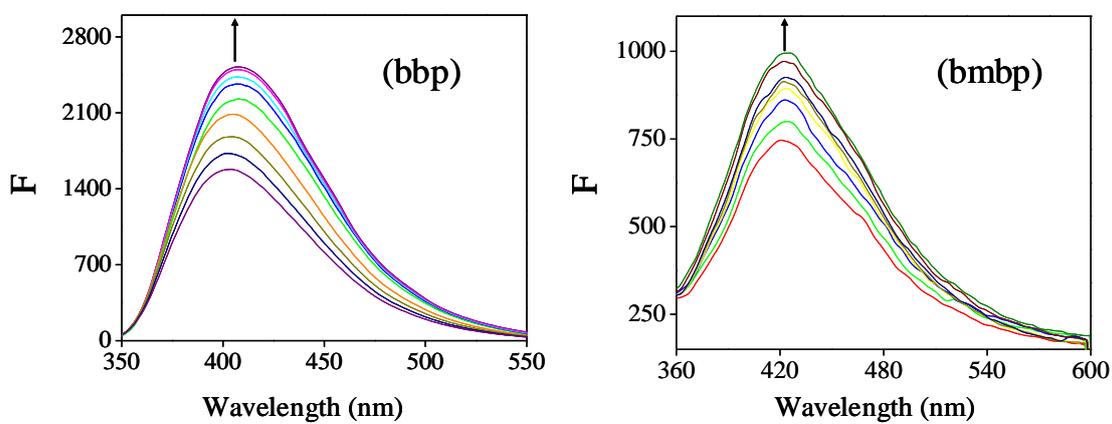


Fig. S2. Emission spectra of ligands bbp and bmbp in 5 mM Tris buffer, pH 7.2 with the absence and presence of different concentrations of CT-DNA.

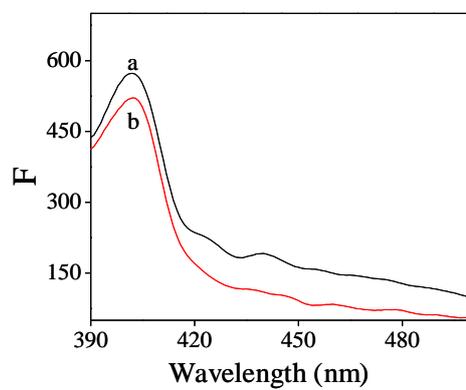


Fig. S3. Emission spectra of DNA-RuBmP in Tris-HCl buffer at 298 K in the absence (a) and presence (b) of Cu^{2+} . $[\text{Ru}] = 20 \mu\text{M}$, $[\text{DNA}] = 14 \mu\text{M}$, $[\text{Cu}^{2+}] = 20 \mu\text{M}$.

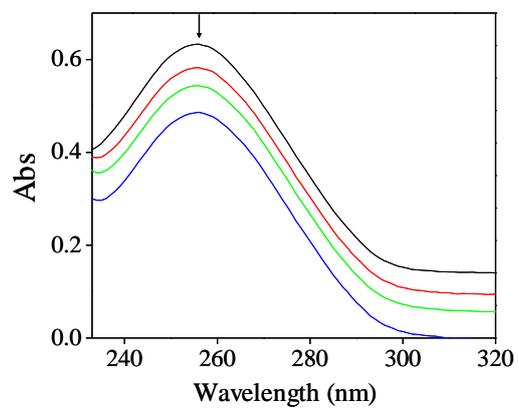


Fig. S4. Absorption spectra of cancer cell chromosomal DNA in 5 mM Tris buffer, pH 7.2 in the absence and presence of RuBmP.

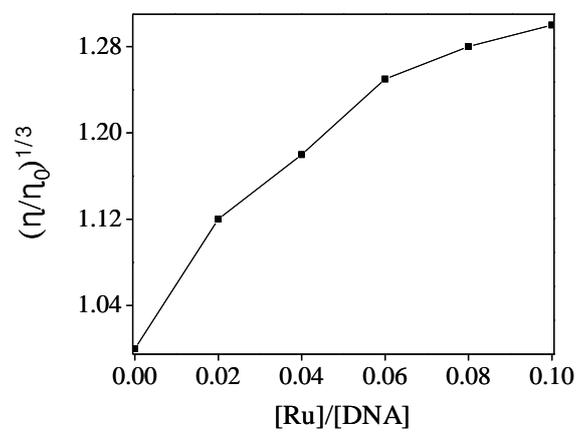


Fig. S5. Effect of EthBr on the relative viscosity of A375 cell chromosomal DNA.