Substituent effects on the biological properties of Zn-salophen complexes

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Supporting Information

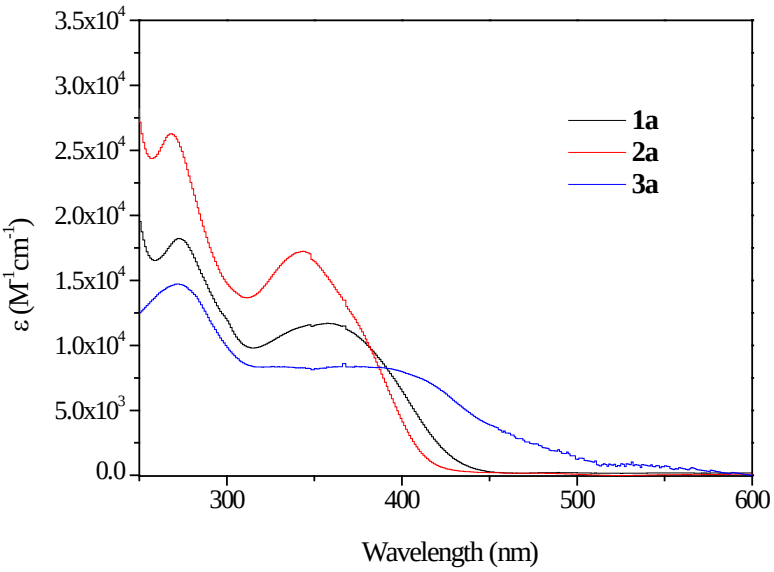


Figure S1. Absorption spectra of **1a**, **2a** and **3a** in ethanol.

λ_{calc} = 340 nm (exp = 354 nm).

HOMO → LUMO transition.

λ_{calc} = 299 nm (exp = 274 nm).

HOMO → LUMO +1 combined with HOMO -1 → LUMO transitions

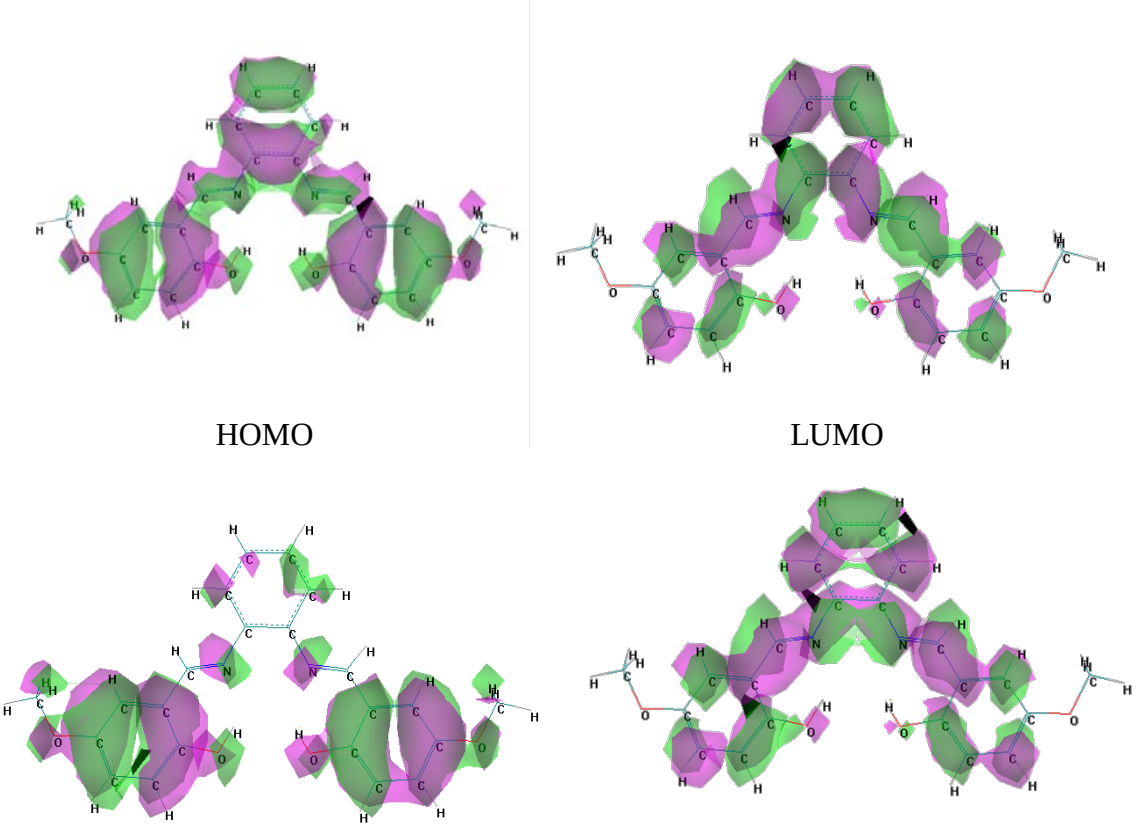


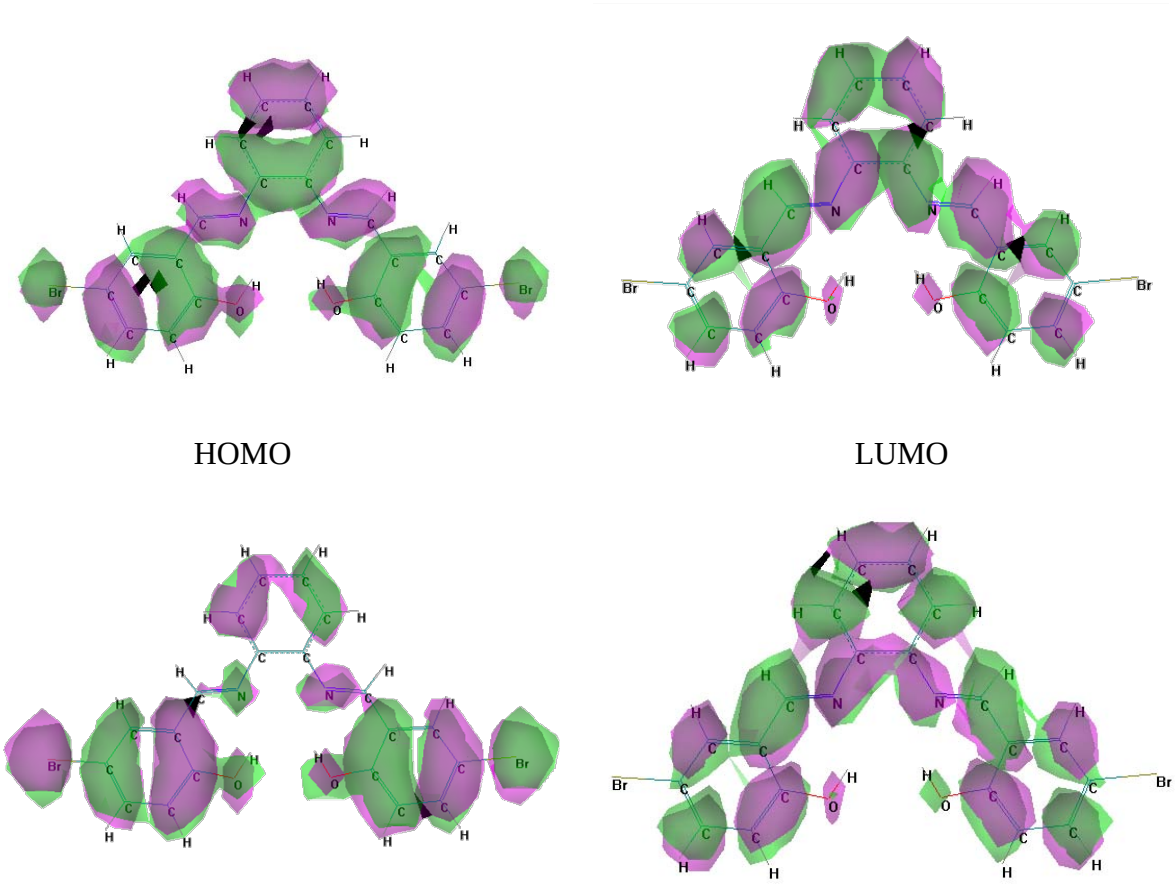
Figure S2. Calculated orbitals involved in the lowest energy absorption transitions of compound **1a**.

λ_{calc} = 336 nm (exp = 341 nm).

HOMO → LUMO transition.

λ_{calc} = 282 nm (exp = 268 nm).

HOMO → LUMO +1 combined with HOMO -1 → LUMO transitions



HOMO LUMO

HOMO -1 LUMO +1

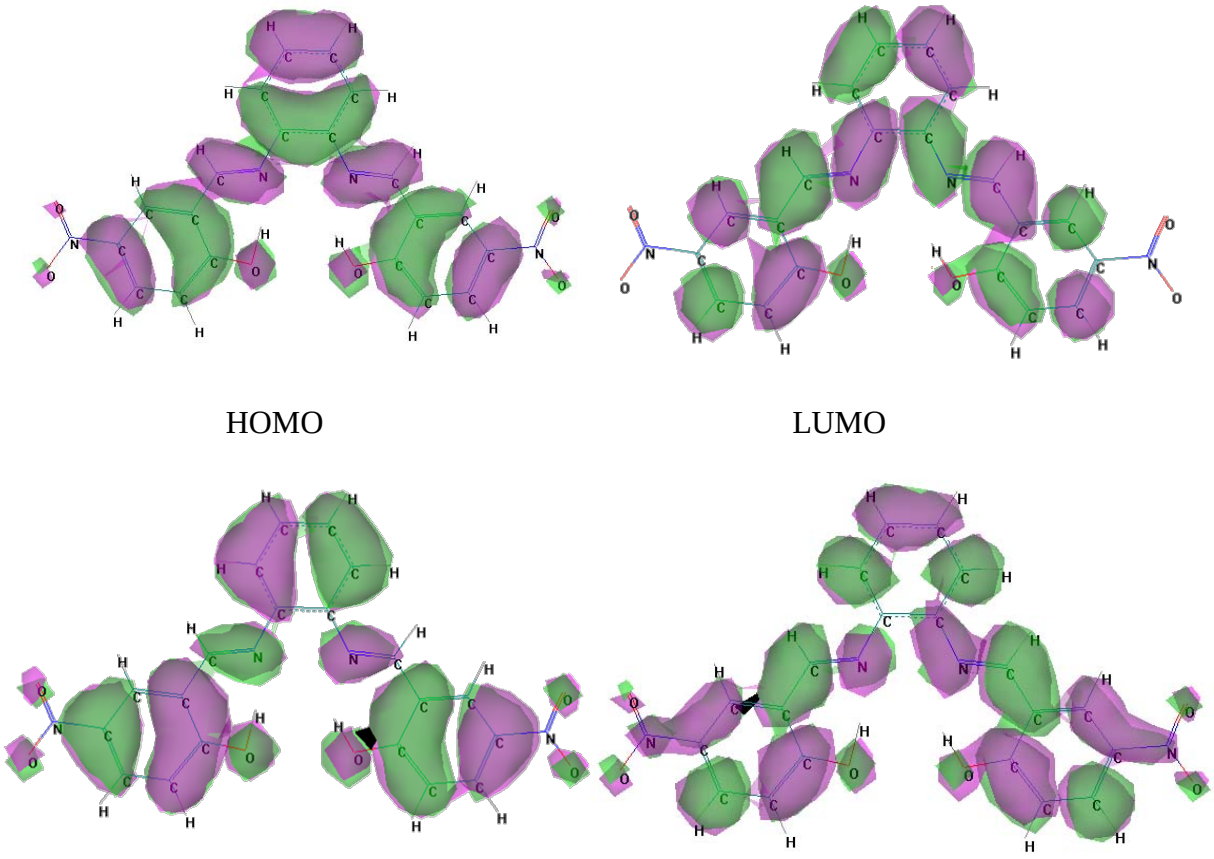
Figure S3. Calculated orbitals involved in the lowest energy absorption transitions of compound **2a**.

λ_{calc} = 392 nm (exp = 404 nm).

HOMO → LUMO transition.

λ_{calc} = 282 nm (exp = 279 nm).

HOMO → LUMO +1 combined with HOMO -1 → LUMO transitions



HOMO LUMO

HOMO -1 LUMO +1

Figure S4. Calculated orbitals involved in the lowest energy absorption transitions of compound **3a**.

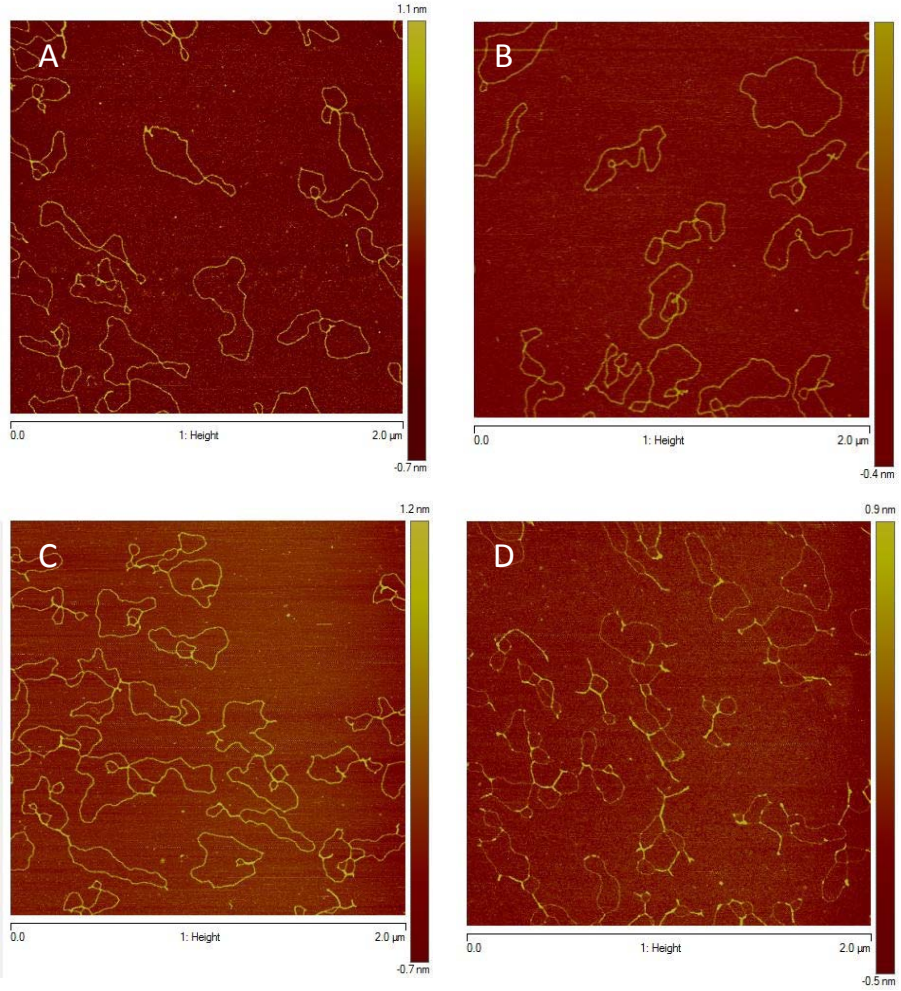


Figure S5. AFM image of pBR322 plasmid DNA (A); pBR322 plasmid DNA incubated with **1a** (B); with **2a** (C) and with **3a** (D).

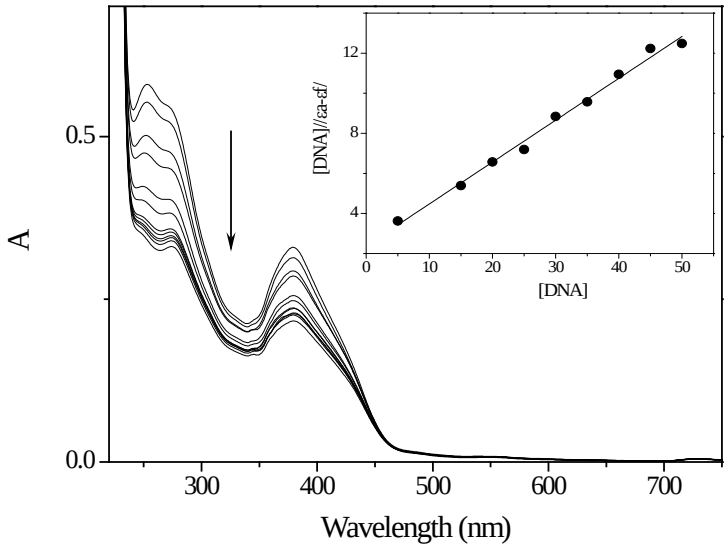


Figure S6. Electronic absorption spectra of complex **1b** in the absence and presence of increasing amounts of DNA. Inset: Plot of [DNA]/(ε_a-ε_f) *vs.* [DNA]).

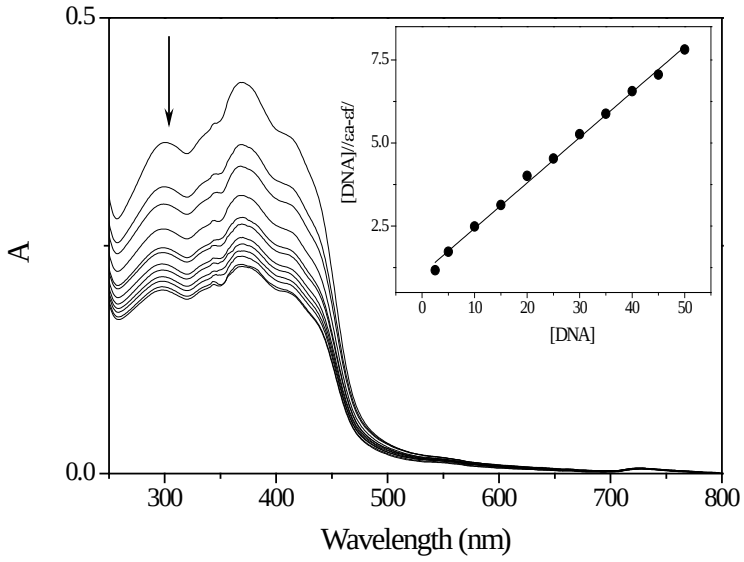


Figure S7. Electronic absorption spectra of complex **2b** in the absence and presence of increasing amounts of DNA. Inset: Plot of [DNA]/(ε_a-ε_f) *vs.* [DNA]).

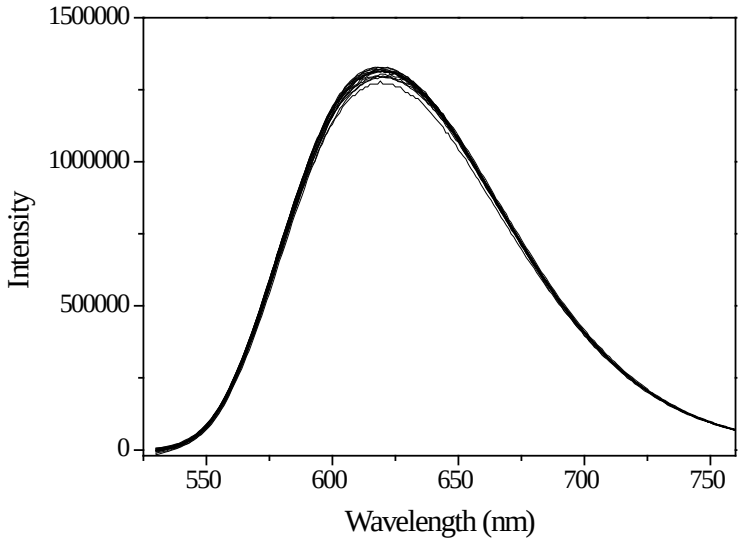


Figure S8. Emission spectra of ethidium bromide (EB) bound to DNA in the absence and presence of increasing amounts of **1b**.

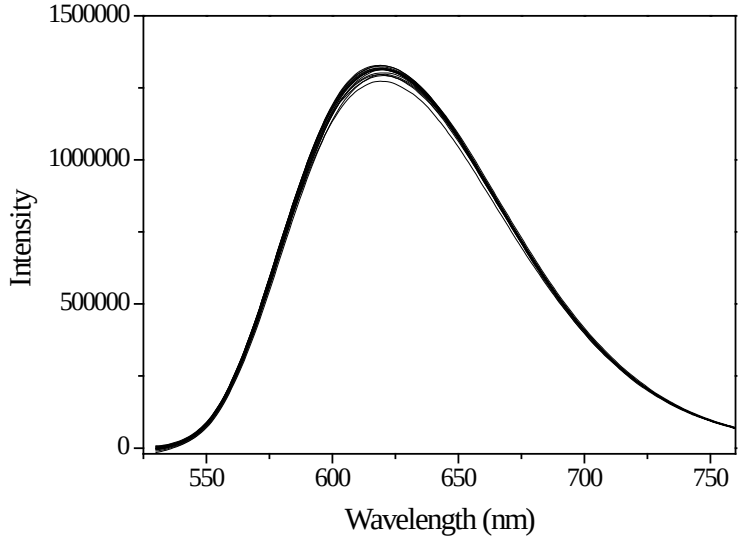


Figure S9. Emission spectra of ethidium bromide (EB) bound to DNA in the absence and presence of increasing amounts of **2b**.

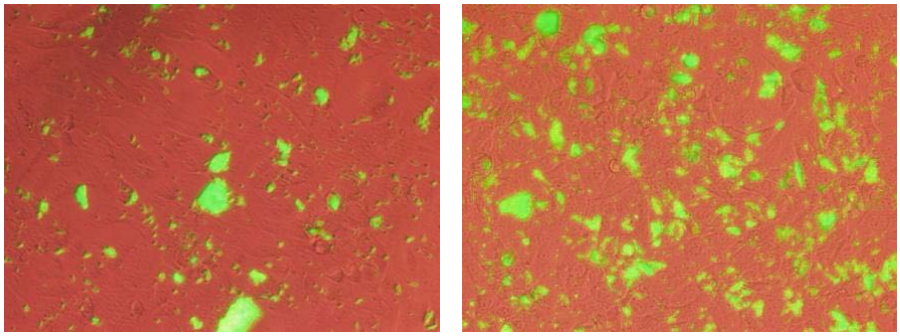


Figure S10. Fluorescence-microscopy images of 3T3 cells incubated for 24 h with 140 μM (left) and 270 μM (right) of compound **2b**. Pink tint represent culture medium; green area represents fluorescent compound **2b**.

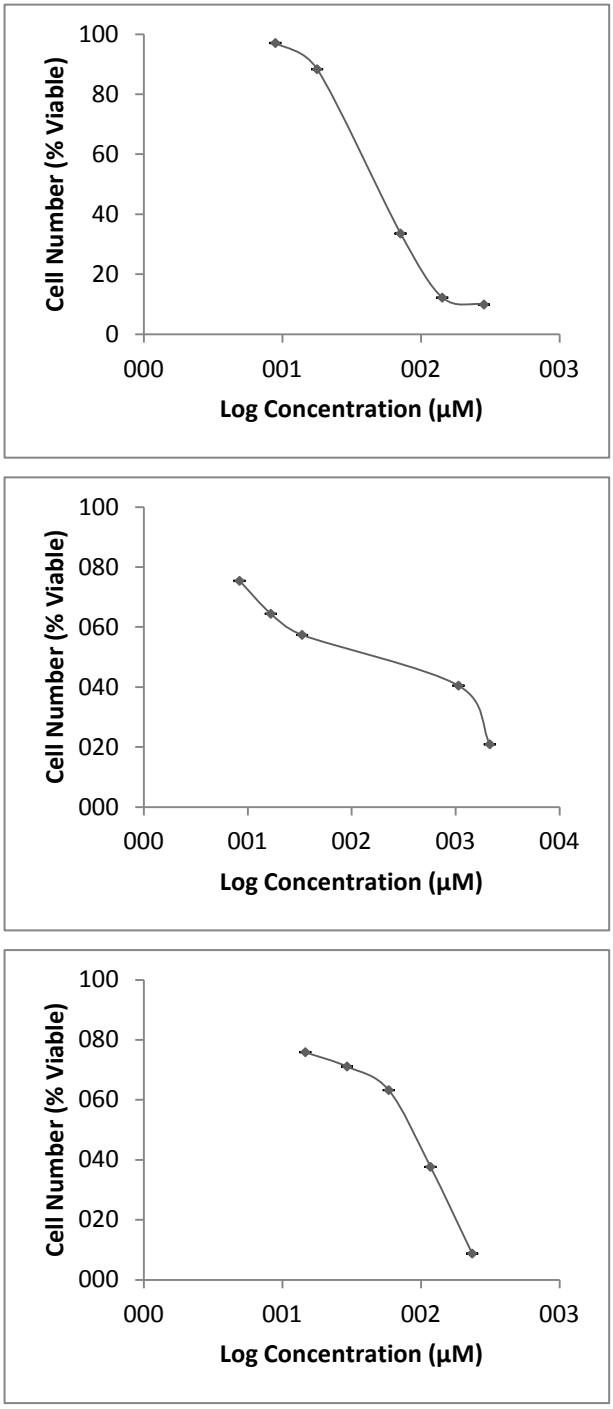


Figure S11. Cytotoxicity dose responses of metal complexes in 3T3 cells for compound **1b** (top), **2b** (middle) and **3b** (down).

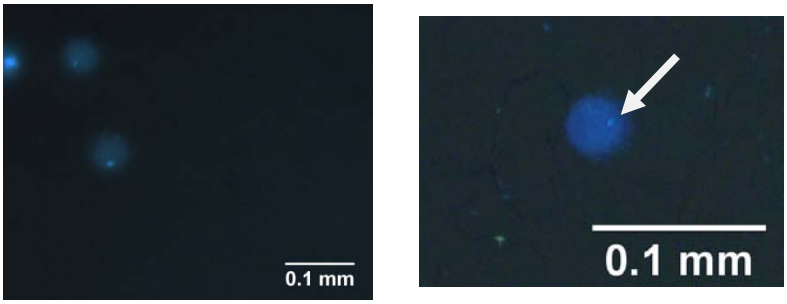


Figure S12. 20x Fluorescence microscopy image of nucleoids incubated with compound **2b** (left) and **3b** (40x, right) at concentration of 113.88 and 93.66 μM respectively and in the presence of DAPI with UV2A filter.

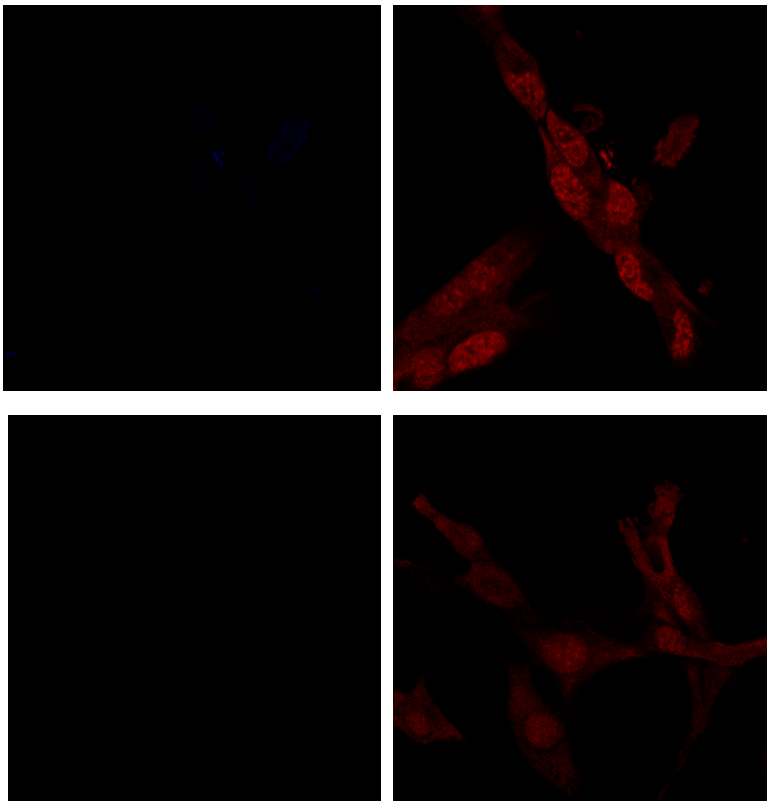


Figure S13. Fluorescence confocal microscopy image of 3T3 incubated cells with Draq5 (red color stain nucleus DNA) and compounds **1b** (concentration of 113.88 μM, blue color, above) and **2b** (concentration 93.66 μM blue color, below). Incubation time: 3 h.