

Supplementary Information

DNA-Interactive and Damage Study with *meso*-Tetra(2-thienyl)porphyrins Coordinated with Polypyridyl Pd(II) and Pt(II) Complexes

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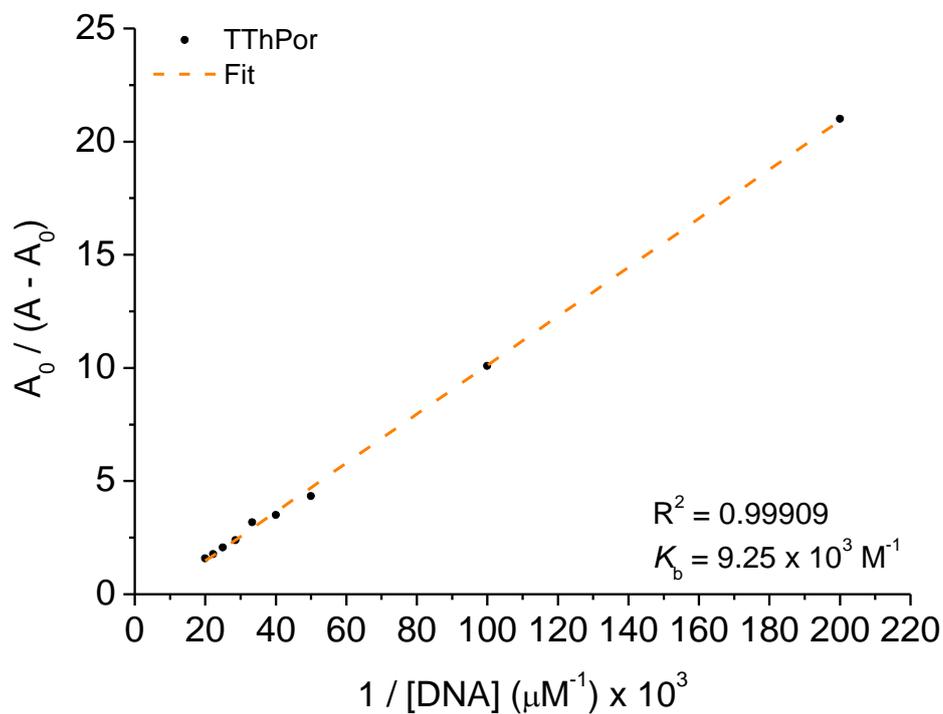
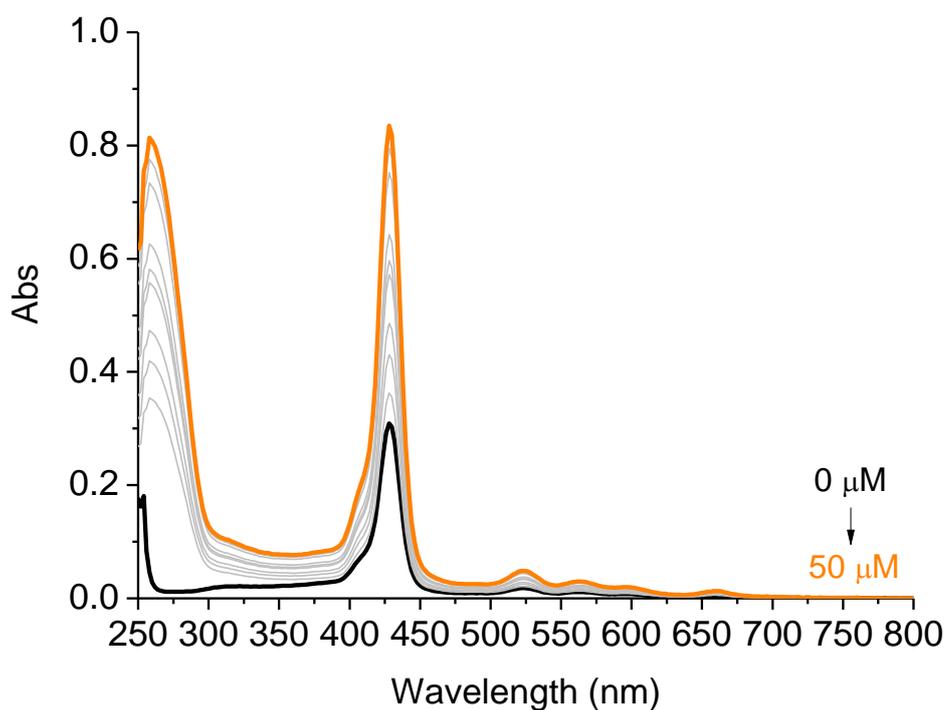


Figure S1. UV-Vis spectra of the **TThPor** upon successive additions of CT-DNA concentrations (0 to 50 μM) in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graph plots of $A_0/(A - A_0)$ versus $1/[\text{CT-DNA}]$.

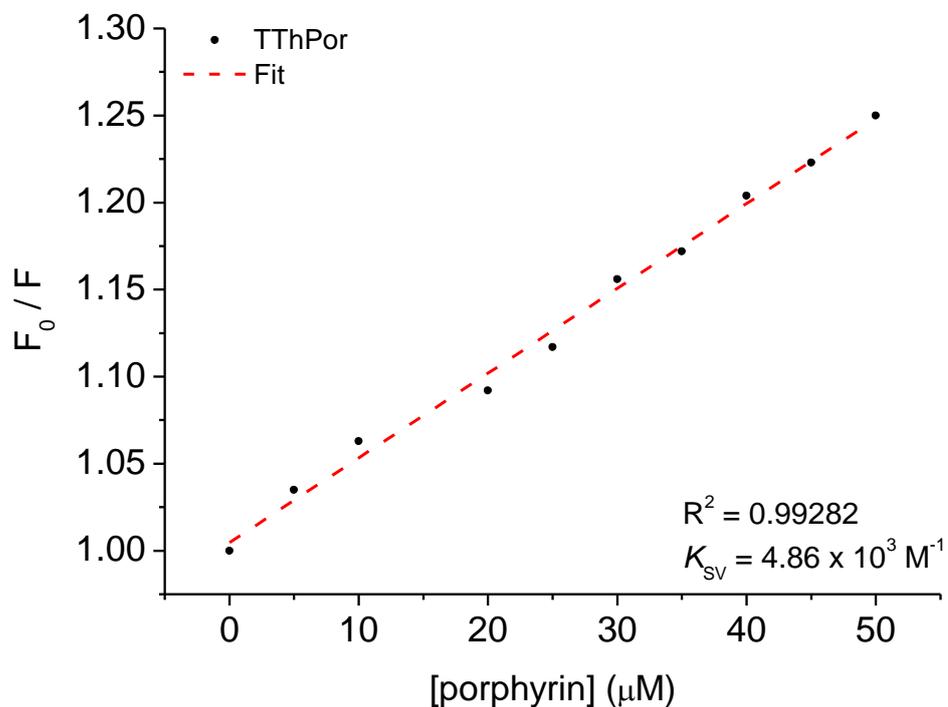
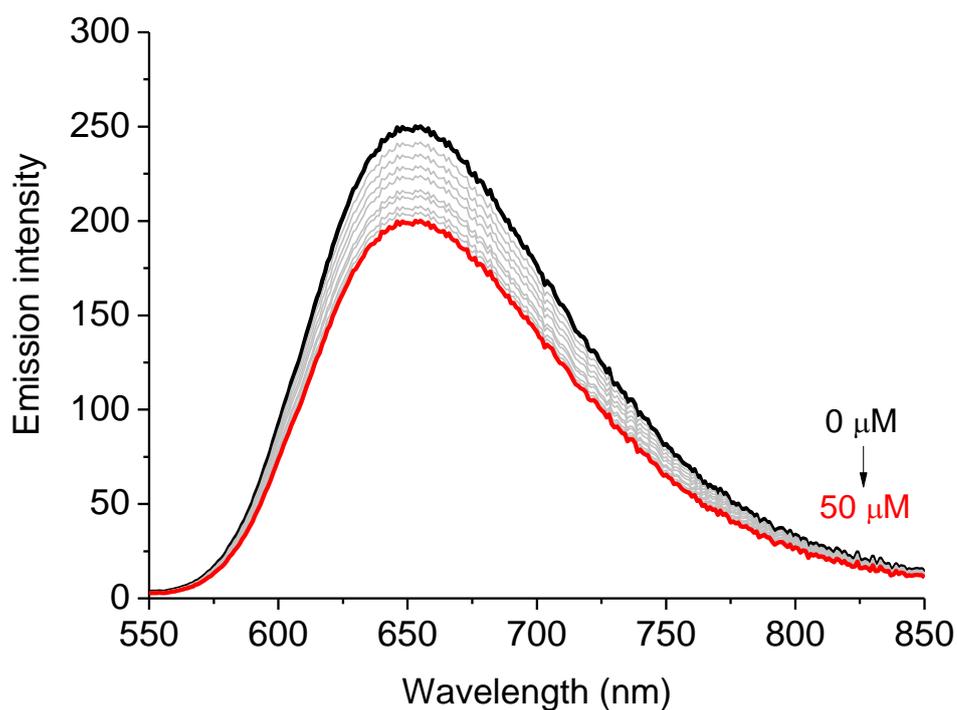


Figure S2. Steady-state fluorescence emission spectra for EB:DNA without and in the presence of porphyrin **TThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus [porphyrin].

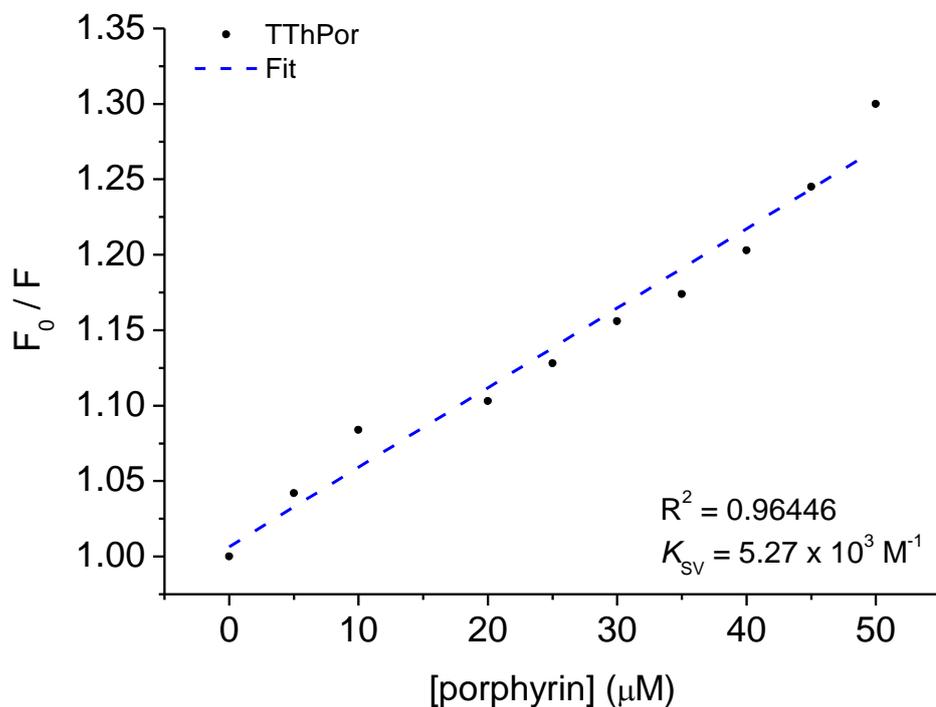
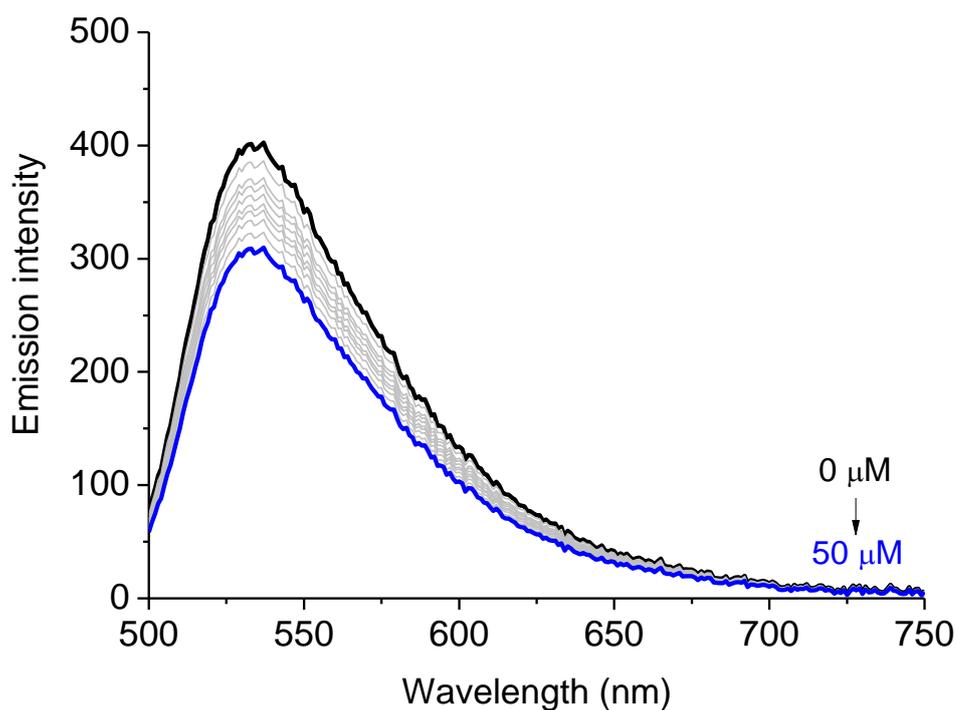


Figure S3. Steady-state fluorescence emission spectra for AO:DNA without and in the presence of porphyrin **TThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus [porphyrin].

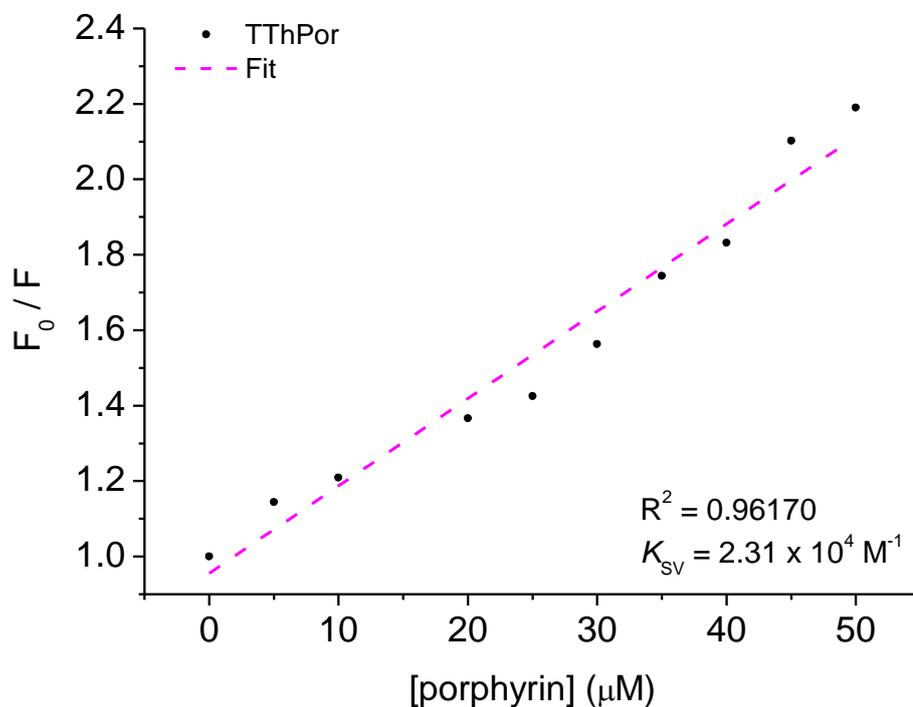
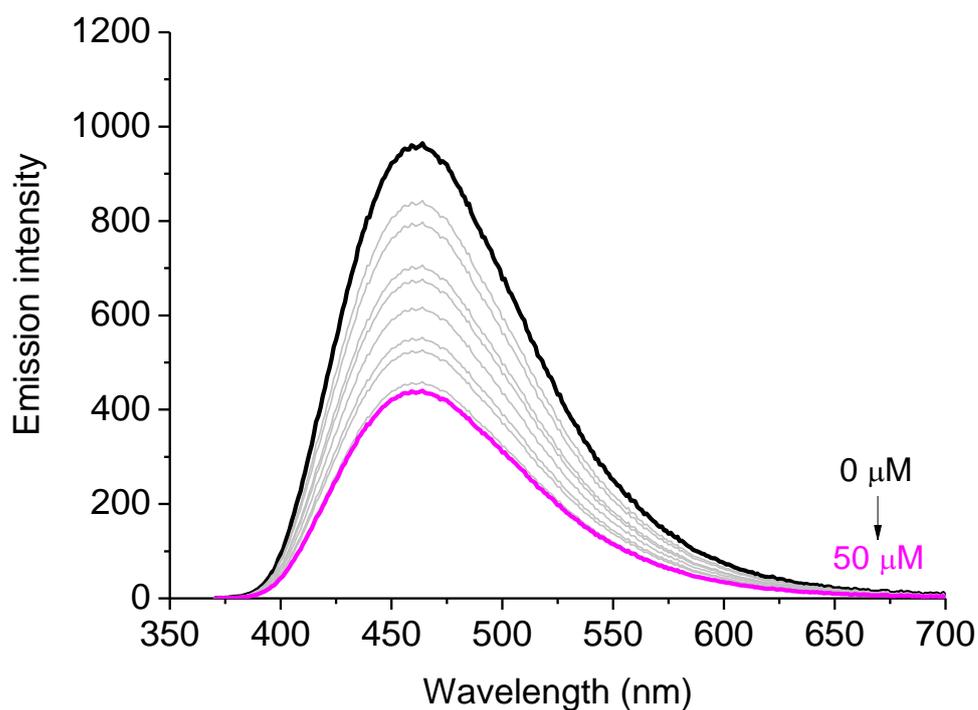


Figure S4. Steady-state fluorescence emission spectra for DAPI:DNA without and in the presence of porphyrin **TThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus $[\text{porphyrin}]$.

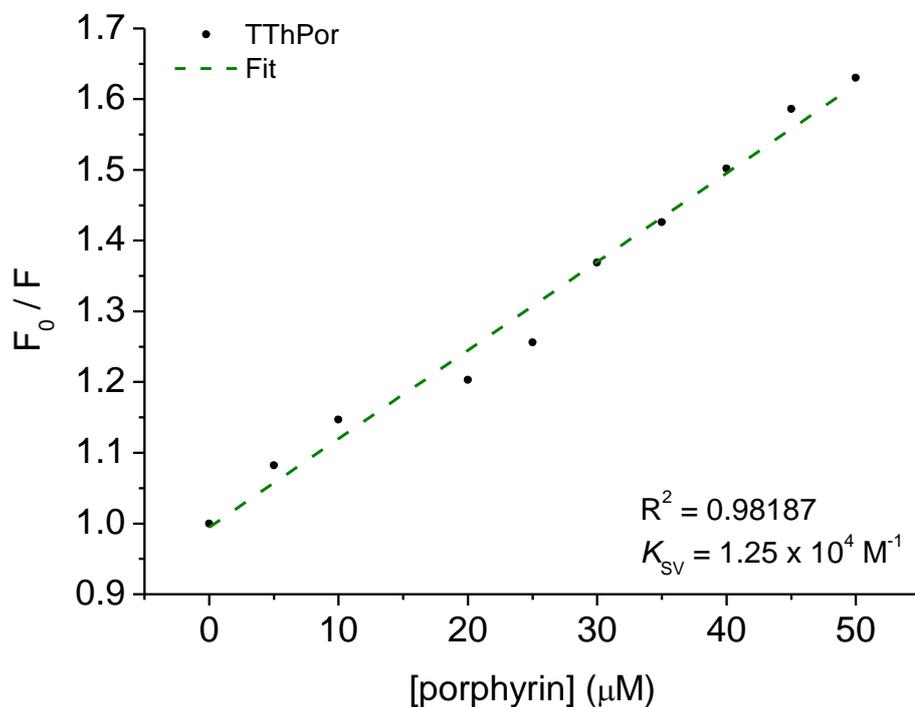
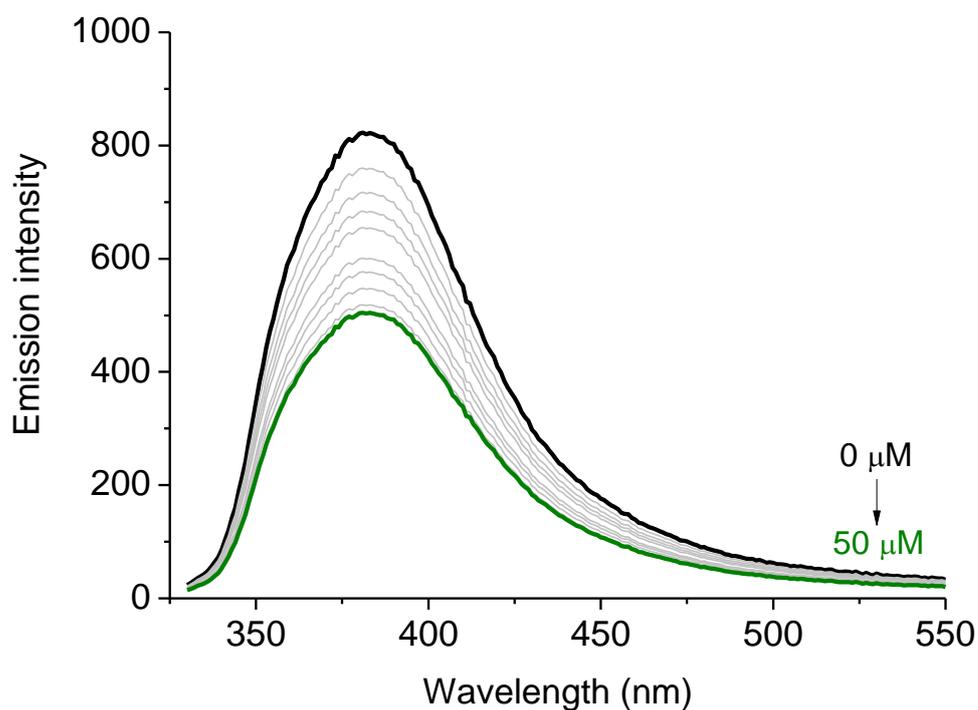


Figure S5. Steady-state fluorescence emission spectra for MG:DNA without and in the presence of porphyrin **TThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus $[\text{porphyrin}]$.

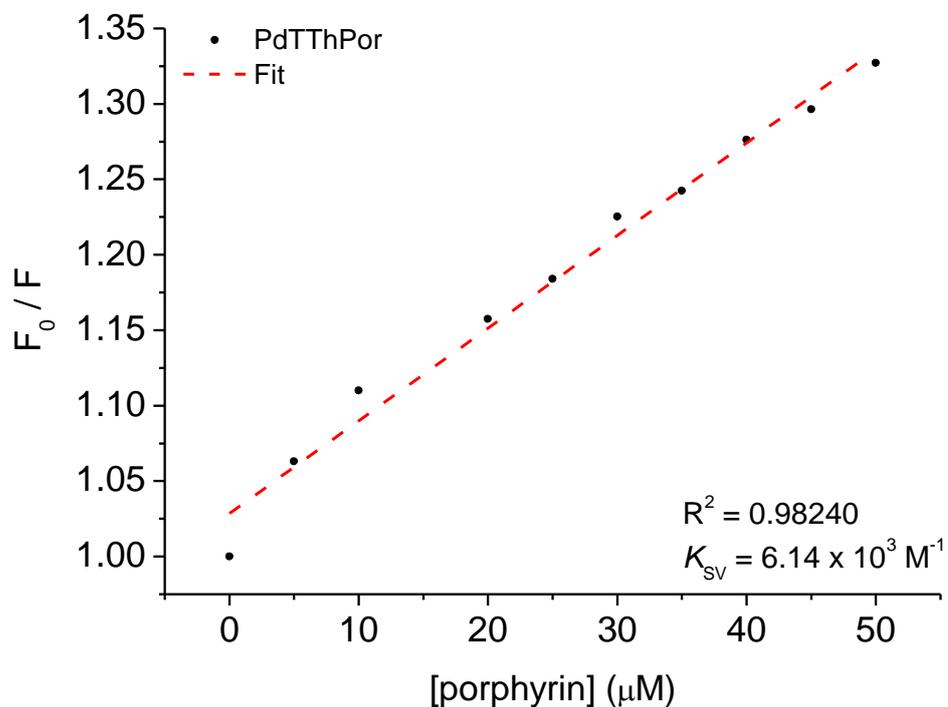
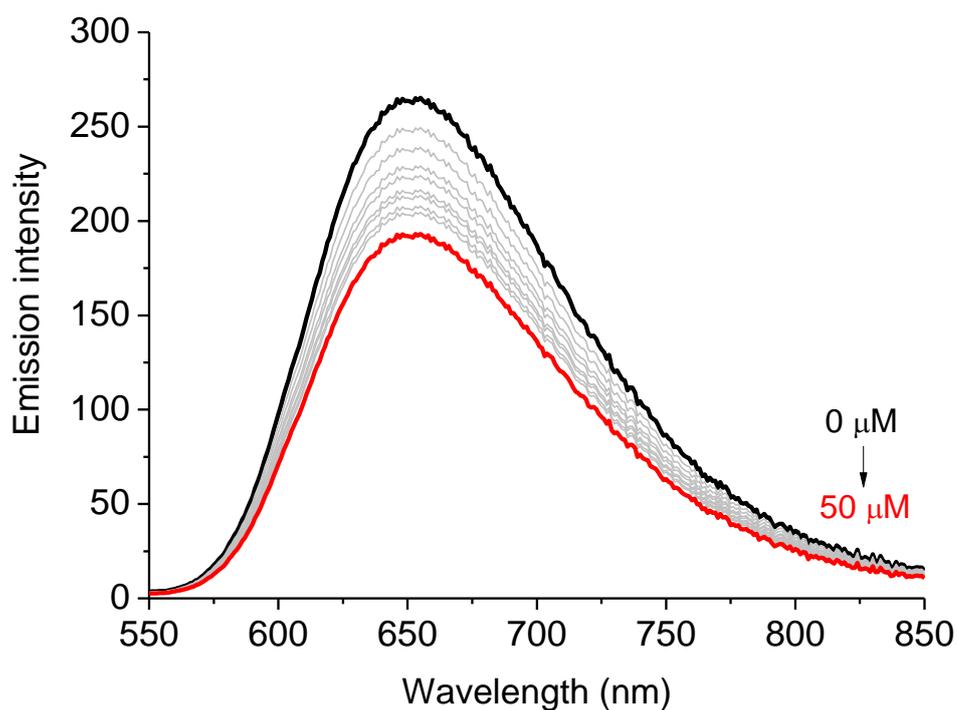


Figure S6. Steady-state fluorescence emission spectra for EB:DNA without and in the presence of porphyrin **PdTThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus [porphyrin].

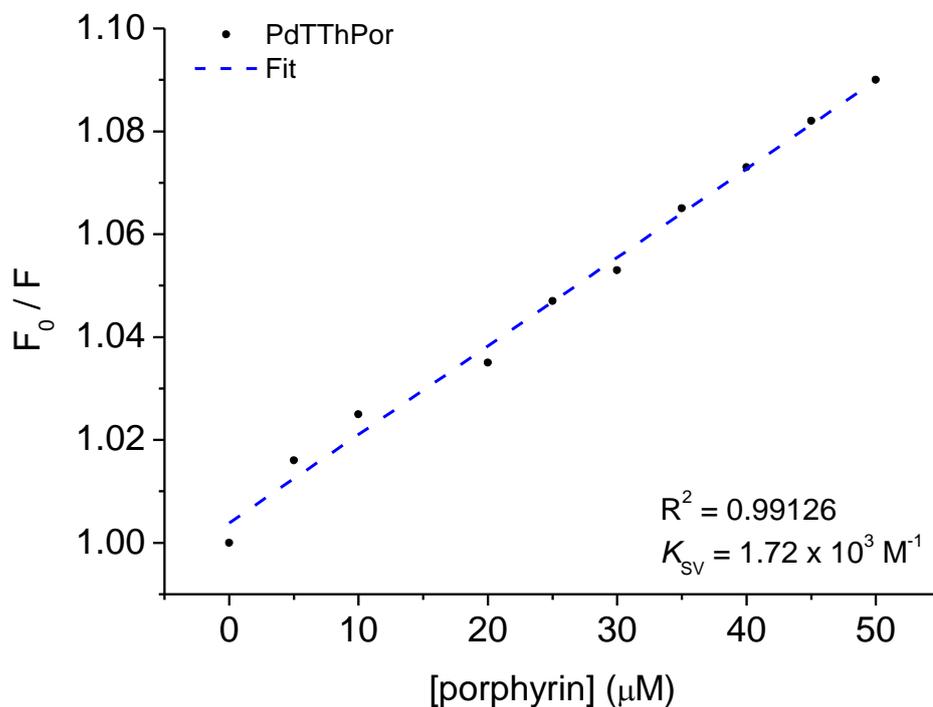
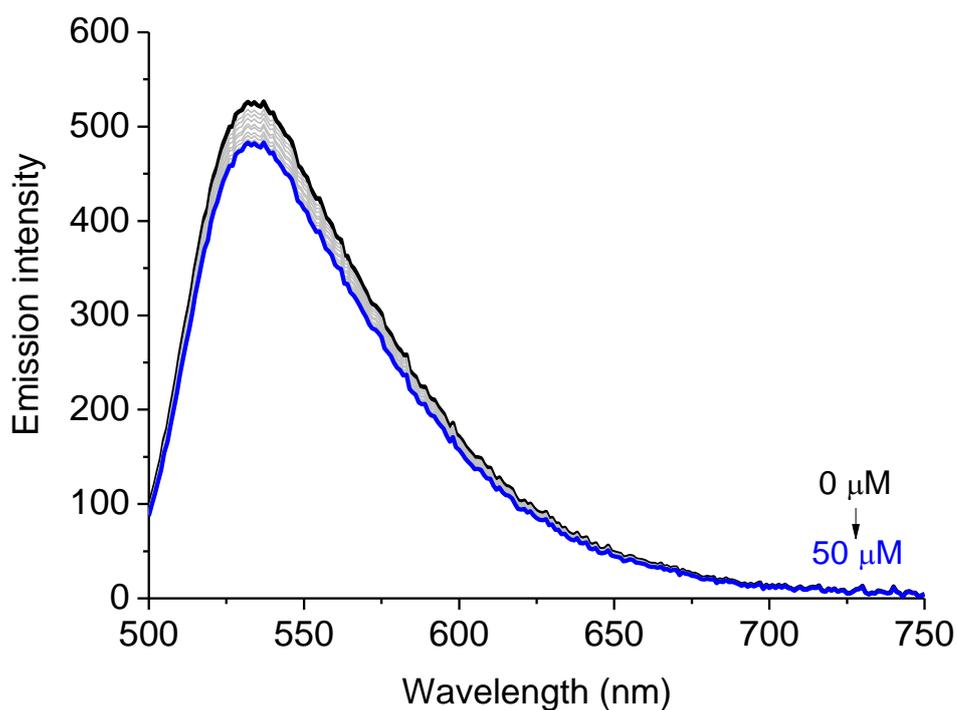


Figure S7. Steady-state fluorescence emission spectra for AO:DNA without and in the presence of porphyrin **PdTThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus [porphyrin].

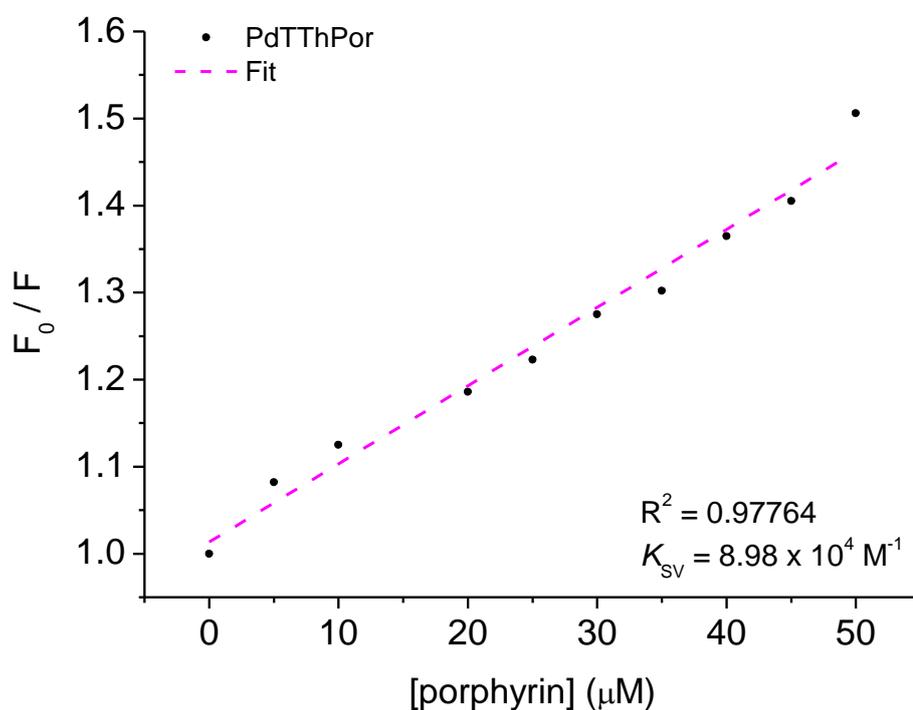
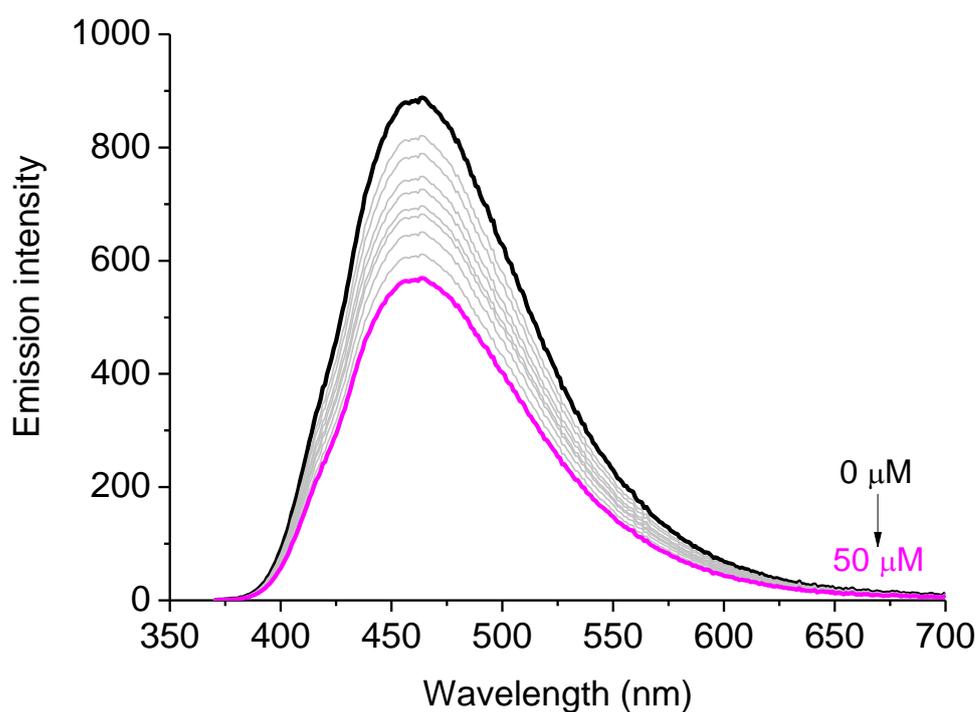


Figure S8. Steady-state fluorescence emission spectra for DAPI:DNA without and in the presence of porphyrin **PdTThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus $[\text{porphyrin}]$.

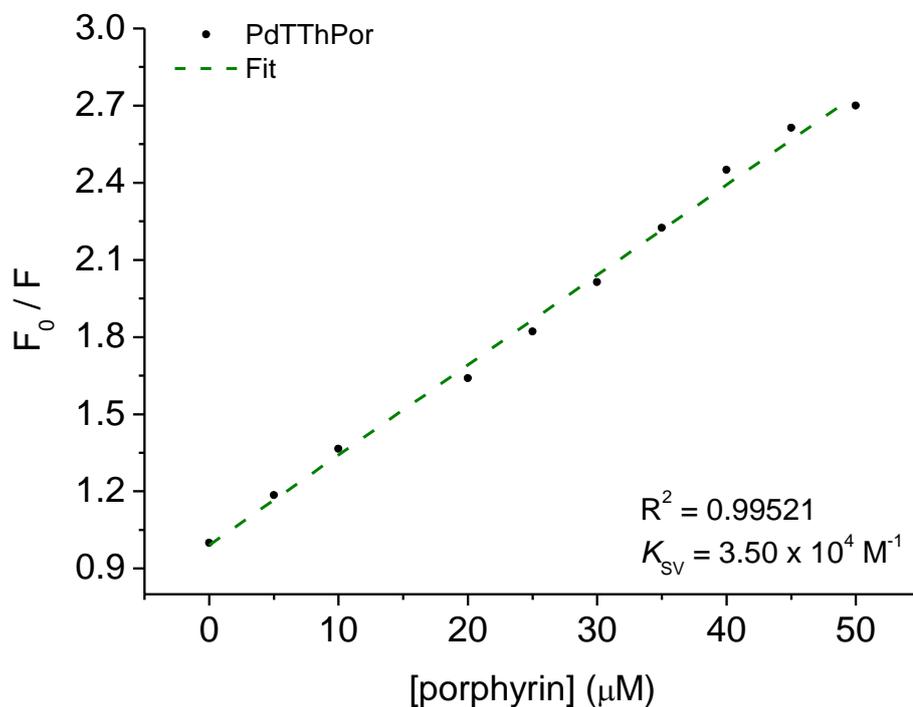
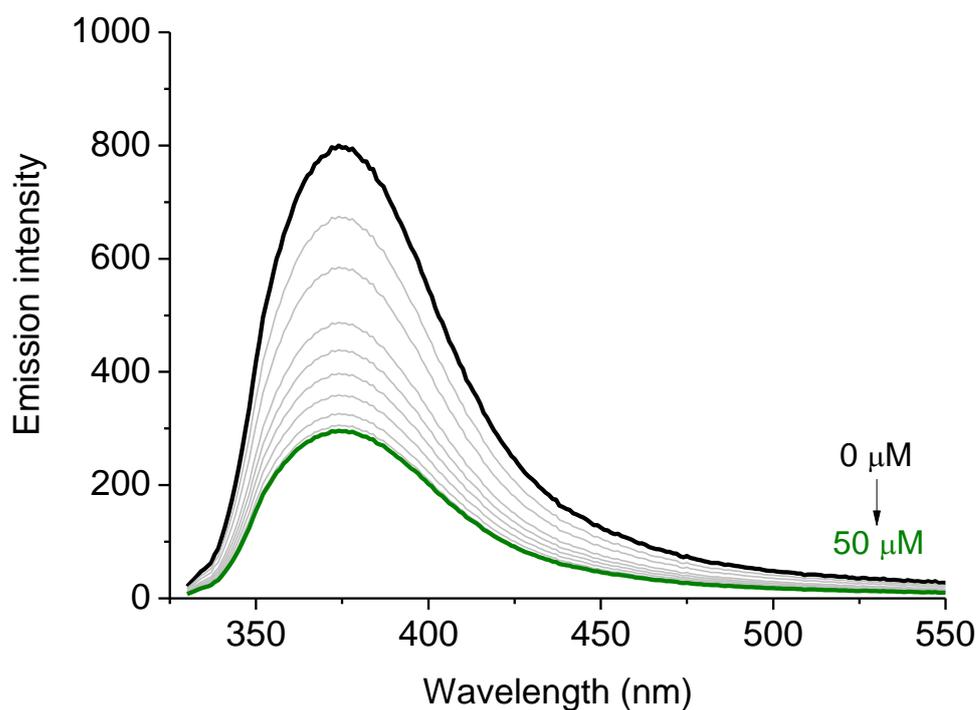


Figure S9. Steady-state fluorescence emission spectra for MG:DNA without and in the presence of porphyrin **PdTThPor**, in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution. Graphs plots shows the F_0/F versus [porphyrin].

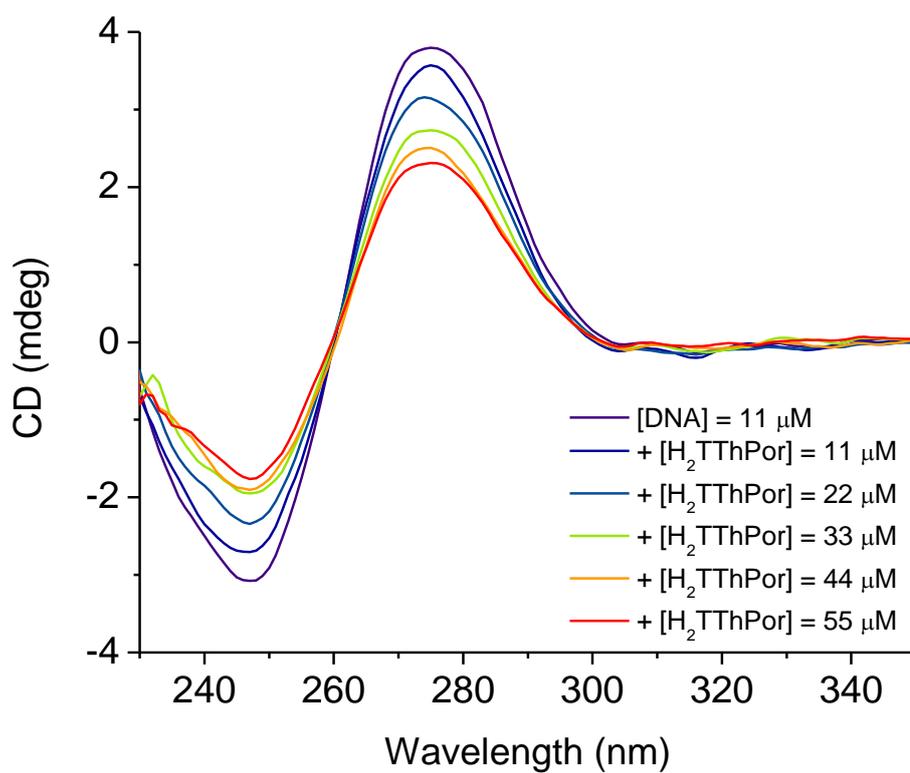
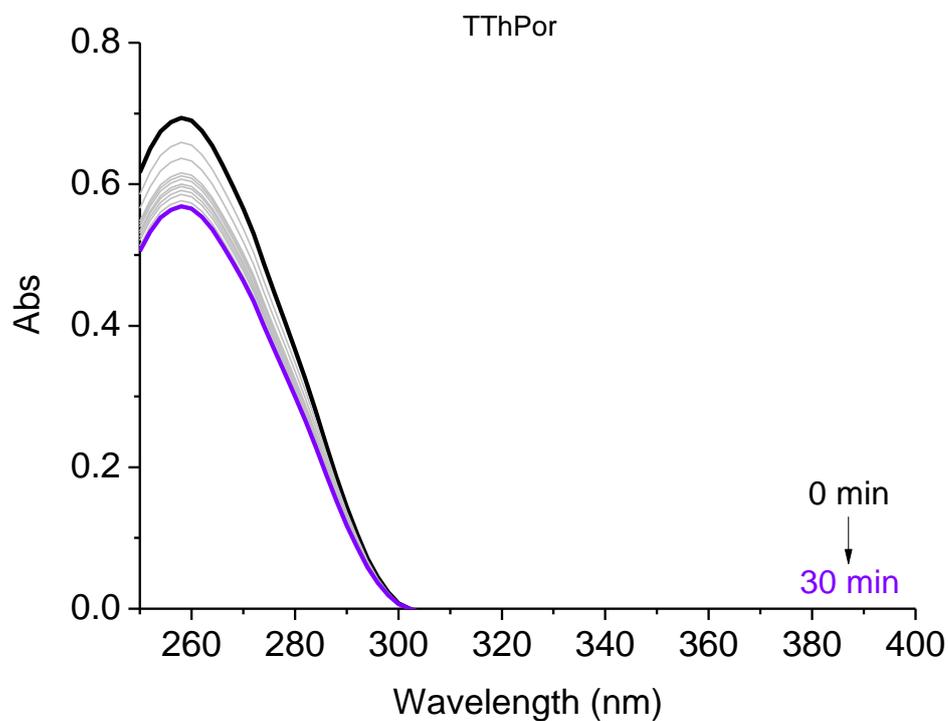


Figure S10. CD spectra for DNA solution in Tris-HCl buffer (pH = 7.4, 1% DMSO) before and after successive additions of porphyrin **TThPor**.



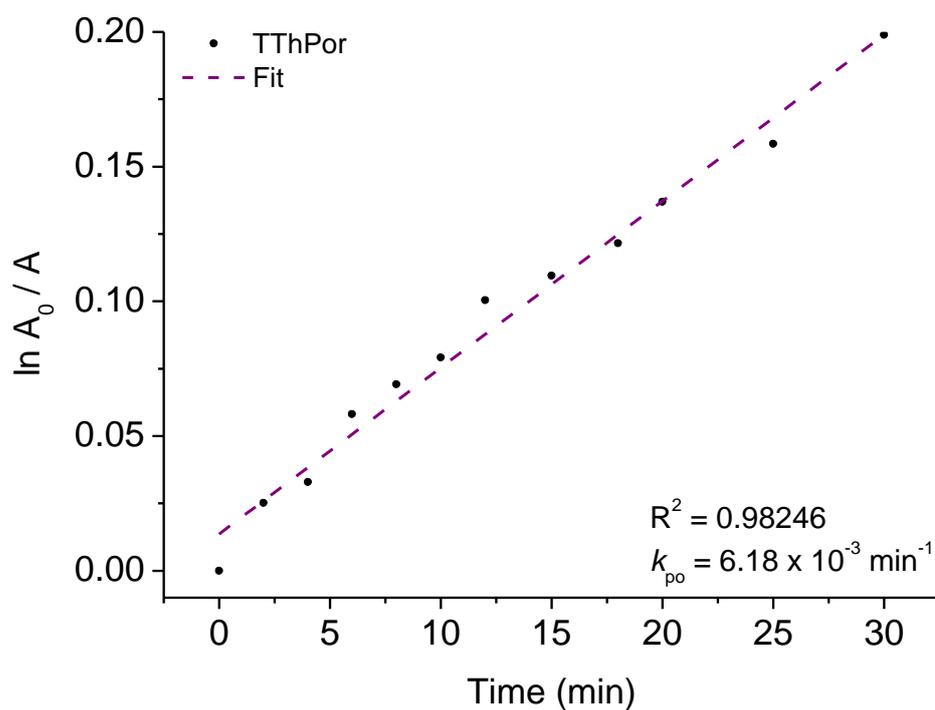
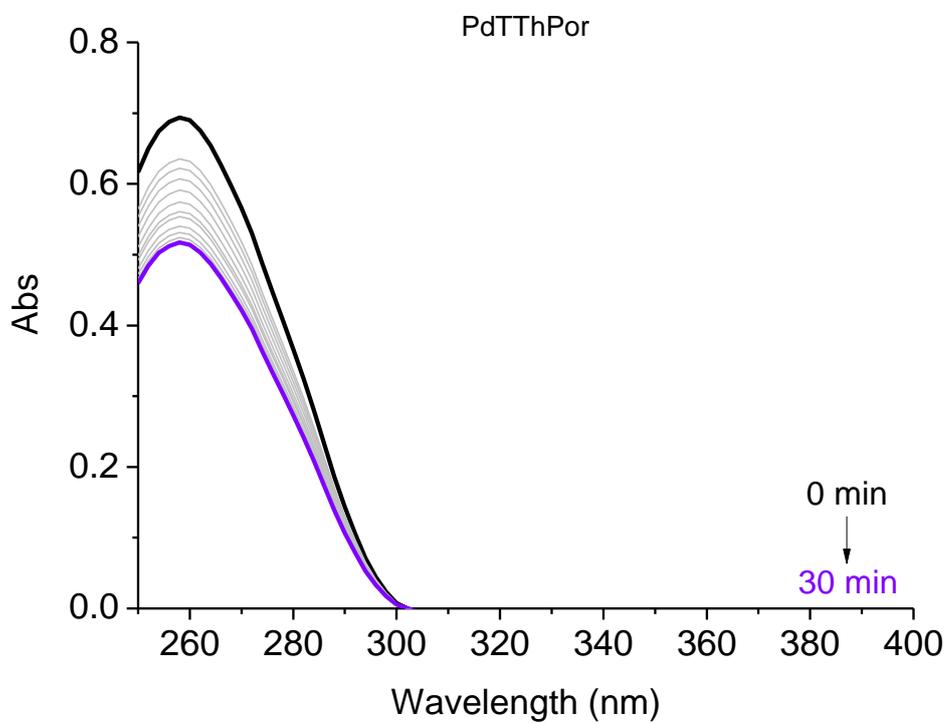


Figure S11. DNA photo-oxidation assay by UV-Vis analysis in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution of porphyrin **TThPor**.



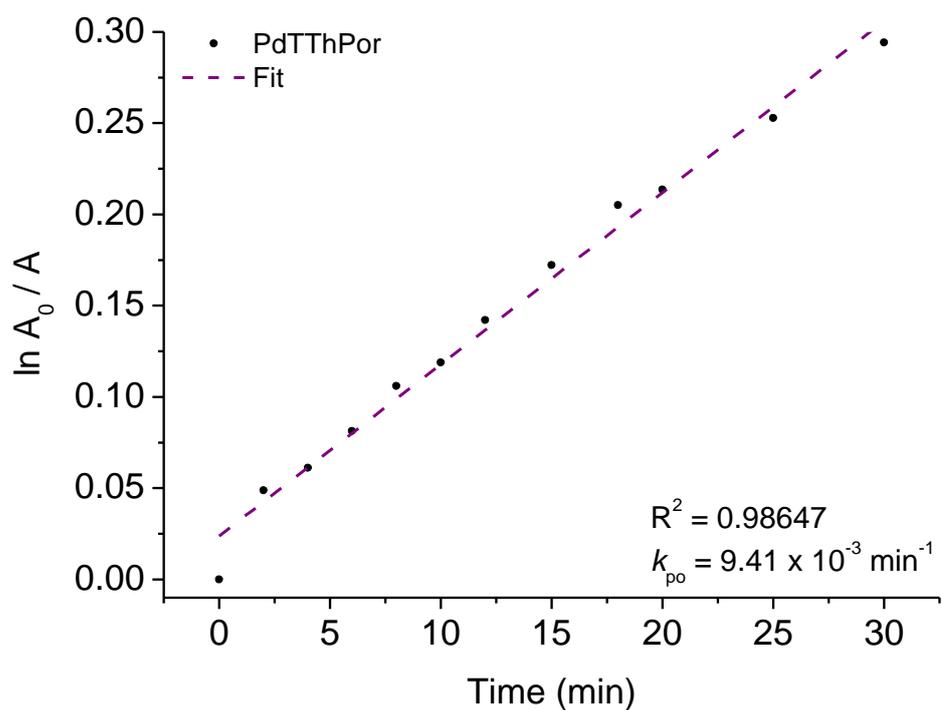
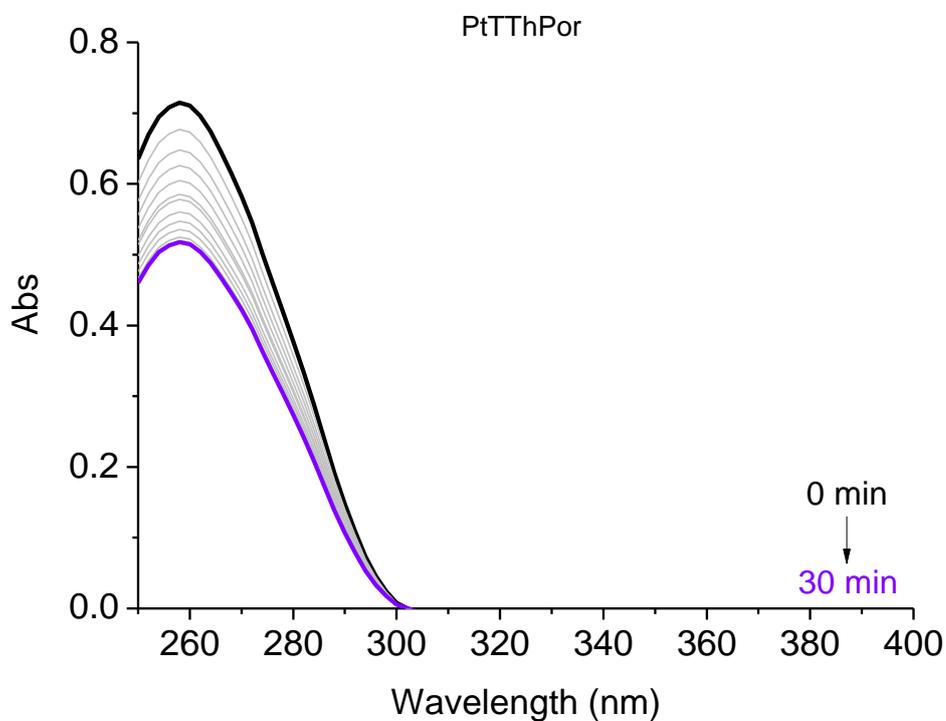


Figure S12. DNA photo-oxidation assay by UV-Vis analysis in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution of porphyrin **PdTThPor**.



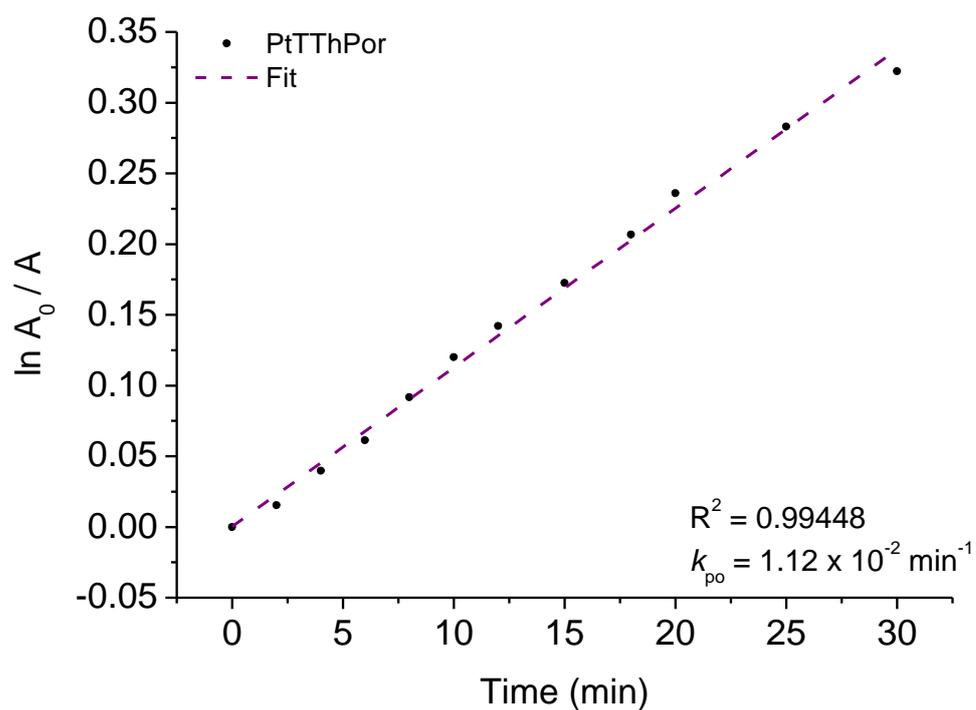


Figure S13. DNA photo-oxidation assay by UV-Vis analysis in DMSO(5%)/Tris-HCl pH 7.4 mixture buffered solution of porphyrin **PtTThPor**.

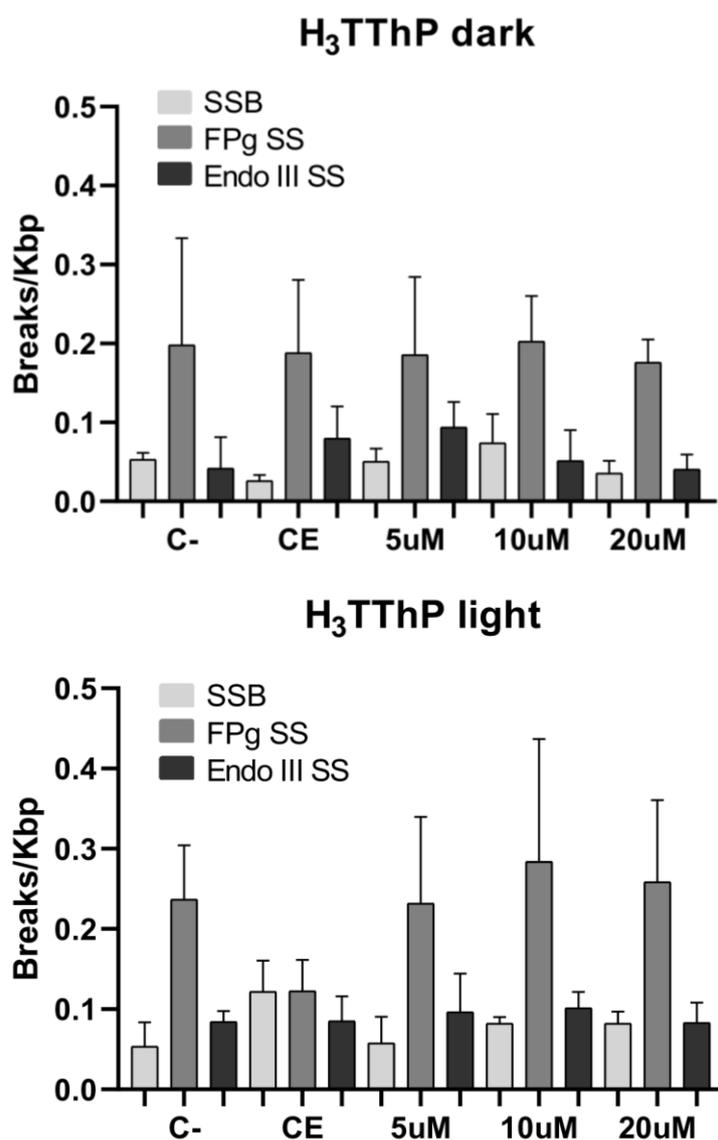


Figure S14. Quantification of DNA lesions generated by porphyrins (a) **TThPor** (dark) and (b) **TThPor** (light), using white-light LED source (irradiance of 50 mW cm^{-2} and a total light dosage of 270 J cm^{-2}) for 90 min. C-: negative control, EC: experiment control. SSB: single-strand breakage of DNA. FPG SS: Formamido-pyrimidine DNA Glycosylase Sensitive Sites. ENDO III SS: Endonuclease III sensitive sites. Mean and standard deviation of three independent experiments. ** $p = 0.0033$; *** $p = 0.0005$; **** $p < 0.0001$.

Table S1. Molecular docking results for the interaction between DNA:TThPor, DNA:PtTThPor, and DNA:PdTThPor in the minor groove.

Code	Nitrogenated bases	Interaction	Distance (Å)
H₂TTP	DA-05	Van der Waals	2.10
	DA-06	Van der Waals	2.70
	DT-07	Van der Waals	2.70
	DT-08	Van der Waals	2.80
	DA-18	Van der Waals	2.40
	DT-19	Van der Waals	2.40
	DT-20	Van der Waals	2.30
PtbpyTTP	DA-06	Van der Waals	3.20
	DT-19	Van der Waals	3.00
	Ribose-DT-20	Van der Waals	3.60
	Ribose-DC-21	Van der Waals	1.90
	Ribose-DG-22	Van der Waals	3.20
PdbpyTTP	DA-06	Van der Waals	2.30
	Ribose-DC-09	Van der Waals	3.30
	DT-19	Van der Waals	3.70
	Ribose-DT-20	Van der Waals	3.10
	DC-21	Van der Waals	2.30
	DG-22	Van der Waals	2.40