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A binuclear Fe(III)/quinizarin complex as a structural model for anthracycline drugs binding to iron

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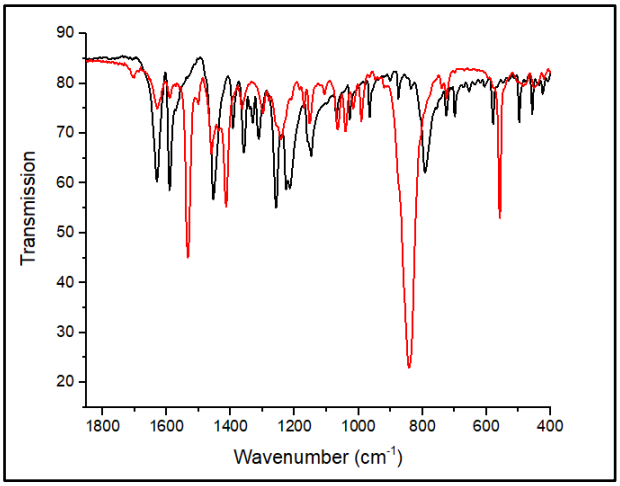

Fig. S1 Infrared spectra of the free Quinizarin (black line) and $[(Fe(cyclam))_2Qz]Cl(PF_6)_3$ (red line) in KBr pellets.

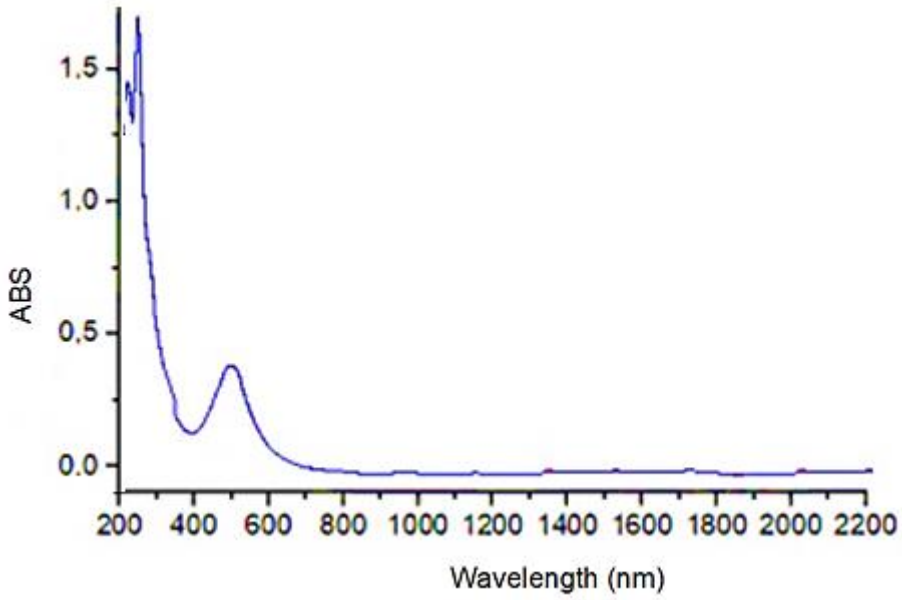

Fig. S2 UV/Vis/NIR absorption spectrum of $[(Fe(cyclam))_2Qz]Cl(PF_6)_3$ complex in CH_3CN.

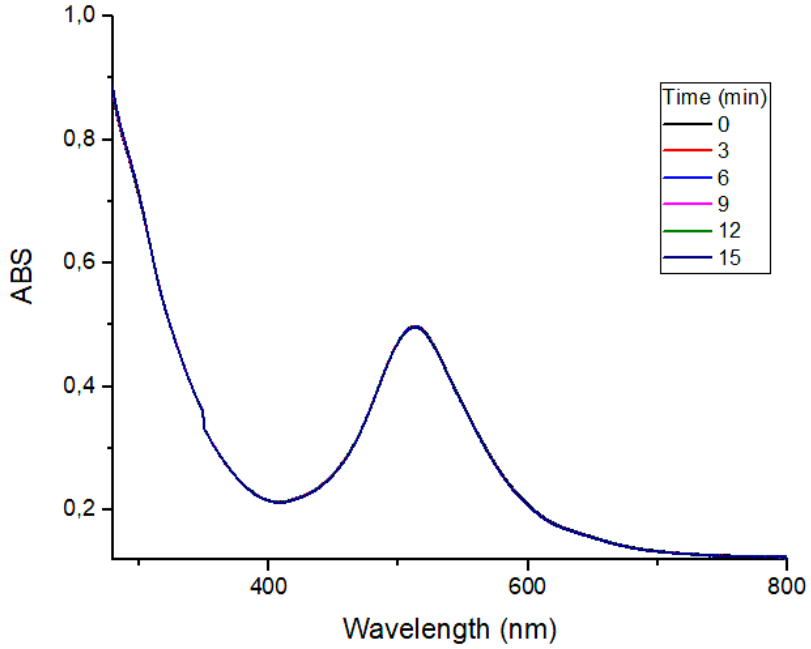

Fig. S3 UV/Vis/NIR spectroelectrochemical response of $[(Fe(cyclam))_2Qz]Cl(PF_6)_3$ upon application of a positive potential (+1000 mV) for 36 minutes in CH_3CN/0.1 M Bu_4NPF_6.

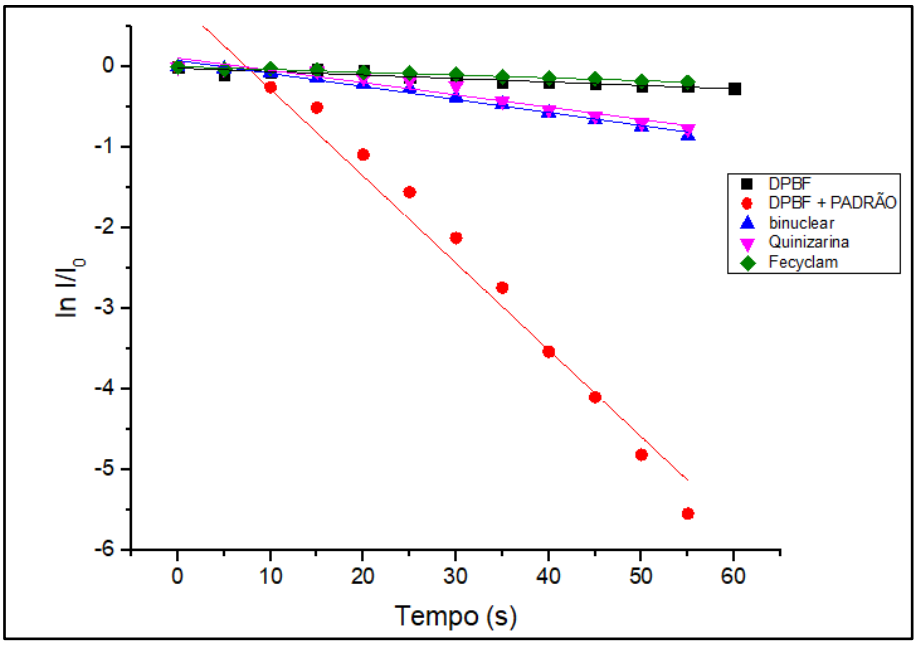

Fig. S4 DPBF consumption (at 20 µmol L^{-1}) as a function of the irradiation time (blue LED) in an air-equilibrated methanol solution, with and without $[(Fe(cyclam))_2Qz]Cl(PF_6)_3$, quinizarin and *cis*–$[Fe(cyclam)Cl_2]Cl$, as indicated (λ_{ex} = 409 nm, λ_{em} = 460 nm).

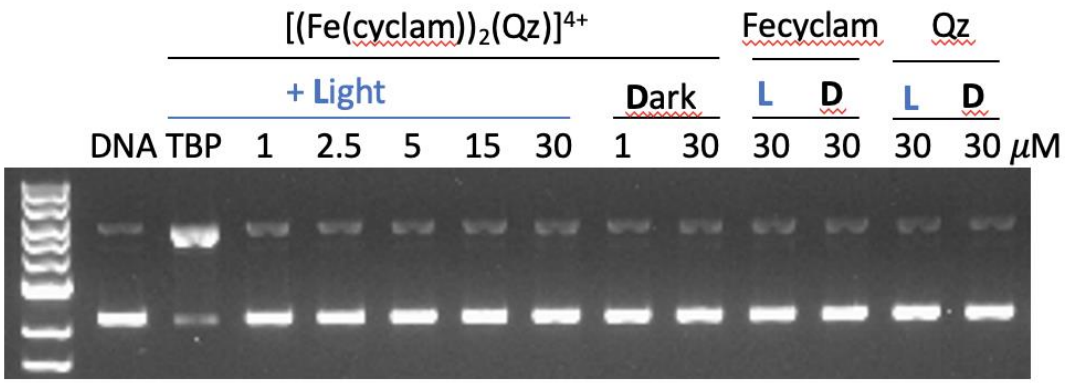

Fig. S5. DNA photocleavage assay. Note that TBP is $[Ru(bpy)_3]Cl_2$ (used at 30 μmol L^{-1}) and Fecyclam is the precursor metal complex ($[Fe(cyclam)Cl_2]Cl$). Samples were kept in the dark (D) or irradiated with blue light (L).

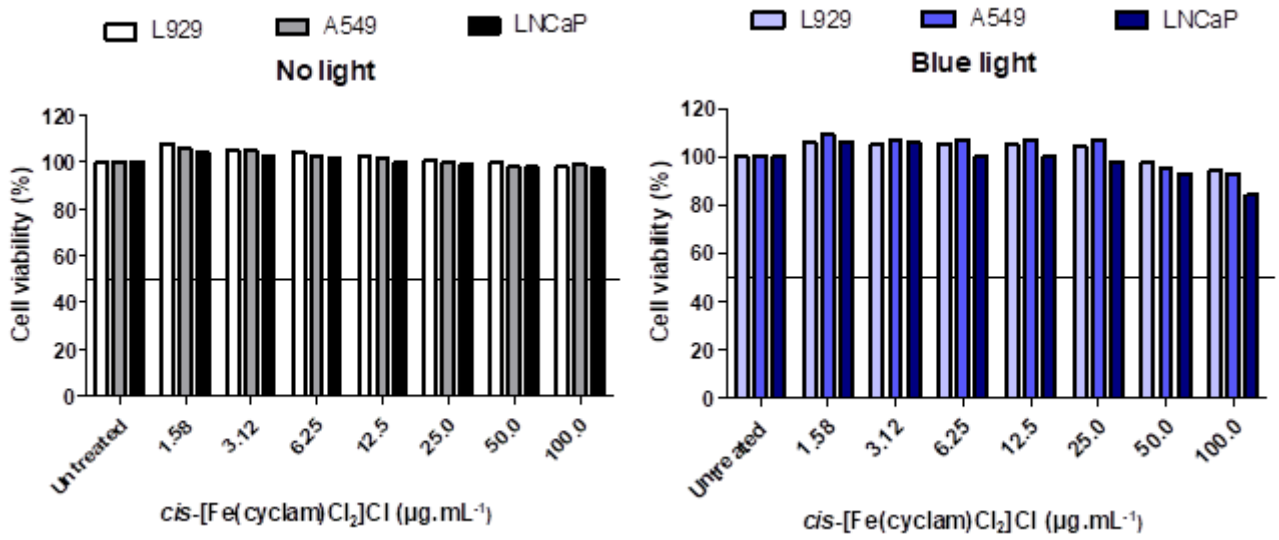

Fig. S6 *cis*-$[Fe(cyclam)Cl_2]Cl$ does not reduce viability of A549 and L929 cell lines, even after irradiation with blue LED (λ_{irr} = 453 nm).