Supporting Information for

Triplet state dynamics of a metalloporphyrin photosensitiser (PtTMPyP4) in the presence of halides and 5'-purine mononucleotides

Páraic M. Keane*^{*a*} and John M. Kelly^{*b*}

Contents

Fig. S1: Lifetime decays and steady-state spectra for quenching of PtTMPyP4 by NaCl

Fig. S2: Lifetime decays and steady-state spectra for quenching of PtTMPyP4 by NaBr

Fig. S3: lifetime and steady-state Stern-Volmer plots for quenching of PtTMPyP4 by NaBr

Fig. S4: UV/vis spectra of Soret band region of PtTMPyP4-GMP complexes

Fig. S5: Benesi-Hildebrand binding plots for PtTMPyP4-GMP complexes

Fig. S6: Stern-Volmer plot for addition of NaCl to PtTMPyP4-AMP complex

Fig. S7: Triplet-triplet decay kinetics for PtTMPyP4 in aerated 50 mM Na-phosphate buffer solution

Fig. S8: Triplet-triplet decay kinetics for PtTMPyP4 with 10 mM AMP aerated 50mM Naphosphate buffer solution

Fig. S9: Stern-Volmer plots for long lifetime component in aerated and deoxygenated PtTMPyP4-GMP complexes derived from T-T absorption kinetics

Fig. S10: Triplet-triplet decay kinetics for PtTMPyP4 in near-IR aerated 50mM Naphosphate buffer solution

Fig S11: Triplet-triplet decay kinetics for PtTMPyP4 with 10 mM GMP in near-IR in aerated 50mM Na-phosphate buffer solution

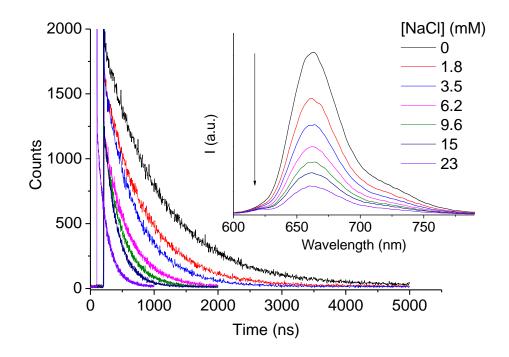


Fig S1: Single-photon counting decays ($\lambda_{exc} = 371 \text{ nm}$, $\lambda_{em} = 665 \text{ nm}$). and inset: steady-state spectra for quenching of 5 µM PtTMPyP4 by NaCl ($\lambda_{exc} = 513 \text{ nm}$) in aerated 50 mM phosphate buffer

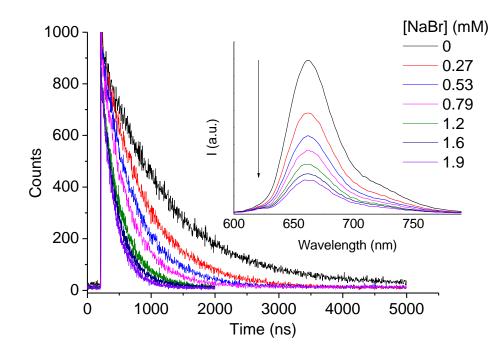


Fig S2: Single-photon counting decays ($\lambda_{exc} = 371 \text{ nm}$, $\lambda_{em} = 665 \text{ nm}$). and inset: steady-state spectra for quenching of 5 μ M PtTMPyP4 by NaBr ($\lambda_{exc} = 513 \text{ nm}$) in aerated 50 mM phosphate buffer

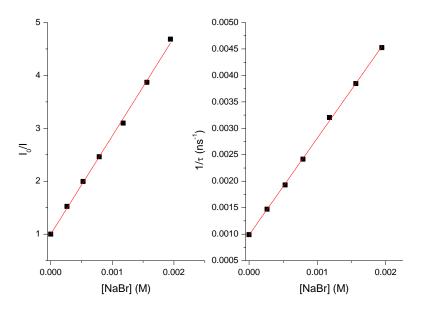


Fig. S3: Stern-Volmer plots for phosphorescence of PtTMPyP4 in the presence of NaBr in 50 mM phosphate buffer for (a) steady-state ($\lambda_{exc} = 513$ nm, $\lambda_{em} = 665$ nm) and (b) time-resolved data ($\lambda_{exc} = 371$ nm, $\lambda_{em} = 665$ nm).

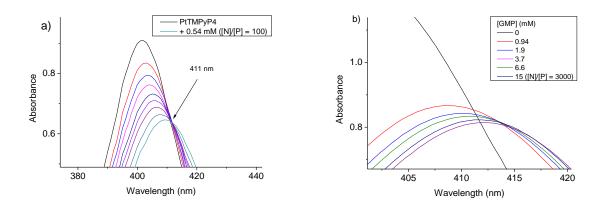


Fig. S4: UV/vis absorption spectra of Soret region of PtTMPyP4 in the presence of GMP in 50 mM phosphate buffer (a) at low GMP conc. (b) at high GMP conc.

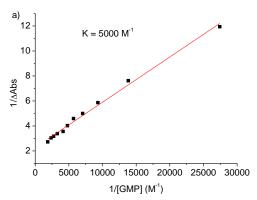


Fig. S5: Benesi-Hildebrand fits to UV/vis absorption spectra of PtTMPyP4 in the presence of low GMP concentrations (< 0.5 mM) in 50 mM phosphate buffer.

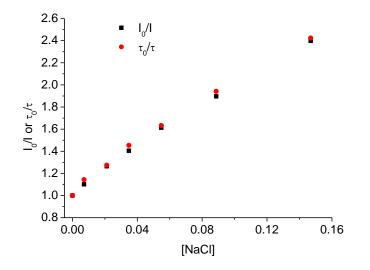


Fig. S6: Combined steady-state ($\lambda_{exc} = 517 \text{ nm}$) and lifetime ($\lambda_{exc} = 370 \text{ nm}$, $\lambda_{em} = 675 \text{ nm}$) Stern-Volmer plots for PtTMPyP4-AMP complex in presence of NaCl in aerated 50 mM phosphate buffer solution. [PtTMPyP4] = 5 μ M, [AMP] = 15 mM.

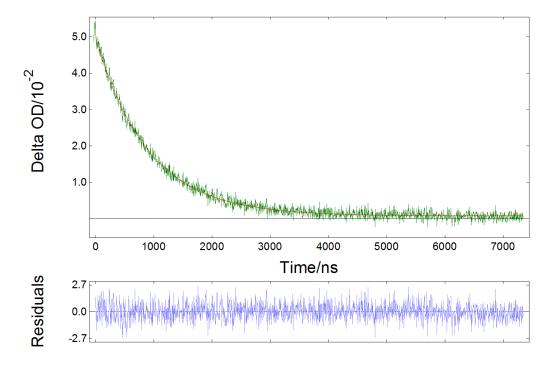


Fig. S7: Monoexponential fit of triplet-triplet absorption spectrum of 6 μ M PtTMPyP4 in aerated 50 mM Na-phosphate buffer solution. Recorded at 440 nm ($\lambda_{exc} = 355$ nm) $\tau = 932$ ns.

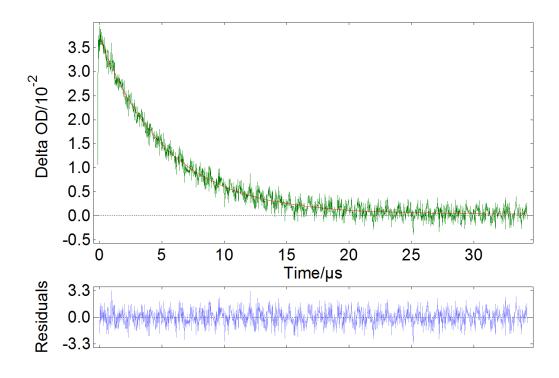


Fig. S8: Monoexponential fit of T-T absorption spectrum of 6 μ M PtTMPyP4 in the presence of AMP (10 mM) in aerated 50mM Na-phosphate buffer solution. Recorded at 460 nm (λ_{exc} = 355 nm) τ = 5650n

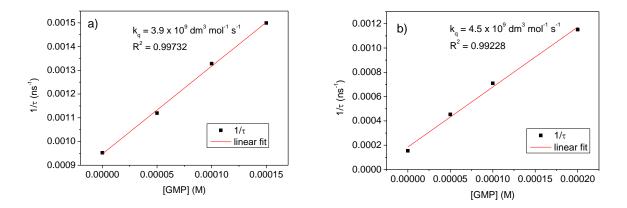


Fig. S9: Stern-Volmer plots for long lifetime component of PtTMPyP4 in presence of GMP calculated from T-T absorption decays at 450 nm in a) aerated solution b) deoxygenated solution. Both in 50 mM Na-phosphate buffer, $\lambda_{exc} = 355$ nm

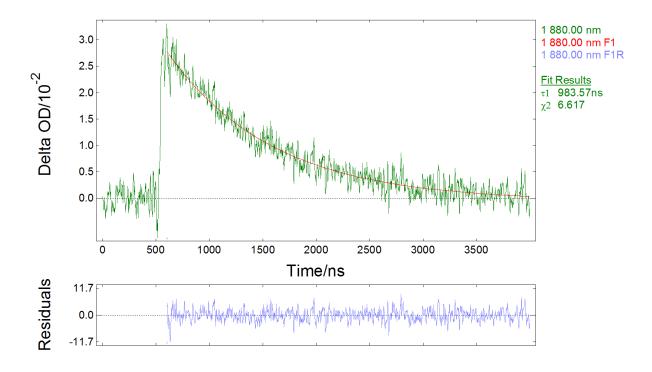


Fig. S10 Monoexponential fit of T-T absorption spectrum of 6 μ M PtTMPyP4 in aerated 50 mM Naphosphate buffer solution. Recorded at 880 nm ($\lambda_{exc} = 355$ nm)

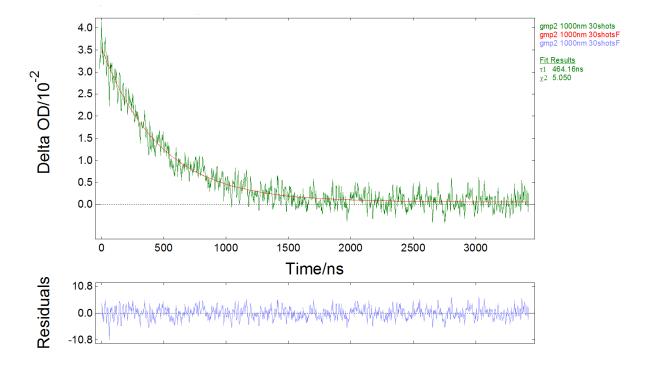


Fig. S11 Monoexponential fit of T-T absorption spectrum of 6 mM PtTMPyP4 in presence of GMP (10 mM) aerated 50mM Na-phosphate buffer solution. Recorded at 1000 nm ($\lambda_{exc} = 355$ nm)