Supplementary Materials: Synthesis, Characterization and Biological Evaluation of Red-Absorbing Fe(II) Polypyridine Complexes

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Figure S1. ¹H NMR spectrum of 4 in CD₃CN, 400 MHz.



Figure S2. ¹³C NMR spectrum of 4 in CD₃CN, 100 MHz.

S2/S11



Figure S3. ESI-HRMS spectrum of 4 (positive detection mode).



Figure S4. ¹H NMR spectrum of 5 in CD₃OD, 400 MHz.

S3/S11



Figure S5. ¹³C NMR spectrum of 5 in CD₃OD, 100 MHz.



Figure S6. ESI-HRMS spectrum of 5 (negative detection mode).



Figure S7. ¹H NMR spectrum of 6 in CD₃OD, 400 MHz.



Figure S8. ¹³C NMR spectrum of 6 in CD₃OD, 100 MHz.



Figure S9. ESI-HRMS spectrum of 6 (negative detection mode).



Figure S10. Normalised Emission Spectrum of 4 in CH₃CN.

S6/S11



Figure S11. Normalised Emission Spectrum of 5 in CH₃CN.



Figure S12. Normalised Emission Spectrum of 6 in CH₃CN.



Figure S13. HPLC chromatogram of Caffeine (internal standard) and **4** after 0 and 48 h incubation in human pooled plasma.



Figure S14. HPLC chromatogram of Caffeine (internal standard) and **5** after 0 and 48 h incubation in human pooled plasma.



Figure S15. HPLC chromatogram of Caffeine (internal standard) and **6** after 0 and 48 h incubation in human pooled plasma.



Figure S16. Temporal change of the UV/Vis spectra of [Ru(bipy)₃]Cl₂ by irradiation at 450 nm in CH₃CN.



Figure S17. Temporal change of the UV/Vis spectra of 4 by irradiation at 450 nm in CH₃CN.



Figure S18. Temporal change of the UV/Vis spectra of 5 by irradiation at 450 nm in CH₃CN.



Figure S19. Temporal change of the UV/Vis spectra of 6 by irradiation at 450 nm in CH₃CN.



Figure S20. Temporal change of the UV/Vis spectra of PpIX by irradiation at 450 nm in CH₃CN.