

Microenvironment-Switchable Singlet Oxygen Generation by Axially-Coordinated Hydrophilic Ruthenium Phthalocyanine Dendrimers

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Supplementary Information

Part I. ¹H NMR Spectra of dendritic pyridine ligands 5-7.

Part II. ¹H NMR Spectra of RuP1-3.

Part III. Phosphorescence at 1140 nm of RuP1-3 in CHCl₃ & D₂O.

**Part IV. Singlet oxygen luminescence at 1270 nm of RuP1-3 in CHCl₃, THF
& D₂O.**

Part I. ^1H NMR Spectra of dendritic pyridine ligands 5-7.

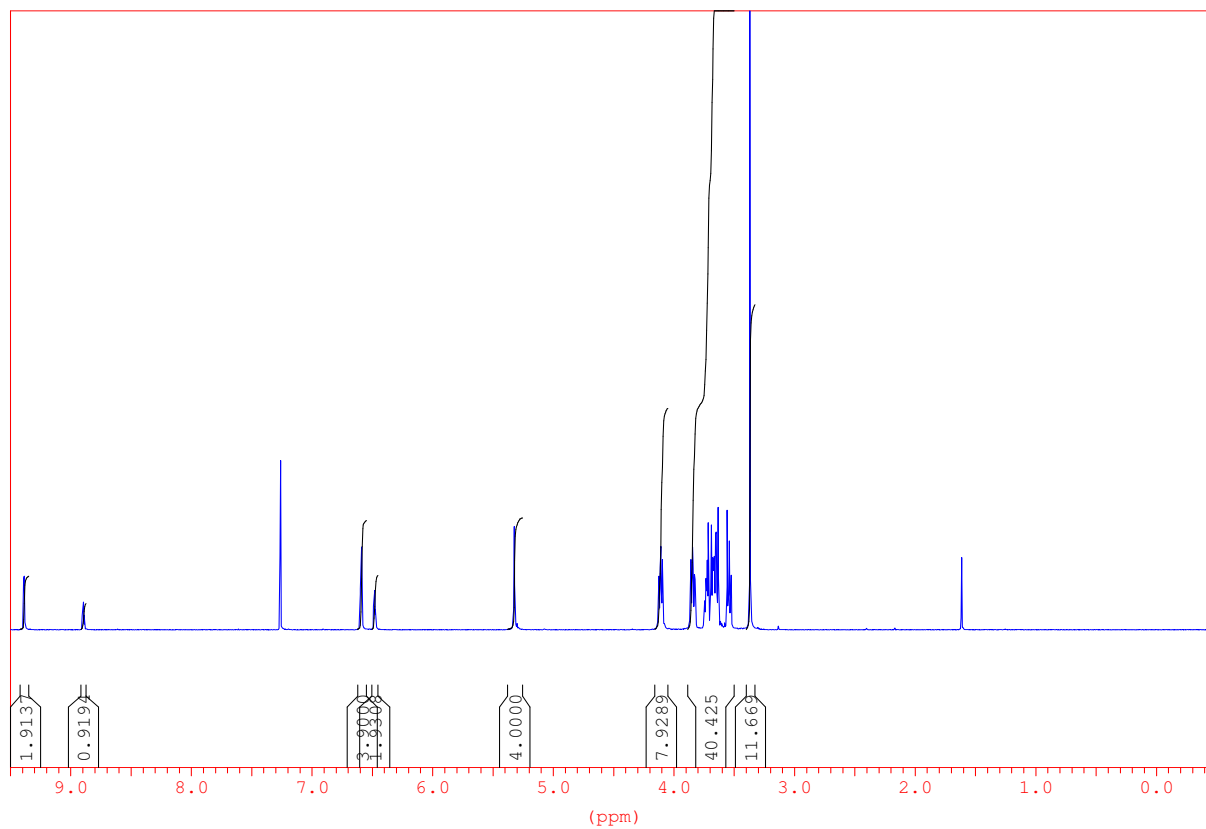


Figure S1. ^1H NMR spectrum of **5** recorded in CDCl_3 .

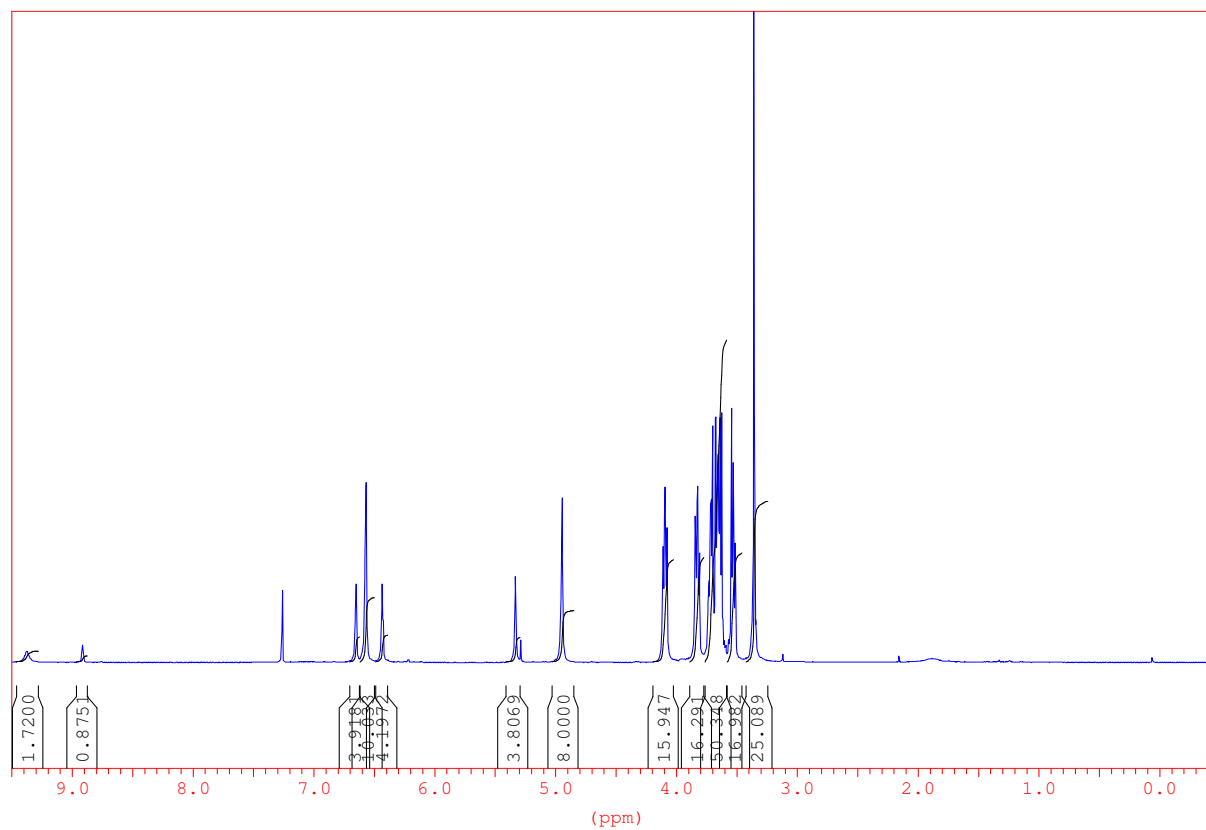


Figure S2. ^1H NMR spectrum of **6** recorded in CDCl_3 .

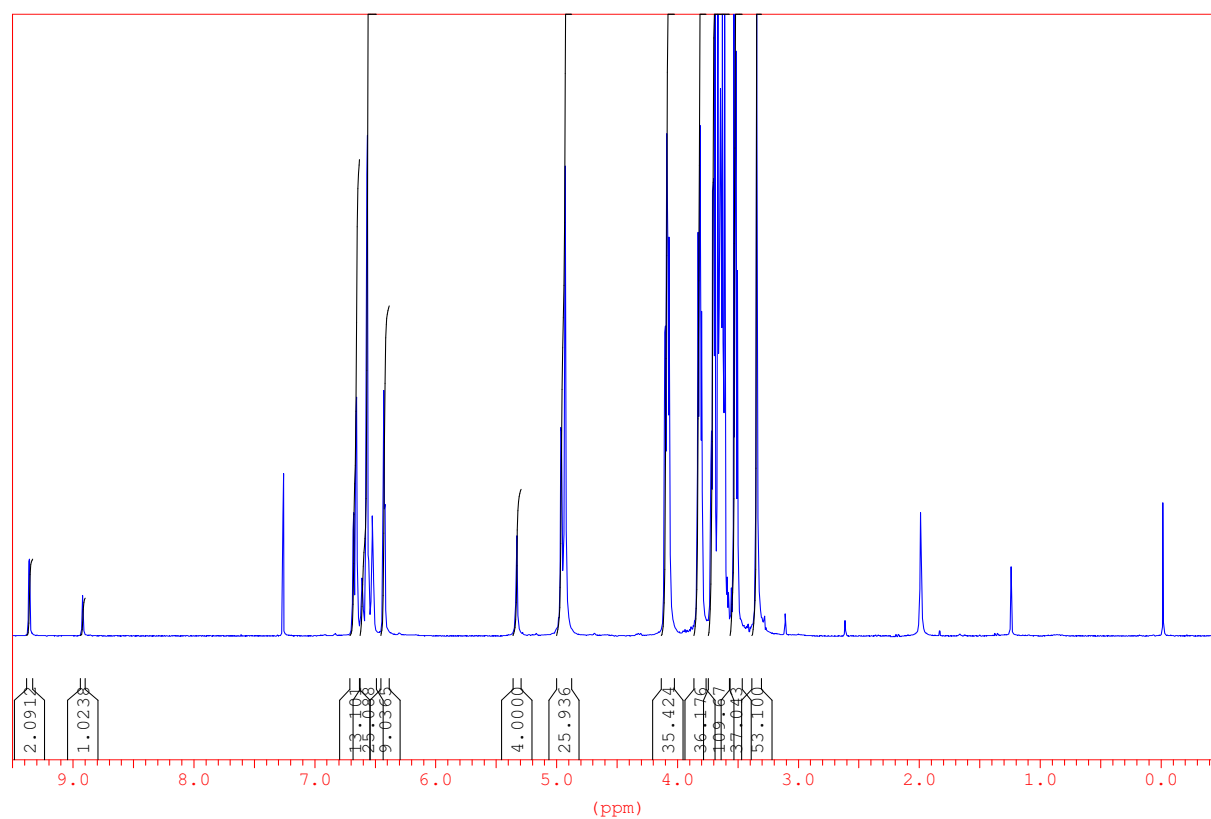


Figure S3. ^1H NMR spectrum of **7** recorded in CDCl_3 .

Part II. ^1H NMR Spectra of RuP1-3.

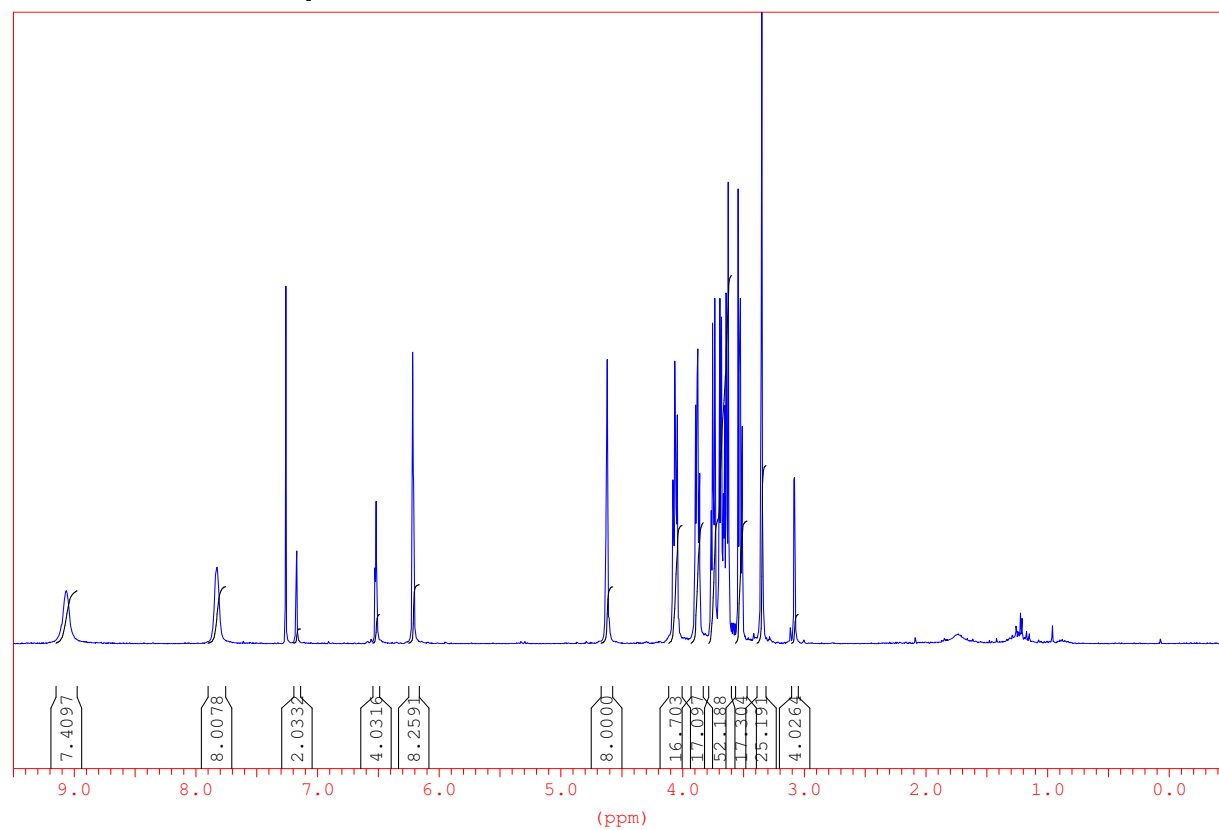


Figure S4. ^1H NMR spectrum of **RuP1** recorded in CDCl_3 .

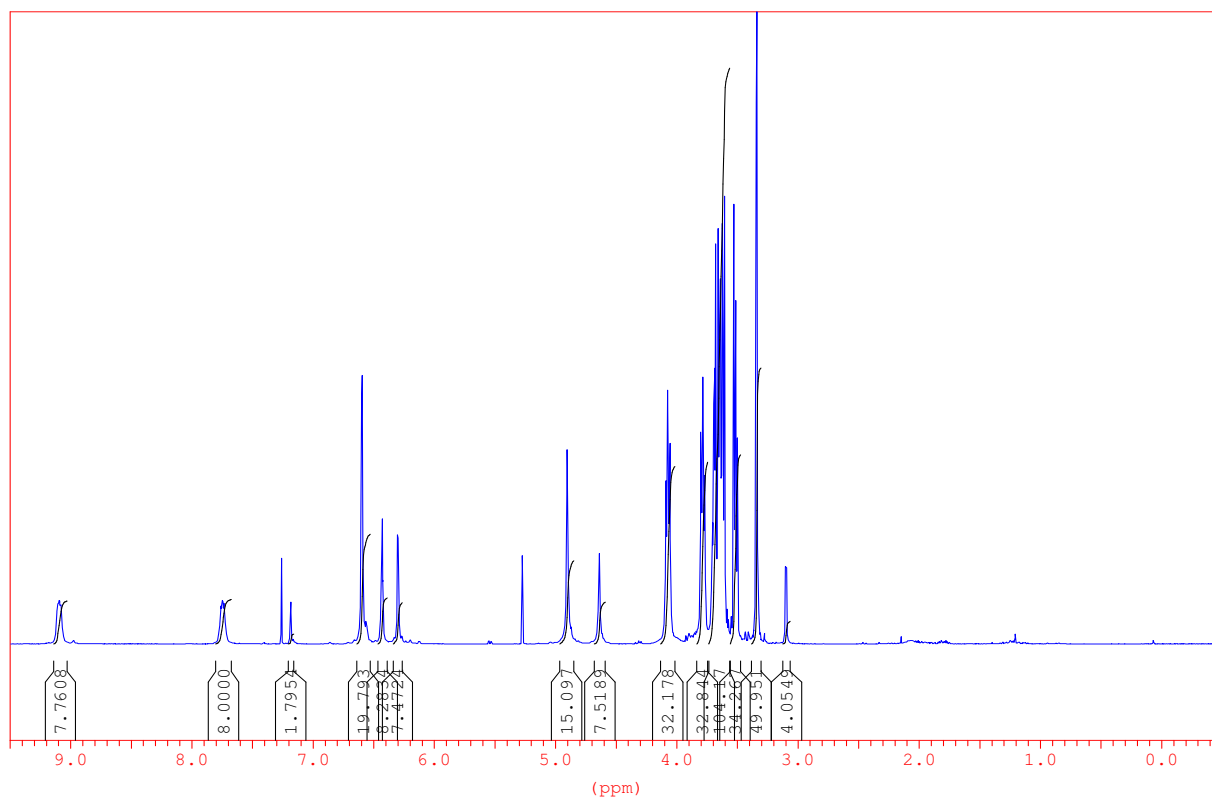


Figure S5. ^1H NMR spectrum of RuP2 recorded in CDCl_3 .

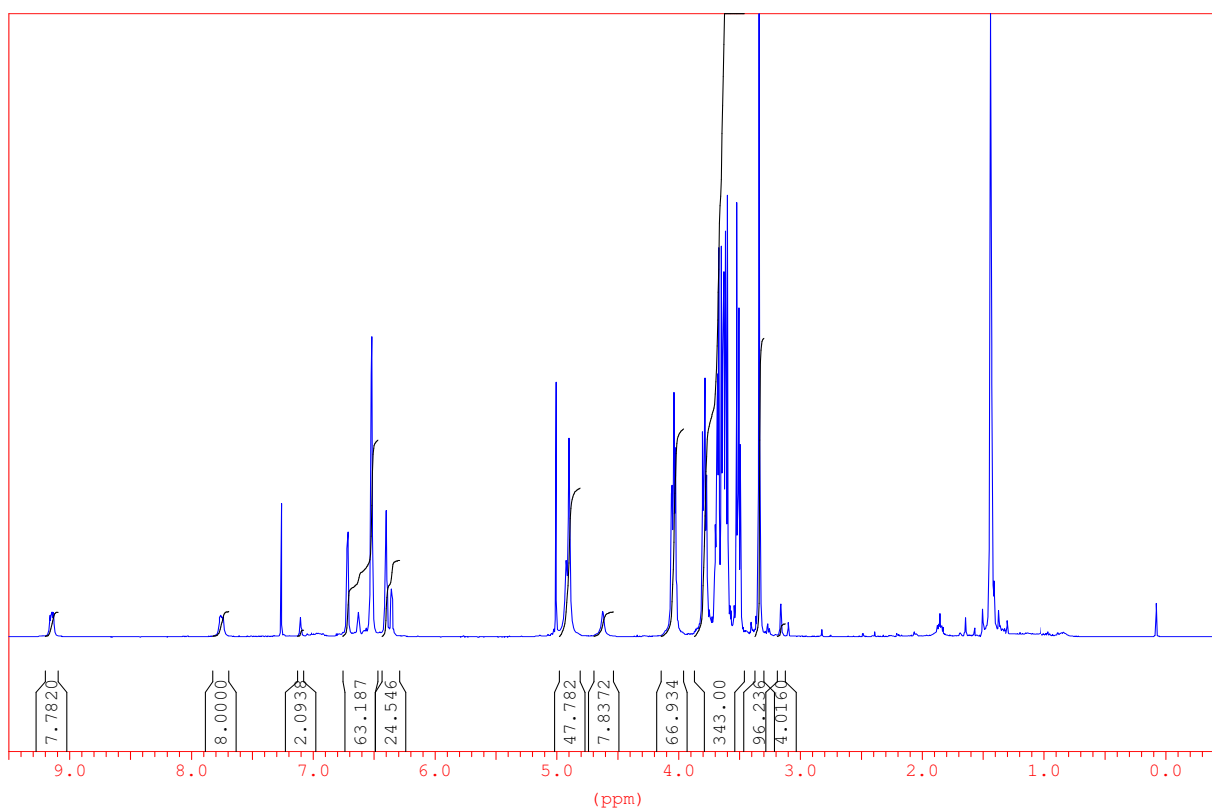


Figure S7. ^1H NMR spectrum of RuP3 recorded in CDCl_3 .

Part III. Phosphorescence at 1140 nm of RuP1-3.

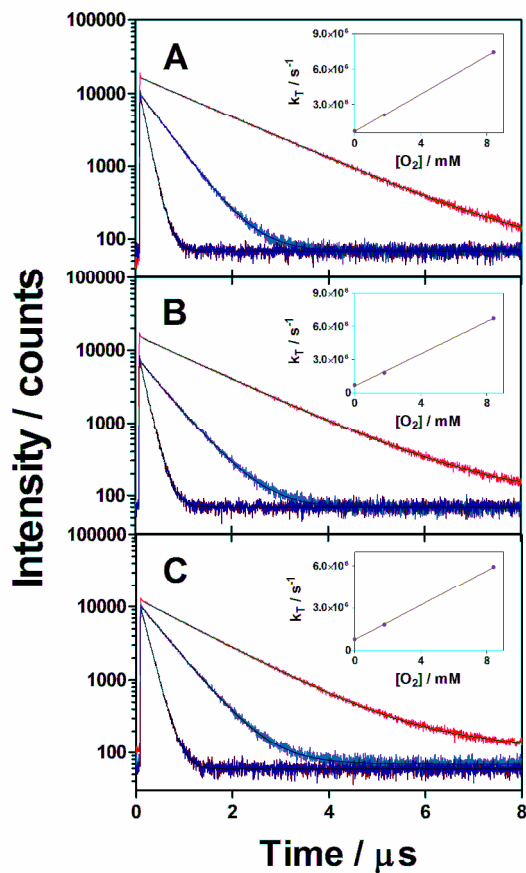


Figure S8. Time-resolved near-IR phosphorescence measurements at 1140 nm for (A) **RuP1**, (B) **RuP2**, and (C) **RuP3** in CHCl_3 , under argon-saturated atmosphere (red), air-saturated atmosphere (green), and oxygen-saturated atmosphere (blue). Insets: Oxygen concentration dependence of the triplet decay rate constant.

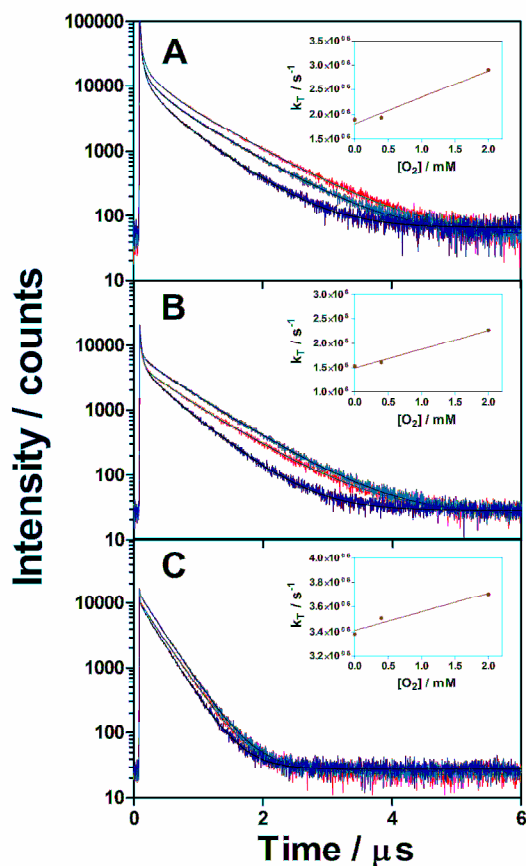


Figure S9. Time-resolved near-IR phosphorescence measurements at 1140 nm for (A) **RuP1**, (B) **RuP2**, and (C) **RuP3** in D₂O, under argon-saturated atmosphere (red), air-saturated atmosphere (green), and oxygen-saturated atmosphere (blue). Insets: Oxygen concentration dependence of the triplet decay rate constant.

Table S1. Triplet decay rate constant values ($k_T \times 10^{-5} / s^{-1}$) of **RuP1-3**.

Atmosphere	RuP1			RuP2			RuP3		
	CHCl ₃	THF	D ₂ O	CHCl ₃	THF	D ₂ O	CHCl ₃	THF	D ₂ O
Argon	6.62	6.99	18.9	6.99	7.25	15.3	7.93	10.8	33.8
Air	20.6	20.3	19.3	18.1	18.7	16.1	18.0	19.2	35.1
Oxygen	74.6	112	29.0	67.6	86.2	22.7	59.2	80.6	37.0

**Part IV. Singlet oxygen luminescence at 1270 nm of RuP1-3 in CHCl₃, THF
& D₂O.**

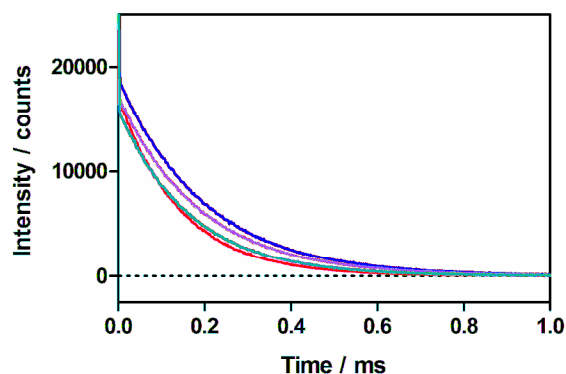


Figure S10. Time-resolved near-IR phosphorescence measurements at 1270 nm in CHCl₃ for TPP (red), **RuP1** (blue), **RuP2** (violet), and **RuP3** (green).

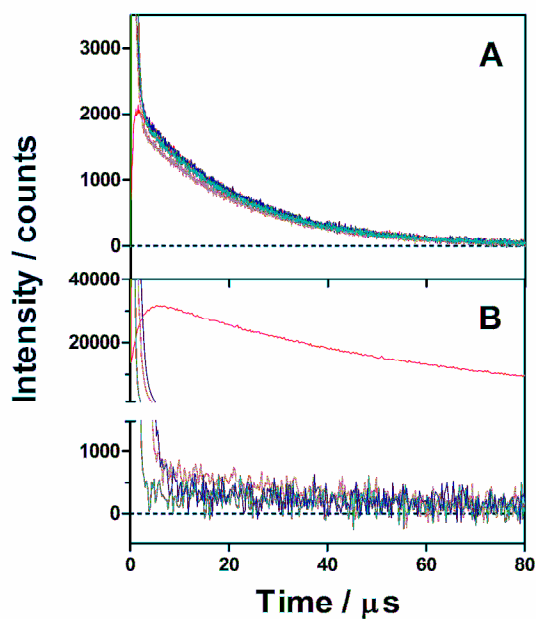


Figure S11. Time-resolved near-IR phosphorescence measurements at 1270 nm in (A) THF and (B) D₂O for the references (red; TPP in THF and TPPS in D₂O), **RuP1** (blue), **RuP2** (violet), and **RuP3** (green).