Supporting Information

Water-soluble Dinuclear Iridium(III) and Ruthenium(II) Bis-terdentate Complexes: Photophysics and Electrochemiluminescence

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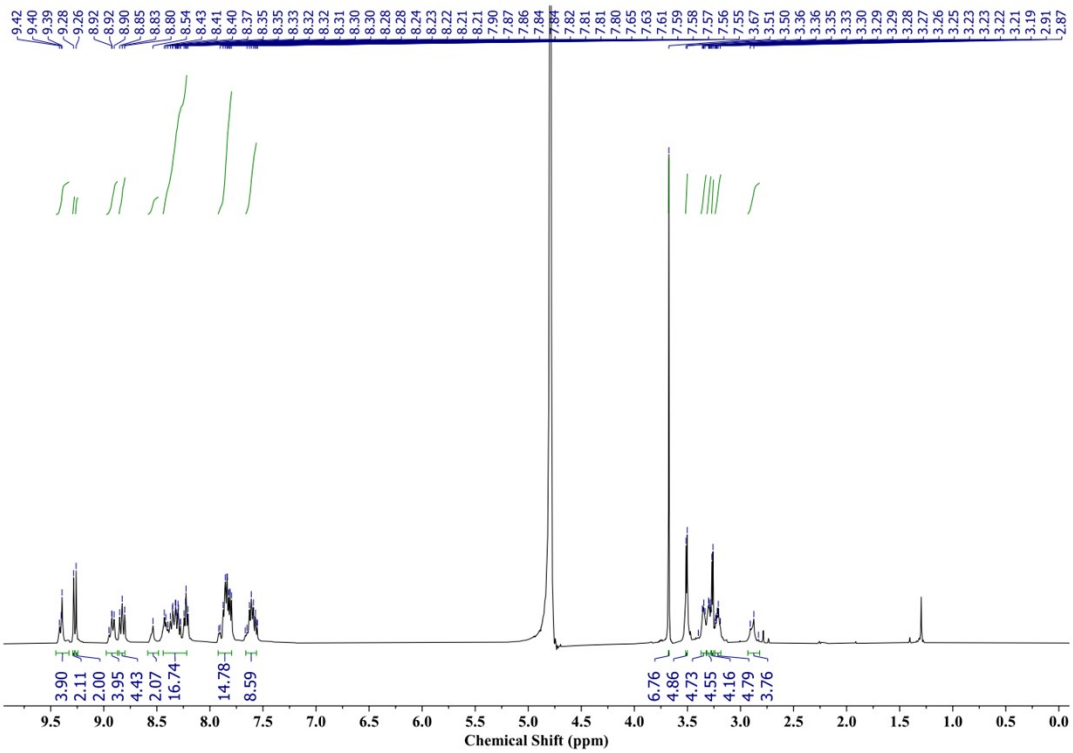


Figure S1. ^{1}H NMR spectrum of complex **1** in D_2O (400 MHz).

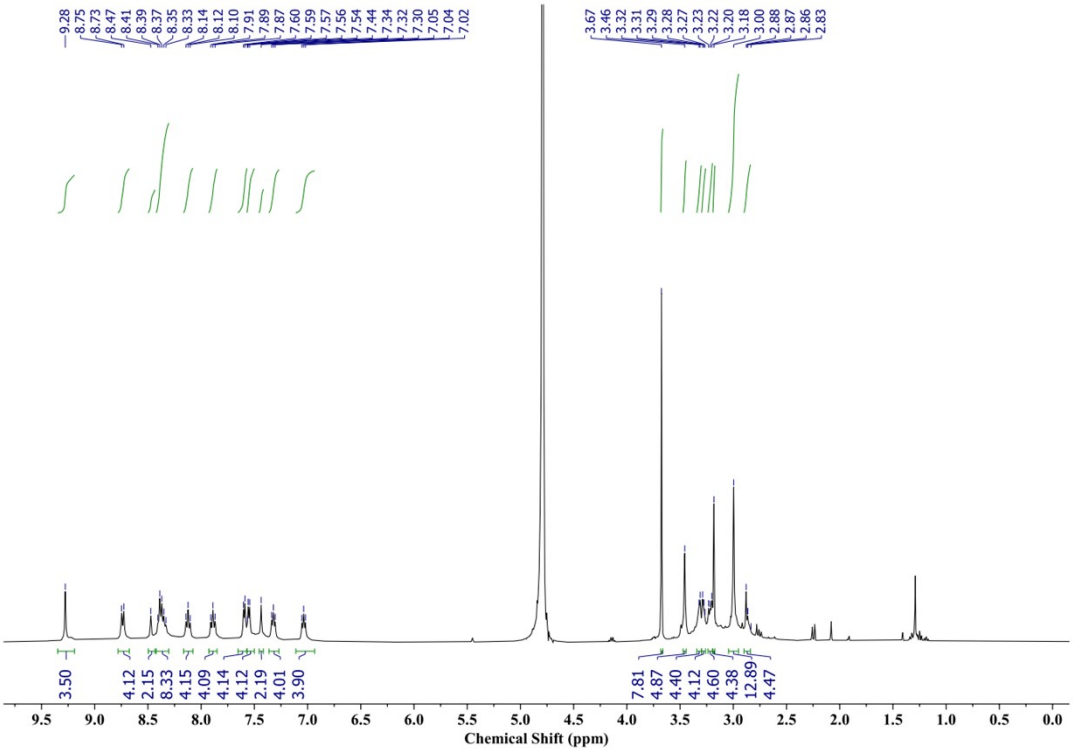


Figure S2. ^{1}H NMR spectrum of **2** in D_2O (400 MHz).

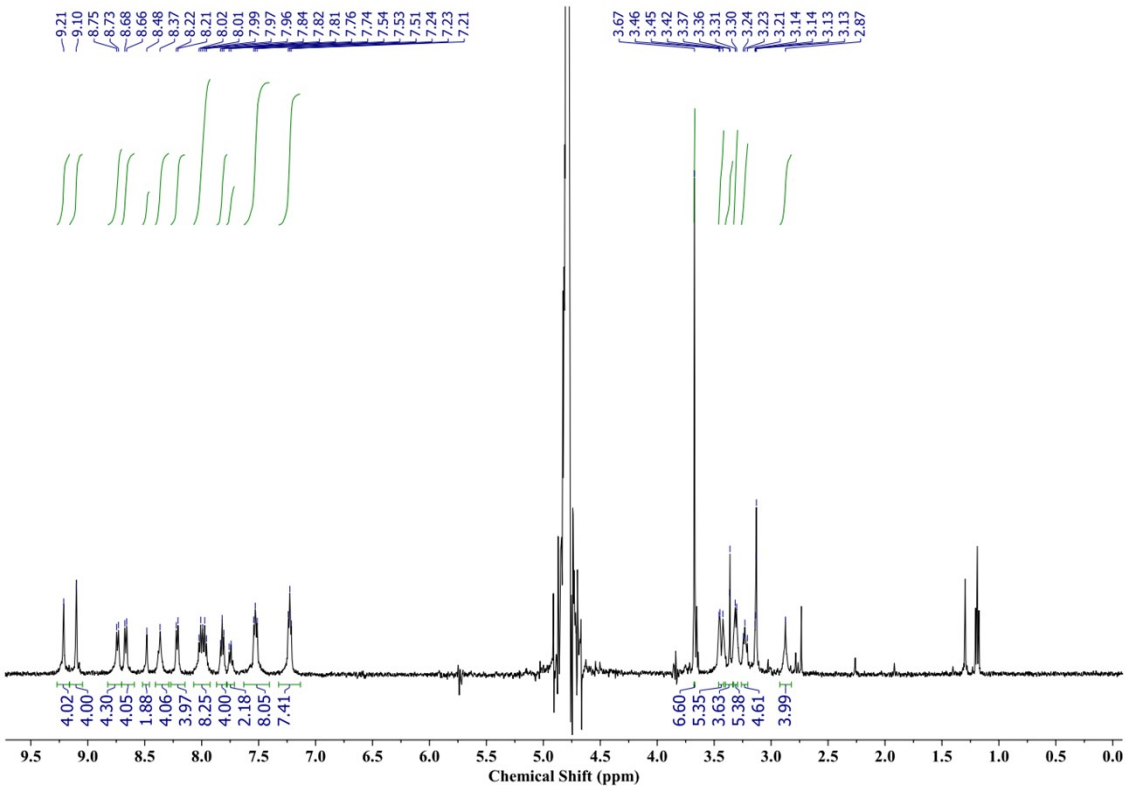


Figure S3. ^{1}H NMR spectrum of **3** in D_2O (500 MHz).

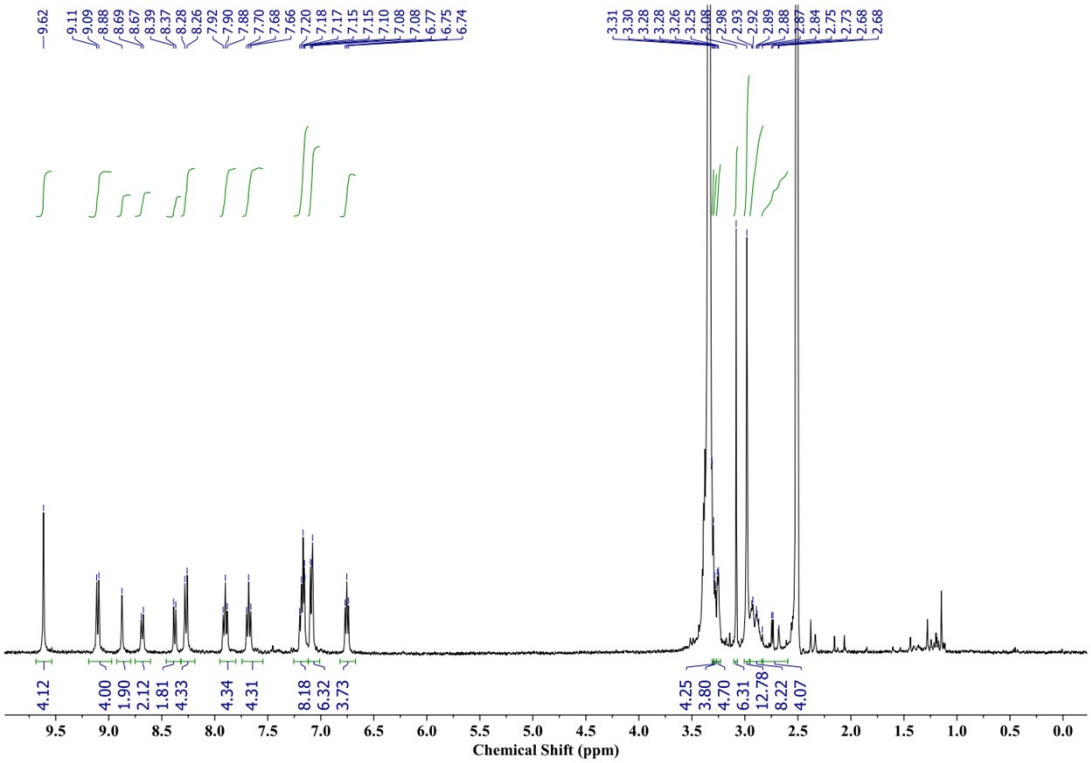


Figure S4. ^{1}H NMR spectrum of **4** in DMSO-d_6 (400 MHz).

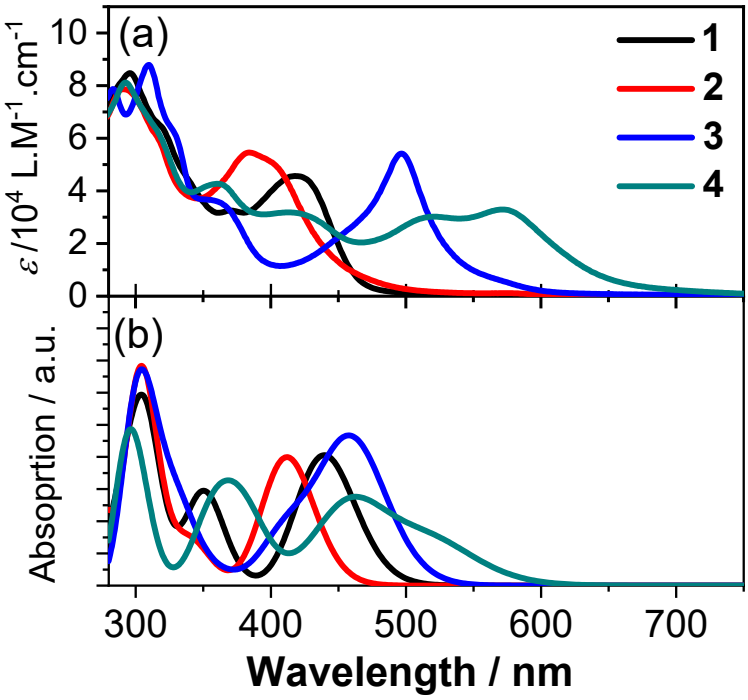


Fig. S5. (a) Experimental and (b) calculated absorption spectra of **1**-**4** in water. The two Ir(III) complexes **1** and **2** were calculated using PBE0 and the two Ru(II) complexes **3** and **4** were calculated using the B3LYP functional.

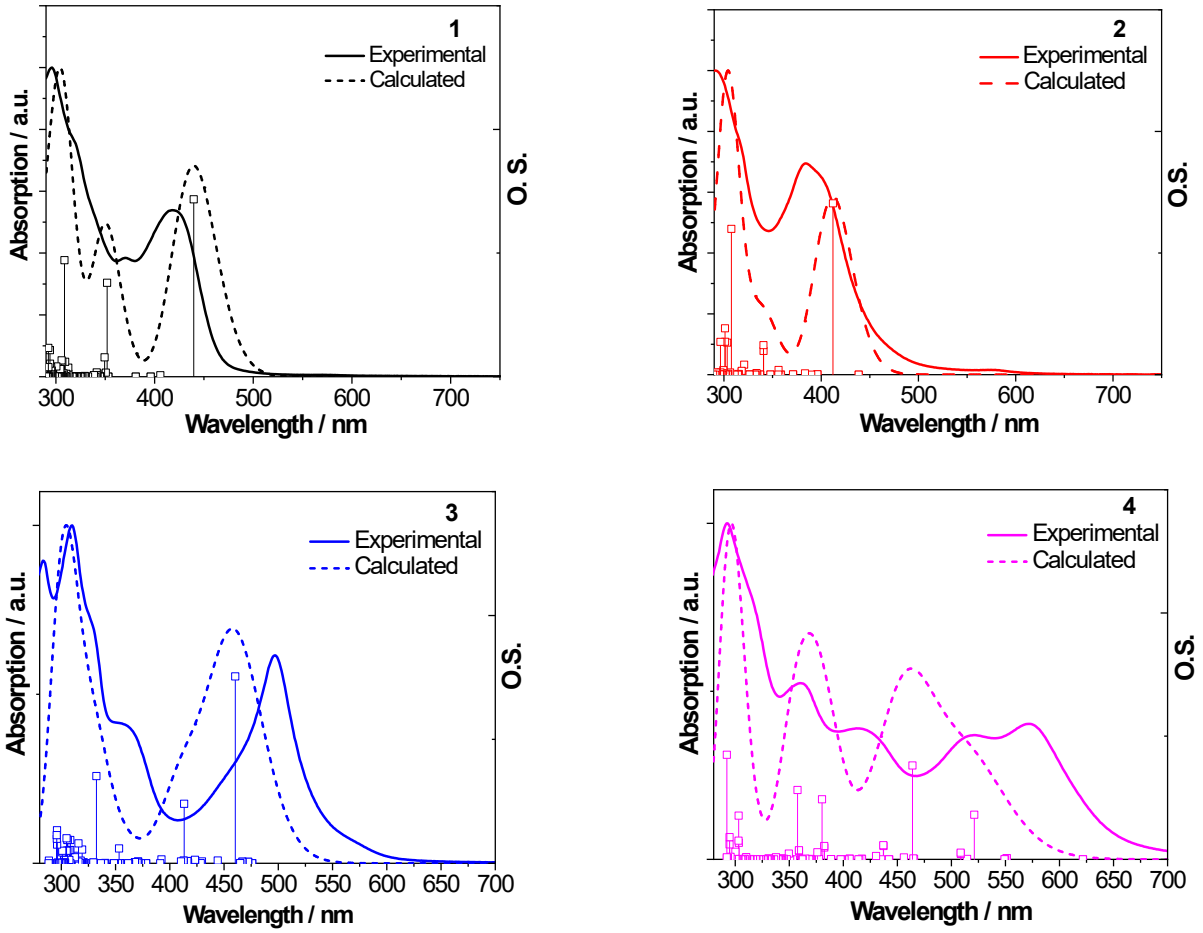


Fig. S6. Comparison of the normalized experimental and calculated absorption spectra for complexes **1**-**4** in water. **1** and **2** were calculated using the PBE0 functional and complexes **3** and **4** were calculated using the B3LYP functional.

Table S1. Natural transition orbitals of the high-energy transitions for complex **1**. The TDDFT calculations were conducted using PBE0 functional, LAN2dz/6-31G* basis set, and water as solvent.

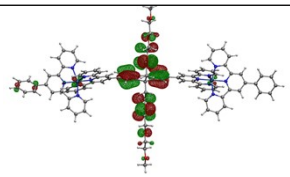
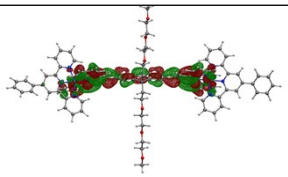
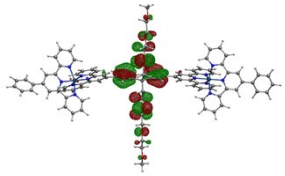
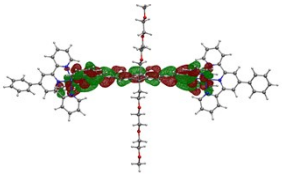
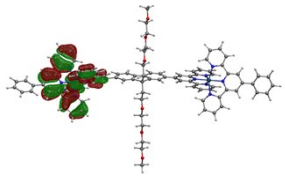
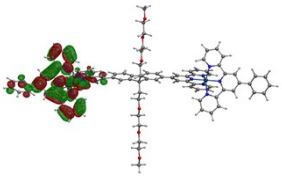
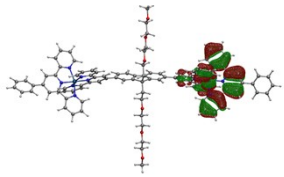
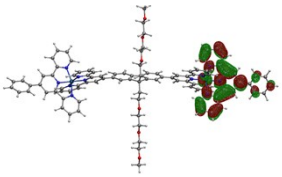
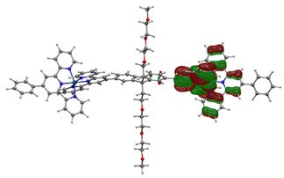
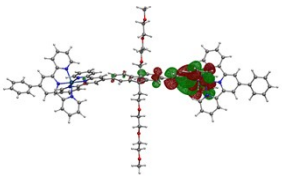
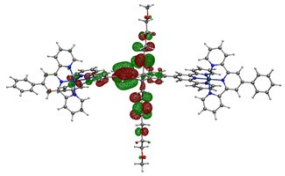
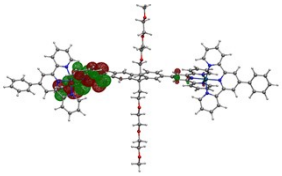
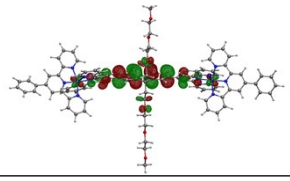
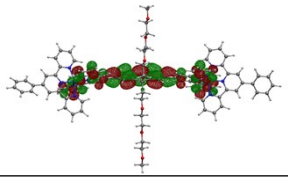
S_n and Properties	Hole	Electron
S_9 352 nm f = 0.759		
S_{11} 349 nm f = 0.156		
S_{14} 342 nm f = 0.022		
S_{15} 342 nm f = 0.027		
S_{16} 341 nm f = 0.035		
S_{41} 313 nm f = 0.023		
S_{49} 309 nm f = 0.942		

Table S2. Natural transition orbitals of the high-energy transitions for complex **2**. The TDDFT calculations were conducted using PBE0 functional, LAN2dz/6-31G* basis set, and water as solvent.

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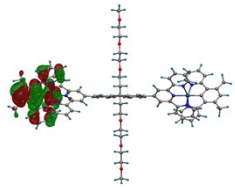
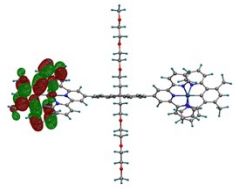
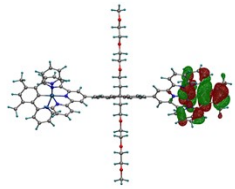
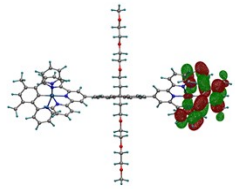
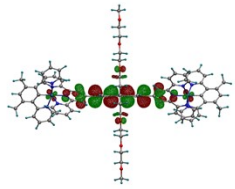
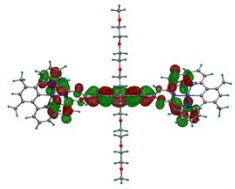
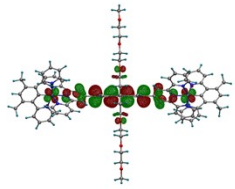
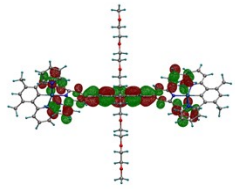
S_{17} 341 nm f = 0.194		
S_{18} 341 nm F = 0.243		
S_{36} 308 nm f = 1.199		
S_{40} 303 nm f = 0.263		

Table S3. Natural transition orbitals of the high-energy transitions for complex **3**. The TDDFT calculations were conducted using B3LYP functional, LAN2dz/6-31G* basis set, and water as solvent.

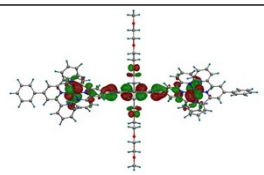
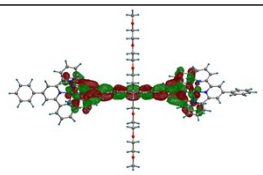
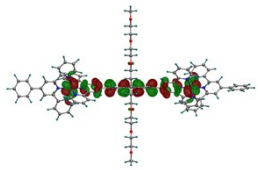
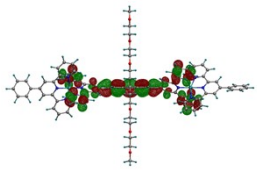
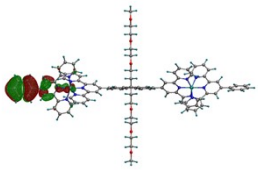
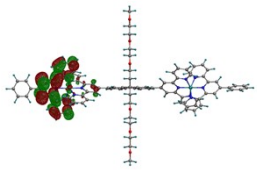
	Hole	Electron
S_{41} 353 nm f = 0.119		
S_{55} 332 nm f = 0.704		
S_{115} 296 nm f = 0.266		

Table S4. Natural transition orbitals of the high-energy transitions for complex **4**. The TDDFT calculations were conducted using B3LYP functional, LAN2dz/6-31G* basis set, and water as solvent.

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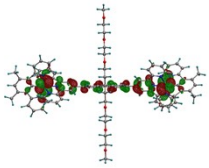
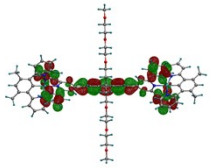
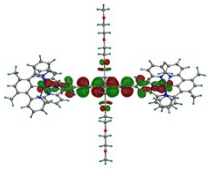
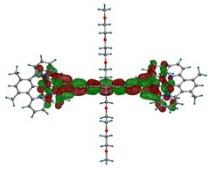
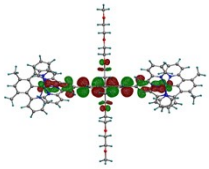
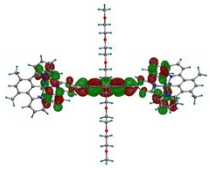
S_{39} 380 nm f = 0.488		
S_{53} 358 nm f = 0.563		
S_{129} 292 nm f = 0.849		

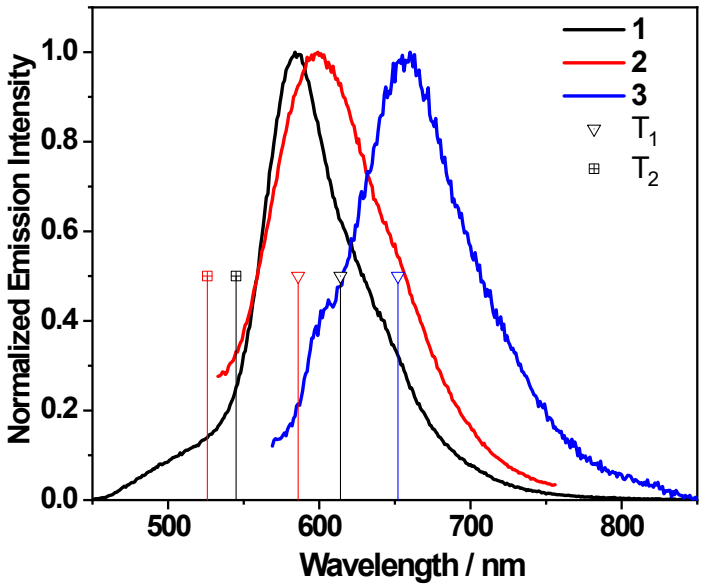


Fig. S7. Experimental emission spectra and calculated emission energies for complexes **1**-**3** in water. Emission energies are calculated by optimizing the triplet state (T_1) using analytical TDDFT method, the PBE0 functional, LAN2DZ/6-31G* basis sets and CPCM solvation method with water being used as a solvent. Bar heights are chosen randomly for a better representation.

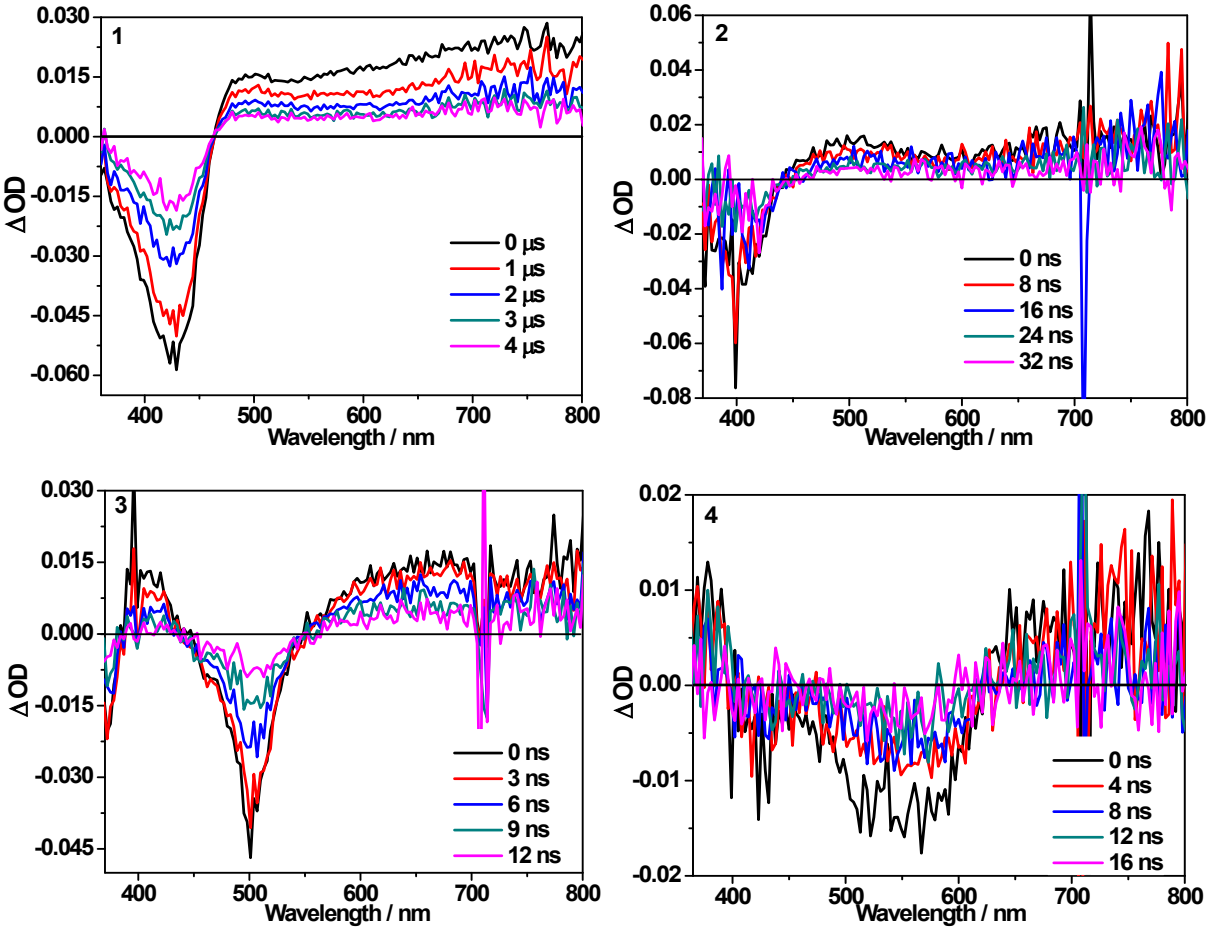


Fig. S8. Time-resolved ns-TA spectra of complexes **1**−**4** in acetonitrile at room temperature after 355 nm laser excitation. A_{355} = 0.4 in a 1 cm cuvette.