

Supporting Information

Synthesis and Photophysics of Reverse Saturable Absorbing Heteroleptic Iridium(III) Complexes Bearing 2-(7-R-Fluoren-2'-yl)pyridine Ligands

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Table S1. Optimized geometries of the singlet and triplet ground states of **1-3** in toluene.

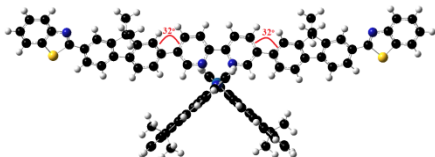
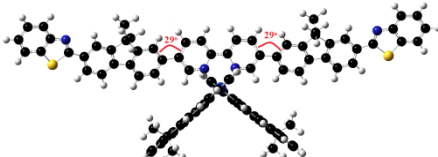
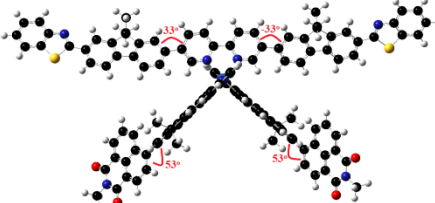
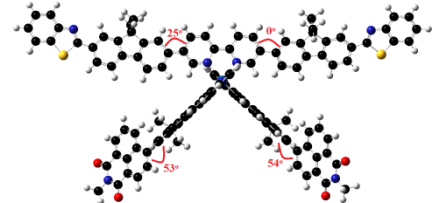
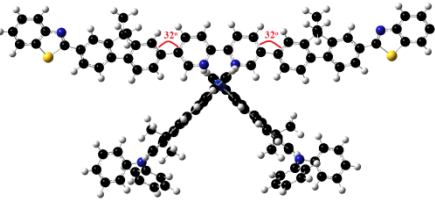
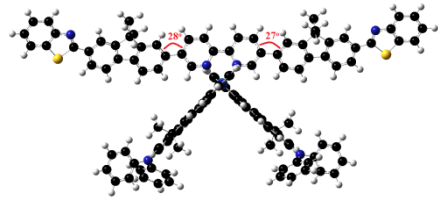
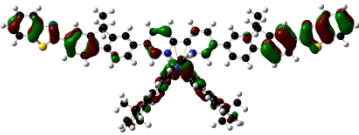
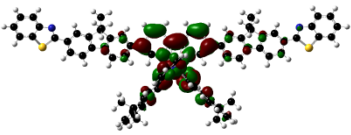
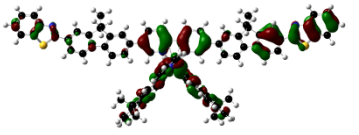
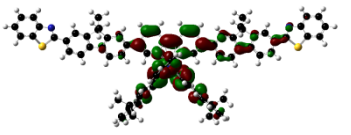
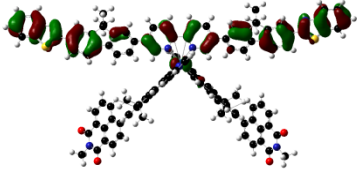
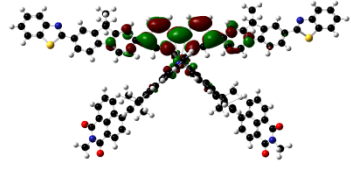
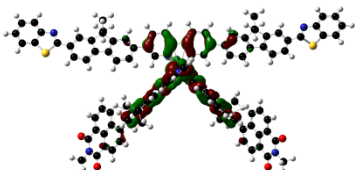
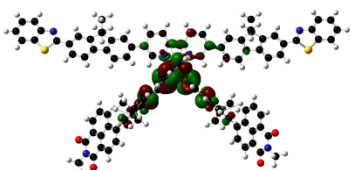
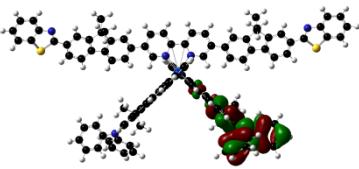
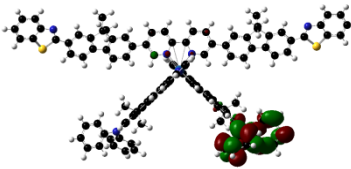
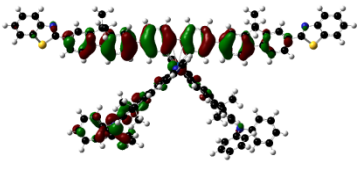
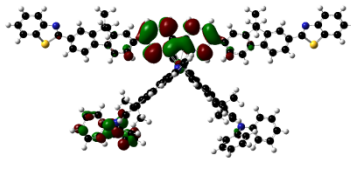
	Singlet	Triplet
1		
2		
3		

Table S2. Natural transition orbitals (NTOs) representing transitions contributing to the high-energy absorption bands of **1-3** in toluene.

Excited state and properties		Holes	Electrons
1	28 th excited state		
	264 nm $f=0.30$		
2	33 rd excited state		
	265 nm $f=0.37$		
3	30 th excited state		
	273 nm $f=0.35$		

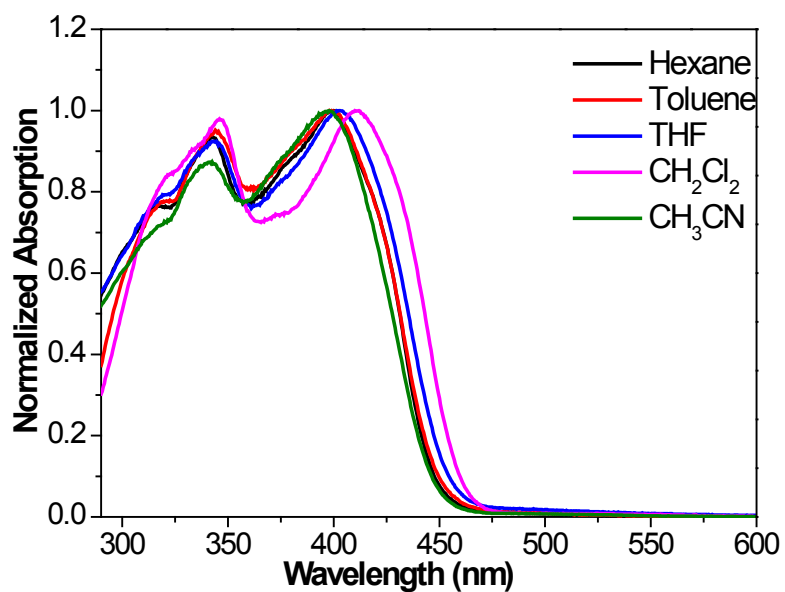


Figure S1. Normalized UV-vis absorption spectra of **1** in different solvents.

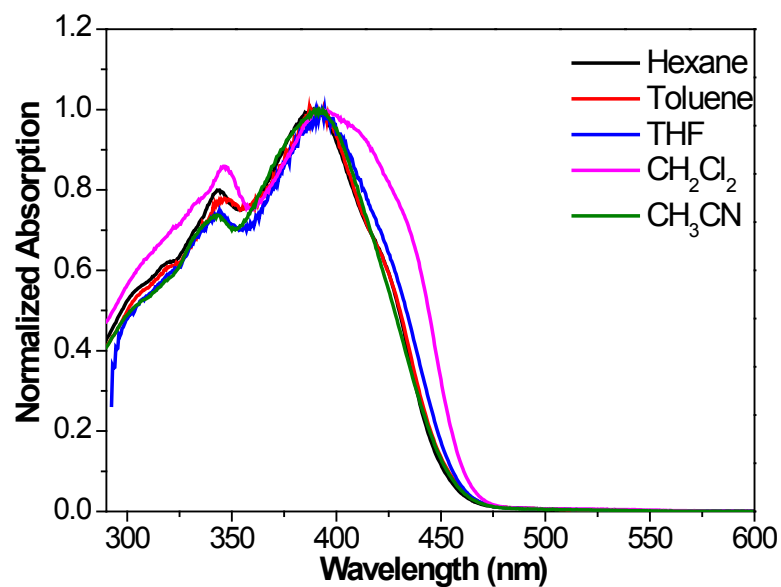


Figure S2. Normalized UV-vis absorption spectra of **2** in different solvents.

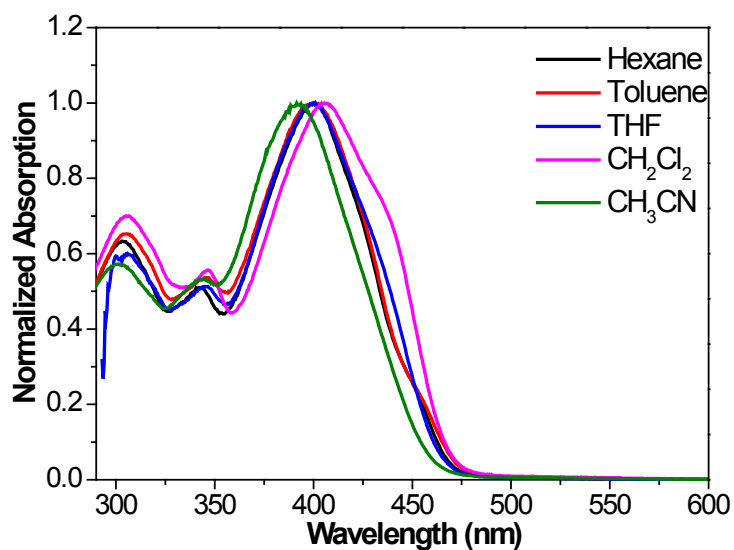


Figure S3. Normalized UV-vis absorption spectra of **3** in different solvents.

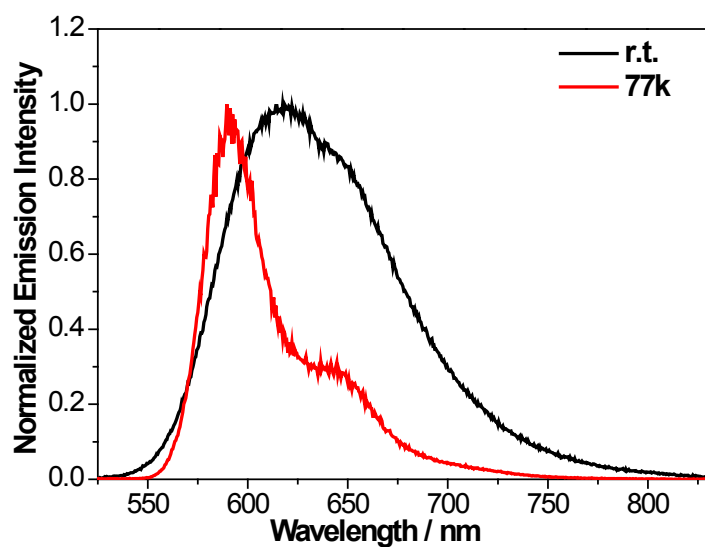


Figure S4. Normalized emission spectra of complex **2** ($\lambda_{\text{ex}} = 420$ nm) at r.t. and 77 K in BuCN.

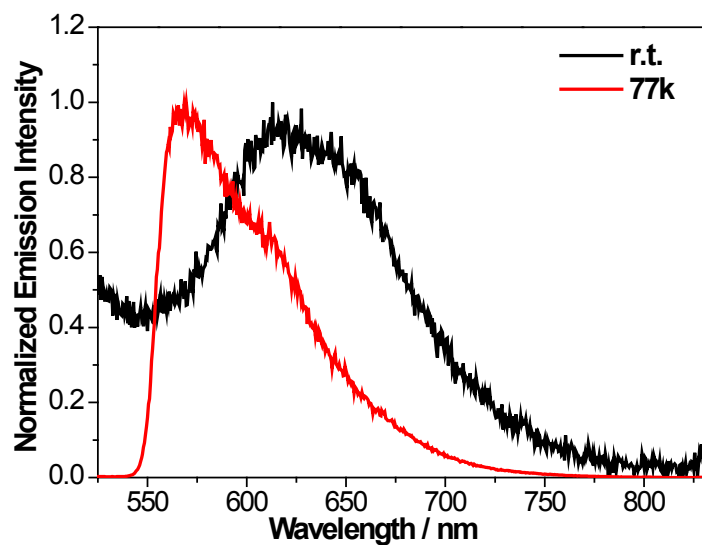


Figure S5. Normalized emission spectra of complex **3** ($\lambda_{\text{ex}} = 420$ nm) at r.t. and 77 K in BuCN.

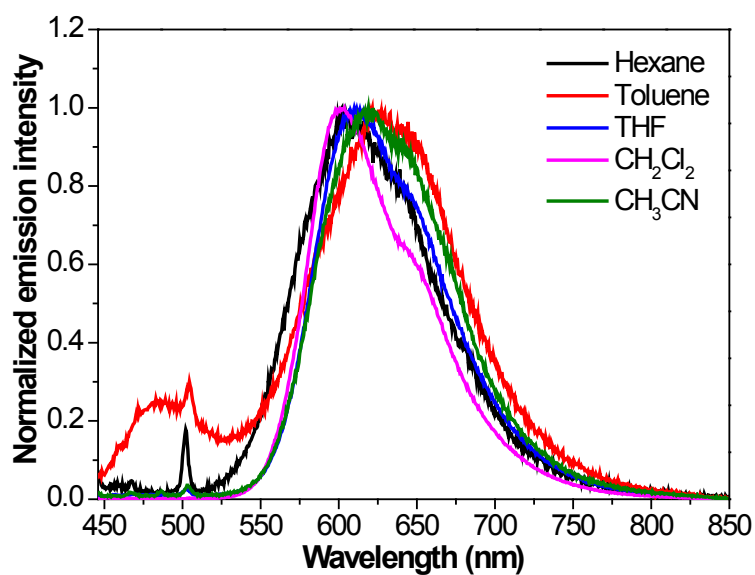


Figure S6. Normalized emission spectra of **2** in different solvents under an argon atmosphere ($\lambda_{\text{ex}} = 436$ nm).

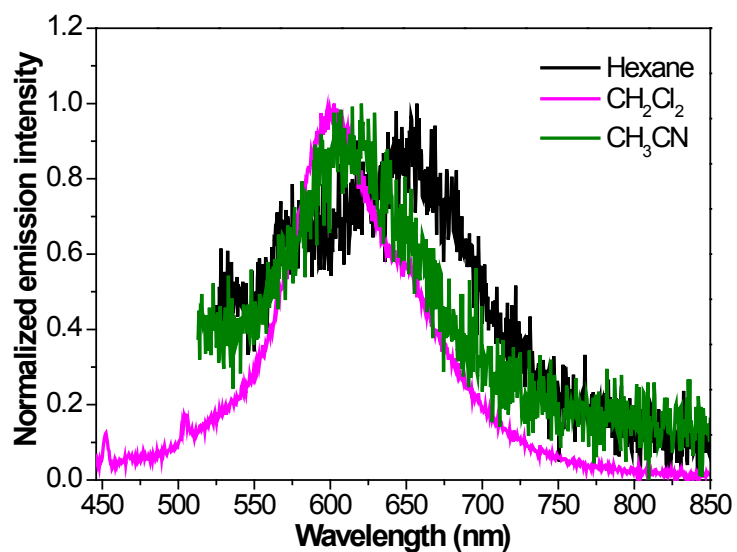


Figure S7. Normalized emission spectra of **3** in different solvents under an argon atmosphere ($\lambda_{\text{ex}} = 436 \text{ nm}$).

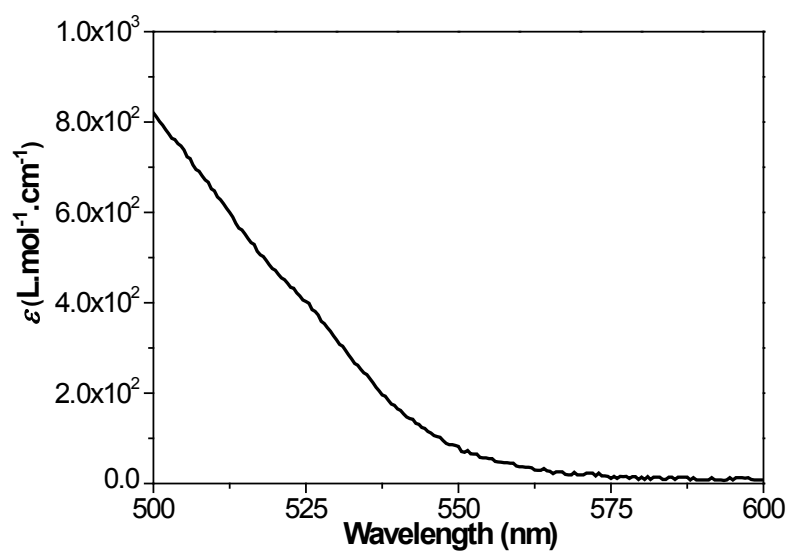


Figure S8. UV-vis absorption spectra of **1** in toluene solvent at 500-600 nm.

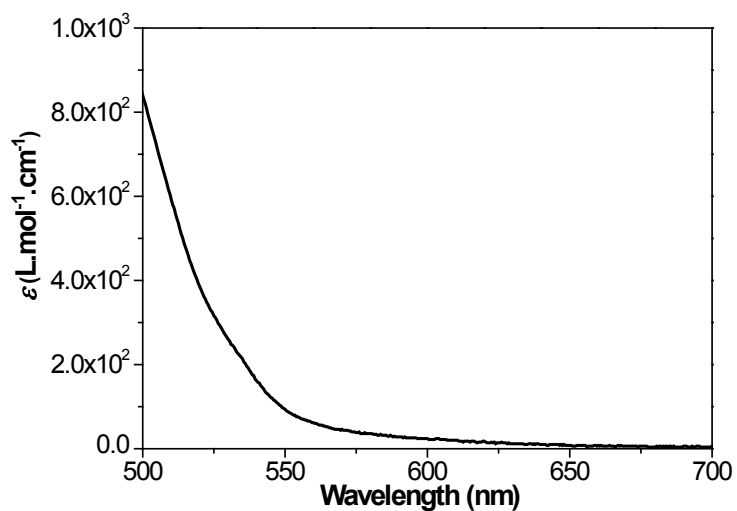


Figure S9. UV-vis absorption spectra of **2** in toluene at 500-700 nm.

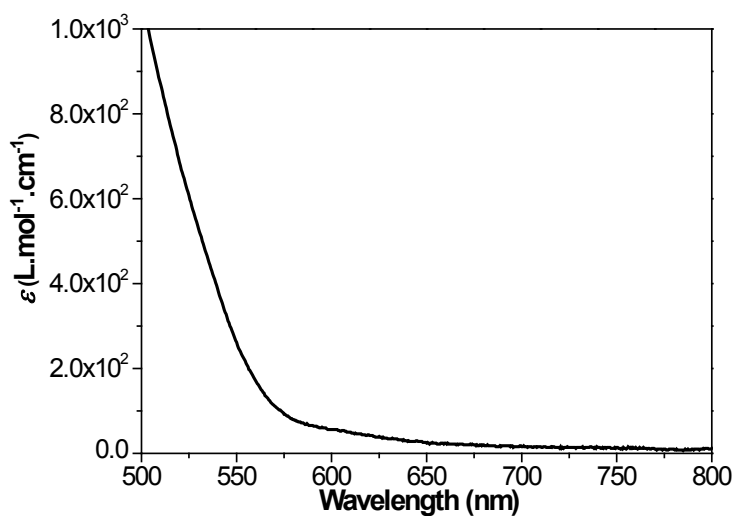


Figure S10. UV-vis absorption spectra of **3** in toluene at 500-800 nm