Electronic Supporting Information (ESI)

Synthesis, Characterization, and Photophysical Properties of Novel BODIPY and [Zn(dipyrrin)$_2$] Complexes from an Asymmetrical Dipyrromethene Ligand

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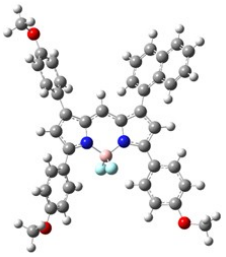
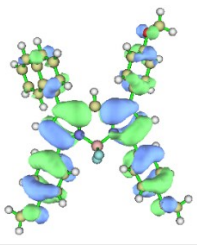
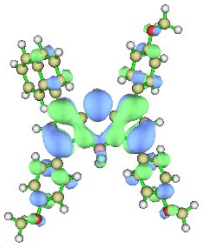
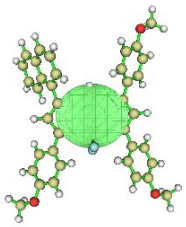
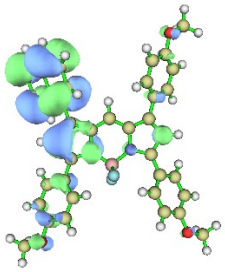
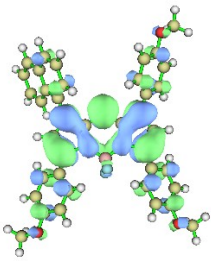
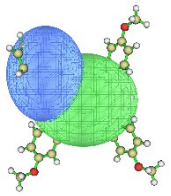
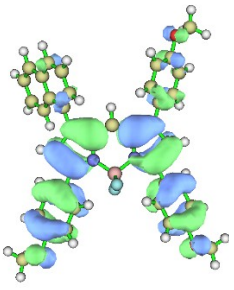
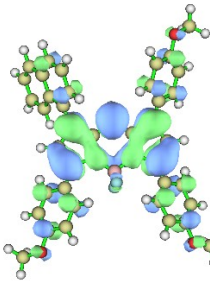
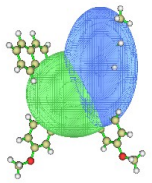
Table S1. Optimized structure**,** Natural transition orbitals (NTOs) for the singlet energy transitions (S_0-S_1, S_0-S_2, S_0-S_3) of the **NafmetBDP** (isosurface value = 0.02 au), centroids of hole and electron (C_{hole} & C_{ele}, isosurface value = 0.0003 au)

Comp.	Transition	Optimized structure	NTOs		C_{hole} & C_{ele}
			Electron	Hole	
NafmetBDP	Dipole moment (μ): 5.99 Debye				
	S_0-S_1 E_E :2.17 eV *t* (Å): -1.683 E_C: 3.66 eV				
	S_0-S_2 E_E : 2.53 eV *t* (Å): 1.775 E_C: 3.09 eV				
	S_0-S_3 E_E :2.65 eV *t* (Å): 1.235 E_C: 3.28 eV				

Blue and green isosurfaces represent C_{hole} and C_{ele} functions, respectively. E_E and *Ec represents the excitation energy and the Coulomb attractive energy, respectively.* The *t*-index quantifies the extent of separation between the hole and electron along the charge transfer direction.

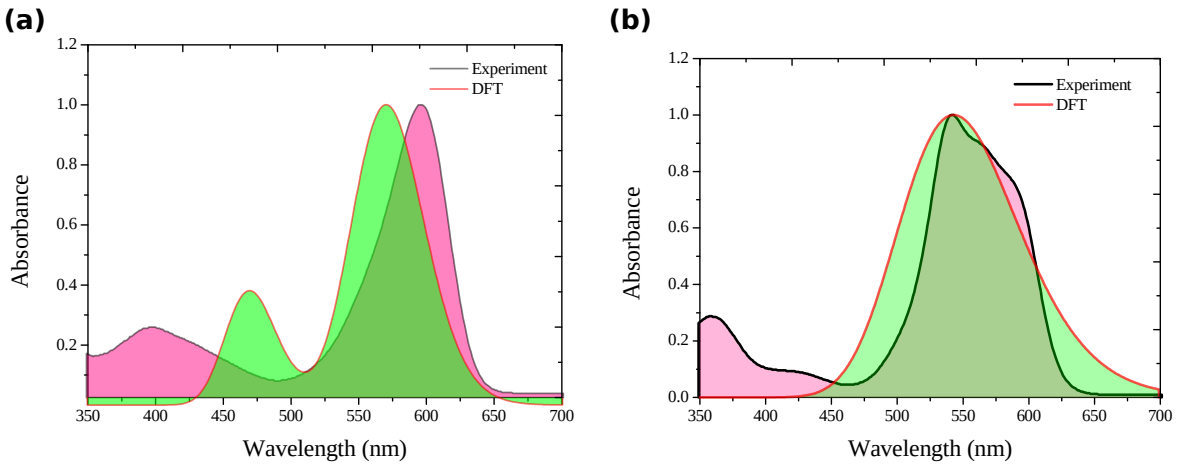


Figure S1. Comparison of experimental and theoretical normalized absorption spectra for the compounds: (a) **NafmetBDP** and (b) **NafmetZn**

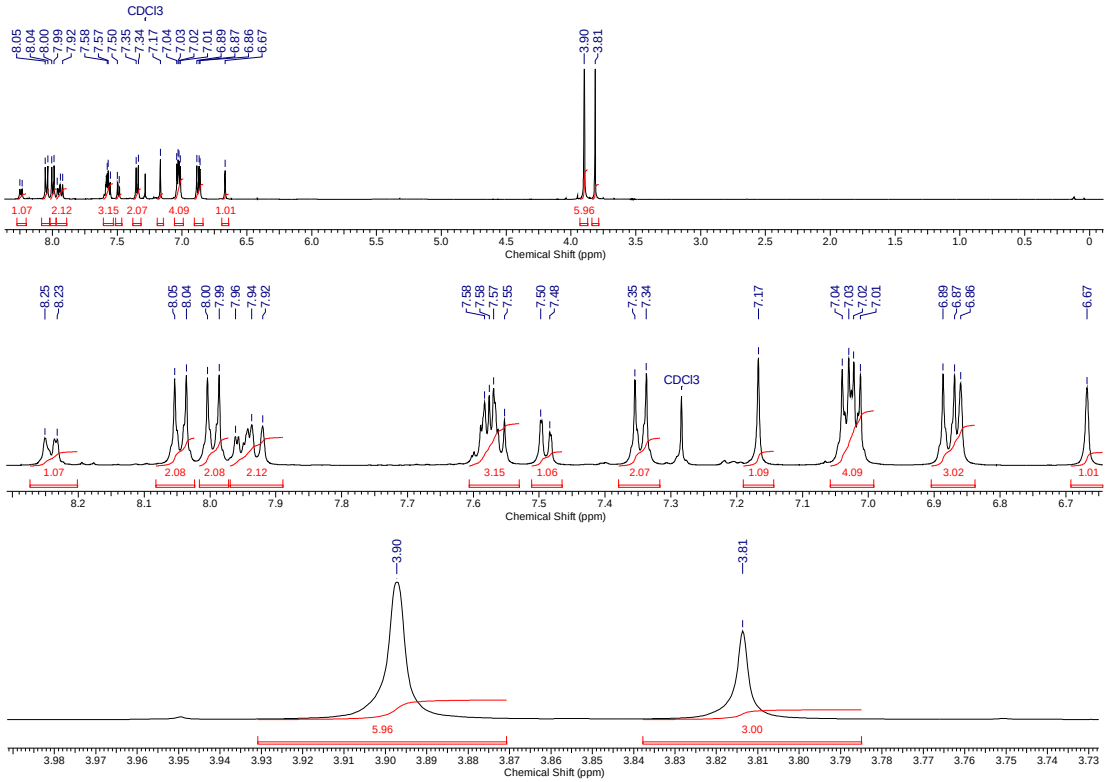


Figure S2. ^{1}H-NMR spectrum of **NafmetBDP** in $CDCl_3$ (500 MHz)

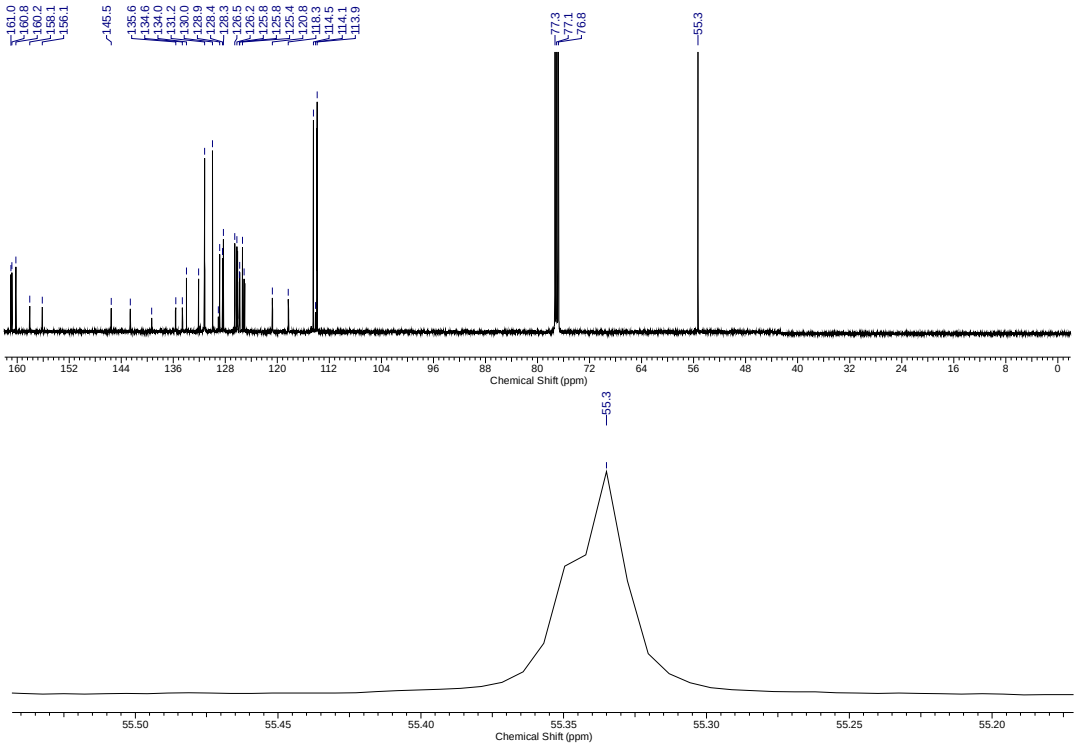


Figure S3. ^{13}C-NMR spectrum of **NafmetBDP** in $CDCl_3$ (125 MHz)

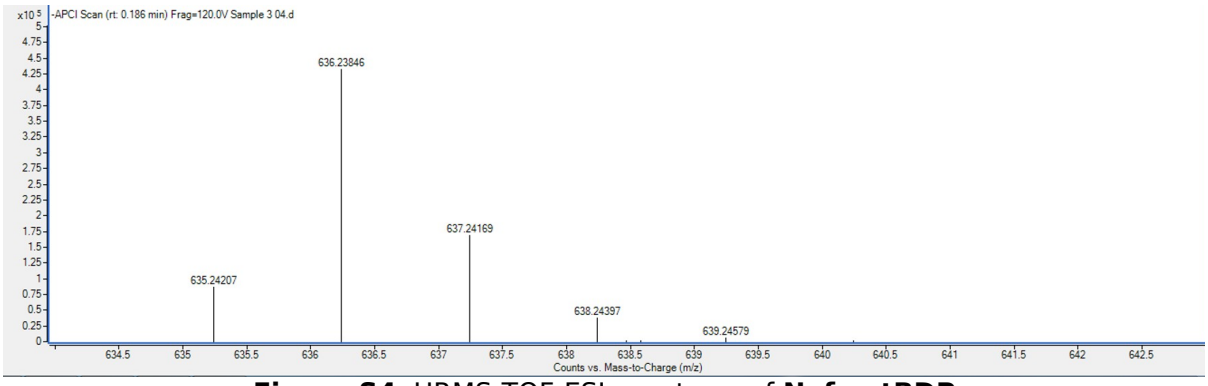


Figure S4. HRMS-TOF-ESI spectrum of **NafmetBDP**

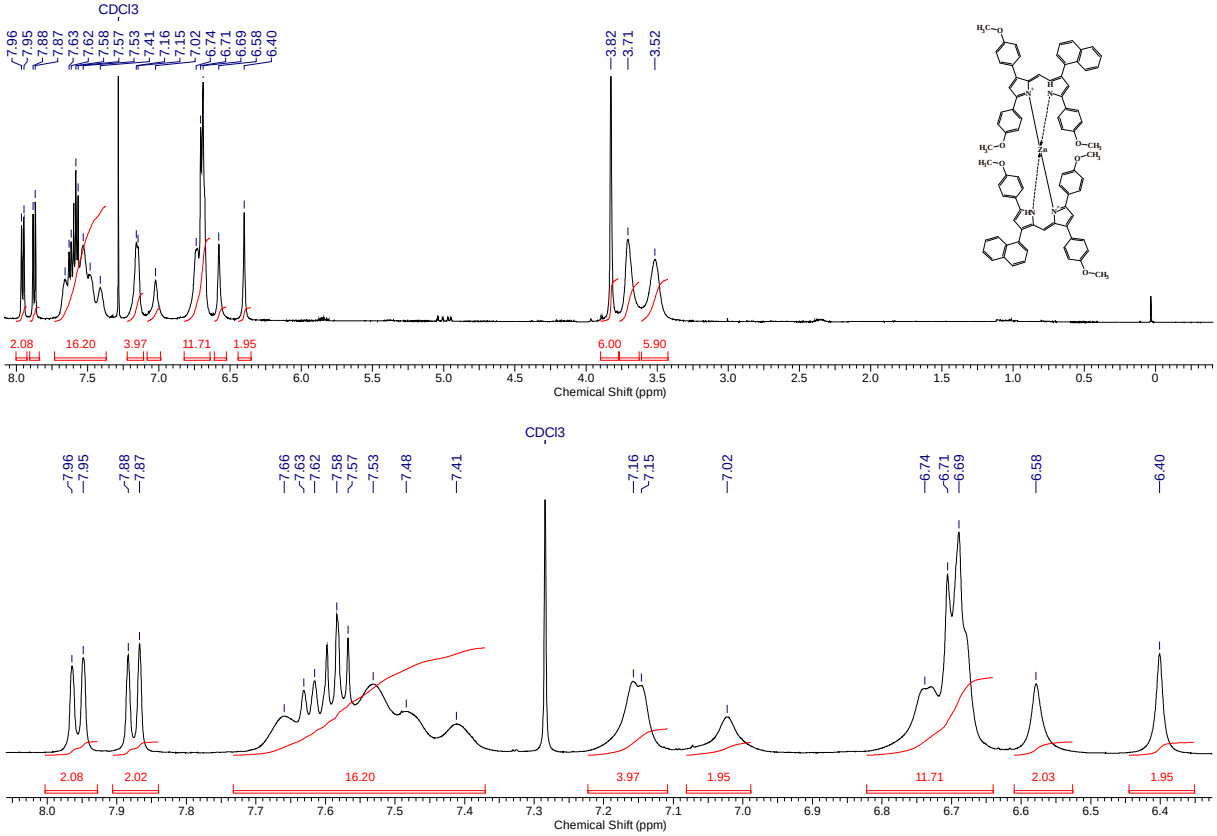


Figure S5. ^{1}H-NMR spectrum of **NafmetZn** in $CDCl_3$ (500 MHz)

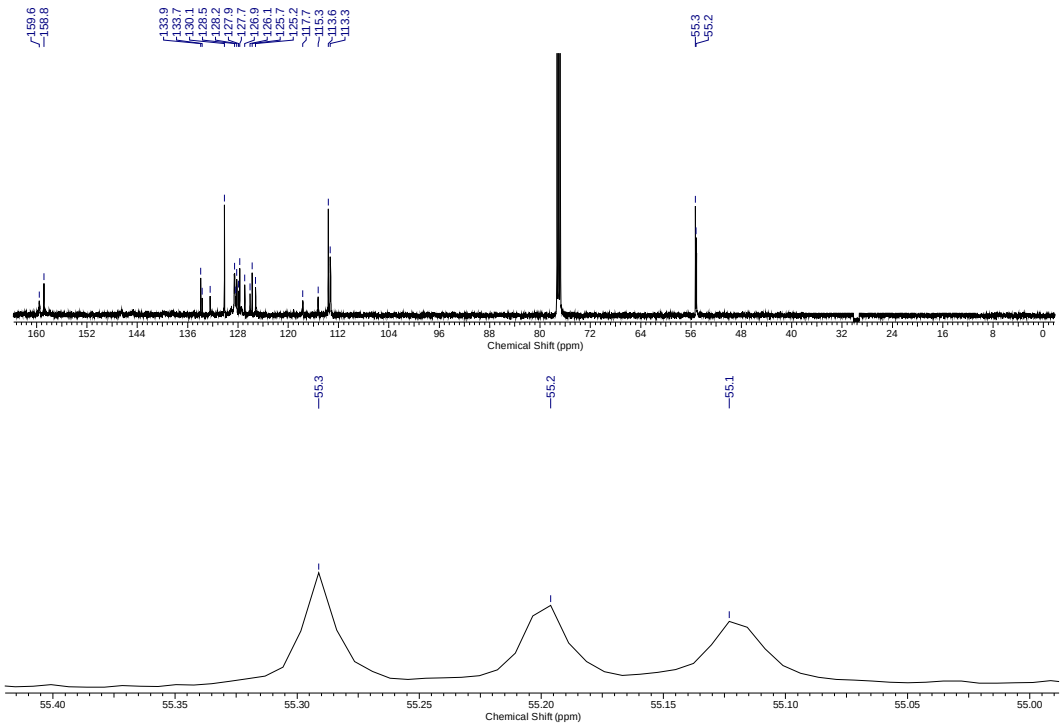


Figure S6. ^{13}C-NMR spectrum of **NafmetZn** in $CDCl_3$ (125 MHz)

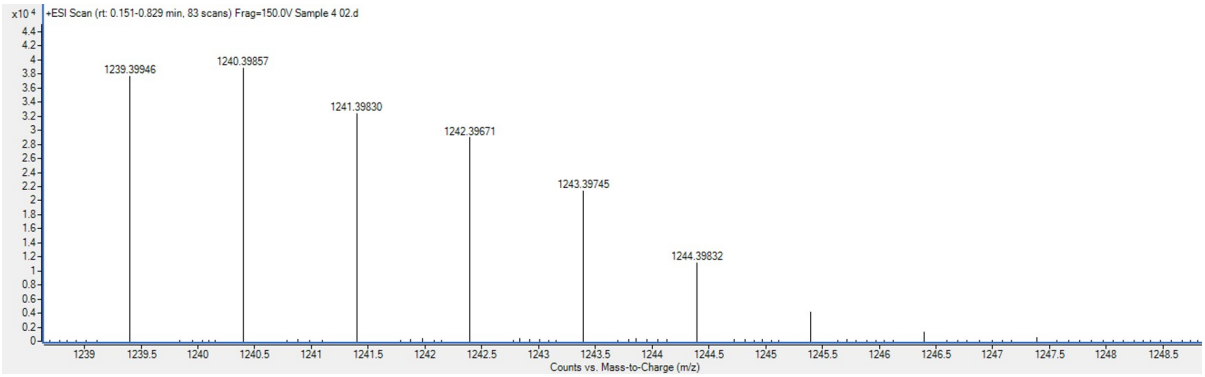


Figure S7. HRMS-TOF-ESI spectrum of **NafmetZn**