

Aggregation-induced emission enhancement (AIEE)-active boron-difluoride dyes with reversible mechanochromic fluorescence

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Table S1. Photophysical data of boron-difluoride dyes

Compound	solvent	λ_{max} , nm	ϵ , $\text{M}^{-1} \text{cm}^{-1}$ ($\times 10^4$)	λ_{em} , nm	Φ_{F}
PHPO-BF₂	hexane	490	0.202	546, 586	0.5%
	chloroform	496	0.318	564	1.3%
	THF	480	0.230	566	0.4%
	acetonitrile	491	0.209	568	0.5%
NHPO-BF₂	hexane	505	0.307	572, 616	0.3%
	chloroform	514	0.304	593	0.7%
	THF	496	0.330	590	0.6%
	acetonitrile	510	0.333	595	0.4%

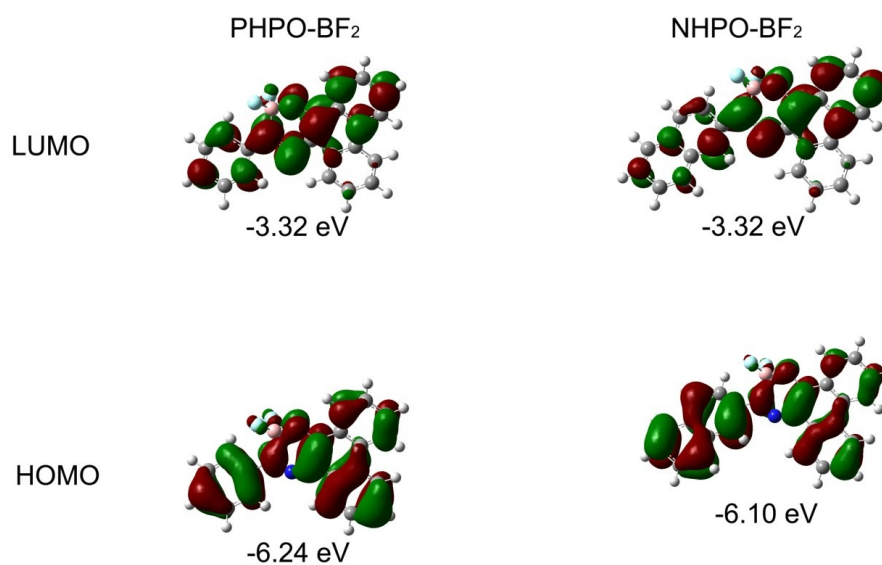


Figure S1. HOMO and LUMO orbitals of **PHPO-BF₂** and **NHPO-BF₂**

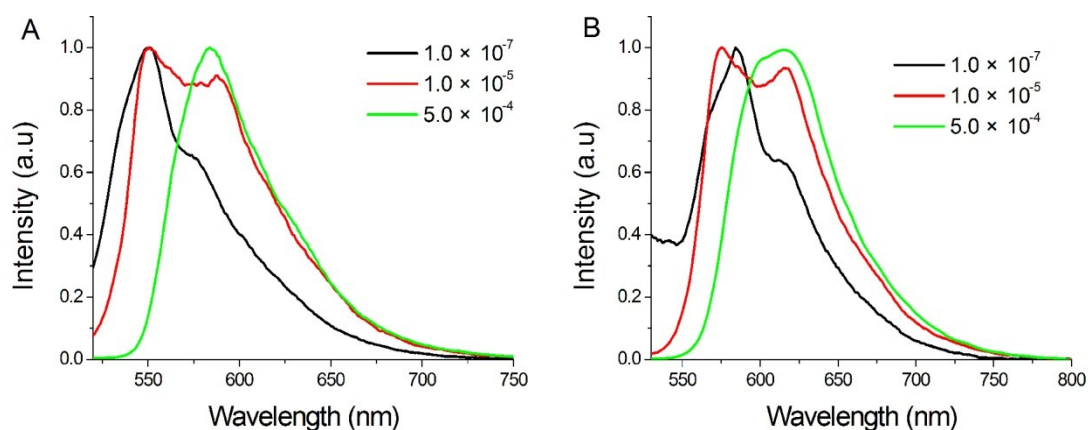


Figure S2. Normalized concentration-dependent fluorescence spectra of **PHPO-BF₂** (A) and **NHPO-BF₂** (B) in hexane

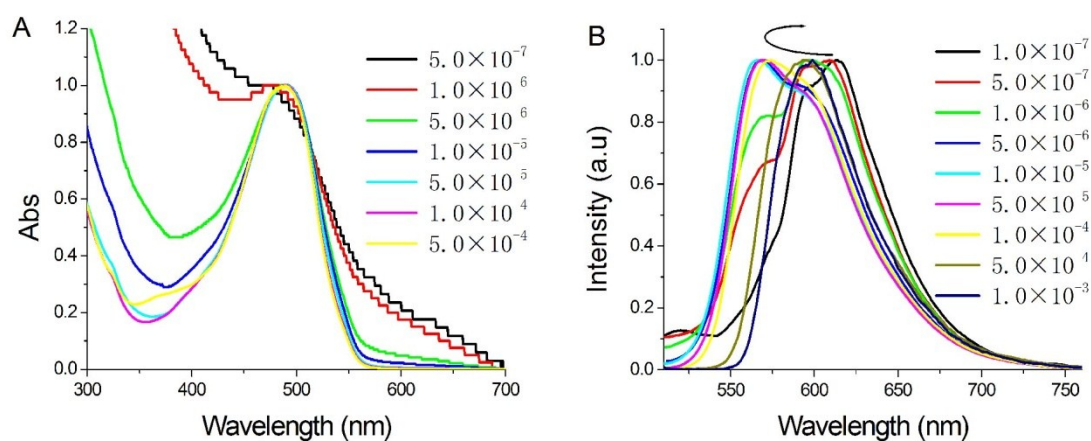


Figure S3. (A) Normalized concentration-dependent absorption and (B) fluorescence spectra of **PHPO-BF₂** in THF

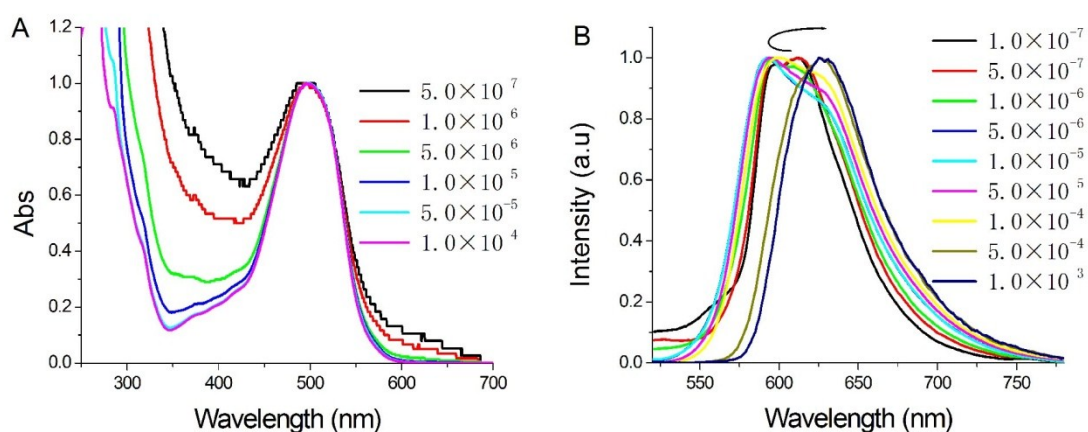


Figure S4. (A) Normalized concentration-dependent absorption and (B) fluorescence spectra of **NHPO-BF₂** in THF

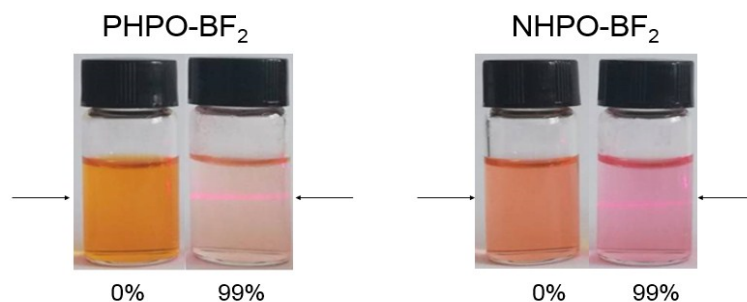


Figure S5. Tyndall effect: (1.0×10^{-5} M, the content of H_2O in THF/ H_2O is 0% or 99%)

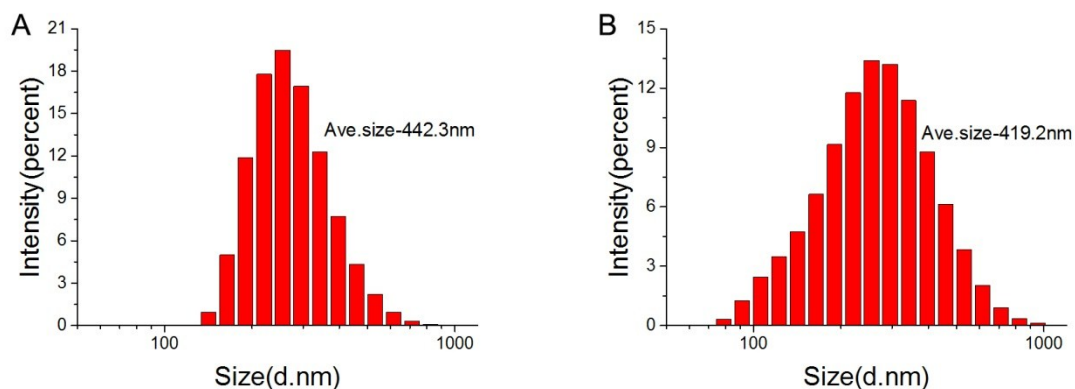


Figure S6. Particle size distribution of **PHPO-BF₂** aggregates from mixture of THF and water (A) THF/ H_2O (v/v 20:80); (B) THF/ H_2O (v/v 1:99)

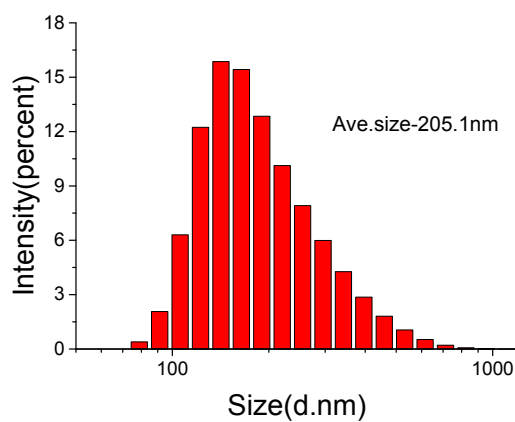


Figure S7. Particle size distribution of **NHPO-BF₂** aggregates from mixture of THF and water (THF/ H_2O , v/v 1:99)

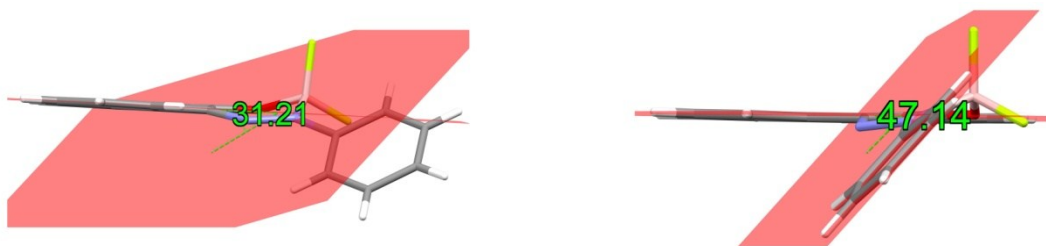


Figure S8. Dihedral angle between different planes in the crystal structure of **PHPO-BF₂**

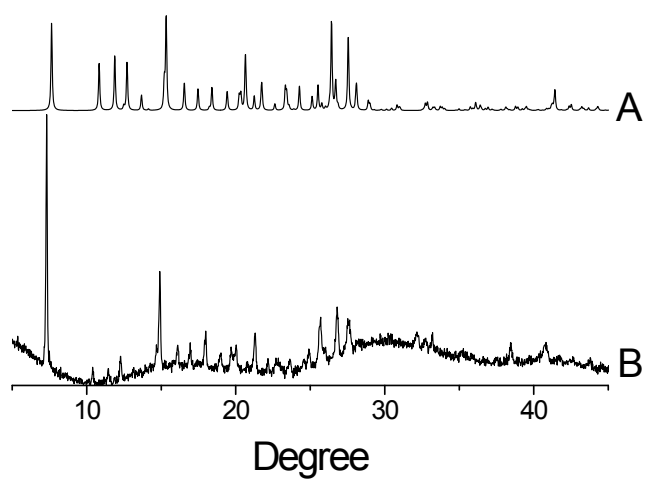


Figure S9. XRD patterns of **PHPO-BF₂** (A) simulated spectra from single crystal structure; (B) initial polycrystalline powder

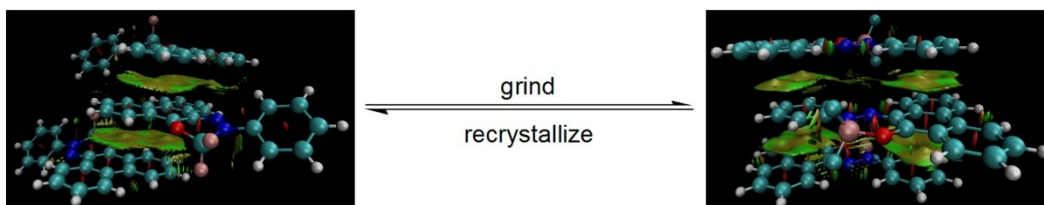


Figure S10. Proposed intermolecular interactions in molecular clusters of **PHPO-BF₂** during the mechanochromism (shown as green cloud)

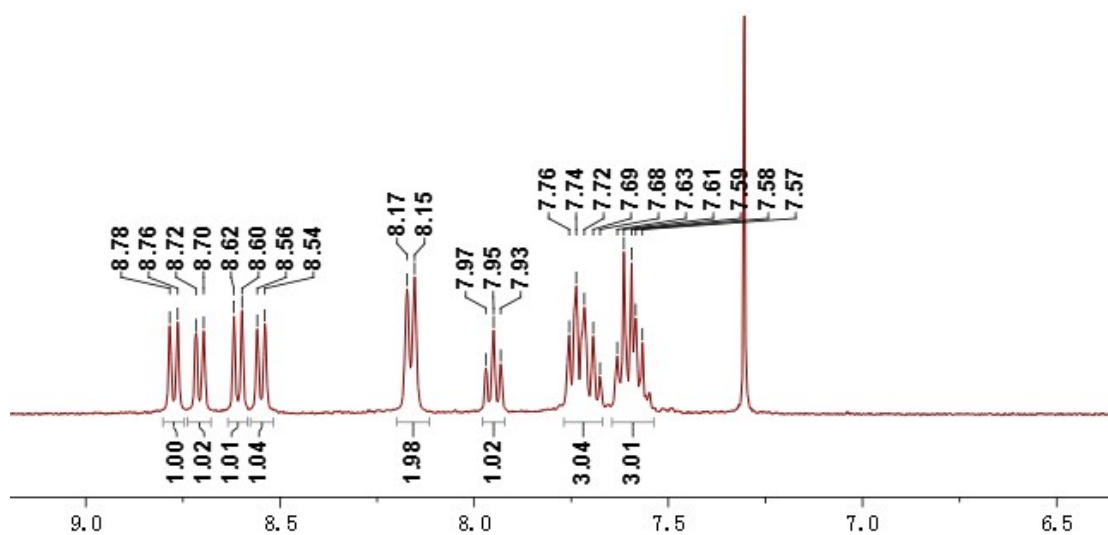


Figure S11. ¹H NMR spectrum of PHPO-BF₂ (400 MHz, CDCl₃)

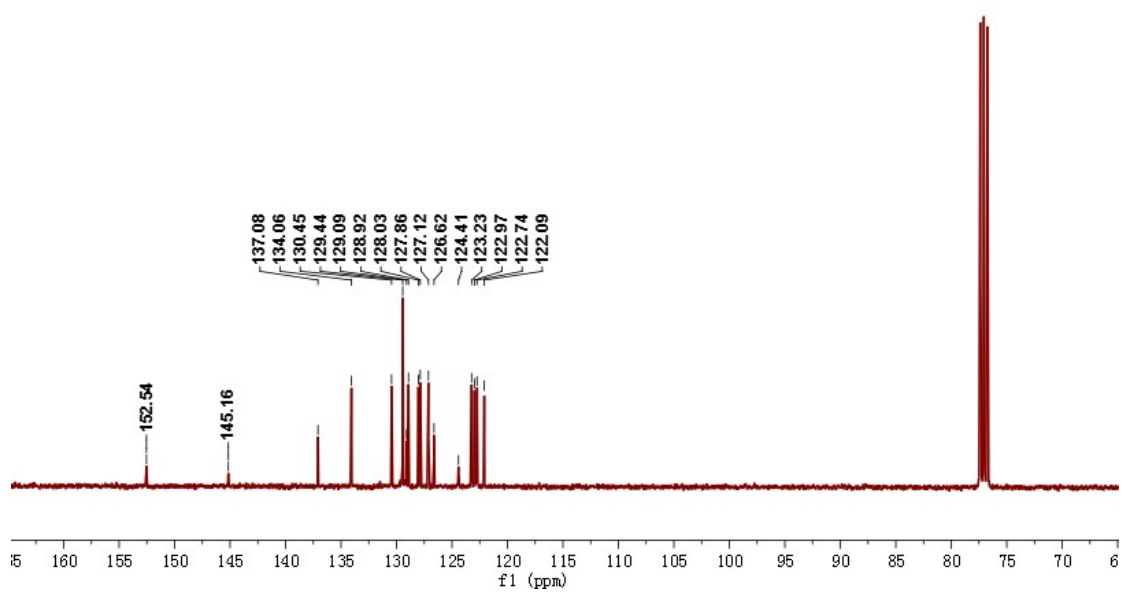


Figure S12. ¹³C NMR spectrum of PHPO-BF₂ (101 MHz, CDCl₃)

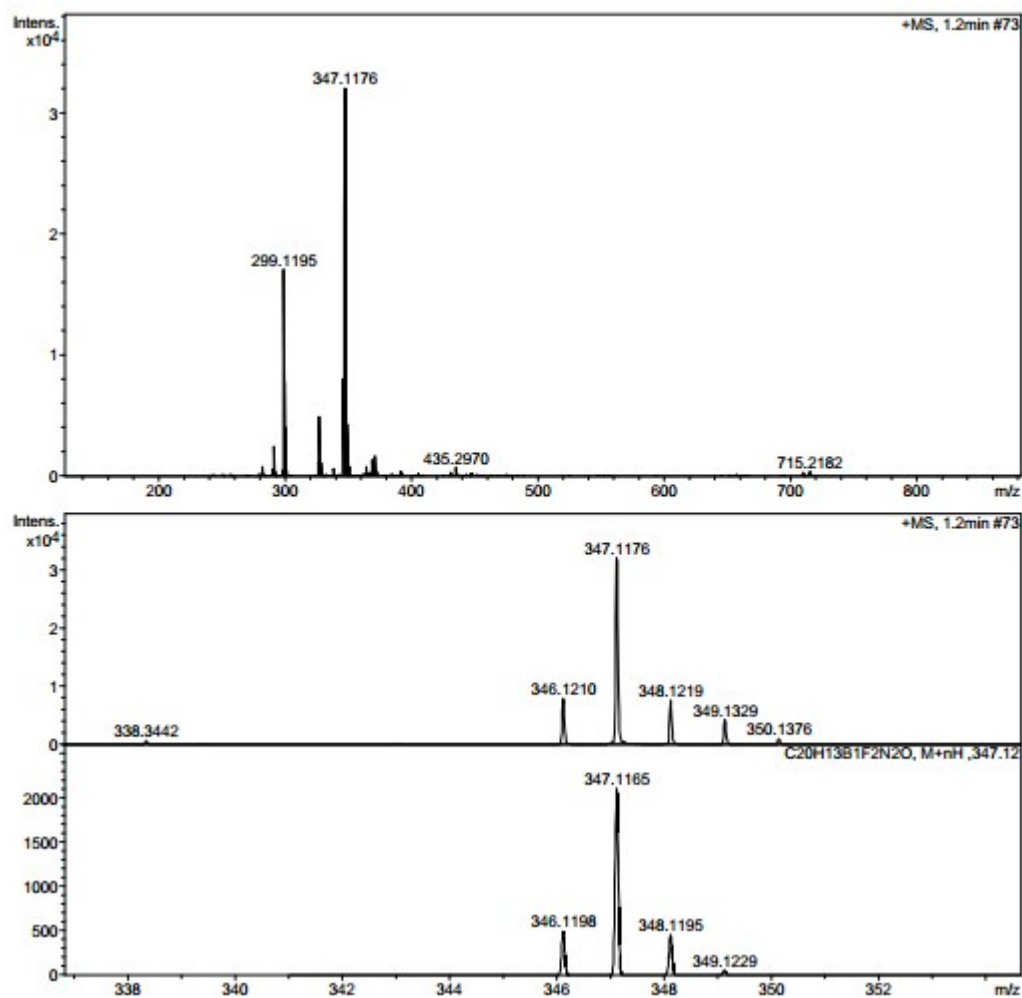


Figure S13. HRMS spectrum of PHPO-BF₂

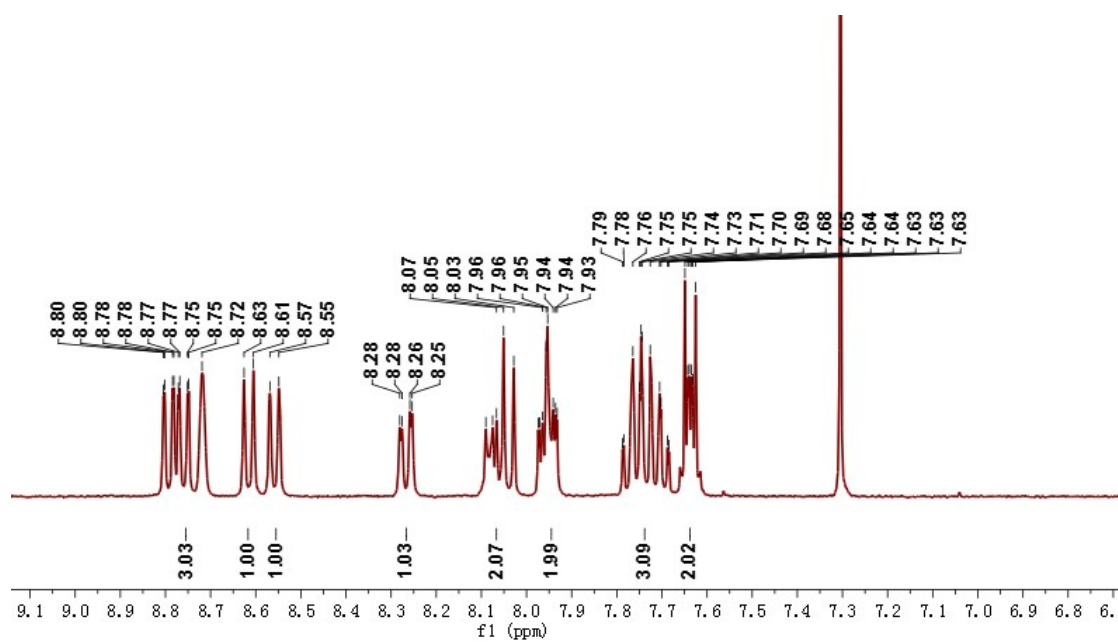


Figure S14. ¹H NMR spectrum of NHPO-BF₂ (400 MHz, CDCl₃)

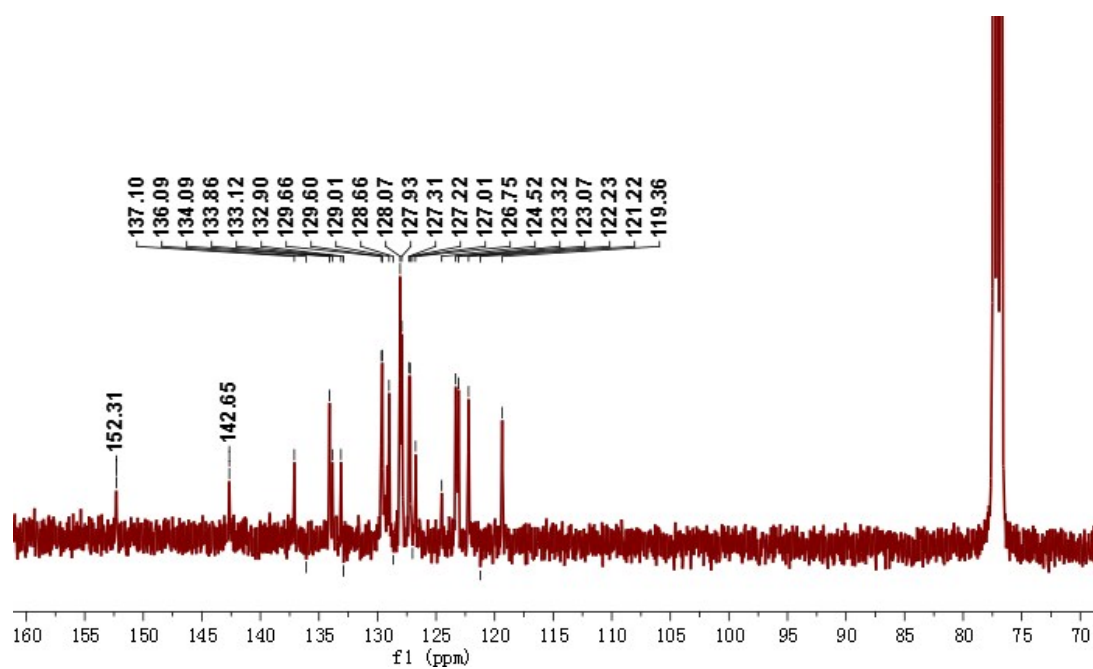


Figure S15. ^{13}C NMR spectrum of NHPO-BF_2 (101 MHz, CDCl_3)

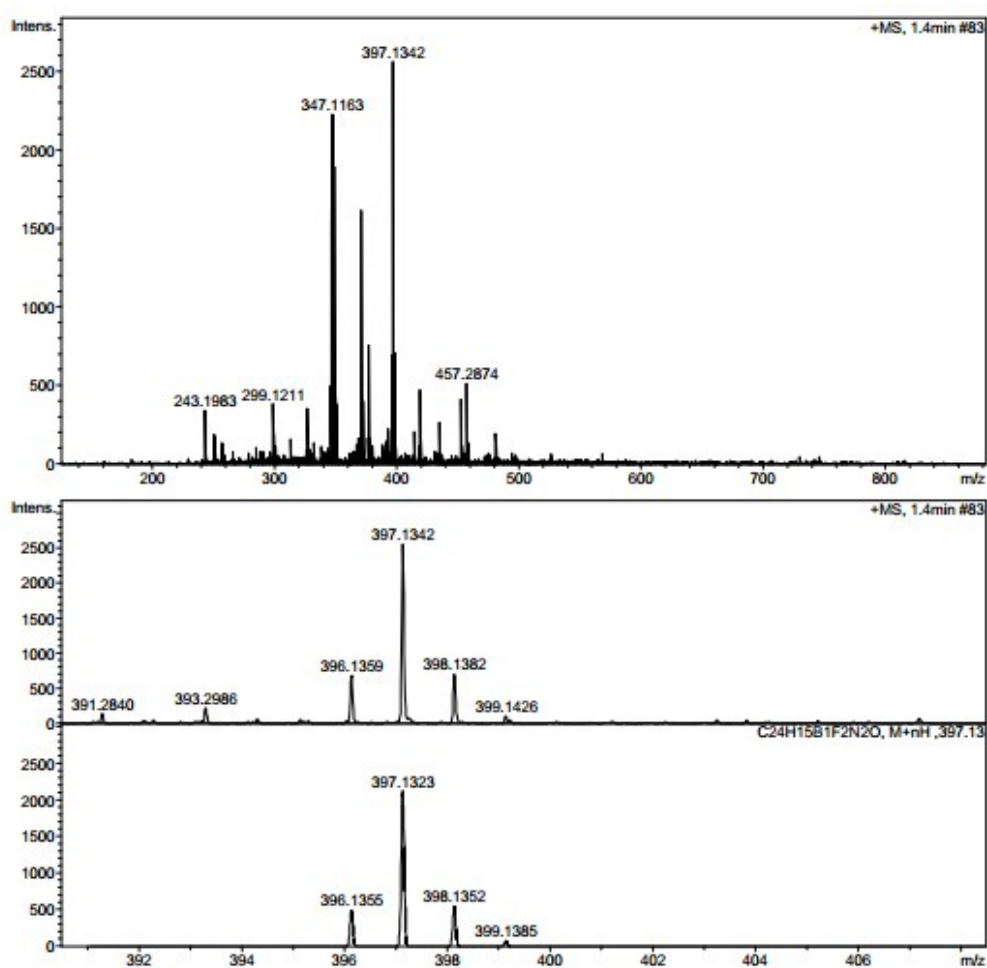


Figure S16. HRMS spectrum of NHPO-BF_2