Benzothiazole appended 2,2'-(1,4-phenylene)diacetonitrile for the calorimetric and fluorescence detection of cyanide ions

Dhanapal Jothi[a], Sathishkumar Munusamy[b], Saravanakumar Manickam[c], Saravanan Enbanathan[a], Selin Manojkumar[a] and Sathiyanarayanan Kulathu Iyer[a]*

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[b]Department of Chemistry, Faculty of Science, Chulalongkorn University, Phayathai Rd., Pathumwan, Bangkok, 10330, Thailand. E-mail: pra3sat@gmail.com

[c]Department of Chemistry, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, (SIMATS), Chennai -602105, Tamil Nadu, India.

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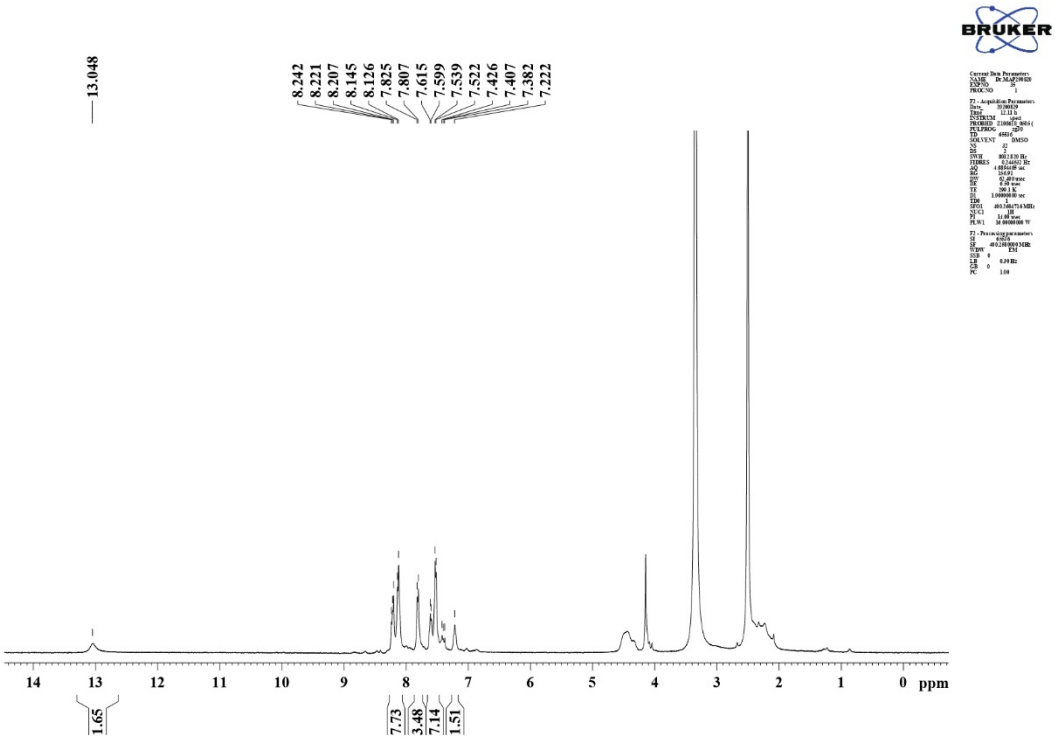


Fig S1 ^{1}H NMR spectra of **PDBT.**

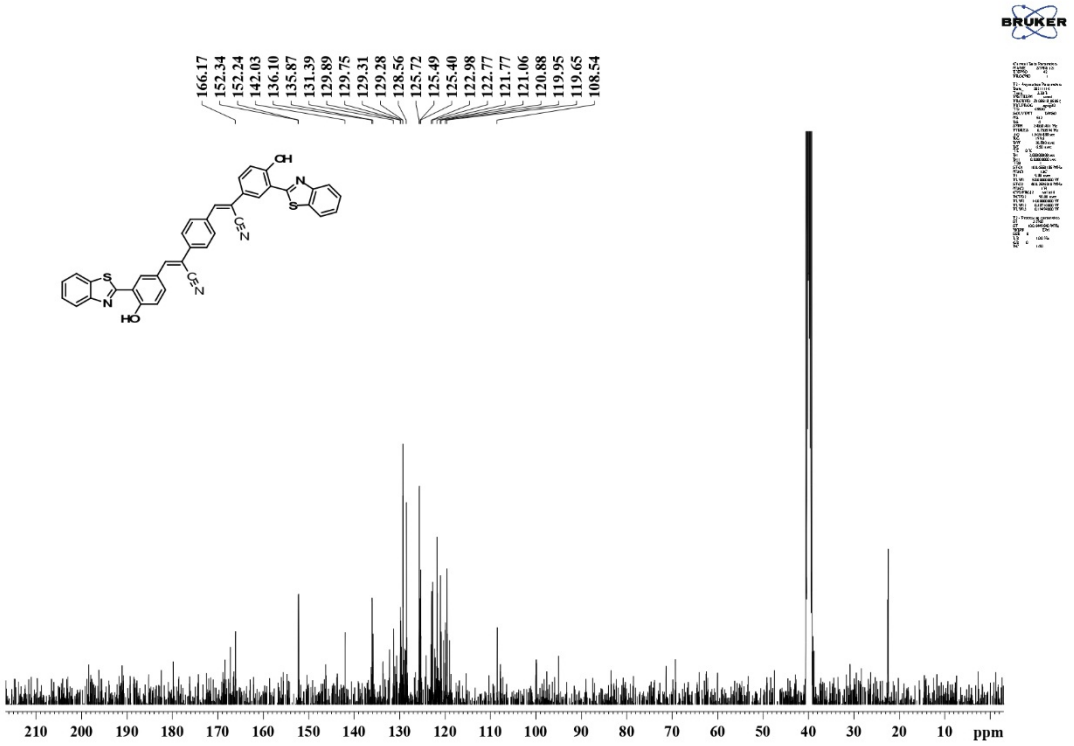


Fig S2 ^{13}C NMR spectra of **PDBT.**

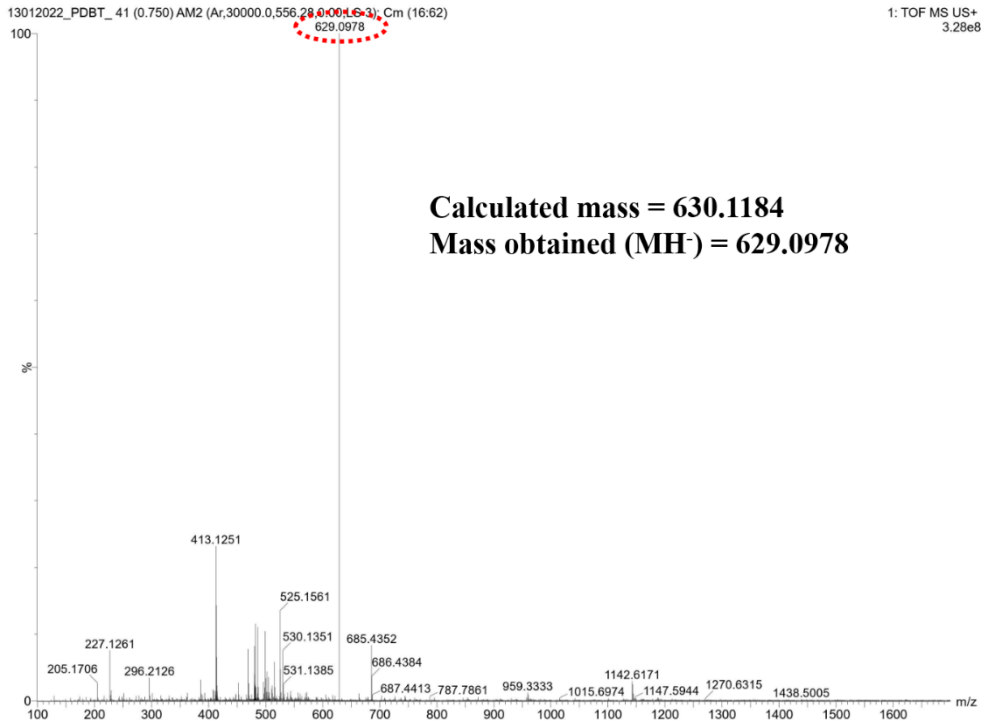


Fig S3 HRMS spectra of **PDBT.**

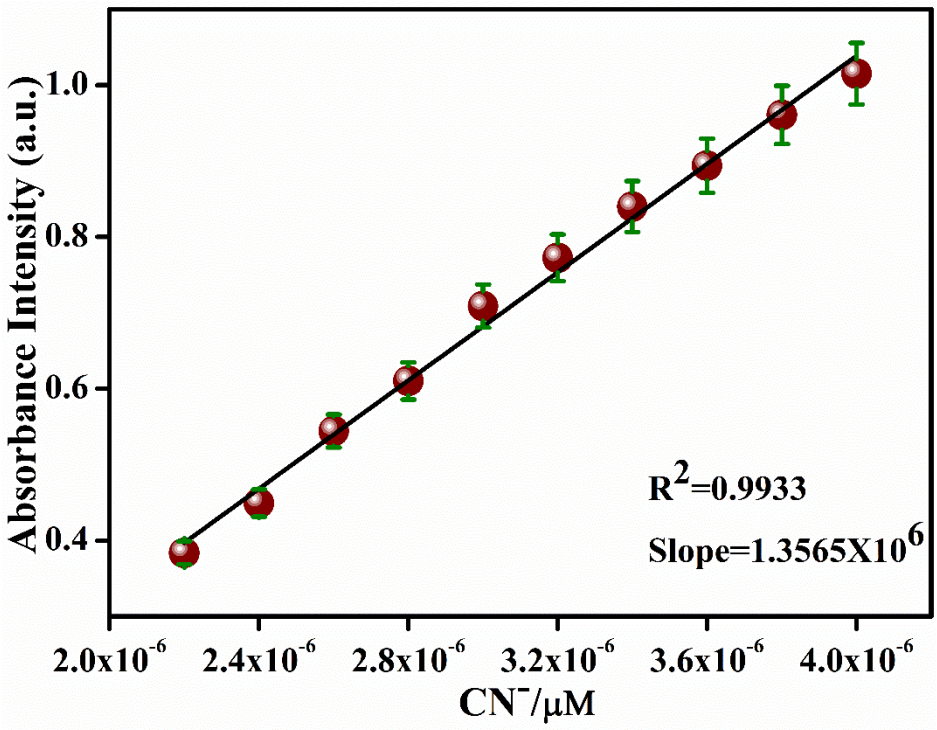


Fig S4. The linear plot of absorption intensity against the concentration of CN^- from 1 to 20 μM in ACN/H_2O (1:1, v/v).

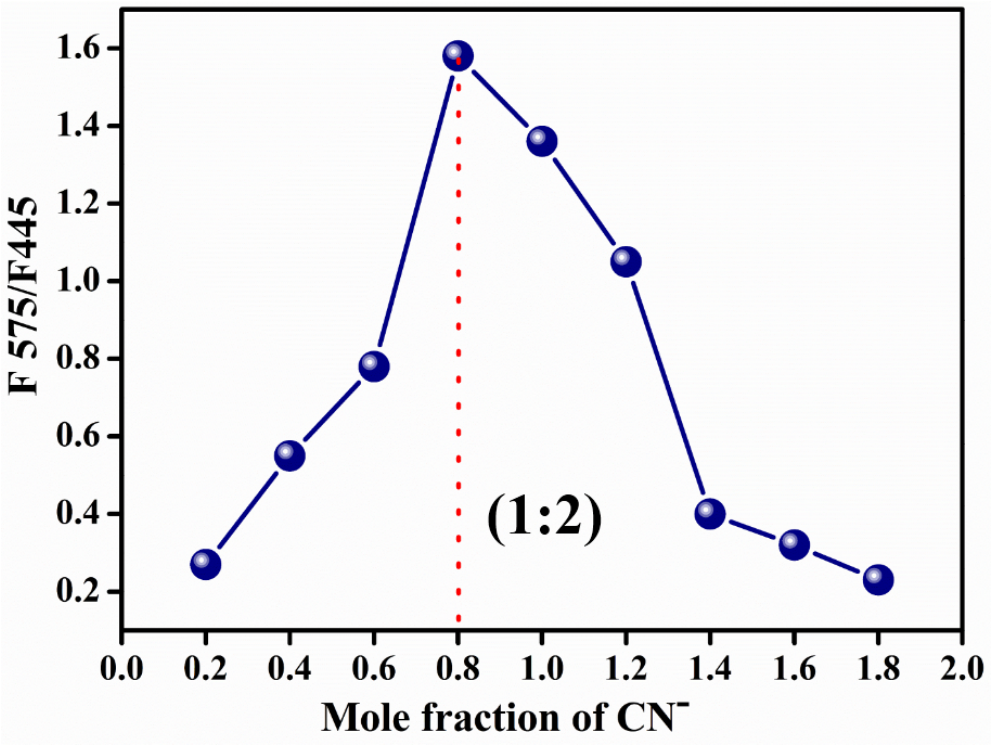


Fig S5. Job's plot for determining the binding stoichiometry of **PDBT** and CN^- ions.

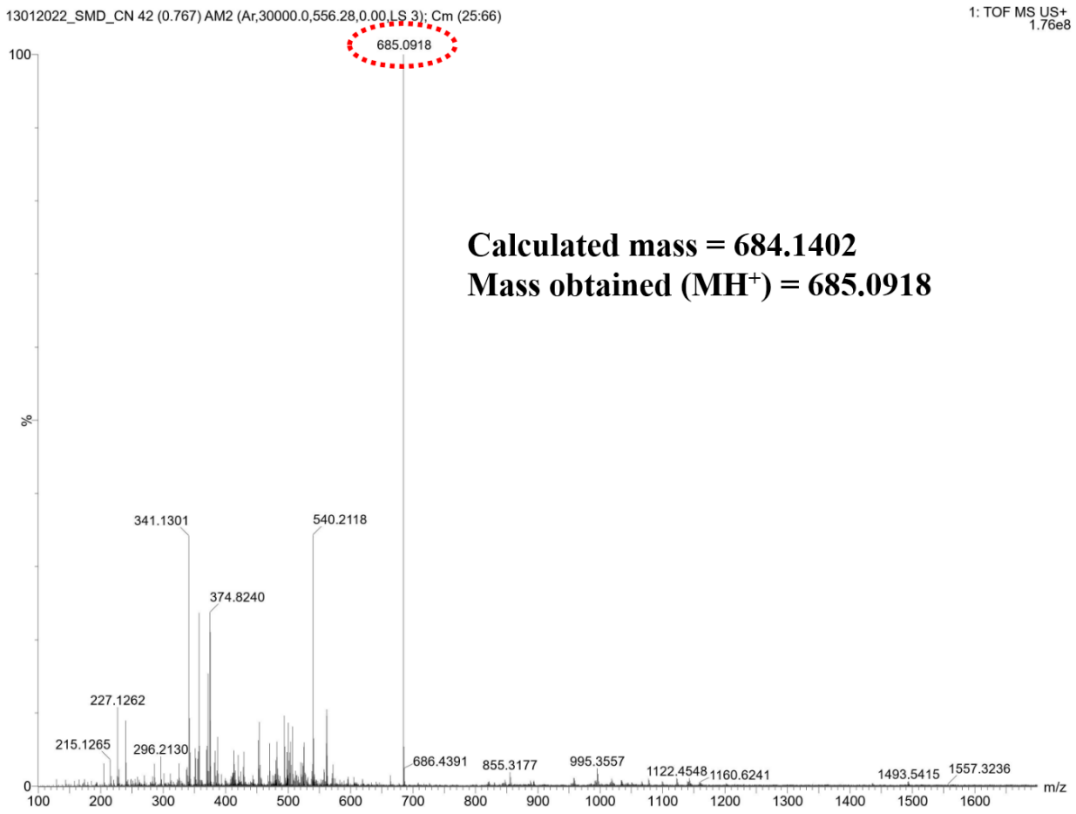


Fig S6 HRMS spectra of **PDBT+CN$^-$.**

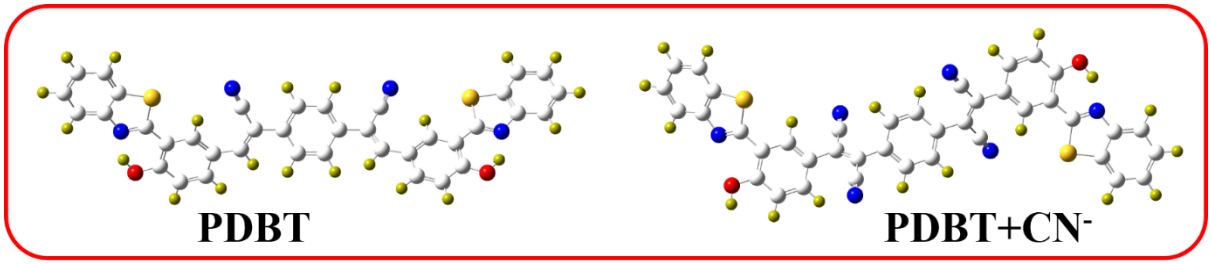
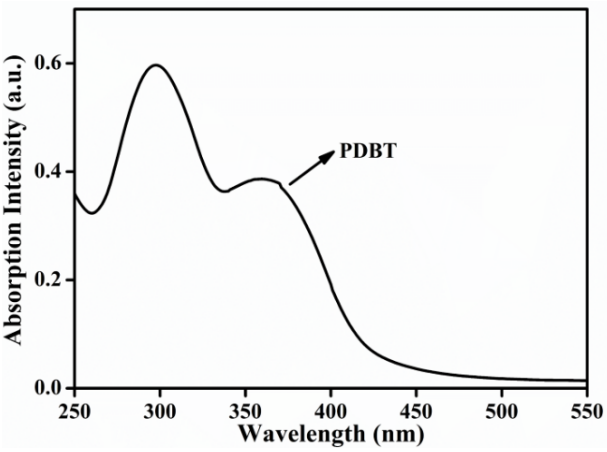
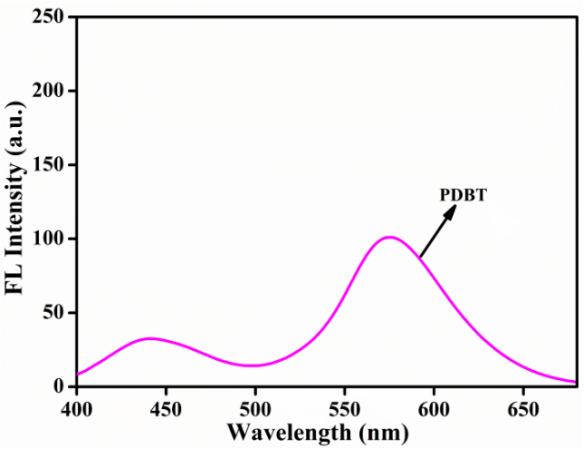


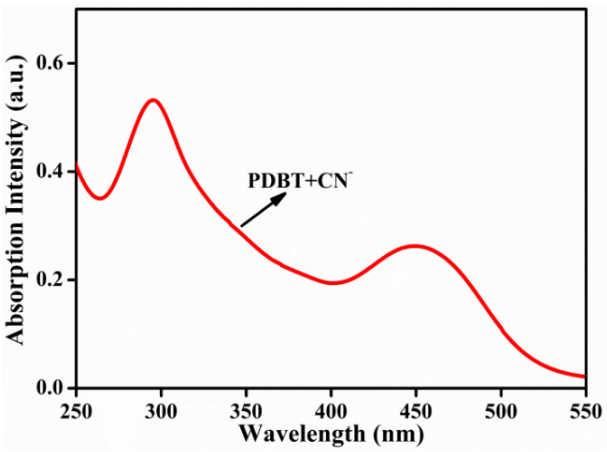
Fig S7. Optimized structures of PDBT and PDBT+CN$^-$.

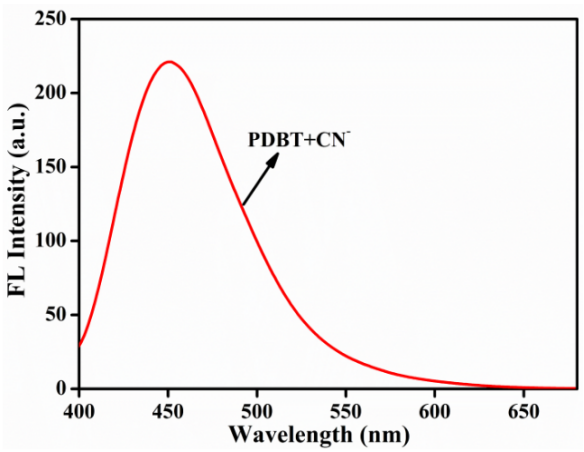
Table S1. Oscillator strengths of important transitions for the **PDBT** and **PDBT** + **CN^-**.

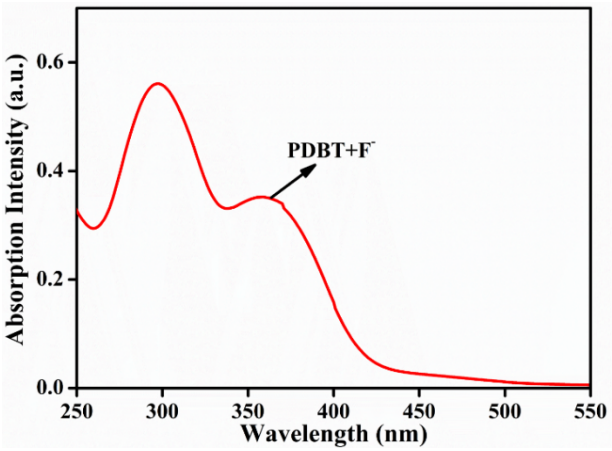
Entry	λ max(nM)	Oscillatory strength	ΔE,Energy(eV)	Selected major transitions
	434.72	1.8799	18.7282	H ⟶ L (47%)
PDBT	370.21	0.0733	17.7472	H ⟶ L_2(42%)
	329.02	0.3664	14.9453	H_1 ⟶ L_1 (30%)
	322.42	0.0675	16.3412	H_3 ⟶ L (36%)
	317.54	0.0310	15.5306	H_5 ⟶ L (32%)
	312.49	0.1017	18.2697	H_1 ⟶ L_3 (45%)
PDBT+ CN^-	474.08	0.8540	18.7559	H ⟶ L (47%)
	402.98	0.0809	13.9161	H ⟶ L_1 (26%)
	387.84	0.0018	18.4784	H_4 ⟶ L (46%)
	351.68	0.0003	18.8697	H_2 ⟶ L_1 (48%)
	303.12	0.1183	8.0216	H_3 ⟶ L_2(8.6%)
	302.85	0.0168	9.8015	H_1 ⟶ L_2 (12%)







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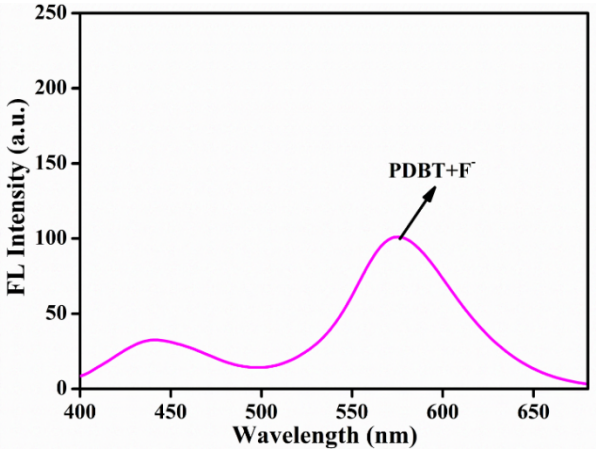
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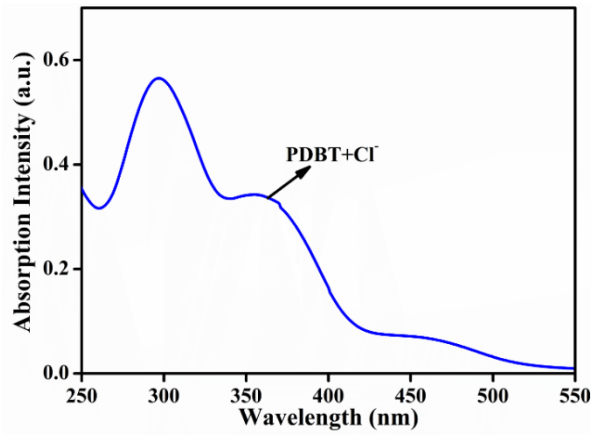
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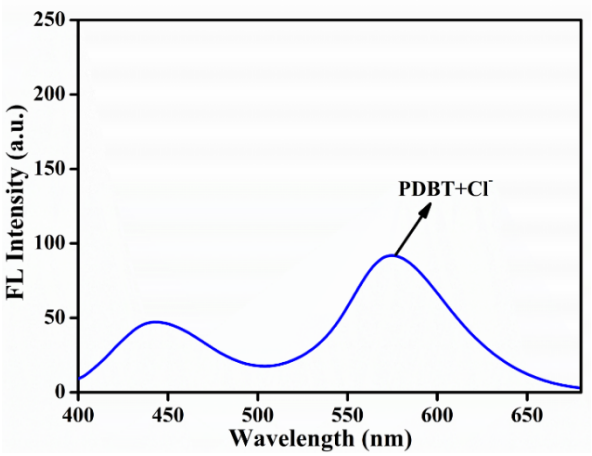
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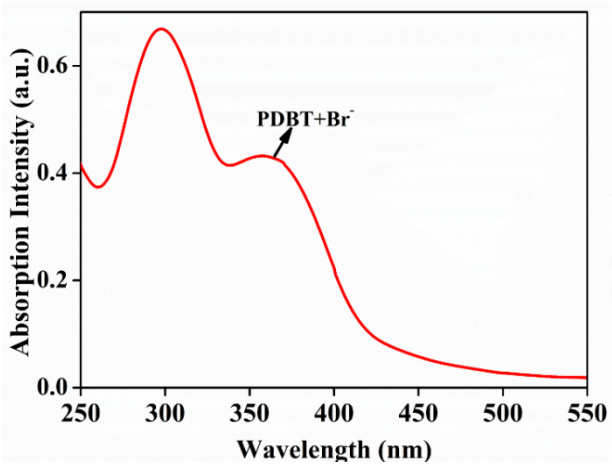
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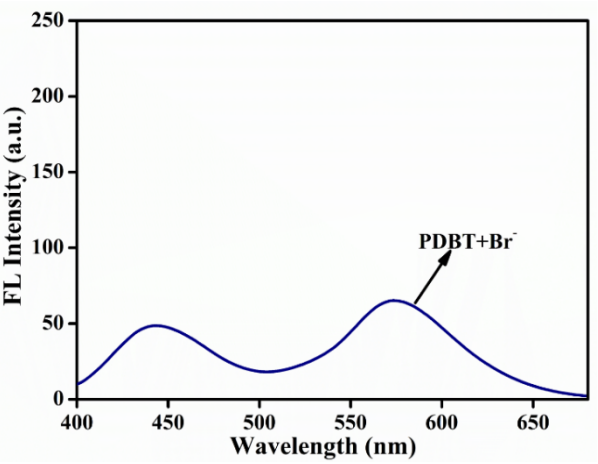
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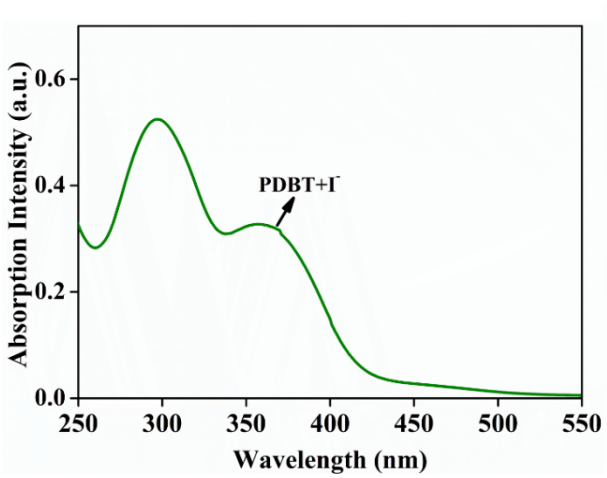
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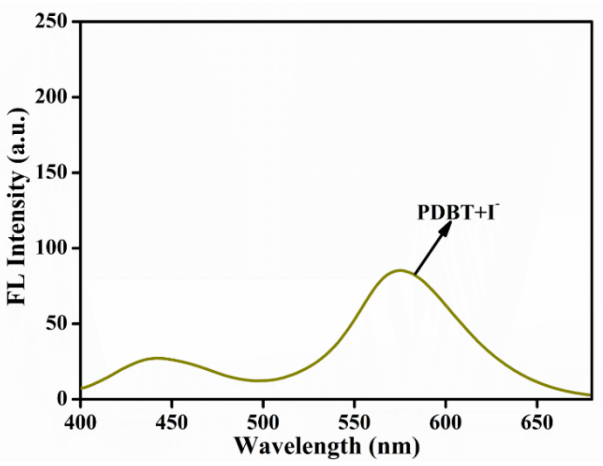
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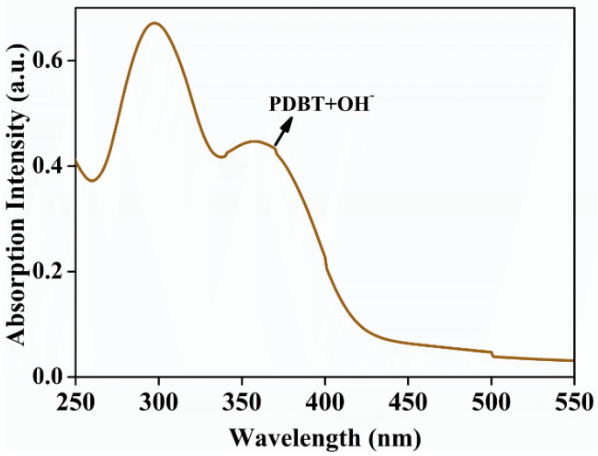
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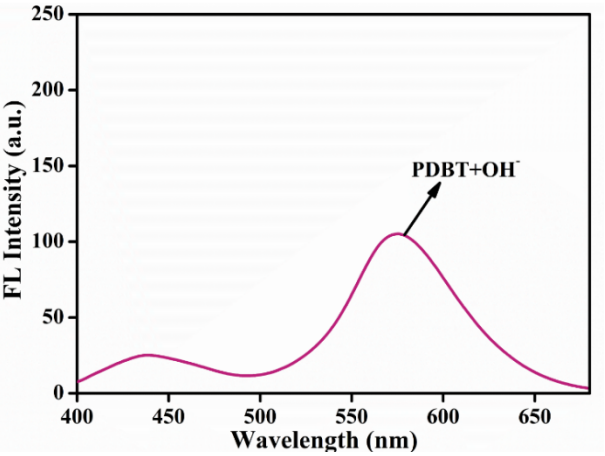
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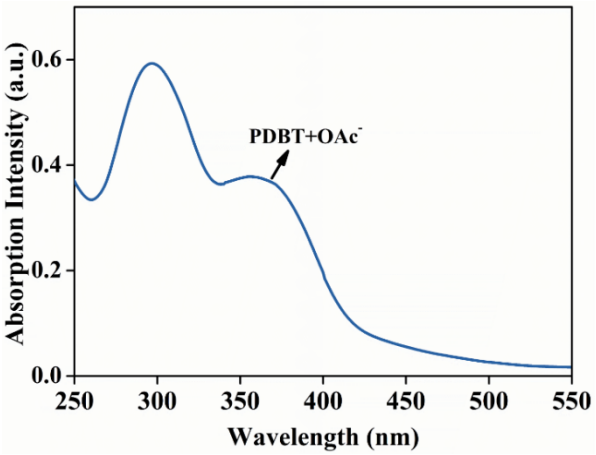
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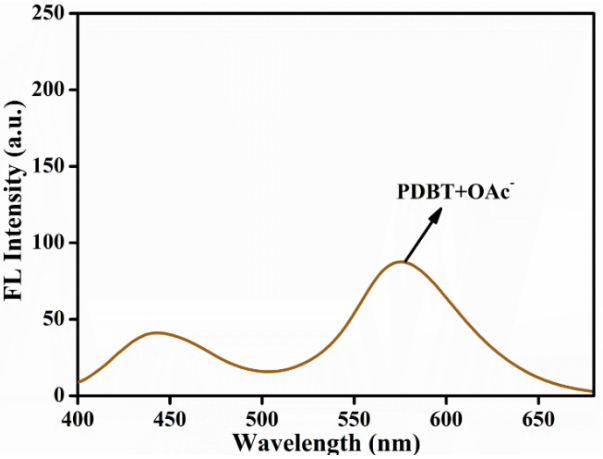
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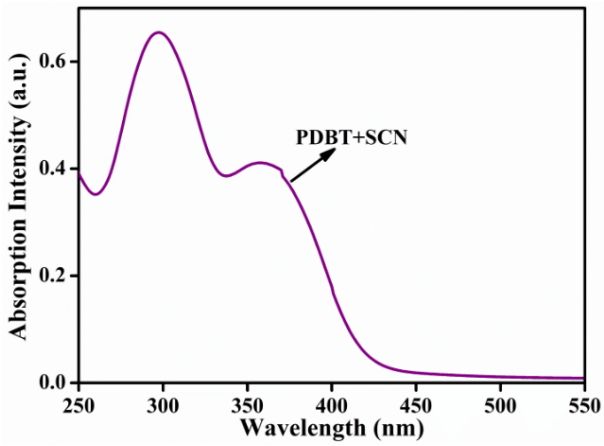
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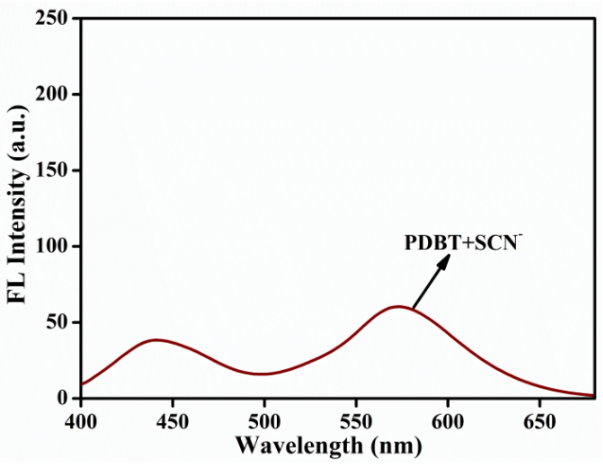
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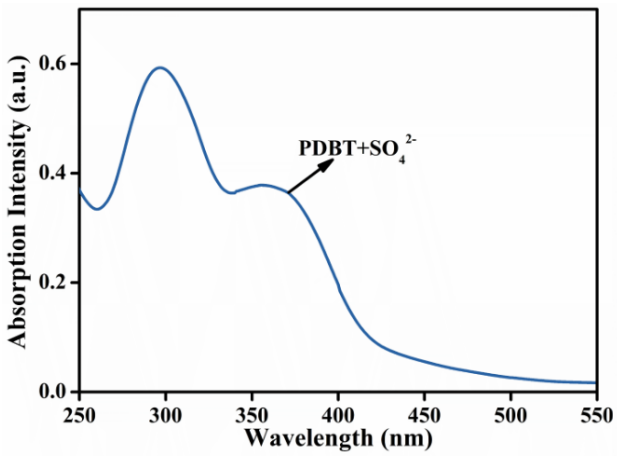
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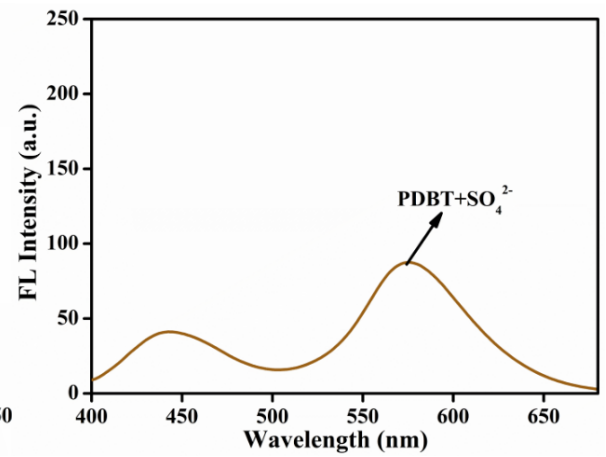
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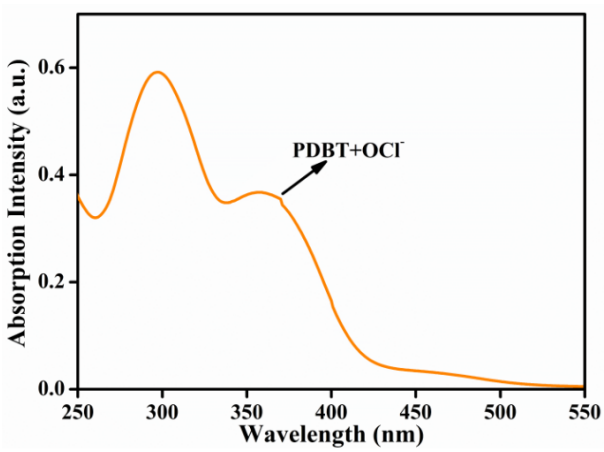
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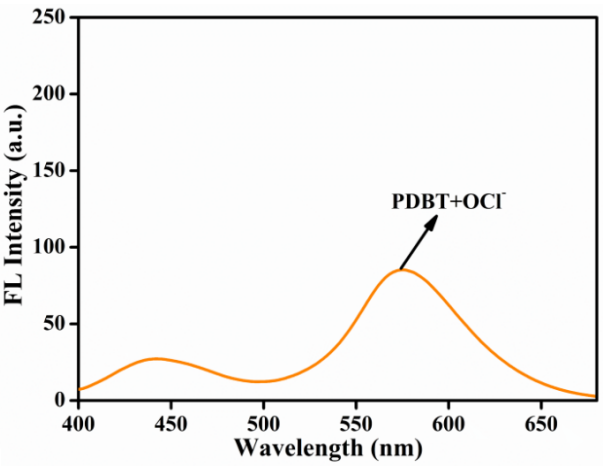
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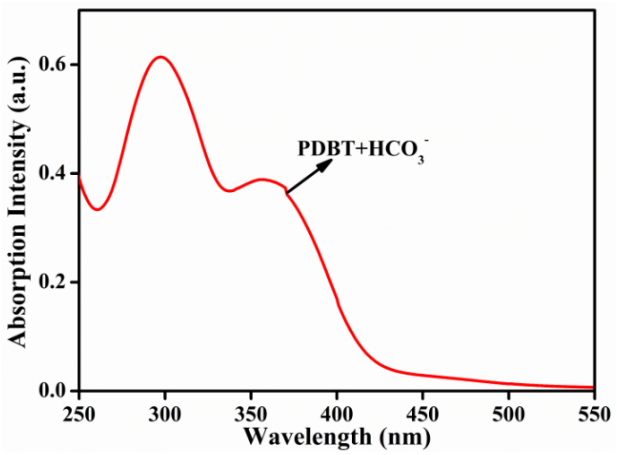
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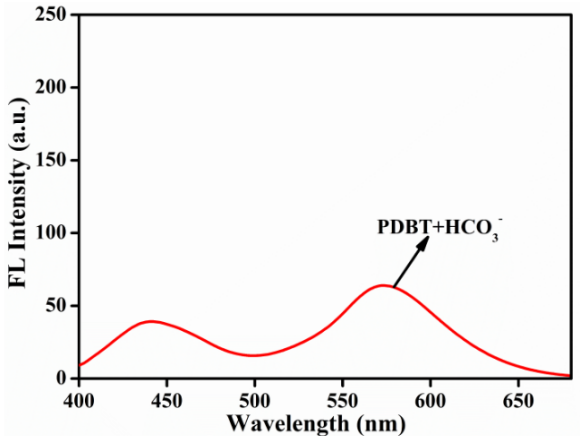
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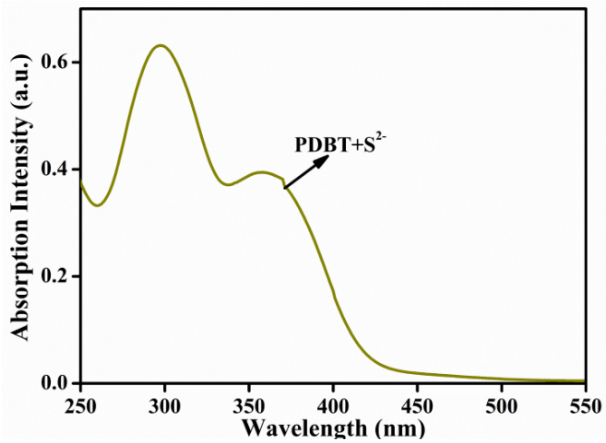
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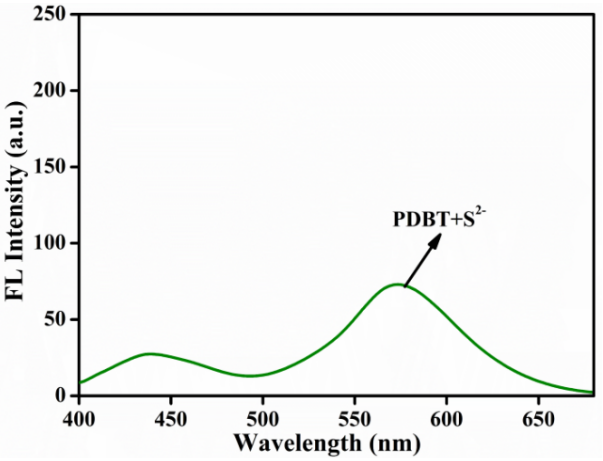
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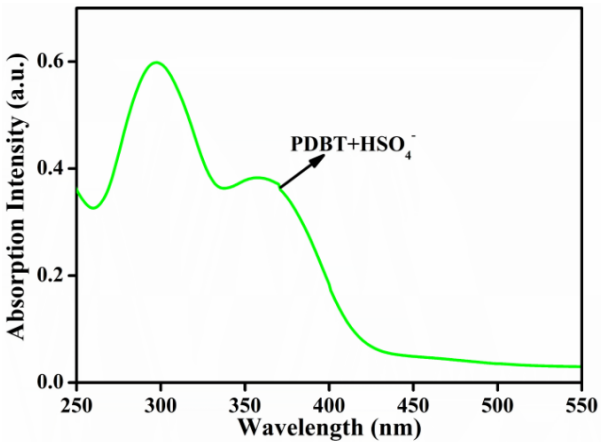
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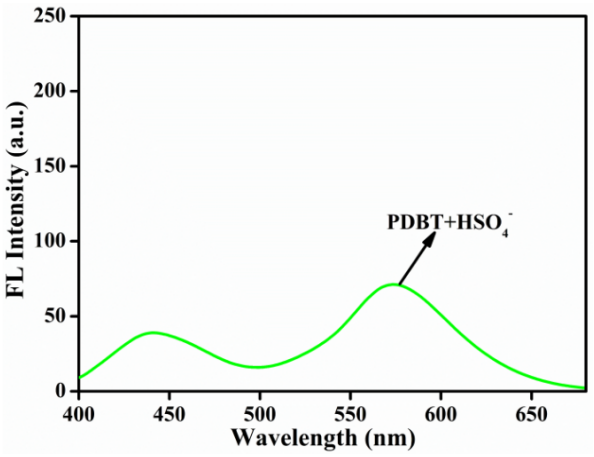
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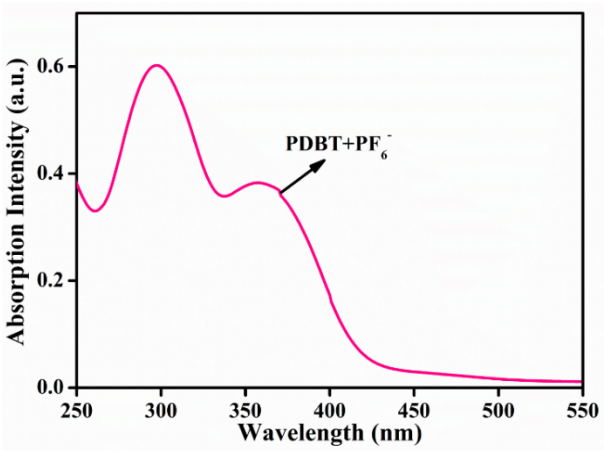
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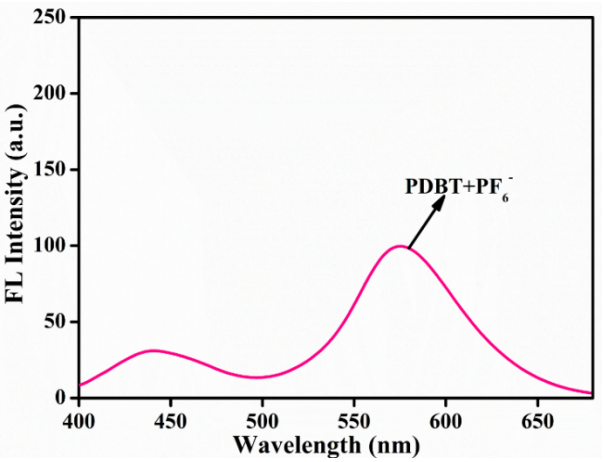
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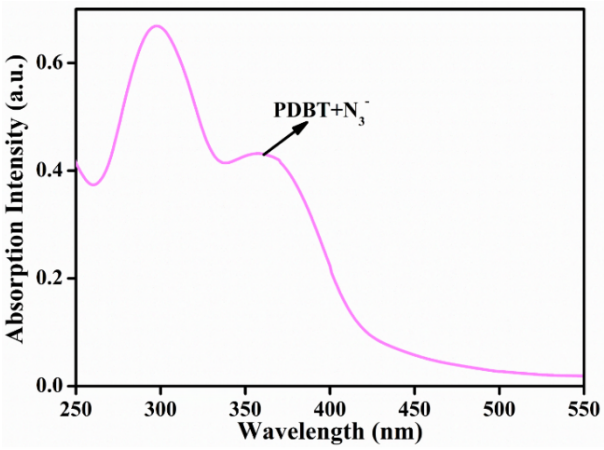
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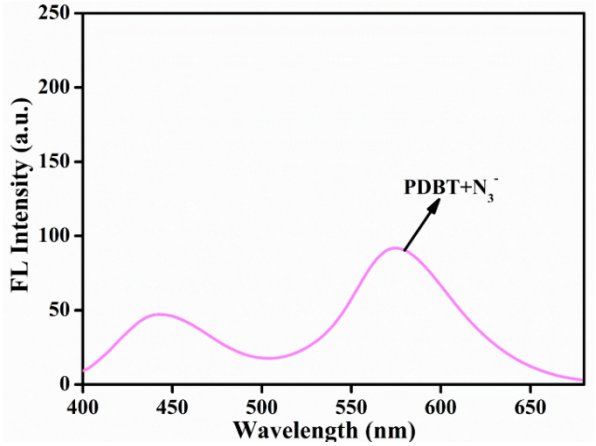
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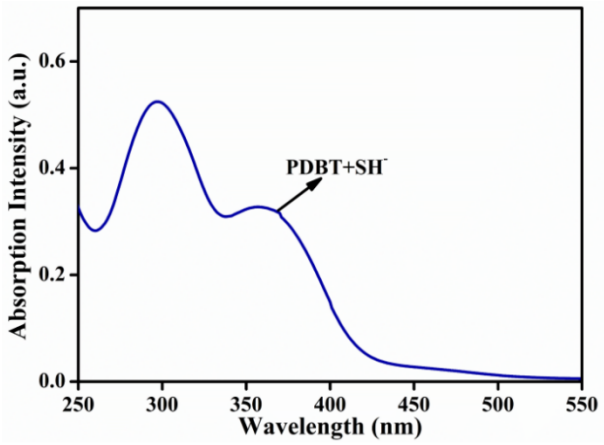
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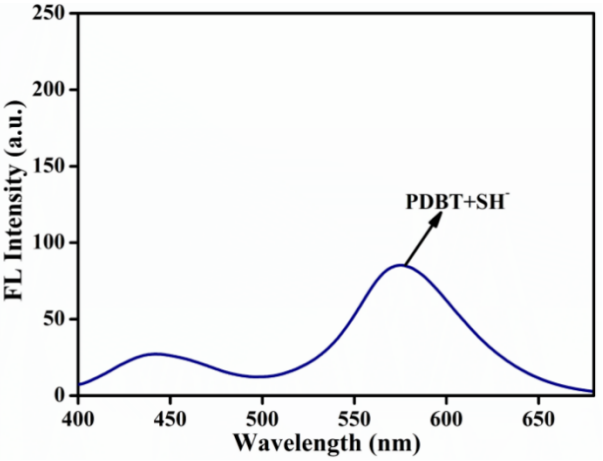
Wavelength (nm)
PDBT+SH-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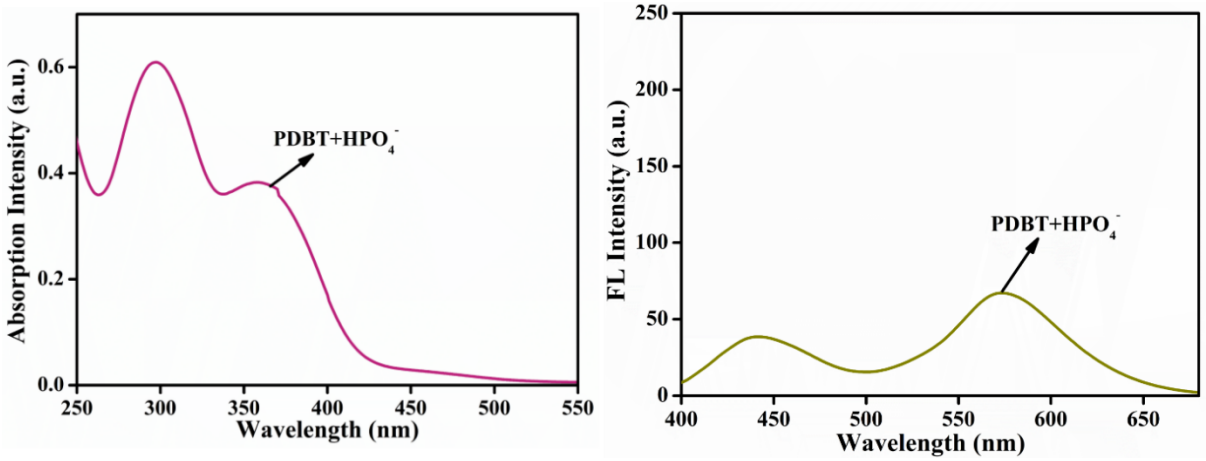

Fig S8. Individual electronic spectra of **PDBT** with various selective anions.

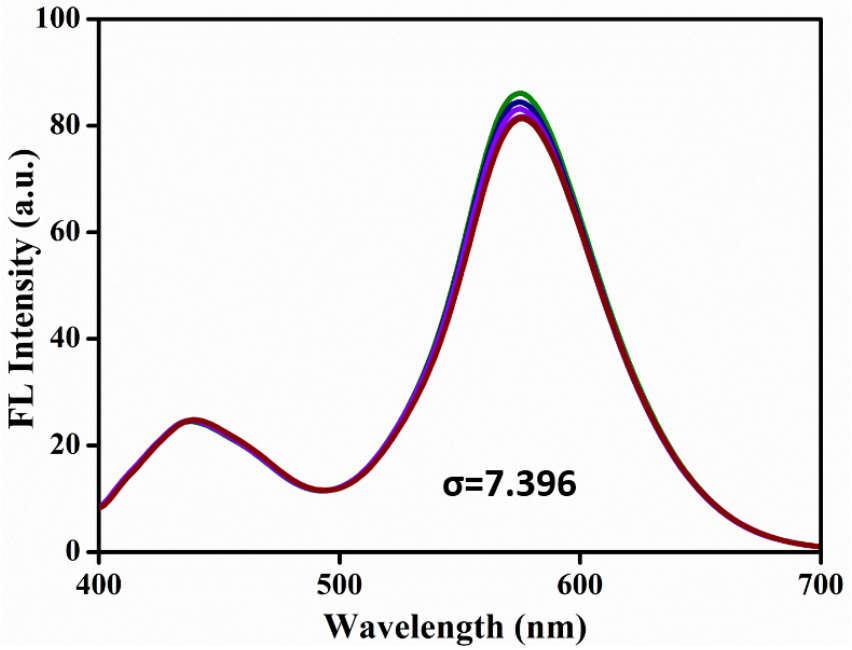

Fig S9. Standard deviation calculation spectra of **PDBT**.