

Pyrano-pyrazole based Schiff Base for Rapid Colorimetric Detection of Arginine in aqueous and Real Samples

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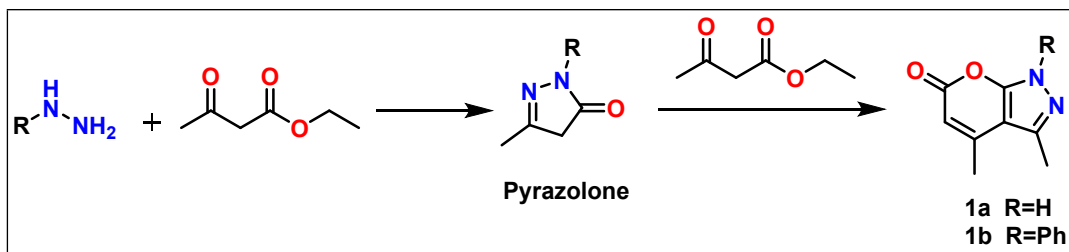
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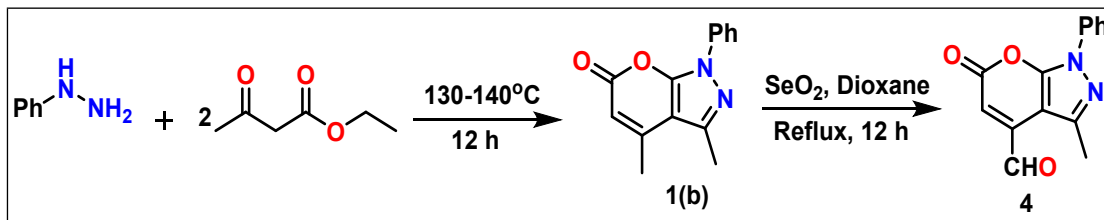
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Table S1: Parameters obtained from the TD-DFT calculations. (f = oscillator strength)



Scheme S1: Synthetic Route to precursors **1a** and **1b**



Scheme S2: Synthetic Route to compound **4**

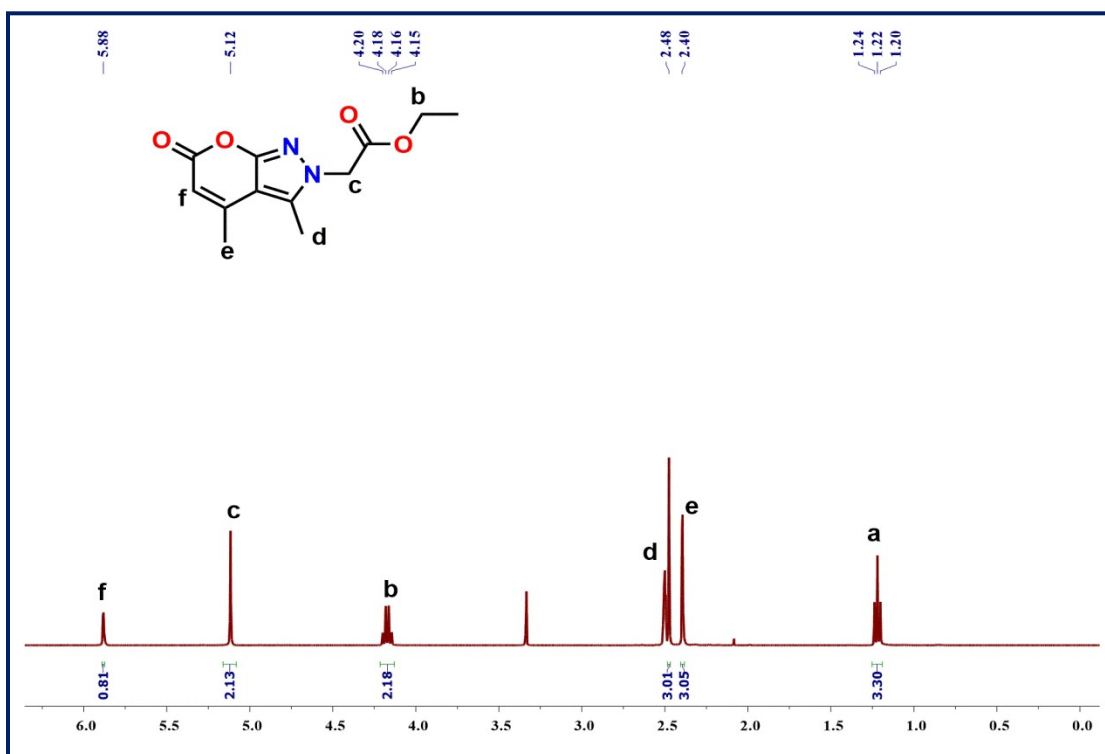


Figure S1: ^1H NMR of **2** in $\text{DMSO-}d_6$

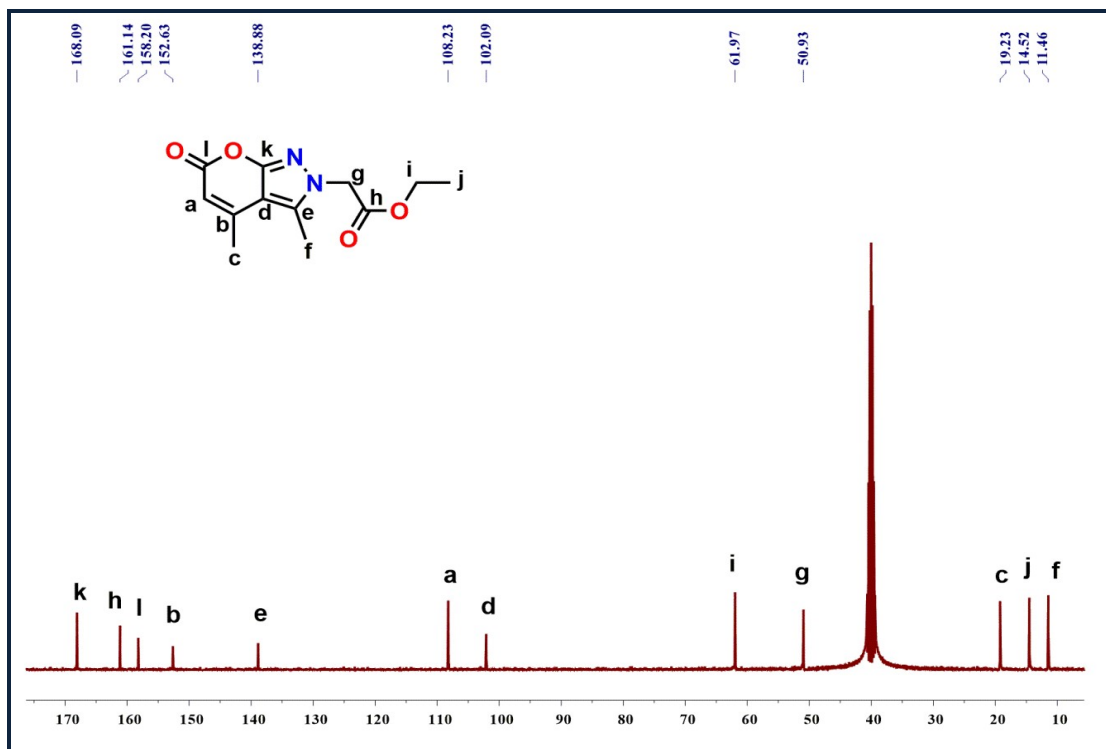


Figure S2: ^{13}C NMR of 2 in $\text{DMSO-}d_6$

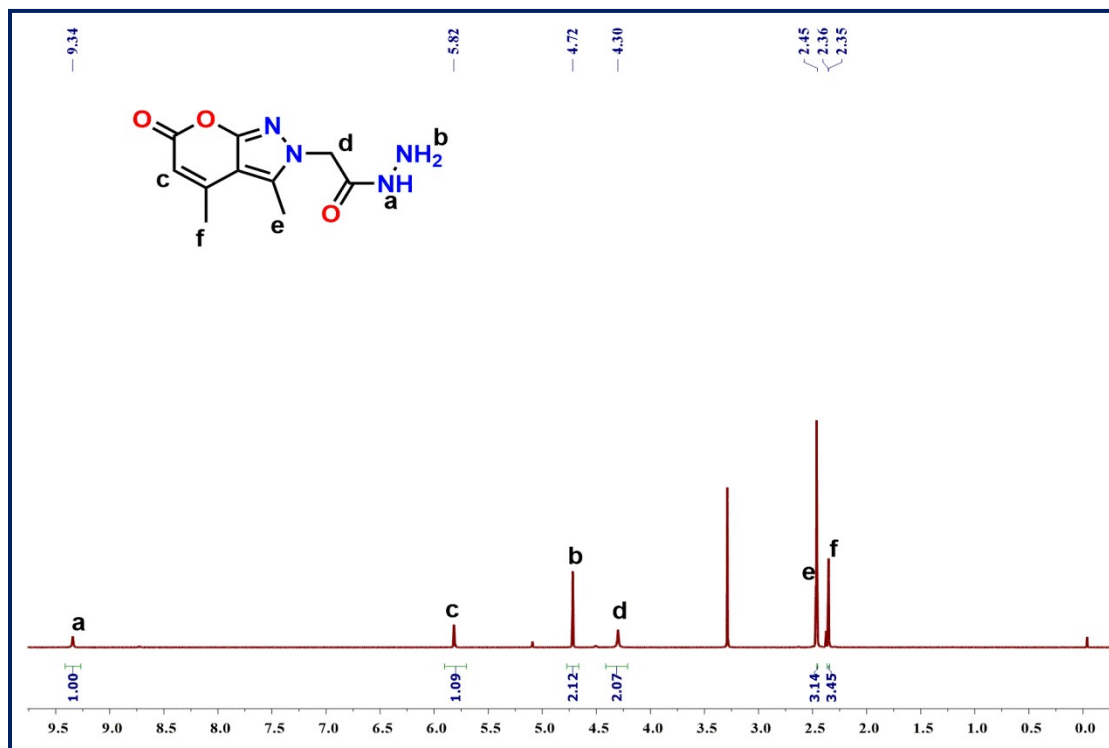


Figure S3: ^1H NMR of 3 in $\text{DMSO-}d_6$

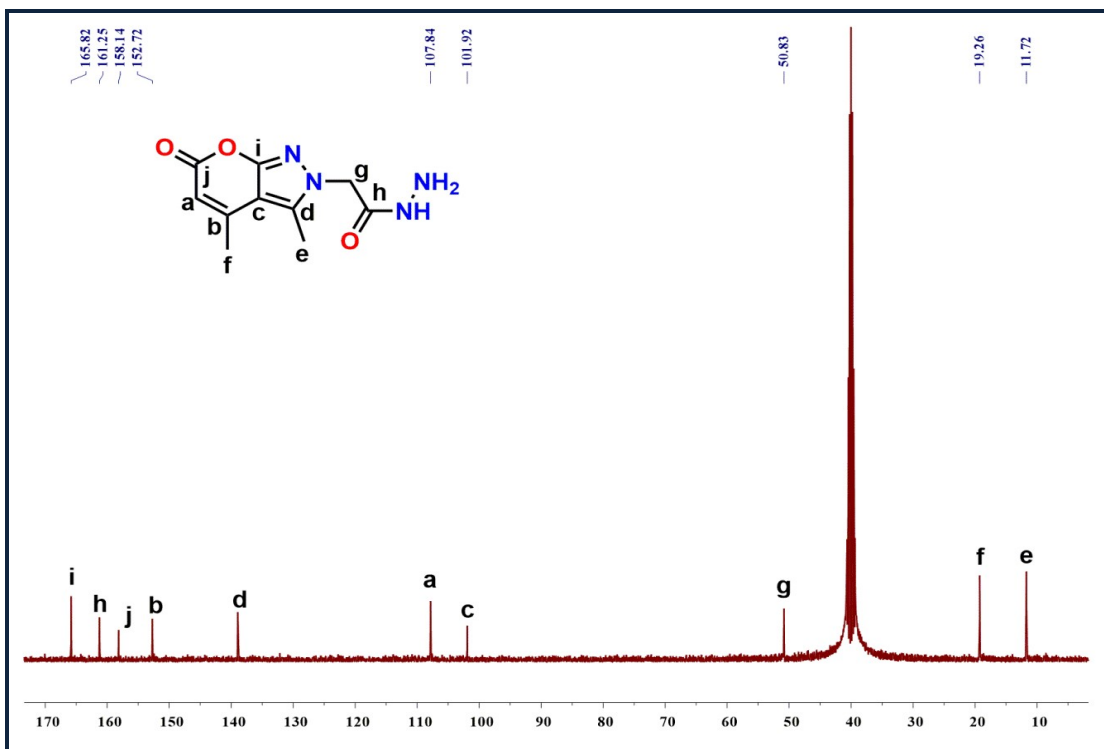


Figure S4: ^{13}C NMR of 3 in $\text{DMSO-}d_6$

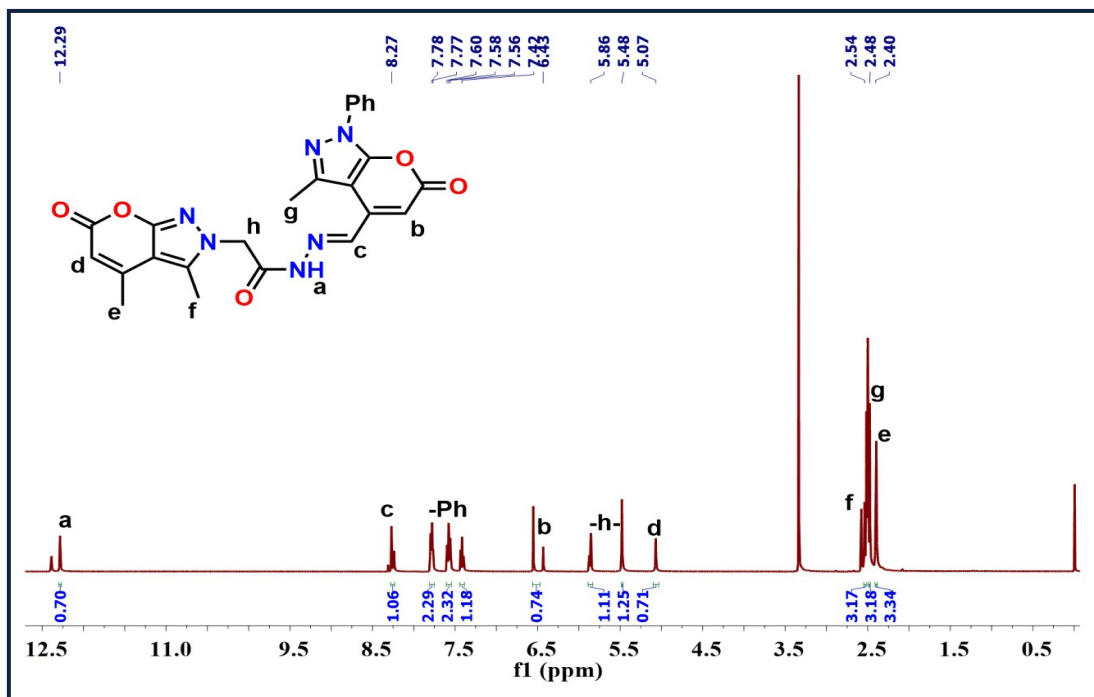


Figure S5: ^1H NMR spectrum of PPS in $\text{DMSO-}d_6$

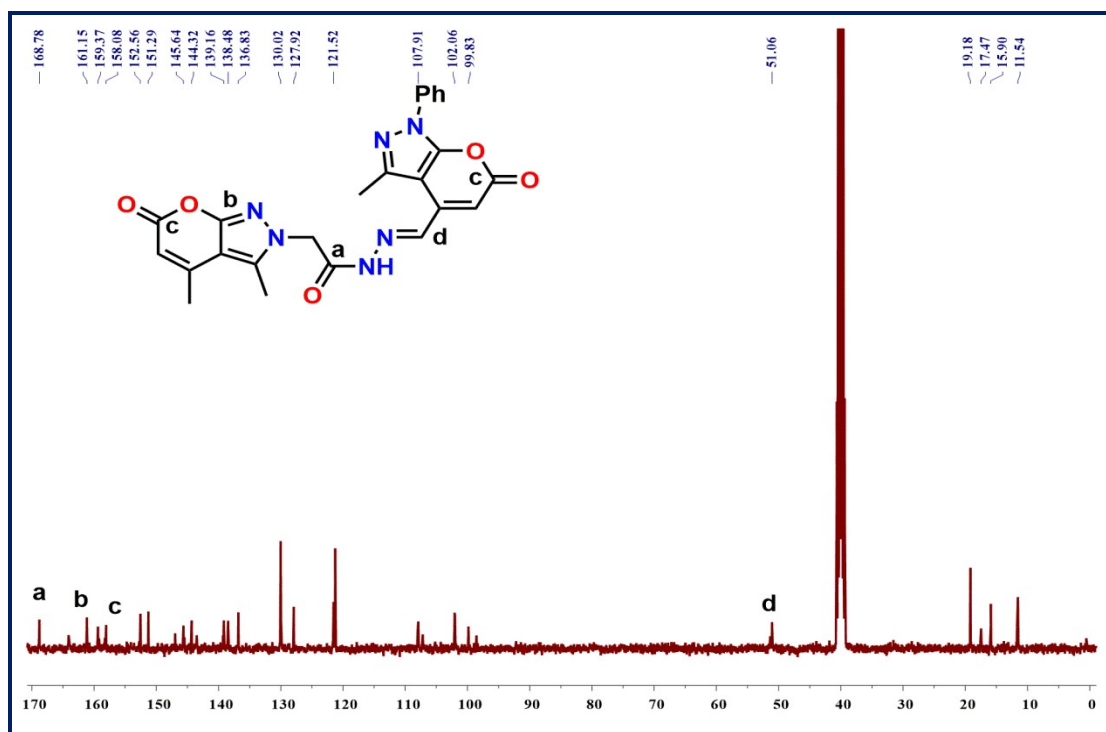


Figure S6: ^{13}C NMR spectrum of **PPS** in $\text{DMSO-}d_6$

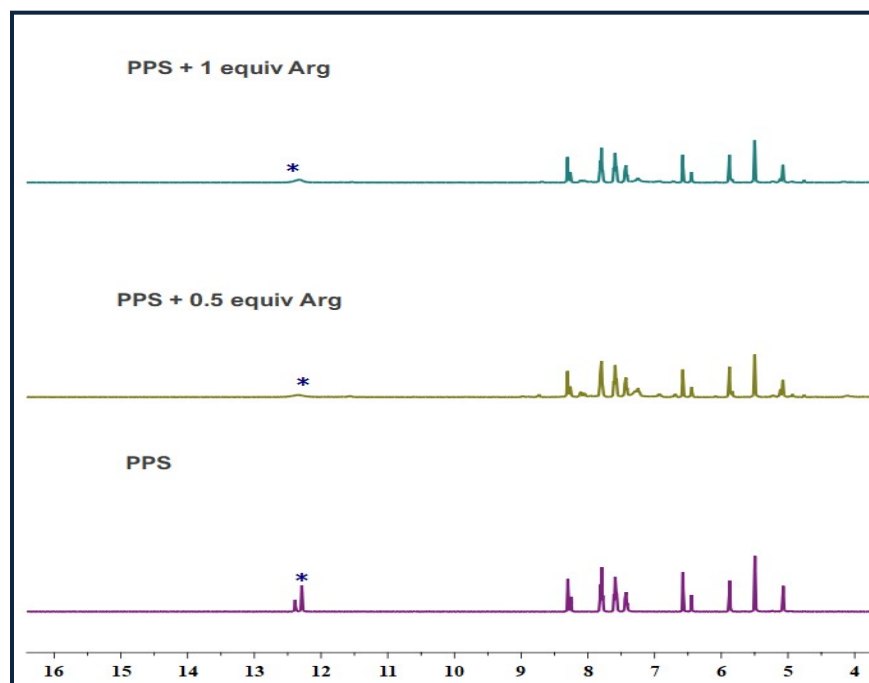
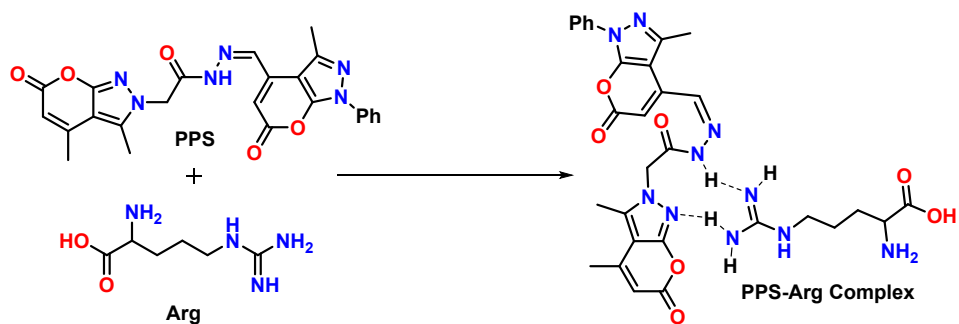


Figure S7: ^1H NMR titration experiment of **PPS** with different equiv. of Arginine in $\text{DMSO-}d_6$



Scheme S3: Plausible binding mechanism of PPS-arginine complex formation

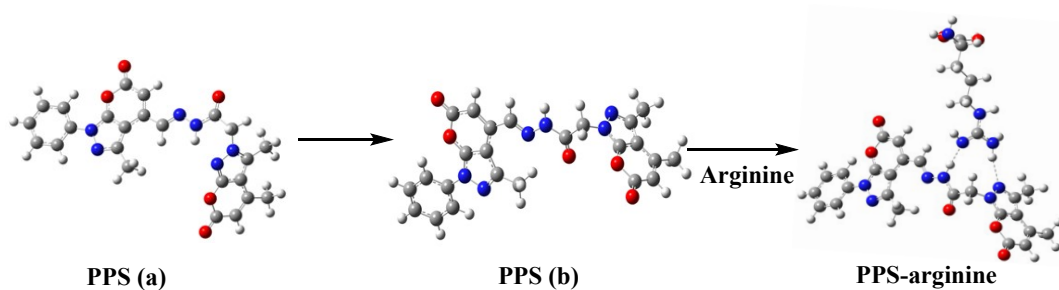


Figure S8: Optimized geometries of PPS and PPS-Arginine

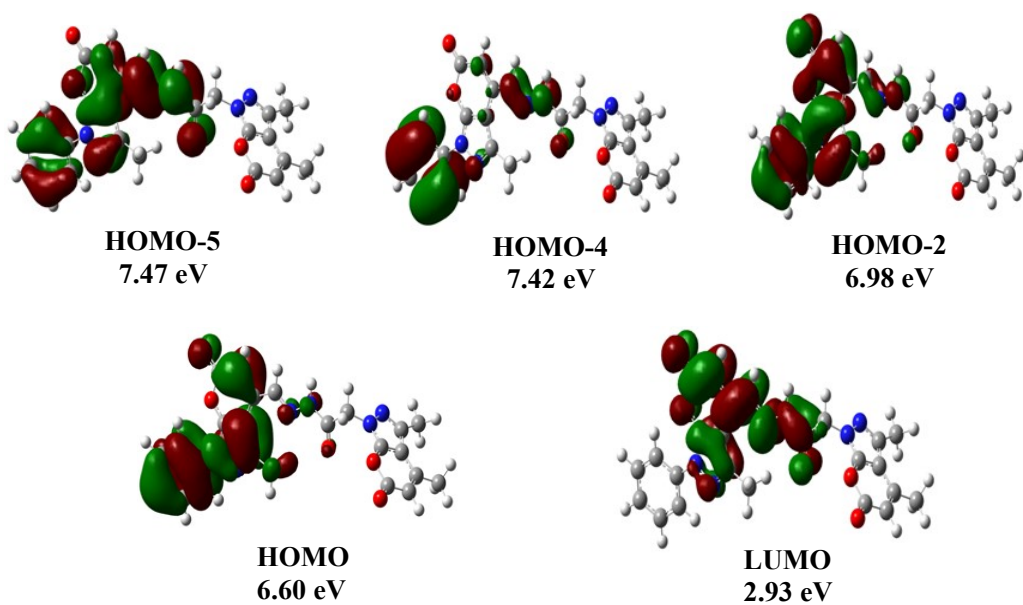


Figure S9: Pictorial representation of different MO's of PPS

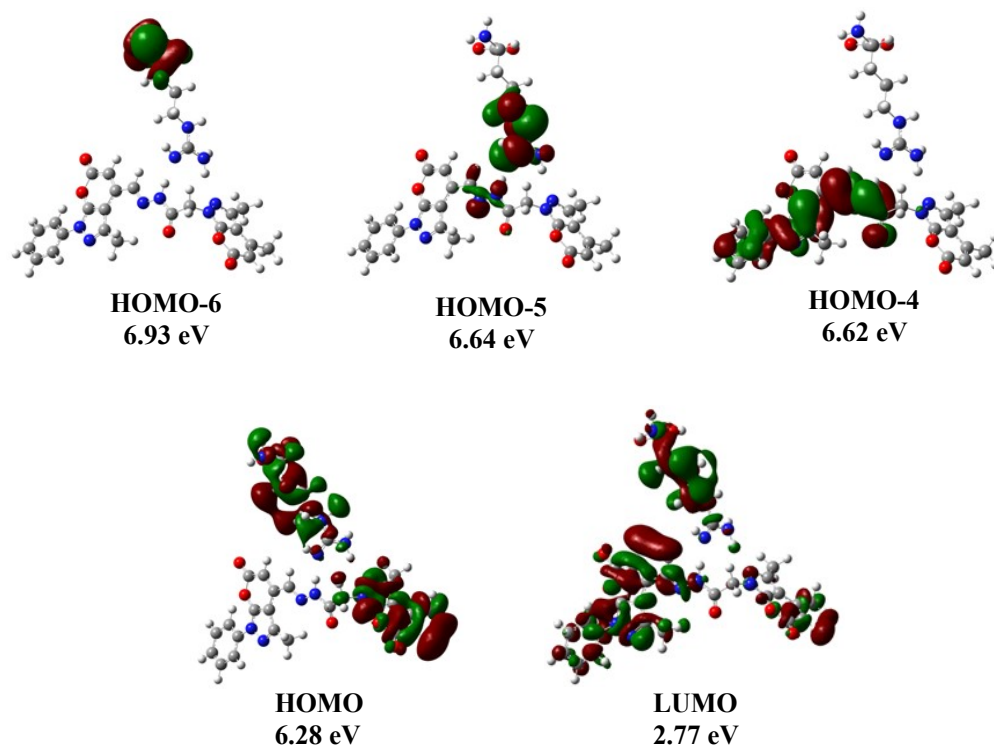


Figure S10: Pictorial representation of different MO's of PPS-Arginine

Table S1: Parameters obtained from the TD-DFT calculations. (f = oscillator strength)

	Experimental λ_{\max} Values	TD-DFT		
		Transition-1	Transition-2	Transition-3
Ligand	310 nm	303.35 nm / 4.08 eV HOMO-5 to LUMO $f = 0.9423$	343.69 nm / 3.60 eV HOMO-2 to LUMO $f = 0.1312$	
Ligand-Arginine Complex	315 nm, 363 nm and 402 nm	319.04 nm / 3.89 eV HOMO-5 to LUMO $f = 0.1814$	349.56 nm / 3.54 eV HOMO-2 to LUMO $f = 0.1381$	382.04 nm / 3.25 eV HOMO to LUMO $f = 0.0682$