Supplementary Information

Synthesis of a redox-active pyrene-F_LF_L-dopamine amphiphile and investigation of their self-assembly at different *p*H leading to microfibrous formation

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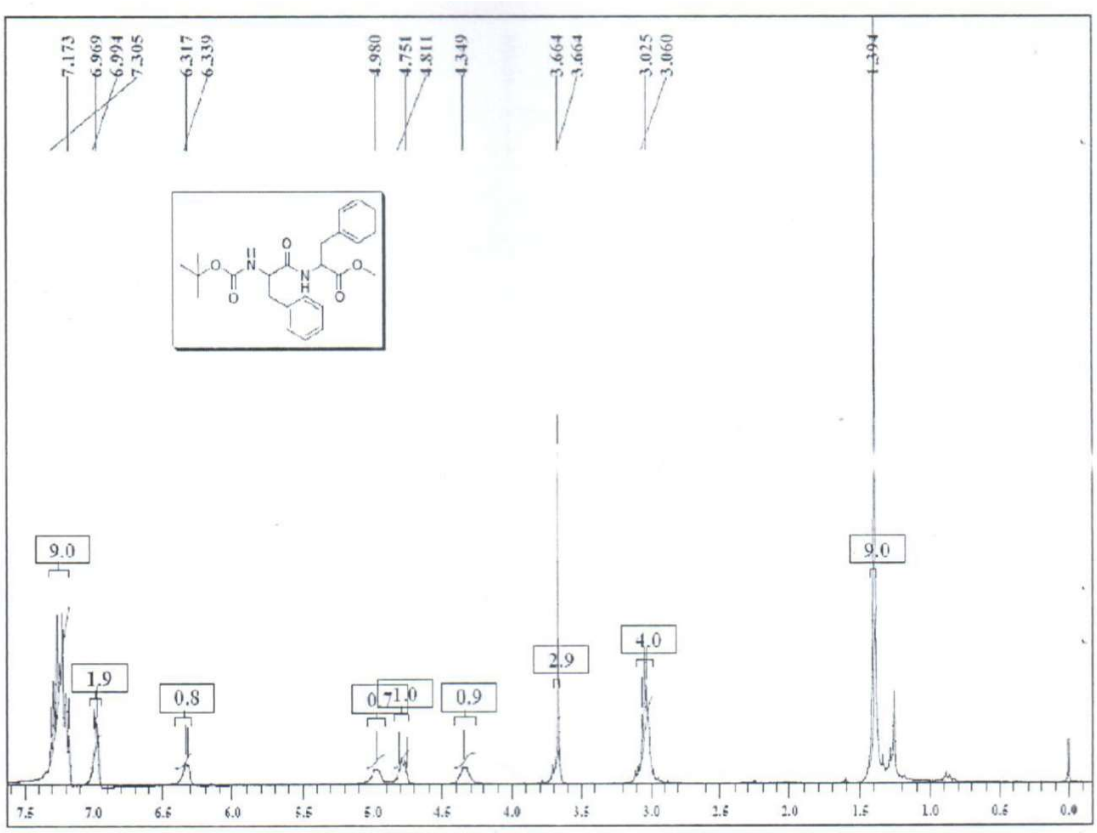


Fig. S1 ^{1}H NMR spectra of compound **3**.

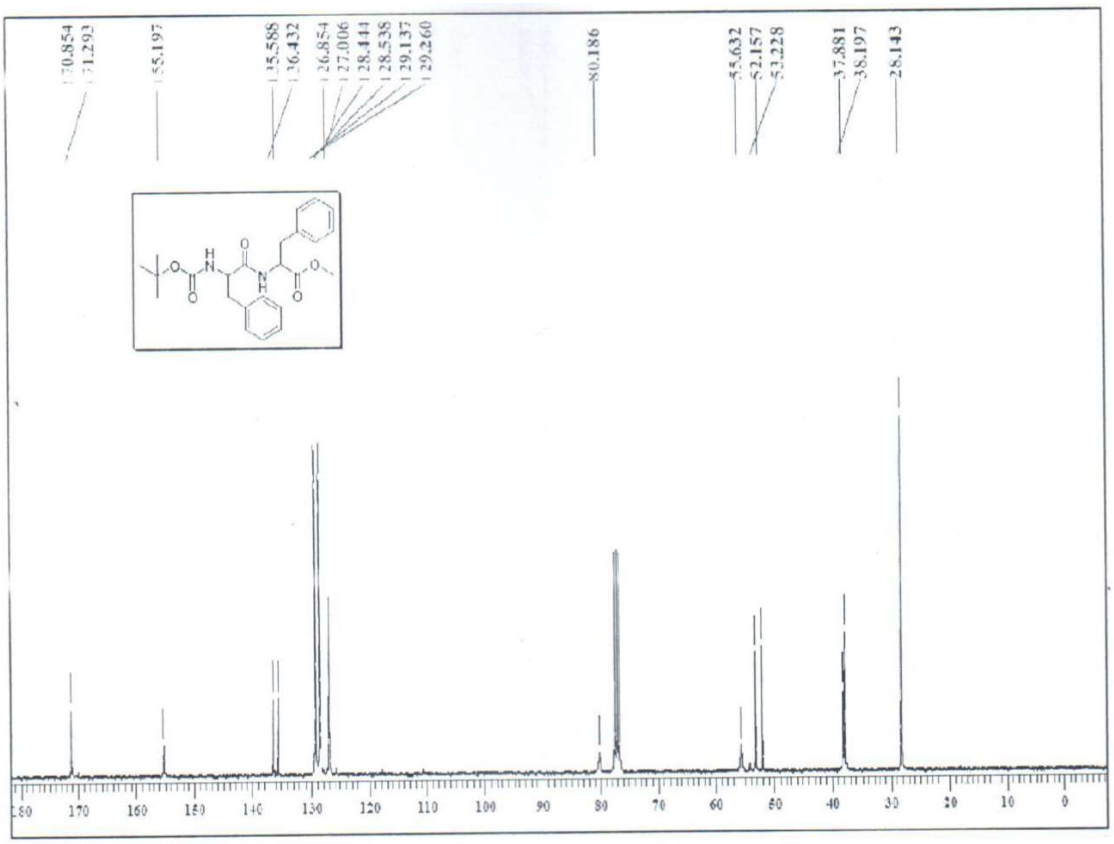


Fig. S2 ^{13}C NMR spectra of compound **3**.

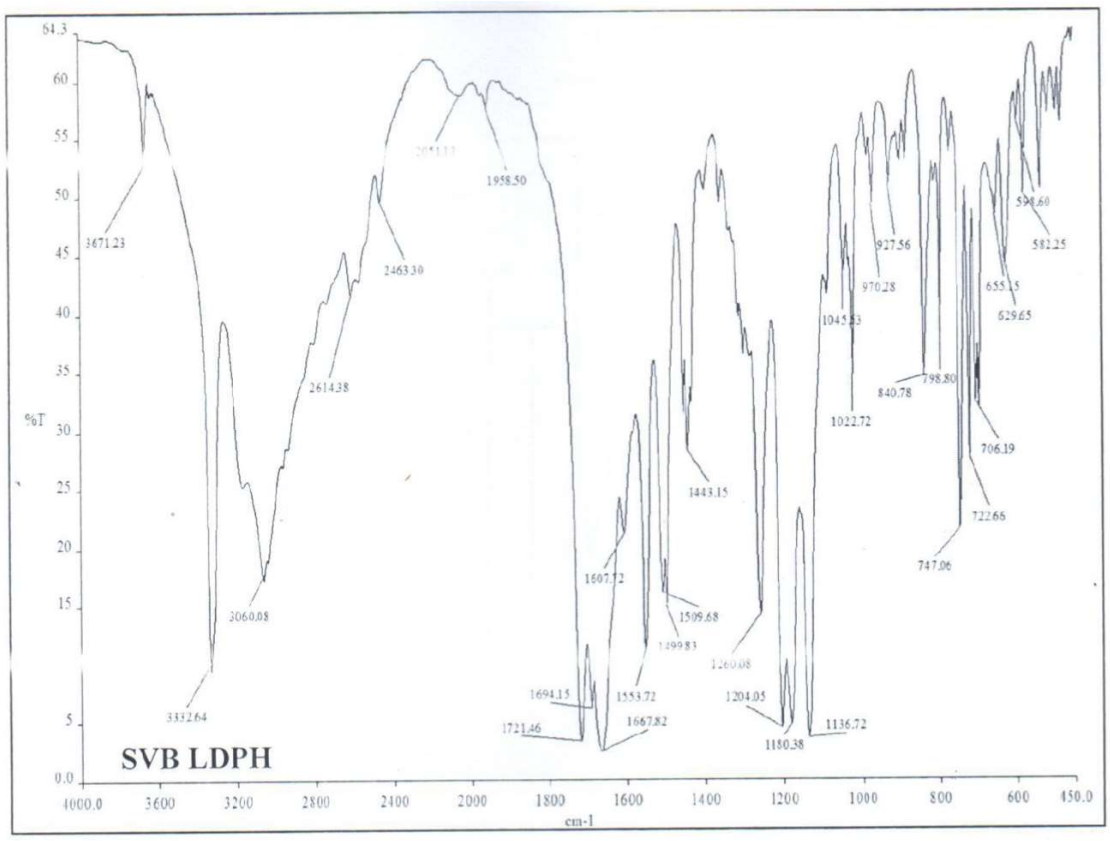


Fig. S3 FT-IR spectra of compound **3**.

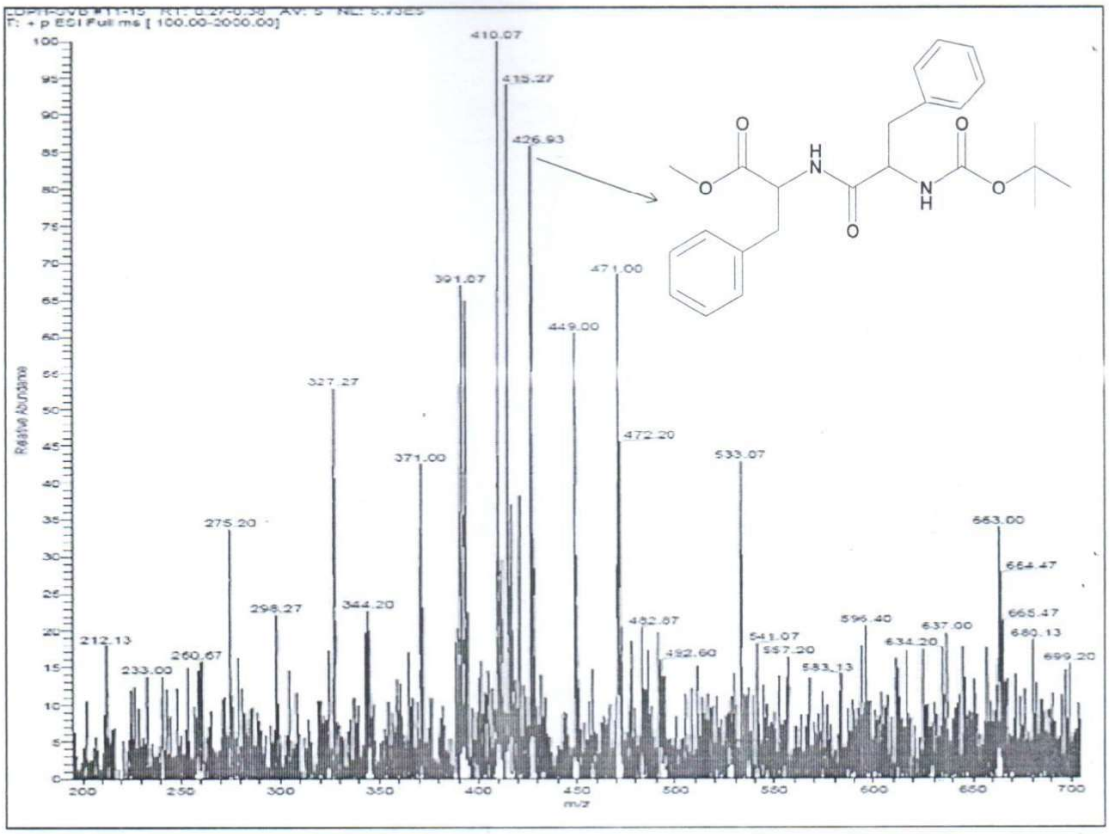


Fig. S4 Mass spectrum of compound **3**.

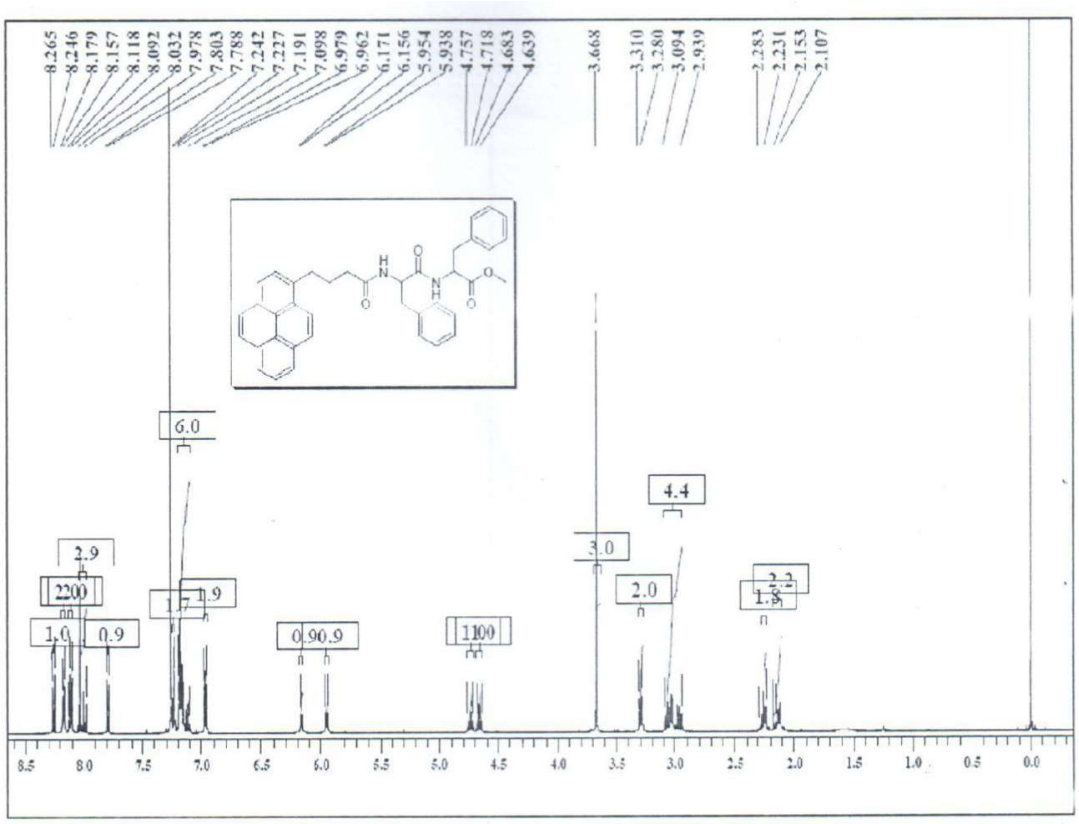


Fig. S5 ^{1}H NMR spectra of compound **5**.

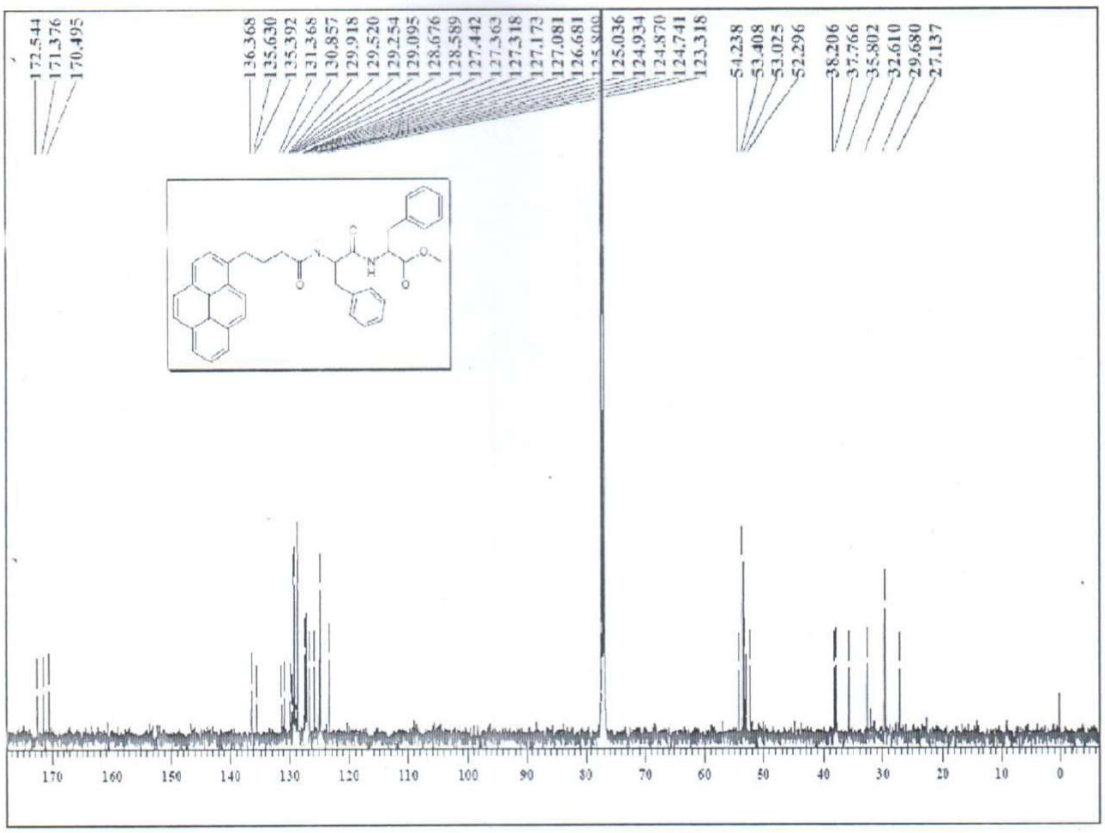


Fig. S6 ^{13}C NMR spectra of compound **5**.

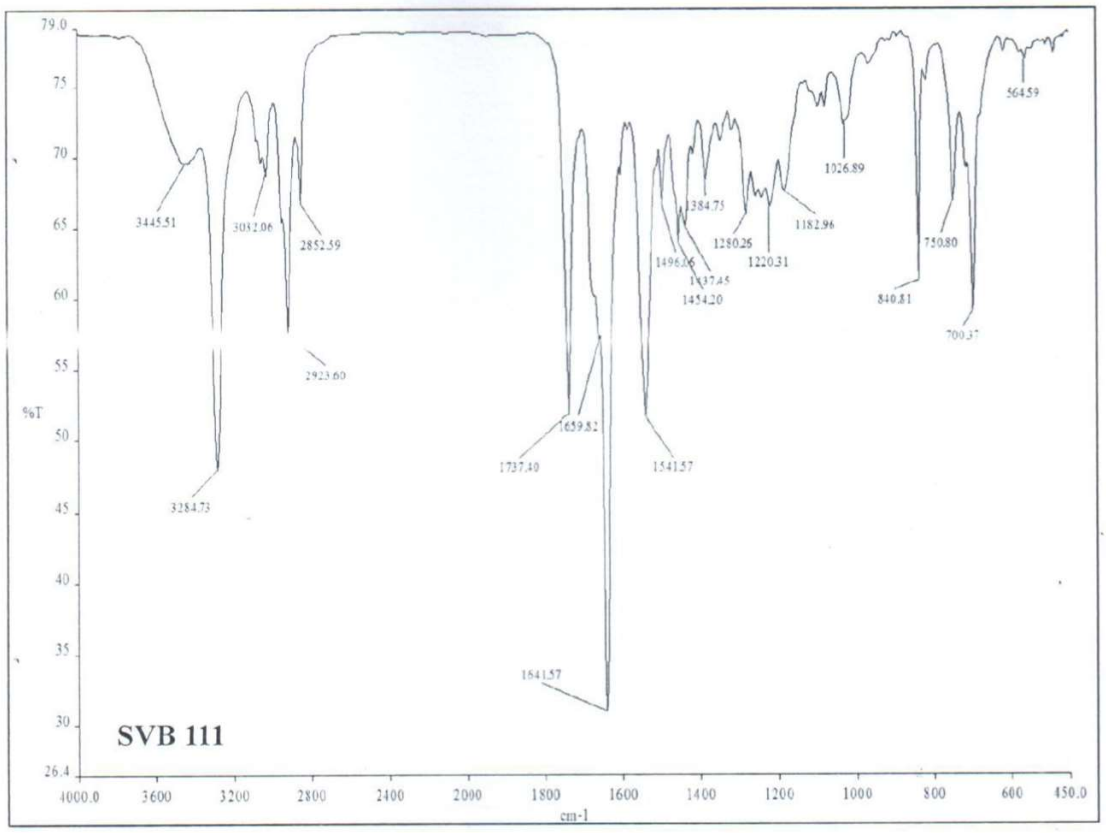


Fig. S7 FT-IR spectra of compound **5**.

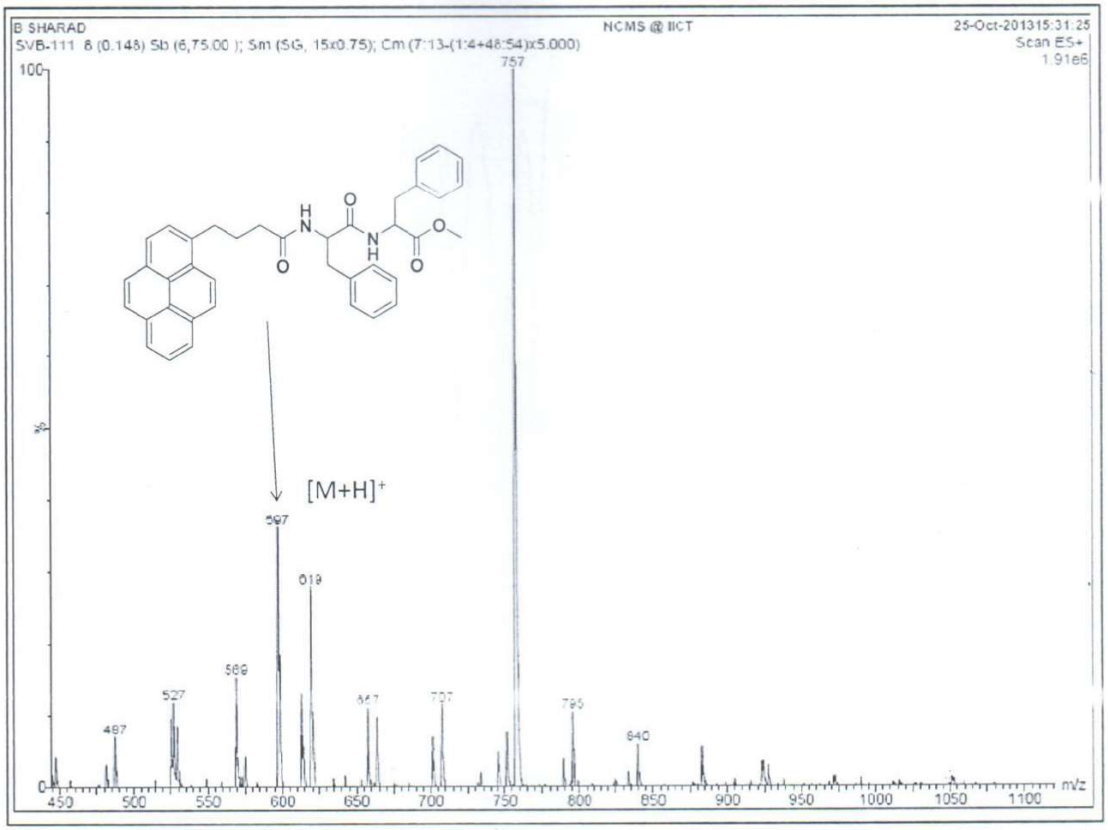


Fig. S8 Mass spectrum of compound **5**.

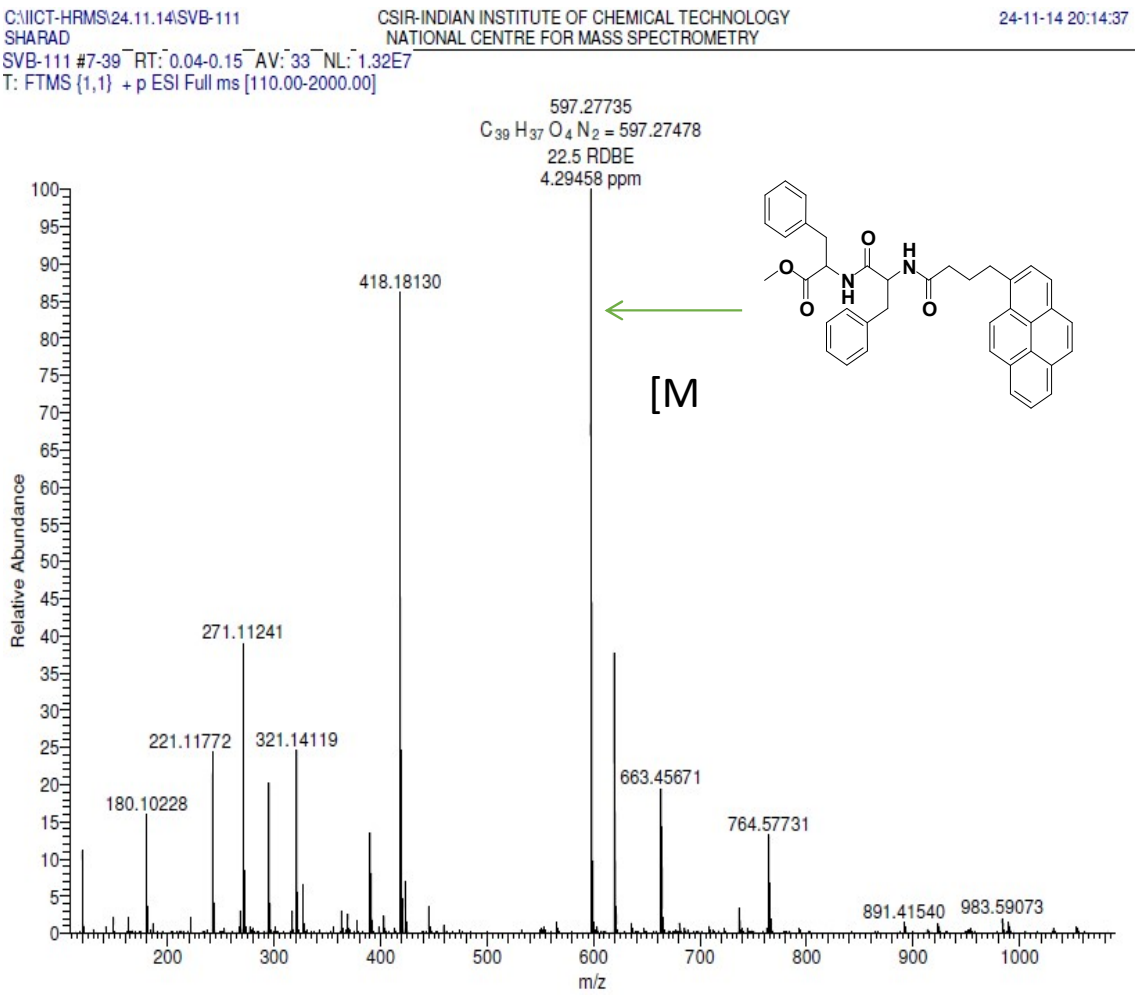


Fig. S9 High resolution mass spectrum (HRMS) of compound **5.**

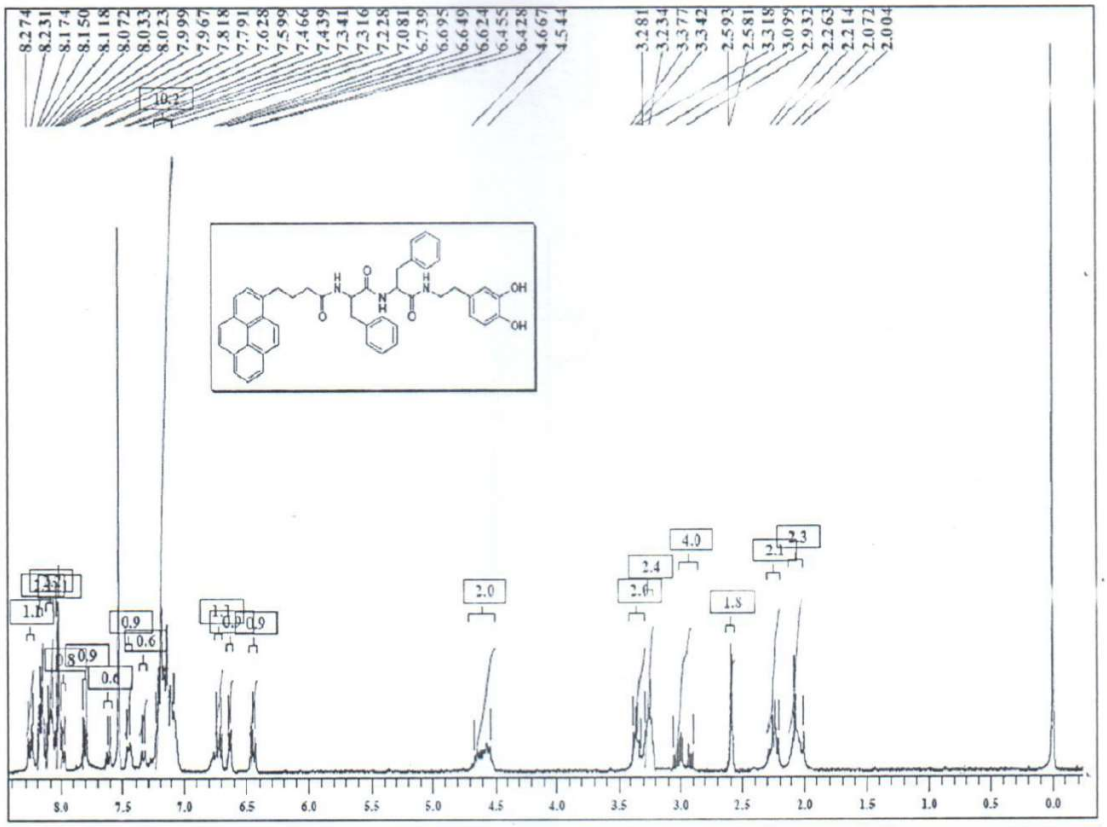


Fig. S10 ^{1}H NMR spectra of compound **Py-F_L-F_L-DP**.

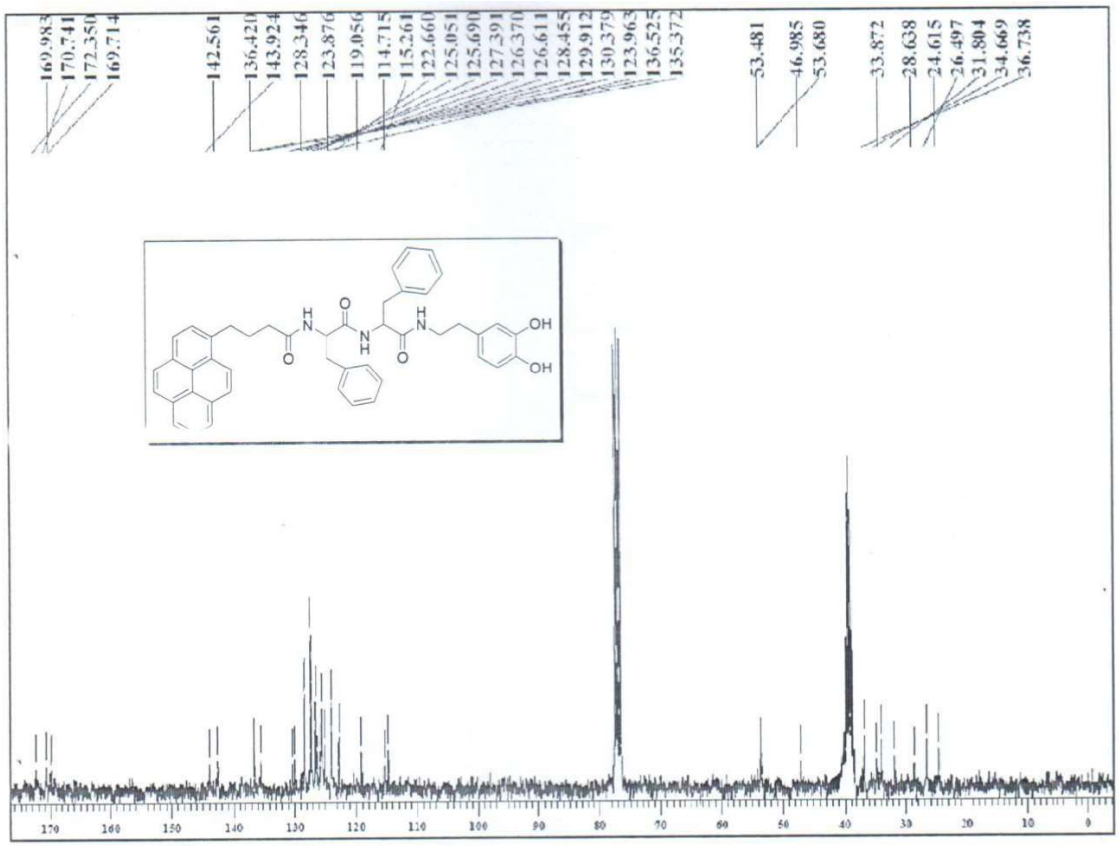


Fig. S11 ^{13}C NMR spectra of compound **Py-FL-FL-DP.**

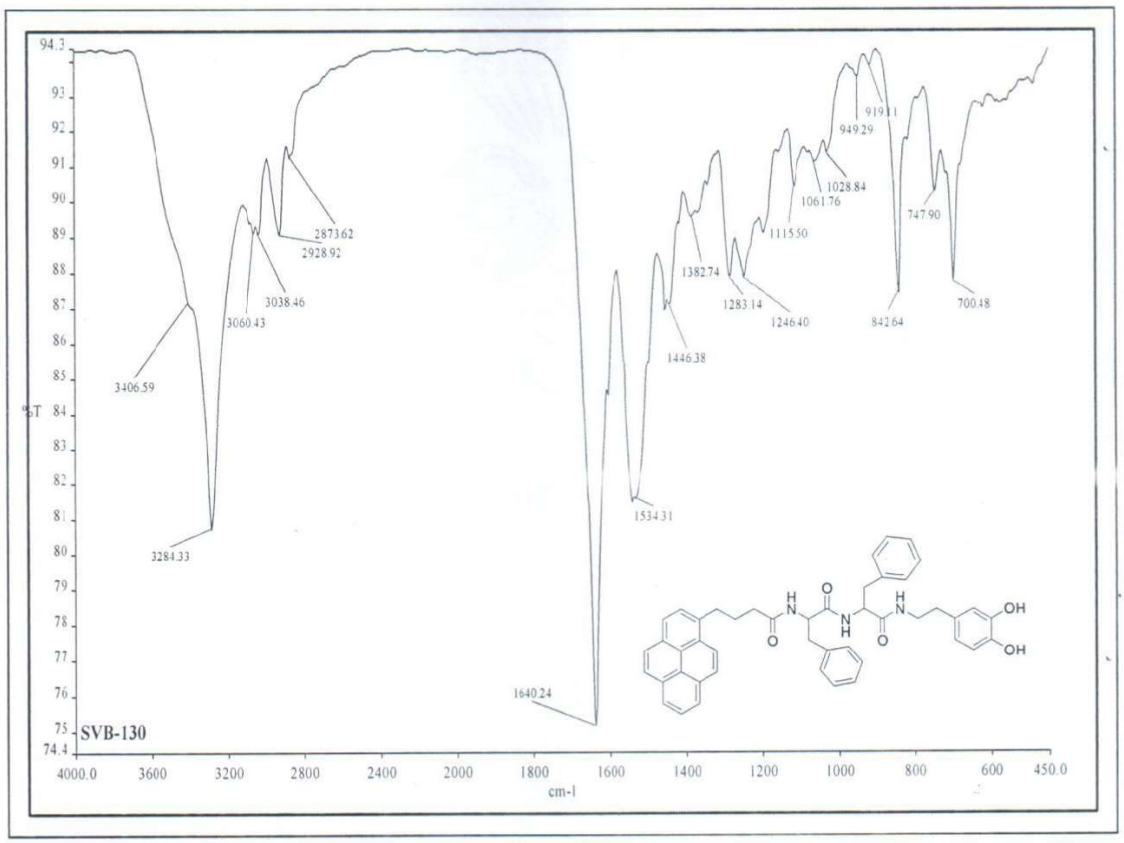


Fig. S12 FT-IR spectra of compound **Py-FL-FL-DP.**

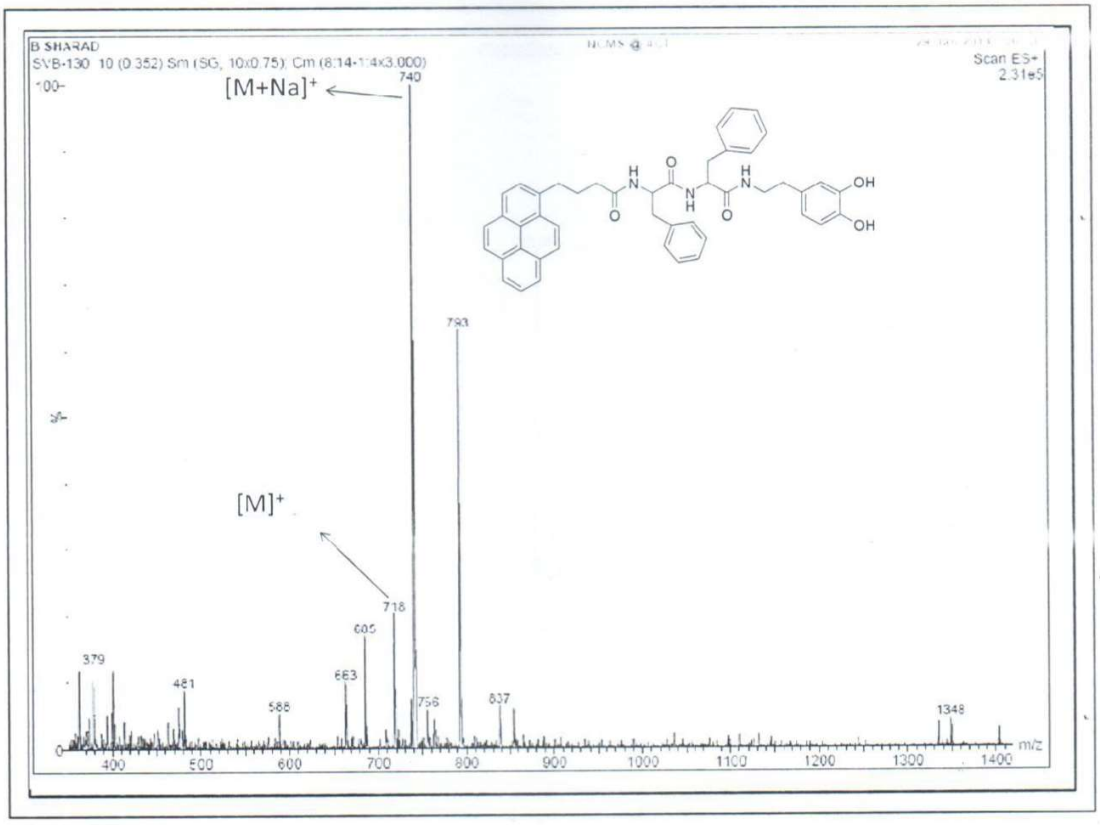


Fig. S13 Mass spectrum of compound **Py-FL-FL-DP.**

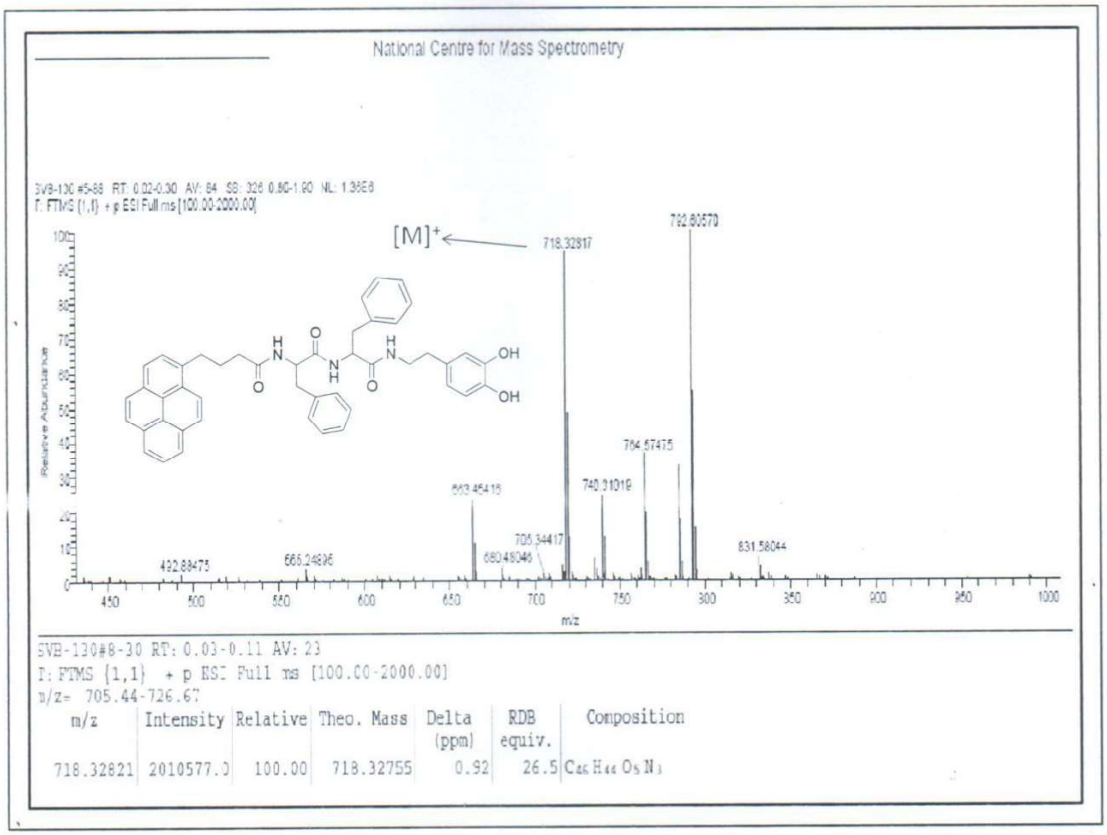
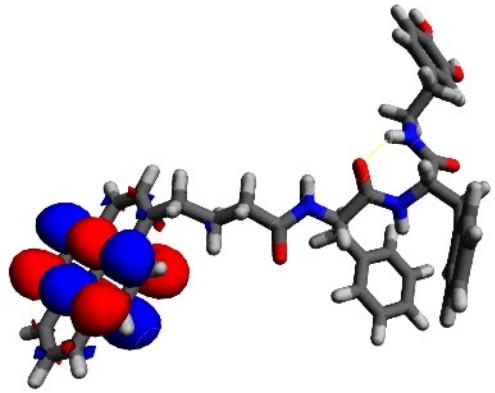
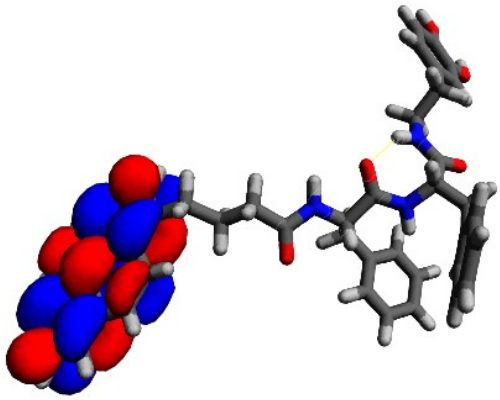
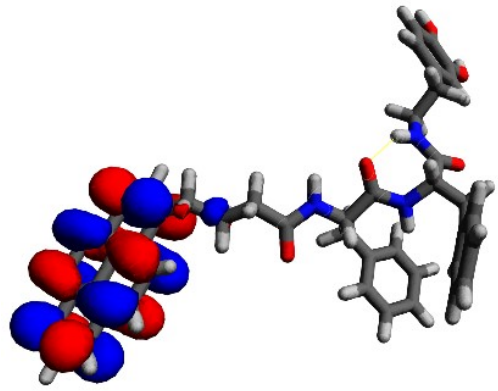
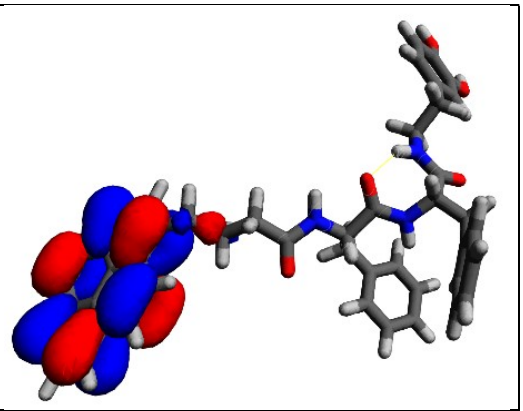
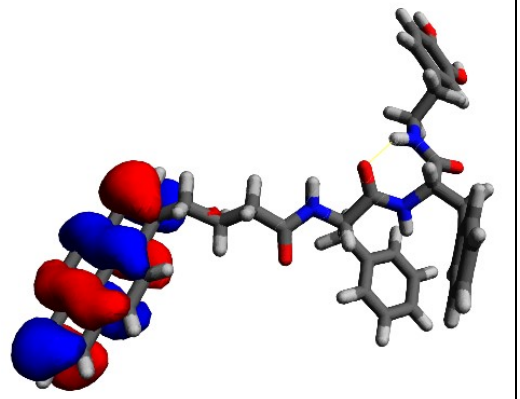
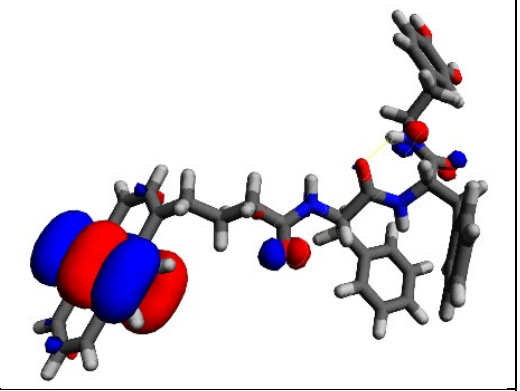


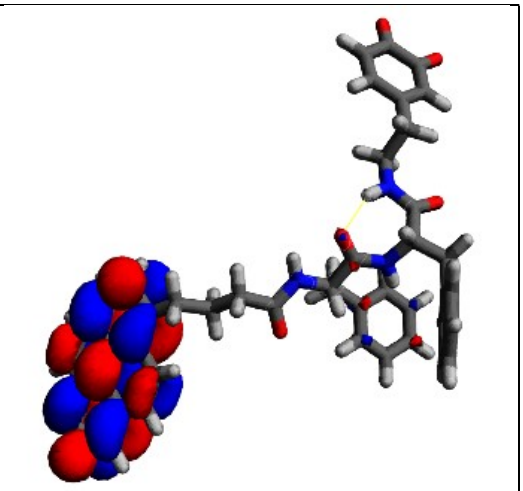
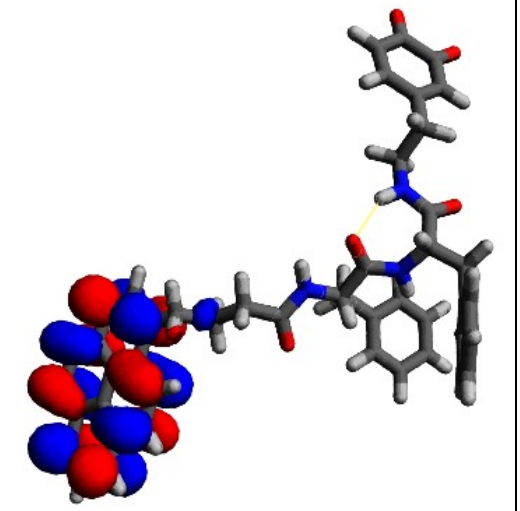
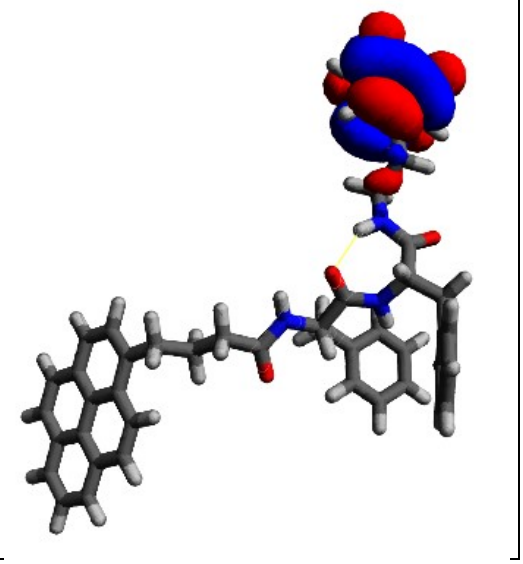
Fig. S14 High resolution mass spectrum (HRMS) of compound **Py-FL-FL-DP.**

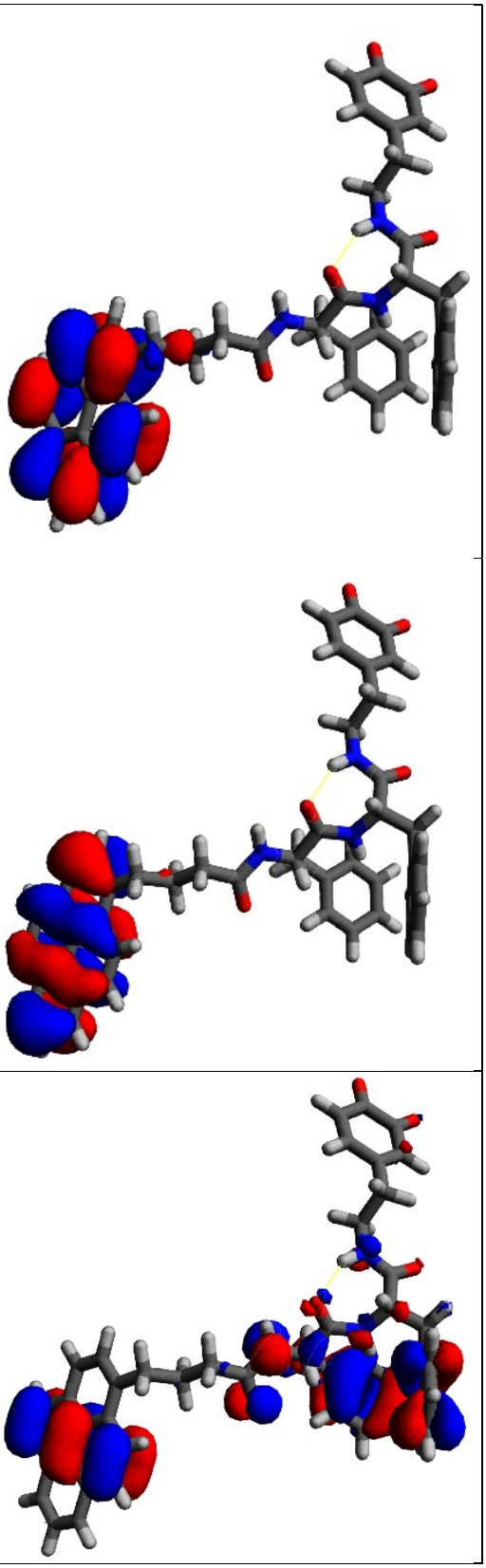
Table S1: Optimised structures, and TD-DFT excitations of **Py-F_LF_L-DP** and **Py-F_LF_L-DQ**

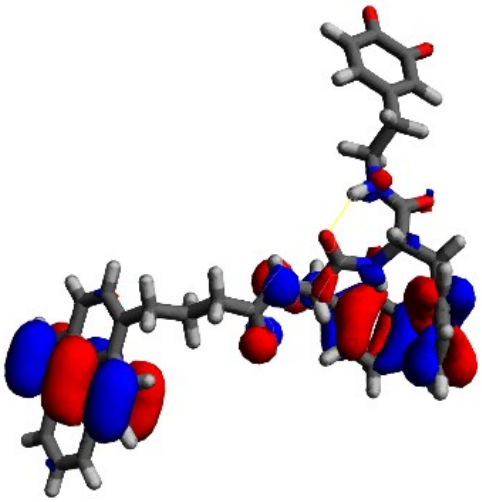
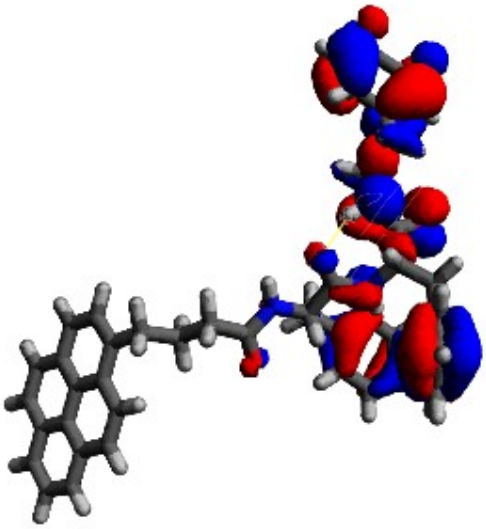
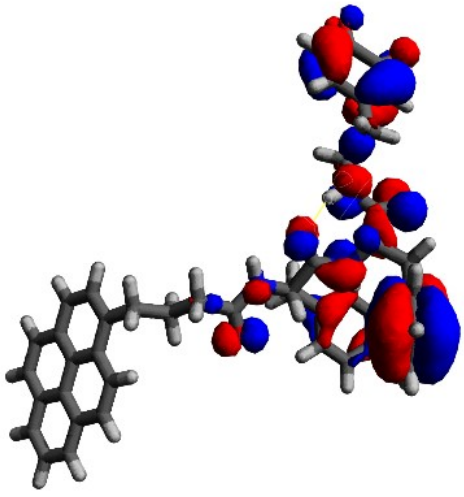
Molecules	**Excitation Energy (eV)**	**Excitation Wavelength (nm)**	**Oscillator Strength (f)**	**Excitations**	**Percentage Contribution for transition**
Py-F_LF_L-DP	3.6335	341.23	0.3301	188 ->192	H-2->L+1 (8%)
				190 ->191	HOMO->LUMO (91%)
	4.6015	269.44	0.1626	182 ->191	H-8->LUMO (39%)
				188 ->191	H-2->LUMO (27%),
				190 ->192	HOMO->L+1 (24%)
				190 ->197	HOMO->L+6 (3%)
	4.6057	269.19	0.1450	182 ->191	H-8->LUMO (43%),
				188 ->191	H-2->LUMO (22%),
				190 ->192	HOMO->L+1 (19%)
				190 ->197	HOMO->L+6 (8%)
Py-F_LF_L-DQ	3.0321	408.91	0.0201	173 ->190	H-16->LUMO (18%)
				181 ->190	H-8->LUMO (20%)
				182 ->190	H-7->LUMO (45%)
				184 ->190	H-5->LUMO (5%)
				185 ->190	H-4->LUMO (7%)
	3.3783	367.00	0.0319	173 ->190	H-16->LUMO (4%),
				176 ->190	H-13->LUMO (34%),
				177 ->190	H-12->LUMO (7%)
				178 ->190	H-11->LUMO (33%),
				180 ->190	H-9->LUMO (19%)
	3.6336	341.22	0.3298	188 ->192	H-1->L+2 (8%)
				189 ->191	HOMO->L+1 (91%)

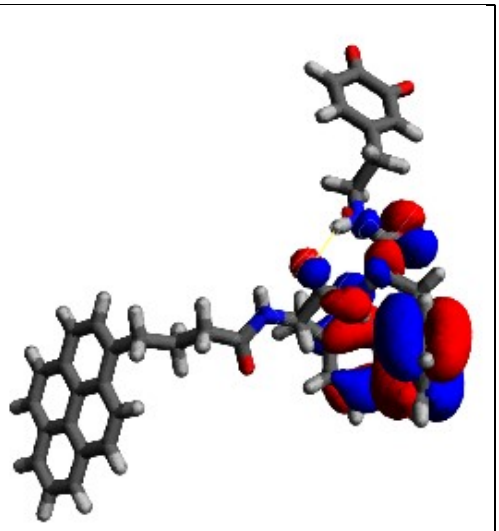
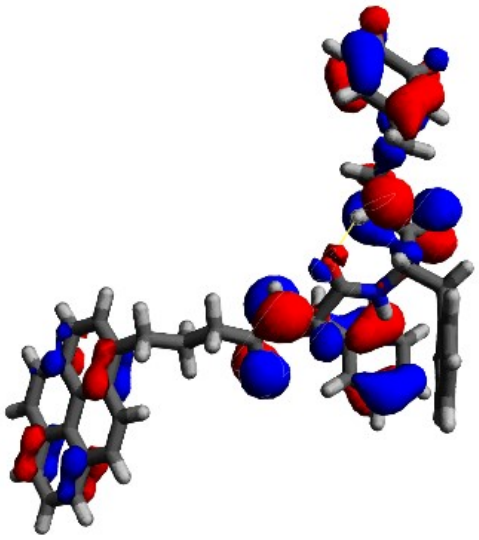
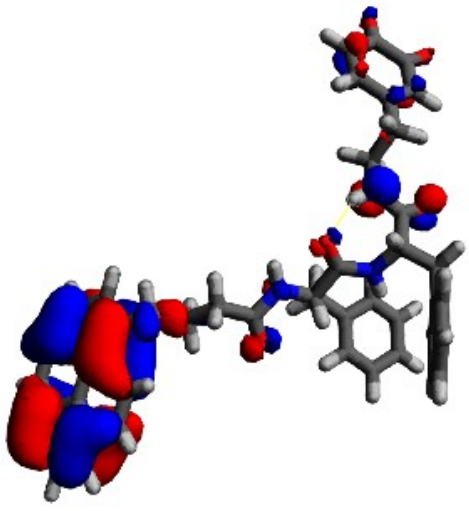
Py-F_LF_L-DP			
Orbital	**Orbital number**	**Energy (eV)**	**Orbital Picture**
L+6	197	+0.012eV	
L+1	192	-0.560eV	
L	191	-1.444eV	

H	190	-5.213eV	
H-2	188	-6.141eV	
H-8	182	-6.798eV	
Py-F_LF_L-DQ			
Orbital	**Orbital number**	**Energy (eV)**	**Orbital Picture**

L+2	192	-0.622eV	
L+1	191	-1506eV	
L	190	-3.415eV	

H	189	-5.274eV	
H-1	188	-6.202eV	
H-4	185	-6.852eV	

H-5	184	-6.857eV	
H-7	182	-6.974eV	
H-8	181	-6.976	

H-9	180	-7.053eV	
H-11	178	-7.279eV	
H-12	177	-7.286eV	

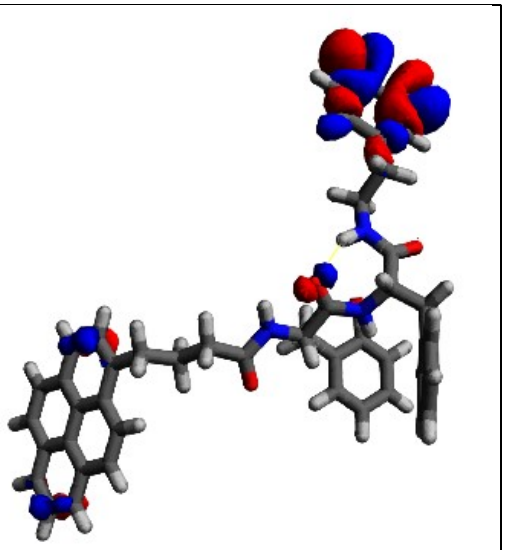
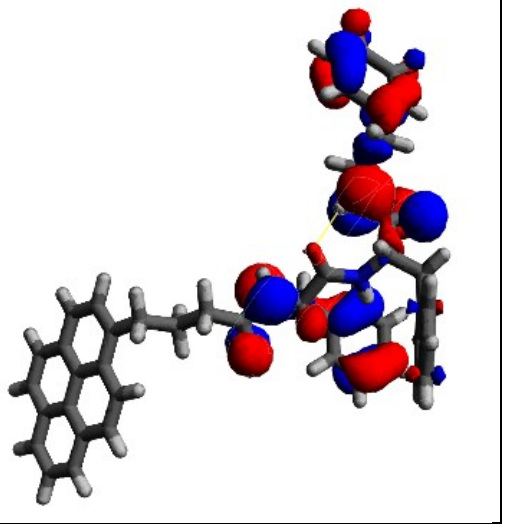
H-13	176	-7.315eV	
H-16	173	-7.962eV	

Fig. S15. Frontier molecular orbitals of **Py-F_LF_L-DP** and **Py-F_LF_L-DQ** with energy in eV**.**

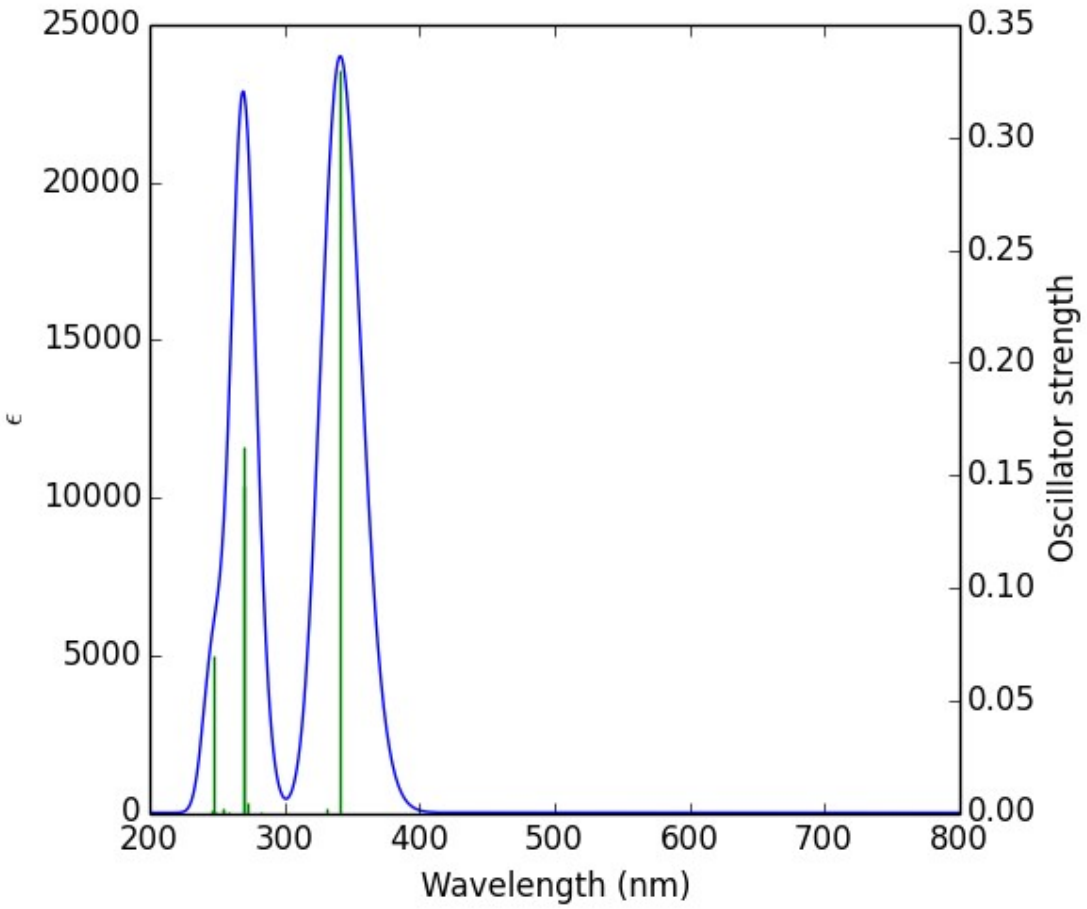


Fig. S16 The computed absorption spectra of **Py-F_LF_L-DP**.

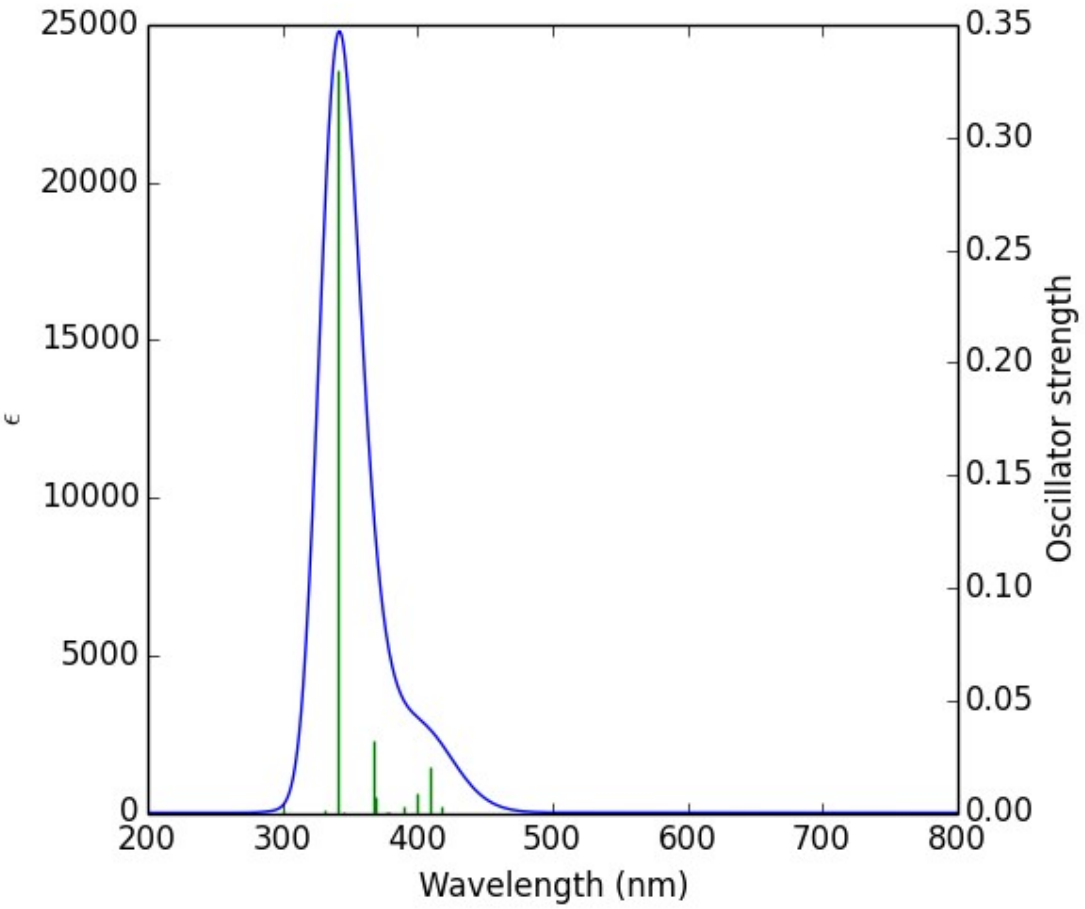


Fig. S17 The computed absorption spectra of **Py-F_LF_L-DQ**.