Supplementary Information

Triphenylamine-merocyanine based D1-A1-π-A2/A3-D2 chromophore system: Synthesis, optoelectronic and theoretical studies

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Keywords: donor-acceptor; cyclic voltammograms; triphenylamine; tetracyanoethylene; 7,7,8,8-tetracyanoquinodimethane

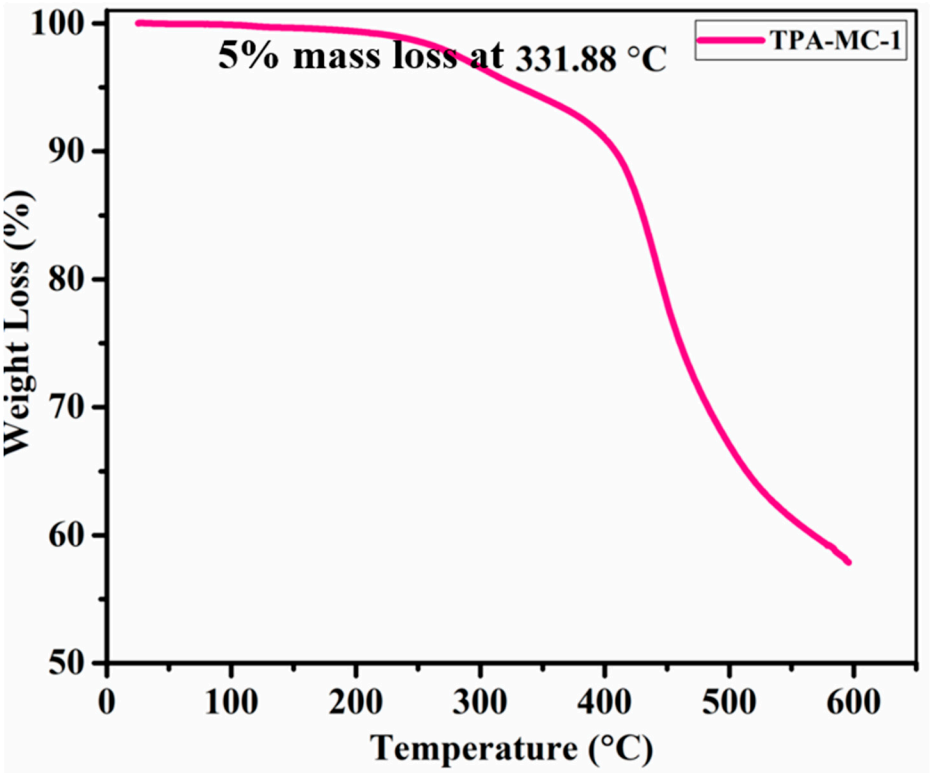


Figure S1. Thermogravimetric analysis (TGA) graph of TPA-MC-1.

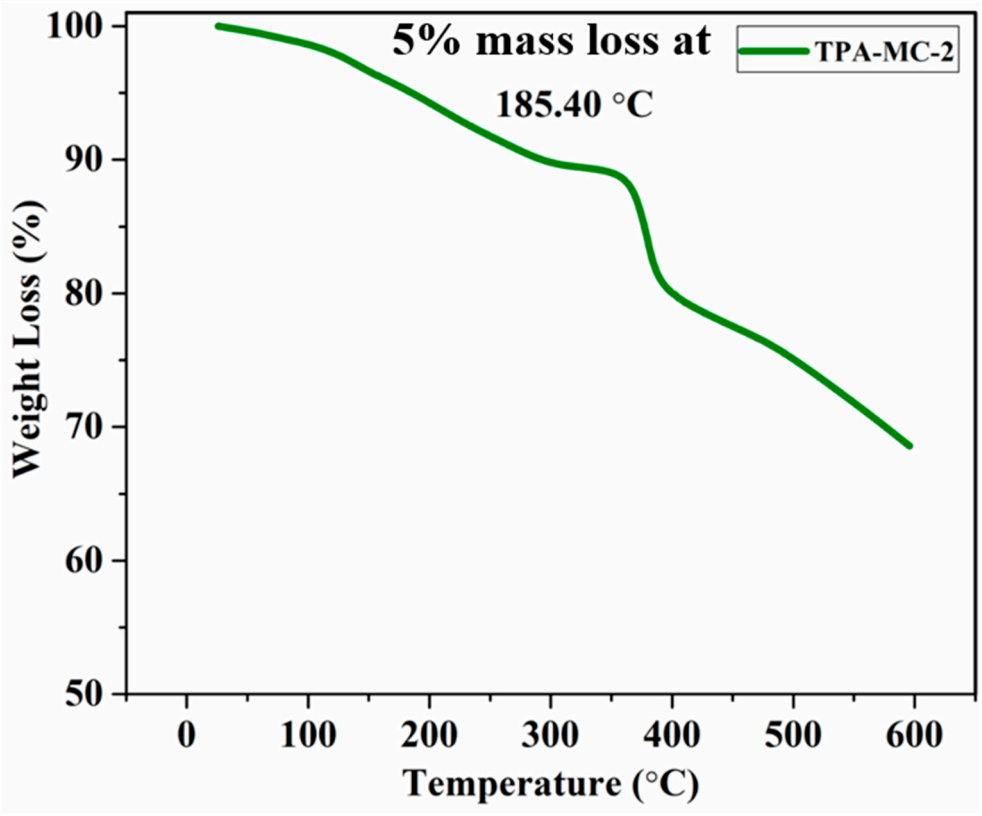


Figure S2. Thermogravimetric analysis (TGA) graph of TPA-MC-2.

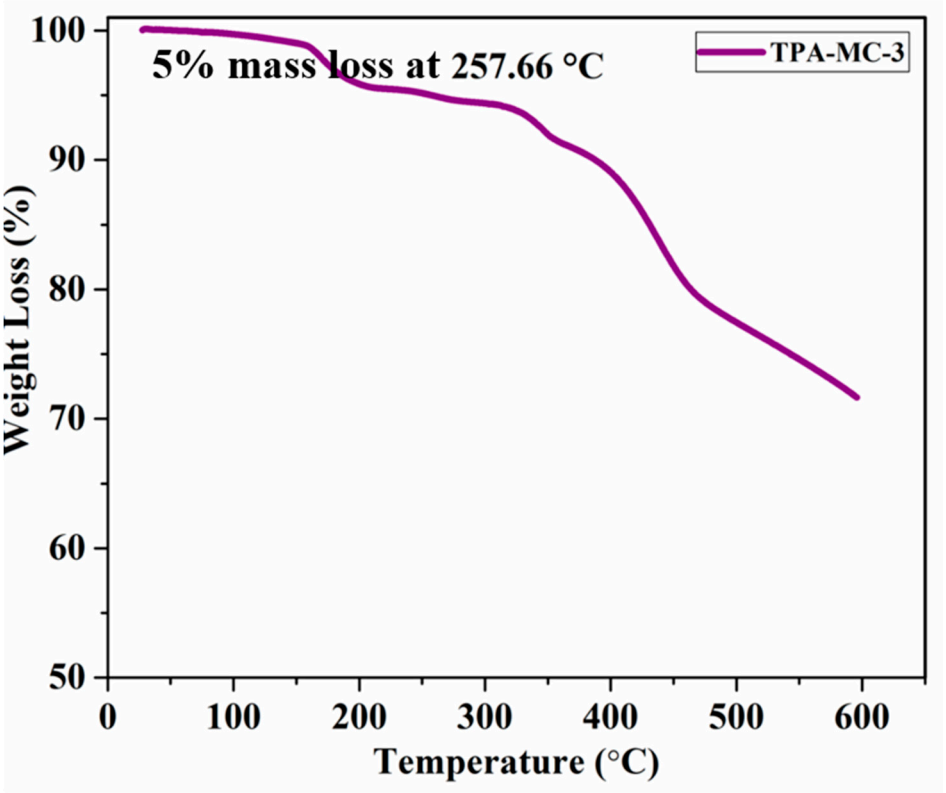
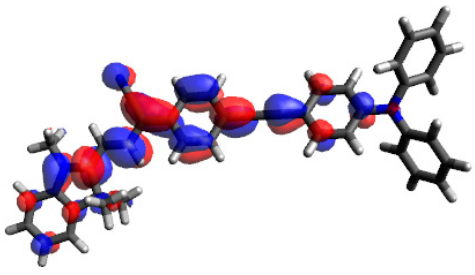
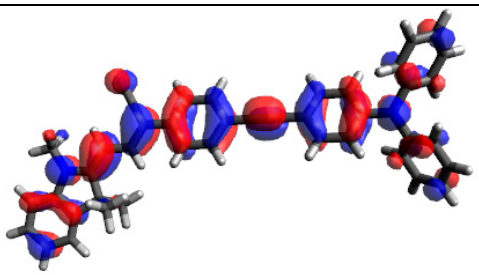
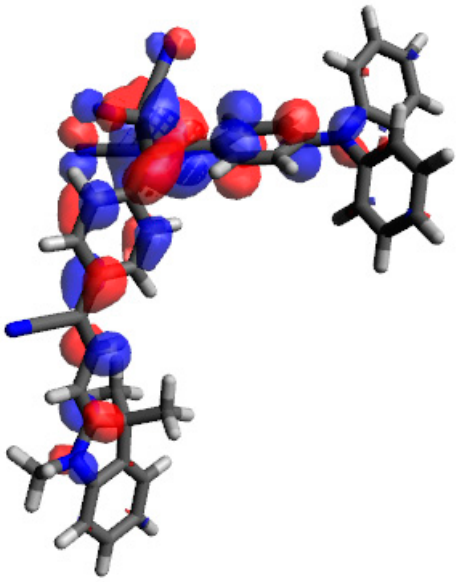
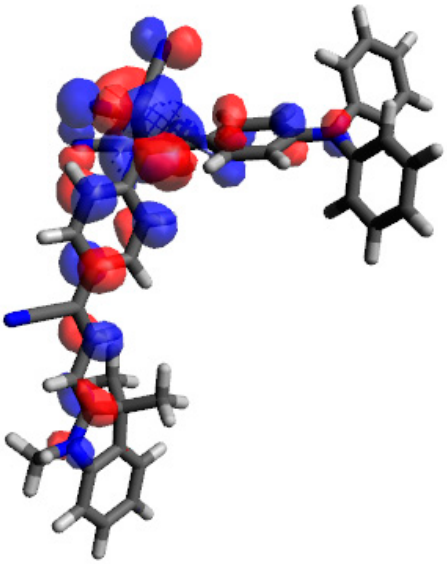


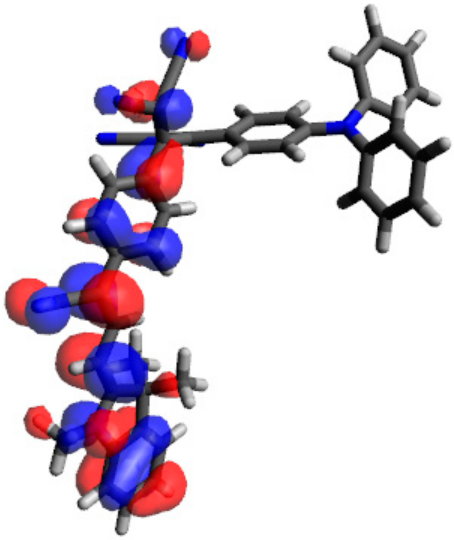
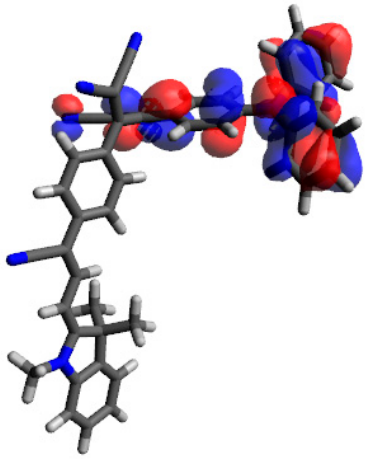
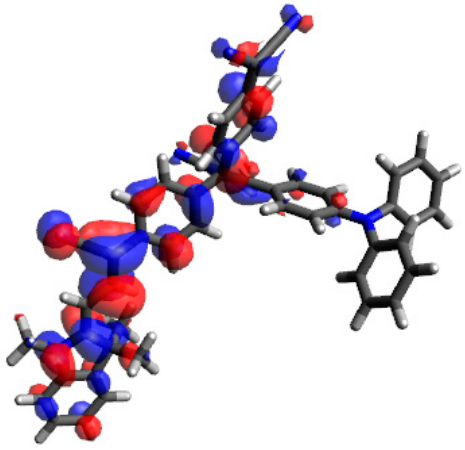
Figure S3. Thermogravimetric analysis (TGA) graph of TPA-MC-3.

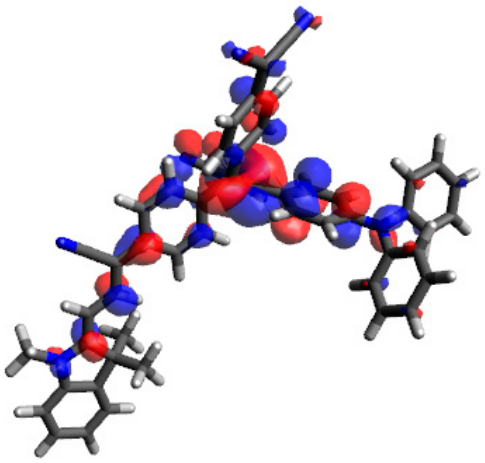
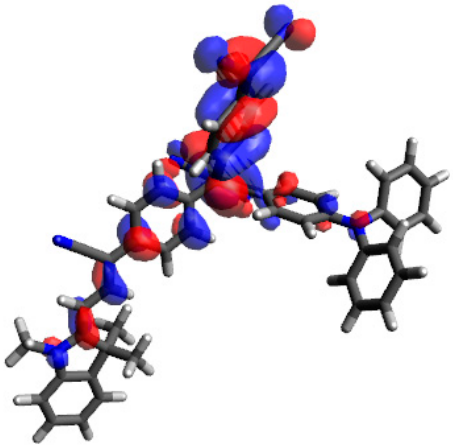
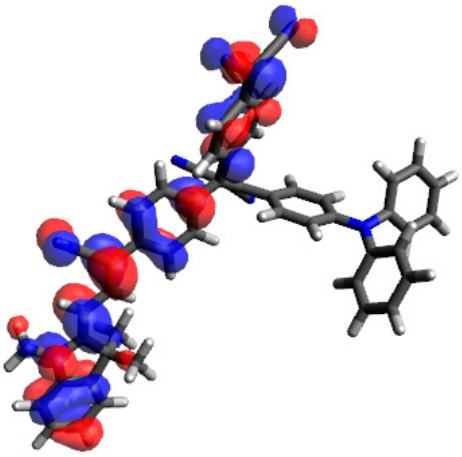
Table S1. Calculated TD-DFT excitation properties of TPA-MC-1, TPA-MC-2 and TPA-MC-3

Molecules	Excitation Energy (eV)	Excitation Wavelength (nm)	Oscillator Strength (f)	Excitations	Percentage contribution for transition
TPA-MC-1	2.5831	479.98	2.1566	150 ->151	HOMO->LUMO (98%)
TPA-MC-2	1.8305	677.34	0.5899	182 ->183	HOMO->LUMO (96%)
				182 ->184	HOMO->L+1 (3%)
	2.2915	541.06	0.7965	182 ->183	HOMO->LUMO (3%)
				182 ->184	HOMO->L+1 (93%)
	2.6517	467.57	0.6391	181 ->183	H-1->LUMO (4%)
				181 ->184	H-1->L+1 (93%)
TPA-MC-3	1.4538	852.85	1.0404	202 ->203	HOMO->LUMO (98%)
	2.2895	541.52	0.9685	200 ->203	H-2->LUMO (50%)
				202 ->204	HOMO->L+1 (44%)
	2.6822	462.25	0.6986	199 ->203	H-3->LUMO (5%)
				200 ->203	H-2->LUMO (2%)
				201 ->204	H-1->L+1 (85%)
				202 ->205	HOMO->L+2 (5%)

TPA-MC-1		**eV**	
L	151	-1.90127	

H	150	-4.81428	
TPA-MC-2			
184	L+1	-2.64034	
183	L	-3.15355	

182	H	-5.25919	
181	H-1	-5.60641	
TPA-MC-3			
205	L+2	-1.93175	

204	L+1	-2.5519	
203	L	-3.57397	
202	H	-5.18	

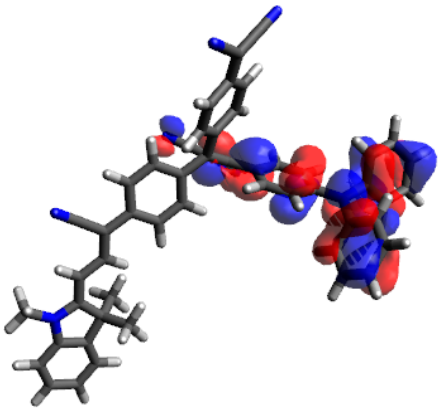
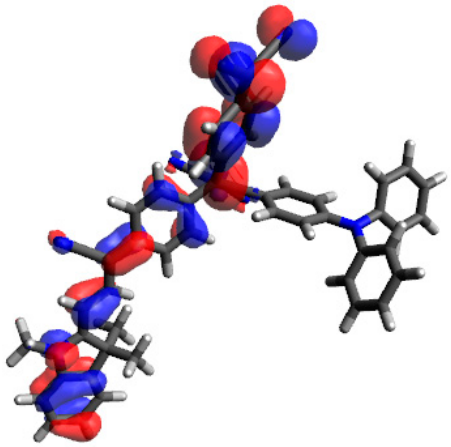
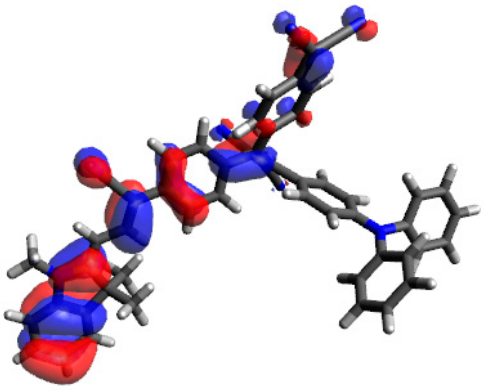
201	H-1	-5.56804	
200	H-2	-5.96533	
199	H-3	-6.78929	

Figure S4. Frontier molecular orbitals of TPA-MC-1, TPA-MC-2 and TPA-MC-3 with energy in eV**.**

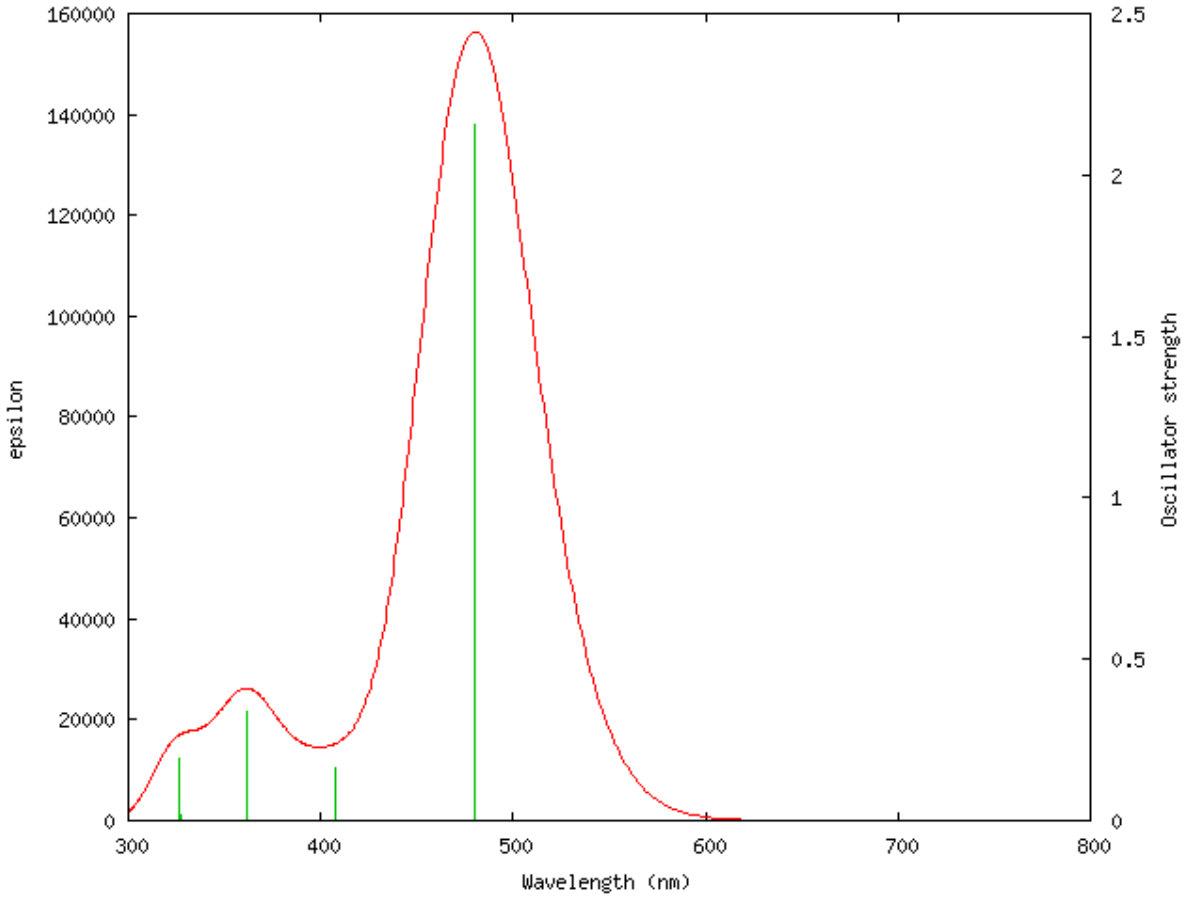


Figure S5. The computed absorption spectra of TPA-MC-1.

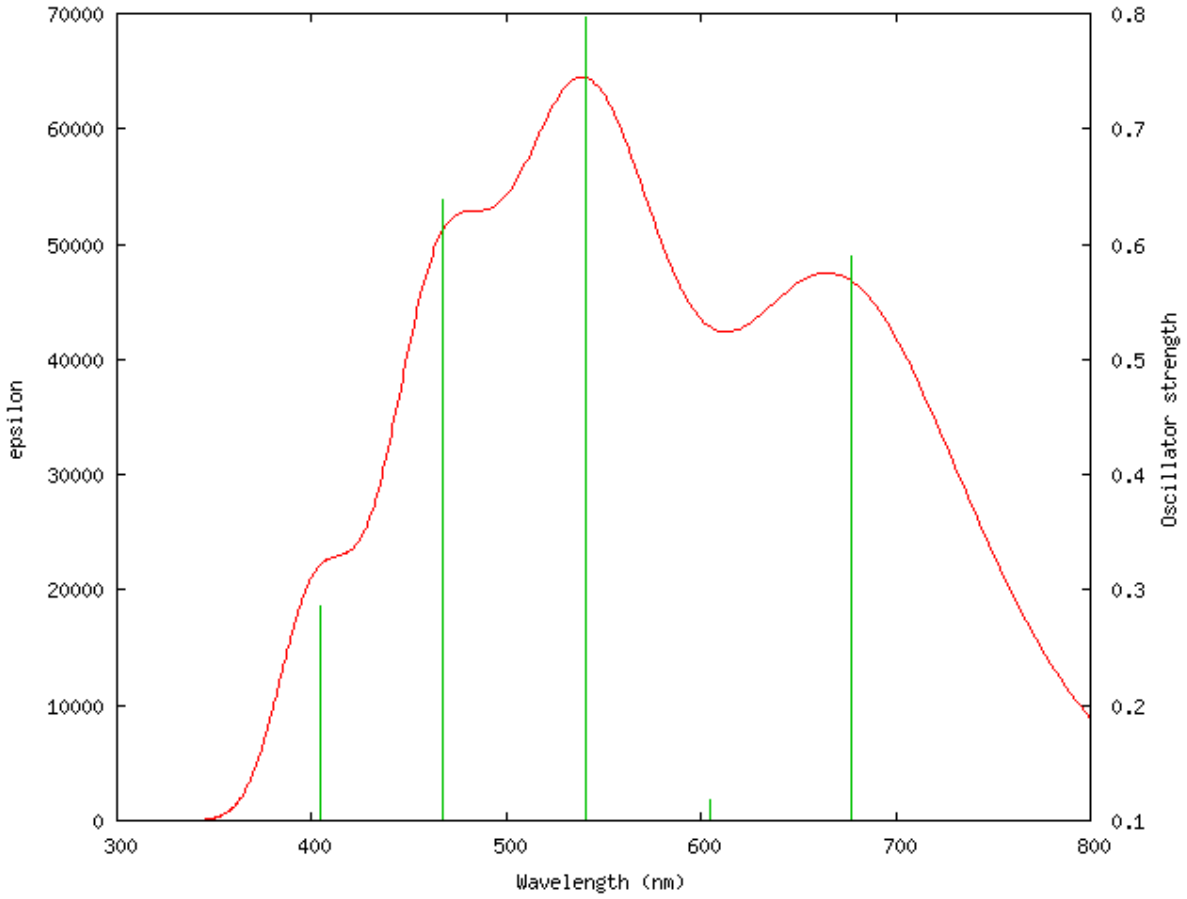


Figure S6. The computed absorption spectra of TPA-MC-2.

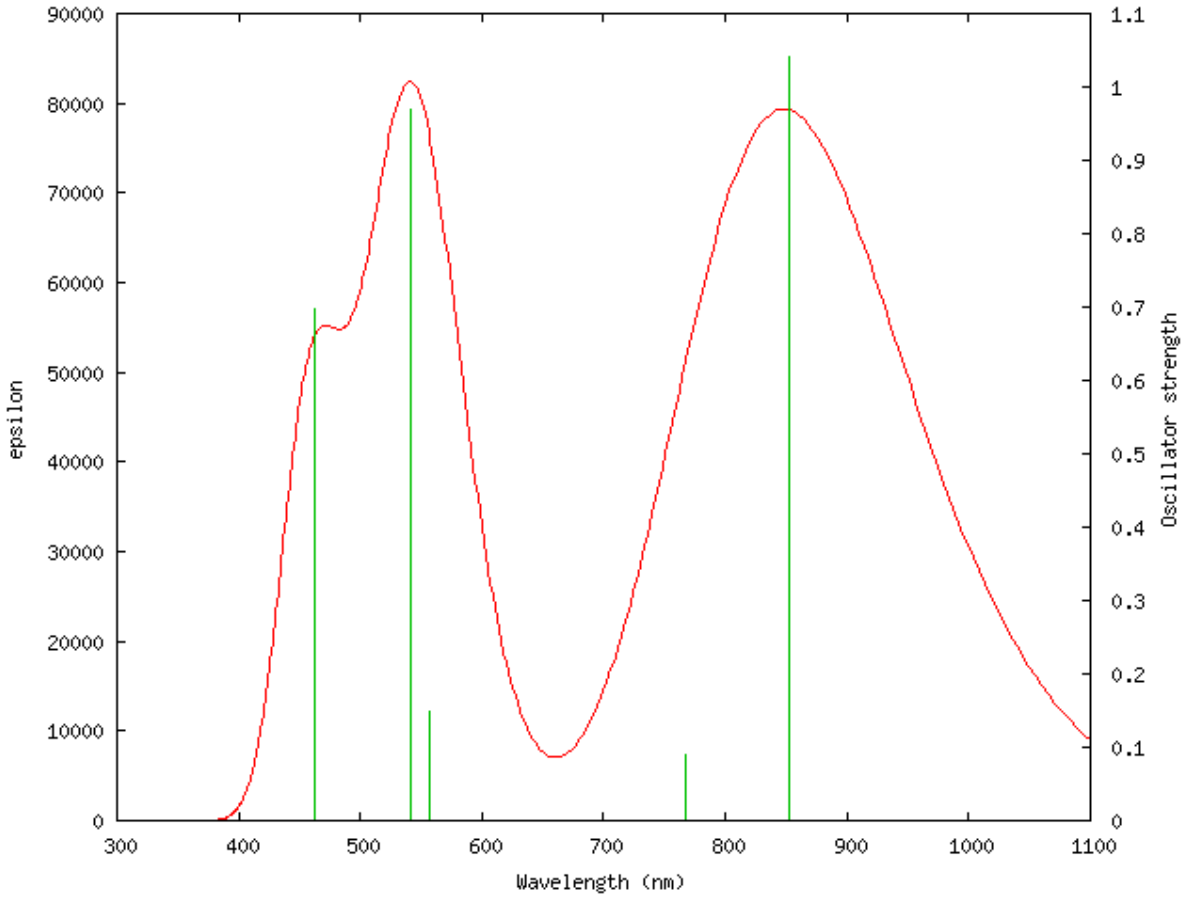


Figure S7. The computed absorption spectra of TPA-MC-3.

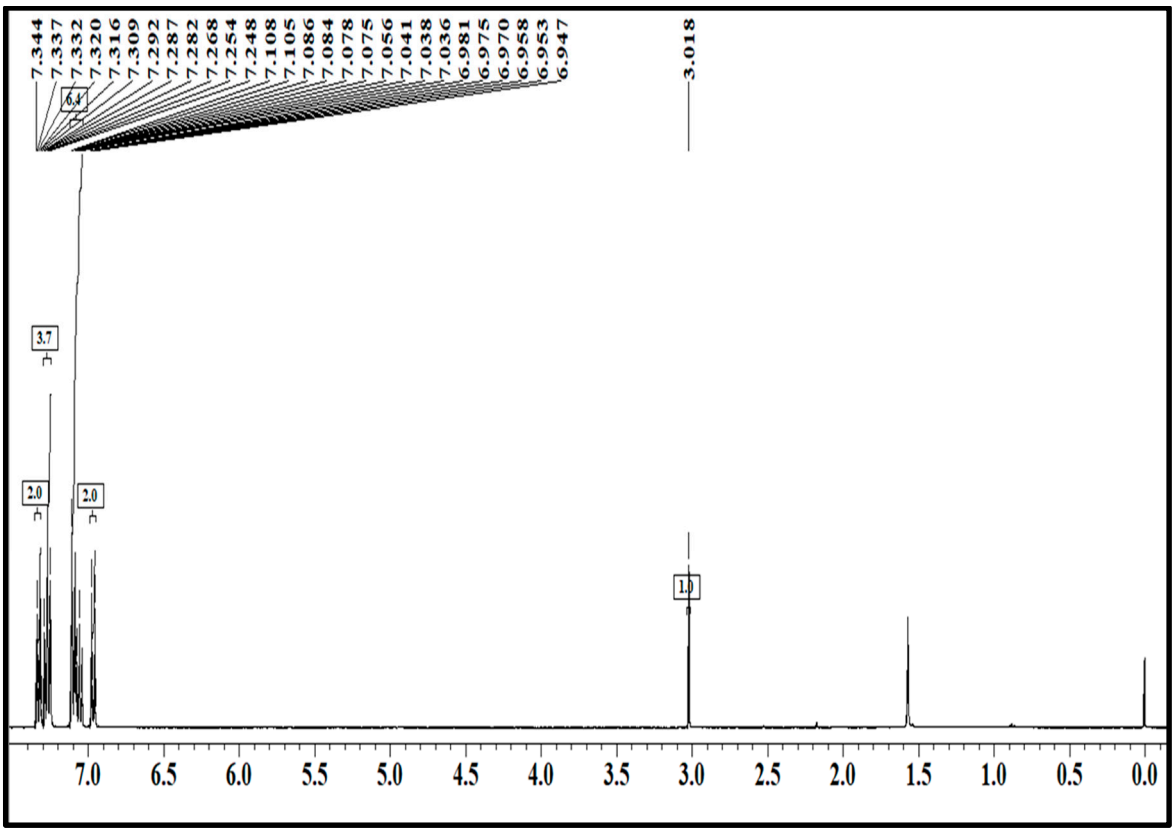


Figure S8. ^{1}H NMR spectra of compound 3.

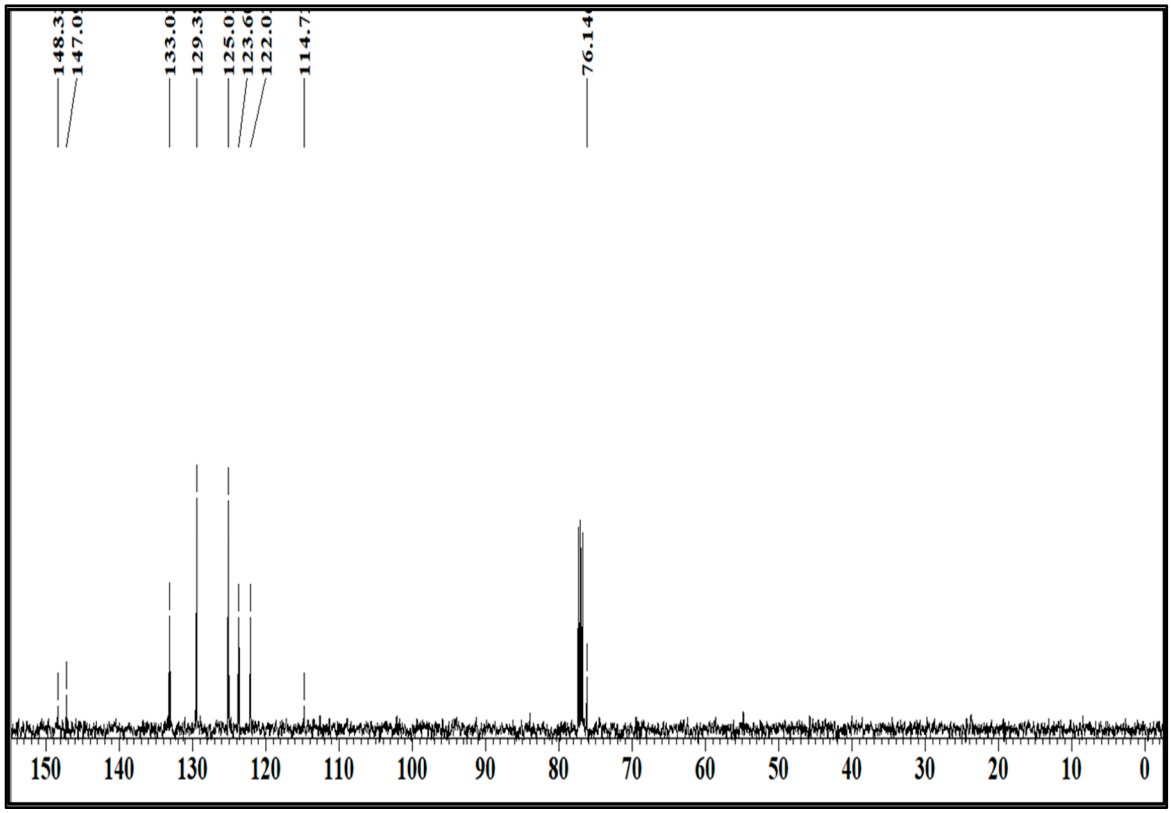


Figure S9. ^{13}C NMR spectra of compound 3.

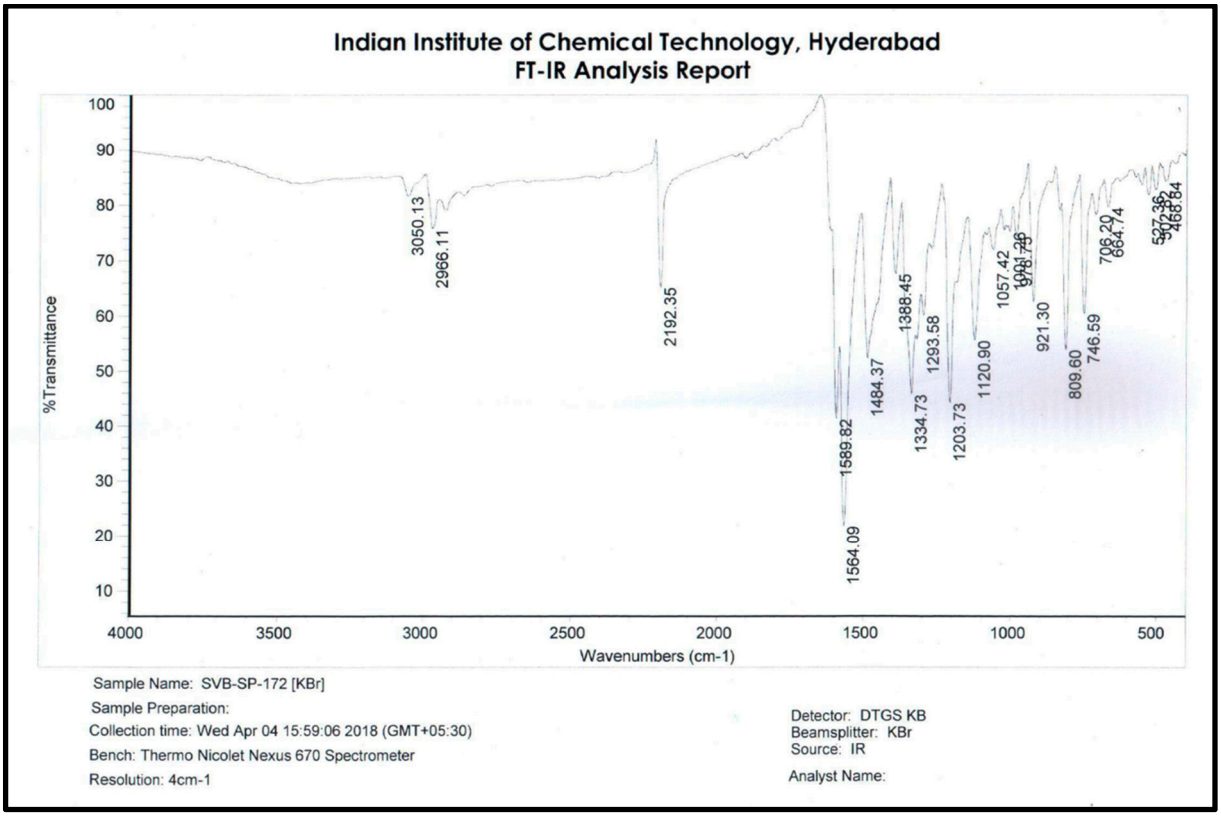


Figure S10. FT-IR spectra of compound 4.

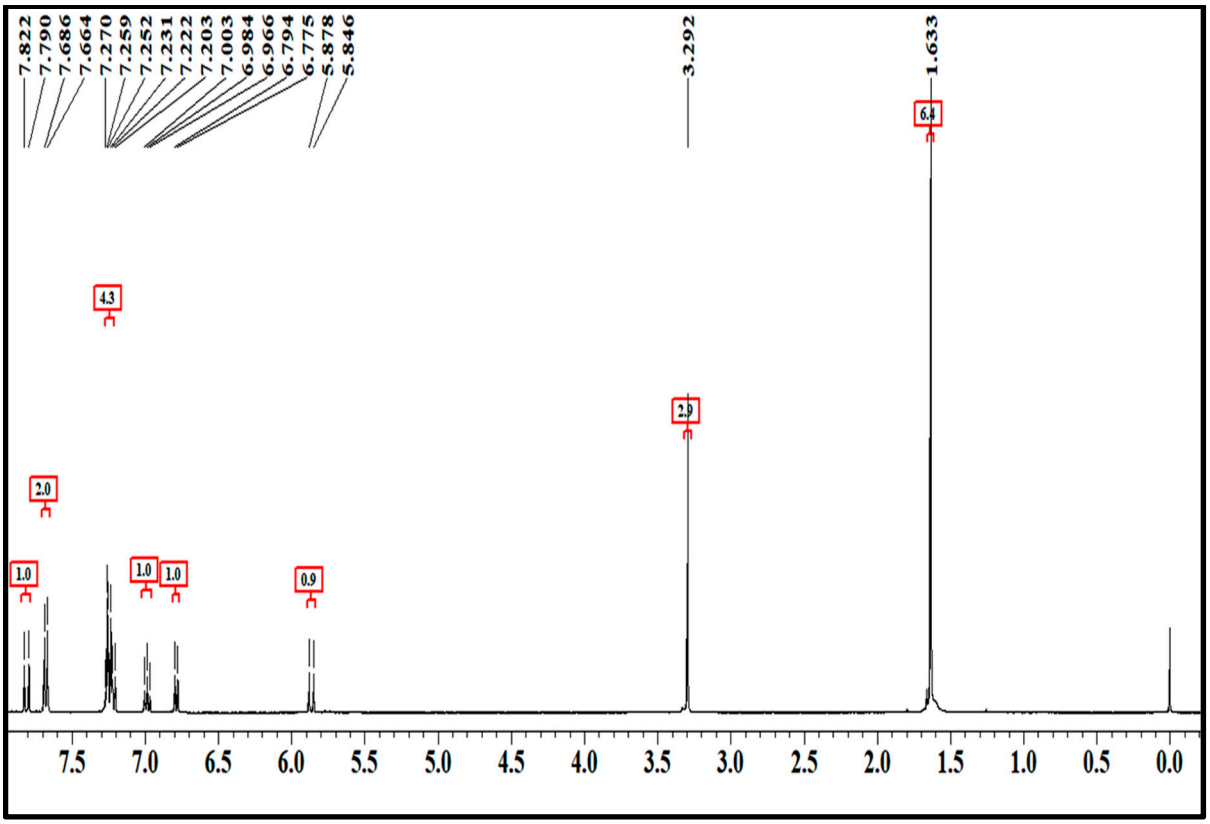


Figure S11. ^{1}H NMR spectra of compound 4.

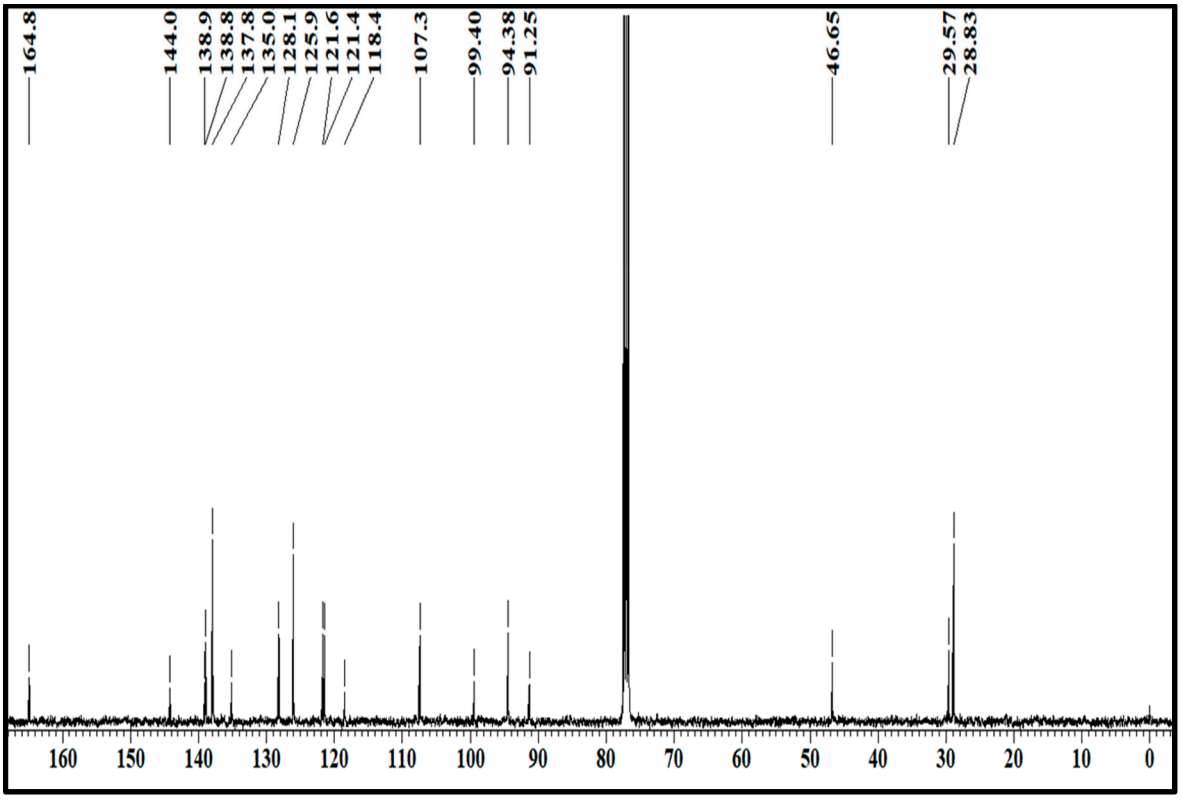


Figure S12. ^{13}C NMR spectra of compound 4.

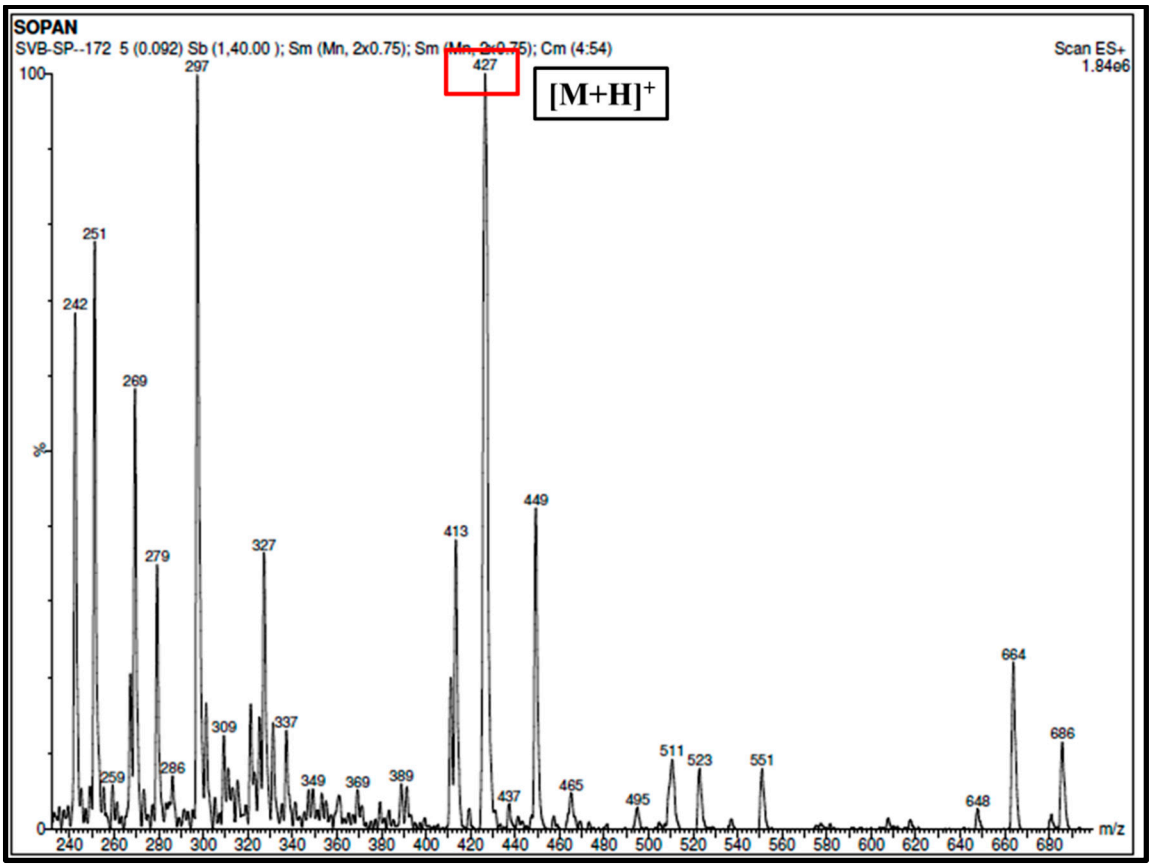


Figure S13. ESI-Mass of Compound 4.

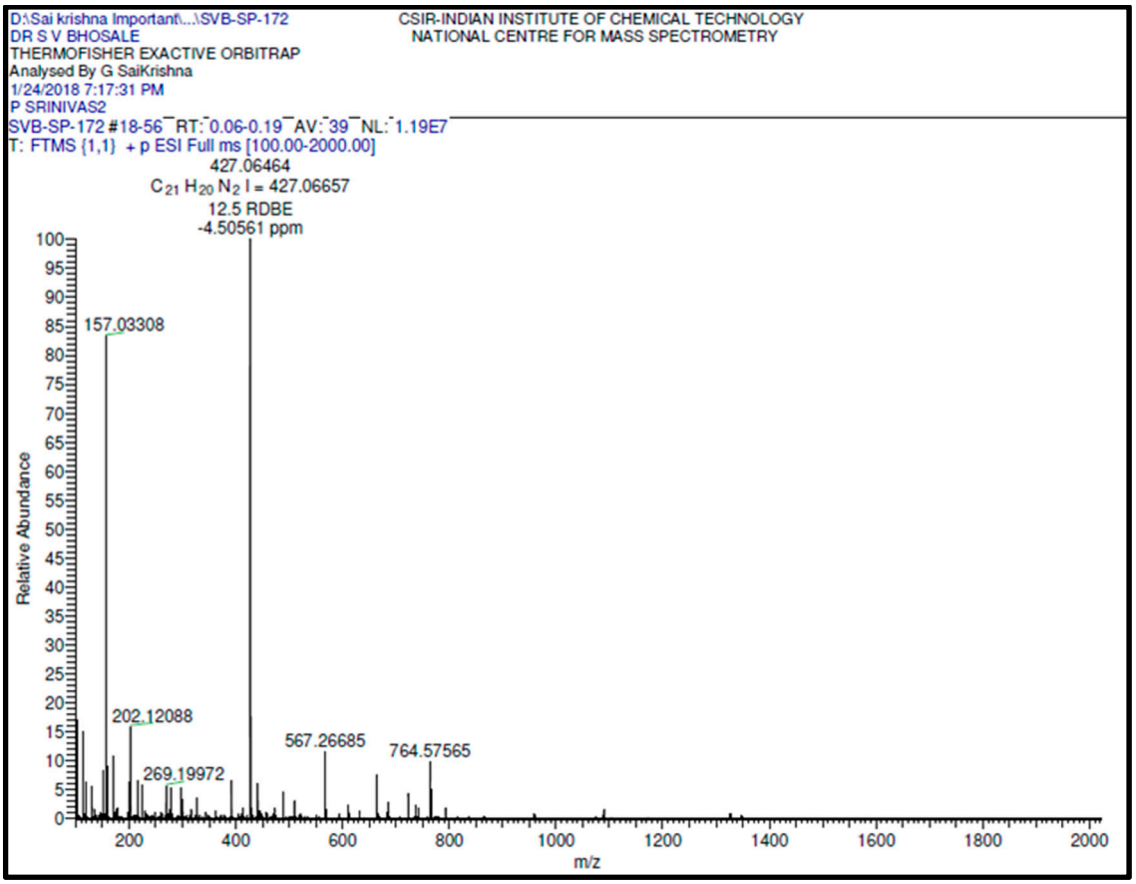


Figure S14. HRMS of Compound 4.

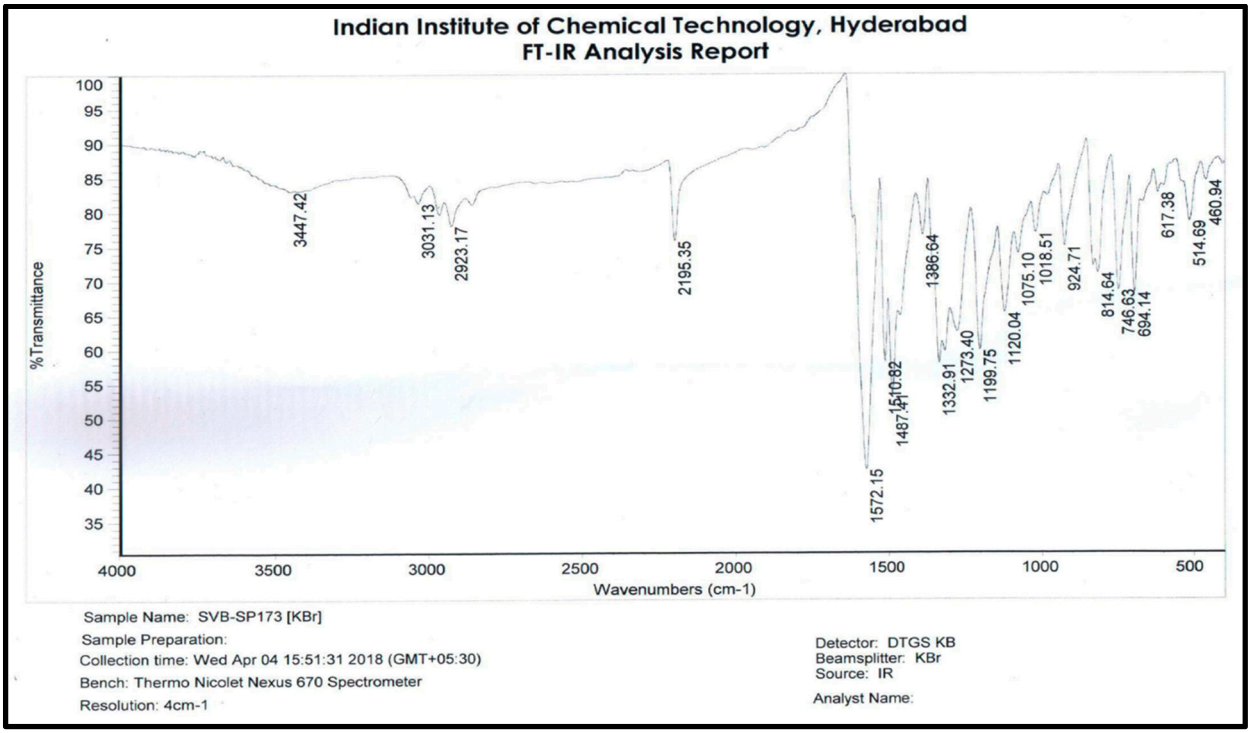


Figure S15. FT-IR spectra of compound TPA-MC-1.

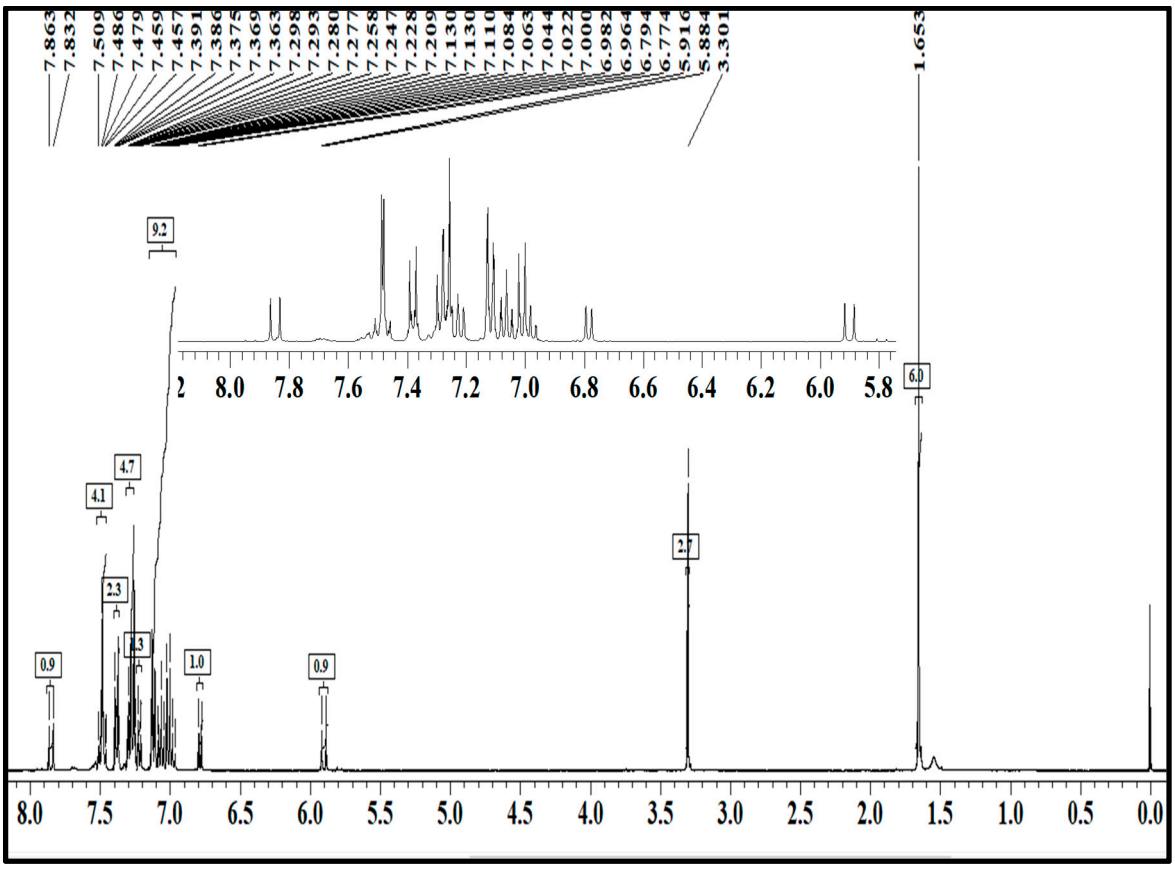


Figure S16. ^{1}H NMR spectra of TPA-MC-1.

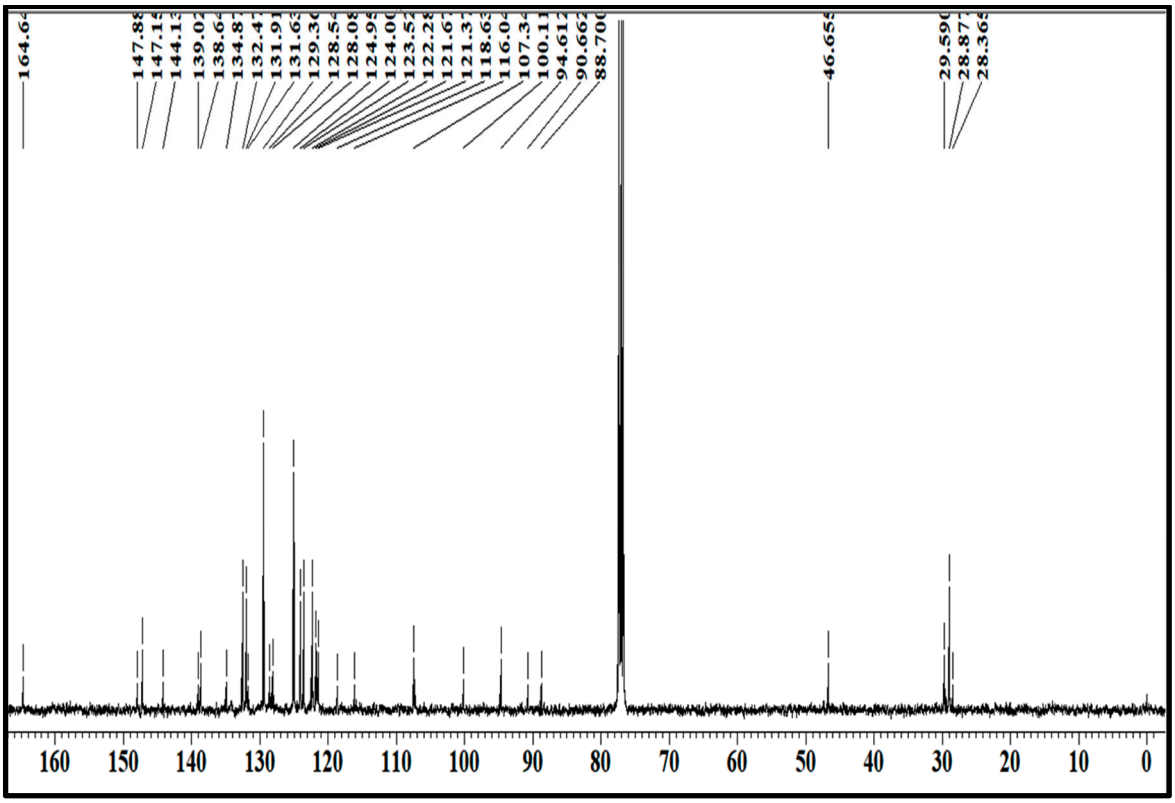


Figure S17. ^{13}C NMR spectra of TPA-MC-1.

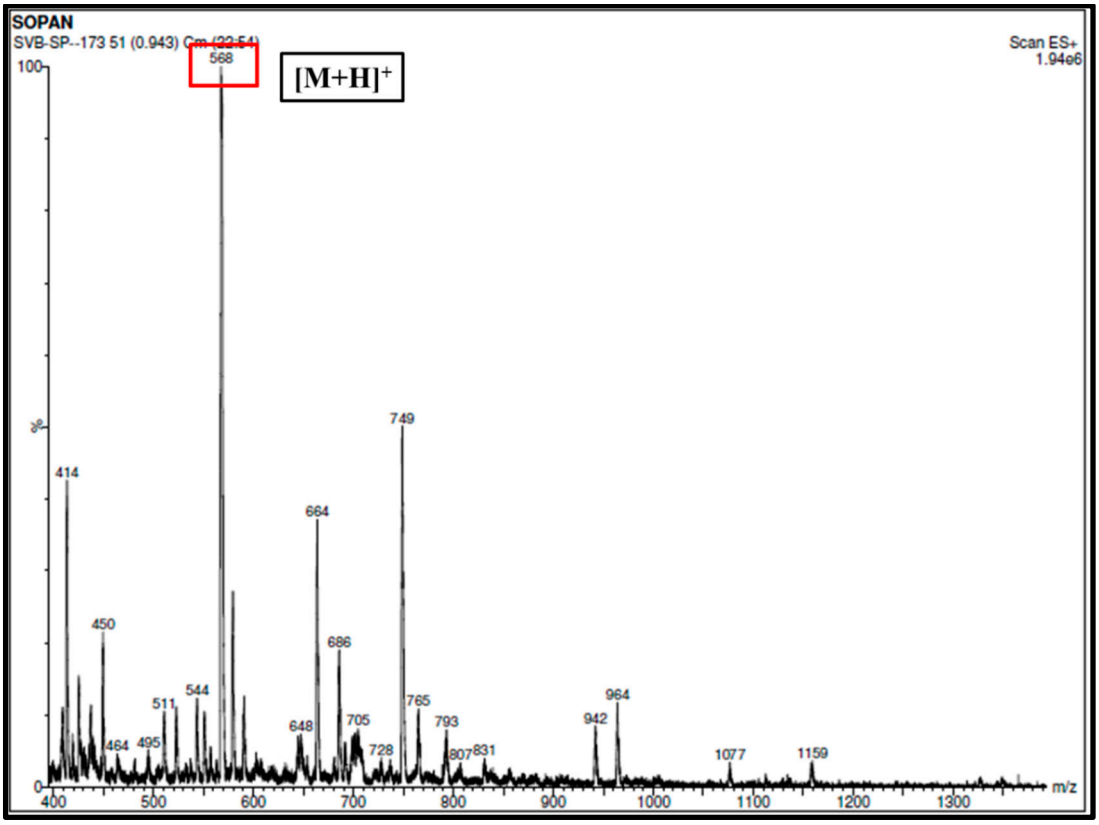


Figure S18. ESI-Mass of TPA-MC-1.

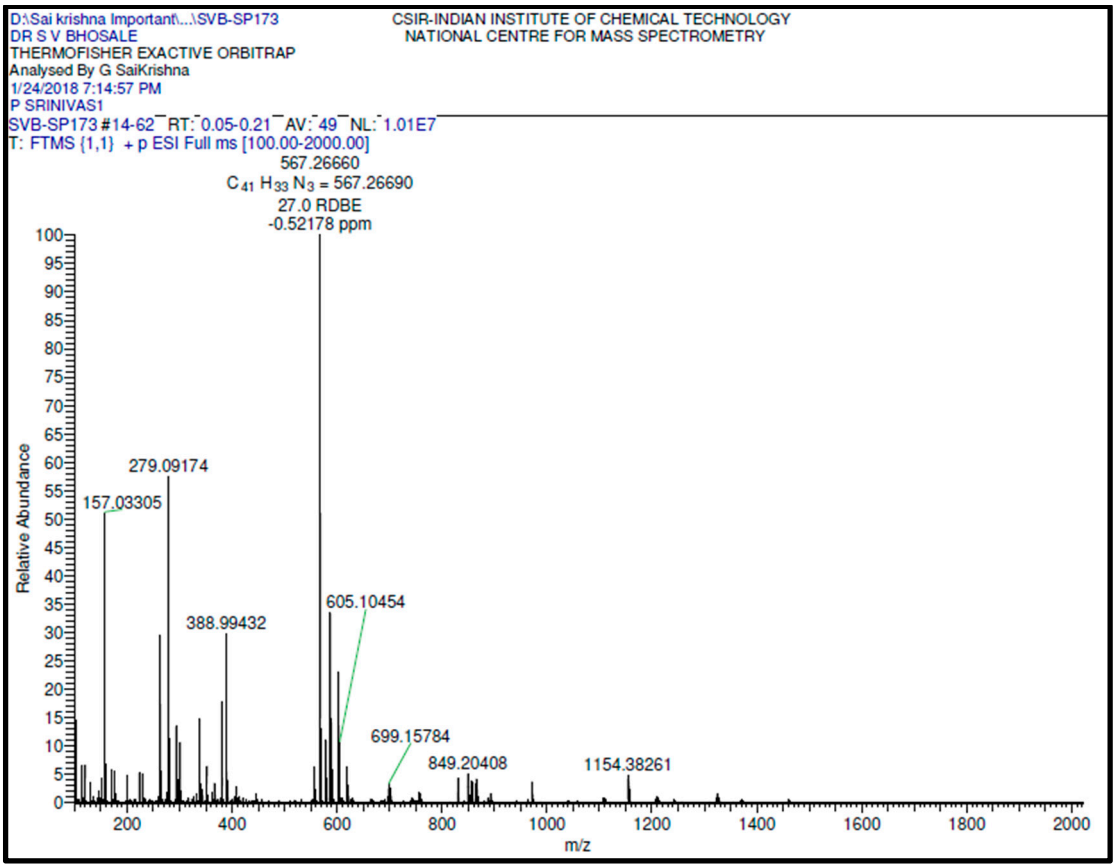


Figure S19. HRMS of TPA-MC-1.

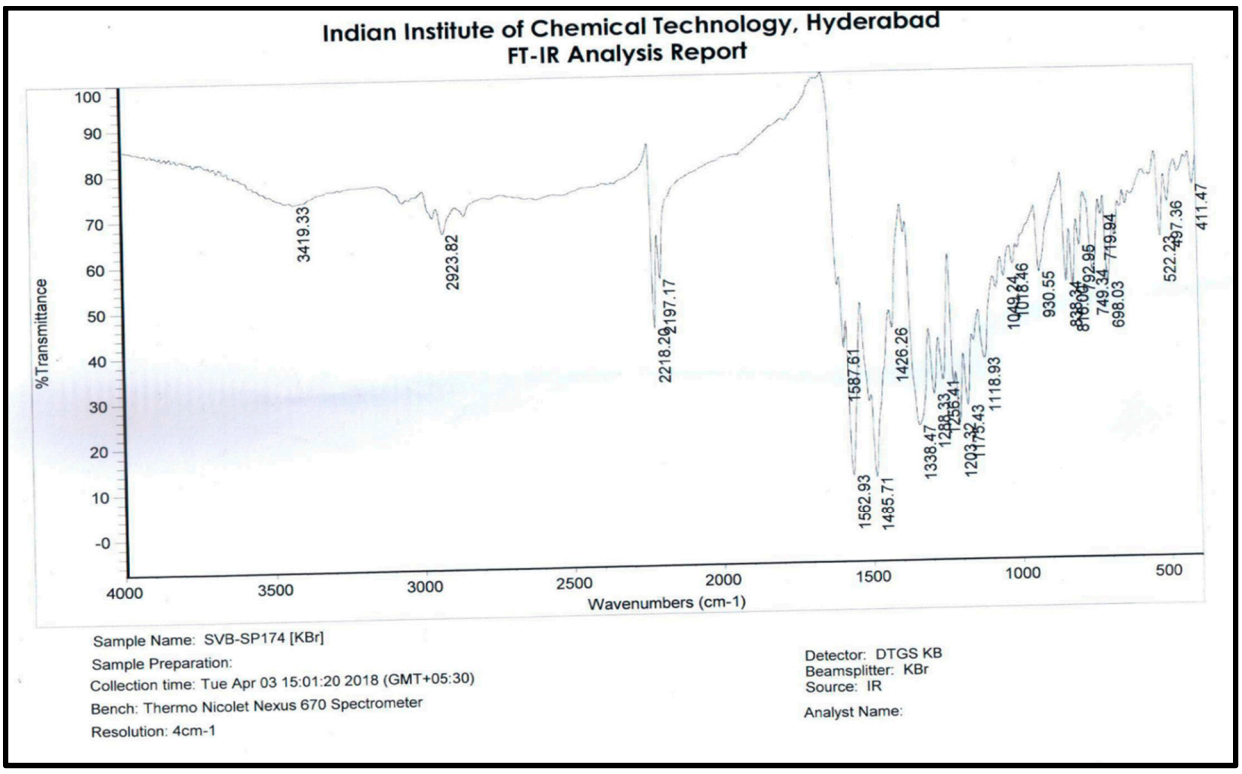


Figure S20. FT-IR spectra of compound TPA-MC-2.

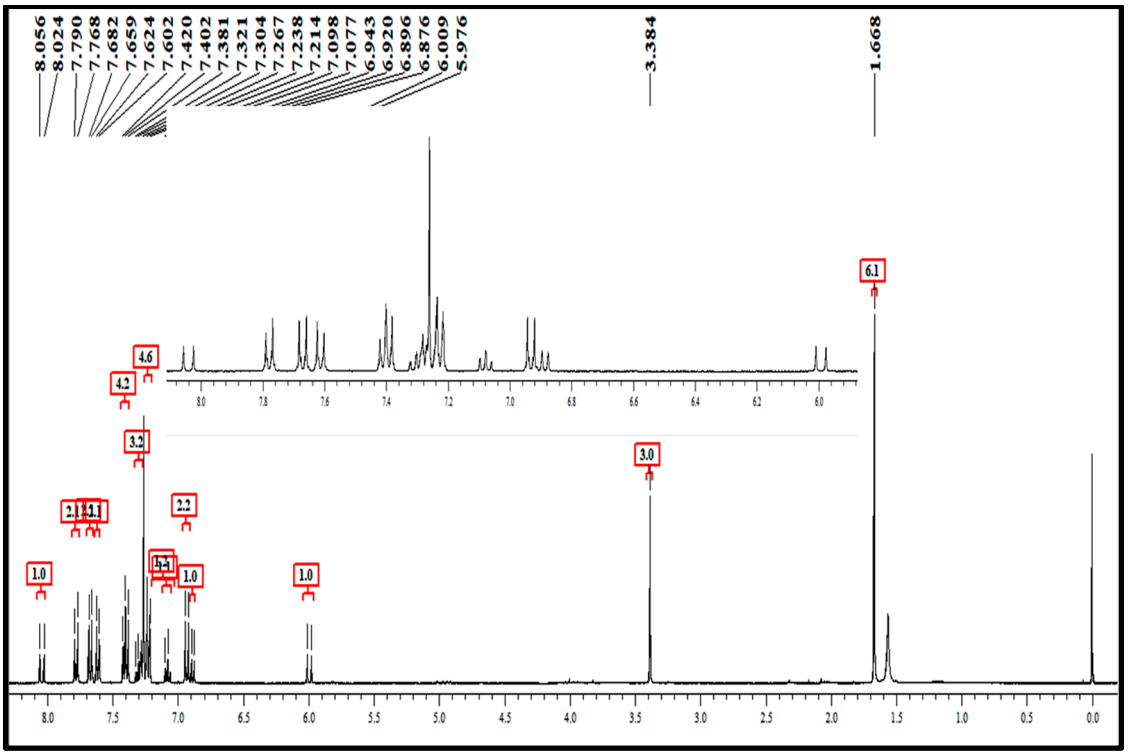


Figure S21. ^{1}H NMR spectra of TPA-MC-2.

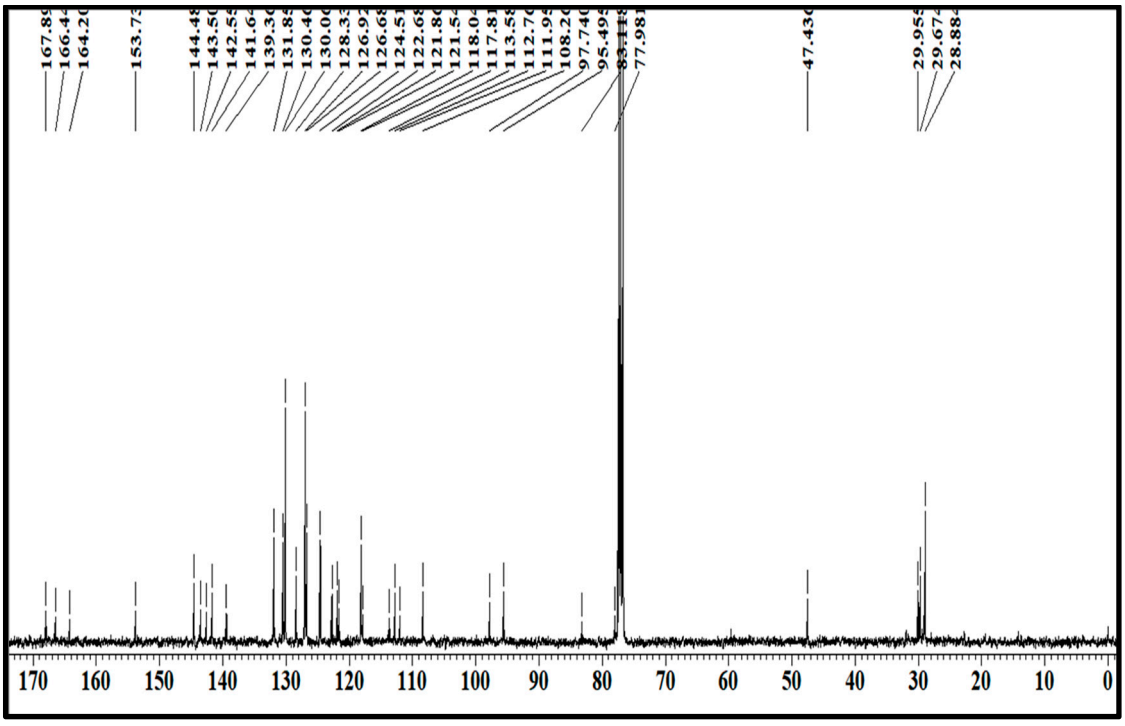


Figure S22. ^{13}C NMR spectra of TPA-MC-2.

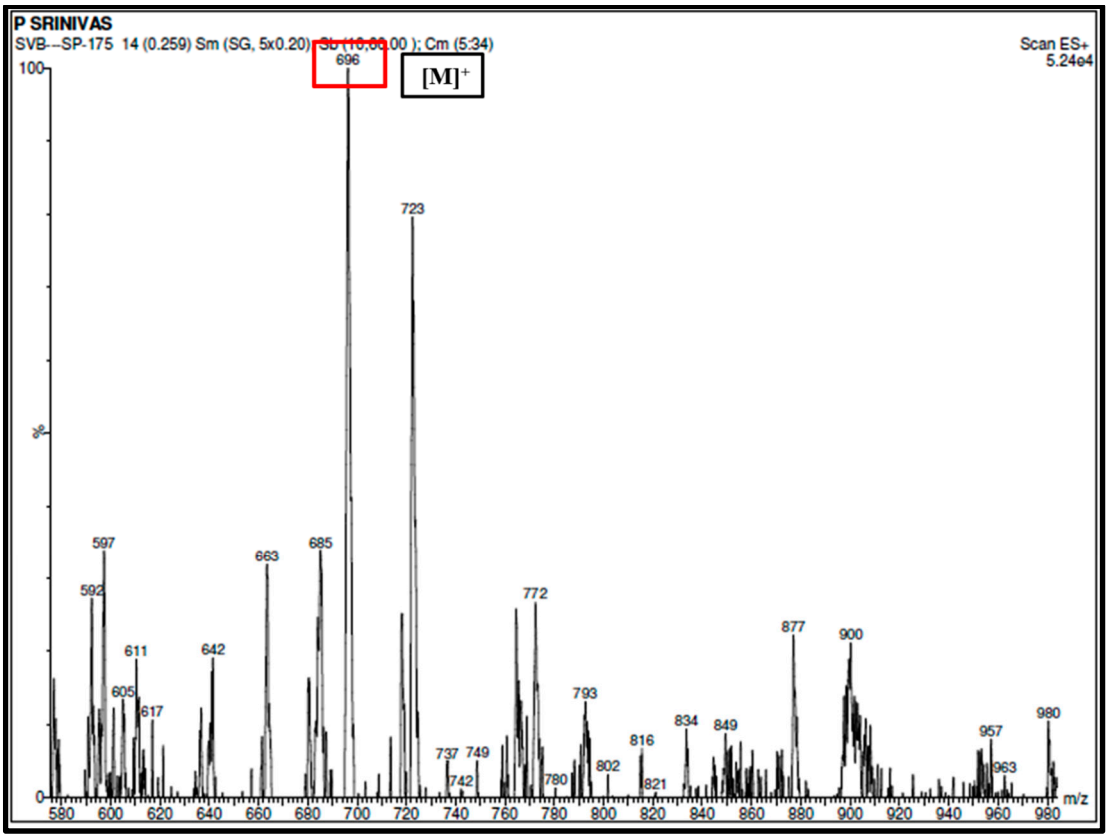


Figure S23. ESI-Mass of TPA-MC-2.

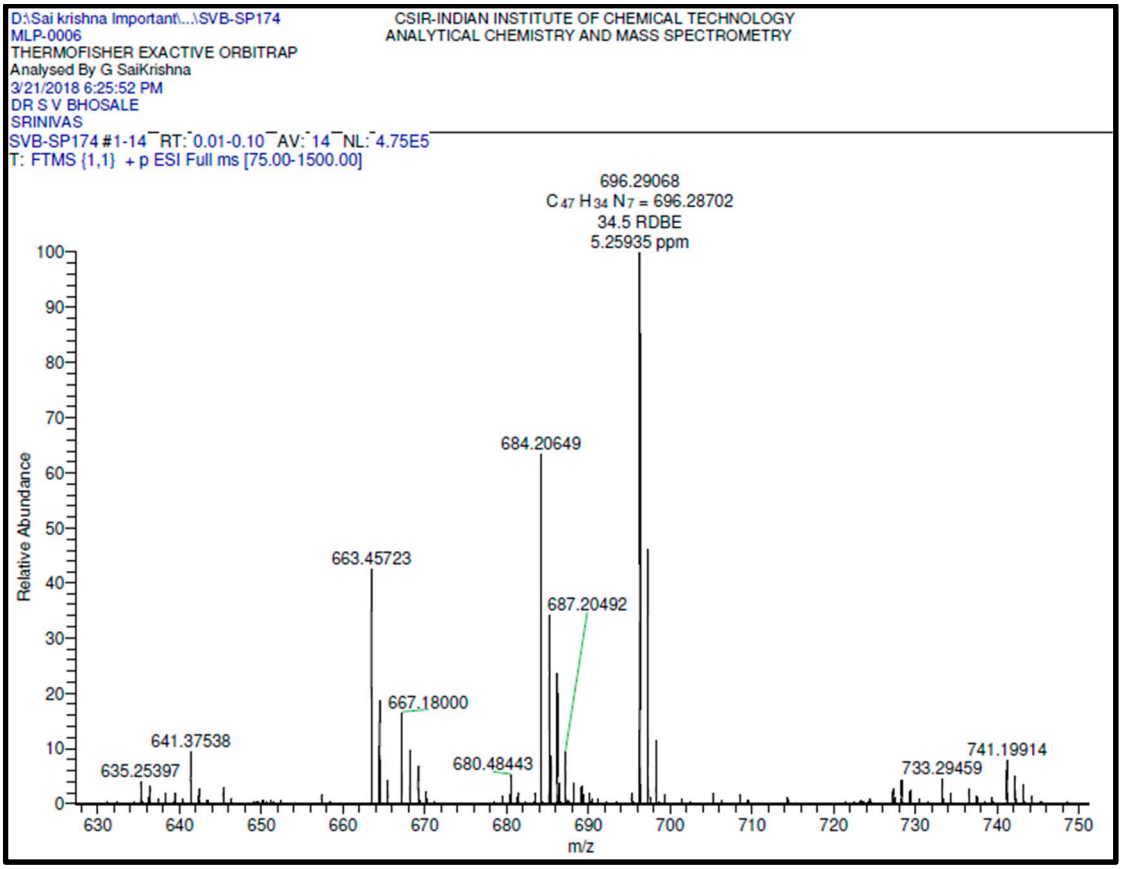


Figure S24. HRMS of TPA-MC-2.

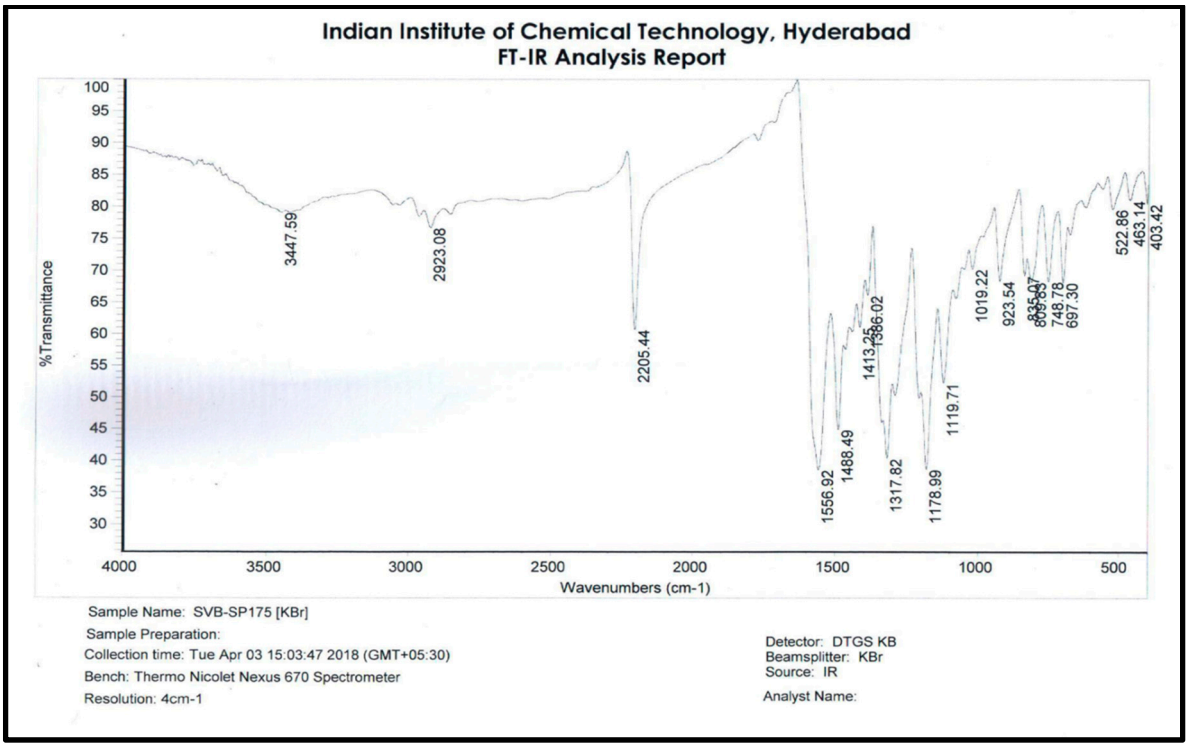


Figure S25. FT-IR spectra of compound TPA-MC-3.

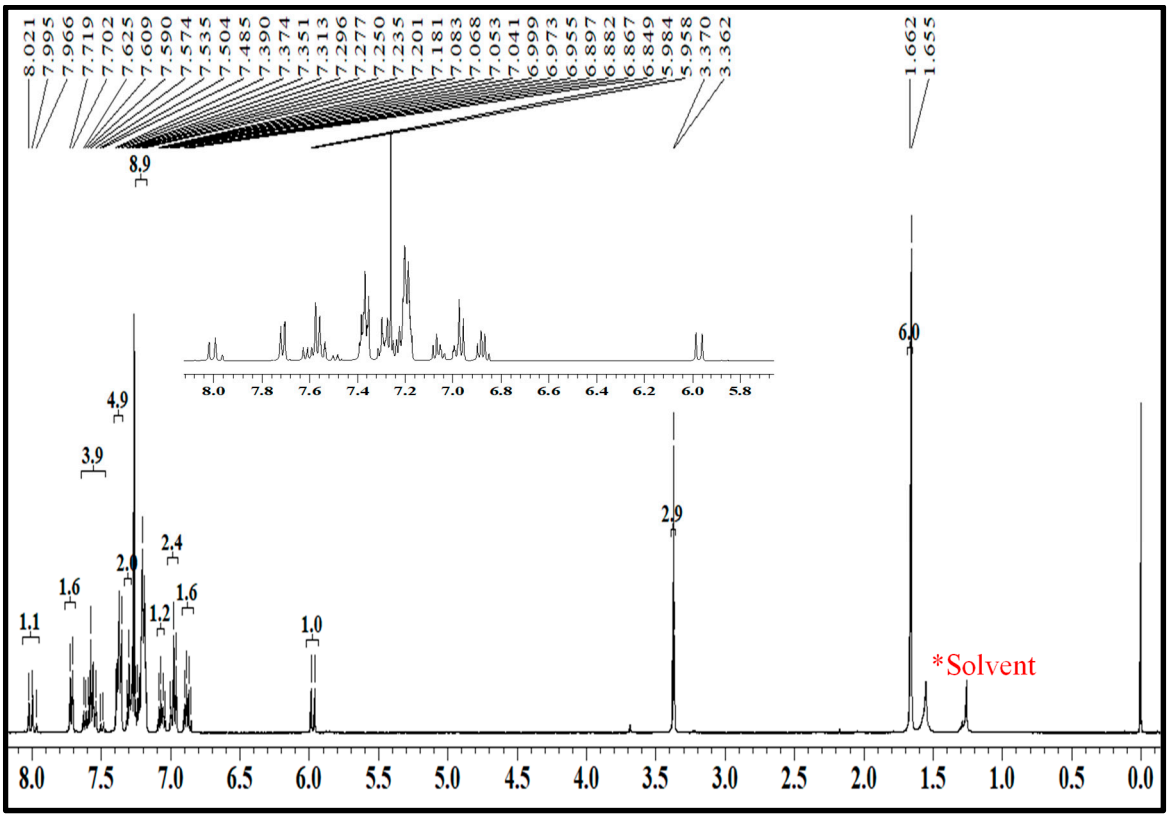


Figure S26. ^{1}H NMR spectra of TPA-MC-3.

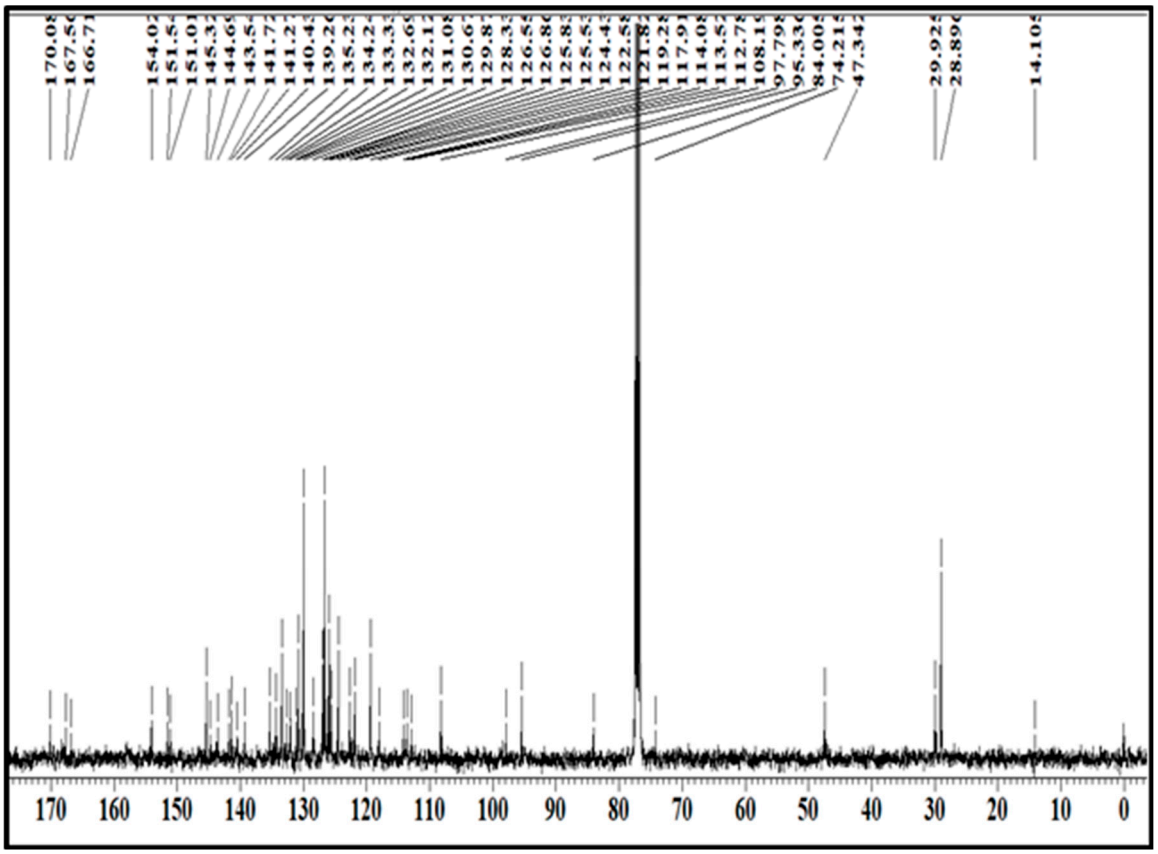


Figure S27. ^{13}C NMR spectra of TPA-MC-3.

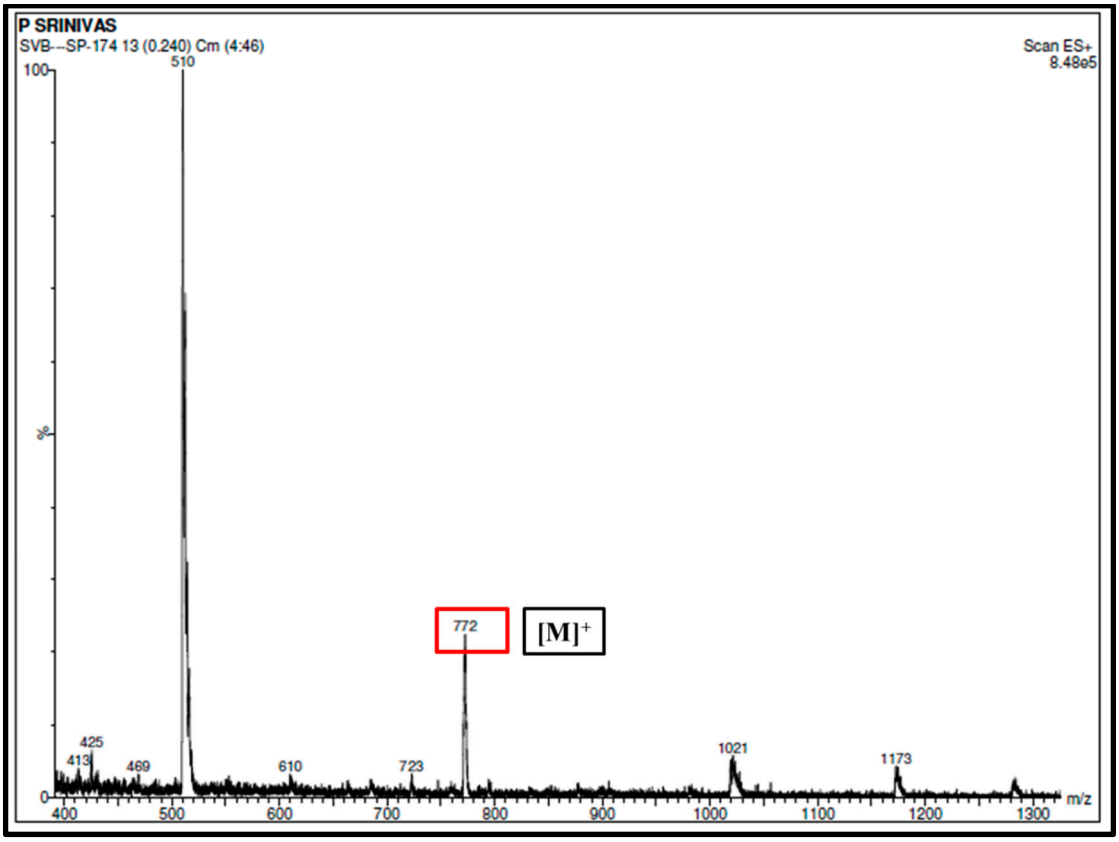


Figure S28. ESI-Mass of TPA-MC-3.

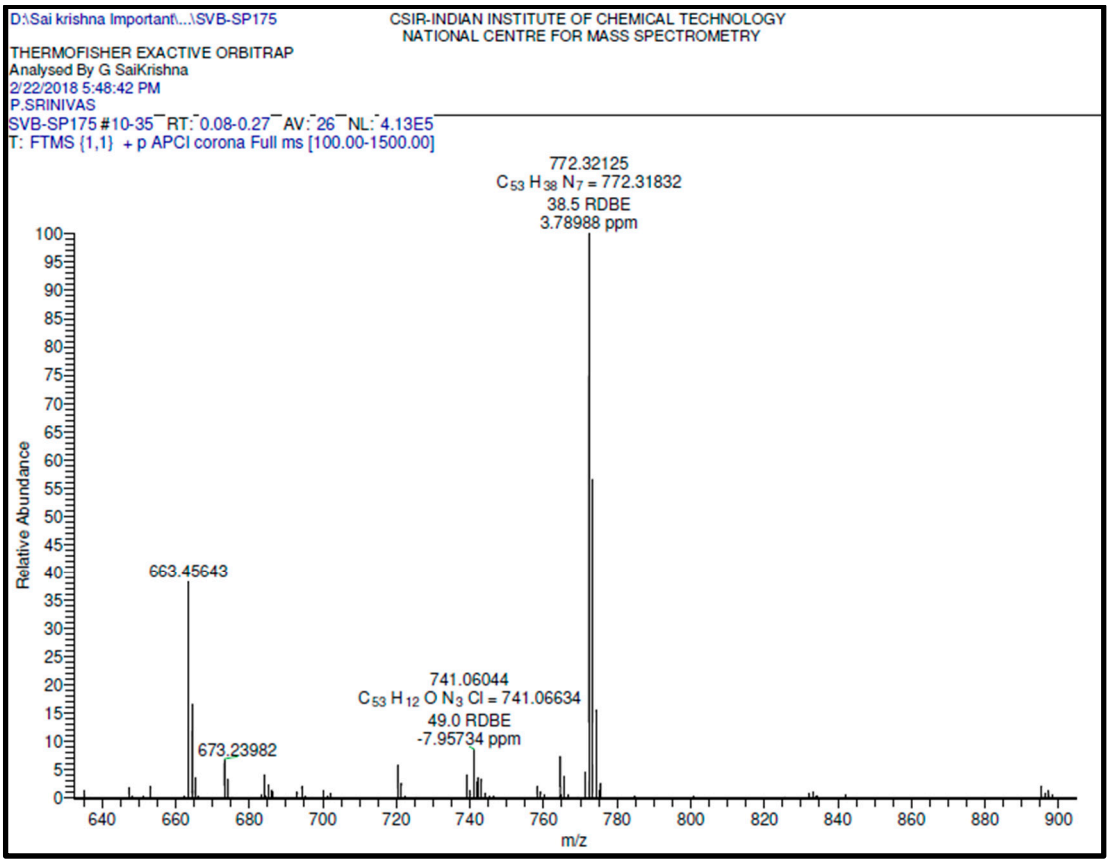


Figure S29. HRMS of TPA-MC-3.