Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Stable and charge recombination minimized π-extended thioalkyl substituted tetrathiafulvalene sensitized dye-sensitized solar cells

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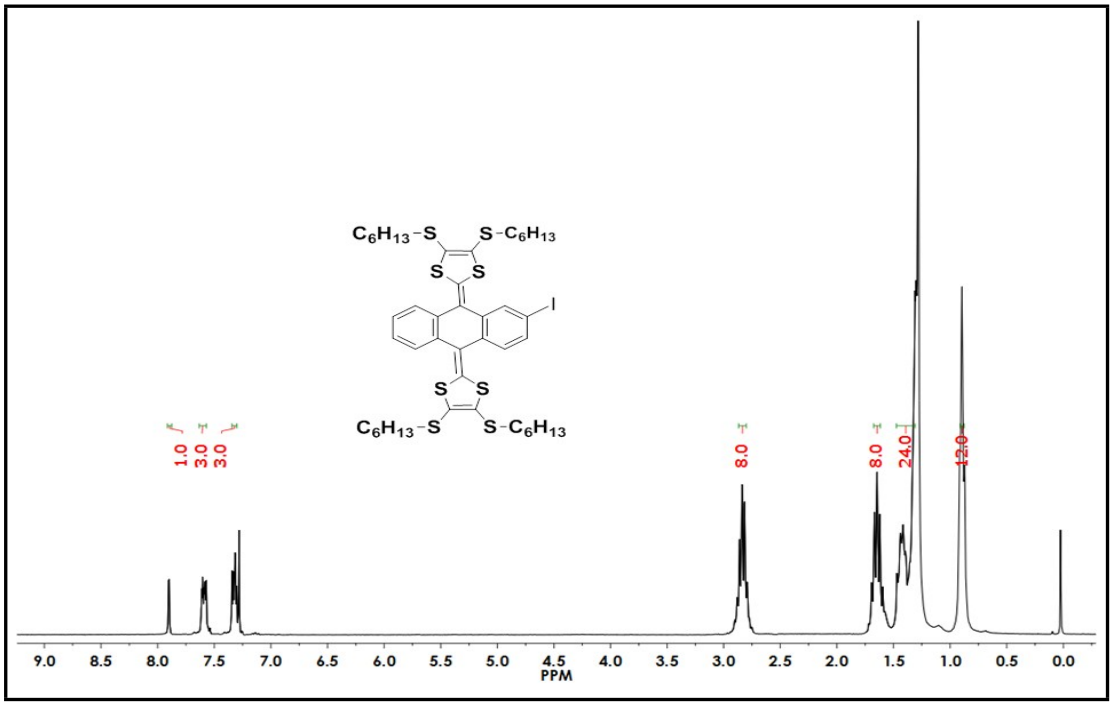


Fig. S1: ^{1}HNMR Spectrum of **(1)** in $CDCl_3$.

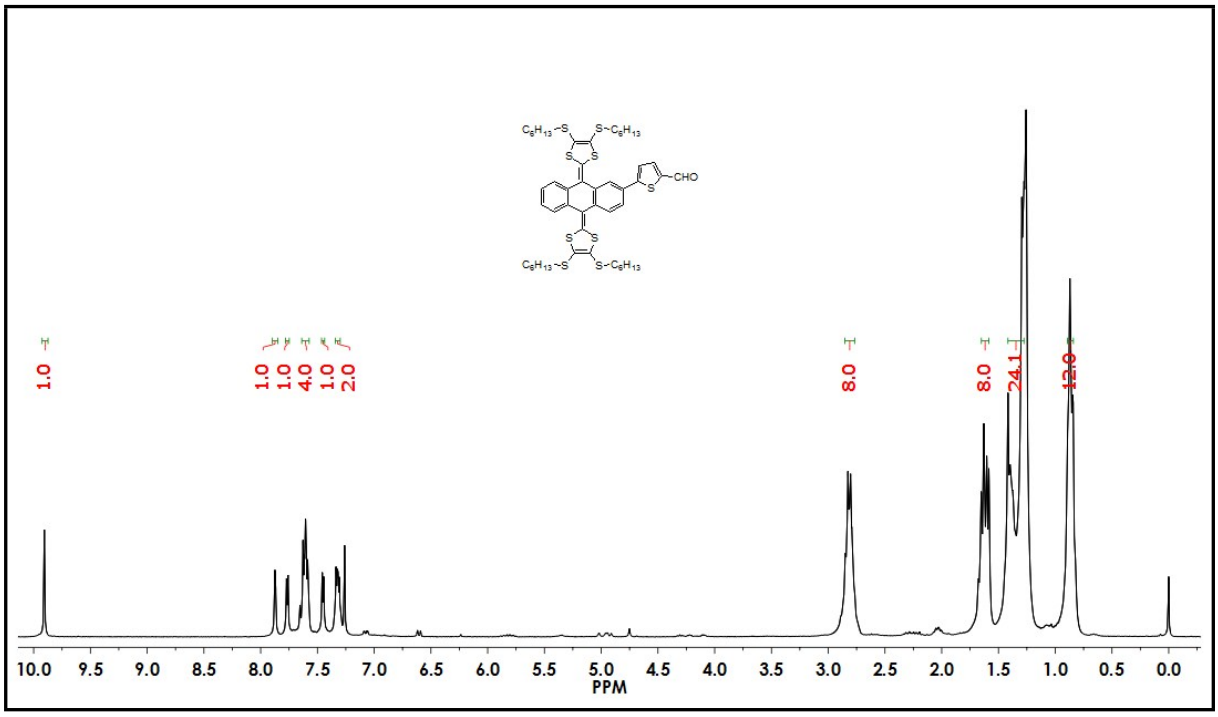


Fig. S2: ^{1}HNMR Spectrum of **(2a)** in $CDCl_3$

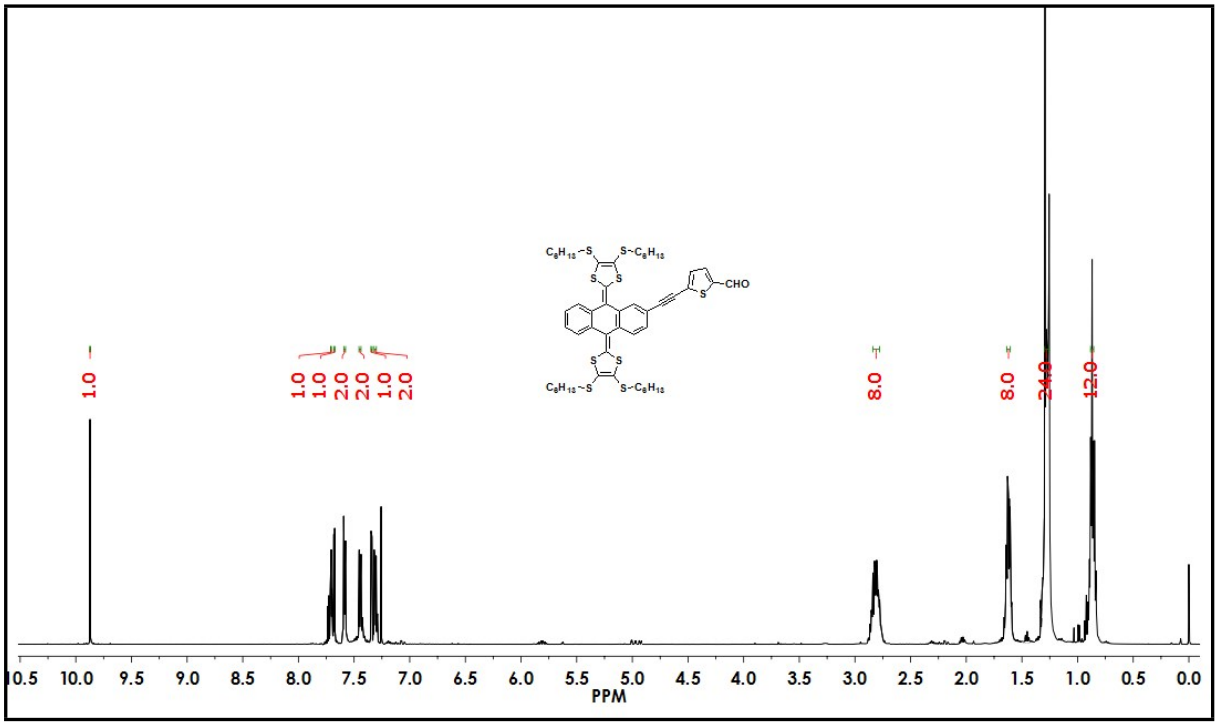


Fig. S3: ^{1}HNMR Spectrum of **(2c)** in $CDCl_3$

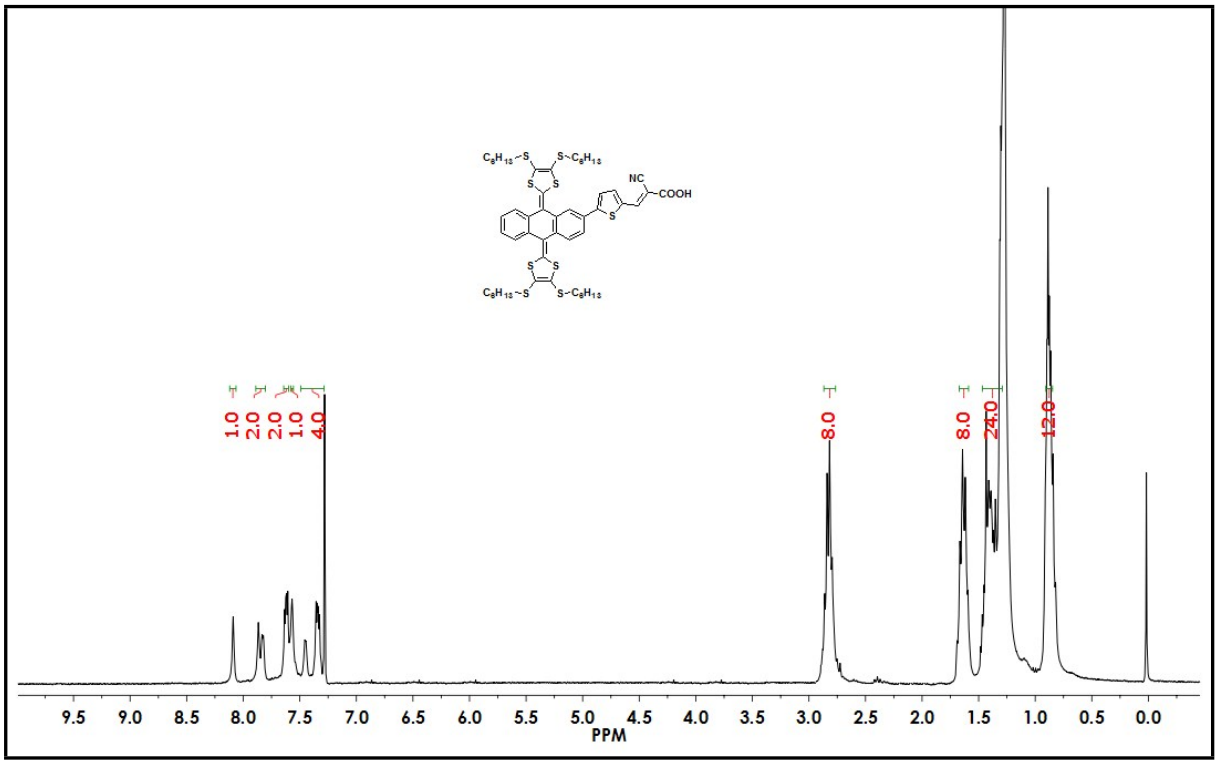


Fig. S4: ^{1}HNMR Spectrum of **(G1)** in $CDCl_3$

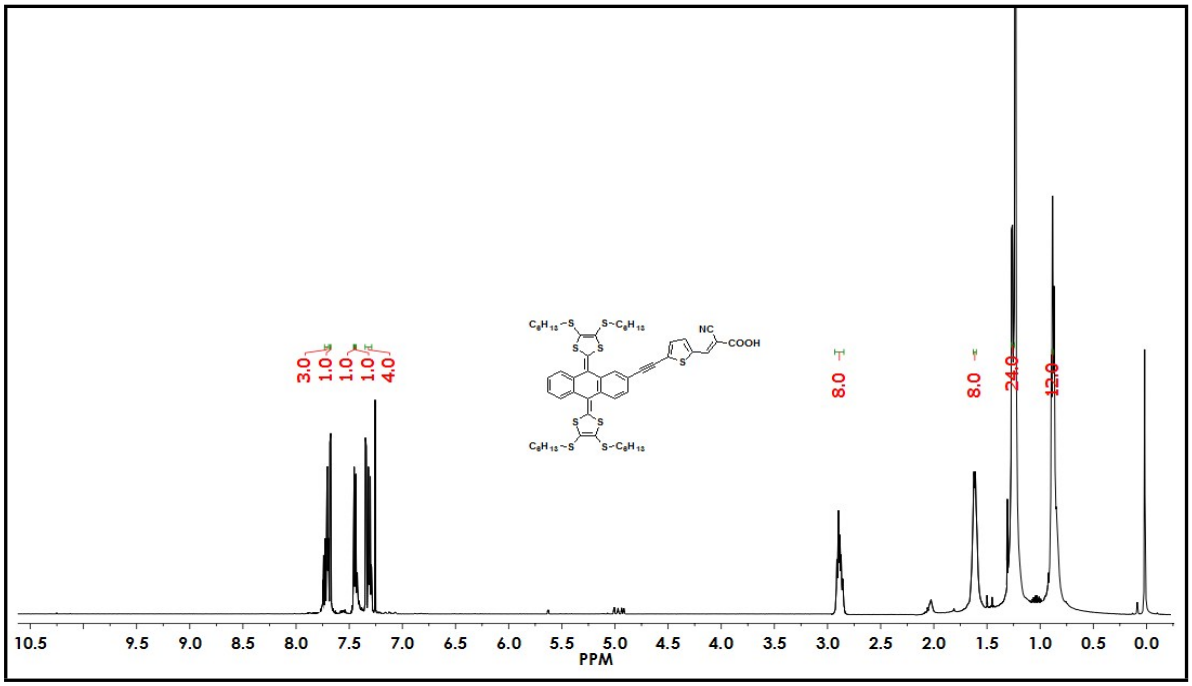


Fig. S5: ^{1}HNMR Spectrum of **(G3)** in $CDCl_3$

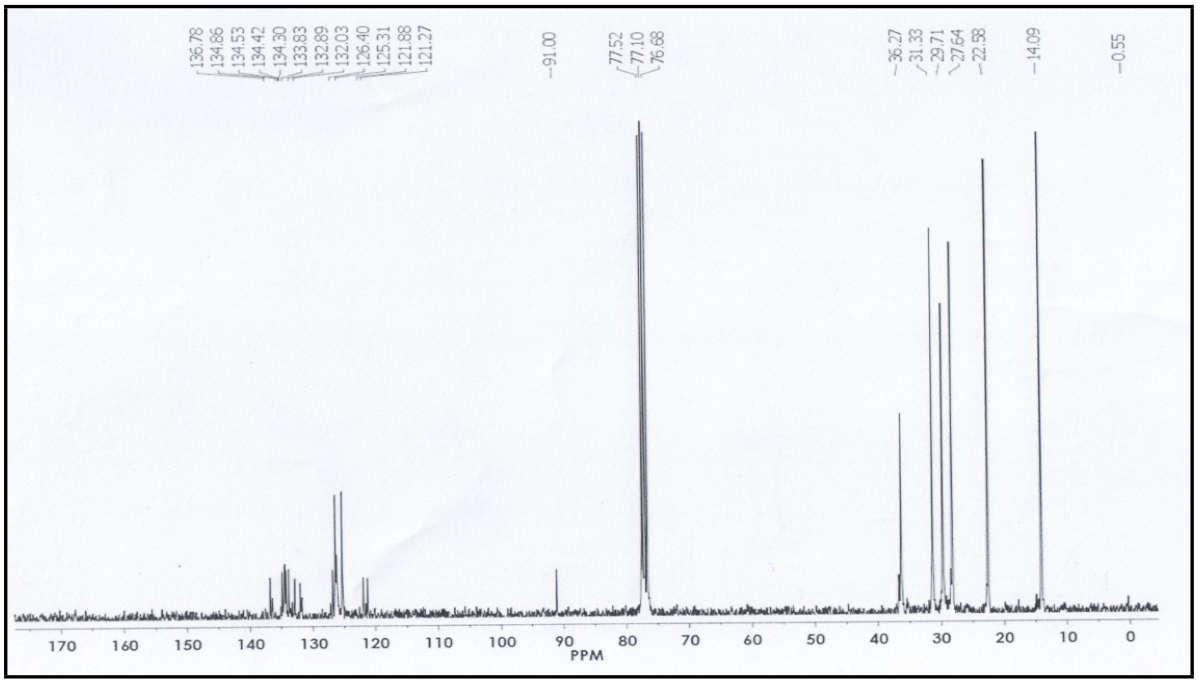


Fig. S6: ^{13}C-NMR Spectrum of **(1)** in $CDCl_3$

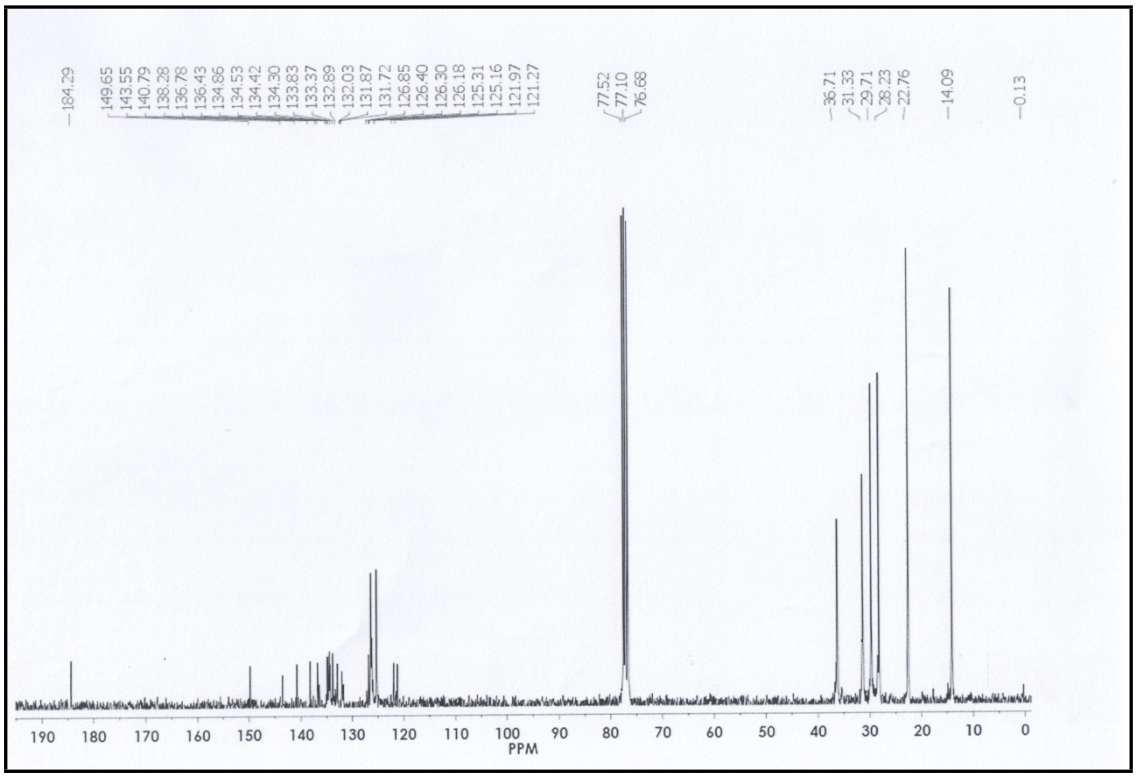


Fig. S7: ^{13}C-NMR Spectrum of **(2a)** in $CDCl_3$

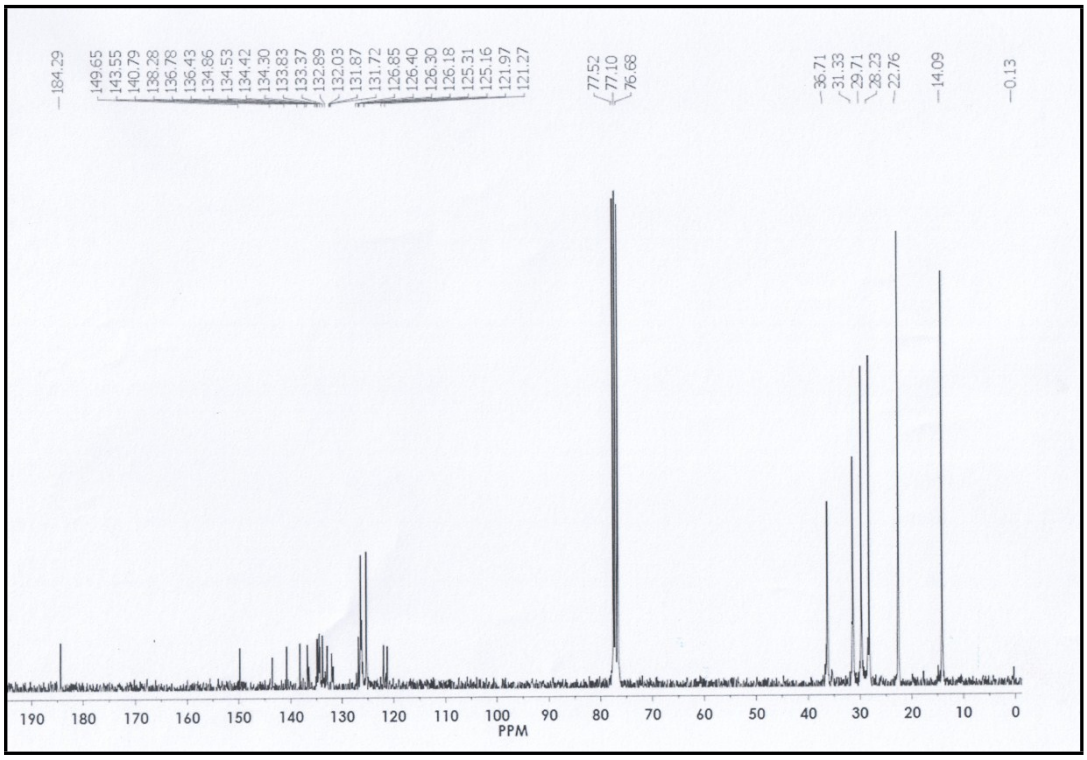


Fig. S8: ^{13}C-NMR Spectrum of **(2c)** in $CDCl_3$

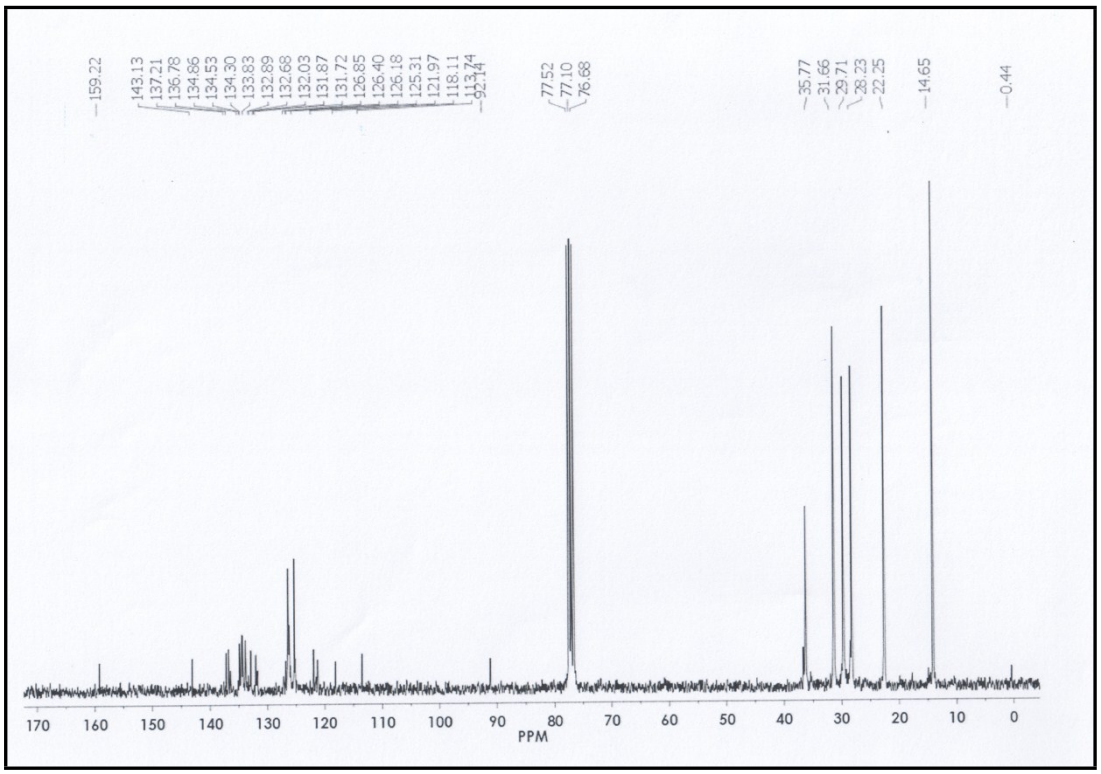


Fig. S9: ^{13}C-NMR Spectrum of **(G1)** in $CDCl_3$

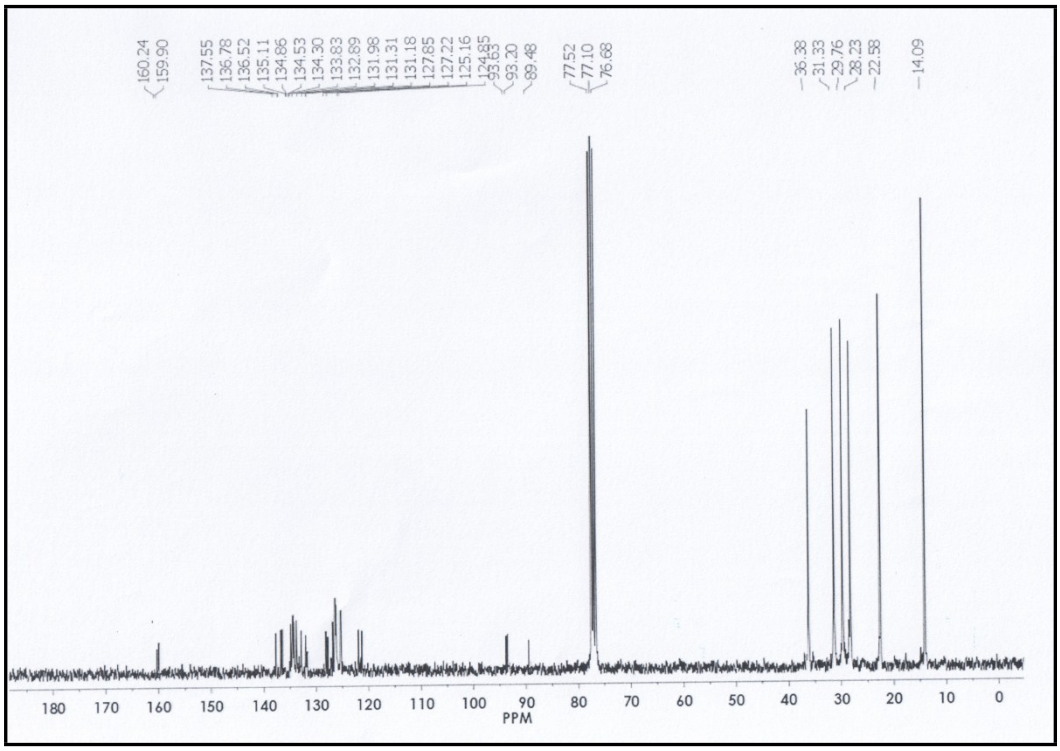


Fig. S10: ^{13}C-NMR Spectrum of **(G3)** in $CDCl_3$

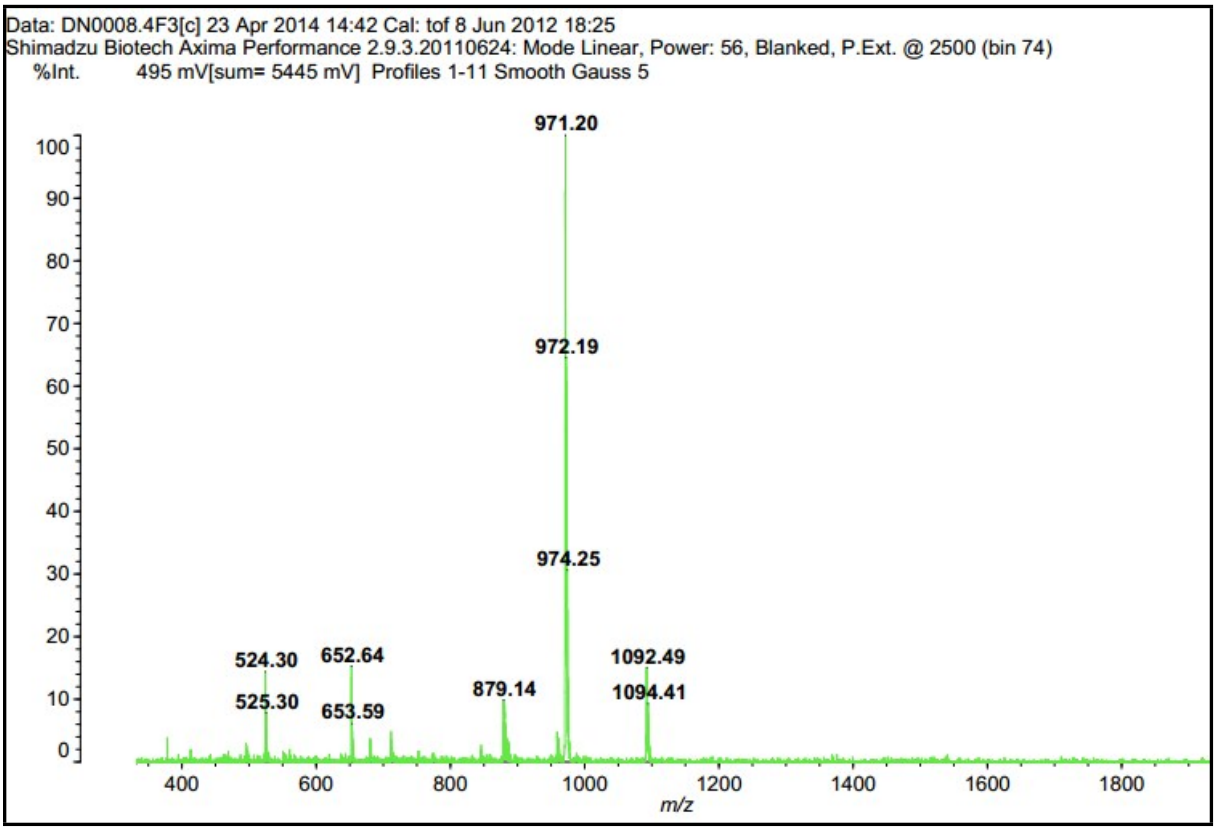


Fig. S11: MALDI-TOF Spectrum of compound **(1)**

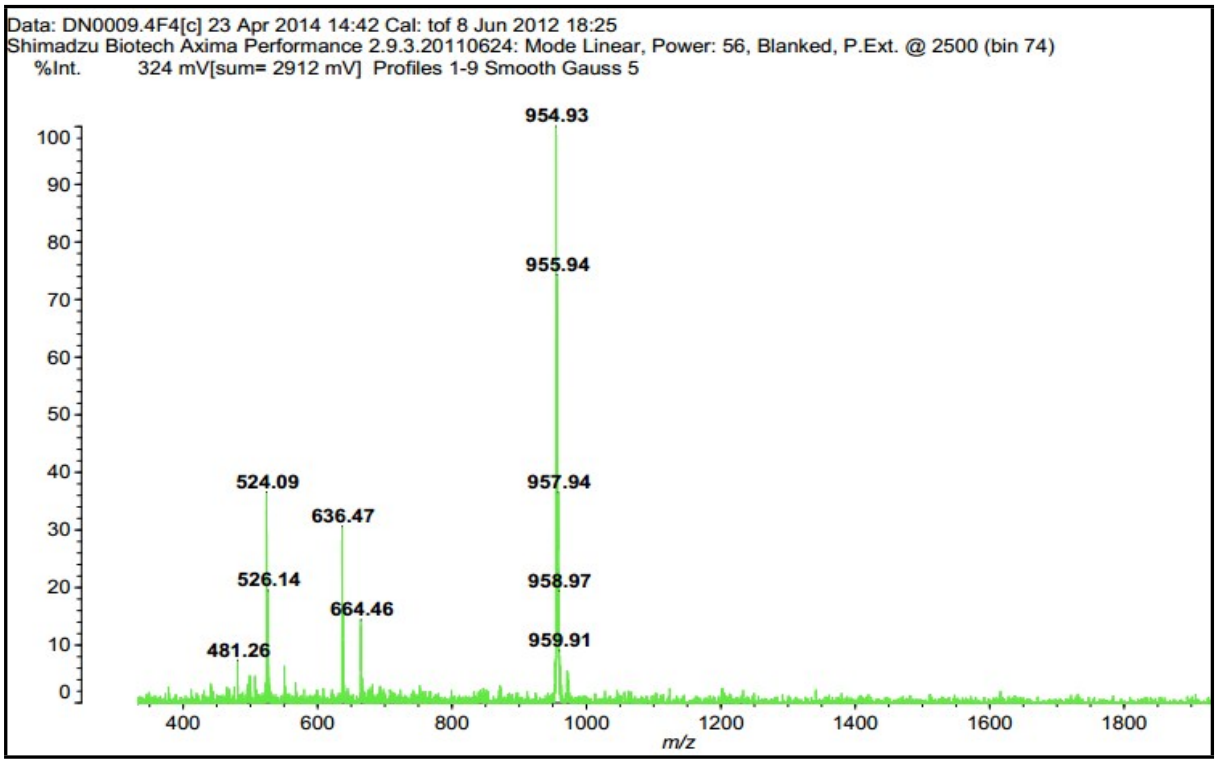


Fig. S12: MALDI-TOF Spectrum of compound **(2a)**

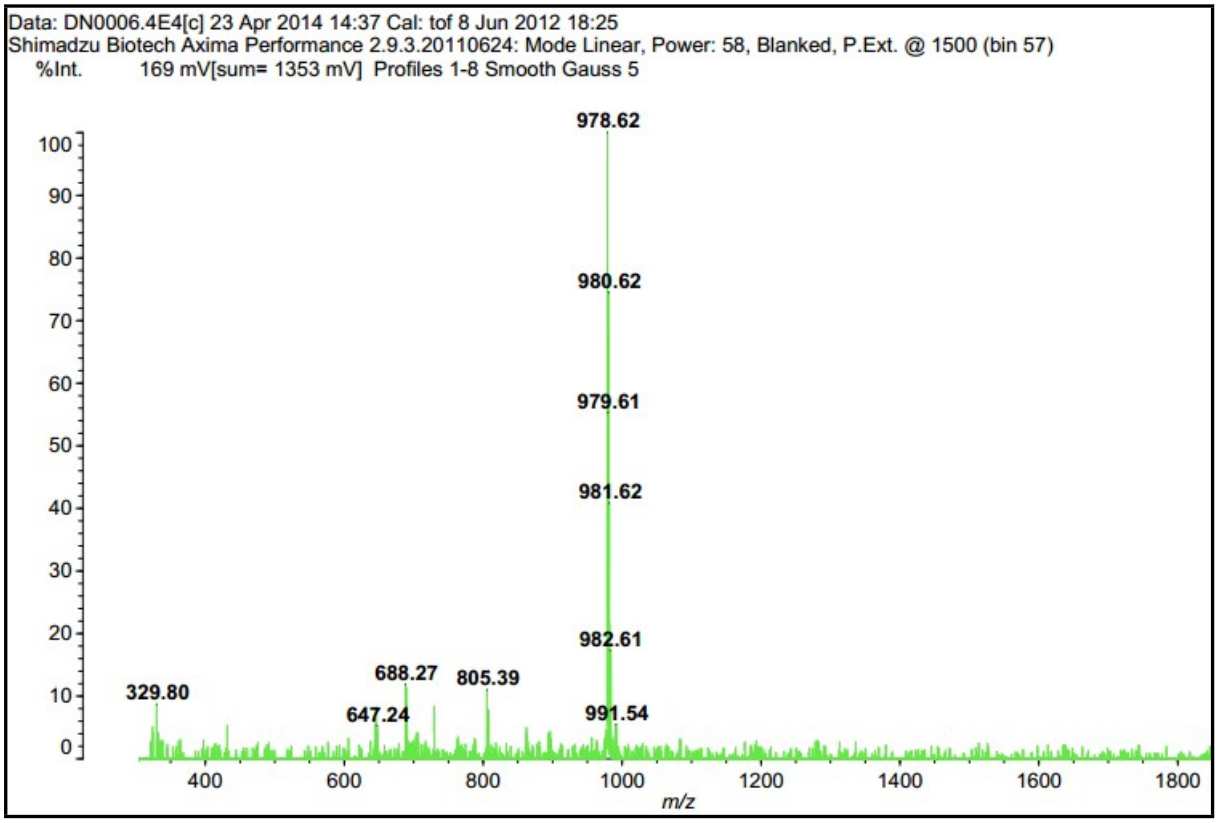


Fig. S13: MALDI-TOF Spectrum of compound **(2c)**

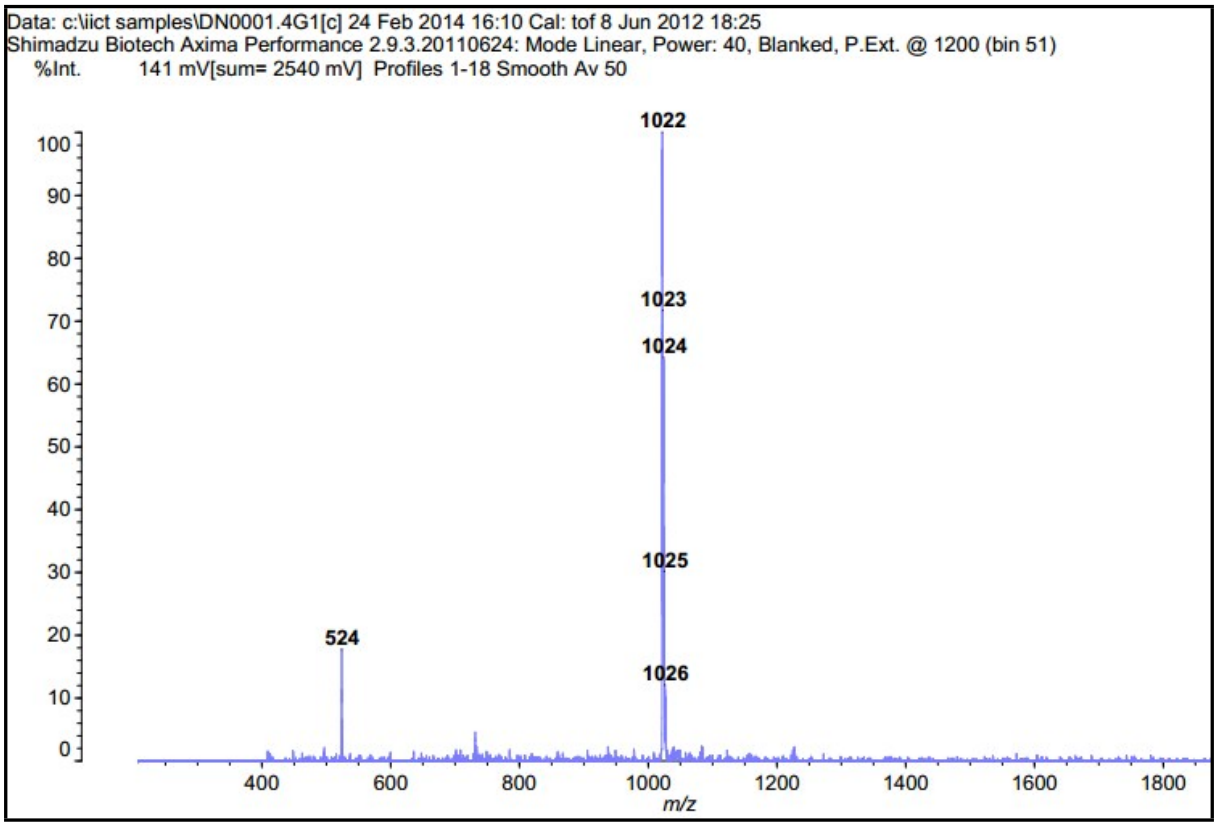


Fig. S14: MALDI-TOF Spectrum of compound **(G1)**

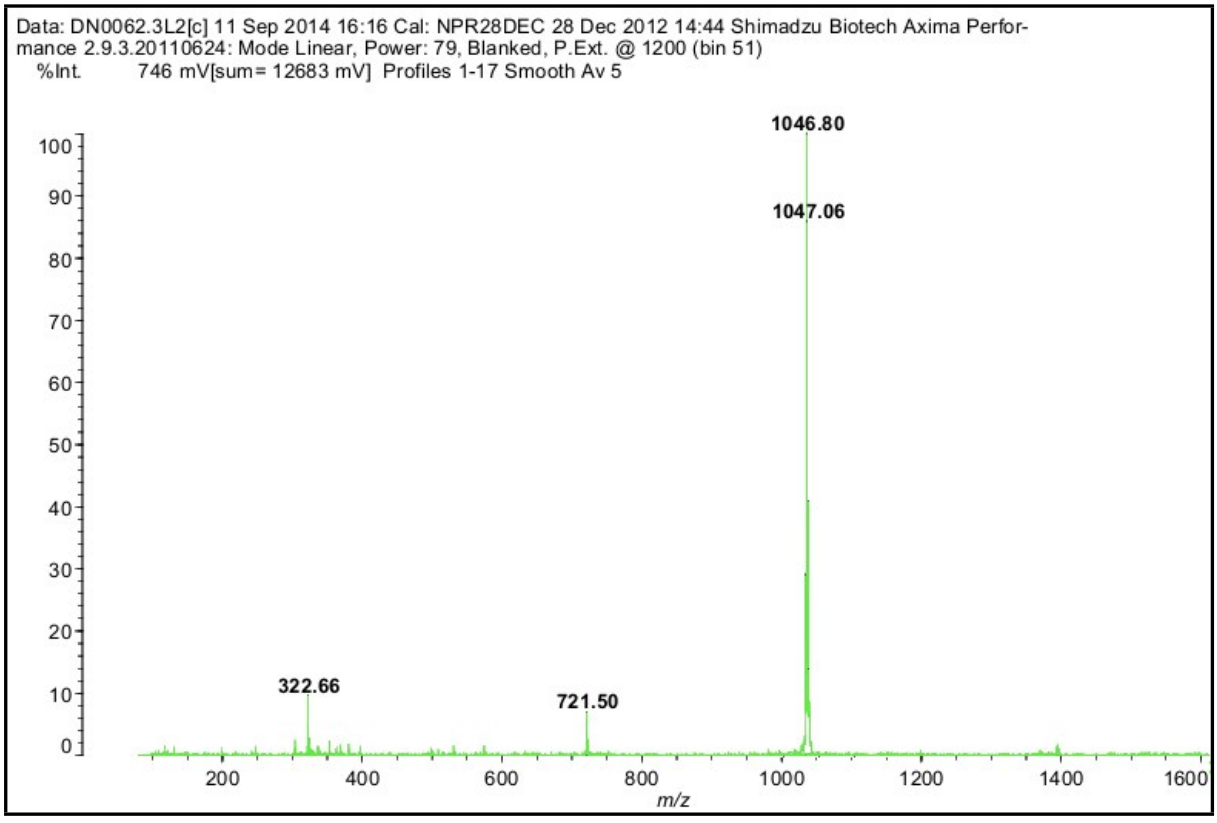


Fig. S15: MALDI-TOF Spectrum of compound **(G3)**

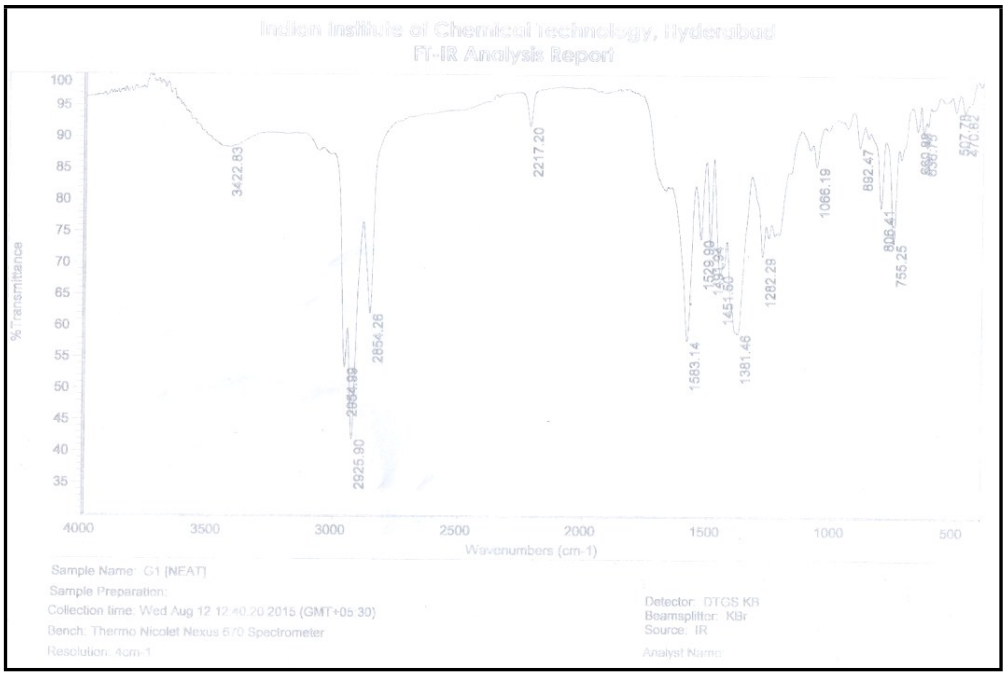


Fig. S16: IR Spectrum of **G1**.

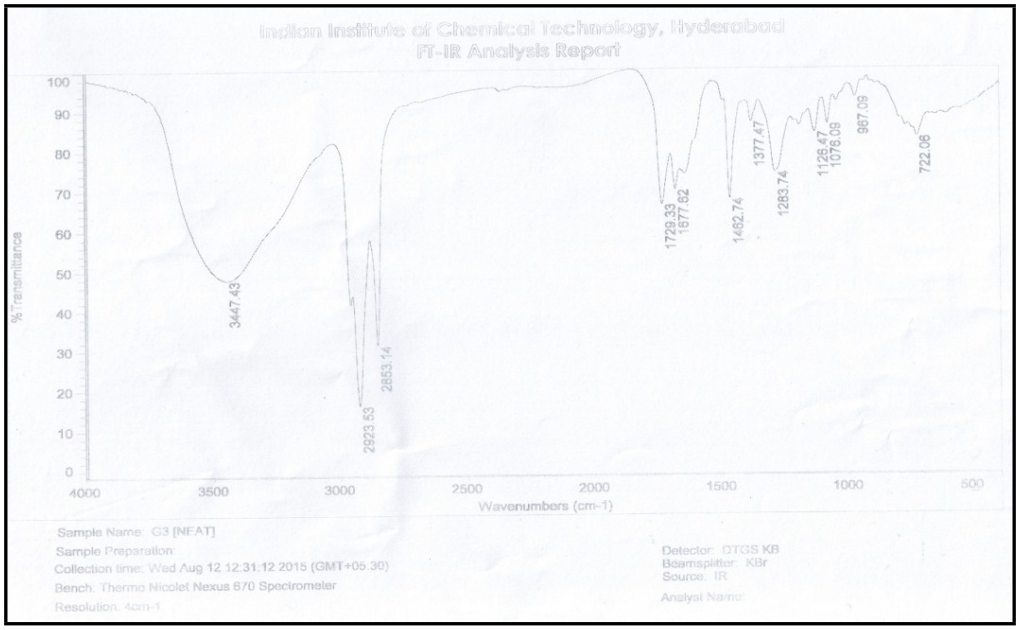
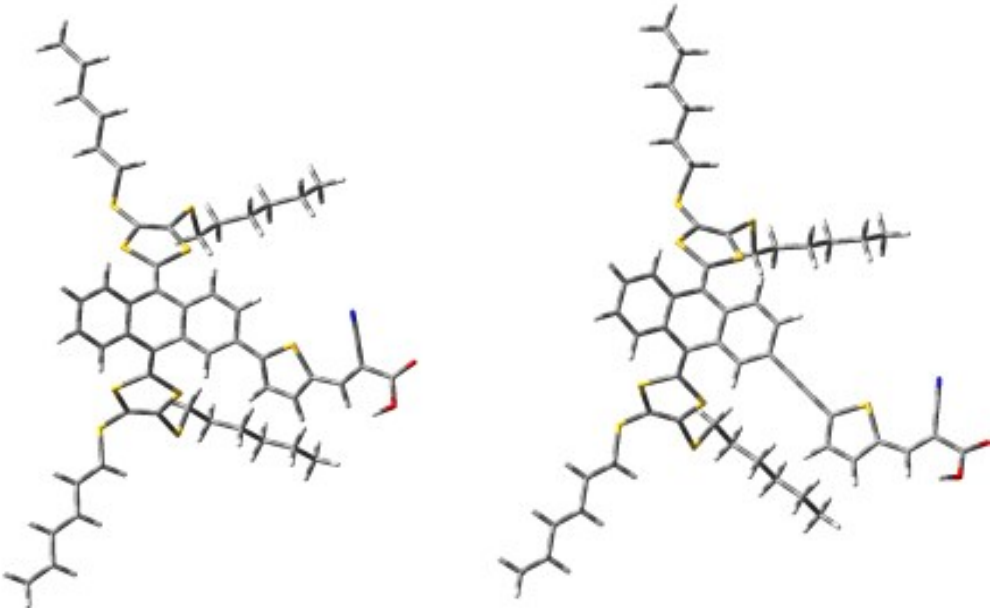


Fig. S17: IR Spectrum of **G3**.



G1 **G3**

Fig. S18: Energy Optimized Structures of **G1**&**G3.**

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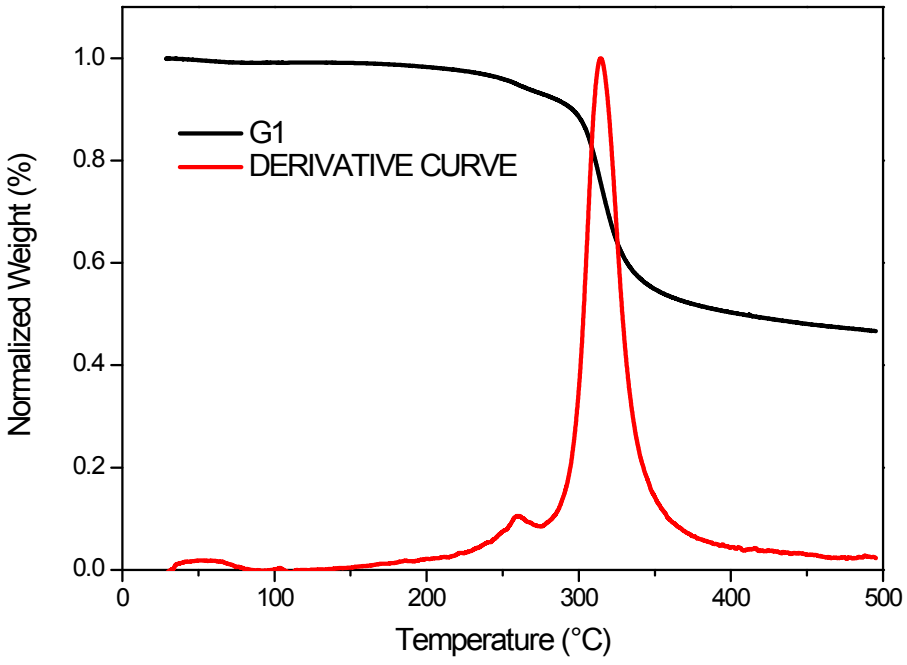

Fig. S19: TG/DTG Curves of **G1** with a heating rate of 10 °C min-1 under nitrogen atmosphere.

Table S1: Comparison of the experimental optical properties with the theoretical data by B3LYP in dichloromethane.

Dye	[a]λ_{max}	[b]λ_{max}	[c]f	[d] E (eV)	% of Molecular Orbital Composition
G1	421	453	0.636	2.73	HOMO->LUMO (82%) H-2->LUMO (5%), HOMO->L+1 (7%)
G3	417	391	0.824	3.16	HOMO->LUMO (29%), HOMO->L+1 (65%)

[a]Recorded absorbance in nm, [b] theoretical absorbance in nm, [c] Oscillation strength, and [d] excited state energy in eV.