Electronic Supplementary Information

Functional π-Conjugated Tetrathiafulvalene Decorated with Benzothiadiazole Organic Sensitizers for Dye Sensitized Solar Cells

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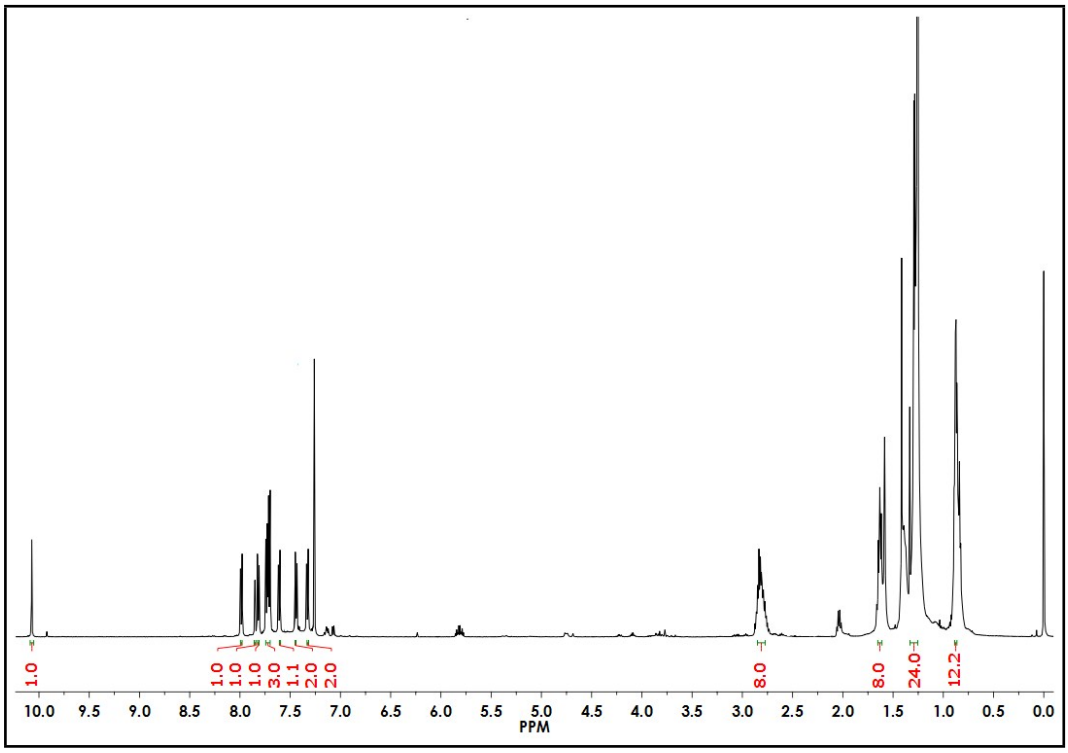


Figure S1: ^{1}H NMR spectrum of **(2)** in $CDCl_3$.

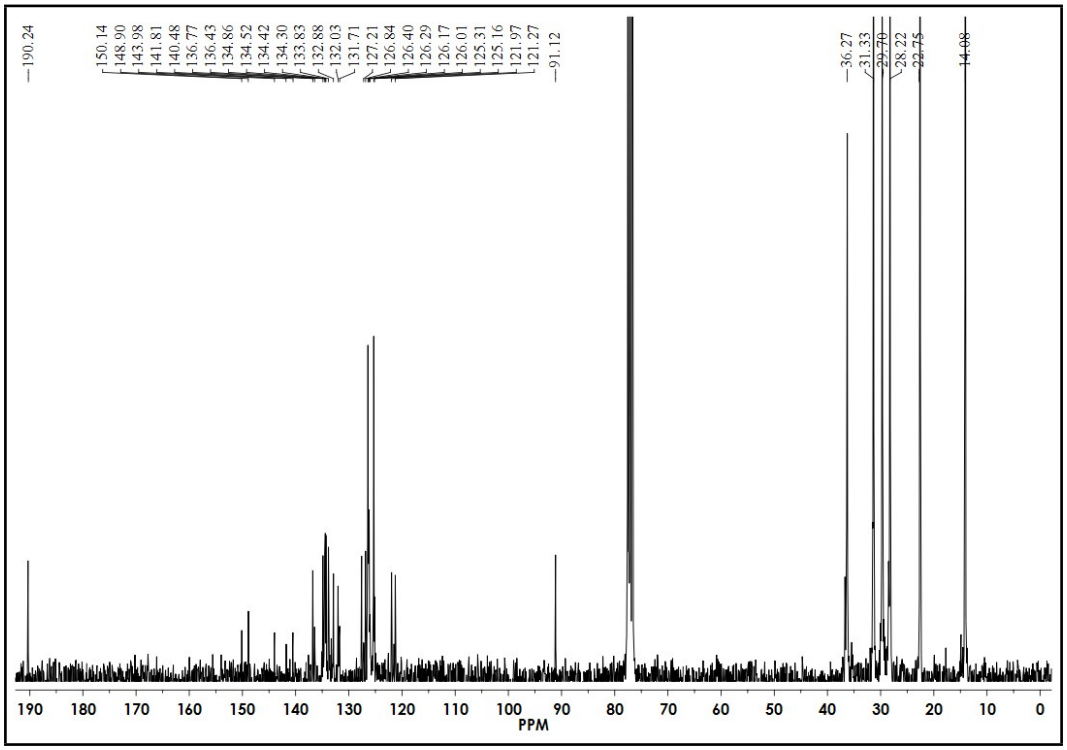


Figure S2: ^{13}C NMR spectrum of **(2)** in $CDCl_3$.

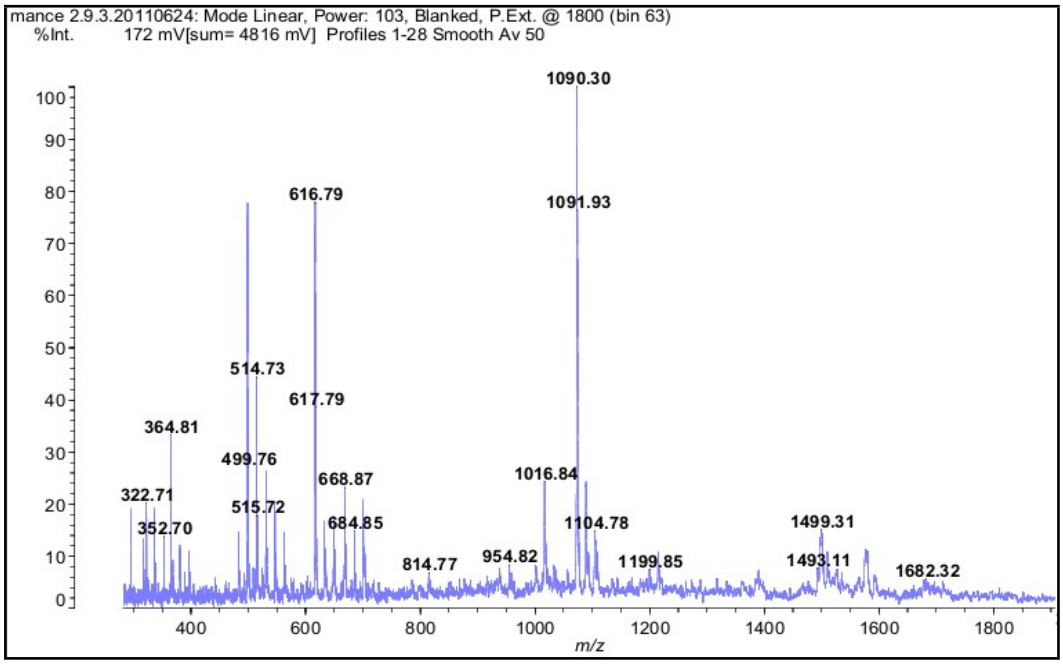


Figure S3: MALDI-TOF Spectrum of compound **(2)**

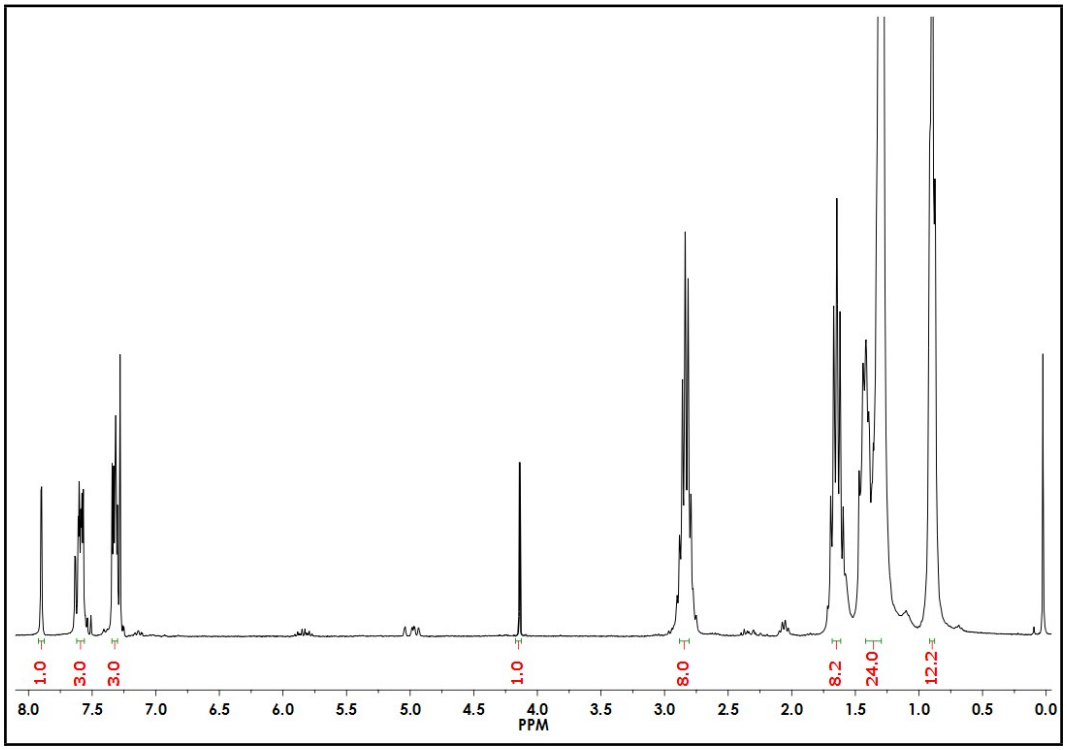


Figure S4: ^{1}H NMR spectrum of **(3)** in $CDCl_3$.

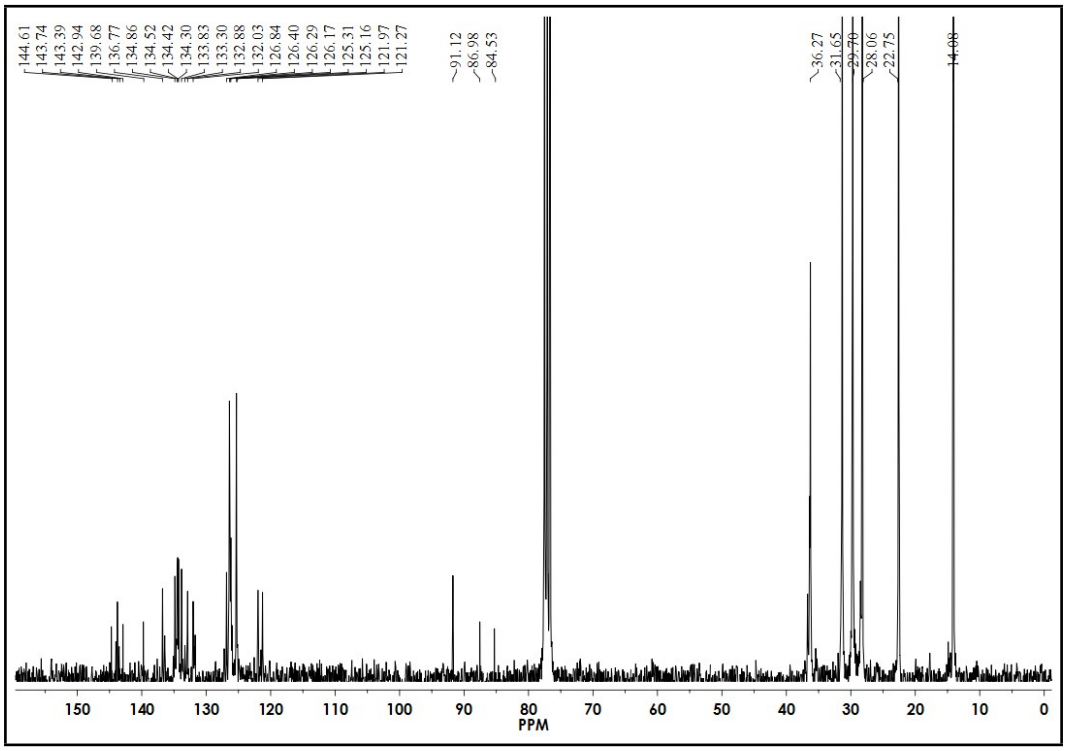


Figure S5: ^{13}C NMR spectrum of **(3)** in $CDCl_3$.

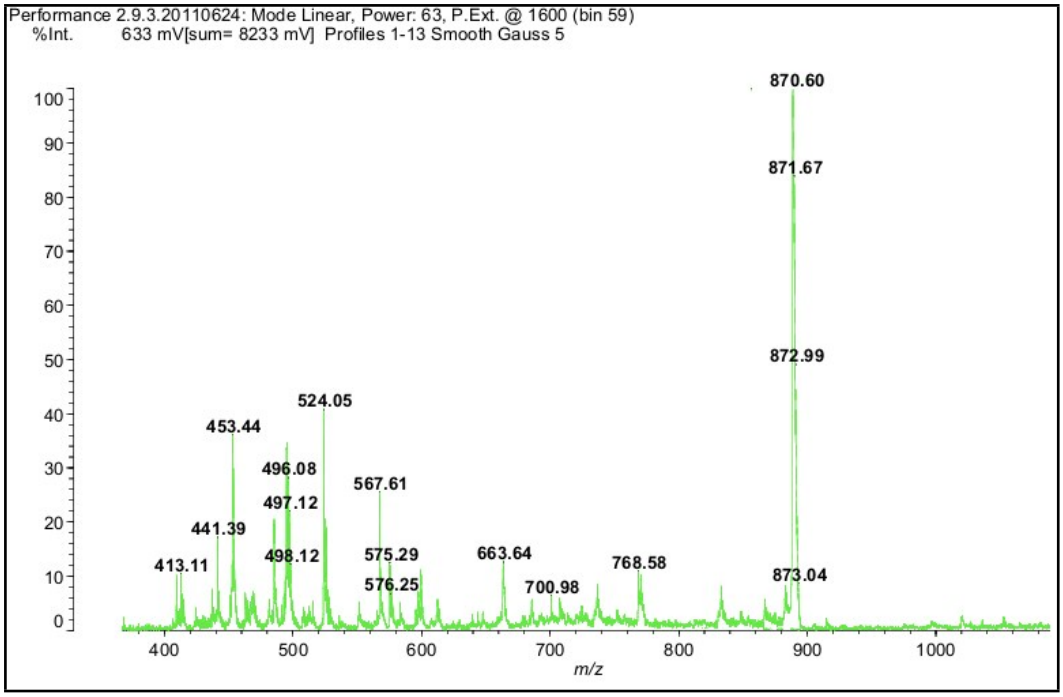


Figure S6: MALDI-TOF Spectrum of compound **(3)**

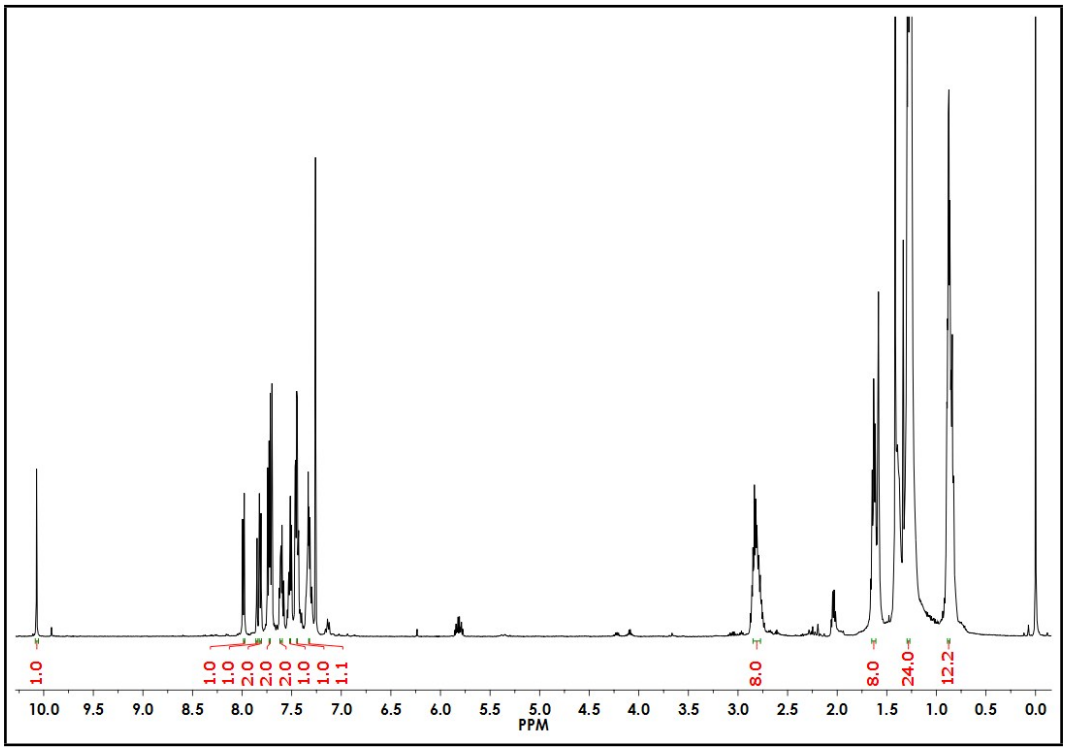


Figure S7: ^{1}H NMR spectrum of **(4)** in $CDCl_3$.

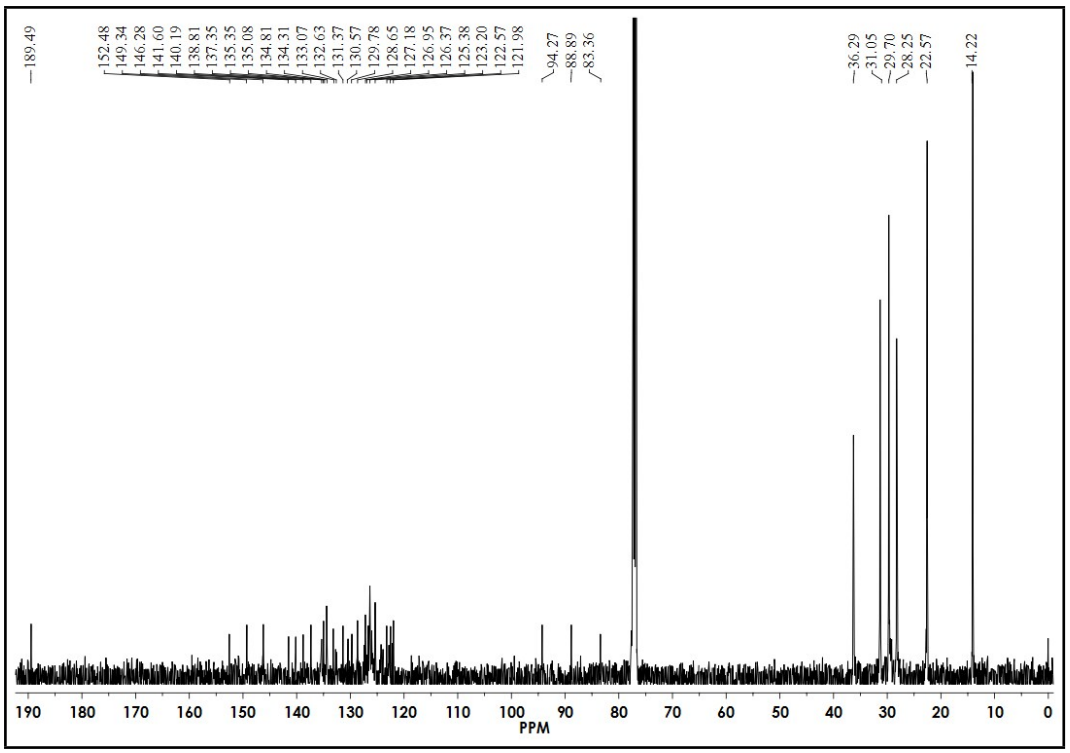


Figure S8: ^{13}C NMR spectrum of **(4)** in $CDCl_3$.

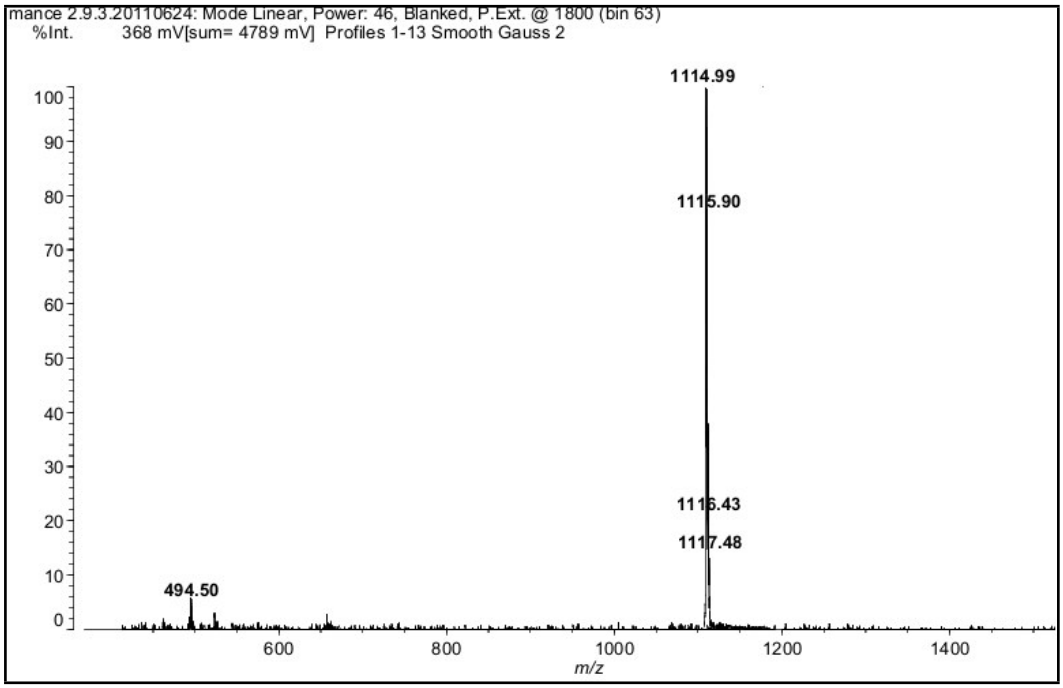


Figure S9: MALDI-TOF Spectrum of compound **(4)**

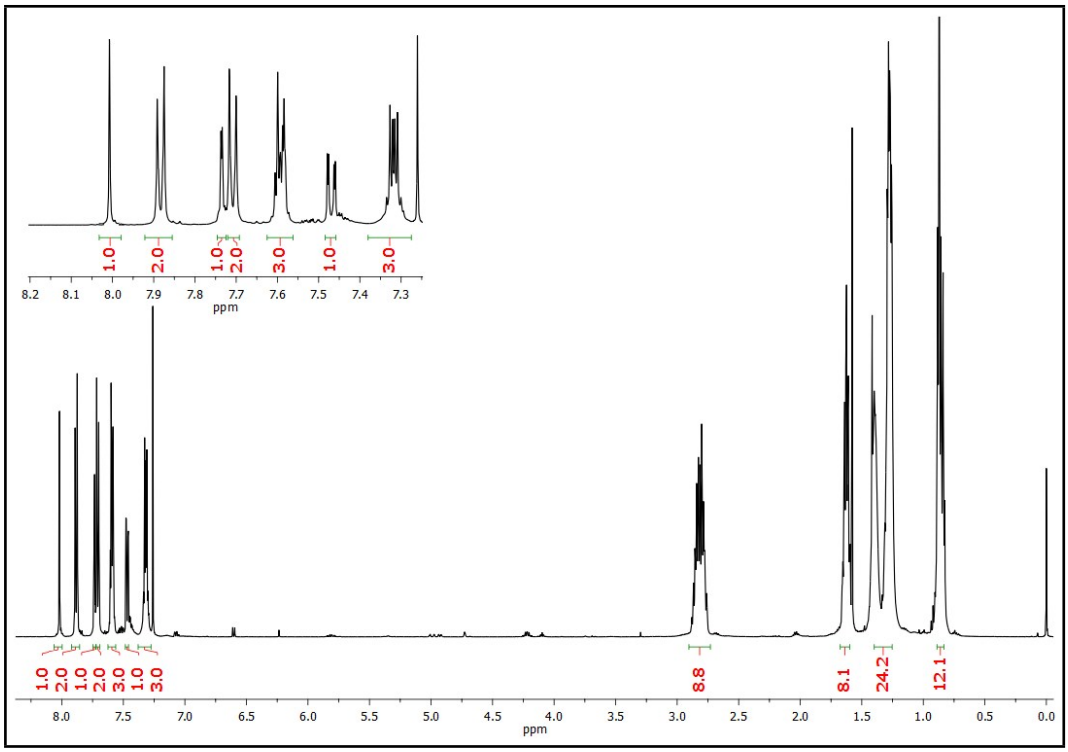


Figure S10: ^{1}H NMR spectrum of **(G7)** in $CDCl_3$.

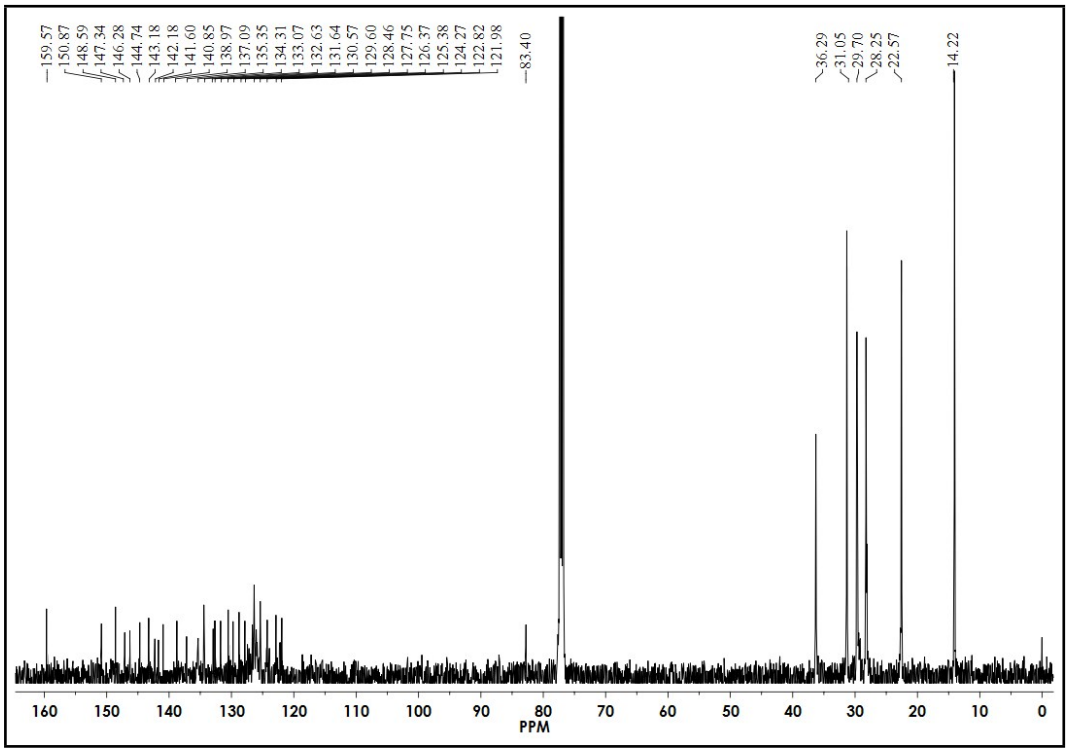


Figure S11: ^{13}C NMR spectrum of **(G7)** in $CDCl_3$.

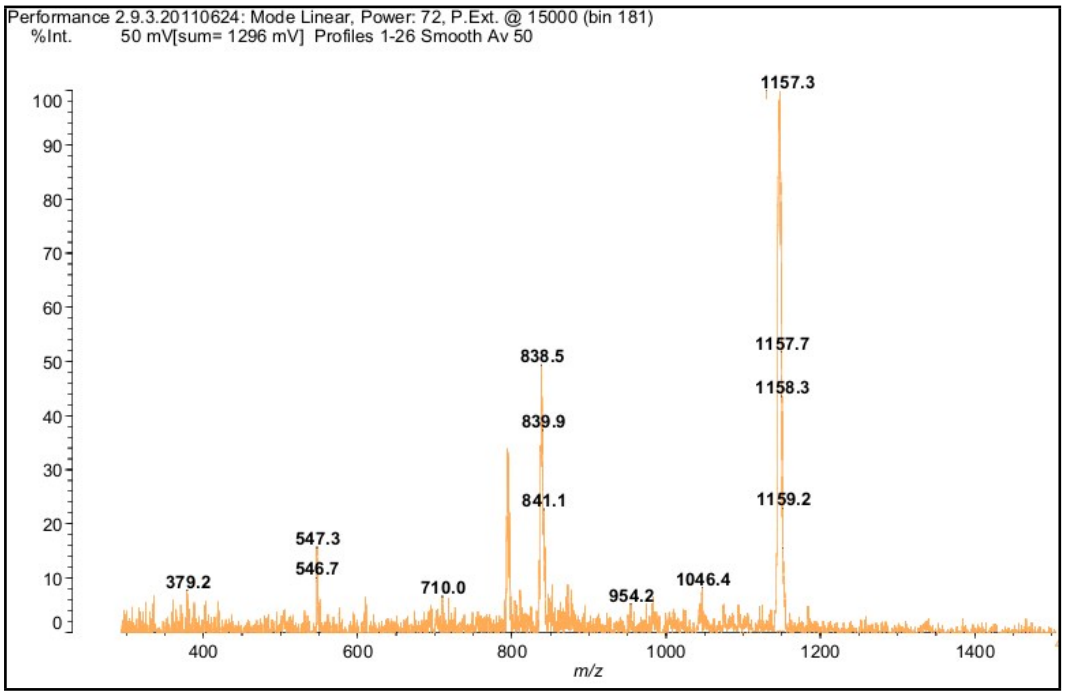


Figure S12: MALDI-TOF Spectrum of compound **(G7)**

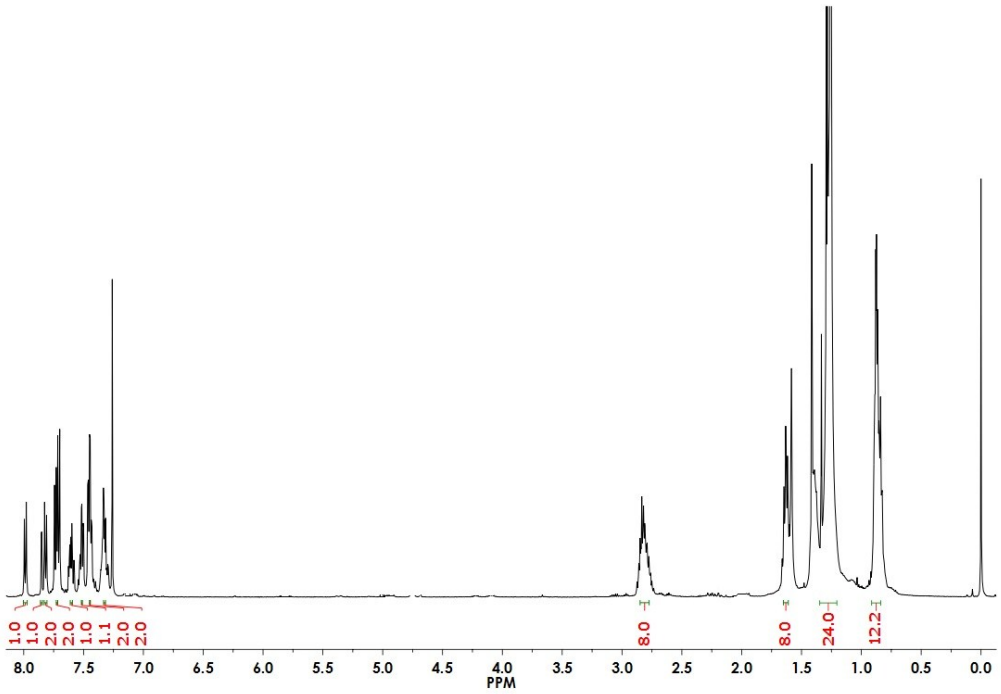


Figure S13: ^{1}H NMR spectrum of **(G8)** in $CDCl_3$.

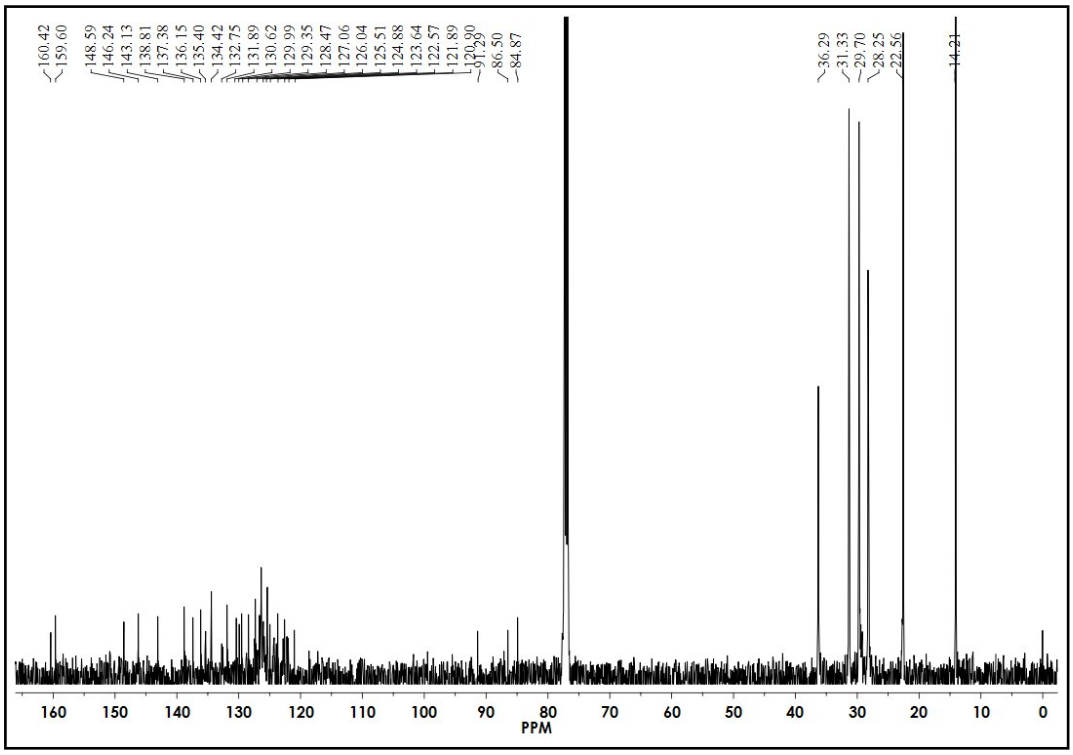


Figure S14: ^{13}C NMR spectrum of **(G8)** in $CDCl_3$.

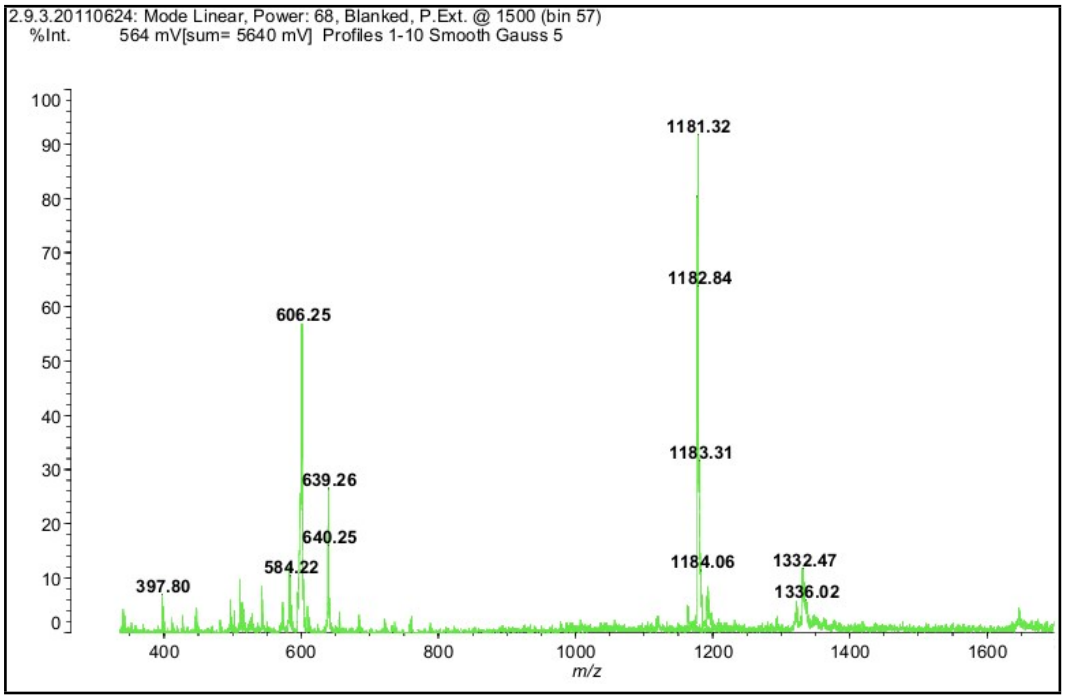


Figure S15: MALDI-TOF Spectrum of compound **(G8)**

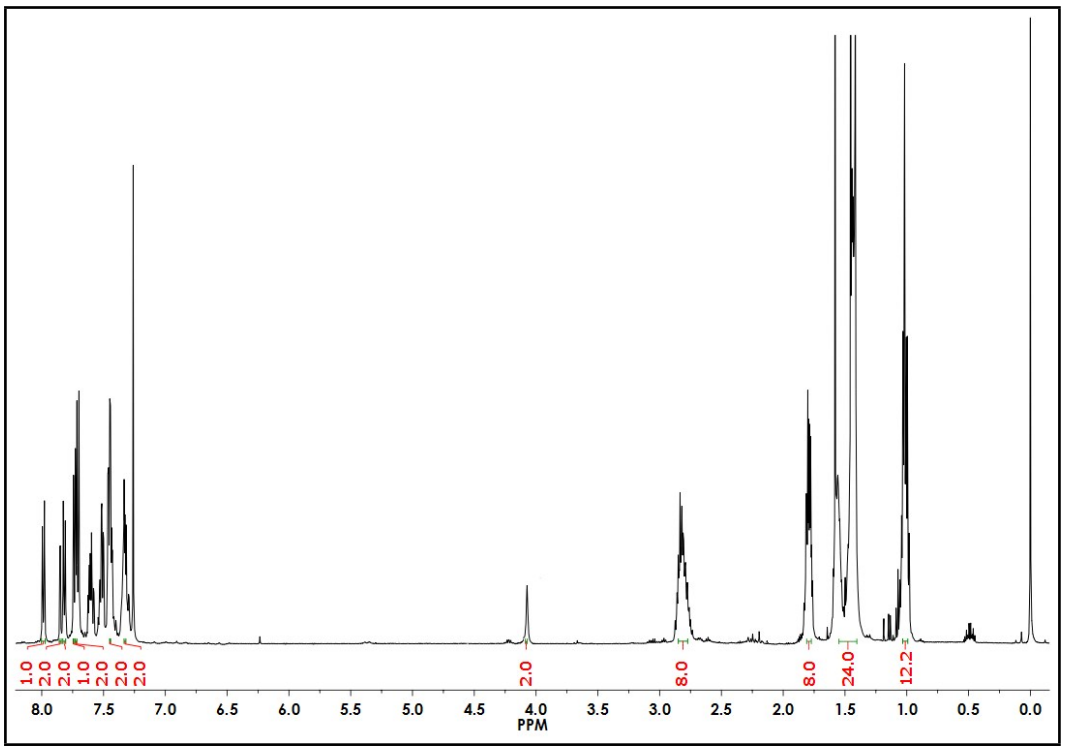


Figure S16: ^{1}H NMR spectrum of **(G9)** in $CDCl_3$.

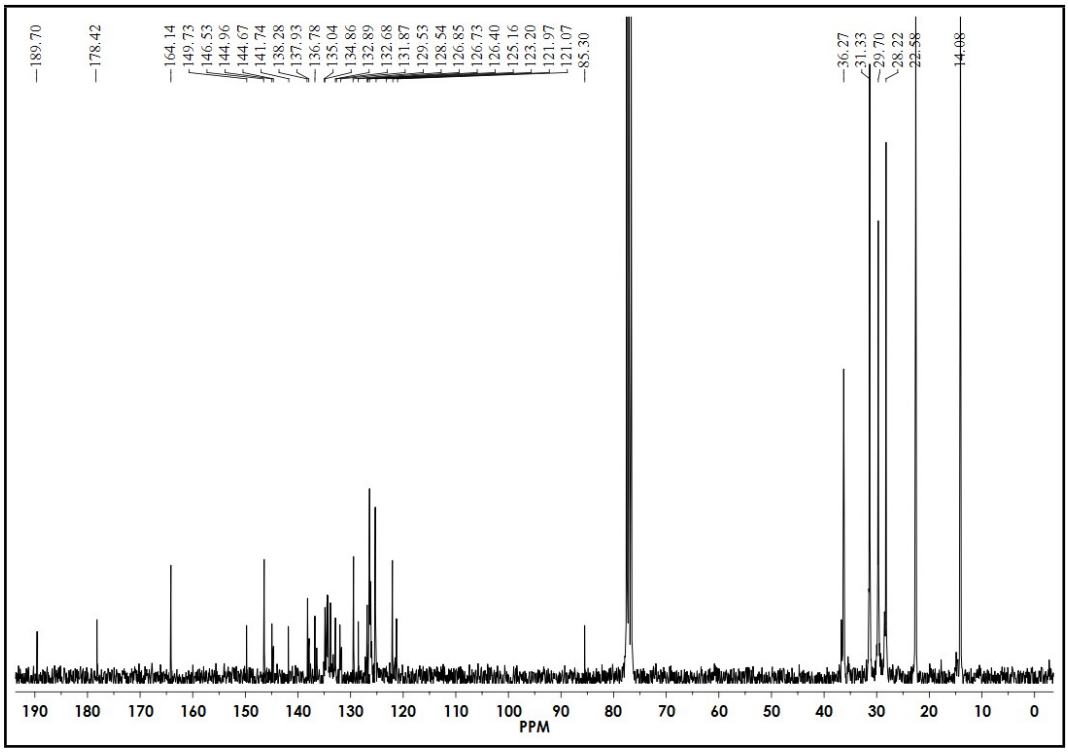


Figure S17: ^{13}C NMR spectrum of **(G9)** in $CDCl_3$.

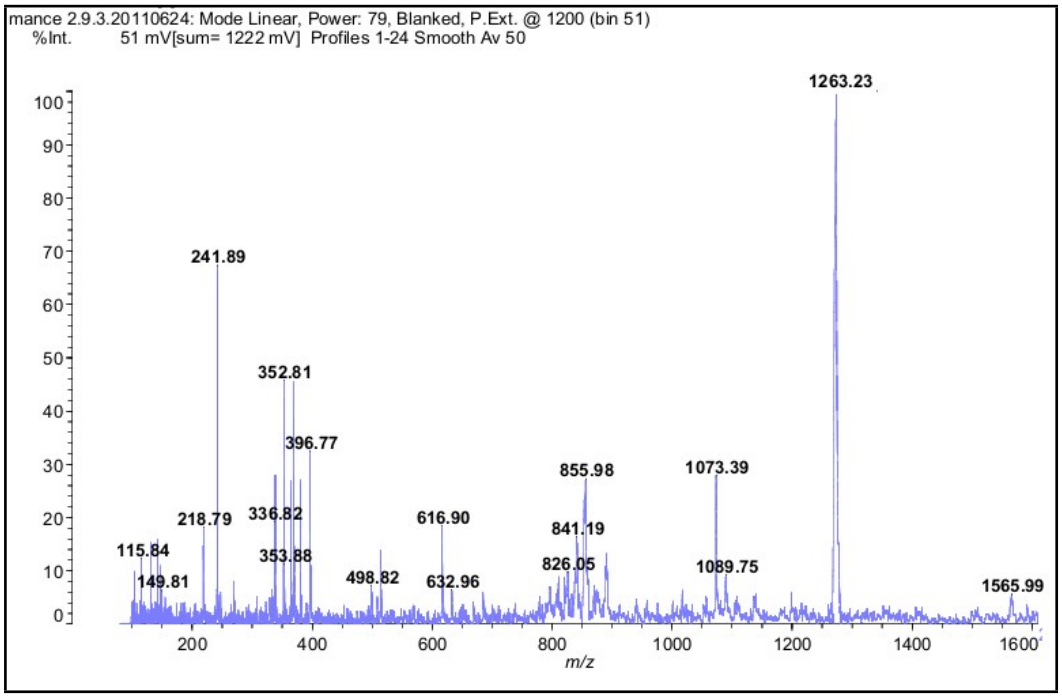


Figure S18: MALDI-TOF Spectrum of compound **(G9)**

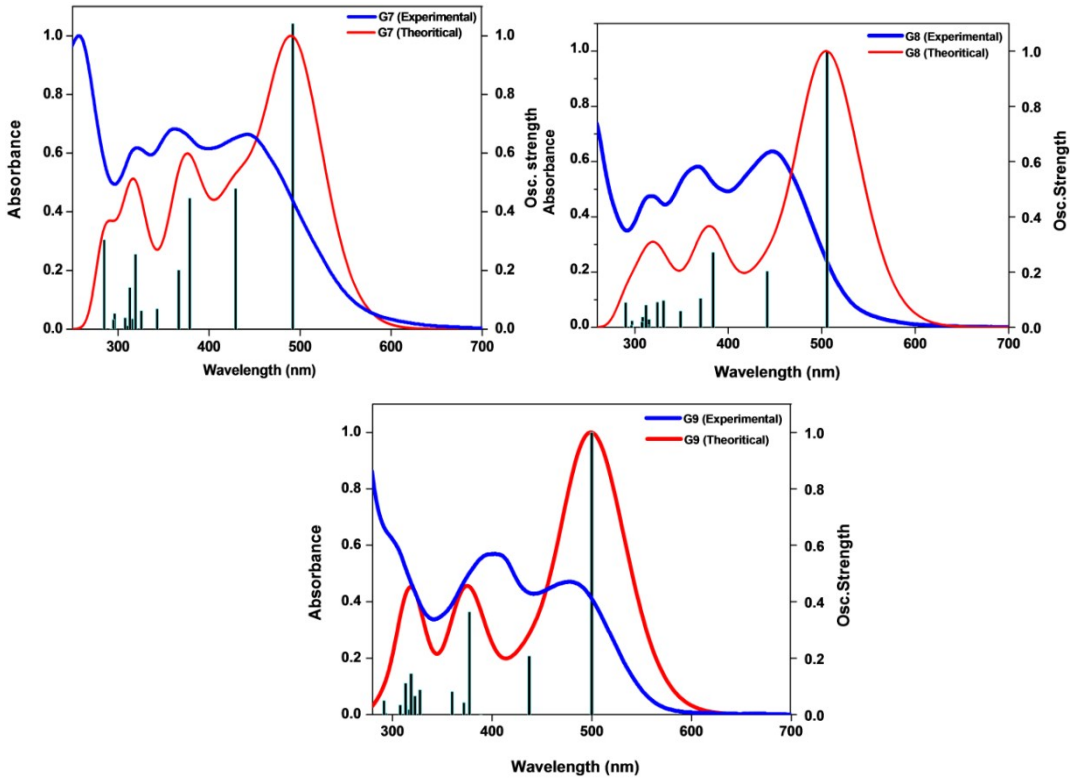


Figure S19: Theoretical and Experimental UV-Visible spectra of G7, G8 & G9 in DMF solvent.

Table S1: The energy values of optimized structure, Optimized structuresand electrostatic potential maps of **G7, G8 & G9** dyes.

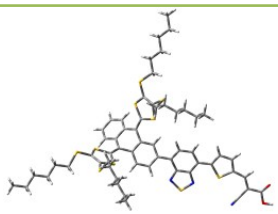
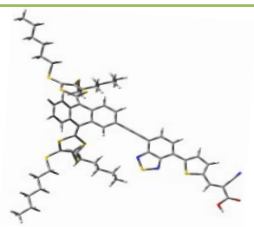
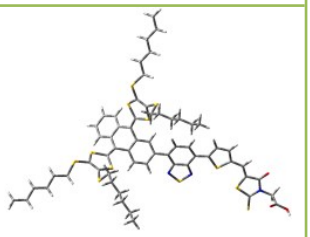
Dye	G 7	G 8	G 9
Minimum energy (in kcal/mol)	4.10 x 10^6	4.15 x 10^6	4.70 x 10^6
Optimized structure			
electrostatic potential maps (ESP)			

Table S2: 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
G7	447	491	1.041	2.52	H-2->LUMO (20%), HOMO->LUMO (68%) H-1->LUMO (4%), HOMO->L+1 (3%)
G8	450	506	1.688	2.45	H-2->LUMO (26%), H-1->LUMO (14%), HOMO->LUMO (54%)
G9	484	498	1.447	2.48	H-2->LUMO (18%), H-1->LUMO (26%), HOMO->LUMO (48%), H-3->L+1 (2%), HOMO->L+1 (3%)

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

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