

Electronic Supplementary Information

Effect of spacer and anchoring group of tetrathiafulvalene based sensitizers influence on the performance of dye sensitized solar cells

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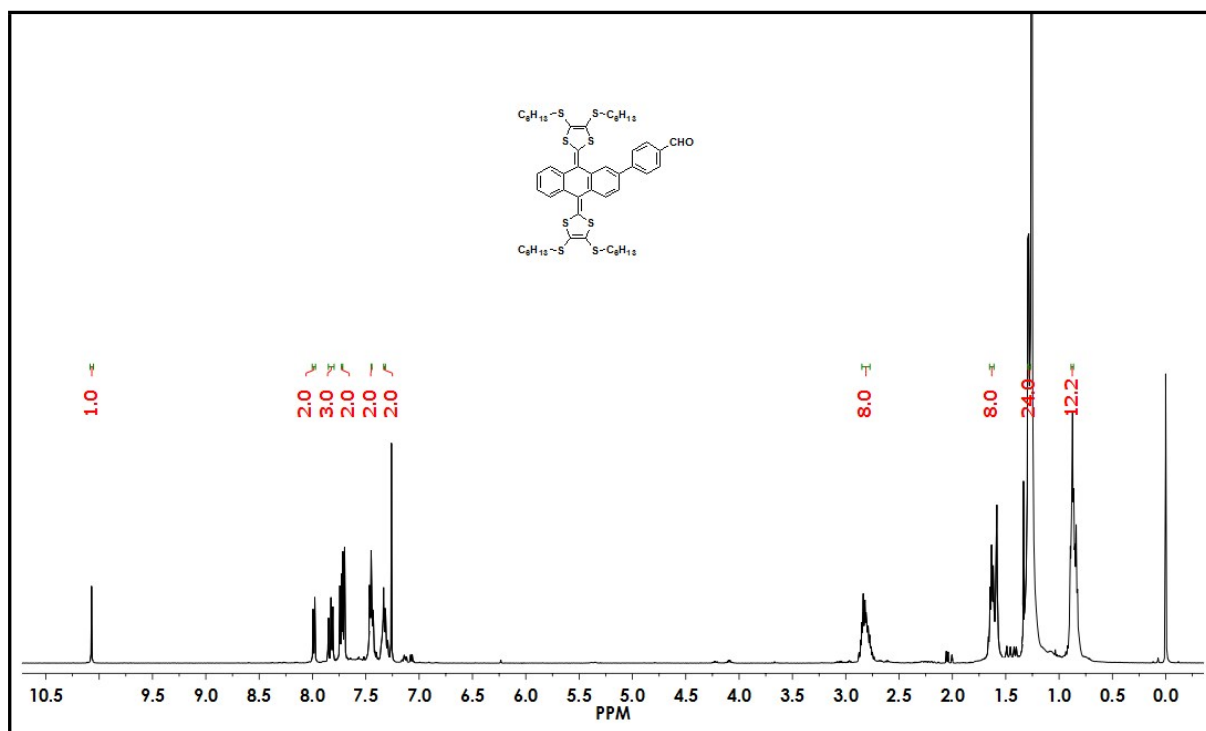


Fig. S1: ¹H NMR Spectrum of (**2b**) in CDCl₃.

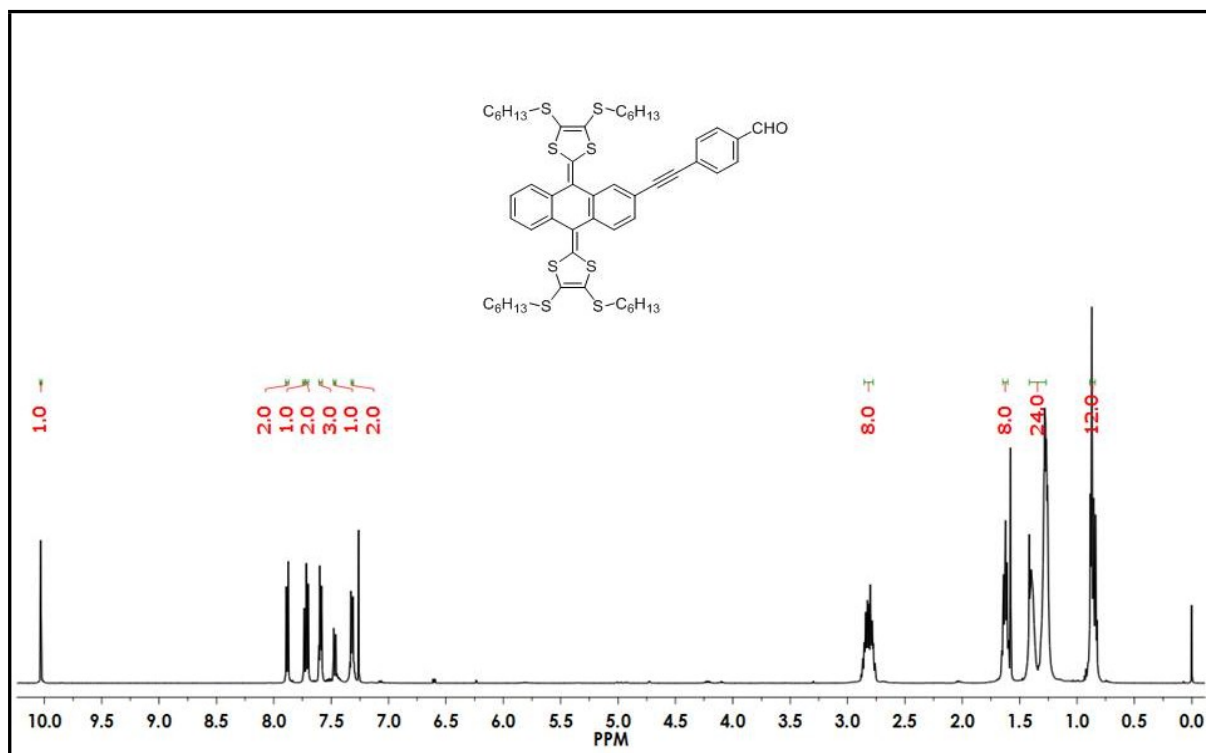


Fig. S2: ^1H NMR Spectrum of (**2c**) in CDCl_3

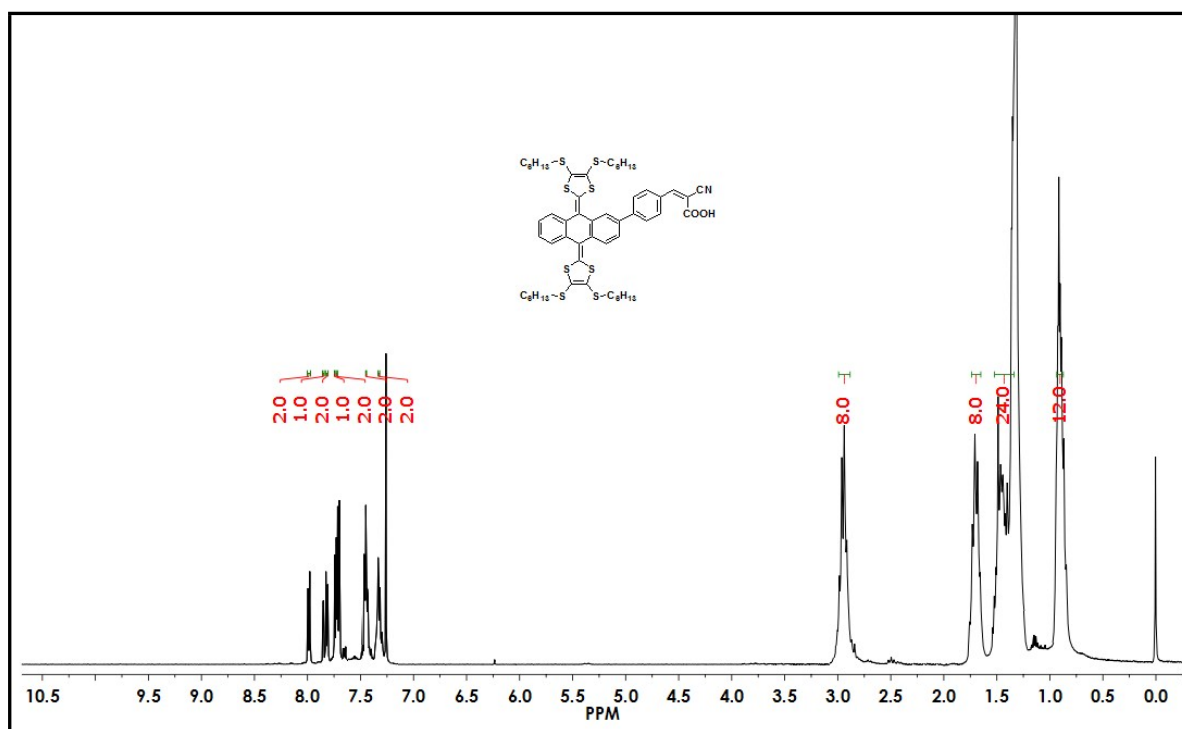


Fig. S3: ^1H NMR Spectrum of (**G2**) in CDCl_3

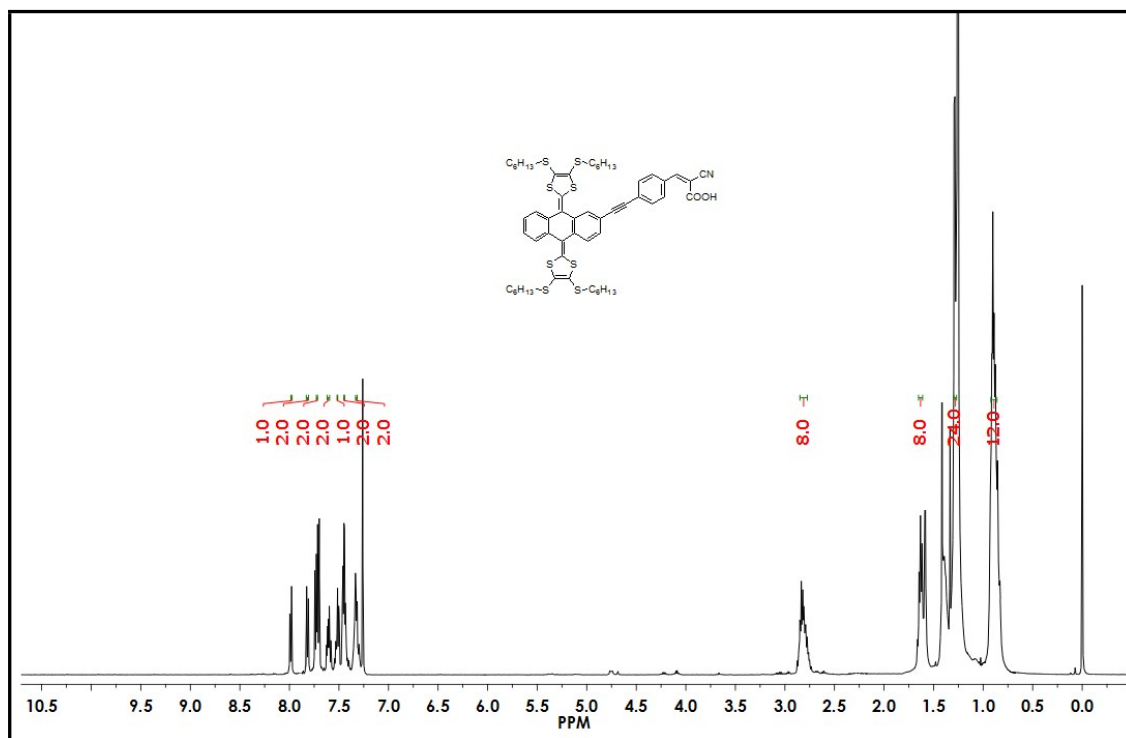


Fig. S4: $^1\text{H NMR}$ Spectrum of (**G4**) in CDCl_3

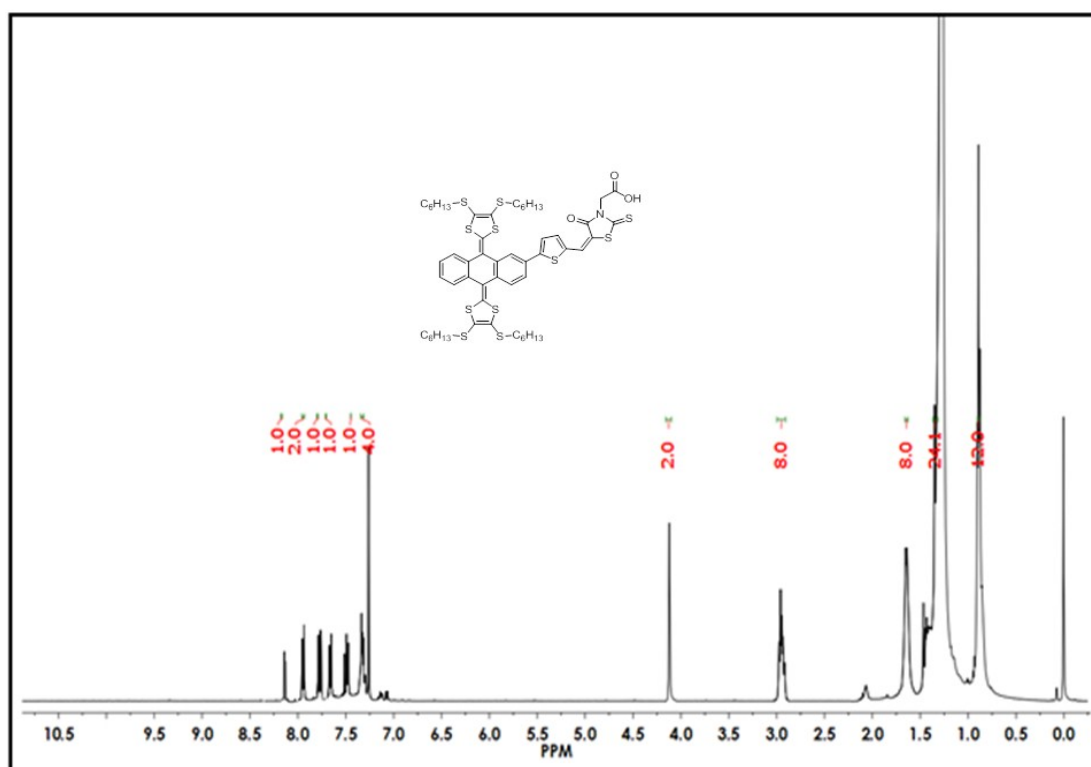


Fig.S5: $^1\text{H NMR}$ Spectrum of (**G5**) in CDCl_3

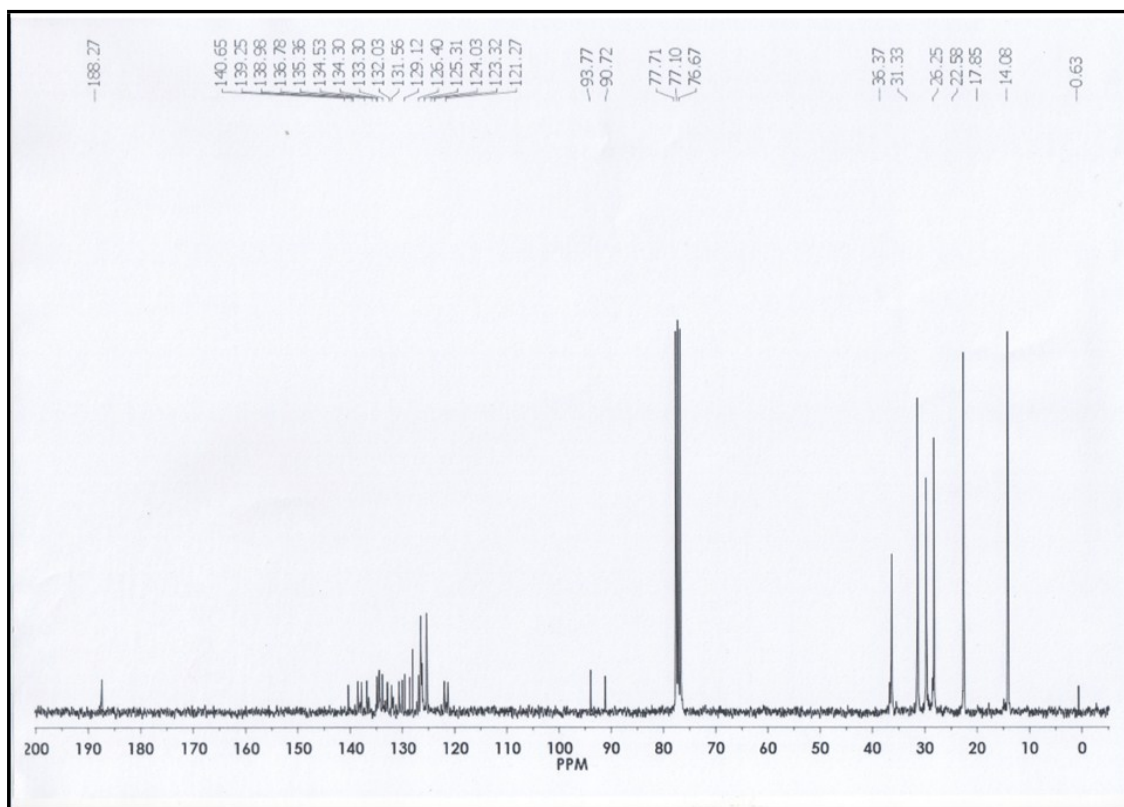


Fig. S8: ^{13}C -NMR Spectrum of (**2c**) in CDCl_3

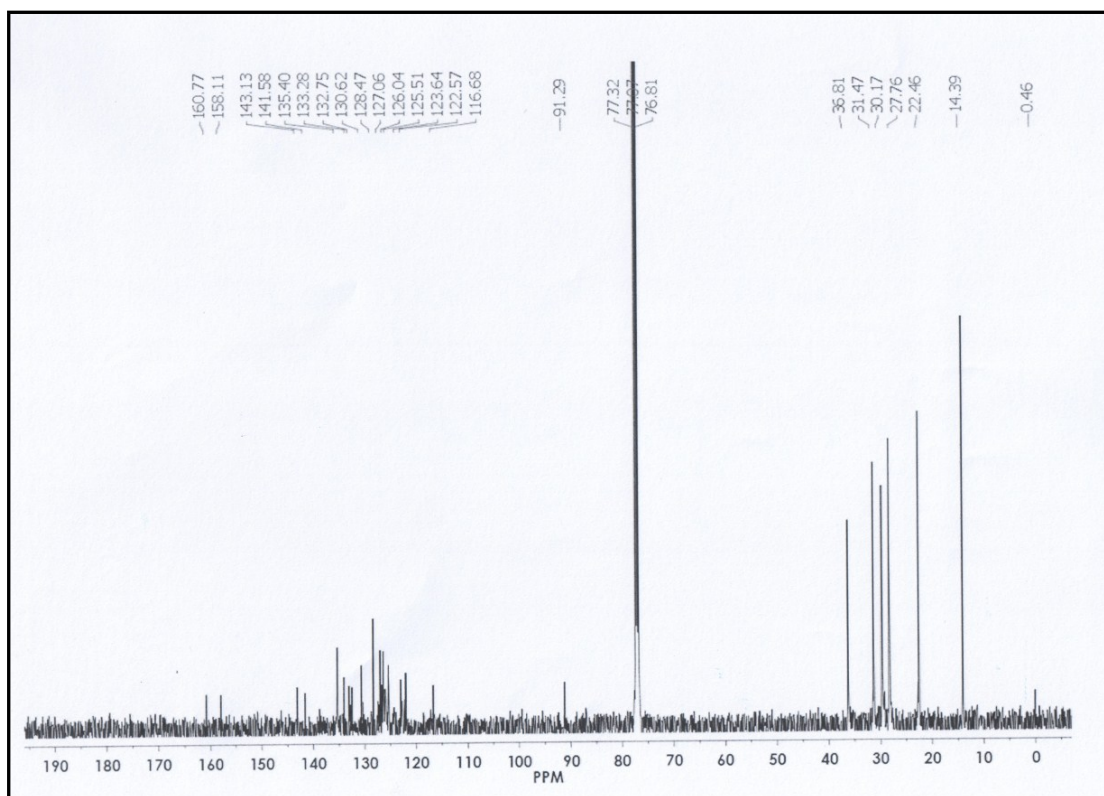


Fig. S9: ^{13}C -NMR Spectrum of (**G2**) in CDCl_3

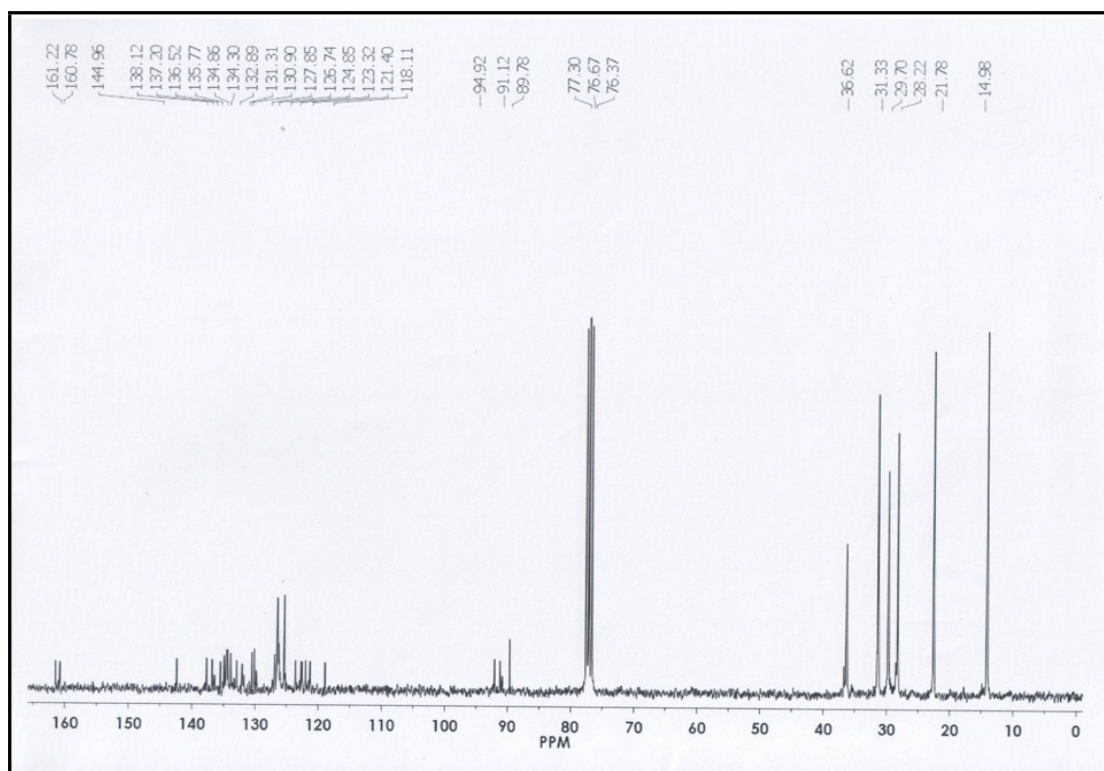


Fig. S10: ^{13}C -NMR Spectrum of (**G4**) in CDCl_3

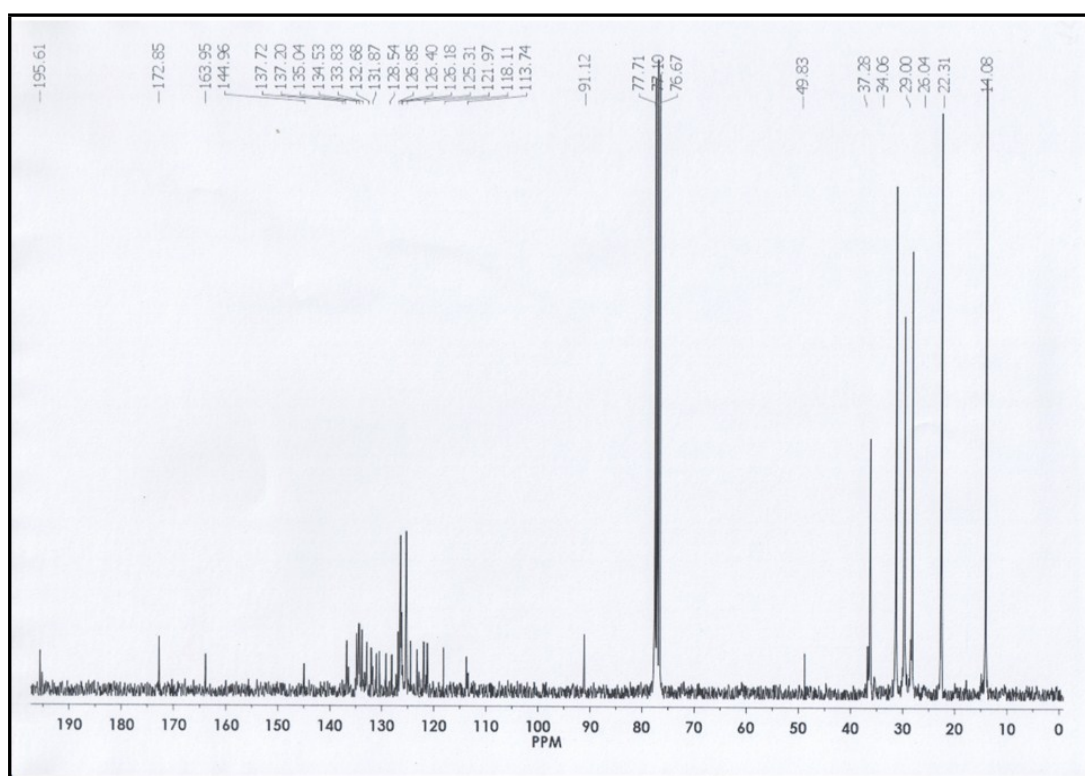


Fig. S11: ^{13}C -NMR Spectrum of (**G5**) in CDCl_3

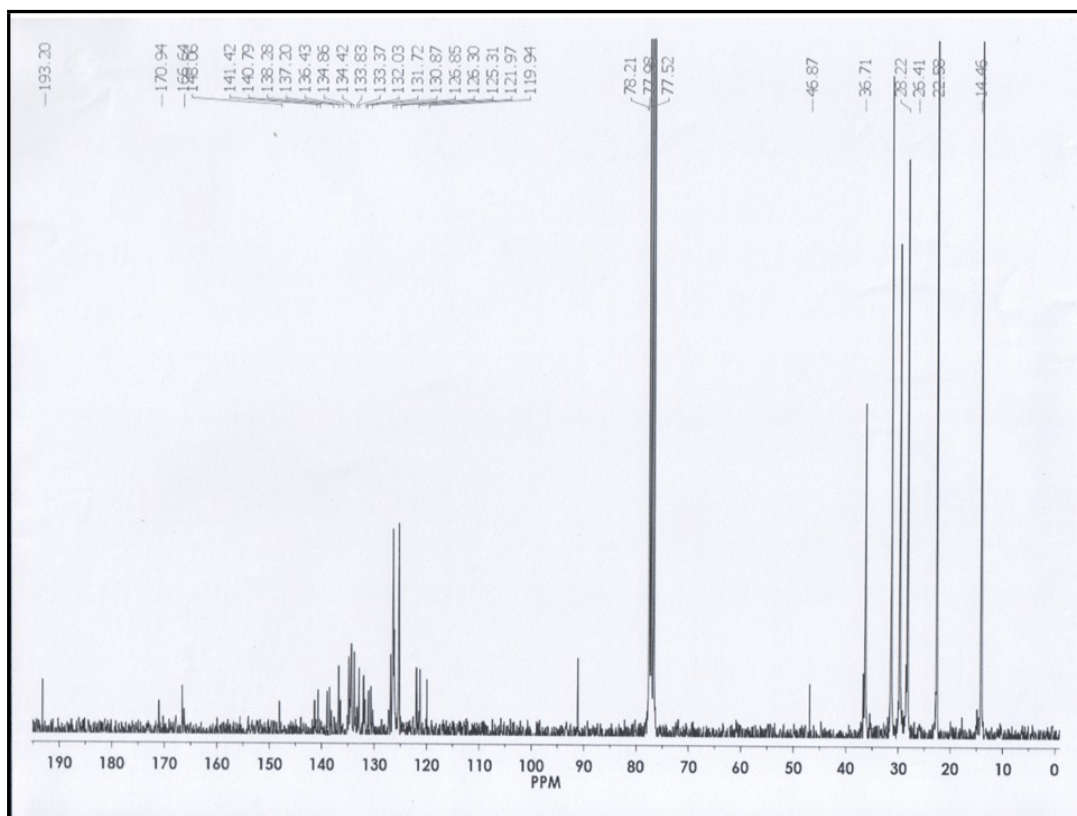


Fig. S12: ^{13}C -NMR Spectrum of (**G6**) in CDCl_3

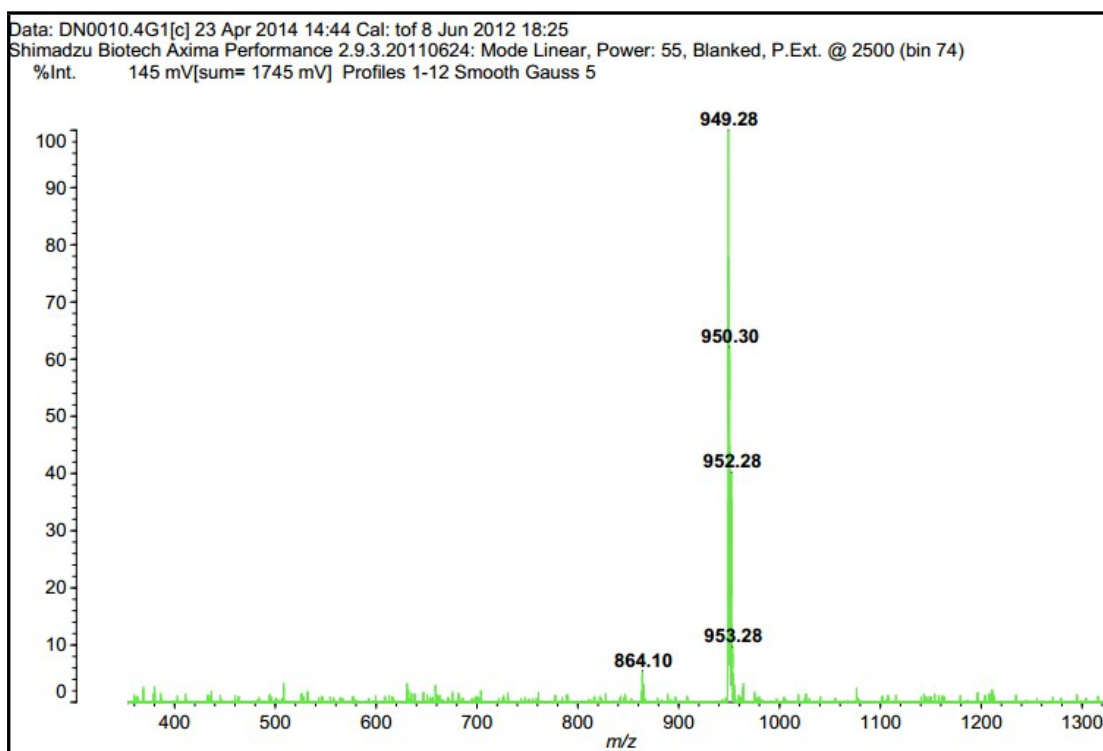


Fig. S13: MALDI-TOF Spectrum of compound (**2b**)

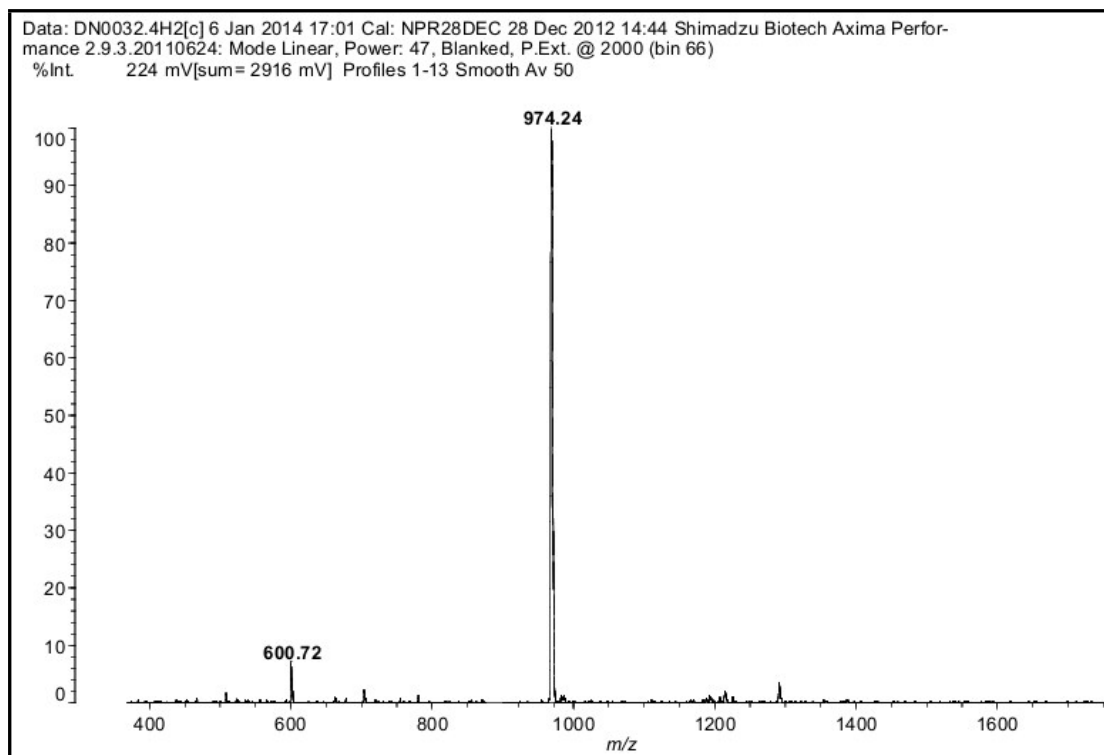


Fig. S14: MALDI-TOF Spectrum of compound (2c)

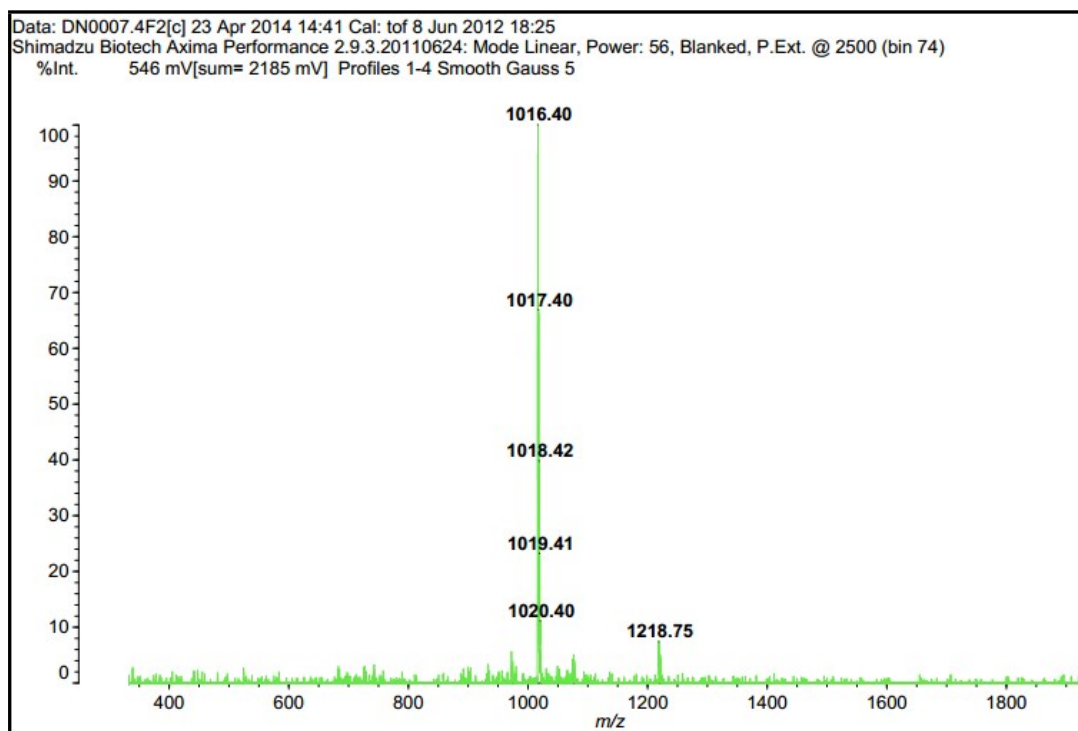


Fig. S15: MALDI-TOF Spectrum of compound (G2)

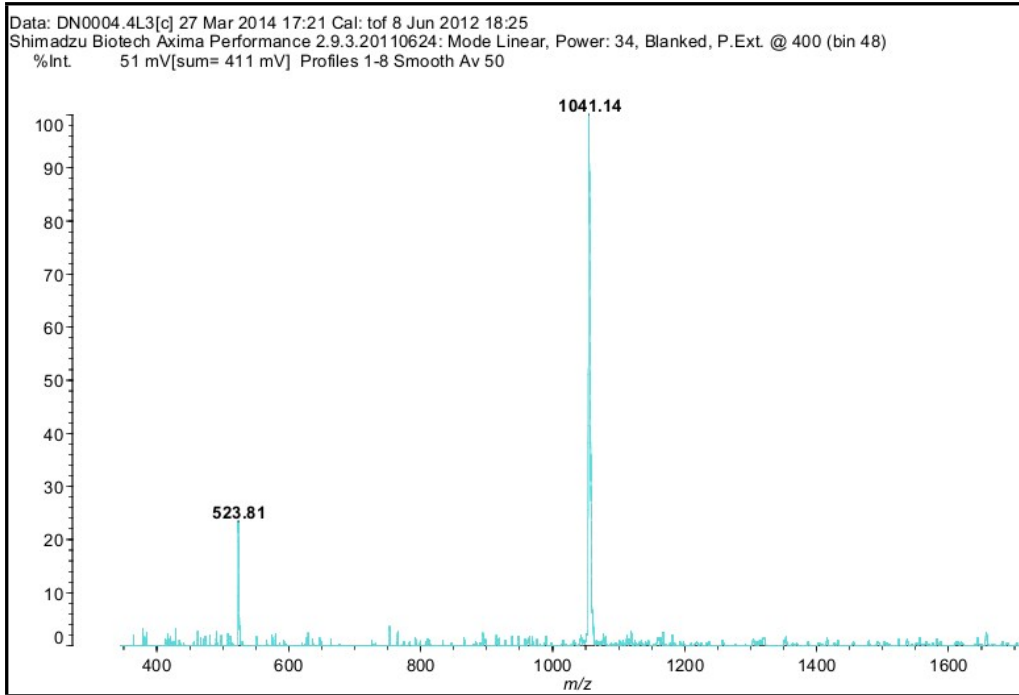


Fig. S16: MALDI-TOF Spectrum of compound (G4)

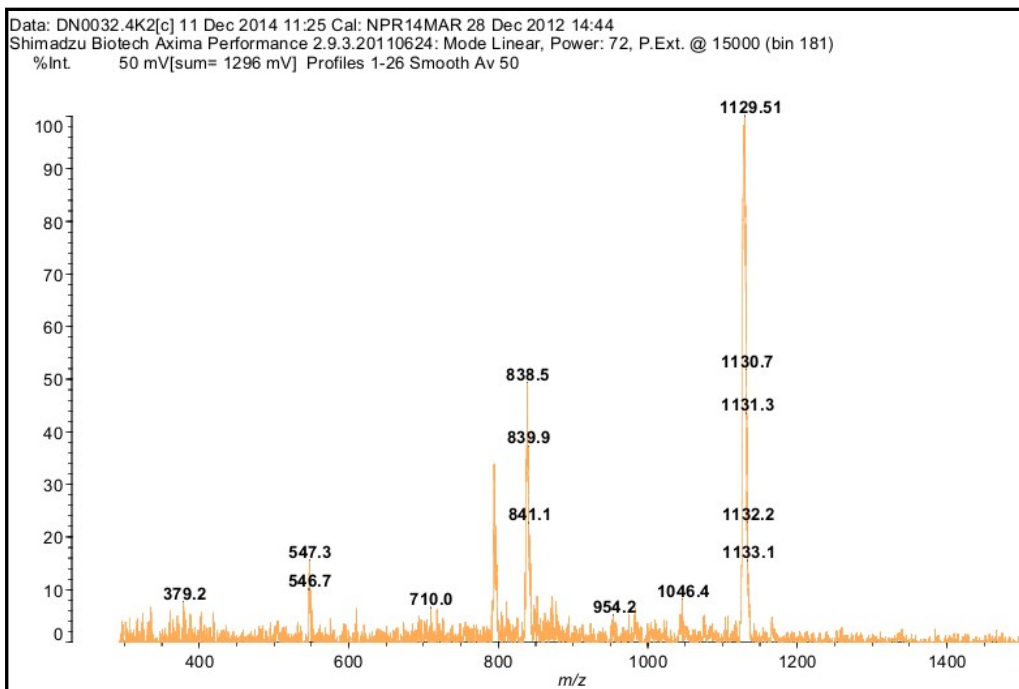


Fig. S17: MALDI-TOF Spectrum of compound (G5)

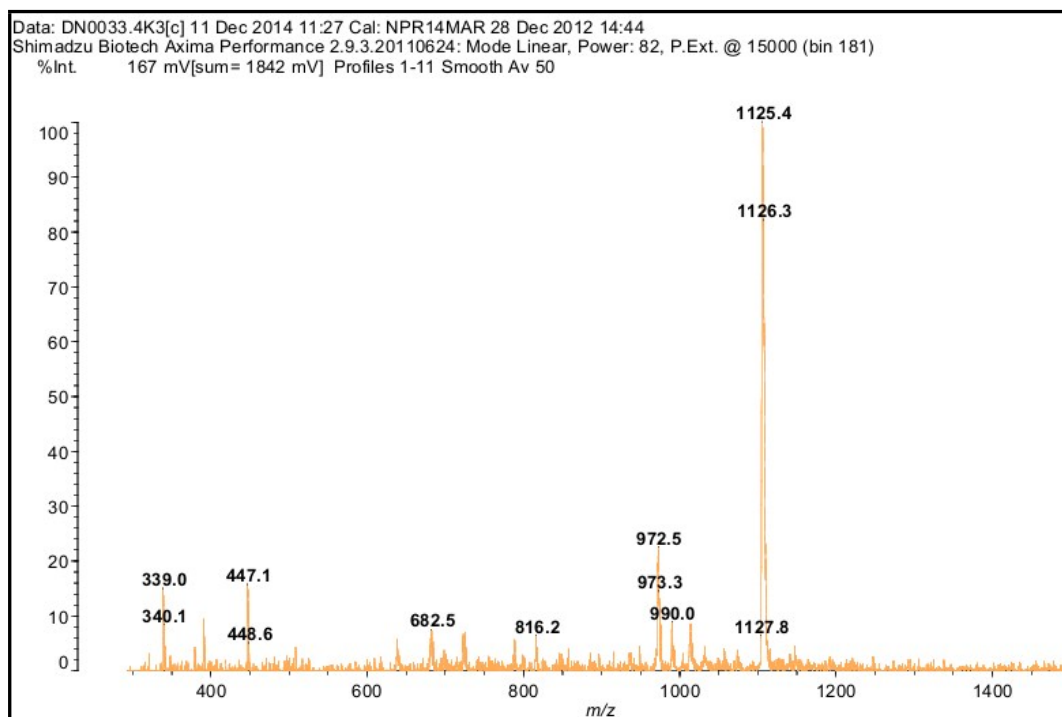


Fig. S18: MALDI-TOF Spectrum of compound (G6)

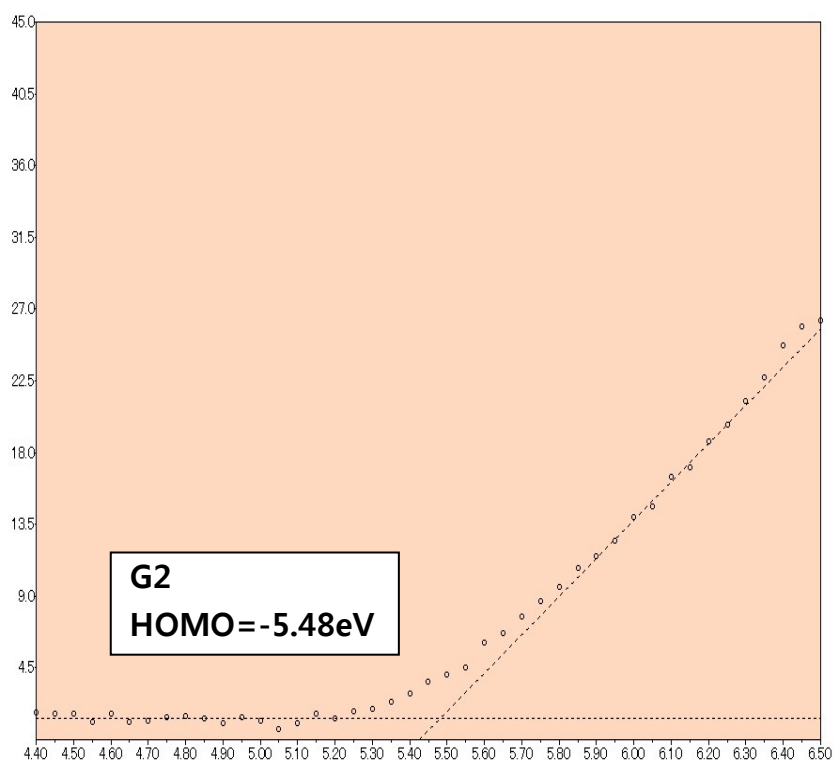


Fig. S19: HOMO energy of G2.

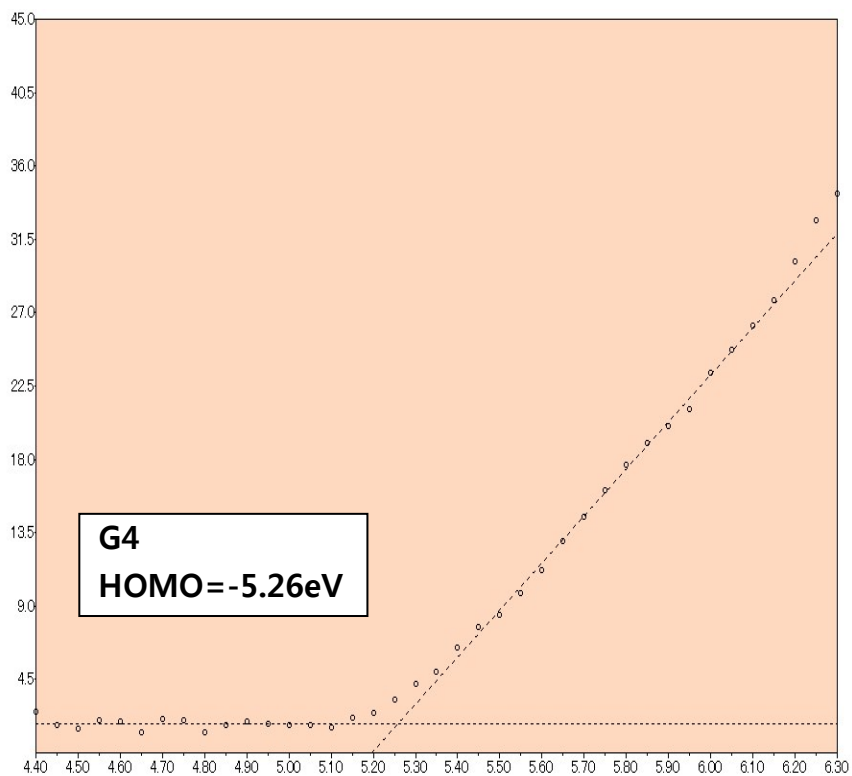


Fig. S20: HOMO energy of G4.

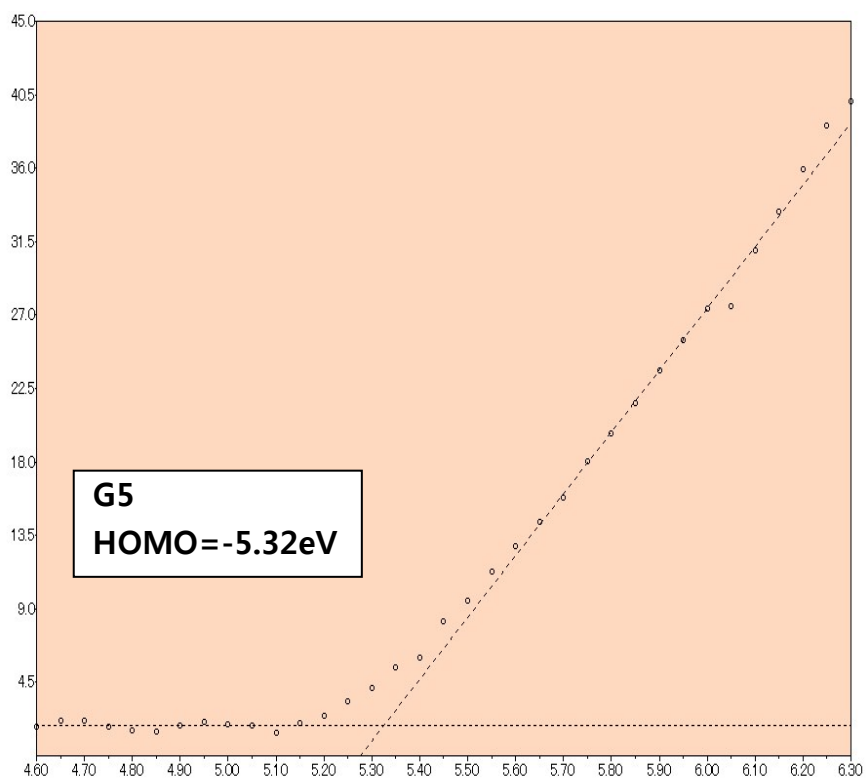


Fig. S21: HOMO energy of G5.

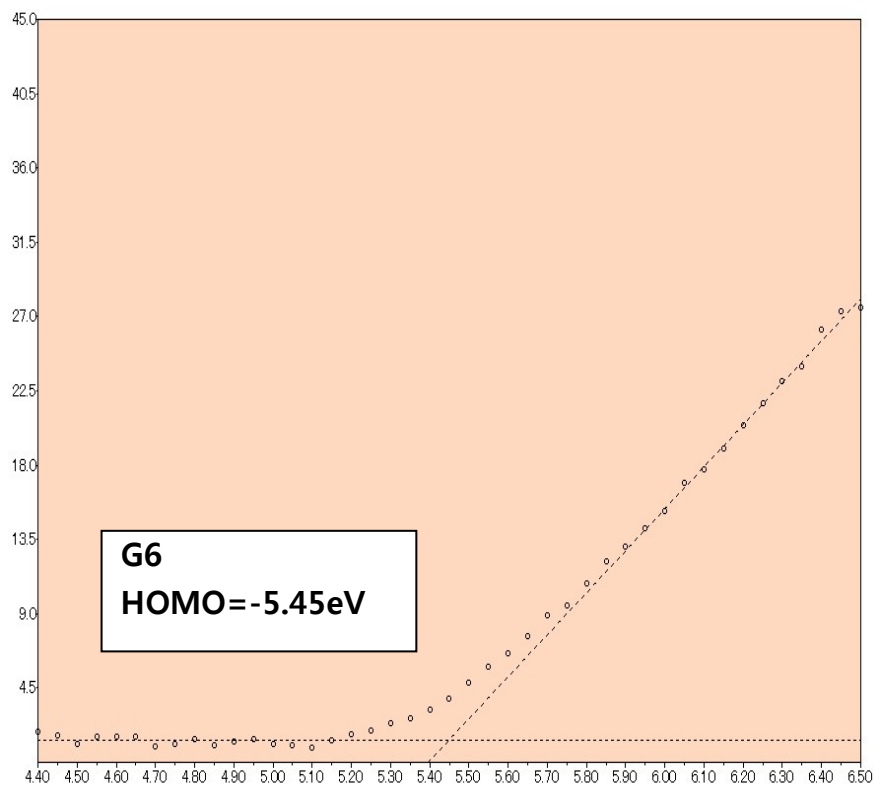


Fig. S22: HOMO energy of G6.

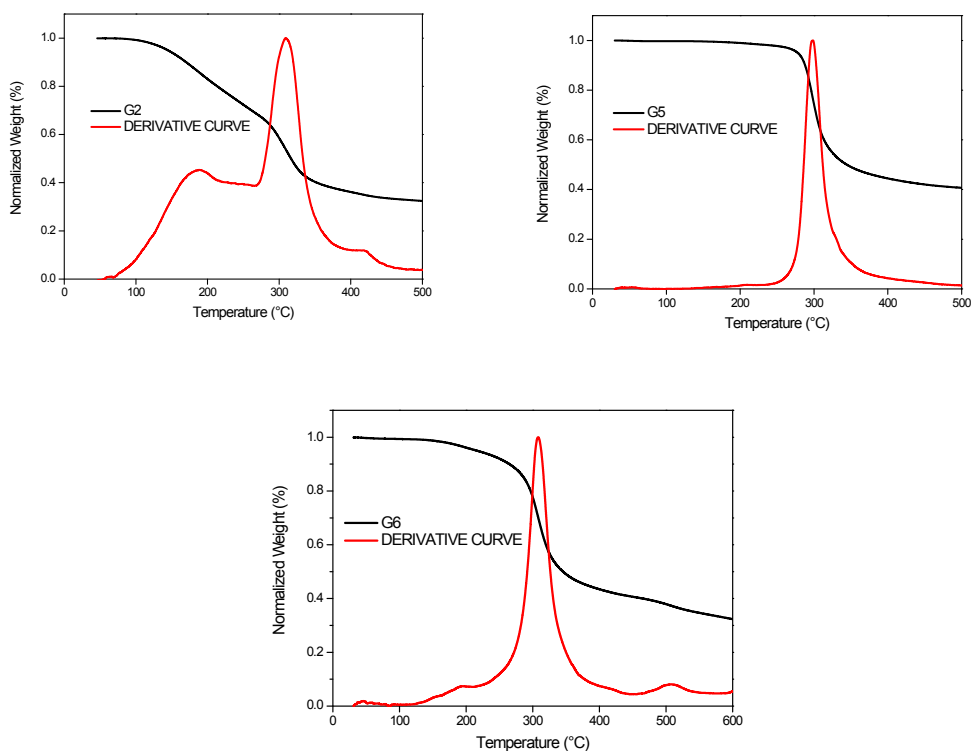


Fig. S23: TG/DTG Curves of G2, G5 and G6 with a heating rate of $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen atmosphere.

Table S1: The optimized structures, Minimum energy and electrostatic potential (ESP) maps of G2, G4, G5 and G6 dyes.

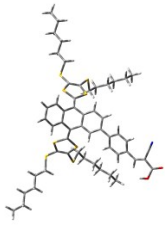
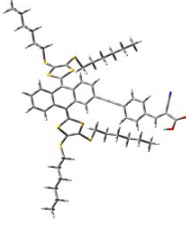
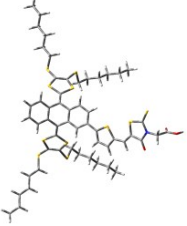
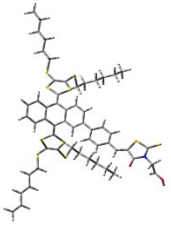
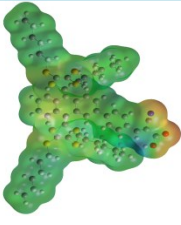
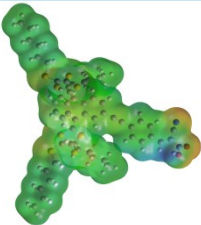
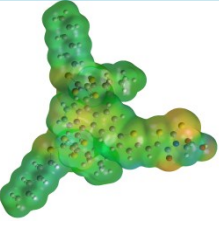

| Dye | G2 | G4 | G5 | G6 |
|--|---|---|--|---|
| Optimized structure And Minimum energy (in kcal/mol) |  3.44×10^6 |  3.49×10^6 |  3.56×10^6 |  4.03×10^6 |
| Electrostatic potential (ESP)map |  |  |  |  |

Table S2: Comparison of the experimental optical properties with the theoretical data by B3LYP in dichloromethane of G2, G4, G5 and G6 dyes.

| Dye | ^a λ_{\max} | ^b λ_{\max} | ^c <i>f</i> | ^d E (eV) | % of Molecular Orbital Composition |
|-----|-------------------------------|-------------------------------|-----------------------|---------------------|---|
| G 2 | 445 | 420 | 0.639 | 2.94 | HOMO→LUMO (75%), HOMO→L+1 (18%) H-2→LUMO (2%) |
| G 4 | 455 | 435 | 0.925 | 2.84 | HOMO→LUMO (71%), HOMO→L+1 (19%) H-2→LUMO (5%) |
| G5 | 440 | 453 | 0.989 | 2.73 | H-2→LUMO (16%), HOMO→LUMO (66%) H-1→LUMO (7%), HOMO→L+1 |
| G 6 | 390 | 413 | 0.860 | 2.99 | HOMO→LUMO (63%), HOMO→L+1 (23%) H-2→LUMO (9%) |

^aRecorded absorbance in nm, ^b theoretical absorbance in nm, ^c Oscillation strength, and ^d excited state energy in eV.