Supporting Information

Regiospecific Protonation of Organic Chromophores

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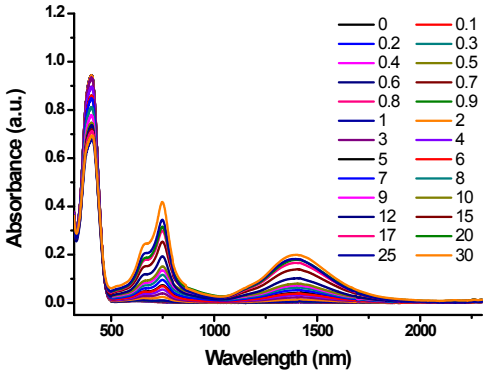


Figure S1. UV-vis-NIR spectrum of chromophore **M3** under different TFA concentration in chloroform solution.

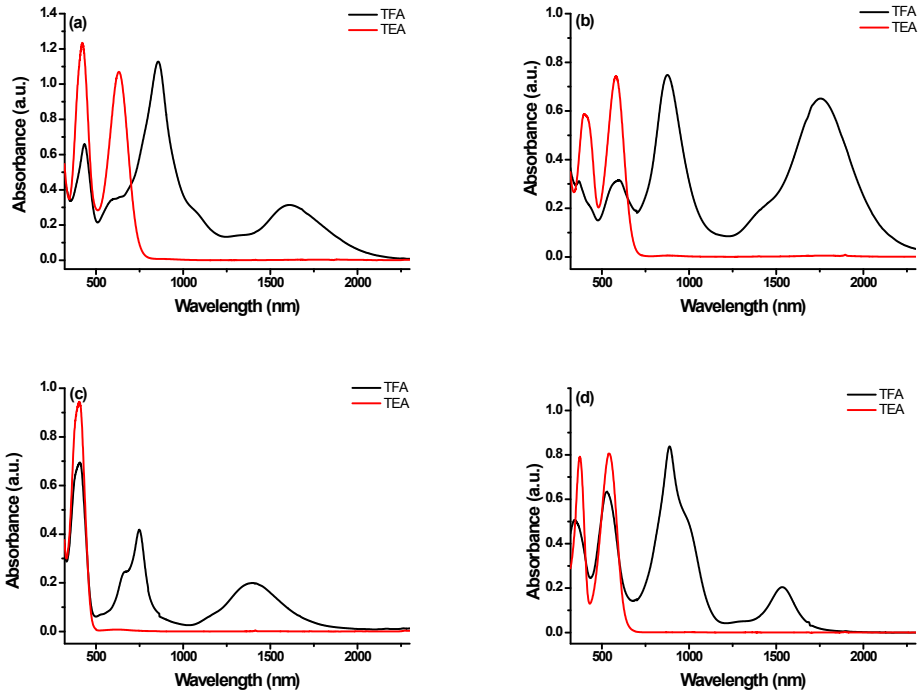


Figure S2. UV-vis-NIR spectrum of chromophores upon the treatment of TFA and then TEA in chloroform solution: (a) **M1**, (b) **M2**, (c) **M3** and (d) **M4**.

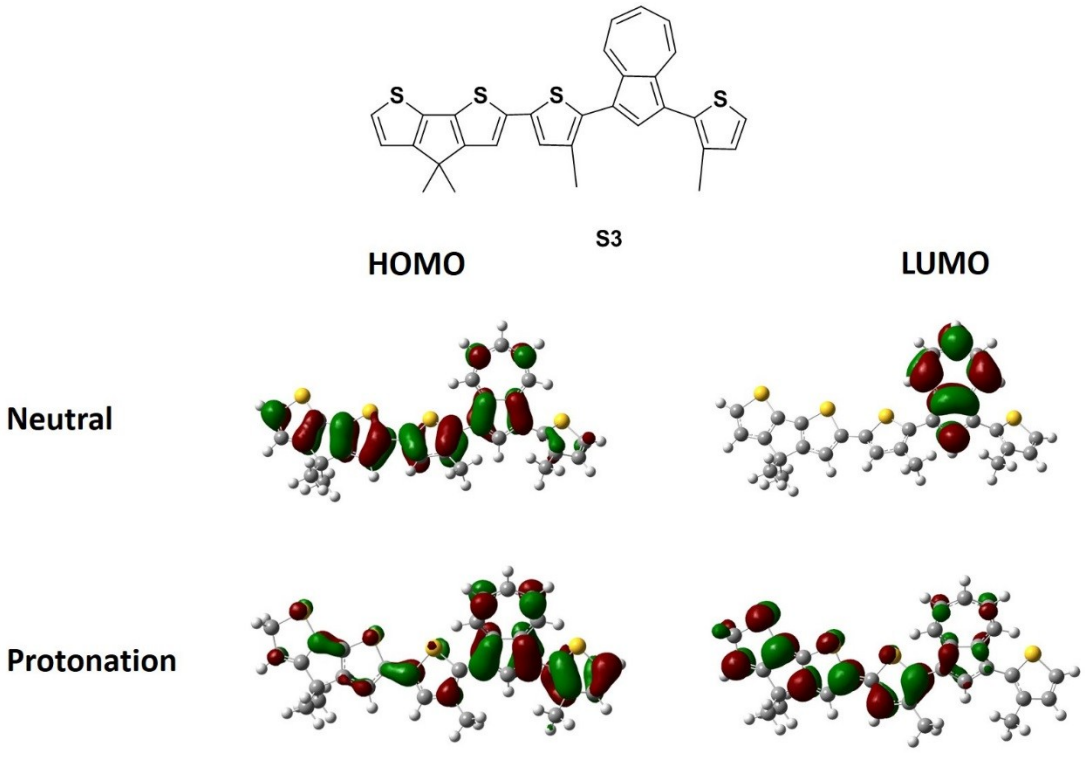
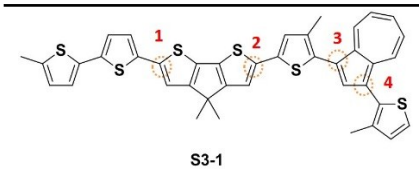


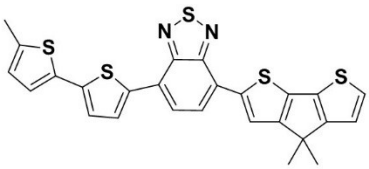
Figure S3. Upper: Simplified monomer **S3** for DFT calculation; bottom: optimized structures of frontier molecular orbitals for model compounds **S3** in their neutral and protonated states.

Table S1. The corrected Zero Point Vibrational Energies (ZPE) and Proton Affinities (PA) calculated by G09 at different sites of Mod-S3-1.

Entry	scaled ZPE (au)	PA (kcal/mol)
P1	0.5765	242.7
P2	0.5760	240.5
P3	0.5749	230.7
P4	0.5751	231.1



S3-1



S4

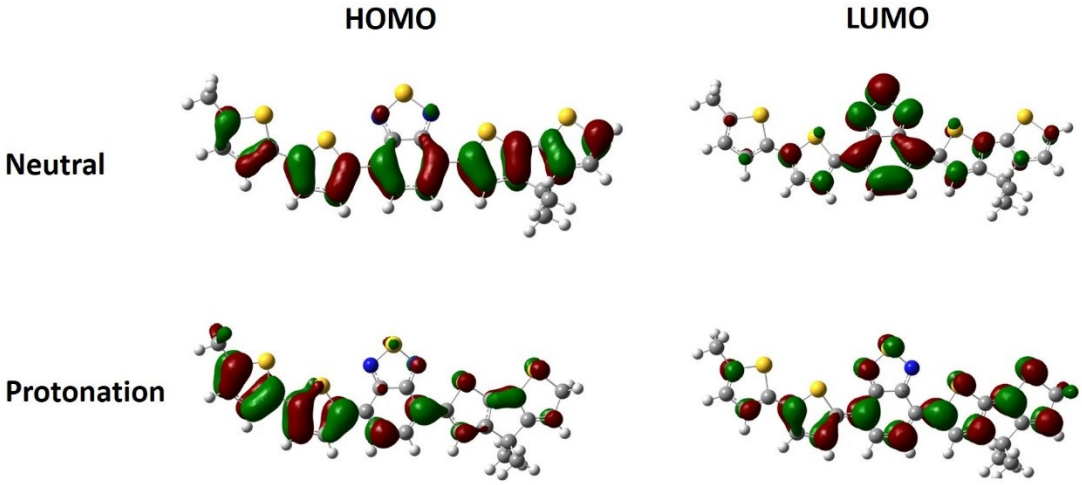
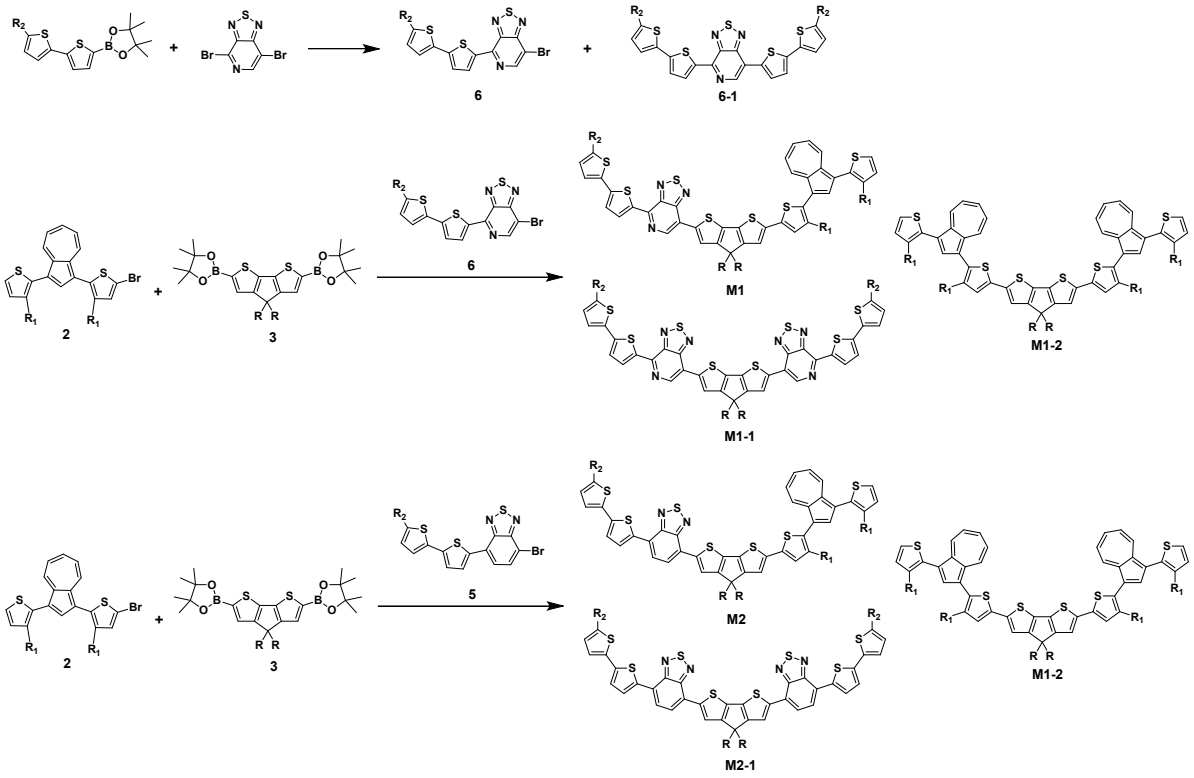
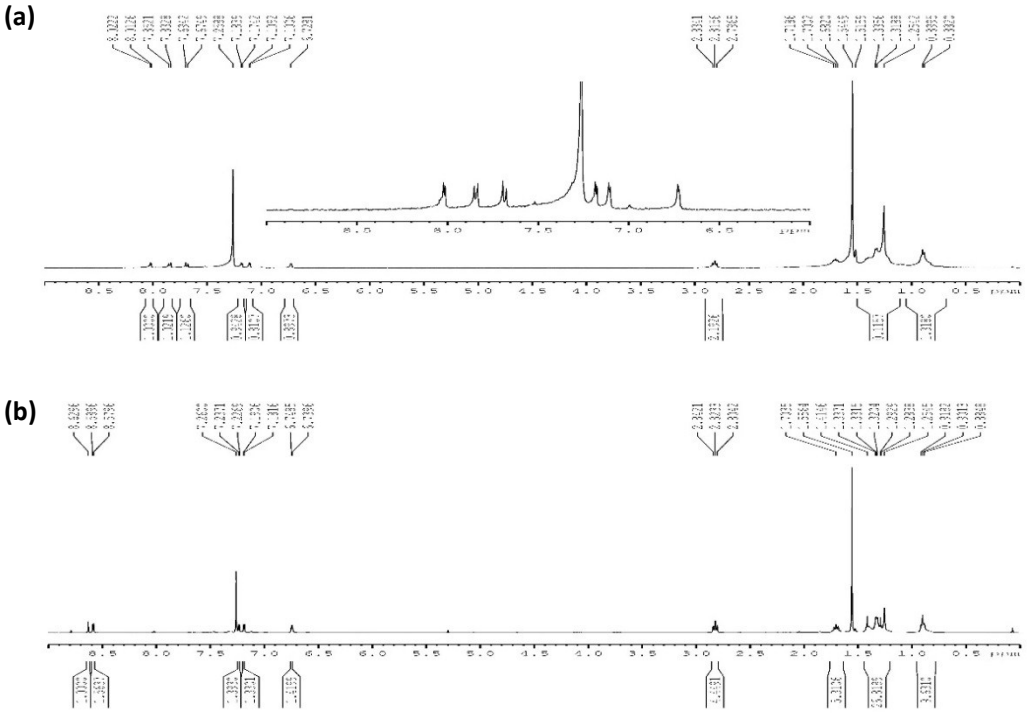


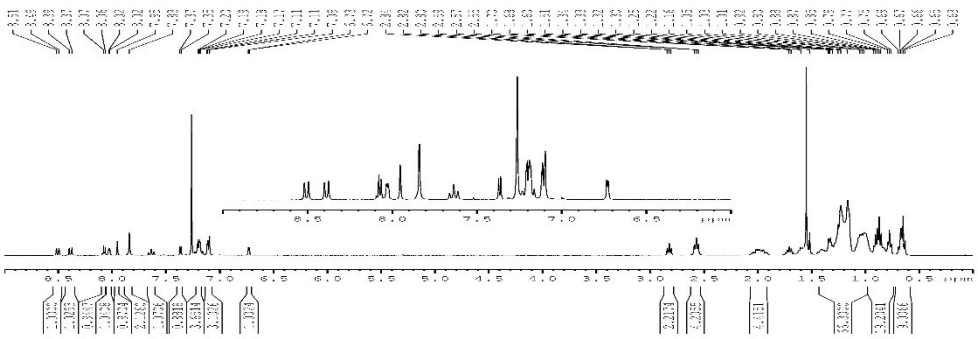
Figure S4. Upper: Simplified monomer **S4** for DFT calculation; bottom: optimized structures of frontier molecular orbitals for model compounds **S4** in their neutral and protonated states.



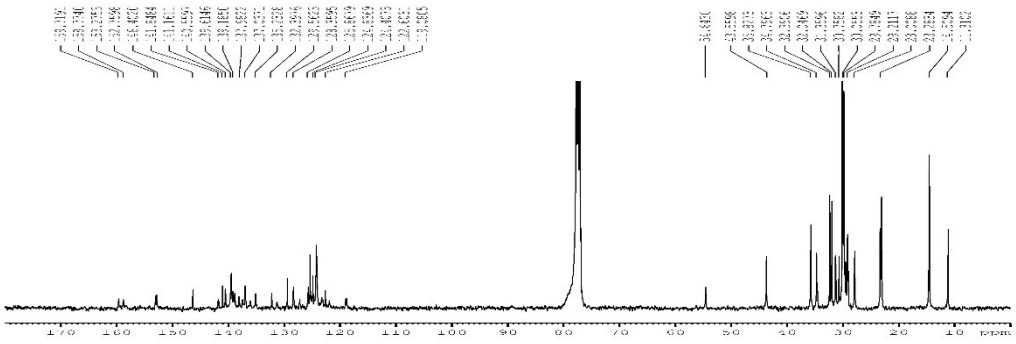
Scheme S1 The possible by-products formation in the Suzuki coupling for compounds **6**, **M1** and **M2**.



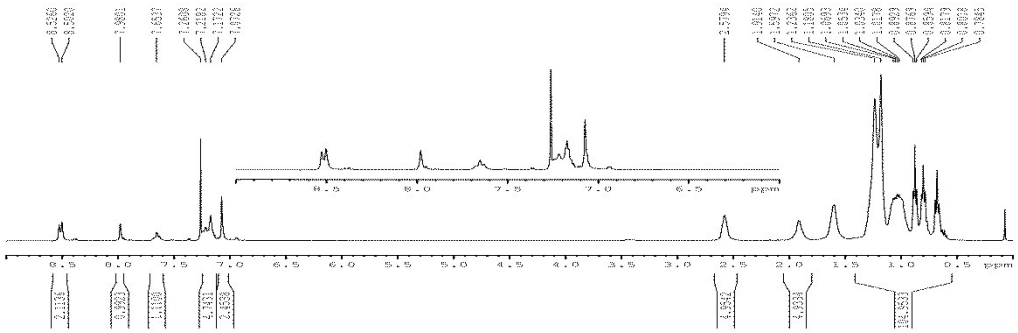
(c)



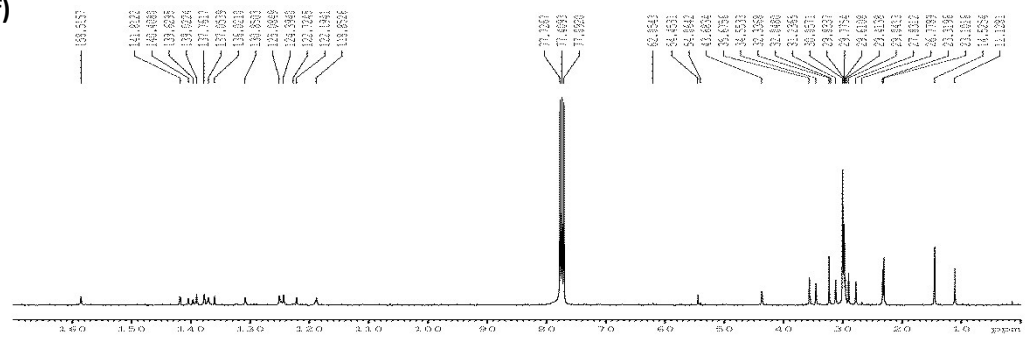
(d)



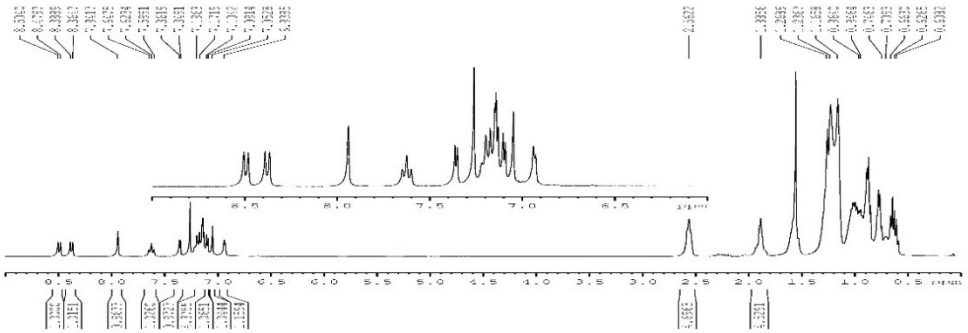
(e)



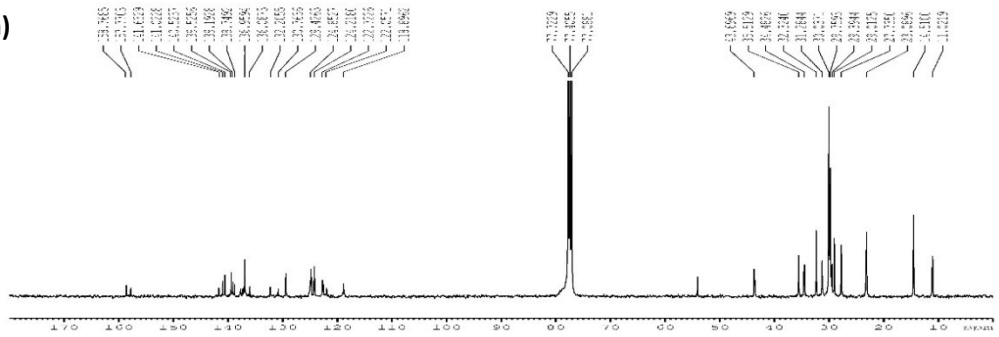
(f)



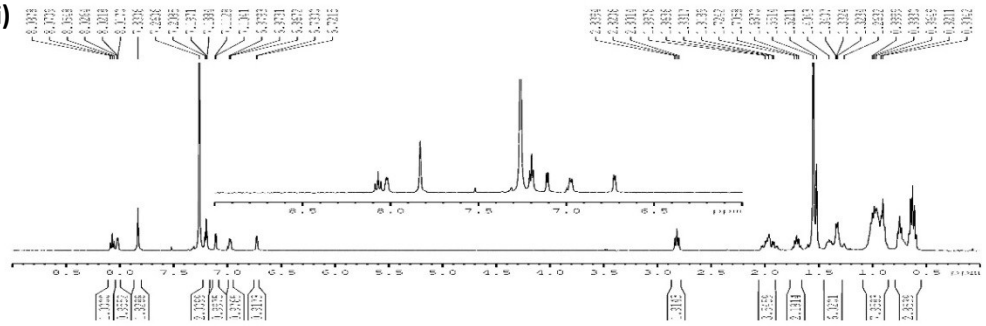
(g)



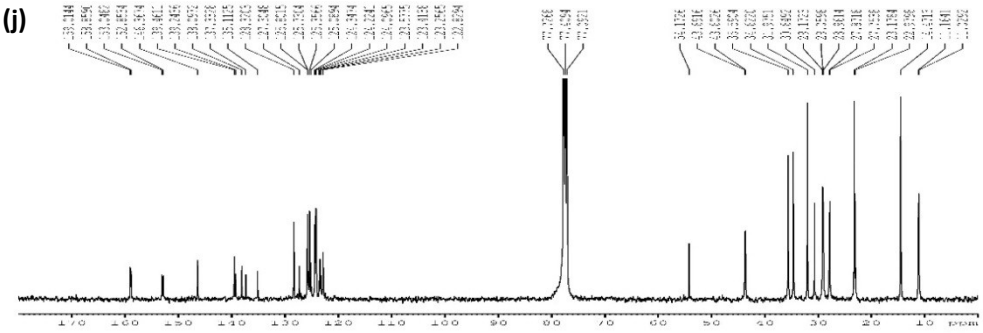
(h)



(i)



(j)



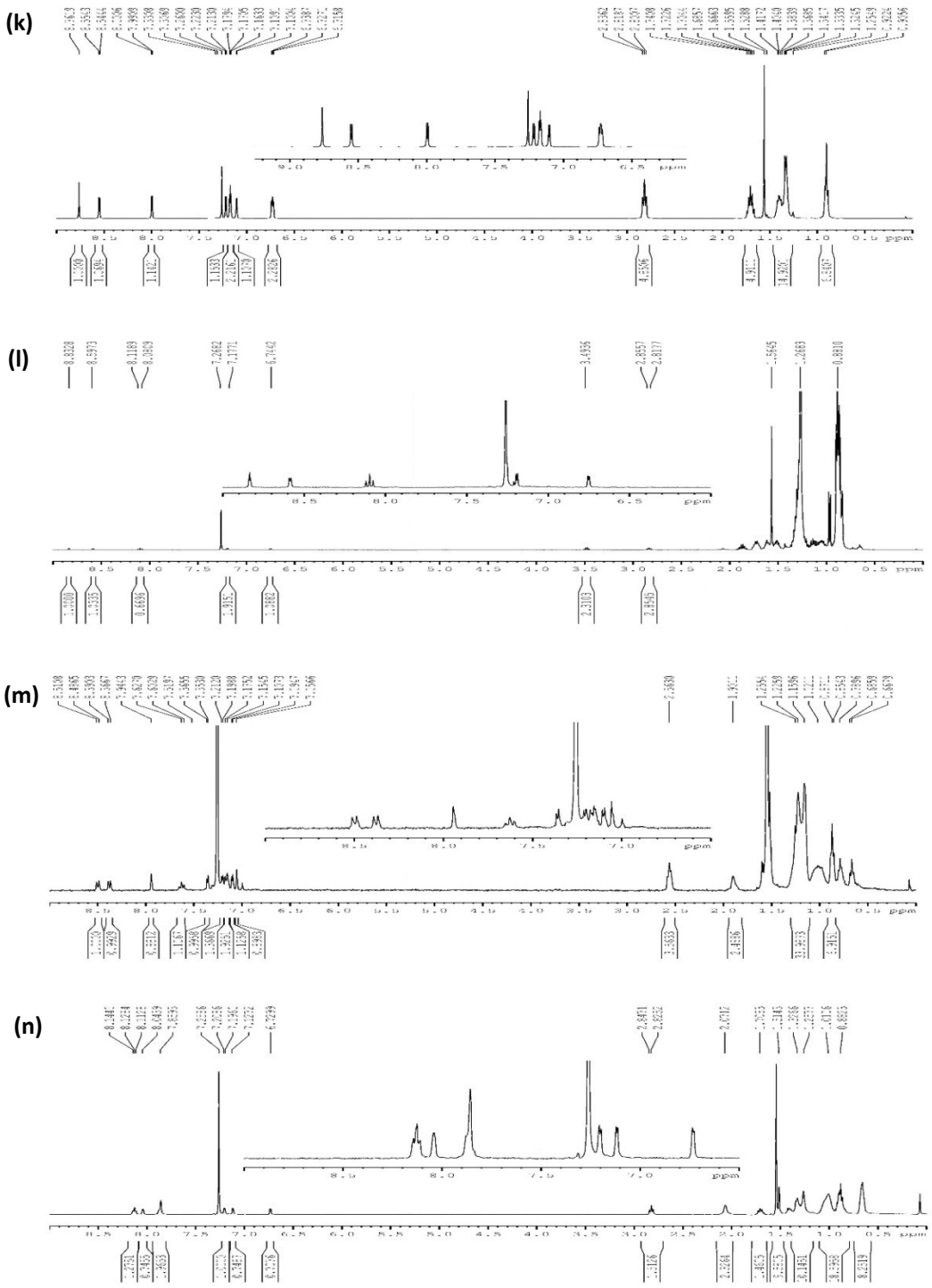


Figure S5. NMR spectra of monomers. (a) ^{1}H-NMR spectra of monomer **5**; (b) ^{1}H-NMR spectra of monomer **6**; (c) and (d), ^{1}H-NMR and ^{13}C-NMR spectra of monomer **M1**; (e) and (f), ^{1}H-NMR and ^{13}C-NMR spectra of monomer **M2**; (g) and (h), ^{1}H-NMR and ^{13}C-NMR spectra of monomer **M3**; (i) and (j), ^{1}H-NMR and ^{13}C-NMR spectra of monomer **M4**; ^{1}H-NMR spectra of monomers: (k) **6-1**, (l) **M1-1**, (m) **M1-2** and (n) **M2-1**.