Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information for "Imidazole and triazole head group containing polydiacetylenes for colorimetric monitoring of pH and detecting HCl gas"

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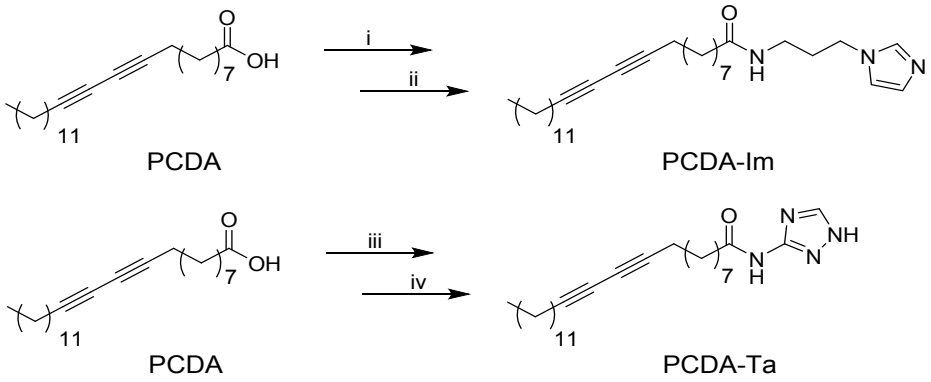

Scheme S1. Preparation of **PCDA-Im** and **PCDA-Ta**. (i) *N,N*-dimethylethylenediamine, *N,N'*-dicyclohexylcarbodiimide, CH_2Cl_2, 24 h. (ii) 1-(3-aminopropyl) imidazole, CH_2Cl_2, 24 h. (iii) Oxalyl chloride, CH_2Cl_2, 5 h. (iv) 3-amino-1,2,4-triazole, CH_2Cl_2, 24 h.

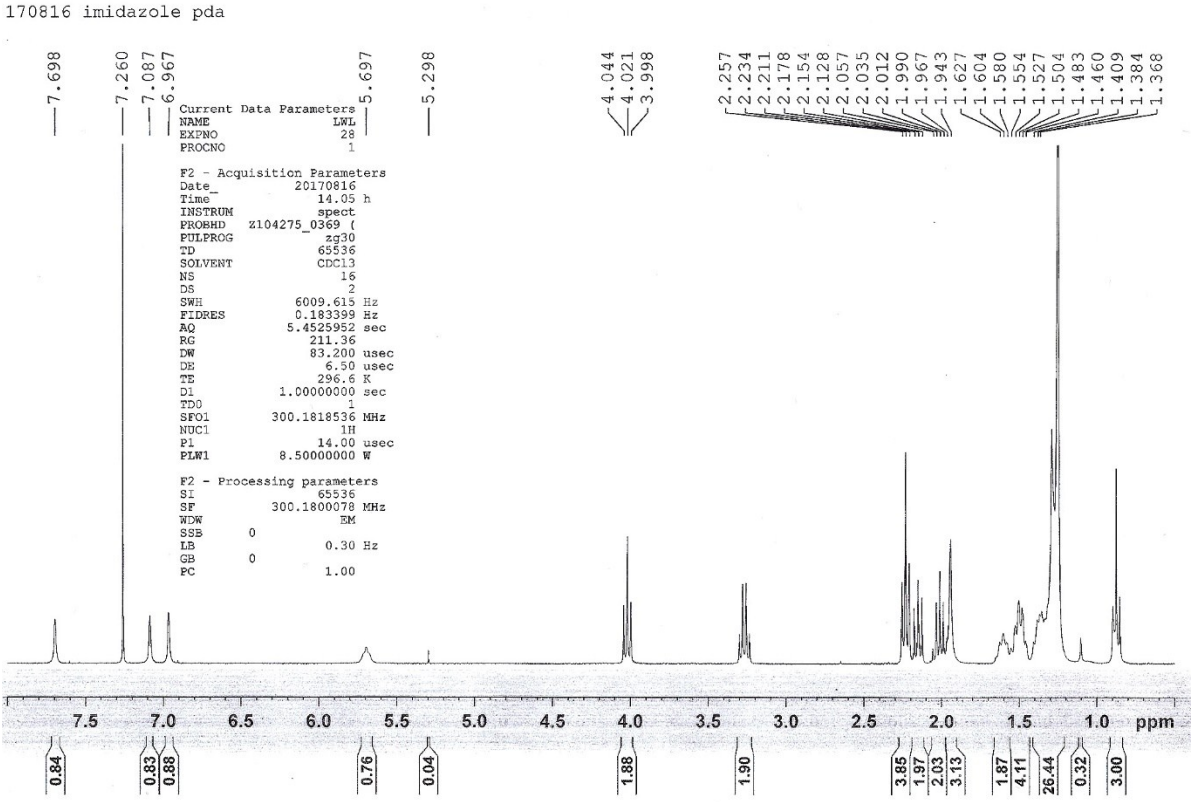

Figure S1. ^{1}H NMR (300 MHz) spectrum of *N*-(3-(1H-imidazol-1-yl) propyl)pentacosa-10,12-diynamide (**PCDA-Im**) in $CDCl_3$.

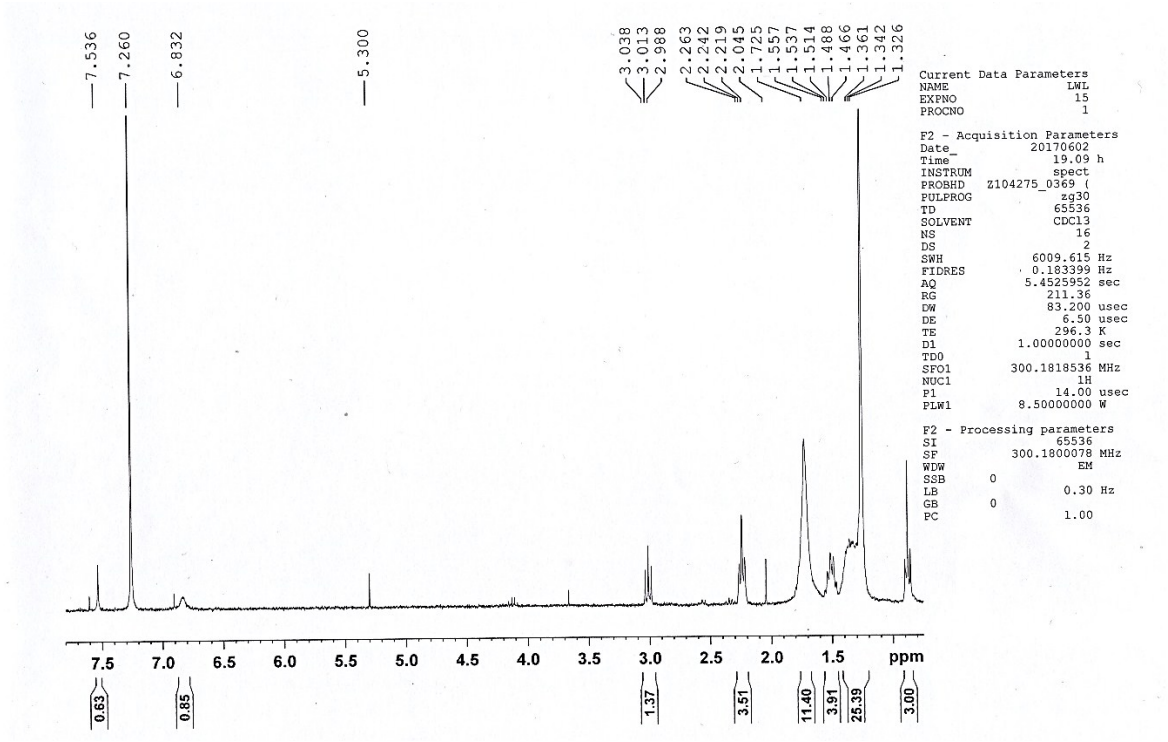

Figure S2. ^{1}H NMR (300 MHz) spectrum of N-(2H-1,2,3-triazol-4-yl)pentacosa-10,12-diynamide (**PCDA-Ta**) in $CDCl_3$.

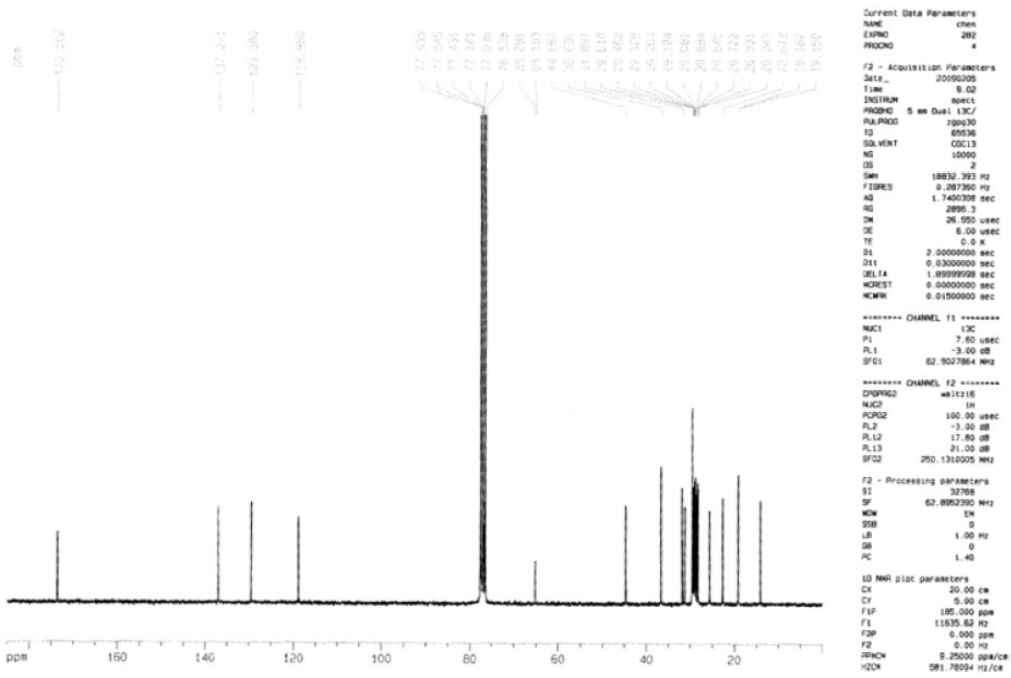

Figure S3. ^{13}C NMR (62.5 MHz) spectrum of *N*-(3-(1H-imidazol-1-yl) propyl)pentacosa-10,12-diynamide (**PCDA-Im**) in $CDCl_3$.

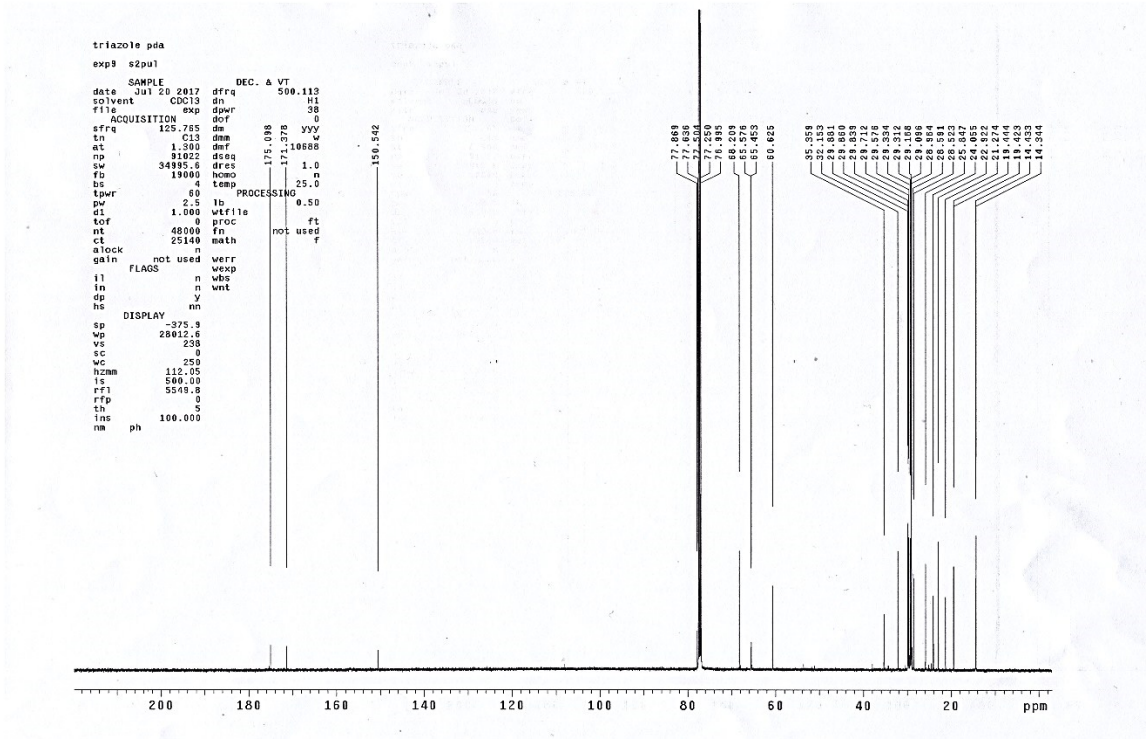

Figure S4. ^{13}C NMR (125 MHz) spectrum of N-(2H-1,2,3-triazol-4-yl)pentacosa-10,12-diynamide (**PCDA-Ta**) in $CDCl_3$.

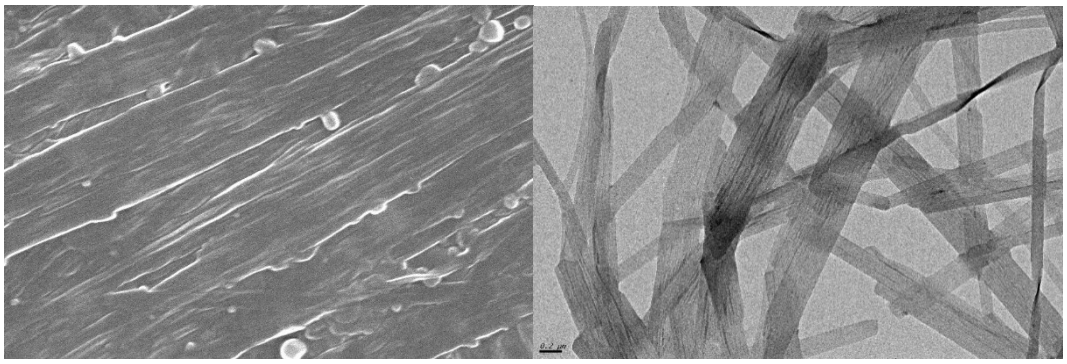

Figure S5. Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM) images of **PDA-Im**.

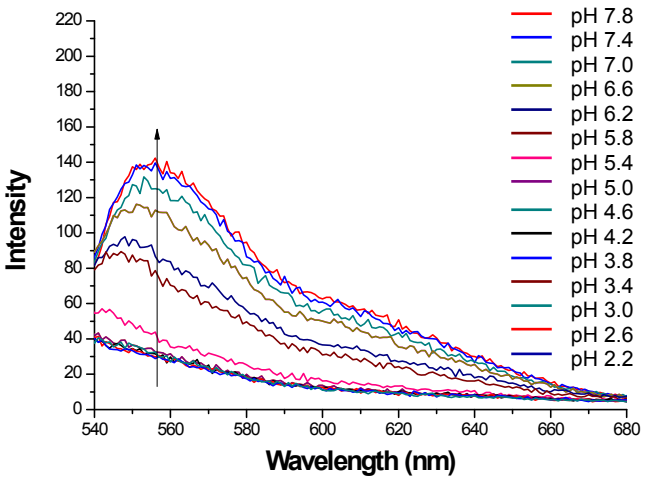

Figure S6. Fluorescence spectra (λ_{ex} = 530 nm, slit widths: 5 nm/5 nm) of **PDA-Im** (10 μM) in different pH (2.2-7.8).

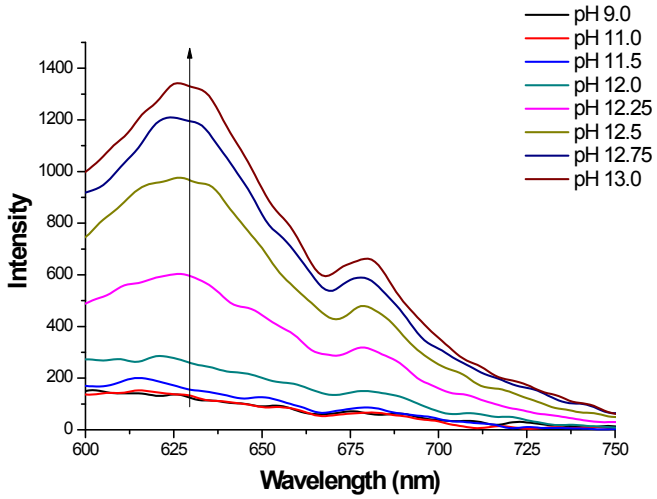

Figure S7. Fluorescence spectra (λ_{ex} = 540 nm, slit widths: 5 nm/5 nm) of **PDA-Ta** (1 mM) in different pH (9.0-13.0).

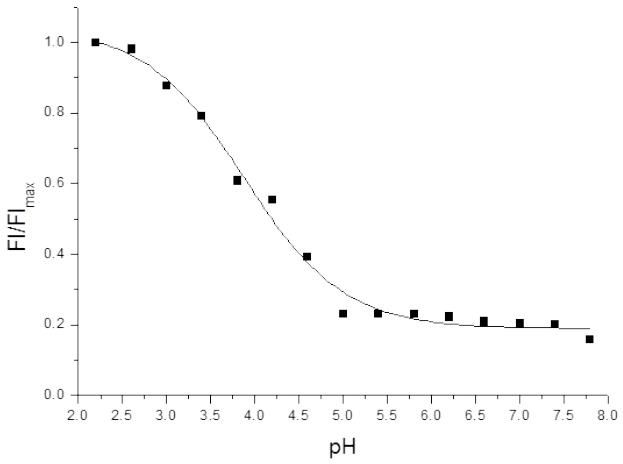

Figure S8. pH titration curve of **PDA-Im** (10 μM), pK_a=4.06.

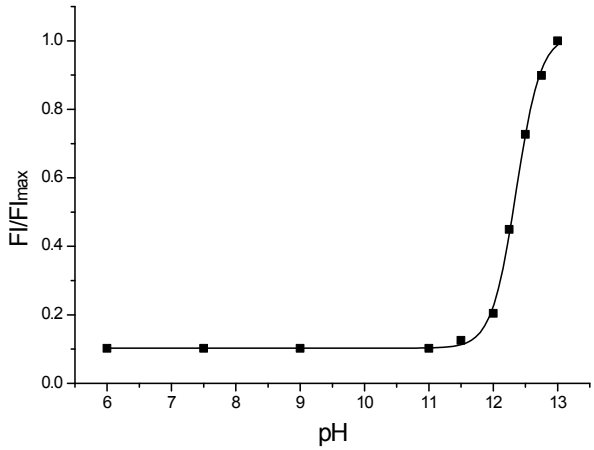

Figure S9. pH titration curve of **PDA-Ta** (1 mM), pK_a=12.3.

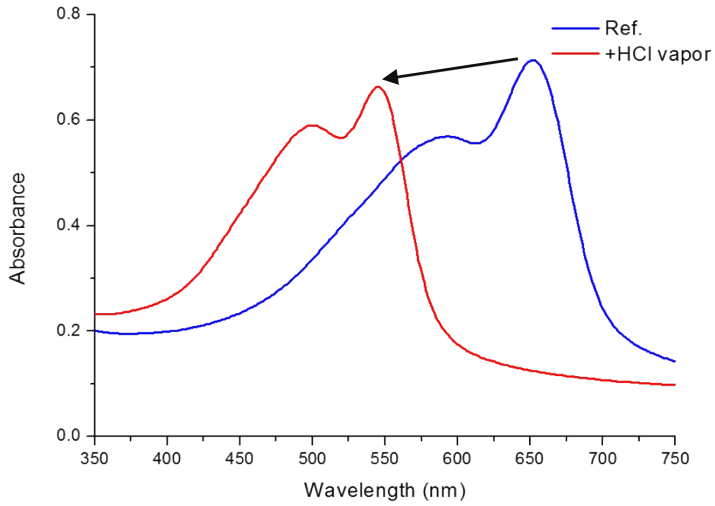

Figure S10. UV absorption spectra of **PDA-Im**-coated glass before and after introducing vapor of 4 μL HCl in 100 mL chamber for 3 sec.

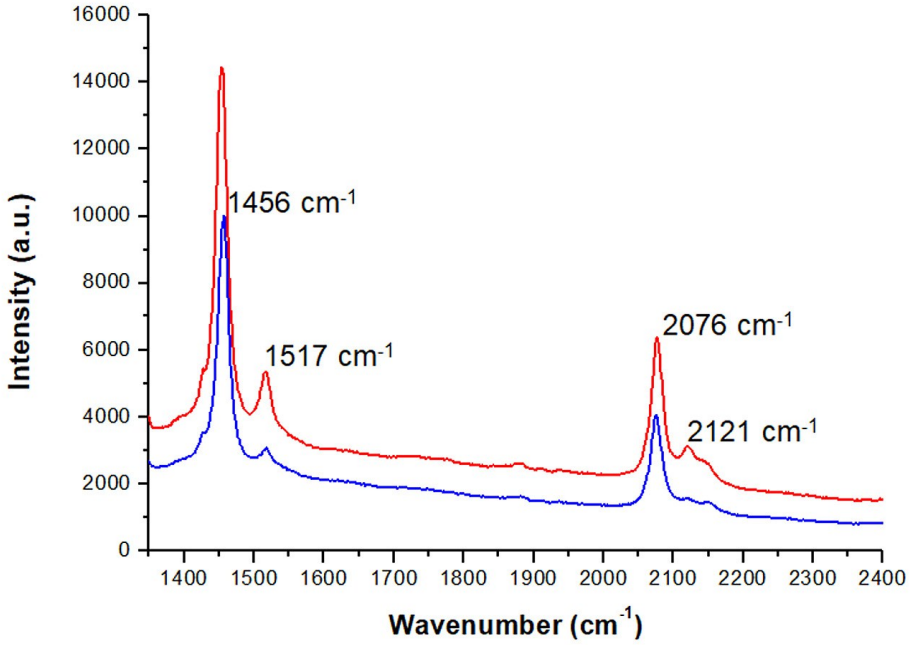

Figure S11. Raman spectra of **PDA-Im**-coated glasses (bottom) and after exposure to HCl gas for 3 s (top).

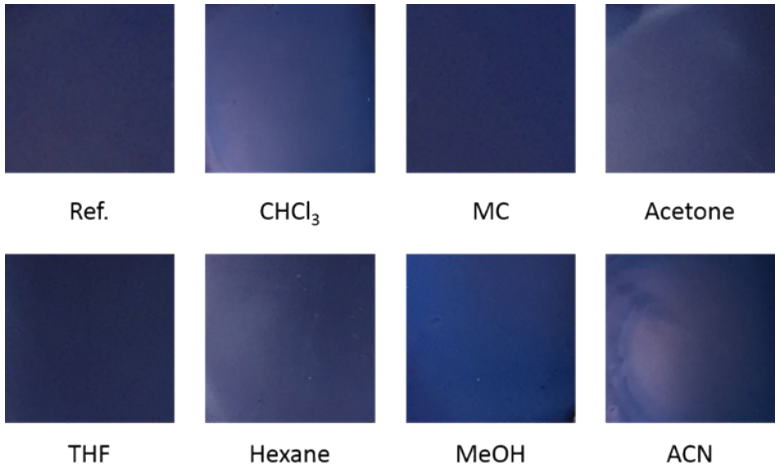

Figure S12. Images of **PDA-Im**-coated glasses after exposure to vapor of various organic solvents (10 μL in 100 mL chamber) for 30 s.