Controllable supramolecular self-assemblies (rods-wires-spheres) and ICT/PET based perylene probe for palladium detection in solution and solid state

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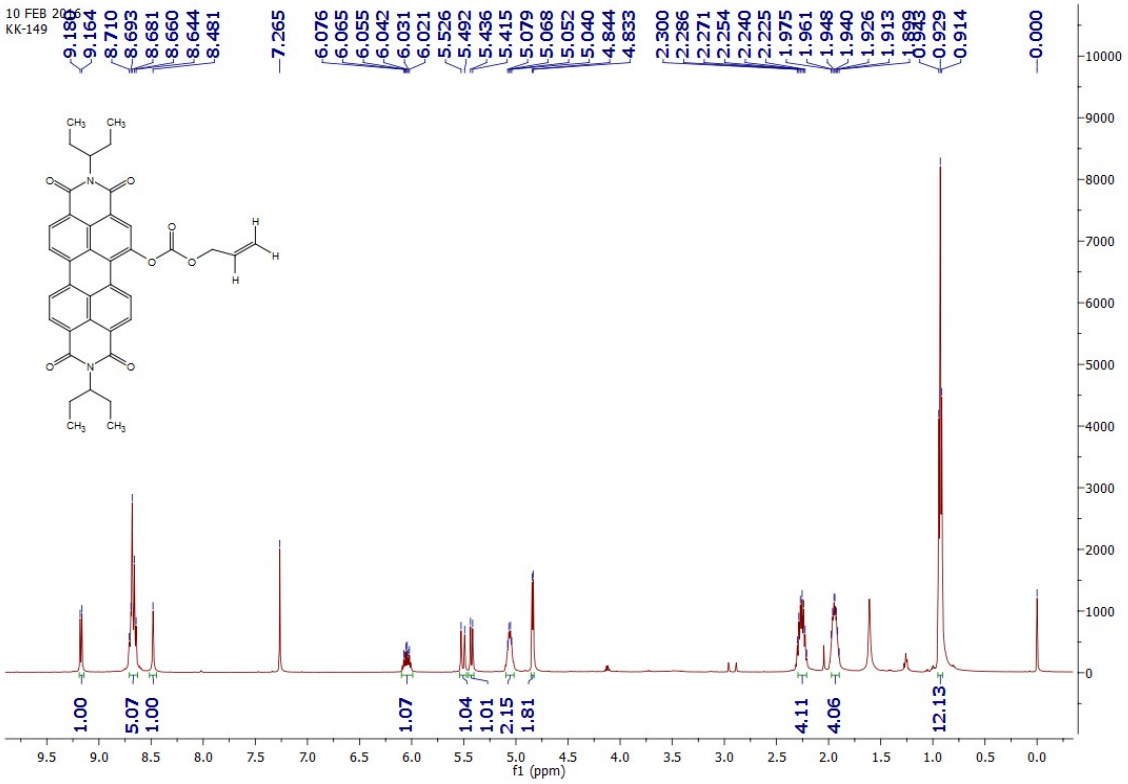
EXPERIMENTAL



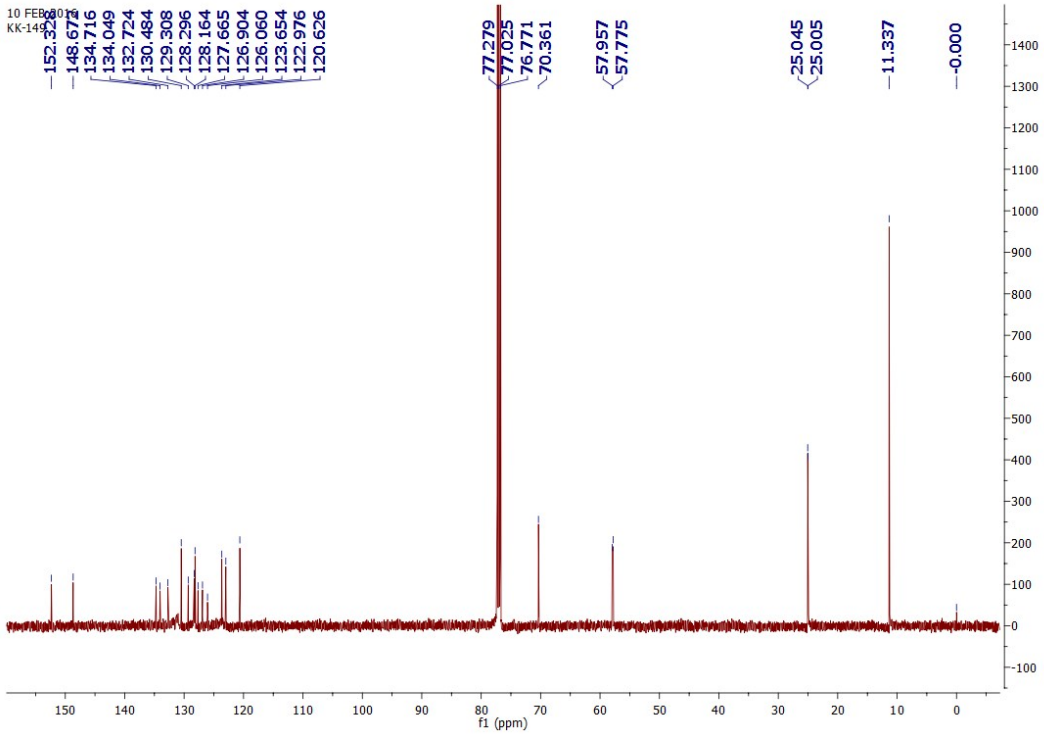


Figure S1a: ^{1}H NMR and ^{13}C Spectrum of **AC-PDI**.

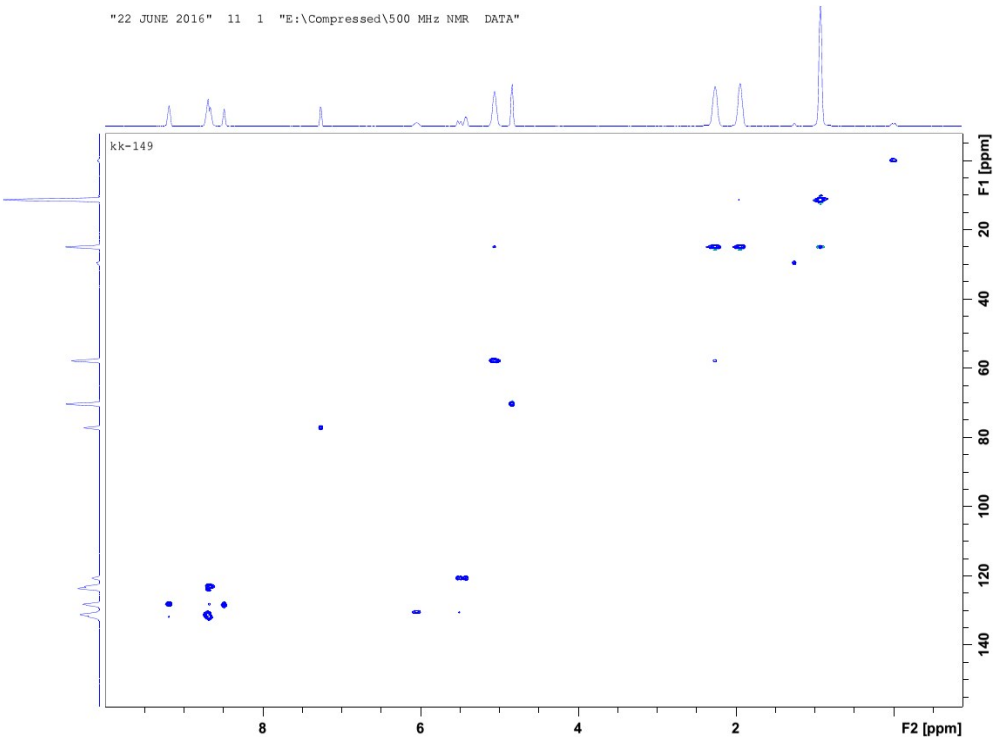


Figure S1b: HSQC spectrum of **AC-PDI**.

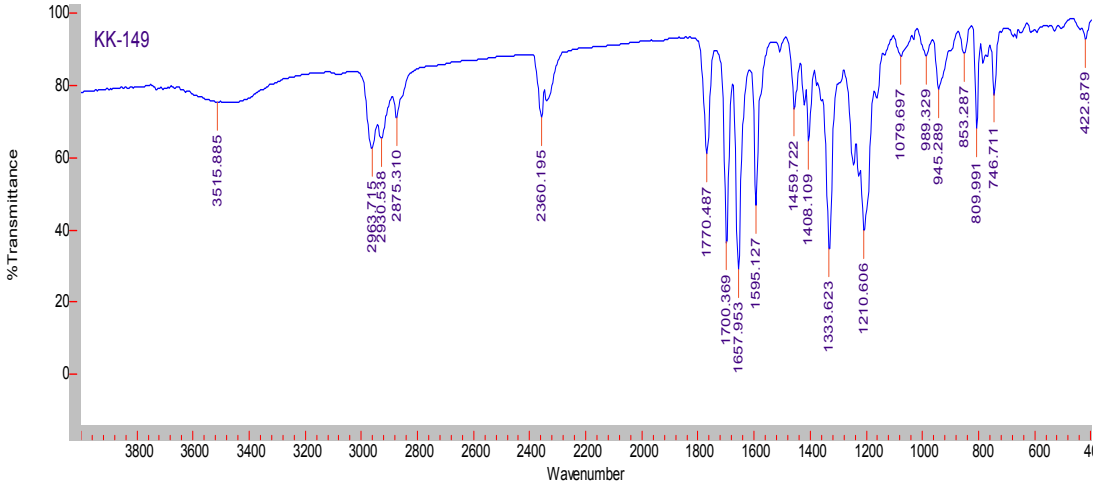


Figure S1c: IR spectrum of **AC-PDI**.

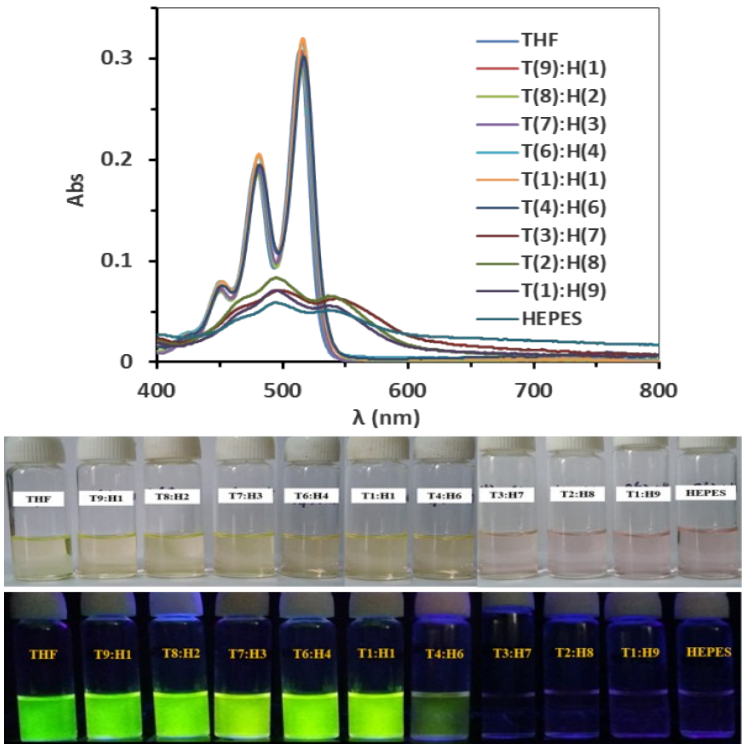


Figure S2 UV-Vis absorption spectra of **AC-PDI** (10 μM) on gradual addition of H_2O in THF (top); room light and after 365 nm UV irradiation photographs showing the visible colour and emission changes of **AC-PDI** in aqueous THF mixture (bottom); T = THF; D = DMF; H = H_2O in v/v ratio.

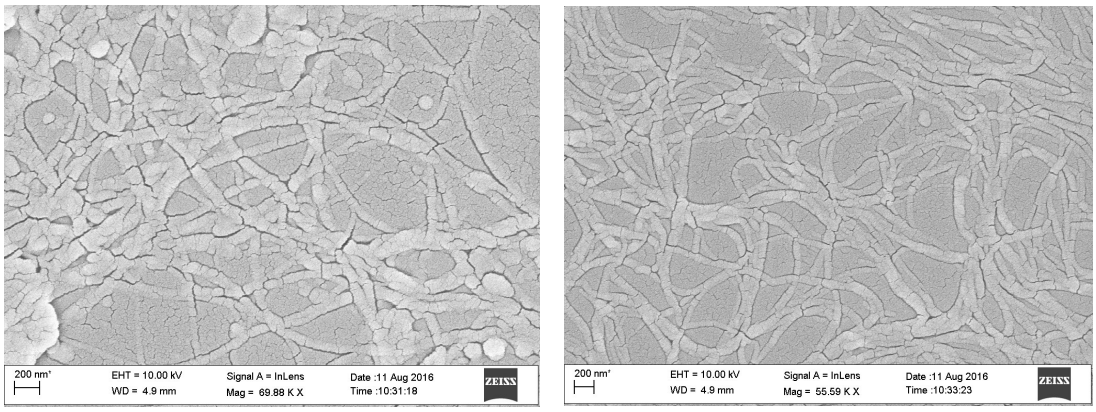


Figure S3 SEM micrographs of self-assembled regular nanorods/tube of **AC-PDI** (10 μM) in methylcyclohexane.

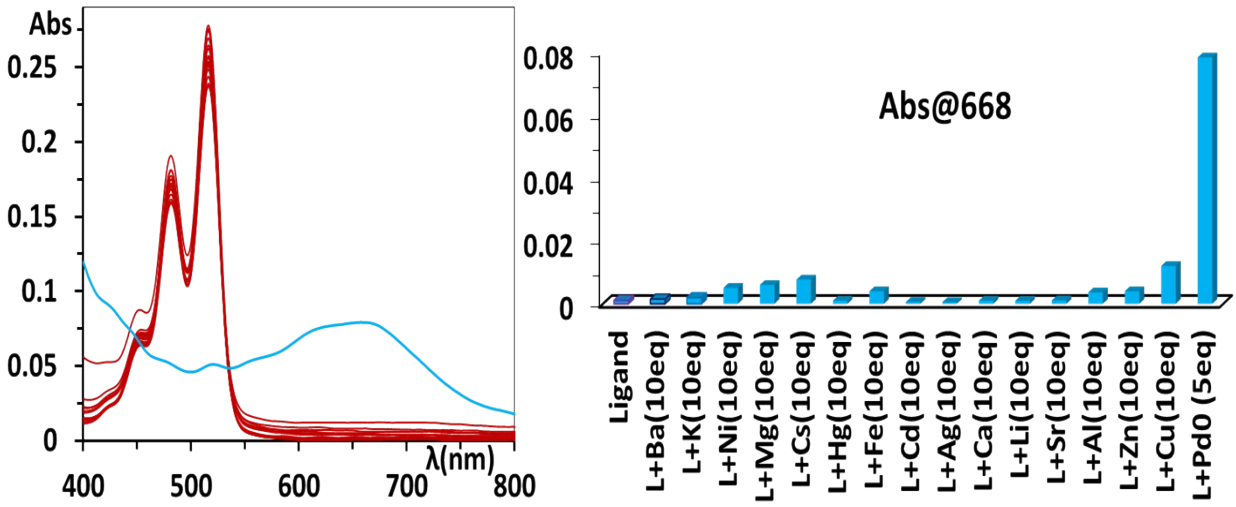


Figure S4a UV-Vis absorption spectrum and (b) bar diagram showing the effect of individual metal ions on the absorption spectra of **ACF-PDI**

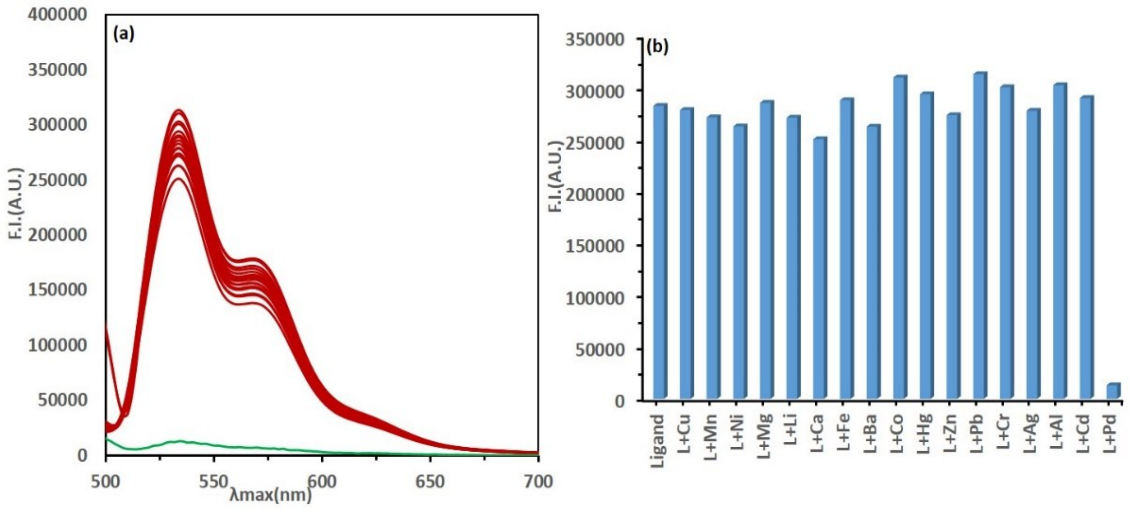


Figure S4b Emission spectra of **AC-PDI** and bar diagram indicating the effect of Pd^0 and other metal ions (λ_{ex} = 490 nm; Ex = 1:1 nm, Em = 0.5:0.5 nm).

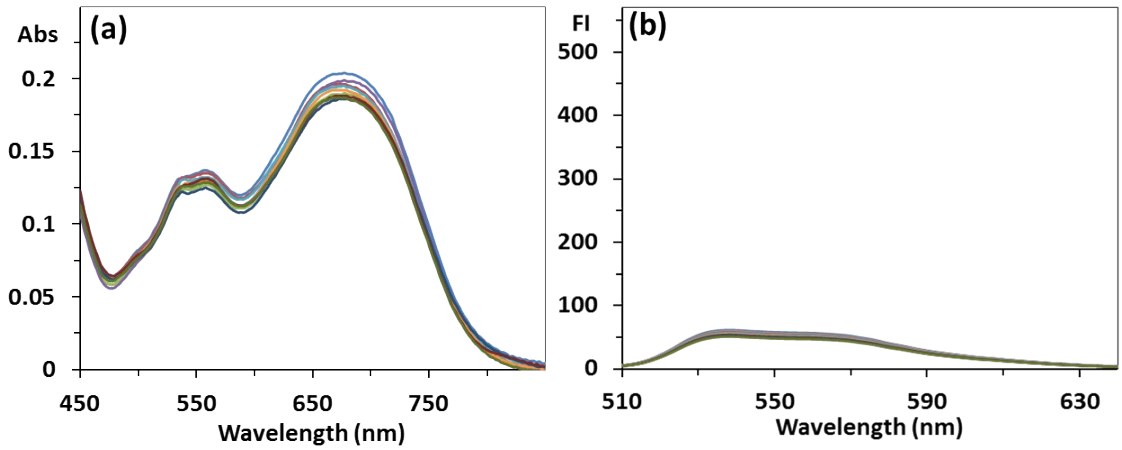


Figure S5 (a) UV-Vis and (b) Fluorescence spectra of **PDI 1** (10 μM) on incremental addition of Pd^0 in HEPES buffer-CH_3CN (1:1, v/v, pH 7.2).

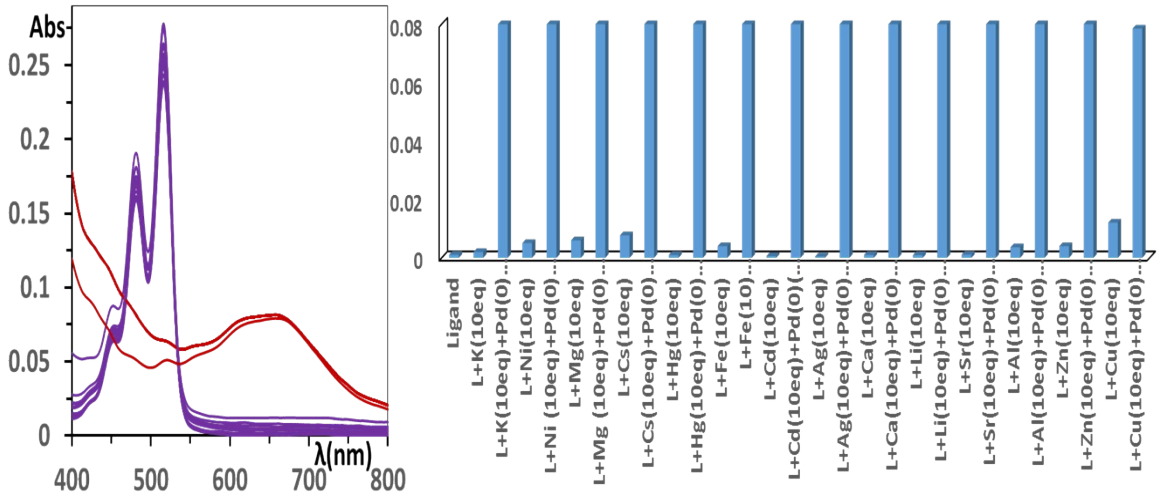


Figure S6a (a) UV-Vis absorption spectra and (b) bar diagram showing the effect of individual metal ions (100 μM) on the absorption spectra of **AC-PDI**.

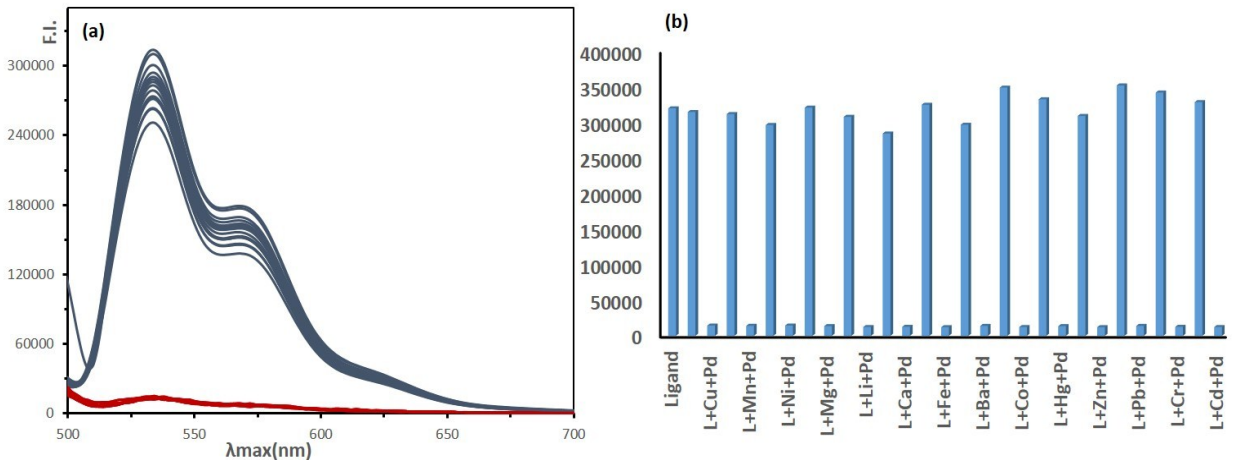


Figure S6b (a) Emission spectra and (b) bar graph of **AC-PDI** representing the response towards Pd^0 in the presence of other metal ions (λ_{ex} = 490 nm; Slit width; Ex = 1:1 nm, Em = 0.5:0.5 nm)

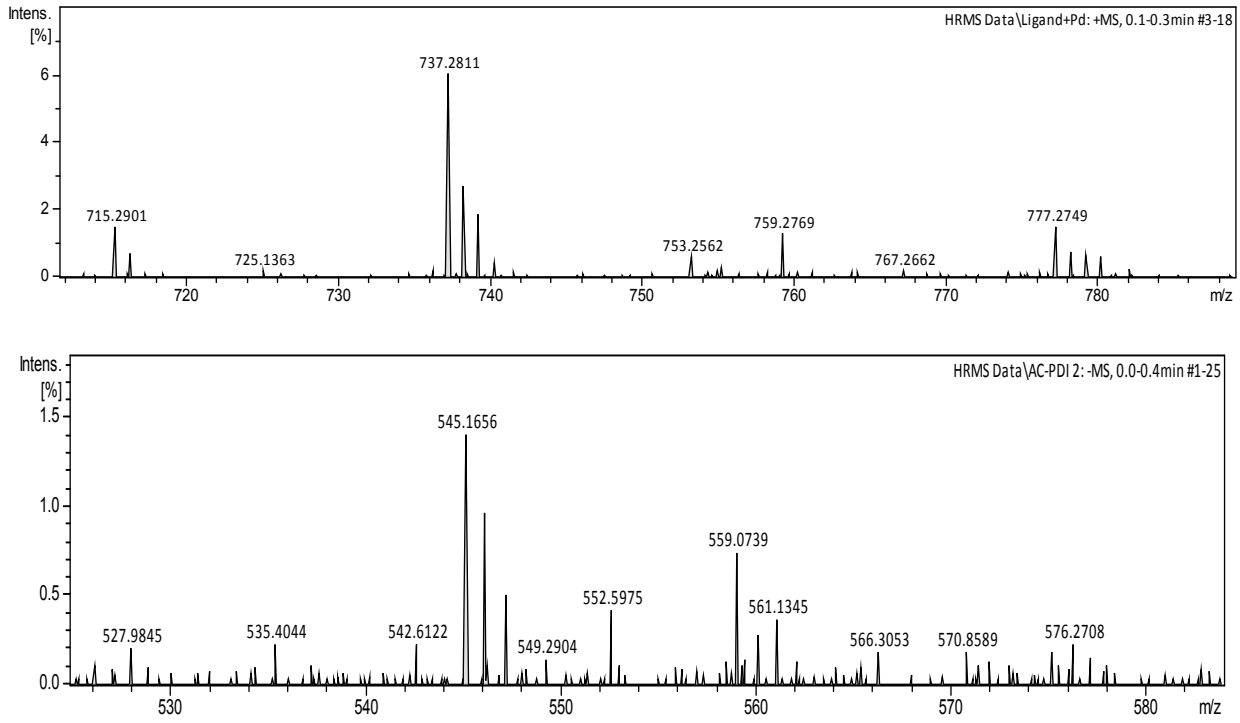


Figure S7 HRMS spectrum of **AC-PDI** + Pd^0 in positive and negative mode.

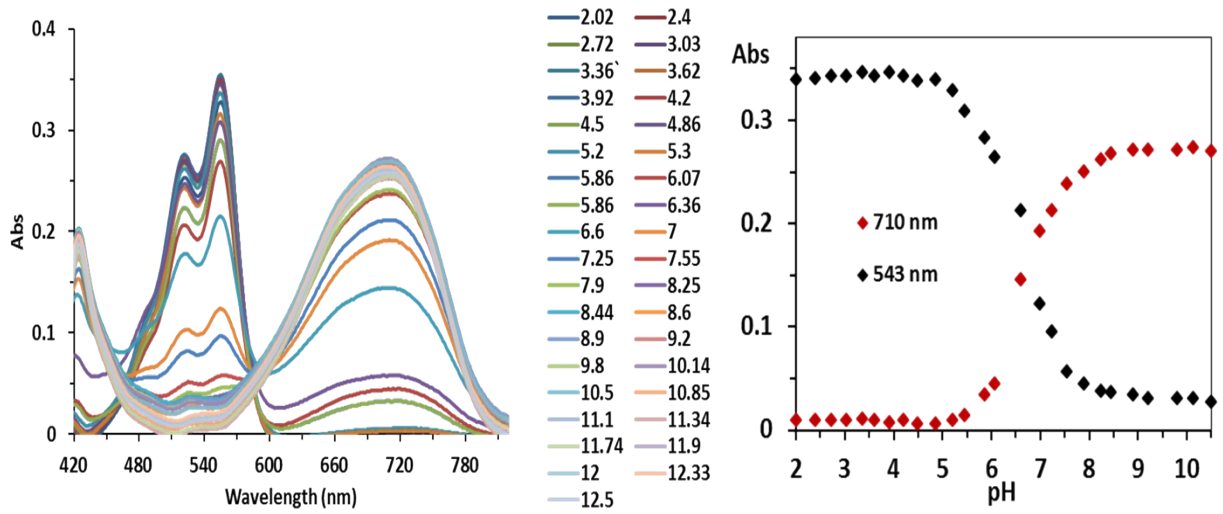


Figure S8. (Left) Effect of pH changes on the UV-Vis absorption spectrum of **PDI-OH** (10 μM) in water (50% THF); (Right) Plot of absorbance at 543 nm and 710 nm vs. change in pH of the solution.

Table S1: Time dependent and concentration dependent absorbance data of **AC-PDI** (10 μM) on addition of Pd^0 in (a) HEPES buffer-THF (1:1, v/v, pH 7.2); (b) HEPES buffer-DMSO (3:7, v/v, pH 7.2).

Conc. of Pd^0	Time taken	50% H_2O:CH_3CN		Conc. of Pd^0	Time taken	30% H_2O:DMSO	
		Rate constant K_1	Rate constant K_2			Rate constant K_1	Rate constant K_2
45 μM	26 min	0.25 min^{-1} (up to 0-4 min)	0.07 min^{-1} (up to 4-18 min)	35 μM	20 min	0.23 min^{-1} (up to 0-8 min)	0.08 min^{-1} (up to 8-20 min)
90 μM	18 min	0.30 min^{-1} (up to 0-4 min)	0.07 min^{-1} (up to 4-16 min)	70 μM	12 min	0.36 min^{-1} (up to 0-4 min)	0.10 min^{-1} (up to 4-12 min)
135 μM	16 min	0.22 min^{-1} (up to 0-6 min)	0.08 min^{-1} (up to 6-14 min)	105 μM	12 min	0.48 min^{-1} (up to 0-4 min)	0.12 min^{-1} (up to 4-12 min)