Electronic Supplementary Information (ESI)

Co-functionalization with phosphate and carboxylate on polydiacetylene for colorimetric detection of calcium ion in serum†

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Optimization of ratio of phosphate and carboxylate groups on PDA

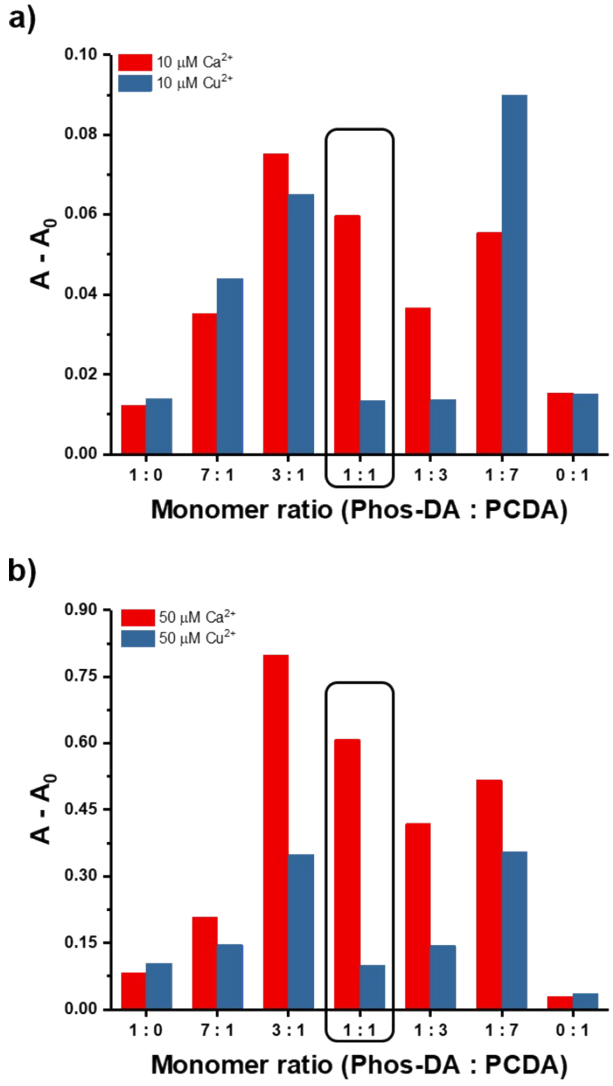

Fig. S1 Absorbance changes of the PDA composed with various ratio (1:0, 7:1, 3:1, 1:1, 1:3, 1:7, and 0:1) of **Phos-DA** and **PCDA** 1 h after the addition of a) 10 μM and b) 50 μM of Ca^{2+} and Cu^{2+}; A_0 and A is absorbance ratio at 543 and 642 nm in the absence and presence of metal ions, respectively.

Time-dependent colorimetric responses of PC-PDA

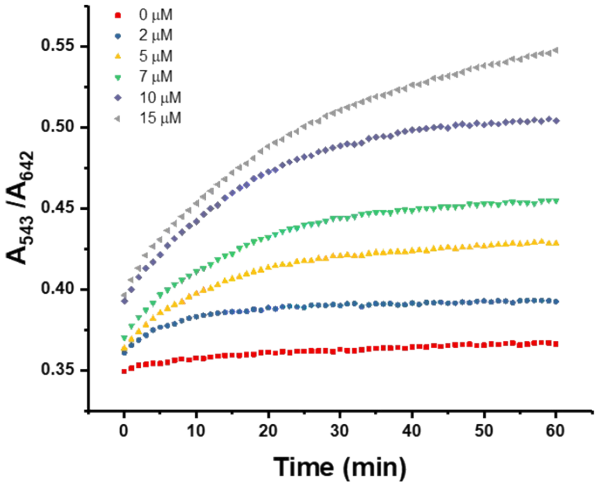

Fig. S2 Plot of absorbance ratio at 543 and 642 nm for 1h after addition of Ca^{2+} to HEPES buffer (20 mM, pH 8.0) containing **PC-PDA** (100 μM).

Limit of detection for Ca^{2+} using PC-PDA

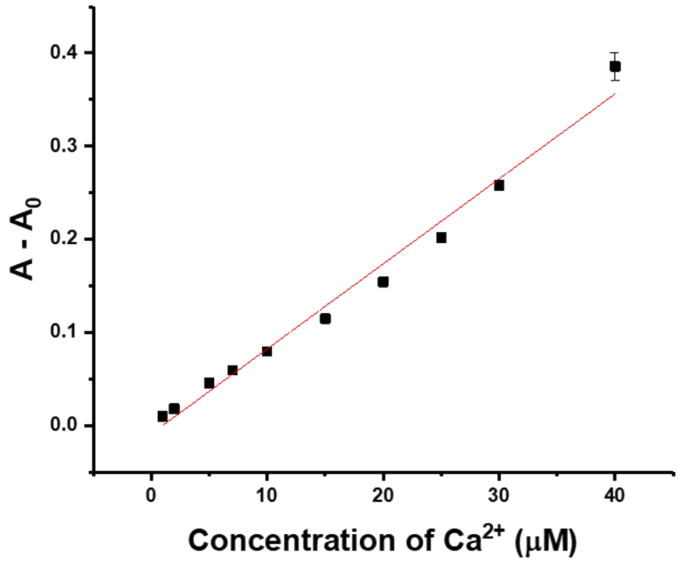

Fig. S3 Plot of absorbance ratio at 543 and 642 nm against Ca^{2+} concentrations (1, 2, 5, 7, 10, 15, 20, 25, 30, and 40 μM) where A_0 and A is absorbance ratio at 543 and 642 nm in the absence and presence of metal ions, respectively.

Intercept = -0.00885

Slope = 0.00913

R^2 = 0.98419

Limit of detection (LOD) = 0.97 μM

Dynamic light scattering (DLS) of PC-PDA

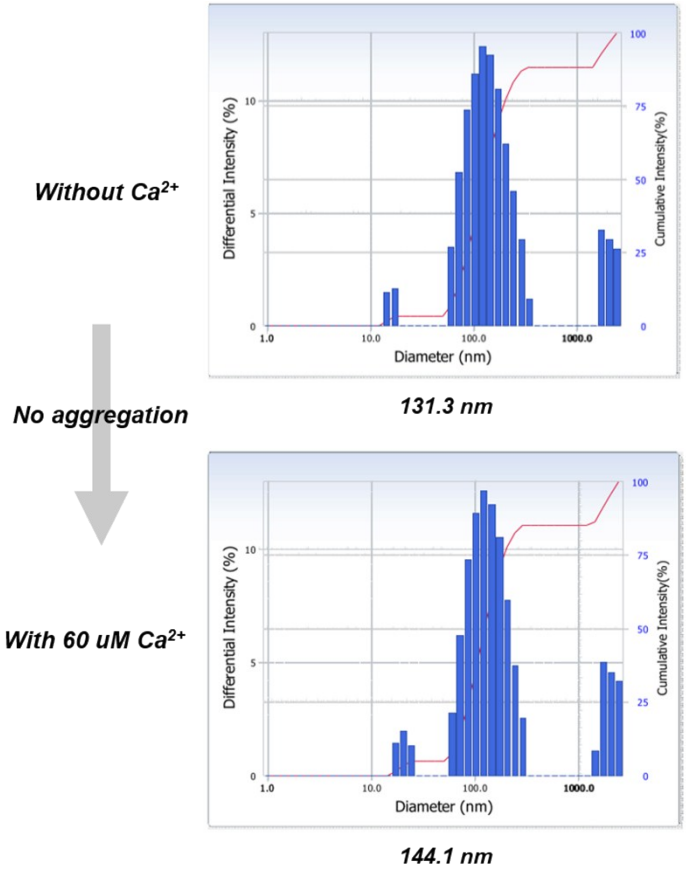

Fig. S4 Size distribution of **PC-PDA** (100 μM) after 1h incubation without or with Ca^{2+} (60 μM).

Characterization of compounds

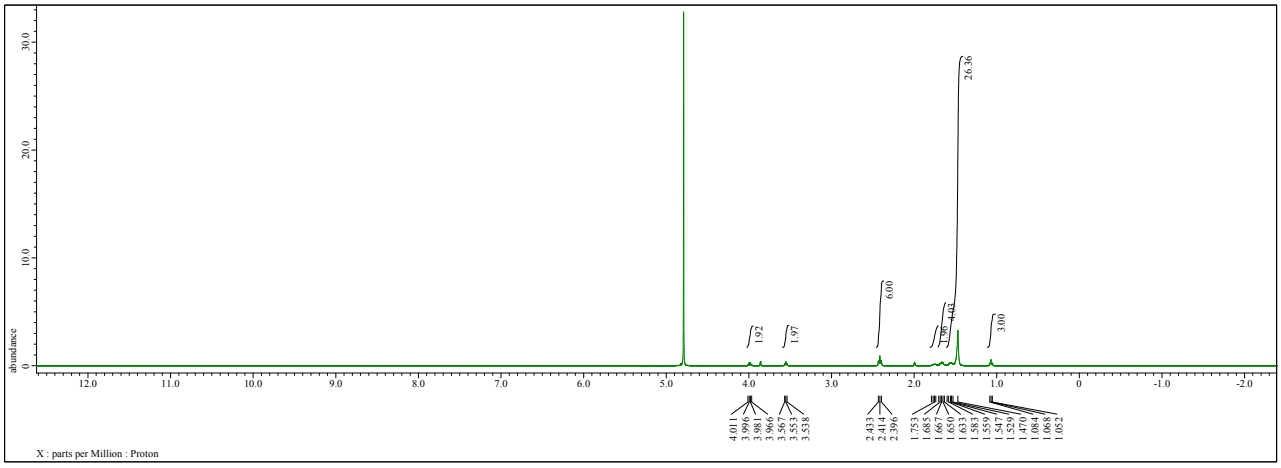

Fig. S5 ^{1}H-NMR spectrum of **Phos-DA** in 0.1 M NaOD in D_2O : THF-d_8 = 1:1.

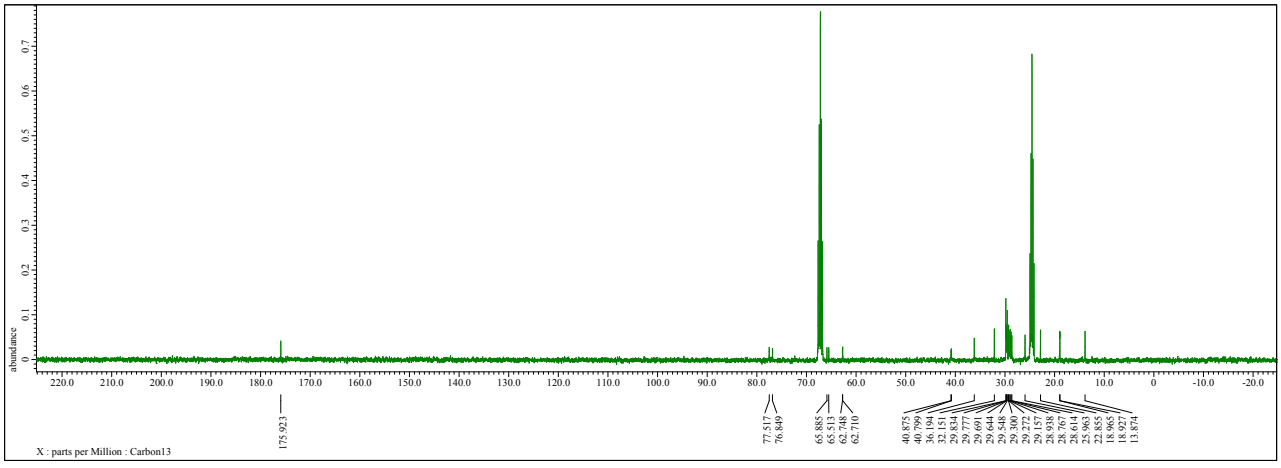

Fig. S6 ^{13}C-NMR spectrum of **Phos-DA** in 0.1 M NaOD in D_2O : THF-d_8 = 1:1.

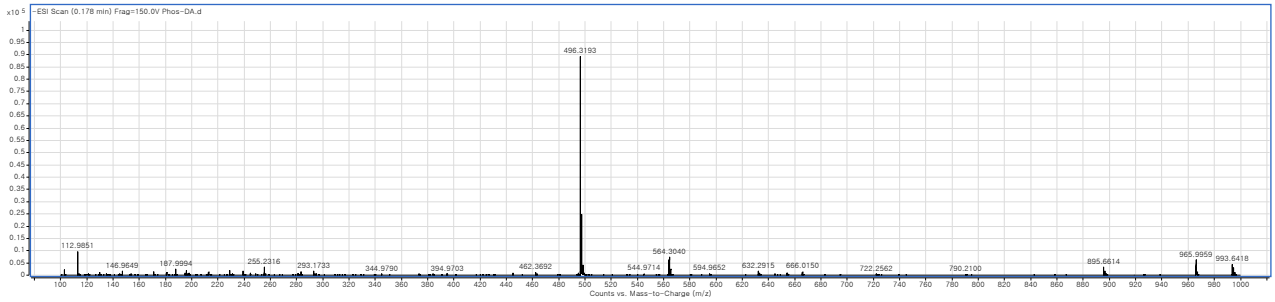

Fig. S7 ESI-MS spectrum of **Phos-DA**.