Supplementary information for

Analyte-Induced Aggregation of Conjugatd Polyelectrolyte: Role of the Charged Moieties and Its Sensing Application

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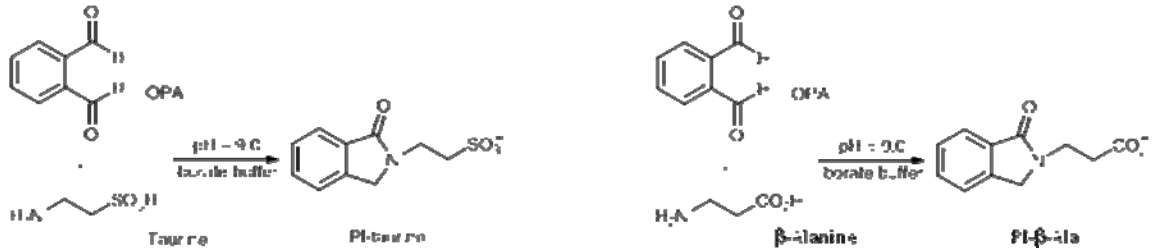
Materials. All chemicals were purchased from Aldrich and Beijing Chem. Reagents Co. (Beijing, China) and were used as received. Water-soluble polythiophene derivative, PMTPA, was synthesized and purified as reported previously.[S1]

Sample Preparation. The i*n situ* premodification reaction of taurine and OPA was performed as the following procedures: stock solutions of taurine and OPA were mixed at 25 ^{o}C to give a mixture with the molar ratio of OPA to taurine, 1.5:1, in 20 mM borate buffer (pH = 9.0).

Control experiments for addressing the specificity of PMTPA toward taurine were carried out under the identical conditions. Sulfur-containing amino acids, Met, Cys, Hcy, Cyt, and aromatic acids, Trp and Tyr were premodified by reacting with OPA for 3 min, respectively, and then the probe PMTPA was added into the OPA/analyte mixture to give a solution containing 0.1 mM PMTPA, 0.5 mM analyte and 0.75 mM OPA. After 5 min, the sample was measured by UV-visible spectrometer.

For NMR measurements, equimolar amount of taurine or β-Ala and OPA (1.0×10^{-3} M) was reacted for 48 h at 25^{o}C in 20 mM borate buffer (pH = 9.0). Then the reaction mixture

was sent to be freezing-dried and the obtained powder was dissolved in deuterated water for NMR measurements. PI-taurine: ^{1}H NMR (D_2O, 300 MHz) (δ): 7.37-7.59 (m, 4H), 4.49 (s, 2H), 3.86 (t, 2H), 3.13 (t, 2H); PI-β-Ala: ^{1}H NMR (D_2O, 300 MHz) (δ): 7.42-7.63 (m, 4H), 4.47 (s, 2H), 3.74 (t, 2H), 2.45 (t, 2H).



Measurements. Absorption spectra were collected by using a Hitachi 3010 UV-visible spectrometer. ^{1}H-NMR spectra were carried out on a JNM-ECA300 spectrometer (JEOL).

Reference

S1 C. Li, M. Numata, A.-H. Bae, K. Sakurai and S. Shinkai, *J. Am. Chem. Soc.*, 2005, **127**, 4548.

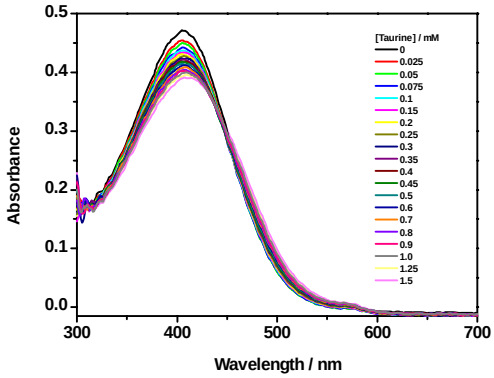


Fig. S1 Variation in the absorption spectra of PMTPA (1.0×10^{-4} M) in 20 mM borate buffer (pH = 9.0) with increasing concentrations of taurine as indicated.

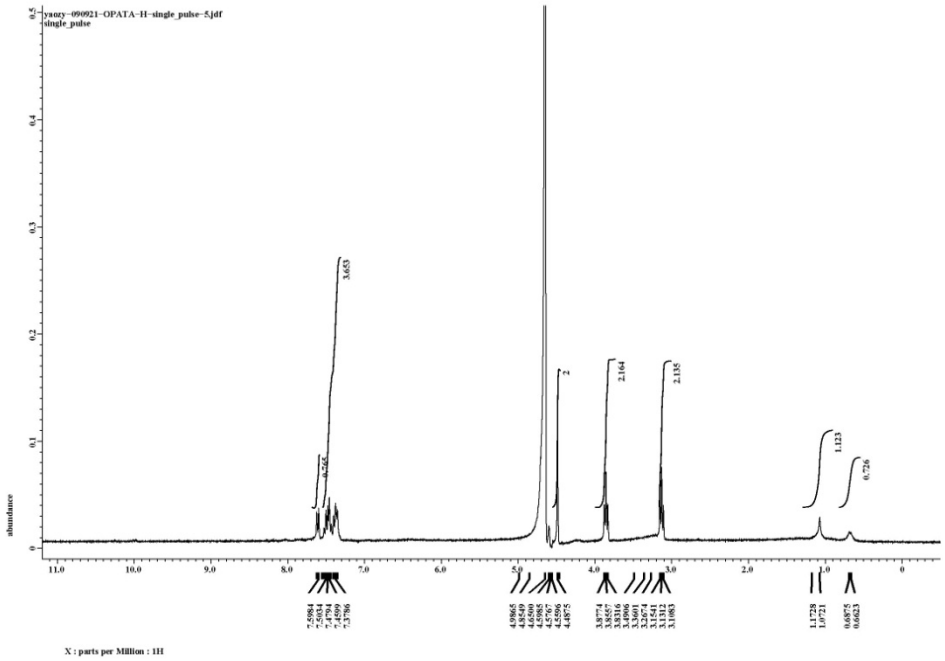


Fig. S2 ^{1}H-NMR spectra of the phthalimidine derivative of taurine (PI-taurine). Solvent: D_2O.

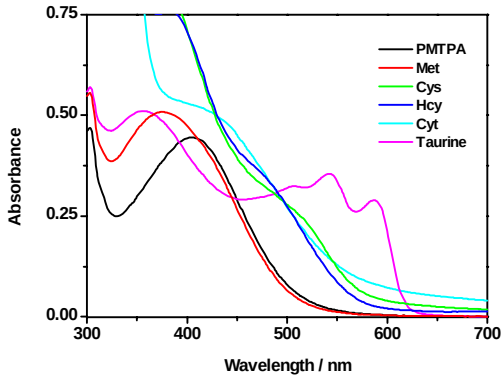


Fig. S3 Absorption spectra of PMTPA (1.0×10^{-4} M) in 20 mM borate buffer (pH = 9.0) in the absence and the presence of sulfur-containing amino acids as indicated.

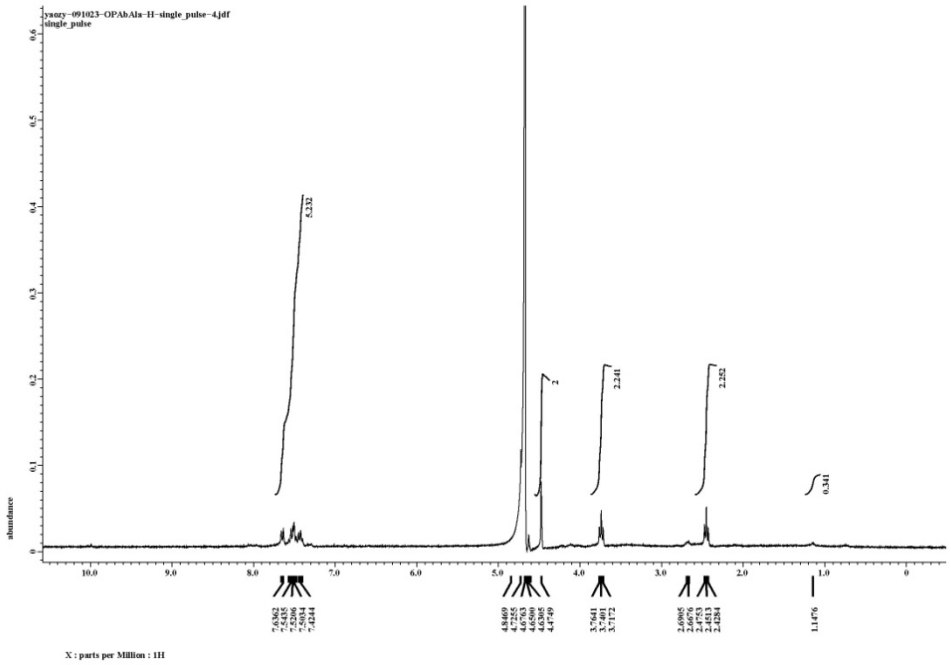


Fig. S4 ^{1}H-NMR spectra of the phthalimidine derivative of β-Ala (PI-β-Ala). Solvent: D_2O.

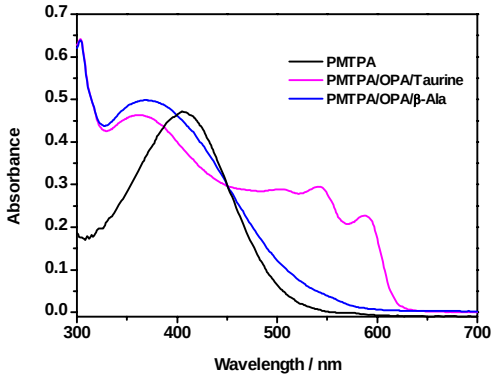


Fig. S5 Absorption spectra of PMTPA (1.0×10^{-4} M) in borate buffer in the absence and the presence of PI-taurine and PI-β-Ala. [OPA] = 1.0×10^{-4} M, [β-Ala] = [taurine] = 5.0×10^{-4} M.

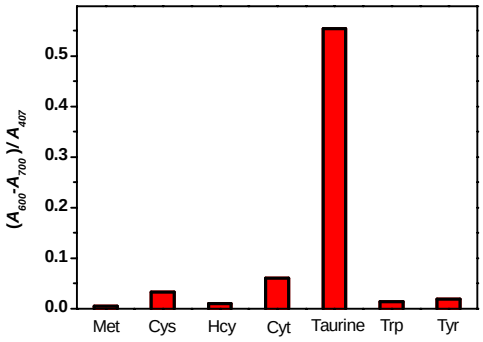


Fig. S6 Relative absorbance of PMTPA (1.0×10^{-4} M) in the presence of OPA (7.5×10^{-4} M) and Met, Cys, Hcy, Cyt, Trp, Tyr and taurine in borate buffer (pH = 9.0). [amino acids] = 5.0×10^{-4} M.

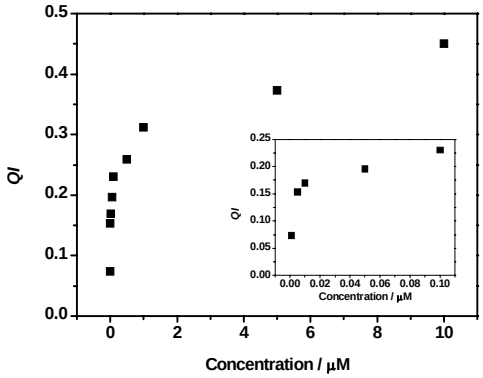


Fig. S7 Fluorescence quenching of PMTPA (1.0×10^{-5} M) by PI-taurine at various concentrations. The fluorescence quenching $QI = [(I_0-I)/I_0] \times 100\%$; I_0 is the fluorescence intensity at 552 nm of a solution of PMTPA (1.0×10^{-5} M); I is the fluorescence intensity at 552 nm of a solution of PMTPA (1.0×10^{-5} M) in the presence of different amounts of taurine. Inset: plot of QI vs taurine concentration at lower concentration. Excitated wavelength λ_{ex} = 450 nm.