Supporting Information

Expanding the Scope of Self-Assembled Supramolecular Biosensors: A Highly Selective and Sensitive Enzyme-Responsive AIE-Based Fluorescent Biosensor for Trypsin Detection and Inhibitor Screening

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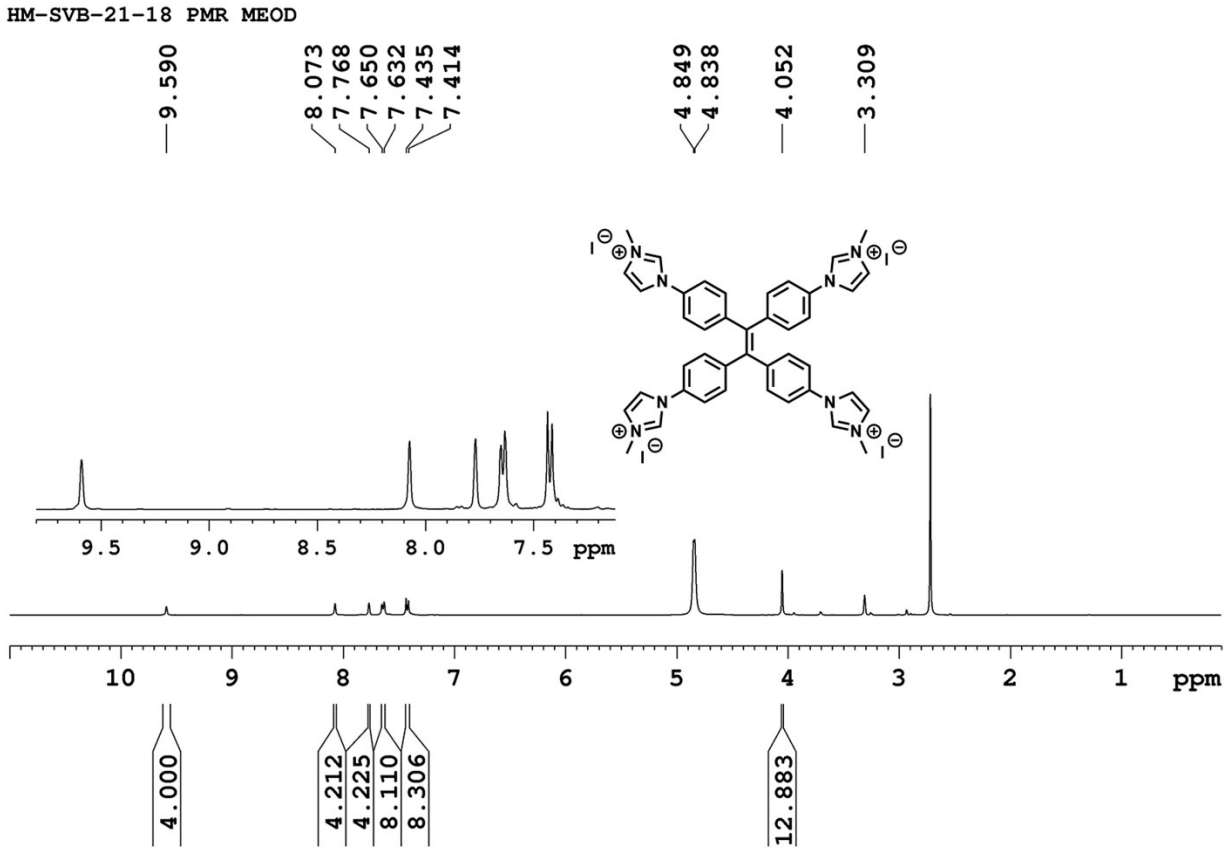

Figure S1. ^{1}H NMR spectrum of TPE-IM

In a 100 mL round bottom flask compound 2 (0.100 g, 0.168 mmol) was dissolved in dimethylacetamide (DMA): acetonitrile (ACN) in 1:2 proportion. Methyl iodide in excess (0.5-0.6 mL, 0.84 mmol) was added dropwise with constant stirring. The reaction mixture was stirred at 60-70 °C. Then compound TPE-IM was precipitated on addition of diethyl ether (50 mL) and filtered and again washed to diethyl ether and hexane leading to pale white solid. Yield 0.156 g (86%)

NMR Data: ^{1}H NMR (400 MHz, MEOD) δ = 9.590 (s, 4H), 8.073 (s, 4H), 7.768 (s, 4H), 7.6425 (d, JH−H = 6.88 Hz, 8H), 7.4262 (d, JH−H = 8.44 Hz, 8H), 4.0532 (s, 12H)

All the ^{1}H NMR data matches with the reported literature data. https://www.frontiersin.org/articles/10.3389/fchem.2019.00493 (accessed April 25, 2023)

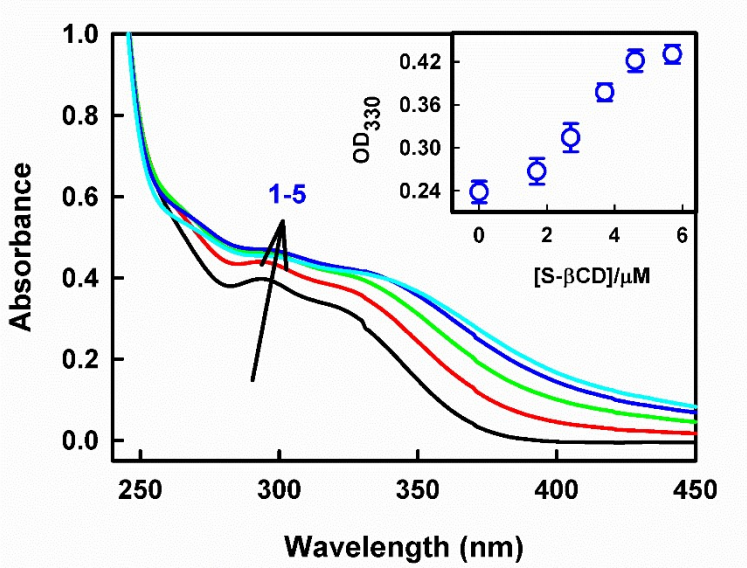

Figure S2. Ground-state absorption spectra of I-TPE (19 μM) at various concentrations of S-βCD (μM) (1) 0 (2) 2.7 (3) 3.7 (4) 4.6 (5) 5.7. Inset: Changes in absorbance at 330 nm at various concentrations of S-βCD. The blue circles correspond to the data points, and the indicated bars represent the standard error (n=3).

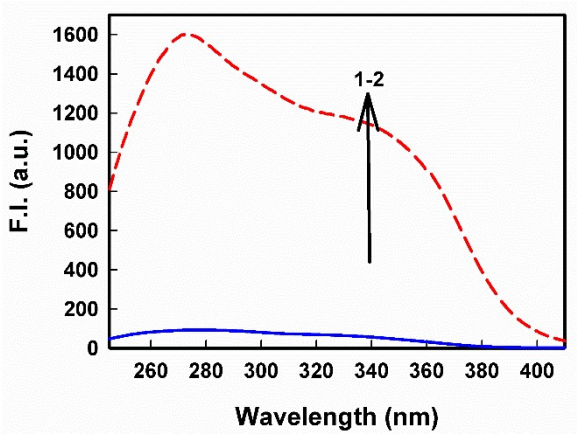

Figure S3: Excitation spectra of TPE-IM/S-βCD at different concentrations of S-βCD (μM) (1) 0 (2) and 2.

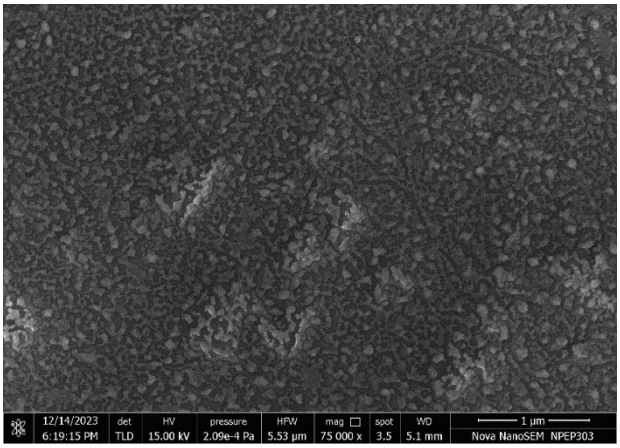

Figure S4: FE-SEM images of TPE-IM/S-βCD system

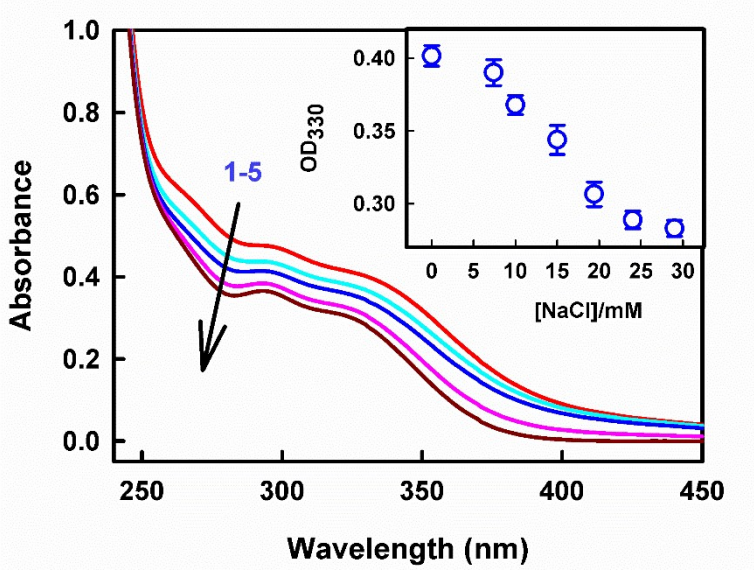

Figure S5. Ground-state absorption spectra I-TPE/S-βCD (I-TPE = 19 µM, S-βCD = 5 µM at various concentrations of NaCl (mM) (1) 0 (2) 10 (3) 15 (4) 19 (5) 29. Inset: Changes in absorbance at 330 nm at various concentrations of NaCl. The blue circles correspond to the data points, and the indicated bars represent the standard error (n=3).

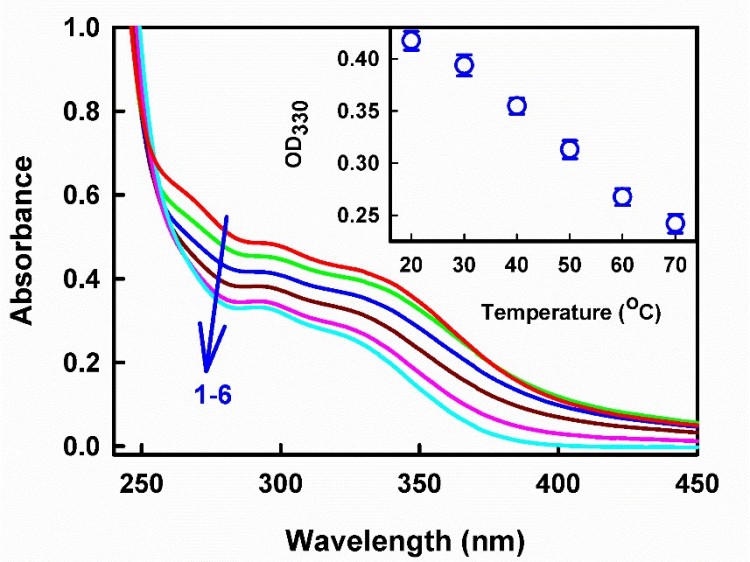

Figure S6. Ground-state absorption spectra I-TPE/S-βCD (I-TPE = 19 μM, S-βCD = 5 μM at various temperatures (° C) (1) 20 (2) 30 (3) 40 (4) 50 (5) 60 (6) 70. Inset: Changes in the absorbance at 330 nm at various temperatures. The blue circles correspond to the data points, and the indicated bars represent the standard error (n=3).

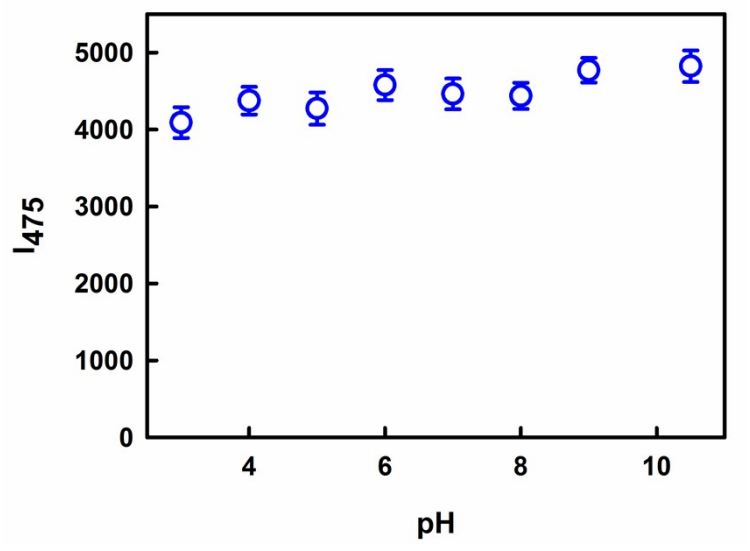

Figure S7. Variation in the fluorescence intensity of I-TPE/S-βCD at 475 nm versus pH.

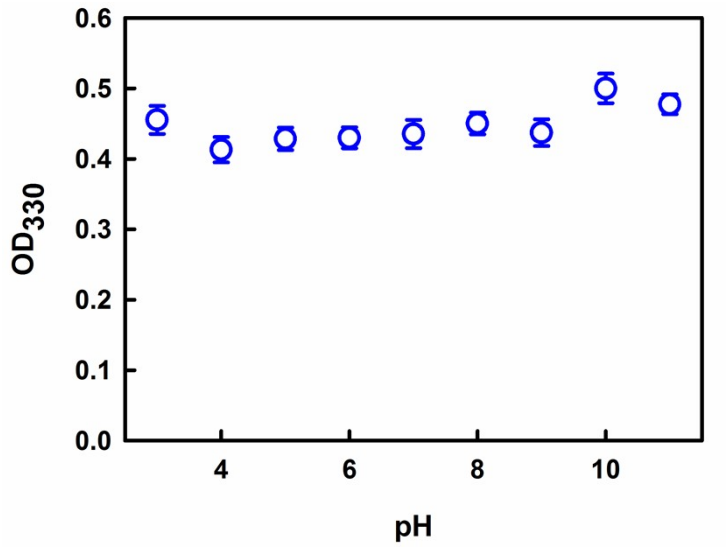

Figure S8. Variation in the absorbance of I-TPE/S-βCD at 330 nm versus pH.

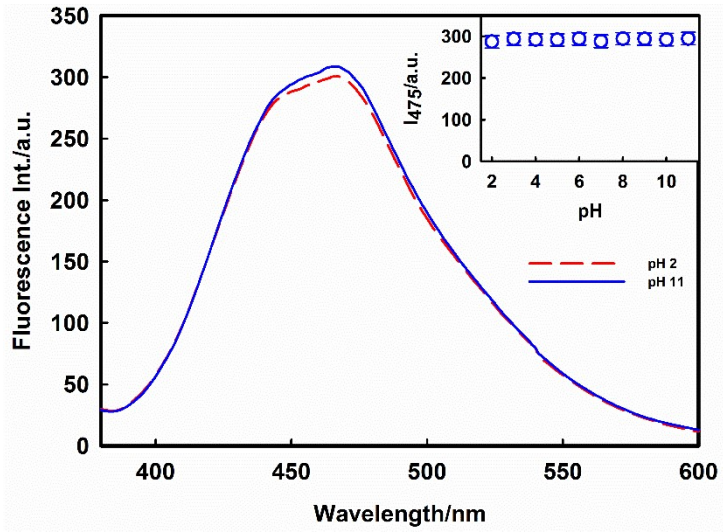

Figure S9: Fluorescence spectra of TPE-IM/S-βCD/PrS (TPE-IM = 19 μM, S-βCD = 5 μM, PrS =4.5 μM, λex = 350 nm) at different pH. Inset: Variation in the fluorescence intensity at 475 nm versus pH.

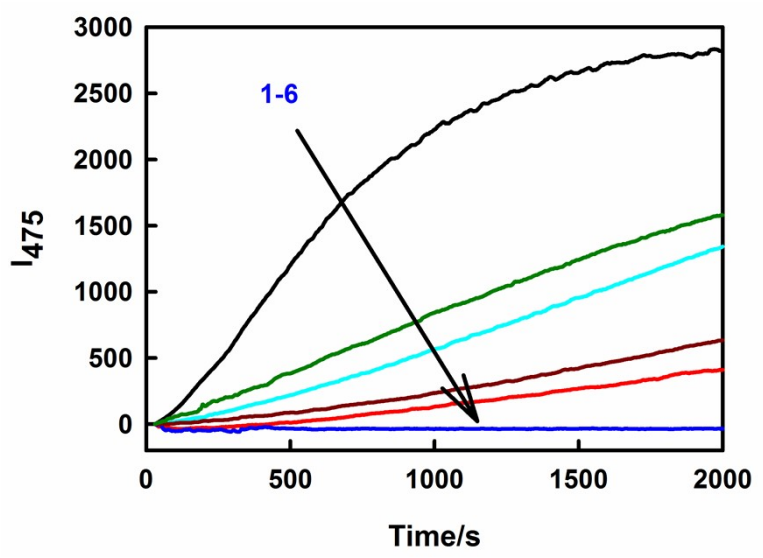

Figure S10. Inhibition of trypsin activity (10 nM) measured as fluorescence decay of I-TPE/S-βCD/PrS complex at 25 ° C, pH 8.2, in the presence of various concentrations of benzamidine (μM) (1) 0 (2) 16 (3) 41 (4) 61 (5) 81 (6) 160.