Electronic Supplementary Information

Hydrogen Bond Assisted Aggregation Induced Emission of Digitonin

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Electronic Supplementary Information, S1:

(A) Calculation of quantum yield:

Quantum yield (QY) of digitonin and base treated digitonin (Φ_s) were calculated using quinine sulfate in 0.1M H₂SO₄ as a standard (Φ_0 = 0.54)¹, according to previously reported procedure.²

	$\Phi_s = \Phi_0 \times \frac{I_s}{I_0} \times \frac{A_0}{A_s} \times \frac{n_s^2}{n_0^2}$								
Sample	Exc. Λ(nm)	Φ_0	A ₀	I ₀	n _o	A _s	Is	n _s	Φs
Digitonin	330	0.54	0.06126	1.7x10 ⁸	1.35	0.081	6.2x10 ⁵	1.35	0.00145
Digitonin- NaOH	380	0.54	0.06126	1.7x10 ⁸	1.35	0.0735	5.1x10 ⁷	1.35	0.135

Where, Φ_0 : Reference QY, Φ_s : Sample QY, I_0 and A_0 are the absorbance and intensity of reference respectively, I_s and A_s are intensity and absorbance of the sample respectively, η_0 and η_s are the refractive index of the solvent used reference and sample respectively.

(B) Calculation of FRET efficiency

(i) Steady State FRET Efficiency (E_S)

$$E_s = 1 - \frac{\Phi_{DA}}{\Phi_D}$$

 Φ_D donor alone quantum yield and Φ_{DA} donor quantum yield in the presence of acceptor

$$E_s = 1 - \frac{0.085}{0.135}$$

 $E_s = 37\%$

(ii) Time Resolved FRET Efficiency (E_T)

$$E_T = 1 - \frac{\tau_{DA}}{\tau_D}$$

 τ_D donor alone lifetime and τ_{DA} donor lifetime in the presence of acceptor

$$E_T = 1 - \frac{5.07}{8.1}$$

$$E_{\rm T} = 37\%$$



Figure S2: PL emission spectra of digitonin (a) and base treated digitonin (b) at a concentration of $10^{\Lambda^{-5}}$ M. Inset: photographs of solid state emission of base treated digitonin under hand held UV light (λ_{ex} : 365 nm).



Figure S3: Plot of PL intensity verses pH of the solution (from pH 2.5 to 14)



Figure S4: Temperature dependent PL emission spectra of aqueous solution of base treated digitonin.



Figure S5: FTIR spectra of digitonin (red trace) and base treated digitonin (black trace).



Figure S6: NMR spectra of digitonin (A) and base treated digitonin (B).



Figure S7: Atomic force microscopy (AFM) images of digitonin (A) and base treated digitonin (B).



Figure S8: Dynamic light scattering measurements depicting average hydrodynamic diameter of digitonin at pH 14.



Figure S9: PL emission spectra of digitonin at pH 14 in the absence and presence of glycerol (viscosity dependent fluorescence study).



Figure S10: PL emission spectra carbohydrates and steroids in the absence (blue) and presence of base (red trace) (A) Glucose (B) Starch (C) Estradiol (D) Carticosterone. Corresponding absorption spectra is shown as inset.



Figure S11: PL emission spectrum of Rhodamine B at 530 nm excitation, photograph under UV light is shown as inset.



Figure S12: Stern-Volmer plot of I_0/I verses concentration of quencher for white light emitting base treated digitonin-Rhodamine mixture.

Reference:

1.W. R. Dawson and M. W. Windsor, J. Phys. Chem., 1968, 72, 3251-3260.

2.Y. Fang, S. Guo, D. Li, C. Zhu, W. Ren, S. Dong and E. Wang, ACS Nano, 2012, 6, 400-409.