Supporting Information of

Turn-on-type emission enhancement and ratiometric emission color change based on the combination effect of aggregation and TICT found in hexaazatriphenylene-triphenylamine dye in an aqueous environment

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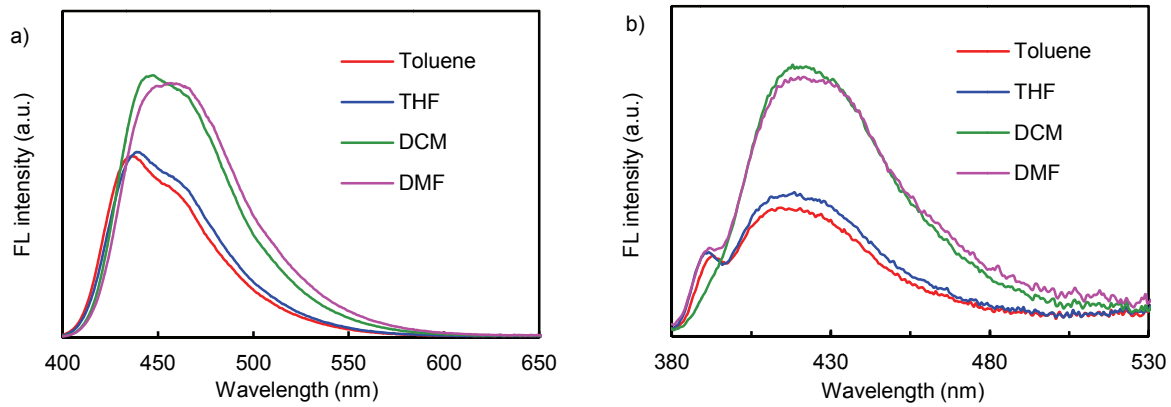

Fig. S1 Fluorescence spectra of **3** (ex. 390 nm) and **4** (ex. 350 nm) in toluene, THF, DCM, and DMF (2.0×10^{-7} M).

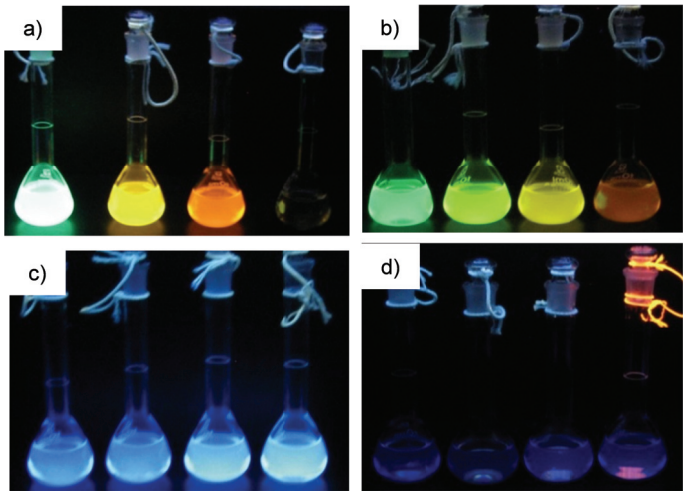

Fig. S2 Fluorescence images of a) **1**, b) **2**, c) **3**, and d) **4** in toluene, THF, DCM, and DMF (from left to right) at 2.0×10^{-6} M under UV light irradiation.

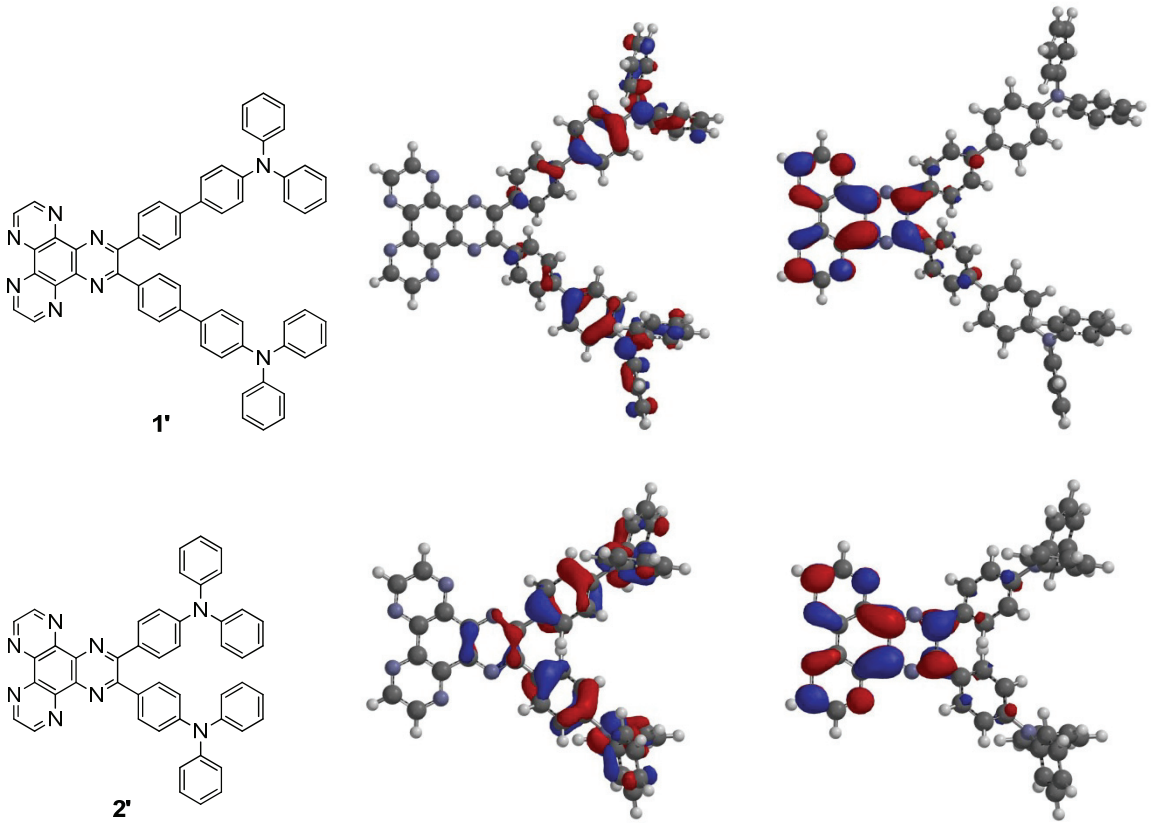

Fig. S3 HOMO and LUMO orbitals of the model compounds **1'** and **2'** (Hartree-Fock 6-31G*, Spartan 10). In the calculation, model compounds **1'** and **2'** bearing only two donor moieties were used, because of the limitation of our calculation soft.

In **1'**, the HOMO orbital was located mainly on the triphenylamine donor moiety, while the LOMO orbital was located on the hexaazatriphenylene acceptor moiety. Thus, the HOMO and LUMO orbitals were separated completely to support the TICT character. In contrast, in **2'** the HOMO and LUMO orbitals were overlapped partially to each other at the one pyrazine ring, indicating the ICT character.

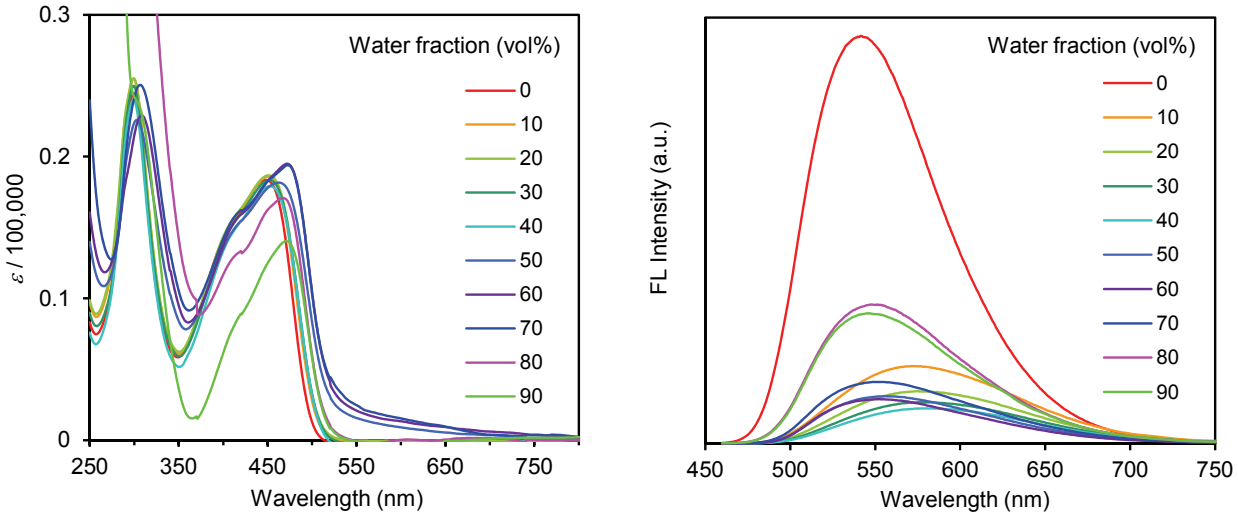

Fig. S4 (a) UV/vis absorption and (b) fluorescence spectra of **2** in THF/water (0, 10, 20, 30, 40, 50, 60, 70, 80, and 90% water fractions) at 2.0×10^{-6} M excited at 440 nm.

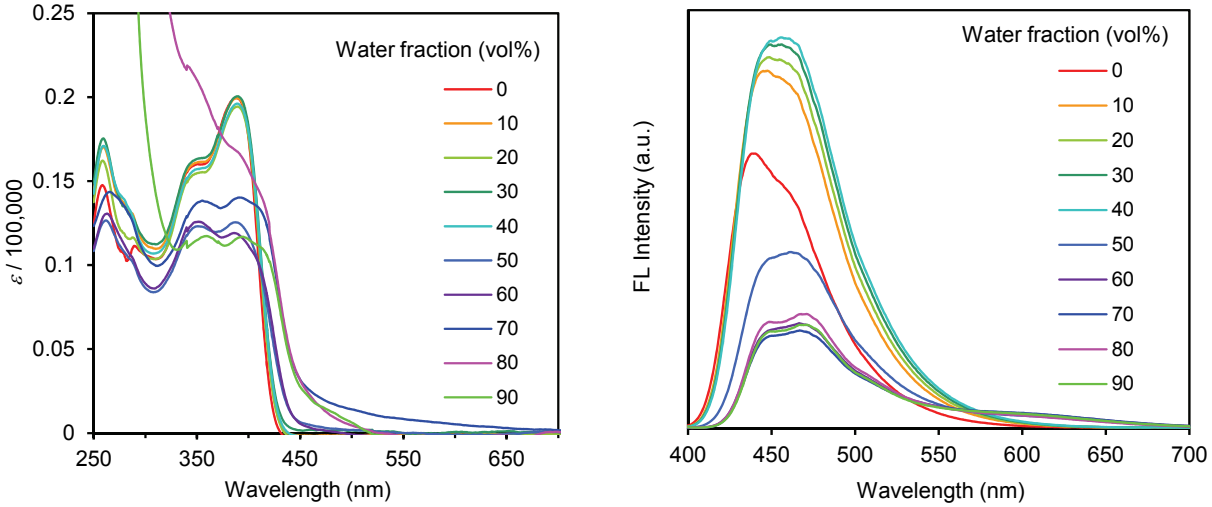

Fig. S5 (a) UV/vis absorption and (b) fluorescence spectra of **3** in THF/water (0, 10, 20, 30, 40, 50, 60, 70, 80, and 90% water fractions) at 2.0×10^{-6} M excited at 390 nm.

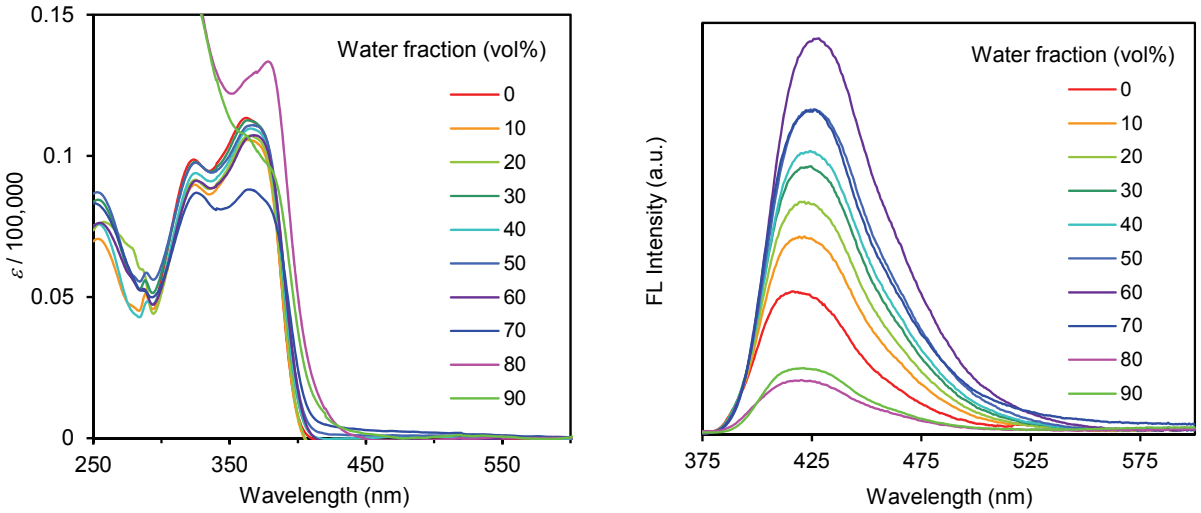

Fig. S6 (a) UV/vis absorption and (b) fluorescence spectra of **4** in THF/water (0, 10, 20, 30, 40, 50, 60, 70, 80, and 90% water fractions) at 2.0×10^{-6} M excited at 350 nm.

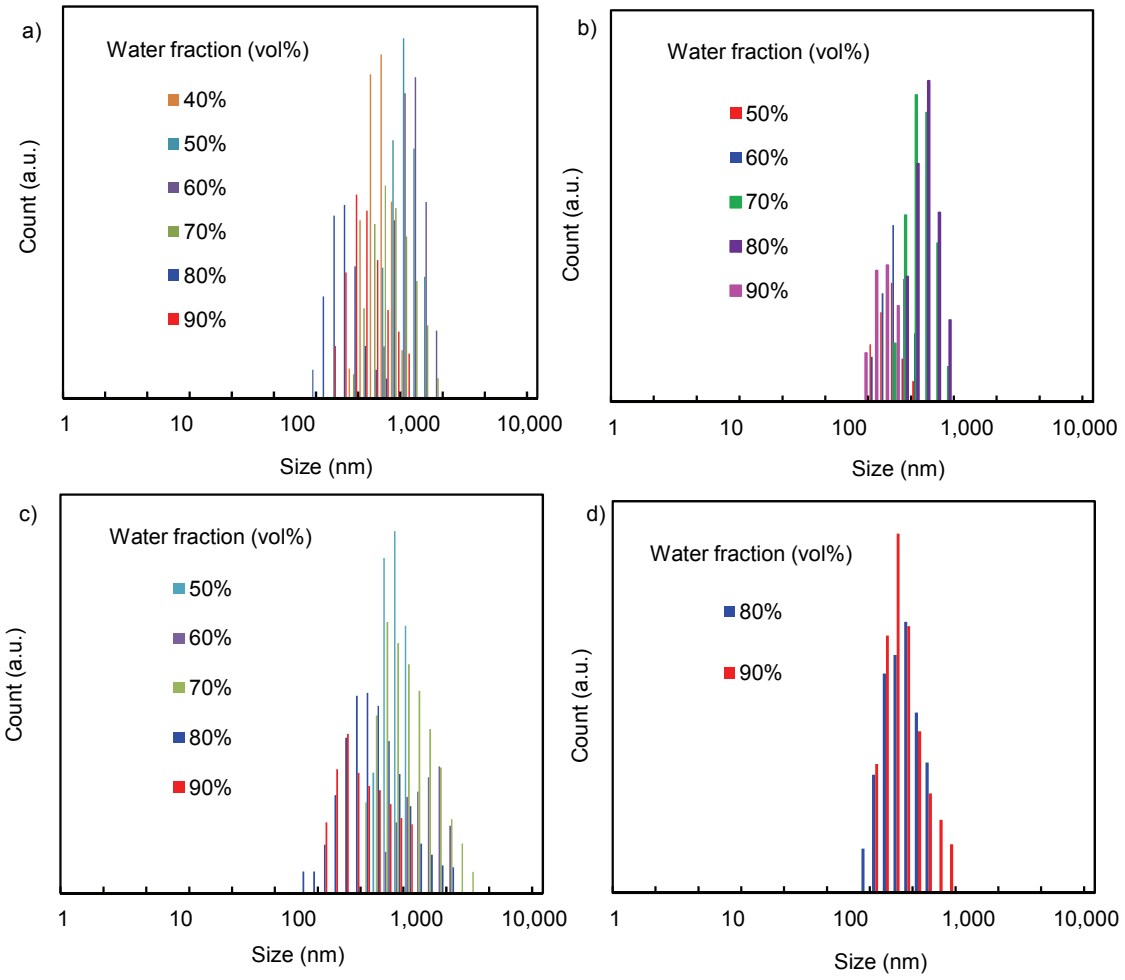

Fig. S7 DSL chart of a) **1**, b) **2**, c) **3**, and d) **4** in THF/water at 2.0×10^{-6} M.

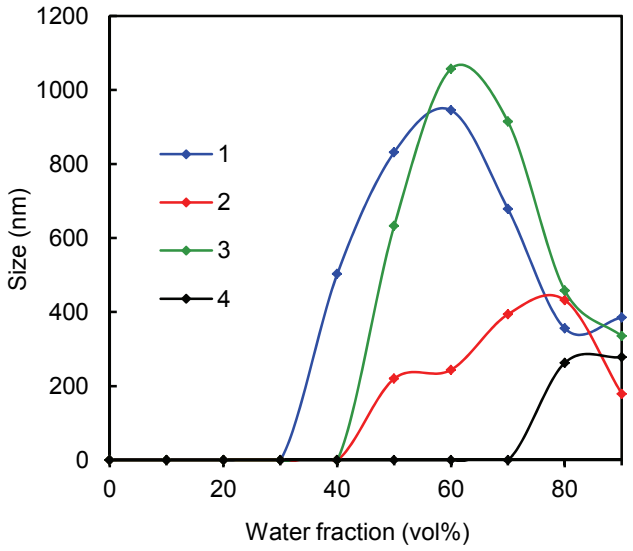

Fig. S8 Plots of aggregate size measured by DLS against the water fraction (vol%) of **1**, **2**, **3**, and **4** in THF/water at 2.0×10^{-6} M. Size at 90%: 390 nm for **1**, 180 nm for **2**, 330 nm for **3**, and 280 nm for **4**.

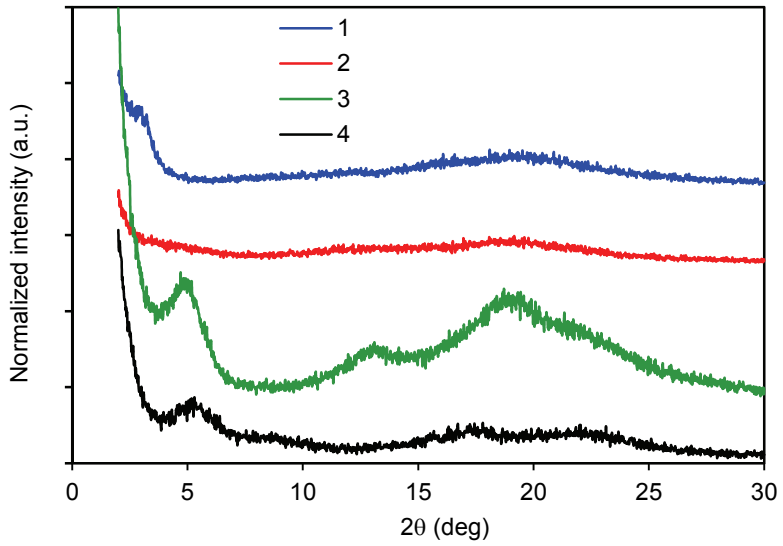

Fig. S9 XRD patterns of **1**, **2**, **3**, and **4**. The samples were obtained by the reprecipitation from the THF/water (90% water fraction) solutions at 1.0×10^{-4} M.