

## Supporting information

### Tuning Excited-State Proton Transfer Dynamics of a 3-hydroxychromone Dye in Supramolecular Complexes via Host-Guest Steric matching

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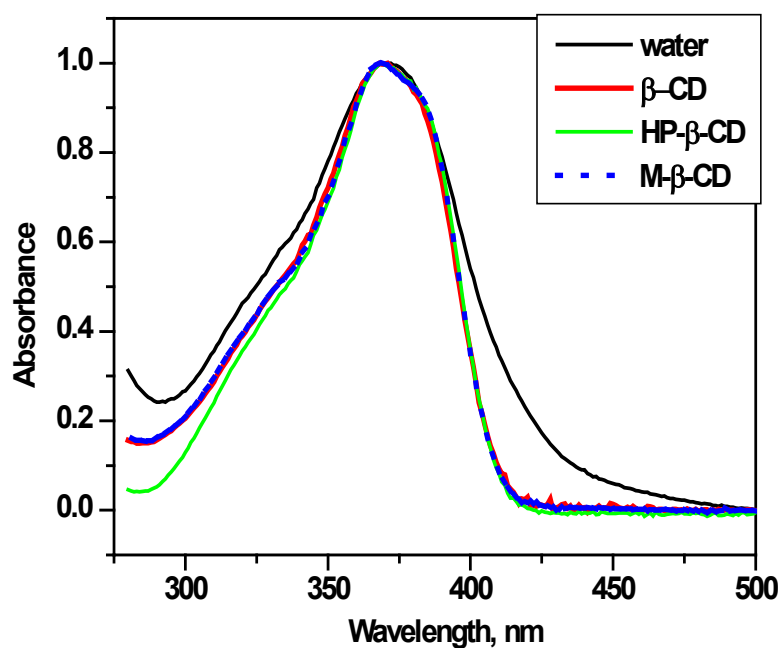


Figure S1. Normalized absorption spectra in water and cyclodextrins, [BFHC] = 5 μM, [CD] = 5 mM

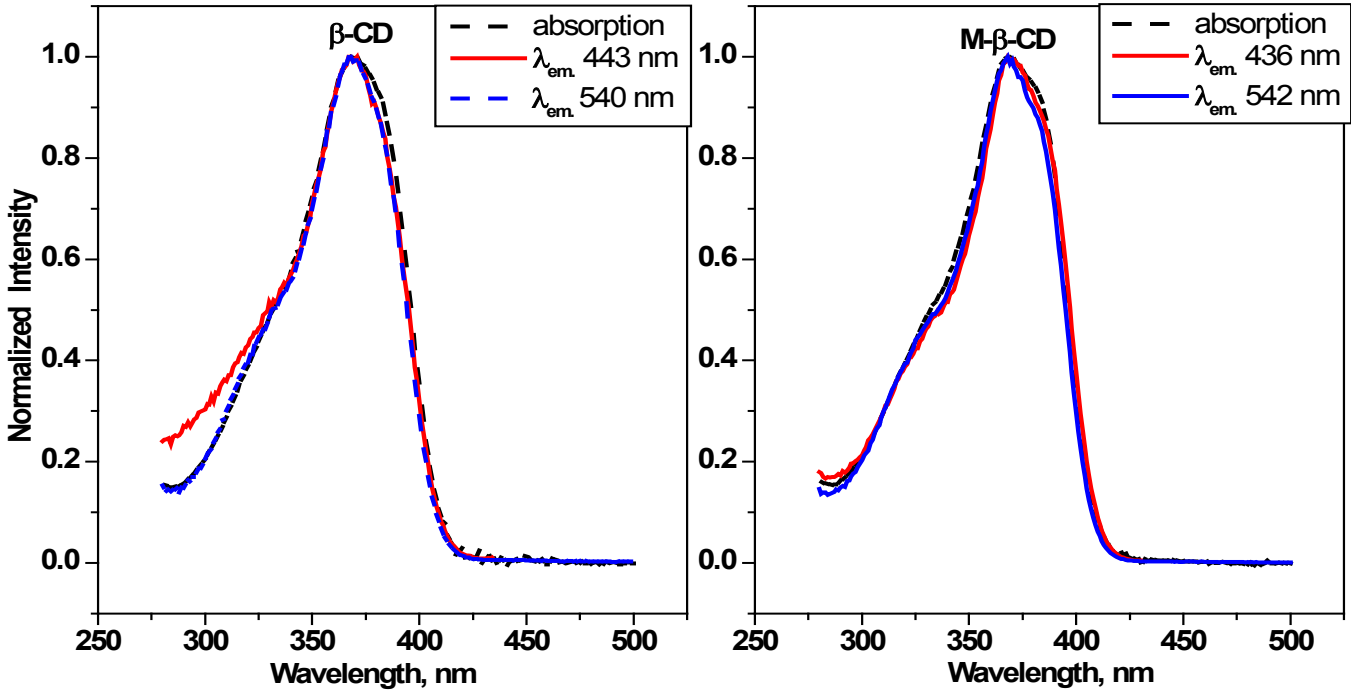
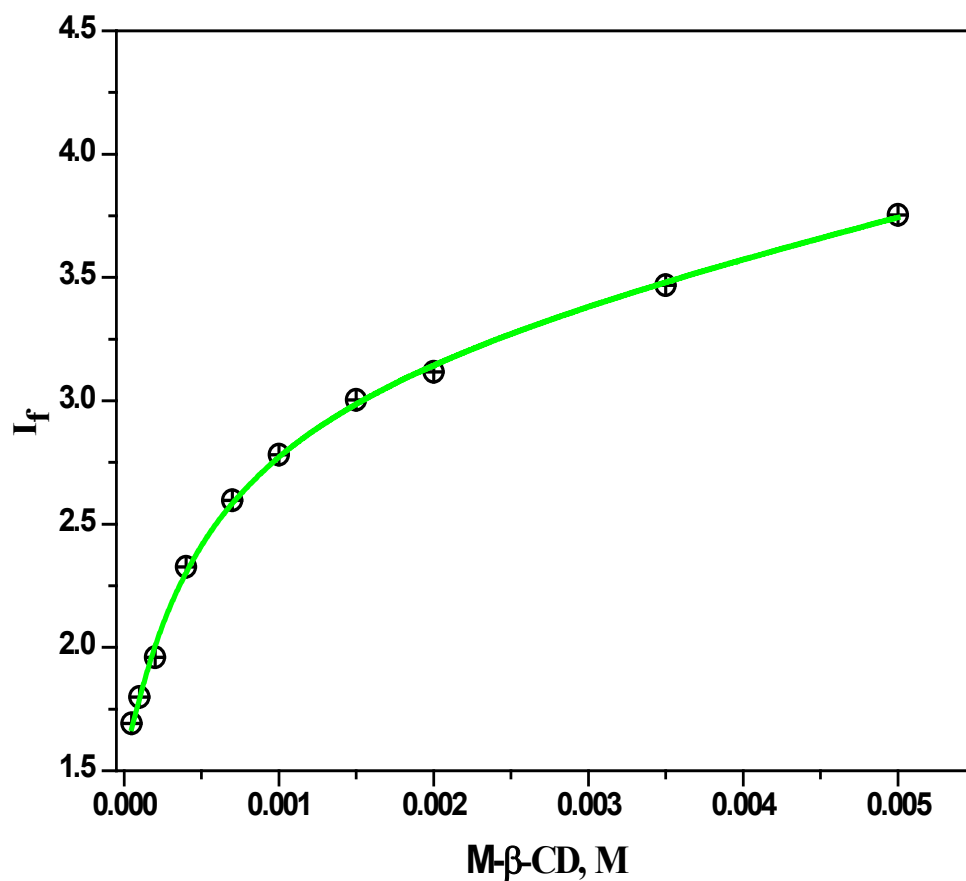
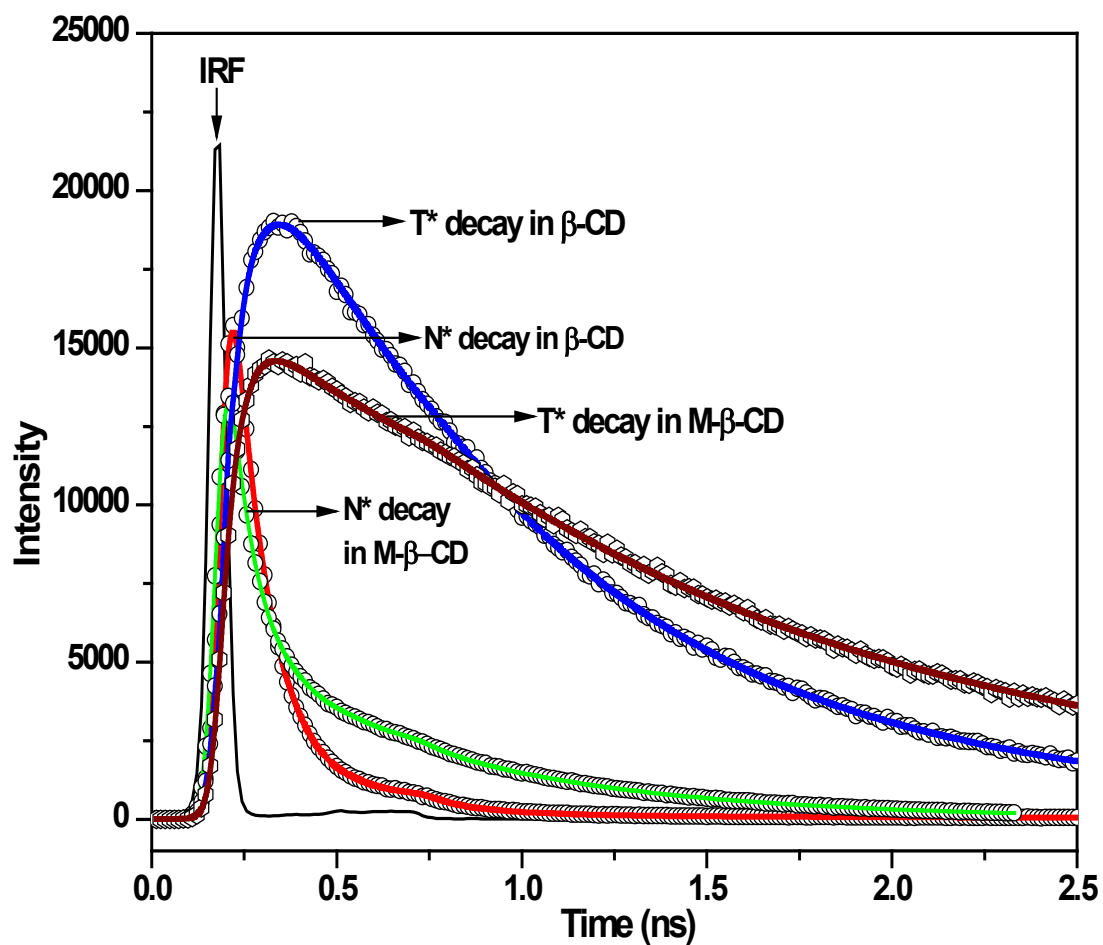


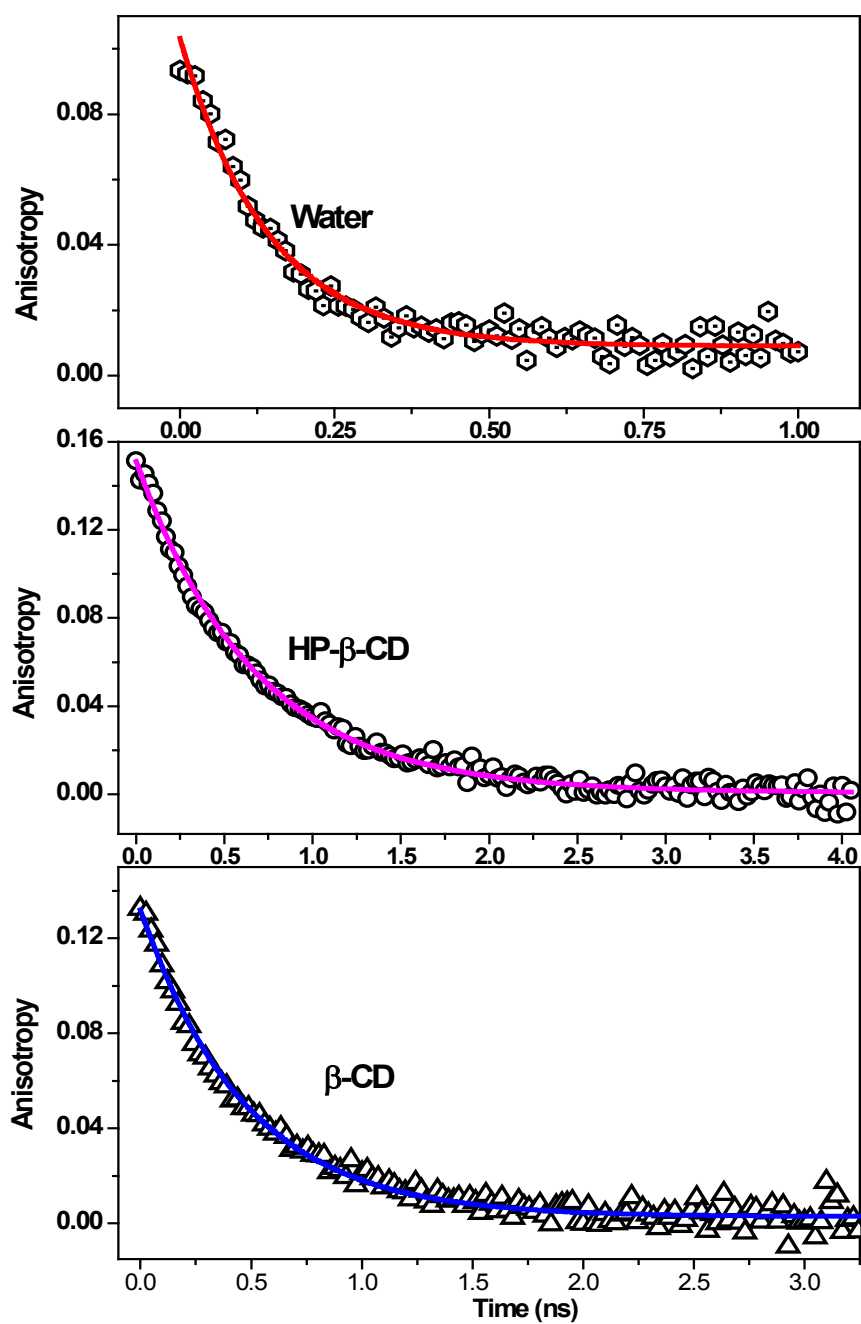
Figure S2. Normalized absorption and excitation spectra in  $\beta$ -CD and M- $\beta$ -CD, [BFHC] = 5  $\mu$ M, [CD] = 5 mM



**Figure S3.** Titration curves of BFHC by M-β-CD in water. The intensity of the T\* band is plotted as a function of the total concentration of the β-CDs. The solid lines are nonlinear regression fits to the experimental data (circles).  $K_1 = 1850 \pm 45 \text{ M}^{-1}$



**Figure S4.** Fluorescence emission decays of BFHC in  $\beta$ -CD and M- $\beta$ -CD at 298K.  $\lambda_{\text{ex}} = 320$  nm (IRF signal is at 320 nm).  $\lambda_{\text{em}}(\text{N}^*) = 435$  nm and  $\lambda_{\text{em}}(\text{T}^*) = 545$  nm. The different coloured continuous curves (—) are the fit of the experimental data ( $\circ$ ).



**Figure S5. Fluorescence anisotropy decay of BFHC ( $\lambda_{\text{ex}} = 320 \text{ nm}$ ,  $\lambda_{\text{em}} = 545 \text{ nm}$ ) in water and 5 mM CDs at 298K**

