Electronic Supplementary Information

Fluorescence quenching by photoinduced electron transfer between 7-methoxycoumarin and guanine base facilitated by hydrogen bond: an *in silico* study

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The labels in Figure S1 have been modified.

Calculation of spectra

The area and height of the spectrum is related to the population on S_0 for absorption (and to the population on S_1 and S_2 for emission from these excited states), the transition dipole moment, and the energy gap between the initial state (S_i) and the final state (S_f). Therefore, a spectrum is calculated as

$$I(\upsilon, t) \propto \sum_{I \in S_i} n_I(t) \times \left| \left\langle \psi_{S_f}(r; \overline{R_I}(t) \middle| \vec{\mu} \middle| \psi_{S_i}(r; \overline{R_I}(t) \right\rangle \right|^2 \times \left(\frac{\left| E_{S_i} - E_{S_f} \right|}{h} \right)^3$$

where the sum is limited by the trajectory basis functions (TBFs) that propagating on S_0 for absorption or on S_1 and S_2 for emission from these excited states, $n_I(t)$ is population of the Ith TBF as calculated from inner product of wave function coefficient, ψ_{S_i/S_f} is S_i/S_f electronic wave function, $\vec{\mu}_{if}$ is S_i/S_f transition dipole moment operator, $\overline{R_I}(t)$ is the center of the Gaussian wave packet for the Ith TBF and E_{S_i/S_f} is the electronic energy on the S_i/S_f state.

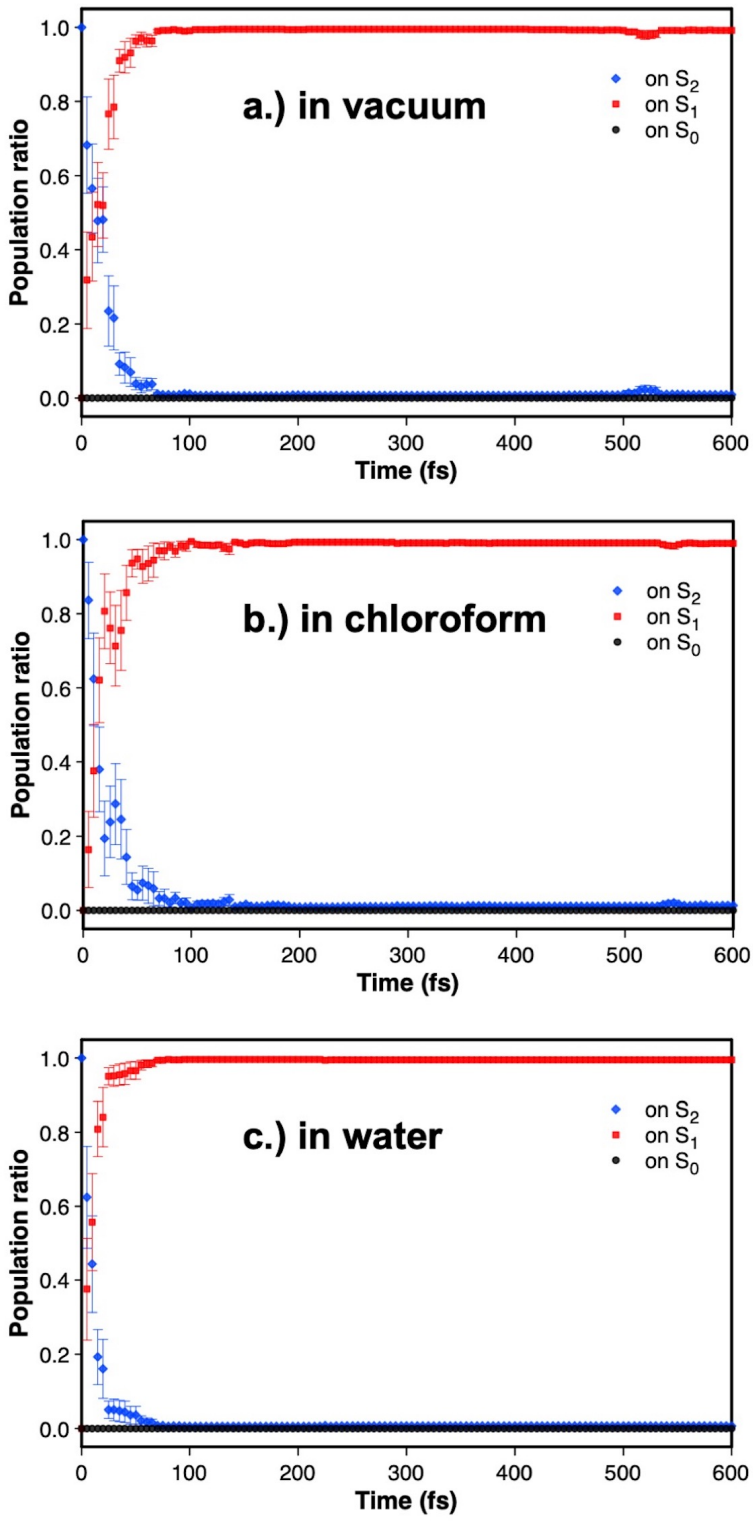

Fig. S1. Averaged (over ten initial conditions) S_2 population decay of free 7MC in vacuum (a), in chloroform (b) and in water (c) obtained from direct dynamics simulations. Error bars are given as standard error of the mean.

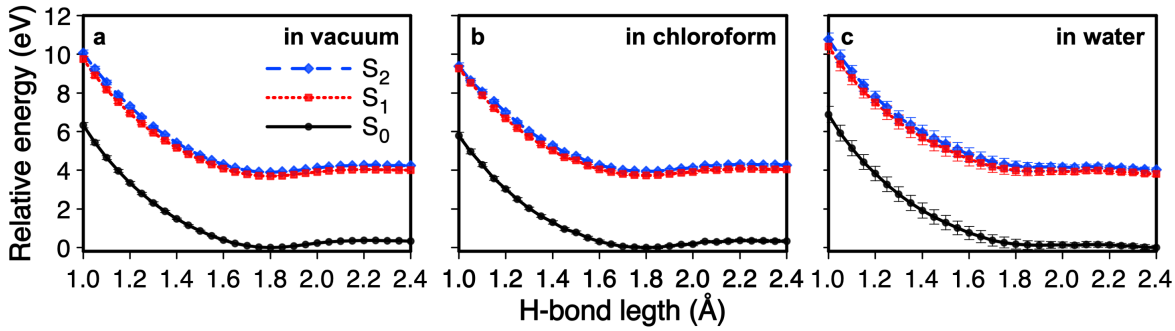

Fig. S2. Relative potential energy variation along H-bond length (d_1) in vacuum (a), in chloroform (b) and in water (c) on S_0 (solid black lines), S_1 (dotted red lines) and S_2 (dashed blue lines)

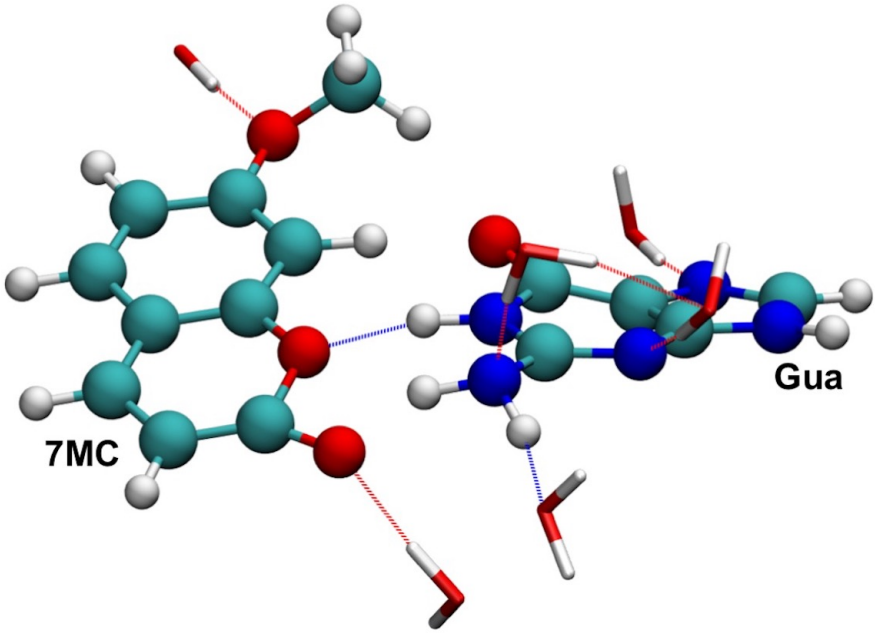

Fig. S3. Water molecules disrupt the H-bonding interaction between 7MC and Gua (this figure is rendered from VMD program[1], the cut-off distance and angle are 3.0 Å and 20°, respectively)

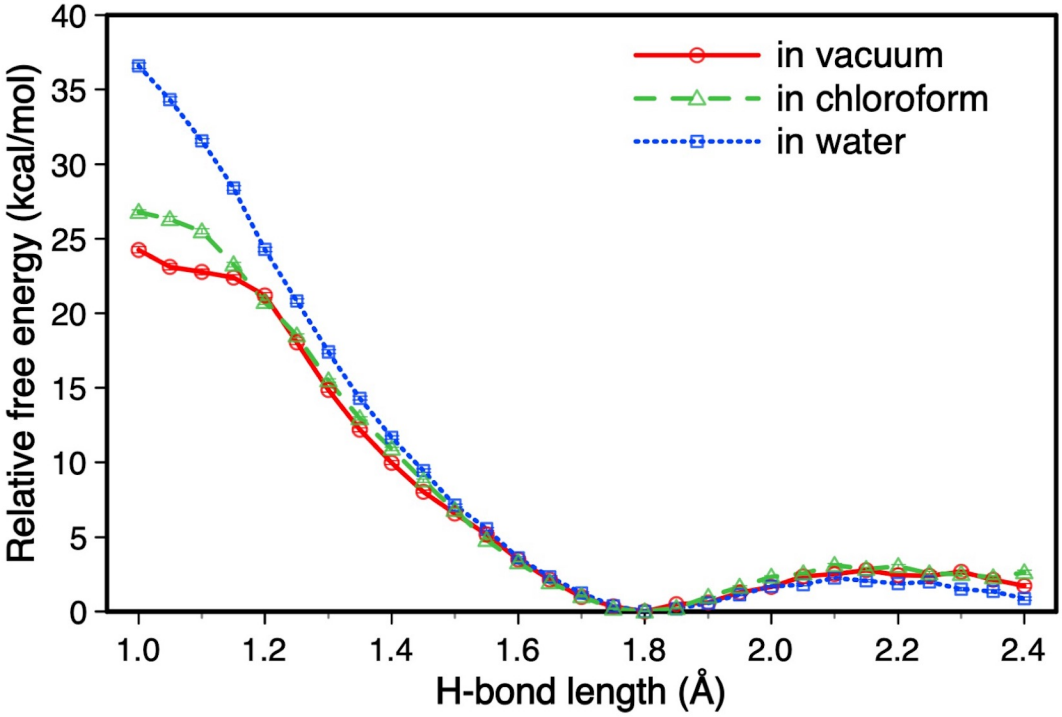

Fig. S4. Relative S_2-free energy curve as a function of the H-bond length (d_1) between 7MC and Gua in vacuum (red solid line), in chloroform (green dashed line) and in water (blue dotted line) obtained from the umbrella sampling technique[2] with the weighted histogram analysis method.[3]

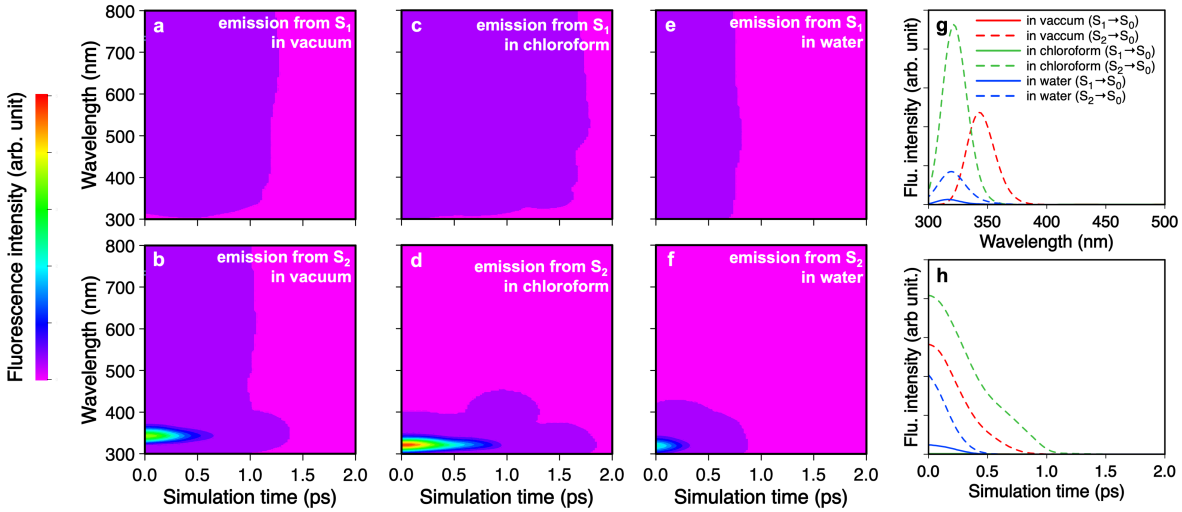

Fig. S5. 2-D contour plots of the time-resolved emission spectra of H-bonded 7MC-complex for emission from S_1 (a) and S_2 (b) in vacuum; emission from S_1 (c) and S_2 (d) in chloroform; emission from S_1 (e) and S_2 (f) in water. The integrated emission spectra (g) and time-resolved total fluorescence emission (h) of free 7MC in vacuum, water and chloroform are shown in red, blue and green colors, respectively, with emissions from S_1 represented as solid lines and emission from S_2 represented as dashed lines.

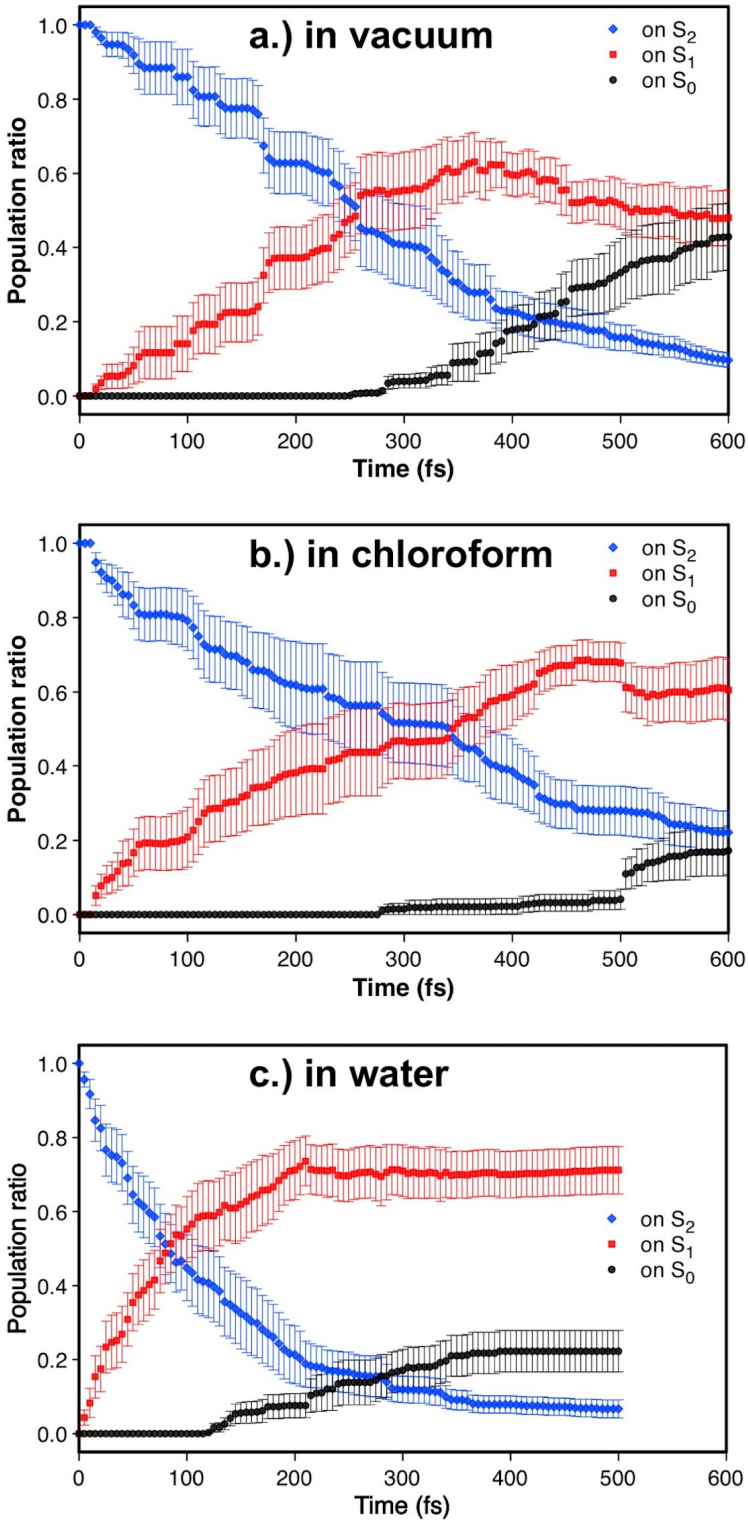

Fig. S6. Averaged (over ten initial conditions) S_2 population decay of H-bonded 7MC-complex in vacuum (a), in chloroform (b) and in water (c) obtained from direct dynamics simulations. Error bars are given as standard error of the mean.

References

1. W. Humphrey, A. Dalke and K. Schulten, *J. Mol. Graph.*, 1996, **14**, 33-38, 27-38.

2. G. M. Torrie and J. P. Valleau, *J. Comput. Phys.*, 1977, **23**, 187-199.

3. S. Kumar, J. M. Rosenberg, D. Bouzida, R. H. Swendsen and P. A. Kollman, *J. Comput. Chem.*, 1992, **13**, 1011-1021.