The Gas-Phase Photophysics of Eosin Y and its Maleimide Conjugate.

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Table S1. Details of the relevant TDDFT results (c.f. Figure 4).

Excited State	KS-Orbital Excitation	TDDFT Coefficient X_{ia}	Spacial Overlap $O_{ia} = \langle \lvert\varphi_i\rvert \lvert\varphi_a\rvert \rangle$
$[EY-2H]^{2-}$			
S_1 (3.1 eV, f=0.8)	HOMO → LUMO	0.7	0.64 (π- π*)
$[EYM-2H]^{2-}$			
S_1 (2.3 eV, f=0.0)	HOMO → LUMO	0.7	0.004 (CT)
S_3 (3.1 eV, f=0.3)	HOMO-3 → LUMO HOMO → LUMO+1	0.49 0.42	0.025 (CT) 0.64 (π- π*)

$[EYM+CA-2H]^{2-}$			
S_1 (3.1 eV, f=0.8)	HOMO → LUMO+1	0.7	0.65 (π- π*)
S_4 (4.07 eV, f=0.0)	HOMO → LUMO	0.7	0.066 (CT)

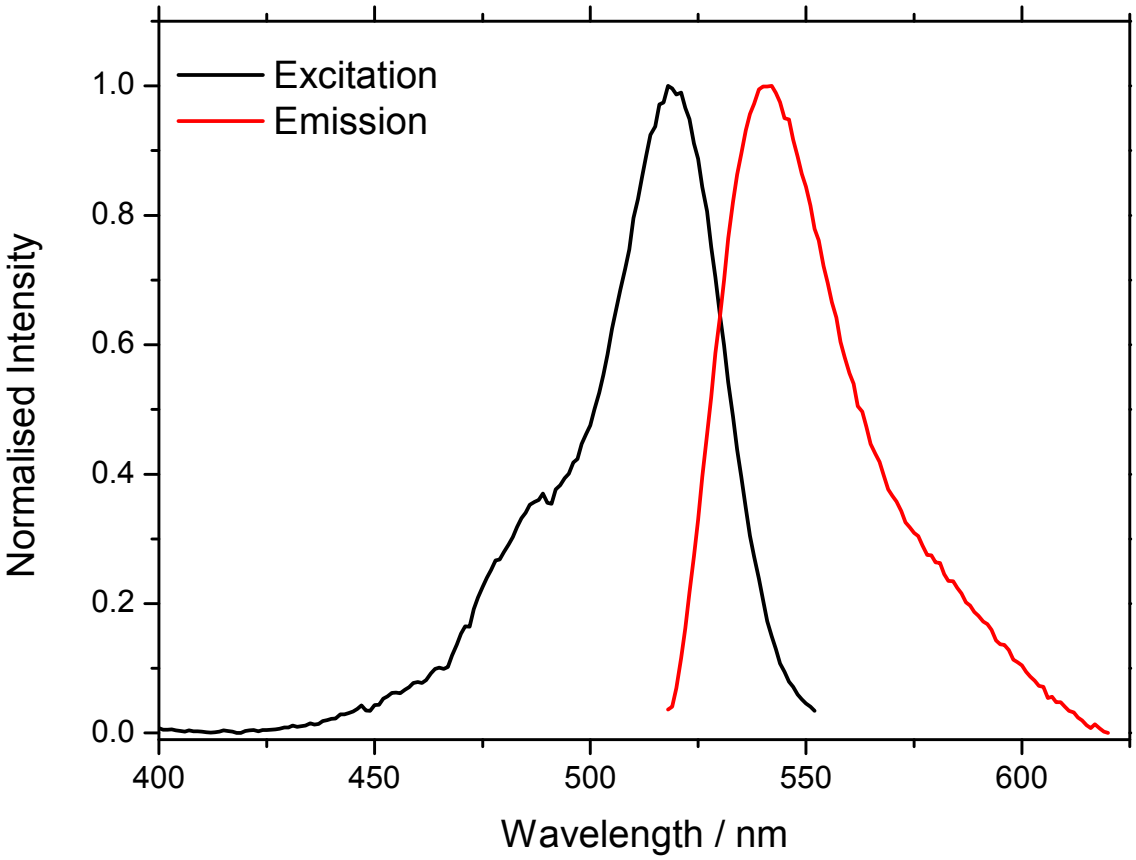

Figure S1. Fluorescence excitation (black) and emission (red) spectra of Eosin Y in H_2O at pH 2.53.

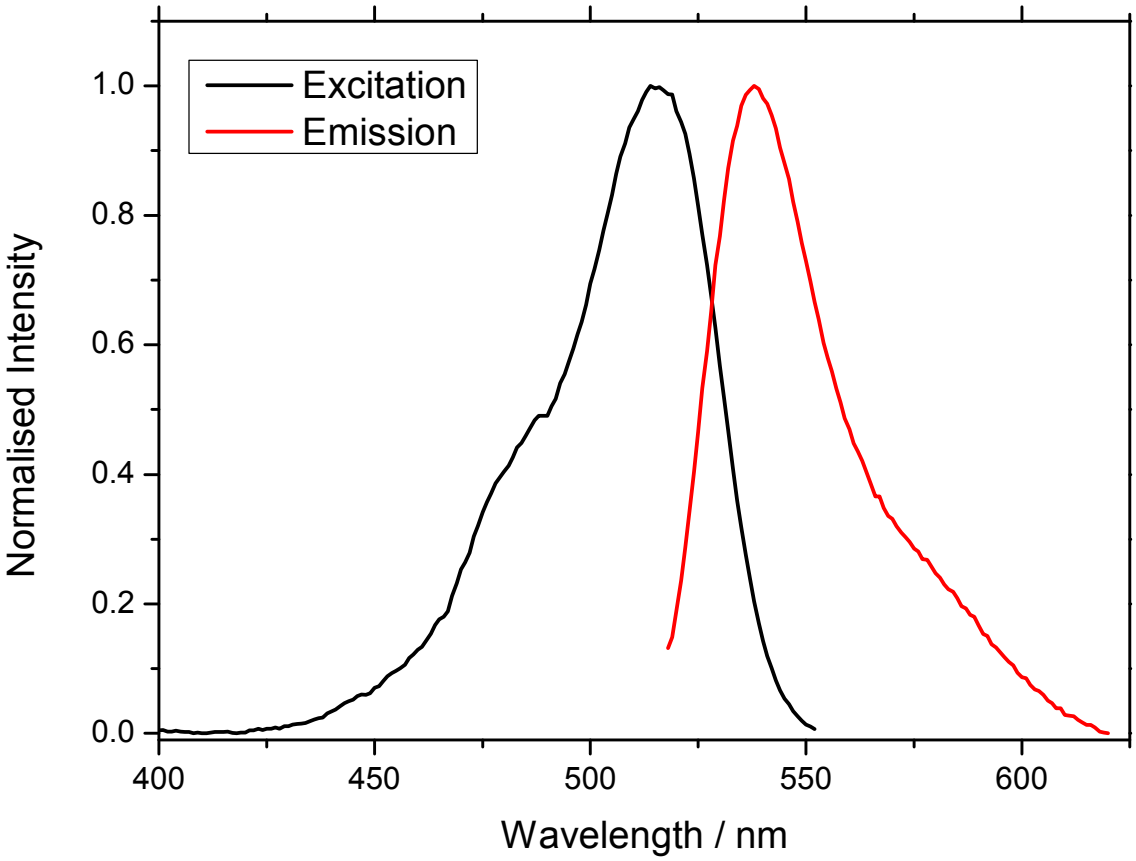

Figure S2. Fluorescence excitation (black) and emission (red) spectra of Eosin Y in H_2O at pH 11.87.

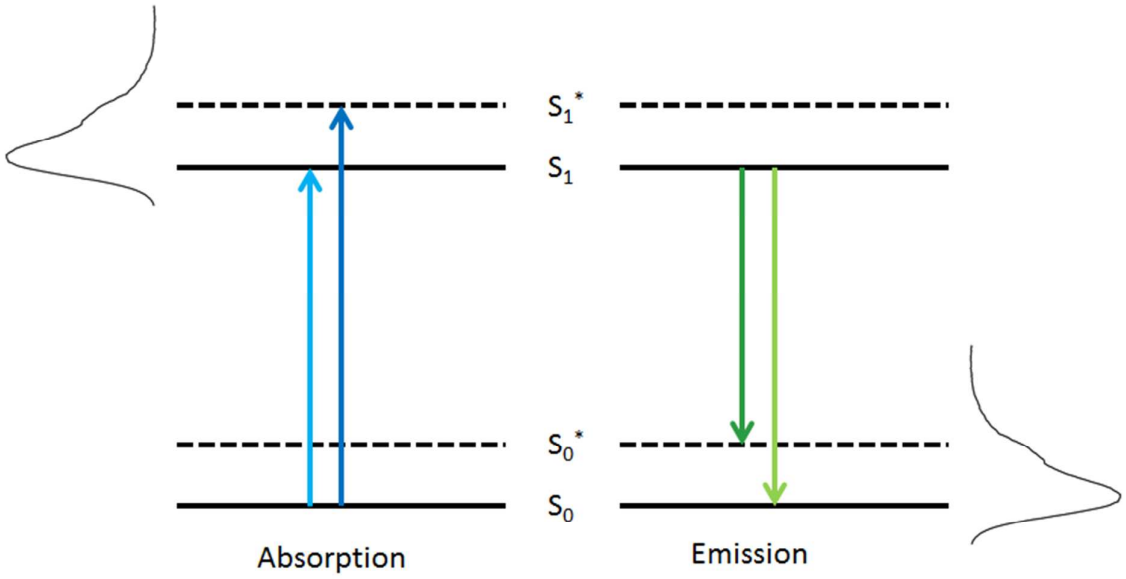

Figure S3. Schematic diagram of the absorption and emission processes leading to the observation of a shoulder in both the absorption and fluorescence spectrum of Eosin Y. Here, S_0 and S_1 refer to the ground and first excited state of the system, and S_0* and S_1* refer to a vibrational level within the ground and first excited state respectively.

Table S2. Fitted values for the fluorescence excitation and emission spectra of Eosin Y in H_2O at different values of the pH.

pH	Excitation (shoulder) / nm	Emission (shoulder) / nm
2.53	520 (492)	541 (567)
11.87	517 (492)	538 (362)