Supporting Information: Comment on "Solvent Effect on the Electronic Spectra of Azine Dyes under Alkaline Conditions"

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1. Computational Methods

All structures were optimized in the solvent phase using the polarizable continuum model[1,2] (PCM) at the B3LYP[3-8] level of theory with the 6-311++G(d,p) basis set;[9,10] no symmetry constraints were imposed during the optimization of the dyes. The structures were optimized in two different solvent (dielectric) environments, water (ε = 78.4) and toluene (ε = 2.4). Time dependent density functional theory[11-13] (TD-DFT) single-point calculations were performed on the optimized structures to obtain the calculated λ_{max} values. The PCM approach was employed within the TD-DFT calculations to model the effect of the respective solvents on the absorption spectra. All calculations were done within the Gaussian 03 program.[14] The charge distribution of methylene blue was determined using the natural bond orbital (NBO) approach.[15]

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2. Figure S1.

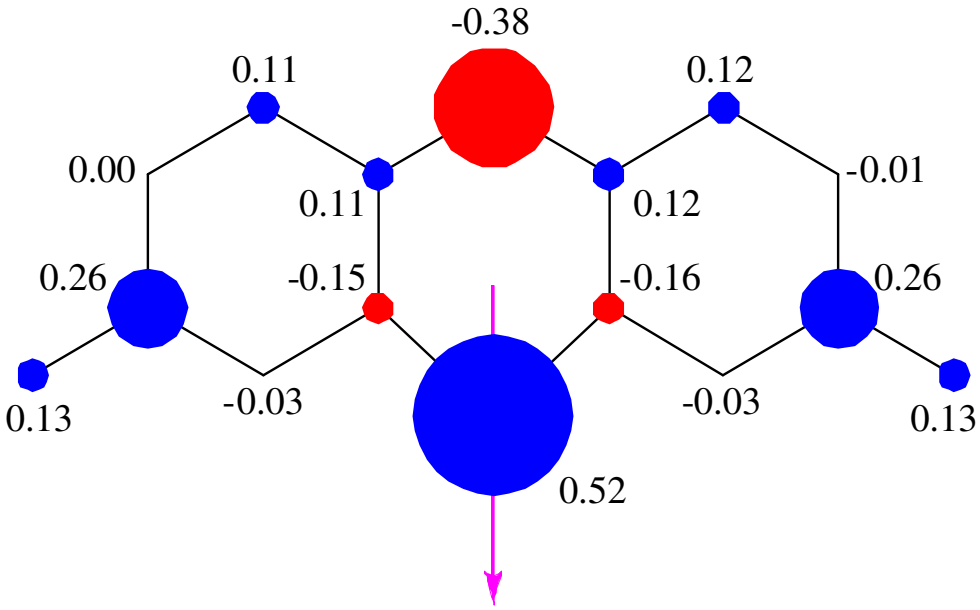

Figure S1. NBO charge distribution on the PCM/B3LYP electronic ground state of MB. See Computational Methods for details. The arrow represents the direction of the molecules dipole moment. Only heavy atoms shown, with charge amalgamated onto the attached C atom, or N atom for methyl groups.