Supporting Information

Photoinduced Generation of the π -Conjugated Zwitterionic State in the ESIPT Fluorophore of 2,4-Bisimidazolylphenol

Ken-ichi Sakai^{*†}, Naoya Miyamoto[†], Mayu Ogawa[†], Keiichi Kawano[†], Tomoyuki Akutagawa^{*‡}

[†]Department of Applied Chemistry and Bioscience, Chitose Institute of Science and Technology (CIST), Chitose 066-8655, Japan,

[‡] Polymer Hybrid Materials Research Center, Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577, Japan



Figure S1. Absorption and fluorescence (λ_{ex} = 365 nm) spectra of 2,4-bImP (a) in ethanol and (b) in acetic acid. The dotted lines are the excitation spectra monitored at the fluorescence maxima.



Figure S2. Fluorescence and excitation spectra of 2,6-bImP in the solid state (red dotted lines), and the absorption and fluorescence spectra of 2,6-bImP in CHCl₃ (blue lines). The dashed line is the absorption spectrum after 1 min UV irradiation of the CHCl₃ solution.



Figure S3. UV light ($\lambda = 365$ nm) irradiation-time-dependent absorption spectra of 2,4-bImP (a) in THF, (b) in EtOH, and (c) in AcOH. The increments are 5 min for (a), 1 min for (b) and (c).



Figure S4. UV light ($\lambda = 365$ nm) irradiation-time-dependent absorption spectra of 2,4-bImP in CHCl₃, in which 2 equiv TFA is added before UV irradiation.



Figure S5. Reversible absorption spectral changes on repeated UV irradiation $(1\rightarrow 2, 4\rightarrow 5)$, 2 equiv TFA addition $(2\rightarrow 3, 5\rightarrow 6)$, and 2 equiv TEA addition $(3\rightarrow 4, 6\rightarrow 7)$.



Figure S6. DFT-calculated HOMO, LUMO, and dipole moments of the enol form (I) and the zwitterion (III).