## SUPPORTING INFORMATION

## Spectra-Structural Effects of the Keto-Enol-Enolate and Phenol-Phenolate Equilibria of Oxyluciferin

Panče Naumov,\* Manoj Kochunnoonny

Department of Material and Life Science, Graduate School of Engineering, Osaka University,

2-1 Yamada-oka, Suita 565-0871, Osaka, Japan



Figure S1. IR spectrum of as-synthesized DHOxyLH in KBr pellet.

**Figure S2 (below, pages S2 through S7)**. Solvent effects on the absorption (left panels) and emission (right panels) spectra of DHOxyLH in solution.













Dimethylformamide (DMF)













Figure S2. Solvent effects on the absorption (left panels) and emission (right panels) spectra of DHOxyLH in solution.



Figure S3. <sup>1</sup>H NMR spectra of DHOxyLH in various solvents (w – water peaks, s – solvent peaks).



Figure S4. <sup>1</sup>H NMR spectra of DHOxyLH in various solvents.



**Figure S5**. <sup>1</sup>H NMR spectra of DHOxyLH in various solvents (w – water peaks, s – solvent peaks).