Electronic supplementary information for:

Mechanistic Insights into Excited State Intramolecular Proton Transfer in Isolated and Metal Chelated Supramolecular Biosensors.

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Figure S1: Minimum energy geometries and dominant orbital excitation accompanying the lowest three singlet electronic transitions of Cd$^{2+}$–HDBO'$^\prime$ (right) and Hg$^{2+}$–HDBO'$^\prime$ (left).
Figure S2: Magnitude and direction of the permanent dipole moment of HBO at the minimum energy geometries of (a) the $S_0$ state, (b) the $S_1$ enol conformer and (c) the $S_1$ keto minimum at planar geometries.