

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' (right) and Hg^{2+} -HDBO' (left).

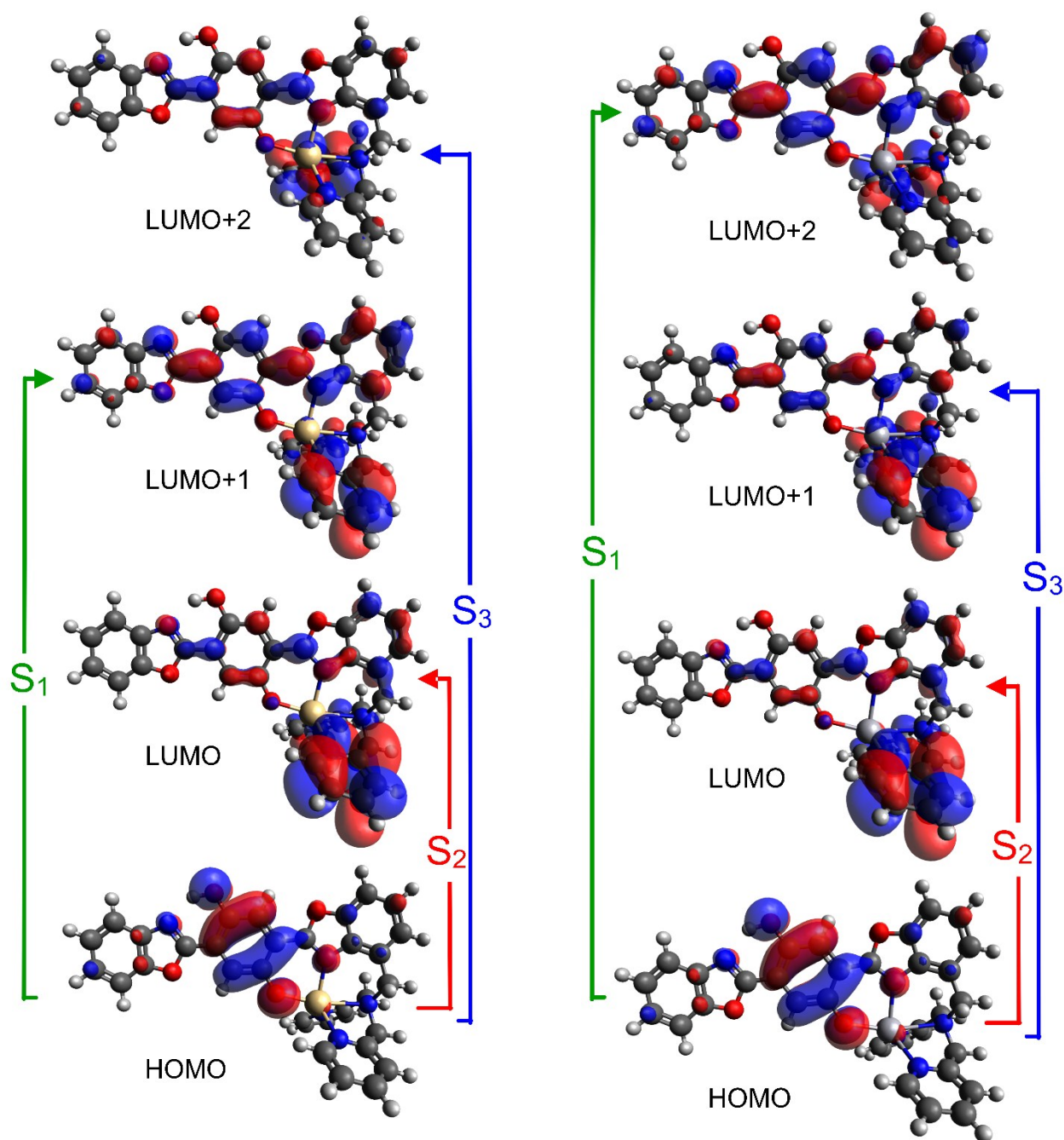


Figure S2: Magnitude and direction of the permanent dipole moment of HBO at the minimum energy geometries of (a) the S_0 state, (b) the S_1 *enol* conformer and (c) the S_1 *keto* minimum at planar geometries.

