Supporting Information for:

Electronic Structure Methods for Simulating Flavin's Spectroscopy and Photophysics: Comparison of Multi-Reference, TD-DFT, and Single-Reference Wave Function Methods

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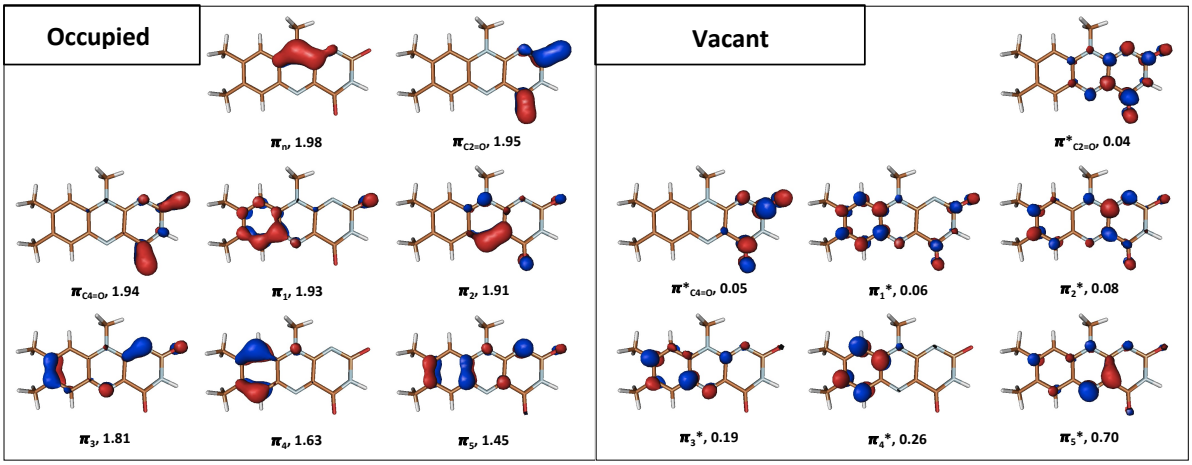
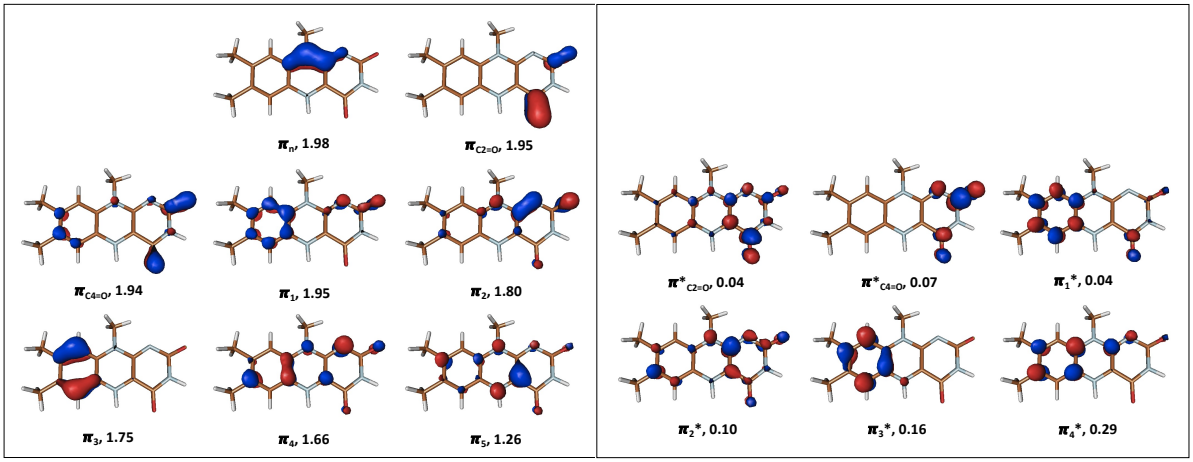
a. Fl



b. FlH$^{\cdot}$



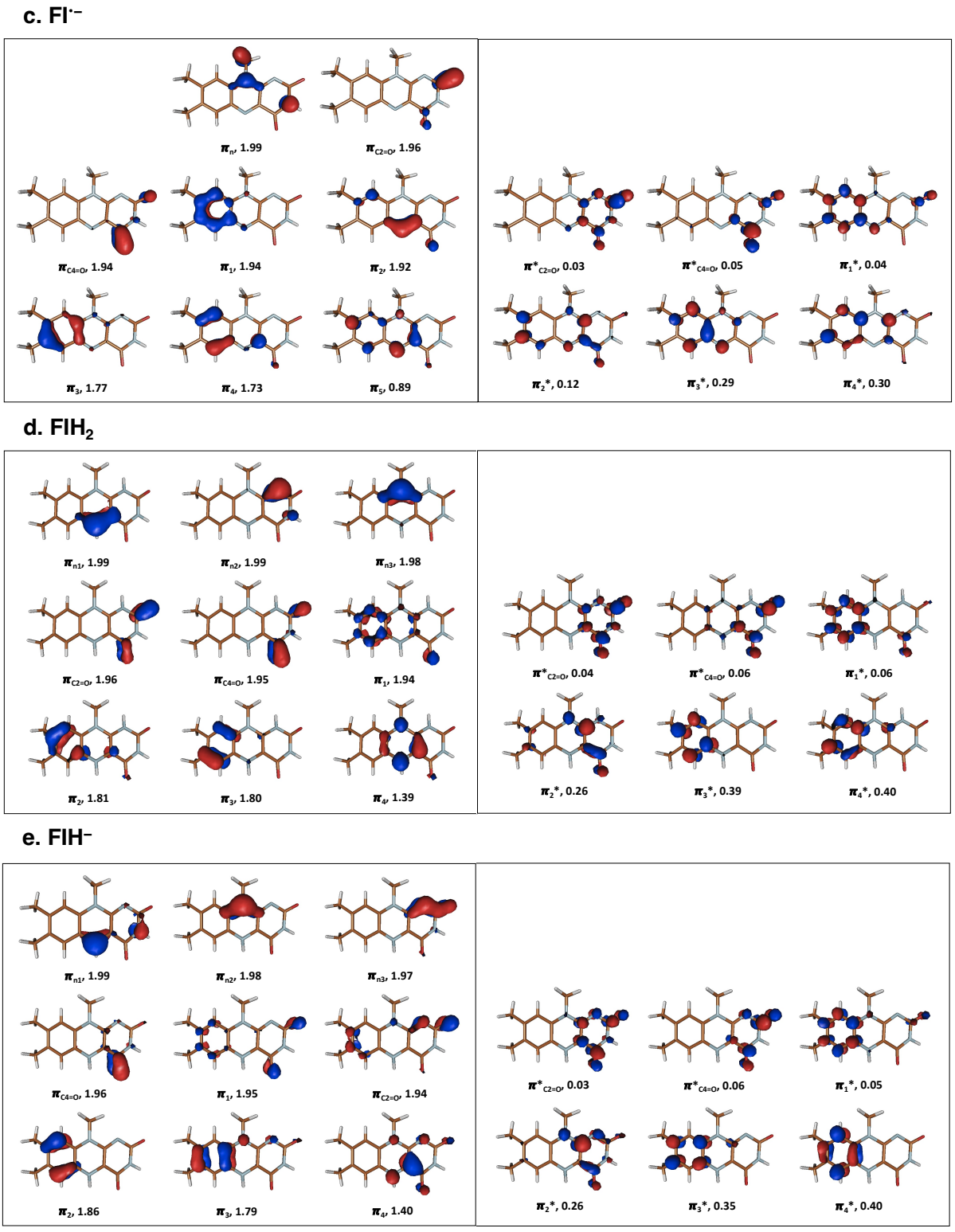


Figure S1. Occupied (left) and vacant (right) orbitals used as a starting point for the active space of flavin in each of five redox and protonation states. **a.** oxidized quinone (Fl), **b.** neutral semiquinone radical (FlH•), **c.** anionic semiquinone radical ($Fl^{\bullet -}$), **d.** neutral hydroquinone (FlH_2), and **e.** anionic hydroquinone (FlH^-).

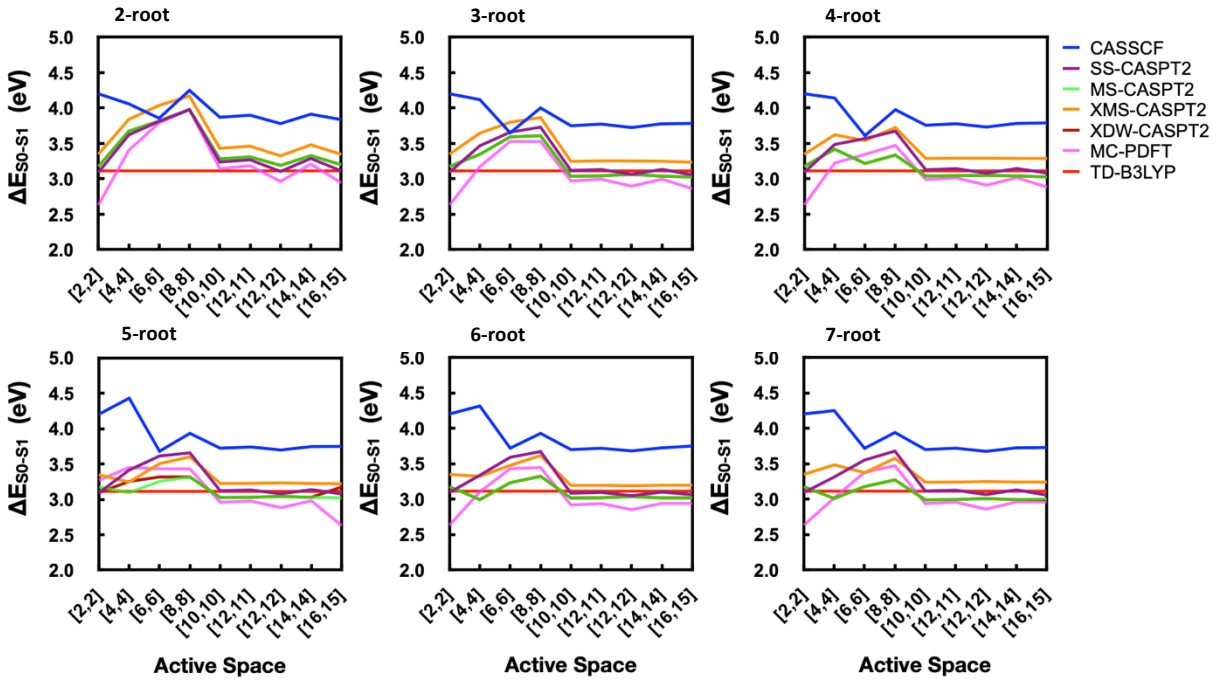


Figure S2. MR-PT2 and CASSCF S_1 excitation energies as a function of active space [number of electrons, number of orbitals] with 2-root averaging, 3-root state averaging, 4-root state averaging, 5-root state averaging, 6-root state averaging, and 7-root state averaging for LF in the oxidized form. The TD-B3LYP excitation energy is shown as a red line for reference.