ELECTRONIC SUPPLEMENTARY INFORMATION

Effect of dynamical fluctuations of hydration structures on the absorption spectra of oxyluciferin anions in aqueous solution

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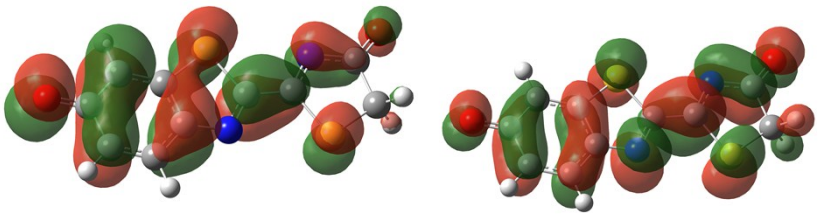
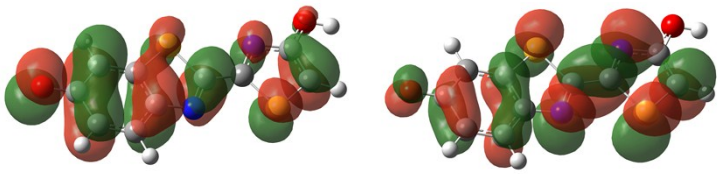


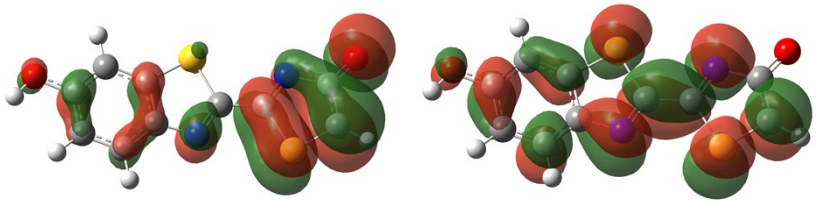
HOMO (64) LUMO (65)

Fig.S1: molecular orbital for phenolate-keto



HOMO(64) LUMO(65)

Fig. S2: molecular orbital for phenolate-enol



HOMO (64) LUMO (65)

Fig.S3 molecular orbital for enolate

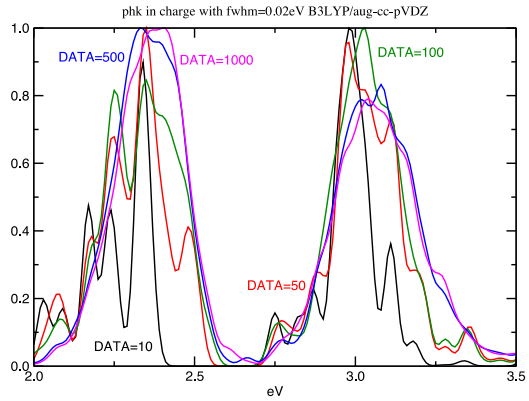


Fig.S4: tQM/MM absorption spectra for phenolate-keto with B3LYP/aug-cc-pVDZ and artificial line width 0.02 eV using 10, 50, 100, 500, and 1000 snapshot from FPMD calculations.

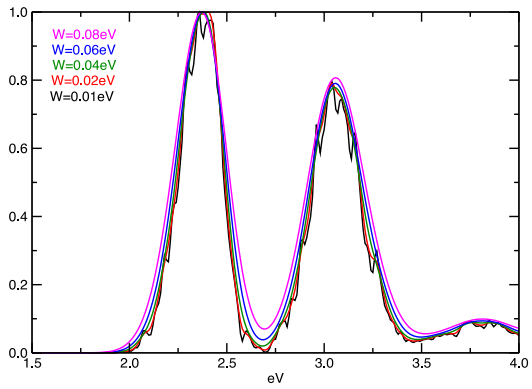


Fig.S5: tQM/MM absorption spectra for phenolate-keto with B3LYP/aug-cc-pVDZ and 1000 FPMD snapshots using the artificial line width: 0.01, 0.02, 0.04, 0.06, and 0.08 eV.

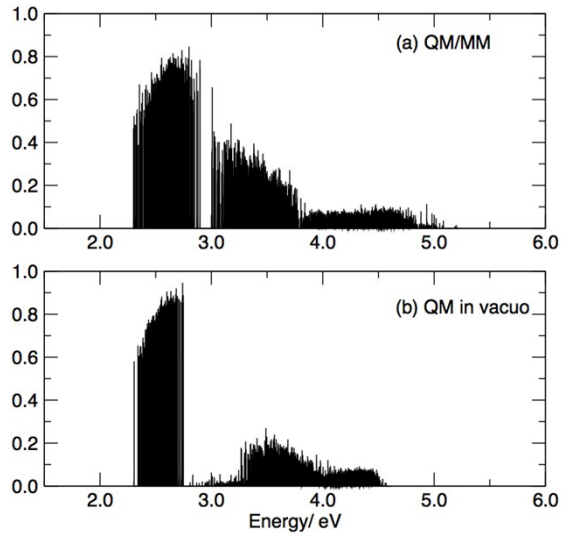


Fig.S6 : Excitation energies and oscillator strength between 1.0 and 5.0 eV using TDDFT cam-B3LYP/aug-cc-pVTZ for phenolate-keto. (a) QM/MM (b) QM in vacuo

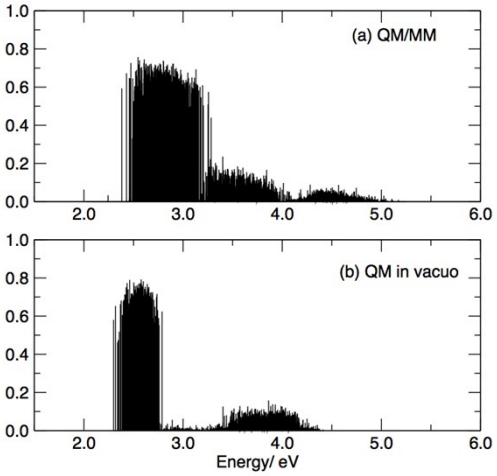


Fig.S7 : Excitation energies and oscillator strength between 1.0 and 5.0 eV using TDDFT cam-B3LYP/aug-cc-pVTZ for phenolate-enol. (a) QM/MM (b) QM in vacuo

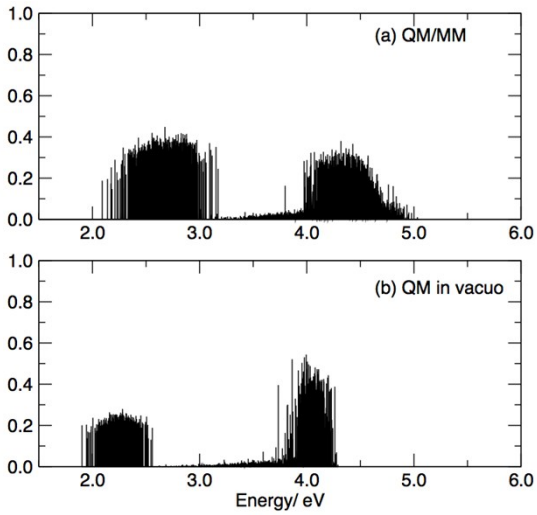


Fig.S8 : Excitation energies and oscillator strength between 1.0 and 5.0 eV using TDDFT cam-B3LYP/aug-cc-pVTZ for enolate. (a) QM/MM (b) QM in vacuo

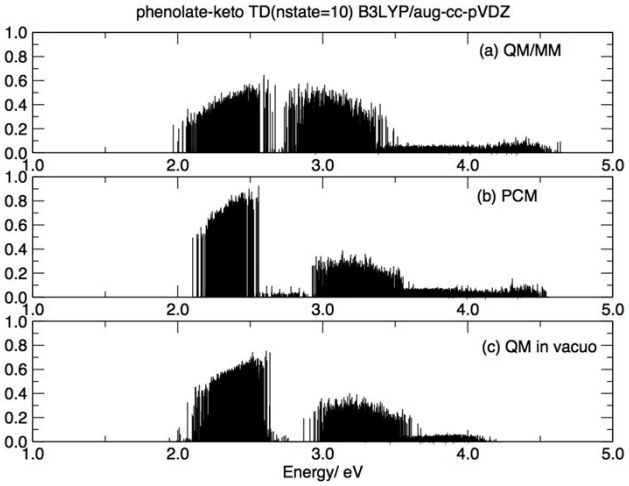


Fig.S9: Excitation energies and oscillator strength between 1.0 and 5.0 eV using TDDFT/B3LYP/aug-cc-pVDZ for phenolate-keto.

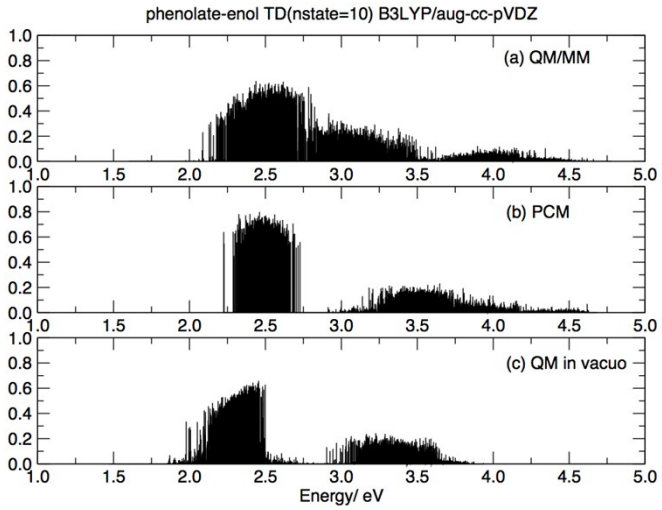


Fig.S10: Excitation energies and oscillator strength between 1.0 and 5.0 eV using TDDFT/B3LYP/aug-cc-pVDZ for phenolate-enol,

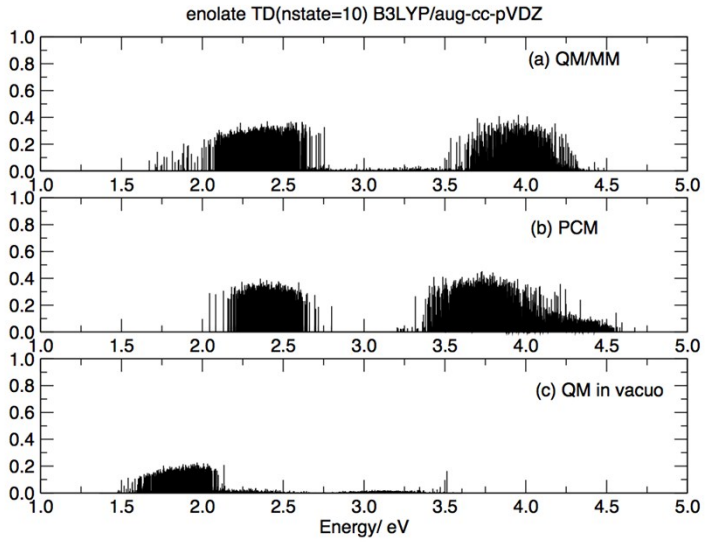


Fig.S11: Excitation energies and oscillator strength between 1.0 and 5.0 eV using TDDFT/B3LYP/aug-cc-pVDZ for enolate.