Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information for

Effects of hydrogen bonding interactions on the redox potential and molecular vibrations of plastoquinone as studied by density functional theory calculations

Ryota Ashizawa and Takumi Noguchi*
Division of Material Science, Graduate School of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8602, Japan.

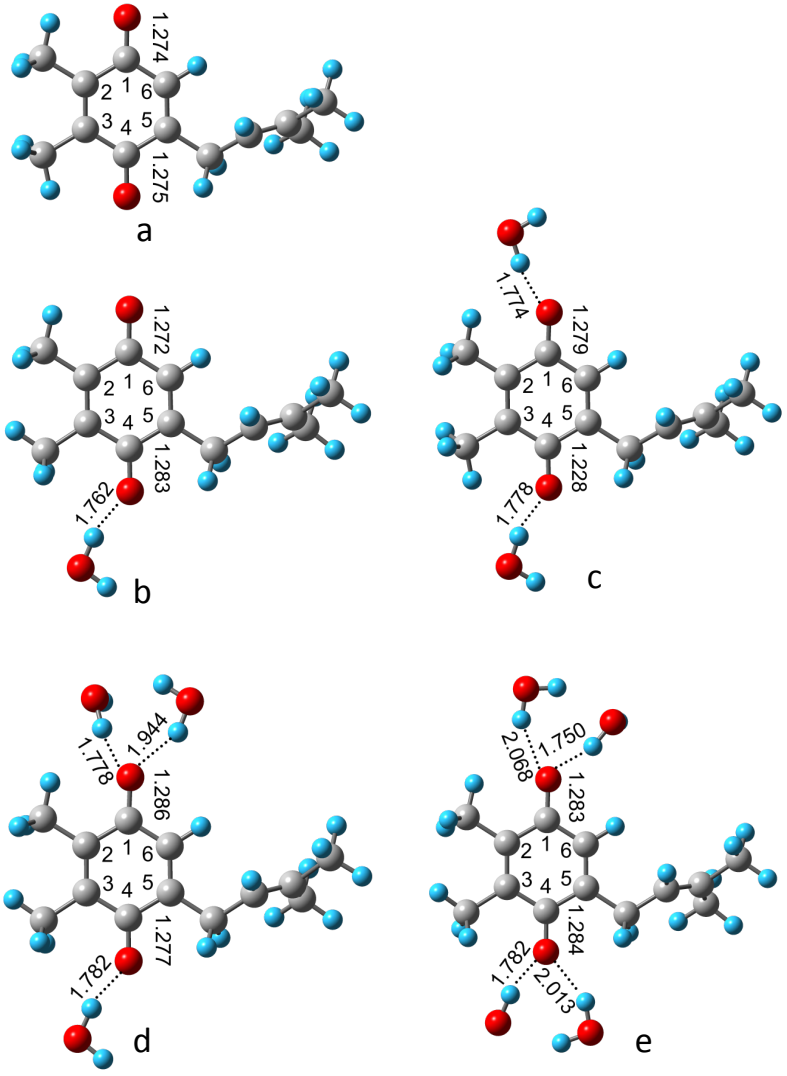

Fig. S1 Optimized geometries of PQ model and its H-bonded complexes with water molecules in the semiquinone anion forms. (a) PQ: free plastoquinone-1, (b) PQ-1H: PQ with one H-bond at C(4)=O, (c) PQ-2H: PQ with two H-bonds (one H-bond at each C=O), (d) PQ-3H: PQ with three H-bonds (two H-bonds at C(1)=O and one H-bond at C(4)=O), and (e) PQ-4H: PQ with four H-bonds (two H-bonds at each C=O). Carbon, oxygen and hydrogen atoms are expressed as gray, red, and cyan balls, respectively.

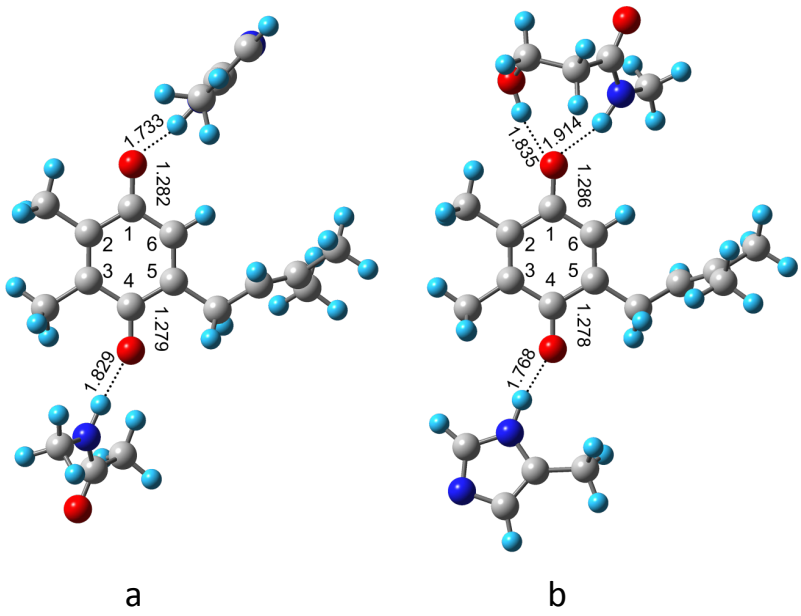

Fig. S2 Optimized geometries of the semiquinone anion forms of PQ complexes H-bonded with amino acids models mimicking the Q_A (a: QA model) and Q_B (b: QB model) interactions in PSII. Carbon, oxygen, nitrogen, and hydrogen atoms are expressed in gray, red, blue, and cyan balls, respectively.