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Computational Calculation of Midpoint Potential of Quinones in the A1 Binding Site of the Photosystem I

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Quinones are oxidants; colorants; electrophiles and involved in the electron transfer process of important biological functions such as photosynthesis, respiration, phosphorylation etc. In earth, photosynthesis is the main biological process which converts solar energy into chemical energy. By producing oxygen and assimilating carbon dioxide, it supports the existence of virtually all higher life forms. It is driven by two protein complexes namely photosystem I and II (PSI and PSII). In PS I, light induces the transfer of electron from P700, a pair of chlorophyll a molecules via a series of protein bound pigment acceptors (A0, A1, FeS) to ferredoxin. In PSI, phylloquinone (PhQ, 2-methyl-3-phytyl-1,4-naphthoquinone) act as a secondary acceptor termed as A1. In menB, a mutant of PS I, a gene that codes for a protein involved in PhQ biosynthesis has been deleted, plastoquinone (PQ9, 2,3-dimethyl-5-prenyl-1,4-naphthoquinone) occupies instead. Recent literature reveals that the PQ9 is weakly bounded in the A1 binding site of menB and can be easily replaced by different quinones both invitro and invivo. The efficiency of light induced electron transfer of quinone is related to the mid potential (E_m) of the quinone in the A1 binding site. For native PSI, the estimated E_m of PhQ is -682 mV. The estimated E_m value of PQ9 in menB is -754 mV, and for the incorporated quinone, 2-methyl-1,4-naphthoquinone, it has been reported to be -718 mV. Interestingly in the case of 2,3-dichloro-1,4-naphthoquinone (DCNQ) incorporated menB, there is no forward electron transfer observed. So far this was the highest positive redox potential quinone incorporated into the A1 site in menB PSI. By keeping this reported E_m values and electron transfer directionality in mind, we intent to find the E_m of the substituted 1,4-naphthoquinones that can be incorporated into A1 binding site. Computation calculations were performed at the B3LYP aug cc-pVTZ level of theory using Gaussian 09 software in linux platform. High performance computer network namely VELA (512 GB RAM per node, 40 core per node, with Turbo-Boost up to 2.4 GHz) in Georgia State University, Atlanta is used through the remote operating system from Qatar University. First the electron affinity (EA) of substituted 1,4-naphthoquinones (NQs) were calculated. From the calculated EA of NQs, we have been able

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to calculate the redox potential of NQs in a solvent and their E_m in the A1 binding site. In order to understand the electronic and structural effects, electron releasing (CH_3 , OCH_3) and withdrawing (Cl, Br) substituted NQs were used in this calculations. Results show that out of seven NQs used, 2-methoxy-1,4-naphthoquinone has the highest negative E_m of -850 mV and the DCNQ has the highest positive E_m of -530 mV in the A1 binding site. Our calculated E_m of DCNQ is in line with the blocking of forward electron transfer reported previously. Our E_m values can be used to explain the directionality of electron transfer reactions past A1 and predict the forward electron transfer kinetics when these NQs are incorporated into the A1 binding site experimentally.