New results from electron paramagnetic resonance showed that the orientations of the PhQ radicals are different which affect the strength of hydrogen bonding between PhQ and the protein backbone. We are investigating these different rates of electron transfer and orientation of PhQ radicals through molecular dynamics simulation and time dependent density functional theory (TD-DFT) methods.

3358-Pos Board B513

A Novel Spectral Marker for Fe-Starvation in Cyanobacteria and its Association with IsiA in the Process of Light-Harvesting

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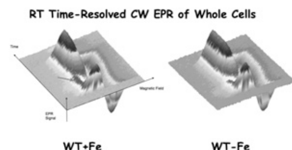
Iron-limiting growth conditions were established for Synechococcus sp. PCC 7002. Time-resolved optical spectroscopy of Fe-starved cells revealed a light-induced 520 nm spectral signal that may represent the electrochromic bandshift of carotenoids. The isiA and isiB were inactivated, respectively. Only the isiA mutant showed differences in growth rate and pigment content relative to the wild type grown in Fe-depleted medium. Further, the signal did not appear in Fe-starved isiA mutant. We conclude the signal serves as a marker for Fe-starvation and is associated with the IsiA protein. Under iron-limitation, IsiA associates with PS I, forms the PS I-IsiA supercomplex and increases the overall light-harvesting efficiency. We propose the spectral signal observed actually arises from the β–carotene near the quinones in PS I when the electron acceptors are transiently reduced by high light intensity. Under the intensity regime employed, the PS I-IsiA supercomplex in Fe-starved cells processes more energy per unit time than the PS I in Fe-replete cells, and thus backs up electrons to quinones more prominently. Time-resolved optical and EPR spectroscopies further demonstrated the carotenoid electrochromic bandshift signal and the semi-quinone signal.



3359-Pos Board B514

Characterization of 2D PSII Crystalline Arrays in Thylakoid Membranes Highly Efficient in Photo-Protective Energy Dissipation by Atomic Force Microscopy

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Non-photochemical quenching (NPQ) is an important mechanism by which photosynthetic organisms balance the light energy necessary for carbon fixation while preventing photo-damage. NPQ requires elaborate dynamic reorganization of the photosystem II (PSII) supercomplex and its closely associated light-harvesting complex II (LHCII). Currently, structural details directly related to NPQ and PSII-LHCII arrangements are scarce and in debate. The suppressor-of-quenching protein SOQ1 has recently been shown to prevent the formation of a slowly relaxing quenching pathway when chloroplasts are exposed to high light. We have used atomic force microscopy (AFM) to characterize the PSII organization in grana thylakoid membranes isolated from Arabidopsis thaliana wild type (wt) and soq1 mutant plants acclimated to different illumination conditions. To analyze the AFM data, we developed sensitive algorithms that automatically detect and discriminate between different types of crystalline packing observed in the membranes. We find that PSII density, extent of PSII array formation, and crystalline packing type depend strongly on illumination and mutant status. Surprisingly, pair correlation function and nearest-neighbor distribution analyses indicate that high-light-acclimated crystalline arrays from wt membranes are similar to those found in low-light-acclimated membranes from soq1 membranes. These different PSII arrangements can be correlated with the high levels of NPQ characteristic of the mutation. A potentially new type of 2D crystalline packing present in the low-light-acclimated soq1 membranes could be associated with slow relaxation of NPQ.

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Protection of Chloroplast *In Vivo* against Oxidative Stress

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For increasing of condition due to that chloroplast in native tissue will be riched by highly reactive oxygen species (ROS) leaves of cucumber and pumpkin plants were spraying with paraquat (methyl-viologen: 1.1’-dimethyl 4.4’-bipyridinium) (MV, 100μM). The states of donor and acceptor sides of Photosystem II (PS II) on the base of different characteristics of the millisecond delayed fluorescence of chlorophyll a (ms-DF) in leaves were analyzed. At the treatment by MV the sharp decay of characteristic value of ms-DF of reaction center of PS II by 80-90%, value of ms-DF, charactering of state donor side of PS II and oxygen-evolving Mn_4O_5Ca-cluster and Y_z by 65-70% was revealed. The changes of different phases of kinetic induction curve of ms-DF indicate that products, possibly ROS, formed in the photosynthetic units surrounding of PS I might bring to damage of PS II. Well known an antioxidant-sodium ascorbate has restored damages appearing under action of MV, possibly by quenching of O_2^- and *OH. Spraying of leaves by paraquat together with Plumbagin - (50mg/l 2 methyl-5hydroxy-1,4-naftoquinone) from (Ceratostigma plumbaginoides) plant roots has restored fast phase of ms-DF induction curve almost to the control value and slow phase representing donor side of PS II more than in three times. At the same time steady state level of fluorescence has increased by 50-75% too. The suggestion is made that plumbagin plays a decisive role in the protection of chloroplasts oxygen-evolving complex possibly on the stage of water oxidation against photooxidative stress by quenching of O_2^- and *OH, being generated under action of paraquat.

3361-Pos Board B516

C-Terminal M4 Peptide Fragment of Albino 3 Interaction with cpSRP-43

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The protein complexes responsible for insertion of light harvesting chlorophyll binding protein into the thylakoid membrane of the chloroplast are the concern of this investigation. Critical for this insertion, the membrane bound protein Albino 3 has been shown to bind a cpSRP-FTSY-LHCP complex. The following study implicates the stromal, c-terminus of Albino 3 as an imperative binding interaction in this process. Isothermal titration calorimetry and 1H-15N HSQC were used to understand the binding of a 16 residue segment from this region of Albino 3 known as M4. The data show that this segment binds with 14uM affinity and that electrostatic interactions with E327 and E356 on the 43kDa subunit of cpSRP are essential for this event. Importantly, significant binding is not observed when two domains of cpSRP-43, CD2 and CD3, are separated. Far UV and intrinsic fluorescence experiments also show that, upon M4 binding, moderate conformational changes in CD2-CD3 occur.

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Theoretical Studies on Excited States of Bacteriochlorophyll *A* in Solutions

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Chlorophylls and bacteriochlorophylls play important roles in photosynthesis, and thus the excited-state properties of chlorophylls and bacteriochlorophylls in solutions and proteins have been studied for a long time both experimentally and theoretically. It is experimentally known that the S_0-S_1 absorption energy of bacteriochlorophyll *a* (BChl *a*) in solution is quite insensitive to solvent, though the BChl *a* has polar functional groups. We investigate the excited-state properties of BChl *a* in several solutions by using QM/MM-RWFE-SCF method (*J. Chem. Theory Comput.* 8 (2012), pp 322-334), in which the geometry of a quantum mechanically treated molecule (BChl *a*, in this case) can be optimized effectively on a free energy surface defined with thermal distribution of the surrounding molecular environment (solvent) obtained by molecular dynamics simulation with a molecular mechanics force field. We employ TDDFT method for the excited-state electronic structure calculation, and find that excited-state properties of BChl *a* strongly depend on the density functional. We can reproduce the solvent insensitivity by adjusting the parameter of the density functional, and find that the solvent insensitivity results from the counterbalance between the redshift due to hydrogen bond interaction and the blueshift due to decrease in dipole moment. It is expected that the density functional with the adjusted parameter can be applied to BChl *a* in proteins.