The Photosystem II Subunit S Dynamics under stress

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The increased spectral range absorption of light exerted by pigments within Light Harvesting Complexes (LHCs) proves an important advantage under low light conditions, in higher plants. However, in the exposure to excess light, oxidative damages and ultimately cell death can occur. It proved, thus, utmost important for the photosynthetic organisms to develop a down-regulatory mechanism called Non-Photochemical Quenching (NPQ). Quantifying this mechanism at the atomic level is still very uncertain. There are several components of the photosynthetic apparatus that are actively involved in NPQ. Apart from the LHCs, and the xanthophyll cycle, the Photosystem II Subunit S (PsbS) is a 22-kDa integral membrane protein that is essential for the response of the photosynthetic apparatus to high-light and it is activated by the protonation of key lumen-exposed glutamate residues. Atomistic details on its involvement in NPQ remain still a mystery. However, It is widely accepted that NPQ (qE) is co-regulated by low lumen pH and ion fluxes (K^+, Ca^{2+}, Mg^{2+}, Cl^-) in Lumen-Stroma areas. It has also been proposed that the activated PsbS may strongly interact with some LHCs enabling quenching by providing an alternative environment for some pigments within these LHCs, or by changing the membrane organization and dynamics. In this study, PsbS (pdb code 4ri2) is embedded in a lipid bilayer model membrane (400-500 POPC lipids, 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine). NPQ conditions are simulated by perturbations in the thylakoid lumen ionic load. Zeaxanthin (Zea) of the xanthophyll cycle that is produced under NPQ is also embedded in the membrane. We employ large-scale Molecular Dynamics simulations to probe the PsbS conformational changes, membrane dynamics, or Zea binding that activate PsbS. We identify two distinct PsbS forms (active-inactive), in response to A) the lumen acidification or ion fluxes, and B) the Zea binding, revealing a PsbS-NPQ relation at the atomic scale.