Available online at www.scholarsresearchlibrary.com

Extended Abstract

Journal of Computational Methods in Molecular Design, 2019, 9(4)
https://www.scholarsresearchlibrary.com/journals/journal-of-computational-methods-in-molecular-design/

ISSN 2231-3176

Study of extrinsic Psb proteins of photosystem II by solution nuclear magnetic resonance

Adriana Rathner

Johannes Kepler Universität Linz

E-mail: adriana.rathner@jku.at

Nuclear magnetic resonance (NMR) is a powerful technique which enables characterization of various biomolecules in solution. This way one is in a position to tune extra precisely the dynamic homes and modifications in the structure over time and various prerequisites (temperature, salt concentration, ligand addition, and pH). Psb proteins of photosystem II are a classification of extrinsic proteins positioned on the cytosolic part of the oxygen evolving center. They assist to keep desirable stipulations for the water splitting response subsequently leading to the release of molecular oxygen. We have studied so far three representatives: PsbP (23 kDa), PsbQ (16 kDa) and PsbO (33 kDa). Using NMR we have been able to determine 3D structures of PsbP and PsbQ in answer including their highly flexible areas whose characterization was hindered with the use of other methods (X-ray and Cryo-electron microscopy). The most interesting information about detailed interplay of these proteins and its dependence on the presence of steel cations has been studied using aggregate of techniques, such as titration and chemical change NMR method (CEST), isothermal titration calorimetry (ITC) and microscale thermophoresis (MST).PsbP (23 kDa) is an extrinsic eukaryotic protein of photosystem II determined in the thylakoid membrane of greater flowers and inexperienced algae. It has been validated to be critical for suited functioning of the oxygen evolving complex. By interaction with other extrinsic proteins (PsbQ, PsbO and PsbR), it modulates the concentration of two cofactors of the water splitting reaction, Ca2+ and Cl−. The crystallographic structure of PsbP from Spinacia oleracea lacks the N-terminal section as properly as two inner regions which had been modelled as loops. Those unresolved parts are believed to be functionally imperative for the binding of PsbP to the thylakoid membrane. In this NMR study we document 1H, 15N and 13C resonance assignments of the spine and facet chain atoms of the PsbP protein. Based on these data, an estimate of the secondary shape has been made. The structural motifs determined in shape the resolved parts of the crystallographic structure very well. In addition, the entire challenge set gives preliminary insight into the dynamic regions. Photosystem II is a multi-protein, -lipid, and -pigment complex, which spans the thylakoid membrane of all photosynthetic organisms. Its protein fraction consists of two major parts, an intrinsic cluster of proteins and a set of extrinsic, “accessory”, proteins. While the intrinsic proteins are distinctly conserved amongst the photosynthetic species, the extrinsic proteins have evolved, possibly from their homologous cyanobacterial precursors, as adaptations to the distinct photosynthetic equipment in eukaryotes as in contrast to prokaryotes. The PsbP protein is placed on the lumenal facet of thylakoids, in the oxygen evolving complicated (OEC) of photosystem II, which is the site of the water-splitting response yielding molecular oxygen. PsbP is section of a barrier of extrinsic proteins, which encompass the reaction centre with the Mn4CaO5 cluster at the lumenal thylakoid surface. In whole four extrinsic proteins have been found in most higher plants: PsbO (30 kDa), PsbP (23 kDa), PsbQ (16.5 kDa) and PsbR (10 kDa). The biggest of these, PsbO, is conserved throughout the all photosynthetic phyla, in contrast to the ultimate three extrinsic proteins. The genuine binding topology and interactions of these proteins nonetheless remain unclear, however recently more experimental records have yielded a clearer picture of the assembly of the complete OEC. One recognized characteristic of PsbP is controlling the concentrations of two co-factors of water oxidation—Ca2+ and Cl−. Binding of PsbP to the thylakoid membrane induces structural changes, which are indispensable for steady oxygen manufacturing in the course of photosynthesis. The N-terminal section of PsbP is crucial for this conformational change to occur. When the PsbP protein is disadvantaged of the 15 amino acids at the N-terminus, it is no longer capable of altering the topology of the membrane and the oxygen production decreases dramatically. In this case, it has been shown that PsbQ can compensate such a defect in the PsbP protein and helps to restoration the stages of oxygen being released. Preliminary studies in our crew have furnished the first answer structure of PsbQ. Horničáková et al. Rathner. The three dimensional structure of PsbP from Spinacia oleracea has been resolved recently by X-ray crystallography at high resolution (1.98 Å). The resolved part of the structure compares very well with an earlier structure of PsbP from Nicotiana tabacum. The electron density was not resolved in the N-terminal residues and in two internal sections, although the crystal did not contain any degradation products. Additional data from Raman spectroscopy and molecular dynamics simulation suggested a dynamic nature for these regions. The N-terminus was modeled to contain a β-sheet element and the two unresolved internal regions to form two loops. Intrinsic disorder of the N-terminal part would be in accordance with its suggested function.

Bottom Note: *This work is partly presented at 10th Edition of International Conference on Structural Biology* March 15-16, 2018 Barcelona, Spain