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Refined structural model of photosystem II from *Thermosynechococcus elongatus*, structural changes in reaction centre.

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Crystal and NMR structures are essential and fundamental in performing almost all molecular modelling techniques. Three dimensions resolution of such structures is certainly one of the most crucial criteria of quality and credibility. Researchers made great effort to prepare crystals of photosystem II (PS II) from algae and higher plants in the last decades. However, till now there are only two experimental crystal structures resolved at adequate resolution. Both are from the same common organism *Thermosynechococcus elongatus*. First was obtained at 3.5 Å (PDB code: 1S5L) [1] and second at 3.2 Å (PDB code: 1W5C) [2] overall resolution. By performing series of molecular dynamics (MD) simulations at appropriate time scales also coupled partially with quantum-chemical calculations, it is possible to increase the model accuracy mainly in the regions, where the probability of spatial orientation of amino acid side chain lacks appropriate electron density or other sources of experimental data. We present here more natural-like, geometrically - optimised structures of extended reaction centre (RC) of PS II.
Recently, changes in excitonic interactions of PS II RC pigments upon light-induced oxidation of primary donor (P680) or reduction of primary acceptor pheophytin *a* (Phe *a*), were analysed using absorption and circular dichroism (CD) spectra [3, 4]. In contrast to the oxidation of primary donor, the light-induced change in the CD spectrum upon primary acceptor reduction was temperature-dependent. This suggests a hypothesis that at a room temperature the reduced Phe *a* induces conformational changes of the RC protein environment, which affects the excitonic interaction of the RC chlorophylls. Having optimised structural models of PS II RC we were able to elucidate and describe some of the details of these processes.

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Iron transport and signal transduction in *Pseudomonas aeruginosa*: crystal structures of the TonB-dependent outer membrane receptors FpvA and FptA.

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The pyoverdine and pyochelin outer membrane receptors, FpvA and FptA respectively, of *Pseudomonas aeruginosa* translocate the ferric-pyoverdine and the ferric-pyochelin across the outer membrane using an energy consuming mechanism involving the proton motive force and the TonB-ExbB-ExbD energy transducing complex from the inner membrane. We solved the crystal structure of FpvA bound to iron-pyoverdine (FpvA-Pvd-Fe) at 2.7 Å resolution and the structure of FptA bound to the iron-pyochelin at 2.0 Å resolution [1]. The FpvA-Pvd-Fe overall structure is composed of 3 domains: a periplasmic signalling domain showing a new fold, a transmembrane 22-β stranded barrel occluded by a domain called the plug domain which contains a mixed 4 stranded β-sheet. FtpA is only composed of the two last domains. The FpvA periplasmic domain involved in the signal transduction to the anti-sigma factor protein FpvR of the inner membrane (and to TonB-ExbB-ExbD) displays a new (β-α-β) fold composed of 2 β-helices sandwiched by 2 β-sheets. One iron-pyoverdine conformer is bound at the extracellular face of FpvA revealing the conformer selectivity of the binding site mainly composed of aromatic residues. The Pch-Fe binding site is mainly composed of hydrophobic residues. The FpvA and FptA extracellular loops do not completely cover the Pvd-Fe and Pch-Fe binding sites. The sequence containing the TonB box involved in interactions with TonB and connecting the signalling domain to the plug domain of FpvA is not defined in the electron density upon Pvd-Fe binding. Similar observation is done for the FptA TonB box. Its high flexibility is probably necessary for signalling through the outer membrane. A comparison of the FpvA-Pvd-Fe structure with that of FpvA-Pvd [2] which is not competent for transport will be also discussed.

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