Molecular Simulation of Photosystem II and Phycobilisome Interactions in Cyanobacteria

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Phycobilisomes (PBS) are the major light harvesting antenna complexes in cyanobacteria and red algae. PBS absorb and transfer light energy to photosynthetic reaction centers, through pigment molecules known as phycocyanobilins. The transfer of energy between PBS and the photosynthetic reaction center, photosystem II (PSII) results in the production of the oxygen we breathe on Earth. Though the relationship between PBS and PSII is well-documented and atomic resolution structures exist for both, little is known about the interactions and energy transfer pathways between the two photosynthetic components. Leveraging existing structural data, we are changing this narrative and exploring the dynamics of a PBS-PSII complex through molecular dynamics simulations. Aligning resolved Synechocystis sp. PCC 6803 PBS and PSII structures from Cryo-EM and utilizing AlphaFold2, we have constructed a 3 million atom system with both photosynthetic components present. Through ~600ns of molecular dynamics simulations with 10 replicas, we observe significant structural changes within the ApcG and rod-core linker proteins. Hydrogen bonding to form the PBS-PSII complex increase over the course of the molecular dynamics simulations, primarily from the ApcE and ApcG residue pair interactions with PsbB and PsbC, respectively. We have also calculated approach distances between phycocyanobilins, chlorophylls, pheophytins, and quinones to predict the impact of thermal motion on excitation energy transfer. Through network analysis of these distances, we identified one key phycocyanobilin with a minimum distance of ~35Å to the closest chlorophyll, the only phycocyanobilin connecting the network of cofactors in the PBS-PSII complex. This minimum distance of ~35Å appears to be comparable to distances found in recent structures, though how efficient this is for energy transfer remains to be seen. This is one of the first looks at the PBS-PSII interface, and we have been able to predict possible interactions within this complex.