UNREVELAING PHOTOPROTECTION MECHANIESMS IN THE FENNA-MATTHEWS-OLSON (FMO) LIGHT-HARVESTING COMPLEX

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Photoprotection is a critical biochemical process that helps organisms to survive cellular damage caused by excessive sunlight. Under sunlight excitation bacteriochlorophyll molecules can undergo intersystem crossing to long living triplet state. In aerobic conditions, the triplet-state (bacterio)chlorophylls can transfer energy to molecular oxygen. This spin-allowed process generates highly reactive singlet oxygen that irreversibly reacts with nearby organic molecules, eventually leading to oxidative stress and damage to living cells.

Many photosynthetic proteins mitigate the damaging effect of excess solar radiation by incorporating carotenoid molecules whose low-lying triplet states become a sink for the excitation energy from which it safely dissipates into heat.

The Fenna-Matthews-Olson (FMO) pigment protein is essential in transferring excitation energy from the chlorosome antenna to the reaction center in green sulfur bacteria. Surprisingly, FMO complex doesn't contain any carotenoids, yet it's found to be exceptionally stable in aerobic conditions. Therefore, our goal is to understand the photoprotection mechanisms of this photosynthetic complex. Implications of this project are a rational design of bio-inspired light-harvesting antennas and the redesign of natural photosynthetic systems, opening new possibilities for regulating these systems in response to excess light.

We explore three possible mechanisms contributing to the photoprotection of FMO. One possibility is a physical barrier photoprotection mechanism that in which the protein backbone acts as a shield to prevent molecular oxygen from reaching BChl sites. To this end, we investigated the distribution of molecular oxygen in molecular dynamics trajectories and computed the binding free energy between O2 and BChls. Furthermore, we studied the energy transfer mechanism between the triplet BChl and O_2 utilizing quantum mechanical calculations, because the fast energy transfer depends on factors such as strong coupling and energy matching between donor and acceptor. Finally, we are investigating whether the photoprotection chemistry in FMO can be attributed to a redox-dependent excitation quenching mechanism and whether specific key amino acids play a role in this redox chemistry.