Computational Mutagenesis: Investigating Single-point Mutation Effects on the Spectra of the Fenna-Matthews-Olson (FMO) complex.

Richmond Arhin[1], Sergei Savikhin[2] and Lyudmila Slipchenko[1]
[1]*Department of Chemistry, Purdue University. West Lafayette, Indiana 47907, USA.*
rarhin@purdue.edu.
[2]*Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA.*
sergei@purdue.edu.
[1]*Department of Chemistry, Purdue University. West Lafayette, Indiana 47907, USA.*
lslipche@purdue.edu.

Pigment-protein complexes involved in light harvesting, such as the Fenna-Matthews-Olson (FMO) protein complex, are renowned for their near-perfect quantum efficiency in capturing and transferring excitation energy to the reaction center (RC). This remarkable occurrence in nature has been investigated by many curiosity-driven researchers and found to result from the intrinsic electronic properties of the individual pigments and the couplings between these pigments. On the other hand, the intricate overlapping of electronic absorptions from numerous pigments that make up the structure of these photosynthetic complexes often leads to ambiguous experimental or spectroscopic assignments of the interactions between the pigments.

Mutagenesis has been widely used to explore intrinsic interactions in proteins and to resolve some of the ambiguities of spectroscopic measurements of wild-type systems. Specifically, in photosynthetic complexes, point mutations in the protein's secondary structures surrounding the pigments revealed significant impacts of the protein environment on the dynamics of the excitation energy transfer process. To gain a deeper understanding of the energy transfer in photosynthetic systems, we are developing theoretical methods that allow for accurate correlations between structure and spectroscopy in these complexes. For example, we have shown that combining classical molecular dynamics, the quantum mechanics/molecular mechanics (QMMM) and quantum mechanics/effective fragment potentials (QM/EFP) methods are highly efficient in predicting the absorption and circular dichroism spectra of the FMO complex and its mutants. In this study, our goal is to create a computationally efficient approach to predict how single-point mutations affect the optical spectroscopy of photosynthetic pigment complexes, using the FMO complex as a test case. This will help establish a workflow for the targeted design of mutations to achieve specific effects on selected protein-pigment components.

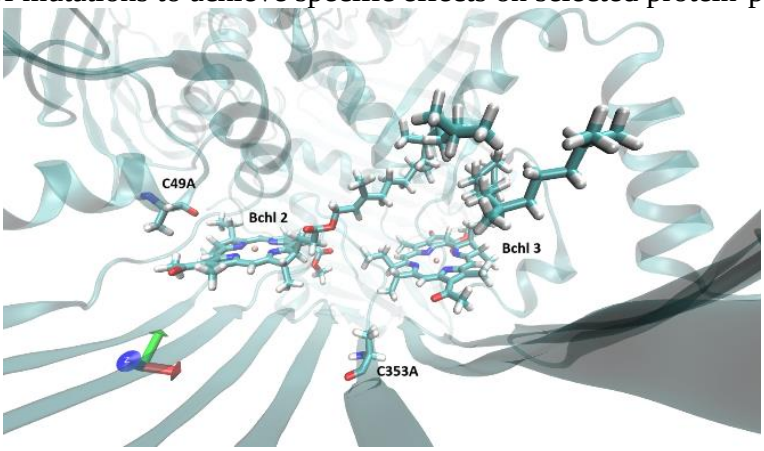

Figure. 01. A structure of the FMO mutant with PDB-ID, 5H8Z showing single point mutations of cysteine residues to alanine at bacteriochlorophyll sites 2 and 3.