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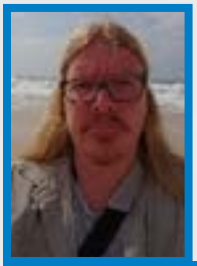

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Modelling/spectroscopy of pigment-protein complexes

Statement of the Problem: Photosynthesis is the most important biological energy conservation pathway on the Earth. Photosynthetic organisms make use of solar energy to create free chemical energy that is used in their metabolic reactions. For light energy to be store by photosynthesis, it must first be absorbed by pigment molecules associated with the photosynthetic apparatus. The light-harvesting (LH) antenna systems collect sunlight and transfer excitation energy rapidly to the photosynthetic reaction centres, where the energy is trapped in an electron-transfer reaction. To investigate these processes both experimental and theoretical methods are needed. There are available only a few experimentally solved atomic-resolution LH structures. Thus, different computational methods together with experimental structural and spectroscopic information are needed to generate three-dimensional pigment-protein LH antenna model structures. The purpose of this study is to generate atomistic model for the LH2 antenna complex of Thermochromatium tepidum and to explain origin of the extraordinary splitting of so called B800 absorption band of the complex.

Methods: Coming from the high protein sequence similarity between LH2 antennae of Thermochromatium tepidum and Phaesporillum molichianum (X-ray structure is known), homology modelling method was used to generate initial LH2 model. After that semi empirical quantum chemical method was used to optimize protein structure. And then density functional method was used to optimise local protein environment around the pigment molecules. At the end, absorption and circular dichroism spectra of the complex were calculated by using molecular exciton theory to verify quality of the model and to explain splitting of the B800 band.

Finding: Origin of the splitting is two different conformations of pigment molecule.

Conclusion & Significance: The study demonstrates that modern computational methods allow producing high quality pigment-protein model structures. Also, it indicates that photosynthetic organisms are able to fine tuning the light-harvesting spectrum by modifying local protein geometry/structure.

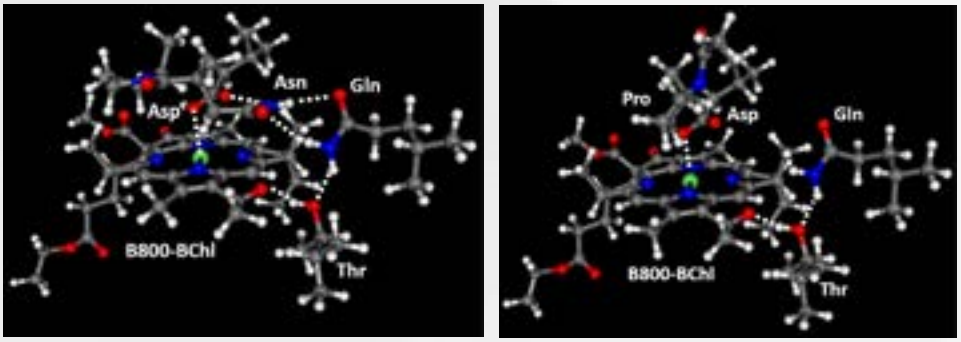

Figure: Two different B800-bacteriochlorophyll a conformers with local protein environments. Coordination bonds and hydrogen bonds are shown as dash lines.

Biography

Juha M. Linnanto is computational/theoretical chemist. His research interests cover various aspects of theory and modelling of electronic, optical, structural and transport properties of photosynthetic pigments, pigment-protein complexes, self-aggregates, dendrimers and metal-organic compounds. His computation competence includes classical molecular mechanic methods; molecular dynamic methods; semi-empirical quantum chemical methods; density functional methods; ab-initio methods; configuration interaction methods; time-dependent Hartree-Fock/density functional methods; and molecular exciton theory. Currently he is an associate professor (Laboratory of Biophysics) at the Institute of Physics of Tartu University.