Photosynthesis and electronic properties of Fenna-Mathhews-Olson light harvesting complexes

Badu, S., Melnik, R., and Prabhakar, S.

Proceedings and Extended Abstracts, IWBBIO 2016 International Work-Conference on Bioinformatics and Biomedical Engineering, ISBN: 978-84-16478-75-0, pp. 202-203, 2016.

Proceedings & EAs, IWWBIO 2016, ISBN: 978-84-16478-75-0

Photosynthesis and Electronic Properties of Fenna-Matthews-Olson Light Harvesting Complexes

Shyam R Badu [1], Roderick Melnik [1,2], and Sanjay Prabhakar [1]

[1]MS2Discovery Interdisciplinary Research Institute, M [2]NeT Laboratory,
Wilfrid Laurier University, Waterloo, ON, N2L 3C5 Canada; rmelnik@wlu.ca
[2] BCAM - Basque Center for Applied Mathematics, E48009 Bilbao, Basque Country - Spain

Photosynthesis is a key process used by plants and other organism to convert light energy from sun to the chemical energy which is then used to fuel the organism. The light harvesting pigment, chlorophyll, is the most abundant in the organism during the process of photosynthesis. It absorbs light from sun as well as converts it into the chemical energy, and the bacteriochlorophyll molecules play a vital role in this. Although they are known to be usually water insoluble, there exists a particular type of bacteriochlorophyll protein which is soluble in water. It is known as the Fenna-Matthews-Olson complex and it is found in the green sulfur bacteria. The particular structure of the Fenna-Matthew-Olson complex is shown in figure 1(a). The FMO protein complex contains seven bacteriochlorophyll (Bchl)a molecules wrapped in a string bag of protein. Many experimental and computational studies have been done on the structure of chlorophyll applying various techniques including solid state and liquid state NMR to understand its role in the photosynthesis [4, 2]

In order to understand the process of photosynthesis in detail, the study on the electronic structure and physical properties of the chlorophyll is essential. In view of this, we have studied energetic and the spectroscopic properties of the seven different types of the bacteriochlorophylls using density functional theory. The presence of the seven different bacteriochlorophylls is demonstrated in the model structure of the FMO complex and Chlorophyll in Figure 1.

Here we note that the chemical shift of a nucleus is defined by the relation [1]

$$\delta = \sigma_{iso} - \sigma, \tag{1}$$

where σ is the shielding tensor which describes the magnetic polarizability of a molecule of the nucleus under the study and the σ_{iso} is the isotropic value of the shielding tensor of the standard reference taken in the NMR experiment. Mathematically, the shielding tensor is defined by the relation

$$\sigma_{\alpha\beta} = \left(\frac{\partial^2 E}{\partial \mu_\alpha \partial_\beta} \right). \tag{2}$$

The calculation of spectra was done by using the functional PBE1PBE of Purdew-Burke-Edword with basis set 6-311G. The structures used in our studies have been taken from the protein data bank which was determined by the X-ray crystallographic method [3]. We have used the Gaussian broadening to calculate the NMR spectra. The geometries obtained from the structures have been optimized using density functional

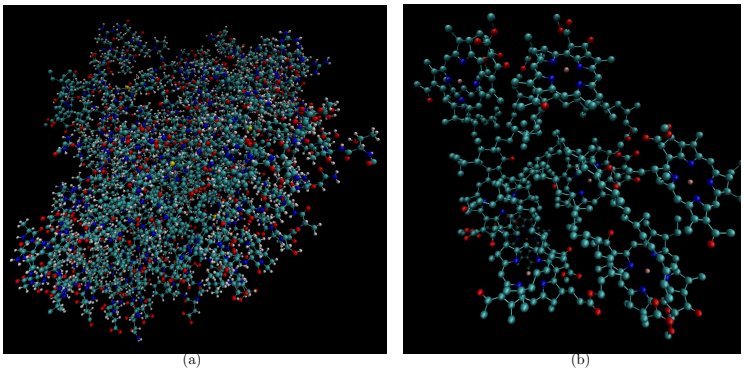

Fig. 1. VMD generated structure of the Fenna-Mathew-Olsen light harvesting complex (a) The whole structure and (b) The model structure for Chlorophyll

theory implemented by the Gaussian 09 set of programs. The chemical shift has been calculated by taking the difference in shielding tensors from the chemical shift of the carbon atom in TMS. Since the crystal structure of the FMO complex was from the X-ray spectra, the missing hydrogen atoms have been added to saturate the dangling bonds. Also, the separation of seven different chlorophylls has been done by using the computational visualization software VMD. In our calculation we have taken the tetra methyl saline (TMS) as a reference system. Furthermore, we also study the infrared spectrum for each of these components using density functional theory. We also determine the energy for all the bacteriochlorophylls present in the FMO complex. In order to address the nuclear properties of the complex and get a better insight into electronic properties, we have estimated the quadrupole coupling constant and the asymmetry parameters for the pyrrole nitrogen and the magnesium at the center of the porphyrin ring of Chlorophyll. The results obtained from our theoretical investigations have been compared to the experimental results available in the literature.

References

1. Facelli, J.C.: Chemical shift tensors: Theory and application to molecular structural problems. Prog Nucl Magn Reson Spectrosc **58**(3-4) (May 2011) 176–201 PMID: 21397119 PMCID: PMC3058154.
2. Taguchi, A.T., O'Malley, P.J., Wraight, C.A., Dikanov, S.A.: Nuclear Hyperfine and Quadrupole Tensor Characterization of the Nitrogen Hydrogen Bond Donors to the Semiquinone of the QB Site in Bacterial Reaction Centers: A Combined X- and S-Band 14,15n ESEEM and DFT Study. J. Phys. Chem. B **118**(6) (February 2014) 1501–1509
3. Tronrud, D.E., Wen, J., Gay, L., Blankenship, R.E.: The structural basis for the difference in absorbance spectra for the FMO antenna protein from various green sulfur bacteria. Photosynth Res **100**(2) (May 2009) 79–87
4. Xu, J., Terskikh, V.V., Huang, Y.: ^{25} mg solid-state NMR: a sensitive probe of adsorbing guest molecules on a metal center in Metal–Organic framework CPO-27-Mg. **4**(1) (January 2013) 7–11

IWBBIO 2016

INTERNATIONAL WORK-CONFERENCE ON BIOINFORMATICS AND BIOMEDICAL ENGINEERING

PROGRAM

20-22 April, 2016
Granada (SPAIN)

A novel divisive iK-means algorithm with region-driven feature selection as a tool for automated detection of tumour heterogeneity in MALDI IMS experiments
Grzegorz Mrukwa, Grzegorz Drazek, Monika Pietrowska, Piotr Widlak and Joanna Polanska

Multigene p-value integration based on SNPs investigation for seeking radiosensitivity signatures
Joanna Zyla, Christophe Badie, Ghazi Alsbeih and Joanna Polanska

Epithelial Mesenchymal Transition Regulatory Network-based Feature Selection in Lung Cancer Prognosis Prediction
Borong Shao and Tim Conrad

PLENARY LECTURE:
Prof. Ferran Sanz

Director, Research Programme on Biomedical Informatics (GRIB) Hospital del Mar Medical Research Institute (IMIM) Dept. of Health and Life Sciences, Universitat Pompeu Fabra

---

Session A.7: "High Performance Computing in Bioinformatics, Computational Biology and Computational Chemistry (Part I)"

Chairman: Dr. Horacio Pérez-Sánchez and Dr. Jose M. Cecilia

The Case for Docker in multicloud enabled bioinformatics applications
Ahmed Abdullah Ali, Mohamed El-Kalioby and Mohamed Abouelhoda

Flexible protein-peptide docking with knowledge about the binding site using CABS-dock
Mateusz Kurcinski, Maciej Pawel Ciemny, Maciej Blaszczyk, Andrzej Kolinski and Sebastian Kmiecik

Computational Modeling and interaction analysis of cannabinoid receptor interacting protein 1a (CRIP1a) with CB1 receptor
Pratishtha Singh, Allyn Howlett and Sudha Cowsik

Real Time GPU-based Segmentation and Tracking of the Left ventricle on 2D Echocardiography
Sidi Ahmed Mahmoudi, Mohammed Ammar, Guillaume Luque Joris and Amine Abbou

Photosynthesis and Electronic Properties of Fenna-Matthews-Olson Light Harvesting Complexes
Shyam Badu, Roderick Melnik and Sanjay Prabhakar

IWBBIO 2016

Organized and supported by