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Fundamental Molecular Complexes of Photosynthesis and Their Biomedical Applications

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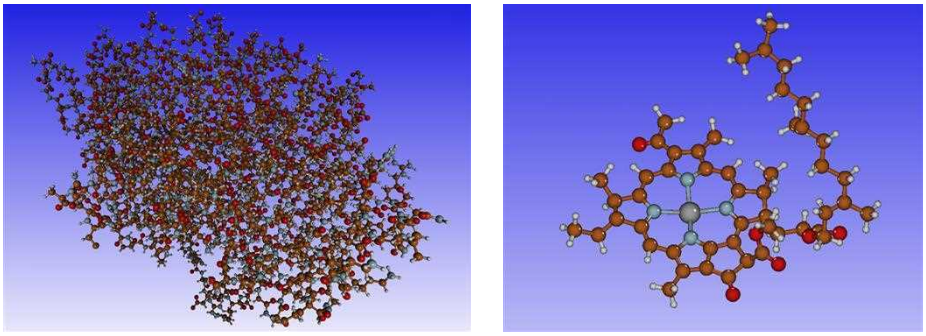
It has been known that photosynthetic bacteria provide an excellent source for producing vitamin B12 which has very important medical applications. Such applications include the treatment of anemia, neuritis, as well as eye problems, to name just a few. Other important applications of photosynthetic bacteria include the production of coenzyme Q10 which is used in the treatment of several kinds of heart disease, brain vascular injury, as well as the anemia. Furthermore, these bacteria can also be used to produce the porphyrin and ribonucleic acid (RNA) which have the potential application in the treatment of several diseases, as well as the deficiencies in the human body [1]. It is also important to note that the photosynthetic chloroplasts are being used for the production of bioactive compounds useful for a range of biomedical applications [1–3].

All these applications motivate us to study fundamental components of photosynthetic light harvesting complexes. While most of such complexes are water insoluble, there exists a particular type of bacteriochlorophyll protein that is soluble in water. This protein is in the focus of the current work, where we further study the properties of the Fenna-Matthews-Olson (FMO) complex, shown in Figure 1(a). The FMO protein complex contains bacteriochlorophyll (Bchl)a molecules wrapped in a string bag of protein. The bacteriochlorophylls contained in the FMO light harvesting complex are the most important components that play a vital role in the photosynthesis process, as well as in critically important biomedical applications mentioned above. Therefore it is imperative to have thorough understanding of the structure of these bacteriochlorophylls at the molecular level.

The bacteriochlorophylls available in the photosynthetic FMO complex consists of a porphyrin ring with the magnesium ion at its center and the magnesium ion is coordinated to four nitrogen atoms which are known as the pyrrole nitrogens. There is a long hydrocarbon chain connected to the porphyrin ring of the bacteriochlorophyll that is known as the phythyl chain. Our model structure for a single bacteriochlorophyll is given in Figure 1(b). Our focus here is on the NMR spectra for a bactriochlorophyll monomer taken from the FMO complex with and without optimization of the geometry using density functional theory (DFT).

Based on DFT, we have studied in detail the NMR spectrum for the bacteriochlorophyll taken from the FMO complex. For this single bacteriochlorophyll molecule, first we have performed the full geometry optimization using density functional theory. As a result of the optimization, the electronic structure of this system will be completely changed from the original structure, directly taken from the FMO protein. For this fully optimized structure of bacteriochlorophyll, we have calculated the NMR spectra by using the same level of DFT approximations, as well as the basis set, as it was done for



(a) (b)

Fig. 1. Molecular structure of the Fenna-Mathew-Olsen light harvesting complex (a) The whole structure with addition of hydrogen and (b) The model structure for a singe bacteriochlorophyll

the original structure. A typical result for the calculated NMR spectra for these two molecular configurations of the same bacteriochlorophyll has been presented in Figure 2. From the obtained results, we observe that the patterns of the NMR chemical shift are same in both cases, but there is a small shift in the peaks of the NMR spectra for the optimized system from the values of the original structure. Among other conclusions, it is important to emphasize that the effect of the protein environment on the bacteriochlorophyll taken from the FMO complex has a significant effect, as seen from the changes in the NMR spectra. This sensitivity of physical properties with respect to the structural change are very important for our better understanding the applications of photosynthetic bacteria in biomedicine, as well as their limitations.

References

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2. A. Z. Nielsen, B. Ziersen, K. Jensen, L. M. Lassen, C. E. Olsen, B. L. Møller, and P. E. Jensen. Redirecting Photosynthetic Reducing Power toward Bioactive Natural Product Synthesis, *ACS Synth. Biol.*, 2 (6): 308—315, March 2013.
3. K. Sasaki, M. Watanabe, Y. Suda, A. Ishizuka, and N. Noparatnaraporn. Applications of photosynthetic bacteria for medical fields. *Journal of Bioscience and Bioengineering*, 100(5):481–488, November 2005.

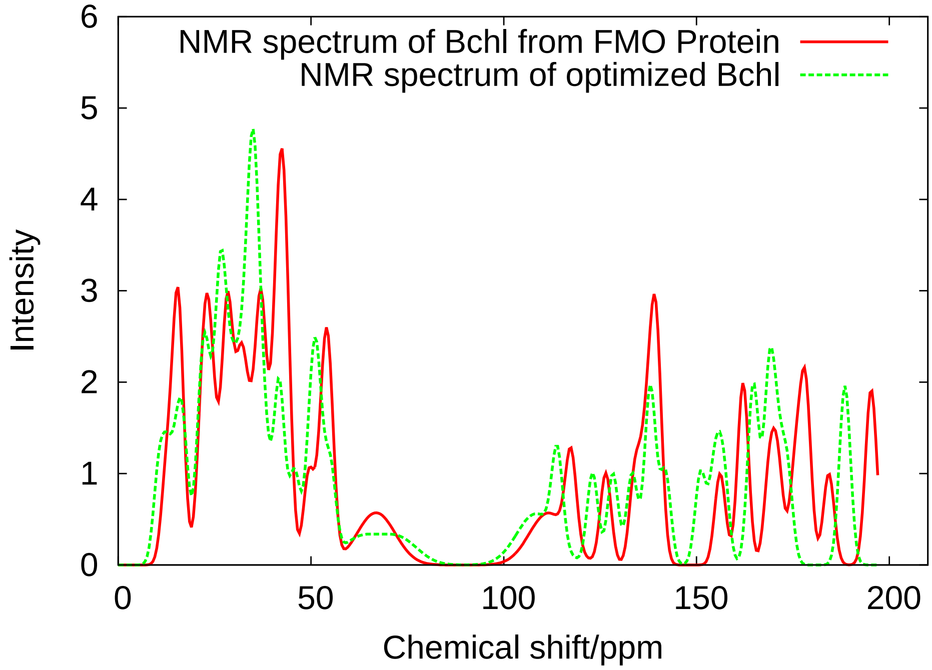

Fig. 2. NMR spectra of the bacteriochlorophyll taken from the FMO complex and its optimized geometry

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PROGRAM

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Scores of Intestinal Fibrosis from Wavelet-Based Magnetic Resonance Imaging Models
Ian Morilla, Magaly Zappa, Eric Ogier-Denis, Sabrina Doblas and Philippe Garteiser

Secret Life of Tiny Blood Vessels: Lactate, Scaffold and Beyond
Michael Sadovsky, Elena Khilazheva, Alla Salmina, Natalia Pisareva, Vladimir Salmin, Andrey Morgun, Elizaveta Boitsova and Pavel Larentiev

Increasing of Data Security and Workflow Optimization in Information and Management System for Laboratory
Pavel Blazek, Kamil Kuca, Jiri Krenek and Ondrej Krejcar

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Tutorial C.1: Half-day GATB Tutorial. The Genome Analysis Toolbox with de-Bruijn graph.

Organizers: Dr. P.Durand,Dr. Lavenier, Dr.R.Chikhi and Dr.G.Rizk

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PLENARY LECTURE:
Prof. Joaquin Dopazo

Fundacion Progreso y Salud, Clinical Bioinformatics Research Area, Sevilla, Spain

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Session A.7: Bioinformatics for healthcare and diseases (Part II)

Chairman: D. Schmude Paul

Biclustering based on collinear patterns
Leon Bobrowski

RISK: a Random optimization Interactive System based on Kernel learning for predicting breast cancer disease progression
Fiorella Guadagni, Fabio Massimo Zanzotto, Noemi Scarpato, Alessandro Rullo, Silvia Riondino, Patrizia Ferroni and Mario Roselli

Variety behavior in the piece-wise linear model of the p53-regulatory module
Magdalena Ochab, Krzysztof Puszynski, Andrzej Swierniak and Jerzy Klamka

Data Mining Analysis of Current and Emerging Synergies Between Biomedical Engineering and Bioinformatics
Jean-Fred Fontaine and Miguel A. Andrade

Multi-omic data integration elucidates Synechococcus sp. PCC 7002 adaptation mechanisms to fluctuations in light intensity and salinity
Supreeta Vijayakumar and Claudio Angione

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