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ORIGINAL PAPER

A PM6 study of *Rhodopseudomonas Acidophila* light harvesting center II B800 bacteriochlorophylls in representative protein environment

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Abstract Bacterial light-harvesting II (LH-II) centers contain two types of Bacteriochlorophylls (Bchl). One is named B800 and found as a single molecule within one monomer of the complex while the other named B850 is found as a dimer. Their names indicate their peak of UV absorbance around red spectrum. Both types of molecules are attached to the protein chain via ligation of their central Magnesium atom to an either Histidine or Deoxymethionine amino acid. They are also coordinated by peripheral hydrogen bonds that they accept with their carboxyl side group. Both the ligation and the hydrogen bonding are thought to have an effect on electronic structure of the Bchl hence its UV absorbance and energy transfer rate. Experiments and theoretic studies performed on this subject support the above idea. This theoretical molecular modeling study case aims to mimic the experimental mutations performed on certain amino acids *in silico* and study its effects on the electronic structure of Bchl. By comparison with experimental results it was observed that the likely place for the nearby Arginine is not below the plane of the Bchl as in the X-ray crystallographic structure but above the plane defined by the four nitrogen atoms and their rings. It was also seen that the coordination of the acetyl group is very sensitive to changes in ligation of the Bchl molecule.

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Introduction

The first implications that photosynthetic units might have been composed of different units originated from experiments performed by Emerson and Arnold in 1932 [1]. They observed that it required more than two thousand chlorophyll molecules to reduce one molecule of CO_2 under saturating light. Further more they demonstrated that samples with low chlorophyll amounts were not easily saturable with even their most intense light sources. These results influenced them and the other scientists working in this area into speculating that only a few chlorophylls in their samples of thousand of chlorophyll molecules were capable of reducing CO_2 when activated with light. They were right and today the distinction is made by naming the light absorbing sections as light harvesting centers and the reducing sections as reaction centers.

Since 1932 researchers have learned a lot about these photosynthetic units. Especially with the advance of X-ray crystallography, the availability of observing these centers in atomic resolution and molecular aspects revealed new perspectives into the field such as possibility of applying ideas and techniques from other fields like computational chemistry and molecular biophysics.

From the information gathered over the years on the subject, a general organizational structure of photosynthetic unit can be deduced, which applies to many cases of plants and purple bacteria. In this model each *reaction center* (RC) is located inside a larger complex called *light harvesting complex I* (LH-I). More over this light complex is itself surrounded by about 12 smaller light harvesting complexes

named *light-harvesting complex II* (LH-II). The chlorophylls that absorb the photons are located in LH-II. Once a photon is received the excitation energy of the absorbing chlorophyll is funneled through arrays of LH-II complexes via random walk until it is captured by a LH-I complex. LH-I is the final destination before the excitation energy caused by a photon is trapped inside a reaction center and utilized for the liberation and flow of electrons (Fig. 1) [2–4].

Molecular structure of light-harvesting center II of *Rhodopseudomonas Acidophila*

The X-ray crystallographic structure for the LH-II of *Rhodopseudomonas Acidophila* at 2.0 Å resolution has been determined in 2003 by Papiz and co-workers [5].

The structure is an oligomaric aggregate of two pairs of alpha and beta apoprotein dimers with each dimer surrounding two carotenoid molecules, a pair of B850 and a single B800 Bchl (Fig. 2b). Each monomer and each constituent of the monomers are held together by noncovalent interactions.

Within these protein dimers, B800 and B850 Bchl form two circles one above the other. B800 molecules are the first step in the energy transfer cascade where they absorb a photon and transfer the energy to the B850 pairs. 800 nm and 850 nm indicate the wavelength at which these Bchls are excited and reveals the energy hierarchy in between. This hierarchy helps funneling the photon energy to the reaction centers (with LH-I complex Bchl absorbing at even higher wavelengths). It is also possible that the absorption of light energy might occur at carotenoids or B850 pairs depending on the wavelength of the photon that reaches these molecules [6].

In the ring of Bchls, the distance between the centers of donor and acceptor molecules plays an important role in

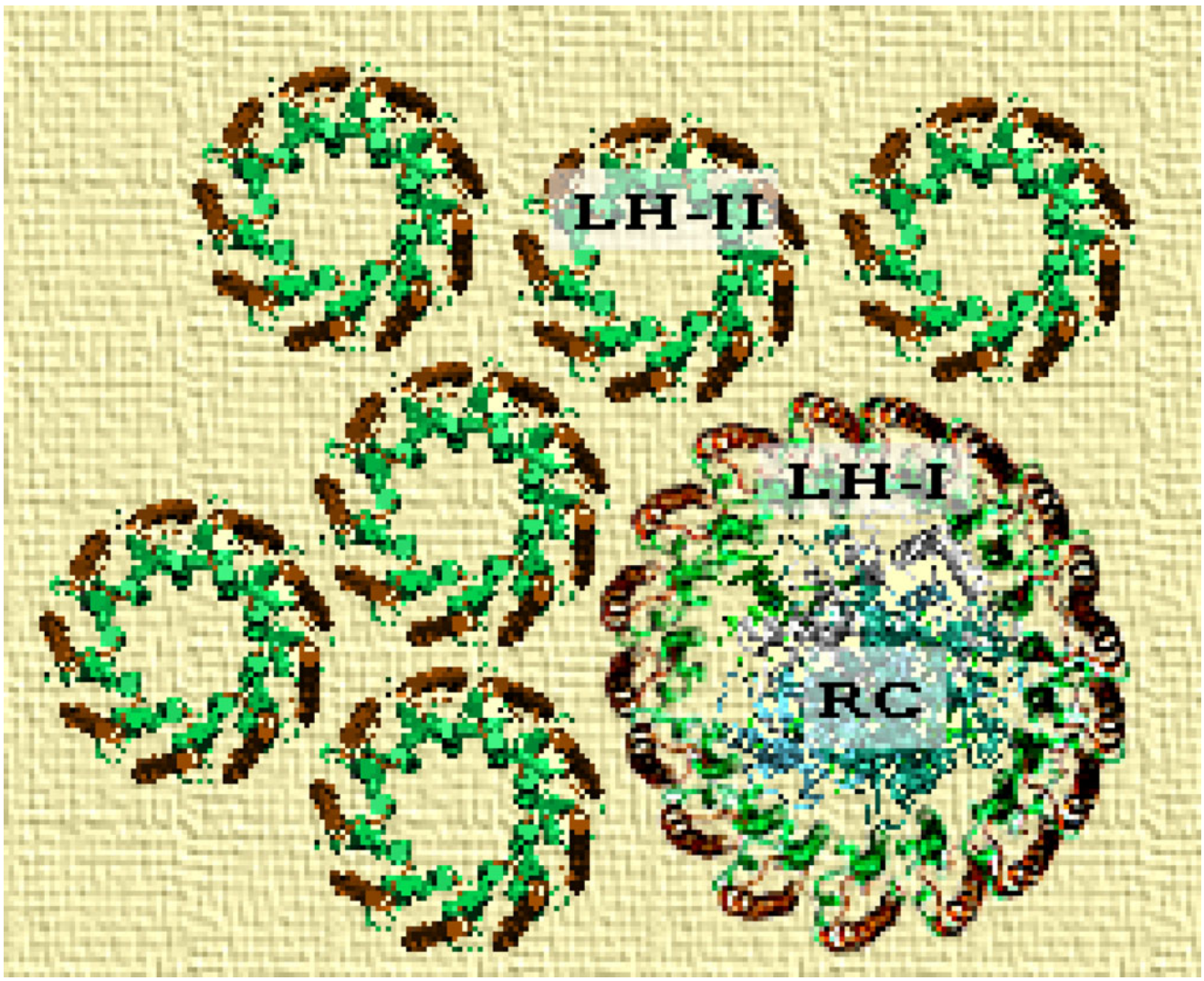

Fig. 1 A representational structure constructed using photosynthetic center structures *for Rhodops. Acidophila* and *Rhodops. Viridis* [5, 10]. Although the general scheme is somewhat universal, the number of monomers (α and β apoproteins etc.) constituting the complexes usually change from organism to organism. The image is created using VMD and Adobe Photoshop [11, 12]

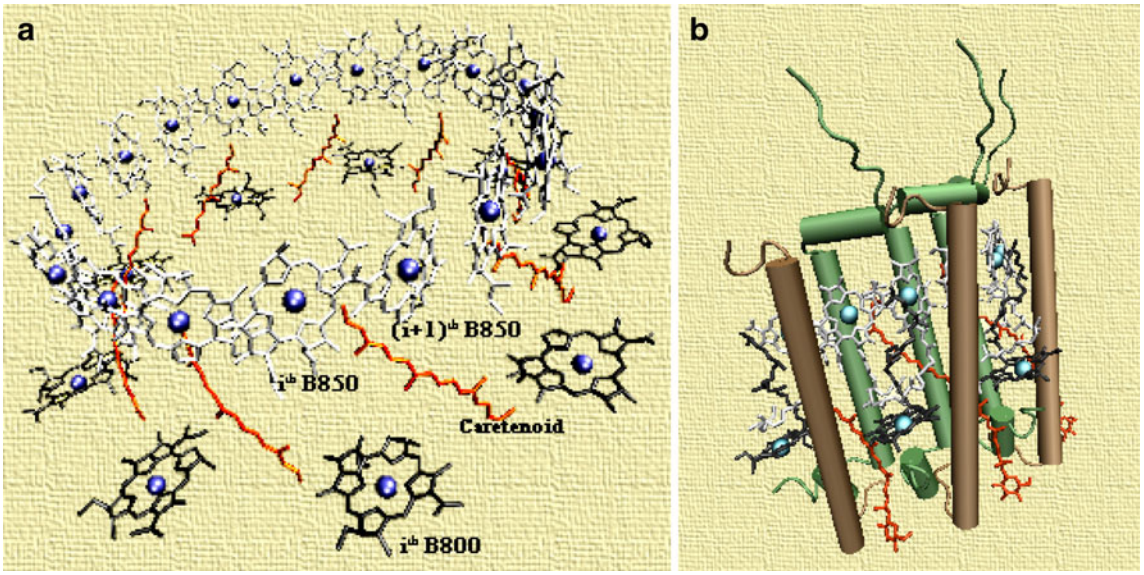

Fig. 2 (**a**) The image represents the ring of Bchls and carotenoids found in a LH-II of Rhodops. *Acidophila* [5]. There is a total of nine B800 and 18 B850 molecules. Besides the nine carotenoid molecules represented here (as orange models) there are nine more carotenoids in the original model, which have been left out along with the phytyl tails of Bchls for simplification. (**b**) Three monomers of the whole *Acidophila* LH-II complex are seen in the image. B800 are represented as the black Bchl models while B850 pairs are the white models and the orange models are the carotenoids. The cylinders represent the α-β apoprotein dimers. Beta chains are shown by the brown cylinders in front while the alpha chains are the green cylinders at the back. Both images were created using VMD and Adobe Photoshop [11, 12]

energy transfer rate. Generally the Mg atoms are accepted as the center of each Bchl; the distance between two neighboring B800 is on the order of 21.20 Å, the distance between two B850 pairs is on the order of 9.00 Å, the distance between i^{th} B800 and i^{th} B850 is on the order of 17.85 Å, the distance between i^{th} B800 and $(i+1)^{th}$ B850 is on the order of 18.48 Å and the distance between i^{th} B850 and $(i+2)^{th}$ B850 is on the order of 19.84 Å (see Fig. 2a) [5].

The Bchls are attached to the protein chains via ligation at their Mg atoms. Each Mg atom, besides ligating the four nitrogen atoms of the poryphorin ring, also ligates an amino acid. In addition to these noncovalent bonds each Bchl, whether B800 or B850, peripherally forms hydrogen bonds to polar amino acid side groups. These interactions are thought to have shifting effects on electronic spectrum of B800 and B850 [7–9, 15].

B800 bacteriochlorophylls

These Bchls, although identical in structure to B850 molecules, exist as single molecules; hence their absorption at a lower wavelength [13, 14]. This property makes them the first excitation donor in the cycle of energy funneling. Like B850 Bchls, they are ligated at the 5′ position of their Mg atom to a Deoxymethionine amino acid, pulling the Mg atom below the plane. The 6th coordination site of the B800 Bchl is occupied by the phytyl tail of the B850 molecules preventing any polar molecule such as water from ligating the Mg center. It is also possible that they might act as a part of a scaffold that keeps B800 molecule in a well defined position. Their acetyl group forms a double hydrogen bond with a nearby Arginine residue. Experimental data suggests that this causes a red-shift in these molecules' spectrum [15] (Fig. 3b).

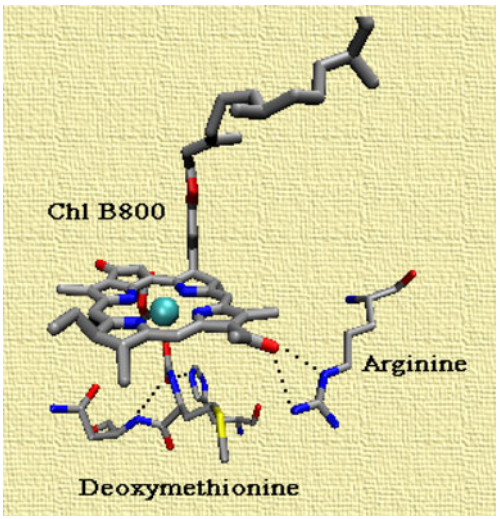

Fig. 3 This figure represents the noncovalent interactions between the bacteriochlorophyll and the polar residues of the protein encapsulating it. The bacteriochlorophyll's acetyl group donates an oxygen bond to two hydrogens from an Arginine functional group. This bacteriochlorophyll is attached to the protein via an interaction with a modified amino acid; Deoxymethionine. There is also a conserved Histidine residue and the nitrogen of this nearby amino acid coordinates this Deoxymethionine by forming a hydrogen bond with it

Methods

Absorption spectrum, determination of configuration interaction (CI) space and a regression equation

The structurally similar molecules Bchl a, b and g all have similar transition wavelengths at Qx, Qy and soret region [16, 17]. Thus these three types of Bchls are used as model molecules to determine a valid CI space and the regression equation for that space (this CI space and the regression equation are then used to calculate the spectroscopic properties of Bchl a in its model protein environment). To calculate spectroscopic properties of Bchl molecules, ZINDO/S as implemented in free molecular modeling software ArgusLab version 4.0.1 [18], is used. Since the spectral data available accounts for the spectral characteristics of Bchl molecules in acetone, a semi-empirical geometry optimization of the Bchls is first carried out with a nearby acetone molecule. Spartan 04 [19] is used for editing the molecules and MOPAC2009 [20] is used to carry out the PM6 calculations. The spectral characteristics of optimized molecules are calculated at (5,5), (10,10), (15,15) (20,20) and (30,30) homo and lumo levels. From each calculation the transition wavelength values for all Bchls are considered as a single data set and plotted against their experimental values. A regression equation is derived from the obtained distribution. The absolute accuracy (closeness of the calculated values to their experimental values) and the relative accuracy (how correctly the differences between the spectral characteristics of the molecules are reflected to the calculated values) of the values are considered together with the parameters of the regression equation (the closer the regression line to an ideal x=y line, the higher the accuracy) for determining the CI space and the regression equation to be used.

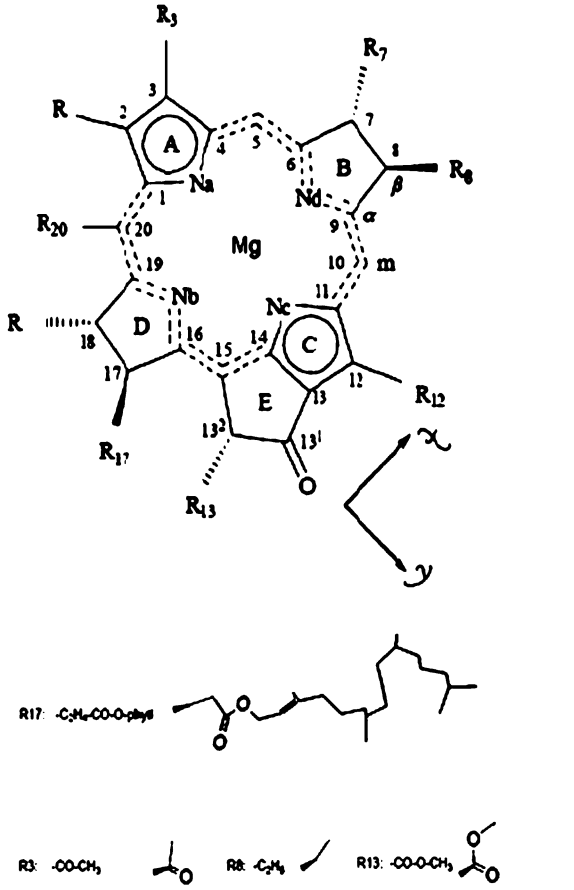

Fig. 4 Molecular structure of isolated B800 is given at the top while the major substituents are given above. Due to alternating double bonds, the inner ring forms a conjugated macrocyclic structure together with ring A and ring B. The β carbons of ring D and ring B do not participate in this conjugation because bonds 17-18 and 7-8 are single bonds. The X and Y molecular axis are defined at the lower right corner. Qx and Qy transition dipole moment vectors are also described according to these axes

Optimization of B800 geometry in different environments

The present study considers B800 molecules as isolated in vacuum, in complex with solvent and as in native and mutated protein environment. The numbering convention for these B800 is given in Fig. 4. The mutated protein environment aims to mimic the experiments performed by Fowler [15] et al. to extract information about Bchl's interaction with its protein environment. While the semi-empirical calculations are carried out with the PM6 method as implemented in MOPAC2009, Spartan is used for molecule editing. The spectroscopic characteristics of these molecules are calculated using ArgusLab by using the CI space and regression model determined as above.

The X-ray structure of LH-II center of *Rhodop. Acidophila* discussed in the introduction part is used as a starting point to obtain a representative model of the protein environment. The model for these calculations include one B800, the phytyl tail of $(i+1)^{th}$ B850, the phytyl tail of i^{th} B850, nearby parts of carotenoids and the amino acid residues at the close vicinity of B800 molecule (see Fig. 5, the model can be obtained from the author as xyz cartesian coordinate files). Most of the protein residues and the pigments other than the B800 are fixed to their coordinates while the B800 and the nearby polar amino acids and some other parts are left free to be optimized. The purpose of these calculations is to see if the effect of changing the environmental conditions and structural properties of Bchls (as tested in lab experiments) can be qualitatively reproduced *in silico* and more information can be extracted from these theoretical experiments.

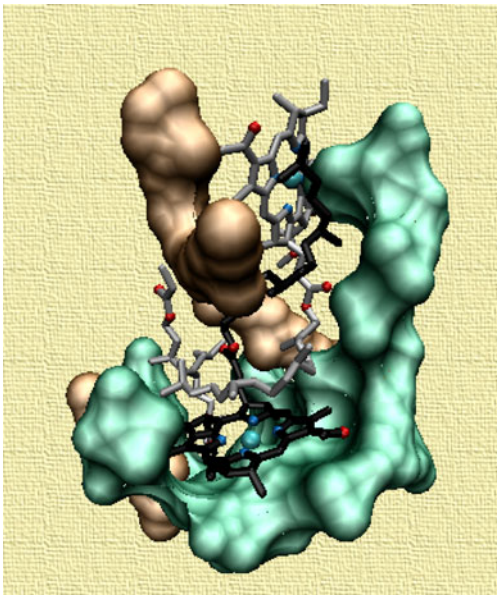

Fig. 5 Sphere representation of the protein scaffold around the B800 that was kept in energy optimization (only the phytyl tail of the B860 Bchl is included in calculations)

Results and discussion

Electronic absorption spectrum, determination of a CI space and a regression equation

The calculated values and their regression model is presented respectively in Tables 1 and 2. It can be seen that increasing the CI space from (5,5) to (50,50) results in divergence of calculated Qy and Qx values from their experimental values and convergence of the soret transition wavelength. Since Qy and Qx are low energy transitions, they can be characterized by Goutermean's four orbital method [21–23]. Thus calculated Qx and Qy values approach experimental values around CI space of (5,5)-(10,10). Soret region transitions, which are the results of interactions between more orbitals, approach their experimental value as CI space is enlarged. However ZINDO/S, as implemented in Arguslab, correctly reveals the relative ordering of absorption wavelengths between different Bchls and between different absorption bands of the same Bchl. Since Qx and Qy calculated values approach their experimental values as the CI shrinks, the regression model converges to a y=x line. Although from this perspective (5,5) CI space might seem as the fittest space, it underestimates the orbitals involved in higher energy transitions, which can not be correctly described by this few number of orbitals. This is one of the reasons why in literature usually CI spaces close to (15,15) or higher are preferred for ZINDO/S calculations [17]. At this point a regression model (as suggested by Petke et al. [24, 25]) can be very useful in estimating transition wavelength values closer to their experimental values while keeping a large CI space that can correctly reveal all the orbitals involved in the transition. As a result (20,20) homo-lumo CI space and the corresponding regression model;

$$\lambda_{est} = 0.735\lambda_{calc} + 141.060\,\eta m$$

is chosen for the spectral calculations to be employed in determination of electronic characteristics of molecules optimized in their local protein environment. It is also noted that when a regression equation is used, the estimated values are not very far from each other for any CI space chosen (since the main purpose of regression equations is to map calculated values into the same set of experimental values). Thus choosing a fit CI space is not more important than one that will correctly describe the orbitals involved in the transitions and hence reveal a correct transition dipole moment. It should also be noted that we are mainly concerned with relative differences of wavelengths in most cases. This regression equation is utilized in the description of UV-absorbance for Bchls optimized in modified protein environments where experimental data is not available. While the solvents and/or nearby amino acids do have an effect on spectroscopic character of Bchls [16, 17], this study is more concerned with the spectral changes arising from the changes in Bchl internal structure. Hence to be able to make a noiseless relative comparison (for which ZINDO/S is a good method), nearby molecules are not involved in spectral calculations.

Optimization of bacteriochlorophyll geometry in different environments

In Table 3 geometrical data of the ring and spectroscopic character is included for some of the runs. The full data for the runs can be obtained from the author. The characteristic properties of the B800 are studied below case by case.

Isolated B800 in vacuum

When the isolated B800 is optimized in vacuum, the carbonyl group of the phytyl tail ligates the magnesium

Table 1 Regression equations for different CI spaces

CI space	Regression equation
5/5	$y = 0.84x + 109.45$
10/10	$y = 0.76x + 134.03$
15/15	$y = 0.74x + 141.08$
20/20	$y = 0.73x + 141.06$
30/30	$y = 0.71x + 148.95$
50/50	$y = 0.69x + 154.19$

Table 2 Transition wavelengths for Bchl a, b and g at various CI spaces

		Exp[a]	5/5 [b]	10/10 [b]	15/15 [b]	20/20 [b]	30/30 [b]	50/50 [b]
Bchl a	Qx	773	786.6	840.9	857.3	866.3	884.9	906.8
	Qy	583	578.6	593.2	596.6	598.0	600.9	605.1
	Soret	394	339.1	342.9	344.7	353.9	351.6	358.1
Bchl b	Qx	796	800.8	847.2	868.4	876.0	892.9	916.3
	Qy	579	589.8	604.5	608.6	610.4	613.1	618.3
	Soret	408	342.6	348.8	352.6	355.0	358.3	364.6
Bchl g	Qx	763	760.7	817.6	831.5	839.1	859.0	880.7
	Qy	566	574.9	593.3	596.5	597.7	601.6	606.5
	Soret	406	333.7	340.6	342.4	343.4	348.8	355.4

[a] Refers to experimental values of Bchls in acetone solution [16, 17]

[b] Refers to values calculated with ZINDO/S as implemented in ArgusLab. X/X orbitals respectively indicate the number of orbitals involved in calculations below homo(included) and above lumo(included)

found in the center of the ring from above (Fig. 6). This causes the magnesium to position itself about 0,321 Å above the plane of the poryphorin ring. The interaction of the Mg atom with the nearby N atoms also causes a steric bending in the ring as observed in the native state of the Bchl. This steric bending can be characterized by the angle between axes defined by C11-C9 and C19-C1, which is 15.7°. Its acetyl group also has a dihedral angle (C_2-C_3-C-O) of about -40 ° which is also approximately the angle with the plane of the nearby poryphorin ring. In native state this group is believed to be in the plane of the ring [26] raising the Q_y wavelength due to its conjugation with the orbitals of the ring.

Isolated B800 in 1:1 and 2:1 water

When B800's Mg is ligated by water from below and optimized, this time magnesium coordinates itself 0.218 Å below the porphyrin plane. In an excess amount of solvent molecules, since Mg can be coordinated by two more sites, it is also possible that it can be ligated from above and below by water molecules. When this condition is simulated, Mg stays on the plane defined by the nitrogen atoms. Similar to the case in vacuum, carbonyl of the phytyl tail is ligated by the water above the ring by hydrogen bond formation. One striking difference is that the acetyl group has a dihedral angle (C_2-C_3-C-O) of about -156°, which results in an angle of about 24° with the plane of the poryphorin ring from the opposite direction in contrast to the case in vacuum. Depending on environmental effects the acetyl group is free to rotate. Also in both of these cases (1 and 2 water coordination), the ring of B800 is almost planar (bending angle close to 0°) and not twisted. Note that in any case (including the cases to follow) the distance between Mg center and the N atoms are quite well-defined while the shape and the twist of the ring can change greatly. This well-defined interaction and the coordination of Mg atom by environmental effects help define the shape of the poryphorin ring, which is also likely to have effects on spectroscopic character of B800 (by changing the internal energy and orbital structure of the molecule). We will mainly consider Qy region since it plays the main role in energy transfer. Indeed, these three molecules optimized under different conditions show varying properties, which can be seen in Table 3. It is seen that the wavelength of self-ligating B800 is 796,46 nm, which is about 20 nm

Table 3 This table contains the essential geometry and spectral data of some of the runs. (C11-C9, C19-C1) is the angle between the axes defined by these carbon atoms while R3(O-C) is the first oxygen and carbon atoms of R3 side group. Center is defined as the center of four N atoms

	Native	In vacuum	1:1 water	Arginine mutated to Isoleucine	Arginine above the plane
Mg-center (A°)	0.30	0.34	0.22	0.37	−0.21
Mg-Na (A°)	2.05	2.03	2.03	2.04	2.06
Mg-Nb (A°)	2.13	2.14	2.16	2.17	2.17
Mg-Nc (A°)	2.06	2.05	2.02	2.04	2.04
Mg-Nd (A°)	2.13	2.13	2.12	2.15	2.14
Mg-ligand (A°)	2.03	N/A	2.08	1.92	1.92
R3(O-C)-C3-C2 (°)	−27.17	−41.41	156.27	−38.93	−12.19
(C11-C9,C19-C1) (°)	4.4	15.7	1.2	5.4	9.4
Na-Nc axis (y-axis)	(-1, 0, 0.15)	(-0.82, -0.004, -0.42)	(-0.97, -0.1, -0.19)	(-0.95, -0.02, 0.12)	(-0.99, -0.02, 0.11)
Qy absorption (nm)	823.9	796.8	777.27	774.63	780.65
Qy dipole direction	(-0.98, 0.09, 0.13)	(-0.81, -0.02, -0,57)	(-0.98, 0.07, -0.21)	(-0.93, 0.208, 0.29)	(-0.97, 0.20, -0.12)

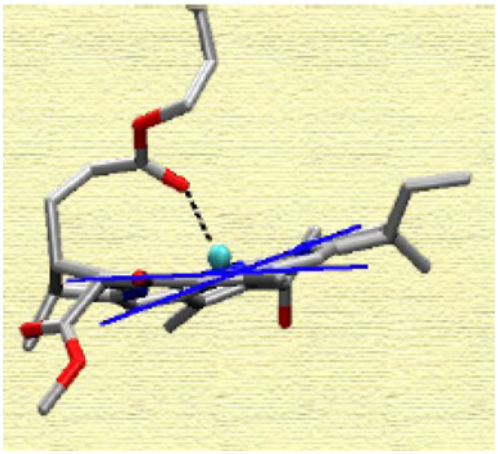

Fig. 6 B800 optimized in vacuum ligates itself. The blue lines refer to the two sides of the ring which twist under the steric effect of Mg-N coordination. The cyan sphere is the Mg atom

higher than the ones in water. This suggests the importance of the coordination of Mg atom in determining spectroscopic character since it interacts with the ring through N atoms. There is also a red shift of 2.5 nm in Qy wavelength in the B800 ligated with two water molecules in comparison to the one ligated with a single water molecule.

It should be noted that the Qy transition dipole moments in each case are approximately aligned in the ŷ axis agreeing with experimental evidence [27]. Also all the B800 Bchls have their dipole moment vectors a few degrees off the plane of the ring, which again agrees with literature [27]. It was also observed that spectroscopic differences increase as the wavelength increases; hence structural changes mainly have an effect on the Qy region.

B800 in native and modified protein environment

The optimization of the B800 in native environment as taken from the X-ray structure leads to a similar structure with the B800 optimized in 1:1 water environment. The Mg atom is about 0.41 Å below the plane due to more polar ligand than the water. The ring is almost planar (1.7° bending angle) and the structures of the poryphorin rings are essentially the same up to 0.1-0.05 Å deviation. It should be noted however that the acetyl dihedral angle is similar to Bchl in vacuum measuring about -23°, being in the same side as that one. The rotation of the acetyl group is interrupted by near by amino acids, which support the idea that the protein environment sterically forces the Bchl away from its minimum energy structure in solution. The angle is smaller due to it is interaction with the Arginine side chain. However it is not in plane with the ring as seen in literature. This suggests that Arginine's native configuration can be above the plane of the ring (in comparison to that of X-ray configuration which is below the plane) thus pulling it upward by hydrogen bonding. This idea is plausible since Arginine lies in the exterior of the isolated LH-II hence it is more exposed to external effects observable during crystallization. The Q_y transition dipole moment is again almost in plane with an angle of about 0.6 °. The Q_y wavelength is 770,96 nm which is far lower than the one optimized in vacuum. This again suggests that the twisted structure introduced to the Bchl due to steric effects might have a role in increasing its Qy absorption wavelength.

Furthermore a series of computational experiments were performed to determine the possible correct position of the Arginine prior to other computational experiments. This was done because there is experimental evidence suggesting that when Arginine is mutated to nonpolar amino acids the Q_y wavelength drops by about 10 nm [15]. Initially the Arginine was mutated to Isoleucine; a nonpolar amino acid that is long enough to still sterically affect the acetyl group but do not participate in hydrogen bonding. In this calculation the structure of the ring remained essentially the same compared to that of the B800 optimized in native protein environment. Only the angle of the acetyl group

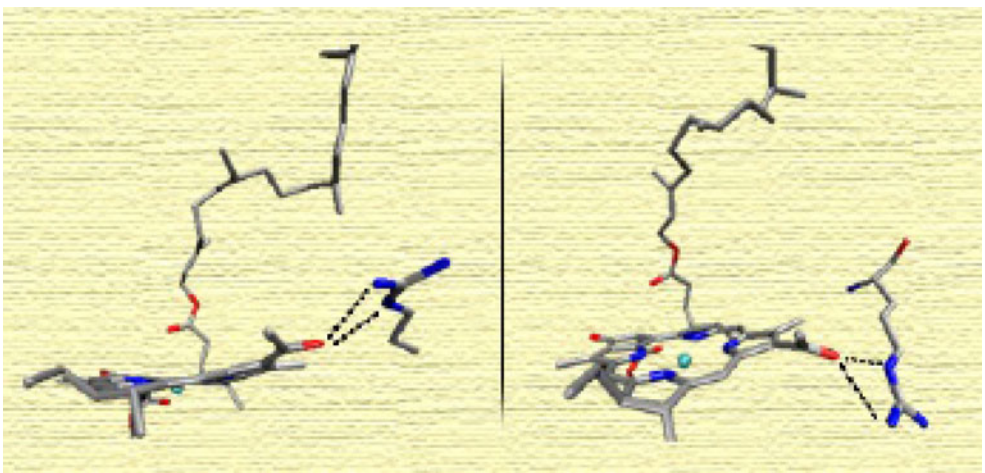

Fig. 7 Respectively B800 optimized with an Arginine in upper plane and in lower plane. The first configuration of the Arginine causes the nearby porphyrin ring to bend, twisting the ring and it also aligns the dihedral of the acetyl group closer to 0°

with the plane of the ring increased to -41.41° when it lost the hydrogen bonds preventing it from rotating to the other side. The spectroscopic characters of the two B800 were also observed to be almost identical. In this configuration Arginine seems to have no spectroscopic effect on the Bchl which is inconsistent with the experiments and the fact that it is a functionally important (conserved) residue.

Along with the fact that the previous optimizations failed to line the acetyl group in plane with the ring and the mutation of the Arginine failed to introduce any spectroscopic differences, we decided to test the hypothesis that Arginine might be located above the plane of the ring in native form (in contrast to the X-ray structure). Calculations were performed with several different conformations of Arginine all above the plane. Most of the calculations resulted in a twisted B800 structure (angle of bending around 9-10°) and a acetyl group which has a much smaller dihedral angle with the nearby porphyrin ring of -12.19° (Fig. 7). In contrast to the B800 minimized with a mutated Arginine, the Qy wavelength also increased by 8-9 nm to the value of 780.51 in this configuration, which is in agreement with the experiments. This result suggests that the Arginine affects the spectroscopic character of the B800 by both aligning the acetyl group with the nearby poryphorin ring and by twisting the structure of the ring and increasing its energy. Since the Arginine residue is on the outer edges of the LHC complex, it is quite likely that its configuration might be effected by the crystallization process and the nearby negatively charged Aspartic acid which is below the plane of the B800.

Next, in lieu of the original X-ray structure, the minimized structure obtained by "above plane configuration" of the Arginine is utilized as the native state for performing the Arginine mutation. When this new configuration is taken and the Arginine is mutated to Isoleucine (previously the Arginine in the structure directly taken from X-ray was mutated), the result is as expected now; the B800 loses its twist, the acetyl group makes an angle of about -38.93° with the plane and Qy wavelength is about 10 nm blue shifted. This also supports our claim in the reverse direction. Furthermore, slight perturbations of the Arginine around its suggested configuration results in the previously obtained structure. This supports that "above the plane" state is a stable local minimum.

The next set of mutations and modifications were performed on the amino acid that ligates Mg to see the effect of ligation on B800 structure. In one experiment, the Deoxymethionine was mutated to normal Methionine while in the second the phytyl tail of the B850 was deleted and a single water molecule was placed at the top of Mg atom. In both cases Mg atom is pulled to the center of the N atoms. While the Arginine still remains above the plane, due to slight sliding of B800 with respect to protein environment, it loses its grip on acetyl group whose dihedral angle increases resulting again in a lower Qy dipole moment. This is suggestive of the scaffolding effect of nearby interacting protein and B860 residue in creating a well defined configuration and relative (to its environment) shape for B800.

Conclusions

In this paper, geometry optimization of B800 in the *Rhodops. Acidophila* LH-II center was carried out with the recent PM6 method and within the nearby protein scaffold (in comparison to previous studies cited in this article). The spectral calculations were performed using ZINDO/S. The main result of this paper is that; computational experiments carried over a large range of modified X-ray structures suggests that the Arginine ligating the acetyl group of B800 molecules in LHII might actually be above the plane in contrast to that of X-ray configuration (in which it is below the plane). It is also seen that scaffolding of protein is required for the B800 to align itself correctly relative to the protein environment thereby gaining the advantage of steric effects required for changing its spectroscopic character.

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