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Crystal structure of the light-harvesting-reaction center core complex from a thermophilic photosynthetic bacterium

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Introduction

In purple photosynthetic bacteria, the light energy is absorbed by two types of light-harvesting complexes (LH1, LH2), and then is transferred efficiently to the reaction center (RC) where the primary charge separation takes place across the membrane and a cyclic electron transport chain occurs. The LH1 complex is located intimately around the RC with a fixed stoichiometric ratio to form the so-called core complex (LH1-RC). LH1 is a large oligomer of a basic structural unit composed of a heterodimer of two small integral membrane polypeptides (α and β, ca. 6 kDa) associated with bacteriochlorophyll (BChl) and carotenoid molecules. *Thermochromatium* (*Tch.*) *tepidum* is a thermophilic purple sulfur photosynthetic bacterium originally isolated from a hot spring in Yellowstone National Park. It grows anaerobically at optimum temperatures of 48 – 50 ºC with an upper limit of 58 ºC, and contains an unusual LH1 complex that absorbs maximally around 917 nm (Q_y transition). In a series of investigations, we found that the *Tch. tepidum* LH1 is highly stable at room temperature, and calcium ions are involved in both the enhanced thermal stability and the large red shift of the LH1 Q_y transition[1, 2].

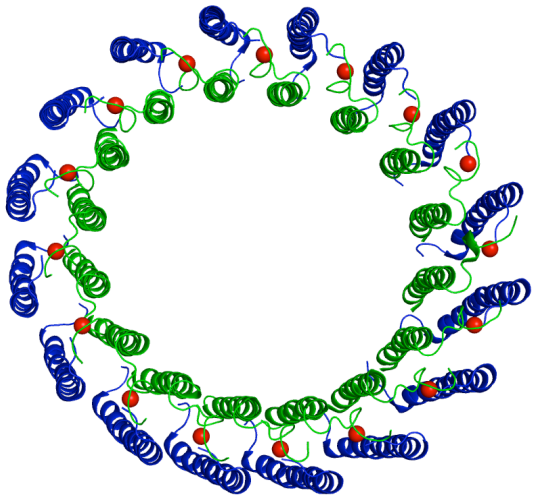
The crystal structure of LH1-RC from *Tch. tepidum* has been determined [3], in which the Ca-binding sites have been identified. Here, we report the structural features on the Ca-binding pockets.

Materials and Methods

Crystallization of the native *Tch. tepidum* LH1-RC complex was performed using sitting-drop vapor-diffusion method at 20 ˚C. The protein solution was mixed with the same volume of precipitant solution (20 mM Tris-HCl, pH 7.5, 3 mM DPC, 50 mM $CaCl_2$, 16% w/v PEG3000).

Results and Discussion

Anomalous difference Fourier maps revealed that there are 16 Ca-binding sites in the LH1 and one in the RC. The Ca^{2+} ions in LH1 distribute in the middle between the inner and outer rings (see the Figure). The Ca^{2+}-binding



sites are located in the C-terminal regions of the α- and β-polypeptides with both chains providing ligands for the coordination. Each Ca^{2+} is coordinated by the main chain oxygen atoms of α-Trp46, side chain of α-Asp49 and α-Asn50, and the C-terminal carboxyl group of the β-Leu46 in the adjacent subunit. Water molecules, whose electron densities have not been clearly identified, may also be involved in the ligation to form a heptacoordinated structure as favoured by the Ca^{2+} ion. Association of the α- and β-polypeptides through the Ca^{2+} stabilizes the LH1 structure and is thought to account for its enhanced thermostability. Since the binding network is positioned close to the BChl *a* molecules, it could modify the configuration of the coupled pigments through the nearby α-Trp46 and β-Trp45 whose side chains are hydrogen-bonded to the C3-acetyl oxygen atoms of BChls *a*. The Ca^{2+}-binding effect is considered to have additional contribution to the larger red-shift of the LH1 Q_y transition in *Tch. tepidum* compared with the Q_y transitions (~ 880 nm) in other species.

References

[1] Y. Kimura, et al., *J. Biol. Chem.*, **283**, 13867(2008)
[2] Y. Kimura, et al., *J. Biol. Chem.*, **284**, 93(2009)
[3] S. Niwa et al., *Nature* **508**, 228(2014)

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