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Structural analysis of the metal-substituted light-harvesting-reaction center core complexes

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1 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 (a and b, 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 915 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. On the other hand, the Ca^{2+} ions in LH1 can be replaced by other divalent metal ions (e.g., Sr^{2+} and Ba^{2+}), resulting in a substituted LH1-RC with the LH1 Q_y in a range of 880 ~ 890 nm [1, 2]. Here, we report structure determination of the Sr- and Ba-substituted LH1-RCs [4].

2 Experiment

Crystallization of the Sr- and Ba-LH1-RCs and post-crystallization treatment were carried out following the same method as describe previously [3]. X-ray diffraction data were collected at BL41XU and BL44XU of SPring-8, and BL1A, BL17A and NE3A of the Photon Factory at 100K. To identify the Sr^{2+}- and Ba^{2+}-binding sites, datasets were acquired at three wavelengths for the Sr-LH1-RC and two wavelengths for the Ba-LH1-RC.

3 Results and Discussion

Anomalous difference Fourier maps obtained at wavelengths of 0.76 Å and 1.5 Å revealed strong electron densities for the Sr- and Ba-LH1-RC crystals, respectively. The strong densities disappeared at 0.78 Å (remote) for the Sr-LH1-RC and largely reduced at 0.98 Å for the Ba-LH1-RC, confirming that they are truly from the Sr^{2+} and Ba^{2+} ions, respectively. Both the Sr^{2+} and Ba^{2+} have the same number and are located at essentially the same positions in the substituted LH1-RCs. These locations are clearly different from, though close to, the Ca-binding sites. Sixteen Sr^{2+} and Ba^{2+} ions are identified in the LH1 complexes. Conformational rearrangement induced by the substitution is limited to the metal-binding sites. Unlike the Ca-LH1-RC, only the α-polypeptides are involved in the Sr- and Ba-coordinations in LH1 (Figure 1). The difference in the thermostability between these complexes can be attributed to the different patterns of the network formed by metal-binding. The Sr- and Ba-LH1-RCs form a single-ring network formed by the LH1 α-polypeptides only, in contrast to the double-ring network composed of both α- and β-polypeptides in the Ca-LH1-RC. Based on the structural information, a combined effect of hydrogen-bonding, structural integrity and charge distribution is considered to influence the spectral properties of the core antenna complex.

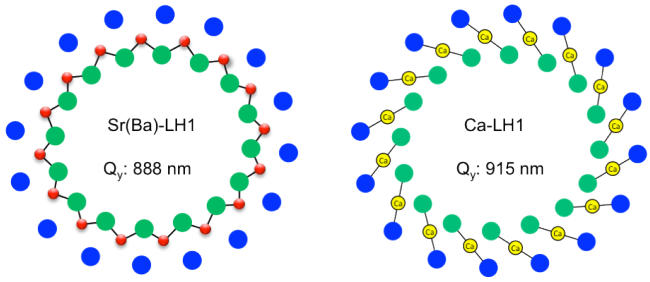

Fig. 1: Schematic illustration showing the difference between Sr(Ba)- and Ca-binding networks formed in LH1s [4].

References

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