Crystallization in lipid mesophases affects pigment composition of photosynthetic reaction center

P-27-027

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Structural studies of membrane proteins are often challenging. One of the popular techniques for this purpose is crystallization using lipid mesophases. It has several advantages over other approaches but we have shown that it has a serious flaw. It turned out that crystal growth in lipid mesophase can affect pigment composition in the resulting x-ray structure. In purple bacteria, the primary process of photosynthesis occurs in a membrane pigment-protein complex termed a reaction center (RC). To obtain structure with the highest resolution, we tried different crystallization techniques. Three specimens of RC crystals were obtained: (i) from detergent conditions without lipids; (ii) from lipid cubic phase (LCP) conditions; (iii) from lipid sponge phase (LSP) conditions. Crystal structures were solved and refined with final resolution of 2.3 Å for “detergent crystals”, 2.0 Å for “LSP crystals”, and 2.1 Å for “LCP crystals”. Comparative analysis of RC structures obtained in lipid and detergent conditions showed several differences. First major difference is the absence of carotenoid spheroidene in “lipid” structures. In this structures carotenoid-binding pocket possess an electron density that does not correspond to a carotenoid molecule. Second major difference is the presence of an unfamiliar molecule in the secondary ubiquinone binding site. Both electron densities most likely correspond to 2-monoolein molecules. 2-monoolein is a monoacylglyceride (MAG) and an isomer of 1-monoolein, the main mesophase matrix lipid. MAGs can undergo spontaneous isomerization over time, therefore, the presence of 2-monoolein in the crystallization mix is highly probable. We assume that during the crystallization process alien molecules can displace natural carotenoid and ubiquinone. This study was supported by the program of the Presidium of the Russian Academy of Sciences “Molecular and Cell Biology and Postgenomic Technologies” and the RFBR (grants 18-02-40008 and 17-44-500828).