regulatory proteins essential for this process. SM proteins are thought to regulate fusion by interaction with the SNARE protein Syntaxin (Sx). Different binding modes for the SM-Sx interaction have been observed: binding to the closed conformation (neuronal system [1]) binding to the N-terminus of the Sx protein (yeast Golgi-ER system [2] and GLUT4 system [3],[4]) and to the SNARE ternary complex (yeast exocytotic system [5]). The role of SM proteins in vesicle fusion has been disputed partly due to the different binding modes. Binding to the closed mode inhibits the formation of the ternary complex, negatively regulating vesicle fusion. Whereas binding via the N-terminus of Sx facilitates binding to the ternary complex and positively regulates fusion [3]. Our research focus is on Munc18c and Sx4, the SM and Sx protein respectively, involved in GLUT4 vesicle transport to the plasma membrane in response to insulin signalling. We have used biophysical techniques such as ITC and small angle scattering (SAS) to further characterize the molecular details of the Munc18c-Sx4 interaction. The findings using these techniques, specifically the possible conformational changes of Sx4 on binding to Munc18c will be discussed.

References:

1. Dulubova I. et al. EMBO 1999 18, 4372
2. Bracher A. and Weissenhorn W. EMBO 2002 21, 6114
3. Latham, C.F. et al. Traffic 2006 7, 1408
4. Hu, S-H. et al. PNAS 2007 104, 8773
5. Carr, C.M., et al. JCB 1999 146, 3334

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Atomic-level models of the bacterial carboxysome shell

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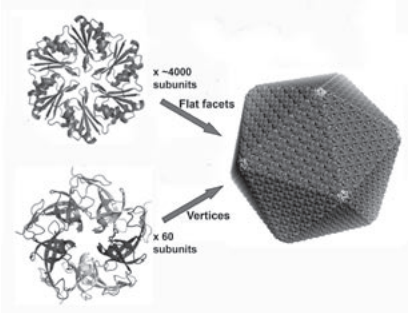
The carboxysome is a bacterial microcompartment, roughly 1000Å in diameter, that sequesters enzymes involved in carbon fixation. The shell is built from several thousand protein subunits and resembles a viral capsid. We have previously solved the crystal structures of hexameric carboxysome shell subunits, which suggest their roles in forming flat facets of the polyhedral shell (Kerfeld, *et al.*, *Science* 2005). There are three structures of homologous hexameric shell proteins solved from one class of carboxysome (beta-type) and one structure solved from another class of carboxysome (alpha-type) (Tsai, *et al.*, *PloS Biol* 2007). The comparison of these hexameric proteins shows interesting characteristics in sheet packing and residue interactions between adjacent hexamers. Furthermore, the recently determined structures of CcmL and CsoS4A subunits from the two classes of carboxysomes possess predominantly β-sheet structures and assemble as pentamers whose size and shape are compatible in forming icosahedral vertices of the protein shell. Combining these pentamers with the hexamers gives two plausible, preliminary atomic models for the carboxysome shell (Tanaka, *et al.*, *Science* 2008).



Keywords: bacterial organelles, carboxysome, CO_2 fixation

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Coordination structure of two Cl^--binding sites in oxygen-evolving photosystem II

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Photosystem II (PSII) performs light-induced electron transfer and water-splitting reactions, leading to the formation of molecular oxygen which is essential for the survival of most of the life on the earth. The components of oxygen-evolving PSII from cyanobacteria include 17 membrane-spanning subunits, 3 hydrophilic, peripheral subunits, and over 70 cofactors such as chlorophylls, carotenoids, Mn, Ca, Fe, and plastoquinones, which give rise to a total molecular mass of 350 kDa for a monomer. The structure of PSII has been reported at 3.8-3.0 Å resolution by X-ray crystallographic analysis. The catalytic center for water splitting of PSII, namely, the oxygen-evolving complex, is located in the membrane surface and composed of 4 Mn atoms and 1 Ca atom coordinated by the protein matrix of PSII. Cl^- is one of the essential cofactors for oxygen evolution of PSII, and is closely associated with the Mn_4Ca-cluster. Its detailed location and function, however, have not been identified. In order to elucidate the coordination structure and function of Cl^- in PSII, we substituted Cl^- with Br^- or I^- in a PSII dimer from *Thermosynechococcus vulcanus*, and analyzed the crystal structure of Br^- or I^--substituted PSII. Our results showed that two Cl^- are bound to each PSII in positions surrounding each side of the Mn_4Ca-cluster at equal distances to the Mn atoms (7.0 Å) as well as to the Ca (10.0 Å). Among these two Cl^-, one is located in the entrance of a proton exit pathway, and another one is located close to the backbone of CP43-Glu354, the side chain of which is coordinated to the Mn_4Ca-cluster. These results well explain the various Cl^--effects on PSII oxygen evolution observed, and provides a basis for fully understanding the mechanism of oxygen evolution.

Keywords: photosynthesis, membrane proteins, anomalous diffraction

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Crystallization and structure determination of the phycobilisome complex

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