MS45-P1 **Crystallization of the photosynthetic core complex of *Blastochloris viridis*** Elin A. Johansson,[a] Weixiao Y. Wahlgren,[a] Ida Lundholm,[a] Linda C. Johansson,[a] Annemarie B. Wöhri,[b] Gergely Katona[a] [a]*Department of Chemistry and Molecular Biology - University of Gothenburg, Sweden,* [b] *Department of Chemical and Biological Engineering - Chalmers University of Technology, Sweden*
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The conversion from solar energy into amenable energy is a fundamental process for all life on Earth, which is performed by the photosynthetic organisms. The photosynthetic core complex of *Blastochloris viridis* is a membrane protein consisting of two parts: a reaction center (RC) and light harvesting complex I (LHI). The RC of 4 subunits is surrounded by a LHI complex, which is constituted of oligomers (16) of three types of polypeptides. The large size of total 440 kDa and its sensitivity to light make not only purification, but also characterization and crystallization of this complex difficult. A high-resolution structure to elucidate the mechanism of electron transfer within the complex is desirable. Several alternative crystal forms using the lipidic sponge phase [1] and bicelle crystallization technique have been produced. Improved crystallization conditions have yielded crystals with X-ray diffraction to 11 Å resolution and an insight to the orientation of the surrounding LHI complex. No high-resolution crystals have been obtained; hence it is necessary to improve the composition and ordering of these crystals. Small-angle X-ray scattering (SAXS) and synchrotron radiation circular dichroism (SRCD) have been used as complementary techniques to provide additional information about the stability and structure of the core complex.

[1] A. B. Wöhri, W. Y. Wahlgren, E. Malmerberg, L. C. Johansson, R. Neutze and G. Katona. Lipidic Sponge Phase Crystal Structure of a Photosynthetic Reaction Center Reveals Lipids on the Protein Surface *Biochemistry* (*2009*) ***48*** (41)

Keywords: membrane protein; bicelle crystallization; X-ray diffraction

MS45-P2 **CCP4 6.3 – new and improved software tools for macromolecular crystallography.** Ville Uski, Charles Ballard, Ronan Keegan, Eugene Krissinel, Andrey Lebedev, David Waterman, Marcin Wojdyr, *Research Complex at Harwell*, *STFC Rutherford Appleton Laboratory, Didcot , United Kingdom*
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The CCP4 software suite provides a comprehensive set of tools for use in the macromolecule structure solution process by X-ray crystallography. CCP4 is a highly collaborative project and derives its contents from the contributions of some of the leading software developers in the field. Our broad community of expert and novice crystallographers, software developers and associated scientists help to engender the continuing development of new ideas and techniques leading to improved performance in the existing software as well as the creation of whole new methods. As a result, the CCP4 software suite undergoes regular updates enabling the distribution of the new software tools to its world-wide user base. Today, tools and packages covering all aspects from data collection through to structure deposition are provided. Here, we present details of version 6.3 of the suite. This release brings updates to many of the key programs, including improved methods for experimental phasing and molecular replacement in Phaser 2.5, new tools for low resolution refinement in Refmac 5.7 and Mosflm 7.0.9 which now has support for Pilatus images. This release also includes several new programs. ViewHKL is a new graphical viewer of reflection data. Aimless, intended as a replacement for Scala, scales together multiple observations of reflections and is considerably faster and better performing than its predecessor. In the area of phasing, version 6.3 includes a beta version of a new program called AMPLE which makes use of ab-initio/de-novo modelling tools such as Rosetta for the generation of search models for use in molecular replacement. There are new model building and refinement tools including Nautilus, which performs automated building of RNA/DNA from electron comparative structural analysis. Some new structure and solution analysis tools are also introduced. Gesamt performs structural alignment allowing for arbitrary selection of residues and Zanuda can be used to check refinement results and validate space group assignment. Building on the legacy of several decades of crystallographic software development, CCP4 6.3 is an indispensable tool for any researcher working in the field of macromolecular crystallography.

Keywords: biological macromolecular X-ray crystallography; software for crystallography; crystal structure determination