optimized. It was shown that oxygen-evolving complex is possible to wash out from thylakoid membrane by contain of different salts. According preliminary crystallization experiments it was shown that success of crystallization trials is dependent on purification steps of this complex. It was shown that degradation of subunits is caused by presence of Na^+, K^+, Ca^{2+} and Mg^{2+} ions, but Ca^{2+} are sufficient additive for crystallization. Our results showed that development of reproducible purification protocol is a crucial step toward reproducible crystallization experiments.

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Keywords: plant photosystem II, oxygen-evolving complex

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ProSMART - procrustes structural matching alignment and restraints tool

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ProSMART (Procrustes Structural Matching Alignment and Restraints Tool) is a tool to aid in the comparative analysis and refinement of protein structures, intended to be complementary to existing resources. Primarily, it is used for conformational invariant/independent pairwise structural alignment, allowing identification of local similarities. The tool provides residue-based dissimilarity scores for assessment of local similarity, identifies rigid substructures, and outputs sets of superposed coordinates. Utilising information from external structures, atomic distance restraints may be generated for subsequent use during crystallographic refinement.

Pairwise structural alignment is achieved by performing an all-on-all comparison of n-residue structural fragments between two chains. Individual structural fragments are compared using Procrustes analysis, quickly achieving local backbone root mean square deviation. A fragment alignment is achieved using a dynamic programming algorithm, which is then further refined. In order to maintain conformation-invariance, the alignment is filtered to enforce global rigidity of neither chains nor domains. This feature makes the tool suited to the analysis of domain movement and other conformational changes, as well as for the identification of structural units that are conserved between seemingly different structures.

Following identification of the alignment, the structures are searched for conserved rigid substructures. For each identified substructure, superposed coordinates are output. ProSMART has a variety of features, useful in different applications. One such feature is the ability to colour (superposed) structures according to various residue-based dissimilarity scores, to be viewed in PyMOL. ProSMART also allows dissimilarity scoring of side chain conformation, relative to local coordinate frame. This feature is of particular use when comparing the side chains of two near-identical structures in different conformations and/or bound states, due to the ability to detect subtle changes.

Given an alignment, ProSMART can be used to generate external restraints on the distances between relatively close, non-bonded, atoms. Using one or more similar structures, the software generates restraints that are intended to help the target protein adopt a conformation that is more reasonable for structures in the class in which it belongs, whilst allowing global flexibility. The assertion is that the target structure's local atomic distances should be reasonably similar to those from similar structures. External restraints from ProSMART can be applied during crystallographic refinement by REFMAC5. These restraints have been found to stabilise refinement in some cases, especially at low resolution (3-6Å) where experimental data alone may not be sufficient. Tests are promising, suggesting that external restraints might be used to improve reliability in future.

ProSMART may be used with data from various methods, including structures from crystallography and electron microscopy, and ensembles from nuclear magnetic resonance and molecular dynamics simulations. A pre-release version of ProSMART is available by contacting the author.

Keywords: alignment, comparison, restraints

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Towards the complete structure of the S-layer protein SbsC

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Monomolecular paracrystalline surface layers (S-layers) are composed of a single (glyco)protein and are the most commonly observed cell surface structures of bacteria and archaea. Because of their diverse properties S-layers have various potential applications in nanobiotechnology [1]. However, detailed structural information on S-layer proteins is very scarce. In order to determine the structure-function relationship of SbsC, the S-layer protein from *Geobacillus stearothermophilus*, deletion mutants were produced. It was shown that the N-terminal part is responsible for binding to the secondary cell wall polymer (SCWP) and that the C-terminal part is essential for self-assembly [2]. Recently, the crystal structure of the C-terminally truncated form $rSbsC_{(31-443)}$ was solved to 2.4 Å [3].

We continued the work with different N-terminal truncations and crystals of 3 different protein constructs were obtained. The structure of one construct was solved by producing different heavy atom derivatives. The structure consists of 3 Ig-like domains connected with the short linker. The refinement of the crystals from two other constructs is in progress.

Small angle X-ray scattering measurement of all constructs was performed. All constructs consist of domains similar in size and shape. We can conclude that the full length SbsC protein consists of 9 domains. The first coiled-coil domain followed by 8 Ig-like domains.

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A study of how different ligands and ph may influence insulin crystallisation by using powder diffraction

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