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X-ray structure of a transmembrane domain from an ABC-transporter dependent system from Neisseria meningitidis in a non-biological state

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Molecular replacement (MR) is the most commonly used method in crystallography to solve the phase problem required to obtain the three dimensional structure of a protein. Traditionally MR uses a search model from a previously determined protein structure. One of the requirements for success by MR is that the amino acid sequences of the search model and the unknown structure should be have at least 35 % identity. When this is not possible, an *ab initio* model can be generated using the sequence of the unsolved protein. In this project, we used the algorithm, tr-Rosetta, from the Rosetta server to obtain *ab initio* models used for use in MR.

CtrC is part of an ABC transporter dependent complex in *Neisseria meningitis*, important for capsule polysaccharide transport. It constitutes the transmembrane domain and associates with a separate nucleotide binding domain, CtrD, making a heterotetramer. CtrC, has been crystallised using the lipidic cubic phase (LCP) method. After data collection using the MX2 beamline at the Australian Synchrotron, the structure has been solved at 2.87 Å by MR using an *ab initio* derived search model.

The structure of CtrC shows a monomeric arrangement in the crystal lattice, unusual for an ABC transporter. A single molecule of the monoolein lipid used in the LCP matrix was found bound within the protein structure. We hypothesize that the presence of the monoolein ligand, and possibly the absence of CtrD, abrogates the ability of CtrC to form the expected dimeric structure.

Level of Expertise

Student

Presenter Gender

Woman

Pronouns

Which facility did you use for your research

Australian Synchrotron

Students Only - Are you interested in AINSE student funding

Yes

Do you wish to take part in the Student Poster Slam

No

Condition of submission

Yes

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