MS01 MX/Cryo-EM software development

MS1-04

Slice'N'Dice: maximising predicted models for structural biologists

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Abstract

With the advent of next generation modelling methods such as Alphafold 2, structural biologists are increasingly using predicted structures as search models for Molecular Replacement (MR) (Barbarin-Bocahu, 2022). Predicted model conformation, especially for multi-domain proteins, is often a key limitation when using predicted models for MR. Slice'N'Dice is a software package designed to solve conformational problems by first slicing models into distinct structural units and then automatically placing these units with Phaser. Predicted models can be clustered based on the xyz coordinates of the C-alpha atoms or, if available, using predicted aligned error (PAE). In a single job, users can select a range of different splits so that the optimal number of splits can be taken forward to MR. Slice'N'Dice is available in CCP4 8.0 and is currently being adapted for cryo-EM.

References

Barbarin-Bocahu, I. & Graille, M. (2022). Acta Cryst. D78, 517-531.