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”MrBUMP: automated search model discovery and preparation for structure solution by molecular replacement”

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MrBUMP is a new automated procedure for structure solution by Molecular Replacement. The aim of MrBUMP is to start from native structure factors and a target sequence, and deliver a positioned and partly refined model, suitable for further model re-building, model completion and/or refinement. In the highest level view, the process consists of three stages. In the first stage, the target sequence is used to search for related proteins in the Protein Data Bank. This gives a list of template chains, domains and multimers, which is passed to the search model preparation stage. Up to three search models are generated for each template, differing in the alignment used and the treatment of side chains. Finally, given a list of putative search models, a subset is passed to the MR stage which uses Phaser or Molrep. Initial restrained refinement of the positioned model is used to assess the putative solution. MrBUMP consists of a set of Python scripts which link together established programs. MrBUMP differs from other molecular replacement pipelines in two ways: Firstly, there is a greater emphasis on the discovery of potential search models. A list of search models is generated and many are tried in molecular replacement with the aim of finding the optimum model. Secondly, Mr Bump is intended for general use within the CCP4 software suite, and is designed to be portable and flexible.

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AutoDep 4.0: A web-based deposition and archival system

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The Macromolecular Structure Database (MSD) (*http://www.ebi.ac.uk/msd/*) [1] group is one of the three partners in the worldwide Protein DataBank (wwPDB) [2], the consortium entrusted with the collation, maintenance and distribution of the global repository of macromolecular structure data. Structures can be deposited at the MSD using AutoDep [3] deposition tool or with the other wwPDB partners using the ADIT system. The latest release of this tool: AutoDep v4.0 (*http://www.ebi.ac.uk/msd-srv/autodep4/*) [4] is a complete rewrite of the original AutoDep system. The new application maintains a superficial similarity to the old AutoDep tool, in order to ensure an easy transition for users from the legacy system, but is a completely new implementation, using a Java servlet framework and XML as a data storage and interchange format. The system is highly customizable, owing to the system of flexible XML-based dictionaries that define all aspects of the user interface and internal data formats. The new system accepts harvest files from commonly used structure determination packages such as CNS and CCP4, in order to automatically populate many data items during the deposition process. The new system also allows a first round of data validation to be applied as data are entered into the system, using validation patterns. Once deposition is complete, a suite of analysis programs are run in order to validate structures before submission to the wwPDB. The AutoDep system allows value-added information to be returned in a safe and secure manner into the password-protected deposition session only accessible to the depositor, following annotation of the structure by curation staff, within 2 days of deposition. These include structure factor validation statistics, quaternary structure assessments, new ligand dictionaries etc., in addition to the annotated PDB file. AutoDep 4.0 is also available for download and installation in-house (*http://msdlocal.ebi.ac.uk/docs/AutodepDistribution/*), where a deposition can be completed and validated before uploading the whole deposition session to the MSD site, where submission to the wwPDB can be completed in minutes. AutoDep 4.0 can also serve as an in-house archiving system into which structures determined can be deposited, validated and written out for analysis as PDB files with annotated headers. With structures being determined at an ever increasing rate, it is imperative that deposition tools keep pace with this exponential growth of data. We believe that the latest release of AutoDep has significantly automated the deposition process, reduced the time taken to deposit a structure, and at the same time harnessed services offered by the MSD group in returning useful information to the depositor.

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