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Modelling Bound Ligands with ARP/wARP

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Once a protein model has successfully been built, the completion step may involve a search of the remaining electron density to fit ligand molecules. Currently most available methods fit one of the largest pieces of remaining density with a sort of template fragment fitting algorithm (e.g. X-Ligand [1], COOT [2], recent work by Terwilliger et al. [3] and by Aishima et al. [4] which uses a skeleton approach). The program module for ligand building that was made available to the community through the release of the version 6.1 of ARP/wARP [5] also fits a model of the ligand to the largest piece of density in a difference density map. The method uses a graph search technique to arrive at the best interpretation of the density in terms of various derived features. The software is quite robust and builds accurate models of ligands (with an r.m.s.d. of less than 1 Å) in about 30% of the cases. We will present further developments of the ligand building module, where several ligands can be built successively, irrespective of the order of their size and independent of the initial knowledge of their identity. One attractive feature is the possibility to automatically build 'the best' ligand from a selection (cocktail) of candidate ligands using a combination of shape recognition techniques. Results will be presented on the application of the software to a large number of cases of building ligands. The potentials and limitations of the method will be discussed.

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ROTFINDER: A Python Graphical User Interface to Perform Molecular Replacement

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Due to the growing number of protein structures present in the Brookhaven Protein Structure Data Bank (PDB) [1], the technique of Molecular Replacement in protein crystallography is retaining importance. A vector-search rotation-function program in Patterson space, OVIONE, has been recently developed in our research group [2]. This program uses image-seeking functions as rotation functions. We present here the development, via python scripting, of ROTFINDER: A Graphical User Interface (GUI) to perform Molecular Replacement in the real space using vector-search rotation functions. With this self-explanatory, widely compatible and user-friendly GUI we expect to open our software to every interested user (both occasional and experts).

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