Conference

Molecular Replacement, new procedures and applications.

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Molecular Replacement is the most used technique to solve macromolecules; an original algorithm called REMO09[1] has been developed and implemented in the software produced by Institute of Crystallography. In order to get a final model as complete and refined as possible, we have developed a pipeline based on the synergy between our phase refinement algorithms[2] and some Automated Model Building programs (AMB) distributed by different scientific teams. Among them we have selected the program Buccaneer,[3] a well known fast and efficient automatic model building program, using it also as a tool for phase refinement: indeed input phases are used for calculating electron density maps which are interpreted in terms of molecular model, from which new phase estimates may be obtained in a cyclic way. This procedure, called CAB,[4] has been implemented in a modified version of Sir2014.[5]

CAB has been tested on 81 protein structures, solved *via* Molecular Replacement, anomalous dispersion and *ab initio* methods. As it is usually done the phases so obtained were submitted to phase refinement and then they have been used as input for CAB. The experimental results were compared with those obtained with the use of Buccaneer alone: it is shown that CAB improves Buccaneer results, both in completeness and in accuracy.

The work is in progress in order to apply such a philosopy to DNA/RNA structures using Nautilus[6] as AMB program.

An example of application to a protein of Molecular Replacement + CAB will be presented.

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Riferimenti

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