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Complete Automation of Molecular Replacement. F. Long, A.A. Vagin, G.N. Murshudov, Chemistry Dept., Univ. of York, York, YO10 5YW, UK.

Analysis of the PDB shows that this year around 67% of all the deposited structures are solved by molecular replacement. With better algorithms and organisation of data bank it can be expected that this number will be substantially higher. This talk will describe a complete automation of molecular replacement. There are three main components of this work: (1) Reorganisation of database of proteins. All entries in the PDB have been analysed and only non-redundant sets of protein structure, domains and tertiary information were stored. Hierarchical database according to sequence identities was organised. It means that search for similar structure is very fast (less than 10 seconds). (2) Automatic molecular replacement system was designed using python. The system requires only experimental data – sequence the reflection data. The system begins searching the database and extracting candidate structures. It also analyses the experimental data and makes such decisions as resolution limit, existence of pseudo-translation. Then the system starts molecular replacement and refinement on the candidate structures using several protocols (3) Programs such as MOLREP, REFMAC. We have already tested more than 1000 cases and success rate is more than 75%. It is expected that more than 80% of structures will be solved completely automatically.