Ab initio protein structure prediction with MOLEGO

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We describe the program MOLEGO [1], a system for the ab initio prediction of the tertiary structure of proteins. Given an amino acid sequence, the program searches the protein conformation with the minimal free energy according to an energy model.

The conformational search of the program is discretized by using a library of short structural fragments. Different fragment libraries were developed in our group by applying clustering techniques to a set of fragments of backbone conformations which were taken from protein structures from the PDB database.We show that we can represent structures of natural proteins within a given accuracy by only using these fragments.

MOLEGO searches the discretized conformational space with a branch and bound algorithm. The used energy model is a contact potential with 26 atom types [2].

Preliminary results of the MOLEGO program were submitted to the CASP3 conference. Tertiary structure predictions of Casp3 targets 59, 61, 65 and 84 were submitted. The structure predictions of the targets 65 and 84 have an rms deviation of equal or less than 5 Ångström to the native protein structure [3].

References

[1] http://www-mp.informatik.uni-mannheim.de/groups/ga/molego.html

[2] Ai-Jun Li, Ruth Nussinov: A Set of van der Waals and Coulombic Radii of Protein Atoms for Molecular and Solvent-Accessible Surface Calculation, Packing Evaluation, and Docking. PROTEINS 32, 111-127 (1998).

[3] Third Meeting on the Critical Assessment of Techniques for Protein Structure Prediction (1998). Conference handout.