P03.07.26

Acta Cryst. (2008). A**64**, C226

Prediction of secondary structure and dihedral angles in proteins

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A method for simultaneous prediction of secondary structure and dihedral angles of the polypeptide backbone in proteins is presented here. Based on a ten-fold cross-validation on a non-redundant set of 2670 protein chains with <= 25% sequence identity, the three-state accuracy (Q3) is 81-82%. Every doubling of the number of non-redundant protein chains used in the training set results in 1% better prediction of secondary structure. With the dihedral angles discretized as 8 or 3 states on the Ramachandran plot, the accuracies for shape symbol prediction are 68.4% and 82.1% respectively. Thus, we show here for the first time that the conformations of all amino acids in proteins can be as accurately predicted as the secondary structure. Out of the residues predicted to be random coils with accuracy of 76.5%, 69.2% of corresponding shape symbols is predicted correctly in 3-state shape classification.

Keywords: structure prediction, secondary structure, dihedral angles

P03.11.27

Acta Cryst. (2008). A**64**, C226

Crystal structure prediction of flexible molecules with genetic algorithms and standard force field

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In this presentation we describe our distributed computing framework for crystal structure prediction, MGAC (Modified Genetic Algorithms for Crystal and Cluster Prediction) and its application to predict the structure of flexible molecules using CHARMM with the Generalized Amber Force Field (GAFF). MGAC is capable of performing crystal structure searches for flexible molecules within any space group and with an arbitrary number of molecules in the asymmetric unit. The distributed computing framework includes a series of tightly integrated computer programs for generating the molecule's force field, sampling possible crystal structures using a distributed parallel genetic algorithm, locally minimization of the structures and classifying, sorting and archiving the most relevant ones. Our results indicate the method can consistently find the experimentally known structures of a set of flexible molecules when GAFF reproduces the torsional energetics of the molecule, but unfortunately in some cases GAFF exhibit serious errors in describing this energetics. For instance the match between the experimental and predicted structures of norephedrine (racemic 2-amino-1-phenyl-1-propanol) has an RMS (root-mean-square) of 0.315 Å over a cluster of 15 molecules using the COMPACK, (Chisholm, J. A. and S. Motherwell, 2005, J. of App. Crystall. 38, 228) method. Both the experimental and predicted structure belong to the P21/c symmetry group, with the predicted cell parameters of (experimental values in parenthesis), a = 12.447 Å (12.507 Å), b = 8.293 Å (8.771 Å), c =7.808 Å (8.130 Å) and β = 104.63° (106.20°).

Keywords: crystal structure prediction, crystal structure software, parallel algorithms

P03.11.28

Acta Cryst. (2008). A**64**, C226

Hybrid genetic algorithm for a full-profile analysis of XRD powder patterns

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The full-profile fitting of powder patterns by Rietveld method is widespread tool for refinement of structural models as well as for quantitative phase analysis. The full-profile fitting is based on non-linear least-square method (NLSM) and is executed for different groups of refinement parameters consecutively. NLSM requires a good initial approximation of refinement parameters. Over the past few years, a genetic algorithm (GA) has been used to determine structural models of powders successfully. The focus of this work is to extend GA to the Rietveld method including full-profile fitting and refinement of crystal structure models and phase content. A hybrid two-level evolutionary genetic algorithm has been developed for this purpose. The hybrid algorithm is based on composition of a conventional GA with a NLSM designed as follows. First-level GA chromosomes comprise values of profile and structure parameters like that are used in the Rietveld method. Second-level GA chromosome is a bit string containing one bit per each parameter. Unit bits define the group of parameters to be refined with the NLSM on a current iteration. GA fitness function is the usual weighted profile R-factor (Rwp). The first-level GA determines initial parameter values of acceptable Rwp. The second-level GA manages NLSM full-profile fitting with found initial parameter values. A number of the parametric masks are used for reduction of dimensionality of the problem. The algorithm was implemented as a shell over the full-profile analysis program DDM [1] and was tested on some powder patterns of single and multi-phases samples with known stable crystal structures.

1. Solovyov L. A. // J. Appl. Cryst. 2004. 37. 743-749.

Keywords: evolutionary algorithm, full-profile analysis, Rietveld method

P03.11.29

Acta Cryst. (2008). A**64**, C226–227

Consistency of particle shape determination from small-angle scattering data: Computer modeling

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Ab initio determination of shape of homogeneous particles from small angle scattering data obtained from monodisperse samples is considered. It was analytically shown that in the case of expansion of shape of homogeneous body in a limited orthogonal series of spherical harmonics the solution ambiguity consists in obtaining