

New Approach for Selecting and Designing Fast Folding Proteins

Dmitry Gridnev and Martin E. Garcia

*Theoretische Physik, FB 18, and Center for Interdisciplinary Nanost
ructure Science (CINSaT), Universität Kassel, Heinrich-Plett-Str. 40,
34132 Kassel, Germany*

garcia@physik.uni-kassel.de

We propose a general algorithm for predicting good folding proteins and for determining their folding temperature. It uses the Monte Carlo dynamics and tests the rate of convergence of a an amino acid chain in the configuration space. The algorithm can be applied to any kind of models (lattice, off-lattice, go-type, atomistic) and does not require the previous knowledge of the native structure. We tested our approach in the framework of the lattice model and obtained several good folders not found before. The algorithm takes considerably less time than the actual folding time of the proteins.