A Genetic Algorithm Study of the Protein Folding Problem

Graham A. Cox*, Thomas V. Mortimer−Jones, Robert P. Taylor and Roy L. Johnston

School of Chemical Sciences, University of Birmingham

Determining the comformation of the "native" state of a folded protein is one of the most challenging problems in science today. Due to the high dimensionality of the conformational space and the complexity of the energy surface, computational searches prove very expensive, therefore simplifed models and search algorithms are employed to investigate the protein folding problem.

In this study protein conformations and intramolecular interactions are modelled using the simplifed HP Bead Model. This work develops a genetic algorithm to search the energy surface to gain an insight into the folding of proteins.