# Predicting Peptides Structure with Solvation Potential and Rotamer Library Dependent of the Backbone

Luis P. B. Scott
CMCC - Universidade Federal do ABC
Rua Catequese, 242 - Jardim
CEP: 09090-400 - Santo André – SP, Brasil
Phone: (55) (11) 4437-1600
Fax: (55) (11) 4437-1600
email: luis.scott@ufabc.edu.br

. The work reported in this paper present the use of Genetic Algorithms (GA) with distinct field forces and rotamer library dependent of backbone to predict the tertiary structure of peptides. We discuss an improved version in which the backbone and side chain were relaxed and a rotamer library dependent of the backbone was used library give the four most probably values of the angles $\chi_i$ for the side chains of each amino acid and for each combination of angles pairs [φ,ϕ]. This library may be find in: *http://www.fccc.edu/research/labs/dunbrack/bbdep.html*.

Two versions of the genetic algorithm were implemented to predict the structure of peptides with different force fields. In both implementations, the population is composed by 440 chromosomes (220 elements). Each element contains information describing a conformation of the side chain and of the backbone in a pair of chromosomes (two parts). The first part is encoded in it as a set of active rotamers for position of the side chains with a specific angle $\chi_i$ and the second part of the information is encoded in chromosome as a set the dihedrals angles **[φ,ϕ].** The algorithm is responsible to keep the chromosome consistency. The set of elements (pairs of chromosome) represents different possible conformations of peptides.

The Genetic Algorithm works with internal coordinates of the backbone and the side chain angles and it uses an initial population completely randomly. The crossover operation is made by exchanging pieces of two chromosomes pairs to search the conformational space (where each pair represents encoded the backbone and side chain representations). The crossover points are selected randomly and it is the same points in both representations. The condition to accept the crossover is the Metropolis test. The algorithm was used to predict the structure of two peptides: polyalanine e polyisoleucine. The both peptide was composed by 20 monomers.

The GA with solvation term found a helix structure to the polyalanine with the lower energy. We could observe that term of implicit solvation is very important to the efficiency of the AG when the backbone is relaxed and a rotamer library is used in this case.

The results, describe in this work, show that the system called YODA-2 can be a tool to prediction 3D and it can help the peptides study. One important topic of this paper is the use of a rotamer library dependent of the backbone and the backbone relaxed. It was possible to verify that this kind of library can be efficient and important to the conformation search. The use of this resource join with a potential solvation allow the GA obtain a good prediction of the polyalanine structure.

In the future, we will be interested to investigate the use of others rotamer library dependent of the backbone. Beside, this GA will be tested with others peptides and molecule segments. Another further work will be to combine the Genetic Algorithms and Dynamic Molecular.

**Aknowledgments**
The authors thank the Fundação de Amparo à Pesquisa do Estado de São Paulo – FAPESP. This work was supported by FAPESP.