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Use of homology information in replica exchange methods for *de-novo* protein fold prediction

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The performance of *ab-initio* methods for protein fold prediction strongly depends on two components: an energy function that is expected to have a stable minimum near the native structure and a method for finding this minimum through the protein conformational space. Monte Carlo replica exchange methods provided a major advance to the latter point, outperforming widely used methods such as the original Monte Carlo Simulated annealing in terms of sampling low-energy states. The Hamiltonian Replica Exchange is one of the most promising among these novel methods. It is accepted that homologous proteins have similar native structures, thus their energy landscapes and therefore their hamiltonians must be similar, at least nearby such conformation. This allowed us to develop, starting from a standard ab-initio protocol implemented using the Rosetta modeling suite, a Replica Exchange method in which the hamiltonians of homologous proteins are used to characterize the replicas. In a pilot study on 40 different domains selected from the SCOP database, we observe that our method is able to improve the exploration of energy landscapes thanks to the exchange of homology information during the Monte Carlo simulation and to reach better solutions in terms of both lower energy and distance from the native structure. These preliminary results show that our novel approach to use homology information can greatly improve the performance of *ab-initio* methods for protein structure prediction, both overcoming errors and approximation in the energy functions, improving the ability of the Monte Carlo method to avoid spurious local minima and allowing for a more efficient search of the conformational space.

Biography

Alfredo Iacoangeli is a Ph.D student at the Molecular Medicine department of the University of Rome, "La Sapienza," Italy. He obtained both his Bachelor's degree (2010) in Physics and his Master's Degree (2012) in BioPhysics at the University of Rome, "La Sapienza," Italy. During his studies he spent one year in the UK at the University of Birmingham, joining an exchange programme, and one year in Spain at the University of Granada as a visiting student. During the final year of his Master's Degree (Sept-2011) he joined the Biocomputing Group (www.biocomputing.it) of Prof. Anna Tramontano, in which he is still working as a Ph.D student (since Nov-2012).

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