Ab initio Protein Structure Prediction with Estimation of Distribution Algorithm and full-atom model

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Estimation of Distributions Algorithms (EDAs) are optimization techniques that are, in general, capable to find the global optimum without using prior knowledge of the problem. They are based on the frequency distribution of variable values to compose new solutions. We proposed an EDA applied to Protein Structure Prediction using full-atom and pure ab initio that minimizes the potential energy of solutions (proteins conformations) in order to find the global minimum. EDA allows finding better solutions than a Genetic Algorithm (GA), since EDAs combine information about promisor solutions to create new individuals, while GA uses information over two or three individuals. The results show that the EDA is capable to predict the same structure as a GA predicts. However, the EDA is capable to find the same solution using less prior knowledge of the problem, reducing the bias of prediction. In order to use such optimization technique for public access, was also developed a web interface that enables the prediction of small proteins online. A web interface shows the energy and the 3D geometry of the best conformation found at each step. The user can visualize the significant changes of protein conformations and to try making some relationship with the real process of the protein folding.

Word Keys: Protein Structure Prediction, Estimation of Distributions Algorithms, ab initio, full atom
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