A Model for HP Folding Prediction Using Increasing Constrain for Spreading in the Process of Making Conformations

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The 3D structure of proteins is the major factor that determines their biological activity. The synthesis of new proteins and the crystallographic analysis of their 3D structure is very slow and very expensive process. If we can predict the 3D structure of many proteins, than only proteins with expected properties have to be synthesized. The main idea, implemented in our research, is not to use lattice cube with constant size to make possible conformations in this space, but to use flexible constrain for spreading away from the center of the formed molecule, which constrain has a coefficient that can vary in the process of folding according the percentage of failing to make possible conformation, caused by lack of space. Less space allowed causes difficulties to make the conformations but the achieved forms are more compact and with lower energy. More space causes making many useless random conformations and more computational time is needed to find the best conformation and to make the same one more times in this random process in order to have bigger probability that it is the best one. This method may be used in every other model for protein folding prediction to improve the computational time and the probability of finding the accurate 3D structure our results show that advantage.

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