CONFORMATION-DEPENDENT SEQUENCE DESIGN: BIO-EVOLUTION MIMETICS APPROACH

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The concept of evolution of primary sequences of biopolymers attends large interest of biologists, chemists and physicists for a long time. The progress in this field will help a lot both in understanding of biological evolution and in creation of synthetic "functional" copolymers.

In the present investigation a new modification of the so-called conformation-dependent sequence design scheme [1] is proposed. A model of step-by-step evolution of a two-letter (HP) copolymer sequence has been studied by means of a coarse-grained Monte Carlo algorithm. The conditions, which have to be satisfied in order to allow a change in the primary sequence, depend on the spatial conformation of HP-copolymer chain. This leads to a coupling between sequence and conformation and to formation of non-trivial primary sequences for some values of parameters of the model. Our approach differs from previously discussed schemes [2]. It does not involve frozen conformations and attempts to find optimum sequence for "target" conformation, but rather performs optimization both in the space of sequences and in the conformational space.

This model can be considered as a "toy" model of the evolutionary process: the rearrangement of unit types corresponds to random mutations in sequences of biopolymers. Here our approach is not involving the attempts to mimic biopolymers at the present stage of biological evolution (for synthetic polymer systems this is definitely too complicated and ambitious task), but rather to understand the principles of biological evolution of sequences at the early stages of evolution and to implement these principles for synthetic copolymers in order to obtain polymer systems with special sophisticated functional properties. This approach can be called bio-evolution mimetics. The proposed method can be easily extrapolated to more complex external conditions and interactions of units.

The financial support from Alexander-von-Humboldt Foundation, Program for Investment in the Future (ZIP), INTAS (project 01-607), and Russian Foundation for Basic Research is highly appreciated.

References:

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