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Conformational alphabets in the study of protein structure

Life science, bringing us ever-growing unexplained data, is attracting increasing interest from physicists. Protein structure is a good subject for physicists to study, being simple enough yet, at the same time, complex enough. Conformational alphabets (CAs) provide discrete representation for the protein local structure. We have proposed an alphabet based on the distribution of three C-alpha pseudobond angles, and constructed its substitution matrix. We have succeeded in developing a fast alignment tool for multiple protein structures by means of our CA. Such alphabets, bridging the secondary and 3D structures, facilitate computations for protein structures. Our focus is on the development of a reliable statistical potential function using CAs, and improving structure prediction.

This is a rich territory for collaboration amongst physicists, computer scientists, mathematicians, and biologists. (I am involved in an ongoing collaboration between the Metagenomics of the Human Intestinal Tract (MetaHIT) program of the European Commission and Beijing Genomics Institute, Shenzhen.)

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