

Protein folding: From simple models to real proteins

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Abstract:

In my seminar I focus on the problem of protein folding and show how simple models help to understand evolution and function of natural proteins through simulations.

I describe the state-of-the-art in computational and experimental protein folding: what we can do and what we want to do in the field. I introduce you to the world of toy proteins that can fold on the cubic lattice, mutate and evolve. In this toy world we simulate evolution with selection favoring rapid folding. We study the properties of emerged rapidly folding proteins and find amino acids crucial for providing rapid folding.

We use these findings to develop an algorithm for identifying such amino acids in real proteins. Experiments show that amino acids found by our algorithm are either responsible for providing fast folding or are involved in the functionally important "super-sites."

The presented analysis also helps to clarify the relation between folding and function, which is apparent for some proteins.