Emergent organisation in complex biomolecular systems - EMBIO

The consortium

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University of **Florence** (Florence, Italy)

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University of **Vienna** (Vienna, Austria)

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Main idea

Biomolecular systems exhibit spontaneous self-organisation that is critical to their function. Examples are protein folding and the self-assembly of membranes. The project aims to develop mathematical and computational approaches primarily to identify the poorly understood principles of this phenomenon. This will provide a basis for modelling of this fundamental property of complex biomolecular systems and will therefore be of great importance to biology, medicine and biotechnology.

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The objectives

The goal of the project is to **quantify the complexity associated with self-organization in bio-molecular systems as a means to understand complex phenomena in systems that exhibit spontaneous emergence.** Specific objectives are:

- to monitor the process of emergent *complexity* by performing all-atom simulations of peptide/protein folding and lipid membrane self-assembly in explicit water;
- to obtain detailed, all-atom data on representative regions of the free energy landscape (*folding funnel)* by simulating biopolymers (proteins and/or RNA) in their denatured and native forms;
- to investigate the *sequence space* of RNA molecular models and its effect on the *kinetics of folding*;
- to study topological, statistical and dynamic properties of *generic* potential energy and fitness *surfaces* in models of polypeptides and in RNA during self-organization;
- to find and characterize the features of the free energy *funnel* for simplified protein-in-water *dynamic models* in order to distinguish between “good” and “bad” folders;
- to define and describe parameters of the folding-unfolding *pathways* on the free energy *funnel* through the experimental mechanical stretching of giant single molecular proteins;
- to reconstruct *dynamic hierarchies* in a model bio-polymer system thus directly detecting the *emergence* of the *dynamic forms* and *information flow* at different scales in the system;
- to calculate the *dynamic complexity* of the system’s trajectories in different regions of the energy funnel as well as the folding process as a whole.

One of the objectives of the project is to collect the approaches and algorithms for quantitative estimation of complexity of a general multidimensional dynamic system. These can be applied to a large variety of complex systems in any branch of natural and social sciences.