

Proteins: an example of supervised dynamics

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Abstract: Proteins are remarkable functional materials produced by living organisms. A ‘simple’ sequence of building blocks, so-called amino acids, encodes information for the construction, the function and the performances of the material upon perturbations.

We will discuss through various case studies, using experimental and network modelling results, how a protein sequence codes for customized spatial packing of amino acids in order to supervise protein multi-scale dynamics.

The dynamics involved in protein function, protein folding and protein misfolding will be explored comparing network features of the structure of the cholera toxin B pentamer (CtxB₅) with the structure of the heat labile enterotoxin B pentamer and with the structures of two proteins, the pore forming toxin aerolysin and the tumor-suppressor p53, known to adopt several conformations¹⁻³ (Fig. 1).



Figure 1. From atomic structures to network models: protein structure plasticity. Left, soluble aerolysin dimer and hydrophobic aerolysin heptamer. Right, the network models of aerolysin dimer and heptamer.

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