

Conférence



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Rational Design of Protein Energy Landscapes

Proteins have found widespread application in research, industry, and medicine because they can mediate complex molecular processes with extreme precision and efficiency. Even so, continued engineering of proteins with tailored functions is essential to enable novel biotechnological applications. Computational protein design (CPD) has enjoyed considerable success in creating protein sequences that stably adopt a single targeted structure. However, attempts to use these methods to generate proteins that can carry out specific functions have mostly failed to match the efficiencies that are found in nature. This is partly due to the fact that most CPD methods evaluate sequence energies in the context of a single structure even though protein function is dictated by the energetic contributions of many conformational states. To increase the accuracy of CPD predictions and thereby design more efficient proteins, we are developing multistate CPD methods that can evaluate sequences in the context of any number of protein conformational states, allowing energy landscapes to be engineered for specific functions. I will show how these methods can be used to design proteins that undergo a specific mode of conformational exchange, as well as *de novo* enzymes for desired chemical reactions.