Exploring the protein assembly space with structural flexibility

Alena Khmelinskaia
Ludwig Maximilian University of Munich

1. Abstract

Recent computational methods have been developed for designing novel protein assemblies with atomic-level accuracy, yet several aspects of current methods limit the structural and functional space that can be explored. For example, the underlying perfect symmetry limits the size and types of architectures that can be designed. I will discuss how local instabilities introduce structural flexibility in protein scaffolds, breaking symmetry and vastly expanding the repertoire of possible target architectures. Then, I'll share with you our ongoing efforts in predicting and controlling local structural flexibility on a sequence level.