Multifunnel energy landscapes - how multiple functions are encoded in biomolecules

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Abstract

Exploration of the energy landscape of biomolecules gives access to all information necessary to calculate structural, mechanistic, thermodynamic and kinetic data. Discrete path sampling (DPS) has been developed to utilise geometry optimisation techniques to allow for efficiently sampling energy landscapes. In this talk I will discuss the recent application of DPS to multifunctional biomolecules. The discussion will include case studies, a descriptions of charachteristic topologies, and implications of our results for experiments and biomolecular design.

Keywords: Multifunctional biomolecules, Multifunnel energy landscapes

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