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New strategy for protein interactions and application to structure-based drug design[1]

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One of the greatest challenges in computational biophysics is to predict interactions between biological molecules, which play critical roles in biological processes and rational design of therapeutic drugs. Biomolecular interactions involve delicate interplay between multiple interactions, including electrostatic interactions, van der Waals interactions, solvent effect, and conformational entropic effect. Accurate determination of these complex and subtle interactions is challenging. Moreover, a biological molecule such as a protein usually consists of thousands of atoms, and thus occupies a huge conformational space. The large degrees of freedom pose further challenges for accurate prediction of biomolecular interactions. Here, I will present our development of physics-based theory and computational modeling on protein interactions with other molecules. The major strategy is to extract microscopic energetics from the information embedded in the experimentally-determined structures of protein complexes. I will also present applications of the methods to structure-based therapeutic design.

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