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Physics-based Visual Characterization of Molecular Interaction Forces

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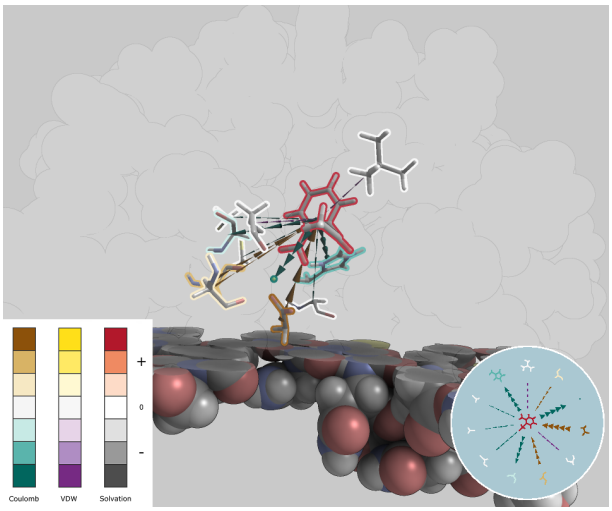

Molecular simulations are used in many areas of biotechnology, such as drug design and enzyme engineering. Despite the development of automatic computational protocols, analysis of molecular interactions is still a major aspect where human comprehension and intuition are key to accelerate, analyze, and propose modifications to the molecule of interest. Most visualization algorithms help the users by providing an accurate depiction of the spatial arrangement: the atoms involved in inter-molecular contacts. There are few tools that provide visual information on the forces governing molecular docking. However, these tools, commonly restricted to close interaction between atoms, do not consider whole simulation paths, long-range distances and, importantly, do not provide visual cues for a quick and intuitive comprehension of the energy functions (modeling intermolecular interactions) involved. In this paper, we propose visualizations designed to enable the characterization of interaction forces by taking into account several relevant variables such as molecule-ligand distance and the energy function, which is essential to understand binding affinities. We put emphasis on mapping molecular docking paths obtained from Molecular Dynamics or Monte Carlo simulations, and provide time-dependent visualizations for different energy components and particle resolutions: atoms, groups or residues. The presented visualizations have the potential to support domain experts in a more efficient drug or enzyme design process.

http://dx.doi.org/10.1109/TVCG.2016.2598825