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Visual Analysis of Protein-ligand Interactions

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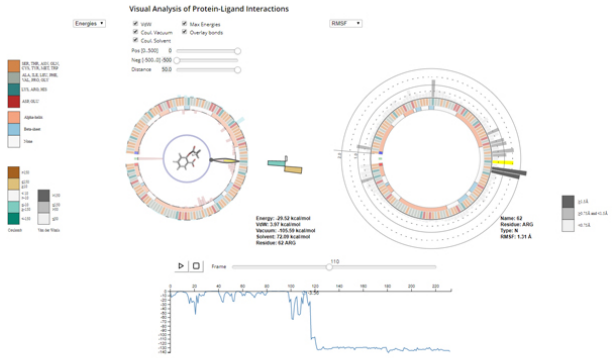

The analysis of protein-ligand interactions is complex because of the many factors at play. Most current methods for visual analysis provide this information in the form of simple 2D plots, which, besides being quite space hungry, often encode a low number of different properties. In this paper we present a system for compact 2D visualization of molecular simulations. It purposely omits most spatial information and presents physical information associated to single molecular components and their pairwise interactions through a set of 2D InfoVis tools with coordinated views, suitable interaction, and focus context techniques to analyze large amounts of data. The system provides a wide range of motifs for elements such as protein secondary structures or hydrogen bond networks, and a set of tools for their interactive inspection, both for a single simulation and for comparing two different simulations. As a result, the analysis of protein-ligand interactions of Molecular Simulation trajectories is greatly facilitated.

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