Visual Computing Forum



Visualizations for conveying biochemical properties across and along protein voids.

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Abstract

Proteins are highly complex systems contributing to all functions in living organisms. Understanding their function helps to reveal the fundamentals of biochemical processes that are taking place in living cells. This search process, however, consumes an enormous amount of time and resources, due to the internal protein dynamics, which constantly change structural and biochemical characteristics of the protein over time. Thus, several in-silico predictive methods already appeared, which focus mostly on the analysis of the protein structure. In this talk we will mainly focus on methods for interactive exploration of protein inner void space including its geometry, physico chemical properties and dynamics to evaluate or modify the reactivity of the protein with other small molecules.

