AnimoAminoMiner: Exploration of Protein Tunnels and their Properties in Molecular Dynamics

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In this paper we propose a novel method for the interactive exploration of protein tunnels. The basic principle of our approach is that we entirely abstract from the 3D/4D space the simulated phenomenon is embedded in. A complex 3D structure and its curvature information is represented only by a straightened tunnel centerline and its width profile. This representation focuses on a key aspect of the studied geometry and frees up graphical estate to key chemical and physical properties represented by surrounding amino acids. The method shows the detailed tunnel profile and its temporal aggregation. The profile is interactively linked with a visual overview of all amino acids which are lining the tunnel over time. In this overview, each amino acid is represented by a set of colored lines depicting the spatial and temporal impact of the amino acid on the corresponding tunnel. This representation clearly shows the importance of amino acids with respect to selected criteria. It helps the biochemists to select the candidate amino acids for mutation which changes the protein function in a desired way. The AnimoAminoMiner was designed in close cooperation with domain experts. Its usefulness is documented by their feedback and a case study, which are included.

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