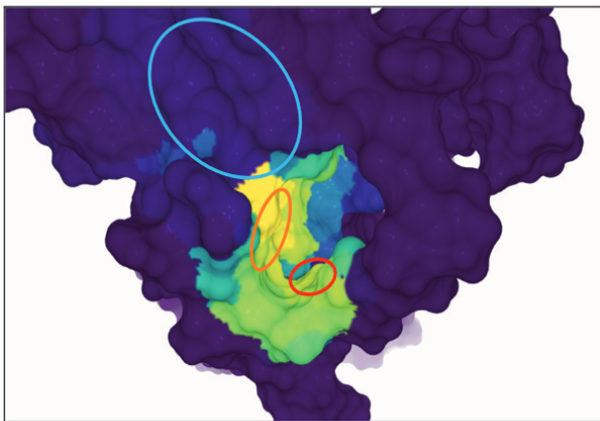


Visual Analysis of Large-Scale Protein-Ligand Interaction Data

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When studying protein-ligand interactions, many different factors can influence the behaviour of the protein as well as the ligands. Molecular visualisation tools typically concentrate on the movement of single ligand molecules; however, viewing only one molecule can merely provide a hint of the overall behaviour of the system. To tackle this issue, we do not focus on the visualisation of the local actions of individual ligand molecules but on the influence of a protein and their overall movement. Since the simulations required to study these problems can have millions of time steps, our presented system decouples visualisation and data

preprocessing: our preprocessing pipeline aggregates the movement of ligand molecules relative to a receptor protein. For data analysis, we present a web-based visualisation application that combines multiple linked 2D and 3D views that display the previously calculated data. The central view, a novel enhanced sequence diagram that shows the calculated values, is linked to a traditional surface visualisation of the protein. This results in an interactive visualisation that is independent of the size of the underlying data, since the memory footprint of the aggregated data for visualisation is constant and very low, even if the raw input consisted of several terabytes.