Studying the patterns of protein interactions is fundamental for understanding the structure and function of biological complexes.

(dva interagující proteiny)

The exploration of the vase space of possible mutual conformations of inereacting proteins is very time consuming and requires non-trivial user experience

(cartoon zobrazení všech 40ti řešení najednou a pak střih na matici, ve které budou tato zobrazení zvlášť)

In this paper we propose a set of novel methods for guided exploration of the conformational space which help the domain experts to select the most biochemically relevant conformations.

(statický obrázek se všema metodama najednou)

These methods were designed to follow the biochemical workflow of the exploration and comparison of the possible conformations.

In the first stage of the workflow the biochemists aim to select a subset of conformations fulfilling given criteria derived from their previous knowledge about the interacting proteins. This step is supported by our Conformation Matrix View and InCo Lens View. These views provide the biochemists with the overview of all conformations by plotting the information about pairs of amino acids from these conformations which are in the interaction distance. Each detected pair contributes to the color of a corresponding cell in the Conformation Matrix View and corresponds to a polyline in the InCo view. This stage helps to select conformations containing the interesting pairs, for example those which are frequently occurring in the input set of conformations.

(video s ukázkou sortování sloupců, výběru a filtrace, interakce s InCo, výběr aminokyselin,…)

These selected conformations can bet further explored in the three-dimensional space using the Conformation Exploded View and Conformation Open-Book View. The Conformation Exploded View serves for comprehensible representation of a set of conformations without any overlaps and occlusion. It enlarges the distance between the interacting proteins and while it maintains the information about the interacting proteins by visualizing a modulated tube between them.

(ukázka rozdílu mezi neexplodovanou a explodovanou variantou, krátký průlet prostorem)

The Conformation Open-Book View servers for detailed exploration of individual conformations. It animates the opening of the conformation thus both parts of its contact zone are visible at once. Additionally, the user can observe the pairing of amino acids and color the contact zones according to different properties of the amino acids, such as their mutual distance, the frequency of their occurrence in the whole set of conformations, or their hydrophobicity.

(animované otevření, ukázky různého barvení, labelling?)

After the detailed exploration of individual conformations, the user can utilize the Conformation List View enabling to compare the lists of amino acids forming the contact zone in a selected set of conformations. The lists can be sorted according to different criteria and help the biochemists to observe the differences in the constitution of the contact zones.

(ukázka list view a různého sortování, porovnání více views vedle sebe)

The proposed visualizations were tested by the domain expert on real datasets and the results confirm that our solutions help to get the insight which was impossible to reach using the existing solutions. In consequence, it helps to understand the interactions in the input conformations and evaluate their biochemical relevance.

(ukázka z těch pěti vybraných řešení)