Protein-Protein Interaction Interactive Exploration

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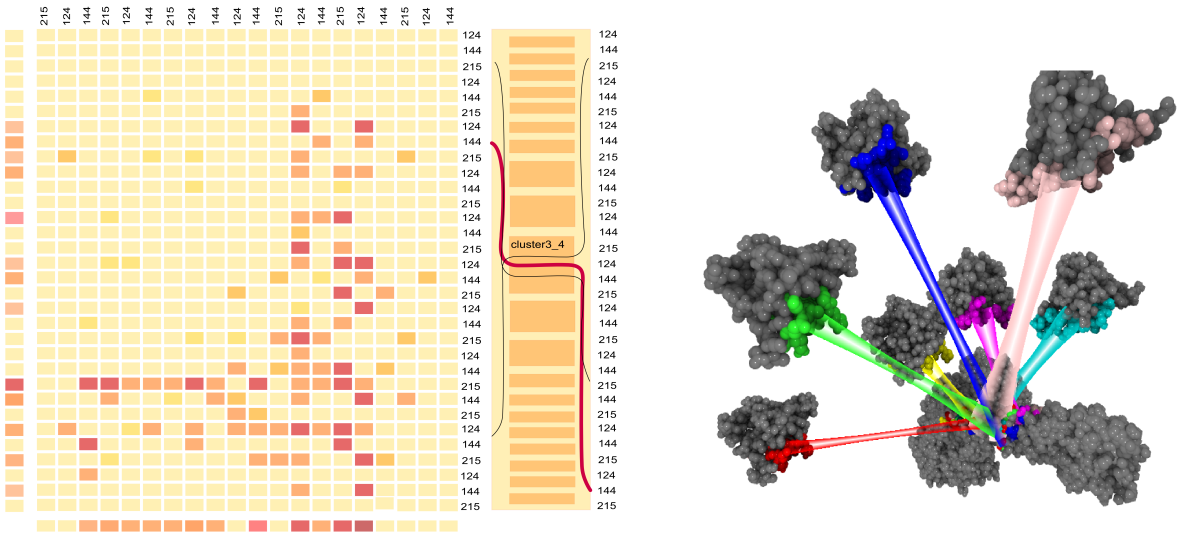

Fig. 1. Visualization methods for exploration of conformations of protein-protein interactions. TODO change image and text.

Abstract—Studying the patterns of protein interactions is fundamental for understanding the structure and function of biological complexes. The exploration of the vast space of possible mutual conformations of interacting proteins and their contact zones is very time consuming and requires non-trivial user experience. Therefore, in this paper we propose three novel methods for guided exploration of the conformational space which help the domain experts to select the most biochemically relevant contact zones and explore them on different levels of detail. The first method, based on customized interactive heat maps, provides the overview of all possible protein conformations and their interactive filtering. The second method enables to traverse the pre-filtered conformations using a lens view. Here the conformation in focus is equipped with the information about interacting amino acids. These techniques are interactively linked with the third proposed method which represents individual conformations in three dimensional space. The problem of high overlaps of the conformations is solved by using exploded views equipped with 2D close-up views showing the details of the contact zone on different levels of abstraction. The usefulness of our methods was evaluated by the domain experts studying the structural maintenance of chromosomes.

Index Terms—Protein-protein interaction, heat plot, exploded view, contact zone.

1 Introduction

Introduction section.

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