Understanding the protein constitution helps to reveal its behavior and function which are crucial in designing new proteins with modified properties. This involves the exploration of the sequence of amino acids forming the protein chain, their grouping into secondary structures, and spatial organization of the chain.

When revealing the properties of a protein chain, one of the most frequent techniques is to compare this chain with other proteins, usually from the same protein family. The similarity between these structures can determine the similarity in their properties as well. However, comparing more protein chains in traditionally used three-dimensional view is very complicated due to occlusion. For these cases the biochemists are using the simple one-dimensional sequential representation which does not possess the information about mutual positions of corresponding secondary structures.

In this paper we proposed a novel visualization which overcomes these problems. It encodes the information about mutual orientation of corresponding secondary structures and thus enables to intuitively reveal the most similar and different parts of the chains. The user can be directly navigated to these significant parts in the three-dimensional view which is also supported by our proposed tool.

The user can interactively explore the superimposed and juxtaposed representations of protein chains, can zoom in and scrutinize the chains in more detail. Moreover, the user can mark a selected chain as the reference one which means that this chain is completely straightened and the remaining chains are aligned to it.

The same approach can be applied to individual time steps of molecular dynamics simulation. In this case the representation encodes the information about the stability and flexibility of the secondary structures over time.

Thank you for watching.