Understanding the protein structure and their reactivity with other molecules helps to design new chemical matters, including new drugs.

One of the most common interactions undergoes between a protein and a small molecule of ligand which enters the deeply buried protein active site.

The trajectory of ligand penetrating from the outer environment to the active site is very complex and the movement is scattered. Therefore, proper understanding of the ligand behavior along its trajectory has to be supported by an exploration tool which helps to reveal the most significant parts of the trajectory. These include parts where the ligand traversed smoothly as well as parts where it got stuck.

In this paper we propose a novel tool for analysis and exploration of ligand trajectories which aims to automatically reveal and explore those interesting parts. Moreover, by untroducing a simplification of the trajectory curve, we are able to convey the main trends in the ligand movement.

First, the user can select an interesting subsection of the whole trajectory. This can be reached by interacting with an overview representation of the whole trajectory which color-codes different positions of the ligand.

Then a selected part of the trajectory can be explored in detail using three linked views – three-dimensional view, scatterplot matrix, and bar charts in combination with line representation of surrounding amino acids.

The three-dimensional view shows the original or simplified trajectory. Selected parts of the trajectory are highlighted by thick tubes. The trajectory can be colored with respect to different criteria.

These criteria, such as ligand speed, distance to the active site, stuckness of the ligand, can be additionaly observed in the scatterplot matrix. Here by interactive brushing the user can select only an interesting part of the trajectory.

Both views are linked with the bar chart representation which enables to show the aggregated information about a given criterion over time. Additionally, the line representation shows the influence of individual amino acids lining the ligand and their changes over time.

Our newly proposed tool was designed in tight cooperation with biochemists and was tested on real simulations of molecular dynamics. The results confirm that our tool helps to navigate the user to the interesting parts of the trajectory and reveal the reasons for such significant behavior of the ligand in those parts.