LassoProt: server to analyze biopolymers with lassos - Supplementary material

Pawel Dabrowski-Tumanski[1,2], Wanda Niemyska[2,3], Pawel Pasznik[2] and Joanna I. Sulkowska*[1,2]

[1] *Centre of New Technologies, University of Warsaw, Banacha 2c, Warsaw, Poland*
[2] *Faculty of Chemistry and Center of New Technologies, University of Warsaw, Pasteura 1, Warsaw, Poland*
[3] *Institute of Mathematics, University of Silesia, Bankowa 14, 40-007 Katowice, Poland*

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1 Identification of piercings in trajectory analysis

In the trajectory analysis we provide two interactive zoomable plots: Lasso type(s) and Atom(s) which pierce the closed loop (Fig. 1). In the first plot the change in lasso type is presented. The second one presents detailed information about change of indices of atoms piercing the surface. The piercings are identified between consecutive frames, resulting in blue (for positively directed) and red (negatively directed) curves.

The identification of piercings in consecutive frames relies on the cut-off sequential distance between essential piercings (10 residues on default). To identify corresponding piercings, first we sort lists of piercings for both frames. Next we cluster together piercings with the same direction if their indices are within the cut-off sequential distance. The piercings left are regarded as new ones (Fig. 2).

Shallow piercings are denoted by dashed lines (Fig. 3). Analysis of piercing appearance and disapearance can reveal much about biopolymer folding. E.g. in Fig. 3 the piercings appear in pairs, which means, that they thread the surface in the slipknot manner.

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*jsulkowska@chem.uw.edu.pl

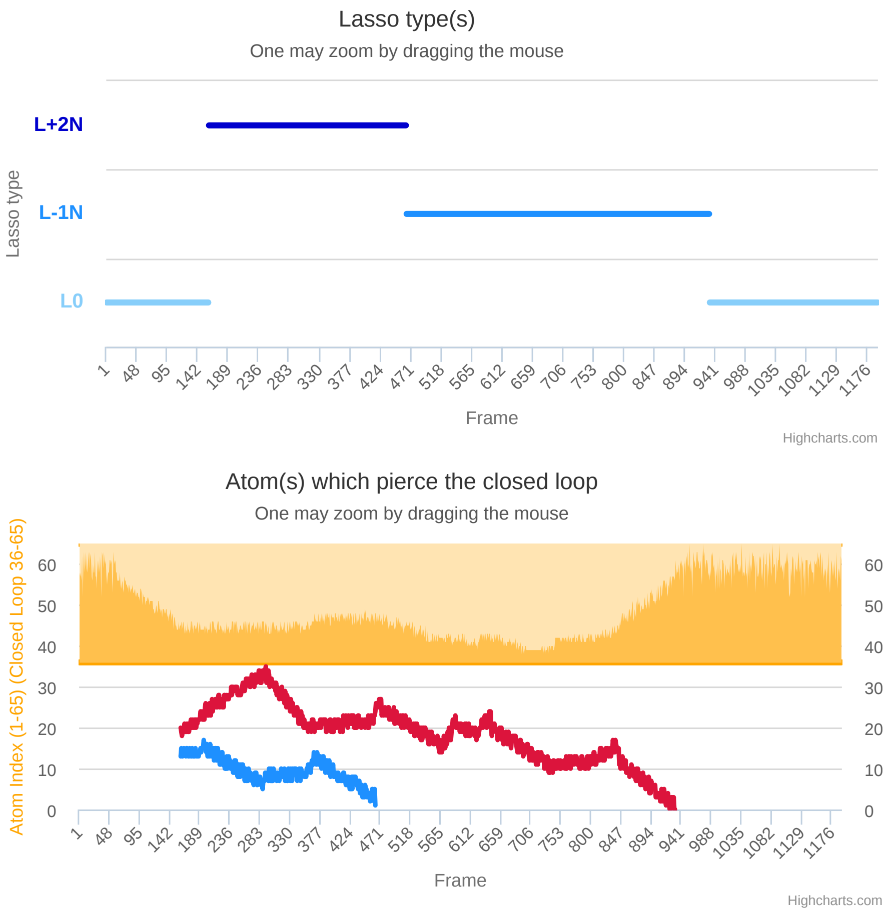

Figure 1: Exemplary charts presenting change in lasso type (upper panel) and change in piercing atom indices (lower panel).

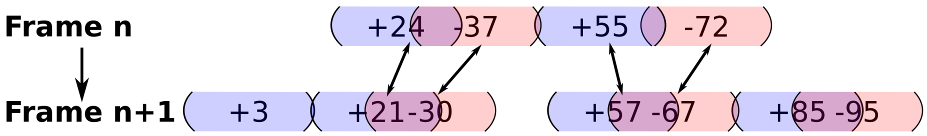

Figure 2: Identification of piercings between two consecutive frames. For each frames the (sorted) list of piercings is printed. The color ovals denote the cut-off sequential distance between essential piercings. The piercings with the same direction falling within cut-off distance are identified (denoted by arrows). Piercings without a corresponding one in previous frame are regarded as new ones. In this case, three new piercings occured.

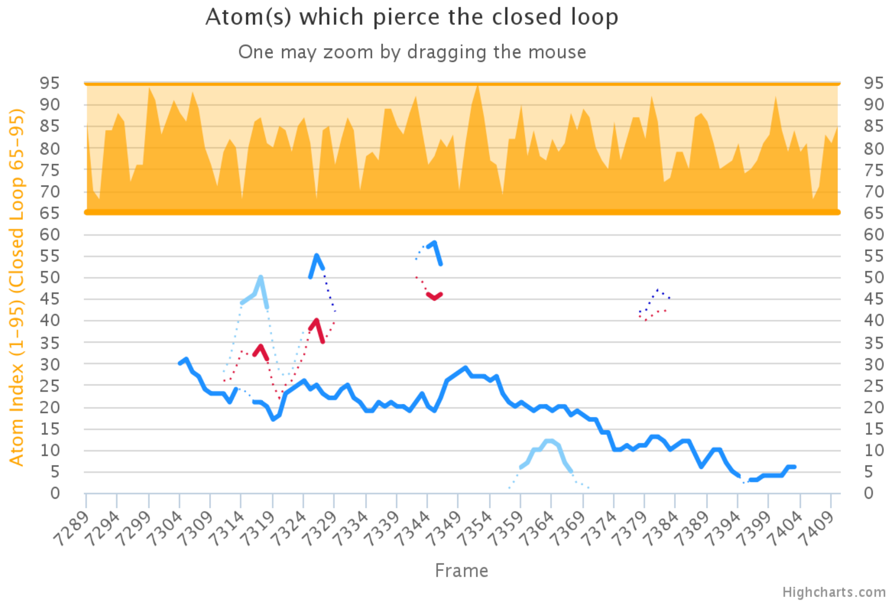

Figure 3: Exemplary plot of indices of atoms piercing the surface. The dashed lines denote shallow piercings.

2 Examples of application of barycentric plot

2.1 Self-crossing surface

The barycentric plots can be especially useful when analyzing complicated, self-crossing surfaces, spanned on large loops. In such case it is sometimes impossible to manually prescribe the direction for each piercing. Moreover, the localization of piercings is hindered. The barycentric plot can be used to localize the piercings and to visualize their direction.

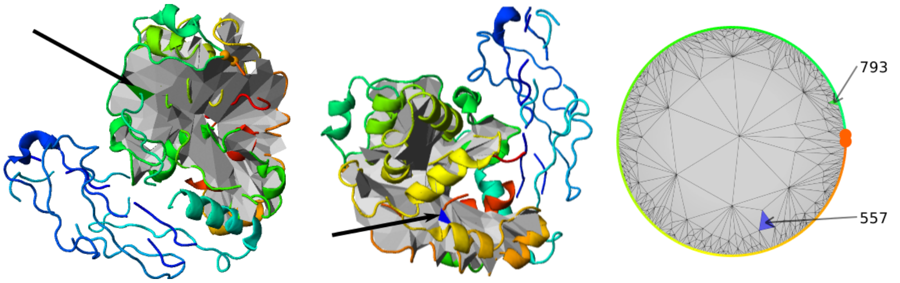

Figure 4: Example of barycentric plot facilitating localization of piercings (hypothetical protein with PDB code 2YHG). The piercing are localized close to the bridge (left panel) and close to the orange part of the chain (central panel). The pierced triangles are denoted by an arrow.

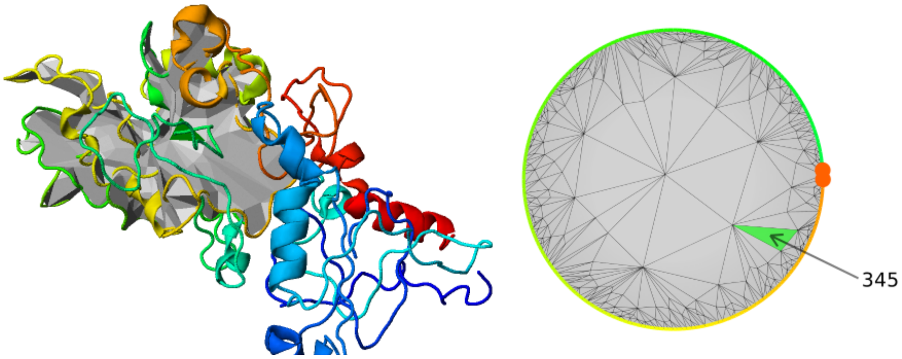

Figure 5: Protein structure and barycentric plot for oxidoreductase with PDB code 4Z80. Barycentric plot shows that pierced triangle locates close to the orange part of the chain.

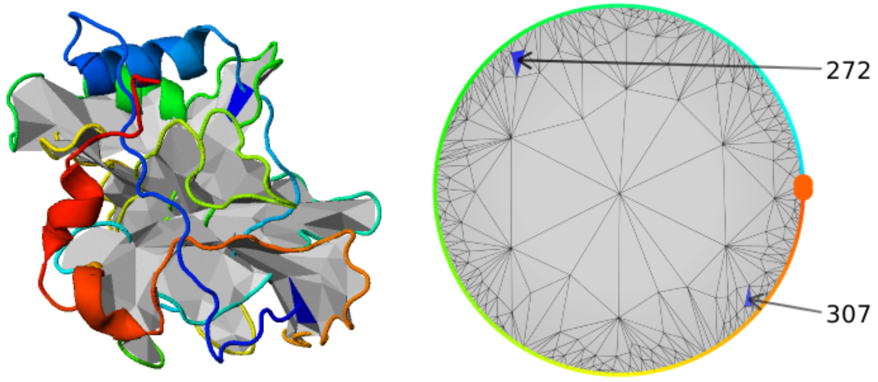

Figure 6: Protein structure and barycentric plot for lyase with PDB code 4XIW. Barycentric plot indicates that the pierced triangles are close to orange and green parts of the chain.

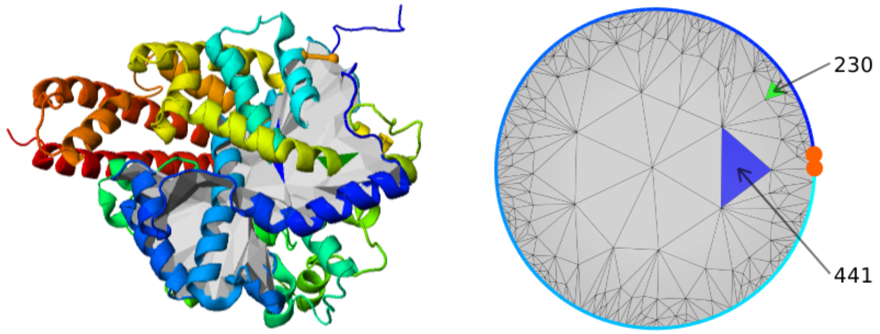

Figure 7: Protein structure and barycentric plot for hydrolase with PDB code 1J36. Barycentric plot indicates that crossings are close to blue fragment of the chain.

2.2 Spatial location of the piercings

The barycentric plot provides also an easy method for selecting structures with piercings spatially closed to each other.

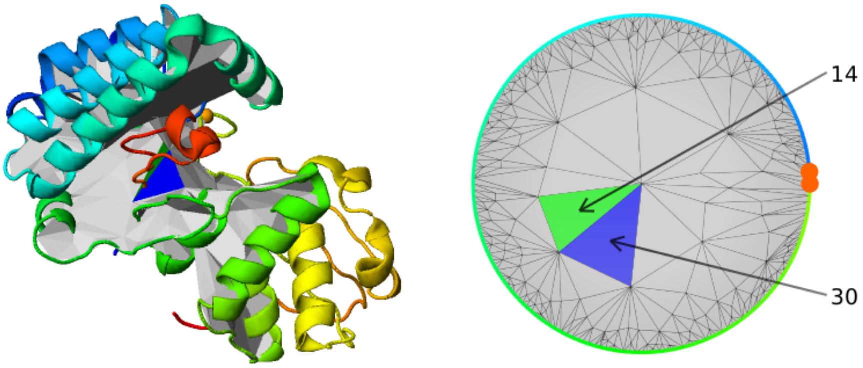

Figure 8: Protein structure and barycentric plot for mevalonate kinase with PDB code 1KKH. Barycentric plot indicates that the piercings (performed by red part of the chain) are spatially close.

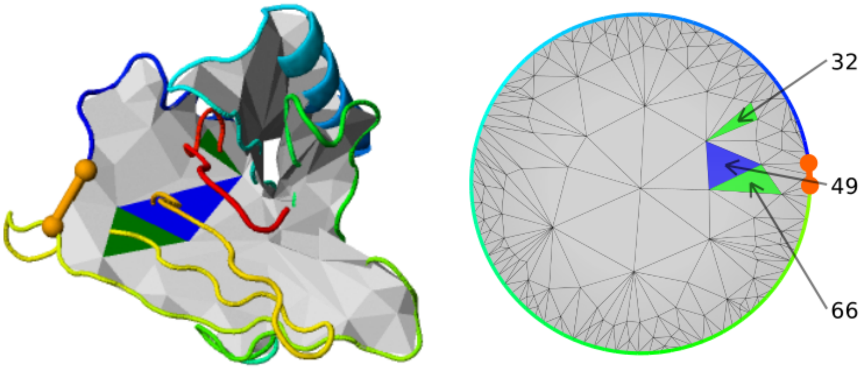

Figure 9: Protein structure and barycentric plot for lipocalin with PDB code 2RA6. Barycentric plot depicts three spatially close piercings.

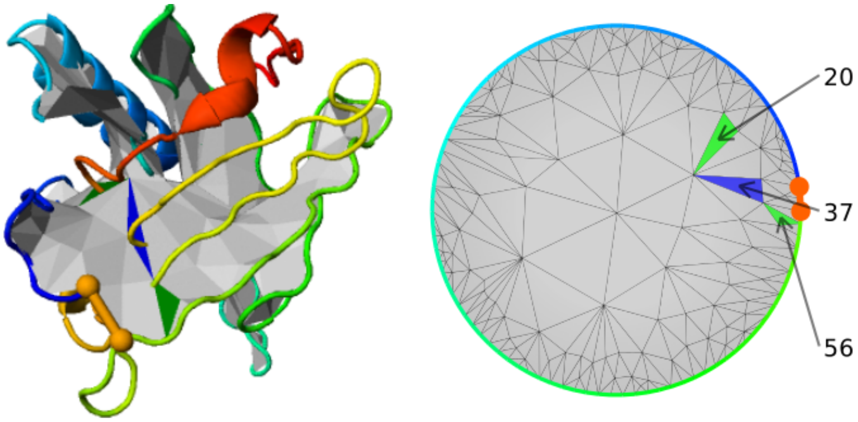

Figure 10: Protein structure and barycentric plot for transport protein with PDB code 3FIQ. Barycentric plot depicts three spatially close piercings.

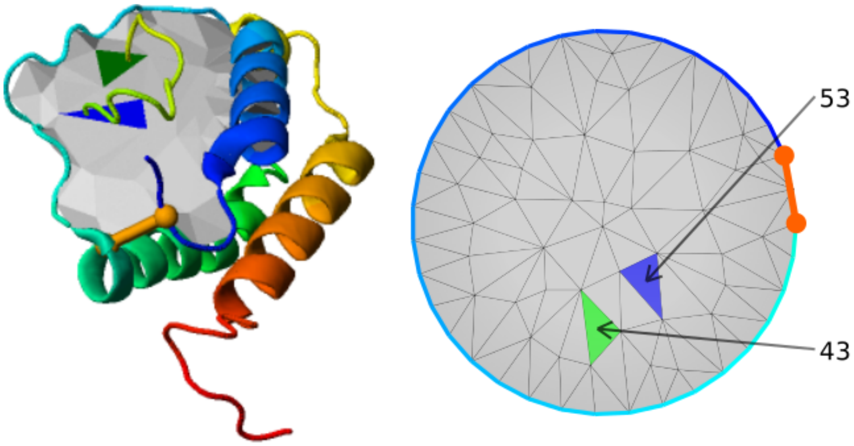

Figure 11: Protein structure and barycentric plot for granulocyte macrophage colony stimulating factor with PDB code 2GMF. Barycentric plot depicts two spatially close piercings.