Contribution ID: **1046** Type: **Oral**

Approaches to the analysis of molecular dynamics trajectories

Monday 24 October 2022 15:30 (15 minutes)

Molecular dynamics (MD) modeling is often becoming a key tool for studying biophysical systems due to increasing computational power and software availability. The MD method makes it possible to study in detail the mobility of molecules, both of their main chains and side chains. As a result of modeling, a large amount of data is generated. The stream of data generated when running an MD simulation even in microseconds is extremely difficult for human perception. Hence, there is a need to adapt already known methods or to come up with new tools for a better understanding of the simulation results. In this work, for these purposes, attempts were made to apply machine learning methods. The current challenge was to analyze in depth the large amount of data generated by the simulations to gain valuable insights and identify general trends.
Some cyclosporins, analogs of cyclosporin A, one of the family of cyclic peptides consisting of 11 amino acid residues, were used as objects. The most variable among them is the second residue.
In this work, high-resolution NMR spectra were preliminarily deciphered, and then MD modeling of various cyclosporine molecules was carried out. Trajectories obtained as a result of molecular dynamics were used for further analysis. Factor analysis was applied to reduce the dimension. Then 33 dihedral angles, which, as a result of factor analysis, became two features, were divided into clusters. The dihedral angles φ and ψ are one of the parameters describing the conformation of the molecule, so that the new division of new components into clusters also indicates that different conformers are present in the model. Python was chosen as the language for implementing the idea, in which we used the built-in method of the sklearn library - K-means.

Author: KOBCHIKOVA, Polina

Co-authors: Mr EFIMOV, Sergey; Mr KLOCHKOV, Vladimir

Presenter: KOBCHIKOVA, Polina

Session Classification: Life Science

Track Classification: Life Science