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AQUA-DUCT – IDEA, IMPLEMENTATION, WORKFLOW AND ANALYSIS

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AQUA-DUCT is a new software dedicated for massive tracing, analysing, and visualisation of molecules movements throughout MD simulations. AQUA-DUCT was developed as a tool for analysis of water molecules movements, but it can be used against any type of molecules. It is implemented in Python 2 programming language. All methods and algorithms are implemented in the library and the driver application provides simple CLI which enables users to perform calculations in steps, provides statistical analysis and visualisation in PyMOL.

During short workshop we would like to familiarize potential users with:

i) idea behind usage of water molecules as a molecular probe for enzyme dynamic description and analysis

ii) implementation of this idea into an easy-to-use tool which enables analysis of the flow of solvent molecules through protein

iii) the workflow of AQUA-DUCT software, its nomenclature including object, scope and tracking molecules definitions, selection of proper methods of clusterization and calculations, and finally

iv) the analysis of results covering general visualizations, detection of preferred entrances to enzymes core, seeking for amino acids important in transport regulation, and statistical data interpretation

Participants should acquire a basic knowledge required for analysis of ligand transportation in enzymes. This should allow to define the penetration pathways in direct and easy way, and can significantly improve understanding of mechanisms controlling enzyme activity. Finally, we aim to present the geometry-based tool which might provide additional information required for successful re-engineering of access pathways leading to active sites buried inside proteins

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Biography

Artur Góra received his PhD degree in Chemistry in 2002 from the Jagiellonian University in Poland. In 2004 he was awarded a JSPS Fellowship, and from 2004 to 2006 he was working at the National Institute of Advanced Industrial Science and Technology in Japan. From 2010 to 2013, he has been a Marie Curie Fellow at the Loschmidt Laboratories of the Masaryk University in Brno, Czech Republic. He is a Leader of Tunneling Group focused on Protein Engineering, Drug Design and Software Development, facilitating molecular dynamic simulations results analysis and interpretation. Since 2016, he is the Vice Director of Biotechnology Centre, Silesian University of Technology in Poland.

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