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CLUSTERIZATION AND PATHS TRIMMING AS A VERSATILE AND UNIVERSAL METHOD FOR ANALYSIS OF SOLVENT FLOW THROUGH THE MACROMOLECULES CORE

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Thousands of single molecules pass through the core of a macromolecule during a course of a molecular dynamic simulation. AQUA-DUCT was developed as an easy-to-use tool which enables to analyze the flow of solvent molecules through any selected region of the macromolecule and group inlets gathered in proximity to surface hollows into separate clusters according to the chosen method of clusterization. Various definitions of the protein surface are provided within the tool, which allows specifying the location of trajectory exits/inlets. AQUA-DUCT stands in for tools which search for tunnels and advanced tools employed for accelerated water flux investigations, optimizing the process of water tracking and yielding clear results. The aim of the study was to examine features offered by AQUA-DUCT used for clusterization and path trimming and to provide a detailed description of water flow through the active site of the protein. The study was performed on a sample simulation of murine soluble epoxide hydrolase structure (PDB ID: 1CQZ). Every option offered by AQUA-DUCT was thoroughly investigated in order to prepare a precise specification of features and explore flow capacity of particular tunnels. The results provide selection of the best methods, which can be potentially useful for analysis of objects dispersed spherically around a macromolecule.

Biography

Agata Raczyńska is a third year Student of Biotechnology at the Faculty of Automatic Control, Electronics and Computer Science at the Silesian University of Technology. She is a member of Tunneling Group at Silesian University of Technology's Biotechnology Centre and within the frames of the group she explored and analyzed features offered by AQUA-DUCT and is involved in project SS-Bridge.

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