EuroSciCon

10th Edition of International Conference on

Structural Biology

March 15-16 2018
Barcelona, Spain

Tomasz Magdziarz, Biochem Mol biol J, Volume 4
DOI: 10.21767/2471-8084-C1-008

WATER FLOW: MOLECULAR DYNAMICS EQUILIBRIUM RELATIONSHIPS

Tomasz Magdziarz

Silesian University of Technology, Poland

Explicit solvent molecular dynamics simulations allow studying biological systems in a very detailed and accurate manner. This proves to be particularly useful for proteins where access of water to the protein core plays a key role in biological functions. In such systems, water, protein and other molecules make one coherent system where all components interact to each other. In the properly set up and performed molecular dynamics simulations, mutual interactions of the system's components can be observed and analyzed. Water-protein interactions are particularly interesting because of their dual nature. Analysis of specific interactions of particular molecules in the key regions of the active site can benefit in better understanding of catalytic function of the enzyme. On the other hand, due to an abundance of water molecules in the simulated system their interaction with protein becomes unspecific. Hence, the flow of water can be used to study the overall behavior of the simulated system and in particular it can be used to detect local equilibrium states. Here, we present application of our newly developed tool, AQUA-DUCT, for the analysis of relationships between water flow and protein local equilibrium states in molecular dynamics simulations. Provided example illustrates how the changes in water transportation reflect changes in protein movements and how it can be used to detect equilibrium states.

Biography

Tomasz Magdziarz received his PhD Degree in Chemistry in 2008 from the University of Silesia in Katowice. From 2007 to 2011, he was working at the Institute of Chemistry in Katowice. In 2011, he joined Molecular-Networks GmbH Computerchemie in Erlangen, Germany. Since 2015, he is the member of Tunneling Group and works at Silesian University of Technology, Biotechnology Centre in Gliwice, Poland.

t.magdziarz@tunnelinggroup.pl