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Water tracking as an alternative method for tunnels search in proteins core - Artur Gora -Silesian University of Technology, Poland

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Abstract

In past years, several tools for porous, tunnels and pathways identification in macromolecules were developed. The most recent ones like CAVER 3.0 or Mole 2.0 can facilitate analysis of molecular dynamic (MD) simulations and allow gathering precise information about the geometry of detected pathways and their prolongation in time. However, the mentioned methods use a spherical probe for tunnels exploration, thus providing an approximation of tunnels to tubes with symmetrical diameter instead of real tunnel picture. Moreover, the knowledge of geometrical properties of existing tunnels can only suggest ways of solvent or ligands molecules entry/exits. It is hard to estimate what are the major factors controlling the solvent flow: tunnel diameter, the length of the tunnel and the properties of amino acids that build the tunnel. It is also unclear how long the tunnel needs to be detected as an open one to provide access for the desired molecule. In principle, MD simulations provide such information.

Simulated protein is immersed in water box and during the entire simulation, water molecules penetrate the protein core. However, the identification and tracking of water molecules which enter regions important for catalysis, require screening of position of thousands dozens of single molecules along several thousands of MD steps. To facilitate analysis of the behaviour of water (and if necessary other solvent molecules or ligands), we have developed AQUADUCT. Here we would like to provide an example of its usage for analysis of water transportation in selected enzymes, which allows defining the water penetration pathways directly and in an easy way distinct the substrate and water pathway.