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VERIFICATION OF LOOP-REBUILDING METHOD

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Epoxide hydrolases belong to alpha/beta hydrolases superfamily; hydrolytic enzymes that share a common fold. The core of these proteins consists of 8 beta-barrels connected by 6 alpha-helices. Their active site is buried inside the protein's core and connected with the environment by tunnels. The accessibility of such active sites could be controlled by a single amino acid or even few amino acids located on an unorganized loop structure. The spatial model of ***Aspergillus niger*** epoxide hydrolase deposited in Protein Data Bank (PDB) database lacks a 9-amino-acids long loop: ^{320}TASAPNGAT^{328}. The missing loop is located near the entrance to the active site cavity, and thus controls access to the active site. The aim of the study was to rebuild the missing loop of ***A. niger*** enzyme, to verify correctness of the model and propose an approach that can be used in similar cases. The stability of construction and examination of loop geometry was validated using standard approaches (RMSD, RMSF, DOPE) and was extended towards analysis of water radial distribution, water flow and tunnels shape and distribution. Such complex analysis was used to provide feedback about importance of the model quality for buried accessibility study.

Biography

Karolina Mitusińska is in her first year of PhD studies at the Chemistry Department of Silesian University of Technology. She is the Project Leader of Dyna-Gate project developed at Tunneling Group at Silesian University of Technology's Biotechnology Centre. In her PhD thesis she will be investigating loop-related accessibility of enzyme's active site.

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