Holyavka M G et al., J Proteomics Bioinform 2016, 9:11(Suppl)
http://dx.doi.org/10.4172/0974-276X.C1.092



# Virtual screening and experimental testing of high affinity ligands for immobilization of some proteases

**Holyavka M G**[1], **Kondratyev M S**[2], **Koroleva V A**[1] and **Artyukhov V G**[1]
[1]Voronezh State University, Russia
[2]Russian Academy of Sciences, Russia

It is known that the immobilization of the enzyme on an insoluble carrier solves several important problems in medicine: Preparing prolonged action formulations due to stabilization and increase half-life of the enzyme; a possibility of obtaining the directed delivery of the drug solution, and its diffusion into the body and; directed regulation of optimums of preparation operation (temperature optimum, pH optimum). Molecules of trypsin (pdb 3UY9), papain (pdb 9PAP) and collagenase (pdb 2CLT) taken from the database of protein structures (PDB) was used as protein models. Virtual screening of ligands for immobilization of some proteases for medical application was performed. The set of ligands included high-molecular compounds (poly-cation and poly-anion exchange fibers) and chitosan. Based on the comparative analysis of the total energy values, the localization of the ligand binding sites and several literature data, we made several suppositions concerning the mechanisms of interaction of the suggested matrices for the immobilization with enzyme molecules and the structural features of such complexes. The adsorptive method of enzyme immobilization on the above matrices proposed here allowed us to keep the enzyme's initial catalytic activity up to 70% for trypsin, papain and collagenase.

## Biography

Holyavka M G is a Senior Researcher and Associate Professor in the Department of Biophysics and Biotechnology at Voronezh State University, Russia. She received her Bachelor's in Science in 2005 and her Master's in 2007. She has completed her PhD in the year 2010. She is currently working on structural & functional properties of homogeneous and heterogeneous biocatalysts on the basis of hydrolytic enzymes.

marinaholyavka@yahoo.com

**Notes:**