

# VIRTUAL SCREENING AND EXPERIMENTAL TESTING OF HIGH-AFFINITY LIGANDS FOR IMMOBILIZATION OF SOME PROTEASES

Holyavka M.G.<sup>1</sup>, Kondratyev M.S.<sup>2</sup>, Koroleva V.A.<sup>1</sup>, Artyukhov V.G.<sup>1</sup>

<sup>1</sup>Voronezh State University Universitetskaya sq. 1, Voronezh, 394018, Russia, holavka@rambler.ru

<sup>2</sup>Institute of Cell Biophysics of the Russian Academy of Sciences Institutskaya st. 3, Pushchino, Moscow region, 142290, Russia, ma-ko@bk.ru

## Introduction

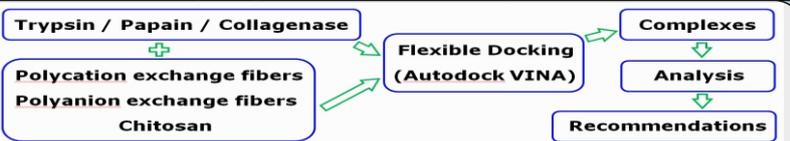
It is known that the immobilization of the enzyme on an insoluble carrier solves several important problems in medicine:

- 1) preparing prolonged action formulations due to stabilization and increase half-life of the enzyme,
- 2) a possibility of obtaining the directed delivery of the drug solution, and its diffusion into the body,
- 3) directed regulation of optimums of preparation operation (temperature optimum, pH optimum).

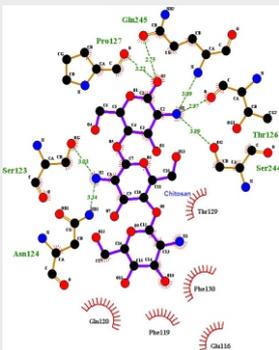
## Results

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. The set of ligands included high-molecular compounds (polycation and polyanion exchange fibers) and chitosan. Based on the comparative analysis of the total energy values and 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.

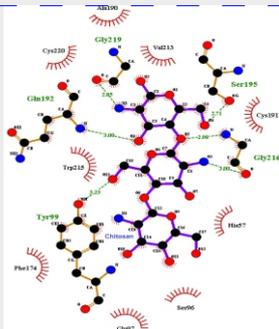
## Methods



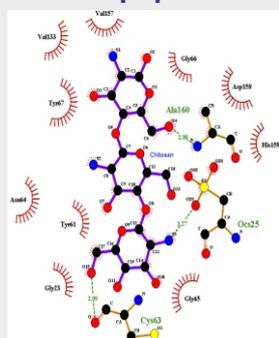
## Interactions for the binding of chitosan and collagenase



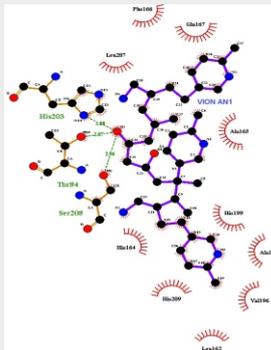
## Interactions for the binding of chitosan and trypsin



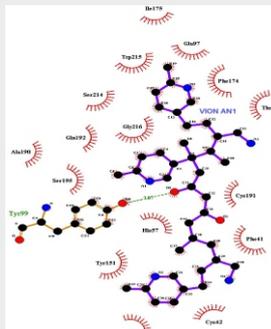
## Interactions for the binding of chitosan and papain



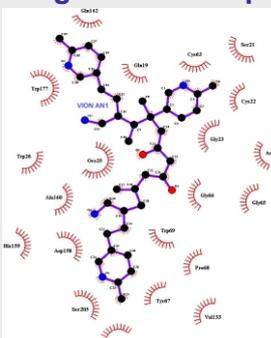
## Interactions for the binding of polyanion exchange fibers and collagenase



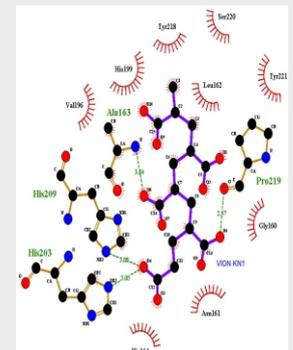
## Interactions for the binding of polyanion exchange fibers and trypsin



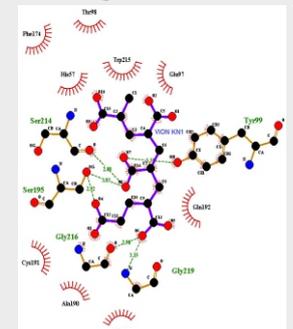
## Interactions for the binding of polyanion exchange fibers and papain



## Interactions for the binding of polycation exchange fibers and collagenase



## Interactions for the binding of polycation exchange fibers and trypsin



## Interactions for the binding of polycation exchange fibers and papain

