In silico design and construction of metal binding hybrid proteins for removal of cadmium on the basis of bacterial pili display on the surface of *E.coli*

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Biotechnology has made high contributions to health care and agriculture and now society is beginning to use the benefits of biotechnology's "third wave"-industrial and environmental biotech.

Modern biotechnology provides new ways for achieving these goals. Without bioinformatics, new research in most fields of medicine and biology would come to be incomplete. Through a combination of bioinformatics and genetics engineering procedures, we have designed a high-affinity metal binding peptides and expressed them on the surface of *E.coli* for sequestration and specific adsorption of cadmium from polluted water.

In this study, cadmium binding motif was identified in databases and the permissive sites of major subunit of *Enterotoxigenic E.coli* pili for insertion of external peptides (metal binding motif) were predicted using bioinformatics tools. By comparing the data obtained from secondary structure prediction servers, secondary structure prediction based on tertiary structure servers, servers displaying protein hydropathy, the permissive sites of the pili subunit were predicted. Fold-recognition servers generated tertiary structure models and the models were analyzed with Vadar software for quantifying and assessing protein structures. After prediction of permissive sites, the metal binding motifs were inserted in this area and hybrid proteins (theoretically) were analysised using previous and other servers.

Swiss-PdbViewer and Discovery Studio Visualizer software were applied for visualizing and structural alignment of predicted structures. The interaction of metal and hybrid proteins were predicted with docking programs. Then the ability and capacity of the recombinant bacteria to absorb the cadmium were evaluated with atomic absorbance procedure which the results were noticeable.

Keywords: metal binding motif, cadmium, surface display and bacterial pili

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