**Computational insights into mercuric reductase to improve Mercury Detoxification**

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Mercury (Hg) pollution poses significant threats to human health and ecosystems worldwide due to its persistence, bioaccumulation, and toxic effects. This study focuses on mercuric reductase from *Pseudomonas fluorescens* (UniProt ID Q51772), a key enzyme involved in detoxifying mercury through reduction to its less toxic elemental form, Hg(0). This study aims to explore the potential of this enzyme for bioremediation applications, focusing on structural insights, functional mechanisms, and biotechnological enhancements to facilitate mercury detoxification. The protein sequence of Q51772 was analyzed using bioinformatics tools to determine its structural and functional attributes. Physiochemical properties, including molecular weight, isoelectric point, and secondary structure predictions, were assessed. Virulence prediction tools confirmed the protein's non-toxic and non-pathogenic nature. Homology modeling and docking studies provided insights into its three-dimensional structure and binding interactions with mercury substrates. Q51772 consists of 548 amino acids and belongs to the Pyridine nucleotide-disulphide oxidoreductase family, class I. It features specific domains crucial for mercury reduction, which were identified through Pfam and InterPro analyses. Physiochemical analysis indicated a stable protein with hydrophilic tendencies conducive to enzymatic function. Structural modeling validated by ProQ and PROCHECK confirmed the reliability of the predicted structure. Molecular docking of organic mercury compound with wild-type and mutant mercuric reductase revealed strong binding affinities, with key hydrogen bonds involving residues Gly95, Thr122, and Asp390. Mercuric reductase Q51772 from *Pseudomonas fluorescens* emerges as a promising candidate for bioremediation of mercury-contaminated environments. Future research should focus on optimizing its performance under diverse environmental conditions to advance sustainable solutions for mercury pollution control.

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