

Development of Bioremediators for Heavy Metal-Contaminated Environments Using Computational Biology on *Saccharomyces cerevisiae* Proteins

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Introduction: Cadmium is a heavy metal that poses serious health hazards due to its entry into the food chain through anthropogenic pathways. Fungal biosorption offers an economically feasible, environmentally sound and effective technology for metal removal and recovery from aqueous solutions. Toxic metals enter cells through the uptake of essential metals or other nutrients. Thus, Alr1p, which is responsible for Mg uptake, may also contribute to Cd tolerance. Alr1p resides in the plasma membrane of yeast and belongs to the CorA-Alr1p-Mrs2p family of magnesium channels. **Objectives:** To develop bioremediators and biosensors using computational biology with proteins from *Saccharomyces cerevisiae*. **Material and Methods:** Comparative and *ab initio* computational modeling was performed, followed by TM-align. Next, the secondary structure was predicted by PSIPRED, Jufo and JPred, and the degree of structural disorder was obtained by MobiDB 2.0 and D2P2. Finally, the models were validated, and the quaternary structure of the best model was predicted by GalaxyGemini. The phylogenetic analysis was performed by ConSurf. **Results and Discussion:** According to the TM-align results, only the structures modeled by the M4T and Swiss-Model programs showed an RMSD < 2.0 and a TM-score > 0.5, but the whole protein was not modeled. The ALR1 protein is almost twice as long as the existing CorA templates, and the non-CorA region could not be modeled due to the lack of homologous proteins and a high degree of disorder. The ALR1 protein was predicted to be a homo-pentamer similar to the known CorA structure, and the ConSurf analysis showed a highly conserved structure. As the M4T model contains 432 AAs and the Swiss-Model models contain only 341 AAs, the M4T model was chosen as the most representative model for further studies. **Conclusions:** Understanding the involvement of proteins implicated in the response to heavy metals in *S. cerevisiae* allows greater understanding and the development of strategies for recovery or the remediation of damage.

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