



Comparative *in Silico* analysis of the behavior of Laccases from marine and terrestrial origin against degradation of industrial dyes

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Abstract : Laccases are multicopper-oxidase enzymes that catalyze one-electron oxidation of phenolic compounds, and other electron-rich substrates with the concomitant reduction of O₂ to H₂O. One of the most important applications of these enzymes can be found in bioremediation processes, for which the search for enzymes derived from marine organisms can be considered strategic due to the physicochemical characteristics of contaminated effluents. In this study, a comparative molecular docking analysis was made considering the behavior of putative laccases of marine and terrestrial origin against six industrial dyes. Using sequences retrieved from NCBI and Uniprot databases, three-dimensional structures were obtained and validated by computational methods. These models were used for docking studies with the dyes Acid Orange 10, Amido Black, Reactive Blue 4, Reactive Yellow 14, Remazol Black B, and Trypan Blue. The results showed an outstanding behavior of the putative laccase from marine-derived bacteria *Pantoea agglomerans*, which showed the best affinity interaction with the dyes Amido Black (-8,2 kcal/mol), Reactive Blue 4 (-9,4 kcal/mol), and Reactive Yellow 14 (-8,6 kcal/mol). Likewise, the putative laccase from marine-derived bacteria *Bacillus stratosphericus* showed the best affinity interaction with the dyes Acid Orange 10 (-7.5 kcal/mol), and Remazol Black B (-8.3 kcal/mol). The findings obtained in the present study demonstrate the potential of microbial enzymes that can be found in marine ecosystems, and establish that specific sequences might be used for further construction of synthetic genes in experimental evaluations.

Keywords: Molecular docking, Multicopper oxidases, Homology modeling, Bioremediation, Textile effluent.