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Unrevealing the Enhanced Laccase Activities of *Phlebiopsis flavidoalba* in the Presence of Lignin-Rich Raw Materials using Molecular Docking**Senavirathna, T.M.Y.H., Perera, P., Attanayake, R.N.****Department of Plant and Molecular Biology, University of Kelaniya, Kelaniya, Sri Lanka***renuka@kln.ac.lk***Abstract**

Laccase, a versatile enzyme that belongs to the multi-copper oxidase family, exhibits extraordinary lignin-degrading capabilities. Among the diverse types of laccases, white-rot fungal laccases are considered some of the best lignin degraders, with various biotechnological and industrial applications. In our previous study, it was found that a wood-decaying white rot fungus, *Phlebiopsis flavidoalba*, is one of the highest laccase producers in vitro in the presence of rice husks as the raw material. However, it is unclear the exact mechanism and whether laccase directly interacts with the raw material, in this case, rice husks and its lignin model compound. Hence, the objective of the current study was to obtain laccase gene sequence from *P. flavidoalba* and subject it to molecular docking with lignin model compounds that are particularly found in rice husks to determine binding affinities to the active sites of enzyme. The laccase gene sequence of *P. flavidoalba* was obtained from the next-generation sequence data set obtained in our previous study and subjected to *in silico* homology modelling and molecular docking using various lignin model compounds reported to be present in rice husks. Firstly, to predict the 3D structure of the laccase of *P. flavidoalba*, homology modelling was performed using SWISS-MODEL. Laccase from *Steccherinum murashkinskyi* was selected as the template for homology modelling using SWISS-MODEL. CB-Dock server was used to perform molecular docking studies with a range of lignin model compounds, including sinapyl alcohol, coniferyl alcohol, ρ - coumaryl alcohol, β -O-4' aryl ether, β -5' phenylcoumaran which are commonly found in rice husks. It was found that the above-mentioned lignin model compounds exhibited strong binding affinities such as -5.9 kcal/mol (sinapyl alcohol), -6.5 kcal/mol (coniferyl alcohol), -8.6 kcal/mol (ρ - coumaryl alcohol), -7.5 kcal/mol (β -O-4' aryl ether), and -7.5 kcal/mol (β -5' phenylcoumaran) with the laccase protein of *P. flavidoalba*. The amino acid residues of modelled laccase in contact with the lignin model compounds forming hydrogen bonds were Gln457, Ile434, Phe432, Arg370, Lys452, Ile365. The insights gained from these docking studies can help uncover the molecular level interactions and the potential of utilizing such low-cost carbon sources for boosting laccase production.

Keywords: Homology modelling, Laccase, Lignin model compounds, Molecular docking, Rice husk