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Evaluation of Lignin Degrading Ability and *In-silico* Analysis and Molecular Docking of Laccase of *Schizophyllum commune* with Lignin

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Abstract

White-rot fungi have a unique and strong ability to degrade lignin, the most abundant and the strongest natural polymer on earth. The ligninolytic enzymes of these fungi comprise of three groups of oxidative extracellular enzymes mainly, lignin peroxidase (LiP), manganese dependent peroxidase (MnP) and laccase. Fungal laccases are considered to be directly involved with the degradation of lignin. Due to the broad substrate specificity and unique ability of biodegradation, fungal laccases have a great value in industrial and biotechnological applications like bioremediation, detoxification of industrial dyes and treatment of other pollutants. The objectives of this study was to evaluate the lignin degradation ability and laccase producing ability of selected fungal isolates originated from decaying hardwoods of Dimbulagala forest reserve, Sri Lanka and to predict the three-dimensional (3D) structure of laccase from *Schizophyllum commune* and its binding to lignin using *in silico* homology modeling and molecular docking. Ten fungal isolates originated from decaying hardwoods were screened for the lignin degradation ability by using lignin amended malt extract plate assay and laccase producing ability by using guaiacol amended PDA plates. Seven isolates showed lignin degradation ability and five of them were laccase producers. Since *S. commune* could produce laccase, degrade lignin and laccase protein sequence is available, it was subjected to homology modeling. Homologous templates were identified using BLASTP across Protein Data Bank from NCBI. Laccase from *Cerrena* sp. was selected as the template for 3D model building of laccase from *S. commune* using Modeller 10.1. The quality of resulted 3D model of the protein was verified by its energy and stereochemical properties. The unstable regions were selected and remodeled by loop modelling using ModLoop web server. The results of evaluation of the remodeled structure by stereochemical quality and energy was found to be improved and showed that predicted model was of good quality due to the presence of maximum residues in the favored region. Later CB-Dock server was used to perform molecular docking studies using lignin model compounds. The amino acid residues of modeled laccase of *S. commune* in contact with the lignin based model compounds were identified. These findings help uncovering the lignin degradation mechanisms by *S. commune* laccases and are useful in biofuel production and bioremediation.

Keywords: Laccase, Homology modeling, Molecular docking, Lignin

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