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In Silico Generation of Protein-Protein Interaction Models of Tubulin and Fungal Laccase

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Abstract—*Over the recent years due to debilitating effects of popular anticancer drug therapies such as radiotherapy and chemotherapy, search for novel anticancer drugs and targets has become imperative. Tubulin protein, a major constituent of microtubule, is a well known target for many commercially available cancer drugs. These drugs, though in clinical use, have debilitating toxicities having a negative impact on quality of life. Tubulin targeting drugs affect microtubular dynamics resulting in apoptosis and necrosis of cancerous cells. Recently laccase, a protein, has shown strong potential as anticancer agent both in vitro and in vivo .The selective activity of laccase targeting only cancerous cells and sparing the normal cells makes it a good target. The aim of the study is to search possible interactions between laccase (isolated from Trametes versicolor) and tubulin. Through in silico methods, using ClusPro, models were generated, visualized using Pymol software and properties of interaction were observed using PDBSum. Two different modes of interaction between tubulin and laccase were observed. In one case, laccase showed interaction with α dimer (I.A.= 145:162 A^2) and β dimer (I.A. = 1006:1017 A^2) interface .Two Hydrogen bonds were observed between A chain of tubulin and 10 Hydrogen bonds between B chain and laccase. Another mode of interaction was laccase interacting only with β tubulin with an improved energy cluster score of -901.1 as compared to -791.2 of former mode. In this case, 4 Hydrogen bonds were observed between tubulin and laccase. Both these models have established that there are laccase binding sites on tubulin heterodimer. Thus, the study indicates possible interaction between tubulin dimer and laccase which can be further explored for potential anticancer activity.*