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In-Silico Fusion of Bacillus Licheniformis Chitin Deacetylase with Chitin Binding Domains from Chitinases

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Abstract : Chitin, the biopolymer of the N-acetylglucosamine, is the most abundant biopolymer on the planet after cellulose. Industrially, chitin is isolated and purified from the shell residues of shrimps. A deacetylated derivative of chitin i.e. chitosan has more market value and applications owing to it solubility and overall cationic charge compared to the parent polymer. This deacetylation on an industrial scale is performed chemically using alkalis like sodium hydroxide. This reaction not only is hazardous to the environment owing to negative impact on the marine ecosystem. A greener option to this process is the enzymatic process. In nature, the naïve chitin is converted to chitosan by chitin deacetylase (CDA). This enzymatic conversion on the industrial scale is however hampered by the crystallinity of chitin. Thus, this enzymatic action requires the substrate i.e. chitin to be soluble which is technically difficult and an energy consuming process. We in this project wanted to address this shortcoming of CDA. In lieu of this, we have modeled a fusion protein with CDA and an auxiliary protein. The main interest being to increase the accessibility of the enzyme towards crystalline chitin. A similar fusion work with chitinases had improved the catalytic ability towards insoluble chitin. In the first step, suitable partners were searched through the protein data bank (PDB) wherein the domain architecture were sought. The next step was to create the models of the fused product using various in silico techniques. The models were created by MODELLER and evaluated for properties such as the energy or the impairment of the binding sites. A fusion PCR has been designed based on the linker sequences generated by MODELLER and would be tested for its activity towards insoluble chitin.

Keywords : chitin deacetylase, modeling, chitin binding domain, chitinases
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