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Structure, Bioinformatics Analysis and Substrate Specificity of a 6-Phospho-β-Glucosidase Glycoside Hydrolase 1 Enzyme from Bacillus licheniformis

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Abstract : In bacteria, mono and disaccharides are phosphorylated during uptake into the cell via the widely used phosphoenolpyruvate (PEP)-dependent phosphotransferase transport system. As an initial step in the phosphorylated disaccharide metabolism pathway, certain glycoside hydrolase family 1 (GH1) enzymes play a crucial role in releasing phosphorylated and non-phosphorylated monosaccharides. However, structural determinants for the specificity of these enzymes still need to be clarified. GH1 enzymes are known to have a wide array of functions. According to the CAZy database, there are twenty-one different enzymatic activities in the GH1 family. Here, the structure and substrate specificity of a GH1 enzyme from Bacillus licheniformis, hereafter known as BlBglH, was investigated. The sequence of the enzyme BlBglH was compared to the sequences of other characterized GH1 enzymes using sequence alignment, sequence identity calculations, phylogenetic analysis, and motif discovery. Through these various analyses, BlBglH was found to have sequence features characteristic of the 6-phospho-β-glucosidase activity enzymes. Additionally, motif and structure comparisons of the three most commonly studied GH1 enzyme-activities revealed a shared loop amongst the different structures that consist of different sequence motifs – this loop is thought to guide specific substrates (depending on activity) towards the active-site. To further affirm BlBglH enzyme activity, molecular docking and molecular dynamics simulations were performed. Docking was carried out using 6-phospho-β-glucosidase enzyme-activity positive (p-Nitrophenyl-beta-D-glucoside-6-phosphate) and negative (p-Nitrophenyl-beta-D-galactoside-6-phosphate) control ligands, followed by 400 ns molecular dynamics simulations. The positive-control ligand maintained favourable interactions within the active site until the end of the simulation. The negative-control ligand was observed exiting the enzyme at 287 ns. Binding free energy calculations showed that the positive-control complex had a substantially more favourable binding energy compared to the negative-control complex. Jointly, the findings of this study suggest that the BlBglH enzyme possesses 6-phospho-β-glucosidase enzymatic activity.

Keywords : 6-P-β-glucosidase, glycoside hydrolase 1, molecular dynamics, sequence analysis, substrate specificity
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