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*Research Article*

# Molecular Phylogeny and Predicted 3D Structure of Plant *beta*-D-*N*-Acetylhexosaminidase

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*beta*-D-*N*-Acetylhexosaminidase, a family 20 glycosyl hydrolase, catalyzes the removal of $\beta$-1,4-linked *N*-acetylhexosamine residues from oligosaccharides and their conjugates. We constructed phylogenetic tree of $\beta$-hexosaminidases to analyze the evolutionary history and predicted functions of plant hexosaminidases. Phylogenetic analysis reveals the complex history of evolution of plant $\beta$-hexosaminidase that can be described by gene duplication events. The 3D structure of tomato $\beta$-hexosaminidase ($\beta$-Hex-Sl) was predicted by homology modeling using 1now as a template. Structural conformity studies of the best fit model showed that more than 98% of the residues lie inside the favoured and allowed regions where only 0.9% lie in the unfavourable region. Predicted 3D structure contains 531 amino acids residues with glycosyl hydrolase20b domain-I and glycosyl hydrolase20 superfamily domain-II including the $(\beta/\alpha)_8$ barrel in the central part. The $\alpha$ and $\beta$ contents of the modeled structure were found to be 33.3% and 12.2%, respectively. Eleven amino acids were found to be involved in ligand-binding site; Asp(330) and Glu(331) could play important roles in enzyme-catalyzed reactions. The predicted model provides a structural framework that can act as a guide to develop a hypothesis for $\beta$-Hex-Sl mutagenesis experiments for exploring the functions of this class of enzymes in plant kingdom.

## 1. Introduction

As a part of the study to elucidate the role of free *N*-glycans and de-*N*-glycosylation mechanism working in plants, we have already characterized the PNGase, ENGase, $\alpha$-mannosidase and $\beta$-hexosaminidase at molecular level [1–3]. The $\beta$-D-*N*-acetylhexosaminidase (EC 3.2.1.52), a member of the glycosyl hydrolase family 20 (GH20), is an enzyme that hydrolyses nonreducing terminal monosaccharide residues of $\beta$-*N*-acetylgalactosaminides and $\beta$-*N*-acetylglucosaminides. It is widely distributed among the animals, insects, plants, fungus, and bacteria. Mammal lysosomal $\beta$-*N*-acetyl-D hexosaminidases are mainly responsible for glycoconjugate degradation in lysosome. HexA is a heterodimer of subunits $\alpha$ (encoded by the gene HexA) and $\beta$ (encoded by the gene HexB), whereas HexB is a homodimer of $\beta$ subunits. The subunits arose through a gene duplication event and the primary sequences are approximately 60% identical. Mutational defects that cause $\beta$-hexosaminidase-A and B deficiency are responsible for Sandhoff and the Tay-Sachs diseases, respectively [4]. Recently, it has been reported that $\beta$-hexosaminidase is a surrogate marker for renal function in autosomal dominant polycystic kidney disease [5]. In insects, it has been postulated to have specialized physiological functions, including posttranslational modification of *N*-glycans, degradation of glycoconjugates, and egg-sperm recognition, suggesting that these enzymes have rather versatile physiological functions in the growth and development of insects [6]. Mammal $\beta$-*N*-acetyl-D-hexosaminidases have been shown to be important for egg-sperm recognition [7], and the enzymes from *Drosophila melanogaster* sperm membrane also participate in the same process [8]. A fungal $\beta$-*N*-acetyl-D-hexosaminidases has been expressed, characterized, and crystallized from