IN SILICO MOLECULAR ANALYSIS OF FRUCTOOLIGOSACCARIDE PRODUCING ENZYMES

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Product Background

- **Putative glycosyl hydrolase (GH) 68 fructosyltransferase (FTase) from *Streptococcus thermophilus* (VUW839976.1) was identified as potential fructooligosaccharides (FOS) producing enzyme.**
- **Computational study using *in silico* molecular analysis was used as alternative approach to discover this potential enzyme.**

Problem Statements

- **Since FOS are prebiotics that good for health, the demand of FOS is forecasted to be gradually increases over the year.**
- **FOS can be manufactured using two types of enzymes which are β-fructofuranosidase (FFase) and fructosyltransferase (FTase) but FTase preferable for industry since FFase required high substrate concentration.**
- **Nevertheless, there was limitation of FTase strains that can produce FOS.**
- **Therefore, it was estimated that this situation could affect the production capacity of FOS in future.**

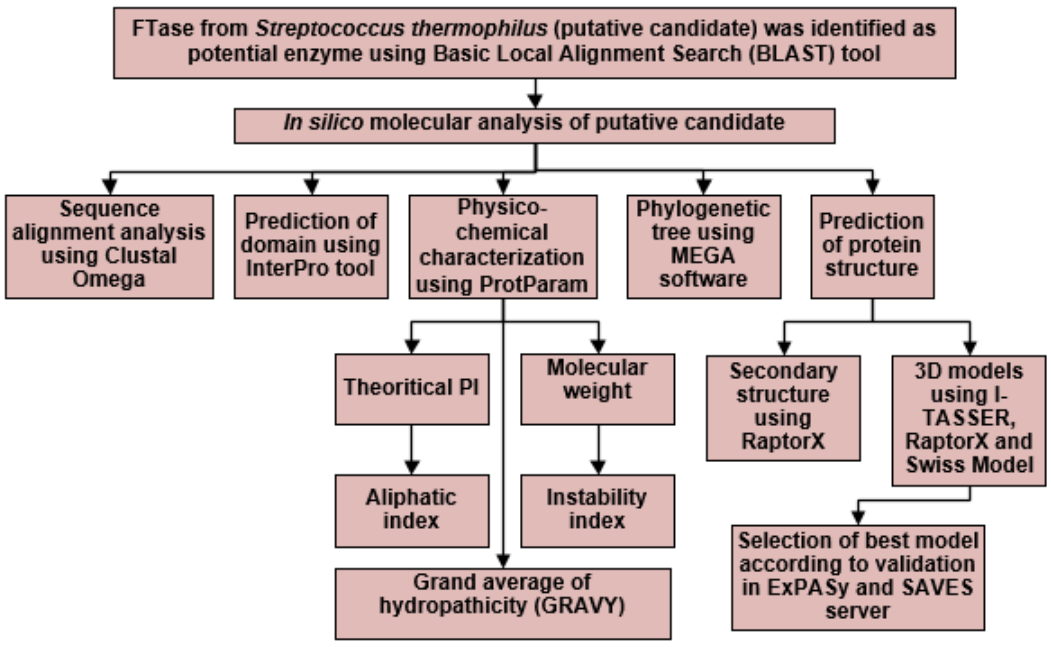
Benefits/Usefulness/Applicability

- **FTase from *S. thermophilus* have high aliphatic index (73.61) indicates that this enzyme is stable in high temperature compared to other FOS producing enzymes.**
- **It is stable in nature because the instability index computed is 35.27 which is less than 40.**
- **The negative GRAVY value (-0.442) indicates this enzyme consists of more hydrophilic residues. Consequently, this enzyme has high affinity for water molecules and hence improves the protein solubility.**

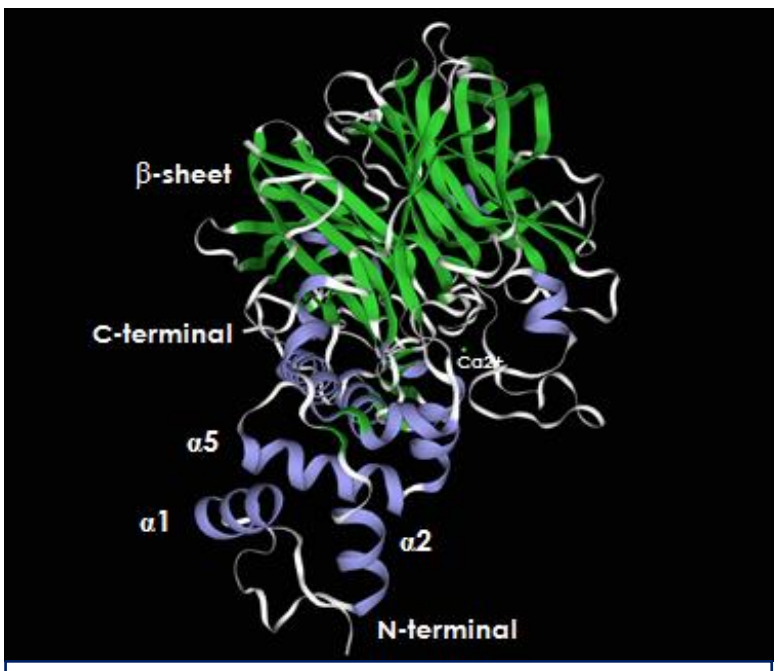
Novelty

- **Previously, FOS producing enzymes are from microorganisms such as *Aspergillus* and *Lactobacillus* sp. However, these microbes are very sensitive towards environment.**
- **From the computational analysis, uncharacterized FTase from *S. thermophilus* have been identified as a useful enzyme for FOS production at industrial scale as it were predicted to be able withstand elevated temperature.**
- **This putative FTase can be proven as FOS producing enzyme by further *in silico* analysis where it shares 55.35% structures and sequences similarity with template FTase, *Lactobacillus johnsonii* NCC533 (AAS08734.1).**
- **Four short conserved motifs of family GH68 FTase were observed in this putative amino acid sequences.**
- **According to phylogenetic tree, this putative FTase also categorized in the same clade with the template FTase.**

Methodology



Product Characteristics and Results



The Selected 3D Model from Swiss Model

- **The 3D model portrays the common structure of the GH68 family which is β-propeller fold.**
- **This is well aligned with the domain prediction analysis where a domain of glycosyl hydrolase with five-bladed beta-propeller domain superfamily is shown to appeared at the position of 180-680 in the amino acid sequence of putative GH68 FTases from *S. thermophilus*.**

Marketability & Commercialisation

- **This FTase from *S. thermophilus* can be commercialize as FOS producing enzyme where it could be segmented into food and beverage, dietary supplements, infant formula, animal feed, and pharmaceuticals.**
- **With the amelioration of advanced computational biology and in vivo studies, this protein will provide a better insight and hold a promising future for FOS production industry.**