

**In silico analysis and structure modelling of heat shock protein HSP70 from
Glaciozyma antarctica PI12 as a model system to understand adaptation
strategies of Antarctic organisms amid adverse climates**

ABSTRACT

The 70-kDa heat-shock proteins (HSP70) are integral components of the cell's folding catalysts. *Glaciozyma antarctica* PI12 is an obligate psychrophilic yeast that possesses six HSP70 genes in its genome. The functions of these HSP70s in *G. antarctica* in terms of similarities and differences are yet to be discovered. The purpose of this study is to determine the structure and function of HSP70 from *G. antarctica*, which will lead to understanding this organism's adaptation strategies through structural and functional annotation. In this study, we utilize the HSP70 genes derived from genome data of *Glaciozyma antarctica* PI12 isolated from the Casey Research Station to characterize and compare structural characteristics which may contribute to their adaptation strategies during global warming. Computational tools such as ExPASy's ProtParam, MEGA 11, SWISS-MODEL, AlphaFold2, and SAVES were used to analyze all the genes via physicochemical analysis, phylogenetic study, homology modelling and structure validation, and superimposition of models. Results showed that reliable 3D models of HSP70 were successfully generated via the homology modelling approach using SWISS-MODEL and AlphaFold2 programs. The proposed model was evaluated as reliable with high confidence based on the structural stereochemical property, verification of protein patterns of non-bonded atomic interactions, compatibility of a 3D model with its amino acid sequence and determination of the protein's native fold. Among the new findings are the molecular signatures such as ionic, aromatic-aromatic, aromatic-sulphur and cation- π interactions that are lesser in the buried residues when compared to their homologs. These interactions are important for maintaining structure stability, flexibility and packing in proteins. This may reflect the yeast response and adaptation strategies during the adverse climate. By studying the structural adaptations of HSP70 proteins in psychrophilic yeast, researchers can gain insights into how these proteins maintain their functionality in changing temperature conditions. This knowledge can inform the development of strategies to mitigate the impact of global warming on cold-adapted organisms and potentially guide the design of novel enzymes with improved thermal stability for biotechnological applications. In conclusion, this comprehensive study provides an in-depth understanding of the structural adaptation and evolution of HSP70 about their thermal resistance to global warming.