

In silico Structural Modelling and Comparative Analysis of β -mannanases from Psychrophilic and Mesophilic *Arthrobacter* sp.

ABSTRACT

Background and Objective: Endo-1,4- β -mannanase (β -mannanase, EC 3.2.1.78) is an industrially important enzyme which catalyses the hydrolysis of mannan-based polysaccharides. This enzyme is produced by psychrophilic and mesophilic groups of *Arthrobacter* sp., yet none of them were structurally characterized. This study aims to decipher the structural features of *Arthrobacter* β -mannanases that might be responsible for their cold adaptation. Material and Methods: Thirty amino acid sequences encoding β -mannanases from *Arthrobacter* sp. were retrieved from GenBank and subjected to a series of analyses including amino acid profiling and structural homology modelling using Phyre2 and SWISS-MODEL. Results: Structural alignment showed that the catalytic residues (2 glutamic acids) were conserved among β -mannanases, suggesting that they share a common catalytic mechanism. Psychrophilic β -mannanases showed remarkable differences from the mesophilic ones in the content of hydrophilic, particularly negatively charged, residues and proline, which were thought to be important for their cold adaptation. Three-dimensional models of all *Arthrobacter* β -mannanases form a classic β -barrel motif consisting of 8 helices and 9 β -sheets, except for psychrophilic ones, which have 8 helices and 8 β -sheets. Conclusion: Adaptation of *Arthrobacter* β -mannanases to cold temperatures involves structural adjustments, particularly in structural flexibility and amino acid distribution.