Title: Structural prediction of a novel laminarinase from the psychrophilic glaciozyma antarctica PI12 and its temperature adaptation analysis

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Abstract: Here, we present a novel psychrophilic ß-glucanase from Glaciozyma antarctica PI12 yeast that has been structurally modeled and analyzed in detail. To our knowledge, this is the first attempt to model a psychrophilic laminarinase from yeast. Because of the low sequence identity (<40 %), a threading method was applied to predict a 3D structure of the enzyme using the MODELLER9v12 program. The results of a comparative study using other mesophilic, thermophilic, and hyperthermophilic laminarinases indicated several amino acid substitutions on the surface of psychrophilic laminarinase that totally increased the flexibility of its structure for efficient catalytic reactions at low temperatures. Whereas several structural factors in the overall structure can explain the weak thermal stability, this research suggests that the psychrophilic adaptation and catalytic activity at low temperatures were achieved through existence of longer loops and shorter or broken helices and strands, an increase in the number of aromatic and hydrophobic residues, a reduction in the number of hydrogen bonds and salt bridges, a higher total solvent accessible surface area, and an increase in the exposure of the hydrophobic side chains to the solvent. The results of comparative molecular dynamics simulation and principal component analysis confirmed the above strategies adopted by psychrophilic laminarinase to increase its catalytic efficiency and structural flexibility to be active at cold temperature.