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## Molecular Modeling and Implications of a *Bacillus* $\alpha$ -Amylase that Acquires Enhanced Thermostability and Chelator Resistance by Deletion of an Arginine-glycine Residue

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Resistance to chelators, as well as thermostability, of an alkaline  $\alpha$ -amylase (AmyK, formerly named LAMY) from an alkaliphilic *Bacillus* sp. strain was significantly improved by deletion of Arg181-Gly182. To clarify the mechanism of thermostability and chelator resistance conferred by the deletion mutation, we constructed models of AmyK with the 3D structure of  $\alpha$ -amylase from *Bacillus amyloliquefaciens* as the template. In the structural models, Ala186 and Asp188 on a loop were both coordinated with a structural calcium ion. Molecular dynamics simulations suggested that the affinity of the Ala186 carbonyl oxygen to the calcium ion in the mutant enzyme was strengthened, thereby causing enhanced thermostability and the chelator resistance.

**Key words:**  $\alpha$ -amylase, homology modeling, molecular dynamics simulation, thermostability, chelator resistance

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