

# **Structural and Substrate Interaction Properties of Alkaline Phosphatase from *Paenibacillus* sp. PSB04: In-Silico Analysis**

## **ABSTRACT**

A Phosphate-Solubilising Bacterium (PSB) of *Paenibacillus* sp. PSB04 was previously isolated from the Sabah tropical rainforest in Malaysia. Interestingly, the genome sequence of the PSB04 strain harbored an Alkaline Phosphatase (AP) (EC 3.1.3.1) gene and was hypothesized to have unique structural characteristics. Therefore, this study aims to determine the AP three-Dimensional (3D) model and catalytic mechanism from *Paenibacillus* sp. PSB04 (PAP). To address this, the 3D model of this protein was built and docked into a model substrate of p-nitrophenyl phosphate. As a result, the best complex was shown to have the lowest binding energy of -5.9 kcal/mol. Furthermore, the complex showed the atomic coordination of catalytic residues of PAP and the substrate was similar to that of AP from *Escherichia coli* (ECAP), which implies that both APs shared a similar catalytic mechanism. In this mechanism, Ser 94 of PAP acted as nucleophilic residues, which were activated by the Zn ion. Arg 145 is predicted to be mobile due to its location in the loop region, which allows this residue to stabilize the substrate through direction or water-mediated secondary interaction. Docking simulation of pNPP indicated that the putative residues involved in the catalysis mainly are Ser 94, Ser 141, Ala 146, Thr 147, Pro 148, Asp 293, and Glu 294. Glu 294 is considered a unique residue corresponding to Lys 328 ECAP, allowing the PAP to have a better affinity to stabilize the substrate in the binding cavity. Accordingly, a unique catalytic mechanism of PAP was proposed.