

## Crystallization and structure elucidation of GDSL esterase of *Photobacterium* sp. J15

### ABSTRACT

GDSL esterase J15 (EstJ15) is a member of Family II of lipolytic enzyme. The enzyme was further classified in subgroup SGNH hydrolase due to the presence of highly conserve motif, Ser-Gly-Asn-His in four conserved blocks I, II, III, and V, respectively. X-ray quality crystal of EstJ15 was obtained from optimized formulation containing 0.10 M ammonium sulphate, 0.15 M sodium cacodylate trihydrate pH 6.5, and 20% PEG 8000. The crystal structure of EstJ15 was solved at 1.38 Å with one molecule per asymmetric unit. The structure exhibits  $\alpha/\beta$  hydrolase fold and shared low amino acid sequence identity of 23% with the passenger domain of the autotransporter EstA of *Pseudomonas aeruginosa*. The active site is located at the centre of the structure, formed a narrow tunnel that hinder long substrates to be catalysed which was proven by the protein-ligand docking analysis. This study facilitates the understanding of high substrate specificity of EstJ15 and provide insights on its catalytic mechanism.

**Keyword:** Crystallization; GDSL esterase; *Photobacterium* sp. J15