Azzmer Azzar, Int J Biotechnol Recent Adv. 2018
http://dx.doi.org/10.18689/2639-4529.a1.004

madridge CONFERENCES
International
Biotechnology and Research Conference
April 25-27, 2018 Rome, Italy

The Mechanistic Role of Active Site Residues in Non-Stereospecific Haloacid Dehalogenase E (Dehe) using Computational Approach

Azzmer Azzar
International Islamic University, Malaysia

Dehalogenase E (DehE) is a non-stereospecific haloacid dehalogenase produced by soil bacteria, *Rhizobium* sp. RC1. This enzyme has been hypothesized to facilitate 'direct attack mechanism' whereby its activated water molecule will directly attack the α-carbon of haloacid compound, thus releasing the halogen. The similar mechanism was proved and identified for Dehalogenase I (DehI) from *Pseudomonas putida* PP3 which also classified under the same group with DehE. For a better understanding of the DehE catalytic mechanism, this enzyme was docked with D- and L- stereoisomer of 2-Chloropropionic acid (2CP) and the their complex structures were simulated using GROMACS 5.1.2 for 50 nano-seconds. Upon completion, the distance of water towards Asn114, Asp189 and the α-carbon of the 2CP were calculated. The same procedure was also applied to DehI as it serves as the benchmark. Analysis of DehE catalysis was revealed information on the presence of water molecule, water activation potential and direct attack mechanism. In this study, the catalytic water was found located nearby Asn114 and a hydrogen bond was formed between these molecules. Asn114 was seen to provide the water molecule that needed for the mechanism and play role as 'water-bearer'. For water activation, the distance of Asp189 towards water molecule was found in the range of ~2 to ~8 Å which is favorable for the activation to occur. This aspartate residue was proposed to activate the catalytic water into hydroxide ion. While for the direct attack, the distance of water molecule towards the α-carbon of 2CP was approximately at 8 Å, which also the similar range that was observed in DehI-2CP. In conclusion, DehE is strongly suggested based on *in silico* analysis to facilitate 'direct attack mechanism' for haloacid catalysis. This study information will provide a platform for isotope labeling experiment and protein engineering for non-stereo haloaciddehalogenase of *Rhizobium* sp. RC1.

Keywords: Dehalogenase E, haloaciddehalogenase, Rhizobial enzyme, molecular docking, molecular dynamics simulation.

Biography:

Azzmer Azzar bin Abdul Hamid obtained his Ph.D from IIUM in Biotechnology and upon completion of his Ph.D, he was appointed as a lecturer at the Department of Biotechnology, Kuliyyah of Science, IIUM Kuantan Campus. Presently, Dr Azzmer is an Assistant Professor at the Department of Biotechnology, Kulliyyah of Science, International Islamic University Malaysia (IIUM) Kuantan Campus. His research work is towards the dehalogenation of toxic compounds by microbial enzyme. Recently, he obtained an endowment grant as a principal researcher and fundamental research scheme grant (FRGS) as a coresearcher. He has published some articles regarding protein modeling, rational design, molecular biology and enzyme kinetics at several journals. Apart from that, he served the Ministry of Education as an examiner for Matriculation programme and also as a reviewer for Journal of Molecular Modeling.