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**Record 1 of 1****Title:** The mechanistic role of active site residues in non-stereo haloacid dehalogenase E (DehE)**Author(s):** Abidin, MHZ (Abidin, Muhammad Hasanuddin Zainal); Abd Halim, KB (Abd Halim, Khairul Bariyyah); Huyop, F (Huyop, Fahrul); Hamid, THTA (Hamid, Tengku Haziyyamin Tengku Abdul); Wahab, RA (Wahab, Roswanira Abdul); Hamid, AAA (Hamid, Azzmer Azzar Abdul)**Source:** JOURNAL OF MOLECULAR GRAPHICS & MODELLING Volume: 90 Pages: 219-225 DOI: 10.1016/j.jmngm.2019.05.003 Published: JUL 2019**Times Cited in Web of Science Core Collection:** 0**Total Times Cited:** 0**Usage Count (Last 180 days):** 4**Usage Count (Since 2013):** 4**Cited Reference Count:** 28

Abstract: Dehalogenase E (DehE) is a non-stereospecific enzyme produced by the soil bacterium, *Rhizobium* sp. RC1. Till now, the catalytic mechanism of DehE remains unclear although several literature concerning its structure and function are available. Since DehE is non-stereospecific, the enzyme was hypothesized to follow a 'direct attack mechanism' for the catalytic breakdown of a haloacid. For a molecular insight, the DehE modelled structure was docked in silica with the substrate 2-chloropropionic acid (2CP) in the active site. The ideal position of DehE residues that allowed a direct attack mechanism was then assessed via molecular dynamics (MD) simulation. It was revealed that the essential catalytic water was hydrogen bonded to the 'water-bearer', Asn114, at a relatively constant distance of similar to 2.0 angstrom after 50 ns. The same water molecule was also closely sited to the catalytic Asp189 at an average distance of similar to 2.0 angstrom, signifying the imperative role of the latter to initiate proton abstraction for water activation. This reaction was crucial to promote a direct attack on the alpha-carbon of 2CP to eject the halide ion. The water molecule was oriented favourably towards the alpha-carbon of 2CP at an angle of similar to 75 degrees, mirrored by the formation of stable enzyme-substrate orientations throughout the simulation. The data therefore substantiated that the degradation of a haloacid by DehE followed a 'direct attack mechanism'. Hence, this study offers valuable information into future advancements in the engineering of haloacid dehalogenases with improved activity and selectivity, as well as functionality in solvents other than water. (C) 2019 Elsevier Inc. All rights reserved.

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Reprint Address: Hamid, AAA (reprint author), IIUM, Dept Biotechnol, Kulliyah Sci, Kuantan 25200, Pahang, Malaysia.**E-mail Addresses:** azzmer@iium.edu.my**Publisher:** ELSEVIER SCIENCE INC**Publisher Address:** STE 800, 230 PARK AVE, NEW YORK, NY 10169 USA**Web of Science Categories:** Biochemical Research Methods; Biochemistry & Molecular Biology; Computer Science, Interdisciplinary Applications; Crystallography; Mathematical & Computational Biology**Research Areas:** Biochemistry & Molecular Biology; Computer Science; Crystallography; Mathematical & Computational Biology**IDS Number:** IE1DO**ISSN:** 1093-3263**eISSN:** 1873-4243**29-char Source Abbrev.:** J MOL GRAPH MODEL**ISO Source Abbrev.:** J. Mol. Graph.**Source Item Page Count:** 7**Funding:**

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