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The mechanistic role of catalytic residues in non-stereo dehalogenase (DehE)

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Introduction: DehE or non-stereospecific dehalogenase from *Rhizobium* sp. RC1 catalyzes the hydrolytic dehalogenation of both isomers of D,L-2-haloacids to produce an inverted configuration of 2-hydroxyl acid. The enzymatic degradation for the removal of halides from haloacid substance has been highlighted since the enzyme itself is a potential candidate as bio-remediation agent. However, the mechanistic role of active site residues for dehalogenase is still unclear, especially for non-stereospecific ones. **Method:** In this study, using computational analysis, the complex structure of DehE docked with catalytic water (DehE-H_2O) was subjected to MD simulation to study the mechanistic role of catalytic residues, especially Asn114 and Asp189 towards catalytic water. **Results:** Our findings confirmed that Asn114 hold the catalytic water at distance of ~4 Å while Asp189 was appropriately oriented towards catalytic water for catalysis reaction throughout the simulation process. **Conclusions:** The results attained here will play important role in elucidating the direct attack mechanism of halogenated compound by non-stereospecific haloacid dehalogenase. Moreover, this research could suggest different solvent that can be used in dehalogenation to produce a beneficial product other than hydroxyl acid.

KEYWORDS: DehE, MD simulation, haloacid dehalogenase, catalytic mechanism