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Mechanistic Analysis of an L-2-Haloacid Dehalogenase (DehL) from Rhizobium Sp. RC1: Computational Approach

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Abstract : Halogenated organic compounds occur in huge amount in biosphere. This is attributable to the diverse use of halogen-based compounds in the synthesis of various industrially important products. Halogenated compound is toxic and may persist in the environment, thereby causing serious health and environmental pollution problems. L-2-haloacid dehalogenases (EC 3.8.1.2) catalyse the specific cleavage of carbon-halogen bond in L-isomers of halogenated compounds, which consequently reverse the effects of environmental halogen-associated pollution. To enhance the efficiency and utility of these enzymes, this study investigates the catalytic amino acid residues and the molecular functional mechanism of DehL, by classical molecular dynamic simulations, MM-PBSA and ab initio fragments molecular orbital (FMO) calculations. The results of the study will serve as the basis for the molecular engineering of the enzyme.

Keywords : DehL, Functional mechanism, Catalytic residues, L-2-haloacid dehalogenase
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