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Biotechnology and Biotechnological Equipment
Volume 28, Issue 4, 22 October 2014, Pages 608-615

Open Access

Insights into the stereospecificity of the d-specific dehalogenase from Rhizobium sp. RC1 toward D-and L-2-chloropropionate (Article)

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Abstract

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Halogenated compounds are recalcitrant environmental pollutants prevalent in agricultural fields, waste waters and industrial by-products, but they can be degraded by dehalogenase-containing microbes. Notably, 2-haloalkanoic acid dehalogenases are employed to resolve optically active chloropropionates, as exemplified by the D-specific dehalogenase from Rhizobium sp. RCI (DehD), which acts on D-2-chloropropionate but not on its L-enantiomer. The catalytic residues of this dehalogenase responsible for its affinity toward D-2-chloropropionate have not been experimentally determined, although its three-dimensional crystal structure has been solved. For this study, we performed in silico docking and molecular dynamic simulations of complexes formed by this dehalogenase and D-or L-2-chloropropionate. Arg134 of the enzyme plays the key role in the stereospecific binding and Arg16 is in a position that would allow it to activate a water molecule for hydrolytic attack on the D-2-chloropropionate chiral carbon for release of the halide ion to yield L-2-hydroxypropionate. We propose that within the DehD active site, the NH group of Arg134 can form a hydrogen bond with the carboxylate of D-2-chloropropionate with a strength of ~4 kcal/mol that may act as an acid-base catalyst, whereas, when L-2-chloropropionate is present, this bond cannot be formed. The significance of the present work is vital for rational design of this dehalogenase in order to confirm the involvement of Arg16 and Arg134 residues implicated in hydrolysis and binding of D-2-chloropropionate in the active site of D-specific dehalogenase from Rhizobium sp. RC1.

Author keywords

Binding energy D-2-chloropropionate D-specific dehalogenase Dehalogenase Hydrogenbond length Interacting residue Stereospecificity

Indexed keywords

D-specific dehalogenase
Dehalogenase
Interacting residue
Rhizobium sp. rc1
Stereospecificity

Engineering main heading: Binding energy

Species Index: Rhizobium sp.

ISSN: 13102818
Source Type: Journal
Original language: English
DOI: 10.1080/13102818.2014.937907
Document Type: Article
Publisher: Diagnosis Press Limited.

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