COMPARISON OF THE STRUCTURAL PROPERTIES OF CHITIN DEACETYLASES SHOWING DIFFERENT ENZYMATIC ACTION PATTERNS.A COMPUTATIONBAL APPROACH

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Within this study we havecomparedand characterizedthe structural and physicochemical properties of chitin deacetylases from fungi (Colletotrichumlindemuthianum, Aspergillusnidulans) and marine bacteria (Vibrio parahaemolyticusVibrio cholera, Arthrobacter SP. AW19M34-1), these enzymes exhibiting distinct deacetylation patterns. Investigated enzymes emphasize reduced sequences identity, but the amino acids belonging to their active sites are conserved. The overall structural identity is low, but the catalytic domains of these enzymesreveal strong structural similarity correlated with their common biological function. Investigated enzymes expose dissimilar local physicochemical propertiesof their catalytic sites (hydrophobicity and electrostatic potential)that could be responsible of their distinct deacetylation patterns.
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