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Molecular Docking Assessment of Pesticides Binding to Bacterial Chitinases

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Abstract : Molecular docking calculations reveal that pesticides provide favorable interactions with the bacterial chitinases. Pesticides interact with both hydrophilic and aromatic residues involved in the active site of the enzymes, their positions partially overlapping the substrate and the inhibitors locations. Molecular docking outcomes, in correlation with experimental literature data, suggest that the pesticides may be degraded or having an inhibitor effect on the activity of these enzymes, depending of the application dose and rate.

Keywords : chitinases, inhibition, molecular docking, pesticides
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