Molecular Docking and In Silico Evaluation of Isochaetominine as a Novel Inhibitor of Helicobacter pylori Urease (1E9Y)

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Abstract:

The virulent urease enzyme enables Helicobacter pylori to thrive in the stomach's acidic environment by elevating local pH, facilitating bacterial colonization and infection. In this in silico experiment, we employed molecular docking (PyRx) and ADME profiling to study a library of 2,431 natural compounds against H. pylori urease (PDB: 1E9Y). We validated the accu-racy of our method with known inhibitors protocatechuic acid (PCA) (-5.9 kcal/mol) and acetohydroxamic acid (AHA/HAE) (-4.9 kcal/mol). Isochaetominine exhibited superior binding (-9.3 kcal/mol), identified as a strong new inhibitor, performing better than the control PCA and showing favorable ADME properties. These results suggest that Isochaetominine could be a promising novel urease inhibitor that could inhibit enzyme activity.

Keywords:

Isochaetominine, urease (1E9Y), molecular docking, ADME.