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Abstract

The Antibacterial Efficacy and Drug Safety Profile of *Trans*-Cinnamaldehyde against *Acinetobacter baumannii*: Bioinformatics and Cheminformatics Approach †

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Introduction: The discovery of antibiotics saves millions of lives worldwide, but in recent years bacterial antibiotic resistance has become a growing global problem as bacteria have become increasingly able to adapt to all known antibiotics. Projections have shown that in 2019, more than 4.9 million people worldwide died directly or indirectly as a result of antibiotic resistance. Therefore, it is crucial to discover new antibacterial agents that have therapeutic potential and are non-toxic and drug-safe so that humanity can successfully fight antibiotic resistance. Since such studies are usually very expensive and disappointing results are a waste of valuable time, the use of bioinformatics and chemoinformatics tools can help overcome these problems.

Methods: SwissADME (http://www.swissadme.ch/citing.php, accessed on 1 April 2024) software was used to assess *trans*-cinnamaldehyde's pharmacokinetics, drug-likeness, and medicinal chemistry friendliness, while potential therapeutic targets in *Acinetobacter baumannii* were assessed using the RCSB Protein Data Bank online platform tools and evaluated with a comprehensive review of the existing literature.

Results: *Trans*-cinnamaldehyde fulfils the requirements for the number of rotatable bonds and proton acceptors, which should be readily absorbed in the gut and can cross the blood—brain barrier, but is not a substrate for P-gp, which contributes to its therapeutic potential as it is not immediately excreted from the body. Theoretically, it should not be hepatotoxic as it has no inhibitory effect on liver cytochromes. It meets all five of Lipinski's rules and, according to these criteria, is a molecule that could have therapeutic effects. The most promising potential targets in *Acinetobacter baumannii* are the proteins AbOmpA and bap, where *trans*-cimetaldehyde could destabilise membrane integrity and disrupt biofilm formation.

Conclusions: Bioinformatics and chemoinformatics tools can help obtain resources for developing new antibiotics. In vitro tests need to be performed to confirm the efficacy of *trans*-cinnamaldehyde as a potential therapeutic agent against *Acinetobacter baumannii*.

Supplementary Materials: The presentation materials can be downloaded at: https://www.mdpi.com/article/10.3390/proceedings2024102011/s1.

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