



Antibacterial activity of *Garcinia* spp. by molecular docking simulations: an overview

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Abstract The plant genus *Garcinia*, which belongs to the Clusiaceae family, was discovered to have excellent sources of bioactive compounds with therapeutic potential and, therefore received significant attention due to its potential for medicinal properties. In the twenty-first century, one of the most crucial threats to global health, food security, and development is antimicrobial resistance (AMR). The alarming surge in AMR transcends geographical and demographic boundaries, impacting individuals of all ages and nationalities. This phenomenon renders previously effective antibiotics increasingly powerless against a growing tide of resistant bacterial infections, posing a significant public health challenge. Notably, the compilation of extract and bioactive compounds from *Garcinia* species that have potent antimicrobial activity against Gram-positive and Gram-negative bacteria strains by the study of previous research reported in this review. Apart from that, the structure-antibacterial activity relationship for the class of specialized

compounds also had been discussed. In addition, this study employed advanced molecular modelling simulations conducted by the authors to explore the mechanism of microbial pathways of isolated compounds that lead to strong antibacterial activity. Based on this comprehensive review, bioactive compounds isolated from *Garcinia* species emerge as promising candidates for spearheading the development of novel antibacterial agents. Their potential merits were further investigated through in vitro and in vivo studies to fully elucidate their efficacy and safety profiles.

Keywords *Garcinia* · Extracts · Bioactive compound · Antimicrobial activity · Molecular modelling simulations

Introduction

The alarming increase in infectious diseases caused by antimicrobial resistance provides a strong impetus for the emergence of new antimicrobial agents (Naves et al. 2019). The discovery of antibiotics heralded a golden age of therapeutic optimism, leading many to believe that infectious diseases were a conquered foe. Unfortunately, since so many bacteria have developed resistance to various antimicrobial agents, the tide of battle appears to be shifting in the bacteria's favor (Reygaert 2018). Elmaidomy et al. (2022) stated that

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