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RESEARCH ARTICLES

Exploring the *in silico* studies of the endophyte fungus *Phoma herbarum* against mur enzymes of *Staphylococcus aureus* – a computational approach

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Abstract
Endophyte fungus *Phoma herbarum* (NFCCI 4035) was previously isolated and identified from healthy leaf tissue of *Meriandra bengalensis* Benth plant from Manipur. We recently established the antibacterial activity of ethyl acetate extracts of endophyte fungus *P. herbarum in vitro* and identified some potentially active components using GC-MS. The current study aims to perform molecular docking of the discovered *P. herbarum* compounds against Mur enzymes (Mur A, Mur C, Mur D, and Mur F) of *Staphylococcus aureus* using Auto Dock Tools 1.5.6. SwissADME online tool was used to calculate the drug-likeness characteristics. According to the findings, only 14 of 23 bioactive compounds evaluated from *P. herbarum* extract adhered to Lipinski's Rule of Five (LRo5) and had binding affinity ranged between − 3.5 to -6.5 (kcal/mol) with at least one of the four targeted Mur enzymes. When compared to all other bioactive compounds that interact with target Mur enzymes, 2-Palmitoylglycerol molecule demonstrated highest binding affinity (-6.5 kcal/mol) with Mur F ligase. However, (1R,2R,3R,5 S)-2,6,6-Trimethylbicyclo[3.1.1]heptan-3-amine has shown excellent binding affinity for all selected target (Mur A, Mur C, Mur D, and Mur F) enzymes. Also, this study confirmed that the bioactive compounds can be developed into more potent inhibitors targeting *S. aureus*-related infections.

Keywords Endophytic fungi · Bioactive chemicals · Mur enzymes · Molecular docking · Drug-likeness

Introduction

Endophytes act as biological archives for unique natural chemicals, opening up new avenues for medication development. In the hunt for novel chemical entities, plant-associated microorganisms, including bacteria and fungi that inhabit the internal tissues of all plant species, are becoming more and more important candidates for bioprospecting (Staniek et al. 2008; Tiwari et al. 2021). Endophytic fungus has been linked to the discovery of numerous significant bioactive compounds (Mousa and Raizada 2013). *Penicillium* and other endophytic fungal species have received more attention than other microbial species ever since the discovery of penicillin. They have strong track record of producing a wide range of chemical compounds that fall into several classes, such as alkaloids, antibiotics, hormones, mycotoxins, etc. (Mousa and Raizada 2013; Frisvad et al. 2013). These species are notable for the presence of particular mycotoxins such as patulin, citrinin, ochratoxin, etc., as well as the large number of pharmacologically significant chemicals that have so far been described from them (Tiwari et al. 2021). The rise of resistance to antibiotics by pathogenic species such as *Staphylococcus aureus*, *Streptococcus pneumoniae*, *Pseudomonas aeruginosa*, etc. has become increasingly common and poses a serious threat to public health. In particular, infections related to *Staphylococcus aureus* (*S. aureus*) pathogens have not only become more prevalent but have also started developing resistance

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