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Research Article

Efficacy of methanolic extract of *Zingiber officinale* against seed-born fungi

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ABSTRACT

This study is focused on determining the efficacy of natural compounds present in *Zingiber officinale* methanolic plant extraction in controlling seed-born fungal pathogens *Aspergillus flavus* and *Rhizopus oryzae*. The maximum percentage inhibition of 94.01% and 90.43% was reported against. *A. flavus* and *R. oryzae* respectively for the crude extract in the poison food agar method. These results were further confirmed by computational investigation. [4]-gingerol, [6]-gingerol, [8]-gingerol, [10]-gingerol, and [6]-dehydroginger phytochemicals identified in the extract were docked to the active sites in chitin synthase from *A. flavus* and squalene epoxidase from *A. flavus* and *R.oryzae,* and to the RNA dependent RNA polymerase (RdRp) enzyme from *R. oryzae*. The highest binding energy (BE) (-8.12 kcal/mol) was noticed between the interactions of squalene epoxidase and [6]-dehydroginger, and this complex was subjected to Molecular Dynamic (MD) analysis. MD simulations were performed on protein-ligand complexes for 10 ns using CHARMM36 force field. The mean radius of gyration (Rg), root mean square deviation (RMSD), and root mean square fluctuation (RMSF) were calculated and hydrogen bond analysis (HBA) was also performed. Rg and RMSD results indicated the stability of the protein-ligand complex throughout the simulation time.

Keywords: *Aspergillus flavus*, molecular docking, molecular dynamic, *Rhizopus oryzae Zingiber officinale*

INTRODUCTION

Sri Lanka's food supply revolves around cereal and legume crops centered on rice, and pulses followed by fruits and vegetables. South Asian nations underwent a dramatic transition in the second half of the 20th century as a result of the green revolution, which caused the production of cereal and legumes to many times. This highlighted the critical role that seeds play in the cultivation of approximately 90% of the world's food crops. The presence of external and internal seed-borne fungi causes negative effects like seed abortion, seed necrosis, loss of seed germination potential, and injury to seedlings (Mughal and Sers, 2020). These effects have been shown to have a major negative influence on agricultural productivity. In Sri Lanka, 46 different fungal species belonging to 26 different genera were reported on rice seeds (Bandara *et al.,* 2017). *Alternaria*, *Cercospora, Fusarium*, *Phytophthora*, and *Rhizoctonia* are the most common fungal pathogens associated with stored seeds. These fungal pathogens are mainly responsible for seed deterioration, reduction in germination potential, and seedling vigor (Chaudhari *et al.,* 2017). Fungal identification is highly involved in determining the most appropriate environmentally friendly

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