Evaluating the potential of selective phytochemicals in the control of rice grain pest *Sitophilus oryzae* L. using molecular docking and visualization

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ABSTRACT

Computer based stimulations allow faster and precise understanding of molecular interactions between a molecular compound and its target protein. In the present study the effect of phytochemicals on significant enzyme receptors are evaluated considering *Sitophilus oryzae* as the target species. The enzyme receptors, Glutathione S Transferase and Alpha amylase, are selected based on their function in the metabolic activities of the target species. The selection of phytochemical ligands was based solely on existing literature describing plant-derived compounds traditionally used in indigenous pest control practices. The compounds selected include Piperin, Curcumin, Gingerol, Zingiberene, Cinnamaldehyde and Shogaol. Molecular docking and visualization techniques are used to stimulate the interactions between these selected receptors and ligands. The analysis of the results showed that all the selected compounds show significant potential as inhibitors of the selected receptors. Thus, they can potentially control the target pest species by interrupting the normal metabolic functions of the insect.

Keywords: alpha amylase, docking, glutathione, phytochemicals, rice pest

1. INTRODUCTION

Rice (*Oryza sativa* L.) is a major staple food crop worldwide and is particularly important in countries such as India, where it contributes significantly to food security. Postharvest losses caused by storage pests, especially the rice weevil *Sitophilus oryzae* (L.), pose a serious problem to grain storage and the agricultural economy. This insect is cosmopolitan in distribution and is responsible for considerable economic losses each year. Adult female weevils bore into rice grains to lay eggs, usually depositing a single egg per grain, which allows larval development to occur within the grain leading to both qualitative and quantitative losses to the grain (Subedi et al., 2009)

Chemical pesticides are commonly used by farmers to manage storage pests. But many farmers lack knowledge of their harmful effects and proper handling practices (Rijal et al., 2018). The choice of chemical pesticides is often influenced by cost and easy availability rather than safety or long-term impact (Sharifzadeh et al., 2018). Prolonged use of synthetic pesticides has been linked to several health problems and negative environmental effects (Nicolopoulou-Stamati et al., 2016). As a result, alternative pest control methods have gained attention. Botanical insecticides have been reported to be suitable for crop production and postharvest protection because they are environmentally safer and pose less risk to human health (Isman, 2006).

Recent advances in computer-based techniques have improved the speed and accuracy of drug discovery. Similar in silico approaches are applied for pest management. In the present study,

computer-based drug design methods were used to evaluate the potential of selected bioactive phytochemicals for the control of *Sitophilus oryzae*. Two key enzymes, Glutathione S-transferase (GST) and alpha-amylase (AA), were selected as target receptors due to their important roles in insect metabolism. GST is involved in detoxification of exogenous materials in insects (Eaton and Bammler, 1999), while AA plays an essential role in digestion (Da, 2018).

The phytochemicals studied are major bioactive compounds found in plant species commonly used in indigenous pest management practices. the plant species clove, cinnamon, turmeric, black pepper, ginger, and karanjin were selected based on documented indigenous pest management practices (Lee et al., 2001; Padmasri et al., 2017; Khanal et al., 2021; Ngegba et al., 2022; Jena et al., 2022). Based on available literature, these plants were reported to contain piperin, curcumin, gingerol, zingiberene, cinnamaldehyde, and pongamol as their most important constituents (Zachariah & Leela, 2018; Stojanović-Radić et al., 2019; Ramteke, 2022; Abdull Rahim et al., 2024). These phytochemicals were therefore selected for the present study. The molecular structures of the target enzymes and ligands were obtained from online databases, and molecular docking simulations were carried out using docking software. The study aims to understand the effectiveness of phytochemicals traditionally used in indigenous pest management practices and to identify eco-friendly compounds with potential for developing safer and more sustainable strategies for the control of rice weevil.

2. METHODOLOGY

2.1 Preparation of receptor and ligand structures

The molecular structure of the receptor Glutathione S- Transferase (1GNW) was downloaded from RCBS PDB (Research Collaborators for structural Bioinformatics Protein Data Bank) database (https://www.rcsb.org/) (Berman et al., 2000). The ligand, selected active components of black pepper was downloaded from Zinc database (https://zinc.docking.org/) which is a free database of commercially available compounds especially prepared for virtual screening (Irwin and Shoichet, 2005). For the present study we download Piperin (ZINC000169711394)

2.2 Molecular docking

Molecular docking was performed to predict the possible molecular interactions between the receptors and the ligand molecules using a docking software, Molegro Virtual Docker (MVD 2010.4.0 for Windows). MVD identifies ligand binding modes by iteratively evaluating a number of candidate solutions (ligand conformations) and estimating the energy of their interactions with the macromolecule (Bitencourt-Ferreira and de Azevedo, 2019).

2.3 Visualization

The data acquired from the docking simulation was further analyzed using visualization software Biovia Discovery Studio. The receptor ligand interactions are visualized using both 3 dimensional and 2 Dimensional images (BIOVIA, 2021).

3. RESULTS and DISCUSSION

Plant-derived phytochemicals traditionally associated with pest management were evaluated for their ability to interact with key metabolic enzymes of the target insect using molecular docking techniques. The results show that all phytochemicals used in the study exhibited negative docking scores against both Glutathione S-transferase (GST) and alpha-amylase (AA), indicating favorable binding interactions with the target enzymes (Fig.1). Molecular docking is a widely used in silico approach for predicting the binding orientation, affinity, and interaction patterns between small molecules and target proteins. It provides insights into the possible inhibitory potential of bioactive compounds by estimating the strength and stability of receptor–ligand interactions. Negative docking scores generally indicate energetically favorable interactions, suggesting that the ligand can bind stably within the active or functional site of the target protein and potentially interfere with its biological activity.

Among the compounds tested, curcumin showed the most favorable docking score against GST, suggesting strong interaction with the detoxification enzyme. In contrast, piperine exhibited the best docking performance against AA, indicating higher affinity toward the digestive enzyme. The variation in binding affinities among the phytochemicals highlights their target-specific interaction.

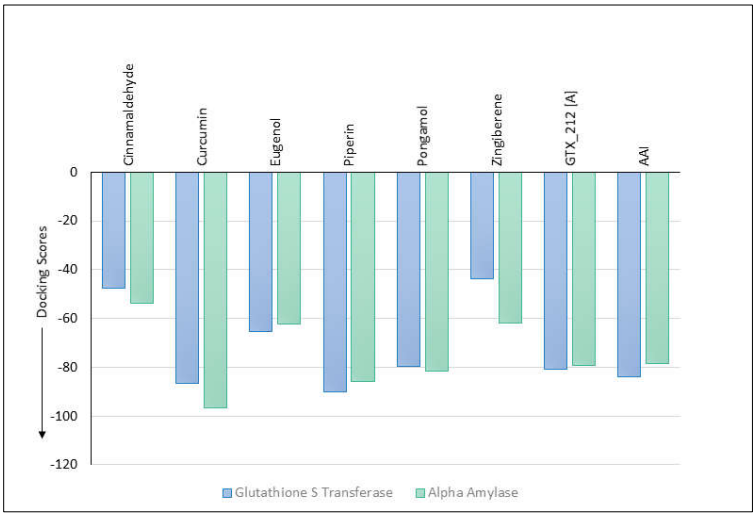

Fig. 1: Graph showing the docking scores of selected phytochemicals against Glutathione S Transferase and Alpha Amylase

Visualization of the receptor-ligand complexes revealed stable interactions involving key amino acid residues of both enzymes (Fig. 2 and Fig. 3). Different interactions were observed including Van der Waals forces, hydrogen bonds, C-H bonds, and non-covalent bonds such as Pi-Alkyl, Pi-pi T shaped, and Pi-Sulfur bonds. The interaction patterns observed suggest that binding of these phytochemicals may interfere with the normal catalytic activity of GST and AA, potentially leading to enzyme inactivation.

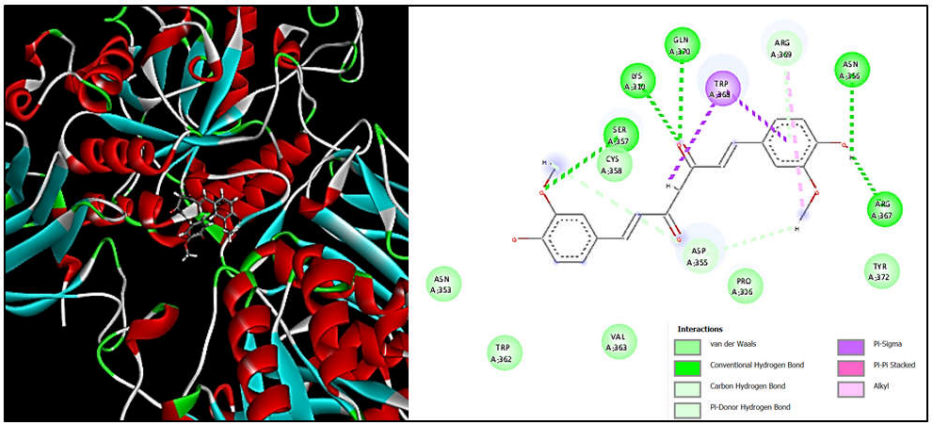

Fig. 2: Interaction between Alpha Amylase and Curcumin observed in 3D and 2D

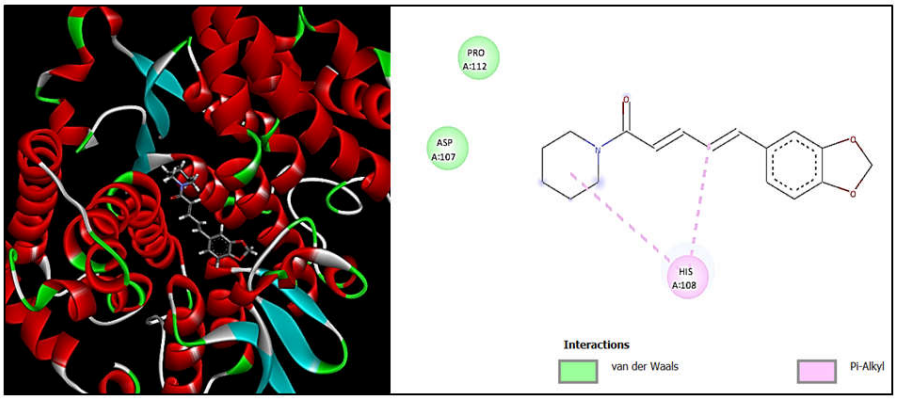

Fig. 3: Interaction between Glutathione S Transferase and Piperin observed in 3D and 2D

The results show the potential of selected phytochemicals to target essential metabolic pathways in *S. oryzae* at the molecular level. Molecular docking has been increasingly applied in pesticide research to predict binding affinities, understand interaction mechanisms, and reduce the time and cost associated with experimental screening of candidate compounds (Hou et al., 2023). This has allowed researchers to improve conventional pesticide discovery towards more targeted and mechanism-based approaches, enabling the rational selection of bioactive molecules with improved efficacy and safety profiles (Desai et al., 2024). Researches ombining bioassays with molecular docking to evaluate plant-derived compounds for stored-product pest management have highlighted the role of in silico approaches in identifying potential insecticidal targets (Hazarika et al., 2025). Molecular docking provides molecular-level insights that support sustainable pest management strategies and contribute to agri-food security (Iñiguez-Luna et al., 2025)

4. CONCLUSION

The present study was undertaken to evaluate the potential of certain bioactive phytochemicals in the control of rice pest Sitophilus oryzae. The selected phytochemicals were bioactive

compounds found in plants that are commonly used in Indigenous pest management practices. It was observed that all the phytochemicals used show The positive interactions of the selected phytochemicals with the target receptors Glutathione S Transferase and Alpha Amylase indicating that they have the ability to suppress their biological functions. The findings provide molecular-level support for the use of phytochemicals traditionally employed in indigenous pest management practices and highlight their promise as eco-friendly candidates for the development of sustainable strategies for rice weevil control.

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