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ORIGINAL RESEARCH

A molecular docking simulation study on potent inhibitors against *Rhizoctonia solani* and *Magnaporthe oryzae* in rice: silver-tetrylene and bis-silver-tetrylene complexes vs. validamycin and tricyclazole pesticides

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Abstract

Rice, well known as the most important staple food source worldwide, is highly susceptible to many infectious diseases, especially rice sheath blight caused by fungus *Rhizoctonia solani* and rice blast caused by fungus *Magnaporthe oryzae*. The inhibitory ability of silver- and bis-silver-tetrylene complexes, including **Ag-E** and **bis-Ag-E** with **E** = C, Si, Ge, onto protein 4G9M in *Rhizoctonia solani* and protein 6JBR in *Magnaporthe oryzae* was theoretically investigated using molecular docking simulation methodology. Two commercial pesticides selected as inhibitory references are validamycin for 4G9M and tricyclazole for 6JBR. The results reveal that bis-silver-tetrylene complexes perform the strongest inhibitory effects towards both proteins. The structures of the complexes exhibit good site–site binding to both proteins given the observations on the hydrogen bond interactions, cation–π bonds, π–π bonds, and ionic interactions, interaction distance between amino acids and ligands, and van der Waals interactions. The inhibitory capacity onto protein 4G9M decreases in the following order: **bis-Ag-C** > **bis-Ag-Si** > **bis-Ag-Ge** > validamycin > **Ag-C** ≈ **Ag-Si** ≈ **Ag-Ge**. The corresponding order observed from the study for protein 6JBR is **bis-Ag-C** > **bis-Ag-Si** ≈ **bis-Ag-Ge** > tricyclazole ≈ **Ag-C** ≈ **Ag-Si** ≈ **Ag-Ge**. The study opens a promising approach to tackle rice blast and rice sheath blight based on a family of silver-tetrylene organometallic chemicals given the theoretical proof of environment-advanced properties and molecule-scaled effectiveness.

Keywords Tetrylenes · *Rhizoctonia solani* · 4G9M · *Magnaporthe oryzae* · 6JBR · docking simulation

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Introduction

Rice (*Oryza sativa* L.) is rich in nutrients, vitamins, and minerals, and by far the most important staple food source for more than 70% of the world's population [1]. The demand for rice production has seen a dramatic increase in recent years due to the rapid growth of the global population. However, rice is vulnerable to many diseases caused by microorganisms such as bacteria, viruses, or fungi, leading to dramatic losses in the crop yield annually. Rice blast and rice sheath blight, caused by fungi *Magnaporthe oryzae* and *Rhizoctonia solani* respectively, are two of the most devastating diseases and result in severe impacts on either rice yield or grain quality.

Sheath blight results in yield loss of 10–25% [2] and up to 50% under favorable environmental conditions [3]. Sheath blight is recognizable by the rapid and irregular appearance

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