Inhibitability of Tetrylene Complexes against *Rhizoctonia solani* and *Magnaporthe oryzae*

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ABSTRACT

Copper carbenes and silylenes are considered for the inhibitory effect of the considered complexes towards *Rhizoctonia solani* (PDB-4G9M) and *Magnaporthe oryzae* (PDB-6JBR) in rice. Quantum chemical calculations of copper carbene and silylene complexes (**Cu-NHC1**, **Cu-NHC2, Cu-NHSi1**, and **Cu-NHSi2**) were obtained using density functional theory (DFT). Their inhibitability towards the targeted proteins (4G9M; 6JBR) was evaluated using molecular docking analysis. Quantum chemical analysis predicts the stability of the studied complexes. Their electronic configurations are justified and highly conducive to intermolecular interaction. Regarding the carbenes/silylenes-4G9M structures, the stability is estimated in the order **[Cu-NHC2]-4G9M** > **[Cu-NHSi1]-4G9M** = **[Cu-NHSi2]-4G9M** > **[Cu-NHC1]-4G9M**; while the order for the carbenes/silylenes-6JBR adducts is **[Cu-NHSi2]-6JBR** > **[Cu-NHC2]-6JBR** = **[Cu-NHSi1]-6JBR** > **[Cu-NHC1]-6JBR**. The findings of this study reveal that copper-carbenes and copper-silylenes have the potential to protect against the infection of fungi *Rhizoctonia solani* and *Magnaporthe oryzae*, which encourages further research.

Keywords*: Carbene; silylene; Rhizoctonia solani; Magnaporthe oryzae; density functional theory; molecular docking simulation.*