

Synthesis and fungicidal activity of hydrated geranylated phenols against botrytis cinerea

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Abstract

Botrytis cinerea is a ubiquitous fungus that affects hundreds of plants, resulting in economic losses to the horticulture and fruit industry. The search for new antifungal agents is a matter of current interest. Thus, in this work a series of geranylated phenols in which the side alkyl chain has been hydrated have been synthesized, and their activity against *B. cinerea* has been evaluated. The coupling of phenol and geraniol has been accomplished under microwave irradiation obtaining the highest reaction yields in the shortest reaction times. Hydration of the side chain was carried out in dioxane with *p*-toluenesulfonic acid polymer-bound as the catalyst. All synthesized compounds were tested against *B. cinerea* using the growth inhibition assay and EC₅₀ values were determined. The results show that activity depends on the number and nature of functional groups in the phenol ring and hydration degree of the geranyl chain. The most active compound is 1,4-dihydroquinone with one hydroxyl group attached at the end of the alkyl chain. Results from a molecular docking study suggest that hydroxyl groups in the phenol ring and alkyl chain are important in the binding of compounds to the active site, and that the experimental antifungal activity correlates with the number of H-bond that can be formed in the binding site. © 2021 by the authors. Licensee MDPI, Basel, Switzerland.

Author keywords

Botrytis cinerea; Docking; Fungicidal; Hydrated geranylated phenols; Synthesis