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ISOLATION, ANTIFUNGAL ACTIVITY, AND MOLECULAR DOCKING ANALYSIS OF AXILLARIN FROM *Tanacetum alyssifolium*

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Abstract

The antifungal activity of axillarin, a polymethoxylated flavone isolated from the methanol extract of *Tanacetum alyssifolium*, was evaluated *in vitro* against several plant pathogenic fungi: *Fusarium oxysporum* f. sp. *radicis-lycopersici* (FORL), *Alternaria alternata* (A.A), *Fusarium oxysporum* f. sp. *niveum* (FON), *Phytophthora infestans*, and *Cylindrocarpon* spp. Antifungal efficacy was assessed at concentrations of 200 and 400 µg/mL using the agar Petri dish method. Axillarin inhibited fungal mycelial growth in a dose-dependent manner, with the highest inhibition observed for *A. alternata* (33.31%), followed by FORL (29.46%), *Cylindrocarpon* spp. (26.64%), and FON (18.21%). No inhibitory effect was detected against *P. infestans*.
To support the experimental findings, molecular modeling was performed using GaussView 5.0 and GAUSSIAN 09 to determine the optimized 3D conformation of axillarin through potential energy surface (PES) analysis. This optimized structure was then used in molecular docking simulations to explore interactions with fungal protein receptors.
The results suggest that axillarin may serve as a natural antifungal agent with potential applications in the development of environmentally friendly alternatives to synthetic fungicides. This approach supports sustainable plant protection strategies and reduces ecological risks associated with chemical pesticide use.

Key words: antifungal activity, axillarin, molecular docking, plant pathogens, *Tanacetum alyssifolium*

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