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Antimicrobial activity and chemical composition of *Syringa vulgaris* L. essential oil and molecular docking simulation of its selected major chemical component

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Syringa vulgaris L. is a well-known ornamental plant used in traditional medicine, but its therapeutic properties and bioactive components have not been sufficiently investigated. Furthermore, there is a lack of detailed research on how the components of *Syringa vulgaris* essential oil (SVEO) interact at the molecular level with target proteins. This study aimed to evaluate the chemical composition and antimicrobial activity of SVEO *in vitro* and in *silico*. GC-MS identified 32 compounds. The most abundant compounds were identified as diethyl phthalate (54.296%), alpha-terpineol (24.141%), and gamma-terpineol (11.389%). SVEO was inactive against nearly all tested bacterial strains in the *in vitro* antibacterial assay but demonstrated varying levels of antifungal activity against yeasts (especially *Candida albicans*) and *Aspergillus* spp. Finally, the binding affinities of the three main components revealed significant potential to inhibit five target receptor proteins crucial to *Candida albicans*, as assessed using the AutoDock-Vina program, which helped determine the antifungal mechanism. SwissADME results for drug-like properties and toxicity prediction showed that these components met the rule of five and exhibited acceptable drug-like properties. Therefore, this study suggests that SVEO is a promising candidate, particularly for treating *Candida albicans* infections and addressing the growing issue of antifungal resistance.

Keywords: lilac oil, essential oil components, GC-MS, antibacterial activity, antifungal activity, prediction of drug similarity

Introduction