

In vitro and in silico evaluation of antifungal activity of cassia (*Cinnamomum cassia*) and holy basil (*Ocimum tenuiflorum*) essential oils for the control of anthracnose and crown-rot postharvest diseases of banana fruits

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Abstract

Anthrachnose and crown-rot postharvest diseases of banana fruit are responsible for major postharvest losses of the fruit. For natural control of these diseases, in vitro antifungal activity of cassia and holy basil essential oils was evaluated by disc volatilization method. Cassia essential oil at 6 μL per plate exhibited 100% growth inhibition of both the causative fungal pathogens, namely *Colletotrichum musae* and *Lasiodiplodia theobromae*. Holy basil essential oil was capable of completely inhibiting the growth of *L. theobromae* at 6 μL per plate, whereas it could inhibit *C. musae* up to 96% at 10 μL per plate. Molecular docking and conceptual DFT studies have been performed to ascertain the components of essential oils responsible for antifungal activity based on their binding affinities to chitin synthase protein and chemical behaviour. Components, such as eugenol, cinnamyl acetate, caryophyllene, humulene and *trans*-calamenene, may most likely be responsible for high activity of the tested essential oils as per the in silico results.