Fabrication and *in vitro* antifungal potential of nanoencapsulated eugenol against fungal contaminants of *Calocybe indica*

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Fungal diseases pose a significant threat to mushroom crops, and the standard approach to controlling these diseases on farms globally often relies on fungicides. However, issues such as the development of pathogen resistance to fungicides due to frequent use and the sensitivity of mushrooms to these chemicals present serious challenges. To address these problems, incorporating herbal agents for disease prevention could contribute to a more sustainable mushroom industry. This study aimed to develop nanoencapsulated eugenol and assess its prolonged antifungal effectiveness. Four fungal competitors *i.e.*, two *Trichoderma spp*, *Penicillium spp* and *Aspergillus spp* were isolated from *Calocybe indica* cultivating industries and identified based on morphological and molecular characteristics. Carboxymethyl cellulose-based nonencapsulated eugenol was synthesized and its physical and chemical properties were determined by Field Emission Scanning Electron Microscopy (FESEM), Zeta sizer, High-Performance Liquid Chromatography (HPLC) and Fourier-transform Infrared (FTIR) spectroscopy. Nanocapsules were found to be nearly spherical in shape with sizes ranging from 139.8 nm to 273.8 nm and possessed encapsulation efficiency of 90.6%. The conical flask paper cone method determined the minimum inhibitory concentration (MIC) of encapsulated eugenol required per centimeter cube. MIC values were recorded as 4.02 µL/cm^3 and 5.0 µL/cm^3 against *Trichoderma spp*, *Penicillium spp* and *Aspergillus spp* respectively. FTIR reports evidenced successful encapsulation of eugenol which might have interacted with CMC *via* intermolecular hydrogen bonding. Further, *in silico* molecular modeling studies also showed CMC-eugenol complex formation by the interaction between the hydrogen atom of hydroxy group of eugenol with the oxygen atom of CMC. The binding energy of the docked structure was calculated to be -2.57 kcal/mol. Molecular docking results well supported the findings of FTIR spectroscopic analysis. The outcome of this study will help the mushroom cultivators prevent economic losses caused by fungal contamination.

Keywords: Molecular docking, Essential oils, Carboxymethyl cellulose, *Trichoderma*, FTIR analysis, Fungal

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