ANTIBACTERIAL POTENTIALS OF ENDOPHYTIC FUNGAL METABOLITES FROM MEDICINAL HERBS; *Carica papaya*, *Mangifera indica* And *Gossypium hirsutum* ON PERIODONTAL ISOLATES.

By

AKINKUNMI, OPEYEMI BAMIDELE (PG/19/0809)

B. Tech (LAUTECH)

A Dissertation submitted to the Department of Microbiology, College of Biosciences, Federal University of Agriculture, Abeokuta in Partial fulfilment of the Requirements for the award of degree in Master of Science in Microbiology

August, 2025

ABSTRACT

The increasing level of multidrug resistance among bacterial pathogens is a major concern in public health sector. This necessitates for more research in search of newer potential drug components. This study aimed at determining the antibacterial potential of endophytic fungal metabolites. The medicinal plants, *Carica papaya, Mangifera indica* and *Gossypium hirsutum* were collected and identified at Botany Department, Federal University of Agriculture, Abeokuta. Fungal isolates were obtained from the plant parts (leaves, roots and stems) by surface sterilization to remove debris and epiphytes present in the plant parts, and were cultured on Potato Dextrose Agar plates. Fungal isolates were characterized using a combination of morphological and molecular techniques. The submerged fermentation was done by sub-culturing the isolates of the filamentous fungi on Potato Dextrose Broth, incubated on a rotary shaker for 18 days for the purpose of the release of their metabolites and finally macerated to obtain the extracts. The obtained extracts were tested by agar well diffusion, Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) for antimicrobial activity against bacteria implicated in periodontal isolates. These include *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, *Escherichia coli*, *Streptococcus pyogenes*, *Proteus mirabilis* and *Enterococcus faecalis*. The crude extracts were analyzed with Gas Chromatography-Mass Spectrometry while pharmacokinetic properties of metabolites were evaluated using *in silico* methods. Data obtained were statistically analysed using one-way ANOVA and values were recorded as mean ±SEM. Four endophytic fungal isolates obtained from the plants were identified as *Trichoderma harzianum*, *Penicillium notatum* and two different strains of *Aspergillus niger*. The zones of inhibition of the fungal extracts ranged from 18.0 ± 1.0 mm to 23.0 ± 1.0 mm where *Aspergillus niger* produced metabolites with the most potent inhibitory properties. However, no zone of inhibition was observed on *E. coli* showing that the *E. coli* strain was resistant to all the extracts used in this

study. The MIC and MBC values ranged from (3.13 µg/mL – 12.50 µg/mL) and (6.25 µg/mL – 5.00 µg/mL) respectively. The GC-MS analysis of the extracts showed the presence of several compounds including acetic acid, oxoprophines, 6-heptenoic acid, ethyl ester, oleic acid, nonanoic acid. It was observed that *A. niger* extracts through GC-MS had the highest peak value of 36.79a.u. *In silico studies* revealed favorable binding interactions between the ligands and the target protein, indicating potential therapeutic applications. Pharmacokinetic studies revealed that all ligands examined in this study passed the Lipinski rule with no violation. The molecular characterization of the fungal isolates revealed *Trichoderma harzianum* NAS120-M44, *Aspergillus niger* AMUAN-1 and *Aspergillus niger* ASP-599. This study showed that the antibacterial activity exhibited by the endophytic fungi and the bioactive compounds of these plants possess a great potential for drug discovery.