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Invitro and Virtual Screening of Bioactive Molecule from Mycelium of *Trichoderma atroviride* Inhibit the UDP-3-*O*-(*R*-3-hydroxymyristoyl)-*N*-acetylglucosamine Deacetylases (LpxC) for Treatment of Bacterial Infection

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Trichoderma species are a rich source of metabolites, but less known for biomedical potential. This work deals with antibacterial and antioxidant potentials of intracellular non-cytotoxic metabolites, extracted from *Trichoderma atroviride* (KNUP001). A total of 53 fractions was collected by column chromatography and tested for cytotoxicity by MTT assay. Only one fraction (F41) was found to be non-toxic to Vero cells with 95.4±0.61% of survival. The F41 was then subjected to chemical analysis, antibacterial and antioxidant assays. The F41 at 500 μg.ml^{-1} showed the total antioxidant of 48.70±2.90%, DPPH radical scavenging activity of 37.25±2.25, nitric oxide (NO) radical scavenging activity of 54.55± 1.95 and H_2O_2 radical scavenging activity of 43.75±3.21. The F41 at 25 μg.ml^{-1} displayed antibacterial activity against *E. coli* (14.25±0.2 mm), *P. mirabilis* (10.4±0.6 mm), *S. dysenteriae* (18.6±03 mm), *S. paratyphi A* (14.1±1.1 mm), *E. aerogenes* (5.6±0.4 mm) and *S. marcescens* (14.25±0.2 mm). GC-MS analysis revealed the dominant presence of oleic acid C 18.1 (63.18%), n-hexadecanoic acid (6.17%), and ethyl oleate (4.93%) and potent molecules such as 8-[(2E)-2-(3-hydroxybenzylidene)hydrazinyl]-1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione, 2-(Dimethylamino)ethyl (1Z)-N-hydroxy-2-(4-morpholinyl)-2-oxoethanimidothioate, Fluorene in the F41, and virtual study revealed that these molecules are likely responsible for the antibacterial activities of F41. Hence, further investigation deserves on purification and characterization of the active metabolites from *T. atroviride* strain KNUP001 towards developing molecular leads to effective antibacterial drugs, and non-toxic to host cells.

Key words: Antibacterial, Antioxidant, Oleic acid, Fluorene, *Trichoderma atroviride*, Virtual screening,