Contribution ID: **245** Type: **not specified**

Antifungal and antibacterial potential of isoflavones from Millettia thonningii

Tuesday, 19 November 2024 16:30 (30 minutes)

This study demonstrates the antifungal and antibacterial potential of isoflavone natural products isolated from the seeds extracts of Millettia thonningii. In an effort to gain bond topological information which may have consequences for the observed bioactivities, the crystal structure of robustic acid was solved and refined using the independent atom as well as the invariom model, and the structures were compared. Robustic acid contains a fused tricyclic unit with a benzopyran moiety, with a phenylene ring substitution on the coumarin ring similar to the alpinumisoflavones isolated from this plant. Two coumarins, robustic acid and thonningine-C isolated from Millettia thonningii, show promising activity against the fungus Candida albicans with minimum fungicidal concentration of 1.0 and 0.5 mg/mL, respectively. Also, at a minimum inhibitory concentration of ˜1 mg/mL, alpinumisoflavone and robustic acid were found to be cytotoxic to Staphylococcus aureus (ATCC 25923) showing a zone of inhibition (ZOI) of ˜9 mm. Molecular modelling against the putative bio-molecular target, lanosterol 14-demethylase (CYP51), revealed a plausible binding mode for the active compounds, in which the hydroxyl group binds with a methionine backbone carboxylic group blocking access to the iron catalytic site. This binding disrupts the synthesis of several important sterols for the survival of fungi. These compounds offer potential new avenues for targeting fungal and bacteria and could be useful as chemical probes for understanding these pathogens in an effort to overcome drug resistance.

Primary authors: KINGSFORD-ADABOH, Robert (University of Ghana); Dr MOSCO, Daniel (University of Ghana); Dr HARRISON, Jerry EK (University of Ghana)

Presenter: KINGSFORD-ADABOH, Robert (University of Ghana)

Session Classification: Plenary

Track Classification: AfLS