Department of Chemistry

Departmental Seminar:
Analytical Chemistry Month

You are cordially invited to a lecture presented by

Portia C. Makhubela

Supervised by Dr Yvette Naudé and Prof Egmont Rohwer

Department of Chemistry, University of Pretoria

Date: Friday, 01 July 2022
Time: 10:30 – 11:20
Venue: **Orbital**
Enquiries: Dr. Madelien Wooding, madelien.wooding@up.ac.za

A non-invasive human skin sampling technique for the detection of volatile organic compounds associated with *Mycobacterium tuberculosis* by comprehensive gas chromatography time-of-flight mass spectrometry (GCxGC-TOFMS)

Tuberculosis (TB) is a communicable disease caused by Mycobacterium tuberculosis. It is one of the leading causes of death globally and yet despite medical and technological advances blood and sputum samples remain the only primary biological materials used in the detection of TB by various diagnostic tests. It is common knowledge that certain diseases are associated with biochemical/metabolic changes; therefore, this suggests that biochemicals/metabolites can be used in a diagnostic context. This study investigated the use of skin volatile organic compounds (VOCs) as

prospective TB diagnostic biomarkers. The use of a non-invasive sampling technique in a non-targeted biochemical screening context was examined to explore biochemical differences between healthy and diseased states. The study cohort consisted of test and control groups both containing male and female participants (n=38). The test group was clinically diagnosed with TB (n=15), without complications and they were sampled before the commencement of the TB drug treatment. The control group (n=23) was clinically proven to be non-TB infected and without respiratory complications. Samples of VOCs from skin emanations of the participants were collected using polydimethylsiloxane (PDMS) silicone rubber loops, worn as a patch, followed by thermal desorption and analysis with comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC-TOFMS). Multivariate analysis was conducted to investigate prospective TB diagnostic biomarkers from skin emanation VOCs, using two approaches; targeted analysis where compounds found in this study were compared to those associated with TB in literature and non-targeted analysis which focused on finding novel compounds. Results established a correlation between compounds found in this study and those associated with TB in literature, in addition to three novel compounds. Predictive modelling achieved sensitivities of 0.867 and 0.830 with specificities of 0.848 and 0.875 for targeted analysis and non-targeted analysis respectively.