Department of Chemistry

Departmental Seminar:
Analytical Chemistry Month

You are cordially invited to a recorded lecture presented by

Daniel T. Pretorius

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

Identifying Markers Of Genus For *Plectranthus* And *Coleus* In Complex Samples Of Foliar Volatile Compounds Using GC×GC-TOFMS And Machine Learning

Plectranthus and *Coleus* are genera of plants from the family Lamiaceae, which includes many species of phytochemical and horticultural importance [1]. Until recently, some species of Coleus were named and subsumed under genus *Plectranthus*, however, genomic analysis has recognised *Coleus* as a sister taxon of *Plectranthus* [2,3]. In this study, profiles of the foliar volatile organic compounds (VOCs) from different species of southern African *Plectranthus* and *Coleus* were obtained by HS-SPME and GC×GC-TOFMS in order to model the data with machine learning, and to identify potential chemotaxonomic markers of genus. The method consists of a pipeline for the pre-

processing of high dimensional datasets, modelling and prediction. Three algorithms (an elastic-net regression, a random forest and a support vector machine) were used to predict the genus (*Plectranthus* or *Coleus*) of unknown samples, and top variables were selected as potential putative markers of genus. With reference to the current study, this presentation will focus on aspects of data processing, modelling and feature selection in the analysis of complex samples of biogenic VOCs.

References

[1] Rice, L.J., Brits, G.J., Potgieter, C.J., Van Staden, J. 2011. Plectranthus: a plant for the future? S. Afr. J. Bot., 77(4): 947-959. https://doi.org/10.1016/j.sajb.2011.07.001.

[2] Paton, A., Mwanyambo, M., Culham, A. 2018. Phylogenetic study of Plectranthus, Coleus and allies (Lamiaceae): taxonomy, distribution and medicinal use. Bot. J. Lin. Soc., 188: 355-376. https://doi.org/10.1093/botlinnean/boy064.

[3] Paton, A.J., Mwanyambo, M., Govaerts, R.H.A., Smitha, K., Suddee, S., Phillipson, P.B., Wilson, T.C., Forster, P.I., Culham, A. 2019. Nomenclatural changes in Coleus and Plectranthus (Lamiaceae): a tale of more than two genera. PhytoKeys, 129: 1-158. https://doi.org/10.3897/phytokeys.129.34988.