

# EMN Live Webinars

THURSDAY, 16<sup>TH</sup> MARCH 2023

13:00 UTC, 14:00 CET



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## Webinar Title: “Overcoming the isomers challenge during metabolite identification by LC-MS technique”

During metabolomics studies, metabolite identification is the most challenging step, requiring in depth understanding of molecular structures. Despite the obvious challenges posed by unknown compounds, isomeric compounds present undisputed analytical challenges. Techniques such as LC-MS and NMR have been used in combination or independently for identification of novel compounds. LC-MS is a powerful technique which exploits the resolution power of the LC technology and the sensitivity and accuracy of the MS detector. As such, LC-MS has been widely applied in the field of metabolomics. However, metabolite identification through LC-MS remains an undisputed challenge because most of the metabolites are not yet characterized and thus, unavailable as references. During LC-MS, isomers, chromatographically elute very close to each other and produce very similar MS fragmentation patterns, further worsening metabolite identification. Herein, we show some innovative strategies developed in our laboratory to overcome challenges associated with isomer differentiation using phenolic compounds (chlorogenic acids and flavonoids) as a study model. Our results show that column chemistry and mass spectrometry settings should be fine-tuned to result in slight differences that can be exploited for isomer differentiation.

## Dr. Ntakadzeni Edwin Madala.

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**Edwin Madala** holds a PhD from the University of Johannesburg under the supervision of Ian Dubery working in the field of plant metabolomics. He is currently an associate professor of biochemistry at the University of Venda. His research interest is on metabolite fingerprinting of under-utilized plants by LC-MS techniques to enhance the pharmacological value thereof. Recently, he also started working on analyses of naturally occurring isomers. Using make-shift UV light photoreactors (mimicking sunlight exposure of plants), he has generated new isomers which he uses as a model for isomer identification through LC-MS. His work has shown that plants contain molecules prone to UV-geometrical isomerization as an evolutionary strategy to protect themselves against excessive sunlight exposure and other stressors.



## Ms. Babra Moyo

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**Babra Moyo** is currently registered for a PhD in Biochemistry at the University of Venda and her research is on the investigation of chemical relationships between host plant and semi-parasitic plants using the UHPLC-q-TOF-MS and molecular networking. She is also working as a Lab Technician in the Department of Food Science and Technology in the same institution. She obtained her MSc Chemistry from the University of Venda, BSc (Hons) Chemistry and BSc Chemistry and Mathematics from the University of South Africa.

