Session 2 - Hyperspectral Imaging (Co-chairs: Devaux/Vermaak)

02-01: Hyperspectral imaging in combination with chemometric data analysis – a powerful duo in the quality control of herbal medicines

Ilze Vermaak[1,2], Sidonie Yankam Tankeu[1], Majolie Djokam[1], Maxleene Sandasi[1], Weiyang Chen[1], Alvaro Viljoen[1,2]

[1]Department of Pharmaceutical Sciences, Tshwane University of Technology, Pretoria, South Africa
[2] SAMRC Herbal Drugs Research Unit, Tshwane University of Technology, Pretoria, South Africa
E-mail: vermaaki@tut.ac.za

The quality control of herbal material is notoriously challenging due to the complex mixture of compounds present in plants. In addition, the variability in phytochemical profiles and toxicity issues associated with herbal products necessitates the development of reliable quality control methods. Analytical methods such as liquid chromatography coupled to mass spectrometry are time-consuming and requires considerable expertise. Hyperspectral imaging (HSI) integrates conventional spectroscopy and imaging to obtain spectral and spatial information from a sample. Once the method has been developed, the visual results are rapidly obtained and easy to interpret. In this study, the use of HSI in combination with chemometric data analysis in quality control will be illustrated using several examples: 1) distinguishing between the whole dried fruit of *Illicium verum* (Chinese star anise) and *Illicium anisatum* (Japanese star anise); 2) *Stephania tetrandra* ('hang fang ji') and its substitution or adulteration with *Aristolochia fangchi* ('guang fang ji'); 3) determining the proportion of each constituent in a tea blend consisting of *Aspalathus linearis* (rooibos) and *Agathoshma betulina* ('buchu'). Hyperspectral images were captured using a shortwave infrared (SWIR) pushbroom imaging system in the wavelength range 920–2514 nm. Multivariate software (Evince® and Matlab®) were used to analyse the data. Principal component analysis was applied to the images to investigate chemical differences between the species. Partial least squares discriminant analysis models were constructed by assigning the clusters to classes. The classification models were used to predict the identity of raw material replicates inserted into the model as well as the levels of adulteration in spiked raw materials. UHPLC-MS as an independent analytical technique was used to confirm chemical differences between the species. For the star anise example, a classification model was developed and used to accurately predict the identity of whole dried fruit of *I. anisatum* and *I. verum*. In the 'fang ji' example, the replicates for each plant species were predicted at a value > 99% for all the samples. Artificially adulterated samples were accurately predicted from as low as 10%. In the herbal tea blend example, the classification model was applied to determine the relative proportions of each blend constituent in intact tea bags. With the increasing need to regulate herbal products and ingredients, emerging technologies are providing alternative methods that allow the holistic analysis of the samples. Hyperspectral imaging in combination with chemometric data analysis is ideally suited as a tool for the quality control of herbal raw material as it is a visual, rapid, accurate and non-destructive method with high prediction ability.