02-06: Visual quality assessment of black cohosh using hyperspectral imaging and chemometrics

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Actaea racemosa (Ranunculaceae), commonly referred to as black cohosh, is a medicinal plant native to North America. Black cohosh is well known for its traditional use in the treatment of gynaecological problems, specifically for symptoms experienced during menopause. However, the American Herbal Products Association reported the plant to be among the top subjects to adulteration. Black cohosh is usually adulterated with Asian cohosh species. This study investigated the use of shortwave infrared hyperspectral imaging (SWIR-HSI) in combination with powerful chemometric methods for data analysis as a fast alternative method to differentiate four cohosh species and investigate 36 commercial products traded as black cohosh. Authentic root material of Actaea racemosa, A. podocarpa, A. pachypoda and A. cimicifuga were purchased from the American Herbal Pharmacopoeia (AHP). Both SWIR-HSI and ultra high performance liquid chromatography coupled to mass spectrometry (UHPLC-MS) analyses were performed on the raw material as well as commercial products. Using Matlab[®] software (2014b) with SWIR-HSI data (920 – 2514 nm), the range containing the discriminating information of the four species was identified as 1204 – 1480 nm. After reduction of the data set range, partial least squares discriminant analysis (PLS-DA) and support vector machine discriminant analysis (SVM-DA) models were created ($R^2 \ge 0.8$). The novel SVM-DA model showed better predictions and was then used to predict the species included in commercial products. Seven out of 36 commercial products were recognised by the SVM-DA model as being true black cohosh while 29 were adulterated black cohosh. Further analysis of the UHPLC-MS data using the OPLS-DA model demonstrated that six commercial products could be true black cohosh. This was confirmed with the investigation of the fragmentation patterns of three black cohosh markers (cimiracemoside C; $12-\beta$, 21-dihydroxycimigenol-3-O-L-arabinoside and 24-O-acetylhydroshengmanol-3-O- β -D-xylopyranoside). Using HSI in conjunction with SVM-DA, it was possible to identify 80% adulteration of commercial products labelled as black cohosh.

