

Abstract

Near infrared spectroscopy can rapidly predict the levels of P57 in *H. gordonii* – a commercially-important dietary herbal substance

Ilze Vermaak, Sias Hamman and Alvaro Viljoen*

Department of Pharmaceutical Sciences, Tshwane University of Technology, Pretoria, 0001, South Africa

*Corresponding author: viljoenam@tut.ac.za

Introduction

Hoodia gordonii (Apocynaceae), indigenous to South Africa and Namibia, was traditionally used by the San tribe to suppress hunger and thirst while on long hunting trips and is currently popularly included in weight-loss supplements. The concentration of the perceived active ingredient P57 is used by industry to assess the quality of raw material. Traditional analytical methods used to quantify P57 such as liquid chromatography coupled to mass spectrometry (LC-MS) are time-consuming and expensive. The potential of NIR spectroscopy in combination with chemometric data analysis to rapidly determine the levels of P57 in *H. gordonii* raw material was investigated.

Materials and Methods

Stem samples (n=146) were collected throughout South Africa and Namibia from cultivated sites as well as natural populations, sliced and air dried. NIR spectra of the powdered samples were collected in reflectance mode from 10000-4000 cm^{-1} on a Büchi NIRFlex N500 spectrophotometer with NIRWare software. The spectra were collected at a spectral resolution of 4 cm^{-1} with 32 scans per sample and the data analysed with Simca-P+12.0 software. The concentration of P57 in these samples were determined with LC-MS analysis and used to develop PLS calibration models.

Results and Discussion

The PLS model with 2nd derivative pre-processing yielded the best calibration model with 6 PLS factors, a correlation coefficient value (R^2) of 0.9629 and a root mean square error of prediction (RMSEP) value of 0.03%. The wavenumbers 10000-7800 cm^{-1} did not contribute to the model as evident from the low absorbance values and were removed from the model, improving the variance of X explained by the model to 42%. The cumulative overall cross-validated R^2X for this model was 75.6% indicating good prediction ability.

Conclusion

NIR spectroscopy in combination with chemometric data analysis can be used as a simple and more cost-effective method of quantification of P57 in *H. gordonii* raw material. The successful implementation of such a quality control technique may contribute to the distribution of high quality *H. gordonii* products.