Abstract

A quality control method for geranium oil (*Pelargonium graveolens* cultivars) based on near infrared spectroscopy

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Introduction

Rose-scented geranium, a cultivar originating from *Pelargonium graveolens* is a high value oil used extensively in flavour and fragrance formulations. The oil is variable in composition with 'Bourbon geranium' (Reunion Island) regarded as the highest quality geranium oil. Quality assessment of essential oils involves profiling seven major volatile constituents (geraniol, citronellol, geranyl formate, citronellyl formate, linalool, isomenthone and guaia-6,9-diene) using gas chromatography (GC) techniques. The aim of this study was to use NIRS together with chemometric algorithms to develop multivariate calibration models for the fast and accurate prediction of the quality of geranium oil.

Materials and Methods

Geranium oil samples (n = 70) were obtained from different suppliers in South Africa, Egypt, India, Reunion Island, China and Madagascar. Reference analysis was performed using gas chromatography coupled to mass spectrometry (GC/MS). NIR spectra of the oils were recorded on a NIRFlex N500 liquid cell spectrometer; spectra were collected in transmittance mode in the wavelength region of 4 000 – 10 000 cm^{-1}. Each sample (50 µl) was transferred into cuvettes and placed on a spacer. A total of 32 scans were accumulated for each sample at a spectral resolution of 4 cm^{-1}. PLS multivariate calibration models were developed using SIMCA-P+ 12.0.

Results and Discussion

NIR calibration models showed very good correlation between the predicted NIRS values and reference data. The correlation coefficients exceeded 0.90 for geraniol (R^2 = 0.93), citronellol (R^2 = 0.95), linalool (R^2 = 0.96), citronellyl formate (R^2 = 0.91) and geranyl formate (R^2 = 0.92). Isomenthone and guaia-6, 9-diene showed lower predictions of R^2 = 0.74 and 0.78, respectively. Generally, the error parameters (RMSEE and RMSEP) after external validation were low (≤ 1.0%) for all compounds guaranteeing reliable predictions.

Conclusion

The results illustrate the potential of NIRS as a rapid and reliable method for predicting the quality of geranium oil.

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