

## **Metabolic changes in different developmental stages of vanilla planifolia pods.**

### **ABSTRACT**

The metabolomic analysis of developing *Vanilla planifolia* green pods (between 3 and 8 months after pollination) was carried out by nuclear magnetic resonance (NMR) spectroscopy and multivariate data analysis. Multivariate data analysis of the <sup>1</sup>H NMR spectra, such as principal component analysis (PCA) and partial least-squares-discriminant analysis (PLS-DA), showed a trend of separation of those samples based on the metabolites present in the methanol/water (1:1) extract. Older pods had a higher content of glucovanillin, vanillin, p-hydroxybenzaldehyde glucoside, p-hydroxybenzaldehyde, and sucrose, while younger pods had more bis[4-(β-d-glucopyranosyloxy)-benzyl]-2-isopropyltartrate (glucoside A), bis[4-(β-d-glucopyranosyloxy)-benzyl]-2-(2-butyl)tartrate (glucoside B), glucose, malic acid, and homocitric acid. A liquid chromatography–mass spectrometry (LC–MS) analysis targeted at phenolic compound content was also performed on the developing pods and confirmed the NMR results. Ratios of aglycones/glucosides were estimated and thus allowed for detection of more minor metabolites in the green vanilla pods. Quantification of compounds based on both LC–MS and NMR analyses showed that free vanillin can reach 24% of the total vanillin content after 8 months of development in the vanilla green pods.

**Keyword:** *Vanilla planifolia*; Vanillin; Pod development; Metabolomic analysis; Nuclear magnetic resonance spectroscopy.