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# High-throughput simultaneous quantitation of multi-analytes in tobacco by flow injection coupled to high-resolution mass spectrometry

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**ABSTRACT**

The high-throughput screening by flow injection coupled to high-resolution mass spectrometry (HTS-FIA-HRMS) is a powerful technique that enables the identification of several types of samples in a short period of time, either with qualitative or quantitative purposes. Sensory attributes of tobacco are affected by its chemical composition, and it is very important to quantify multi-analytes in a high-throughput methodology. HTS-FIA-HRMS coupled to multivariate analysis was used to create calibration models for 27 analytes, or group of compounds, of tobacco sensory interest. The models were validated by different approaches, including permutation test to avoid overfitting, evaluation of the equipment repeatability by control samples, reproducibility comparison of results from two different equipment and analysts, and with a blind test analysis. All tests demonstrated a good response to the proposed method. No statistical difference between the errors of both equipment was observed, with less than 7% error from the control samples, and a blind test error between 5.96 and 20.10%. The partial least squares (O-PLS) regression models were applied to 815 samples, and a principal component analysis (PCA) was performed from the predicted concentration values, aiming at the non-supervised classification based on tobacco type. We expect that this proposed methodology shows not only the applicability in tobacco samples, but also demonstrates a guideline to an efficient performance of multi-analytes target analysis using the flow injection mass spectrometry with reliable and robust validation steps.