

BOOK OF ABSTRACTS

11th International Symposium on **RECENT ADVANCES IN FOOD ANALYSIS**

**November 5-8, 2024
Prague, Czech Republic**

Jana Pulkrabová, Monika Tomaniová, Stefan van Leeuwen, Michele Suman,
Michel Nielen and Jana Hajšlová

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DEVELOPMENT AND VALIDATION OF A RAPID AND GREEN ANALYTICAL TOOL FOR TOMATO PUREES AUTHENTICATION BY HIGH RESOLUTION MASS SPECTROMETRY BASED FLOW INJECTION ANALYSIS

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Among fruits and vegetables, tomatoes are commonly valued for their sensorial and nutritional properties due to the high content in antioxidants and bioactive compounds. Over the last decade, several metabolomic approaches were proposed to investigate tomato varieties. The aim of this study was to develop and validate a rapid analytical tool for Datterino purees authentication by flow injection analysis based on high resolution mass spectrometry detection (FIA-HRMS). In addition, a preliminary marker analysis for varietal discrimination will be presented.

The approach was developed on a set of 40 puree samples equally distributed into two groups: (A) labelled as 100% Datterino, (B) low-cost alternative purees with no varietal specifications. The sample preparation was designed to be time-effective and optimized to involve only green solvents. The metabolite extracts were analysed by FIA-HRMS in both polarity modes on a hybrid quadrupole/orbitrap MS. The total run time, including sample preparation and detection, was below 30 min. Three independent extracts were prepared for each puree sample under optimized conditions to build up the final data set (n=120). The spectra were averaged over a 30s-time range, background subtracted and grouped into accurate peaks lists. The lists were processed by MetaboAnalyst v6.0 for peak matching, imputation of missing values, data filtering and normalization. PCA by NIPALS algorithm with a V-fold cross-validation (V=7) was used as unsupervised approach to evaluate the presence of outliers and establish the number of significant PCs best describing the multivariate system. These latter provided a total explained variance of 96,2% ($R^2X(\text{Cum})$) and predicted variance of 96,1% (Q^2), with a barely valuable grouping of cases. The significant PCs were used as input for supervised pattern recognition by Linear Discriminant Analysis (LDA) with external validation. The LDA model achieved a prediction ability of 100% for the analysis set and 95% for the testing set in both groups A and B. Markers discovery by multivariate exploratory ROC (Receiver operating characteristic) analysis was carried out, with conservative filters applied for matrix preparation excluding non-informative and low intensities features. The multivariate ROC curves were automatically generated based on three multivariate algorithms: support vector machines (SVM), partial least squares-DA (PLS-DA), and random forests (RFs). All the three classification methods applied with Monte-Carlo cross-validation provided the best modelling with 100 features. With the SVM algorithm, the predictive accuracy was 96,5% with an area under the curve of 0,986 and a 95% confidence interval of 0,895-1. Comparable performances were obtained with PLS-DA (10 latent-variables) and RFs classification methods. The three lists of ranked important features were evaluated to match common candidates, and MS/MS-based identification of such candidate markers was accomplished.

Keywords: tomato authenticity, rapid method, green technology, high resolution mass spectrometry, flow injection analysis

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