

Abstract

# Berry-Based Products Classification by FIA–HRMS Fingerprinting and Chemometric Analysis <sup>†</sup>

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**Abstract:** In recent years, nutraceuticals prepared with cranberry (*Vaccinium macrocarpon*) have gained special attention because of their beneficial effects on human health (e.g., antioxidant activity and antimicrobial activity against bacteria involved in a wide range of diseases), which are mainly attributed to the high content of specific polyphenols in cranberry. However, these products present a risk of fraud consisting of the total or partial substitution of cranberry extracts with cheaper and more abundant fruit extracts. Therefore, in this study, flow injection analysis coupled with high-resolution mass spectrometry (FIA–HRMS) fingerprinting was proposed as a rapid high-throughput analytical approach to address the classification of berry-based products through chemometrics, focusing on cranberry-based products authentication. Thus, several berry-based natural products (including 18 based on blueberry, 25 on grape, 12 on raspberry, and 28 on cranberry) and 21 cranberry-based nutraceuticals were analyzed. Sample treatment consisted of a simple solid–liquid extraction method, using acetone:water: hydrochloric acid (70:29.9:0.1, v/v/v) as the extracting mix. After both negative and positive electrospray ionization FIA–HRMS sample analysis, raw data were processed with mzMine 2.53 software to obtain the corresponding fingerprints. In this line, four different data matrices including negative, positive, low-level data fusion (LLDF), and mid-level data fusion (MLDF) FIA–HRMS fingerprints—were then subjected to principal component analysis (PCA) and partial least squares regression-discriminant analysis (PLS-DA) using Solo 8.6 chemometrics software. PCA results allowed the identification of specific sample groups and trends. Subsequently, the complete sample classification was segregated through a classification decision tree—consecutive two-input class PLS-DA models—leading to excellent assignment accuracies after external validation according to sample botanical origin (independently of the employed data matrix). The poster of this work is provided in the supplementary materials.

**Keywords:** berries; cranberry; FIA–HRMS; chemometrics; data fusion



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**Supplementary Materials:** The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/Foods2021-10916/s1>, Poster: Berry-based products classification by FIA–HRMS fingerprinting and chemometric analysis.

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