

GAS CHROMATOGRAPHY – MASS SPECTROMETRY BASED METABOLITE PROFILING OF SEEDS FROM CULTIVATED BERRY FRUITS



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Introduction

Berry seed oils are good source of essential fatty acids and bioactive compounds that could be potentially used as functional ingredients in food, cosmetic and pharmaceutical industry. Fruit processing produces large amounts of by-products in the form of seeds and their better utilization is promising and economically attractive field. Therefore, more information about seeds and their composition are required.

The object of this work is characterization of 37 different genuine Serbian strawberry, raspberry, blueberry, black currant, blackberry and gooseberry cultivars according to fatty acid profile and determination of its authenticity regards their botanical origin. Gas chromatography - mass spectrometry (GS-MS) analysis was applied for the separation and identification of the fatty acid methyl esters, while pattern recognition methods were applied for classification of investigated berries cultivars according to their botanical origin.

Experimental part

Sample preparation

Fatty acid methyl esters (FAME) were obtained from extracted oil using trans-methylation under alkaline conditions, according to ISO 12966-2:2012. Extracted oil was dissolved in 2 mL *n*-hexane, afterward 1 mL of 2 mol/L methanolic potassium hydroxide solution was added and vortexed for 2 min at room temperature. Neutralization of hexane phases was done by adding 1 g of sodium hydrogen sulphate monohydrate.

GC-MS analysis

Oven temperature program was as follows: initial temperature 50 °C (1 minute), then 25 °C / min to 200 °C and finally 3 °C / min to 230 °C (18 minutes). Injection volume was 1 µL and the injector was in split mode (50:1). Helium was used as the carrier gas (1 mL/min). Fatty acid methyl esters were identified by comparison of the retention times with known standards and the resulting mass spectra to those in database.

Results and discussion

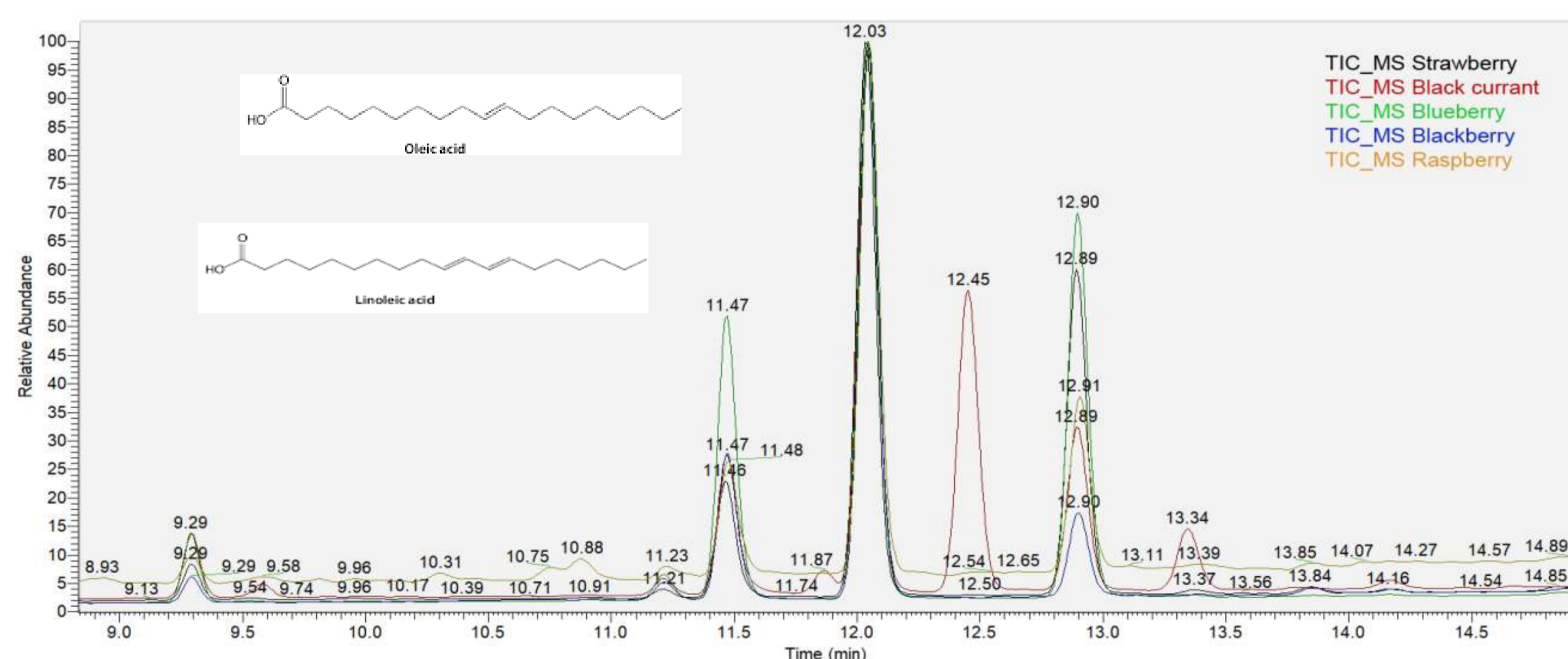


Figure 1. Fatty acid methyl esters chromatograms of some of investigated berry species.

A set of chromatographic signals as unique multivariate fingerprint was used for sample characterization (Figure 1). In order to extract maximum useful information from the profiles and look for possible trends among data, principal component analysis was applied. The score plot indicated differentiation of samples according to botanical origin (Figure 2a). Blackberry, strawberry, black currant, raspberry and blueberry seed samples formed five compact clusters suggesting uniform free acids profiles within certain cultivar. Variables that potentially have the highest influence on separation along axis are presented on Figure 2b,c.

Conclusion

Resulted fatty acid profiles within the same fruit species showed specific pattern, only intensity of the signals differ among cultivars. The most abundant fatty acid in berry seed oils was linoleic acid, followed by oleic, α -linolenic and palmitic acids.

Pattern recognition methods applied for classification of cultivated berries cultivars confirmed their botanical origin. This kind of investigation can contribute to the inter-cultivar discrimination and enhancing the possibilities of acquiring an important authenticity factor.

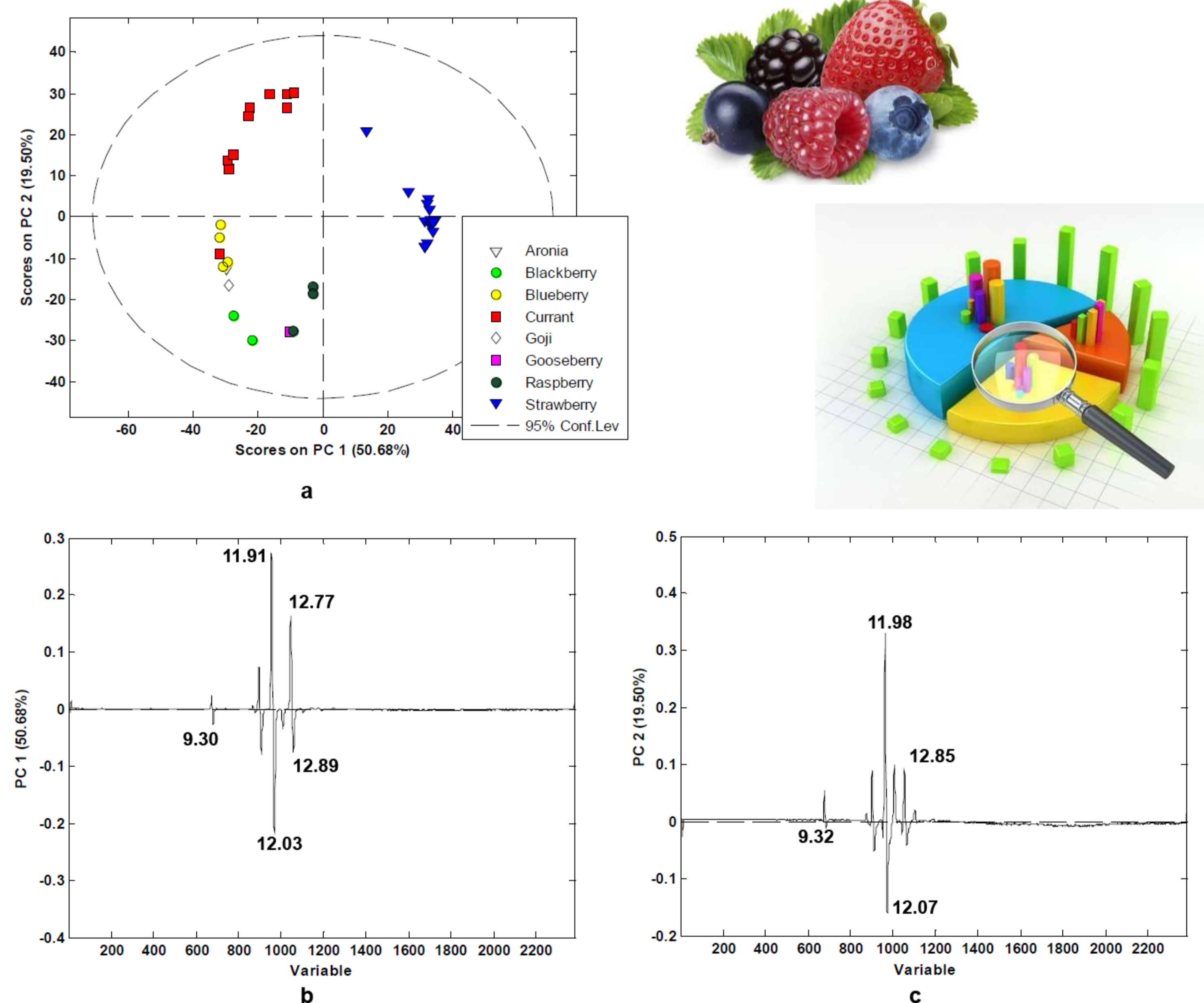


Figure 2. PCA analysis performed on data obtained from fatty acids profiles of seeds from berry cultivars, a) score plot, b,c) loading plots.

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