

Abstract

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Title of Graduation Thesis: A comparison of ESI and APCI ionization during the development of UHPLC-MS/MS method for the determination of phenolic acids.

Phenolic acids are aromatic secondary metabolites which are widely spread in the whole plant kingdom. The thesis deals with the development of the method for the determination of the group of phenolic acids by ultra high performance liquid chromatography coupled with triple quadrupole mass spectrometry. Chromatographic column BEH C₁₈ (1.7 µm; 2.1 x 100 mm) was used for the separation of analytes. The optimization of the mass spectrometry parameters was conducted for electrospray ionisation (ESI) and atmospheric pressure chemical ionization (APCI). Sensitivity, linearity and repeatability of this method were finally assessed.

The full scan of mixture of analytes was firstly performed and suitable precursor ions were chosen. In the following step the ion source (ESI⁻ and APCI⁻) was optimized. The next step was scanning of product ions and choosing suitable ion transitions for quantification mode SRM and optimizing their collision energies. The repeatability after the optimization of the parameters (RSD < 1% for retention time; RSD < 10% for the area under the curve, except for isoferulic, cinnamic, sinapic acid), sensitivity (LOQ = 0,007 – 6,600 µg·ml⁻¹ for ESI⁻ and 0,007 – 6,600 µg·ml⁻¹ for APCI⁻) and linearity (of all analytes r² ≥ 0,9900 except for isoferulic, cinnamic, sinapic acid) were measured.

Electrospray in negative mode was found to be more suitable for the analyses of the mixture of phenolic acids. The sensitivity for acids was found to be low for: vanillic, isoferulic and cinnamic.

The keywords: shikimic acid, gallic acid, protocatechuic acid, gentisic acid, chlorogenic acid, vanillic acid, caffeic acid, syringic acid, p-coumaric acid, o-coumaric acid, m-coumaric acid, ferulic acid, isoferulic acid, sinapic acid, rosmarinic acid, cinnamic acid, UHPLC-MS/MS, phenolic acids.