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Assessment and quantification of new metabolites in quinoa (*Chenopodium quinoa* Willd.) using UHPLC-Q-Orbitrap mass spectrometer

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Abstract

Quinoa (*Chenopodium quinoa* Willd.) is a pseudo-cereal originating from the mountain region of South America. Quinoa possesses excellent nutritional quality and contains numerous secondary metabolites acting as plant protection. Many of the metabolites also display biological activities and potential health benefits. The two principal groups of secondary metabolites in quinoa are phenolic acids and flavonoids. In this study, 56 various quinoa genotypes grown in the climatic conditions of the Czech Republic during the year 2021 were subjected to metabolomic analyses using a UHPLC-Q-Orbitrap high-resolution tandem mass spectrometer. Obtained data were processed in Xcalibur Quan Browser and Compound Discoverer software and compared to available scientific literature. As a result, eight flavonoids, two phenolic compounds, and one phenolic amid were detected and quantified in quinoa samples. The majority of them have never been quantified in quinoa before. The concentration of all 11 compounds was compared among red- and yellow-coloured seed samples of the same genotype. Red seeded genotypes had higher mean concentration rates of analysed metabolites than yellow seeded genotypes. Chemicals identified in absolutely all quinoa samples were isoquercetin, naringenin, pinocembrin, emodin, isorhamnetin from the flavonoid group, and salicylic acid as a phenolic compound. Isoquercetin was the metabolite with the highest concentration ranging from 0.138–9.907 g/g in dry weight (DW). The lowest concentration was identified for naringenin, ranging from 0.002–0.179 g/g DW. Three flavonoids were detected only in some genotypes – quercitrin (identified in 26 genotypes), taxifolin (identified in 25 genotypes), and vitexin (identified in 1 genotype), all of them having relatively low concentrations. Two chemicals, namely 4-hydroxybenzaldehyde (0.576–4.233 g/g DW), a phenolic compound, and N-feruloyloctopamine (0.092–4.993 g/g DW), a phenolic amid, have never been identified or quantified in quinoa before. Both are additionally the first compounds found in the genus *Chenopodium* and the family *Chenopodiaceae*. These findings showed that quinoa metabolomics is a potential area for further investigations since the variability of chemical compounds has not been fully explored yet.

Keywords: Flavonoids, liquid chromatography-mass spectrometry, metabolites, quinoa