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BOOK OF ABSTRACTS



P52 - CHARACTERIZATION OF SIMPLE PHENOLIC COMPOUNDS IN COCOA PRODUCTS USING HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY COUPLED TO HIGH RESOLUTION MASS SPECTROMETRY (Q-ORBITRAP)

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Different studies revealed that the consumption of cacao-based products has positive effects on human health, because cocoa is considered a major dietary source of antioxidants due to its high content of phenolic compounds [1,2]. Phenols are studied not only for their physiological health benefits, including antioxidant, anti-inflammatory and cardioprotective effects [3], but also because they seriously affect the sensory and nutritional qualities of food products [4].

Combining an on-line SPE clean-up for reducing matrix interference and a rapid chromatographic detection performed with an UHPLC coupled with a Quadrupole/High-Resolution Mass Spectrometry (Orbitrap), a new targeted analytical method was developed for the quantification of 56 simple phenols.

On-line concentration/purification was performed with a HyperSep™ Retain PEP spe cartridge, while the chromatographic separation was performed with an Acquity UPLC BEH C18 analytical column, managing a water-acetonitrile gradient elution in 22 minutes from 5% to 100% of organic solvent.

Mass spectra were acquired in full MS-data dependent MS/MS analysis (full MS-dd MS/MS) at mass resolving power of 140.000. The mass spectrometer operated using the following parameters: spray voltage, 2.80 kV; sheath gas flow rate, at 30 arbitrary units; capillary temperature, at 310 °C.

The method is linear up to concentration of 10000 µg L⁻¹ with a R² at least of 0,99. Limits of detection are generally low (0.1-1 µg L⁻¹) and suitable for analytical requirements in tested matrices.

Thanks to the on-line SPE and to the mass high resolving power, the proposed approach allowed a satisfactory characterization of the phenolic content in about 60 cocoa products. The most abundant phenolic compounds were: catechin and epicatechin among flavanols; 4-hydroxy-benzoic acid, vanillic acid and protocatechuic acid among hydroxybenzoic acids; caffeic and ferulic acids among hydroxycinnamic

acids; protocatechuic aldehyde and vanillin among hydroxybenzaldehydes; 4-vinyl phenol and 4-methylsyringol among alkyl- and alkylmethoxyphenols.

References

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