



40th International Symposium on Capillary Chromatography and 13th GCxGC Symposium

Chairman
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May 29 - June 03, 2016

*Palazzo dei Congressi,
Riva del Garda
Italy*

ABSTRACT BOOK

INFORMATION

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The Forum on Microcolumn Separations

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Publisher: Chromaleont S.r.L.
Viale Bocchetta 70
98122 Messina, Italy

Edited by: L. Mondello and P. Dugo

ISBN: 978-88-941816-0-9

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UNTARGETED ANALYTICAL METHOD FOR GLYCOSYLATED SIMPLE PHENOL PROFILING BY ON-LINE SOLID PHASE EXTRACTION AND LC-HIGH RESOLUTION MASS SPECTROMETRY (Q-ORBITRAP)

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Free simple phenols are intensively studied not only for their physiological health benefits, including antioxidant, anti-inflammatory and cardioprotective effects, but also because they influence remarkably the organoleptic profile of many natural products, contributing to delineate aroma and nutritional properties. Glycosidically bound simple phenols are considered a natural stock of these compounds, because they can be hydrolyzed to the corresponding free forms during the food transformation, representing a possible additive contribution to the final sensory perception.

A new untargeted approach, offering new opportunities for a detailed description of the bound phenol profiles, was developed combining on-line SPE clean-up for reducing matrix interference with ultra-high liquid chromatography coupled with hybrid quadrupole-high resolution mass spectrometry (Q-Orbitrap). On-line purification was performed with a HyperSep™ Retain PEP spe cartridge, the chromatographic separation was performed with an Acquity UPLC BEH C18 analytical column, managing a water-acetonitrile gradient from 5% to 100% of organic solvent. Mass spectra were acquired in full MS-data dependent MS/MS analysis at mass resolving power of 140.000, in negative ion mode and with a heated electrospray.

The untargeted approach, validated using glycosidic precursors, was aimed to characterize the phenolic composition of different natural matrices (cocoa, vanilla extracts and food tannins), and to tentatively identify the glycosylated precursors in the forms of -hexoside, -pentoside, -hexoside-hexoside, -hexoside-pentoside, -pentoside-hexoside and -pentoside-pentoside.