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Il contributo della scienza delle separazioni alle
problematiche alimentari ed ambientali

BOOK OF ABSTRACTS

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TARGETED METABOLOMICS METHODS FOR THE SEPARATION AND QUANTIFICATION OF MULTIPLE CLASSES OF PHENOLICS: APPLICATION IN FOOD AND NUTRITIONAL STUDIES

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Compelling evidence of the health benefits of phenolic compounds and their impact on food quality have stimulated the development of analytical methods for the separation and quantification of these compounds in different matrices in recent years. The complexity and remarkable diversity of phenolics has challenged the analytical performances of separation and detection methods in terms of resolving power, selectivity and sensitivity for the identification and quantification of these compounds in different matrices. Targeted metabolomics is a strategy based on the use of predefined metabolite-specific signals, such as MRM transitions, that can be used to accurately determine the concentrations of a wide range of known metabolites.

A targeted metabolomics method [1] has been developed for the quantification >150 phenolics, such as benzoates, phenylpropanoids, coumarins, stilbenes, dihydrochalcones, and flavonoids, using an UPLC/MS/MS system. Reverse-phase chromatography was optimised to achieve separation of the compounds over 15 min, reducing possible ion suppression effects and resolving many isomeric compounds and MRM transitions were selected for accurate quantification.

Recently a new targeted metabolomics method [2] was developed for the quantification of 23 metabolites/catabolites related to the consumption of polyphenols and associated to the microbial digestion made by the gut microflora. The present new method was developed the analysis of complex matrix with SPE purification before the UPLC separation. Then it was validated and applied for human/animal biofluids or tissues.

The validated methods were applied to the analysis of fruits and wine polyphenols as well as in nutritional studies providing a valuable tool for food quality evaluation and nutritional relevant bioactive compounds profiling. The short duration of the analysis and the straightforward sample preparation make the methodology suitable for high-throughput screening studies for analysis of food as well as its application in nutritional studies to biofluids.

References:

[1] Vrhovsek U. et al., *J. Agric. Food Chem.* **60**, 8831, (2012).

[2] Gasperotti M. et al., unpublished data