

UHPLC-MS/MS ANALYSIS OF POLYPHENOLIC COMPOUNDS IN PLANT MATERIAL: FROM THE FOOD QUALITY TO THE PHYSIOLOGIC RESPONSE

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Phenolic and polyphenolic compounds are a very large group of plant secondary metabolites, synthesized by plants to protect themselves against insect pests, but also in response to biotic and abiotic stress [1]. These compounds are well-known for their health protecting attributes, as anti-inflammatory [2], anti-hypertensive [3], anti-microbial [4] and anti-cancer agents [5,6].

Currently, ultra-high performance liquid chromatography coupled with advanced tandem mass spectrometric techniques (UHPLC-MS/MS) is without doubts the most powerful analytical technique for polyphenol analysis. In fact, atmospheric pressure ionization sources provide a soft ionization of target analytes, which is particularly recommended for structure elucidation of polar, non-volatile and thermally labile compounds, such as flavonoids and other phenolic-based bioactive compounds. Moreover, the use of tandem mass spectrometry (MS/MS) enables to obtain important structurally-related information through the fragmentation of parent molecules [7]. In this context, the adoption of high-resolution mass spectrometry (e.g. time-of-flight based instruments), allows for obtaining accurate mass read-out, thus facilitating the assignment of an elemental formula to the parent molecule and/or to the fragments and its fragmentation characteristics [8].

In this lecture, some examples of application of UHPLC-MS/MS to the identification of phenolic and polyphenolic compounds in plants are presented, in order to highlight the wide applicability of this technique for the unequivocal or putative attribution of unknown compounds in plant materials. Some important results obtained in relation to phenolic identifications and quantification are also shown. These examples concern the investigation of the nutraceutical value of various fruits, with particular reference to small berries, but also the plant response to different stress.

References

- [1] Del Bubba, M., Ancillotti, C., Checchini, L., Ciofi, L., Fibbi, D., Gonnelli, C. & Mosti, S. (2013). Chromium accumulation and changes in plant growth, selected phenolics and sugars of wild type and genetically modified *Nicotiana langsdorffii*. *Journal of Hazardous Material*, 262, 394–403.
- [2] Kim, J., Lee, K., Lee, H., Watson, R. R., Preedy, V. R., & Zibadi, S. (2014). Polyphenols suppress and modulate inflammation. *Polyphenols in Human Health and Disease*, 1, 393–408.
- [3] Rodrigo, R., Gil, D., Miranda Merchak, A., & Kalantzidis, G. (2012). Antihypertensive role of polyphenols. *Advances in Clinical Chemistry*, 58, 225–254.
- [4] Daglia, M. (2012). Polyphenols as antimicrobial agents. *Current Opinion in Biotechnology*, 23, 174–181.
- [5] Paller, C. J., Ye, X., Wozniak, P. J., Gillespie, B. K., Sieber, P. R., Greengold, R. H., Stockton, B. R., Hertzman, B. L., Efros, M. D., Roper, R. P., Liker, H. R., & Carducci, M. A. (2013). A randomized phase II study of pomegranate extract for men with rising PSA following initial therapy for localized prostate cancer. *Prostate Cancer and Prostatic Diseases*, 16, 50–55.
- [6] Wang, L.-S., & Stoner, G. (2008). Anthocyanins and their role in cancer prevention. *Cancer Letters*, 269, 281–290.
- [7] Del Bubba, M., Checchini, L., Chiuminatto, U., Doumet, S., Fibbi, D., & Giordani, E. (2012). Liquid chromatographic/electrospray ionization tandem mass spectrometric study of polyphenolic composition of four cultivars of *Fragaria vesca* L. berries and their comparative evaluation. *Journal of Mass Spectrometry*, 47, 1207–1220.
- [8] Ancillotti, L., Ciofi, L., Rossini, D., Chiuminatto, U., Stahl-Zeng, J., Orlandini, S., Furlanetto, S. & Del Bubba, M. (2016). Liquid chromatographic/electrospray ionization quadrupole/time of flight tandem mass spectrometric study of polyphenolic composition of different *Vaccinium* berry species and their comparative evaluation. *Analytical and Bioanalytical Chemistry*, in press.