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CHEMOMETRICS AND DIRECT INJECTION ANALYSIS OF VOLATILE COMPOUNDS BY PTR-TOF-MS: A TOOL FOR METABOLOMIC INVESTIGATIONS**Luca Cappellin¹, Eugenio Aprea², Pablo Granitto³, Andrea Romano⁴, Flavia Gasperi⁵, Franco Biasioli^{6*}**^{1 2 3 4 5 6} *Fondazione Edmund Mach, San Michele a/A, Italy***Corresponding author - E-mail: franco.biasioli@iasma.it, Phone: + 39 0461 615 187*

Sample classification and “explanatory” variable selection is a cutting edge problem in metabolomics. Among direct injection methods for the detection of volatile compounds, Proton transfer reaction-mass spectrometry (PTR-MS) is becoming more and more spread, especially after the coupling with time of flight detectors (PTR-TOF-MS). PTR-MS was proposed almost two decades ago for the rapid and high sensitivity monitoring of volatile compounds. It was immediately evident that food science and technology was one of its most interesting field of application given the role that volatile compounds play in food production, storage and consumption. We show that modern chemometric and data mining techniques, such as Random Forest, Partial Discriminant Analysis, Support Vector Machine, are well suited for addressing multiclass problems starting from fruit flavour profiles (by GC-MS) or fingerprints (by PTR-TOF-MS). Marker identification is successfully performed by recursive strategies such as Random Forest Recursive Feature Elimination. Moreover, regression methods, for instance LASSO and PLS, proved to be useful to link headspace, nose-space and sensory data from different analysis techniques. We present results from metabolomic studies by GC-MS and PTR-TOF-MS on i) raspberries: several cultivars having diverse levels of Botrytis susceptibility have been classified by the mentioned chemometric strategies and markers of Botrytis resistance have been identified; ii) apple cultivars and clones: markers for the discrimination of the apple clones based on their flavour profile have been identified; iii) grana cheeses and olive oils: we investigate the link between GC-MS profiles and PTR-TOF-MS fingerprint. Through these examples we will discuss the characteristics of the proposed strategy and show that it can provide a powerful tool for metabolomic.

Keywords: PTR-ToF-MS, volatile compounds, chemometrics, data mining, metabolomics

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