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Advancements in lc direct-eims: State of the art and applications

Achille Cappiello
University of Urbino, Italy

Mass spectrometry (MS) is renowned for its impressive identification potential especially when it is coupled to a separation technique such as liquid chromatography (LC-MS) or gas chromatography (GC-MS). Direct-EI LC-MS interface, developed in our lab, is a powerful technique that combines, in a single instrument, the identification advantages of library searchable, electron ionization (EI) spectra with the separation power of an LC column, without the drawbacks of matrix effects or the polarity limitations typical of electrospray ionization. Non target analyses are of increasing importance in food safety, environmental, forensic and many other applications where the complexity of the matrix is a troubling factor. The advantage of EI for tentative identification is unparalleled. Expansion of EI fragmentation to a wider variety of molecules in a liquid phase provides an attractive alternative to identification and offers a complementary technique to high-resolution/high-mass accuracy LC-MS instrumentation and atmospheric pressure techniques. The simple interfacing process make it compatible with any LC separation technique and with any solvent combination, including non-volatile buffers and UHPLC methods. The gas-phase ionization process and the negligible matrix effects allows direct injections of samples even without column separations. In this presentation, the basic principles of compound identification in various applications and the advantages offered by an MS/MS analyzer in combination to HPLC and UHPLC separations will be presented. New instrumental developments involving the use of ceramic coatings and membrane probes for additional sensitivity and flexibility will be also shown.

achille.cappiello@uniurb.it

Endogenous and exogenous volatile compounds in breath as detected byPTR-MS

Franco Biasioli
Fondazione Edmund Mach, Italy

Among the different approaches to volatile organic compound (VOC) profiling, Proton Transfer Reaction Mass Spectrometry (PTR-MS),shows intriguing peculiarities: it is fast, non-invasive and can provide very high sensitivity. Moreover, recent technological advancements partly overcome its limitations in compound identificationand quantification. Here,the use of PTR-MS for the real time measurement of the concentration ofVOCs in breath is discussed with reference to two studies: i) the monitoringof exogenous flavor compounds during food consumption and ii) the monitoring of endogenous compounds as possible markers of diseases or diet. In the first study the nose-space concentration during coffee drinking has been compared with dynamic sensory methods to investigate the perceived effect of different roasting. Data indicates that nose-space concentration can be used to distinguish different coffee samples and different assessors and to identify markers of sensory quality which clearly show multimodal characteristics.In the second series of studies the breath of human and rats has been measured to assess whether VOC concentration can be related to diseases (cirrhosis and coeliac disease) or diet. Data indicates that markers of cirrhosis can be identified by breath analysis and that they are correlated with serum bilirubin while no evidence of breath markers can be found for coeliac disease if the patience follow a gluten free diet.In conclusion: PTR-MS allows the real time analysis of breath VOCs and can be used both for exogenous or endogenous compounds analysis to investigate flavor perception or markers of disease or diet.

franco.biasioli@fmach.it