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ABSTRACT BOOK

INFORMATION
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The Forum on Microcolumn Separations

DEVELOPMENT OF A GAS CHROMATOGRAPHY TANDEM MASS SPECTROMETRY METHOD FOR MULTIPLE FLAVOURS QUANTIFICATION

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The chemical study of food and beverage aroma needs nowadays the accurate quantification of an always larger number of flavour compounds from different chemical classes. Generally flavours are analyzed by GC-FID [1] or GC-MS, after a procedure of purification and concentration (SPE, SPME) [2,3]. These two techniques could present low sensibility and selectivity, to avoid this problem, long chromatographic separations were generally proposed with great loss of time [4].
An answer to these problems can be given coupling gaschromatography with a triple quadrupole mass spectrometer (GC-QqQ-MS) configured in multiple reaction monitoring (MRM) mode. Compared to the single quadrupole used in SIM mode, the noise of a triple-quadrupole used in MRM mode is considerably reduced, the sensitivity increased, and the selectivity can be considerably augmented by choosing appropriate transitions. The greater specificity makes possible in many cases to resolve co-eluted peaks even using a less accurate chromatographic separation, and to save time with routine analysis.
Flavour compounds were extracted by adsorption on a SPE cartridge (ENV+) [4], eluted with CH_2Cl_2, concentrated using a Vigreux apparatus and then injected into the GC-MS/MS. The MS/MS parameters, transitions and collision energy, were studied using commercial standards, and their optimization was a compromise between signal intensity and specificity. The developed method permitted ,in wines and spirits, the quantification of 8 acids, 18 alcohols, 39 esters, 13 aldehydes, 10 ketones, 6 phenols, 12 norisoprenoids, 32 terpenols, 11 lactones and 14 sesquiterpens for a total of 163 compounds in only 40 minutes of GC run instead of the classical 90-120 minutes [4]. The number of quantified compounds is definitely higher than many classical routine methods considering also the short time of analysis. The method has shown a satisfactory reproducibility and a good linearity for all the target compounds with R^2 higher than 0.99 for all/ almost all compounds. The proposed GC-QqQ-MS method is an important starting point for routine quantitative multiple aroma analysis in complex matrix like wine and spirits because of his rapidness and specificity.

References

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