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OP2. Novel analytical tool for a univocal flavor and fragrance identification: Gas chromatography coupled with condensed-phase FTIR and TOF mass spectrometry

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The correct identification of flavor and fragrance (F&F) compounds in real samples is still a challenge despite the huge number of different instruments available. Only a slight structural difference can cause a very different sensory profile, for example in the case of geometric isomers, it is generally considered that (*Z*)-isomers have a more pleasant and natural odor than (*E*) ones.

The most frequently used instrument for the analysis of volatiles is gas chromatography (GC) coupled with mass spectrometry (MS). MS may still fail to adequately identify compounds because of the lack of specificity of spectra (terpenes, isomers). MS spectral searches can be supported with linear retention index (LRI) information which, although not in all cases, could resolve the problem of possible misidentification of target molecules.

Condensed phase FTIR can be a complementary detection system to MS, and its application could allow a very detailed structural elucidation. The novelty of this instrument is that the separated compounds are condensed in small, singular spots on a rotating disc, thus the distortion of spectra is eliminated, giving an excellent spectral resolution. Through the specificity of the "fingerprint" region around 1100 cm^{-1}, even positional isomers and diastereomers could be distinguished.

Coupling condensed-phase FTIR after a simple post-column split to a GC-TOF MS, three independent analytical information can be obtained about the target compound: retention behavior (LRI), MS and FTIR spectra. Exploiting the enhanced resolution of the TOF MS and discriminating power of FTIR a unique TOF MS/FTIR spectral library with more than 1500 F&F compounds was developed, including also experimental LRI. Boosting this comprehensive information collection, a universal post-run software, namely CromatoPlus Spectra, performs the library search using the FTIR spectral similarity and LRI filter, simultaneously. A GC-TOF MS/FTIR method was optimized for the analysis of real essential-oil and perfume samples. Using the F&F library with embedded LRI, a reliable peak assignment was obtained for each separated compound.

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