

Side product analysis of minor constituents in perfumery raw materials using two-dimensional gas chromatography coupled to mass spectrometry

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Large volume perfumery raw materials have to be investigated more and more thoroughly and registered with traces down to 0.1%. Mainly for terpene derived chemicals this can represent a tremendous analytical challenge, due to the complexity of the mixture at this concentration level. Comprehensive two-dimensional gas chromatography (GCxGC) provides an increased separation power compared to one-dimensional GC and has proved useful for essential oil analysis [1]. Its capability for the side product analysis of Javanol® [2], a derivative of campholenaldehyde with a natural sandalwood-oil scent, was tested. GCxGC separations were conducted on apolar x polar and polar x apolar column sets using a longitudinally modulated cryogenic system (LMCS, Chromatography Concepts). Mass spectra were recorded using a quadrupole mass spectrometry (qMS, Agilent) system with an electronic upgrade for faster scanning (up to 10000 amu/s) allowing an acquisition rate of 20 Hz. By comparing GCxGC-qMS with GC-qMS data (slower scanning), improved spectral quality due to reduction or absence of interferences with coeluting compounds or column bleed was observed but with reduced sensitivity. Nevertheless, identification of known constituents by library searches was possible. Structure elucidation of unknowns by mass spectral interpretation, however, was further facilitated by the 'structured separations' of components in the 2-D plane compared to the 1-D retention of single column GC analysis. At the moment significant effort is required to interpret 2-D data because of the lack of an integrated GCxGC-qMS system with dedicated MS software. Nevertheless, GCxGC-MS proved to be a powerful technique for this kind of analysis.

[1] R. Shellie and P. Marriott, *Flavour Fragr. J.* 2003, 18, 179.

[2] J.A. Bajgrowicz, et al., *Helv. Chim. Acta* 1998, 81, 1349.