

OT2 Studies in comprehensive two-dimensional gas chromatography/mass spectrometry

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GC×GC, time-of-flight MS, incense, petrochemicals, doping control drugs

GC×GC separation with MS gives much better molecular identification for complex sample sets

Comprehensive 2D GC (GC×GC) brings together two of the premier tools for volatile chemical analysis: gas chromatography (GC) and mass spectrometry (MS). However, whilst the GC step offers one of the highest resolution platforms currently available, in GC×GC technology the MS step has certain limitations, imposed by the speed of data acquisition that is required.

Time-of-flight technology with unit mass resolution meets these needs, and we have demonstrated this technology for a diverse range of applications, e.g. incense smoke analysis [1], petrochemicals, sterols [2], and atmospheric particulates with isotope dilution [3]. Quadrupole MS may be contrasted with TOFMS [4], and suggests that some measure of qualitative data may be generated, but it also suggests that accurate mass MS and isotope ratio MS could be more problematical. Finally we have demonstrated that off-line NMR analysis with GC [5] can be usefully employed as a complementary tool for structural assignment.

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