Recent developments in comprehensive two-dimensional gas chromatography (GC × GC) IV. Further applications, conclusions and perspectives☆

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We review the literature on comprehensive two-dimensional gas chromatography (GC × GC), emphasizing developments in the period 2003–2005. The review opens with a general introduction, the principles of the technique and the set-up of GC × GC systems. It also discusses theoretical aspects, trends in instrumentation, column combinations, and detection techniques – notably mass spectrometric detection. We devote attention to a wide variety of applications and to analytical performance.

Keywords: Application; Complex sample; Comprehensive two-dimensional gas chromatography; Detection; GC × GC; Mass spectrometry; Modulation; Review

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3.3. Food, fat, oils and fragrances

Over the years, an increasing number of food and beverage, fat, essential oil and fragrance samples have been subjected to GC × GC in order to detect and/or quantify trace-level constituents or contaminants, or to unravel their composition [239,240]. Most of these categories are discussed in the present section (see Table 13). However, studies on vegetables and fruits (mainly analyzed to detect organic micro-contaminants) and fish (where organohalogens are almost invariably the target compounds) are included in Sections 3.4.3 (below) and 3.2 (Part III), respectively.

3.3.1. Fats and oils

Fatty acids (FAs) can be classified as saturated, mono-unsaturated and poly-unsaturated fatty acids (PUFAs). Fats containing PUFAs are liquid at room temperature and are called oils. Saturated FAs are mainly present in animal fat, while vegetable oils contain PUFAs with two or three double bonds, and fish oils contain a large proportion of PUFAs having five or six double bonds. The location of the double bonds is also different, with vegetable oils mainly containing the ω-6 series, and fish oils the ω-3 series of FAs.

FAs are almost invariably analyzed by means of 1D-GC, after their transesterification and hydrogenation to methyl esters (FAMEs). Because of the complexity of many samples, an adsorption LC separation (e.g., on silica) is sometimes used to effect a fractionation prior to the GC analysis. Specifically, when minor FAs eluting close to much more abundant homologues are of interest, MDGC is preferred as a more selective technique.

Ordered structures were prominently present in the first GC × GC paper on biological oil samples [19] and, after the improved presentation in [92], it was clear that, in a conventional system:

(i) FAMEs with the same number of carbon atoms elute as clusters with a gradual increase of the first-dimension retention times with increasing carbon number; and,

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Table 13. Papers on GC × GC of food, fat, oils and fragrances[c]

Subject matter	Detector	Refs[a,b]
Fats and oils		
Group-type separation of natural fats and oils	FID	[130]
Evaluation of fast GC and GC–MS of lipids	FID	[131]
Fatty acids in biological oil	FID	[**19**, 77]
Fatty acids in lanolin	ToF-MS	[241]
Flavors in dairy spread and sour creams	ToF-MS	[**117**]
Flavor compounds in butter	FID, ToF-MS	[**242**]
'Reversed-type' GC × GC of vanilla and olive oil	FID, ToF-MS	[**123**]
GC × GC–qMS of olive oil	qMS	[**184**]
GC × GC for fast screening of wash oils	FID	[243]
Fragrances		
Suspected allergens in fragrances	FID	[**180**, **244**]
Target terpenes in perfume mixtures	FID	[**199**]
Alcoholic beverages		
Trans-resveratrol in wine	FID	[**245**]
Methoxypyrazines in wine	NPD, ToF-MS	[**200**]
Amino acids in wine, beer and honey	ToF-MS	[**129**]
Positional isomers (2- and 3-methyl isomers of butanol)	FID	[138]
Essential oils		
Sesquiterpene and oxygenated sesquiterpene hydrocarbons	FID	[78]
Volatiles in tea tree and lavender oils	FID	[79]
Lavender essential oils	FID	[**80**]
Lavender volatiles	ToF-MS	[81]
Ginger volatiles	FID	[191]
Volatiles in peppermint and spearmint oil	FID	[82]
Enantioseparation of monoterpenes	FID	[25, **23**]
Australian sandalwood oil	FID, ToF-MS	[**246**]
Sub-critical water extraction of essential oils from *Thymbra spicata*	ToF-MS	[247]
Volatiles in *Pistacia vera L.*	ToF-MS	[248]
Hop volatiles	ToF-MS	[119]
Odorants in coriander and wild coriander leaves	ToF-MS	[249]
Zedoary volatile oil	ToF-MS	[134,133]
Volatile oils in Chinese medicines	FID	[250]
Volatile oils in Chinese medicines	ToF-MS	[132]
Profiling of volatile oils in herbal mixtures	FID	[251]
Pulp properties of Eucalyptus clones and leaf volatiles	FID	[252]
Asian and American ginseng	FID, qMS	[**183**]
Volatiles in *Pelargonium graveolens*	qMS	[181]
Quantification of compounds in tobacco essential oils	ToF-MS	[253]
Tobacco essential oils	ToF-MS	[254]
Volatiles in *Ziziphora taurica subsp. taurica*	ToF-MS	[255]
Volatiles in essential oil samples	FID	[91]
Miscellaneous		
Roasted coffee beans		
Volatiles in roasted coffee beans	FID	[126]
Volatiles in roasted coffee beans	ToF-MS, qMS	[124]
Volatiles in roasted coffee beans	NPD, ToF-MS	[172]
Strawberry volatiles (enantiomers)	FID	[139]
Flavors in garlic powder	FID, ToF-MS	[83]

[a]Papers on organohalogens in food (mainly fish) are included in Table 10 (Part III).
[b]**Bold**: analytical performance reported.
[c]For a recent review of the role of GC × GC in food analysis, see [101].