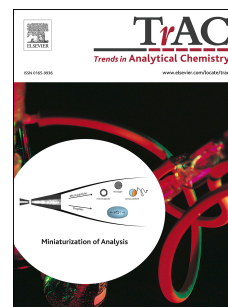


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## Comprehensive two-dimensional gas chromatography in forensic science: A critical review of recent trends

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### ABSTRACT

Comprehensive two-dimensional gas chromatography (GC×GC) has become accepted as one of the most powerful separation techniques in several application areas. In forensic investigations, however, it has not yet been entirely established due to limitations regarding standardized methodology, data interpretation and consistency of results. Nevertheless, GC×GC allows for target analysis, compound class analysis and chemical fingerprinting of samples and is therefore increasingly applied in forensic analytics. In this review, recent and significant advances in GC×GC for application to forensic studies including human scent, arson investigations, security-relevant substances and environmental forensics are discussed. The discussion includes a brief overview of the latest trends and evolutions with regard to the various forensic applications and data evaluation as well as limitations. This leads to the conclusion that the full potential of the comprehensive data sets can only be achieved by implementing standardized analysis and data processing methods.

### KEYWORDS

Human scent; arson investigations; security-relevant substances; environmental forensics; mass spectrometry; GC×GC-MS; targeted analysis; discovery-based analysis; group-type analysis; chemical fingerprinting

### ABBREVIATIONS

μECD, Micro-electron capture detector; <sup>1</sup>D, One-dimensional; <sup>1</sup>t<sub>R</sub>, Primary retention times; <sup>2</sup>D, Two-dimensional; <sup>2</sup>t<sub>R</sub>, Secondary retention times; ANOVA, Analysis of variance; CBRN, Chemical, biological, radiological, nuclear; CWAs, Chemical warfare agents; DDTs, Dichlorodiphenyltrichloroethanes; DoE, Design of experiments; EI, Electron ionization; ENCI, Electron capture negative chemical ionization; FFF, Fracturing, flowback and drilling fluids; FID, Flame ionization detection; FRs, Fisher ratios; GC, Gas chromatography; GC×GC, Comprehensive two-dimensional gas chromatography; HCA, Hierarchical cluster analysis; HR, High-resolution; HS-SPME, Headspace solid-phase microextraction; KMD, Kendrick mass defect; kNN, k nearest neighbor classification; LC, Liquid chromatography; MCCPs, Middle-chained chlorinated paraffines; MOECC, Ministry of the Environment and Climate Change; MS, Mass spectrometry; MW, Macondo Well; NAFCs, Naphthenic acids fraction compounds; NPD, Nitrogen phosphorus detection; PBDEs, Polybrominated diphenyl ethers; PCA, Principal component analysis; PCBs, polychlorinated biphenyls; PCDD/Fs, Polychlorinated dibenzo-p-dioxins and dibenzofurans; PCNs, Polychlorinated naphthalenes; POPs, Persistent organic pollutants; qMS, Quadrupole-MS; qTOF, Quadrupole-TOF; RFF, Reverse fill/flush; SCCPs, Short-chained chlorinated paraffines; TAS, Triaromatic steroids; TD, Thermal desorption; TIC, Total ion current; TOF, Time-of-flight; US, United States; VOCs, Volatile organic compounds; VX, O-ethyl S-2-diisopropylaminoethyl methylphosphonothiolate

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