Gas Chromatography–Time-of-Flight Mass Spectrometry in Food Analysis

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Gas chromatography (GC) coupled to time-of-flight mass spectrometry (TOF-MS) offers unique solutions for various analytical applications including the analysis of food quality, authenticity and safety markers. This article provides a general overview of TOF-MS basic features, highlighting its advantages and limitations compared with GC using conventional mass analysers. Examples of recent results obtained for selected food contaminants and flavour components are described to illustrate the potential of this recently introduced technique.

Hyphenation of gas chromatography (GC) with mass spectrometry (MS) allows identification and quantification of a wide range of trace amounts of GC-amenable compounds in complex matrices. Until now, low-resolution (unit mass) mass spectrometric detectors employing either single quadrupole or ion trap mass analysers have been used in most of the food analysis applications.

While quadrupole is mainly operated in selected ion monitoring (SIM) mode for enhanced sensitivity in ultra-trace analysis, the ion trap (except for full scan mode) is used in MS–MS (tandem-in-time) mode to increase selectivity. In addition, triple quadrupole (tandem-in-space) or high-resolution magnetic double-focusing sector instruments can be employed for specific analyses.

Recent progress in instrumentation design (optics mainly) as well as the use of fast recording electronics (which were not available or were too expensive until a few years ago) together with improvements in signal-processing techniques has led to the renaissance of time-of-flight (TOF) mass analysers for the determination of a wide range of both target and non-target organic components occurring in various biotic matrices.

Time-of-Flight Mass Spectrometry (TOF-MS)

There are numerous ways that mass spectrometers separate molecules of different masses. Some systems measure the deflection of an ionized and accelerated beam of analyte in a magnetic or electric field. Another applied approach employs separation of the ion beam by passing it through a high frequency electrical field. Contrary to these principles, as the name implies, a TOF mass analyser identifies sample molecules by measuring their flight time in a field-free tube.

The gaseous ions generated in an ion source from the neutral molecules of an analyte are in the first phase accelerated to get constant kinetic energy and then ejected into a mass analyser

using pulsed electric-field gradient oriented orthogonally to the ion beam (orthogonal acceleration TOF), which has a positive influence on mass resolution of the instrument. Further enhancement of mass resolution is obtained by using a reflectron (ion mirror). This device consists of a series of ring electrodes with increasing voltage creating retarding fields. After reaching the reflectron area, ions with higher energy penetrate more deeply inside, extending the time when they are reflected. As a consequence of this phenomenon, the ions of the same *m/z* value with different initial energies hit the detector at almost the same time. In addition, the mass resolution is substantially improved by making the ions pass twice along a TOF flight tube before reaching the detector. The flight times of the ions separated in a field free region are proportional to the square root of respective *m/z* values. For the detection of ions a microchannel plate (MCP) detector is preferred. The outgoing pulses are registered either by a time-to-digital converter (TDC) or by an analogue-to-digital (ADC)-based continuous averager, also called a digital signal averager (DSA) or integrating transient recorder (ITR).[1]

The effort to exploit the unique features of the rapidly developing TOF-MS technique resulted in the introduction of two types of spectrometers differing in their basic characteristics:

- Instruments using high-resolution analysers characteristic with only moderate acquisition speed.
- Unit-resolution instruments that feature a high acquisition speed.

The application potential of these approaches is obviously complementary. The technical features of current available GC–TOF-MS systems are summarized in Table 1.

Applications of GC–TOF-MS in Food Analysis

Recently GC–TOF-MS employing both high-resolution (HR) and high-speed (HS) detectors has been demonstrated as a powerful and highly effective analytical tool in various fields such as analysis of food and environmental contaminants, flavour components, drugs screening, petrochemical analysis, or metabolomics studies.

Thanks to the availability of spectral information even at very low levels for a particular compound (high mass analyser efficiency), this technique can be used not only for quantification/confirmation of target analytes but also for identification of non-target sample components even in very complex mixtures.[2–11] This article will describe examples of TOF-MS performance in challenging applications, including determination of pesticide residues, polybrominated diphenyl ethers (PDBEs), acrylamide and volatiles in different food matrices.

Recent progress in instrumentation design has led to the renaissance of time-of-flight (TOF) mass analysers for the determination of a wide range of both target and non-target organic components occurring in various biotic matrices.

Pesticide residues, occurring in food crops as a consequence of their protection against various pests and weeds, represent a typical example of troublesome analytes. Unbiased, highly sensitive analysis of multiple residues possessing a wide range of physicochemical properties in a single run is a difficult task.

The EU legislation (2003/13/EC) sets the uniform limit for any pesticide residue potentially present in processed cereal-based foods and baby foods for infants and young children as low as 0.01 mg kg^{-1} (for several pesticides with high toxicity, even lower maximum residue limits (MRLs) are enforced).

Figure 1 illustrates the main advantage of using the HRTOF-MS instrument (GCT, Micromass, Manchester, UK) in the fast GC analysis of low level (0.01 mg kg^{-1}) chlorpyrifos. When using 1 Da mass window (setting corresponding to a unit mass resolution instrument) the peak-to-peak:signal-to-noise (PtP:S/N) ratio was only 6:1. Moreover, interference at the target ion occurred, thus baseline integration was not possible. On the other hand, setting the mass window as narrow as 0.02 Da led to a distinctly improved value of PtP:S/N of 87:1. Thanks to the high mass resolution and monitoring of the exact mass of target analyte, chemical noise originating from various sources (e.g., matrix coextracts, column bleed) can be significantly reduced, resulting in an improved limit of quantification (LOQ). It should also be noted, that the mass

Table 1: Characteristics of current GC–TOF-MS systems.

Instrument (company)	Upper mass limit (Da)	Mass resolution	Maximal acquisition rate (spectra s^{-1})	Mass accuracy (ppm)	Linearity (Orders of magnitude)	Acquisition system	Ionization technique	
							EI	CI
GCT (Micromass) *	1500	7000 fwhm	10	5	3	TDC	+	+
GCT Premier (Waters)	1500	7000 fwhm	20	5	4	TDC	+	+
JMS-T100GC (JEOL)	2000	5000 fwhm	25	5	4	ADC	+	+
Kronus (Scientific Analysis Instruments)	2000	Unit mass	100	ns	4	ADC	+	+
Pegasus 4D (Leco) *	1000	Unit mass	500	ns	4	ADC	+	–
Tempus (Thermo)	1000	Unit mass	60	ns	4	ADC	+	+

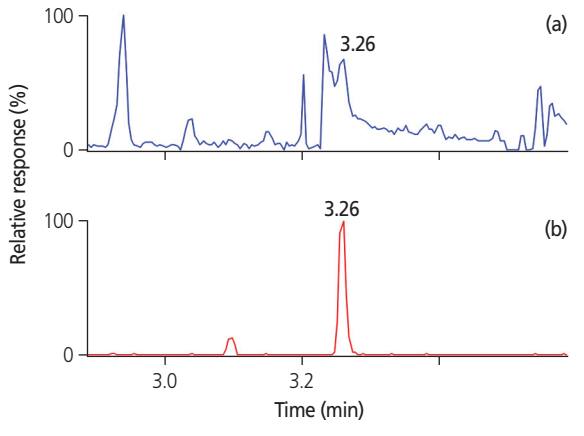
* Instruments used in this paper.
fwhm = full width at half maximum, ns = not specified.

measurement accuracy allowed determination of the mass of quantification ion with the error as low as −1.5 ppm. Experimentally determined mass of this pesticide was 198.9170 Da versus a theoretical mass of 198.9173 Da that corresponds to chlorpyrifos quantification ion with an elemental composition of $C_5H_2NO^{35}Cl_2{}^{37}Cl$. Using this approach, the identification of the analyte can be based not only on retention time and mass spectrum (as traditionally used in GC–MS) but thanks to the exact mass measurement also on elemental composition determination, which brings a new dimension in the identification/confirmation process.[2]

Analysis of phosalone (0.01 mg kg^{-1}) in apple extract shown in Figure 2 demonstrates outcomes facilitated by a HSTOF-MS instrument (Pegasus, Leco Corp., St Joseph, Michigan, USA) when coupled to comprehensive two-dimensional (2D) gas chromatography (GC×GC). The most abundant ions of this analyte are *m/z* 182, 184 and 367. In conventional one-dimensional (1D) GC separation, the presence of chemical noise led to its poor detectability. This problem can be eliminated by increased separation power obtained by GC×GC set-up.

Employing the combination of a non-polar column (5% phenyl polysilphenylenesiloxane) in the first dimension and a more polar one (50% phenyl polysilphenylenesiloxane) in the second dimension, a much lower detection limit for phosalone was achieved. Improvement of detectability was a result of cryofocusing of the effluent from the first column by the modulator as well as the separation of the analyte from the background interferents (chemical noise) exhibiting different retention behaviour on the second dimension column.[3]

Figure 1: GC–HRTOF-MS chromatograms of chlorpyrifos (t_R = 3.26 min) at a concentration of 0.01 mg kg^{-1} in apple baby food. Target ion *m/z* 198.9173 extracted using a mass window of (a) 1 Da and (b) 0.02 Da. Experimental conditions: Ethyl acetate extraction followed by GPC clean-up used for sample preparation.[2] Injection: 2 µL PTV (solvent vent, 15 s, 20 mL min^{-1}), injector temperature programme: 70 °C (15 s), 10 °C s^{-1} to 280 °C. GC separation: RTX–5 Sil MS column 10 m × 0.53 mm × 0.5 µm connected to a 3 m × 0.15 mm i.d. non-coated restriction column; oven temperature programme: 90 °C (1 min), 60 °C min^{-1} to 280 °C (2.83 min); column pressure: 14 psi (90 °C) linearly increased to 24 psi (280 °C). MS detection: EI mode; acquisition rate: 4 spectra s^{-1}.



It should be noted that separation on a short microbore (second dimension) column is so fast that only a HSTOF-MS provides sampling rates relevant to the very narrow eluting peaks (0.1–0.2 s). If a less expensive, rapid-scanning quadrupole instrument is employed for detection in GC×GC, broader peaks (0.2–1 s in the second dimension) have to be obtained by setting a less steep temperature programme to get a sufficient number of points per chromatographic peak.[12] As a result of this, not only speed of analysis but also detection sensitivity is sacrificed.[5] Compensation of the latter drawback by reduction of the monitored mass range is possible, but might be insufficient since the mass analyser efficiency of quadrupole operated in full scan mode is significantly lower compared with HSTOF-MS.

Polybrominated diphenyl ethers (PBDEs) belong to a group of brominated flame retardants, which are chemicals widely used in various products, for example plastics, textiles, furnishing foams to prevent a fire hazard. Currently, there is a growing interest in PBDE analysis in environmental and food samples because of the continual increase in the levels of these compounds in the general environment and human tissues during the last decade. Similarly to other persistent organic pollutants, such as, for example, polychlorodibenzo-*p*-dioxins and -furans (PCDDs/Fs) and/or polychlorinated biphenyls (PCBs), these contaminants are lipophilic and considerably resistant to degradation processes.[13] Considering PBDEs accumulation potential and with regard to the growing toxicological concerns, unbiased control of PBDEs occurrence in the environment is recommended by the recently introduced EU regulation (2003/11/EC). Figure 3 shows negative ion chemical ionization (NICI) chromatograms obtained by

Figure 2: Separation of phosalone at 0.01 mg kg^{-1} in apple extract by (a) 1D–GC–HSTOF-MS and (b) GC×GC–HSTOF-MS. Experimental conditions: Ethyl acetate extraction followed by GPC clean-up used for sample preparation.[2] Injection: 1 µL splitless at 250 °C. 1D–GC separation: DB-5ms column 30 m × 0.25 mm × 0.25 µm; oven temperature programme: 60 °C (1.5 min), 20 °C min^{-1} to 280 °C (12.10 min); column flow 1 mL min^{-1}. GC×GC separation: DB-5ms column 30 m × 0.25 mm × 0.25 µm coupled to BPX-50 column 1.2 m × 0.10 mm × 0.10 µm; primary oven temperature programme: 60 °C (1.5 min), 20 °C min^{-1} to 280 °C (20.50 min); secondary oven temperature: +10 °C above the primary oven temperature; modulator offset: +30 °C above the primary oven temperature; modulation period: 5 s (hot pulse 1 s); column flow: 1 mL min^{-1}. MS detection: EI mode; acquisition rates: 5 spectra s^{-1} (1D–GC), 100 spectra s^{-1} (GC×GC).

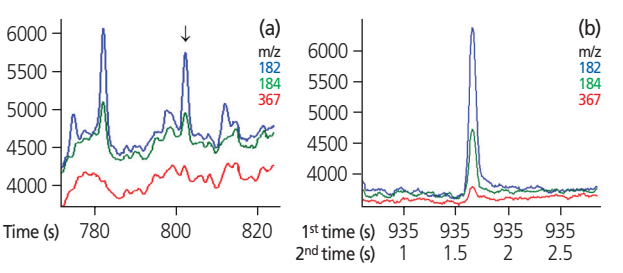


Figure 3: GC–HRTOF-MS chromatograms of PBDEs in (a) fish (perch) extract and (b) standard at concentration 0.1 ng mL^{-1}. Target ion *m/z* 80.9163 extracted using a mass window of 0.02 Da. Experimental conditions: Soxhlet extraction and GPC clean-up used for sample preparation.[4] Injection: 1 µL pulsed splitless at 280 °C. GC separation: DB-XLB column 30 m × 0.25 mm × 0.10 µm; oven temperature programme: 110 °C (1.5 min), 45 °C min^{-1} to 210 °C, 20 °C min^{-1} to 300 °C (5 min). MS detection: NICI mode; acquisition rate: 2 spectra s^{-1}.

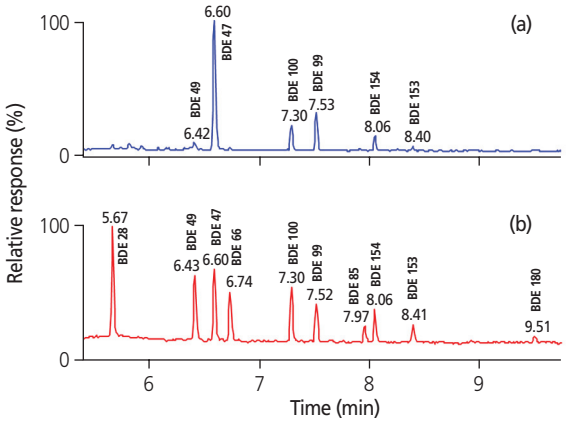
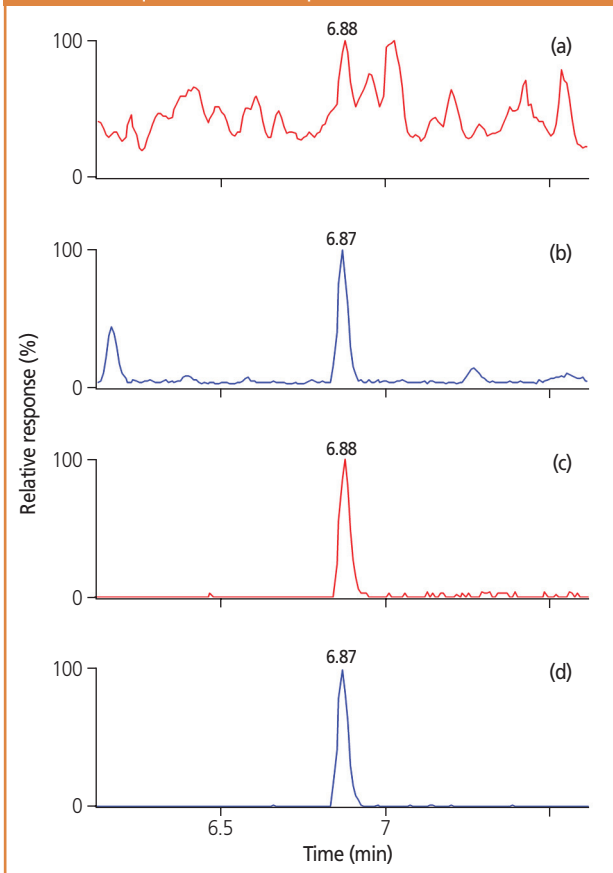


Figure 4: GC–HRTOF-MS chromatograms of acrylamide (t_R = 6.88 min) in potato chips sample (0.7 mg kg^{-1}) and d_3-acrylamide (t_R = 6.87 min, internal standard). Target ions *m/z* 71.0371 for acrylamide (a)+(c) and *m/z* 74.0559 for d_3-acrylamide (b)+(d) extracted using a mass window of (a)+(b) 1 Da and (c)+(d) 0.01 Da. Experimental conditions: sample preparation described in reference 15. Injection: 1 µL pulsed splitless at 250 °C. GC separation: HP-Innowax column 30 m × 0.25 mm × 0.25 µm; oven temperature programme: 70 °C (1 min), 20 °C min^{-1} to 240 °C (10.5 min). MS detection: EI mode; acquisition rate: 2 spectra s^{-1}.



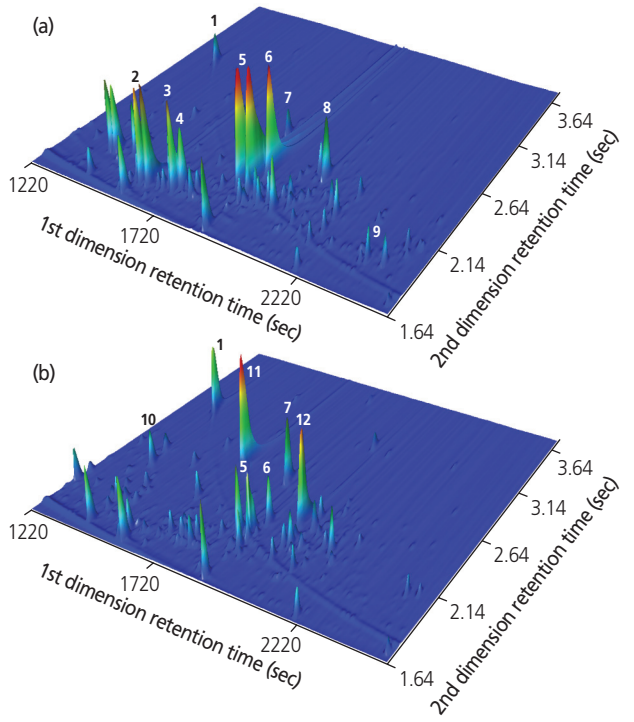
HRTOF-MS examination of purified fish (perch) extract and standard of PBDEs. In our recent study, we demonstrated that operating the instrument in the NICI mode provides not only more sensitive detection (20–100-fold) compared with electron ionization (EI) but also results in increased selectivity. Although the low *m/z* bromine ions used for identification/quantification of target analytes may not seem specific enough (compared with high molecular ions produced by the EI), their selectivity is relatively high since only a limited number of GC-amenable compounds potentially present in food samples are prone to yield ions capable of efficient electron capture in NICI.

Moreover, thanks to the availability of full spectral information other analytes (particularly case major PCB congeners) occurring in this sample could be determined without any instrumental modification, simply by retrieval of stored data. To obtain comparable LOQs by quadrupole operated in SIM mode (ions *m/z* 79 and 81 monitored only) as those achieved by HRTOF-MS, a ten times higher sample equivalent had to be introduced into the system. In other words, HRTOF-MS was more sensitive by one order of magnitude in the analysis of PBDEs.[4]

Another challenging use of GC–HRTOF-MS is demonstrated in the analysis of acrylamide, a recently reported processing carcinogen that originates in heat-treated starch-rich foods. Since the majority of GC–MS methods employs unit resolution mass analysers, laborious and time consuming derivatization (bromination) is usually performed prior to the determination step to obtain the form of target analyte yielding more specific ions (higher *m/z*).[14] The narrow mass window setting enables significant reduction of chemical noise, even in the low mass region (Figure 4), hence direct determination of acrylamide by GC–HRTOF-MS is possible as in the other widely used LC–MS–MS methods.[15]

A wide range of volatile compounds occurs in food headspace, including components responsible for typical flavour, off-flavour and other quality/safety parameters. Solid-phase microextraction (SPME) in combination with the GC–MS technique is a conceivable method of choice.[16] Application of the SPME–GC×GC–HSTOF-MS technique can be illustrated by the analysis of volatiles in honey. Figure 5 shows largely differing three-dimensional (3D) GC×GC plots of aroma compounds sampled by solvent-free SPME technique from headspace of honey samples collected in two different localities (Brazil and Austria). Thanks to high resolution power of this system, both chromatographic (higher peak capacity) and spectral (higher spectral match), even minor volatile components could be identified compared with a 1D–GC set-up. Coupling of SPME with a GC×GC–HSTOF-MS system undoubtedly results in a very promising tool for food profiling and other applications.

Figure 5: A part of the GC×GC chromatograms of volatiles isolated by SPME from floral honey from (a) Brazil and (b) Austria. Experimental conditions: 0.5 g honey and 0.5 mL water in 10 mL SPME vial; DVB/CAR/PDMS (50/30 µm) fibre; incubation time: 10 min; incubation temperature: 40 °C; agitator speed: 500 rpm; extraction time: 30 min; desorption: 2 min (splitless). GC×GC separation: HP-VOC column 60 m × 0.2 mm × 1.1 µm coupled to Supelcowax–10 column 2.5 m × 0.10 mm × 0.10 µm; primary oven temperature programme: 40 °C (2.0 min), 5 °C min^{-1} to 250 °C (5 min); secondary oven temperature: +5 °C above the primary oven temperature; modulator offset: +20 °C above the primary oven temperature; modulation period: 5 s (hot pulse 1 s); column flow: 1 mL min^{-1}. MS detection: EI mode; acquisition rate: 100 spectra s^{-1}. Marked compounds: (1) furan-2-carbaldehyde; (2) lilac alcohol isomers; (3) 3-ethenyl-2,5-dimethyl-hexa-1,4-diene; (4) ipsdienol; (5) linalool oxide isomers; (6) hotrienol; (7) 2-phenylacetaldehyde; (8) epoxylinalol; (9) megastigma-4,6,8-triene isomers; (10) hexan-1-ol; (11) benzaldehyde; (12) isophorone.



Advantages and Limitations of GC–TOF-MS

Table 2 gives the overview of specifications for selected commercial GC–MS benchtop instruments with different mass analysers. The choice of a mass analyser determines the key operating parameters such as the mass range, mass resolution, sensitivity, acquisition rate and linear dynamic range. The following paragraphs summarize advantages and limitations of TOF-MS instruments allowing comparison with conventional scanning MS detectors.[1,2,17]

Acquisition speed: Generally, 1–500 spectra s^{-1} during the GC run are stored in a computer depending on the type of TOF-MS instrument. The moderate acquisition rates of the HRTOF instruments predetermine their use as the detector for conventional and fast GC; the HSTOF instruments are suitable for detection of very narrow chromatographic peaks generated by very fast and ultra-fast GC or GC×GC.

Mass resolution: HSTOF-MS instruments provide only a unit mass resolution, whereas HRTOF analysers offer resolution as high as 7000 full width at half maximum (fwhm) and even more. The advantage of high resolution is the possibility of partially or completely resolving matrix components yielding ions with the same nominal mass as that of the target analyte, hence, significantly reducing background interferences and, consequently, improving the analyte identification.

Mass measurement accuracy: Typically, the HRTOF-MS instruments achieve mass accuracy as low as 5 ppm. Under these conditions, the determination of elemental composition is possible; also the specificity for the identification of unknowns is enhanced.

Acquisition of complete spectra: Mass analyser efficiency of the TOF-MS instruments is as high as 25% in full spectra acquisition. This value is significantly higher compared with that obtained by a scanning instrument such as quadrupole (~0.1%). This fact implies availability of spectral information even at the ultra-trace level of a particular compound and, consequently, the possibility of identifying it on the basis of a library search.

Absence of spectral skew: There are no changes in the ratios of analyte ions across the peak during the acquisition of the mass spectrum and, consequently, no spectral skew (observed commonly by scanning instruments) is encountered. This allows automated deconvolution of partially overlapped peaks on the basis of increasing/decreasing ion intensities in collected spectra and background subtraction followed by identification using a library search. We should note that deconvolution function (employing software correction for spectral skewing) is currently available also for scanning

Table 2: Comparison of different GC–MS benchtop instruments.

Mass analyser	Upper mass limit (Da)	Mass resolution	Maximal acquisition rate[(V)]	Linearity (Orders of magnitude)	Instrumental limit of detection (LOD)	Estimated cost (K€)
Quadrupole[(I)]	1050	Unit mass	15.3 scans s^{-1}	6	pg (fg in SIM)	60–100
Ion trap[(II)]	1000	Unit mass	5.6 scans s^{-1}	5	pg	60–100
HSTOF[(III)]	1000	Unit mass	500 spectra s^{-1}	4	pg	170–220
HRTOF[(IV)]	1500	7000 fwhm	20 spectra s^{-1}	4	fg–pg	190–240

(I) 5975 MSD (Agilent); (II) Polaris Q (Thermo); (III) Pegasus 4D (Leco); (IV) GCT Premier (Waters); (V) Mass range 50–500 Da.

instruments in AMDIS software (Automated Mass Spectral Deconvolution and Identification System).[18] However, the low signal intensity during full spectra acquisition as well as the relatively low acquisition rate of common scanning instruments are parameters that make this feature of high importance in fast GC analysis (i.e., under conditions of lower chromatographic resolution of eluted components).

Extended mass range: Although there is theoretically no upper mass limit for the TOF-MS analysers, this parameter is not critical in combination with GC, because volatility/thermolability of target compounds effectively dictates the scope of this technique. Compared with common mass analysers with an upper mass limit of *m/z* 600–1050, the TOF analysers coupled to GC operate up to *m/z* 1000–2000.

Detector: On the contrary to many scanning instruments, in which an electron multiplier is integrated as a detection device, the TOF-MS employs the MCP detector, that allows simultaneous analysis of all masses across the whole mass range within a few microseconds. However, one must be aware of its limited lifetime, that is 1–3 years (the replacement of a conventional electron multiplier is required in a 5–7 year period).

Depending on the frequency of the instrument use, the potential to detect compounds at ultra-trace concentrations is dropping during the time; the key factor in this context is the value of voltage set to the MCP. In general, sensitivity improvement requires a higher MCP voltage setting, which unavoidably leads to a reduced lifetime of the MCP.

Linear dynamic range: The linear dynamic range of common scanning instruments varies between 5–6 orders of magnitude. The current TOF-MS instruments generally suffer from the limited linear dynamic range compared with conventional MS instrumentation. The ITR (based on ADC) offers linear dynamic range of four orders of magnitude but, at low analyte signal intensities, noise becomes a limiting factor of its use. The TDC, on the contrary, is very suitable for detection of weak signals, which is the case of analytes at ultra-trace levels. Although the linear dynamic range of this device typically does not exceed two orders of magnitude, it can be expanded to approximately three orders of magnitude by application of the dead time correction function (for an explanation see references 2 and 4).

Moreover, because of the continuing improvements in both hardware and software features the dynamic range of some recent instrument employing the TDC is as high as four orders of magnitude. Application of a high voltage to a specific focusing lens reducing the intensity of ions passing into the TOF analyser represents a technical solution that allows replacement of saturated data in a mass spectrum with unsaturated ones acquired when the ion beam has been defocused by the lens.

Cost of the instrument: An important factor when considering a TOF-MS system purchase is undoubtedly its cost. Unfortunately, the cost of TOF-MS is still substantially higher (approximately 2–3 times) compared with low-resolution quadrupole or ion trap instruments. However, in line with dropping cost of sophisticated electronics integrated in these instruments, prices may fall.

Conclusions

Over the past few years, there has been substantial progress in technologies employing the orthogonal acceleration time-of-flight mass spectrometry for improved performance. High-resolution and high-speed time-of-flight analysers represent complementary approaches for target as well as non-target analysis of a wide range of (semi)volatile organic compounds present in food. The availability of sophisticated data systems and data processing algorithms has enabled automated and faster data handling, which is an important requirement for implementation of this mass spectrometric technique into routine use.

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