MARKES international

IngenieríaAnalítica
Chromatography & Spectrometry

BenchTOF

High-performance time-of-flight mass spectrometry for gas chromatography

BenchTOF

The BenchTOF™ range of time-of-flight mass spectrometers connect to any GC and offer major sensitivity and productivity advantages for a broad range of GC–MS applications.

Designed from first principles for optimum performance, and complemented by comprehensive and innovative software, BenchTOF instruments equip GC–MS laboratories to meet the demands of increasingly complex applications, and so significantly extend the range of services they offer.

BenchTOF-HD™

Ground-breaking analytical performance enhanced by the exceptional power and productivity of TOF-DS GC–MS software.

BenchTOF-Select™

BenchTOF-Select unites the power of BenchTOF-HD with Select-eV – Markes' revolutionary variable-energy ionisation technology.

High-definition mass spectrometry

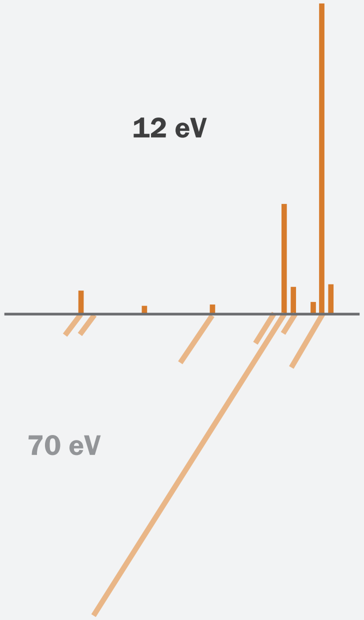
BenchTOF offers a unique and synergistic combination of attributes that deliver a powerful 'high-definition' MS solution for the most challenging GC applications:

- **SIM-level sensitivity with full spectral information**, delivering outstanding results for trace-level analysis of targets *and* unknowns.
- **Reference-quality spectra** simplify component identification by enabling reliable searching against large commercial libraries such as NIST.
- **Long-term stability of analyte response**, and a greatly reduced need for cleaning or maintenance, optimise uptime and productivity.
- **High-speed spectral acquisition** provides information-rich datasets for enhanced data-mining and compatibility with fast GC and GC×GC.
- **Sub-unit mass resolution** allows selective elimination of interferences, and enhanced detection of trace analytes in complex matrices.

The high-definition analytical performance of BenchTOF is now matched by the elegance and ingenuity of **TOF-DS control software** – including the innovative **ChromCompare module** – and by the option of ground-breaking **Select-eV ion-source technology**.

Variable-energy ionisation technology

Select-eV delivers the ability to switch between conventional 70 eV ionisation and lower, softer energies without losing sensitivity, and without the need for reagent gases or source exchange.



Select-eV

Revolutionise your analysis

> **"The impressive sensitivity, speed and spectral integrity of BenchTOF has enabled us to address research questions that literally 'escaped' our previous set-up"**

Dr Carsten Müller
School of Biosciences,
Cardiff University, UK

Innovative technology, elegant design

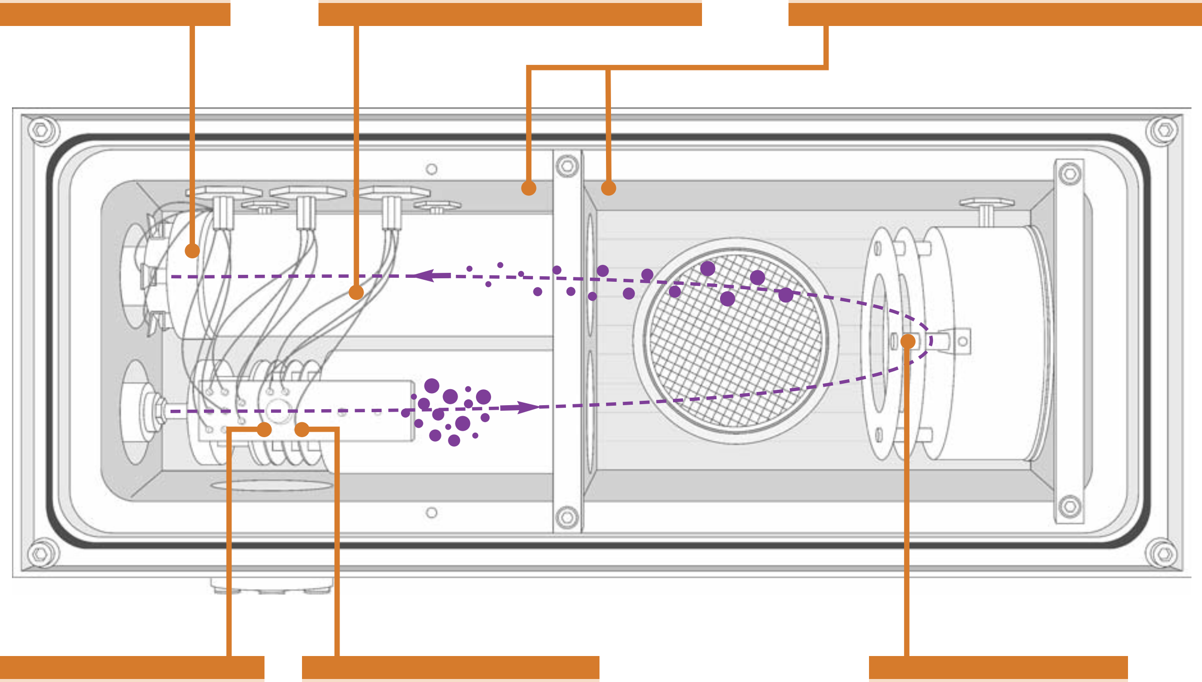
BenchTOF is engineered from first principles, to provide reliable detection and outstanding analytical performance for all major models of GC.

Systems are rugged, requiring minimal intervention for routine applications, but at the same time offering expert users the performance and flexibility required for specialist research work.

A research-grade turbo-pump (three-way, split-flow) allows you to be back up and running within as little as 30 minutes after venting, while the absence of polymers from the vacuum housing minimises organic chemical background noise.

A high-temperature model (with maximum temperatures of 400°C in the source and 450°C in the transfer line) further improves performance for analysis of high-boilers.

Designed from first principles for optimum performance



Micro-channel plate detector: Optimised design delivers spectra free from discrimination.

Unsheathed point-to-point conductors minimise trapped moisture and volatiles, and allow fast equilibration following a vent.

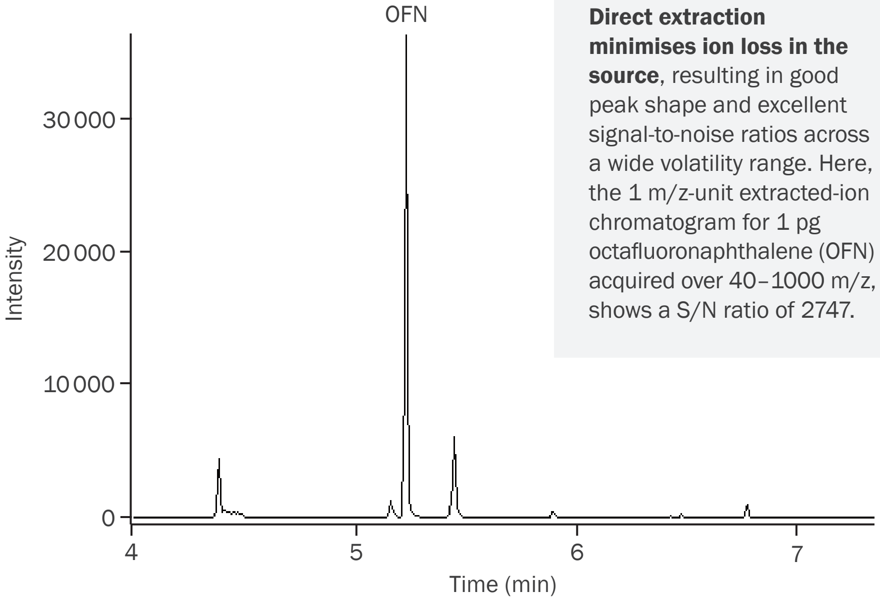
Differentially pumped source and analyser chambers mean that any pressure changes are confined to the source chamber and do not affect ions in the flight tube.

High operating voltages virtually eliminate the need for manual source cleaning, optimising uptime.

Direct extraction design minimises ion loss and improves sensitivity.

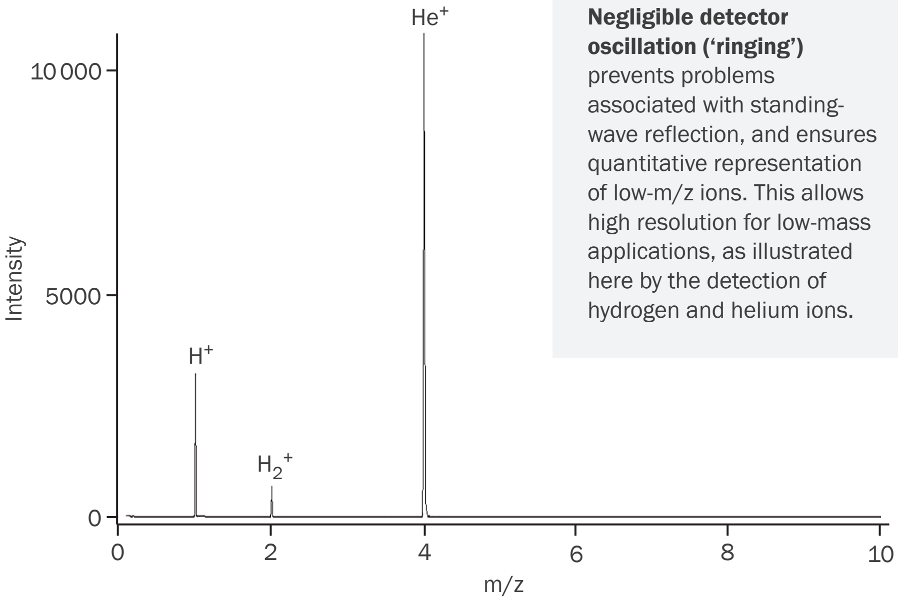
Two-stage reflectron optimises resolution.

Direct extraction optimises sensitivity



Direct extraction minimises ion loss in the source, resulting in good peak shape and excellent signal-to-noise ratios across a wide volatility range. Here, the 1 m/z-unit extracted-ion chromatogram for 1 pg octafluoronaphthalene (OFN) acquired over 40–1000 m/z, shows a S/N ratio of 2747.

High resolution at low mass



Negligible detector oscillation ('ringing') prevents problems associated with standing-wave reflection, and ensures quantitative representation of low-m/z ions. This allows high resolution for low-mass applications, as illustrated here by the detection of hydrogen and helium ions.

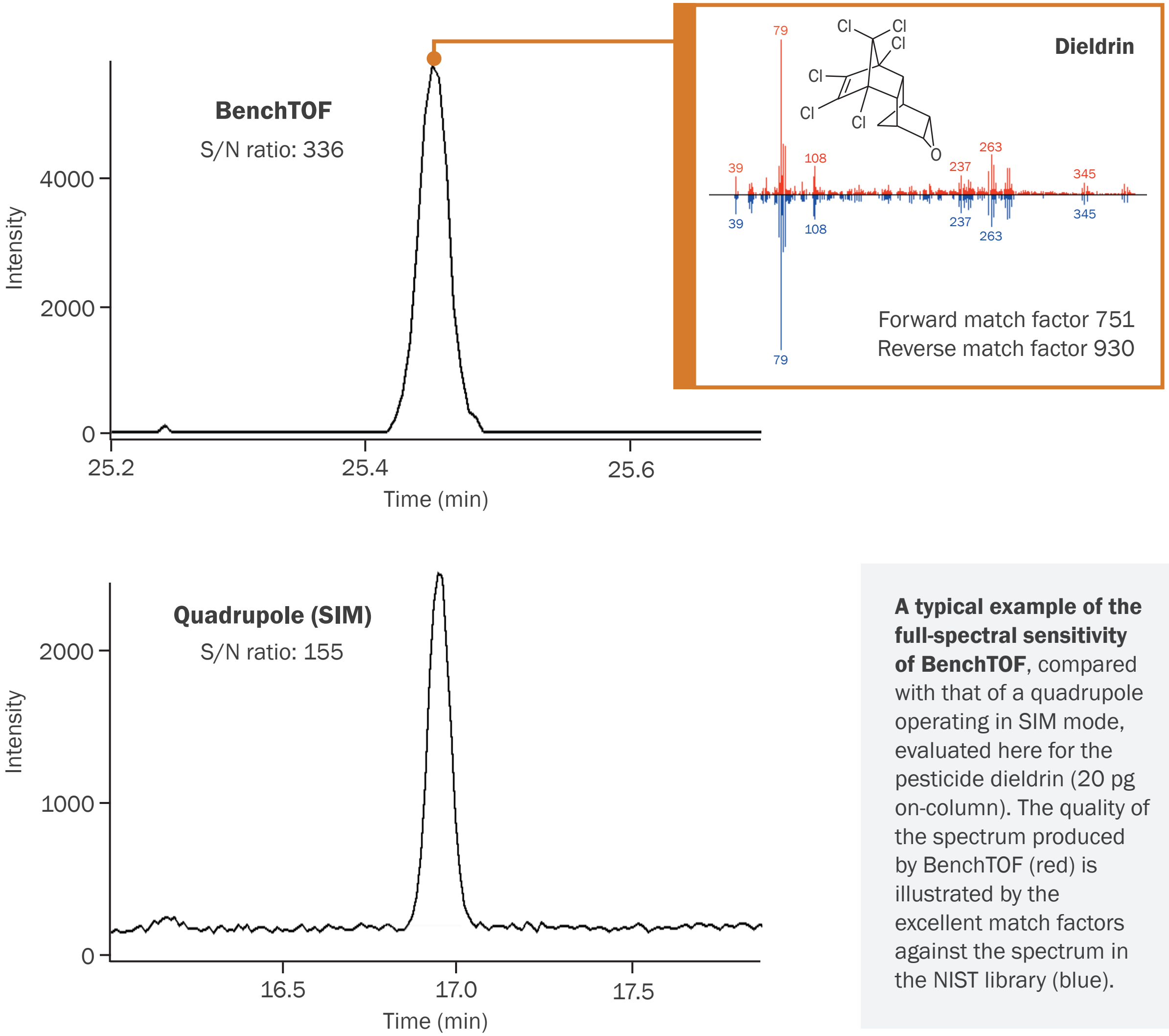
Exceptional sensitivity and spectral quality

Innovative direct-extraction technology minimises ion loss by ejecting ions straight from the source and into the flight tube. This allows BenchTOF to acquire full-range spectra (1–1500 m/z) with **outstanding sensitivity** – comparable or better than those obtained using a traditional quadrupole MS in selected ion monitoring (SIM) mode.

The **reference-quality 70 eV spectra** produced by BenchTOF show none of the bias (discrimination) against high (or low) masses exhibited by other TOF designs. This enables automated peak matching against standard commercial libraries, such as NIST and Wiley, or against custom libraries of quadrupole spectra built up over many years.

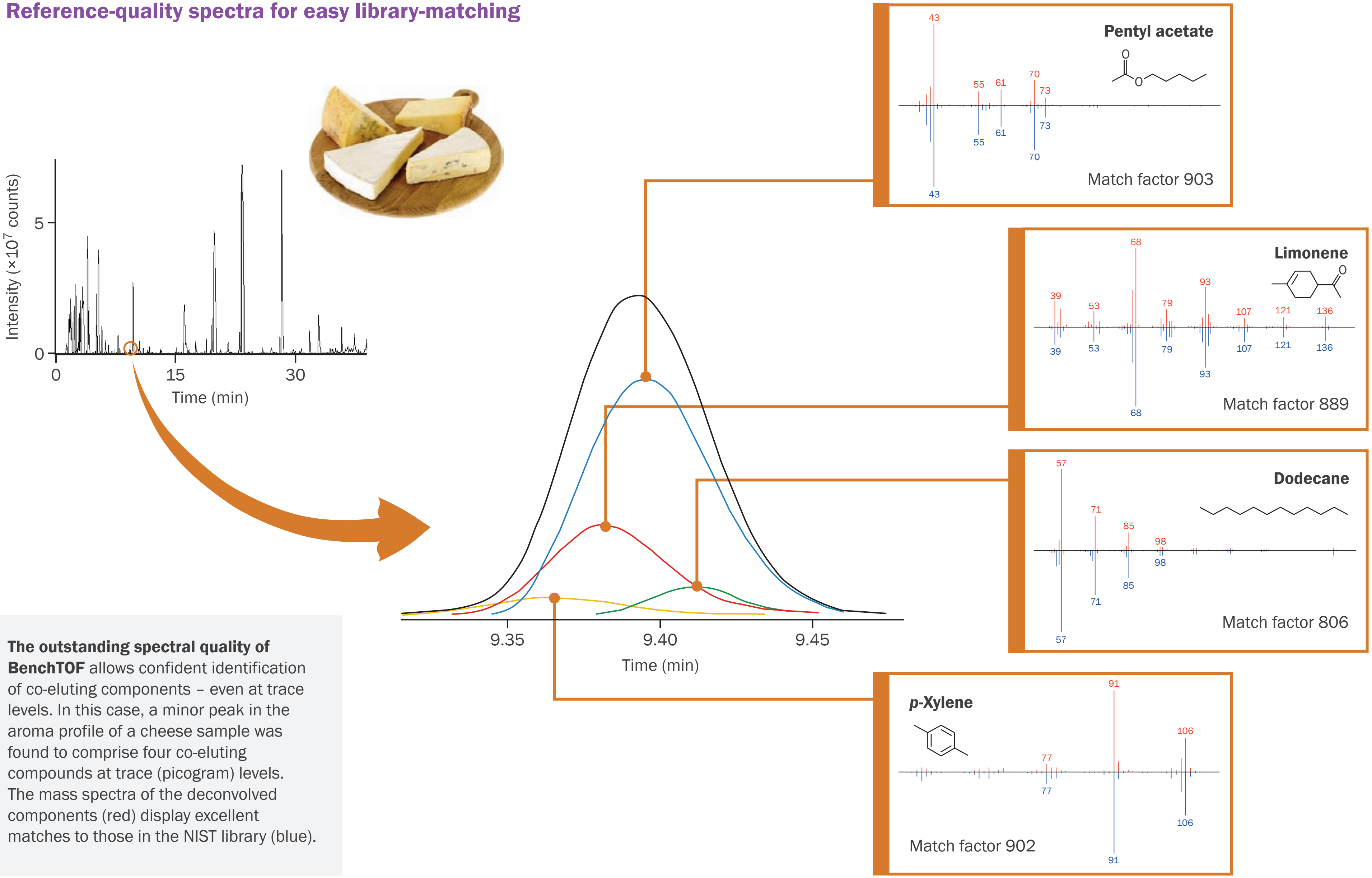
This powerful combination of sensitivity and spectral quality allows BenchTOF users to confirm the identity of trace target compounds and unknowns in a single analysis, thus optimising laboratory efficiency.

Sensitivity comparison for dieldrin



A typical example of the full-spectral sensitivity of BenchTOF, compared with that of a quadrupole operating in SIM mode, evaluated here for the pesticide dieldrin (20 pg on-column). The quality of the spectrum produced by BenchTOF (red) is illustrated by the excellent match factors against the spectrum in the NIST library (blue).

Reference-quality spectra for easy library-matching



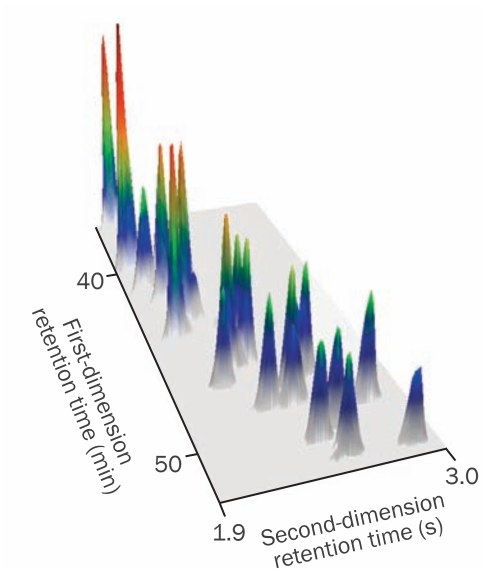
The outstanding spectral quality of BenchTOF allows confident identification of co-eluting components – even at trace levels. In this case, a minor peak in the aroma profile of a cheese sample was found to comprise four co-eluting compounds at trace (picogram) levels. The mass spectra of the deconvolved components (red) display excellent matches to those in the NIST library (blue).

Ultimate performance and productivity

As well as enabling simultaneous analysis of trace target compounds and unknowns, the **high sensitivity** of BenchTOF allows laboratory workflow to be vastly improved. Smaller sample sizes (and more dilute samples) enhance laboratory productivity and reduce turnaround times by simplifying sample preparation and minimising routine maintenance requirements.

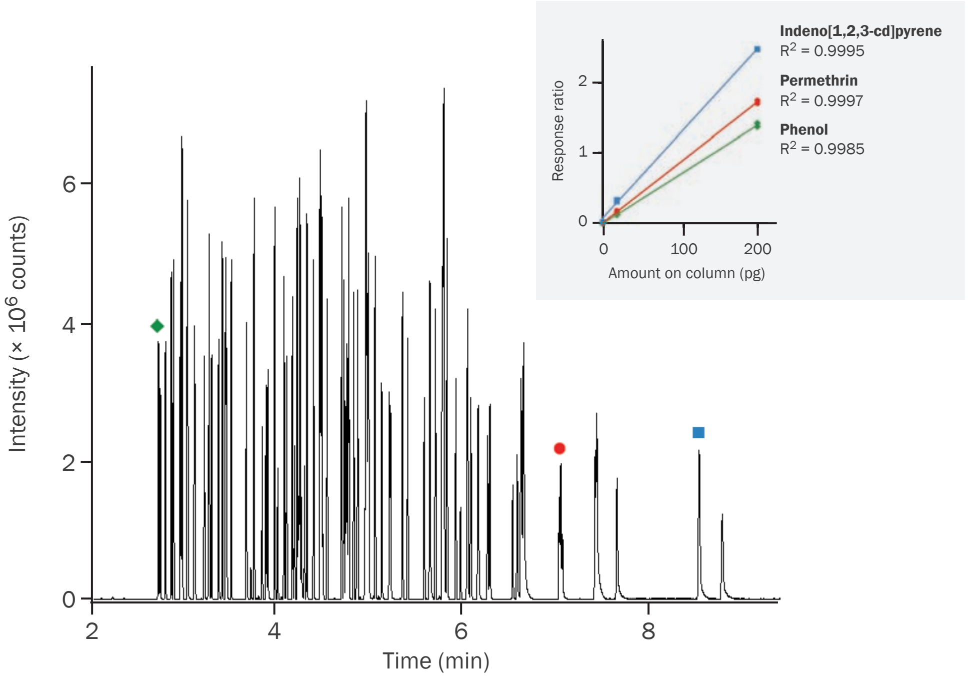
The inherent speed of BenchTOF (10 000 full spectra per second) also allows coupling to fast GC and GC×GC – meaning that complex samples can be analysed in minutes rather than hours.

The speed of BenchTOF enables GC×GC...



The high spectral acquisition rate of BenchTOF results in excellent peak shape and peak-to-peak resolution for challenging GC×GC analyses, such as this set of dichloro- to heptachlorobiphenyls.

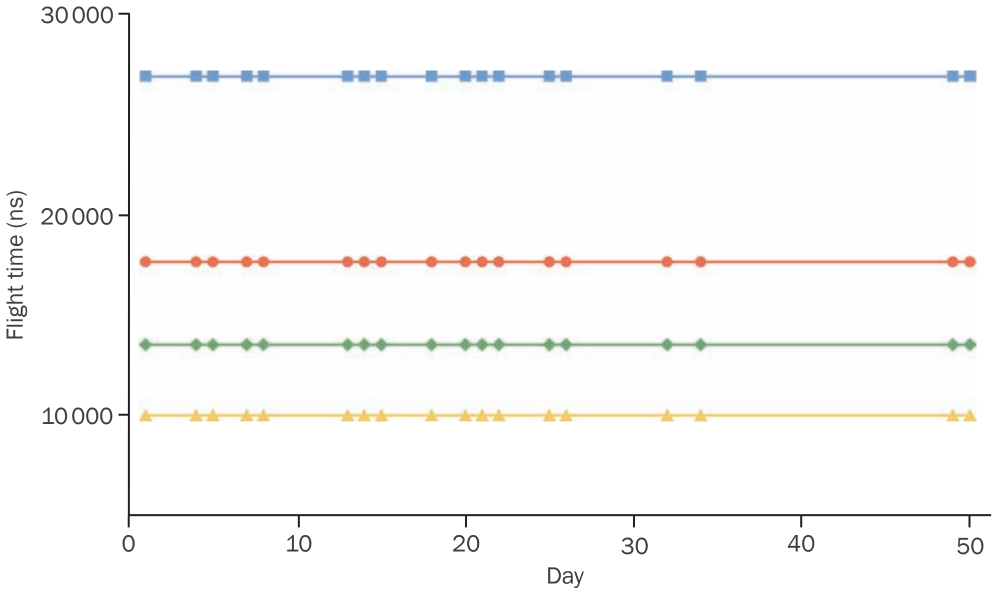
...and fast chromatographic analysis



This 95-component mix of environmental contaminants and pesticides (20 pg on-column) was analysed in less than 10 minutes using BenchTOF. The inset demonstrates that excellent linearity was obtained across the analyte range. The mean signal-to-noise ratio for all 95 compounds in the 20 pg standard was 2252 and in the associated 2 pg standard was 719.

Long-term mass stability enhances productivity

Innovative engineering makes BenchTOF uniquely stable, with an exceptional duty cycle. This means **reliable performance for weeks or even months**, optimising uptime and sample throughput.

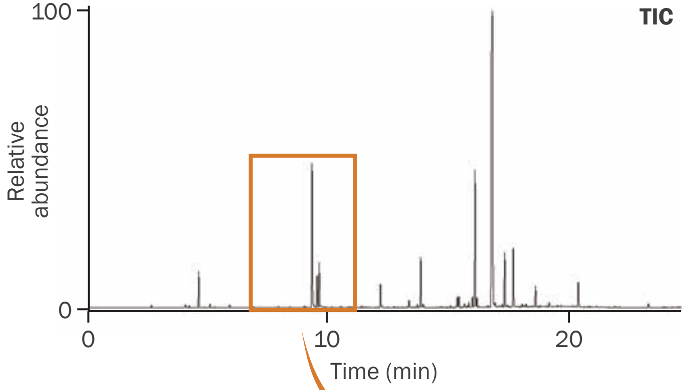


Fragment ion	m/z	RSD (n = 18)
$C_9F_{20}N^+$	501.971	0.006%
$C_4F_9^+$	218.986	0.004%
$C_3F_5^+$	130.992	0.004%
CF_3^+	68.995	0.004%

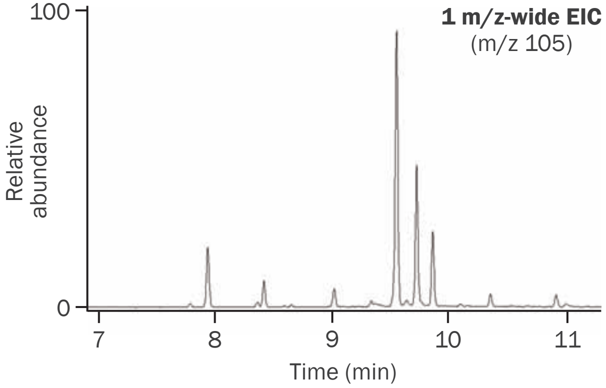
The exceptional stability of ion arrival times at the BenchTOF detector over a 50-day period is demonstrated here for four fragment ions of PFTBA (perfluorotributylamine).

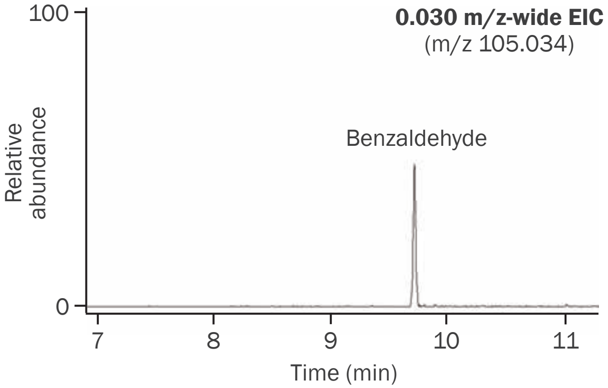
Selectivity and enhanced data confidence

Removing interferences enhances trace-level detection



Sub-amu selectivity can eliminate matrix interferences, allowing precise identification of target compounds, as illustrated here for the emission profile of plastics used in a car stereo.





Sub-unit mass resolution enables BenchTOF to deliver enhanced selectivity.

By allowing selective elimination of matrix interferences, sub-unit mass resolution dramatically improves signal-to-noise ratios, enabling unambiguous detection of trace target compounds in complex matrices.

Revolutionise your analysis with Select-eV®

The capability of BenchTOF is further extended by Select-eV – ground-breaking ion-source technology that allows the energy of electron ionisation to be varied without loss of sensitivity.

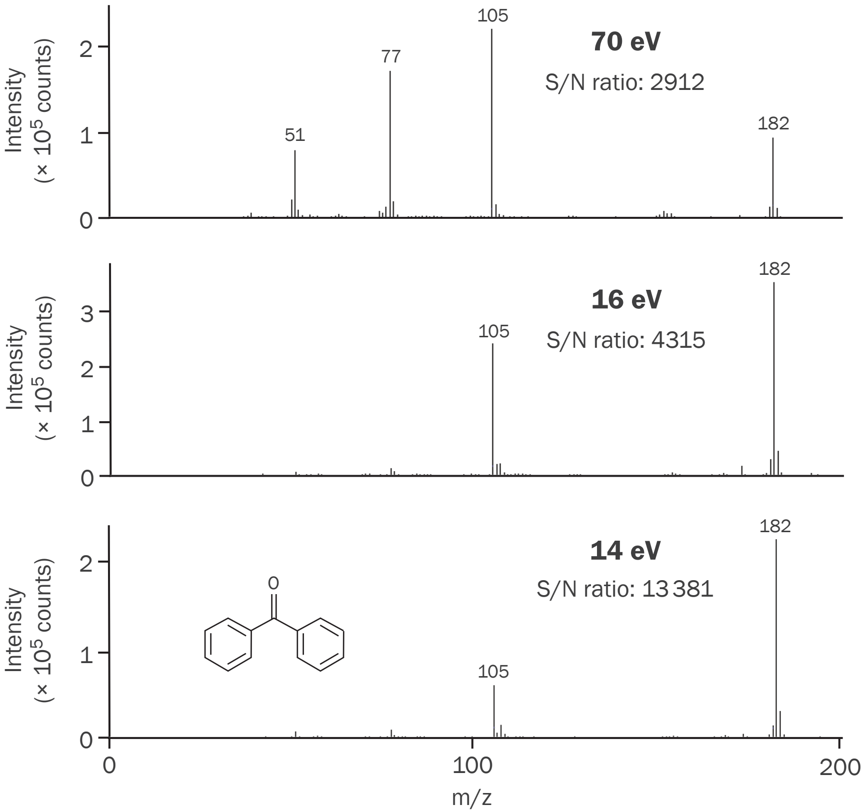
Electron ionisation energies can be changed on a sliding scale, anywhere from the 70 eV used conventionally down to 10 eV, within a single automated sequence, and without the hassle and expense associated with other soft ionisation techniques.

Select-eV is available as an upgrade for BenchTOF-HD, and is integrated as standard in BenchTOF-Select.

Differentiate your laboratory with Select-eV.

Revolutionary BenchTOF-Select ion source incorporating Select-eV technology.

Enhanced molecular ion signal at lower energies

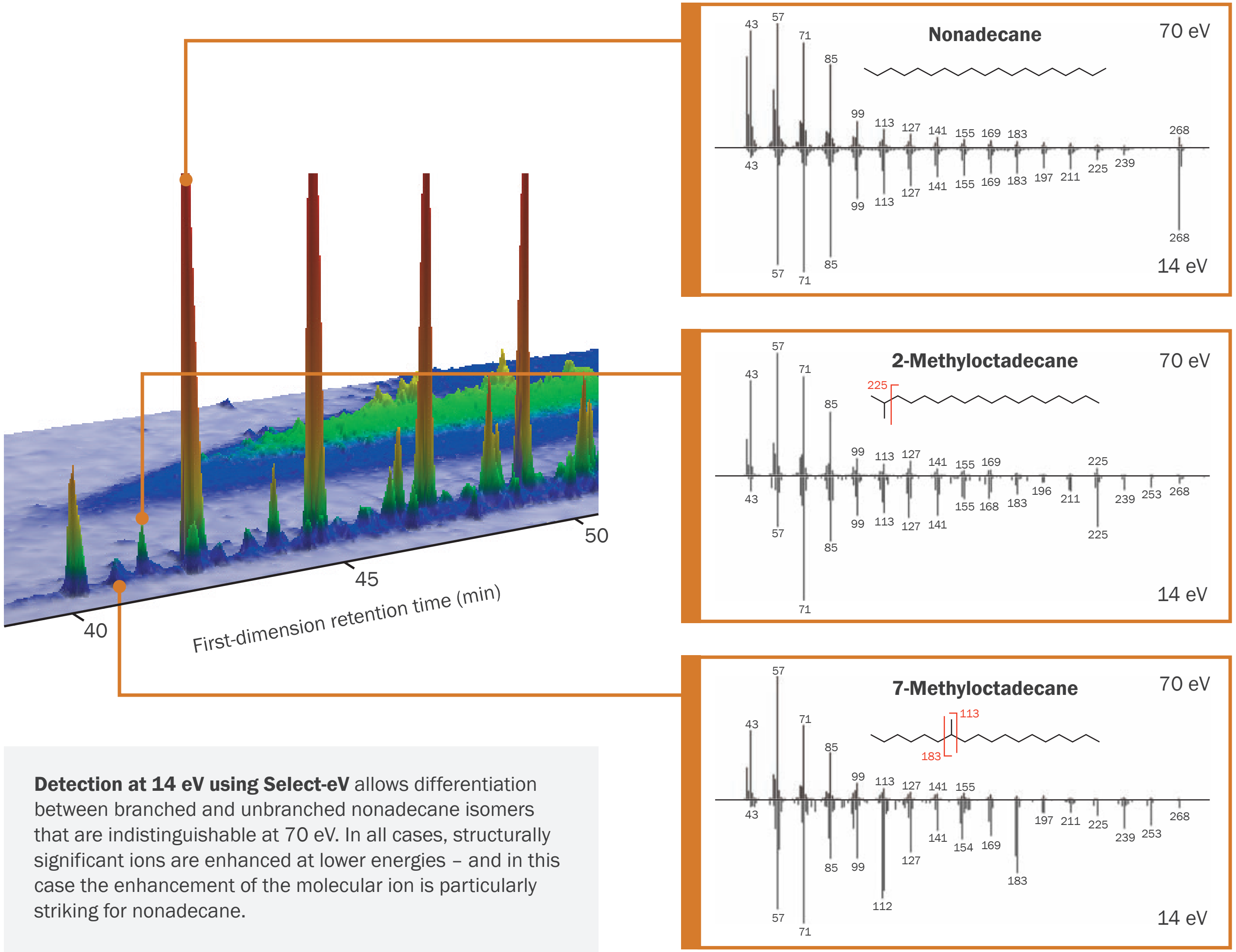


The ability of Select-eV to enhance the molecular ion stands out in this set of spectra for benzophenone (MW 182). Note the enhancement of sensitivity at lower ionisation energies, and the ability to optimise intensities of fragment or molecular ions by a slight change in the energy used for soft ionisation.

An extra dimension of confidence in component identification

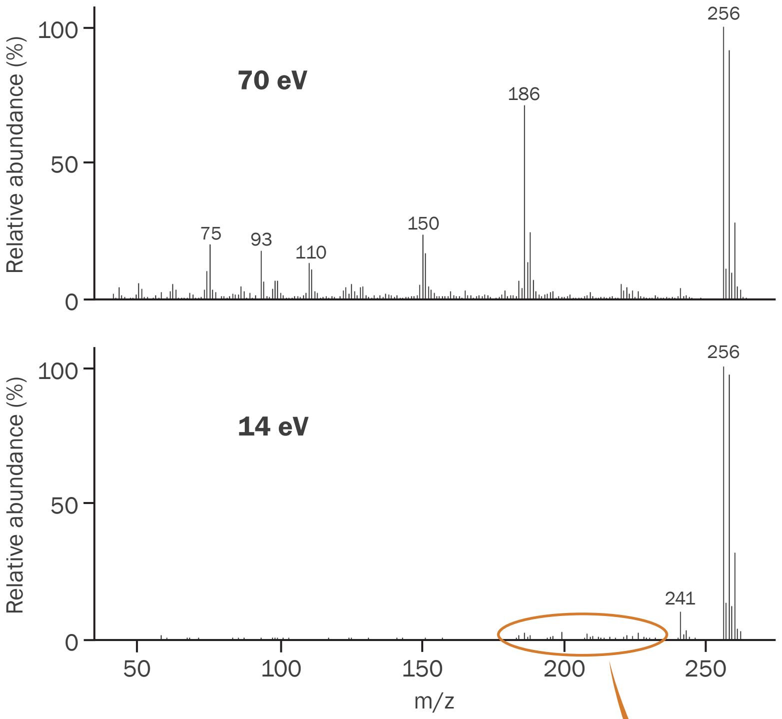
Select-eV results in a degree of fragmentation even at the lowest energies, aiding compound identification.

This is particularly useful for challenging forensic and petrochemical applications, which require accurate distinction between similar species such as hydrocarbon isomers.



Detection at 14 eV using Select-eV allows differentiation between branched and unbranched nonadecane isomers that are indistinguishable at 70 eV. In all cases, structurally significant ions are enhanced at lower energies – and in this case the enhancement of the molecular ion is particularly striking for nonadecane.

Enhanced selectivity with Select-eV



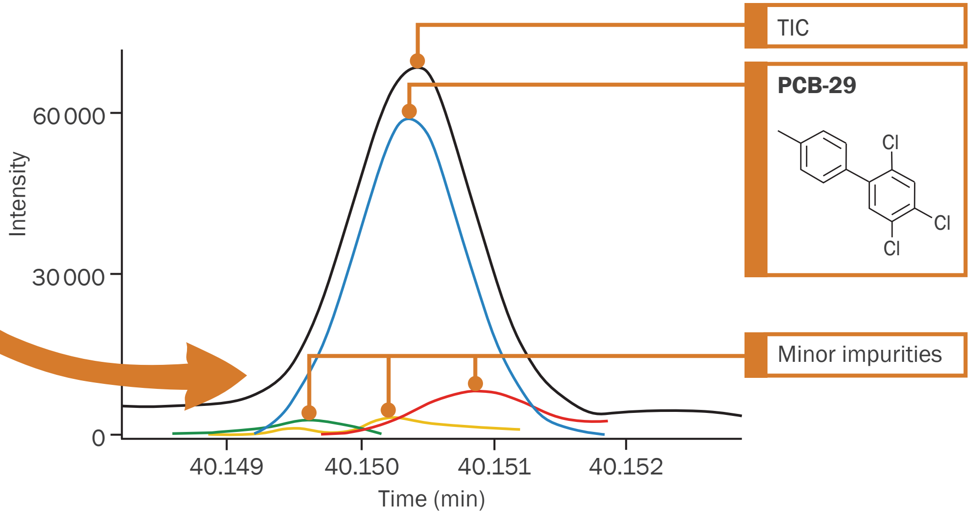
The speed and sub-amu selectivity offered by every BenchTOF is complemented by the ability of Select-eV to detect and visualise co-eluting components. In this GC×GC analysis of PCB-29, the complexity of the 70 eV spectrum makes it difficult to visualise minor impurities. The reduced fragmentation at 14 eV makes it easy to detect and deconvolve these components.

Convenient soft ionisation

Select-eV is more economical and easier to run than other soft ionisation techniques for GC–MS, because it doesn't demand reagent gases, pressurisation of the ion source, or changes to the hardware setup.

The required ionisation energy is simply selected as part of the GC–MS method, allowing the construction of an automated sequence of runs at different energies.

Another advantage of Select-eV is that spectra are **consistent and repeatable** at any given ionisation energy. This allows searchable libraries of reference spectra to be built up for each ionisation energy of interest, aiding rapid and reliable structural elucidation of the most challenging analytes.

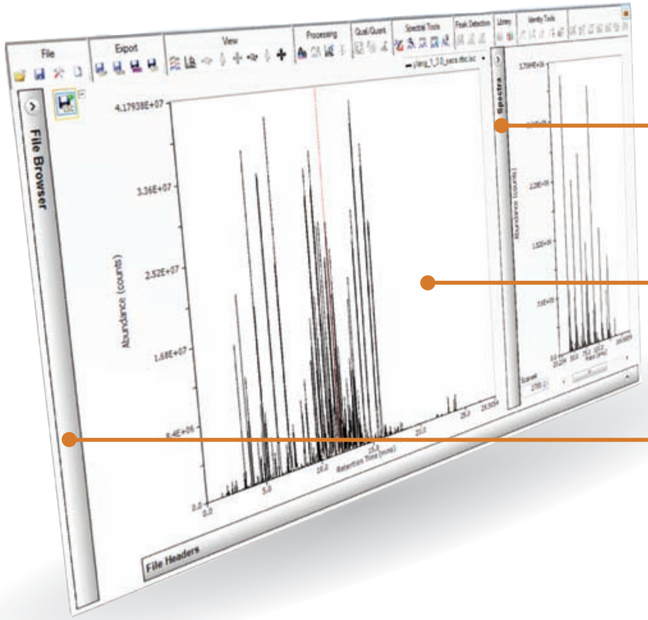


TOF-DS – Innovative software for BenchTOF

TOF-DS™ software has been developed to optimise GC–MS productivity and complement the power and flexibility of BenchTOF. In one intuitive package, it offers full system control, combined with comprehensive qualitative and quantitative analysis, plus a suite of innovative productivity enhancements.

The labour-saving functionality of TOF-DS allows the analyst to speed up method development, streamline routine operation and carry out advanced data-mining of complex chromatograms – both post-run and in real-time.

Elegant and dynamic user interface



Customisable screen layout with collapsible panels makes viewing multiple data-files easy.

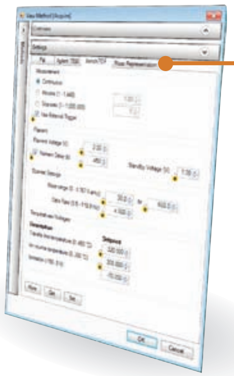
Uncluttered screens ease navigation and visualisation of complex data.

File browser previews chromatograms and their headers for instant access to stored data.

Intuitive method development

The ability to ‘unlock’ method parameters and vary them through a sequence of runs eliminates the need to build and link multiple methods.

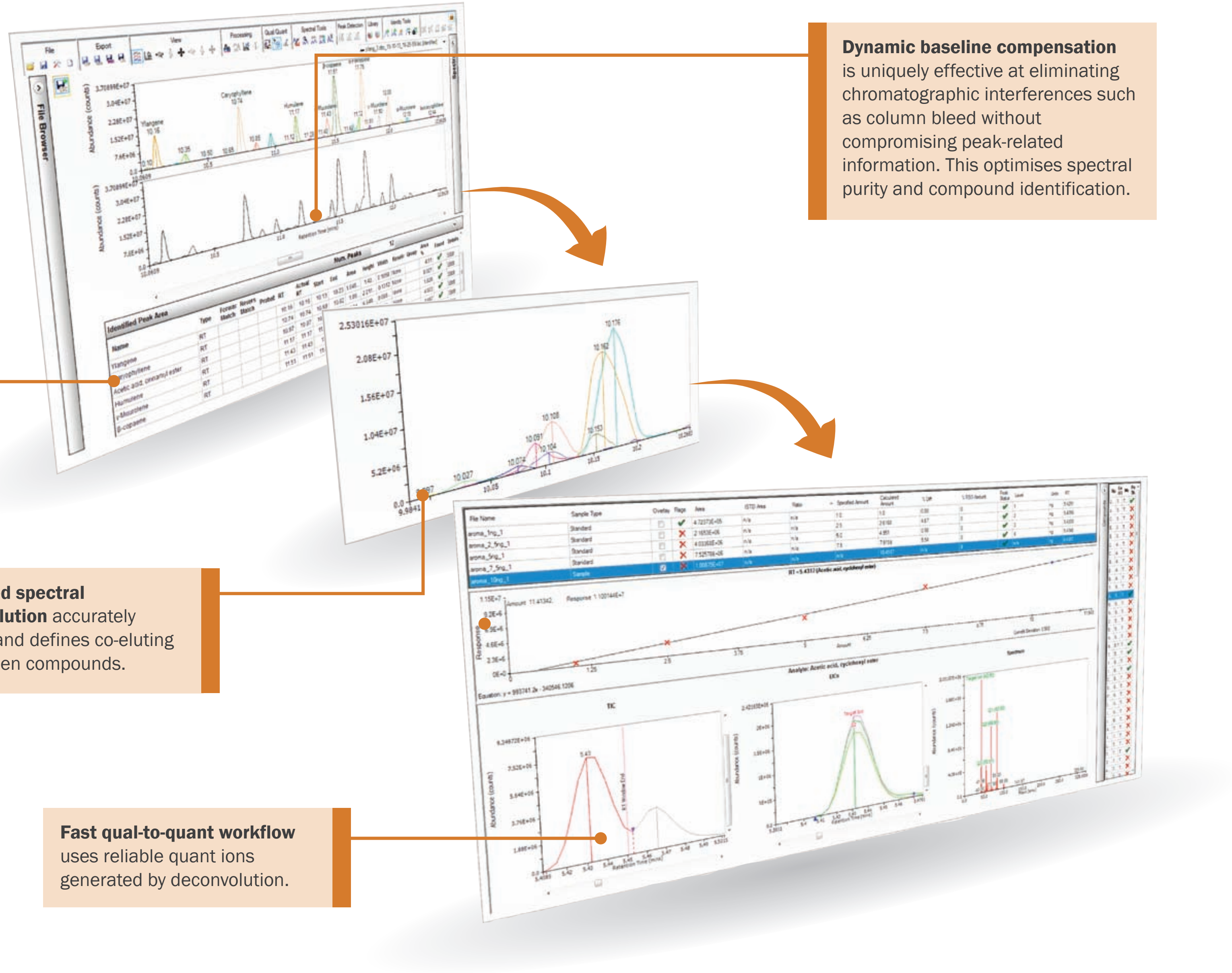
Global method development including GC, TOF and autosampler.



Easy manipulation of GC–TOF parameters.

The sophisticated data-mining capabilities of TOF-DS software perfectly complement the speed and quality of spectra generated by BenchTOF.

Programmed from the ground up for uniquely powerful processing



Dynamic baseline compensation is uniquely effective at eliminating chromatographic interferences such as column bleed without compromising peak-related information. This optimises spectral purity and compound identification.

Auto-propagating peak tables show identifications based on customisable target libraries or full commercial libraries.

Advanced spectral deconvolution accurately detects and defines co-eluting and hidden compounds.

Fast qual-to-quant workflow uses reliable quant ions generated by deconvolution.

Real-time capability

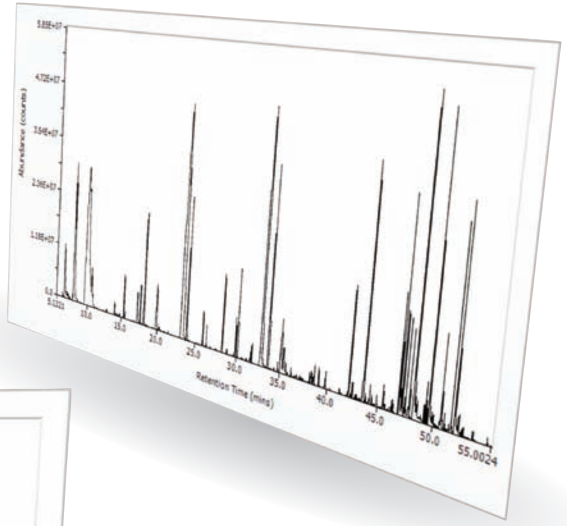
The advanced data-mining functions of TOF-DS are also available in real-time – aiding on-the-fly method development and speeding up the review of urgent samples.

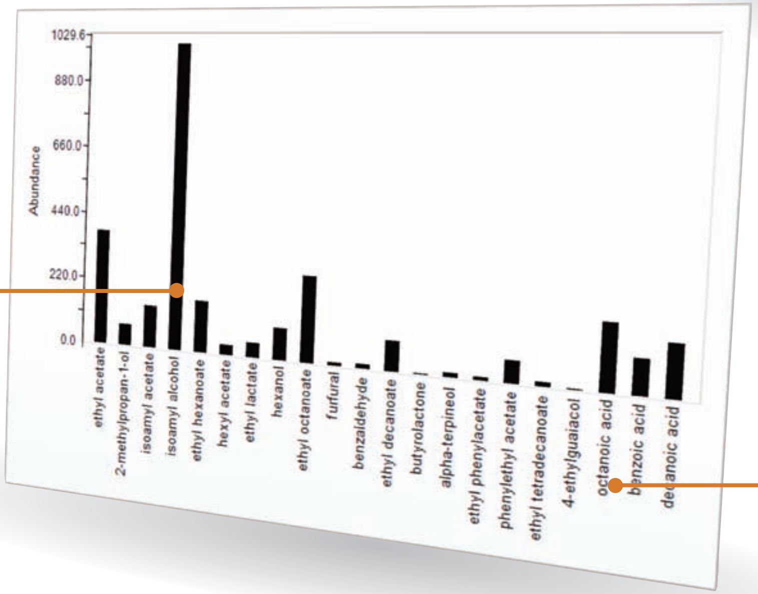
Sample screening made easy with ChromCompare®

Integral to TOF-DS is ChromCompare – an innovative module that saves time and effort when comparing chromatographic profiles.

ChromCompare distils the information-rich chromatographic data sets generated by BenchTOF into ‘H-Plots’ that are understandable at a glance. Libraries of H-Plots can then be created to characterise future unknown samples.

Rapid and reliable extraction of peak abundance data





User-selected components that appear in the H-Plot are displayed with bar heights that are proportional to the peak areas, as shown here for a sample of red wine.

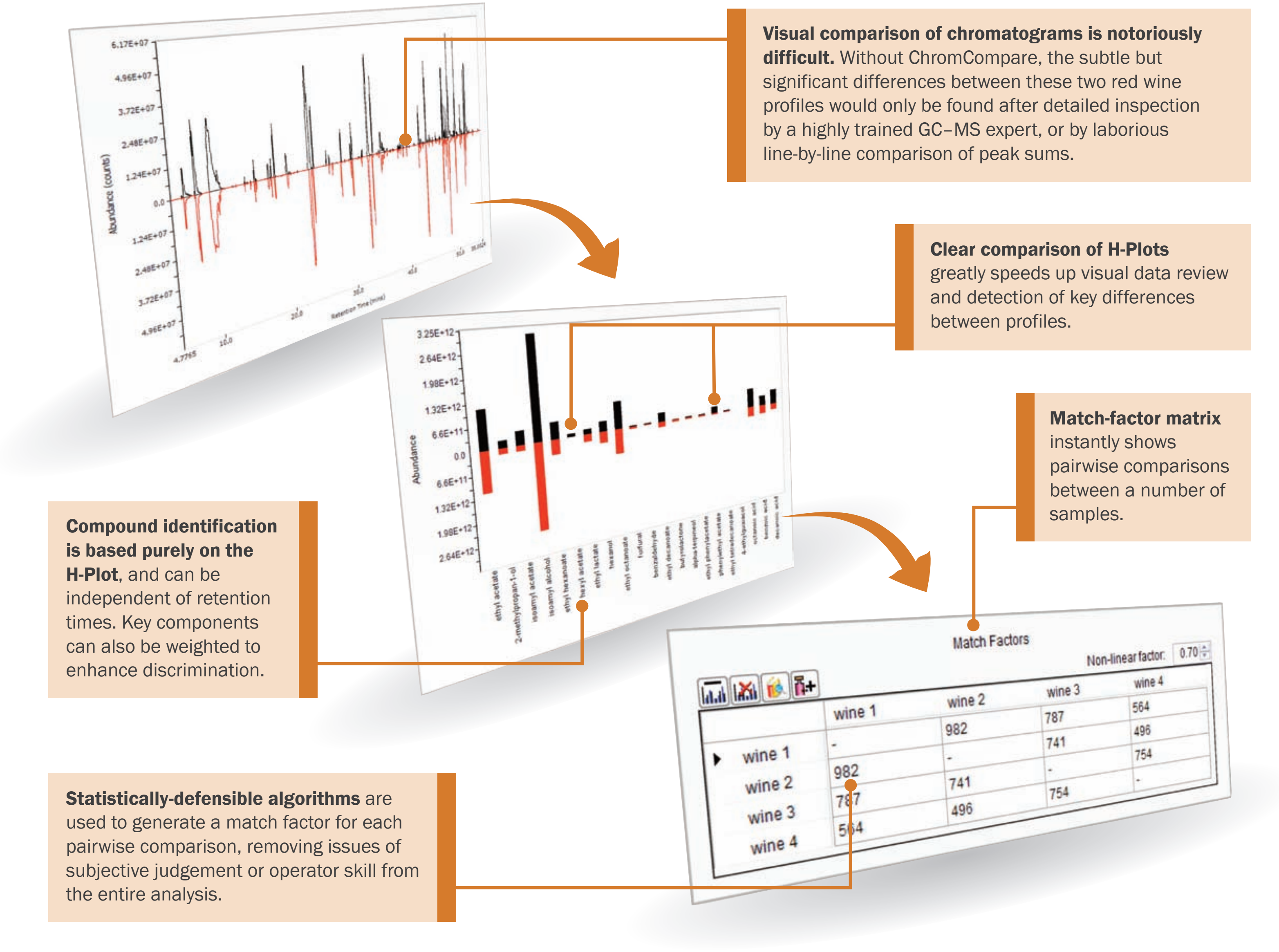
H-Plots can be ordered by compound group or by any other parameter, rather than retention time, to aid comparison with stored data generated under different conditions, for example on different systems or using alternative GC columns.

ChromCompare improves productivity and data confidence, both when comparing GC–MS profiles and when screening large numbers of chromatograms for target compounds.

Fast and accurate screening of thousands of datafiles is further helped by the ability to average and store multiple H-Plots as a single entry – for example, to account for natural variation across a large number of control samples.

In addition, the ability to apply weighting to trace-level components known to have a disproportionate impact on product quality is of particular value for aroma and fragrance profiling.

Simple and objective comparative analysis



Visual comparison of chromatograms is notoriously difficult. Without ChromCompare, the subtle but significant differences between these two red wine profiles would only be found after detailed inspection by a highly trained GC–MS expert, or by laborious line-by-line comparison of peak sums.

Clear comparison of H-Plots greatly speeds up visual data review and detection of key differences between profiles.

Match-factor matrix instantly shows pairwise comparisons between a number of samples.

Compound identification is based purely on the H-Plot, and can be independent of retention times. Key components can also be weighted to enhance discrimination.

Statistically-defensible algorithms are used to generate a match factor for each pairwise comparison, removing issues of subjective judgement or operator skill from the entire analysis.

Match Factors

Non-linear factor: 0.70

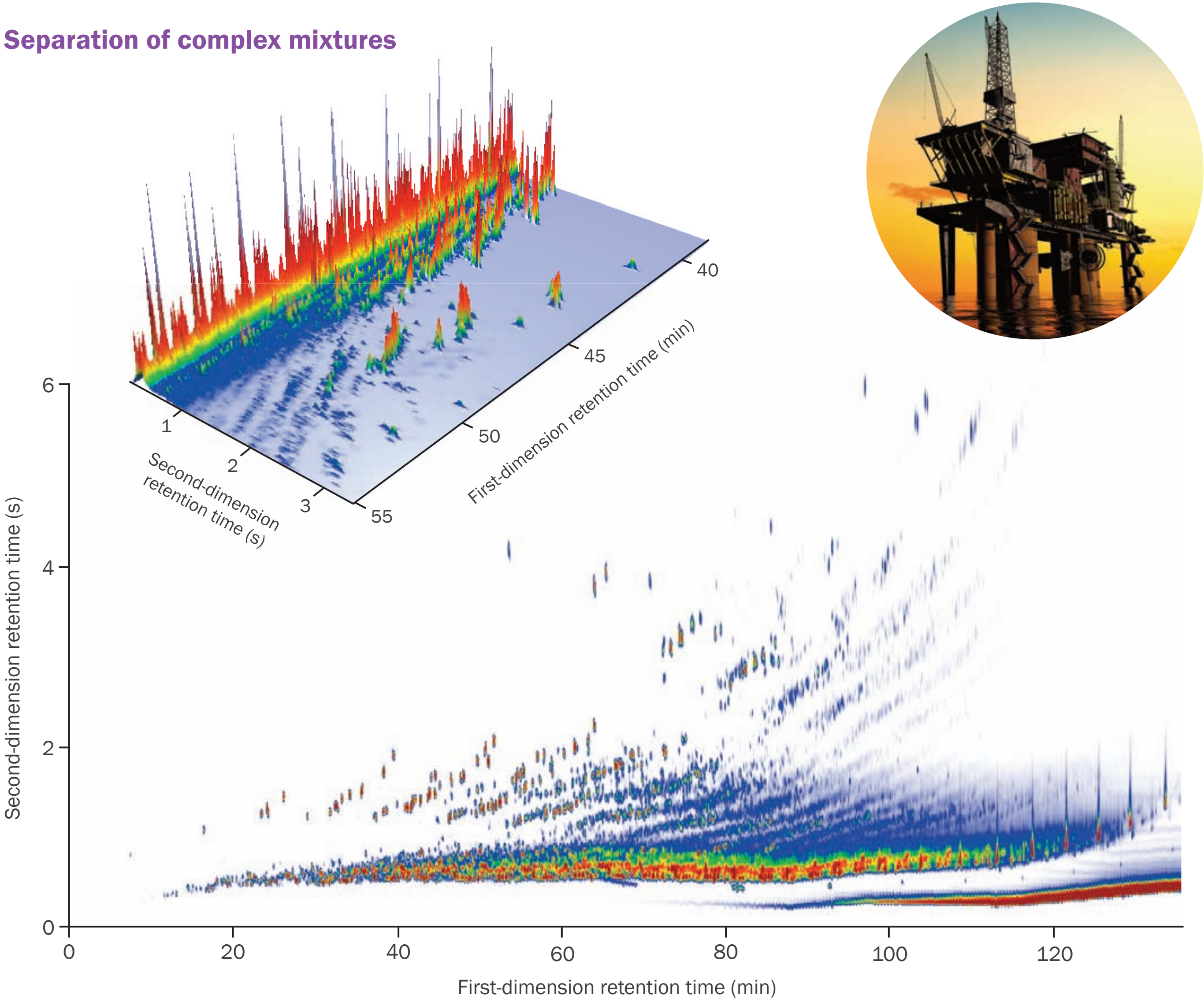
	wine 1	wine 2	wine 3	wine 4
▶ wine 1	-	982	787	564
wine 2	982	-	741	496
wine 3	787	741	-	754
wine 4	564	496	754	-

Outstanding analytical power for demanding applications

BenchTOF is fundamentally versatile, offering an unbeatable combination of innovative hardware and intelligent software design to streamline and enhance the capability and throughput of your GC–MS laboratory.

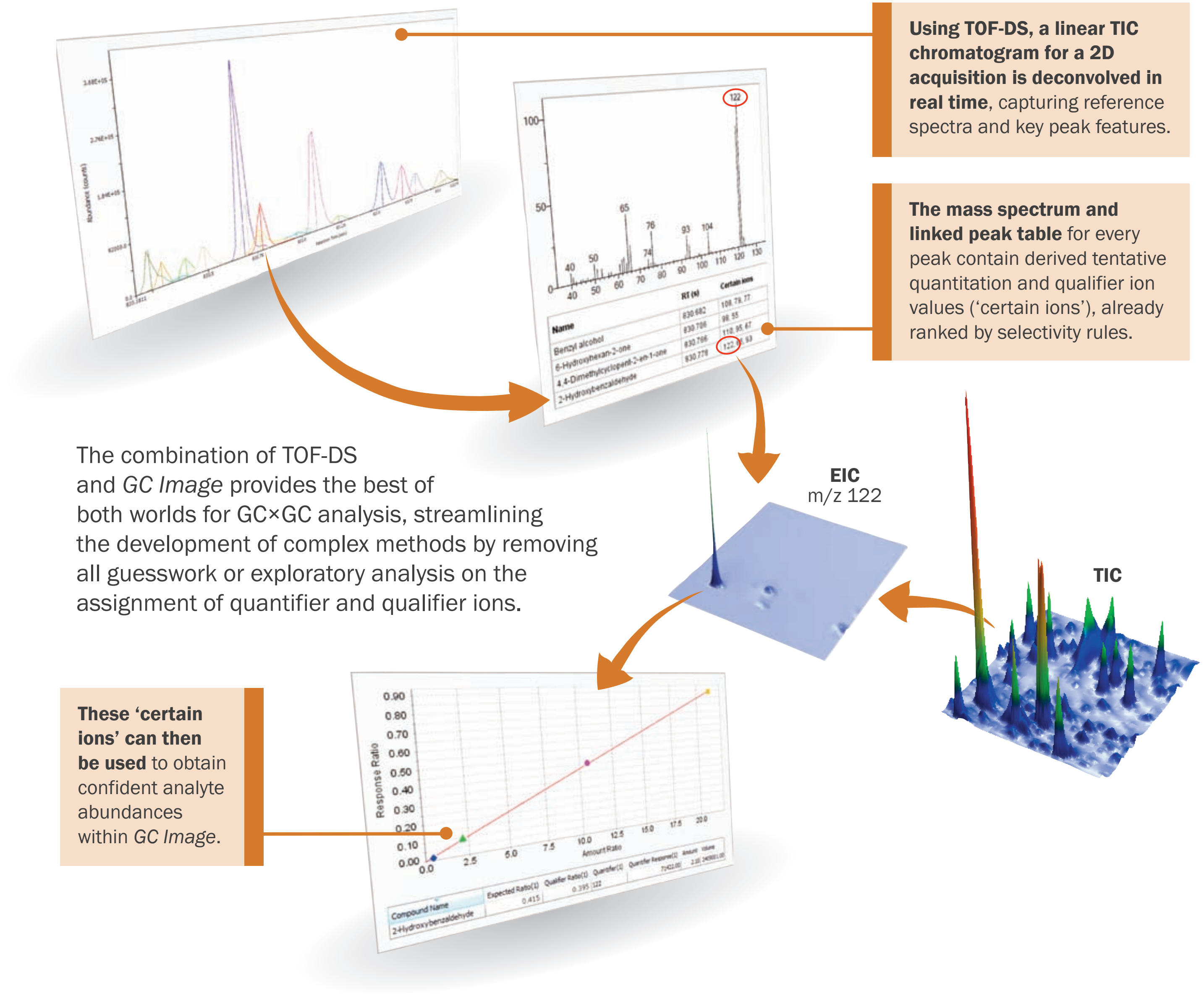
In particular, BenchTOF is compatible with the latest advances in two-dimensional chromatography, including thermally- and flow-modulated technology.

Separation of complex mixtures



The separating power of GC×GC, combined with the speed, sensitivity and spectral excellence of BenchTOF, allows the detection and identification of the most challenging compounds in the most complex matrices, as illustrated here for diesel. The structured ordering and excellent peak shape allow identification of all chemical classes in a single run.

TOF-DS: High-productivity workflow for quantitative GC×GC–TOF MS



Using TOF-DS, a linear TIC chromatogram for a 2D acquisition is deconvolved in real time, capturing reference spectra and key peak features.

The mass spectrum and linked peak table for every peak contain derived tentative quantitation and qualifier ion values ('certain ions'), already ranked by selectivity rules.

Name	RT (s)	Certain ions
Benzyl alcohol	830.682	108, 79, 77
6-Hydroxyhexan-2-one	830.706	98, 55
4,4-Dimethylcyclopent-2-en-1-one	830.766	110, 95, 67
2-Hydroxybenzaldehyde	830.778	122, [illegible], 93

The combination of TOF-DS and *GC Image* provides the best of both worlds for GC×GC analysis, streamlining the development of complex methods by removing all guesswork or exploratory analysis on the assignment of quantifier and qualifier ions.

These 'certain ions' can then be used to obtain confident analyte abundances within *GC Image*.

Compound Name	Expected Ratio(1)	Qualifier Ratio(1)	Quantifier(1)	Quantifier Response(1)	Amount	Volume
2-Hydroxybenzaldehyde	0.415	0.395	122	71422.00	2.10	[illegible]

Markes International

Leaders in instrumentation for trace organic analysis

BenchTOF-HD and BenchTOF-Select are examples of exceptional instrumentation developed by Markes International.

With centres in the UK, US and Germany, Markes manufactures a range of innovative and labour-saving instruments for extraction, pre-concentration and analysis of trace organic chemicals. These include the world's leading brand of thermal desorption systems, BenchTOF technology, and a range of complementary software platforms for optimising GC–MS data analysis.

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