



# BenchTOF-dx



**A high performance, bench-top, time-of-flight (TOF) mass spectrometer for GCMS analysis of trace organic chemicals**

# BenchTOF-dx™



***BenchTOF-dx offers a unique combination of high-performance & affordability to any GCMS user interested in trace detection***

## BenchTOF-dx Main Features

- State-of-the-art ion optics and direct-extraction technology maximise sensitivity. **Full scan data at quadrupole SIM sensitivity levels** (>800:1 s/n for 1 pg OFN while scanning over full mass range)
- Enhanced detection of trace target analytes
- **High speed spectral acquisition (10,000 Hz)** for compatibility with fast GC, GCxGC (2D GC) and complex conventional GC profiles. 100 "scansets" written to disc every second
- Mass range of **1 to 1000 amu**, with mass resolution of 1000, ensures compatibility with every GC application
- **0.01 amu spectral display** for <sup>12</sup>C/<sup>13</sup>C isotope resolution
- Long term mass & detector-response stability reduces tuning/calibration frequency and optimises system productivity
- **Uniquely powerful noise reduction software** minimises requirement for manual data manipulation
- **Integrates with existing third-party GCMS data analysis software** to minimise operator learning curve or uses own comprehensive data processing software package
- Optimum versatility: **Compatible with any make of GC** and a wide range of hyphenated techniques
- Low cost, **compact** technology that operates in standard laboratory environments ensuring fast return on investment

## BenchTOF-dx

BenchTOF-dx is a fast, high performance reflectron time of flight (TOF) mass spectrometer (MS) for analysing ultra-trace level volatile and semi-volatile organic chemicals in complex real-world samples. Novel architecture and proprietary noise reduction algorithms offer an unrivalled combination of:

- Sensitivity
- Compound resolution
- Spectral quality, and
- Robust operation

All clear advantages for trace analysis.

This affordable bench-top MS platform can be interfaced to any major brand of gas chromatograph (GC).

Moreover, integration can include transfer of BenchTOF-dx data into various GCMS data systems, enabling the performance enhancements of BenchTOF-dx to be realised within a familiar GCMS operating environment.

BenchTOF-dx offers a unique combination of high-performance and affordability to any GCMS user with an interest in trace detection. Offering compatibility with conventional and high-speed GC, key applications include chemical agent monitoring, flavour/fragrance profiling and monitoring low-level environmental pollutants.



### Flavour/fragrance profiling

Detecting trace olfactory components



### Chemical agent monitoring

Counter-terrorism & civil defence



### Environmental monitoring

Measuring trace toxic & odorous chemicals

# No other affordable bench-top MS can compete with BenchTOF-dx sensitivity in full scan mode

## High performance trace analysis

Innovative engineering allows BenchTOF-dx to go beyond the traditional TOF applications of fast GC and GCxGC. In addition to high speed scanning, BenchTOF-dx offers users full-scan capability at conventional single ion monitoring (SIM) detection limits. It, therefore, provides a robust, high-sensitivity alternative to quadrupole MS technology for the most demanding conventional GC-MS measurements, such as aroma profiling, chemical agent detection (counter-terrorism) and trace environmental analysis.

## Sensitivity

In quadrupole MS instruments only a proportion of the ions produced in the ion source actually reach the detector because the technology utilises a mass filter which only allows one mass unit through to the detector at a time. This reduces the inherent sensitivity of the quad MS technology. The impact on sensitivity is worsened with increasing scan speed and mass range. Optimum sensitivity is obtained from a quad during SIM operation, *e.g.* monitoring between one and three individual mass ions, but this means most spectral information is lost.

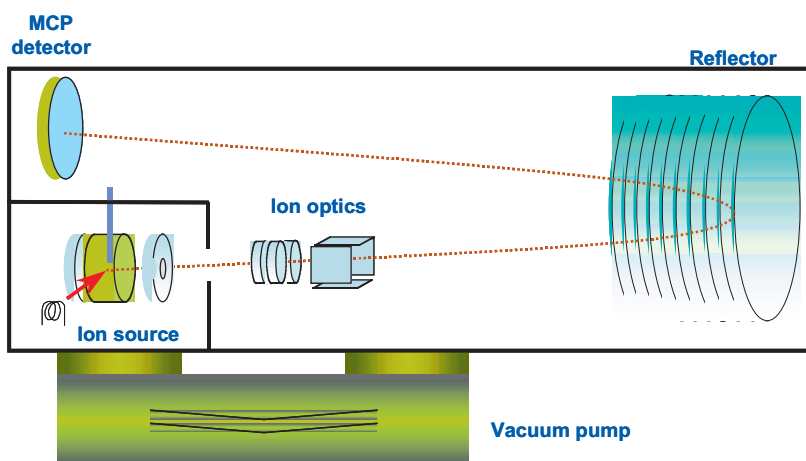
## Enhanced sensitivity with direct extraction (dx)

TOF MS operates on an entirely different principle with all the ions entering the flight tube 'flying' directly to the detector without filtering. This has the potential to allow full spectral acquisition at the same sensitivity levels as SIM mode in quads. However, this theoretical sensitivity advantage is not fully realised in traditional TOF MS designs because of the need to first transfer the ions from the source to a separate extraction area to preserve mass resolution. This 'orthogonal extraction' process results in a loss of ions and reduced sensitivity.

Using innovative ion optics, BenchTOF-dx dispenses with the orthogonal extraction of ions and adopts a cutting-edge and highly effective direct extraction (dx) approach.

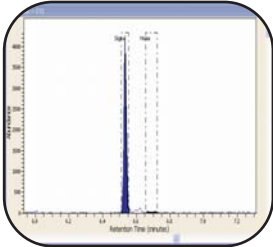
With dx technology, ions are directly extracted from the ion source and are transferred to the flight tube and detector with minimal loss of ions or mass resolution. The result is enhanced sensitivity over other TOF systems using orthogonal extraction.

**No other affordable bench top mass spectrometer can compete with BenchTOF-dx sensitivity in full scan mode.**



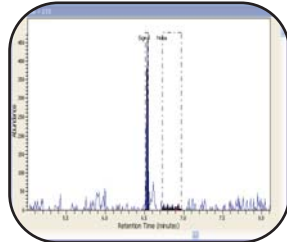
# Full scan spectral acquisition at typical SIM detection limits ...

Octafluoronaphthalene (OFN) mass ion 272 amu



1pg OFN S/N (RMS) > 800:1

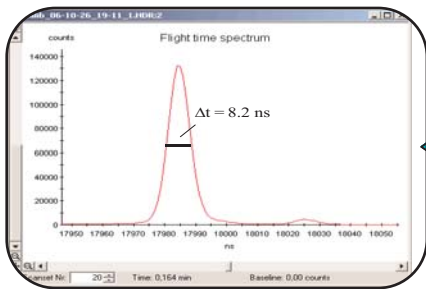
OFN <sup>13</sup>C isotope (mass 273 amu)



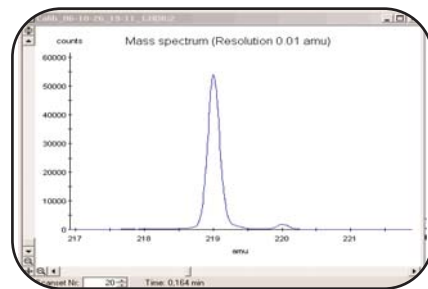
<sup>13</sup>C isotope (equivalent ~110 fg) S/N > 80:1

BenchTOF-dx provides a mass resolution of ~1000 across the full mass range without the need for orthogonal extraction. This enables high sensitivity to be combined with greater than unit mass resolution. Mass ion spectra can be displayed with 0.01 amu resolution allowing accurate assessment of <sup>12</sup>C/<sup>13</sup>C isotope separation. For example, for tuning mass ions 219/220. It also facilitates improved identification of mass ion values at peak apex.

## ... without compromising mass resolution ...



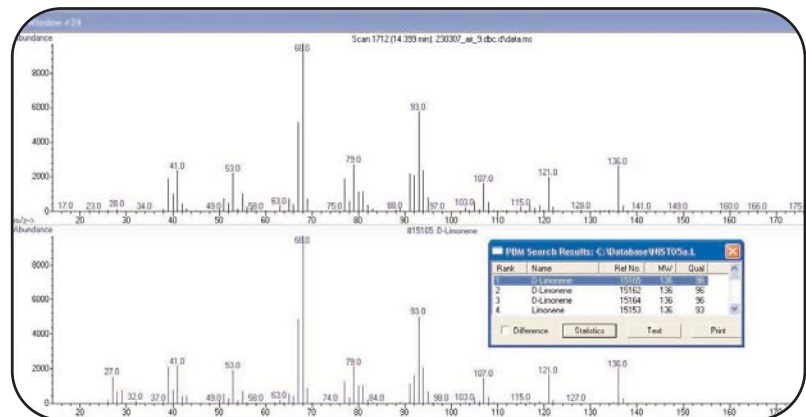
For mass 219 the mass resolution = 1096  
R = 17984 (ns)/16.4 (ns)



Mass spectrum display in 0.01 amu resolution

## ... and with excellent spectral quality

100 ppt D-limonene taken from a 1000 ml air sample, monitored using a UNITY-Air Server thermal desorption system with GC and BenchTOF-dx. This equates to 100 pg limonene with a library match quality of 98%



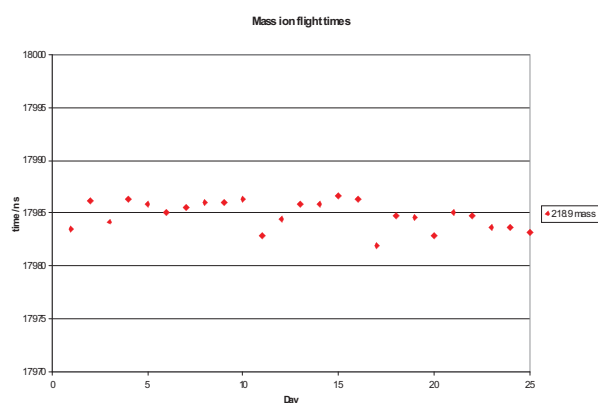
## BenchTOF-dx: Robust answer for demanding GCMS applications

BenchTOF-dx is designed for intuitive operation and optimum productivity in busy, routine GCMS laboratories. Maximum uptime and throughput is ensured by:

- Mass ion stability: Unaffected by diurnal temperature variations and other factors
- Linear for 4 orders of magnitude which reduces error and minimizes calibration frequency
- Robust mechanical design with easy component access for routine maintenance
- Comprehensive yet intuitive control software
- Automation of key system control parameters (e.g. detector optimization)

### Mass ion stability

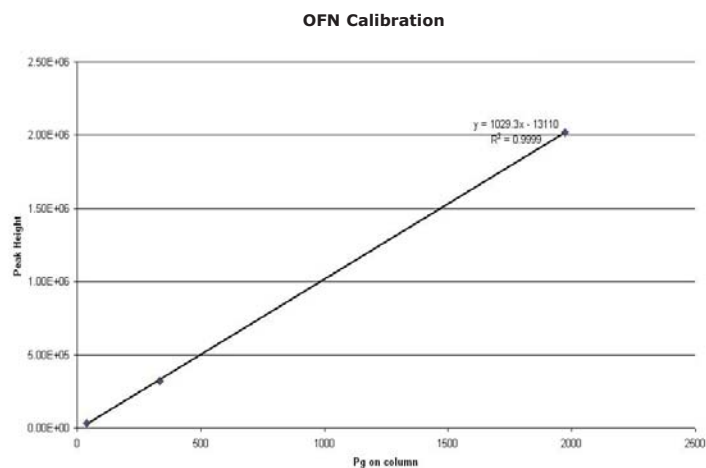
Many TOF MS systems require frequent tuning to calibrate for drift in the flight time of mass ions. Instability can be triggered by laboratory temperature variations, voltage fluctuations within the ion optics and changes in vacuum control. The innovative system architecture of BenchTOF-dx makes it far more tolerant of variations in these parameters and allows it to provide the required level of stability for routine applications.



**Variation in flight time for mass ion 219 amu of perfluorotributylamine (PFTBA) recorded over one month. Equating to a negligible 2 ns drift within the 25-day period. (0.008 % RSD)**

### Linear working range

BenchTOF-dx offers excellent linearity of four orders of magnitude. System parameters can also be optimized to ensure compatibility with the widest possible range of applications. Samples from sub-pg to high-ng quantities can be comfortably accommodated.



**OFN – Linearity (mass ion 272) from pg to ng**

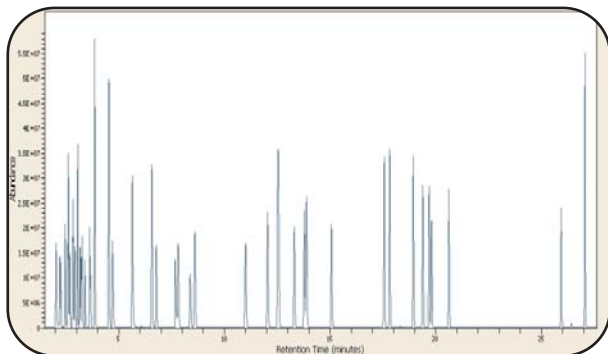
# Excellent linearity, stability & reproducibility

## Reproducibility

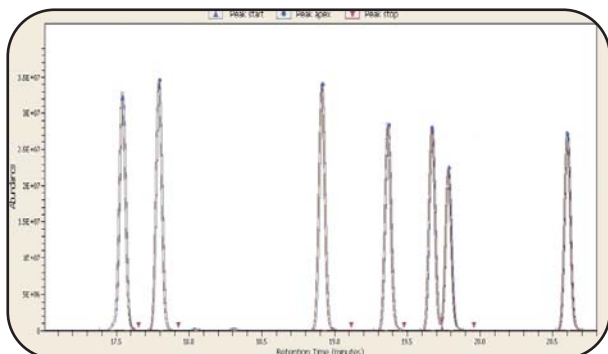
The data generated by BenchTOF-dx has excellent reproducibility, even at trace levels.

This is illustrated with the analysis of a trace level US EPA 'air toxic' standard comprising 63 components. One litre of a 1 ppb gas-phase standard was introduced to the BenchTOF-dx using a Markes series 2 UNITY-Air Server system.

A series of five repeat samples, shown overlaid and in close-up illustrate excellent reproducibility in terms of both peak height and area for this type of samples. RSDs are between 1 and 6 %.



**Total ion chromatogram (TIC) of the 1 ppb level air toxics standard run using a Markes International UNITY-Air Server with GC & BenchTOF-dx**



**Overlay in close-up of five repeat trace level air toxics standard runs showing excellent run-to-run reproducibility. Average mass per compound: 4.5 ng**

## Easy access to key hardware components

BenchTOF-dx is designed for ease of access. This enables routine maintenance procedures, such as cleaning the ion source or replacing a filament, to be simplified for system users.



**Removable self-aligning plug in ion source and detector modules designed for easy maintenance**

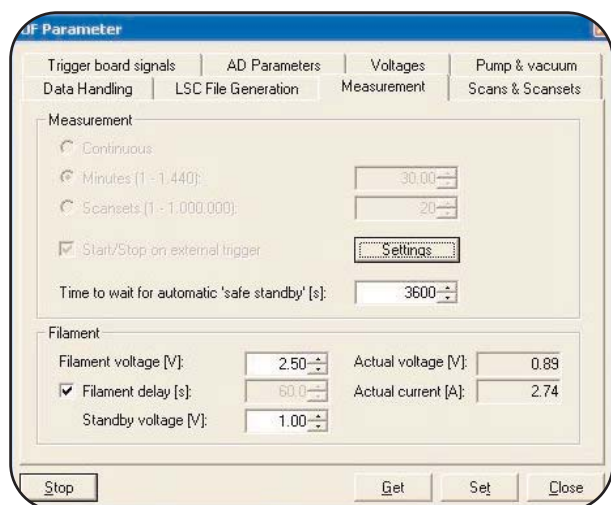
# Spectral display resolution at 0.01 amu facilitates enhanced diagnostics

## Intuitive control software

BenchTOF-dx control software is loaded onto the same PC as that controlling the rest of the analytical system and is operated *via* an intuitive user interface. The functions available in BenchTOF-dx operating software include: control of ioniser voltages, source & transfer line temperatures and turbo pump operation.

Data collection may be continuous or programmed for a fixed period of time for direct on-line measurements.

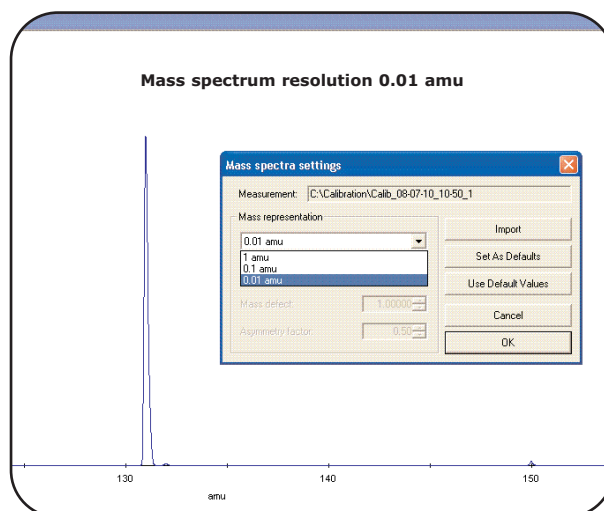
For normal chromatographic operation, data collection is synchronised to the GC run time as defined in the GC method and analytical sequence.



## Enhanced diagnostics

Whilst presenting traditional line spectra (1 amu resolution), BenchTOF-dx software also allows data to be displayed as a continuous mass spectrum at 0.1 or 0.01 amu.

A display resolution of 0.01 amu allows the  $^{12}\text{C}/^{13}\text{C}$  isotope separation to be assessed for important tuning masses, such as 502/503 amu for the calibration compound perfluorotributylamine (PFTBA). This is a useful indicator of system performance; the merging of these masses indicates that the system needs re-tuning or the ion source cleaning.



## Remote access

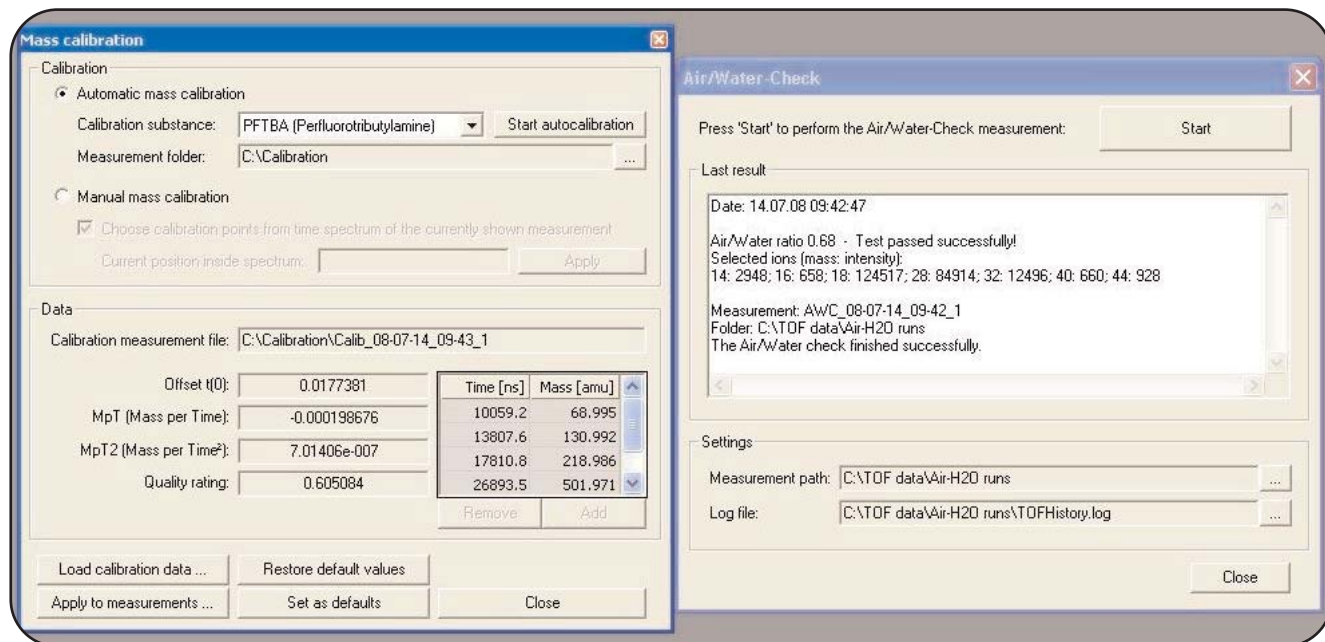
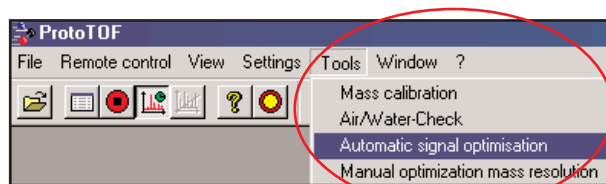
Operating parameters of the BenchTOF-dx are also accessible *via* LAN communication (TCP/IP), if and when required. This allows remote operation and facilitates off-site support. Wherever your BenchTOF-dx system is installed in the world trained service engineers can access your system remotely allowing faults to be diagnosed and rectified as quickly and efficiently as possible.



## Full automation of routine checks & signal optimisation

Key system checks and operations, *i.e.* air/water background, mass tuning/calibration and optimisation of signal intensity, are all fully automated within the BenchTOF-dx control software.

Each operation is set up *via* an intuitive on-screen dialogue helping experienced and inexperienced GCMS users alike to optimize system operation and maintain this level of performance for extended periods of time.



Mass calibration & background air water check utilities

## Automatic signal optimisation

# Compatible with fast GC, GCxGC & conventional GC

## High throughput solution for conventional & high-speed GC

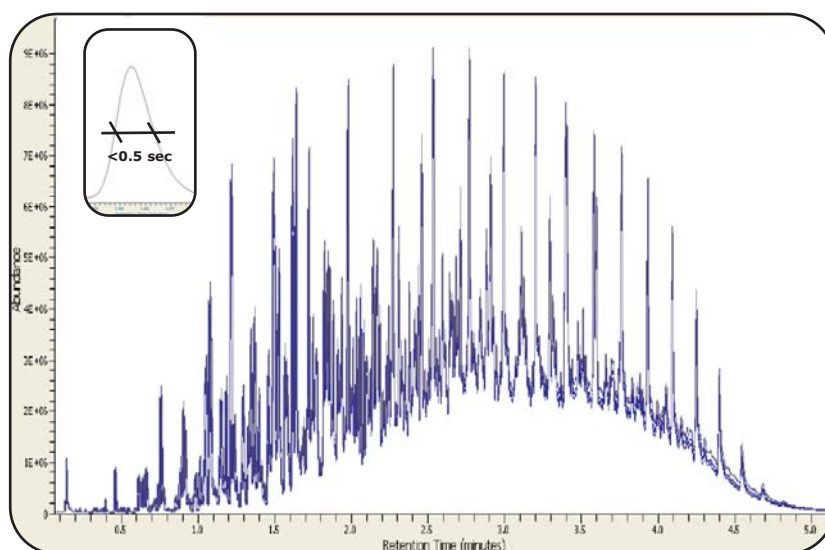
The combination of full-scan capability at traditional SIM levels with uncompromised spectral quality and robust operation makes BenchTOF-dx an ideal high performance MS workhorse for conventional capillary GC systems, irrespective of configuration or manufacturer.

Additionally, it also offers the speed required for compatibility with the latest advances in high throughput configurations such as fast GC and GCxGC (2D GC).

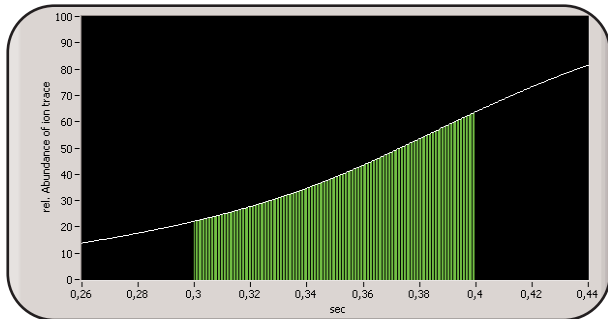
### How can one system meet the requirements of these very different applications?

- BenchTOF-dx constantly accumulates mass spectral data at an incredible speed regardless of the application. **It acquires 10,000 full mass range spectra (all 1-1000 amu) every second** which is perfect for the fastest GC separations. When compared to the performance of the fastest conventional bench-top quadrupole MS technology running at 10,000 amu/second. A single scan of typical 300 mass range (e.g. 30-330 amu) would take 30 ms. In contrast, BenchTOF-dx would have collected 300 full scans over this time and without any spectral compromise.

- The 10,000 full mass range spectra acquired every second by BenchTOF-dx are 'packaged' together into "scansets" to minimize data storage requirements and provide the familiar GCMS data points.
- Conventional chromatography produces peak widths, at base, in the region of 6 seconds. Sampling 2 - 3 data points per second is, therefore, usually sufficient to accurately quantify a peak. At this sampling rate each data point in BenchTOF-dx comprises the sum of 3000 - 5000 direct extraction spectra.
- For high speed analysis, with peak widths of the order of 0.5 seconds or less, BenchTOF-dx may be programmed to acquire 20 data points per second; more than sufficient to define these narrow peaks. Even at such fast sampling rates, each data point comprises the sum of 500 spectra, each recorded without loss due to mass filtering or orthogonal extraction; the result of the highly powerful direct extraction technology.



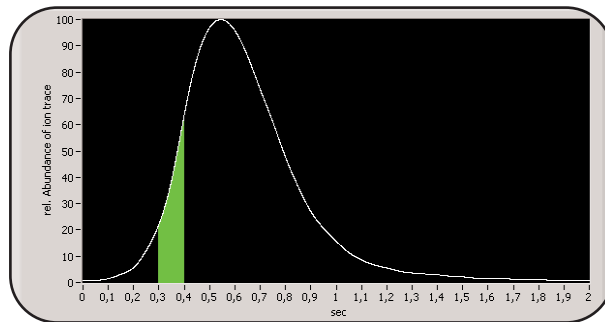
High-speed analysis of a diesel sample.  
Inset peak has a peak width at base < 0.5 seconds



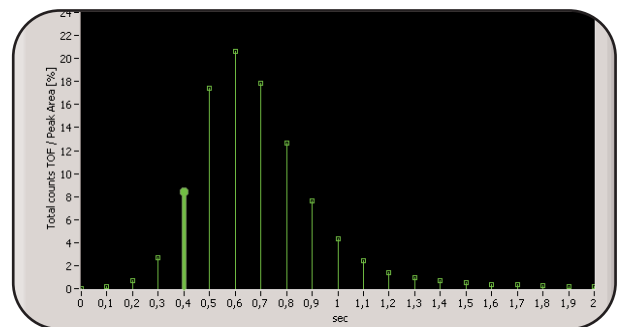
1000 scans in 0.1 sec

BenchTOF-dx acquires 10,000 scans every second. These are packaged in "scansets" for ease of data transfer and written to hard disc.

In this example, 1000 scans are added to one "scanset" every 0.1 secs and are saved to hard disc at a "scanset" rate of 10 Hz.



One "scanset" comprising 1000 scans



"Scanset" rate of 10 Hz

**Acquires 10,000 full mass range spectra every second ... ultimate sensitivity with full spectral information**

# Interfaces with any make of GC & with existing GCMS software

## Uniquely flexible data analysis

BenchTOF-dx offers the option of using its own comprehensive data analysis software (**dx-View™**) or integration with the data analysis systems of major brands of GCMS *via* **dx-Connect™**

## dx-Connect

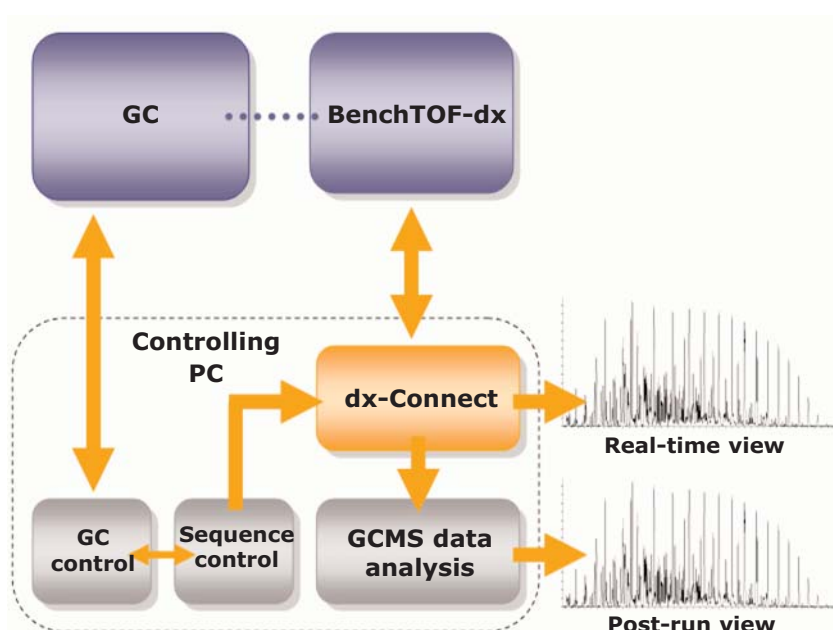
dx-Connect offers users access to the enhanced performance of BenchTOF-dx without the burden of familiarisation and validation of a new GCMS data processing package. It allows laboratories, that are already equipped with one or more major brands of GCMS, to simply install BenchTOF-dx with the GC configuration of choice and interface system control and data processing to the GCMS data analysis packages already used in the laboratory. This minimises the learning curve for laboratory staff.

Compatible third-party GCMS analysis options include: Agilent Technologies ChemStation, Thermo Fisher XCalibur® and Shimadzu GCMS Solutions.

dx-Connect allows BenchTOF-dx to interface with the GC parameter and sequence control of the existing operating system. It offers:

- Real time data view capability
- Synchronization with the GC sequence
- Flexible data format output options

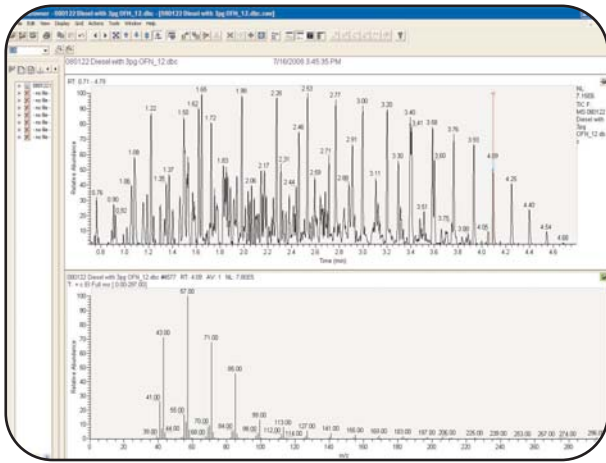
Using BenchTOF-dx and the dx-Connect facility, GC parameters and analytical sequence development are all set up and controlled using the appropriate existing software in the same way as other GCMS systems in the laboratory.



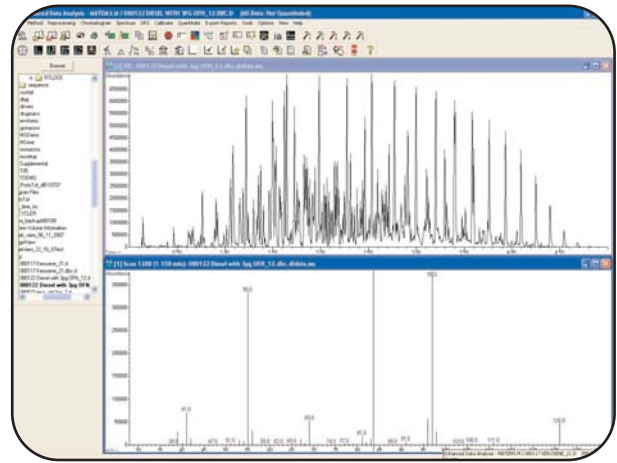
## Data processing with existing software

For data processing, dx-Connect allows BenchTOF-dx data (whole runs or 'snapshots') to be stored in a variety of file formats for analysis within a third-party GCMS data processing environment. For example, Agilent Technologies ChemStation format (\*.d), Thermo Fisher XCalibur® format (\*.raw) and the universal AIA (\*.cdf) format utilised by manufacturers such as Shimadzu and Varian.

File header information and key operating parameters from BenchTOD-dx are stored along with the converted (\*.d, \*.raw, \*.cdf) data file. This maintains the association with the original stored raw BenchTOF-dx data. Any subsequent data manipulation (e.g. library searching, integration and quantification) can then be carried in the familiar operating environment of the preferred GCMS data processing package.



Thermo Xcalibur® - Fast GC data



# DBC: Uniquely powerful background elimination - operates automatically & in real-time

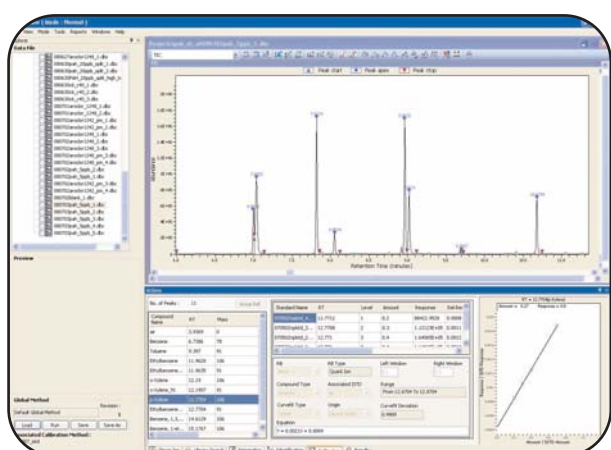
## dx-View

dx-View is the proprietary data-processing software package for BenchTOF-dx. It can be used as an alternative to third-party GCMS data processing packages accessed *via* dx-Connect (see above).

dx-View incorporates database technology enabling large quantities of complex data to be stored, accessed and rapidly processed. On completion of an analysis, or creation of a real-time snapshot, data from dx-Connect is imported into dx-View for processing.

Imported (\*.lsc) data files may be categorised by project and assigned as 'Calibration' or 'Sample' for ease of identification. Preview TIC data is shown for rapid selection of stored data files. The layout in dx-View is intuitive with independent access to tabs for: Chromatographic display > Library Search > Integration > Identification > Calibration > Results.

## Versatile display functions



The chromatographic display window shows TIC data, extracted ion chromatograms and mass fragmentation patterns. Data files may be overlaid (normal or inverted) for comparison in TIC or EIC formats.

EIC plots can include single ion response, multiple (user-) selected ions or ion ranges. Specific mass ions can also be excluded from the TIC/multi-ion EIC profiles. TIC data can be library searched using a variety of libraries either singularly or in multiples.

## Data-processing and calibration

Peak area values are calculated using defined integration parameters and compounds are assigned a name based on library search results or manual input. Data is saved within the method file.

Response factors may be applied to each compound based on single quantitative ions, multiple ions, ranges of ions or the complete spectrum. The implementation of dynamic background compensation (see below), to minimise chromatographic background interference, often allows more ions to be selected for quantification thereby increasing signal/sensitivity.

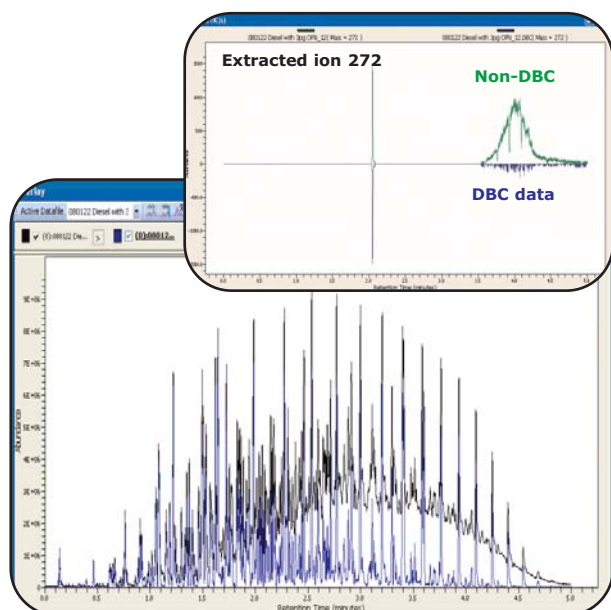
Ultimately, a global data-processing method is created and saved containing all relevant parameters. This can then be used to process subsequent data files.

## Enhanced data quality: Dynamic Background Compensation

Dynamic Background Compensation (DBC) is an innovative real-time data processing algorithm implemented as standard on BenchTOF-dx. Those using BenchTOF-dx with dx-Connect and their preferred third-party data processing package will see two converted (\*.d, \*.raw, \*.cdf, etc) data files for each run; one with and one without dynamic background compensation. Those using the proprietary dx-View data processing package will see two \*.lsc data files for each run; again one with and one without DBC.

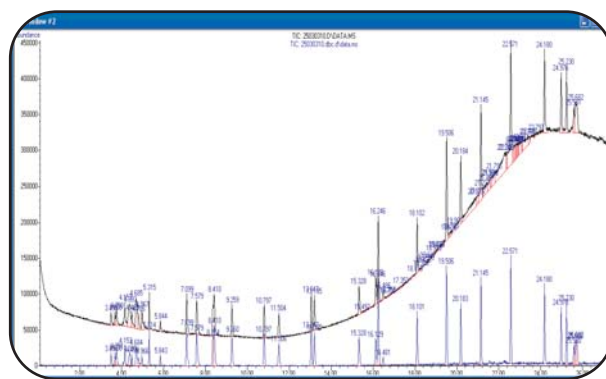
DBC uses an innovative mathematical approach to distinguish and eliminate background interference from real chromatographic peaks, even at the lowest levels. It accommodates conventional and high-speed chromatography and is a dynamic process, compensating for the chromatographic background as it changes throughout a run, but without compromising any peak-related information.

For example, extracted ion (mass 272) data for a sample of 3 pg octafluoronaphthalene (OFN) in diesel was analysed using fast GC with BenchTOF-dx. The compensated and uncompensated data files show identical results (area counts) for the OFN peak, but efficient removal of the mass 272 contribution to the GC background later in the run.

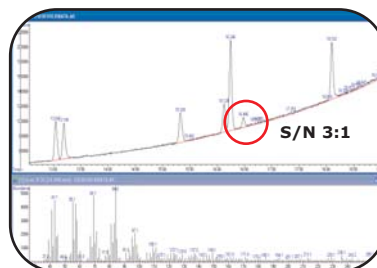


## Improving spectral purity and signal-to-noise ratios

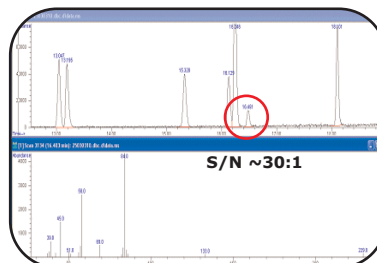
DBC offers GC-BenchTOF-dx users significantly **enhanced spectral purity and analytical sensitivity without compromising quantitative data**. It allows accurate and automatic peak identification (without manual background subtraction) and improves signal to noise ratios by as much as a factor of 10.



High bleed total ion chromatogram (black trace) and DBC acquired data file (blue trace)



Thiophene peak (S/N 3:1) cannot be identified in the original data without manual background subtraction



With DBC the S/N ratio of thiophene improves to 30:1 and the component is confidently identified by automatic library search

TIC of fast GC analysis of diesel containing 3 pg of OFN. With DBC (blue) & without DBC (black)

# Improved spectral purity simplifying automatic identification of trace compounds

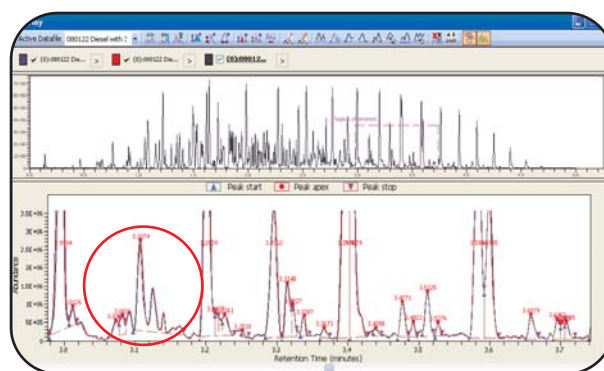
## Quantitation

By selectively eliminating interfering background ions DBC also simplifies integration, improving both quantitative accuracy and run-to-run reproducibility.

The improved run-to-run reproducibility of the DBC processed data even allows sophisticated, time-dependent integration events to be implemented within a GCMS data analysis method and applied to all the runs in a data set. The area reproducibility, as shown, is 4%; remarkable for summed peaks and manual integration.

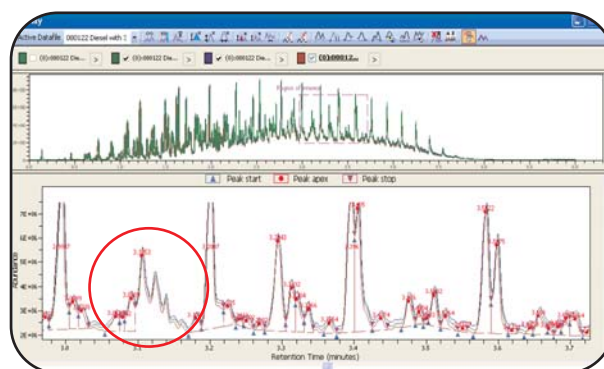
Note that the effect of DBC on the diesel analysis is to eliminate the background ion contributions comprising an unresolved 'hump' of material from the sample itself. In such cases, the advantage of having both files (compensated and uncompensated) becomes apparent. The uncompensated data can be used, for example, for simulated distillation determinations or for calculating total-VOC levels in material emissions data, while the compensated data is much better for detailed speciated analysis.

With DBC



Three overlaid DBC (ClearView) high speed GC-BenchTOF-dx analyses of OFN-spiked diesel TICs with a single manually drawn baseline (highlighted by circle). Excellent y-axis reproducibility (4%).

Without DBC



No DBC (ClearView) produces large y-axis variation and prevents use of certain manual integration events for baseline construction

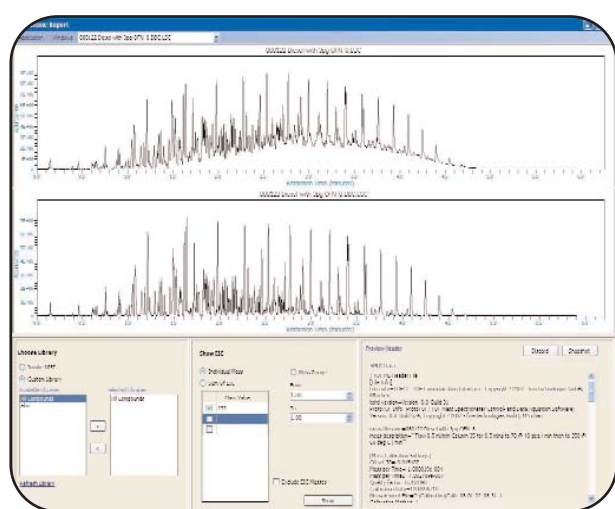


## Flexible real-time data manipulation options

The dx-Connect facility allows real-time viewing of analyses that are underway. Users integrating BenchTOF-dx with their preferred third-party data processing software will see a highly desirable difference between results from BenchTOF-dx and those from other GCMS systems in the laboratory: Every analysis carried out using BenchTOF-dx generates two files, one DBC (compensated) and one non-DBC (uncompensated) in real time.

Both DBC and non-DBC compensated real-time data files can utilise a sophisticated range of functions, which are generally only available post-run (*i.e.* on stored GCMS data). Functions available, in real-time using BenchTOF-dx, include: zooming, viewing the mass ion fragmentation pattern (spectrum) at any point on either DBC or non-DBC data files, library searching spectra to identify peaks as they elute and viewing extracted ion profiles.

Should quantitative data be required during a run for any peaks in the partial DBC or non-DBC chromatograms, dx-Connect creates "snapshot" files for integration with dx-View or with any of the dx-Connect supported data analysis systems.



Original TIC data *without* DBC compensation

Original TIC data *with* on-line DBC compensation

Data handling options: Library search, extracted ion chromatograms (EIC), etc.

## ClearView™

ClearView is the generic, stand-alone version of BenchTOF-dx's DBC facility that lets you apply the advantages of DBC to other standard GCMS systems in the laboratory network.

Using ClearView, conventional stored **GCMS data files can be reprocessed**, singly or in batches, to remove chromatographic background interference thus improving spectral purity and system sensitivity for trace compounds.

Reprocessed data is stored in a separate file and can be validated against original results at any stage.

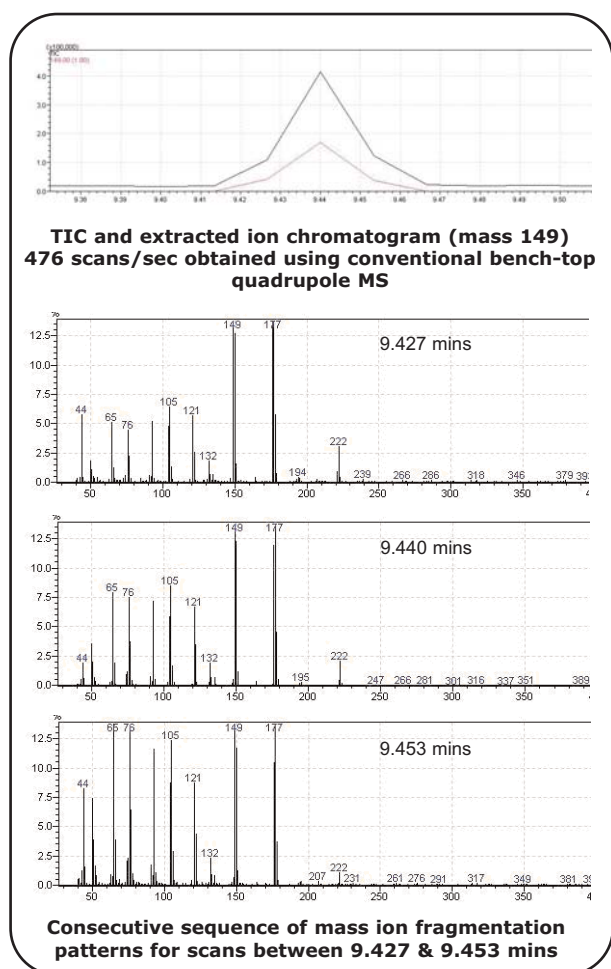
The ability to apply the advantages of dynamic baseline compensation to both BenchTOF-dx and conventional GCMS systems in a network enables DBC/ClearView to be incorporated into standard laboratory operating procedures when appropriate.

# Elimination of spectral skew aids library identification

## Improving resolution & identification of trace target compounds

The speed of BenchTOF-dx spectral acquisition (10,000 full scans every second) makes it the ideal MS platform for resolving individual components in complex total ion chromatographic (TIC) profiles.

This is partly because the scan speed of BenchTOF-dx **totally eliminates spectral skew** within and across a peak.



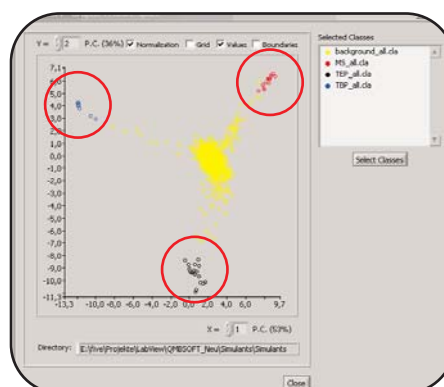
Typical spectral skew observed using quadrupole MS technology is shown here for diethyl phthalate

Skew occurs in slower scanning systems such as quadrupole MS instruments because the ratio of ions eluting from the column changes during the finite time that it takes to scan across the mass range. Spectral skew can be reduced using quadrupole MS instruments at higher scan speeds, but as higher scan rates reduce the dwell time on each mass ion, this compromises sensitivity for trace components.

BenchTOF-dx eliminates spectral skew without compromising instrument sensitivity. This improves the match quality of library search data from scans at the start or end of peaks, thereby aiding the identification of analytes of interest.

In practice, the effect of spectral skew is rarely significant in conventional capillary GCMS, but it can adversely impact the quality of quadrupole MS data for fast GC *i.e.* for peaks less than 1 second wide. Moreover, eliminating spectral skew is of universal benefit when applying mathematical processes such as spectral deconvolution and chemometric techniques to enhance detection/identification of trace components.

Chemometric (pattern recognition) techniques such as Principle Component Analysis (PCA) for example, perform best on peaks with a uniform mass ion fragmentation pattern (spectrum) from start to end. Such mathematical approaches play an increasingly important role in de-skilling rapid characterization of complex data and are likely to become more widely used in the future.



PCA analysis of mass spectral data from BenchTOF-dx for 3 components (methyl salicylate, tri-ethyl phosphate and tri-butyl phosphate) across a wide concentration range - 5 ng (at peak apex) to 2pg (at peak tail.) Data shows tight clustering indicating excellent spectral uniformity across the peak

## **BenchTOF-dx: Summary**

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Whatever the field of application, BenchTOF-dx provides a state-of-the-art and highly reliable system which will extend the capabilities of any GCMS laboratory ...

- **Ultimate sensitivity with full spectral information**
- **Uncompromised spectral quality and optimum resolution for multi-component mixtures**
- **Compatibility with high-speed, GC, GCxGC and conventional capillary GC**
- **Excellent linearity, stability, repeatability**

... and with the robustness and eas of maintenance required by routine, high throughput laboratory environments.

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