micrOTOF II

The Powerful, Flexible Analysis Solution
Accurate, with “sub-ppm” Confidence

Being fully furnished with convincing mass accuracy, a high dynamic range and speed of analysis, micrOTOF II is the first choice for:

- Molecular Formula Verification
- De novo Formula Generation
- Multi-Target Screening
- Biomarker Discovery
- Intact Protein Analysis

Highest flexibility

The micrOTOF II is the first high resolution TOF-MS which can be used in combination with GC and LC, providing unequalled flexibility with remarkable mass accuracy.

Certainty in formula generation

The identification and subsequent quantitation of unknown substances requires exact mass determination with highest reliability and great confidence in your analytical system.

Integrity in multiple target ID

micrOTOF II electrospray ionization time-of-flight (ESI-TOF) system gives the right answers. It generates results with high specificity from high mass accuracy and mass resolution for multiple targets simultaneously: Multi-targeting with hrEICs (high resolution Extracted Ion Chromatograms).

Significance in biomarker profiling

Metabolic profiling is a key technology in the study of drug efficacy, toxicology or clinical biomarkers. Capabilities to comprehensively analyse ingredients enhances plant and nutrition sciences to new levels.

Speed in protein projects

micrOTOF II gives easy access to fast LC-MS and CE-MS applications for refined elucidation of intact proteins.
**Molecular formula generation**

Mass accuracy, chemical knowledge and SmartFormula™ clearly limit the number of possible formulae in molecular formula generation for confident determination of the elemental composition of a given peak.

This invaluable sub-ppm confidence is available for formula determination in pharmaceutical impurity analysis, metabolite identification as well as in pesticide screening, toxicology & doping analysis.

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**De novo sum formula generation**

Replacing the established approach of just using the measured mass for formula determination, the micrOTOF II adds a second dimension into the routine: Analysis of the isotope profile provides a “True Isotopic Pattern” (TIP) which is automatically matched against the measured spectrum – leading to real chemical information on a confidence level below 1 ppm: SmartFormula.

*De novo* sum formula generation achieves sub-ppm confidence through SmartFormula enhancement of stable mass accuracy across an LC-peak. Almost without restrictions on time or concentration, < 1-2 ppm mass accuracy is rendered to a < 1 ppm confidence by the application of chemical knowledge and Bruker Daltonics’ unique SmartFormula.

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**Detection of C_{21}H_{24}ClFNO_{2} Haloperidol with SmartFormula:** The correct formula has the best Sigma-ranking (isotope pattern matching factor). Top spectrum: Measured, lower spectrum: Calculated theoretical isotopic distribution.
A Dynamic Range that is Impressive

More than five orders of magnitude dynamic range

The micrOTOF II knows how to impress with excellent stability of mass measurement over a wide dynamic range without tedious recalibration routines – key for screening applications.

Confidence by 3D mass accuracy

The micrOTOF II defines stability in all 3 relevant dimensions of dynamic range: With one single calibration, the instrument provides mass accuracy for long time periods, for large concentration changes over up to 5 orders of magnitude and over a wide mass range essential for development of LC-MS applications. All these features are available simultaneously, without the need for recalibration.

Intra-spectra dynamic range

High Intra-spectra dynamic range of mass accuracy allows for correct simultaneous detection of high and low abundant components.

Quantitative and qualitative analysis for forensics, doping control, and residue analysis

Screen hundreds of compounds

The solution is able to screen hundreds of compounds from a single sample LC/ESI-TOF run and enables screening for large compound libraries with a confidence level and reproducibility unsurpassed by any other system. This workflow saves significant time when running multi-target applications such as drugs/metabolites in urine, food safety analysis, forensic toxicology or environmental testing.

ID of unknowns

Retrospective in silico screening for new or unexpected compounds is possible because, unlike in triple-quad based MRM methods, the full scan information content in addition to the target library specific information is retained. Read more: Application Note ET-12.
hrEIC Enables Multi-Target Screening

Results with high specificity

Mass accuracy over a long period, high mass resolution and a wide dynamic range are prerequisites for high resolution Extracted Ion Chromatograms with 2mDa mass window.

hrEIC Enables Multi-Target Screening

Mass traces (hrEIC) of a complex pesticide mixture detected with a mass window of 2 mDa (left) with one single run. Resulting search in TargetAnalysis database (top, detail shown) based on accurate mass, isotope pattern and retention time identified more than 250 compounds in a mass range from m/z 100 to m/z 1000.
Mass traces (hrEIC) of a pesticide mixture in CH$_2$Cl$_2$, detected with a mass window of 2 mDa. 28 pesticides were identified at a concentration of 100 μg/l.

Identification of a volatile reaction intermediate by SmartFormula and the GC-micrOTOF II from a GC peak (Base Peak Chromatogram is shown).

**Coupling with LC or GC for widest range of analytes**

The micrOTOF II is the only TOF mass spectrometer that can be coupled either to LC or to GC using the same, uniquely designed APCI interface. Gone is the need for an expensive dedicated GC-TOF/MS.

This option makes the micrOTOF II the ideal tool for labs which occasionally need a GC/TOF-MS for the identification of unknown peaks in a GC chromatogram or for resolving complex mixtures.

The APCI source has been designed to optionally add an excimer laser for applications such as PAH analysis or polymer research where laser ionisation (APLI) is required.

**GC-TOF/MS-Coupling**

The system can be up-and-running within minutes, giving unrestricted access to the full range of micrOTOF II features such as accurate mass, high resolution extracted ion chromatogram (hrEIC) and SmartFormula™.
Capillary electrophoresis and micrOTOF II

Complementing LC methods and as an additional separation technique, Capillary Zone Electrophoresis (CZE) is being increasingly utilized due to its high separation efficiency and speed. Bruker offers sophisticated coupling techniques to gain full advantage from CZE, delivering a uniquely powerful combination of separation efficiency and accurate mass determination (see Application Note ET-05: Capillary Electrophoresis-ESI-TOF MS: Combining separation efficiency with the mass accuracy of the micrOTOF™).

Interface to all popular LC systems

The sophisticated Hystar LC integration software enables micrOTOF II to seamlessly interface with all leading Liquid Chromatography systems including Agilent 1200, Waters Alliance and CapLC, VWR LaChrom and Dionex Ultimate 3000.

The high acquisition speed of micrOTOF II also makes ultra-high performance systems such as UPLC ideal partners and this is fully supported by our integration software.

For proteomics applications the Bruker easy nLC nano HPLC system is recommended and fully supported to offer seamless integration.

Bruker EASY-nLC is the ideal HPLC system for Proteomics applications.

Setup of CE with micrOTOF II

Simple, sensitive and robust coupling of the micrOTOF II with capillary electrophoresis.
**Technical Specifications**

**Sophisticated micrOTOF focus technology**
- Worldleading combination of mass accuracy, resolution, and sensitivity
- SmartFormula is the unique combination of accurate mass with True Isotopic Pattern (TIP)
- Automated determination of elemental composition, the “formula finder”
- Footprint 640 x 640 mm, height 1220 mm, weight 130 kg

**TOF analyzer**
- Mass range 50 – 20,000 m/z
- Mass resolution 16,500 FWHM with micrOTOF focus
- Mass accuracy of < 1-2 ppm (RMS) error with internal calibration
- Mass Stability & Dynamic Range proven by better than 2mDa hrEICs (high resolution Extracted Ion Chromatograms)
- Sub-ppm confidence by application of SmartFormula algorithm
- Acquisition rate of 40 Hz (100-3,000 m/z profile mass spectra to disk)
- Polarity switching for both, positive and negative ions

**Source options**
- ESI orthogonal electrospray source
- APCI orthogonal atmospheric pressure chemical ionization source
- Multimode source (ESI/APCI)
- APPI Atmospheric pressure photo ionization source
- Online NanoElectrospray source for nano LC applications, flow down to 50 nL/min
- Offline NanoElectrospray source, typical flow rates of 25 nL/min
- CE-MS coupling with grounded ESI needle
- GC/APCI/APLI source for coupling with LC and GC

**Software**
Compass software environment for integrated LC/MS control and data processing including:
- Generate molecular formula module
- ChargeState and optional MaxEntropy Deconvolution
- Optional application software and solutions:
  - TargetAnalysis
  - Compass Security Pack allows for support of ER/ES (Electronic records & signatures)
  - Compass OpenAccess
  - Compass OA/QC
  - MetaboliteTools
  - ProfileAnalysis

**Support of:**
- Bruker EASY-nLC nano HPLC
- HPLC systems from the following vendors:
  - Agilent, Waters (incl. UPLC), Dionex, VWR/Hitachi
- Autosamplers from CTC
- LC-NMR/micrOTOF coupling

For research use only. Not for use in diagnostic procedures.

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www.bdal.com  Bruker Daltonik GmbH  Bruker Daltonics Inc.
Bremen · Germany  Billerica, MA · USA
Phone +49 (421) 2205-0  Phone +1 (978) 663-3660
Fax +49 (421) 2205-104  Fax +1 (978) 667-5993
sales@bdal.de  ms-sales@bdal.com