BRUKER

Bruker Daltonics

micrOTOF-Q

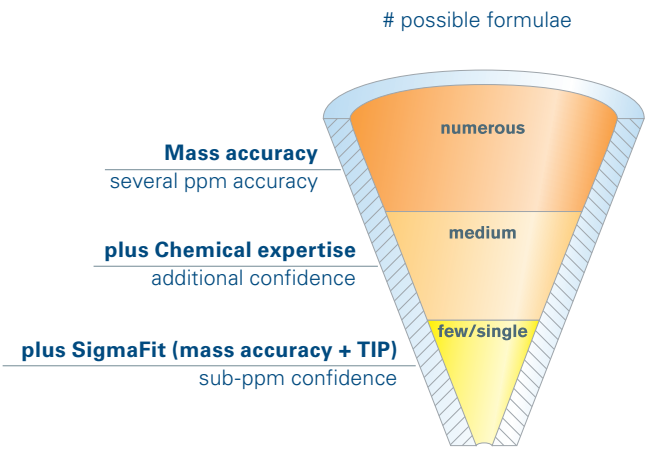
- Cutting Edge Performance with Sub-ppm Confidence

think forward

ESI-Qq TOF

The advantage of ultimate confidence

Do you need maximum confidence in your analytical system?
Bruker Daltonics' new micrOTOF-Q™ ESI-Qq-TOF mass spectrometer features the very lastest technology developments to provide maximum certainty in your research in Small Molecule Identification, Metabolomics or Proteomics.



Simultaneously three dimensions of information promote your analytical tasks to unrivaled heights of confidence:

- Measure with unequalled accurate mass.
- Validate with True Isotopic Pattern (TIP) analysis.
- Benefit from accurate mass and TIP also in fragments analysis in MS/MS mode.

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

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

Unique Power³ – simultaneously without compromise

It has never been this easy to use: Cutting-edge performance is now available in a comprehensive bench top package.

sensitivity

Experience market leading sensitivity with the next-generation Apollo II™ ion funnel ESI source, dramatically improving ion transmission.

mass accuracy

Be impressed by a mass accuracy of better than 3 ppm over an exceptionally wide dynamic range.

resolution

Be amazed from superb focus resolving power exceeding a resolution of 15,000 FWHM.

fragment analysis

Featuring a superb quadrupole mass filter and a quadrupole collision cell for accumulation of parent and fragment ions prior to mass analysis, the micrOTOF-Q expands the renowned micrOTOF's advanced performance on the analysis of molecule fragments, adding a third level of confidence to the two dimensions of accurate mass and True Isotopic Pattern analysis with SigmaFit™.

A convenient, highly stable, external one-step calibration for automated data output with a mass accuracy of 3 ppm makes this instrument your easy-to-use companion with superior performance to all other (ESI)-TOF instruments.

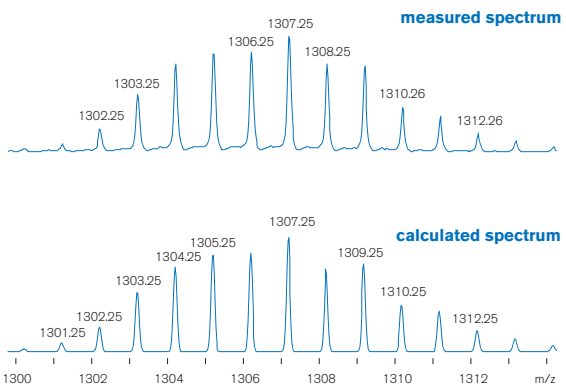
Achieve simultaneously reliable MS and MS/MS accuracy, independent of whether calibration was performed in MS or MS/MS mode.

Thus, for chemical formula determination, a detailed formula suggestion is only three clicks away.

Raise your research to higher power with all these skills available concurrently!

Unprecedented Certainty

Isotopic Pattern Analysis



MS analysis of Pd-Complex ($C_{61}H_{65}N_4O_{15}$) in synthetic chemistry. Isotopic Pattern of measured spectrum and calculated spectrum (SigmaFit) show outstanding homogeneity, providing a superior sigma value for enhanced confidence in structural analysis.

Precision in Organic Chemistry

Accurate mass and Bruker Daltonics' proprietary SigmaFit™ True Isotopic Pattern analysis algorithm provide unrivalled certainty for the identification of unknowns.

Due to an extraordinarily wide dynamic range, the entire mass range is covered with a high mass accuracy – resulting in unambiguous molecular formula generation.

Mass accuracy is not enough: Using isotopic patterns for enhanced identification

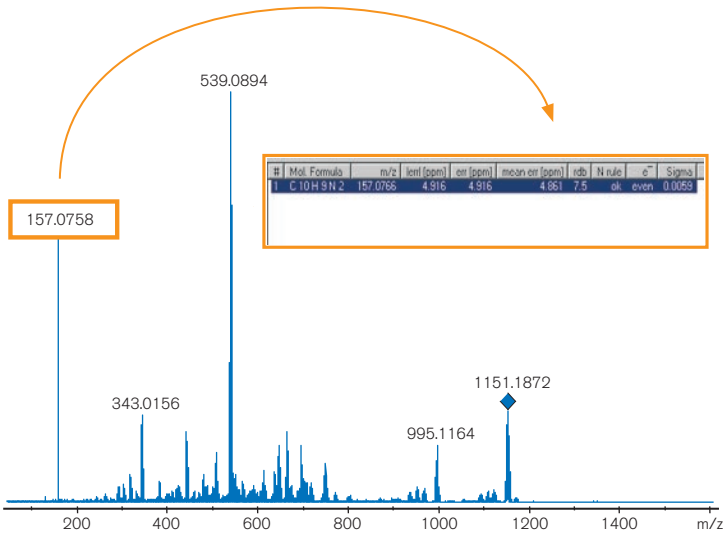
After generation of a list of possible formulae within 5 ppm mass accuracy, the measured isotopic pattern is compared with the theoretical isotopic pattern – resulting in a stastistical match factor, SigmaFit.

micrOTOF-Q's capability to deliver correct isotopic patterns discriminates over 200 possible formulae from 5 ppm mass accuracy alone to one single formula with a SigmaFit < 0.01.

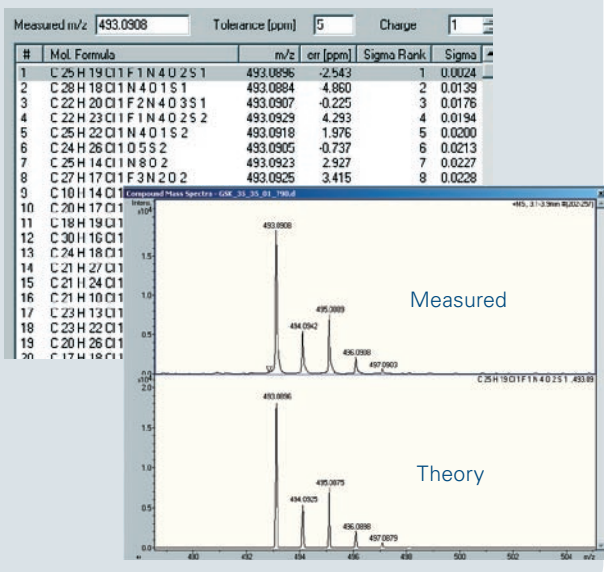
ISCID-MS/MS analysis of Pd-Complex in synthetic chemistry. A fragment m/z 157.0758 reveals a mass error of < 5 ppm for reading out a formula with a sigma value of < 0.006. Parent ion was m/z 1307, see above.
The micrOTOF-Q covers the whole mass range with high mass accuracy.

SigmaFit: Combining accurate mass with True Isotopic Pattern (TIP) capabilites of the micrOTOF-Q. Only one in over 200 possible formulae has a fit better than 0.01

Formula Generation from MS/MS Fragment



SigmaFit Delivers the Correct Formula



Accurate mass, SigmaFit and MS/MS

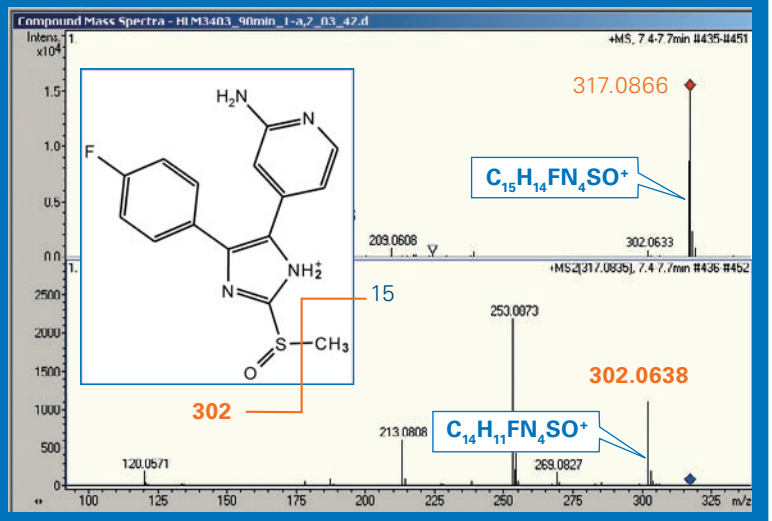
Advancing Metabolomics Research

Metabolic profiling promotes biomarker discovery to the metabolome level to address profiles that are powerful sensors reflecting situations at physiological endpoints.

Identify small molecule biomarkers with the power of accurate mass, TIP and fragments analysis for evaluation of disease state, following drug treatment or to monitor toxic response.

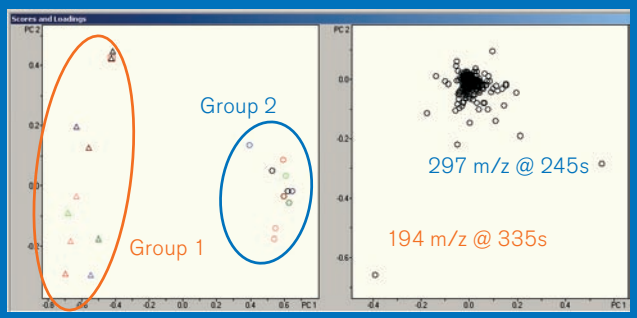
Tailored tools for pattern recognition, metabolite MS and MS/MS identification complete the solution package for metabolome research.

Metabolic Fragment ID and Statistical Analysis



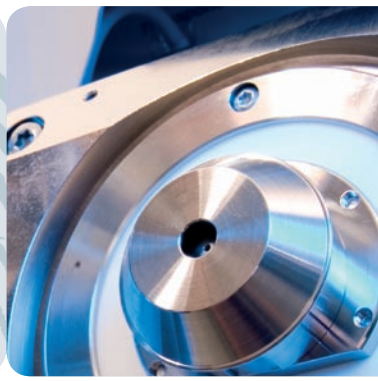
Auto MS^2 of a Metabolite m/z 317 and the fragmentation of a methylgroup from the molecule increase confidence of identification by fragments analysis and allows to study the fragmentation pathway, e.g. amine- or methylgroup.

A clear separation of groups in the PCA analysis: Scores and Loadings Plot of rat urine samples From groups receiving different levels of food. (with friendly permission from Organon).



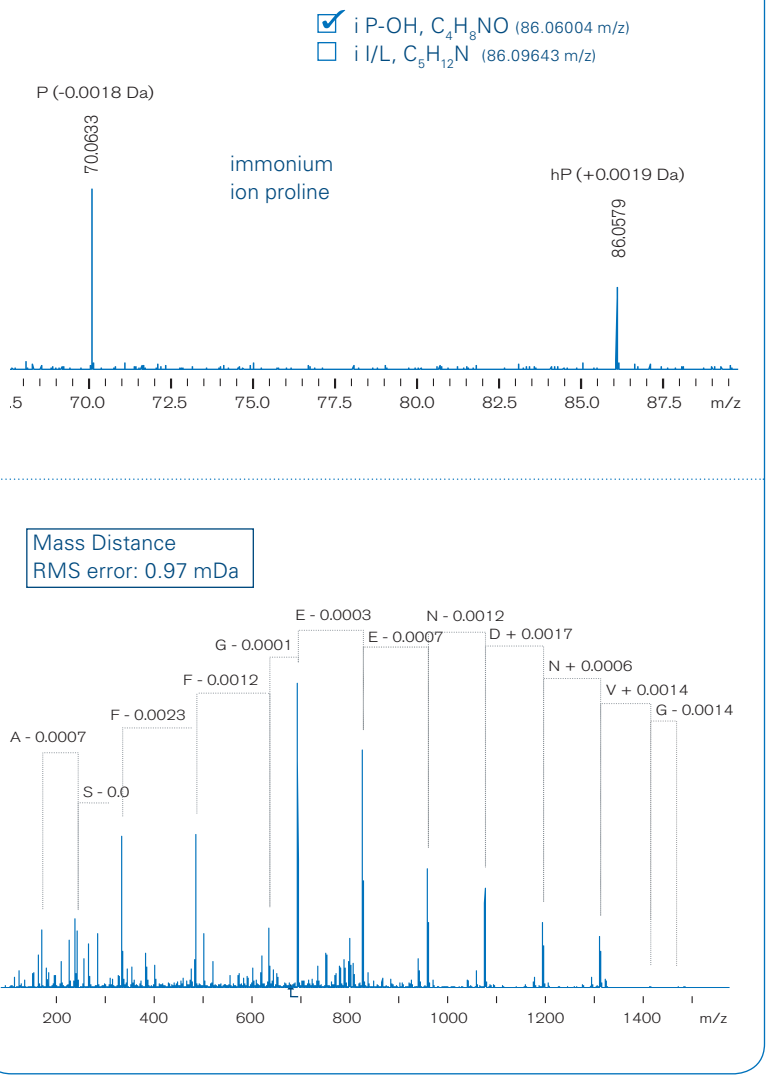
Super-sensitive ion funnel source

The new state of the art Apollo II™ ion funnel ESI electrospray source provides 10x more ions – significantly improving sensitivity by an order of magnitude. This leads to substantial progress for applications such as detailed structural studies of low-abundance protein modifications, PTMs or natural products! All ions are collected by a radial RF field and smoothly directed towards the funnel exit. In the second funnel, CID energy can be freely selected for optimal performance of the experiment.



Information-Rich In Depth Analysis

De novo Sequencing Down to Low Masses



The *de novo* Sequencing Machine

The micrOTOF-Q is the ideal instrument to achieve outstanding mass accuracy including low masses, a prerequisite for successful de novo sequencing.

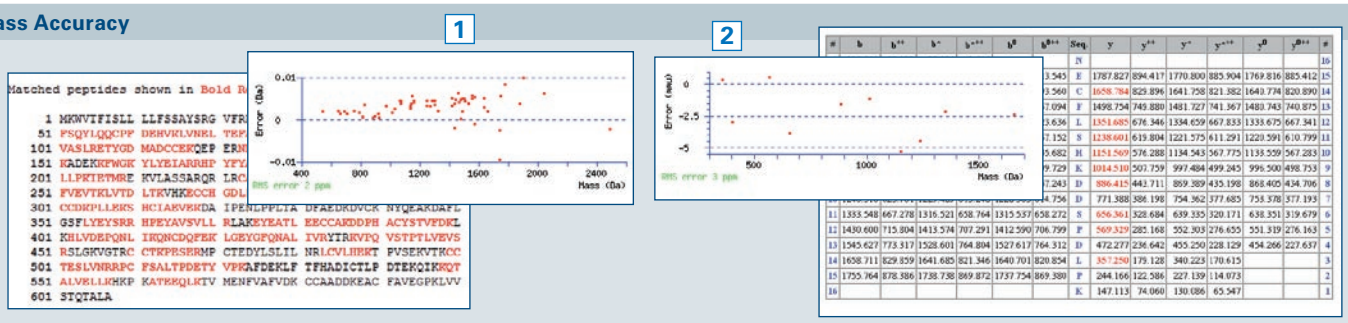
Immonium Ions of proline ($C_5H_9NO_2$) in a MS/MS measurement of m/z 626.2862+: *De novo* sequencing down to low masses – only the unique micrOTOF-Q can provide information on immonium ions in one spectrum.

MS/MS spectrum of GluFib m/z = 785.8. Exceptional mass accuracy leads to outstanding *de novo* sequencing results.

Powerful Identifications over a wide Dynamic Range

High mass accuracy is available on both the peptides and fragments levels. Impressive mass accuracy on all peptides [1] meets unrivalled mass accuracy on fragments [2] a feature delivering the highest reliability for proteomics research.

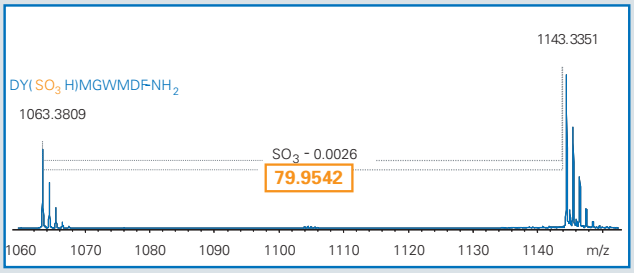
Mass Accuracy

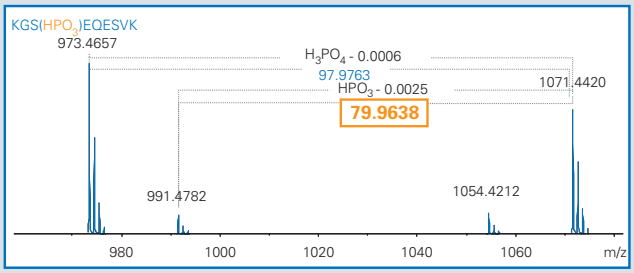


Reproducible mass accuracy: 50 fmol BSA on a Waters UPLC™ column are measured with an RMS error of only 2ppm (1). Even fragments are reliably analyzed (2) with only 3 ppm RMS error (20 fmol BSA) from a single external calibration.

Proteomics Applications without Compromise

Accurate Mass Measurements of PTMs





Distinction of sulfation and phosphorylation with micrOTOF-Q's accurate mass measurement capabilities.

Sulfation? Phosphorylation? Explore the Difference!

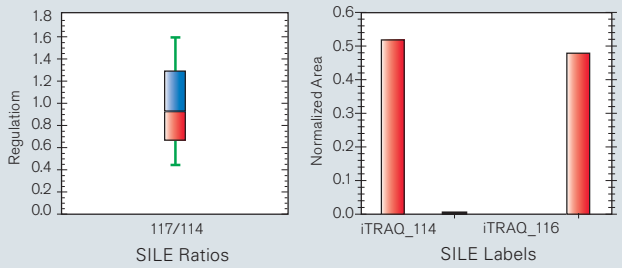
Understanding proteomes requires knowledge about posttranslational modifications. Detailed insights into the molecule's structure is achieved with the excellent mass accuracy of the micrOTOF-Q – even with minor mass differences.

Count on the Ability to Quantitate

Stable isotopic labeling using iTRAQ™ or the newly invented technology ICPL™ allow fast and convenient, yet easy-to-use, quantitative proteomics research. Due to the ion funnel ESI source design, excellent sensitivity is achieved, coupled with highest confidence by true isotopic pattern (TIP™) analysis.

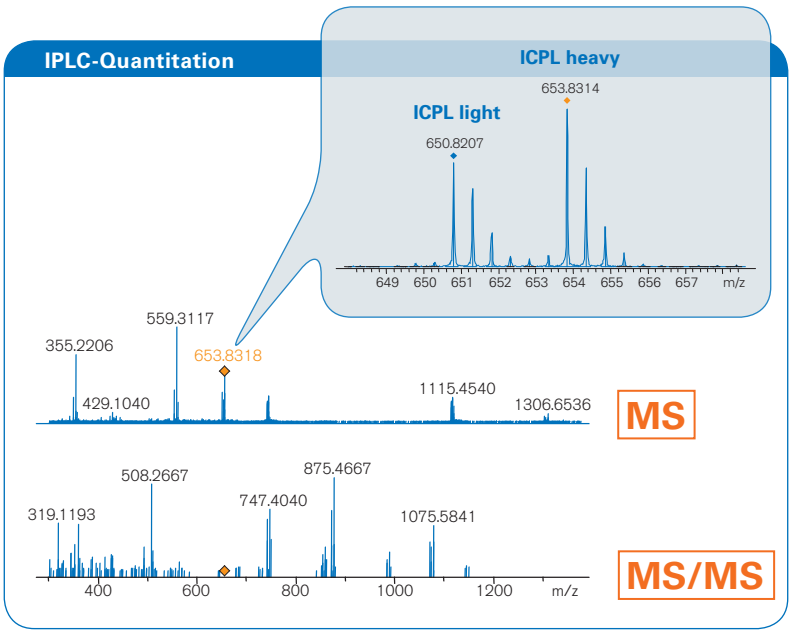
High sensitivity, high mass accuracy and high resolution over the whole mass range is the instrument's contribution to an integrated solution for Quantitation from Bruker Daltonics: WARP-LC, a system providing automatic workflows from chromatography to quantitation.

Quantitation with WARP-LC



WARP-LC quantitation analysis: Box-and-whisker plot of an iTRAQ labeled protein. For validation, the statistical distribution is shown.

IPLC-Quantitation



ICPL quantitation on the micrOTOF-Q in MS and MS/MS mode.

Resolution and Sensitivity

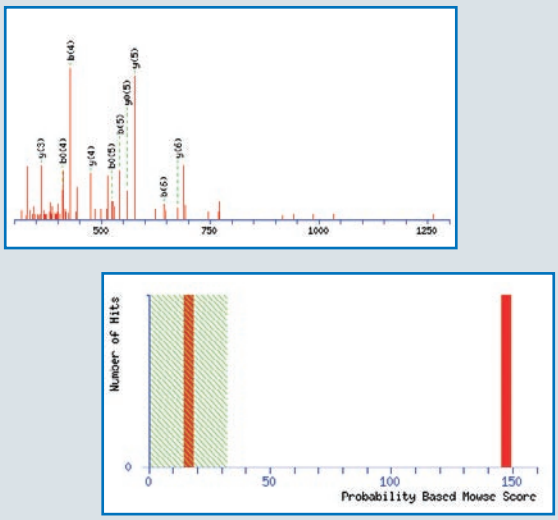
Sensitivity

Ultimate sensitivity is demonstrated with a 500 amole digested BSA sample. Even for this low sample amount, solid peptide identifications are possible.

Mass resolution

Both small molecules and intact proteins are analyzed with excellent mass resolution. Isotopic resolution is achieved even for deconvoluted spectra. The simulated pattern fits perfectly to the measured mass spectrum.

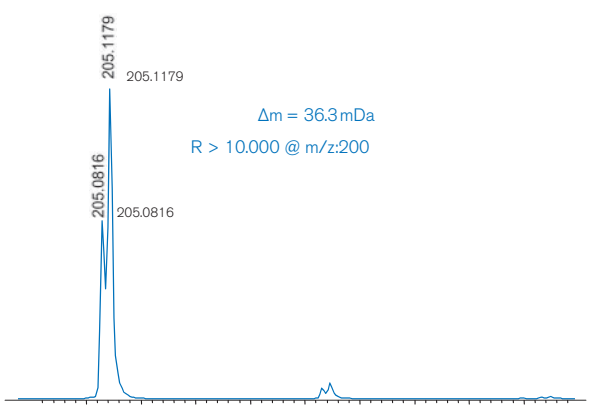
MS/MS ID from 500 amol BSA



Analysis of 500 amol BSA digest on column. MS/MS of peptide 788.46 (1+), ion score 29 and the corresponding Mascot™ search result.

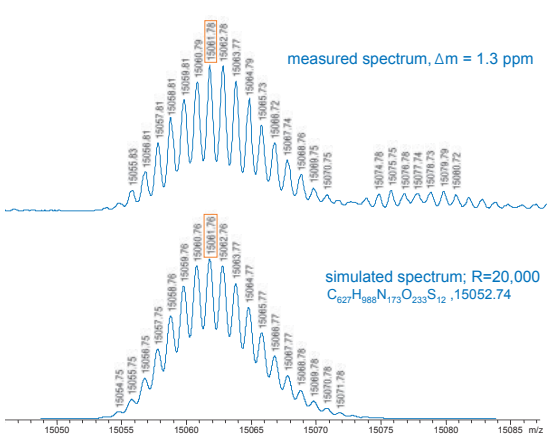
Differentiation of isobaric dipeptides.
$C_7H_{13}N_2O_5$ (AD) MW physical = 205.0819
$C_8H_{17}N_2O_4$ (SV) MW physical = 205.1183
delta MW = 0.0364 Da.
For separation of the dipeptides at m/z 200, a resolution > 10,000 is achieved.

Resolution of Isobaric Peptides



Ribonuclease B. A spectrum of the intact protein acquired with the micrOTOF-Q. The mass difference to the calculated mass is only 1.3 ppm. A resolution of 20,000 FWHM is achieved.

Intact Protein Mass Resolution

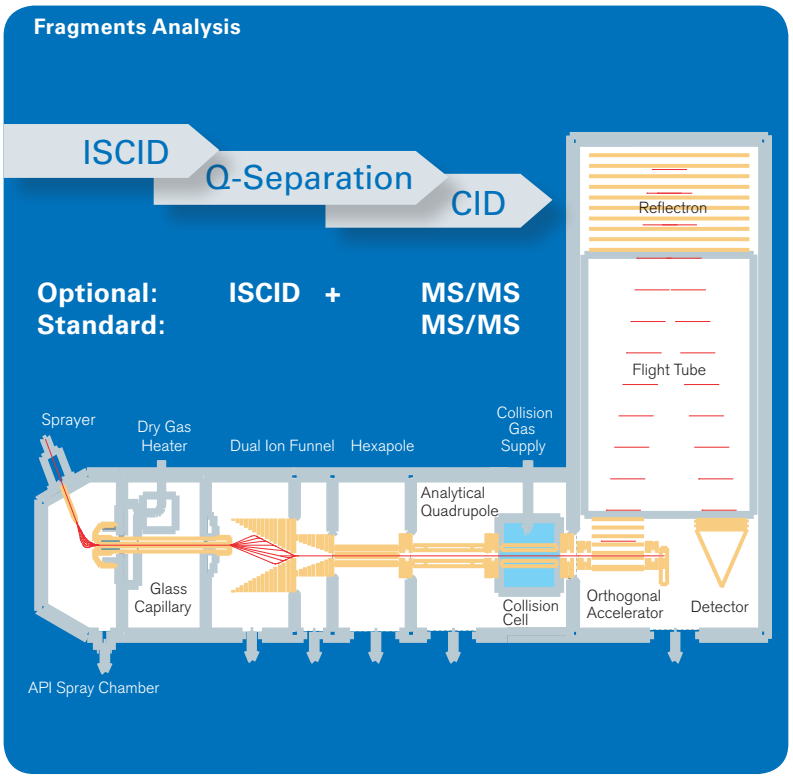


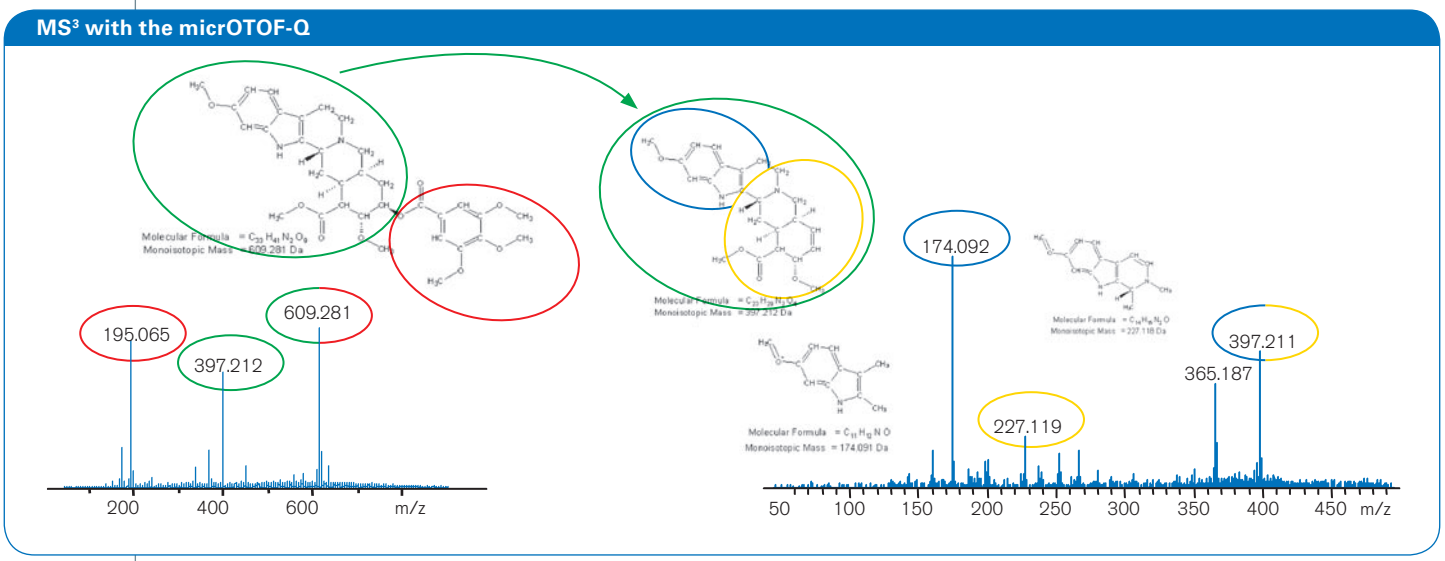
Ultimate Performance with Superiour Detection Power

Fragments Analysis

The micrOTOF-Q provides exceptional mass accuracy in MS/MS for metabolite and protein identification.

Achieve optional additional fragmentation performance with a source designed for ion fragmentation prior to the quadrupole (In-Source CID). After isolation in the analytical quadrupole, the ISCID fragments can be further fragmented in the collision cell (CID).

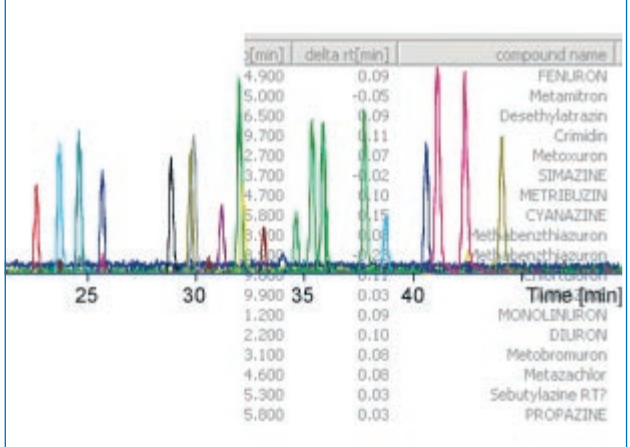




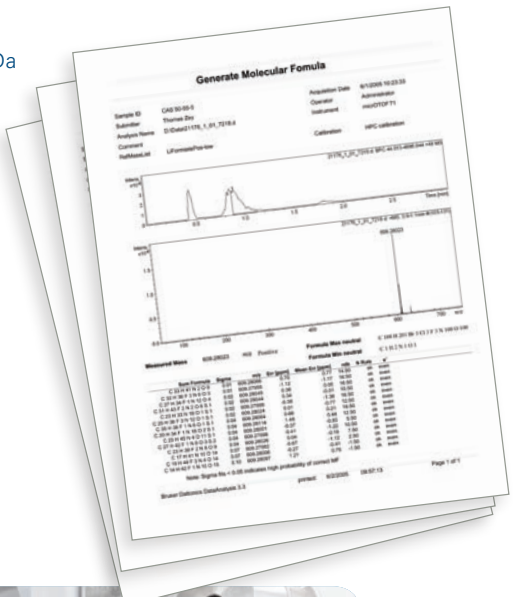
Reserpine: In-Source CID, Isolation of ISCID ions and fragmentation: MS^3.

Outstanding Solutions and Software Environment

Target Screening



Multitarget Pesticide Screening: EIC of detected compounds with ± 0.002 Da mass window.



Combine Multi Target screening with general unknown ID:

- Screen for multiple targets (up to several 100)
- Archive the whole sample-information
- ID unknowns with MS/MS

Confident Quantitative and Qualitative Multi-Target Screening – Forensics, Doping control, and Residue Analysis

The TargetAnalysis™ application allows multi-target compound screening in complex matrices, providing high specificity and enhanced SigmaFit™ molecular formula determination.

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 like drugs/metabolites in urine, food safety analysis, forensic toxicology or environmental testing.

Create Own Libraries

Users are enabled to create their own application-specific accurate mass libraries. The unique AMIC (accurate mass ion chromatogram) technique, with a tolerance down to +/- 0.002 Da, dramatically reduces chemical background interference and greatly improves specificity.

ID of Unknowns

Retrospective in silico screening for new or unexpected compounds is possible because unlike in triple-quad based MRM methods, the full molecular information content in addition to the target library specific information is retained .

Empowering accessories

Chemical Formula Generation

Compass OpenAccess™ provides a automated walk-up LC/MS system for chemical formula generation, molecular formula confirmation and generic LC/MS measurements.

This client-server based software supports LC/MS workflows especially for chemists in laboratories with various level of instrumental analysis experience.

Metabolic Profiler™

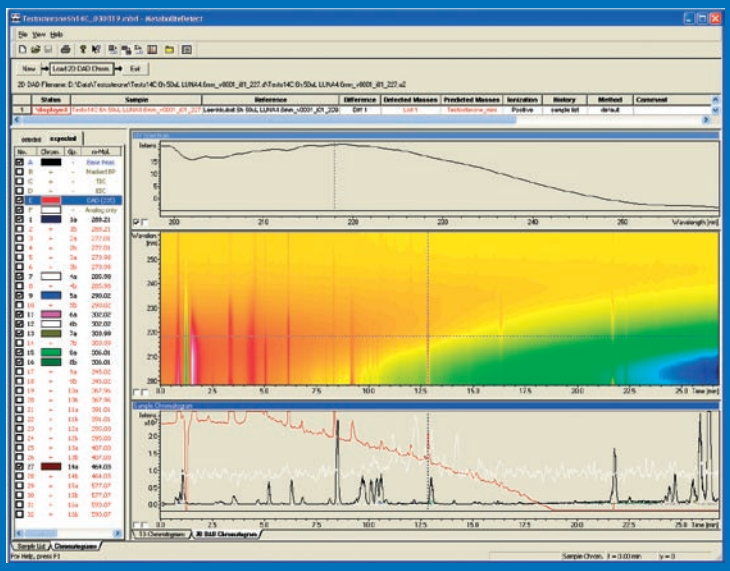
Advance biomarker profiling to the metabolome level to address metabolomic profiles that are powerful sensors reflecting situations at physiological endpoints. An application feasable with the micrOTOF-Q in nutraceutical, pharmaceutical and clinical research.

Metabolite ID

Metabolite and small molecule prediction and detection is performed by MetaboliteTools™, allowing detailed evaluation of samples and sample batches based on the sophisticated eXpose™ detection algorithm and accurate mass capabilities of micrOTOF-Q.

MetaboliteTools predicts possible metabolites from a given drug structure, and extracts relevant information on existing metabolites for LC-MS data.

Metabolite ID User Interface



Proteomics Screening and in-depth Analysis

Translate mass spectra into knowledge. ProteinScape with WARP-LC™ and BioTools™ provides unique software backbones to mass spectrometric proteome and protein analysis. Visualization tools for validation, such as the LC-SurveyViewer or quantification box-plots, are accompanied by protein identification tools, de novo sequencing support and PTM discovery.

The Unified Software Environment

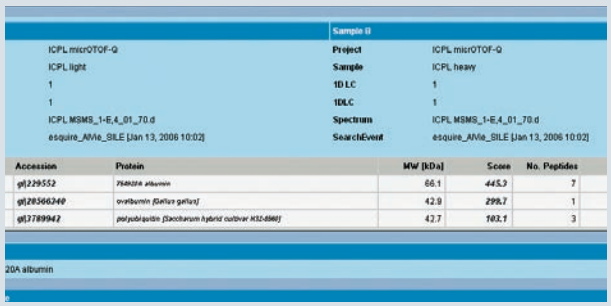
Our unified Compass™ software environment for all our life science instruments integrates instrument control, data acquisition, processing and interpretation – speeding research and enhancing productivity.

Regulatory Compliance

Compass Security Pack™ provides all necessary functions for work in compliance with FDA and EU regulations (21CFR part 11/Annex 11):

- electronic signatures
- audit trailing
- user management
- result history
- system protection during breaks

ProteinScape Quantitation Result



Technical specifications

Cutting-edge Performance

Advanced micrOTOF-Q Technology

- World-leading combination of mass accuracy, resolution and sensitivity without compromise
- SigmaFit™, the unique combination of accurate mass with True Isotopic Pattern (TIP™)
- Wide dynamic range for ultra-stable accurate mass
- High-performance Q-q-front end
- Footprint 640 x 949 x 1320 mm, weight 160 kg

Source Options

- Apollo II ion funnel ESI Electrospray source (1 µl – 1 ml/min)
- APCI atmospheric pressure chemical ionization source (100 µl – 1,5 ml/min)
- APPI atmospheric pressure photo ionization source
- online / offline NanoElectrospray source
- CE/MS coupling with grounded ESI needle

Analytical Performance

- Mass range 20 – 40,000 m/z
- Mass accuracy in MS and MS/MS 3 ppm RMS Error (internal), 5 ppm RMS Error (external)
- Mass resolution in MS and MS/MS 15,000 (FWHM)
- Temperature compensated
- Acquisition rate (2GHz sampling rate) 20 Hz (profile and peak detected spectra to disk)

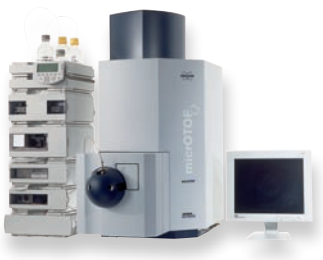
Compass Software Suite

Integrated LC-MS/MS control and data processing

- Generate formula module using SigmaFit
- BioTools™/RapiDeNovo™ software for protein data interpretation
- MetaboliteTools™ for metabolite identification
- ProteinScape™ database system for proteome project management

The micrOTOF-Q seamlessly integrates in Bruker Daltonics' System Solutions:

- TargetAnalysis – for multi-target compound screening
- Compass OpenAccess™: Walk-up LC/MS chemical formula generation
- Metabolic Profiler™: The ideal tool for Metabolic Studies
- PROTEINEER™: 2D Gel-MS/MS-based Proteomics Suite
- PROTEINEER-LC™: LC-MS/MS-based Proteomics Suite



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