

Bruker Daltonics



micrOTOF-Q II

- 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 II™ ESI-Qq-TOF mass spectrometer features the very latest technology developments to provide maximum certainty in your research in Small Molecule Identification, Metabolomics or Proteomics.

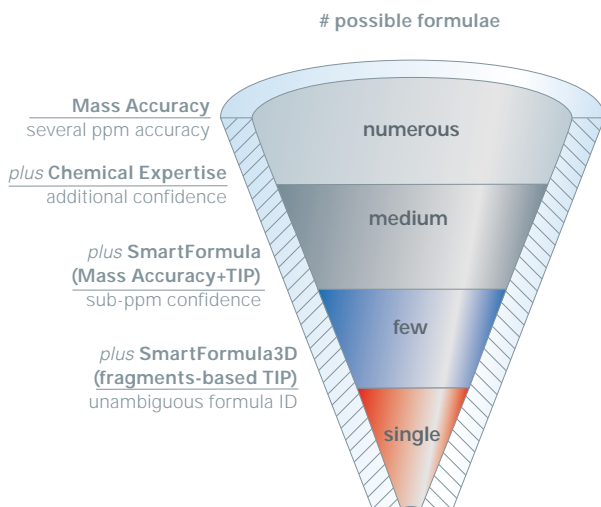
SmartFormula determination

Three dimensions of information simultaneously raise your analytical tasks to unrivaled heights of confidence:

- Measure with unequalled accurate mass
- Validate with True Isotopic Pattern (TIP) analysis
- Also benefit from accurate mass and TIP in analysis of fragments in MS/MS mode

Mass accuracy, chemical knowledge and SmartFormula 3D™ clearly limit the number of possible formulae in molecular formula generation: for confident determination of the elemental composition of a given peak.

This valuable 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

Cutting-edge performance has never been this easy to use:

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 1 – 2 ppm over an exceptionally wide dynamic range.

Resolution

Be amazed by superb focus resolving power exceeding a resolution of 17,500 – 20,000 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 II expands the renowned micrOTOF's advanced performance in the analysis of molecule fragments, adding a third level of confidence to the two dimensions of accurate mass and True Isotopic Pattern analysis with SmartFormula 3D.

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

Simultaneously achieve reliable MS and MS/MS accuracy, independent of

whether calibration was performed in MS or MS/MS mode.

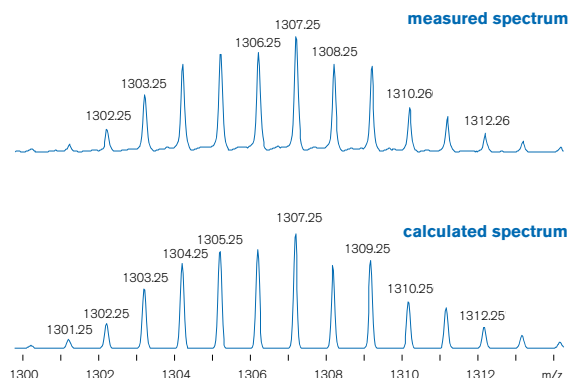
Thus, for chemical formula determination, a detailed formula suggestion is only a keystroke away.

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



Unprecedented Certainty

Isotopic pattern analysis



MS analysis of Pd-Complex ($C_{61}H_{64}N_4O_{15}Pd_2$) in synthetic chemistry. Isotopic Pattern of measured spectrum and calculated spectrum show outstanding homogeneity, providing a superior SmartFormula scoring for enhanced confidence in structural analysis.

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

After generation of a list of possible formulae, the measured isotopic pattern is compared with the theoretical isotopic pattern – resulting in a statistical match factor, the Sigma factor used for SmartFormula.

microTOF-Q II's capability to deliver correct isotopic patterns discriminates over typically 50 possible formulae from 2-5 ppm mass accuracy alone to one single formula by SmartFormula scoring.

Precision in organic chemistry

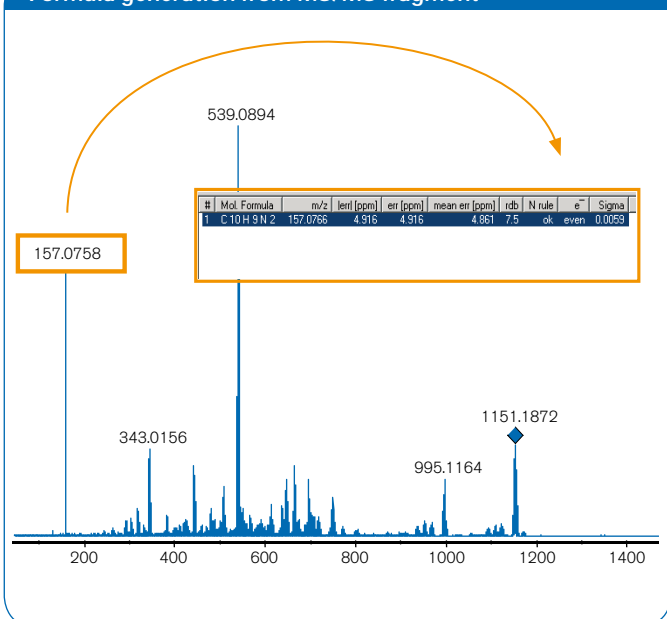
Accurate mass and Bruker Daltonics' proprietary SmartFormula 3D True Isotopic Pattern analysis algorithm provide unrivalled certainty for the identification of unknowns.

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

ISCID-MS³ analysis of Pd-Complex in synthetic chemistry. A fragment m/z 157.0758 reveals a mass error of < 5 ppm (external calibration) for reading out a formula by SmartFormula scoring. Parent ion was m/z 1307, see above. The ion was fragmented insource followed by a CID experiment of the fragment m/z 1151. microTOF-Q II covers the whole mass range with high mass accuracy.

SmartFormula 3D: Combining accurate mass with True Isotopic Pattern (TIP) capabilities of the microTOF-Q II. 15 possible sum formulae candidates from MS analysis are condensed down to one, Minocycline. (see Technical Note TN-26).

Formula generation from MS/MS fragment



SmartFormula 3D delivers the correct formula

#	Mol. Formula	m/z	err [ppm]	Sigma Rank
1	C ₂₃ H ₂₈ N ₃ O ₇	458.1922	1.2	1
2	C ₂₀ H ₂₀ N ₃ O	458.1908	1.8	2
3	C ₂₄ H ₂₄ N ₇ O ₃	458.1935	4.1	
4	C ₂₁ H ₃₃ N ₈ O ₈ P	458.1938	4.8	
5	C ₁₉ H ₂₄ N ₉ O ₅	458.1895	4.7	
6	C ₁₉ H ₃₄ N ₅ O ₂ P ₂ S	458.1903	2.9	6
7	C ₂₇ H ₃₀ N ₃ P ₂	458.1909	1.5	7
8	C ₁₈ H ₂₅ N ₁₁ O ₂ P	458.1925	1.8	8
9	C ₂₅ H ₃₃ N ₃ O ₃ P ₅	458.1913	0.7	9
10	C ₂₇ H ₂₈ N ₃ O ₂ S	458.1897	4.3	10
11	C ₁₈ H ₃₃ N ₇ O ₃ P ₅	458.1920	0.8	11
12	C ₂₀ H ₂₈ N ₉ S ₂	458.1904	2.8	12
13	C ₂₄ H ₃₂ N ₃ O ₂ S	458.1930	3.1	13
14	C ₃₂ H ₂₈ N ₅			
15	C ₃₅ H ₂₄ N			

SmartFormula hit list

SumFormula	m/z calc	err [ppm]	mSigma
<input checked="" type="checkbox"/> C ₂₃ H ₂₈ N ₃ O ₇	458.1922	1.2	4.3

SmartFormula 3D:
One single formula

● Accurate Mass, SmartFormula and MS/MS

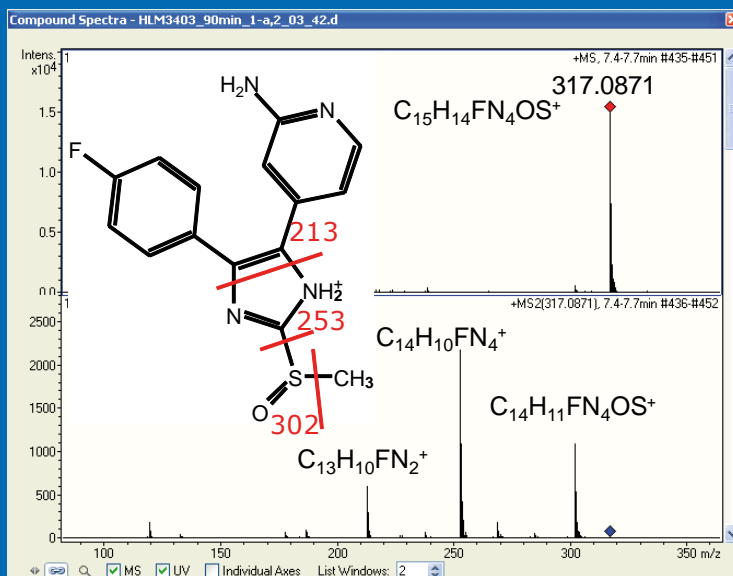
Advancing metabolomics research

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

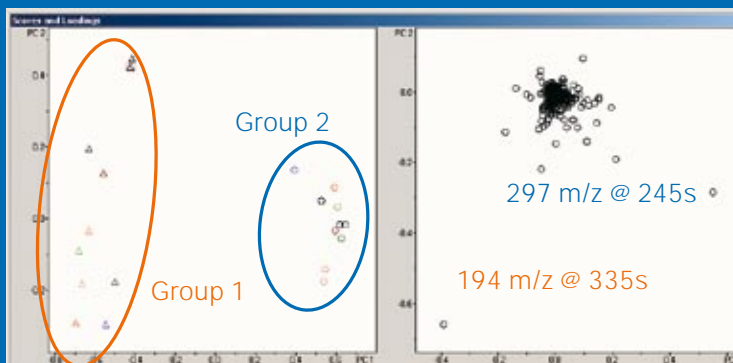
Identify small molecule biomarkers with the power of accurate mass, TIP and fragments analysis for evaluation of disease state, following drug treatment or to monitor toxic response.

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

Metabolic fragment ID and statistical analysis



Assignment of fragments in metabolite identification is made easy based on the Smart Formula results. AutoMS² of metabolite with m/z 317 exhibits e.g. the following losses: methyl radical and the entire sulfenyl group.



A clear separation of groups in the PCA analysis: Scores and Loadings Plot of rat urine samples from groups receiving different levels of food (reproduced with kind 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

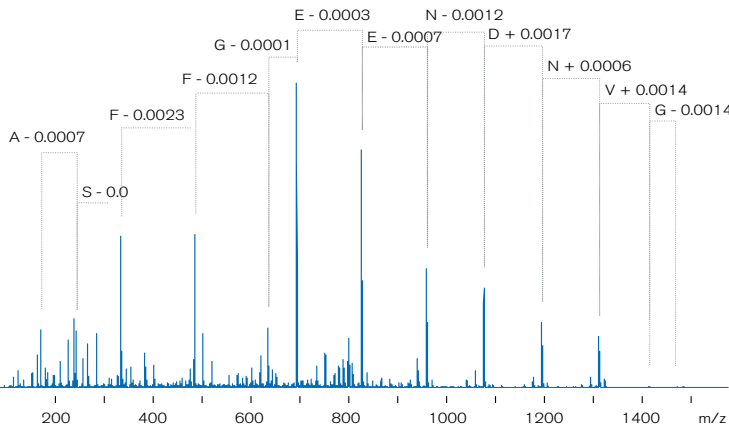
modifications, PTMs or natural products! All ions are collected by a radial RF field and smoothly directed towards the funnel exit. Between the first and the second funnel, ISCD energy can be freely selected for optimal performance of the experiment.



Information-Rich in Depth Analysis

De novo sequencing

Mass Distance
RMS error: 0.97 mDa



The *de novo* sequencing machine

The micrOTOF-Q II is the ideal instrument to achieve outstanding mass accuracy over a broad mass range, a prerequisite for successful *de novo* sequencing – from low-mass immonium ions to high-mass fragment ions.

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.

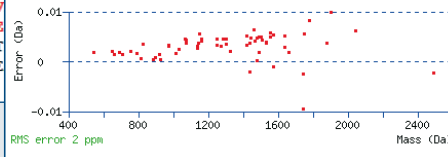
Mass accuracy

Matched peptides shown in **Bold Red**

```

1 MKWVTFISLL LFFSSAYSRG VFRDRTHKSE IAHRFKDLGE BHFKGLVLIA
51 FSQYLQCCPF DEHVKLVNEL TEFARTCVAD ESHAGCEKSL HTLFGDELCK
101 VASLRETYGD MADCCCKQEP ERNECFLSHK DDSPLPKLK PDPNTLCDEF
151 KADEKIFWKG YLYEIAARRH YFYAPELLEY ANKYNGVFQE CCQAEDRGAC
201 LLPKIETMRE KVLASSARQR LRCASIQKFG ERALKAWSVA RLSQKFPKAE
251 FVEVTKLVTD LTKVHKECCG GDLLCCADDR ADLAKYICDN QDTISSKLEK
301 CCDKPLLEKS HCIAEVEKDA IPENLPPLTA DFAEDKDVCK NYQEAKDAFL
351 GSFLYEYSRR HPEYAVSVLL RLAKYEATL EECCKADD
401 KHLVDEPQNL IKQNCQPEK LGEYGFQNAL IVRYTRKV
451 RSLGKVGTRC CTKPESERMP CTEDYLSLIL NRLCVLHE
501 TESLVNRRFC FSALTPEDETY VPKAFDEKLF TFHADICT
551 ALVELLKHKP KATEEQLKIV MENFVAFVDK CCAADDKE
601 STQTALA
    
```

1

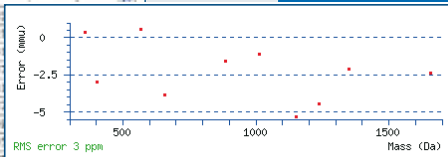


Reproducible mass accuracy: 50 fmol BSA separated by Waters UPLC™ is measured with an RMS error of only 2ppm (1).

Even fragments are reliably analyzed (2) with only 3 ppm RMS error (20 fmol BSA) from a single external calibration.

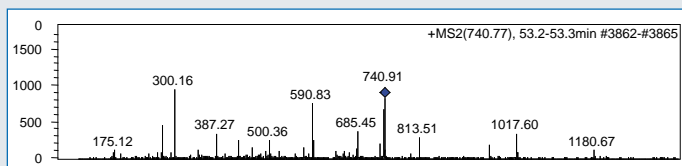
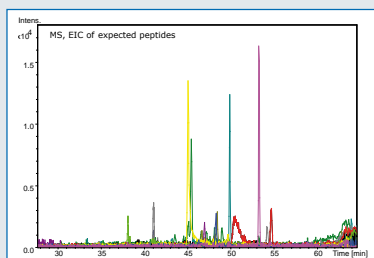
#	b	b ⁺⁺	b ⁺	b ⁺⁺	b ⁺	Seq	y	y ⁺	y ⁺⁺	y ⁺	y ⁺⁺	#		
1	115.050	58.029	98.020	49.515		N						16		
2	244.093	122.550	227.055	114.037	226.062	113.545	E	1787.827	894.417	1770.800	885	16		
3	484.123	202.563	387.097	194.052	386.113	193.540	C	1678.784	829.896	1641.758	811	16		
4	551.192	276.100	534.185	267.586	533.181	267.034	F	1430.754	749.880	1481.727	741	16		
5	664.276	332.642	647.243	324.126	646.245	323.616	L	1391.687	676.345	1374.659	667	16		
6	751.398	376.158	734.281	367.644	733.297	367.152	W	1239.603	619.804	1221.575	611	16		
7	888.367	444.687	871.340	436.174	870.356	435.612	H	1151.565	576.280	1134.543	571	16		
8	1016.462	508.733	999.433	500.221	998.431	499.729	K	1014.510	507.759	997.484	491	16		
9	1131.480	566.248	1114.482	557.735	1113.478	557.243	D	886.487	443.711	869.589	441	16		
10	1246.516	623.761	1229.489	615.248	1228.505	614.756	D	771.388	386.198	754.362	377	16		
11	1333.548	667.270	1316.521	658.764	1315.537	658.272	E	676.541	328.684	659.335	329.171	658.351	319.619	16
12	1430.600	715.804	1413.576	707.291	1412.590	706.799	P	569.329	285.158	552.303	276.655	551.319	276.163	16
13	1545.627	773.317	1528.601	764.804	1527.617	764.312	D	472.273	236.642	455.250	228.129	454.266	227.637	16
14	1658.713	829.859	1641.813	821.346	1640.791	820.854	L	387.250	179.128	340.223	173.613	333	16	
15	1755.764	878.386	1738.732	869.872	1737.754	869.381	P	244.164	122.596	227.139	114.073	221	16	
16							K	147.113	74.060	130.086	65.547	111	16	

2



Sensitivity, Dynamic Range & Resolution

MS/MS ID from 100 amol BSA



Analysis of 100 amol BSA digest on column. BSA was unequivocally identified by five peptides. Left: Extracted Ion Chromatograms of identified peptides.

Sensitivity

Ultimate sensitivity is demonstrated with a 100 amol digested BSA sample. Even for this small sample amount, solid peptide identification is possible.

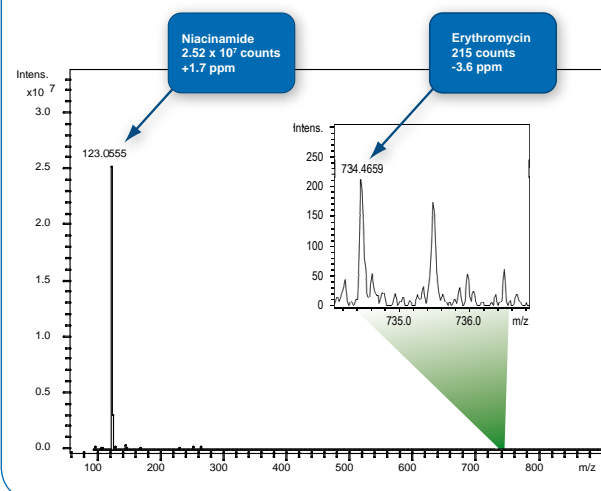
Dynamic range

More than 5 orders dynamic range - excellent stability of mass measurement without tedious recalibration routines is key for screening and LC-MS applications and enables the simultaneous detection of high and low abundance compounds.

Mass resolution

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

More than 5 orders dynamic range

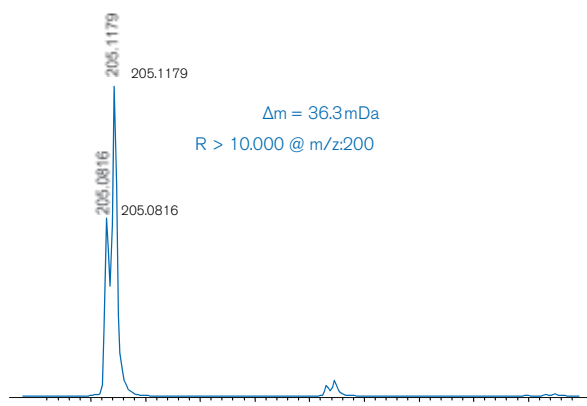


Real measured intraspectrum dynamic range of 5.1 demonstrate the exceptional capabilities of the micrOTOF-Q II.

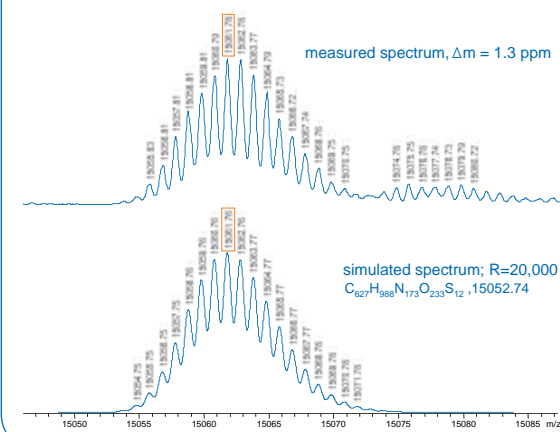
Differentiation of isobaric dipeptides. C₇H₁₃N₂O₅ (AD) MW physical = 205.0819, C₈H₁₇N₂O₄ (SV) MW physical = 205.1183 delta MW = 0.0364 Da. For separation of the dipeptides at m/z 200, a resolution > 10,000 is achieved.

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

Resolution of Isobaric peptides



Intact protein mass resolution

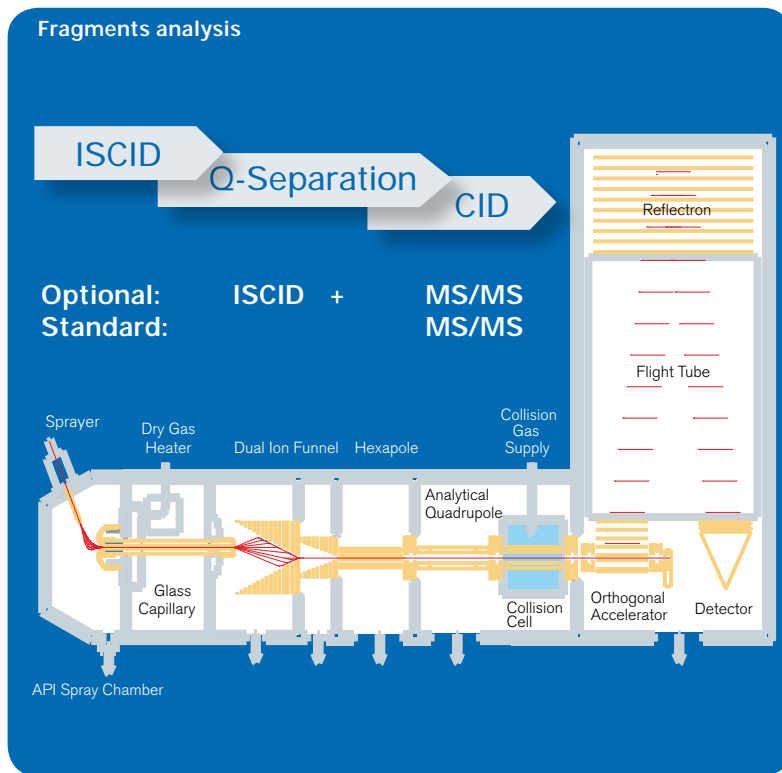


● Ultimate Performance with Superior Detection Power

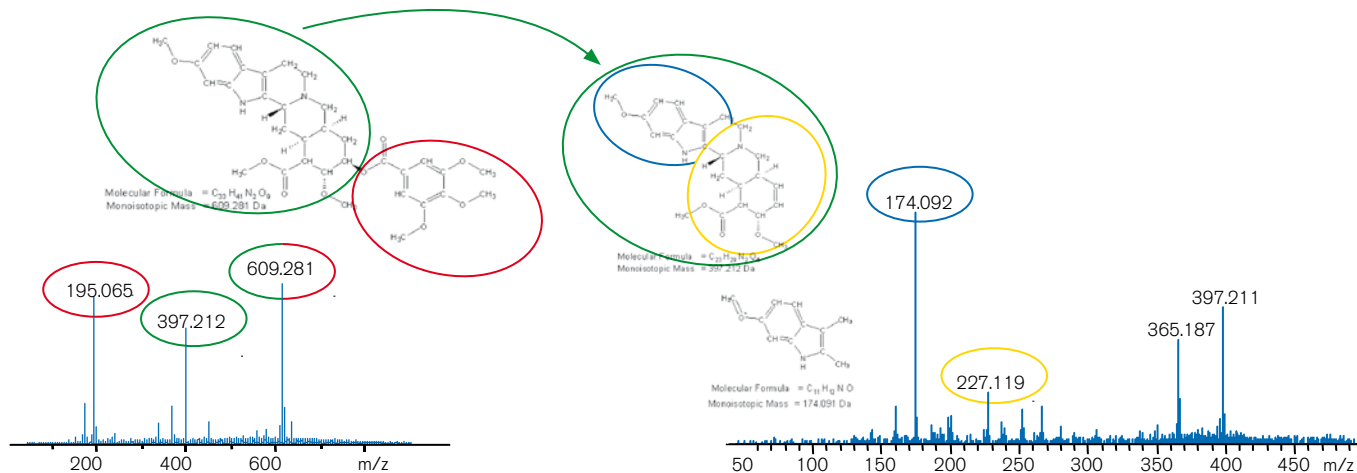
Fragment analysis

The micrOTOF-Q II 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).



MS³ with the micrOTOF-Q II



Reserpine: In-Source CID (left), Isolation of ISCID ions and fragmentation: MS³ (right).

● Empowering Accessories

Chemical formula generation

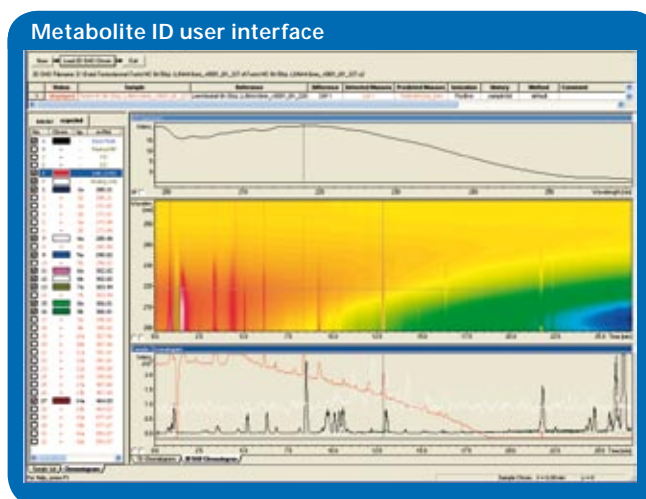
Compass OpenAccess™ provides an automated walk-up LC/MS system for chemical formula generation, molecular formula confirmation and generic LC/MS measurements. This client-server based software supports LC/MS workflows especially for chemists in laboratories with various levels of instrumental analysis 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 feasible with the micrOTOF-Q II 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 II. MetaboliteTools predicts possible metabolites from a given drug structure, and extracts relevant information on existing metabolites for LC-MS data.



Proteomics screening and in-depth analysis

Translate mass spectra into knowledge. ProteinScope 2 and BioTools™ provide unique software backbones to mass spectrometric proteome and protein analysis. Visualization tools for validation, such as the LC-SurveyViewer or quantification box-plots, are complemented with protein identification tools, *de novo* sequencing support and PTM discovery. ProteomeQuant, the label-free quantitative solution for discovery, identification, and targeting of regulated proteins allows differential proteome analysis of putative biomarkers in a comprehensive system.

The unified software environment

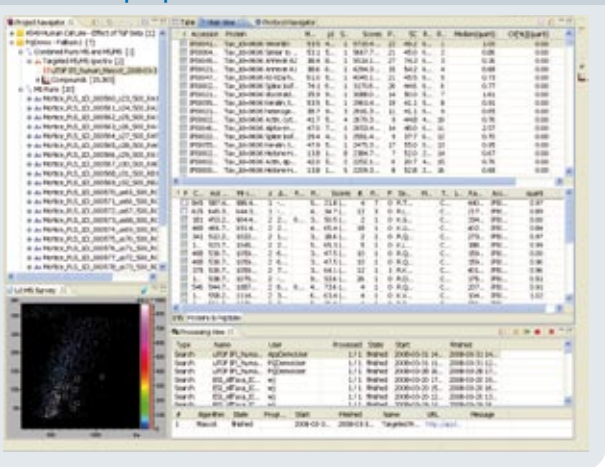
Our unified Compass™ software environment for all our life science instruments integrates instrument control, data acquisition, processing and interpretation – speeding research and enhancing productivity.

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

ProteinScope quantitation result



Technical Specifications

Cutting-edge performance

- Advanced micrOTOF-Q II technology
- World-leading combination of mass accuracy, resolution and sensitivity without compromise
- SmartFormula 3D™, the novel combination of accurate mass of parent and fragment ions with True Isotopic Pattern (TIP™)
- Wide dynamic range for ultra-stable accurate mass
- High-performance Q-q-front end
- Dimensions 640 x 949 x 1320 mm, weight 160 kg

Source options

- Apollo II ion funnel ESI Electrospray source
- APCI atmospheric pressure chemical ionization source
- ESI/APCI multimode source
- APPI atmospheric pressure photo ionization source
- Online / offline NanoElectrospray source
- CE/MS coupling with grounded ESI needle

Analytical performance

- Mass range 50 – 20,000 m/z
- Mass accuracy 1 - 2 ppm RMS Error (internal), 5 ppm RMS Error (external)
- Mass resolution 17,500 (FWHM), typically 20,000 FWHM at LC-speed
- Temperature compensated
- Acquisition rate (2GHz sampling rate) 20 Hz (profile and peak detected spectra to disk)

Compass & application software suites

Integrated LC-MS/MS control and data processing

- SmartFormula and novel SmartFormula 3D
- BioTools™ / RapiDeNovo™ software for protein data interpretation
- MetabliteTools™ for metabolite identification
- ProteinScape™ database system for proteome project management
- TargetAnalysis™ – for multi-target compound screening
- Compass OpenAccess™: Walk-up LC/MS chemical formula generation

The micrOTOF-Q II seamlessly integrates into Bruker Daltonics' system solutions:

- Metabolic Profiler™: The unique NMR-MS solution for Metabolomic Studies
- PROTEINEER™: 2D Gel-MS/MS-based proteomics suite
- ProteomeQuant™: LC-MS/MS-based proteomics suite
- LC-NMR/micrOTOF-Q II coupling

Support of:

HPLC and sample inlet systems from the following vendors: Bruker EASY-nLC, Advion TriVersa NanoMate, Agilent, Dionex, VWR/Hitachi, Waters (incl. UPLC), Autosamplers from CTC

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

micrOTOF-Q II, SmartFormula 3D, SmartFormula, TIP, Apollo II, Compass, Compass OpenAccess, Compass Security Pack, Metabolic Profiler, MetabliteTools, eXpose, BioTools, RapiDeNovo, PROTEINEER and ProteomeQuant are trademarks of Bruker Daltonics corporation. ICPL is a trademark of TopLab GmbH. iTRAQ is a trademark of Applied Biosystems. ICAT is a trademark of the University of Washington. MASCOT is a registered trademark of Matrix Science Ltd., EASY-nLC™ is a trademark of Proxeon A/S, Odense, Denmark



www.bdal.com

● **Bruker Daltonik GmbH**

Bremen · Germany
Phone +49 (421) 2205-0
Fax +49 (421) 2205-103
sales@bdal.de

Bruker Daltonics Inc.

Billerica, MA · USA
Phone +1 (978) 663-3660
Fax +1 (978) 667-5993
ms-sales@bdal.com