BRUKER

# What will you identify today?

## Industrial Microbiology

## MALDI Biotyper

- Fast & Accurate Identification of Microorganisms

MALDI-TOF

Innovation with Integrity

# High Quality Identifications in just a Couple of Minutes

The MALDI Biotyper System:

- Sequence Quality Data
- Comprehensive Libraries
- Open Microbiology
- 21CFR part 11 support
    - Audit Trail
    - User Management
    - Data Security
    - Electronic Signature
- IQ/OQ/PV
- Robust and Easy to Use
- Compact Bench Top System

## A Powerful Technology for Industrial Microbiology Applications

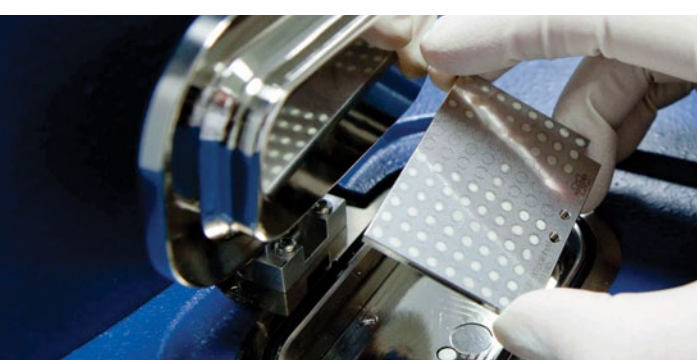
To help solve the challenges of performing microbiology in the industrial market, Bruker has utilized its wealth of experience to create the truly innovative MALDI Biotyper system.

Over the past 5 years the MALDI Biotyper has revolutionised how microorganism identification is performed in more than 700 laboratories around the world.

## Identifying Microorganisms by Their Molecular Fingerprint

The MALDI Biotyper identifies micro-organisms using MALDI-TOF (Matrix Assisted Laser Desorption Ionization-Time of Flight) Mass Spectrometry to measure a unique molecular fingerprint of an organism.

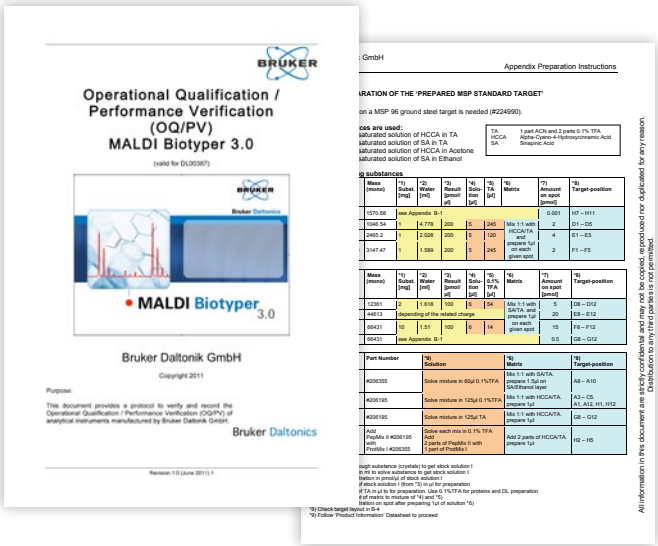
This coupled with extensive libraries covering environmental and clinical isolates provides extremely broad coverage of microorganisms found in Food, Pharmaceutical and Water industries.



# Installation, Operational and Performance Qualifications

Already in use in a number of Industrial microbiology laboratories, the MALDI Biotyper provides a very rapid and specific microorganism identification with resolution comparable to molecular sequencing techniques with significantly less effort, time and cost.

The implementation and validation of the MALDI Biotyper is assisted by IQ/OQ/PV documentation and 21 CFR Part 11 compliant software.




# Quality Assurance

Drawing upon over 20 years of experience in the manufacture of reagents used in Mass Spectrometry, Bruker supplies both certificates of Analysis and Traceability for the Bacterial Test Standard and the HCCA Matrix.

The Bacterial Test Standard is a typical *E. coli* extract containing additional proteins that can be used for instrument mass calibration and as a performance verification standard.


Further reading

McDaniel, A. Validation of an Automated Microbial Identification System, In Microbial Identification: The Keys To A Successful Program. Griffin M. & Reber D. (Eds.) PDA Chapter 5,87-106

# Technical Specifications

| Dimensions & Operating Parameters | |
|---|---|
| LxWxH: | 510 x 680 x 1093mm [20.1" x 26.8" x 43"] |
| Weight: | 84kg (185 lb) net weight |
| Noise: | <30 dB under normal operating conditions |
| Temp Range: | 10-30°C (50-86°F) |
| Operating Humidity: | 15-85% non-condensing @ 30°C |

## Instrument: Microflex LT

- Nitrogen Laser with 60Hz repetition rate
- Full Spectrum Resolution (FSR) with broadband focusing mode (PAN™)
- Smart Spectra Acquisition™
- Perpetual Ion Source™ with IR-laser self-cleaning functionality
- FlashDetector™
- Whispermode™
- Oil-free membrane pre-vacuum pump and turbo pump
- Manufactured under QSR regulations

## Microbial Identification Applications:

- Gram +/- Bacteria, Yeast, Moulds, Fungi and Mycobacteria
- Direct from Liquid media

## Computer, Software & Database:

- Windows 7 operating system with Quad-Core CPU 2.66 GHz, Laser printer and Remote Service Capability via 128-bit SSL
- **MALDI Biotyper** Database
- **MALDI Biotyper** Client Server

## Optional System Upgrades and Accessories:

- GPR kit for direct processing of liquid samples
- IQ/OQ/PV
- Security pack

## Sample Targets:

- Reusable Polished Stainless Steel Targets: 48 & 96 position with and without barcode
- Disposable 48 position Biotargets with individual barcode
- 24 and 96 position BigAnchorChip™ Targets

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

# solarıx

- Optimized FTMS Solutions for the Most Challenging Applications

Qq-FTMS

Innovation with Integrity

# Dedicated to the Most Challenging Applications

solariX, the next-generation line of hybrid Qq-FTMS systems, is the culmination of key technology enhancements that provide unique capabilities in mass spectral performance and versatility.

### The technological advances encompassed by solariX provide:

- Superior Sensitivity
- Unmatched Mass Accuracy and Broadband Resolution
- Widest range of structural tools, including Electron Transfer Dissociation (ETD)
- Expansive Mass Range
- Selective Ion Enrichment and Enhanced Dynamic Range
- Application Directed and Optimized Solution Packages

### Common applications for solariX

The analytical power and performance of FTMS is well suited to address some of today's most challenging and complex samples. Drawing on years of applications experience, we have combined our unique FTMS instrumentation and comprehensive software tools to provide turn-key solutions for the following areas:

- High End Proteomics Studies (Top-down and Bottom-up workflows)
- Molecular Imaging of Tissue - Distribution of Drugs, Metabolites, and Biomarkers
- Petroleum Product Analysis
- Complex Environmental sample analysis
- Metabolomics Research

# Performance Beyond Compare

At the core of the solariX is dramatically improved sensitivity and dynamic range. This allows researchers to identify and analyze a much wider range of molecules than ever before, and to delve deeper into complex mixtures and analyze lower abundance species.

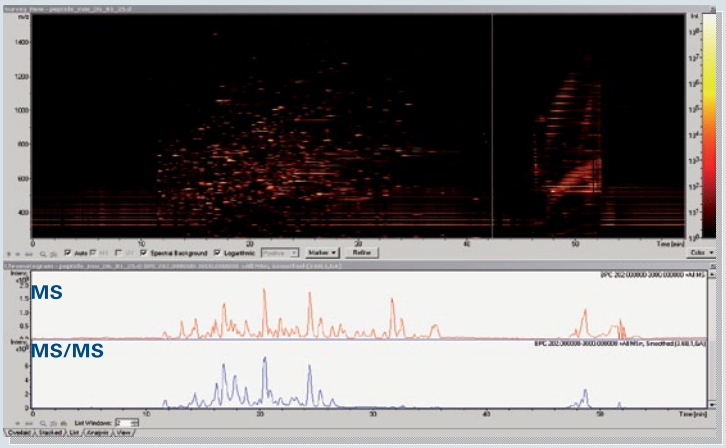
## More power for greater complexity

The broadband, ultra high resolving power (increased 8-fold) and superb mass accuracy of solariX is more powerful than previously possible with any other mass spectrometer. This extraordinary increase in the number of available m/z channels is essential for addressing complex problems such as petroleomics and environmental samples which require resolving powers of greater than 400,000 for effective analysis.

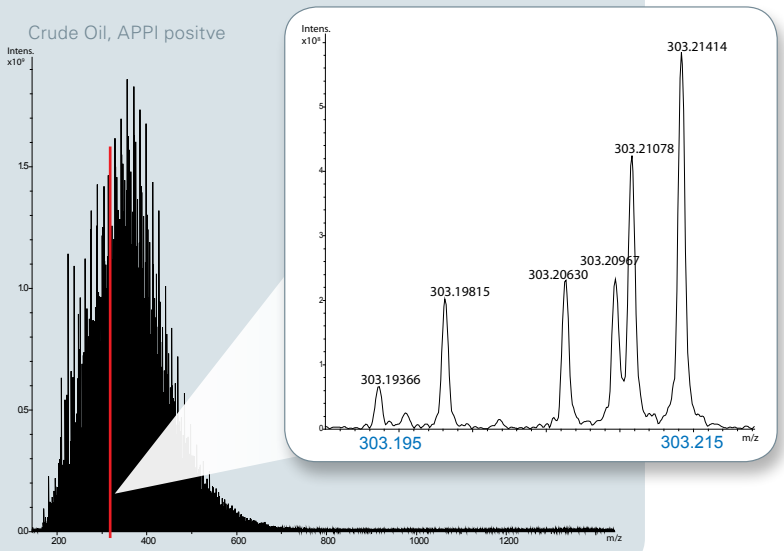
## Faster and more advanced LC-MS and LC-MS/MS operation

The new data acquisition functionality enables smarter modes of data dependent operation. Here, spectral acquisition parameters such as data set size or starting mass may be adjusted on-the-fly in a mass dependent mode of operation. Smaller data sets can be selected for MS/MS acquisitions making the overall data acquisition rate faster, while maintaining the high fidelity measurements for the MS precursor acquisitions. Moreover, super stable mass accuracy is maintained throughout the LC-MS analysis using Bruker's proprietary Ion Charge Control (ICC™) mode.

**Base Peak Chromatogram for LC-MS and LC-MS/MS of protein mixture**




**Effective analysis of complex problems**



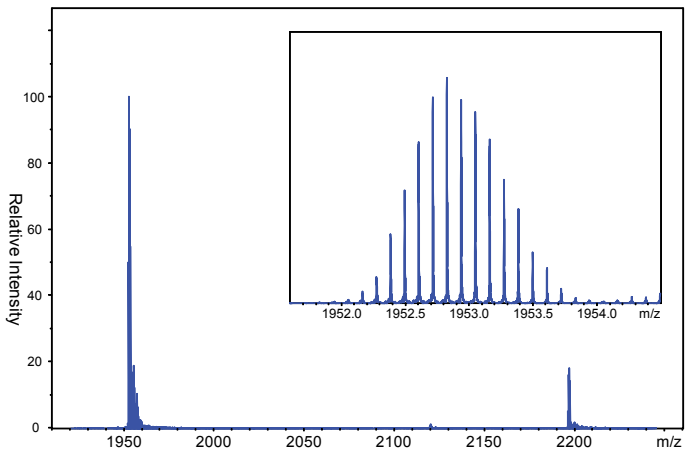

Broad band spectrum of a crude oil measured by APPI in positive ion mode. Insets illustrate the extreme high resolving power (> 550,000) of the solariX-CM.

# New Horizons for Biomolecule Analysis

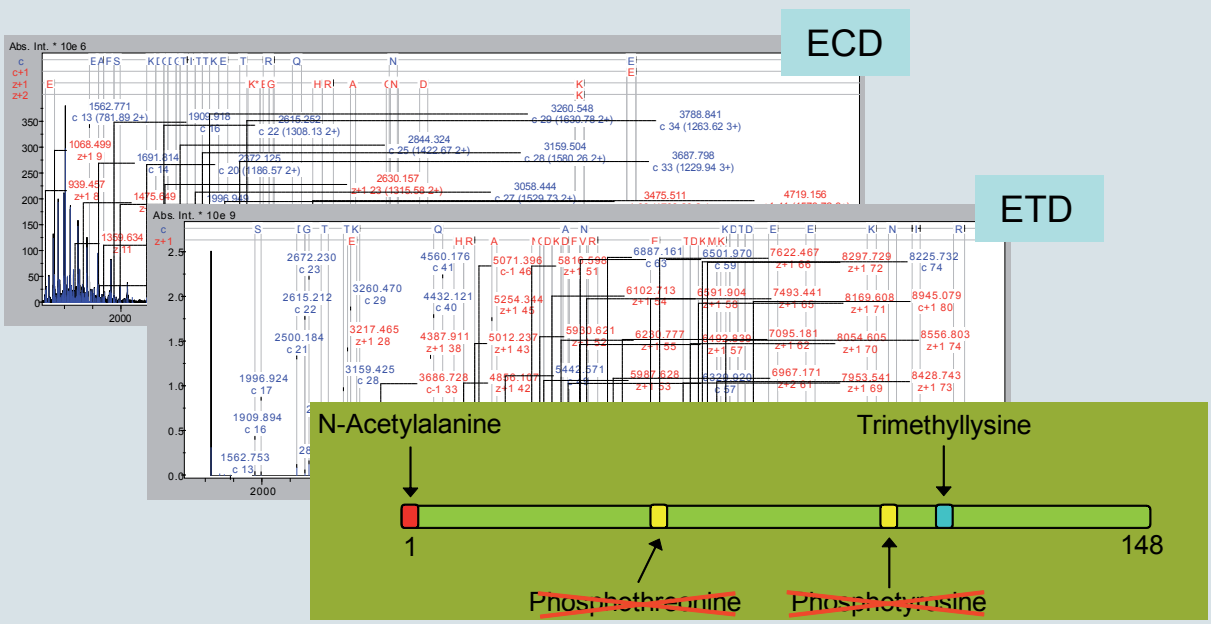
## Expanded capabilities for biomolecule analysis

Adding to the existing arsenal of structural fragmentation tools, solariX is fully enabled with Electron Transfer Dissociation (ETD). This exciting new technique is superb for in depth, comprehensive analysis of proteins and peptides and their subtle, posttranslational modifications. For instance, the gentle molecular dissociation chemistry associated with ETD enables researchers to elucidate subtle post-translational modifications such as glycosylation and phosphorylation at levels of accuracy and resolution previously unavailable for such de-novo approaches. Furthermore, ETD can be automated, and combined with LC-MS/MS schemes in combination with quadrupole fragmentation (Q-CID).

**Myoglobin, non-denaturing MS conditions**
Resolving Power = 450,000 @ m/z 1953



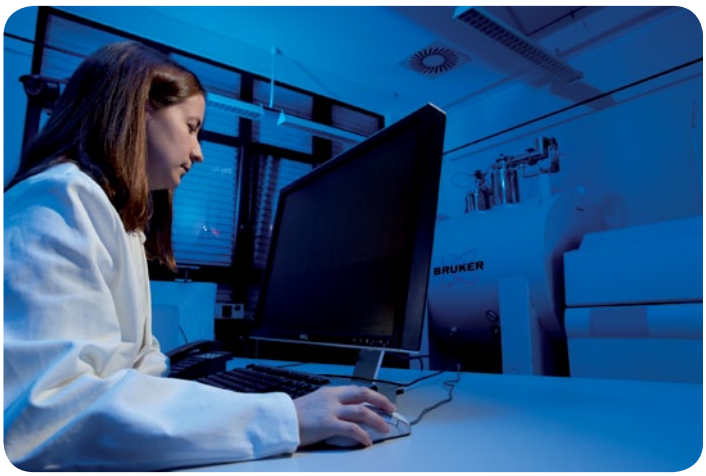

**ETD + ECD of Calmodulin**




The combination of ECD and ETD performed on Calmodulin. As illustrated above, the expected phosphorylations are not present and the lysine at position 116 is trimethylated.

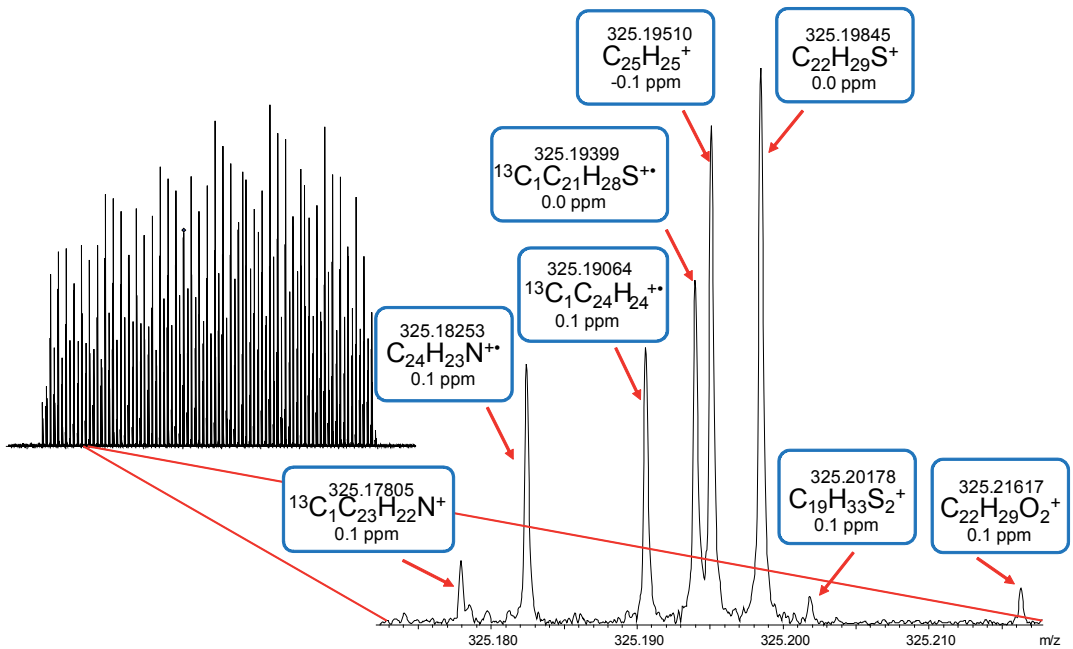
## Definitive molecular identification

With the solariX, high sensitivity, superior quality, exact mass measurements are only a mouse click away. Leveraging sub-ppm levels of mass accuracy for both intact precursor (MS) and product ions (MS/MS) combined with accurate isotope patterns, SmartFormula3D™ provides definitive elemental composition and molecular formula information. This level of confidence is readily achieved without internal standards or recalibration and the high resolution data inherently mitigates the complications resulting from other chemical interferences.




**Molecular formulae determination of components in crude oil**

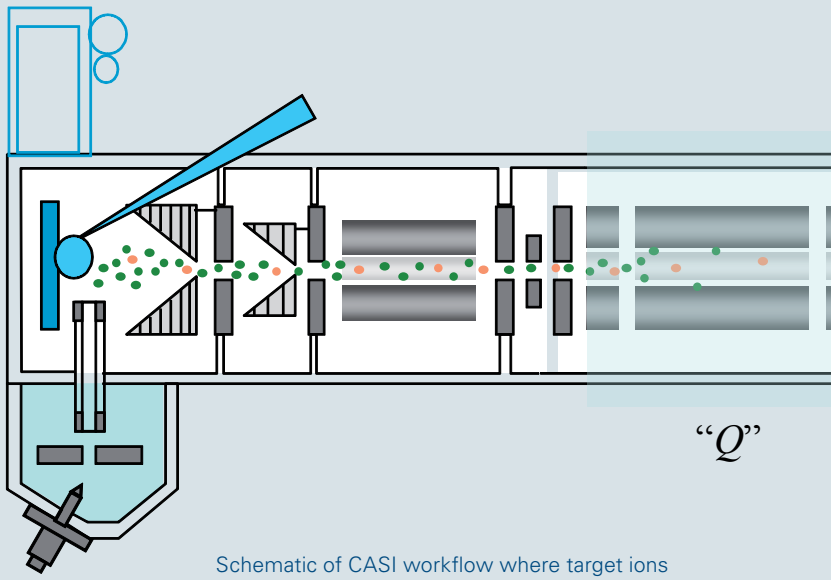
High resolution spectrum of crude oil by APPI demonstrating broadband resolving power of 950,000 with average mass measurement error below 100 ppb.



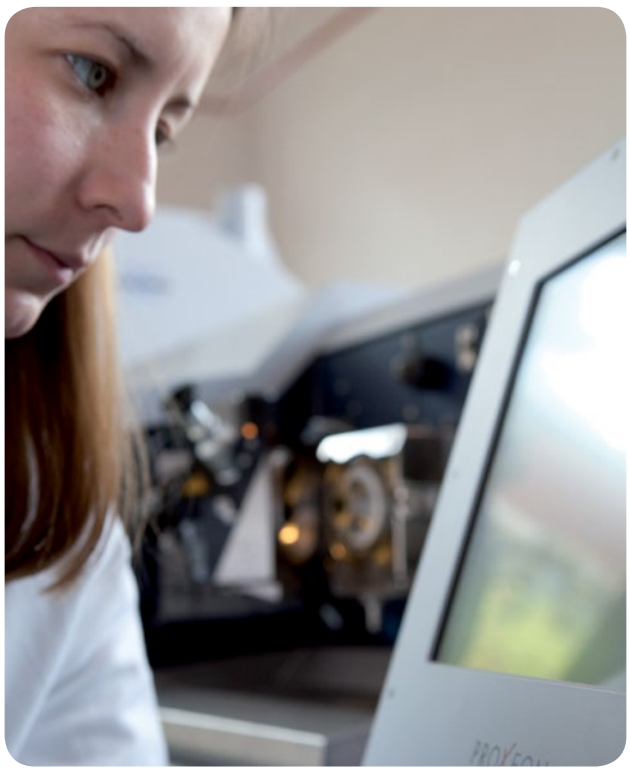
## CASI™: For rapid, enhanced selectivity and dynamic range

The unique Qq-FTMS geometry of the solariX can enrich lower abundant or trace species for detection and structural interrogation via MS and MS/MS, respectively. This mode, known as Continuous Accumulation of Selected Ions (CASI), is essential for tissue imaging, analyzing low-copy PTMs, and to extend the general dynamic range of almost any measurement. This can improve signal intensities by as much as an order of magnitude.

**CASI Figure**



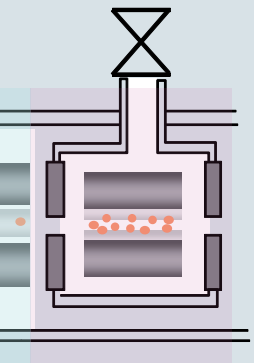

Schematic of CASI workflow where target ions are selected and enriched in the collision cell.



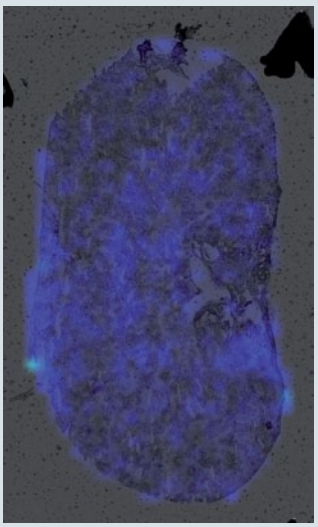
## Solution packages optimized for a variety of applications

The solariX product line features a series of tailored solutions around specific applications. Each solution comprises the appropriate hardware, ion source options, and application level software for a turn-key analytical platform. Whether your primary application is complex mixtures (e.g. petroleomics) or high resolution tissue imaging, a solariX package is designed to meet your needs. For laboratories having unique or multiple analysis needs, Bruker will work with you to prepare an appropriate, customized configuration.

# High-End Performance for any Analytical Laboratory

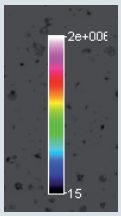


"q"

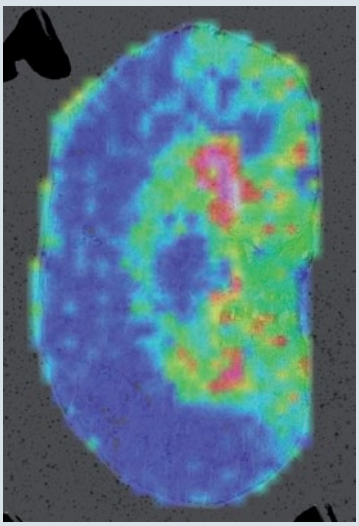


Full mass range MS

m/z = 313.1485




CASI boosts sensitivity, enabling the detection of drug and metabolites at lower concentrations



CASI - 20 m/z window

Molecular imaging of olanzapine in kidneyDosage – 5 mg/kg, 6h post dosage analysis.

The solariX FTMS is as intuitive and easy to use as a benchtop instrument. Bruker's Compass™ software enables the researcher to harness the analytical power and versatility with ease so that the focus is on the application and not on the instrumentation.

**Weekly cryogen "fills" become annual…**

Bruker's patented refrigerated magnet technology means nitrogen-free compact superconducting magnets with very low helium losses to minimize instrument maintenance and service. Patented active shielding technology minimizes the stray magnetic field levels for compact installations and maximum laboratory safety. These magnets are available for the full range of magnetic field strengths (7T, 9.4T, 12T, and 15T).

# Unique Features of solariX

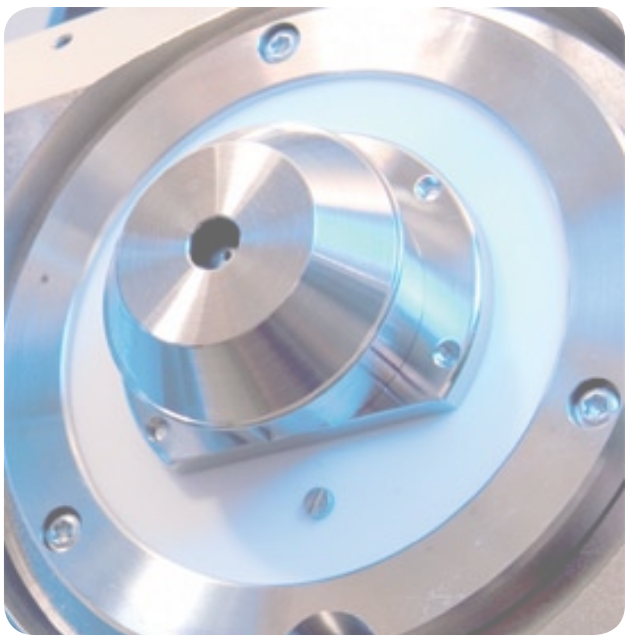
## Ultimate versatility in structural analysis

The solariX leverages the complementary nature of traditional quadrupole based Collisional Induced Dissociation (CID), and now Electron Transfer Dissociation (ETD). Additionally, precursors of complex mixtures may be isolated and fragmented using high front-end resolution, in-cell isolation followed by Electron Capture Dissociation (ECD) or Sustained Off-Resonance Irradiation (SORI)-CID. Whether your application is natural product, peptide/protein, carbohydrate, orpetroleum product analysis, solariX has an array of fragmentation tools to address practically any compound class.

## Ion source flexibility

While FTMS is ideally suited to liquid introduction, Bruker Daltonics offers the unique dual ESI/MALDI source. This is based on patented Ion Funnel technology for maximum sensitivity which allows effortless switching between ESI and MALDI – all at the touch of a button! The intermediate pressure MALDI source offers exquisite sensitivity, and preserves molecular ion fidelity throughout the complete FTMS detection process. The efficiency of the dual ESI/MALDI source combined with the new ion optics of the solariX provides a marriage of ultra-high resolution with high-end "MALDI-TOF sensitivity".

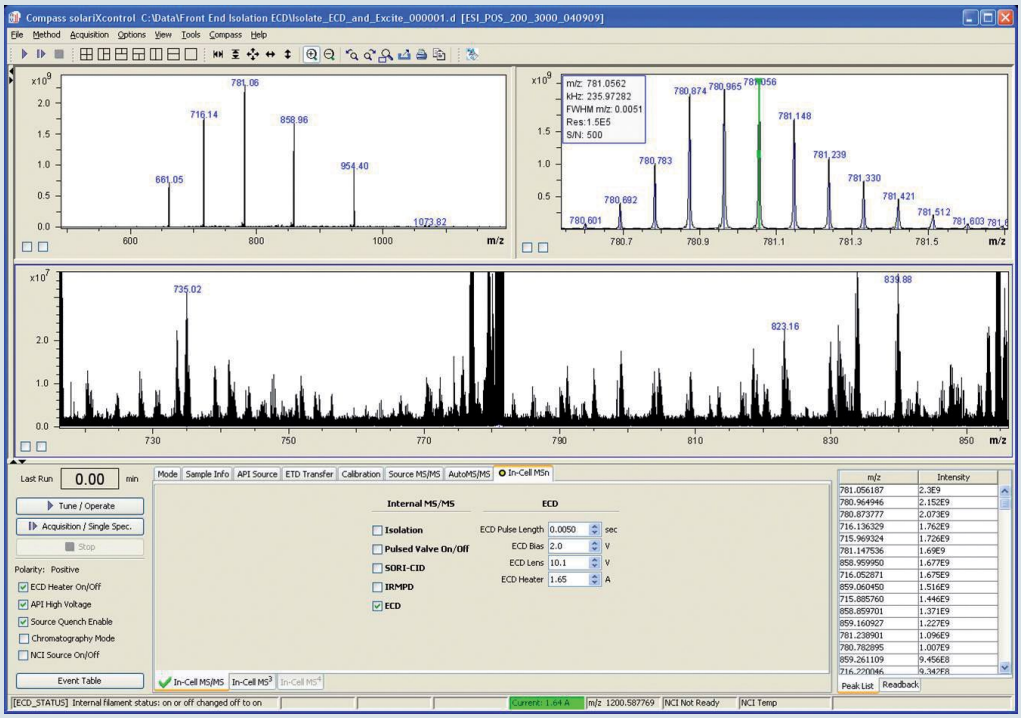
Along with our array of atmospheric pressure ionization sources (ESI, nano-ESI, APCI, and APPI), Bruker now offers GC-APCI capability.



# Flexible Front-end Solutions

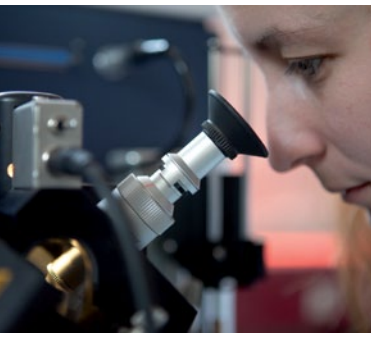
## Compass

The powerful Compass software enables the operation of a range of industry standard HPLC and u-HPLC platforms with the solariX. This includes comprehensive system control and seamless integration of mass spectral and UV data.




solariXcontrol™ - the instrument control software for solariX

# Technical Specifications



| | |
|---|---|
| **Magnet 7.0T/US/R refrigerated magnet** | |
| Field strength | 7.0T |
| **Analytical Performance** | |
| Mass Range | 100 – 10,000 m/z (transmission with RF only)<br>100 – 6,000 m/z (mass selective) |
| **MS/MS Operation** | |
| Isolation efficiency (Qh-Interface)<br>(LHRH, [M+2H]2+) | > 60% |
| MS/MS Efficiency (Qh-Interface)<br>(LHRH, [M+2H]2+) | > 50% conversion from isolated precursor |
| Multistage MS (MS3 guaranteed)<br>(LHRH) | LHRH MS/MS (collision cell) -><br>MS/MS/MS (Infinity Cell™) |
| Mass Dependent MS/MS | Automated isolation and MS/MS of the most intense ions in an LC-MS/MS run (scan ratio set to five) |
| Sensitivity ECD<br>(Substance P) | S/N > 10:1 for 5 fmol (consumed).<br>c5 fragment @ m/z 624 |
| **ESI** | |
| Mass accuracy<br>(Calibration on any 8 Q-CAD fragments for Angiotensin 1. checked on 4 different masses) | <1.0 ppm, m/z range 100 - 1500 (internal)<br><1.5 ppm, m/z range 100 – 1500 (external)<br>*Spec is based on average of errors |
| Resolving Power @ m/z 400 (lincomycin) | > 1,000,000 (FWHH) |
| Sensitivity<br>(Ubiquitin) | S/N > 10:1 for <100 amol (consumed) |
| High mass<br>(BSA 0,1mg/ml) | S/N > 10:1 |
| Negative ions | Functionality shown on Fibrinopeptide B |
| **ESI Source Options** | |
| Electrospray (standard) | (1 µl/min – 1 ml/min) |
| On-Line Nanospray (standard) | (100 nl/min – 500 nl/min) |
| EZ Nanospray (standard) | Zero – Adjust Off line Nanospray |
| APCI (optional) | Optional accessory |
| APPI (optional) | Optional accessory |
| Off-Line Nanospray (optional) | Optional accessory |

For research use only.
Not for use in diagnostic procedures.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# micrOTOF-Q III

- The bench-mark in accurate mass LC-MS/MS

ESI-Qq-TOF

Innovation with Integrity

# The Advantage of Confidence in Routine


The micrOTOF-Q range is widely acknowledged in setting standards in performance and reliability by which all other accurate mass ESI mass spectrometers are judged. micrOTOF-Q III demonstrates the best performance standard in its class:

- 20,000 full sensitivity resolution
- Low picogram sensitivity
- 2 ppm mass accuracy

Each performance parameter whether it is mass accuracy, resolution, or sensitivity is top in its class. Uniquely in the market, micrOTOF-Q III makes no compromise in delivering the best - all parameters are simultaneously delivered for fullest possible insight into your sample.

Complete applications solution software allows your micrOTOF-Q III to become your dedicated partner whatever your challenge in routine formulae confirmation, advanced screening and identification, or intact proteins and biopharmaceutical analysis.

# Your Partner in Innovative Chemistry

## 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.

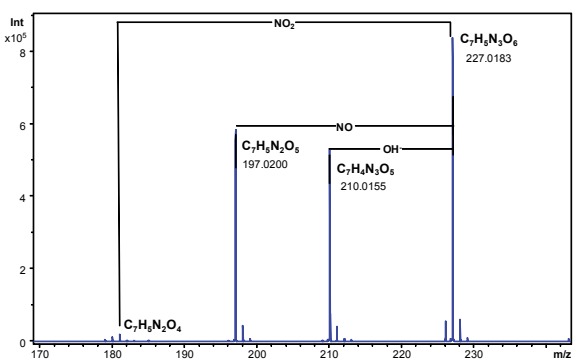
## GC-APCI

The GC-APCI source enables the combination of LC-QTOF MS with both LC and GC. The micrOTOF-Q III system provides exact mass accuracy and resolving power to expand the horizon for GC-MS based analyses. Data acquisition rates of 20Hz and faster are mandatory for typical GC peak widths of < 2 s (FWHM). The unambiguous formula ID from the GC-TOF-MS run is determined using SmartFormula™.

### Compass OpenAccess job results

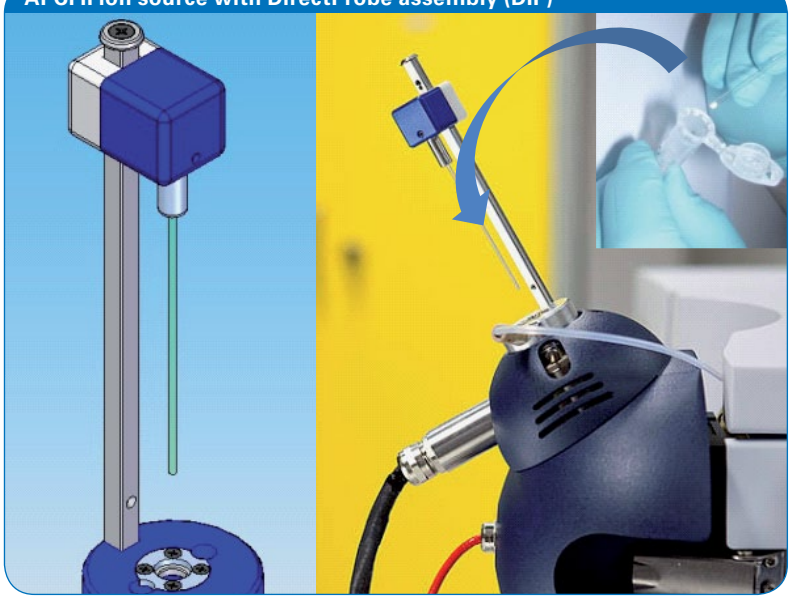

| Sample | ExpectedFormula | Project | meas. m/z | theo. m/z | \|err\|[ppm] | sigma | Review |
|---|---|---|---|---|---|---|---|
| Oxybutynin | C22H31NO3 | XW1 | 358.237543 | 358.237670 | 0.356 | 0.005 | |
| Terfenadine | C32H41NO2 | XW2 | 472.320032 | 472.321006 | 2.063 | 0.006 | |
| Erythromycin | C37H67NO13 | XW3 | 734.467653 | 734.468518 | 1.177 | 0.006 | |
| Sulfadimethoxine | C12H14N4O4S | SU1 | 311.079894 | 311.080852 | 3.081 | 0.002 | |
| Sulfachloropyridazine | C10H9ClN4O2S | SU2 | 285.020004 | 285.020750 | 2.618 | 0.007 | |
| Sulfamethizole | C9H10N4O2S2 | SU3 | 271.031605 | 271.031793 | 0.695 | 0.004 | |
| Sulfamethazine | C12H14N4O2S | SU4 | 279.090340 | 279.091023 | 2.448 | 0.001 | |
| Oxybutynin | C22H31NO3 | XW1 | 358.236997 | 358.237670 | 1.879 | 0.002 | |
| Oxybutynin | C22H31NO3 | XW1 | 358.237377 | 358.237670 | 0.819 | 0.004 | |
| Terfenadine | C32H41NO2 | XW2 | 472.321037 | 472.321006 | 0.066 | 0.011 | |
| Erythromycin | C37H67NO13 | XW3 | 734.467581 | 734.468518 | 1.276 | 0.004 | |

### Compound ID of TNT




Negative ion APCI spectra of the explosive TNT measured on an DirectProbe API-TOF system. Here, the accurate mass values allow the direct verification of the compound and its fragment ions.

### APCI II ion source with DirectProbe assembly (DIP)



The DirectProbe assembly (left) is an add-on to the Bruker APCI II ion source. Sample preparation involves simply dipping the disposable glass capillary (green) into the solid or liquid sample and sliding it into the APCI II source where vaporization and ionization takes place.

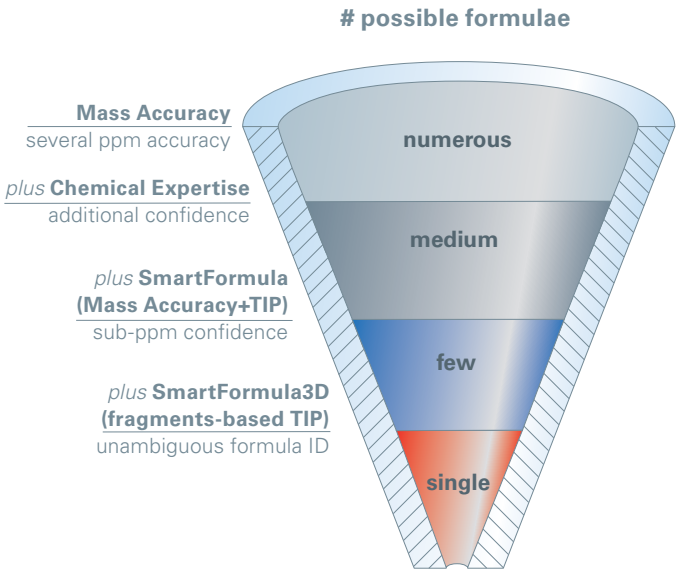
## SmartFormula determination

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.

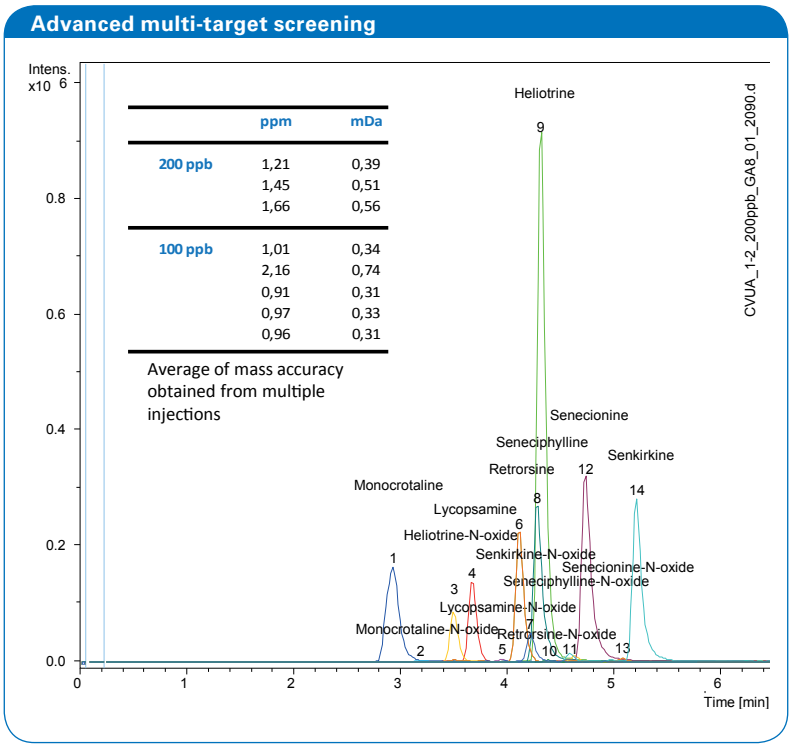
This valuable sub-ppm confidence is available for formula determination in pharmaceutical impurity analysis, metabolite identification, pesticide screening and toxicology & doping analysis.




## Advanced multi-target screening

Confident quantitative and qualitative multi-target screening for forensics, doping control and residue analysis. Due to a full-scan accurate-mass approach in combination with application specific high-quality screening libraries thousands of compounds are identified and confirmed by SmartFormula3D from 1 single LC-ESI-TOF run.

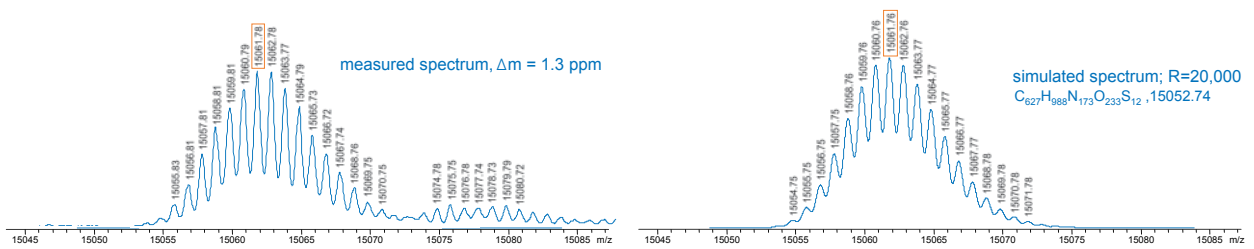
Retrospective *in-silico* screening for new or unexpected compounds is possible because, unlike in triple-quad based MRM methods, the full molecular information content is retained.




High resolution chromatogram (hrXIC) identifying Pyrrolizidin-Alkaloides 200 ppb each in honey.

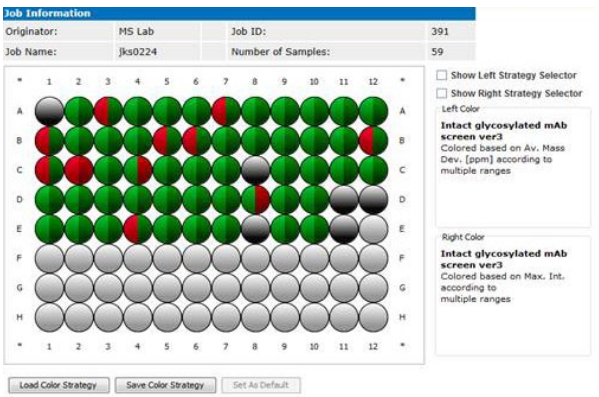
# Top-Down Analysis of Intact Proteins and Antibodies

**Intact protein mass resolution**

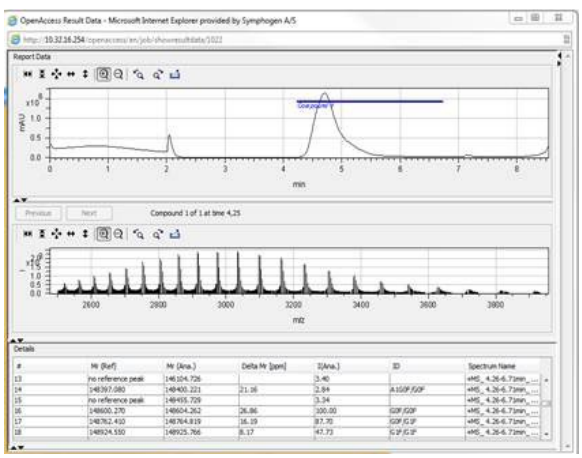



Ribonuclease B. A spectrum of the intact protein acquired with the micrOTOF-Q III. The mass difference to the calculated mass is only 1.3 ppm. A resolution of > 20,000 FWHM is achieved.

**BioPharma Compass results**




**Reports and data accessible from Internet Browser**



## Automated analysis of monoclonal antibodies

Result view of the intact mass workflow for identity testing of discovery mAbs.

The identity of 54 different antibodies coming out of discovery are confirmed here.

Color coding defined by user. Shown here according to average mass accuracy of 50 ppm (left) and an intensity of 3000 counts in the deconvoluted spectrum. For gray, the reference mass was not yet available.

Raw data are available from the Compass OpenAccess server immediately after the analysis, and are accessible to all with a password to the server. In addition, the quantitative data can be exported to Excel.

Data with courtesy of Symphogen A/S, Lyngby, Denmark

# Technical Specifications

## Best in its class performance

- Proven micrOTOF-Q technology
- Class-leading combination of mass accuracy, resolution and sensitivity without compromise
- SmartFormula3D, the unique combination of accurate mass and true isotopic pattern of both, parent and fragment ions
- Wide dynamic range for ultra-stable accurate mass
- High-transmission dual ion funnel Q-q-front end
- Dimensions 640 x 949 x 1320 mm, weight 160 kg

## Source options

- APCI atmospheric pressure chemical ionization source
- APPI atmospheric pressure photo ionization source
- Direct probe option
- Direct GC coupling
- CryoSpray Source
- CaptiveSpray NanoElectrospray source
- CE/MS coupling with grounded ESI needle

## Analytical performance

- Mass range 20 – 40,000 m/z
- Mass accuracy 1 - 2 ppm RMS Error
- Mass resolution 20,000 (FWHM) at LC-speed
- Advanced temperature compensation
- Up to 40 Hz Acquisition rate (2GSample/sec sampling rate)

## Compass & application software suites

- Integrated LC-MS/MS control and data processing
- Compass OpenAccess: Walk-up LC-MS chemical formula generation
- MetaboliteTools™ – metabolite and impurity identification
- TargetAnalysis™ – multi-target compound screening
- ProfileAnalysis™ – LC-MS based profiling and label-free quantitation
- ProteinScape™ – the bioinformatics platform

Support of – HPLC and sample inlet systems from the following vendors:

Bruker nano-Advance LC, Advion TriVersa, NanoMate, Agilent, Dionex, Shimadzu, VWR/Hitachi, Waters (incl. UPLC), Autosamplers from CTC

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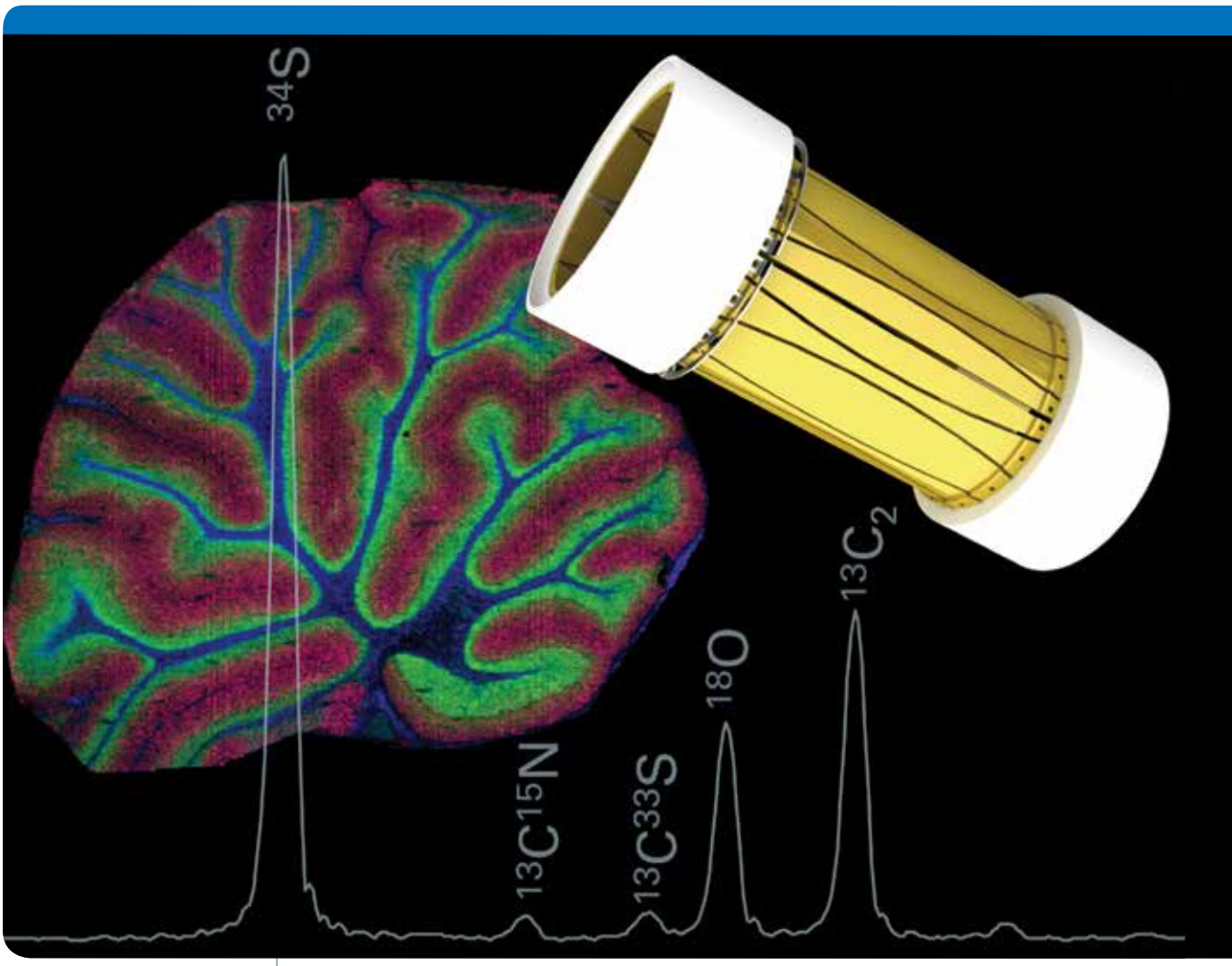
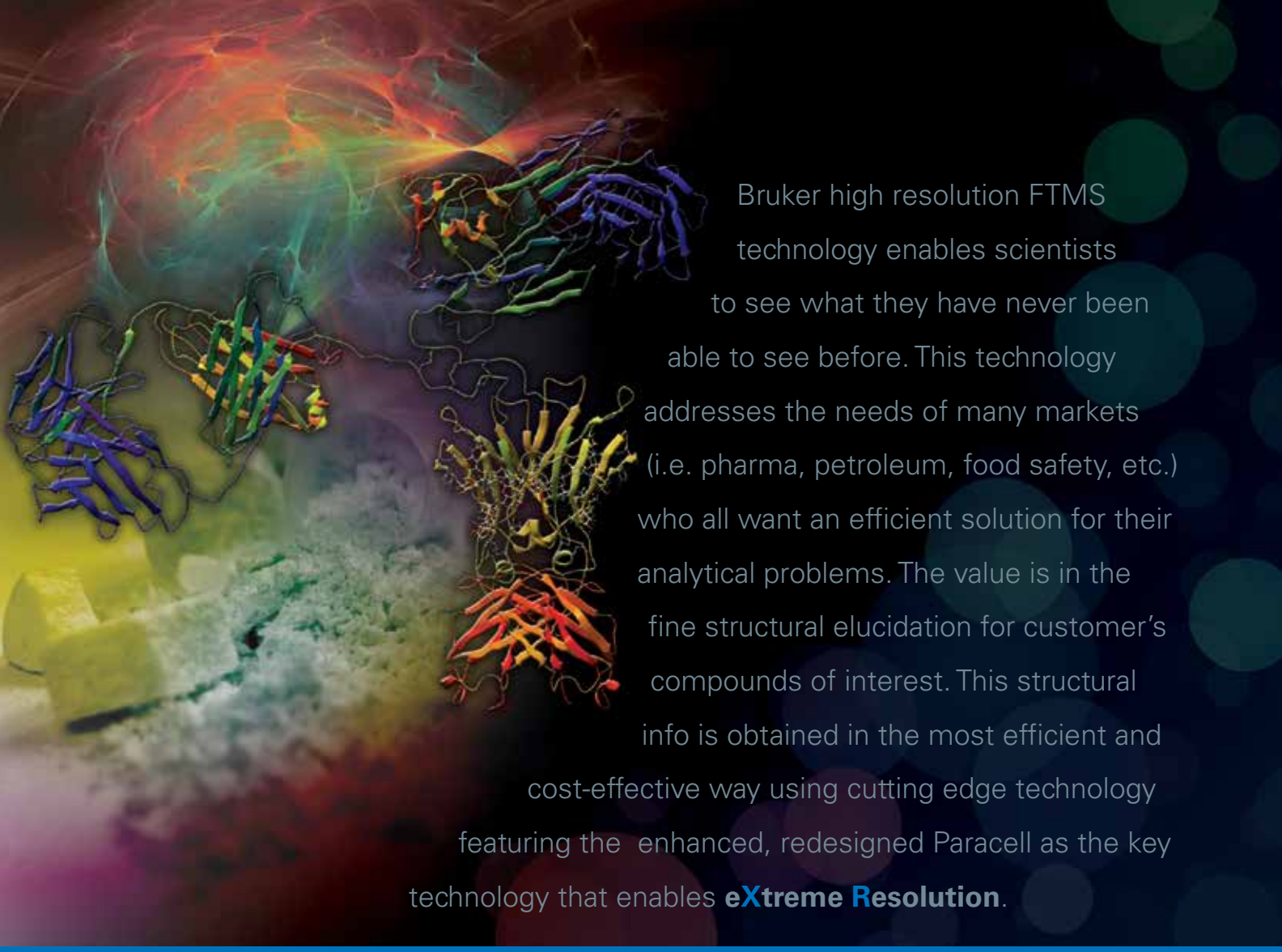



# solarıx XR

- A New Era in Mass Spectrometry

Qq-FTMS

Innovation with Integrity



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**eXtreme Resolution** is the ability of the **solariX** to provide "razor thin" peaks in the mass spectrum resulting in significantly greater information content and peak capacity. **eXtreme Resolution** enables interrogation of complex mixtures or compounds very close in mass without the need for spatial separation providing simpler and more efficient analytical workflows. This is achieved with a combination of technological breakthroughs introduced in the **solariX XR**.

# Key Benefits

- ***Analytical power***—unmatched in commercial mass spectrometry provides the capability to create new workflows and explore the chemical landscape in ways not conceivable before.

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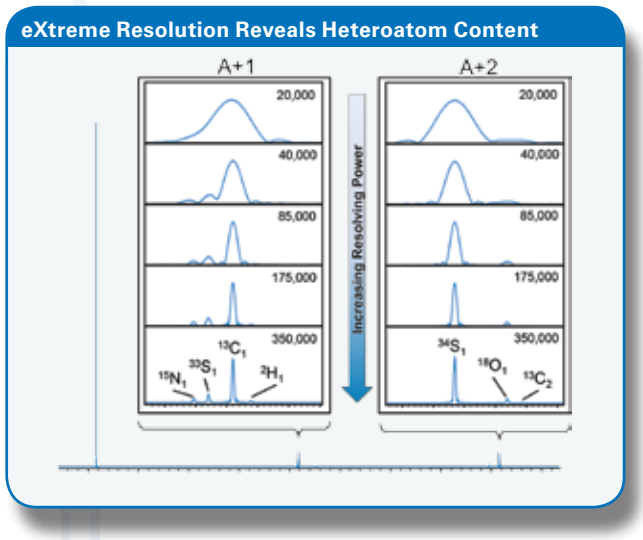


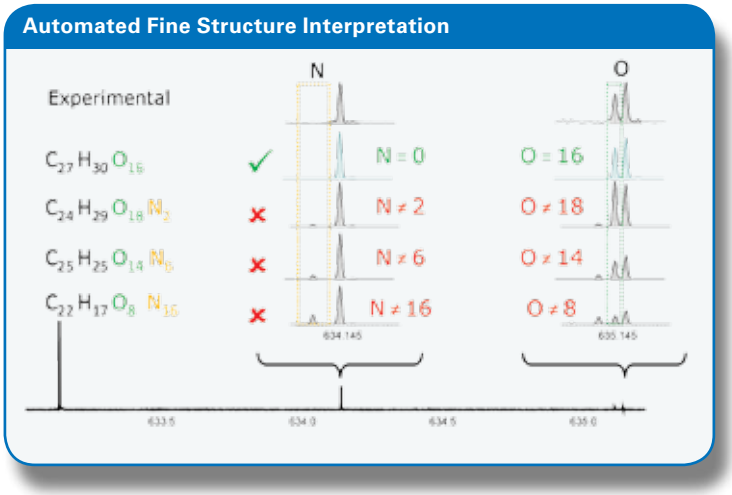


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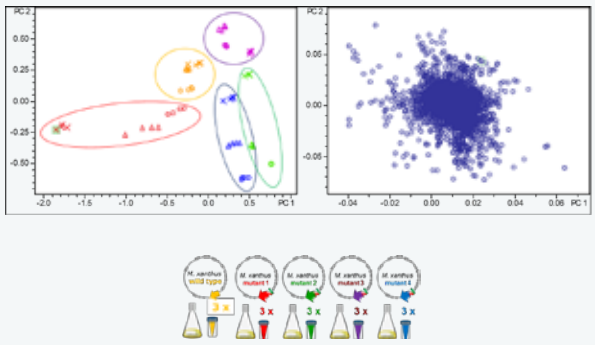

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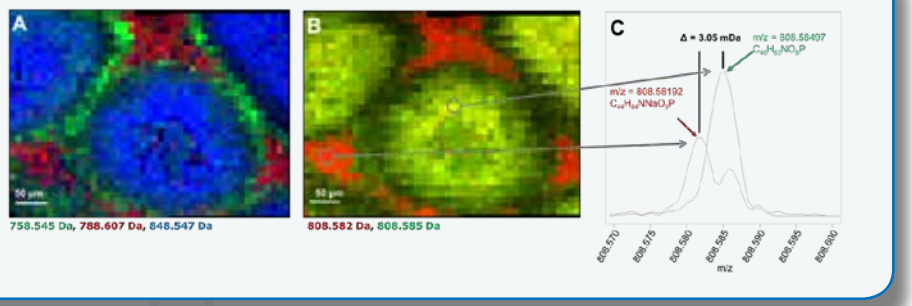


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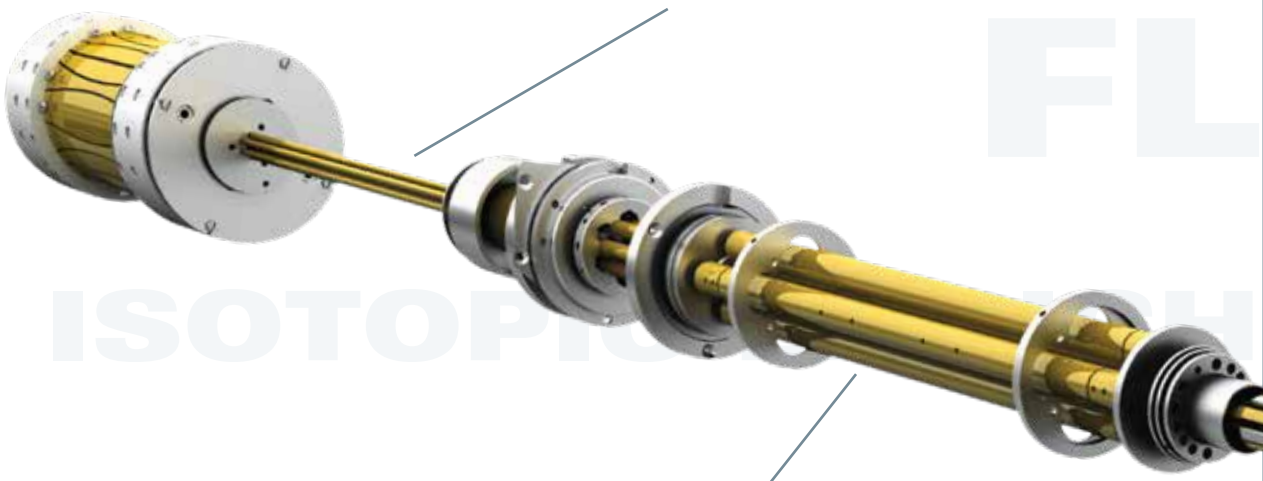

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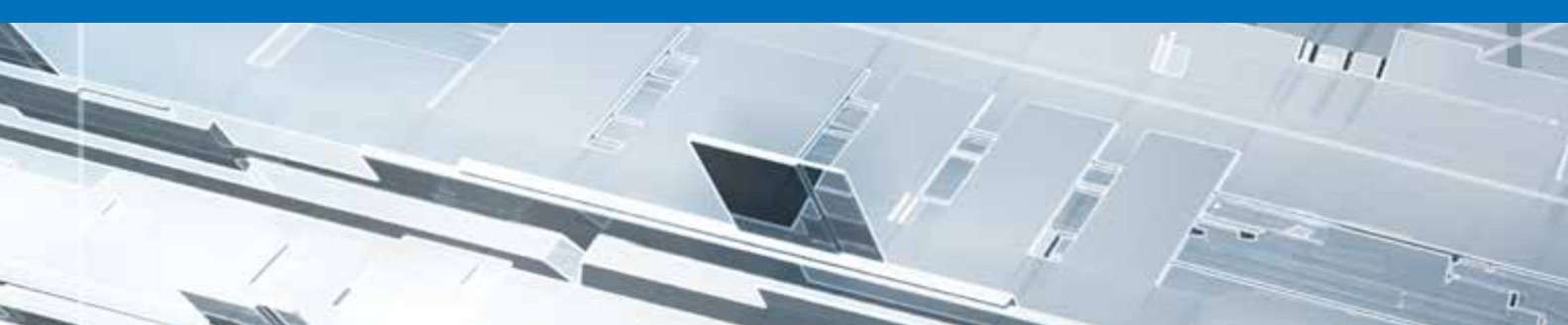

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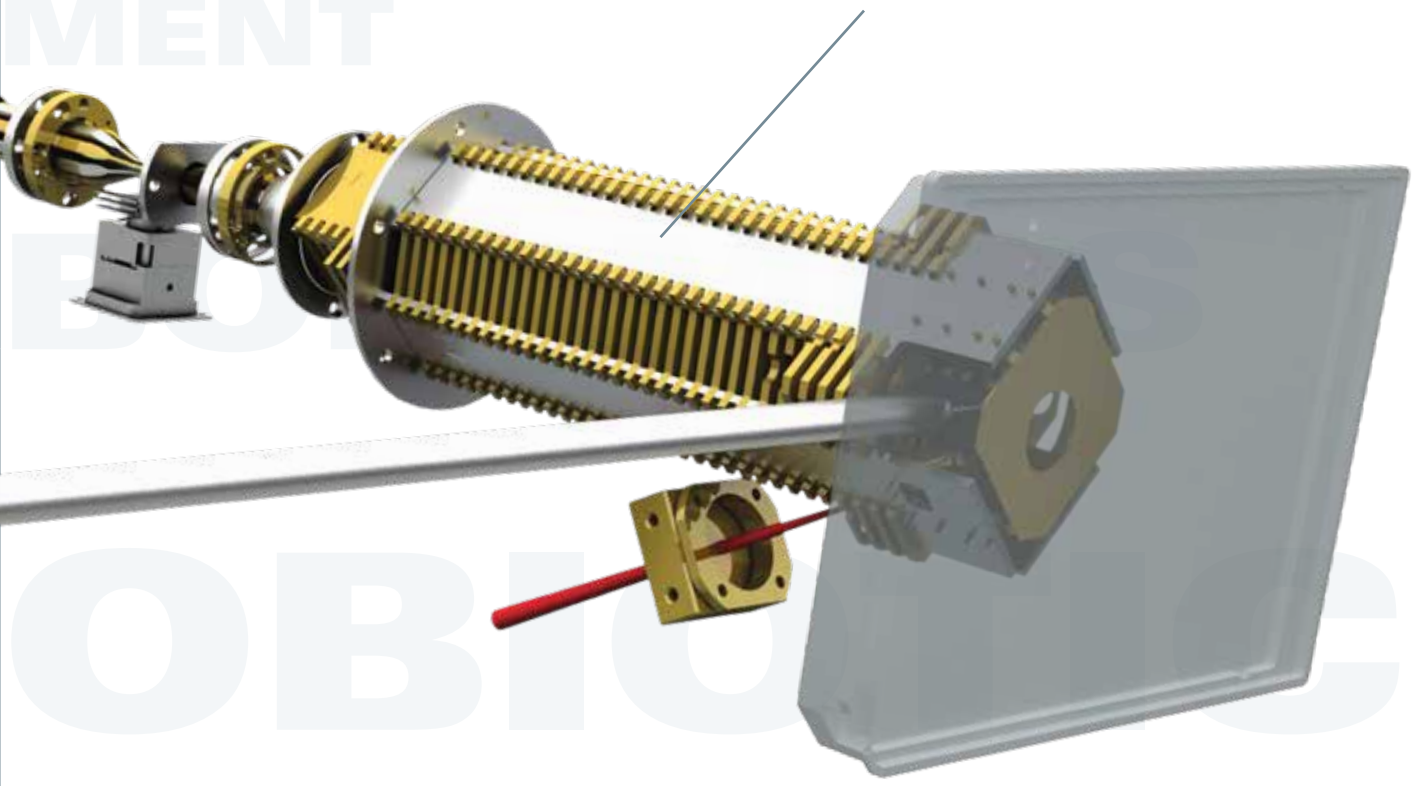

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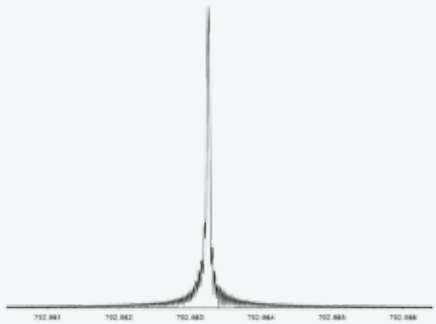

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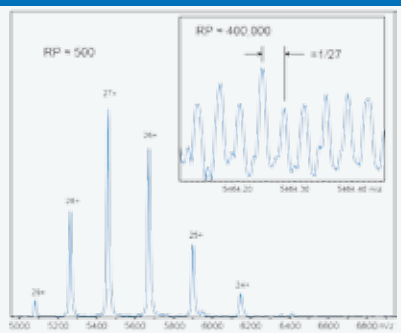
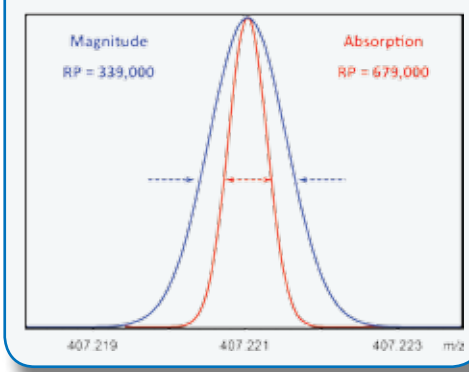



**~700,000 Resolving Power at 1 Hz Duty Cycle**




Whether it is increasing the duty cycle or providing additional resolving power, Absorption Mode Processing (AMP) comes with no cost in processing/acquisition time and can provide resolving power in excess of 650,000 at m/z 400 in a 1 second scan.

# Simple, Efficient, and Dramatically Robust

The dual stage ion funnel innovates through simplicity. Reducing the number of tunable DC elements means ***easy operation*** by switching samples and polarity without the need for additional tuning.

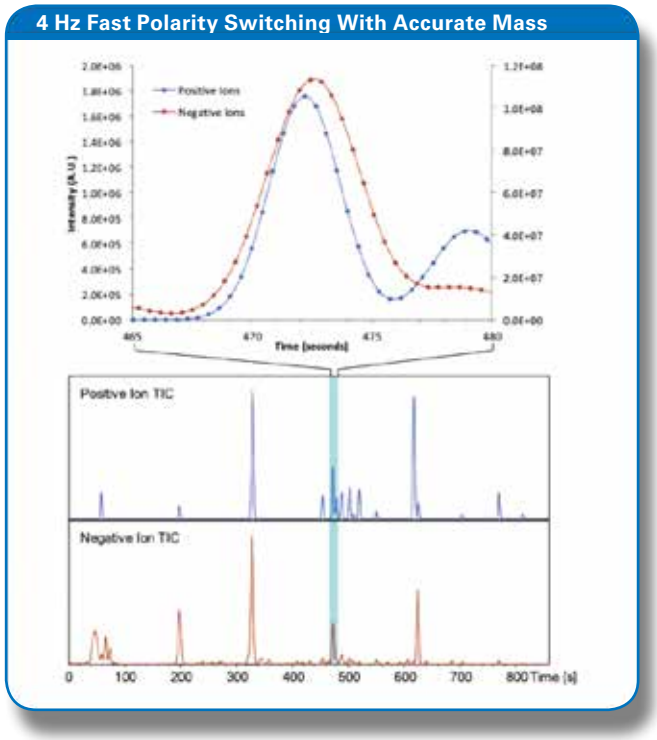
The ***robust*** orthogonal design also eliminates the need for frequent cleaning as contaminants are directed away from the ion optics and removed from the system. Less tuning and ***more uptime*** means more concentrating on what matters most.

MALDI has never been easier as the target sits coincidentally in the beam path with the API source, "switching" sources is a thing of the past providing maximum throughput for methods that involve both MALDI and ESI.

## Fast polarity switching

### Fastest in the industry for high mass accuracy

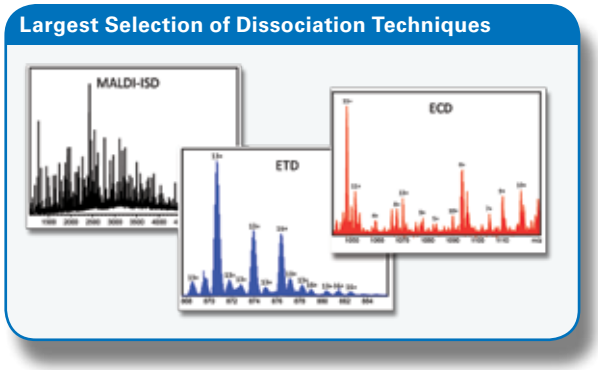
"***Zero Delay Alternating Polarity***" adds to the overall efficiency by providing a 4 Hz polarity switching capability at mass accuracies typical of ultra high performance mass spectrometers, providing the only solution to ultra high resolution and high mass accuracy polarity switching.

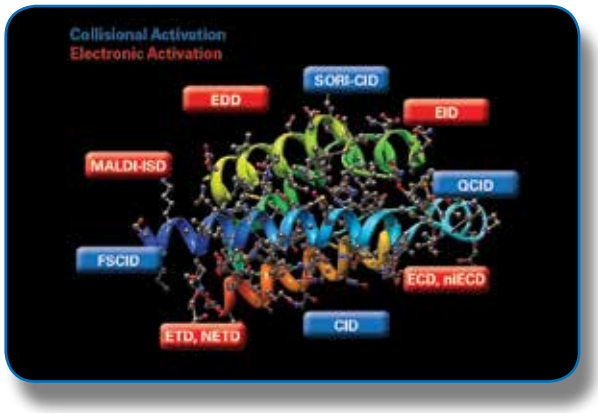


# Flexible Biomolecule Analysis

The new solariX XR is the most ***flexible*** mass spectrometry platform for the characterization of biomolecules. The solariX XR platform offers:

- The ***largest variety*** of collisional- and electron-dissociation techniques available on any mass spectrometry platform.
- ***Highest mass accuracy*** and ***resolving power*** of all mass spectrometers.
- ***Wide m/z range***, from m/z 100 – 10,000.
- Wide variety of ***ion sources***, including MALDI, ESI, nanoESI, APPI, and APCI.

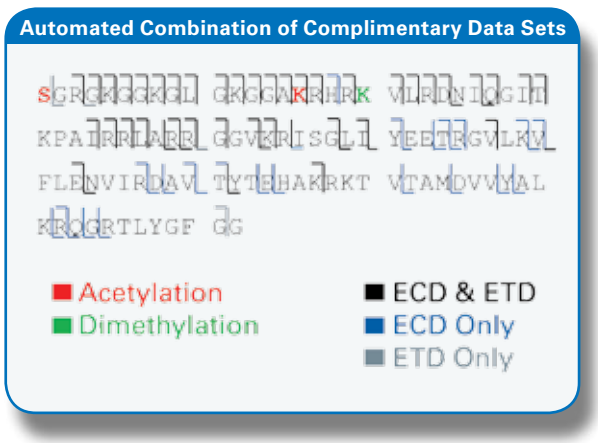



## Automated data processing

***Automated*** processing rapidly characterize the complex, often overlapping dissociation products.

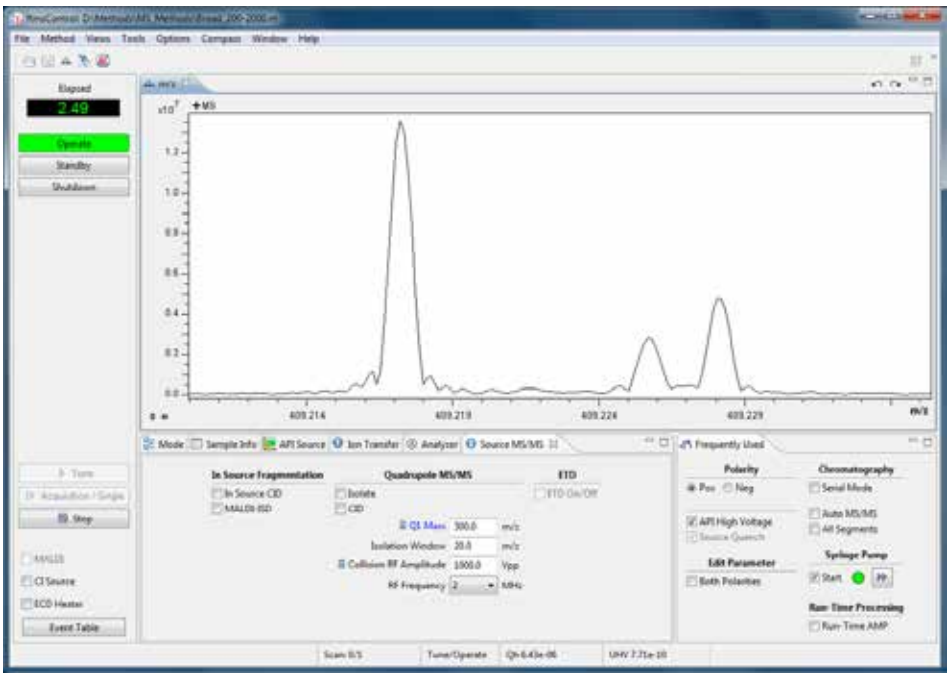
- Monoisotopic m/z and charge deconvolution.
- Quickly ***combine data sets*** from multiple dissociation techniques into an accurate picture of biomolecule sequence, structure, and modifications.



# Dynamic Source Configuration

In addition to the included MALDI and ESI sources, **solariX XR** supports a wide range of source options from Bruker and third party vendors, all switchable within seconds.


## New easy-to-use software to complete the newest innovations



## ftmsControl Features:

- Absorption mode processing
- Accumulation during detection
- Online data reduction
- Online calibration
- Online readback traces
- +/- mode calibration
- User customizable workspaces
- Integrated system diagnostics

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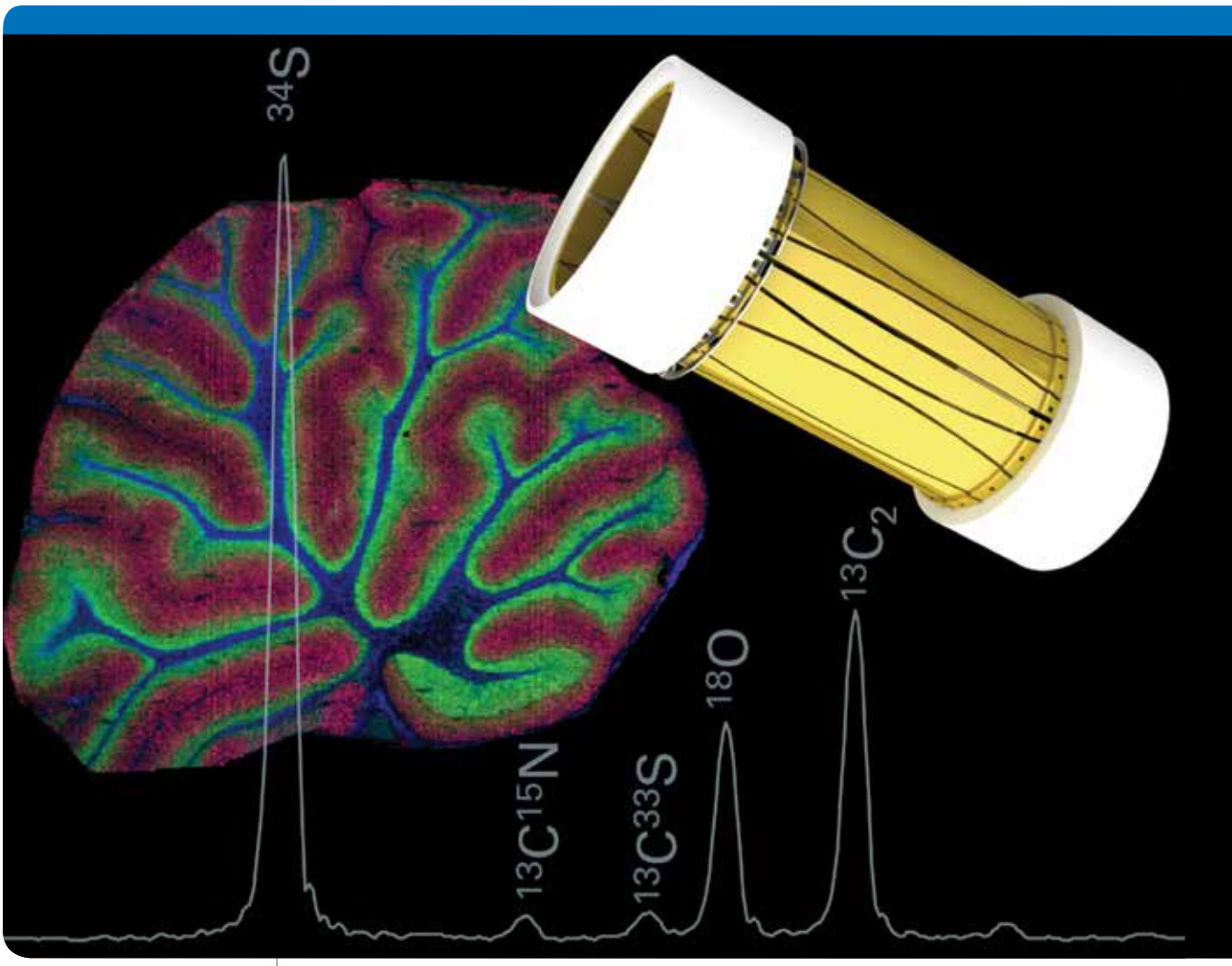


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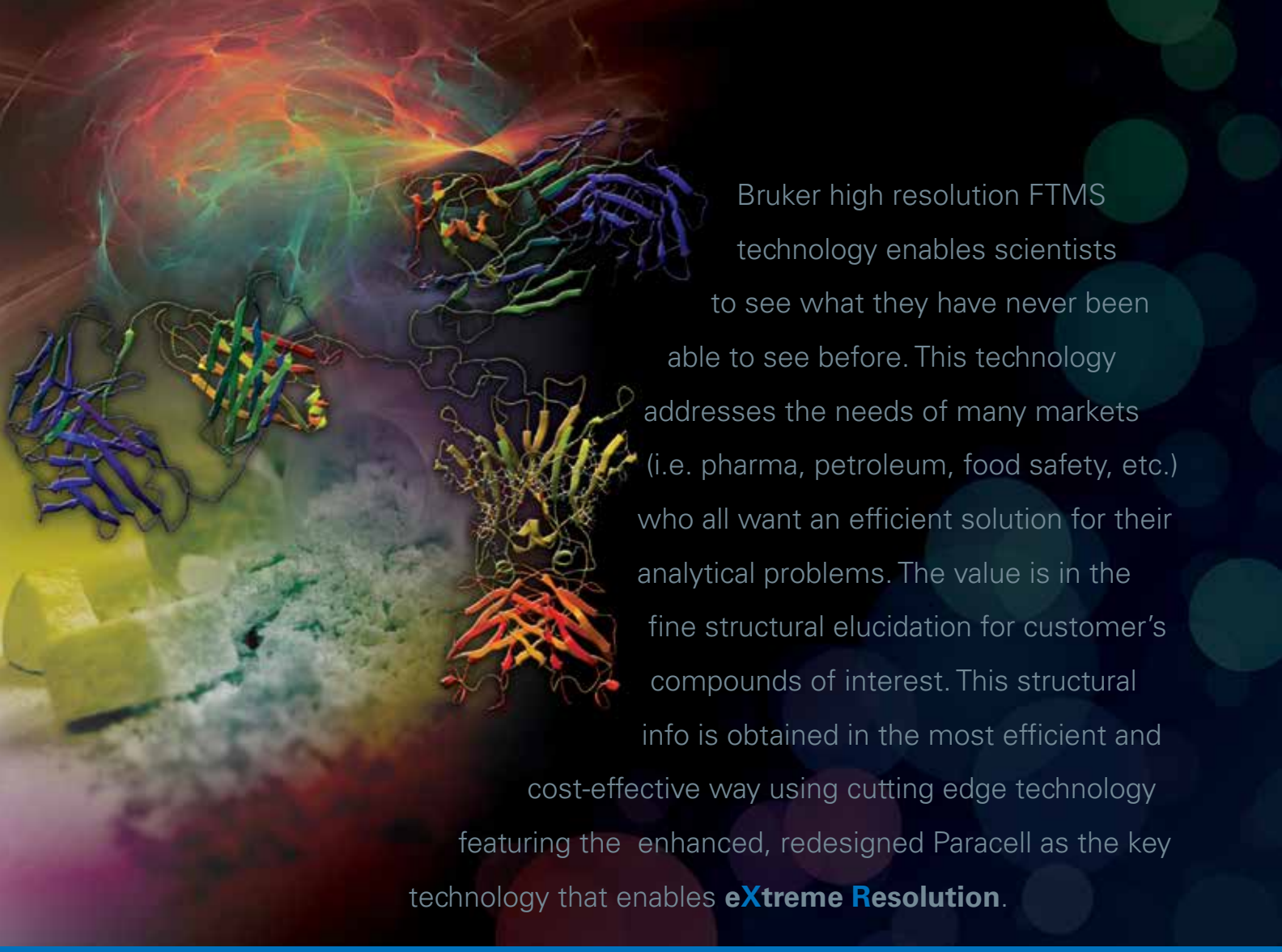

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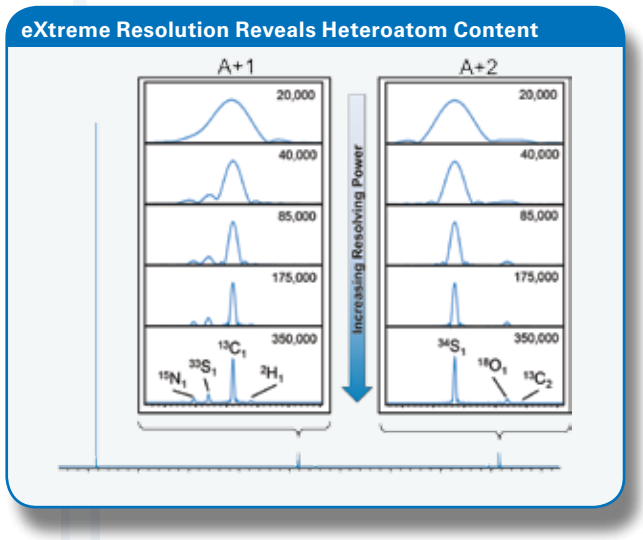


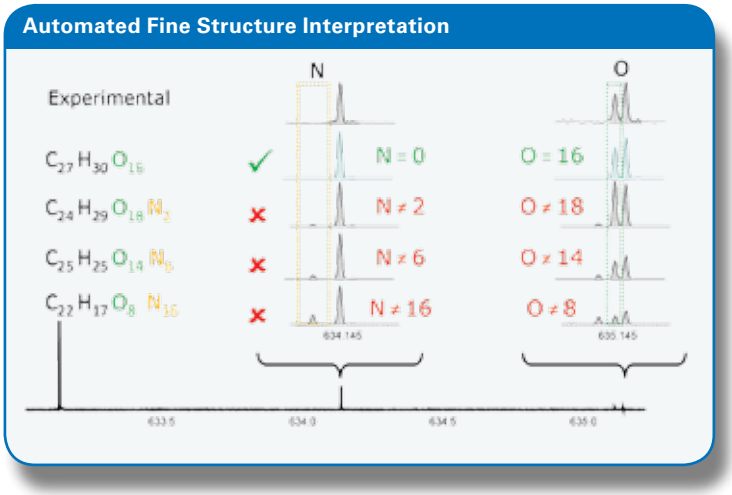


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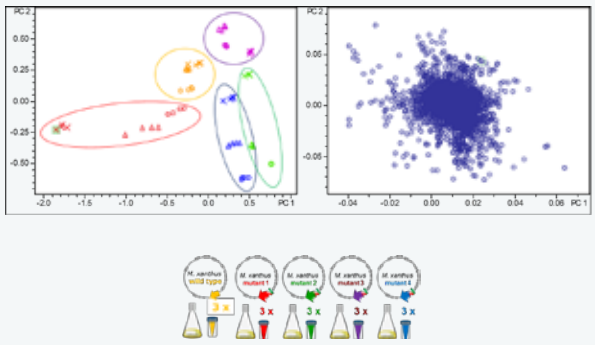

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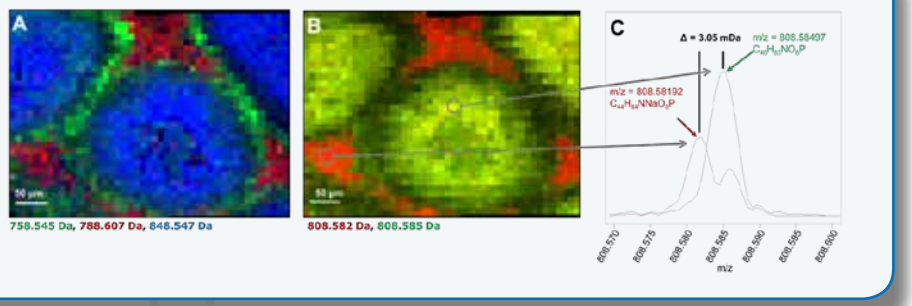


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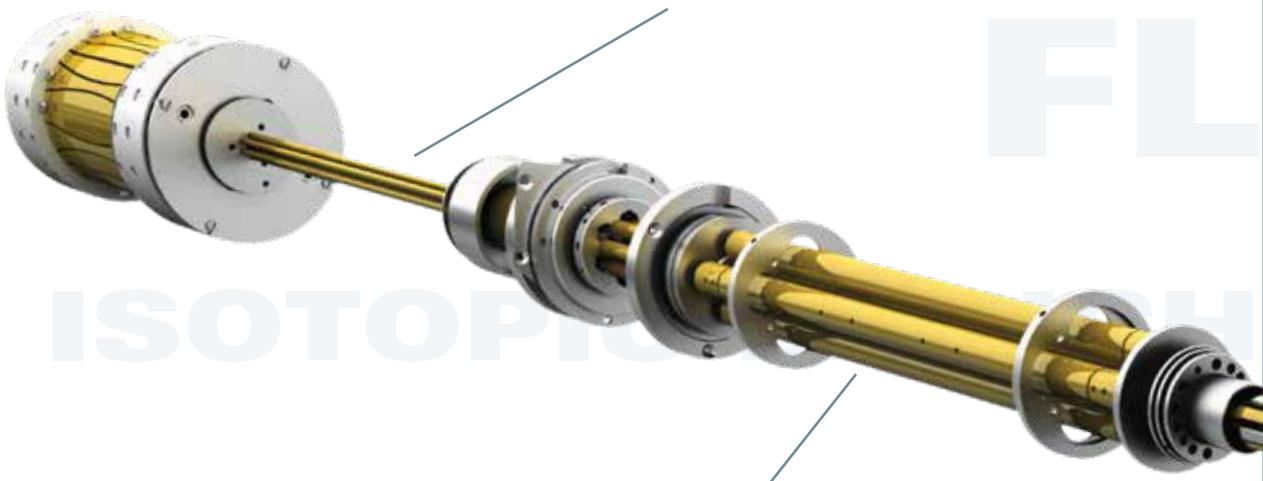

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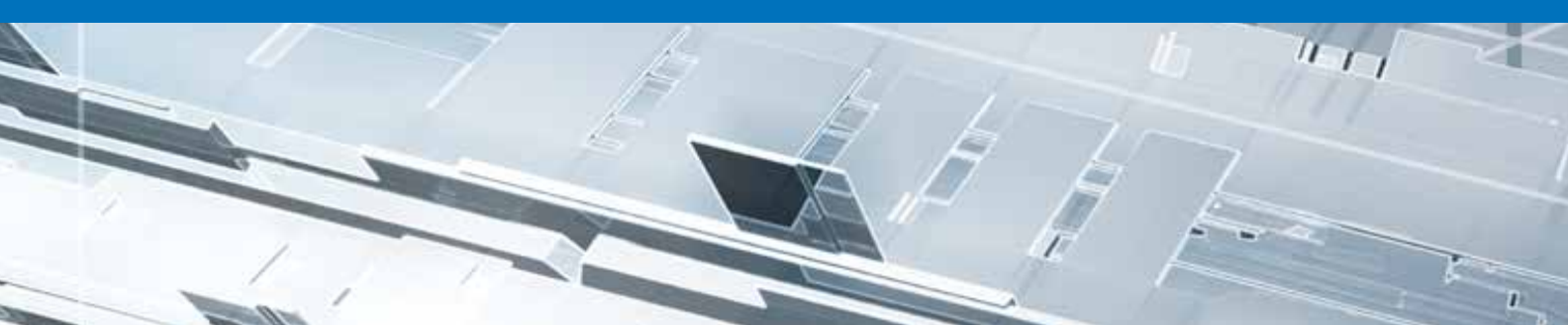

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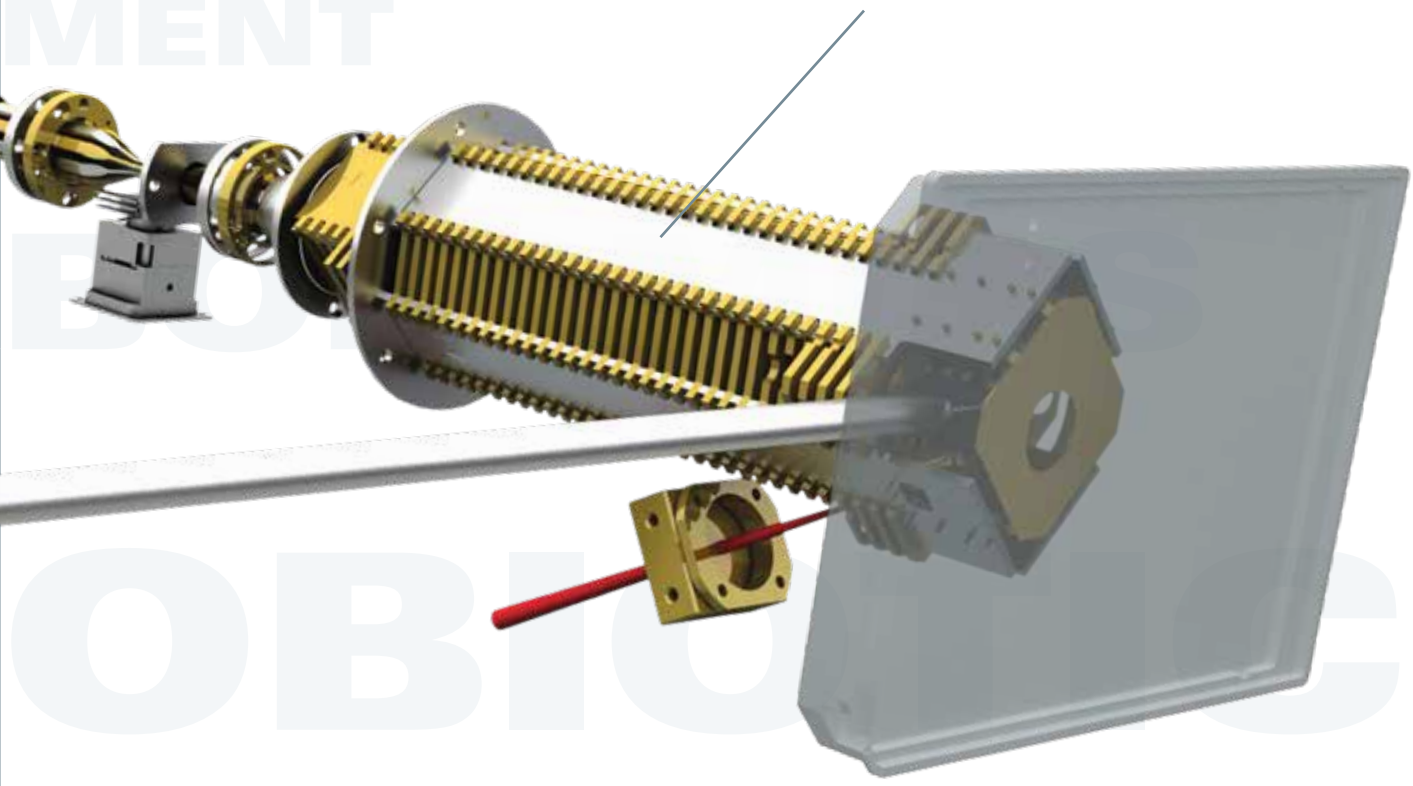

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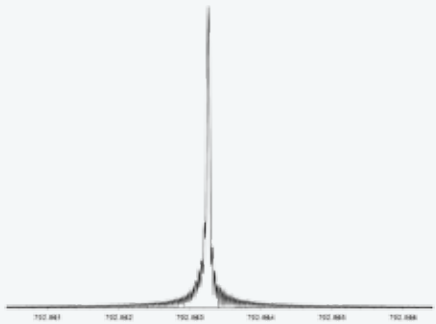

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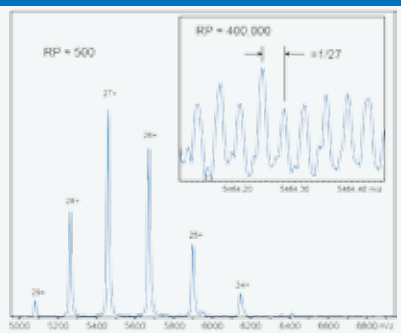
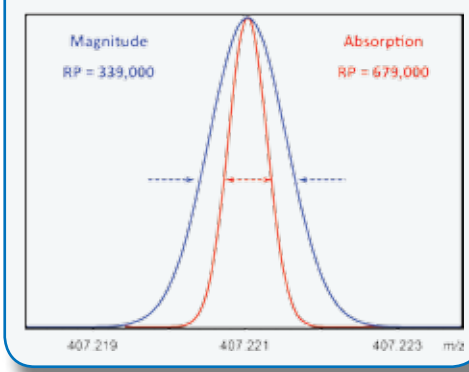



**~700,000 Resolving Power at 1 Hz Duty Cycle**




Whether it is increasing the duty cycle or providing additional resolving power, Absorption Mode Processing (AMP) comes with no cost in processing/acquisition time and can provide resolving power in excess of 650,000 at m/z 400 in a 1 second scan.

# Simple, Efficient, and Dramatically Robust

The dual stage ion funnel innovates through simplicity. Reducing the number of tunable DC elements means ***easy operation*** by switching samples and polarity without the need for additional tuning.

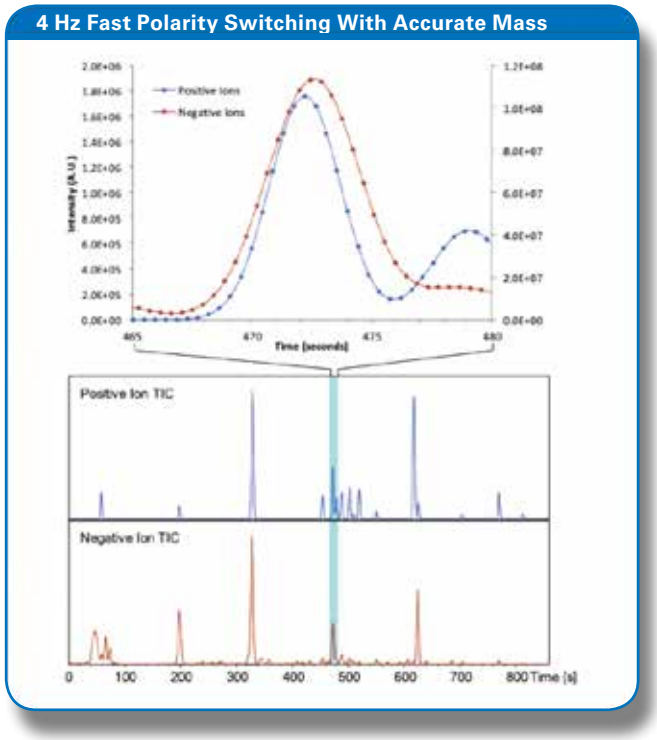
The ***robust*** orthogonal design also eliminates the need for frequent cleaning as contaminants are directed away from the ion optics and removed from the system. Less tuning and ***more uptime*** means more concentrating on what matters most.

MALDI has never been easier as the target sits coincidentally in the beam path with the API source, "switching" sources is a thing of the past providing maximum throughput for methods that involve both MALDI and ESI.

## Fast polarity switching

### Fastest in the industry for high mass accuracy

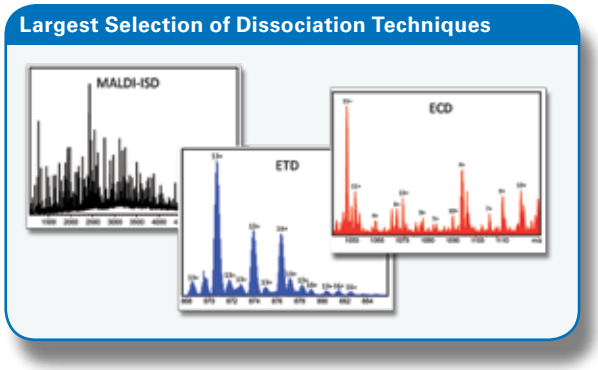
"***Zero Delay Alternating Polarity***" adds to the overall efficiency by providing a 4 Hz polarity switching capability at mass accuracies typical of ultra high performance mass spectrometers, providing the only solution to ultra high resolution and high mass accuracy polarity switching.

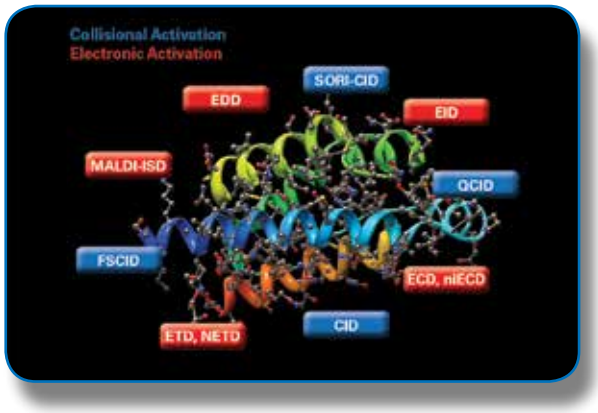


# Flexible Biomolecule Analysis

The new solariX XR is the most ***flexible*** mass spectrometry platform for the characterization of biomolecules. The solariX XR platform offers:

- The ***largest variety*** of collisional- and electron-dissociation techniques available on any mass spectrometry platform.
- ***Highest mass accuracy*** and ***resolving power*** of all mass spectrometers.
- ***Wide m/z range***, from m/z 100 – 10,000.
- Wide variety of ***ion sources***, including MALDI, ESI, nanoESI, APPI, and APCI.

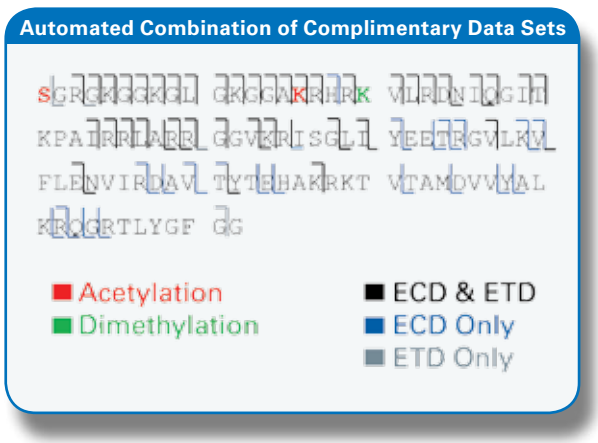



## Automated data processing

***Automated*** processing rapidly characterize the complex, often overlapping dissociation products.

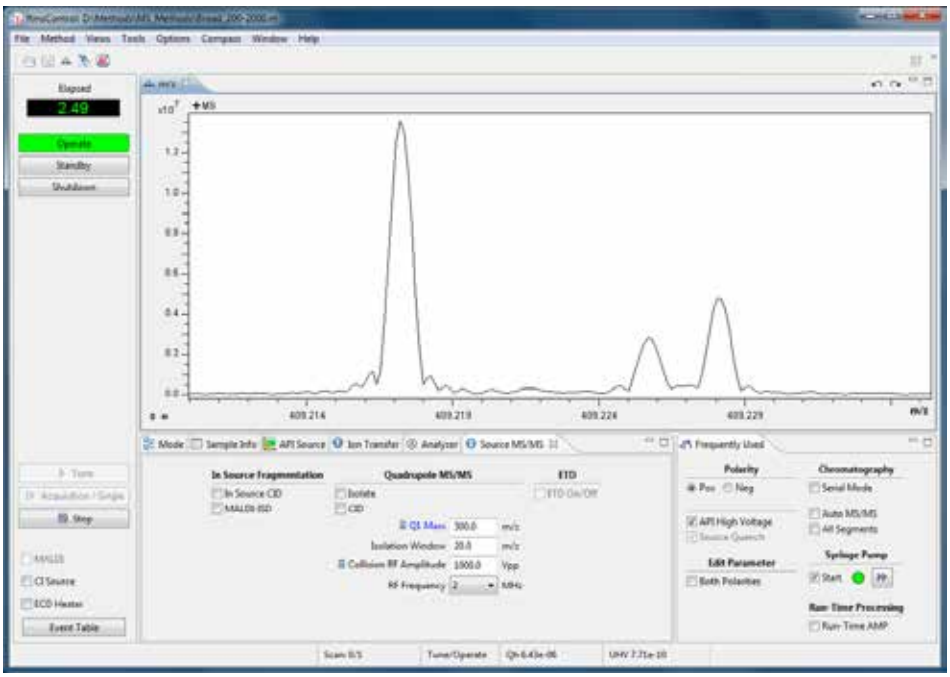
- Monoisotopic m/z and charge deconvolution.
- Quickly ***combine data sets*** from multiple dissociation techniques into an accurate picture of biomolecule sequence, structure, and modifications.



# Dynamic Source Configuration

In addition to the included MALDI and ESI sources, **solariX XR** supports a wide range of source options from Bruker and third party vendors, all switchable within seconds.


## New easy-to-use software to complete the newest innovations



## ftmsControl Features:

- Absorption mode processing
- Accumulation during detection
- Online data reduction
- Online calibration
- Online readback traces
- +/- mode calibration
- User customizable workspaces
- Integrated system diagnostics

For research use only. Not for use in diagnostic procedures.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Coming soon!

BRUKER

# MALDI Biotyper Galaxy

Automated target preparation system for use with the MALDI Biotyper


- **Quality Control**
  Using patented light sensor technology the system scans the target positions before and after matrix is deposited, ensuring that each spot is optimally prepared for the MALDI Biotyper workflow.
- **Traceability**
  Seamless integration with the MALDI Biotyper server coupled with on-board barcode reading ensures that target plates are matched to their corresponding projects using both the barcode and a date/time stamp.
- **Reproducibility**
  A two channel micro volume delivery system not only facilities support for the extended direct transfer method, but also ensures that the correct volume of matrix is added to each spot thus minimizing the need for further processing of samples.

## Completing the workflow ... Pilot your way to the NEW Galaxy !


### Multiple Work Benches Supported

Each work bench can access the server using the Satellite software and create projects.

### Completely Barcode Driven Workflow

Target barcodes are automatically read by the system and the associated project downloaded from the MALDI Biotyper server.

### Traceability Always Assured

Just like the Galaxy, the prepared MALDI target barcode is automatically read by the MALDI Biotyper system and the matching project is selected and processed.


**For further information and availability in your country please contact your local Bruker office.**

MALDI Biotyper Galaxy: For research use only. Not for use in diagnostic procedures.

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# 450-GC

**Specification Sheet**

### Dimensions and Weights
Size*: Height: 53 cm (20.9 in.),
Width: 66 cm (26.0 in.),
Depth: 56 cm (22.0 in.)
Weight*: 43 kg (95 lb)
* Typical values

### Environmental Conditions
Operating temperatures: 10 °C to 40 °C.
Operating humidity (relative): 5 % to 95 %
Line voltage requirements: 101 V, 120 V, 230 V
(±10 % nominal)

### Column Oven
Dimensions: 28 cm (w) x 20 cm (d) x 28 cm (h)
Temperature range:
- Ambient +4 °C to 450 °C
- With liquid $N_2$: -100 °C to 450 °C
- With liquid $CO_2$: -60 °C to 450 °C

Temperature program ramps/holds: 24/25
Maximum temperature ramp rate: 120 °C/min for all voltages
Cool down rate: 400 °C to 50 °C in 4.5 minutes
Temperature set-point resolution: 1 °C

### General Specifications
GC Control:
- External events (digital output):
  - 7 standard
  - 8 optional
- Max number of timed events: 15 x 99
- Heated zones: 7 (including column oven)

Methods:
- Maximum stored methods: 50 (max 30 alphanumeric characters)

Logging:
- Run log file (stored with the chromatogram when using Galaxie™ or MS Workstation)
- Error log file

- Local Display:
  - TFT full color screen
  - VGA resolution (640 x 480)
  - Size 8.4" (20 cm)


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- Local Control:
  - Touch screen
  - Hard keys

- Languages: English, German, French, Spanish, Italian, Portuguese, Cyrillic, Kanji, Chinese, Thai and Korean (Other languages on request)

Local automation:
- Method lines: 25
- Modes:
  - Infinite looping
  - Dual and duplicate injection

System operational qualities:
- High Inertness: sample path UltiMetal treated, optional
- Low level detection assurance: purged valves, optional

### Communication

Ethernet: Protocol: TCP/IP
Data rate: 100 Mbps
Control: GC control and method parameters
Analog output (optional):
- Number of channels: 3
- Time programmable steps: 25
- Output (set individual):
  - 0-1 V (default)
  - 0-10 V

Synchronization signals with other devices and data systems:
- Ready in
- Start out

Data Handling and System control:
- GC: Galaxie™ Chromatography Data System (CDS)
- GC/MS: MSWS (see the GC/MS brochure and datasheet for more information)

### Certifications

- CSA:
  - C22.2 61010-1
  - UL 61010-1
- IEC: 61010-1
- EMC:
  - 47 CFR part 15
  - ANSI C63.4
  - EN 61326

### Injector Options

Maximum injectors: three, operating concurrently
Pneumatics: Electronic Flow Control (EFC), or manual
Injector types:
- 1177 S/SL Split/Splitless injector
- 1079 PTV Programmable Temperature Vaporizing
- 1093 COC Cold On-Column injector
- 1061 Flash injector
- 1041 PWOC Packed/Wide bore On-Column injector


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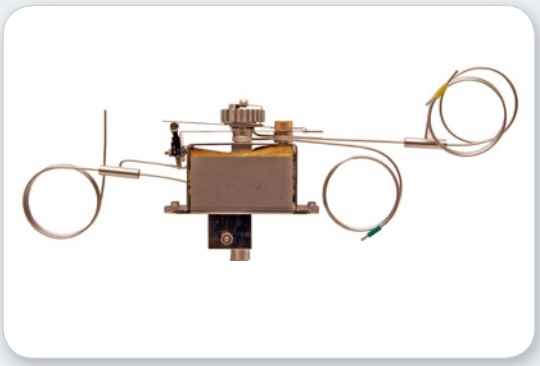
### 1177 S/SL Split/Splitless Injector
Pressure range: 0-150 psi
Total flow: 500 mL/min at 10 psi
1500 mL/min at 10 psi (He)
Maximum temperature: 450 °C
Split range: 1-10,000 (column dependent)

Suited for columns:
- Wide bore: (0.53 mm)
- Narrow bore: (0.05 to 0.32 mm)



1177 S/SL Injector

### 1093 COC Cold On-Column Injector
Pressure range: 0-150 psi
Total Flow: 50 mL/min (Type 23 EFC)
500 mL/min (Type 24 EFC)

Temperature range:
- Ambient +10 °C to 450 °C using air cooling
- -60 °C to 450 °C using liquid $CO_2$ cooling
- -160 °C to 450 °C using liquid $N_2$ cooling

Maximum temperature: 450 °C
Maximum temperature ramp rate: 200 °C/min
Temperature ramps/holds: 24/25

Suited for columns:
- Wide bore (0.53 mm)
- Narrow bore (0.32 mm)

### Sample Preconcentration Trap (SPT)
Trace level analysis of volatiles in gases
Fully integrated

Temperature range:
- -60 °C to 450 °C using liquid $CO_2$ cooling
- -185 °C to 450 °C using liquid $N_2$ cooling

Temperature rate:
- Ballistic for instant release of adsorbed volatiles

Available traps:
- Two lengths
- A wide range of standard packings and custom packings

### Quick-Switch Valve Option
Instantly switch between injectors/columns and detectors
Configurations: automated or manual, factory or field installed

### 1079 PTV Programmable Temperature
Vaporizing Injector
Pressure range: 0-150 psi
Total flow: 500 mL/min at 10 psi

Temperature range:
- Ambient + 10 °C to 450 °C using air cooling
- -160 °C to 450 °C using liquid $N_2$ cooling
- -60 °C to 450 °C using liquid $CO_2$ cooling

Maximum temperature ramp rate: 200 °C/min
Temperature ramps/holds: 24/25
Split range: 1-10,000 (column dependent)

Operational modes:
- Large volume injection
- Temperature ramped splitless
- Cold on-column
- Split and splitless
- ChromatoProbe solid sample introduction optional

Suited for columns:
- Wide bore (0.53 mm)
- Narrow bore (0.05 to 0.32 mm)

Maximum injection volume: 250 µL (LVI mode)

PFPD Detector

### 1061 Flash Injector

Pressure range: 0-150 psi

Total flow:
- 50 mL/min (Type 23 EFC)
- 500 mL/min (Type 24 EFC)

Maximum temperature: 450 °C
Suited for columns:
- Wide bore (0.53 mm)
- Packed (1/8 " to 1/4 ")

### 1041 PWOC Packed/Wide-bore On-Column Injector

Pressure range: 0-150 psi
Total flow: 50 mL/min (Type 23 EFC)
500 mL/min (Type 24 EFC)
Maximum temperature: 450 °C

Suited for columns:
- Wide bore (0.53 mm)
- Packed (1/8 " to 1/4 ")

### Electronic Flow Control: Injectors (EFC)

Module types: 4 injector-specific modules
Pressure: 0.1 % Full Scale
Flow: 0.5 % Full Scale and 3% Measured Value
Resolution: 0.1 psi or 0.1 mL/min

### Detector Options

Maximum detectors: three: operating concurrently
Pneumatics: Electronic Flow Control (DEFC) or manual

Detector types:
- FID Flame Ionization Detector
- TCD Thermal Conductivity Detector
- ECD Electron Capture Detector
- TSD (NPD) Thermionic Specific Detector
- PFPD Pulsed Flame Photometric Detector
- PDHID Pulsed Discharge Helium Ionization Detector
- MS Mass Spectrometry
  (see GC/MS brochure and datasheet)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### FID Flame Ionization Detector

Maximum temperature: 450 °C
Detectivity: 2 pg °C/sec
Linear dynamic range: $10^7$

Flame tip type: ceramic (patented)
Operational quality:
- Flame-out detection
- Auto re-ignition

### TCD Thermal Conductivity Detector

Maximum temperature: 450 °C
Detectivity: 300 pg/mL (Butane)
Linear dynamic range: $10^6$

Operational quality:
- Filament protection
- Automatic bridge balancing

### ECD Electron Capture Detector

Maximum temperature: 450 °C
Detectivity: 7 fg/s Lindane
Linear dynamic range: $10^4$
Radioactive source: 63Ni - 15 mCi (555 Mbq)

### TSD Thermionic Specific Detector

Maximum temperature: 450 °C

Detectivity:
- N: 100 fg N/sec (Azobenzene)
- P: 100 fg P/sec (Malathion)

Linear dynamic range:
- N: $10^5$
- P: $10^4$

Operational quality: self-aligning bead

### PFPD Pulsed Flame Photometric Detector

Photomultiplier tube:
- S/P
- S/P/N

Maximum temperature: 450 °C

Detectivity:
- S: 1 pg S/sec (S/P tube)
- P: 100 fg P/sec (S/P tube)
- N: 20 pg N/sec (S/P/N tube)

Linear dynamic range:
- S: $10^3$
- P: $10^4$
- N: $10^2$

Up to 23 elements can be detected


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### PDHID Pulsed Discharge Helium Ionization Detector

Detectivity: 50 ppb (Methane)
Linear dynamic range: $10^4$ (Methane)
Operational quality:

- Gold plated connections
- Welded column connections

### Detectors (DEFC)

Module types: 6 detector-specific modules
Accuracy: ± 7 % set point flow
Resolution: 0.1 or 1 mL/min

### Automation Options

### CP-8410 Auto Injector

Sample capacity:

- 10 x 2 mL vials
- 6 x 5 mL vials
- 5 x 10 mL vials

Large solvent wash vial: 2 x 120 mL*
Dual and duplicate mode
Internal standard addition

Modes of operation:

- Liquid
- Ambient headspace*
- SPME (Solid Phase MicroExtraction)*
- Sample heating and cooling*

Pre-programmed modes of injection Syringes:

- 1 µL, 2 µL, 5 µL, 10 µL, 100 µL, 250 µL for liquid injection
- SPME

### CP-8400 AutoSampler

Sample capacity: 100 x 2 mL vials
Large solvent wash vial: 2 x 120 mL*
Dual and duplicate mode
Internal standard addition

Modes of operation:

- Liquid
- Ambient headspace*
- SPME*
- Sample heating and cooling*

Pre-programmed modes of injection

Syringes:

- 1 µL, 2 µL, 5 µL, 10 µL, 100 µL, 250 µL for liquid injection
- SPME

* Optional


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**Combi PAL AutoSampler**
Sample trays: two standard and expandable to four
Tray types:
- 98 x 2 mL vials
- 200 x 1 mL vials
- 32 x 10 mL/20 mL vials
- 96-well plates

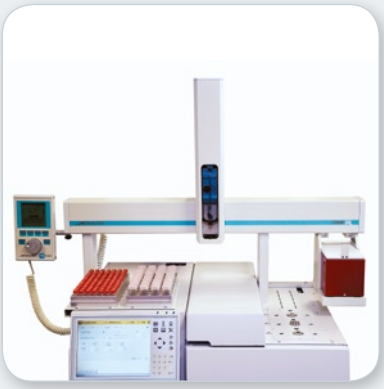
Dual and duplicate mode
Internal standard addition

Modes of operation:
- Liquid
- Heated headspace*
- SPME*

Sample heating and cooling
Optional modules: additional sample trays, micro-well plate holders, wash station, SPME fiber bake-out station, dilutor, barcode readers, and flowcell

* Optional

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



For laboratories requiring even greater sample throughput or more extensive sample preparation automation options, Bruker offers the CombiPAL system.

The CP-8400. Automatic access to two injection ports allows you to double your throughput. These can be installed in addition to gas or liquid Sample injection valves for optimum flexibility.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# SCION 456-GC

**Specification Sheet**

### Dimensions and Weights
Size*: Height: 57 cm (22.5 in.)
Width: 66 cm (26.0 in.)
Depth: 56 cm (22.0 in.)
Weight*: 43 kg (95 lb)
* Typical values

### Environmental Conditions
Operating temperatures: 10 °C to 40 °C.
Operating humidity (relative): 5 % to 95 %
Line voltage requirements:, 120 V, 230 V (±10 % nominal)

### Column Oven
Dimensions: 28 cm (w) x 20 cm (d) x 28 cm (h)
Temperature range:
- Ambient +4 °C to 450 °C
- Liquid $N_2$: -100 °C to 450 °C
- Liquid $CO_2$: -60 °C to 450 °C

Temperature program ramps/holds: 24/25
Maximum temperature ramp rate: 150°C/min for all voltages and 180 °C/min with oven insert accessory

| Temperature Range (°C) | 456-GC Rates (°C/min) |
|---|---|
| 50 -70 | 150 |
| 70 - 115 | 95 |
| 115 - 175 | 70 |
| 175 - 300 | 45 |
| 300 - 450 | 30 |

Cool down rate: 400 °C to 50 °C in 4.5 minutes
Temperature set-point resolution: 0.1 °C
Ambient temperature reject <0.01°C change in oven for 1°C change in ambient temp
Retention time Repeatability <0.008% or < 0.0008 min, based on Pentadecane under temperature program conditions
Area repeatability < 1% RSD

### General Specifications
Up to 9 EFC modules total, injector, detector and auxiliary
Optional backflush
GC Control:
- External events (digital output):
  - 8 standard
  - 8 optional, total 16
- Max number of timed events: 16
- Heated zones:
  - Standard 5
  - 4 optional, 9 total
- Two power outlets 24V (1A max. each)

Methods:
- Maximum stored internal methods: 50 (max. 30 alphanumeric characters)


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Logging:
- Run log file (stored with the chromatogram when using CompassCDS)
- Error log file

Local Display:
- TFT full color screen
- WVGA resolution (800 x 480)
- Size 23 cm (9")

Local Control:
- Touch screen
- Hard keys

Languages:
- English, German, French, Spanish, Italian, Portuguese, Cyrillic, Kanji, Chinese (standard and traditional), Thai, Korean and Dutch.

Local automation:
- Method lines: 25
- Modes:
  - Infinite looping
  - Dual and duplicate injection

**Communication**

Ethernet: Protocol: TCP/IP
Data rate: 100 Mbps
Control: GC control and method parameters
Analog output (optional):
- Number of channels: 3
- Time programmable steps: 30
- Output software selectable (set individual):
  - 0-1 V (default)
  - 0-10 V

Synchronization signals with other devices and data systems:
- Ready in and out
- Start in and out

Data Handling and System Control:
- CompassCDS Chromatography Data System

**Certifications**
- CSA:
  - C22.2 61010-1
  - UL 61010-1
- IEC: 61010-1
- EMC:
  - 47 CFR part 15
  - ANSI C63.4
  - EN 61326


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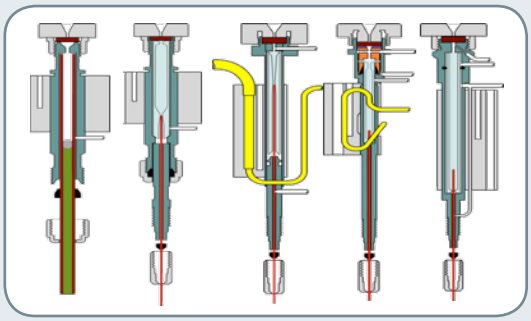
### Injector Options

Maximum injectors: three, operating concurrently
Pneumatics: Electronic Flow Control (EFC), or manual
Injector types:

- S/SL Split/Splitless injector*
- PTV Programmable Temperature Vaporizing*
- COC Cold On-Column injector*
- Flash injector
- PWOC Packed/Wide bore On-Column injector

*Including septum purge



### S/SL Split/Splitless Injector

Pressure range: 0-150 psi
Total flow:

- 500 mL/min for $N_2$/Ar
- 1500 mL/min for He/$H_2$

Maximum temperature: 450 °C
Split range: 1-10,000 (column dependent)

Suited for columns:

- Wide bore: (0.53 mm)
- Narrow bore: (0.05 to 0.32 mm)

### COC Cold On-Column Injector

Pressure range: 0-150 psi
Total Flow: 50 mL/min (Type 23 EFC)

Temperature range:

- Ambient +10 °C to 450 °C using air cooling
- -60 °C to 450 °C using liquid $CO_2$ cooling
- -160 °C to 450 °C using liquid $N_2$ cooling

Maximum temperature: 450 °C
Maximum temperature ramp rate: 200 °C/min
Temperature ramps/holds: 24/25

Suited for columns:

- Wide bore (0.53 mm)
- Narrow bore (0.32 mm)

### PTV Programmable Temperature

Vaporizing Injector
Pressure range: 0-150 psi
Total flow:

- 500 mL/min for N2/Ar
- 1500 ml/min for He/H2

Temperature range:

- Ambient + 10 °C to 450 °C using air cooling
- -160 °C to 450 °C using liquid $N_2$ cooling
- -60 °C to 450 °C using liquid $CO_2$ cooling

Maximum temperature ramp rate: 200 °C/min
Temperature ramps/holds: 24/25
Split range: 1-10,000 (column dependent)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Operational capabilities:
- Large volume injection
- Temperature ramped splitless
- Cold on-column
- Split and splitless
- ChromatoProbe solid sample introduction optional

Suited for columns:
- Wide bore (0.53 mm)
- Narrow bore (0.05 to 0.32 mm)

Maximum injection volume: 250 µL (LVI mode)

**Flash Injector**

Pressure range: 0-150 psi
Total flow:
- 50 mL/min (Type 23 EFC)

Maximum temperature: 450 °C
Suited for columns:
- Wide bore (0.53 mm)
- Packed (1/8" to 1/4")

**PWOC Packed/Wide-bore On-Column Injector**

Pressure range: 0-150 psi
Total flow:
- 50 mL/min (Type 23 EFC)

Maximum temperature: 450 °C

Suited for columns:
- Wide bore (0.53 mm)
- Packed (1/8" to 1/4")

**Electronic Flow Control: Injectors (EFC)**

Module types: 4 injector-specific modules
Pressure: 0.1 % Full Scale
Resolution pressure set points is 0.001psi
Flow sensor accuracy 2% of measured or 0.2% of full scale
Flow sensor repeatability 0.5%

**Sample Preconcentration Trap (SPT)**

Trace level analysis of volatiles in gases
Fully integrated

Temperature range:
- -60 °C to 450 °C using liquid $CO_2$ cooling
- -185 °C to 450 °C using liquid $N_2$ cooling

Temperature rate:
- Ballistic for instant release of adsorbed volatiles

Available traps:
- Two lengths
- A wide range of standard packings and custom packings


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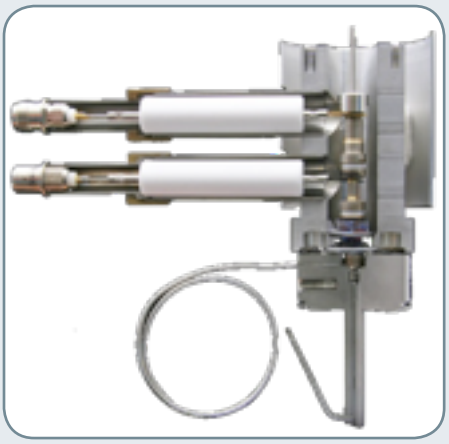

### Quick-Switch Valve Option
Instantly switch between injectors/columns and detectors
Configurations: automated or manual, factory or field installed

### Detector Options
Maximum detectors: four: operating concurrently (one of which is a Single or Triple Quad MS)
Pneumatics: Electronic Flow Control (DEFC) or manual

Detector types:
- FID Flame Ionization Detector
- TCD Thermal Conductivity Detector
- ECD Electron Capture Detector
- NPD (TSD) Nitrogen-Phosphorus Detector
- PFPD Pulsed Flame Photometric Detector
- PDHID Pulsed Discharge Helium Ionization Detector
- MS Mass Spectrometry (see GC/MS brochure and datasheet)

Note: Data Acquisition Rate : 600Hz for all detectors, exception is the PFPD

### FID Flame Ionization Detector
Maximum temperature: 450 °C
Detectivity: 2 pg C/sec
Linear dynamic range: $10^7$

Flame tip type: ceramic (patented)
Operational quality:
- Flame-out detection
- Auto re-ignition

### TCD Thermal Conductivity Detector
Maximum temperature: 450 °C
Detectivity: 300 pg/mL (Butane)
Linear dynamic range: $10^6$

Operational quality:
- Filament protection
- Automatic bridge balancing

### ECD Electron Capture Detector
Maximum temperature: 450 °C
Detectivity: 7 fg/sec Lindane
Linear dynamic range: $10^4$
Radioactive source: 63Ni - 15 mCi (555 Mbq)

### NPD (TSD) Nitrogen-Phosphorus Detector
Maximum temperature: 450 °C
Detectivity:
N: 100 fg N/sec (Azobenzene)
P: 100 fg P/sec (Malathion)

Linear dynamic range:
- N: $10^5$
- P: $10^4$

Operational quality: self-aligning bead

### PFPD Pulsed Flame Photometric Detector

Photomultiplier tube:
- S/P
- S/P/N

Maximum temperature: 450 °C

Detectivity:
- S: 1 pg S/sec (S/P tube)
- P: 100 fg P/sec (S/P tube)
- N: 20 pg N/sec (S/P/N tube)

Linear dynamic range:
- S: $10^3$
- P: $10^4$
- N: $10^2$

Up to 23 elements can be detected

### PDHID Pulsed Discharge Helium Ionization Detector

Detectivity: 50 ppb (Methane)
Linear dynamic range: $10^4$ (Methane)
Operational quality:
- Gold plated connections
- Welded column connections

### Detectors (DEFC)

Module types: 6 detector-specific modules
Accuracy: ± 7 % set point flow
Resolution: 0.1 or 1 mL/min

### Automation Options

### CP-8410 Auto Injector

Sample capacity:
- 10 x 2 mL vials
- 6 x 5 mL vials
- 5 x 10 mL vials

Large solvent wash vial: 2 x 120 mL*
Dual and duplicate mode
Internal standard addition

Modes of operation:
- Liquid
- Ambient headspace*
- SPME (Solid Phase MicroExtraction)*
- Sample heating and cooling*

Pre-programmed modes of injection Syringes:
- 1 µL, 2 µL, 5 µL, 10 µL, 100 µL, 250 µL for liquid injection
- SPME


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**CP-8400 AutoSampler**
Sample capacity: 100 x 2 mL vials
Large solvent wash vial: 2 x 120 mL*
Dual and duplicate mode
Internal standard addition

Modes of operation:
- Liquid
- Ambient headspace*
- SPME*
- Sample heating and cooling*

Pre-programmed modes of injection syringes:
- 1 µL, 2 µL, 5 µL, 10 µL, 100 µL, 250 µL for liquid injection
- SPME

* Optional

**PAL Combi-xt AutoSampler**
Sample trays: two standard and expandable to four
Tray types:
- 98 x 2 mL vials
- 200 x 1 mL vials
- 32 x 10 mL/20 mL vials
- 96-well plates

Dual and duplicate mode
Internal standard addition

Modes of operation:
- Liquid
- Heated headspace*
- SPME*
- ITEX*

Sample heating and cooling
Additional optional modules: further sample trays, micro-well plate holders, wash station, SPME fiber bake-out station, dilutor, barcode readers, and flowcell

* Optional


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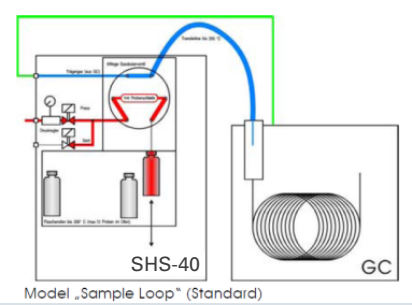
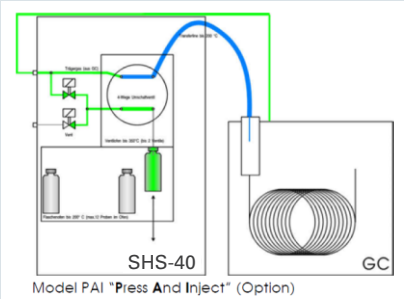
SHS-40 Headspace Sampler

## Fixed Sample Volume Configuration



Model „Sample Loop" (Standard)

## Press and Inject Configuration



Model PAI "Press And Inject" (Option)

## System Features

| | |
|---|---|
| Sample Capacity | Up to 40 vials; 20mL<br>or 10 mL w/adaptor<br>Crimp or Screw Top Vials |
| Injection Modes | Fixed Sample Volume<br>Press and Inject |
| Injection Valve | 6 Way Electric Actuated<br>1 mL Sample Loop<br>Heat up to 350°C |
| Incubator | Up to 12 Samples<br>40-200°C in 1°C increments<br>Integrated Shaker |
| Instrument Control | Remote with Compass CDS<br>Stand alone |
| Sample Recognition and Detection | Automated |
| Carrier Gas Control | Direct from GC |
| Optional Accessories | Additional Sampling Valve<br>Reactant Gas<br>Catalytic Converter |

- Sample Capacity: 40 x 20ml (10ml vials with adaptors).
- Fully integrated
- Sample path inert
- Automated vial queuing system
- Automated Gas Sampling Valve- Electric actuated 6-way injection valve (VICI) with 1 ml sample loop. This entire module may be separately heated up to 350°C.
- Heated incubation oven for 12 samples (40°C - 200°C, in 1°C-steps
- Integrated Shaker
- Automatic sample detection/recognition
- Compatible with Crimp and Screw Top Vials
- Carrier gas controlled direct from the GC
- AUX gas pre-set internally.
- Up to 9 different parameter sets can be stored.
- Adaptable to different injectors
- Multiple Headspace Extraction mode via single puncture
- Flexible transfer line
- Option: Sample Transfer Line Kit (direct connection to carrier gas, insertion of transfer line via injector no longer required)
- Control: Stand alone or remotely via Compass CDS software
- Voltage: 110V or 230V
- Dimensions: Width: 29cm (12in) Height: 46cm (18in) Depth: 62cm (25in)
- Weight: 21kg (47lb)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## Description

# amaZon SL Dual Funnel Ion Trap Mass Spectrometer System

BDAL #294445

**Easy-to-use high performance bench top LCMS system for HPLC detection.**
High performance ion trap with dual funnel ion guide.

## amaZon SL Ion Trap System

**High sensitive small molecule LC/MS$^n$ system with fast polarity switching.**

The amaZon SL is a robust high performance Electrospray Ion Trap Mass Spectrometer for HPLC detection in routine work.

**Compact, small footprint system enclosure for ion trap mass analyzer, ESI source, electronics, and vacuum pumps, containing:**

**A. Bruker research-grade mass analyzer:**

- Advanced multipole **H**igh **C**apacity ion **T**rap for ultra-fast, high-sensitivity scanning with good resolution
- High sensitivity conversion dynode detector with. For positive and negative ion detection.
- Systems enclosure footprint: width 76 cm x depth 91 cm

**B. Robust, computer-controlled APOLLO II electrospray ionization (ESI) source with minimal adjustment and easy maintenance:**

- **Apollo II Electrospray Ionization Source with ion funnel**
- 
- Highly sensitive ESI Source with proprietary ion funnel guide for gentle mass independent ion focusing and high ion transmission efficiency
- ESI source with grounded needle for safety and easy sample introduction and CE-coupling
- Heated counter current drying gas for gentle and efficient drying
- Pneumatic off-axis nebulization for flow rates up to 1 ml/min., with gradients from 100% aqueous to 100% organic
- SW control of flow and heater of counter current N2 drying gas
- SW control of high voltage
- High-sensitivity RF ion guide
- Ion lens system including in Source collision induced dissociation possibility (IS-CID)
- Combined Funnel-Octopole-Cartridge with front access for easy maintenance
- Ion lens housing and vacuum system
- Robust setup with easily cleanable glass capillary
- Positive / negative ion operation
- Fast polarity switching for obtaining data of both ion species in a single LC/MS run
- Divert valve option: User exchangeable valve head to suit nano scale or analytical scale applications
- Suitable for HPLC and U-HPLC coupling

### C. Vacuum System

- Four-stage pumping system for high ion transmission
- Vacuum system equipped with low maintenance split flow drag pump and single mechanical single stage fore line pump (34 $m^3/h$)
- All gas inlets are fully SW controlled
- Software integrated pressure gauges

### D. Research-grade Digital and RF Electronics

- Ultra-stable high-voltage RF generator for high m/z-range
- Low-noise preamplifier for high MS and $MS^n$ sensitivity
- Monoisotopic isolation capability in the m/z range 50-2200

**High-performance and high-throughput features:**

### E. Modes of Operation

- **ultraScan™**Standard Resolution scan from 70-2200 m/z with 32,000 u/sec at 0.6 u FWHM
- **Enhanced Resolution Scan** from 50-2200 m/z with 8,100 u/sec at 0.35 u FWHM
  for isotopic resolution of up to triply charged ions, optimized for both scan speed and resolution
- **Extended scan range:** 200-4000 m/z with a scan speed of 27,000 u/sec

- **SmartICC™** (ion charge control) unique patented ion charge control for optimal ion trap filling and extended dynamic range for quantification without the need of pre-scans.

**Operation modes**

- **$MS^n$ ($n \leq 11$)**
- Selected Reaction Monitoring (**SRM**) and Multiple Reaction Monitoring (**MRM**) for quantitation in complex matrices
- SIM for up to 10 channels
- **Data-depending Auto-MS/MS** and auto-$MS^n$ ($n \leq 5$) for alternating MS and MS/MS detection on-the-fly in HPLC runs. $MS^n$ detection can be applied for a fixed number of ion signals.
-

### F. Syringe pump

- Low pulsation syringe pump
- Fully integrated in GUI
- User exchangeable syringes
- Flow from 50 nl/min to 1.5 ml/min
- Volume control
- Stall detection
- One 500µL syringe included

**G. Data system:**

- Workstation: HP z400 or successor
- Windows XP professional pre-installed on image DVD, US English localization
- prepared for installation into LAN
- 3,0 GHz quad core processor, 1333 MHz front side bus
- 4 GB RAM, 1000 GB hard disk
- DVD+/-RW writer 16x DL LightScribe, DVD-ROM 16x
- 2x Ethernet, optical Mouse, Keyboard, Nero 7 Essentials Suite 1
- easy to use emergency backup software Acronis.
- Monitor: HP LP2205wg 22" TFT wide screen display or successor
- Printer: HP LaserJet P3015p USB+parallel or successor

**H. Applications software: Compass 1.3 SR2 for amaZon**

- Fully integrated software package **Compass 1.3 SR2** for HPLC and Trap control, data acquisition, post processing, and data analysis.

**Consisting of:**

- **trap control 7.0:**
  - **SmartSuite™** for automated optimization of all instrument parameters without the need of expert skills:
    - **Smart Parameter Setting** (SPS): Auto-adjusting of acquisition parameters to a target mass.
    - **SmartCal**: Auto-Calibration
    - **SmartRamp**: Automated tuning (ramping) of all parameters for best performance, used for easy method development
    - **SmartFrag**: Ramps the collision energy for most efficient and reproducible MS/MS fragmentation
    - **Scheduled Precursor List:** allows defining component specific AutoMS(n) experiments based on known retention times of sample compounds.
    - **Smart Time Segment Editor (STS):** Enables intuitive setup of an LC/MS/MS method with optimized acquisition parameters based on an initial LC/MS run
  - **Expert mode**: extended control over instrument parameters for interactive system optimization of sophisticated $MS^n$ methods

- **Data dependent Scans modes:**
  - **ActiveExclusion™**
  - **PassiveExclusion™**
  - Preferred Mass List: contains masses or m/z ranges which should be preferentially selected for AutoMS(n).
  - Preferred Charged State: selection of defined charge states of precursor ions for most efficient AutoMS(n). Avoids as well the fragmentation of the same precursor in various charge states.

- **HyStar 3.2 SR2:** For integrated control of most popular HPLC systems and automation systems. e.g. Bruker EASY-nLC II, Agilent 1100 and 1200 series (also rapid resolution), Dionex/LC Packings Ultimate plus and UltiMate3000, Waters 2795 and Acquity UPLC, LaChrome Elite (Hitachi), Eksigent nanoLC

- **Data Analysis software DA 4.0 SP 4**, including:
  - Advanced data processing with a high degree of automation
  - New QuantAnalysis™ quantitation package
  - LibrarySearch ™ module for search of MS/MS and $MS^n$ spectra with advanced matching algorithm
  - Charge deconvolution module
  - Neutral loss scans
  - Survey view for density plots of MS and UV-DAD data
  - Export of peak reports to dBase or MS-Excel
  - Export of spectra and ion current profiles as Windows metafiles to word-processing programs

- One SW License ESI Compass 1.3 (incl. esquire control, Data Analysis, LibrarySearch, QuantAnalysis, Dissect)
- One SW License ESI Compass 1.3 charge deconvolution
- One SW License HyStar 3.2 LC/MS (incl. post processing)

**I. Set of manuals and reference CD-ROMs**
**J. Installation**
**K. Familiarization upon installation**
**L. 1 year warranty**
**M. Voucher for a factory-training course - valid for 2 participants.**

**Performance Specifications**

**amaZon SL Dual Funnel Ion Trap Mass Spectrometer System**

BDAL #294445

| | |
|---|---|
| Size | Benchtop:<br>89 x 76 cm x 51 cm (Height) |
| Weight | ~ 86 kg |
| Vacuum System | 4 stages, 34 $m^3$/h rough pump |
| Apollo II ion funnel electrospray source | Flow rate: 1 µL/min – 1 mL/min |
| Polarity switching | Fast Polarity switching < 80 ms |
| Stages of MS(n) | MS(n) for n = 1 through 11 |
| Stages of AutoMS(n) | AutoMS(n) for n = 1 through 5 |
| Mass accuracy in MS and MS/MS | +/- 0.15 u<br>within the calibrated standard mass range at ultraScan resolution in full scan mode, with proper calibration, ICC target and ion statistics, and thermal equilibrium of electronics and ion source |
| Sensitivity Specification | The following system sensitivity specifications are only applicable when a Agilent 1200 Series HPLC system is purchased together with the amaZon SL System and this LC system is installed in conjunction with the amaZon SL System |
| Full scan sensitivity in MS | Reserpine 5 pg/µL@ S/N>10: 1<br>Signal-to-noise ratio of the extracted ion chromatogram of the protonated molecular ion (m/Z 609) as the result of an injection of 1 µL Reserpine (5 pg/µL), measured in positive ion mode, at a flow rate of 200 µL/min when the mass spectrometer is operated in full scan mode using the Enhanced Resolution Mode, scanning from m/z 250 to 750. |
| Full scan sensitivity in MS/MS | Reserpine 125 fg/µL @ S/N>50: 1<br>Signal-to-noise ratio of the extracted ion chromatogram of the transition of the protonated molecular ion (m/Z 609) to the most abundant product ion as the result of an injection of 2 µL Reserpine (125 fg/µL), measured in positive ion mode, at a flow rate of 200 µL/min when the mass spectrometer is operated in full scan MS/MS mode scanning the product ion spectrum from m/z 250 to 650 using the Enhanced Resolution Mode. |

| Scan Mode | Mass Range (m/z) | Resolution FWHM (u) | Scan Speed (u/sec) |
|---|---|---|---|
| ultraScan | 70-2200 | 0.6 | 32,000 |
| Enhanced Resolution Mode | 50-2200 | 0.35 | 8,100 |
| Extended Mass Range | 200-4000 | 3 | 27,000 |

**Optional accessory**

| | |
|---|---|
| Bruker EASY-nLC | Split-free nano-flow HPLC system |
| Switching valve analytical scale | Optional accessory |
| APCI | Optional accessory |
| CE/MS interface | With grounded needle for easy CE-MS set-up (Optional accessory) |



**Descriptions and specifications supersede all previous information and are subject to change without notice**

# aurora M90

**Specification Sheet**

### Design Overview

The aurora M90 systems is compact, floor-mounted inductively coupled plasma mass spectrometers (ICP-MS) with full PC control of all instrument settings and compatible accessories. It features patented [1] 90 degree reflecting ion optics system for gigahertz sensitivity (1000 Mc/s/mg/L) and low background and interferences. The aurora M90 system includes a sample introduction system, solid state 27 MHz RF generator, and patented [2] Turner Interlaced Coils. Full PC control of plasma positioning, triple stage vacuum system, all plasma gas flows, mass analyzer, and Discrete Dynode Electron Multiplier (DDEM) detector is also included. The vacuum system is fully contained within the instrument for a small instrument footprint. Unique DDEM detector provides nine decades of dynamic range in an all-digital pulse design. Fully web-integrated ICP-MS Expert software uses Bruker's worksheet concept for ease of use and rapid operator training. The aurora M90 system also features a unique and patented [3] Collision Reaction Interface (CRI) providing fast, flexible, interference-free analysis using simple collision and reaction gases.

### Instrument Hardware

#### Sample introduction - ESIA

External Sample Introduction Assembly (ESIA) with Peltier-cooled spraychamber, nebulizer, and peristaltic pump mounted outside the torch box to eliminate temperature-induced drift. Features rapid start-up, easy access for maintenance and cleaning, and rapid switchover to accessories.

- Low-flow (400 µL/min) glass concentric nebulizer. Optional inert PFA nebulizer and a range of low-flow, inert microconcentric nebulizers
- Peltier-cooled spraychamber with variable temperature control for enhanced stability and reduced oxide ion interferences. PC-controlled temperature from -15 °C to room temperature, insulated with inert polypropylene foam
- Fully PC-controlled peristaltic pump, variable speed from 0–50 rpm, three independently pressure adjustable channels for sample, drain, and internal standards or diluent
- Standard one-piece, low flow, ball-and-socket connection torch. Optional semi-demountable torch and inert PFA transfer tubes available

#### Gas control

- One button automated optimization of all gas flows, including CRI gases
- Standard sheath gas flow allows aerosol dilution of high matrix samples
- Optional external MFC gas control (nitrox 500), for online addition of nitrogen and oxygen to the plasma

#### RF generator

- 27.12 MHz solid-state, air-cooled, crystal locked RF generator in main instrument housing, 600–1600 W in 10 W increments. Optimum power settings defined and stored within each method for different sample types
- Automatic ignition and shutdown. User-customizable ignition sequence for different accessories and plasma types

#### Plasma

- Optimize plasma parameters according to specified performance targets (sensitivity, interferences, etc.)
- Full PC control of horizontal, vertical and sampling depth (Z position) of plasma for maximum sensitivity and minimum polyatomic interferences
- Spacious plasma compartment simplifies routine maintenance

#### Cool plasma

- Patented Interlaced Coils minimize polyatomic interferences without the use of a mechanical torch shield

## Instrument Hardware continued

### Collision Reaction Interface

- Reduces interferences by injecting simple collision and reaction gases (hydrogen or helium) into the plasma as it passes through the orifice of the cones
- All CRI gas flows controlled by mass flow controllers
- Rapid switchover between gas on and gas off, or between different collision and reaction gases

### Plasma interface

- Easy access and removal of sampler and skimmer cone from simple threaded mounts
- One set of high performance nickel cones as standard. Optional high performance platinum cones for corrosive acids and solvents
- Orifice diameters: 1.1 mm sampler, 0.5 mm skimmer
- Water-cooled plasma interface for stability including individual and independent cooling of the cones for faster warm-up, improved stability, and faster cool down

### Ion optics

- Patented ion mirror reflects analyte ion beam through 90 degrees while photons and neutrals pass to the vacuum system. Ion mirror creates parabolic electrostatic field to focus the analyte ions with optimum efficiency at the quadrupole entrance aperture. Results in gigahertz sensitivity (1000 Mc/s/mg/L)
- Features easy access to extraction lens 1 and 2 for cleaning without breaking the vacuum
- Auto-optimization of all ion optics settings, including ion mirror, based on selected optimization criteria such as signal and interferences
- Quadrupole mass analyzer is off-axis using patented [4] curved stainless steel entrance rods to ensure low background by further eliminating excited neutrals before the quadrupole

### Vacuum system

- Pumps consist of two rotary (SD602 and SD302) and two V-301 turbomolecular pumps for efficient pumping and to eliminate excessive pump wear
- Choice of standard rotary pumps for general applications or inert rotary pumps for more corrosive acids and solvents
- Rotary pumps mounted on forward facing pull-out slides for easy inspection of oil levels and easy access and changing of oil
- All vacuum components located in the main housing of the instrument to reduce noise in the laboratory and eliminate the requirement for extra floor or bench space
- Turbomolecular pumps feature maintenance-free ceramic bearings. First turbopump is positioned immediately behind the ion mirror and skimmer cone for maximum pumping efficiency and removal of unwanted neutrals and particles
- Pneumatic vacuum isolation gate between the first and second vacuum stages. Gate automatically closes in the event of a power failure


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### Quadrupole

- Precision-machined, stainless steel, round rods manufactured to micrometer tolerances and locked into ceramic mounts for a near-perfect hyperbolic field. Stainless steel construction permits determination of Hg without high memory. Patented curved entrance rods provide a double off-axis design and low background signals
- Easy access to mass analyzer and detector for cleaning or detector replacement. All voltages are fully interlocked and under PC control
- Solid-state air-cooled power supply
- Built-in, on board multi-channel scaler provides up to 40 channels per mass
- Range of 3 to 256 amu with 'zero blast' protection. Resolution adjustable from 0.5 to 1.2 amu
- Mass calibration stability: 0.05 amu per day
- Quadrupole RF frequency: 3.0 MHz
- Scan speed: 2000 amu/s
- Minimum dwell time: 200 µs

### Detector

- All-digital ETP AF250 Discrete Dynode Electron Multiplier (DDEM) as standard provides nine decades of linear dynamic range in an all-pulse-counting detector. No complex, time-consuming analog-to-digital cross calibrations
- Measuring dynodes mounted off-axis for reduced background

### Performance

The performance data is typical unless otherwise noted.

| | | |
|---|---|---|
| High sensitivity mode, Mc/s/mg/L) | $^{9}Be$ | >50 |
| | $^{115}In$ | >1000 |
| | $^{232}Th$ | >500 |
| Precision (10 replicates, 20 minutes) | | <3% |
| Oxide ions | $CeO^{+}/Ce^{+}$ | <3% |
| Doubly charged ions | $Ba^{++}/Ba^{+}$ | <3% |
| | $Ce^{++}/Ce^{+}$ | <2% |
| Background at 5 amu | | <5 c/s |
| Normal sensitivity mode, Mc/s/mg/L) | $^{9}Be$ | >15 |
| | $^{115}In$ | >120 |
| | $^{232}Th$ | >100 |
| Precision (10 replicates, 20 minutes | | <3% |
| Long term stability (10 µg/L multi-element standard aspirated for 4 hours) | | <4% |
| Oxides | $CeO^{+}/Ce^{+}$ | <2% |
| Doubly charged ions | $Ba^{++}/Ba^{+}$ | <3% |
| | $Ce^{++}/Ce^{+}$ | <2% |
| Background (at 5 amu) | | <2 c/s |
| Abundance sensitivity | $10^{-6}$ low, $10^{-7}$ high on $^{23}Na$ | |
| Isotope ratio precision | <0.1% ($^{107}Ag/^{109}Ag$) | |
| CRI interference reduction | 1 µg/L As readback in 1% HCl 1 µg/L ± 0.1 µg/L | |


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## Instrument Software

Easy-to-use, web-integrated design. Features wizards that guide users through method and sequence development, and method templates for rapid development of commonly used methods.

### Features include

- Quantitate analytes on any possible combination of isotopes
- Fully editable interference correction equations
- A range of internal standard assignment options
- Multiple condition sets allowing different element suites to be determined under different conditions with a single sample measurement, including CRI modes, hot plasma, cool plasma, etc.
- Calibration routines for multi-element external calibration, method of standard additions, and isotope ratios
- Automatic method optimization, including ion optics, plasma and CRI gasses and aerosol dilution
- Automatic monitoring and adjustment of nominated elements/isotopes in real time for optimal rinse out
- High speed Time Resolved Signal (TRS) capability for interfacing to chromatographic (such as HPLC) and other separation techniques
- Seamless LC-ICP-MS integration
- Fully editable sample label list of up to 1000 samples for analysis per worksheet
- Autosampler rack and tube positions can be edited for true random access sampling
- Calibrations can be programmed at a user specified rate either amongst the sample tubes or from centralized calibration tubes (rate driven)
- Sequence options include full control of reporting actions at the end of the run, exporting of results at the end of the run, emailing of results, calibration, recalibration and resloping error actions, and saving mass scans during the analysis
- Fully automated instrument initialization (start-up) routine, including instrument stabilization time, plasma X/Y position adjustment, mass calibration, and quadrupole resolution
- Simultaneous real-time graphical display of signal as full mass scan, segments of mass scan, and signal response vs time for multiple isotopes or ratios
- Post-run retrospective data editing
- Wide variety of reporting and exporting options
- Comprehensive set of instrument diagnostics and performance tests
- Comprehensive help system


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## Accessories

### Autosamplers
- Compatible with a wide range of commercially available autosamplers and laboratory racks

### Productivity Pack
- Optional four-port Switching Valve System (SVS) immediately rinses the sample introduction system while the next sample is being introduced to the instrument
- Reduces carryover, increases sample throughput, and decreases cost per analysis

### Integrated speciation (LC-ICP-MS)
- Seamless LC-ICP-MS integration including real-time display of time resolved chromatographic signals
- Full control of LC injections, pumps, autosamplers and data acquisition

### High Sensitivity Pack
- Includes non-CRI cones optimized for maximum mid-to-high mass sensitivity when operating the ICP-MS in high sensitivity mode
- Ideal for research applications requiring ultra-low detection limits on non-interfered isotopes

### nitrox 500
- Adds oxygen to the plasma to eliminate carbon deposition on the injector tube and sampler cone when analyzing organic solvents.
- Adds nitrogen to the plasma for better detection of elements with high ionization potential (eg. As, Se)

### Clean Room Pack
- Includes o-ring free, inert sample introduction system, platinum-tipped cones, and additional exhaust outlet panel
- Removes all exhaust air from the instrument, maintaining the integrity of the highly sensitive clean room environment
- Allows analysis of corrosive samples and acids, such as hydrofluoric acid

### Inert sample introduction kits
- Semiconductor kit includes low contamination and inert PFA nebulizer, spraychamber and transfer tubing, platinum-tipped cones and platinum torch injector.
- Chemical kit includes inert PFA nebulizer, spraychamber and transfer tubing, platinum-tipped cones and sapphire torch injector.

### Microconcentric nebulizer
- Compatible with a range of microconcentric nebulizers for sample volume limited applications

### Laser ablation
- Fully compatible with a range of laser ablation accessories


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### ICP-MS Installation Requirements

For details of Bruker ICP-MS installation requirements refer to the pre-installation manual, Bruker publication number 8510206700.
Installation qualification (IQ) and operational qualification (OQ) protocols are available for the Bruker ICP-MS.

### Bruker Customer Support Policies

#### Warranty

12 months, though this may vary by location. One-year warranty on DDEM detector with pro-rata warranty on replacements.

#### Hardware support period

Eight (8) years from date of last unit manufacture. After this time, parts and supplies will be provided if available.

#### Software support

Software upgrades to fix nonconformances or safety issues will be issued free of charge. Software upgrades for additional functionality will require a fee. Availability of remote diagnostic support may vary according to location.

### Further Details

**For further details on the following**

- PC configurations
- Installation/Operational Qualification
- Accessory specifications and application information
- Part numbers and other ordering information

Please consult your Bruker office or supplier, or our Web site at www.bruker.com.

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

[1] US Patent 6,614,021 B1
[2] US Patent 5,194,731
[3] US Patent 7,329,863 B2
[4] US Patent 6,762,407 B2


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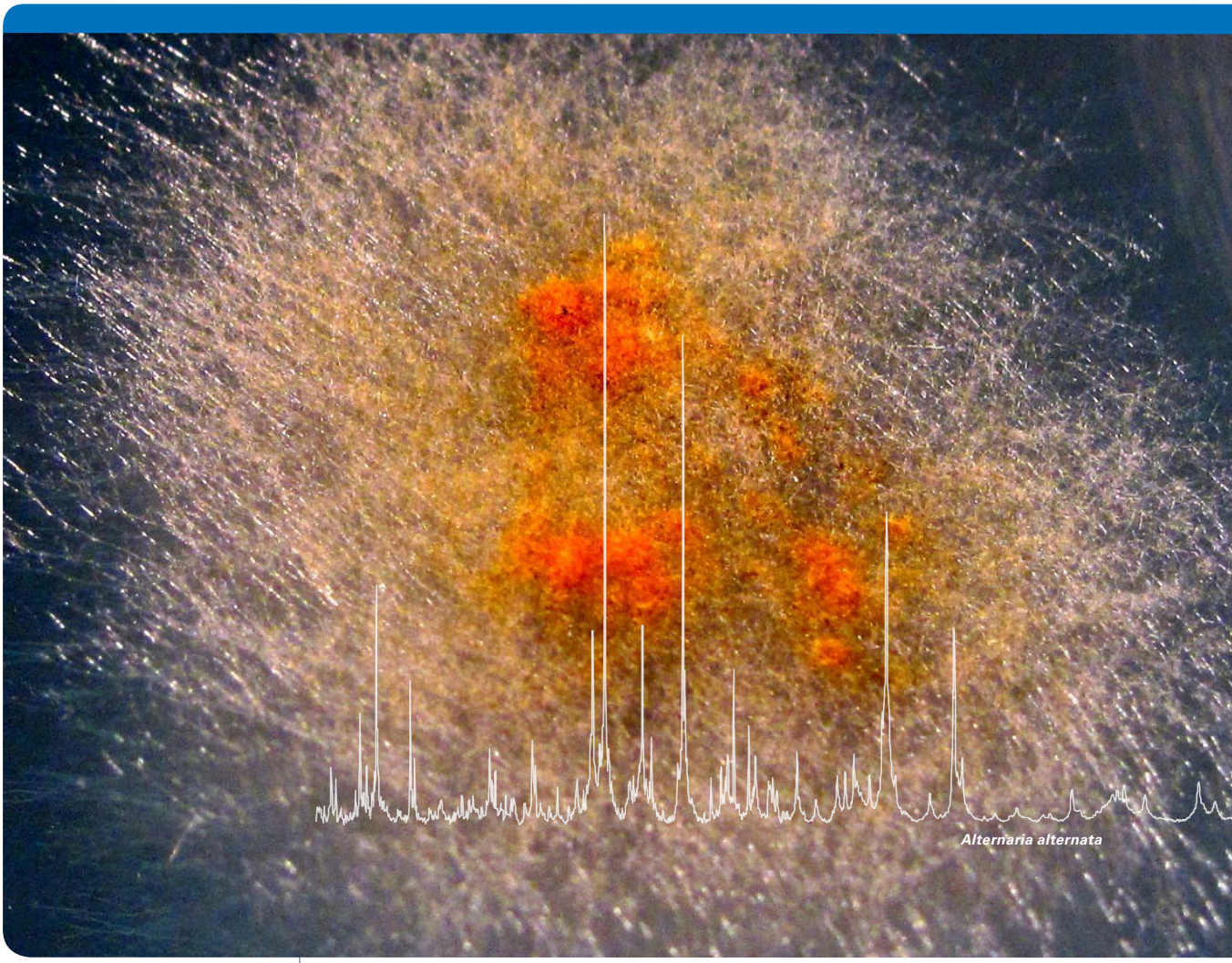



# Fungi Library

- MALDI Biotyper

MALDI-TOF MS

Innovation with Integrity

# Expanding MALDI Biotyper's Libraries with the Addition of Filamentous Fungi

The identification of moulds and multicellular fungi has always been one of the most challenging aspects of clinical microbiology. Whilst MALDI-TOF has over recent years revolutionised the identification of bacteria & yeasts, it has had little impact on the identification of filamentous fungi. This has been mainly due to the effect of culture conditions. Bruker has now developed a cultivation method that ensures a stable physiological status and prevents the germination process and the formation of spores.

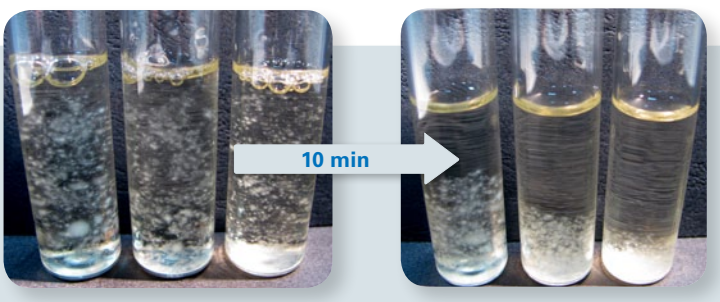
## Standardised liquid cultivation with constant rotation for library construction

In order to reduce the effects of culture conditions and aid in the production of a uniform mycelium, a liquid based cultivation method has been developed which standardises the physiological status. The method has then been used to create library entries. In essence tubes are inoculated with the fungi and placed on a rotator and incubated overnight or until enough biological material is observed.


Rotator SB2

## Sample preparation

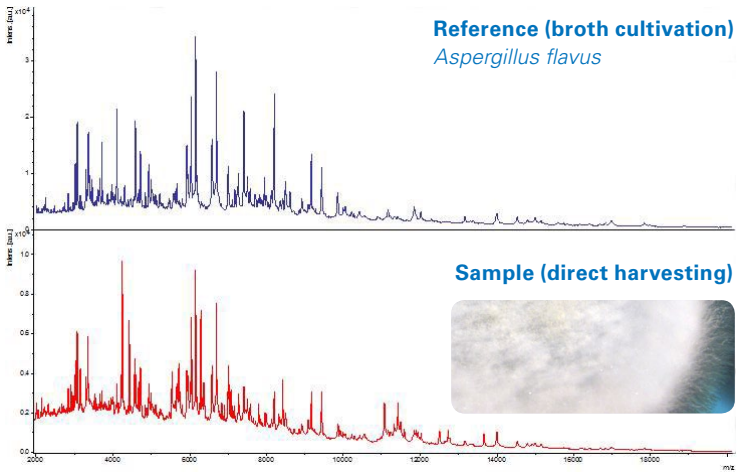
- Remove cultivation tubes from the rotator and wait for 10 minutes until filamentous fungi sediment to the bottom of the tube
- Harvest up to 1.5 ml from the sediment and centrifuge for 2 min at full speed (e.g. 13,000 upm)
- Carefully remove the supernatant
- Add 1 ml water to the pellet and vortex for one minute, repeat washing and vortexing twice
- Ethanol extract



# Daily Routine Workflow – Analysis Possible Direct from Agar

As in this example if a "front mycelium" is clearly visible and can be harvested then it is possible to sample directly from the agar and using the simple ethanol extraction method, good results can usually be obtained without the need for liquid cultivation for most of the samples. In cases were direct harvesting is difficult then the liquid cultivation method should be used.

**Typical MALDI Biotyper mass spectra**



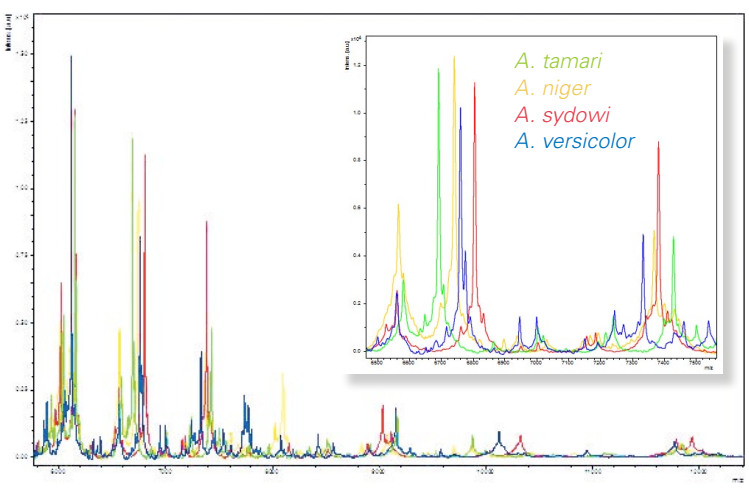

Top spectrum is achieved after liquid cultivation of *Asgergillus flavus* and the bottom spectrum is achieved by direct harvesting of *Asgergillus flavus* from agar. Note from the image that the "front mycelium is both clearly visible and can be easily harvested.

## International fungi consortium

The goal of this consortium was firstly to test the reliability of the liquid based cultivation and sample preparation and then provide securely identified fungi strains for creation of the library.

Currently contributions have been received from over 20 laboratories across 8 countries with an aim of creating an initial library covering >100 species from approximately 40 different genera.

**Different species of the genus *Aspergillus***




MALDI Biotyper spectra overlay of various species of *Aspergillus*.

# Fungi Library

The filamentous fungi library currently includes more than 110 species from approximately 40 different genera. As with other Buker MALDI Biotyper libraries we will continue to grow and maintain this library.

## Material

- Rotator SB2, Order-No. Y549.1, Carl Roth GmbH & Co. KG
- Rotator dish for Rotator SB2, Order-No. Y552.1, Carl Roth GmbH & Co. KG
- Sabouraud Liquid Broth, Modified, 8 ml, Order-No. 221014, Becton Dickinson (BD)

**Prof. Dr. med H. Hof • Mycology Lab**
**Laboratory of Limbach, Heidelberg, Germany**

"The identification of multicellular fungi to the species level is one of the most challenging tasks of many microbiological laboratories in medicine, hygiene as well as food industries. In cooperation with Bruker's dedicated microbiology team we worked as part of an international group of fungi experts on the identification of fungi using the MALDI Biotyper approach. Based on Bruker's existing development on fungi sample preparation procedure, we contributed, established and validated a reference library of a large panel of the most important fungal strains. Our common efforts during the last years's have shown that MALDI-TOF based molecular fingerprints of fungi provide a high differentiation power both at species and strain level. The analytical performance of the MALDI Biotyper when used with the fungi library is a major technological breakthrough and practical improvement when compared to more conventional approaches and technologies using microscopy and sequencing methods only."

## Genera list

- Acremonium
- Alternaria
- Arthrinium
- Aspergillus
- Aureobasidium
- Botrytis
- Chaetomium
- Chrysosporium
- Cladosporium
- Cunninghamella
- Curvularia
- Epicoccum
- Epidermophyton
- Eurotium
- Fenellia
- Fusarium
- Geomyces
- Lecythophora
- Lichtheimia
- Microsporum
- Monilinia
- Mucor
- Paecilomyces
- Penicillium
- Phaeoacremonium
- Phialemonium
- Phialophora
- Phoma
- Rhizopus
- Scedosporium
- Schizophyllum
- Scopulariopsis
- Scytalidium
- Thanatephorus
- Trichoderma
- Trichophyton
- Trichurus

Order information: Fungi Library 1.0 – #700281

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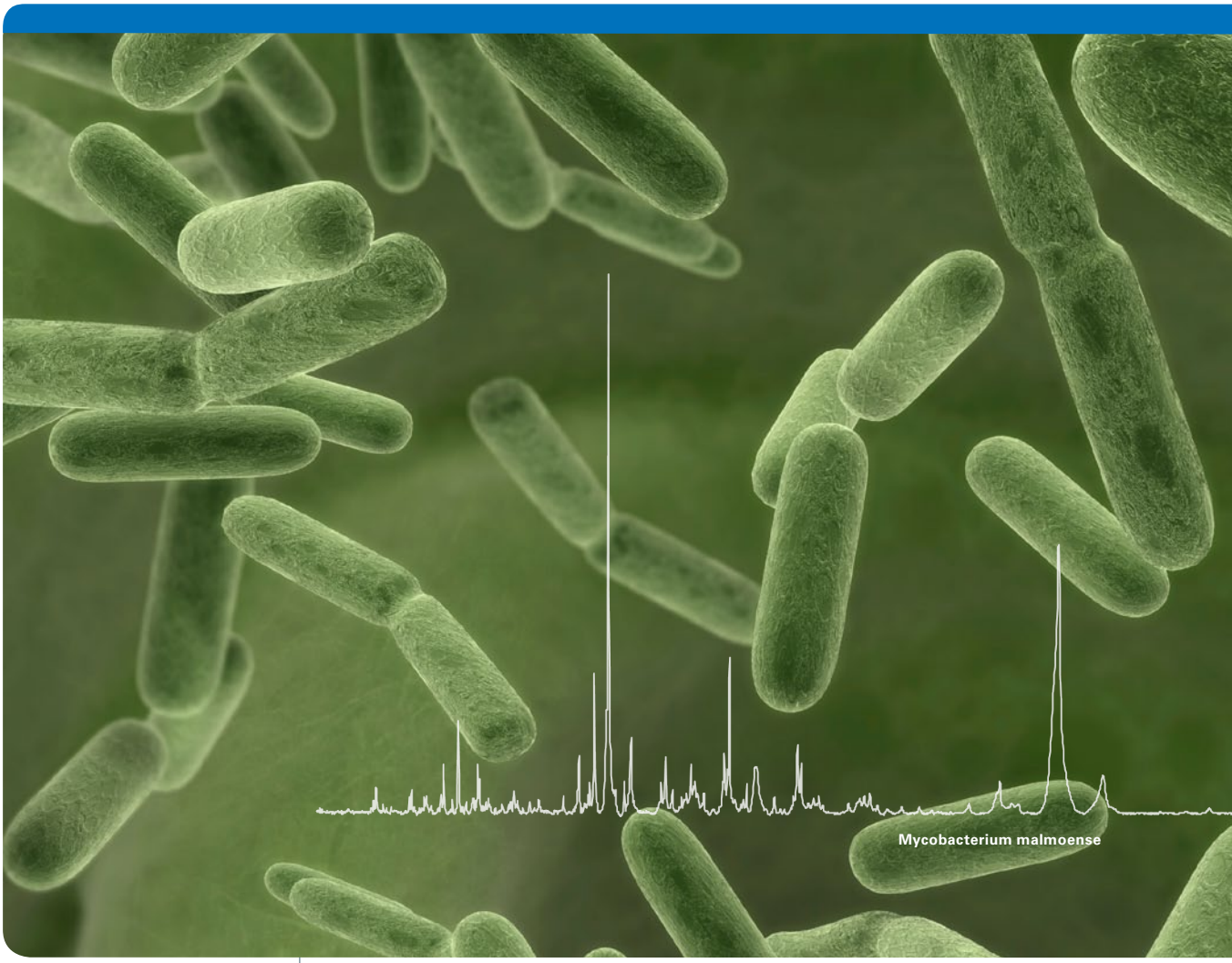



# Mycobacteria Library

- MALDI Biotyper

MALDI-TOF MS

Innovation with Integrity

# Generation of a *Mycobacterium* Species Library

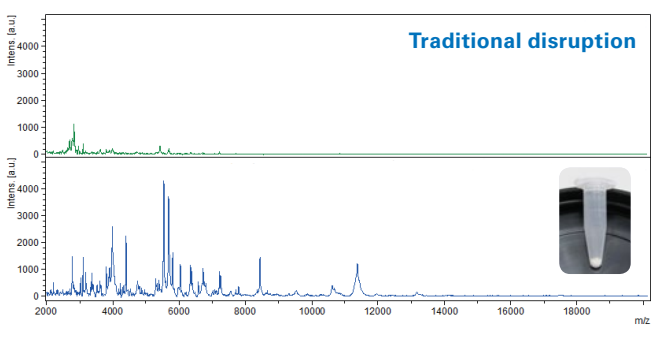
Next to the clinical important *Mycobacterium tuberculosis complex (MTC)* Nontuberculosis Mycobacteria (NTM) are pathogens especially in immunocompromised and senior people. Species identification is important for diagnosis and optimal treatment. Conventional MALDI-TOF identification of mycobacteria using simple extraction methods or direct smearing approaches yield low quality spectra and are unsafe. Hence an inactivation & preparation method for mycobacteria has been optimised using silica beads, which yields high quality spectra and leads to reproducible identifications at the species level. This approach has been used to generate the library entries.

## Optimized method using silica beads

- Biomass of mycobacteria in 75% ethanol, centrifugation
- Washing step, 500 µl water
- Resuspend pellet in 50 µl of water, 30 min heating 95C
- Addition of 1,2 ml ice cold ethanol
- Centrifugation, discard supernatant
- Suspend dried pellet in acetonitrile
- Addition of silica beads (0.5 mm)
- Vortex for 1 min
- Addition of 70% formic acid
- Vortex for 10 sec
- Centrifugation
- 1 µl of supernatant on a MALDI target

As can be seen here using two different sample extraction methods, the only extraction that yielded a good quality mass spectrum is the one using silica beads. Hence an optimized method for sample preparation and inactivation using silica beads has been developed to facilitate the generation of good quality mass spectra of every species for library entries.

**Mass Spectra of *Mycobacterium gastri* DSM 44505$^T$**



# One Library – Two Sample Cultivation Methods Supported

As can be seen here, it is possible to analyse samples cultured either in liquid media BACTEC™ MGIT™ (Becton Dickinson Company) or from Löwenstein-Jensen media.

Identification of *Mycobacterium* sp. by MALDI-TOF using just 1 ml of BACTEC™ MGIT™ culture is possible.

**Spectra of *Mycobacterium peregrinum* DSM 43271$^T$**

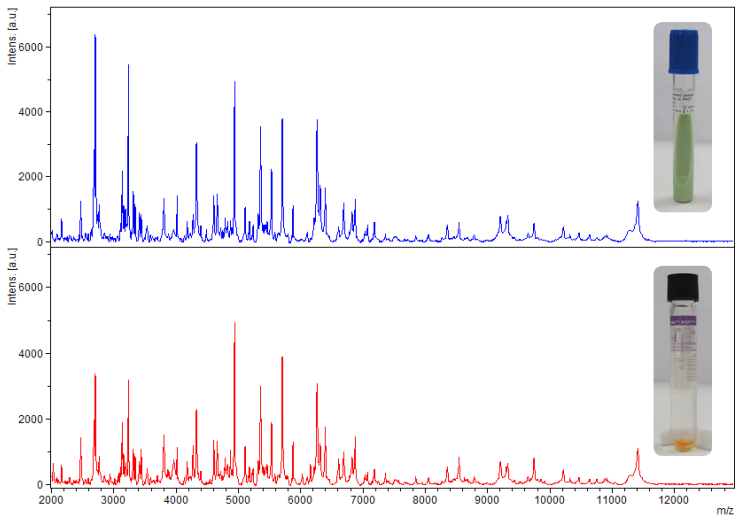



Figure 1: Spectra of *Mycobacterium peregrinum* DSM 43271$^T$ cultivated on Löwenstein-Jensen medium (top) and in MGIT™ tube (bottom), using "Mycobacterium bead preparation" method.

## International mycobacteria consortium

The goal of this consortium was firstly to develop and refine an extraction procedure that works for both liquid and solid media as well as safely inactivating the mycobacterium. And then to provide securely identified mycobacteria strains for creation of the library.

Currently contributions have been received from over 17 laboratories across 9 countries with an aim of achieving both complete species coverage and strain diversity coverage.

**Dendrogram**

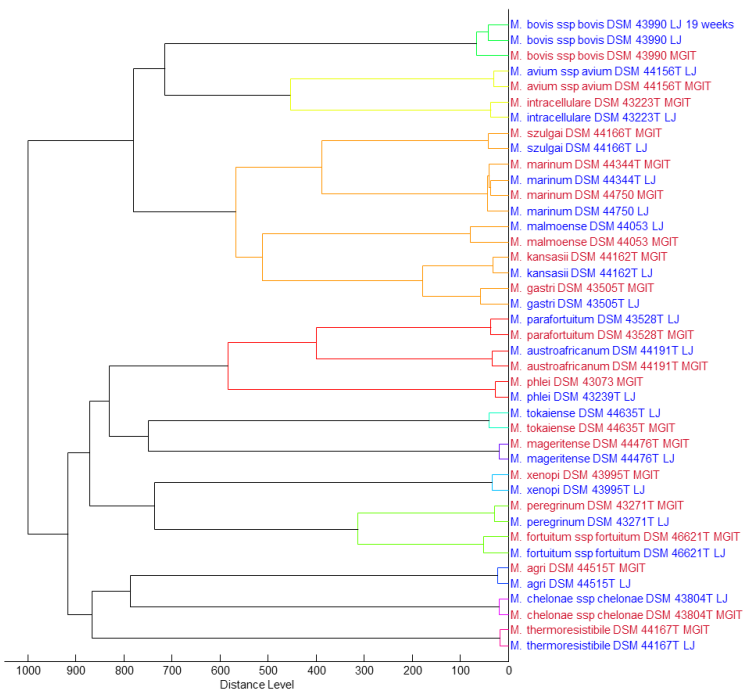



Figure 2: The Dendrogram of 19 different species of mycobacterium cultivated on Lowenstein-Jensen medium (blue) and in MGIT™ tubes (red) demonstrates that the same species always cluster together and are well resolved from other species.

# Mycobacteria Library

**Prof. Dr. Dag Harmsen • Head of R&D Policlinics for Parodontology, WWU Münster**

"MALDI-TOF mass spectrometry has been shown to have major clinical impact by a very fast species identification with a very broad species coverage. However, the technology was not readily available for the very demanding analysis of Mycobacteria. In the past years I have been deeply involved in molecular characterization of Mycobacteria, for example by means of sequencing approaches. I am glad to see that now with the new Mycobacteria library of Bruker´s MALDI Biotyper, this further dimension of molecular characterization by a proteomic fingerprint is also available for Mycobacteria."

## Mycobacteria library

The first version of the mycobacteria library contains more than 90 species and will continue to grow in both species coverage and number of strains per species.

### Mycobacteria Library

| | | | |
|---|---|---|---|
| M. abscessus ssp abscessus | M. colombiense | M. intermedium | M. pseudoshottsii |
| M. abscessus ssp bolletii | M. conceptionense | M. intracellulare | M. pulveris |
| M. agri | M. confluentis | M. kansasii | M. rhodesiae |
| M. alvei | M. conspicuum | M. kumamotonense | M. saskatchewanense |
| M. arosiense | M. cosmeticum | M. lacus | M. scrofulaceum |
| M. arupense | M. diernhoferi | M. lentiflavum | M. senegalense |
| M. asiaticum | M. elephantis | M. mageritense | M. senuense |
| M. aurum | M. farcinogenes | M. malmoense | M. seoulense |
| M. austroafricanum | M. florentinum | M. mantenii | M. septicum |
| M. avium subsp. avium | M. fortuitum subsp. acetamidolyticum | M. marinum | M. setense |
| M. avium subsp. paratuberculosis | M. fortuitum subsp. fortuitum | M. monacense | M. shimoidei |
| M. avium subsp. silvaticum | M. gastri | M. montefiorense | M. shottsii |
| M. boenickei | M. gilvum | M. mucogenicum | M. simiae |
| M. bohemicum | M. goodii | M. neoaurum | M. smegmatis |
| M. botniense | M. gordonae | M. neworleansense | M. szulgai |
| M. bovis | M. haemophilum | M. nonchromogenicum | M. thermoresistibile |
| M. branderi | M. hassiacum | M. novocastrense | M. tokaiense |
| M. brumae | M. heckeshornense | M. parafortuitum | M. triplex |
| M. brisbanense | M. heidelbergense | M. parascrofulaceum | M. tuberculosis |
| M. canariasense | M. hiberniae | M. paraseoulense | M. vaccae |
| M. celatum | M. hodleri | M. parmense | M. wolinskyi |
| M. chelonae subsp. chelonae | M. houstonense | M. peregrinum | M. xenopi |
| M. chimaera | M. immunogenum | M. phlei | |
| M. chitae | M. insubricum | M. phocaicum | |
| M. chlorophenolicum | M. interjectum | M. porcinum | |

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Order information: Mycobacterium Library 1.0 – #700279


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BRUKER

# SCION™ SQ Series GC-MS

The Gas Chromatographers' Detector

GAS CHROMATOGRAPHY

Innovation with Integrity

# Introducing the SCION SQ GC-MS

Bruker's long tradition of innovation and product reliability have combined to create a new industry standard for gas chromatography single quadrupole mass detection – the SCION SQ series. By designing the GC-MS systems to exceed the most critical performance and reliability needs of GC users, Bruker has delivered systems that are especially for, and all about, the ultimate success of the GC users. The SCION SQ Select, Prime, and Premium models are designed to meet many important user specific requirements – reliable performance, ease-of-use and simple maintenance – all in a small footprint that saves valuable bench space.

## SCION SQ GC-MS Benefits

**Easy to Use and Maintain**

- Simple tuning due to "lens-free" ion-path design
- No multiplier calibration required

**Robust**

- An inert ion source that requires less frequent cleaning

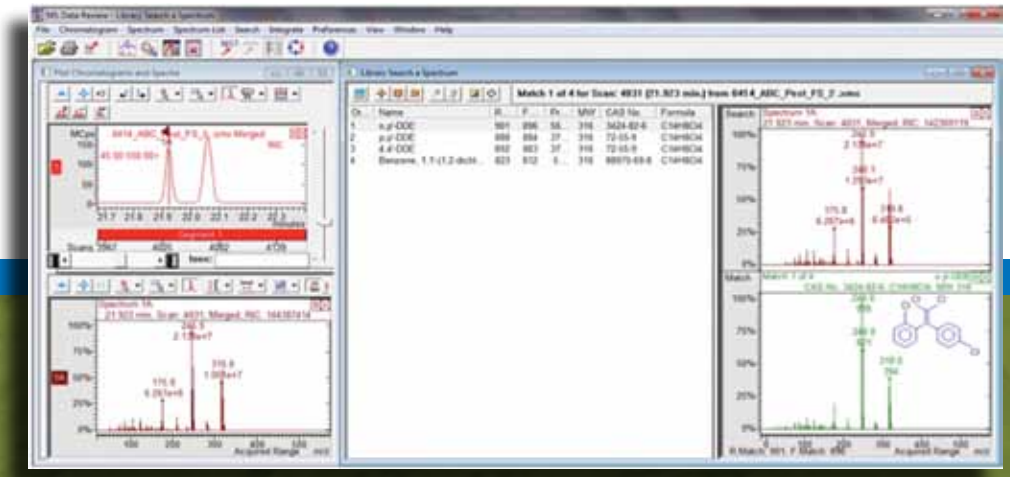
**Sensitive**

- Optional active-focusing q0 uses He atoms to focus ions

# Enhanced Library Searching through Cleaner EI Spectra

The SCION SQ models are designed to analyze thousands of samples from complex matrices. With an upper mass limit of m/z 1200, they are exceptionally capable of handling almost any GC application. The innovative lens-free design, combined with the robustness of the axial ion source, delivers unmatched stability and ultra-high sensitivity on a routine basis.

- One-click search of multiple spectral databases
- User-created spectral libraries and full support of spectral libraries such as NIST, Wiley, and Maurer/Pfleger/Weber (MPW)
- Adjustable spectral search parameters to streamline library searches
- Automated workflow to build a SIM method from a full scan data file
- Flexible and easy to use



Flexible and powerful library search showing matching of sample peak to o,p'-DDE in the NIST library

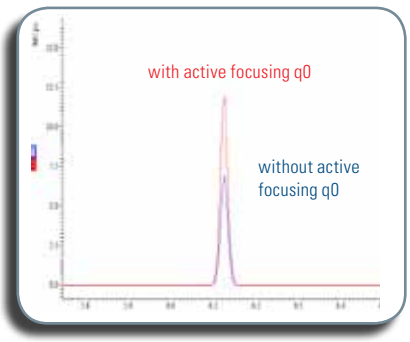
# Why Choose the SCION SQ?

The SCION SQ series delivers exceptional performance for a single quadrupole mass spectrometer: a robust axial ion source, ultra-high sensitivity, cleaner spectra, and virtually-zero neutral noise. The series includes the SQ Select, Prime, and Premium GC-MS models.

For routine EI-only applications, the **SCION SQ Select** delivers the best value. It comes with an industry leading 400 L/s high-capacity turbo pump that enables fast pump-down time for quick maintenance, and the use of high carrier gas flow for fast GC separations.

The EI-only **SCION SQ Prime** model comes with the split-flow, ultra-high capacity turbo pump (300-400 L/s) for added robustness and ease of use. It comes with the innovative active-focusing q0 ion optics that delivers enhanced sensitivity.

The **SCION SQ Premium** model comes CI-ready and therefore is the most versatile GC-MS SQ platform. The active-focusing q0 optic is heated for the demanding analysis that requires the ultimate robustness.



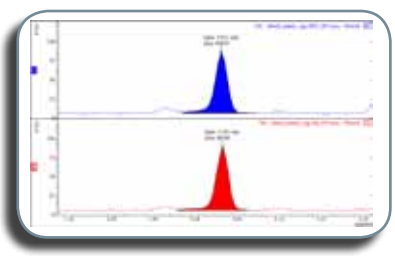

Effect of active-focusing q0 on SIM of Hexachlorocyclopentadiene



**Extended Dynamic Range (EDR) Detector**
- Integrated-Quad design for maximum sensitivity
- Superior negative ion performance
- No multiplier calibration required

**Lens-Free Ion Path**
- Simplifies tuning
- Increases mass stability
- Reduces maintenance

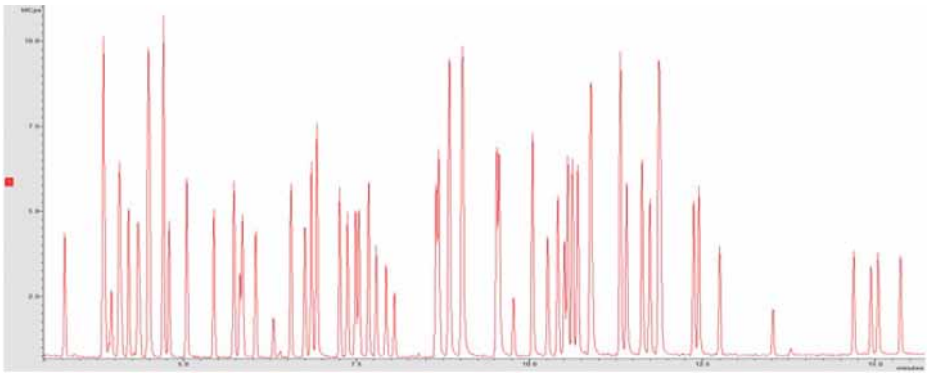
**Axial Ion Source**
- Dual Filament with Rebound Electron Beam technology
- Plug'N'Play for fast exchanges
- Inert for high robustness



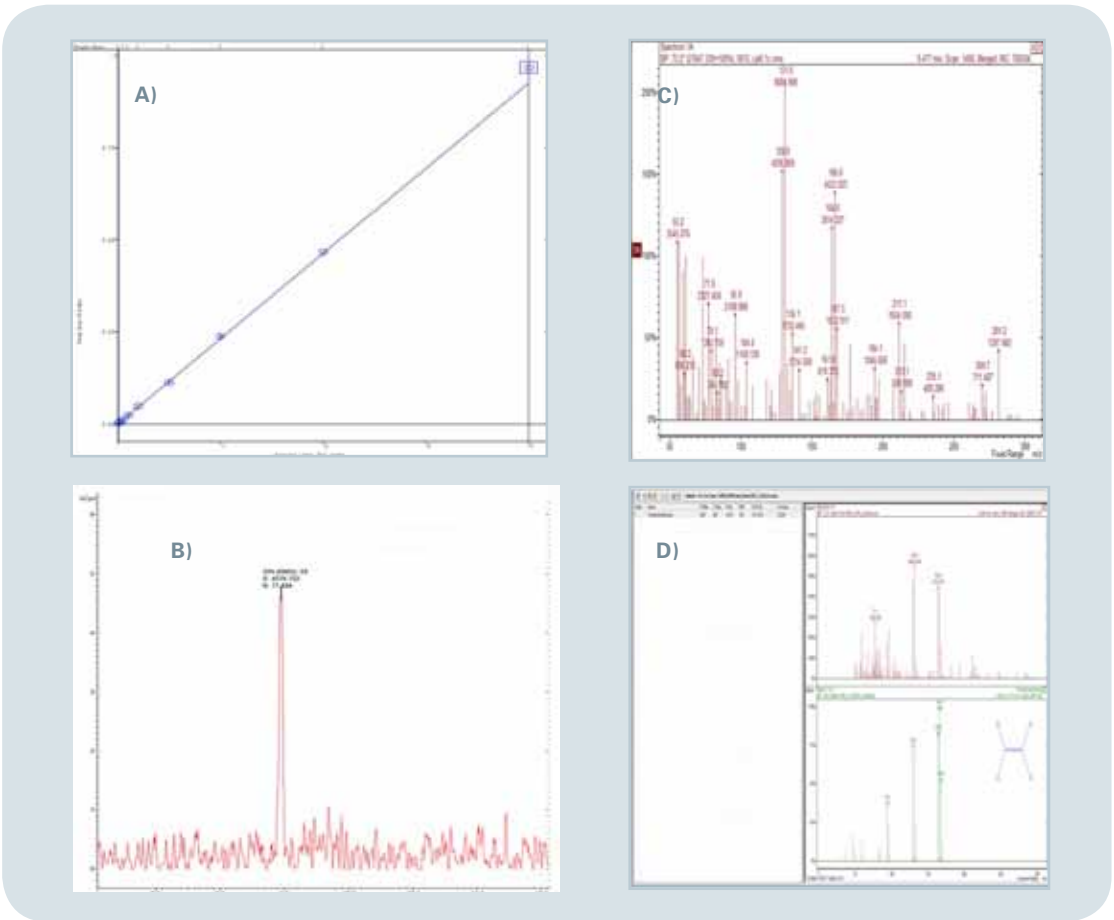
Robustness demonstrated by 350 consecutive injections of 1 pg octafluoronaphthalene (OFN) in 1% Diesel Oil matrix on Scion SQ Select system in Selected Ion Monitoring (SIM) mode

# Linearity, Sensitivity, and Spectral Matching Using the SCION SQ for US EPA Methods

**TIC Chromatogram**



TIC chromatogram of a 5 mL water sample containing 84 VOCs at 10 µg/L (ppb) by US EPA Method 524.3




(A) Excellent linearity of Tetrachloroethylene from 0.1 to 40 ppb with the purge-and-trap, (B) good sensitivity, (C) high quality spectra, (D) down to 0.1 ppb level and showing good match to the NIST library.

# Gas Chromatographs

## An Infusion of Innovation with a Legacy of Reliability

The GC is a key part to the reliability, robustness, and sensitivity of any GC-MS analysis. Bruker's philosophy of innovation is highlighted by the introduction of two new GCs built to support the ultra-sensitive SCION SQ. The compact SCION 436-GC and the versatile SCION 456-GC can accommodate two columns in the oven and are available with new backflush technology and the innovative ChromatoProbe™. The new GCs are also equipped with the multi-language touchpad display supporting 13 languages and enabling MS control.

### SCION 436-GC

Compact design for those focused on routine applications requiring maximum throughput using one or two injectors

- Select up to 2 injectors: Split/Splitless (SSL), Programmable Temperature Vaporization (PTV), Cold-on-Column (COC), Flash and Packed/Wide bore On-Column (PWOC)
- Support one GC detector and the mass spectrometer
- High precision electronic pressure control
- All temperature zones up to 450 °C
- Automated with Model 8400/8410 or CTC liquid/headspace autosampler

### SCION 456-GC

Versatile design with additional injector and detector options for laboratories seeking multipurpose analysis using both GC and GC-MS

- Select up to 3 injectors: SSL, PTV, COC and PWOC
- Add up to 3 GC detectors-FID, ECD, TCD, PFPD, NPD (TSD)
- High precision electronic pressure control
- All temperature zones up to 450 °C
- Automated with Model 8400/8410 or CTC liquid/headspace autosampler

Bruker has now set the industry standard for ease-of-use: Basic operation of SCION GC-MS systems can be directly controlled from the multi-language touchpad on the gas chromatograph. Automatic tuning, along with tune-to-target for meeting specific USEPA methods can be done with a touch of a button. And the MS can be vented and pumped down from the interface for the ultimate in easy maintenance.


SCION 436-GC

SCION 456-GC

# Additions to Enhance System Capability and Performance

### SHS-40 Automated Headspace Sampler

- Perfect for analyzing VOCs in solid or liquid samples
- 40/125 sample capacity – Crimp cap or screw cap 10 or 20 mL vials
- 12 position oven for increased throughput
- 200 °C sample heating for extended range
- Injection with 1 mL sample loop, designed for EPC GCs MHE mode via single puncture ensuring no leaks

### ATOMX® Purge and Trap (P&T) System from Teledyne Tekmar

- Automated VOC Sample Prep System
- Combine an autosampler and purge and trap concentrator into a single platform
- Unique Automated Methanol Extraction (ME) features for high level soil samples
- 80-position carousel design for optimal throughput
- TekLink™ software with fully optimized user interface including diagnostic tools and benchmark tests for instrument validation

The perfect addition for the SCION SQ PTV inlet is the backflush option. Complex sample matrix can quickly ruin the chromatographic performance of your GC column. However, the PTV with Bruker's "backflush" technique can reliably divert the higher boiling sample matrix away from the column. The benefits of this accessory are many:

- Run more samples per day – decrease analysis times as the heavy components are quickly eliminated
- Save time by eliminating column bakeout
- Preserve column performance for extended period of time

### ChromatoProbe™

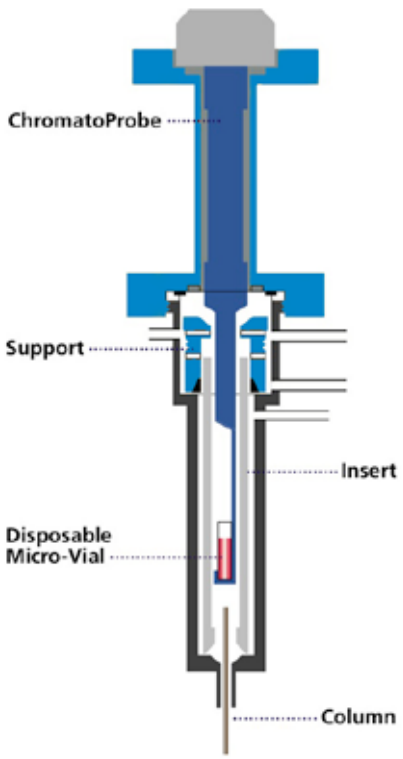
Added versatility for superior analysis of solids, liquids, and slurries

Compounds such as street drugs, industrial solids, synthetic organic products, and plant tissues that normally are not considered amenable to GC-MS analysis can be easily investigated with the ChromatoProbe.

Samples are introduced into the PTV injector via disposable micro-vials. Non-volatile or thermally degraded components from the sample remain in the micro-vial allowing the system to remain clean.

ChromatoProbe benefits:

- Increase uptime
- Minimize system contamination with disposable micro-vials
- Directly desorb samples in the PTV injector without added hardware



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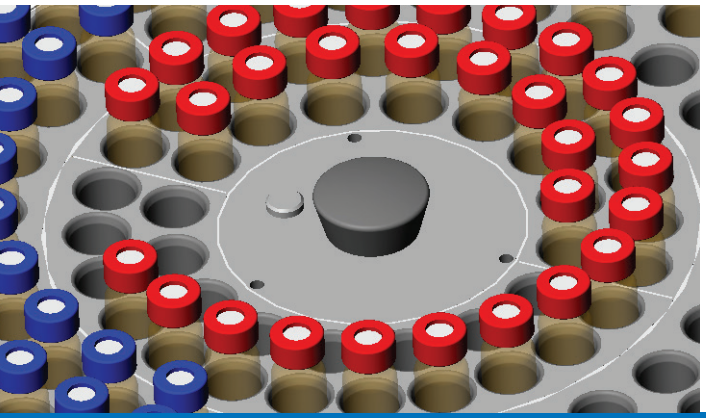
# DHA Analyzer Family

- Optimized Solutions for Detailed Hydrocarbon Analysis

Innovation with Integrity

Gas Chromatography



The DHA Analyzer is a complete high resolution gas chromatography solution for the analysis of hydrocarbons in petroleum streams. It is capable of performing all of the standard methods including the analysis of light petroleum streams and crude oil light end.

## Key Benefits include:

- **Compliant with all industry standard methods**
  Be confident using Bruker's DHA Analyzers, which are configured in accordance with all the established standard methods including ASTM D6729, D6730, D6733, D5134, IP 344/DHA "Front End"and "Fast DHA".
- **Complete and fully integrated solution**
  DHA Analyzers come complete with everything you need to be up and running quickly.
- **Powerful and easy-to-use analyzer**
  With relatively little training, operators can generate outstanding analysis results day after day.
- **Save time**
  Easily generate reports with a few mouse clicks and reduce analysis time using "Fast DHA", increasing lab productivity.
- **Single vendor solution**
  Bruker's GC analyzers are built and tested at Bruker's factory, as well as installed and performance-verified on-site by Bruker trained and certified engineers. Rest assured that our analyzers can meet or exceed your needs throughout the instrument's lifetime.

Detailed hydrocarbon analysis is often the preferred technique to fully characterize petroleum streams. The technique is based on the identification of individual components using high performance, high resolution capillary gas chromatography.

## Software Ensures Accurate Identification

To successfully apply gas chromatography to detailed hydrocarbon analysis (DHA) the analyzer must be able to correctly identify a large number of components (many eluting very closely to one another) in a complex chromatogram. The identification is based on a comparison of their individual retention index values to those in a pre-established database. Therefore, it is extremely important that the analyzer functions in a highly repeatable manner.

Due to the high number of possible components in hydrocarbon streams, even though analyzed on a high resolution column, it cannot prevent coelution of some hydrocarbons. However, the presence of certain hydrocarbons depends on the type of sample stream. For example the presence of naphthenes is more common in Naphtha than in Reformate where aromatics are more dominant. The DHA analyzer allows presetting a sample type within the DHA method. By setting a component identification preference for a coelution, the most likely main component is assigned and sample characterization is improved. The software also allows defining additional sample presets in case new sample types become available.

| KRI or LRI* | Component | Hydrocarbon Type | Component Present in: | | |
|---|---|---|---|---|---|
| | | | Reformate | Naphtha | Alkylate |
| 721.4 | 1,1,3-Trimethyl cyclopentane | Naphthenic C8 | - | + | - |
| | 2,2-Dimethylhexane | iso paraffin C8 | ++ | + | - |
| 751.1 | Toluene | Aromatic C7 | +++ | + | - |
| | 2,3,3-Trimethylpentane | Iso paraffin C8 | - | + | ++ |
| 877.9 | o-Xylene | Aromatic C8 | +++ | + | - |
| | 1,1,2-Trimethylcyclohexane | Naphthenic C8 | - | + | - |
| * KRI = Kovats REtention Index. LRI = Linear Retention Index. | | | | | |

**Table 1:** For some sample streams a single component assignment is possible due to the assumed absence of one of the coeluting components.

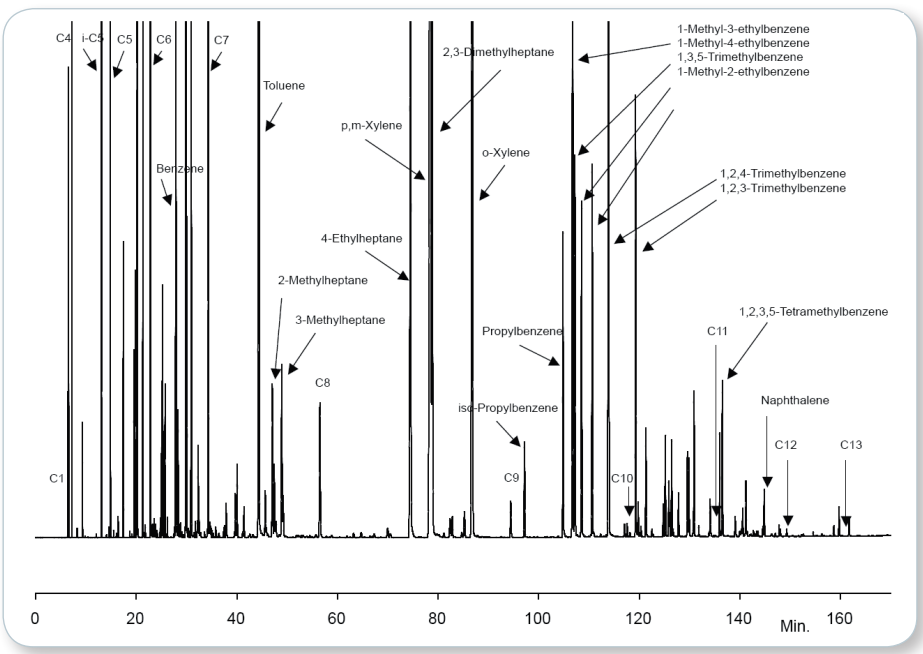



**Figure 2:** Detailed hydrocarbon analysis of a reformate sample showing aromatics identification according ASTM D6730

# Standard Methods

## Selecting Individual Peaks and Updating the Database

The DHA software includes a Peak Select and Database Update function to make identification of unknown peaks as straightforward as possible. The system automatically provides the operator with detailed comparative retention index information for each "unknown" peak including a highlighted "best fit" indicator, making it easy for the operator to determine the ID.

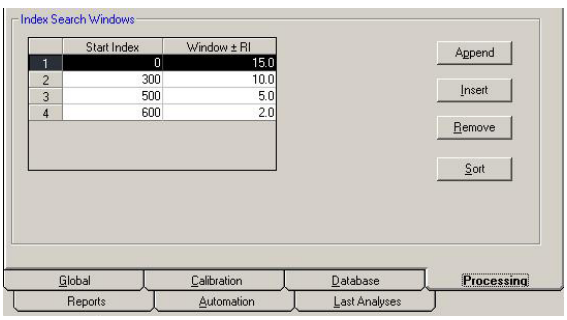



**Figure 3:** Assigning custom peak matching criteria is easy.

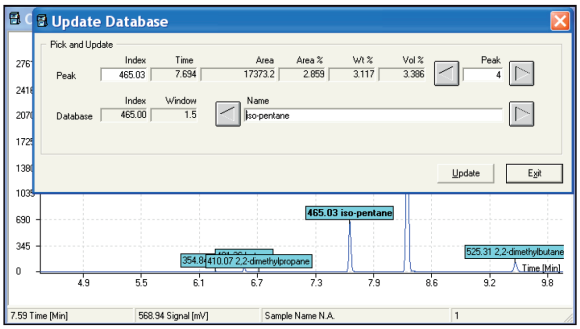



**Figure 4:** DHA provides an easy-to-use graphical means to select peaks and update the database

## Integrated Standard Test Methods

Bruker's DHA analyzers are compliant with the following methods:

- ASTM D6729
- ASTM D6730
- ASTM D6733
- ASTM D5134
- "Fast" DHA
- IP 344 "Front end"

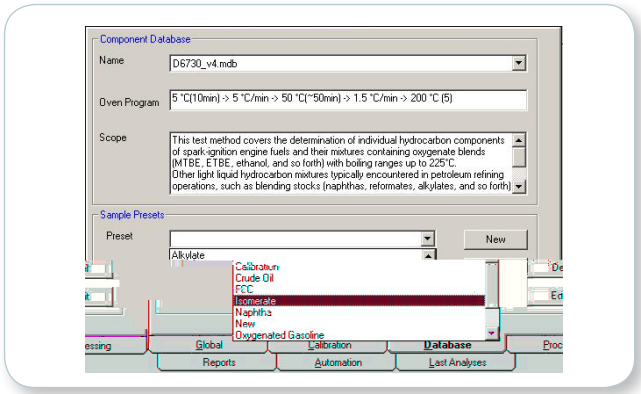



**Figure 5:** Choosing a preferred standard method is easy with the DHA software

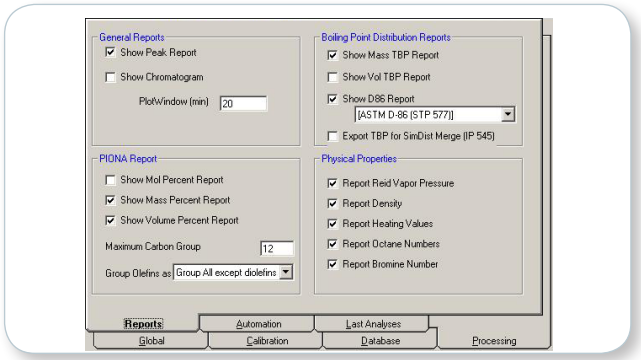



**Figure 6:** Choosing report options is simple

Although each DHA analyzer is configured, tested and certified at the factory for a standard method specified by the customer, the DHA software permits the operator to utilize any of the other popular standard methods as well. And, because of the outstanding performance and flexibility of the Bruker GC and CompassCDS software design, Bruker is able to quickly modify the existing methods or add new ones if required as a result of the on-going "dynamic" industry standard processes.

## Powerful Reporting is Built-in

Bruker's DHA software includes several report options to accommodate the standard methods and/or to meet the customer's special needs. These include:

- Carbon number distribution
- PIONA report; (weight and volume percentage by hydrocarbon group)
- Physical properties calculations; specific gravity and molecular weight
- True distillation profile
- RON/MON specification

# Reduce Sample Analysis Time With “Fast DHA”

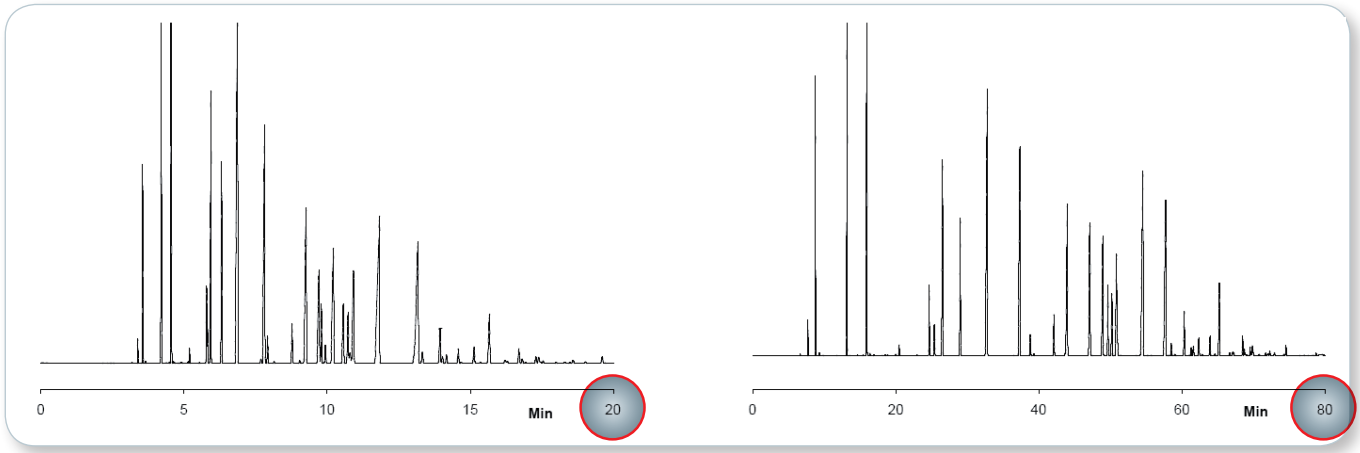
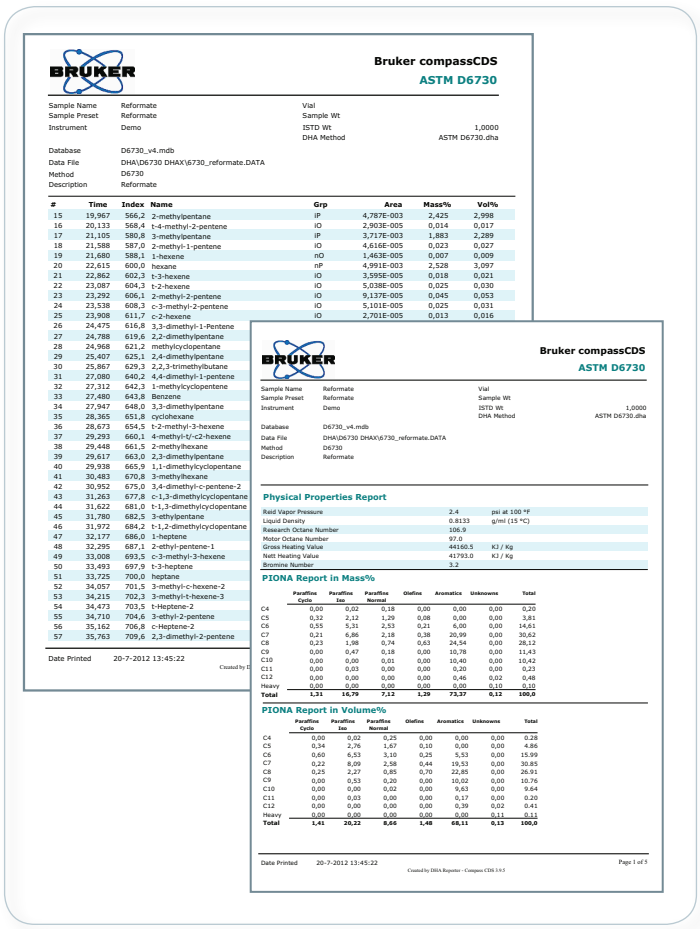



**Figure 7:** These chromatograms illustrate the decreased analysis time using the “Fast DHA” method. Chromatogram of a naphtha sample run on a 40 m X 0.10 mm X 0.2 µm film BR-DHA using the “Fast DHA” method (left). Chromatogram of the same sample, but run on a 100 m X 0.25 mm ID X 0.5 µm film BR-DHA column using standard method D6729 (right). Note reduced analysis time from ~80 minutes to ~20 minutes; almost four-fold.

## DHA Analyzer Includes These Key Components

- Bruker GC high performance gas chromatograph equipped with:
  - Split/splitless capillary injection port
  - High performance capillary column (dependent on specified method on order)
  - Flame ionization detector (FID)
  - Full electronic flow control (EFC) of all gases
- State of the art backflush capabilities for the IP 344 “Front End” method
- CP-8400 or CP-8410 automatic liquid sampler
- CompassCDS for system control, data acquisition and report generation
- CompassCDS based DHA application software
- Computer/monitor
- Pre-loaded standard methods
- Factory test
- Reference chromatogram
- Reference standard for use in conducting on-site performance verification


BRUKER

Bruker compassCDS

ASTM D6730

| | | | |
|---|---|---|---|
| Sample Name | Reformate | Vial | |
| Sample Preset | Reformate | Sample Wt | |
| Instrument | Demo | ISTD Wt | 1,0000 |
| | | DHA Method | ASTM D6730.dha |
| Database | D6730_v4.mdb | | |
| Data File | DHA\D6730 DHAX\6730_reformate.DATA | | |
| Method | D6730 | | |
| Description | Reformate | | |

| # | Time | Index | Name | Grp | Area | Mass% | Vol% |
|---|---|---|---|---|---|---|---|
| 15 | 19,967 | 566,2 | 2-methylpentane | iP | 4,787E-003 | 2,425 | 2,998 |
| 16 | 20,133 | 568,4 | t-4-methyl-2-pentene | iO | 2,903E-005 | 0,014 | 0,017 |
| 17 | 21,105 | 580,8 | 3-methylpentane | iP | 3,717E-003 | 1,883 | 2,289 |
| 18 | 21,588 | 587,0 | 2-methyl-1-pentene | iO | 4,616E-005 | 0,023 | 0,027 |
| 19 | 21,680 | 588,1 | 1-hexene | nO | 1,463E-005 | 0,007 | 0,009 |
| 20 | 22,615 | 600,0 | hexane | nP | 4,991E-003 | 2,528 | 3,097 |
| 21 | 22,862 | 602,3 | t-3-hexene | iO | 3,595E-005 | 0,018 | 0,021 |
| 22 | 23,087 | 604,3 | t-2-hexene | iO | 5,038E-005 | 0,025 | 0,030 |
| 23 | 23,292 | 606,1 | 2-methyl-2-pentene | iO | 9,137E-005 | 0,045 | 0,053 |
| 24 | 23,538 | 608,3 | c-3-methyl-2-pentene | iO | 5,101E-005 | 0,025 | 0,031 |
| 25 | 23,908 | 611,7 | c-2-hexene | iO | 2,701E-005 | 0,013 | 0,016 |
| 26 | 24,475 | 616,8 | 3,3-dimethyl-1-Pentene | | | | |
| 27 | 24,788 | 619,6 | 2,2-dimethylpentane | | | | |
| 28 | 24,968 | 621,2 | methylcyclopentane | | | | |
| 29 | 25,407 | 625,1 | 2,4-dimethylpentane | | | | |
| 30 | 25,867 | 629,3 | 2,2,3-trimethylbutane | | | | |
| 31 | 27,080 | 640,2 | 4,4-dimethyl-1-pentene | | | | |
| 32 | 27,312 | 642,3 | 1-methylcyclopentene | | | | |
| 33 | 27,480 | 643,8 | Benzene | | | | |
| 34 | 27,947 | 648,0 | 3,3-dimethylpentane | | | | |
| 35 | 28,365 | 651,8 | cyclohexane | | | | |
| 36 | 28,673 | 654,5 | t-2-methyl-3-hexene | | | | |
| 37 | 29,293 | 660,1 | 4-methyl-t/-c2-hexene | | | | |
| 38 | 29,448 | 661,5 | 2-methylhexane | | | | |
| 39 | 29,617 | 663,0 | 2,3-dimethylpentane | | | | |
| 40 | 29,938 | 665,9 | 1,1-dimethylcyclopentane | | | | |
| 41 | 30,483 | 670,8 | 3-methylhexane | | | | |
| 42 | 30,952 | 675,0 | 3,4-dimethyl-c-pentene-2 | | | | |
| 43 | 31,263 | 677,8 | c-1,3-dimethylcyclopentane | | | | |
| 44 | 31,622 | 681,0 | t-1,3-dimethylcyclopentane | | | | |
| 45 | 31,780 | 682,5 | 3-ethylpentane | | | | |
| 46 | 31,972 | 684,2 | t-1,2-dimethylcyclopentane | | | | |
| 47 | 32,177 | 686,0 | 1-heptene | | | | |
| 48 | 32,295 | 687,1 | 2-ethyl-pentene-1 | | | | |
| 49 | 33,008 | 693,5 | c-3-methyl-3-hexene | | | | |
| 50 | 33,493 | 697,9 | t-3-heptene | | | | |
| 51 | 33,725 | 700,0 | heptane | | | | |
| 52 | 34,057 | 701,5 | 3-methyl-c-hexene-2 | | | | |
| 53 | 34,215 | 702,3 | 3-methyl-t-hexene-3 | | | | |
| 54 | 34,473 | 703,5 | t-Heptene-2 | | | | |
| 55 | 34,710 | 704,6 | 3-ethyl-2-pentene | | | | |
| 56 | 35,162 | 706,8 | c-Heptene-2 | | | | |
| 57 | 35,763 | 709,6 | 2,3-dimethyl-2-pentene | | | | |

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BRUKER

Bruker compassCDS

ASTM D6730

| | | | |
|---|---|---|---|
| Sample Name | Reformate | Vial | |
| Sample Preset | Reformate | Sample Wt | |
| Instrument | Demo | ISTD Wt | 1,0000 |
| | | DHA Method | ASTM D6730.dha |
| Database | D6730_v4.mdb | | |
| Data File | DHA\D6730 DHAX\6730_reformate.DATA | | |
| Method | D6730 | | |
| Description | Reformate | | |

**Physical Properties Report**

| | | |
|---|---|---|
| Reid Vapor Pressure | 2.4 | psi at 100 °F |
| Liquid Density | 0.8133 | g/ml (15 °C) |
| Research Octane Number | 106.9 | |
| Motor Octane Number | 97.0 | |
| Gross Heating Value | 44160.5 | KJ / Kg |
| Nett Heating Value | 41793.0 | KJ / Kg |
| Bromine Number | 3.2 | |

**PIONA Report in Mass%**

| | Paraffins Cyclo | Paraffins Iso | Paraffins Normal | Olefins | Aromatics | Unknowns | Total |
|---|---|---|---|---|---|---|---|
| C4 | 0,00 | 0,02 | 0,18 | 0,00 | 0,00 | 0,00 | 0,20 |
| C5 | 0,32 | 2,12 | 1,29 | 0,08 | 0,00 | 0,00 | 3,81 |
| C6 | 0,55 | 5,31 | 2,53 | 0,21 | 6,00 | 0,00 | 14,61 |
| C7 | 0,21 | 6,86 | 2,18 | 0,38 | 20,99 | 0,00 | 30,62 |
| C8 | 0,23 | 1,98 | 0,74 | 0,63 | 24,54 | 0,00 | 28,12 |
| C9 | 0,00 | 0,47 | 0,18 | 0,00 | 10,78 | 0,00 | 11,43 |
| C10 | 0,00 | 0,00 | 0,01 | 0,00 | 10,40 | 0,00 | 10,42 |
| C11 | 0,00 | 0,03 | 0,00 | 0,00 | 0,20 | 0,00 | 0,23 |
| C12 | 0,00 | 0,00 | 0,00 | 0,00 | 0,46 | 0,02 | 0,48 |
| Heavy | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,10 | 0,10 |
| **Total** | **1,31** | **16,79** | **7,12** | **1,29** | **73,37** | **0,12** | **100,0** |

**PIONA Report in Volume%**

| | Paraffins Cyclo | Paraffins Iso | Paraffins Normal | Olefins | Aromatics | Unknowns | Total |
|---|---|---|---|---|---|---|---|
| C4 | 0,00 | 0,02 | 0,25 | 0,00 | 0,00 | 0,00 | 0,28 |
| C5 | 0,34 | 2,76 | 1,67 | 0,10 | 0,00 | 0,00 | 4,86 |
| C6 | 0,60 | 6,53 | 3,10 | 0,25 | 5,53 | 0,00 | 15,99 |
| C7 | 0,22 | 8,09 | 2,58 | 0,44 | 19,53 | 0,00 | 30,85 |
| C8 | 0,25 | 2,27 | 0,85 | 0,70 | 22,85 | 0,00 | 26,91 |
| C9 | 0,00 | 0,53 | 0,20 | 0,00 | 10,02 | 0,00 | 10,76 |
| C10 | 0,00 | 0,00 | 0,02 | 0,00 | 9,63 | 0,00 | 9,64 |
| C11 | 0,00 | 0,03 | 0,00 | 0,00 | 0,17 | 0,00 | 0,20 |
| C12 | 0,00 | 0,00 | 0,00 | 0,00 | 0,39 | 0,02 | 0,41 |
| Heavy | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,11 | 0,11 |
| **Total** | **1,41** | **20,22** | **8,66** | **1,48** | **68,11** | **0,13** | **100,0** |

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Page 1 of 5

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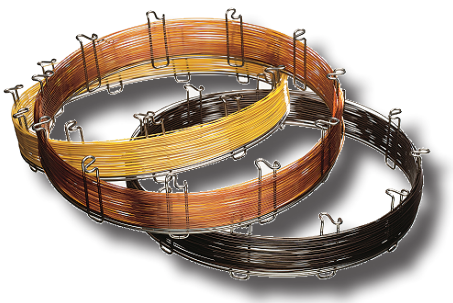
**Figure 8:** Physical properties and detailed hydrocarbon report

# Bruker-Certified Consumables for Your SCION GC Series

Bruker GC columns span a broad range of column diameters, stationary phases, and capillary column materials: Fused Silica (FS) and Inert Steel (IS). Ideal for either routine or research type analyses.

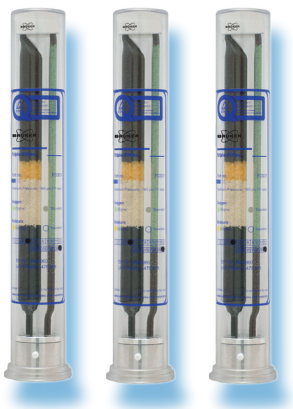


Bruker GC column offerings bridge across many important applications and include a number of offerings such as:

- Standard WCOT (Wall Coated Open Tubular)
- Solid Stationary Phase PLOT (Porous Layer Open Tubular)
- Inert Steel Micro-Packed and Packed

## Super Clean™ Gas Filters

Bruker Gas Purification Systems have the range to satisfy your needs from individual to combination filters, from Ultra purity combined with Ultra capacity, to all in one solution kits. Innovative features designed into the product yield extensive benefits to the user.



- Ultra-high capacity for long life, less change and improved productivity
- High-purity output ensures 99.9999% Pure Gas
- "Quick connect" fittings for easy, leak-tight filter changes
- Glass internals prevent diffusion; plastic externally for safety
- Easy-to-read indicators for planned maintenance and improved up-time

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

www.ScionHasArrived.com

www.Bruker.com

**www.bruker.com/scion**

# Natural Gas Analyzer

- A Family of optimized GC Solutions

Gas Chromatography

Innovation with Integrity

# Bruker Natural Gas Analyzers

Natural gas is bought and sold as a bulk commodity with price based on its energy content. It is very important for all stakeholders in the natural gas supply and consumer chain to accurately determine the heating value of their streams. Bruker offers a full range of GC based solutions for the analysis of natural gas. The analyzer family is designed to offer superior results through the use of industry proven hardware, software, optimized columns and consumables, and is backed by a team of global sales and support specialists.

## Key Benefits include:

- A complete range of natural gas analysis (NGA) solutions. Bruker offers many different NGA gas chromatography analyzers to meet the broadest range of stream sample types and throughput needs, whether the analysis is conducted in a laboratory, at-line or in the field.
- Easy to operate, powerful GC solutions. Bruker's GC with CompassCDS Chromatography Software, form a powerful combination and do not require a high degree of skill to be used successfully.
- Flexibility to analyze natural gas, liquified petroleum gas or natural gas liquids (NGL). Bruker's GC based NGA analyzers can be configured to measure the composition of LPG or NGL streams through the use of specialized sample conditioners, ensuring sample integrity is constistently maintained.
- Operational procedures are fully documented. All Bruker NGA analyzers not only incorporate proven GC hardware and software, but arrive with the pre-loaded analysis method(s) and documentation specific to the application.
- Comprehensive single-vendor solution. Bruker is proud to provide complete solutions. The hardware, software, application optimization, documentation, installation and performance verification are all delivered by Bruker.


Figure 1: The Bruker GC based Natural Gas Analyzer.

# Solutions for Natural Gas Analysis

Gas chromatography offers a proven means to determine the composition and heating value of natural gas and related streams quickly and cost effectively. Bruker's natural gas analyzers (NGAs) are standard 'turnkey' systems pre-configured and tuned at the factory to ensure their compliance with standard methods used to determine the heating value of natural gases and related streams. They can also be specially configured to determine other components of interest (eg. sulfur compounds), to ensure suitability for use in downstream processes. The analyzers are based on the Bruker GC gas chromatograph platforms and Bruker's CompassCDS Chromatography Software. All systems employ a proven and optimized multi-channel/multi-dimensional approach to determine the heating/calorific value of natural gas, as well as quantify individual components.
Bruker offers several NGA systems to meet the widest range of analysis needs.

## Basic NGA (System A)

This is the simplest of all available natural gas analysis systems. As shown in Figure 3, the system employs a single valve column designed for simplicity, a Thermal Conductivity Detector (TCD) and Flame Ionization Detector (FID). The TCD is used for the determination of $O_2$, $N_2$, $CH_4$, $CO_2$ and Ethane, while the FID, connected in series, determines hydrocarbons in low concentrations, i.e. C3-C5 and C6+ back-flushed grouping peak (late back-flush). A single unheated 4 port Liquid Sampling Valve (LSV) is available for LPG type samples.

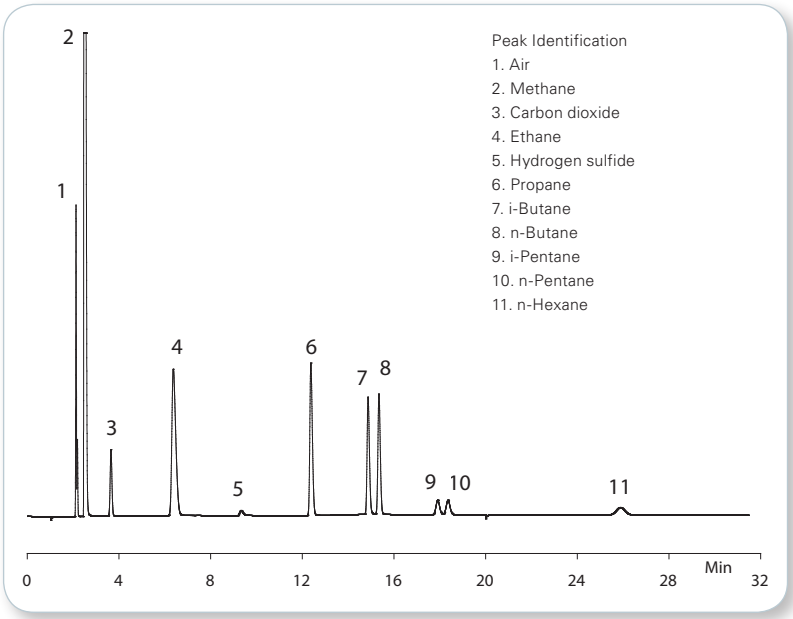



Figure 2: Chromatogram of natural gas sample from 'System A'. Up to 10 Min TCD signal, 10 to 31 Min FID signal.

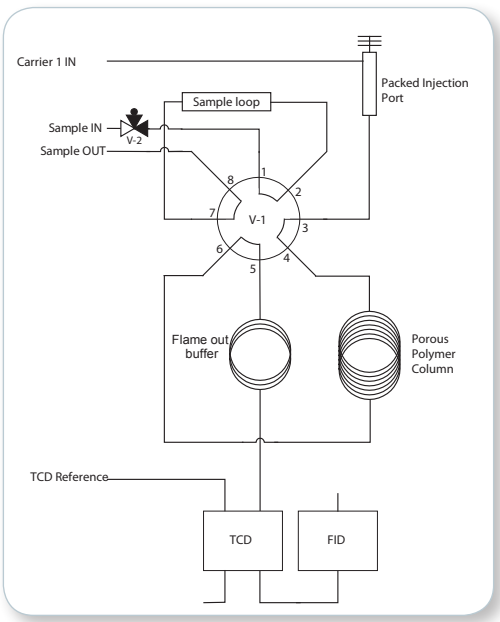



Figure 3: System configuration schematic diagram for Natural Gas Analyzer 'A'.

# Natural Gas Analysis

## NGA/Natural Gas Liquids (System B)

This system is optimized for the analysis of natural gas or de-methanized hydrocarbon matrices. For natural gas, the components of interest are typically oxygen, nitrogen, carbon dioxide, methane, ethane, propane, butane, isobutane, pentane, hydrogen sulfide, and C6+ as a composite peak. For de-menthanized streams (liquid natural gas) the components of interest are typically carbon dioxide, ethane, propane, butane, iso-pentane, hexane, and C7+ as a composite peak.

The system is configured with a 10 and 12 port valve (a third liquid sampling valve is added if liquid streams are to be analyzed) and three analysis columns connected to TCD and FID detectors (Figure 4). The system simultaneously injects the stream onto two column systems, a Molsieve column for the determination of $O_2$ and $N_2$ without the use of coolants, and short/long Non-Polar columns for the analysis of hydrocarbons and $CO_2$. The Non-Polar columns are set up for early back-flush, which optimizes sensitivity while reducing run time (from 25 minutes using the system 'A' configuration to less than 15 minutes) (Figure 5). The System „B" is extendable with two standard options. For the analysis of de-methanized liquefied natural gas distillates (i.e. propane, butanes and pentanes) an automated 4 port Liquid Sampling Valve is available to inject the sample as a Liquid. For the analysis of hydrogen and helium in natural gas a $He/H_2$ channel is available as extra GC channel.

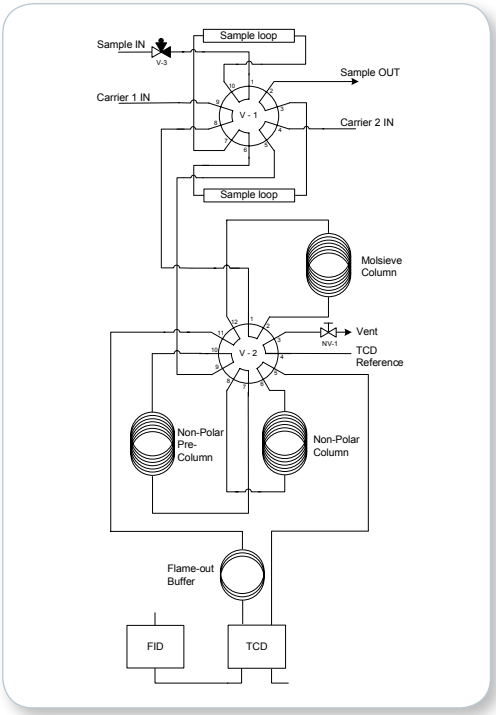



Figure 4: System configuration schematic for Natural Gas Analyzer 'B'.

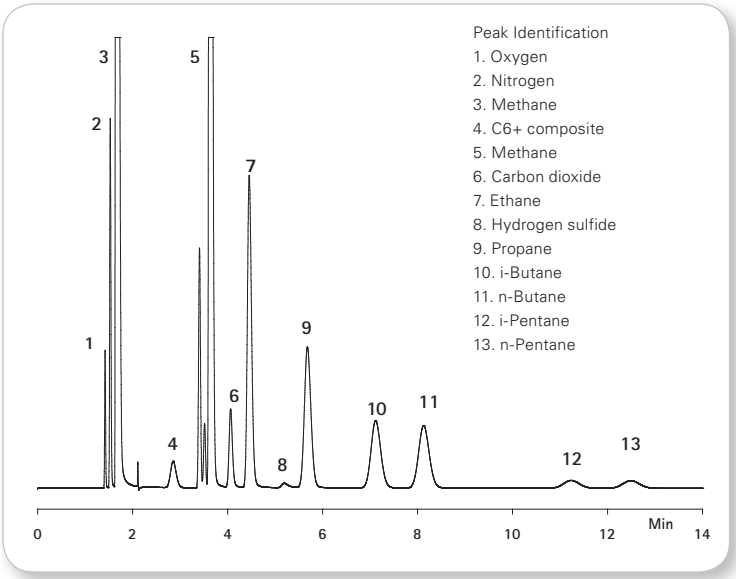



Figure 5: Chromatogram of natural gas samples from 'System B'. Note separation of oxygen and nitrogen.

# "Rich" Natural Gas Analysis

## NGA/Natural Gas Liquids - Extended Analysis (System C)

This system is specifically designed to analyze 'rich' natural gas or natural gas liquid streams by separating all hydrocarbon components up to C16. As with System B, it separates and quantifies oxygen and nitrogen, as well as measuring hydrogen sulfide down to ~100 ppm.

The system is configured with a 14 port valve and 6 port valve. The 14 port valve enables the system to introduce the sample stream simultaneously to three independent columns with automated detector switching which provides high sensitivity detection of all components of interest. The valves are installed in the multi-valve oven for flexible operation of the conventional column oven. Two of the sample paths flow onto Molsieve and porous polymer columns to separate oxygen, nitrogen and carbon dioxide, ethane, methane, ethane and $H_2S$, and the other via a 'splitter' onto a high performance non-polar capillary column to separate the hydrogen components up through C16. The 6 port valve is used to direct the separated components fraction to the TCD detector while components remaining on the Molsieve column are flushed to vent. If natural gas liquids are to be analyzed, a third valve (liquid sampling) is added to the configuration described above. For natural gas containing hydrogen and helium a He/$H_2$ channel is configured additionally.

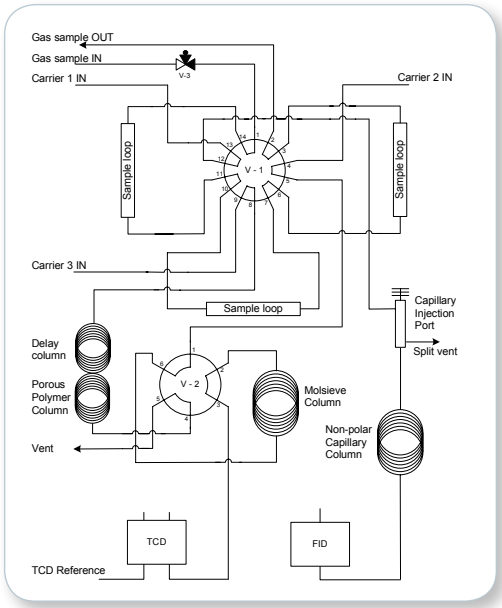



Figure 7: System schematic for Natural Gas Analyzer 'C'

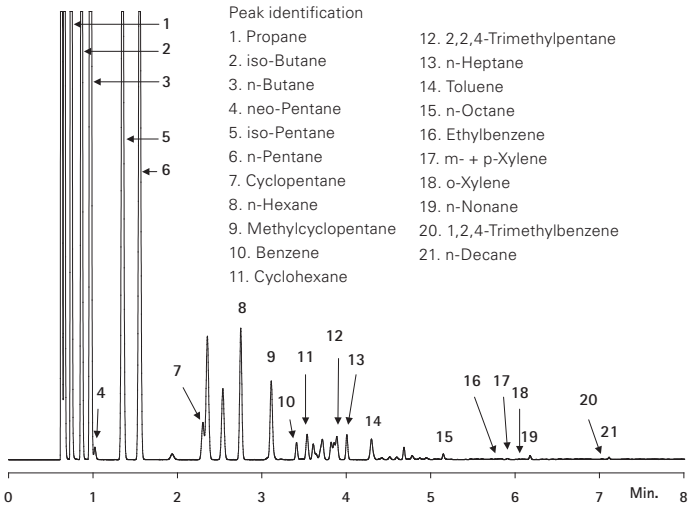



Figure 6: Chromatogram showing natural gas sample from 'System C' FID channel. Note individual separation of C6+ components

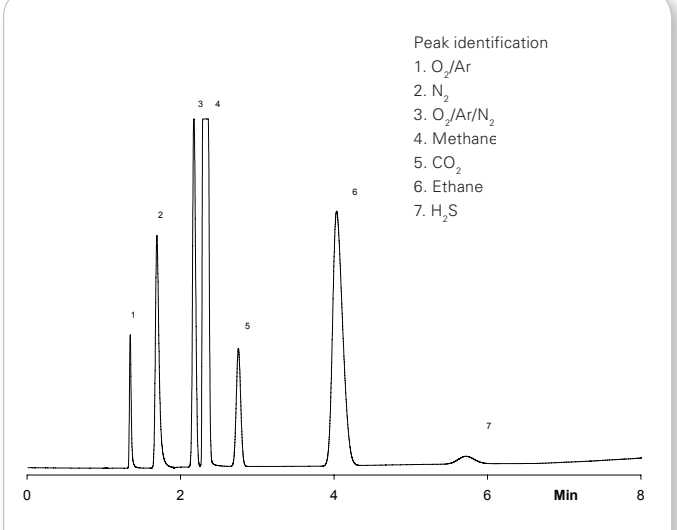



Figure 8: Chromatogram showing natural gas sample from 'system C' TCD channel.

# Base Natural Gas Analysis Systems

| Analyzer Characteristic | Bruker GC System 'A' | Bruker GC System 'B' | Bruker GC System 'C' |
|---|---|---|---|
| **Gas Components Measured** | | | |
| $O_2$, $N_2$, $CO_2$, $CH_4$ | YES | YES | YES |
| Ethane, Propane, Butane, Iso-butane, Neo-pentane, Pentane, Iso-pentane | YES | YES | YES |
| C6+ as a composite peak | YES | YES | YES |
| C7+ as a composite peak | YES | YES | YES |
| $O_2/N_2$ Separation | YES[1] | YES | YES |
| $He/H_2$ Separation | NO | YES[3] | YES[3] |
| Max hydrocarbon number speciated | C6 | C7 | C16 |
| LPG | YES[4 or 5] | YES[4 or 5] | YES[4 or 5] |
| De-methanized natural gas/natural gas liquids | NO | YES[4] | YES[4] |
| Typical analysis to analysis repeatability % RSD | <1.0 | <1.0 | <1.0 |
| Analysis time | 30 min | 14 min | 15-20 min |
| **Standard Gas Methods** | | | |
| IP-345 | YES | | |
| GPA 2172 | | | |
| GPA 2177 | | YES | |
| GPA 2261 | | YES | |
| GPA 2286 | | YES | YES |
| GPA 2186 | | YES | YES |
| ASTM D5504 | | | YES[5] |
| ASTM D6228 | | | YES[5] |
| **Natural Gas Calculation Methods** | | | |
| ISO 6974 | | Contact Bruker, several configuration possibilities | |
| ISO 6976 | | | |
| GOST-22667 | | | |

[1] Requires liquid nitrogen or liquid $CO_2$ oven cooling
[2] Requires 3rd dedicated channel
[3] Requires additional channel including valve, columns and TCD
[4] Requires LSV to be additionally installed
[5] This method is specifically for sulfur components in natural gas, therefore a sulfur selective detector must be used such as a PFPD

# Sulfur components in Natural Gas

**CompassCDS Chromatography Data System**

**Extended Natural Gas Analysis Report**

| | |
|---|---|
| **Run File** | NGC.DATA |
| **Method** | Nat Gas C |
| **Sample Name** | NGC |

| Component | Mole % | MW | kJ/Mole (Superior) | kJ/Mole (Inferior) |
|---|---|---|---|---|
| 3,3-Dimethylpentane | 0.9586 | 0.83 | 40.14 | 37.17 |
| trans 1,2-Dimethylcyclopentane | 0.6972 | 0.60 | 29.22 | 27.06 |
| 2,2-Dimethylhexane | 0.6100 | 0.53 | 25.50 | 23.60 |
| Nitrogen | 1.4815 | 0.42 | 0.00 | 0.00 |
| Methane | 65.3595 | 10.49 | 582.41 | 524.61 |
| Carbon Dioxide | 0.5229 | 0.23 | 0.00 | 0.00 |
| Ethane | 8.2789 | 2.49 | 129.52 | 118.28 |
| Hydrogen Sulphide | 4.3573 | 1.48 | 24.50 | 22.57 |
| Propane | 3.7037 | 1.63 | 82.23 | 75.68 |
| i-Butane | 2.3529 | 1.37 | 67.51 | 62.31 |
| n-Butane | 2.4401 | 1.42 | 70.24 | 64.84 |
| neo-Pentane | 1.0458 | 0.75 | 36.77 | 33.99 |
| i-Pentane | 2.2658 | 1.63 | 79.99 | 73.98 |
| n-Pentane | 2.4401 | 1.76 | 86.31 | 79.84 |
| n-Hexane | 1.6558 | 1.43 | 69.49 | 64.36 |
| 2,2-Dimethylpentane | 1.0458 | 0.90 | 49.35 | 40.47 |
| Methylcyclopentane | 0.7843 | 0.68 | 32.86 | 30.43 |
| **Totals** | 100.0000 | 28.63 | 1,406.03 | 1,279.18 |

| | | | |
|---|---|---|---|
| **MJ/kg (Superior)** | 49.11 | **Sample Ideal Relative Density** | 0.9885 |
| **MJ/kg (Inferior)** | 44.68 | **Sample Real Relative Density** | 0.9948 |
| **MJ/m3 (Superior)** | 59.46 | **Sample Ideal Absolute Density** | 1.2069 kg/m3 |
| **MJ/m3 (Inferior)** | 54.10 | **Sample Real Absolute Density** | 1.2151 kg/m3 |
| **Sample Compressibility** | .9932 | **Sample Wobbe Index** | 59.62 |

**Base Conditions: Temperature = 15 C, Pressure = 101.325 kPa**
**Reference: ISO 6976: 1995(E)**

Figure 9: Natural Gas Report - 'System C' generated using Bruker's CompassCDS Chromatography Data Software

There are several methods specifically used for the analysis of sulfur components in natural gas, e.g. ASTM D5504 and ASTM D6228. Bruker's natural gas analyzers can be modified to measure sulfur components through the addition of an extra, fully inert channel, dedicated for the determination of lowlevel sulfur components only. This sulfur channel will be equipped with the Pulsed Flame Photometric Detector (PFPD), a sulfur specific detector. The systems can also be configured and tested exclusively for the analysis of sulfur components as per standard methods, or enterprise specific requirements.

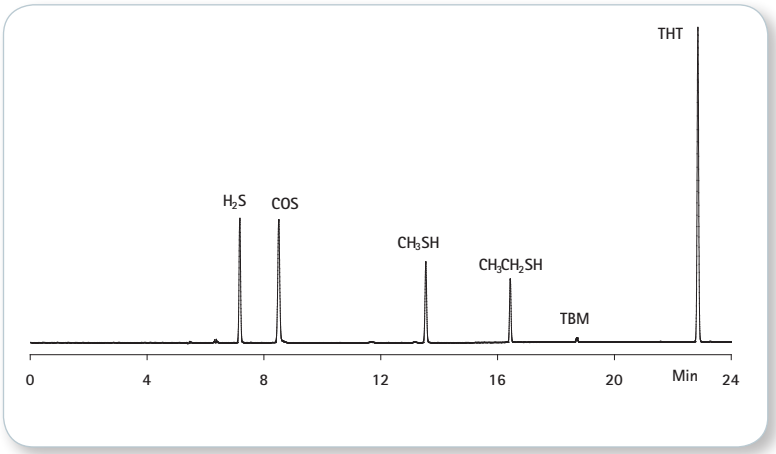
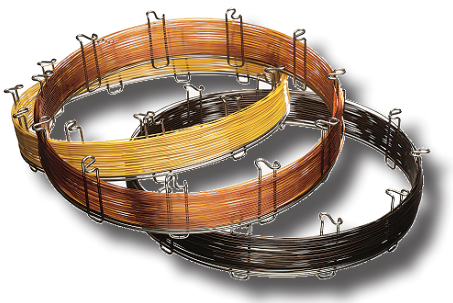



Figure 10: Detection of trace level sulfur components using the 450-GC, specially treated with Inert Steel surface deactivation and Pulsed Flame Photometric Detector (PFPD).

# Bruker-Certified Consumables for Your SCION GC Series

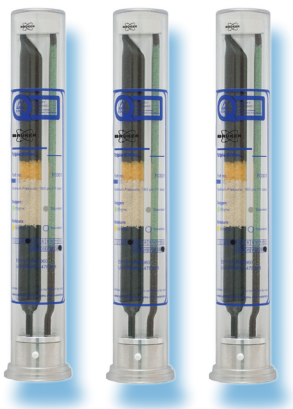
Bruker GC columns span a broad range of column diameters, stationary phases, and capillary column materials: Fused Silica (FS) and Inert Steel (IS). Ideal for either routine or research type analyses.



Bruker GC column offerings bridge across many important applications and include a number of offerings such as:

- Standard WCOT (Wall Coated Open Tubular)
- Solid Stationary Phase PLOT (Porous Layer Open Tubular)
- Inert Steel Micro-Packed and Packed

## Super Clean™ Gas Filters



Bruker Gas Purification Systems have the range to satisfy your needs from individual to combination filters, from Ultra purity combined with Ultra capacity, to all in one solution kits. Innovative features designed into the product yield extensive benefits to the user.

- Ultra-high capacity for long life, less change and improved productivity
- High-purity output ensures 99.9999% Pure Gas
- "Quick connect" fittings for easy, leak-tight filter changes
- Glass internals prevent diffusion; plastic externally for safety
- Easy-to-read indicators for planned maintenance and improved up-time

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

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# Refinery Gas Analyzer

- Optimized GC Analysis Solutions

Gas Chromatography

Innovation with Integrity

# Bruker Refinery Gas Analyzers

The source and composition of refinery gases varies considerably. Measuring gas composition precisely and accurately is a significant challenge in today's refinery operations. Bruker's refinery gas analyzers are designed to deliver superior, reliable results for a wide range of sources and analysis throughput requirements.

- A range of refinery gas analysis (RGA) solutions. Bruker offers RGA solutions to meet the broadest range of stream sample types and throughput requirements.
- A powerful, easy to use GC solution. Bruker's 456-GC and CompassCDS chromatography software is a very powerful combination designed to achieve the best possible results. In addition, these systems do not require a high degree of operator skills.
- A highly flexible solution for analysis. The Bruker RGA solutions can optional be configured to analyze high pressurized gas and liquefied petroleum gas (LPG) through the use of a fully integrated Micro-Gasifier, giving the flexibility to accommodate a wide range of stream types.
- Operational procedures are fully documented. Bruker RGA analyzers not only incorporate proven GC hardware and software but also arrive pre-loaded with analysis methods, and include documentation specific to the application required.
- A comprehensive, single vendor solution. Bruker provides complete solutions. The hardware, software, application optimization, documentation, installation and performance verification are all provided by Bruker, offering an all inclusive, convenient analysis solution.


Figure 1: The 456-GC RGA has outstanding flexiblity, analytical power and robustness.

# Key Benefits

## Bruker solutions for refinery gas analysis

Typical sources for refinery gases include atmospheric or FCC overheads, ethylene, propylene production, fuel gas, stack gas and off gas from desulfurization. The physical stream types range from gas to highly pressurized gas or liquefied gases. Bruker's refinery gas analyzers (RGA) are 'turnkey' systems pre-configured and tuned at the factory to conform to industry standard methods including: UOP 539, DIN-51666 and ASTM D2163. The RGA systems are based on the Bruker 456-GC. To perform good analysis, the RGA is optional equipped with an integrated micro-gasifier. This sample conditioning device ensures complete vaporization of LPGs and high pressures samples to prevent any sample discrimination prior injection.

The Analyzers employ a proven and optimized multi-channel approach. They determine the concentration of individual saturated and unsaturated hydrocarbon components up to and including C5 (C6 and higher components as a composite peak) and all permanent gases, including hydrogen and hydrogen sulfide in a single analysis. Included in every system is Bruker's powerful CompassCDS chromatography software to provide complete analyzer control, data acquisition and flexible report generation.

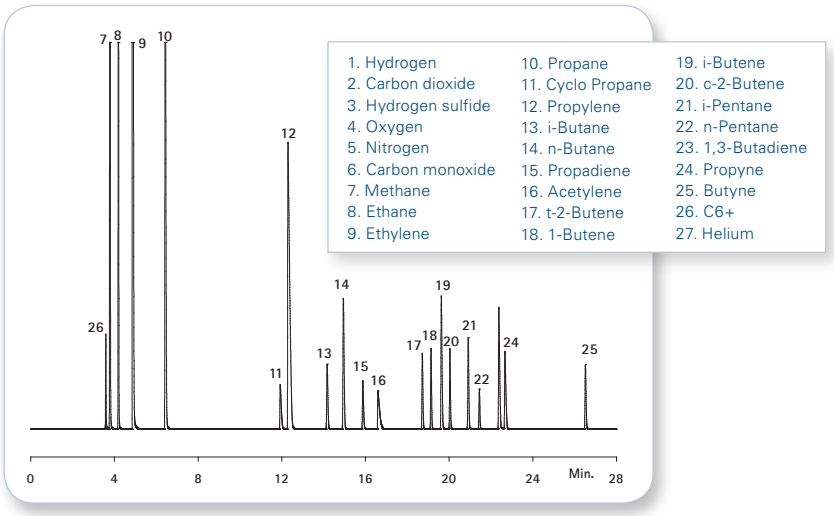


Figure 2: The separation of light hydrocarbons using the Standard RGA.

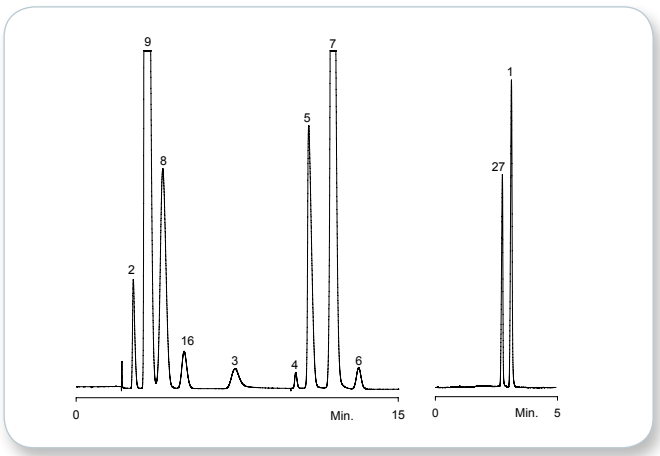


Figure 3: The analysis of the permanent gases and hydrogen (and helium) using the Standard RGA.

| | | | | |
|---|---|---|---|---|
| **FCC Overhead** | **Ethylene** | **Propylene** | **Propane** | **Butylene** |
| **Butanes** | **Fuel Gas** | **Stack Gas** | **Off Gas from Desulphurization** | **Reformer Gas** |

Figure 4: The RGA analyzers are applicable to a variety of different hydrocarbon streams.

## Bruker offers two RGA systems to meet the widest range of analysis requirements:

- Standard RGA: A three channel 456-GC with a multi-valve design using both capillary and packed columns. The first channel is optimized for the analysis of permanent gases, the second is designed for light hydrocarbons, and the third specifically for hydrogen. The system is configured and fully tested in accordance with industry standard methods. Total analysis time for all components is less than 25 minutes.
  The standard RGA analyzer is the most powerful tool to analyze the widest range of RGA type streams. This includes sample streams with a high % level of components as in ethylene, propylene and butylene streams.

- Rapid RGA: A three channel 456-GC that utilizes a multi-valve design in which the packed columns used in the Standard RGA are replaced by micro-packed columns in both the hydrogen and permanent gas channels. Since the micro-packed columns are installed in a separate heated zone, the capillary columns located in the GC oven can be temperature programmed in a more aggressive manner. For high sample analysis demand, the Rapid RGA Analyzer concept provides a substantial reduction in overall analysis time of 5 minutes ( 7 minutes with $H_2S$) compared to the 25 minutes with the standard RGA.

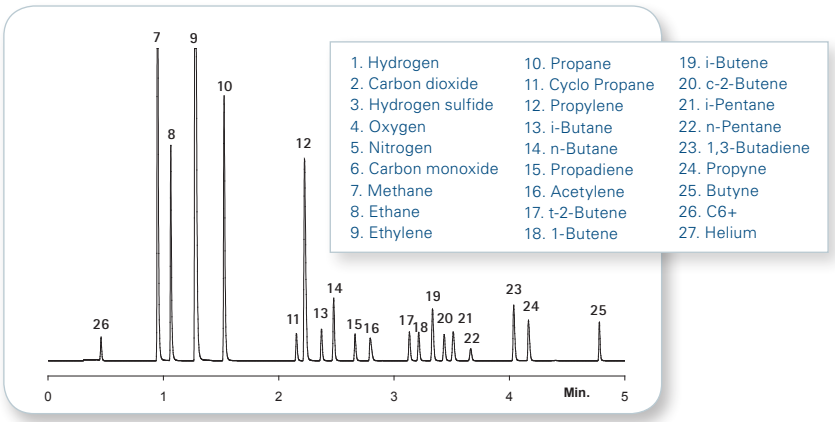


Figure 5: The analysis of light hydrocarbons using the Rapid RGA, with complete separation in less than five minutes.

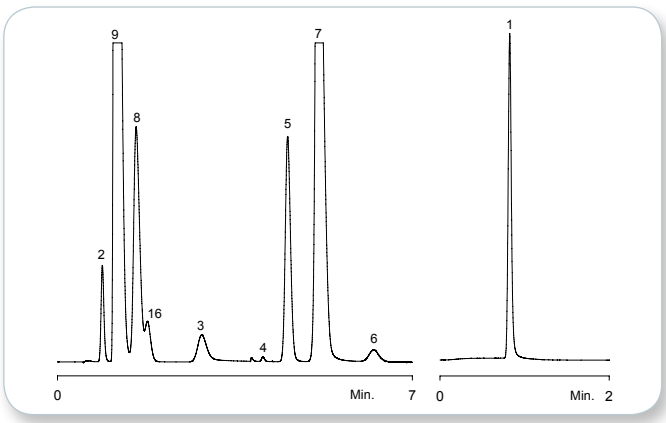


Figure 6: The analysis of permanent gases and hydrogen using the Rapid RGA.

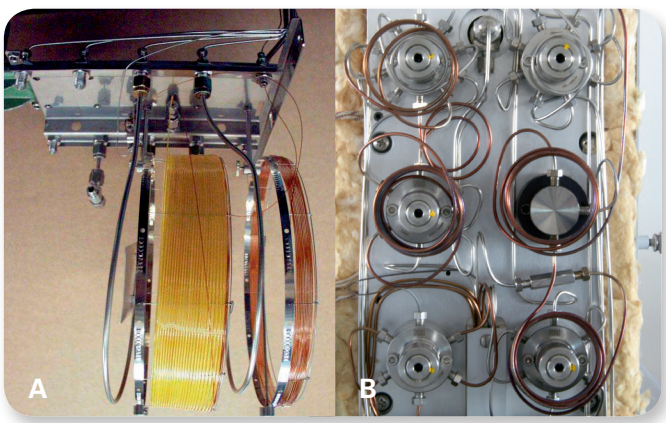


Figure 7: A shows a 'traditional' RGA with all columns mounted in oven. B shows the micro-packed columns mounted in the separate heated zone in the Rapid RGA.

# Bruker Refinery Gas Analyzers

Table 1: RGA Analyzer Characteristics.

| Characteristics | Standard RGA | Rapid RGA |
|---|---|---|
| No. of Channels/Detectors Used | 3 | 3 |
| No. of Column Ovens | 1 | 2 |
| Analysis Time | 25 min | 5 min (7 min with $H_2S$) |
| Repeatability | <1% | <1% |
| Linear Bench Space Required | 66 cm/26 in. | 66 cm/26 in. |
| Minimum Component Detection Level | 0.01% all components except $H_2S$ = 0.05% | 0.01% all components except $H_2S$ = 0.05% |
| **Suitability** | | |
| Typical Refinery Gas | Excellent | Excellent |
| Impurities in Bulk Ethylene | Excellent | Excellent |
| Impurities in Bulk Propylene | Excellent | Good |
| Impurities in Bulk C4 | Good | Good |

Table 2: Multiple channels of data are conveniently combined into a single analysis report.

| Peak No. | Peak Name | Channel | RT (min.) | Result (g/l) | Norm. (%) | Area (uV/Sec.) |
|---|---|---|---|---|---|---|
| 1 | Hydrogen | Middle (TCD) | 1.6967 | 36.0300 | 22.7681 | 390257 |
| 2 | Carbon dioxide | Front (TCD) | 2.6000 | 0.1000 | 0.0632 | 13376 |
| 3 | Hydrogen sulfide | Front (TCD) | - | 0.0000 | 0.0000 | 0 |
| 4 | Oxygen | Front (TCD) | 9.9200 | 0.0000 | 0.0000 | 37325 |
| 5 | Nitrogen | Front (TCD) | 10.3267 | 1.1990 | 0.7577 | 2122071 |
| 6 | Carbon monoxide | Front (TCD) | - | 0.0000 | 0.0000 | 0 |
| 7a | Methane | Front (TCD) | 11.1917 | 11.9900 | 7.5767 | 1394584 |
| 7b | Methane | Rear (FID) | 3.7350 | 11.9900 | 7.5767 | 1492388 |
| 8a | Ethane | Front (TCD) | 3.5367 | 17.9900 | 11.3682 | 2867688 |
| 8b | Ethane | Rear (FID) | 4.1283 | 17.9900 | 11.3682 | 4480322 |
| 9a | Ethylene | Front (TCD) | 2.9550 | 29.9800 | 18.9449 | 4139442 |
| 9b | Ethylene | Rear (FID) | 4.7217 | 29.9800 | 18.9449 | 7411134 |
| 10 | Propane | Rear (FID) | 6.1933 | 0.1990 | 0.1258 | 71402 |
| 11 | Cyclo Propane | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 12 | Propylene | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 13 | i-Butane | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 14 | n-Butane | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 15 | Propadiene | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 16a | Acetylene | Front (TCD) | 5.0283 | 0.5020 | 0.3172 | 49786 |
| 16b | Acetylene | Rear (FID) | 16.4331 | 0.5020 | 0.3172 | 121300 |
| 17 | t-2-Butene | Rear (FID) | 18.5050 | 0.0990 | 0.0626 | 138647 |
| 18 | 1-Butene | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 19 | i-Butene | Rear (FID) | 19.5167 | 0.0990 | 0.0626 | 44492 |
| 20 | cis-2-Butene | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 21 | 1,3-Butadiene | Rear (FID) | 22.1367 | 0.0000 | 0.0000 | 16165 |
| 22 | Propyne | Rear (FID) | - | 0.0000 | 0.0000 | 0 |
| 23 | C5+ | Rear (FID) | 2.9217 | 0.1000 | 0.0632 | 58164 |
| Totals | | | | 158.2480 | 100.0000 | |

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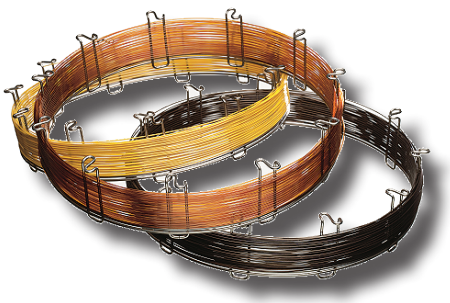

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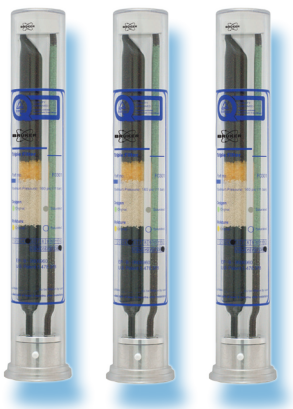

- Ultra-high capacity for long life, less change and improved productivity
- High-purity output ensures 99.9999% Pure Gas
- "Quick connect" fittings for easy, leak-tight filter changes
- Glass internals prevent diffusion; plastic externally for safety
- Easy-to-read indicators for planned maintenance and improved up-time

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

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Technical Note # CA-270111

# Principles and performance of the Collision Reaction Interface for the aurora M90

Bruker's patented 90 degree ion optics provides unsurpassed efficiency of transfer of ions from the interface to the mass analyzer, which enables the aurora M90 ICP-MS to achieve a sensitivity of more than 1000 million c/s per mg/L of analyte, while maintaining oxide ratios ($CeO^+/Ce^+$) below 3%. The aurora M90 ICP-MS is also equipped with Bruker's unique and patented interference management system, the Collision Reaction Interface (CRI). This CRI technology reduces common polyatomic interferences on elements such as As, Se, Cr, V and Fe, thus achieving lower detection limits in hot plasma, even for samples with complex matrices.
Unlike other interference management systems, the CRI does not use a pressurized multipole prior to the mass analyzer. Instead, reaction and collision gases are injected directly into the plasma through the tips of the interface cones. This innovative approach reduces/removes interferences before the interfering and analyte ions are extracted into the ion optics. Due to highly efficient pumping within the interface region, switching between CRI and normal mode (no CRI gas) is very rapid, enabling multiple condition sets to be run on a single solution.

## Basic Principles of Collision Reaction Interface (CRI)

As shown in Figure 1, the CRI works simply by injecting the reactive/collision gases into the plasma through the tips of the sampler and/or skimmer cones to induce collisions and/or ion-molecule reactions with interfering ions. Plasma conditions at the interface cone apertures are ideal for collisions and reactions to occur. The high plasma density and high temperature should lead to a high collision/reaction frequency between the interfering ions and the injected gases. As a result, most argon-based polyatomic interferences are destroyed or removed before they are extracted into the ion optics. Hydrogen and helium are used as CRI gases, as these gases provide efficient interference attenuation, and avoid the need to use expensive or corrosive gases such as methane or ammonia.
When a collision/reaction gas is added to the plasma, a number of processes occur including charge transfer, proton transfer, electron-ion reactions and ion-molecule interactions. For example, when hydrogen is injected, a polyatomic interfering ion such as $Ar_2^+$ (that interferes with $^{80}Se$ determinations) collides with a hydrogen molecule. A proton is transferred from the $H_2$ molecule to the $Ar_2^+$ ion, forming $ArH^+$, a neutral H atom and a neutral Ar atom. The $ArH^+$ ion then collides with another $H_2$ molecule and a proton is transferred from the ion to the molecule, forming a neutral Ar atom and an $H_3^+$ ion. The $H_3^+$ ion (m/z = 3 amu/unit electronic charge) does not interfere with any isotopes of interest in ICP-MS.

**Enhanced gas injection of the CRI**

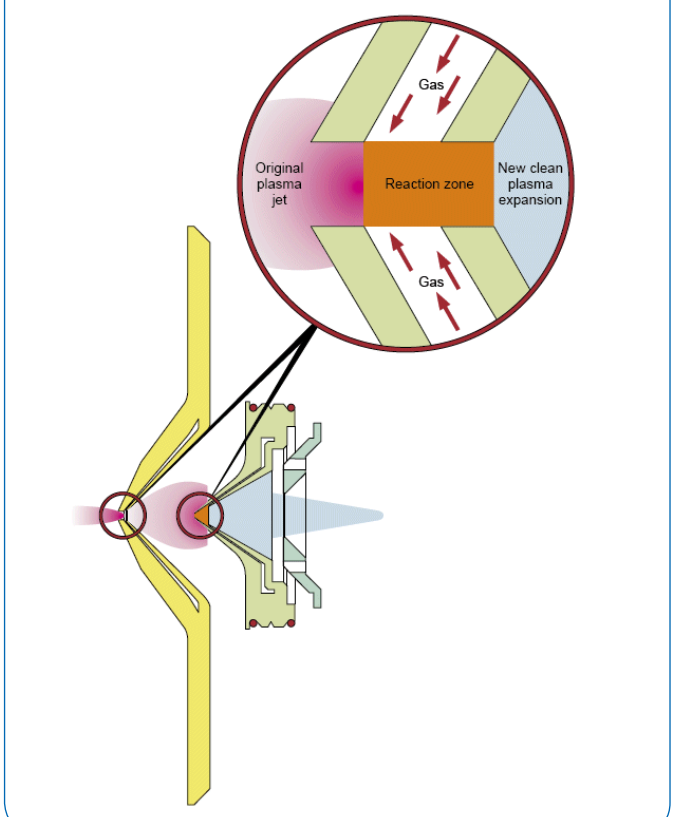


Figure 1: Schematic diagram of the Bruker CRI system

When helium is injected, interaction between the electron clouds of the helium atoms and those of interfering polyatomic ions can make a large polyatomic interfering ion such as $^{35}Cl^{16}O^+$ (which interferes with $^{51}V$) rotationally and vibrationally excited. In subsequent collisions, an excited $^{35}Cl^{16}O^+$ ion can receive sufficient energy to bring about its dissociation, removing the $^{35}Cl^{16}O^+$ interference from the $^{51}V$ determination. In general, the analyte ions are not removed by the CRI technique; they simply lose energy as they collide with the CRI gases. Polyatomic ions, in contrast, are destroyed and removed when colliding with the CRI gases, mainly due to the charge transfer reactions, or collisional excitation-dissociation processes.

## The Effect of Injecting CRI Gas at the Skimmer and Sampler Cone

Experimental results obtained so far suggest that gas injected into the plasma from the aperture of the sampler cone has less effect on the interferences reduction/removal. Figure 2 is a 3-D graph showing typical results of interference reduction experiments, where the sensitivities for $^{75}As$ and $^{89}Y$ were measured at various CRI gas flow rates through both the skimmer and sampler cones. The test solution (Var-IS-1) contains 10 µg/L Y in 0.5% $HNO_3$ and 0.5% HCl matrix solution, and helium was used as the CRI gas. Since no arsenic was present in the solution, the measured sensitivity for $^{75}As^+$ is entirely due to the interfering polyatomic ion $^{40}Ar^{35}Cl^+$.

It is clear from Figure 2 (A), that the apparent signal for $^{75}As$ (actually from $^{40}Ar^{35}Cl^+$) is decreasing with increasing He flow into the skimmer. At a flow rate around 120 mL/min, the interference from $^{40}Ar^{35}Cl^+$ is completely removed. The efficiency of interference removal is demonstrated in Figure 2 (B), where the signal ratio of $^{89}Y/^{75}As$ (i.e., ratio of a real analyte ion to the signal from an interfering ion) is improving with increasing He flow rate into the skimmer. In contrast, the He flow at the sampler cone has very little impact on either the $^{40}Ar^{35}Cl^+$ signal or the $^{89}Y/^{75}As$ ratio, as shown in Figure 2. Most of the results shown in this report were obtained with the CRI gases injected into the plasma at the aperture of the skimmer cone.

**CRI removes interferences**

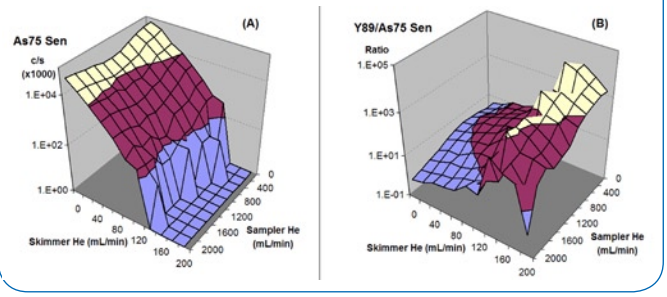


Figure 2: Typical 3-D graph of isotope sensitivity versus CRI gas flow at both skimmer and sampler apertures

## Interference Reduction by using the CRI

As a simple example of using the CRI technique to remove the $Ar_2^+$ interferences, Figure 3 shows a time scan graph for $^{115}In^+$ and $^{80}Se^+$ (i.e., $Ar_2^+$), where the CRI gas flow is increasing stepwise.

Also shown in Figure 3 is the signal ratio of $^{115}In^+/^{80}Se^+$. The time scan was carried out with a test solution (Var-IS-1) containing 10 µg/L of internal standard elements (Bi, In, Li, Sc, Tb, and Y). During the time scan, the $H_2$ gas was injected into the plasma through the CRI skimmer cone tip. The $H_2$ flow rate was stepped from 0, 20, 50, 80, 100, to 120 mL/min with about 50 seconds between each step. The efficiency of interference reduction/removal using CRI is clearly demonstrated in Figure 3, in which the signal for the interfering species $Ar_2^+$ (scanned as $^{80}Se^+$) is progressively decreasing with increasing $H_2$ gas flow rate, while the signal to interferent level (determined as the ratio $^{115}In^+/^{80}Se^+$) is continuously improving. As seen in Figure 3, at a $H_2$ flow rate around 120 mL/min, the interference from $Ar_2^+$ has been completely removed, and the sensitivity for the analyte $^{115}In^+$ is still maintained at a high level (i.e., over 50 000 c/s per 1 µg/L of indium).

Another example of using the CRI technique to effectively reduce or remove some common plasma-based polyatomic interferences is shown in Figure 4, which shows mass spectra of high purity water in the m/z range from 42 to 78 amu/unit electronic charge. One spectrum is obtained under the conventional ICP-MS operation mode ('normal mode'), and the other is obtained under the CRI mode where $H_2$ gas is injected through the skimmer cone into the plasma at a flow rate of 120 mL/minute.

**Interference removal**

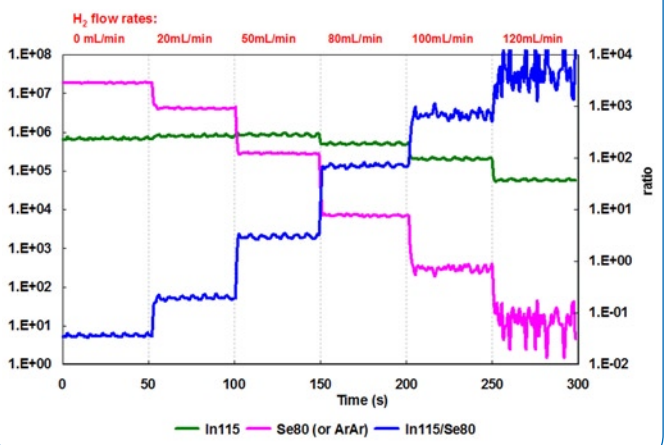


Figure 3: Time scan for $^{115}In^+$, $^{80}Se^+$ (i.e., $Ar_2^+$), and the ratio of $^{115}In^+/^{80}Se^+$ with increasing $H_2$ gas flow

**Removal of plasma-based polyatomic**

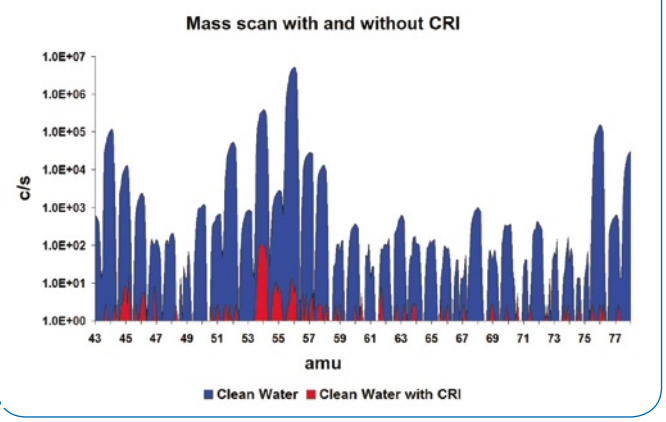


Figure 4: Mass spectra of pure water obtained under conventional ICP-MS and CRI-ICP-MS conditions

**Calibration curves**

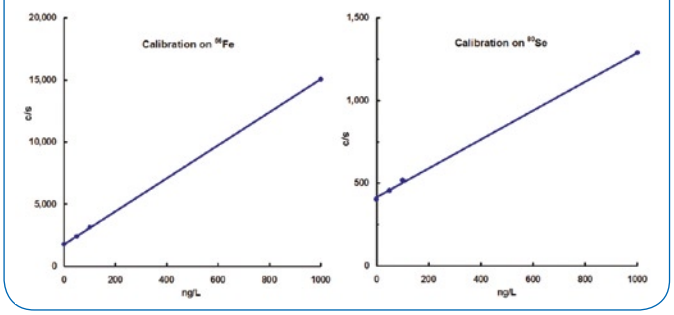


Figure 5: Typical calibration curves for $^{56}$Fe and $^{80}$Se, with hydrogen gas added at the skimmer at 100 mL/min, calibration standards; 0 ng/L, 50 ng/L, 100 ng/L and 1000 ng/L of Fe and Se

## Typical detection limits in CRI mode

The principal benefit of using the CRI technique is to reduce common polyatomic interferences on elements such as As, Se, Cr, V and Fe, thereby improving the detection limits for these elements in hot plasma. Table 1 lists the typical detection limit (DL) measured in the CRI mode. All DLs were determined as the concentration corresponding to 3 times the standard deviation of 10 replicates of a blank (i.e., 1% $HNO_3$). The measurements were made under routine analytical laboratory, not 'clean-room', conditions. Hence, the DL values listed in Table 1 can be routinely achieved outside a 'clean-room' in a clean laboratory.

In addition to the DLs, the background equivalent concentrations (BECs) when the DLs were determined under the CRI mode, are listed in the table. Hydrogen was used as the CRI gas, and it was injected into the plasma through the skimmer cone at a flow rate 80 mL/min for most of the elements listed in the table.

In some cases, the amount of the CRI gas required to remove the interferences can vary depending on the sample. In general (if the interfering ion is formed from the sample matrix), the greater the concentration of sample matrix, the more the CRI gas will be needed.

## Determination of Iron using $^{56}$Fe, and Selenium using $^{80}$Se

In a traditional ICP-MS analysis, both Fe and Se are regarded as difficult elements to determine at trace level. Interferences from $ArO^+$ and $Ar_2^+$ make it impossible or extremely difficult to determine trace levels of Fe using the most abundant isotope ($^{56}$Fe) or trace levels of Se using the most abundant isotope ($^{80}$Se). In some cases, the cool plasma technique may be used. However, the cool plasma technique is subject to matrix effects that restrict its areas of application. The CRI technique removes polyatomic interferences before the ions enter the ion optics. Hence, even using hot plasma conditions; it is now possible to determine Fe and Se at trace level using their most abundant isotopes. Figure 5 shows typical calibration curves of Fe and Se at sub-µg/L levels.

## Determination of Iron in High Calcium Matrices

Another potential interference for $^{56}$Fe is $^{40}Ca^{16}O^+$ from calcium in the sample matrix. Calcium is a common matrix element in most environmental waters, and its level can vary significantly depending on the source of the water samples. The CRI can effectively remove the $CaO^+$ interference allowing trace level determinations of Fe using the $^{56}$Fe isotope. Figure 6 shows the recovery of 1 µg/L of iron in the presence of various concentrations of calcium.

Table 1: Typical CRI DLs and BECs for selected isotopes

| Isotope | CRI ($H_2$) DL (ng/L) | Non CRI DL (ng/L) | CRI ($H_2$) BEC (ng/L) | Isotope | CRI ($H_2$) DL (ng/L) | Non CRI DL (ng/L) | CRI ($H_2$) BEC (ng/L) |
|---|---|---|---|---|---|---|---|
| $^{9}$Be | 0.5 | 3 | 1.1 | $^{59}$Co | 0.2 | 0.2 | 0.8 |
| $^{23}$Na | 13 | 200 | 252 | $^{60}$Ni | 10 | 2 | 68 |
| $^{24}$Mg | 0.5 | 2 | 4.7 | $^{63}$Cu | 1 | 0.3 | 5.3 |
| $^{25}$Mg | 1 | 5 | 5.3 | $^{65}$Cu | 1 | 2 | 7.0 |
| $^{27}$Al | 0.8 | 2.0 | 7.9 | $^{66}$Zn | 1.5 | 5 | 15 |
| $^{39}$K | 43 | 500 | 328 | $^{68}$Zn | 1.2 | 20 | 17 |
| $^{40}$Ca | 2.5 | - | 23 | $^{75}$As | 0.6 | 20 | 2.2 |
| $^{44}$Ca | 6.5 | 500 | 81 | $^{78}$Se | 1.5 | 400 | 26 |
| $^{49}$Ti | 1.3 | 3 | 3.2 | $^{80}$Se | 8.8 | - | 193 |
| $^{51}$V | 0.15 | 3 | 1.7 | $^{98}$Mo | 0.7 | 0.4 | 2.7 |
| $^{52}$Cr | 0.6 | 8 | 13 | $^{107}$Ag | 0.2 | 0.6 | 1.2 |
| $^{53}$Cr | 1.5 | 3 | 23 | $^{111}$Cd | 0.2 | 0.2 | 0.2 |
| $^{55}$Mn | 0.4 | 2 | 10 | $^{206,7,8}$Pb | 0.1 | 0.3 | 1.9 |
| $^{56}$Fe | 1.5 | 4000 | 167 | $^{232}$Th | 0.08 | 0.04 | 0.9 |
| $^{57}$Fe | 44 | 300 | 2146 | $^{238}$U | 0.01 | 0.06 | 0.07 |

## Determination of Arsenic in Chloride Matrices

In a chloride matrix, the $^{40}Ar^{35}Cl^+$ ion interferes with $^{75}As^+$ (the only naturally-occurring arsenic isotope). Conventional correction equations may be used, but the resulting detection limits are often inadequate. The CRI efficiently removes the $ArCl^+$ ion from the plasma before it is extracted into the ion optics, and allows routine detection of As at low ng/L levels. Figure 7 shows the recovery of 1 µg/L As in various HCl concentrations, with and without CRI. Correction equations were not applied in this experiment. Under the CRI mode, $H_2$ was added through the skimmer cone at a flow rate of 105 mL/min.

## Long Term Stability Performance in the CRI Mode

Figure 8 shows the long term signal stability in a high total dissolved solids matrix in the CRI mode. The stability was tested over a period of 5 hours using a solution containing 0.1% w/v (1000 mg/L) NaCl spiked with 1 µg/L of various analytes. The results in Figure 8 show that the aurora M90 ICP-MS, running in the CRI mode, was extremely stable over 5 hours, even in a matrix solution containing 1000 mg/L NaCl (i.e., TDS=0.1%). The relative standard deviations (RSD) of the measured signals for most analytes did not exceed 5% over the 5 hours. Similar results were also obtained using helium as the CRI gas.

## Summary

The aurora M90 ICP-MS provides a simple, but very effective approach to removing common polyatomic interferences in ICP-MS analysis. The unique CRI technology used on the aurora M90 ICP-MS reduces common polyatomic interferences on elements such as As, Se, Cr, V and Fe, thus achieving lower detection limits in hot plasma, even for samples with complex matrices.


| Keywords |
|---|
| ICP-MS |
| Collision Reaction Interface |
| Detection Limits |

| Instrumentation |
|---|
| aurora M90 ICP-MS |


**1 µg/L iron recovery**

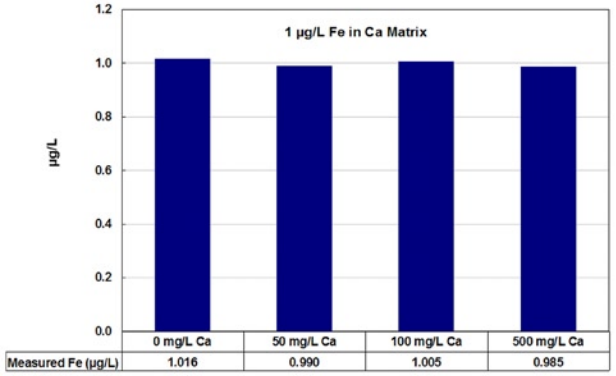


Figure 6: Recovery of 1 µg/L Fe in various Ca concentrations; $H_2$ added through the skimmer at 120 mL/min

**As recovery**

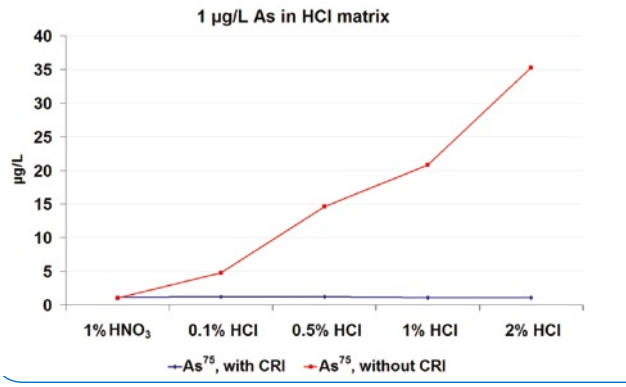


Figure 7: Recovery of 1 µg/L of As in various HCl concentration levels, with and without CRI

**CRI mode: Long-term stability**

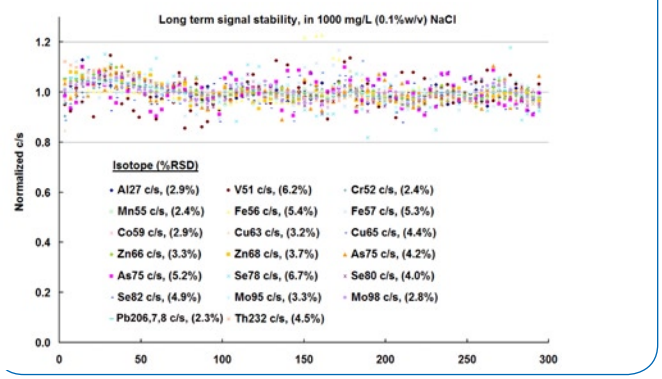


Figure 8: Long-term signal stability in 1000 mg/L NaCl; CRI gas $H_2$; flow rate 100 mL/min at the skimmer



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# EVOQ Elite LC Triple Quadrupole Mass Spectrometer

**Specification Sheet**

### Performance Specifications

| Mode | Test | Specification |
|---|---|---|
| Positive ESI MRM | 50 fg of reserpine injected | S/N≥2000:1 |

*The Signal-to-Noise ratio S/N values are based on RMS*

### Dimensions (H x W x D) and Weight

- Mass Spectrometer: 53 cm (H) x 45 cm (W) x 70 cm (D), 193 lbs/68kg
- UHPLC Advance: 71 cm (H) x 76 cm (W), 56 cm (D), 75lb/34kg

### Analyzer – EVOQ Elite Specifications

- Scan modes: Full Scan with Q1; Precursor, Product, Neutral Loss/Gain Monitoring, Selected Ion Monitoring (SIM), Multiple Reaction Monitoring (MRM)
- Standard ionization modes: Heated Electrospray Ionization, Atmospheric Pressure Chemical Ionization (APCI)
- Ion source: Fixed 90° spray, single housing for HESI to APCI
- Cone gas orifice temperature up to 400 °C
- HESI and APCI Source temperature: Up to 750 °C
- Mass filters: quadrupole with pre- and post-filters
- Collision cell: 180° curved path with lens-free design
- Collision cell gas: Argon with adjustable pressure up to 2 mTorr
- Collision energy: selectable up to 75 eV
- Mass range (m/z): 10 to 1250 Da
- Scan rate: up to 14,000 Da/sec
- Minimum dwell times: 1 ms
- Maximum acquisition MRM rate: 500 MRM's/sec
- Resolution: adjustable from Unit (0.7 Da) to 4 Da, also with three selectable settings (Unit, Standard, Open) on both Q1 and Q3.
- Mass axis stability: <±0.1 Da over 24 hours with normal temperature variations (+/- 3°C)
- Manifold temperature: 40-50 °C
- Detector: Electron multiplier with ±5 kV post acceleration and with an option for on-the-fly multiplier gain optimization for Extended Dynamic Range (EDR); direct ion collection onto multiplier for negative ion detection without dynode loss
- Turbo molecular pump: Three stage, 25/300/400 L/sec


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- Roughing pump: Two single stage 40 meter³/hour pumps
- Gas Requirements:
  Nitrogen (nebulizing gas, cone gas and probe gas) 32 L/min @ 80 psi
  Compressed air 50 L/min @ 80 psi
  Argon (collision cell) high purity gas @ 20-50 psi
- Power requirements:
  For mass spectrometer: 16A, 200 - 240V
  For roughing pump control box, 20A, 200-240 V.
- Operating environment temperature: 15 °C to 30 °C
- Operating environment humidity: 20% to 80% relative humidity (without condensation)
- Syringe Pump: eVol handheld syringe drive
- Divert Valve: six port integrated valve and software controlled

### Software

- Bruker MS Workstation equipped with the Compound Base Scanning (CBS) MRM library for data acquisition, data handling and reporting
- PACER data processing with Exception Based Review

### Liquid Chromatograph (Bruker Advance)

- Standard Injection Volume Range: 1 - 100 ul
- Injection Precision: <0.25% RSD
- Standard Sample Capacity: 6 deepwell or 6 microplate or 6x 54 2 ml vials
- Sample Temperature Range: 4- 40 °C
- Column Heater: 5 °C above room temperature to 90 °C
- Heater Capacity: Single <250 mm column
- Injector: UHPLC Capable
- Carryover: Less than 0.003% (30 ppm)
- Solvent Channels: 2 binary gradient, with optional third isocratic pump
- Flow Range: 0.005 - 2.5 ml/min
- Max Pressure: HPLC - 8000 PSI, UHPLC - 15,000 PSI
- Dead Volume: <100ul
- pH Range: 2-12
- Degasser: 2 Channel (3 with optional third isocratic pump)
- Flow Rate Precision: 0.06% RSD
- Flow Rate Accuracy: 1%
- Line Voltage: 100 – 240 VAC, ± 10%
- Line Frequency: 50 or 60 Hz, ± 5%
- Power Consumption: 400 VA Maximum
- Communication: USB


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# EVOQ Qube LC Triple Quadrupole Mass Spectrometer

**Specification Sheet**

### Performance Specifications

| Mode | Test | Specification |
|---|---|---|
| Positive ESI MRM | 200 fg of reserpine injected | S/N≥2000:1 |

*The Signal-to-Noise ratio S/N values are based on RMS*

### Dimensions (H x W x D) and Weight

- Mass Spectrometer: 53 cm (H) x 45 cm (W) x 70 cm (D), 193 lbs/68kg
- UHPLC Advance: 71 cm (H) x 76 cm (W), 56 cm (D), 75lb/34kg

### Analyzer – EVOQ Qube Specifications

- Scan modes: Full Scan with Q1: Precursor, Product, Neutral Loss/Gain Monitoring, Selected Ion Monitoring (SIM), Multiple Reaction Monitoring (MRM)
- Standard ionization mode: Heated Electrospray Ionization, Atmospheric Pressure Chemical Ionization (APCI)
- Ion source: Fixed 90° spray, single housing for from HESI to APCI
- Cone gas orifice temperature up to 400 °C
- HESI and APCI Source temperature: Up to 750 °C
- Mass filters: quadrupole with pre- and post-filters
- Collision cell: 180° curved path with lens-free design
- Collision cell gas: Argon with adjustable pressure up to 2 mTorr
- Collision energy: selectable up to 75 eV
- Mass range (m/z): 10 to 1250 Da
- Scan rate: up to 14,000 Da/sec
- Minimum dwell times: 1 ms
- Maximum acquisition MRM rate: 500 MRM's/sec
- Resolution: adjustable from Unit (0.7 Da) to 4 Da, also with three selectable settings (Unit, Standard, Open) on both Q1 and Q3.
- Mass axis stability: <±0.1 Da over 24 hours with normal temperature variations (+/- 3°C)
- Manifold temperature: 40-50 °C
- Detector: Electron multiplier with ±5 kV post acceleration and with an option for on-the-fly multiplier gain optimization for Extended Dynamic Range (EDR); direct ion collection onto multiplier for negative ion detection without dynode loss
- Turbo molecular pump: Three stage, 25/300/400 L/sec


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- Roughing pump: One single stage 40 meter³/hour pump
- Gas Requirements:
  Nitrogen (nebulizing gas, cone gas and probe gas) 32 L/min, @ 80 psi
  Compressed air @ 80 psi
  Argon (collision cell) high purity gas @ 20-50 psi
- Power requirements:
  For mass spectrometer: 16A, 200 - 240V
  For roughing pump control box: 10A, 200-240 V.
- Operating environment temperature: 15 °C to 30 °C
- Operating environment humidity: 20% to 80% relative humidity (without condensation)
- Syringe Pump: eVol handheld syringe drive
- Divert Valve: six port integrated valve and software controlled

### Software

- Bruker MS Workstation equipped with the Compound Base Scanning (CBS) MRM library for data acquisition, data handling and reporting
- PACER data processing with Exception Based Review

### Liquid Chromatograph (Bruker Advance)

- Standard Injection Volume Range: 1 - 100 ul
- Injection Precision: <0.25% RSD
- Standard Sample Capacity: 6 deepwell or 6 microplate or 6x 54 2 ml vials
- Sample Temperature Range: 4- 40 °C
- Column Heater: 5 °C above room temperature to 90 °C
- Heater Capacity: Single <250 mm column
- Injector: UHPLC Capable
- Carryover: Less than 0.003% (30 ppm)
- Solvent Channels: 2 binary gradient, with optional third isocratic pump
- Flow Range: 0.005 - 2.5 ml/min
- Max Pressure: HPLC - 8000 PSI, UHPLC - 15,000 PSI
- Dead Volume: <100ul
- pH Range: 2-12
- Degasser: 2 Channel (3 with optional third isocratic pump)
- Flow Rate Precision: 0.06% RSD
- Flow Rate Accuracy: 1%
- Line Voltage: 100 – 240 VAC, ± 10%
- Line Frequency: 50 or 60 Hz, ± 5%
- Power Consumption: 400 VA Maximum
- Communication: USB


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Application Note # CA-270109

# High Matrix Sample Analysis with the aurora M90 ICP-MS using the Collision Reaction Interface (CRI)

## Introduction

Inductively Coupled Plasma Mass Spectrometry is a powerful tool for a wide range of applications. The excellent sensitivity, multi-element capability and the wide analytical range give this technique the ability to analyze trace levels in a variety of environmental samples.

The unique design of the aurora M90 ICP-MS features a patented 90-degree ion mirror [1] that significantly reduces the background signals. It allows photons and neutrals to pass directly though the hollow structure of the mirror while analyte ions are directed into the mass analyzer. The amount of analyte passing through the skimmer cone to the quadruple is over 80%, which provides excellent ion transmission efficiency [2].

The new aurora M90 ICP-MS, in addition to the benefits of the ion mirror, has also been designed to reduce/eliminate interferences. The unique Collision Reaction Interface (CRI) introduces a new era of interference management for ICP-MS systems.

This application note demonstrates the capability of the aurora M90 system to determine sub-µg/L concentrations of a large number of elements in solutions containing high amounts of total dissolved solids (often defined as "high matrix" samples) as waste extracts or digests.

## Instrumentation

All measurements were carried out using the aurora M90 ICP-MS equipped with Collision Reaction Interface (CRI) and a Sample Preparation System, SPS3. The system operations of the aurora M90 are fully controlled by Bruker's Quantum software. The software provides one-step instrument setup, optimization, and method development. By using the auto-optimization routine supplied in the Quantum software, the instrument was automatically tuned to chosen CRI conditions.

## Materials and reagents

All calibration standards were prepared by diluting multi-element stock standards (Var-Cal-1 and Var-Cal-2, Inorganic Ventures, Inc., Lakewood, NJ, USA) with 1% v/v nitric acid (Ultrapur® $HNO_3$ 60%, Merck, Kilsyth, Victoria, Australia). Working standards below 10 µg/L were prepared immediately before the measurement. An internal standard solution, containing 100 µg/L of $^{6}Li$, $^{45}Sc$, $^{115}In$, $^{89}Y$, $^{159}Tb$, and $^{209}Bi$, was prepared by diluting a 100 mg/L of internal standard stock (Var-IS-1 Inorganic Ventures, Inc., Lakewood, NJ, USA).

## Sample preparation

High matrix samples were prepared to match the EPA 6020 interference check sample matrix (ICS A) [3]. Samples and spikes were prepared by dilution of a stock solution (6020ICS-A, Inorganic Ventures, Inc., Lakewood, NJ, USA) and then spiked to a final concentration of 0.5 µg/L with the multi-element stock standard (Var-Cal-1 and Var-Cal-2, Inorganic Ventures, Inc., Lakewood, NJ, USA). Table 1 lists the elemental concentrations of the high matrix sample (ICS A) and the spiked solution (ICS AB).

The EPA 6020 method requires MDLs to be determined using a spiked, fortified blank solution. That is, a sample at low levels with no matrix. By using ICS-AB to determine the MDLs, the data below shows that even with a highly demanding sample (with a high matrix) the aurora M90 ICP-MS can easily meet the required control limits.

Table 1: Composition of high matrix sample and spike.

| | Concentrations in µg/L | |
|---|---|---|
| Analytes | ICS A | ICS AB |
| Al | 100,000 | 100,000 |
| Ca | 100,000 | 100,000 |
| Fe | 100,000 | 100,000 |
| Mg | 100,000 | 100,000 |
| K | 100,000 | 100,000 |
| Na | 100,000 | 100,000 |
| C | 200,000 | 200,000 |
| Cl | 1,000,000 | 1,000,000 |
| P | 100,000 | 100,000 |
| S | 100,000 | 100,000 |
| Mo | 2,000 | 2,000 |
| Ti | 2,000 | 2,000 |
| As | | 0.5 |
| Cd | | 0.5 |
| Co | | 0.5 |
| Cu | | 0.5 |
| Mn | | 0.5 |
| Ni | | 0.5 |
| Ag | | 0.5 |
| Zn | | 0.5 |
| Sb | | 0.5 |
| Ba | | 0.5 |
| Pb | | 0.5 |
| Se | | 0.5 |
| Tl | | 0.5 |
| V | | 0.5 |

Table 2: ICP-MS conditions for analyses of interfence check samples.

| Parameters | CRI 1 | CRI 2 |
|---|---|---|
| Skimmer gas | $H_2$ | He |
| Sampler gas | none | none |
| Skimmer flow (mL/min) | 90 | 180 |
| Sampler flow | 0 | 0 |
| Outer flow | 16.5 | 16.5 |
| Intermediate flow | 1.65 | 1.65 |
| Sheath gas | 0.2 | 0.2 |
| Nebulizer flow | 0.95 | 0.98 |
| RF power (kW) | 1.3 | 1.3 |
| Sampling depth (mm) | 6.5 | 6.5 |
| Pump rate (rpm) | 3 | 3 |
| Stabilization delay (s) | 60 | 60 |
| Spray chamber (°C) | 3 | 3 |
| First extraction lens (V) | -1 | -1 |
| Second extraction lens (V) | -21 | -75 |
| Third extraction lens (V) | -195 | -235 |
| Corner lens (V) | -177 | -197 |
| Mirror lens left (V) | 39 | 38 |
| Mirror lens right (V) | 35 | 39 |
| Mirror lens bottom (V) | 23 | 24 |
| Entrance lens (V) | 0 | -2 |
| Fringe bias (V) | -2.5 | -3.5 |
| Entrance plate (V) | -29 | -28 |
| Pole bias (V) | 0 | 0 |
| Scan mode | Peak hopping | Peak hopping |
| Dwell time (ms) | 20 | 20 |
| Points per peak | 1 | 1 |
| Scans/Replicate | 20 | 20 |
| Replicates/Sample | 5 | 5 |

## Conditions

For the analysis of all samples in this work, normal sensitivity mode was used. Two condition sets were used in this study. Both sets used CRI conditions. The method parameters used for the two conditions sets are summarized in Table 2.

## Discussion

In order to verify corrections for elemental and polyatomic isobaric interferences EPA Method 6020 requires the analysis of two interference check samples, ICS A and ICS AB, at the beginning of the analysis run.

In this work, the ICS AB solution (0.5 µg/L) was analyzed to evaluate a lower working range in the presence of a high matrix. Table 3 summarizes the found results for the ICS A and ICS AB solutions and recoveries of the 0.5 µg/L spike for the different CRI conditions.

This spike level of 0.5 µg/L is 40 times lower than EPA 6020 requires (20 µg/L). This was done to make the analysis more demanding.

The Method Detection Limits (MDLs) and Method 6020 control limits are also listed. Seven subsequent reading of the ICS AB solution were used to calculate MDLs for each of the selected isotopes.

Table 3. Results summary for Interference check samples spike recoveries.

| Element | Isotope (m/Z) | Spike level | | With CRI | | |
|---|---|---|---|---|---|---|
| | | ICS AB (µg/L) | Recovery % | MDL* (µg/L) | CRDL (µg/L) | CRI condition |
| V | 51 | 0.50 | 94 | 0.183 | 5 | [2] |
| Cr | 53 | 0.50 | 110 | 0.259 | 5 | [2] |
| Mn | 55 | 0.50 | 101 | 0.103 | 5 | [2] |
| Co | 59 | 0.50 | 98 | 0.032 | 5 | [2] |
| Ni | 60 | 0.50 | 103 | 0.089 | 5 | [2] |
| Cu | 63 | 0.50 | 107 | 0.297 | 10 | [1] |
| Zn | 66 | 0.50 | 145 | 0.253 | 10 | [1] |
| As | 75 | 0.50 | 101 | 0.292 | 1 | [1] |
| Se | 78 | 0.50 | 105 | 0.257 | 5 | [1] |
| Ag | 107 | 0.50 | 99 | 0.050 | 5 | [2] |
| Cd | 111 | 0.50 | 102 | 0.107 | 1 | [2] |
| Sn | 118 | 0.50 | 99 | 0.100 | 1 | [2] |
| Sb | 121 | 0.50 | 102 | 0.027 | - | [2] |
| Ba | 137 | 0.50 | 102 | 0.031 | 5 | [1] |
| Tl | 205 | 0.50 | 94 | 0.038 | 5 | [2] |
| Pb | 206+7+8 | 0.50 | 97 | 0.036 | 10 | [1] |

[1] Skimmer $H_2$, [2] Skimmer He
* MDL were calculated using SD of seven subsequent readings of interference check sample spike (ICS AB) multiplied by 3.14

## References


[1] I. Kalinitchenko, Ion Optical system for a Mass Spectrometer, Australian Patent 750860, 14 November 2002

[2] S. Elliott, M. Knowles and I. Kalinitchenko, "A New Direction in ICP-MS", Spectroscopy, 19(1), 30 (2004)

[3] EPA Method 6020 Inductively Coupled Plasma – Mass Spectrometry, www.epa.gov/epaoswer/hazwaste/test/pdfs/6020.pdf



| Keywords |
|---|
| ICP-MS |
| Collision Reaction Interface |
| High Matrix |
| Multiple Condition Sets |

| Instrumentation & Software |
|---|
| aurora M90 ICP-MS |
| Bruker Quantum |


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# aurora M90

- A new era in ICP-MS

Innovation with Integrity

ICP-MS

# Your Partner in ICP-MS Solutions

Bruker continues to find new and novel ways to meet your changing needs. As a leader in elemental analysis you can be assured that when you buy a Bruker ICP-MS, you're buying more than just an instrument. You're buying a relationship with one of the most respected and experienced instrument companies in the world.

# ICP-MS: It's never been Easier

## Bruker innovation, making ICP-MS easier

If you've ever wished that ICP-MS could be simpler, wish no more. The aurora M90 makes light work of it. No matter what your requirements, with a Bruker ICP-MS, you can tackle any application with ease.

Key benefits of aurora M90 include:

- Bruker's patented high-efficiency 90 degree ion optics and double off-axis quadrupole delivers exceptionally low background noise and unmatched sensitivity – at more than 1 million counts per second for 1µg/L.
- Tunable from normal to high sensitivity, the aurora M90 is perfect for both routine and research-grade applications – Flexibility at your fingertips.
- The aurora M90 delivers industry leading detection limit performance. Collision/reaction interface (CRI) technology makes setup of complex cell systems a thing of the past. Simply turn on the gas flow to remove interferences. It's that simple.
- Featuring the only all-digital ICP-MS detector, covering more than nine decades of dynamic range in pulse counting mode, the aurora M90 delivers fast and accurate multi-element analysis from ultra-trace to major levels in a single measurement.

## Let Bruker Quantum work for you

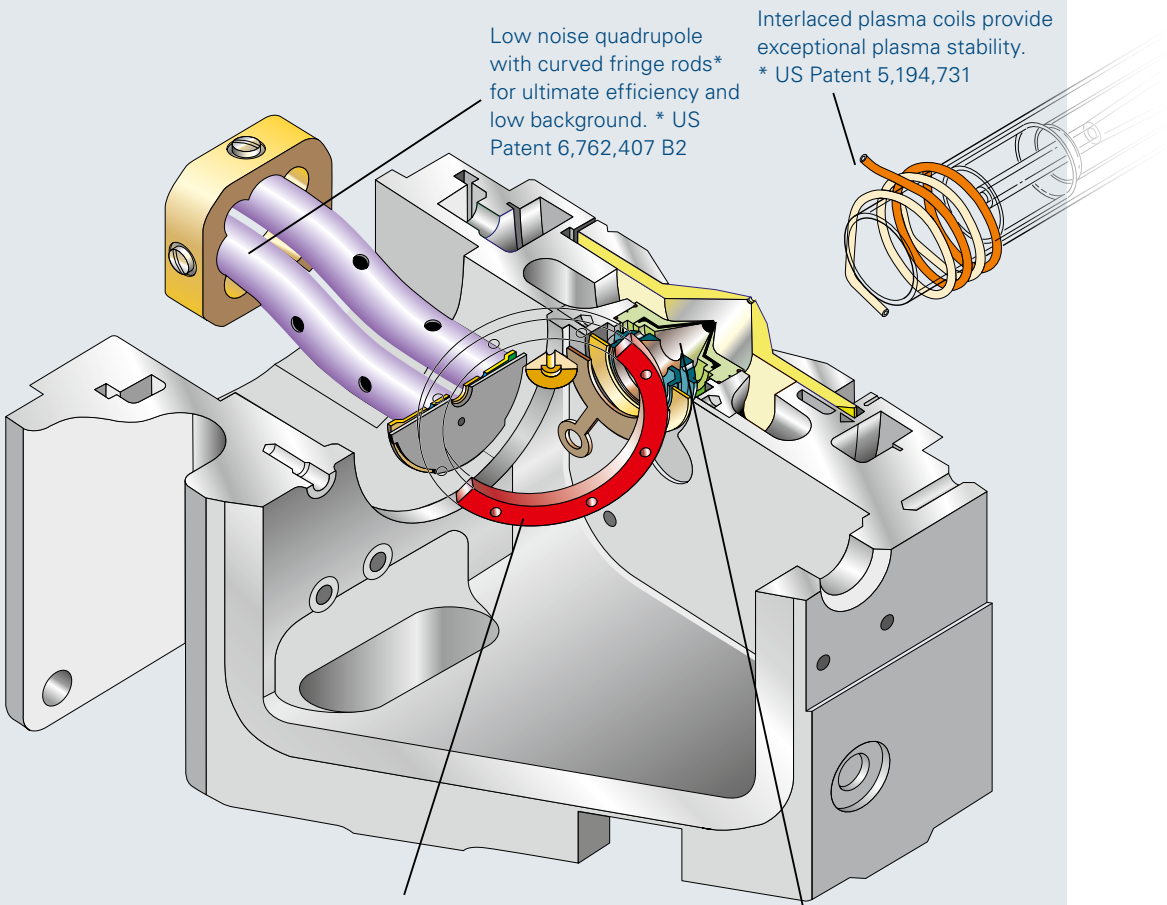
If your goal is to spend less time creating methods and optimising conditions, and more time running samples, Bruker Quantum software delivers. Enjoy accurate results in less time with an intuitive yet flexible user interface that takes the hard work out of ICP-MS.

- With auto-tuning of all instrument parameters, you can spend less time on instrument setup and more time on sample analysis. Saving you valuable time and money.
- Fully automated, aerosol dilution extends the high dissolved solids tolerance of your ICP-MS allowing you to directly analyze challenging samples without additional sample preparation.

# Innovation you can trust

- Patented 90 degree ion mirror and low noise double off-axis quadrupole provide industry leading sensitivity and background for lowest detection limits.
- New and improved Collision Reaction Interface (CRI II) provides even simpler and more effective removal of trouble–some interferences for interference-free analysis of your samples.
- Robust, high-efficiency plasma system and patented Interlaced Coils break down your toughest sample matrices, reduce matrix effects, and minimize ion energy spread for maximum sensitivity and stability.
- All-digital extended range detector – means fewer dilutions, and longer detector lifetime for greater productivity and lower running costs.

## Our 90 Degree Reflecting Ion Optics Revolutionizes ICP-MS Performance



# Fast, Flexible, Interference-Free Analysis

Bruker is proud to bring you CRI II, now even simpler to use and more effective at removing troublesome interferences from your sample analysis.

The CRI injects helium (He) and hydrogen ($H_2$) collision and reaction gasses directly into the plasma as it passes through the orifice of the skimmer cone.

This innovative approach suppresses interferences before the analytes are extracted into the ion optics.

It's that simple!

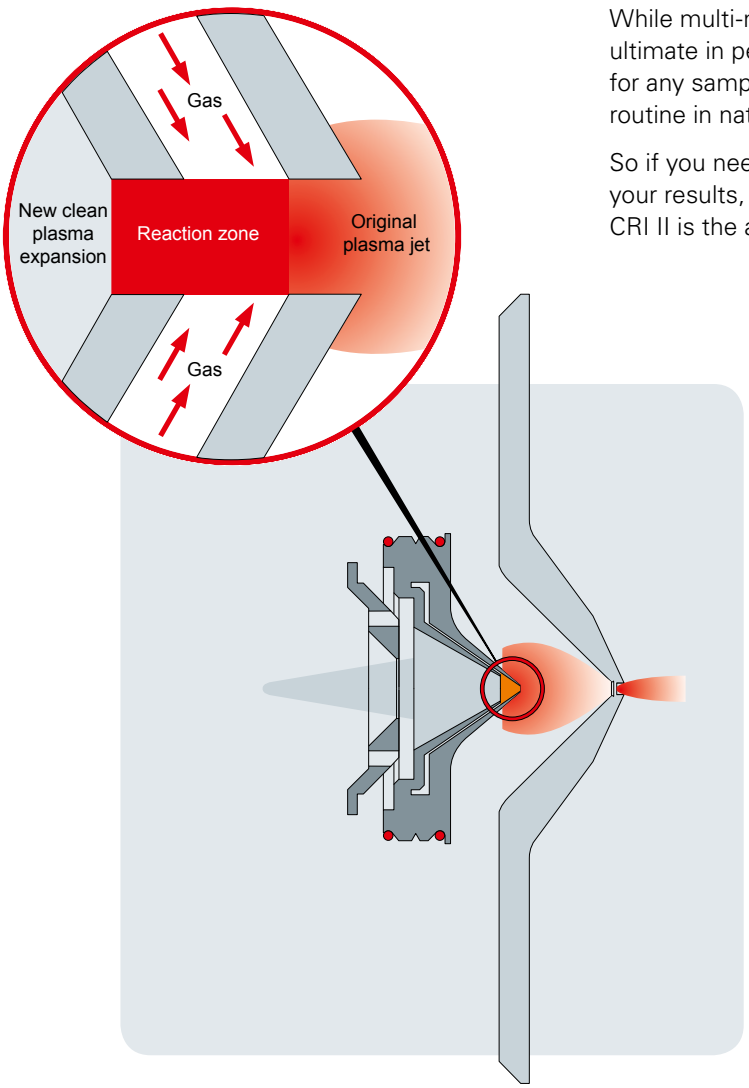
- No need for expensive or corrosive gasses such as ammonia or methane, so laboratory costs are reduced.
- No additional cleaning as CRI forms part of the cone interface, making this interference management system maintenance-free.

## Choose your analysis mode

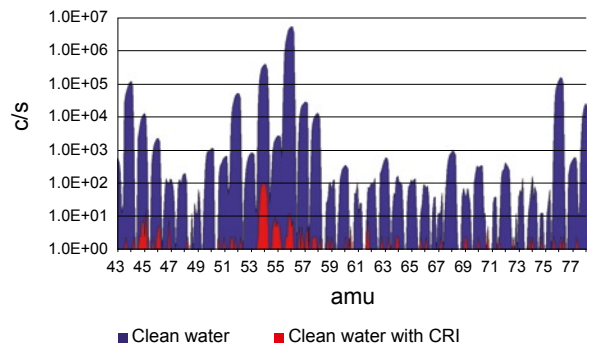
CRI II universal analysis mode provides fast and accurate results for samples routinely encountered across the wide range of environmental and industrial monitoring processes.

While multi-mode delivers the ultimate in performance and flexibility for any sample type including those less routine in nature.

So if you need absolute confidence in your results, no matter what the sample, CRI II is the answer.




**Mass scan with and without CRI**



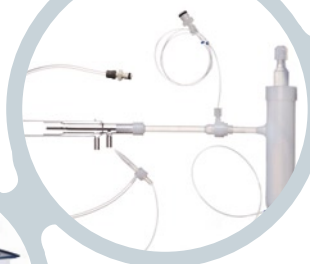

Dramatically reduce or eliminate troublesome plasma and sample matrix based interferences, using CRI II.

# The solution to your application needs

With a vast range of options to choose from, Bruker has the solution to your application. Choose from

- CRI II for fast, accurate interference-free analysis of your samples.
- High sensitivity interface. Ideal for research applications on non-interfered isotopes, pushing your detection capability to levels never seen before.
- Make simple work of your most challenging samples. Upgrade to the inert vacuum pump system for low maintenance, high performance ICP-MS operation.
- Clean room package is suited to applications in the semiconductor industry and provides an inert and contamination-free environment for ultra-trace analysis.
- Application-specific sample introduction systems for routine analysis of geochemical and petrochemical samples.
- A range of autosampler and productivity-enhancing accessories provide you with fast, unattended operation of your ICP-MS.
- The nitrox 500 accessory allows online addition of nitrogen or oxygen gas to the plasma. Add nitrogen to lower your detection limits on key elements like As and Se. Add oxygen for routine analysis of organic solvents.
- Fully-integrated speciation options for the analyst wanting to know more about their samples.
- The aurora M90 is compatible with a wide range of laser ablation systems providing you with solution-free analysis.

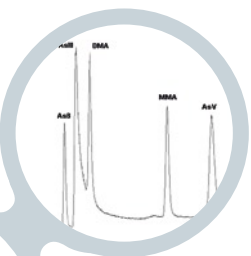
Clean room package helps semiconductor labs attain clean room conditions for ultra-trace analysis.



All PFA sample introduction kits allow direct analysis of samples containing free HF acid.

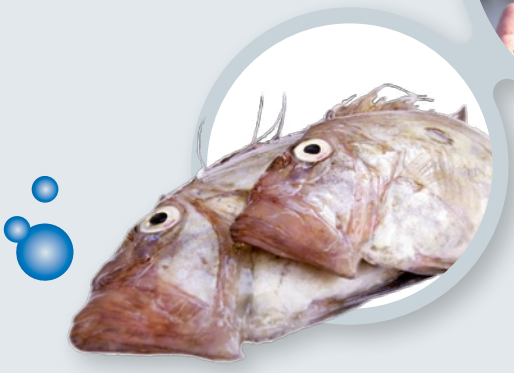
Choose from a range of accessories to meet your sample handling requirements.


Boost the performance of your aurora M90 by adding the nitrox 500.



Fully-integrated HPLC interface makes light work of speciation applications.

# The Benchmark in Analytical Performance



## Quickly and reproducibly reduce interferences

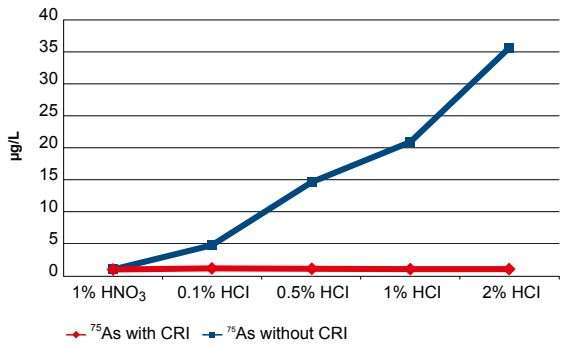
With CRI II you can quickly switch from CRI to non-CRI, or between different collision and reaction gases.

Multi-mode delivers the ultimate in performance and flexibility for any sample.

## Determination of As in Cl containing samples

Use CRI II in $H_2$ mode to remove the ArCl interference when determining As in high chloride containing samples like blood, serum and urine.

**1 µg/L As in HCl matrix**

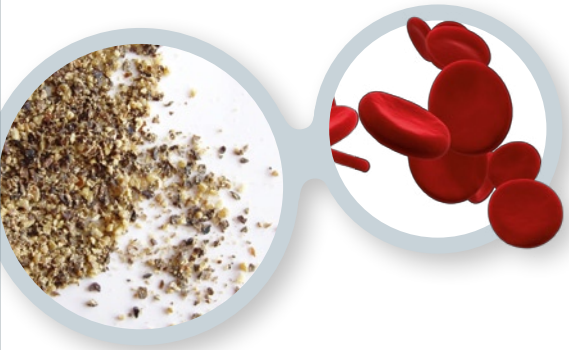



Comparison plots showing 1 µg/L spike recoveries for $^{75}As$ without correction equations. ArCl interferences are removed, allowing accurate trace level quantification of As.

| | Certified range µg/L | Measured value µg/L |
|---|---|---|
| $^{27}Al$ | 13 – 21.2 | 20 |
| $^{51}V$ | 0.27 – 0.37 | 0.29 |
| $^{52}Cr$ | 0.42 – 0.78 | 0.42 |
| $^{56}Fe$ | 404 – 460 mg/L | 420 mg/L |
| $^{75}As$ | 1.4 – 2.2 | 1.8 |
| $^{78}Se$ | 74.4 – 85.2 | 77.2 |
| $^{206, 207, 208}Pb$ | 26.2 – 29 | 27.6 |
| $^{238}U$ | 0.16 – 0.18 | 0.17 |

Obtain accurate results in complex biological matrices. Above, certified and measured values for Reference Whole Blood Seronorm WB1 show that trace and major levels can be determined with accuracy and confidence using CRI II.

# Unrivalled Performance



## Maximum dynamic range for food samples

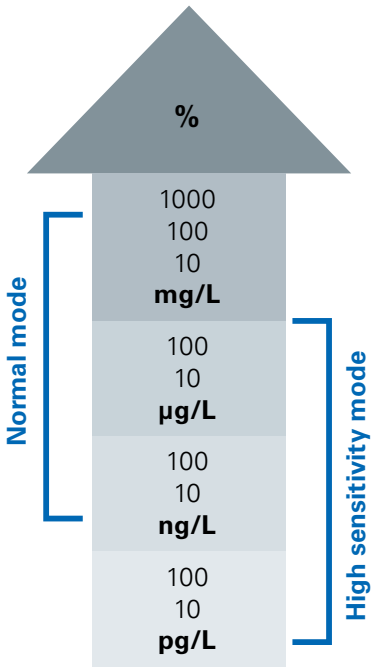
Determine toxic, essential and nutritional elements in a single, all-digital measurement for optimum accuracy and precision.

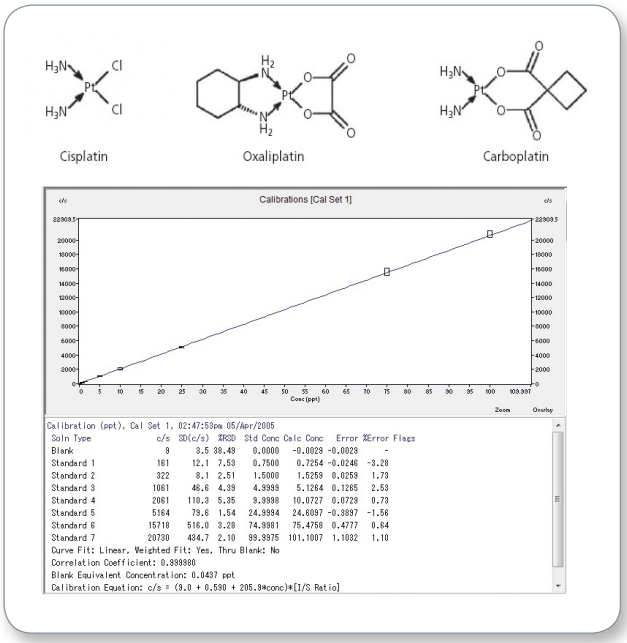
| Element | Units | Measured | Certified |
|---|---|---|---|
| $^{24}$Mg | mg/kg | 513 | 500 |
| $^{39}$K | mg/kg | 3128 | 3100 |
| $^{44}$Ca | mg/kg | 422 | 410 |
| $^{56}$Fe | mg/kg | 39.0 | 40.7 ± 2.3 |
| $^{75}$As | mg/kg | 0.024 | (0.023) |
| $^{78}$Se | mg/kg | 0.026 | (0.025) |
| $^{114}$Cd | mg/kg | 0.0270 | 0.0284 ± 0.0014 |
| $^{206\text{-}8}$Pb | mg/kg | 0.182 | 0.187 ± 0.014 |

Above, certified and measured values for brown bread reference material BCR-191 showing accurate measurement from ultra-trace to major levels.

## Unequalled high sensitivity performance

The aurora M90's unique high sensitivity mode opens up a world of new possibilities in research.



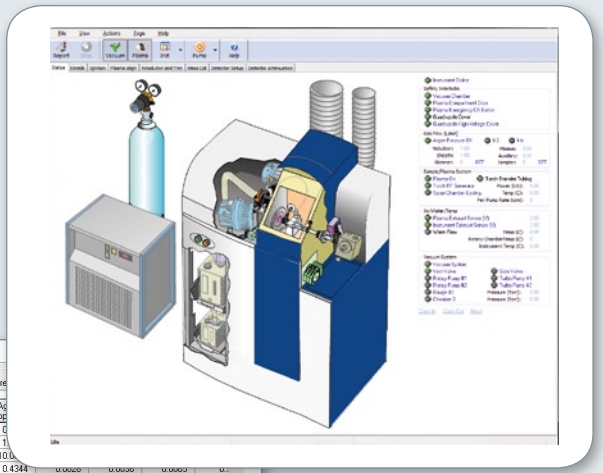

Achieve levels of detection never seen before in ICP-MS. Above, a typical calibration for $^{194}$Pt in chloroplatinin acid in the ng/L to sub-ng/L range used in the determination of pharmacologically active Pt tracers of anti-cancer drugs.

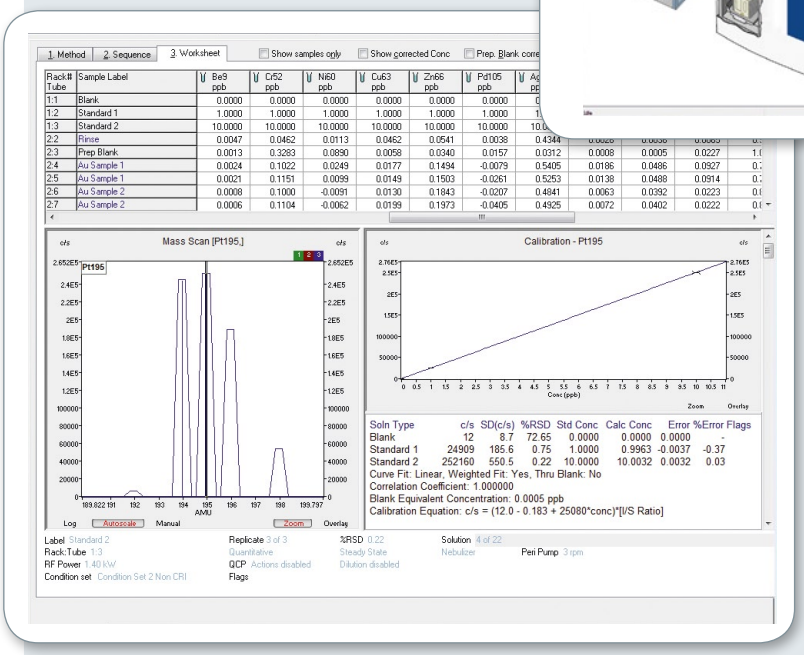
# Setting the Benchmark for Ease-Of-Use

## Bruker Quantum software

Bruker redefines ease-of-use with our Web-integrated ICP-MS worksheet software. Quantum features a range of automated options, including setup and initialization routines, such as plasma alignment, mass calibration and resolution tests. Bruker's AutoMax makes method development easy by automating all ion optics, nebulizer and plasma settings for optimum results. Including auto-optimization for Aerosol Dilution, Bruker Quantum makes light work of your most difficult samples.

The dynamic Instrument Status window provides a quick visual check of the status of all system components. It is an excellent diagnostic tool that maximizes instrument up time.






Each worksheet cell provides all the results you need – including concentrations, intensities, statistics, replicate readings and graphical mass scans.

Bruker Quantum switches automatically between multiple method condition sets within a single sample, giving optimum performance for specific element suites, without having to re-run samples.

# Chemical Analysis Solutions

## Laboratory gas chromatography systems

The 400 Series consists of two gas chromatographs and an associated range of analyzers and solutions designed for leading applications. These systems allow chemists and engineers to employ standard methods and/or high quality trace sample analysis, in the petrochemical, agrochemical and environmental industries.

The 450-GC is a highly affordable and powerful analytical instrument that offers robust operation in an easy-to-use package. The system gives users a broad choice of injectors, detectors, switching and sampling valves up to three channels. The high resolution color touch screen is intuitive and supports local languages. The Bruker 430-GC offers the same outstanding performance as the 450-GC but in a compact, single channel package that occupies about half the bench space of conventional multi-channel GC.

## Triple quadrupole mass spectrometer

The Bruker 320-MS GC/MS stands at the forefront of configurable triple-quadrupole mass spectrometer systems. It offers: femtogram sensitivity, 10 – 2000 Da mass range, and a wide array of chromatographic and ionization configurations to uniquely match your needs - all in less than 72 cm. (28 in.) of linear bench space! In minutes, the 320-MS can be changed from EI to CI modes of operation. Easily, the 320-MS is the most sensitive, robust, and flexible triple-quadrupole MS system currently available.

For research use only.
Not for use in diagnostic procedures.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**www.bruker.com/chemicalanalysis**

# impact HD LC-MS System


**Description**
**Part Number: # 1819695**

Bench-top High-Definition UHR Time-of-Flight Mass Spectrometer

Easy-to-use, instant expertise™ Ultra-High-Resolution electrospray ionization quadrupole time-of-flight LC/MS/MS mass spectrometer designed for exact mass and true isotopic measurements in both MS and MS/MS mode.

**Bench-top, small footprint Mass Spectrometer system for exact mass and highest mass resolution at U-HPLC speed in both MS and MS/MS mode:**

- Unique FSR technology with Full Sensitivity @ Maximum Resolution achieved without any time constraints, in MS and MS/MS mode
- Outstanding Mass Resolution and Accuracy in both MS and MS/MS
- High-resolution extracted ion chromatograms capabilities
- High performance hyperbolic quadrupole and collision cell for compound fragmentation
- True Isotopic Measurements

**A. Apollo II (ESI) Source**

- Highly sensitive ESI Source with proprietary dual ion funnel guide for gentle mass independent ion focusing and high ion transmission efficiency
- Combined Funnel-Hexapole-Cartridge with front access for easy maintenance
- Grounded needle for safety and easy sample introduction
- Suitable for U-HPLC, HPLC and CE coupling
- Heated counter current drying gas for gentle and efficient drying
- Ion lens system including in Source collision induced dissociation control (IS-CID)
- Pneumatic off-axis nebulization for flow rates up to 1 ml/min., with gradients from 100% aqueous to 100% organic
- Flow rate 1µl/min to 1ml/min
- Coated glass capillary for physical and electrostatic isolation
- Processor controlled HV and gas controller



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**B. High Mass Quadrupole Mass Filter:**

- Hyperbolic quadrupole mass filter
- Ultra stable monolithic design
- RF-generator for monoisotopic precursor ion selection

**C. Novel high-transmission CID Collision cell:**

- Hyperbolic quadrupole broad-mass bandwidth design
- Fast radial ion ejection enabling fast MS/MS cycle
- RF-Generator with fast amplitude switching
- Collision gas controller

**D. Orthogonal pulsed ion extraction and Time-of-Flight Mass Analyzer**

- Interface housing and ion lens system
- In-line detector system for easy maintenance
- Ultra-stable high voltage switches with up to 20 kHz repetition rate and appropriate power supplies.
- TOF analyzer with orthogonal mounted ion source
- In-flight refocusing optics for uncompromised sensitivity
- Dual stage ion reflectron with increased mass resolution and accuracy
- Ultrafast 5 GS/sec 10 bit digitizer
- High-sensitivity and fast ion detector system, mechanical adjustment in micrometer range
- Positive and negative ion modes
- Ultra-stable high voltage power supplies for TOF analyzer and detector

**E. Vacuum system**

- Analyzer vacuum housing
- Vacuum system with 5 differential pumping stages
- One roughing pump 28 m^3/h, tri- and dual-stage turbo pumps for ESI source and UHR-TOF analyzer
- Vacuum measurement and pump control unit

**F. Syringe pump**

**G. Modes of Operation**

- TOF Mass ranges 20-40,000 m/z
- Internal calibration (MS and MS/MS)
- External calibration (MS and MS/MS)
- Exact mass measurements independent from sample concentration over a wide dynamic range without second sprayer.

**H. High-resolution-performance and accurate mass features**

- Patented ion funnel source
- One-shot acquisition mode, no tuning for mass range optima
- Enhanced low mass sensitivity
- Superior MS/MS sensitivity
- Ultra broad mass-bandwidth



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- Long term and ultra stable mass axis stability in MS and MS/MS
- Exact mass independent from sample concentration charge state and collision energy
- Combined calibration for both MS and MS/MS
- Wide dynamic range for quantitation
- Advanced temperature compensated flight tube
- Positive / negative ion operation

**I. Data system:**

- PC Workstation with 2.66 GHz Single-CPU-Quad-Core-processor, 12 GB RAM, 2 TB hard disk, Ethernet connection for external networks
- DVD-ROM drive
- R/W DVD-ROM drive DL
- ≥ 24" flat screen colour monitor
- Windows™ 7/32 operating system
- Laser printer
- Remote Service capability via 128-bit SSL-security web connection

**J. Applications software**

Software package Compass 1.6 for HPLC and MS control, data acquisition, post processing, and data analysis:

- Operation system Windows 7/32
- Compass / HyStar 3.2 for integrated control of most popular U-HPLC and HPLC systems and auto samplers and automation
- Instant Expertise™ features for intelligent autoMS/MS workflows
- Expert mode: extended control over instrument parameters for interactive system optimization of sophisticated exact mass methods
- Compass / Data Analysis software DA 4.1, including:
    - Advanced data processing with a high degree of automation
    - SmartFormula 3D™: Automated sum formula determination using MS and MS/MS data with both, accurate mass and isotopic fit.
    - QuantAnalysis™ quantitation package
    - LibrarySearch ™ module for search of MS, MS/MS and MSn spectra with advanced matching algorithm
    - Charge deconvolution module
    - Export of spectra and ion current profiles as Windows metafiles to word-processing programs
- SW License DataAnalysis 4.1
- SW License Charge Deconvolution for DA 4.1
- SW License MaxEntropy Deconvolution as an option

**K. Set of manuals and reference CD-ROMs**
**L. Installation**
**M. Familiarization upon installation**
**N. 1 year warranty**
**O. Training course - for 2 participants.**



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# impact HD LC-MS System

**Specification Sheet**
**Part Number: # 1819695**

Impact HD UHR Time-of-Flight Mass Spectrometer System


| | |
|---|---|
| Size | Bench-top:<br>64cm x 118cm (Footprint)<br>198cm (Height) |
| Weight | ~ 210 kg |
| Vacuum System | 5 stages, 28 $m^3$/h rough pump |
| Apollo II ion funnel electrospray source | Flow rate: 1 µL/min – 1 mL/min |
| Mass Range | 20 – 40,000 m/z |
| Quadrupole isolation | Up to 3,000 m/z |
| Quadrupole Mass Range | Up to 40,000 m/z |
| Mass accuracy in MS and MS/MS | With internal calibrant: better than 800ppb RMS Error<br>With external calibrant: better than 2 ppm RMS Error |
| Calibration | ONE calibration valid for MS and MS/MS analysis. Calibration is independent from charge state of calibrant mass |
| Mass resolution | 40,000 FSR (full sensitivity resolution) |
| Isotopic pattern | The true isotopic pattern is maintained due to TIP™ technology (True Isotopic Pattern) and allows three dimensional chemical characterizations of analytes via SmartFormula™3D algorithm using exact mass, TIP, and MS/MS fragment data. |
| SmartFormula™3D | Enables unambiguous formula determination at "sub-ppm" confidence level up to 1000 Da. |



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| | |
|---|---|
| Mass stability & dynamic range | hrXIC (high resolution Extracted Ion Chromatogram) technology with better than +/- 1.0 mDa stability on centroid data values over an typical LC peak. |
| Full scan sensitivity in MS | ESI: Reserpine 1 pg S/N>100:1 RMS<br>With Ion-Booster (optional): Reserpine 100 fg S/N>100:1 RMS |
| Full scan sensitivity in MS/MS | The signal height obtained from a consumption of 2.5 fmol of Glu-Fibrinopeptide B will be better than 100 counts on the most intense y' sequence ion from the MS/MS spectrum of the doubly charged precursor ion. This shall correspond to a signal to noise ratio better than 50:1. The MS/MS sensitivity specification is met while using quadrupole isolation of the precursor ion demonstrating that there is minimal transmission loss through the isolating quad.<br>A solution of 100 fmol/µL Glu-Fibrinopeptide B shall be introduced at a flow rate of 3 µL/min. |
| TOF repetition rate | Up to 20 kHz |
| Temperature compensation | Yes |
| Digitizer | 5Gsample/sec ADC with 50 Gbit/sec |
| Dynamic range | 10 bit ADC for high quantitative dynamic range |
| Acquisition rate | up to 50 Hz MS<br>50 Hz MS/MS (profile and peak detected spectra to disk) |

## Optional accessory

| | |
|---|---|
| IonBooster | Optional ion source |
| APCI II | Optional ion source |
| APPI II | Optional ion source |
| GC-APCI | Allows for direct GC coupling (Optional ion source) |
| APLI | Optional ion source |
| CryoSpray | Optional ion source |
| Bruker CaptiveSpray nanoBooster | Optional ion source |
| On-/Off-Line Nanospray | Optional ion source |
| CE/MS interface | With grounded needle for easy CE-TOF set-up (Optional) |
| DIP | Direct Probe (Optional ion source) |



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# Lock-out specifications for an Ultra High Resolution- Time of flight (UHR-TOF) system**maXis HD**

**System description**:

Complete, factory-new, working and ready-to-use LC-MS/MS system including:

1. mass spectrometer with ESI source allowing positive and negative ion detection; the needle of the ESI source has to be on ground potential. (2,3)
2. floorstanding ultra high resolution reflectron Time-of-Flight mass spectrometer with small footprint (maximally 1 by 1,50 m.(2,3)) and near-orthogonal electrospray ion source.
3. The spectrometer has to include the following parts:
    a. Ion lens system with possibility to perform In Source-CID experiments;
    b. quadrupole/quadrupolesystem for ion isolation and fragmentation for MS/MS experiments;
    c. ion transfer line with patented dual ion funnel system for maximum transmission (1,2,3)
    d. A hyperbolic quadrupole mass filter
    e. New HDC Collision Cell with DC Gradient (1,2,3,4)
    f. New 50 Gbit/sec Digitizer(1,2,3,4)
    g. Ultra high resolution TOF analyzer with dual stage reflectron, in-flight refocusing optics and advanced temperature compensation.
    h. Fast and robust detector with linear response for high dynamic range
    i. Five-stage pumping system, incl. >28 m3 rough pump.
    j. Needs to run with single rough pump (1,3)
    k. detection system with an New 10 bitanalog-to digitizer converter unit allowing recording of the complete analog ion signal (1,2,3,4)
    l. PC-station with complete software (including Windows operating system and LC-MS control software) that allows acquisition, processing and exporting data + LCD-screen + laser printer;

**Required parameters and features:**

1. Analyzer resolution in single-reflection mode better than 75'000 (FWHM) at m/z 1222 without the need of multiple ion reflection at 50Hz acquisition rate, available without a loss of sensitivity (compared with the respective instrument specification);([1],[2],[3],[4])
2. Analyzer resolution in single-reflection mode better than 30'000 (FWHM) at m/z 118 without the need of multiple ion reflection at 50Hz acquisition rate, available without a loss of sensitivity (compared with the respective instrument specification); (1,2,3)
3. MS and MSMS mass accuracy not worse than 600 ppb (calibrated internally) and 2 ppm (calibrated externallyand without the use of any additional lock-spray) in a wide dynamic range i.e. independent from sample concentration. (1,2,3,4)
4. Long term and ultra-stable mass axis stability in MS and MS/MS, both with full sensitivity!
5. In scan Dynamic range ≥ 4-5 orders of magnitude at 1Hz acquisition (2,3) without any need to split the ion beam dynamically (2;4) and without any need to switch the digitizer into under sampling mode (1).
6. Asingle calibration must be valid and applicable for both MS and MSMS measurements;
7. Possibility to use any substance for calibration chosen by the user (within available mass range); (3)
8. Mass range not less than 20 – 40'000 m/z; (3,4)
9. Possibility to select MS/MS precursors with m/z values up to 3000 (quadrupole isolation)(4)
10. Scan Speed: MS and MS/MS acquisition rate 50 Hz written to disc in 1 sec (1,2,3,4)
11. Fully automated isotope pattern matching with the generation of a list for the sum formula from both mass accuracy as well as the isotope pattern matching - it has to use both MS and MSMS data (3,4)
12. Possibility to maintain the isotopic pattern with an error of less than 2%.
13. Possibility to analyze intact proteins at m/z values> 4000 to obtain most comprehensive information (3,4)
14. Possibility of remote service diagnostics via secured Internet connection;
15. Possibility to create high resolution Extracted Ion Chromatograms within +/- 0,5 - 1,0 mDa error for screening of complex mixtures (4)
16. Possibility to save the hrEIC to disk (2,3).
17. Flexibility to control HPLC systems of various vendors (Dionex (Ultimate 3000), Waters (UPLC), Agilent, VWR/Hitachi, Shimadzu, Proxeon) within the original MS vendor software offered here (START/STOP signal is insufficient). (1,2,3)

[1] Against Agilent 6538, 6540
[2] Against Waters Synapt G2 SI
[3] Against Thermo OT velos
[4] Against AB Sciex 6500 TripleTOF

18. Flow rate of 1uL/minute-1mL/minute to facilitate flow injection as well as LC-driven experiments (1[6540])
19. MS sensitivity at reserpine of better than S/N 100:1 RMS at 1 pg Reserpine(at FIA flow rate >= 200 uL/min) at full instrument resolution.With Ion-Booster (optional): better than S/N 100:1 RMS at 100 fgReserpine (1,2)
20. MS/MS sensitivity equal to or better than a consumption of 2.5 fmol peptide at S/N 100:1 when a solution of 100 fmol/µLGlu-Fibrinopeptide B is introduced at a flow rate of 3 µL/min.
21. Comfortable Charge-state-ruler (1,2,3,4)
22. Possibility to upgrade the system to an LC-NMR-MS setup (4, 2,3)
23. Possibility to upgrade the system with an atmospheric pressure source to couple a GC system (3,4)
24. Changing of API sources from ESI to nano-spray and back without breaking vacuum (4)
25. Possibility to upgrade the system with a CaptiveSpray source with patented nano-booster
26. Possibility to upgrade the system with DIP (direct probe) to analyze insoluble compounds without the need for any sample preparation (1,3,4).
27. The software has to support and allow the quantitative analysis of proteins by the use of all protein labeling techniques, as well as of label-free experiments;
28. The software has to be able to combine results of several proteomics databases like Mascot and Phenyx in order to improve protein identification rates, under strict false positive rates for peptide identifications (1,2,3)
29. package dedicated for small molecules analysis allowing i.a.:
    - statistical comparison analyses of different sample groups
    - prediction of metabolites on the basis of biotransformation rules
    - differential display of LC-MS runs on samples taken from one organism at different times
30. package dedicated for multi-target compound screening allowing i.a.:
    - generation of extracted ion chromatograms (EIC)
    - automated generation of a compound list from those EIC
    - automated comparison of the detected compounds with a predefined target list
    - target list containing drugs, metabolites, natural and toxic products as well as pesticides
31. package for statistical analysis allowing i.a.: (3)
    - PCA analysis;
    - different normalization options;
    - data validation by test set and cross-validation;
    - data recalibration before post-processing;
    - evaluation results visualization;

# maXis HD LC-MS System

**Specification Sheet**
**Part Number: # 1820746**

maXis HD UHR Time-of-Flight Mass Spectrometer System


| | |
|---|---|
| Size | Floorstanding:<br>80 x 132 cm (Footprint)<br>290 or 320 cm (Height) |
| Weight | ~ 500 kg |
| Vacuum System | 5 stages, 28 $m^3$/h rough pump |
| Apollo II ion funnel electrospray source | Flow rate: 1 µL/min – 1 mL/min |
| Mass Range | 20 – 40,000 m/z |
| Quadrupole isolation | Up to 3,000 m/z |
| Quadrupole Mass Range | Up to 40,000 m/z |
| Mass accuracy in MS and MS/MS | With internal calibrant: better than 600ppb RMS Error<br>With external calibrant: better than 2 ppm RMS Error |
| Calibration | ONE calibration valid for MS and MS/MS analysis. Calibration is independent from charge state of calibrant mass |
| Mass resolution | 75,000 FSR (full sensitivity resolution) |
| Isotopic pattern | The true isotopic pattern is maintained due to TIP™ technology (True Isotopic Pattern) and allows three dimensional chemical characterizations of analytes via SmartFormula™3D algorithm using exact mass, TIP, and MS/MS fragment data. |
| SmartFormula™3D | Enables unambiguous formula determination at "sub-ppm" confidence level up to 1000 Da. |



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| | |
|---|---|
| Mass stability & dynamic range | hrXIC (high resolution Extracted Ion Chromatogram) technology with better than +/- 0.5 - 1.0 mDa stability on centroid data values over an typical LC peak. |
| Full scan sensitivity in MS | ESI: Reserpine 1 pg S/N>100:1 RMS<br>With Ion-Booster (optional): Reserpine 100 fg S/N>100:1 RMS |
| Full scan sensitivity in MS/MS | The signal height obtained from a consumption of 2.5 fmol of Glu-Fibrinopeptide B will be better than 1000 counts on the most intense y' sequence ion from the MS/MS spectrum of the doubly charged precursor ion. This shall correspond to a signal to noise ratio better than 50:1. The MS/MS sensitivity specification is met while using quadrupole isolation of the precursor ion demonstrating that there is minimal transmission loss through the isolating quad.<br>A solution of 100 fmol/µL Glu-Fibrinopeptide B shall be introduced at a flow rate of 3 µL/min. |
| TOF repetition rate | Up to 20 kHz |
| Temperature compensation | Yes |
| Digitizer | 5Gsample/sec ADC with 50 Gbit/sec |
| Dynamic range | 10 bit ADC for high quantitative dynamic range |
| Acquisition rate | up to 50 Hz MS<br>50 Hz MS/MS (profile and peak detected spectra to disk) |

## Optional accessory

| | |
|---|---|
| IonBooster | Optional ion source |
| APCI II | Optional ion source |
| APPI II | Optional ion source |
| GC-APCI | Allows for direct GC coupling (Optional ion source) |
| APLI | Optional ion source |
| CryoSpray | Optional ion source |
| Bruker CaptiveSpray nanoBooster | Optional ion source |
| On-/Off-Line Nanospray | Optional ion source |
| CE/MS interface | With grounded needle for easy CE-TOF set-up (Optional) |
| DIP | Direct Probe (Optional ion source) |



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# maXis impact

- Maximum Impact – Definitive Answers

UHR-TOF MS

Innovation with Integrity

# Redefining Accurate Mass LC-MS/MS

Until now, mass spectrometry technologies have forced scientists to choose between performance characteristics for a given application. Often, a system is designed for qualitative work, sacrificing quantitation performance in the process.

There is no need to make compromises in mass spectrometry anymore. The maXis impact™ sets a new technology standard where industry leading performance values are all simultaneously available in a single acquisition at full sensitivity.

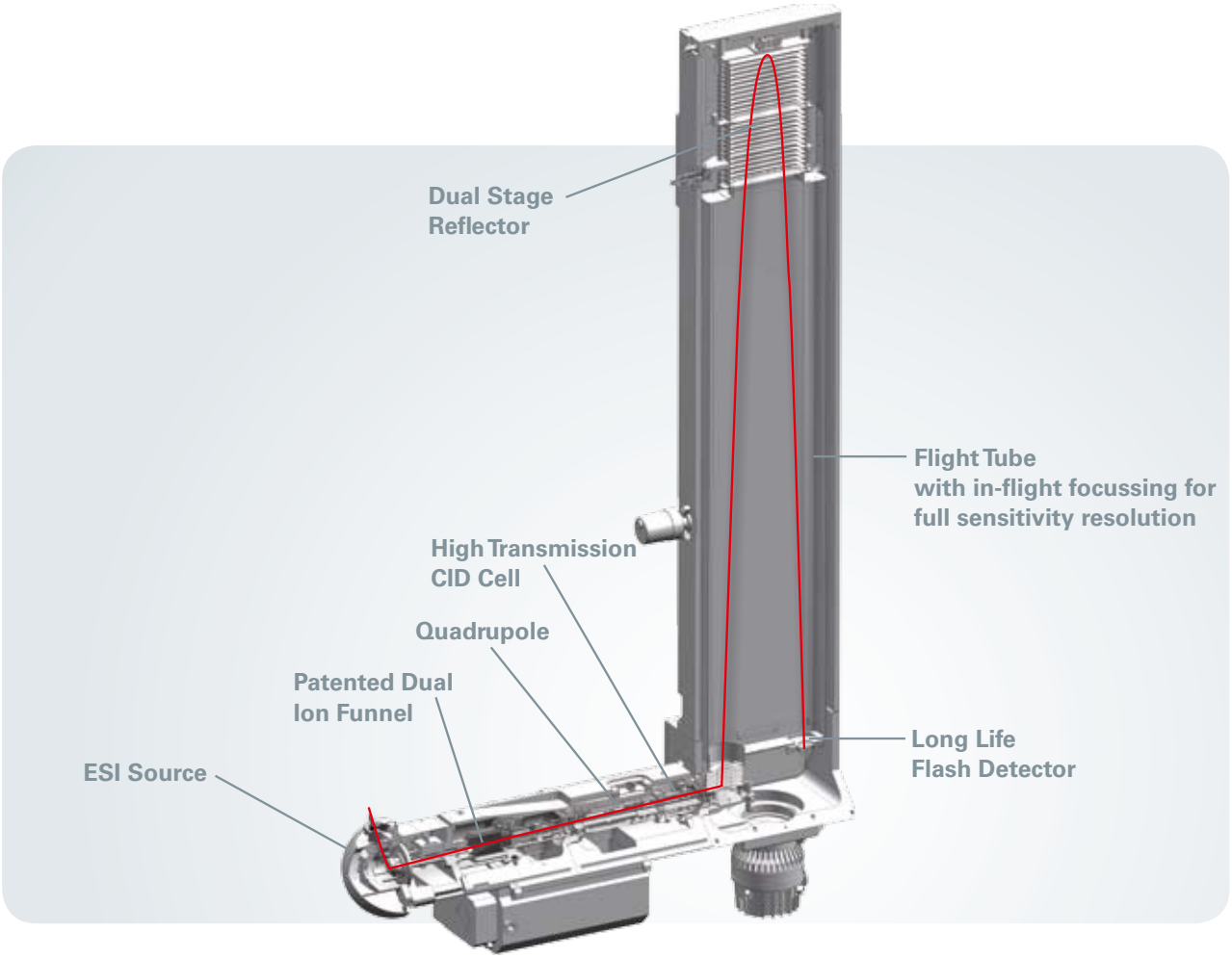
Powered by a series of patented technology innovations, the maXis impact simply provides the very best results without compromise in a cost effective, benchtop format.

**maXis impact: Qualitative and Quantitative results from a single LC/MS analysis**

- Sub-ppm mass accuracy and 40,000 full sensitivity resolution
- Extreme sensitivity across the entire mass range from very small molecules to intact proteins
- High speed MS/MS capability with full U-HPLC compatibility
- Simultaneous analysis of major and trace sample components
- Isotopic fidelity for definitive molecular formulae determination
- Robust and easy to operate system

**And all in an economical and compact design!**

# Unparalleled Performance Now in a Bench-top Package




## The only no-compromise full sensitivity and full resolution UHR-TOF on the market

A game changing step forwards in TOF technology featuring nine new patents. The maXis impact is powered by a number of outstanding technology innovations including:

- Unique Full Sensitivity Resolution (FSR) technology in all modes
- Proven Bruker UHR-TOF technology in bench-top format
- New broadband transmission CID cell providing ground-breaking sensitivity
- Fast 4 G sample/sec digitizer enabling data acquisition at up to 50 Hz
- Long life FLASH Detector
- Flexible choice of API sources including new CaptiveSpray™ and solid sample (DIP) and GC inlets

## Refining capabilities across the analytical world

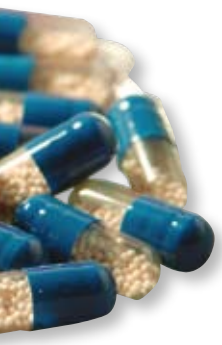
With it's unique capabilities, the maXis impact liberates your work from restriction and compromise. Whether the need is for small or large molecule analysis, quantitation or molecular identification, the maXis impact is more than capable of providing the results needed to make decisions first time, every time.

Let the maXis impact achieve your goals in:

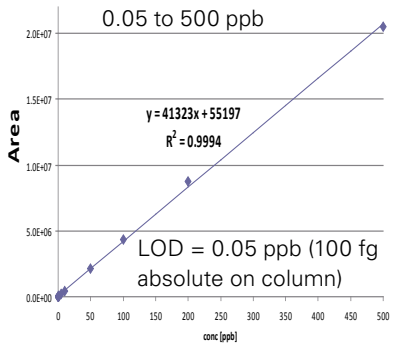
- Forensics, toxicology & doping control
- Food & environmental testing
- Synthetic chemistry support
- Drug metabolite and impurity identification and quantitation
- Metabolomics
- Intact protein analysis & characterization of biophamaceuticals
- Biomarker discovery & validation

# One-Shot Certainty for Qual/Quant Analysis

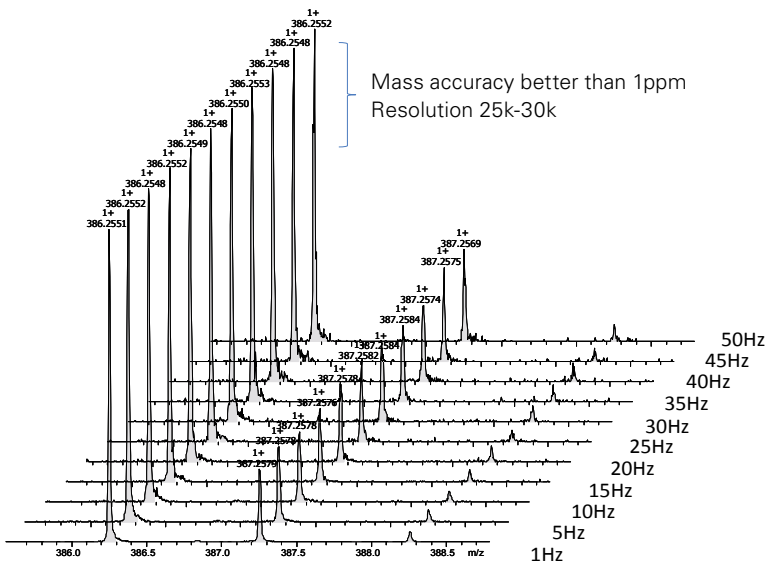
maXis impact captures the full picture of your sample in one analysis alleviating the need for multiple runs. More than 4 orders of fundamental dynamic range achieved without artificial compensators allows simultaneous measurement of major and trace sample components in a single analysis - even if coeluent.



**Buspirone MS/MS linearity**

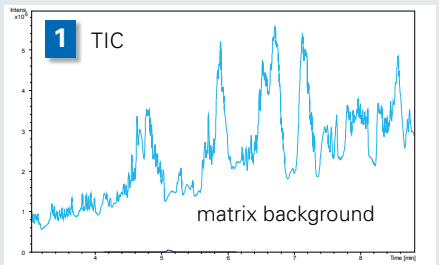


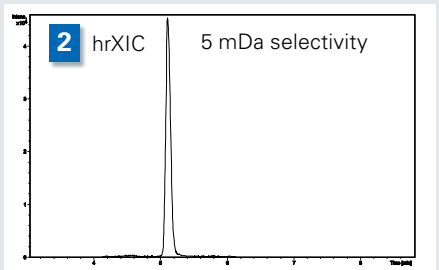

**Ultra fast acquisition speed up to 50 Hz**

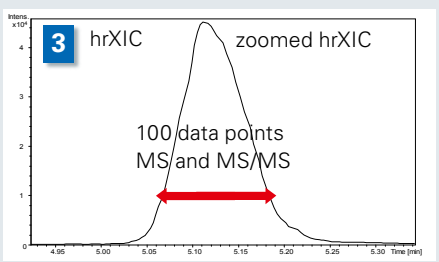


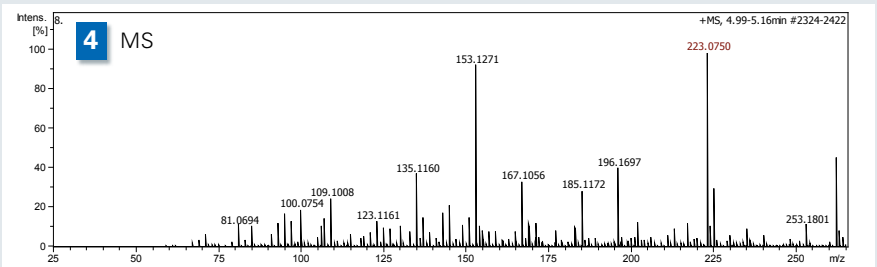

MS of Buspiron acquired at 1Hz up to 50 Hz spectra to disk.
Resolution and spectral accuracy maintained even at maximum speed

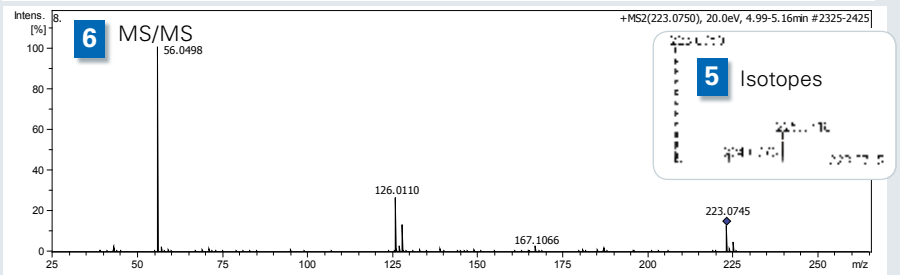
**Qualitative and quantitative results from a single auto MS/MS run**




1. TIC from complex sample (60 pesticides spiked into ginger extract (QuEChERS)).
2. High resolution extracted ion chromatogram (hrXIC) of m/z 223.0745 with 5mDa discrimination width (Acetamiprid).
3. Magnified LC peak. High speed acquisition rate in MS and MS/MS mode (MS: 100ms, MS/MS: 20ms spectra time). 100 data points across this LC peak allows precise quantitation.
4. High resolution survey MS with m/z 223.0745 selected as precursor.
5. High spectral accuracy means isotopic fidelity for identification certainty.
6. High sensitivity MS/MS spectrum even at very low MW (56.0498 m/z) for confirmation by fragment information.

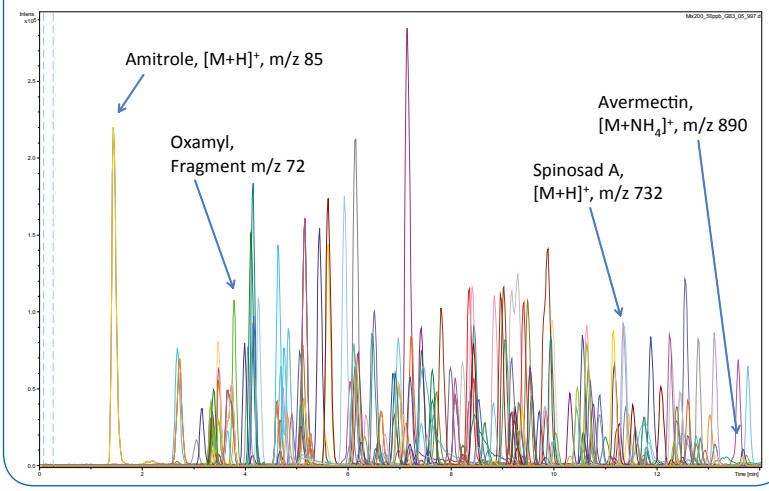
# Precisely Targeted Small Molecule Analysis

## Ideally suited for broad band multi-target screening

Resolve and identify multiple compounds from extremely complex mixtures across a wide mass range even at low analyte concentrations. With these key performance attributes, the maXis impact is an ideal fit for rapid, high target number screening tasks such as food testing or forensic analysis.

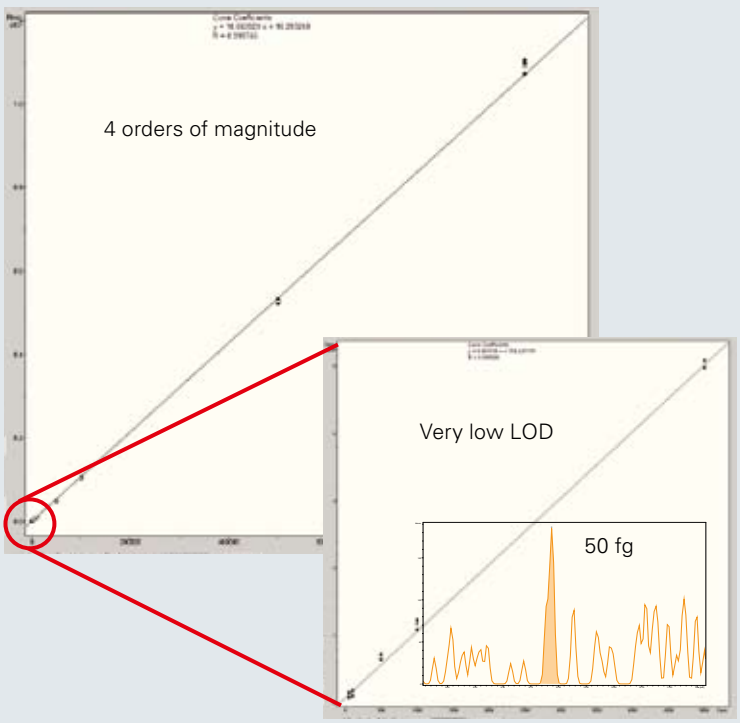
For the laboratory challenged with rapid response to novel analytes, retrospective *in-silico* screening of complete datasets using TargetAnalysis™ software makes maXis impact the most agile screening tool available.

### Multi-target screening at 2mDa hrXIC selectivity




2 mDa high resolution XIC from 200 pesticides. Each color represents the hrXIC of one pesticide. Sample at a concentration of 50 ppb each separated with U- HPLC maXis impact.

### Triple quad sensitivity and quantitation with high-res, accurate mass




Fluoxastrobin (m/z 459) has been quantified over 4 orders of magnitude in concentration from 1ng down to 50fg. The linearity is R=0.9996 with an ultra low LOD coupled with accurate mass certainty.

The maXis impact encapsulates the capabilities of low fg range sensitivity with more than four orders of magnitude dynamic range and quantitative capacity along with the performance of an exceptional high resolution accurate mass instrument. The simultaneous combination of attributes is ideal for many discovery, development, screening and drug metabolism applications which often require both the identification and quantitation of sample components that vary widely in both structure and concentration.

Excellent for use in the analysis of both known and unknown compounds, the maXis impact represents a new level of achievement in the challenge to provide one step qualitative and quantitative data in a single rapid analysis.

# Small Molecule ID & Structure Elucidation

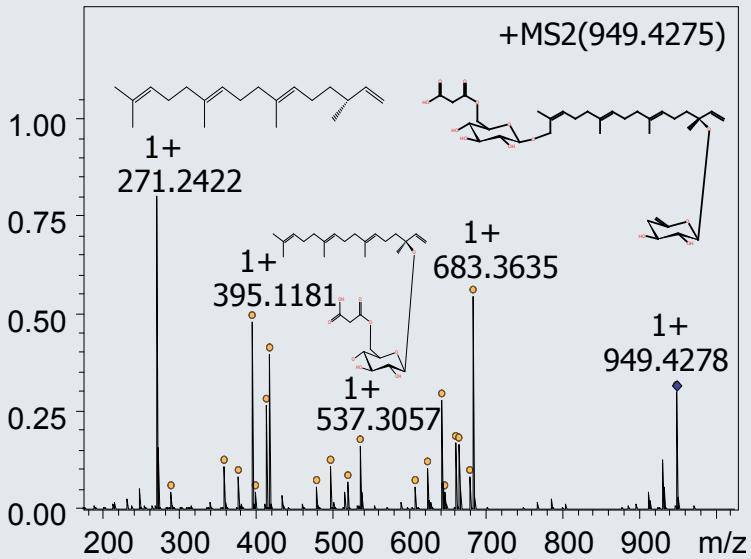
## Impacting Metabolomics results

A key bottleneck in metabolomics research is structural confirmation and elucidation of metabolites. Diterpene glycosides (DTGs) are abundant plant defence compounds with largely unknown modes of action. Outstanding MS and MS/MS data for Nicotiana attenuata (tobacco) DTGs acquired on a maXis impact enabled the rapid identification of the entire compound family. To achieve this, the fragmentation results are visualized and interpreted using Bruker´s novel FragmentExplorer™.

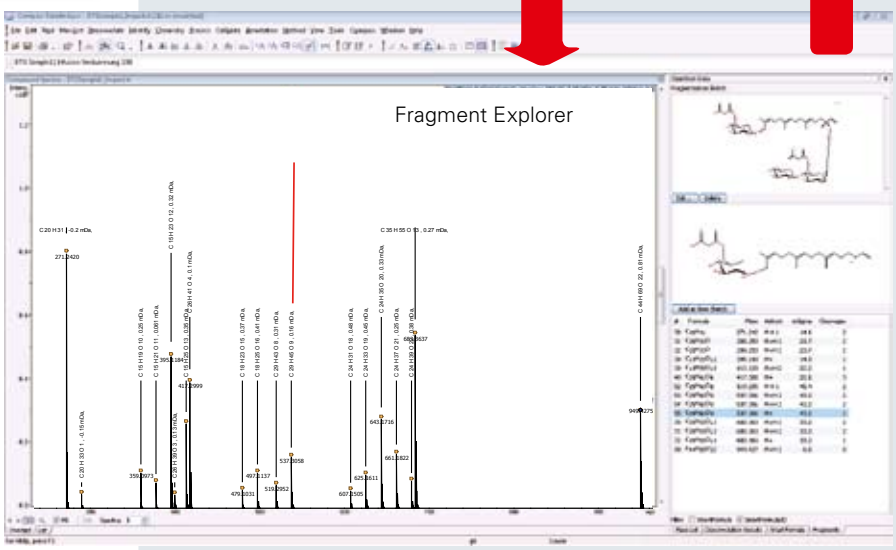
The FragmentExplorer has been especially designed for faster interpretation of MS/MS data.
It provides an interactive link between SmartFormula 3D™ results, mass spectra and molecular structures.

SmartFormula3D™ co-developed with Pfizer, utilizes maXis impact high isotopic fidelity in MS and MS/MS in a unique relational algorythm to assign molecular formulae of unknown analytes without prior knowledge or assumptions.

### Compound identification and structure confirmation



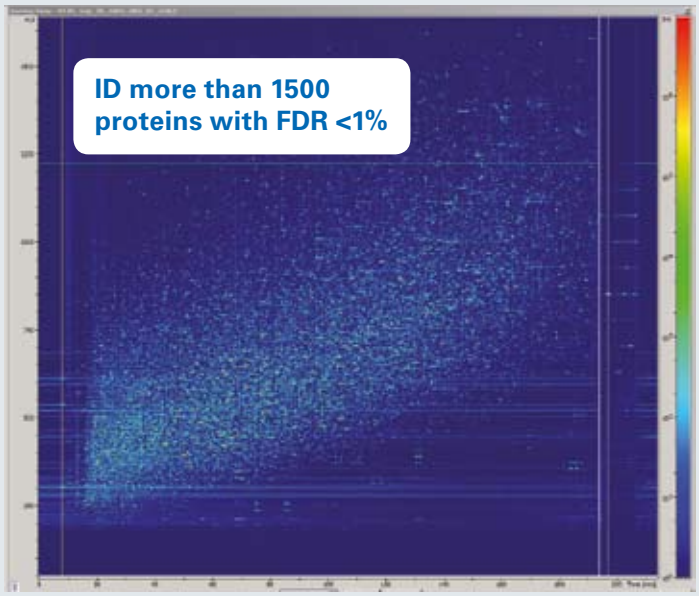

SmartFormula3D




FragmentExplorer with embedded ChemDraw expertly assists fragment assignments.

# Biomarker Discovery and Validation

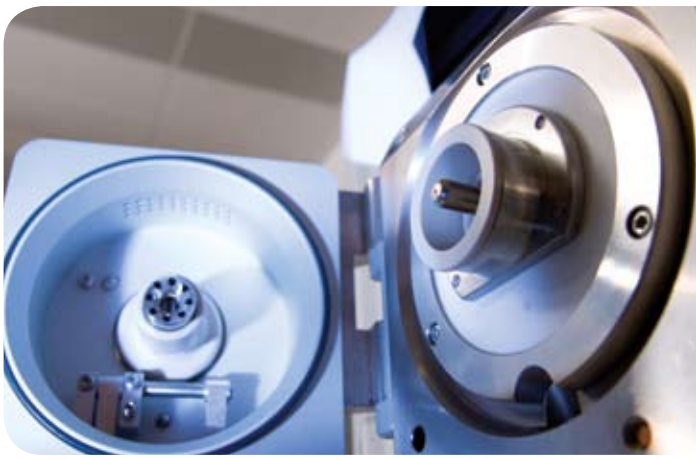
## In-depth qualitative analysis of complex proteomics samples




LC auto MS/MS survey. The human cell line HT29 is an established model system to study colon cancer progression. A 1 µg digest of HT29 cells was separated on a RSLCnano system (3 h gradient, 25 cm column) and measured on a maXis impact with a captive spray source.

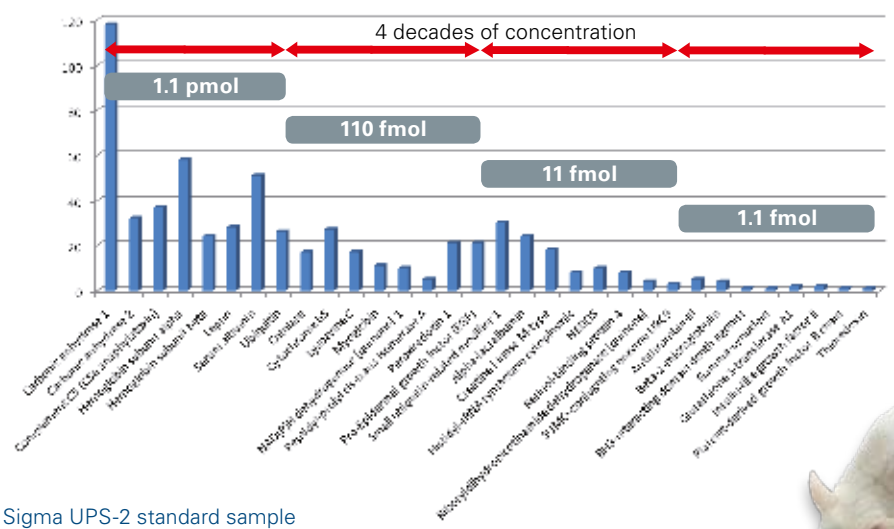
### Get full performance first time, every time

The CaptiveSpray is a revolutionary LC-MS source that combines the sensitivity of nanospray with the ease of use and robustness of electrospray. CaptiveSpray utilizes patented technology to capture and sweep sample ions into the MS independent of LC flow rate.



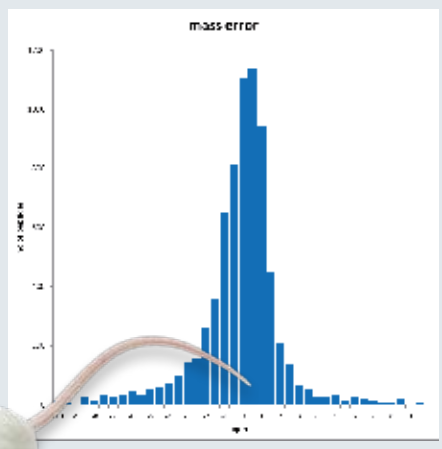
CaptiveSpray LC-MS source

## Identification over a dynamic range of 4 decades of concentration from complex samples




Sigma UPS-2 standard sample

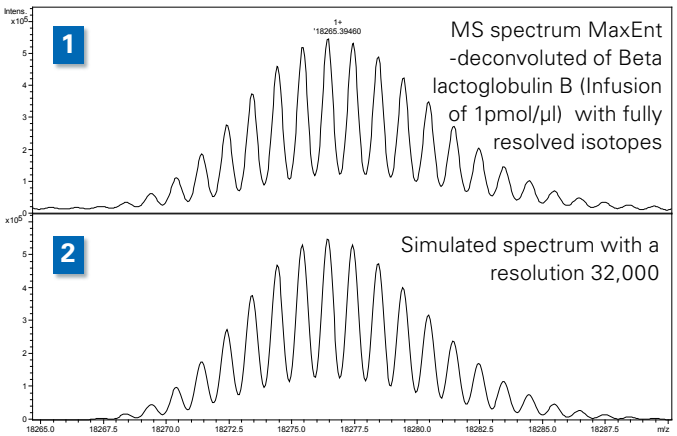
## Real-life MS mass accuracy




Plot of all peptides from a digest of 200ng E.coli

# BioPharma QC

**Isotopic resolution of intact proteins**




## Quantum leap in data quality for biopharmaceutical characterization

With 30k-40k resolution for intact proteins @ full sensitivity with true isotopic patterns, the maXis impact allows you to simultaneously characterize, impurity detect and quantify your biopharmaceutical products. Combined with MS& MS/MS accuracy < 1ppm the maxis impact ensures certainty first time every time, allowing you to report your results with confidence.

## Source Options

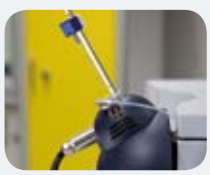
Wide choice of ionization and coupling techniques for a broad range of sampling including insoluble compounds:

- GC-MS coupling
- APCI II (atmospheric pressure chemical ionization) source with direct probe
- APPI II (atmospheric pressure photo ionization) source
- CaptiveSpray LC-MS source
- CE-MS coupling with grounded needle

## LC Options

Bruker fully supports and integrates a wide range of leading HPLC systems, autosamplers and accessories.

GC-MS coupling



Solid probe mounted on an APCI II source

APPI II source

For research use only. Not for use in diagnostic procedures.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**www.bruker.com/maXis**

# Description

## maXis impact bench-top UHR Time-of-Flight Mass Spectrometer System

BDAL #282000

Easy-to-use, Ultra-High-Resolution electrospray ionization quadrupole time-of-flight LC/MS/MS mass spectrometer designed for exact mass and true isotopic measurements in both MS and MS/MS mode.

**Bencch-top, small footprint Mass Spectrometer system for exact mass and highest mass resolution at U-HPLC speed in both MS and MS/MS mode:**

- Unique FSR technology with Full Sensitivity @ Maximum Resolution achieved without any time constraints, in MS and MS/MS mode
- Outstanding Mass Resolution and Accuracy in both MS and MS/MS
- High-resolution extracted ion chromatograms capabilities
- High performance hyperbolic quadrupole and collision cell for compound fragmentation
- True Isotopic Measurements

### A. Apollo II (ESI) Source

- Highly sensitive ESI Source with proprietary ion funnel guide for gentle mass independent ion focusing and high ion transmission efficiency
- Combined Funnel-Octopole-Cartridge with front access for easy maintenance
- Grounded needle for safety and easy sample introduction
- Suitable for U-HPLC, HPLC and CE coupling
- Heated counter current drying gas for gentle and efficient drying
- Ion lens system including in Source collision induced dissociation control (IS-CID)
- Pneumatic off-axis nebulization for flow rates up to 1 ml/min., with gradients from 100% aqueous to 100% organic
- Flow rate 1µl/min to 1ml/min
- Ni coated glass capillary for physical and electrostatic isolation
- Computer controlled HV and gas controller

### B. High Mass Quadrupole Mass Filter:

- Hyperbolic quadrupole mass filter
- Ultra stable monolithic design
- RF-generator for monoisotopic precursor ion selection

### C. Novel high-transmission CID Collision cell:

- Hexapole broad-mass bandwidth design
- Fast radial ion ejection enabling fast MS/MS cycle
- RF-Generator with fast amplitude switching
- Collision gas controller

### D. Orthogonal pulsed ion extraction and UHR Time-of-Flight Mass Analyzer

- Interface housing and ion lens system
- In-line detector system for easy maintenance

- Ultra-stable high voltage switches with up to 20 kHz repetition rate and appropriate power supplies.
- UHR-TOF analyzer with orthogonal mounted ion source
- Novel in-flight refocusing optics for uncompromised sensitivity
- Dual stage ion reflectron with increased mass resolution and accuracy
- High-sensitivity and fast ion detector system, mechanical adjustment in micrometer range
- Positive and negative ion modes
- Ultra-stable high voltage power supplies for TOF analyzer and detector

**E. Vacuum system**

- Analyzer vacuum housing
- Vacuum system with 5 differential pumping stages
- One roughing pump and quadruple stage turbo-drag pumps for ESI source and UHR-TOF analyzer
- Vacuum measurement and pump control unit

**F. Syringe pump**

**G. Modes of Operation**

- TOF Mass ranges 20-40,000 m/z
- Internal calibration (MS and MS/MS)
- External calibration (MS and MS/MS)
- Exact mass measurements independent from sample concentration over a wide dynamic range without second sprayer.

**H. High-resolution-performance and accurate mass features**

- Patented ion funnel source
- One-shot acquisition mode, no tuning for mass range optima
- Enhanced low mass sensitivity
- Superior MS/MS sensitivity
- Ultra broad mass-bandwidth
- Long term and ultra stable mass axis stability in MS and MS/MS
- Exact mass independent from sample concentration charge state and collision energy
- Combined calibration for both MS and MS/MS
- Wide dynamic range for quantitation
- Advanced temperature compensated flight tube
- Positive / negative ion operation

**I. Data system:**

- PC Workstation with 2,66 GHz Dual-Pentium Processor, 4 GB RAM, system hard-disk drive plus 1000 GB hard-disk drive for data, 1.44 Mb 3.5" floppy diskette drive
- DVD-ROM drive
- R/W DVD-ROM drive
- 20" flat screen colour monitor
- WinXP OS
- Laser printer

## J. Applications software

Software package Compass 1.4 for HPLC and MS control, data acquisition, post processing, and data analysis:

- Operating system Windows XP
- Compass / HyStar 3.2 for integrated control of most popular U-HPLC and HPLC systems and auto samplers and automation
- Expert mode: extended control over instrument parameters for interactive system optimization of sophisticated exact mass methods
- Compass / Data Analysis software DA 4.1, including:
    - Advanced data processing with a high degree of automation
    - SmartFormula 3D™: Automated sum formula determination using MS and MS/MS data with both, accurate mass and isotopic fit.
    - QuantAnalysis™ quantitation package
    - LibrarySearch ™ module for search of MS, MS/MS and MSn spectra with advanced matching algorithm
    - Charge deconvolution module
    - Export of spectra and ion current profiles as Windows metafiles to word-processing programs
- SW License Compass 1.3
- SW License Charge Deconvolution for DA 3.4
- SW License MaxEntropy Deconvolution as an option

**K. Set of manuals and reference CD-ROMs**
**L. Installation**
**M. Familiarization upon installation**
**N. 1 year warranty**

**Voucher for a factory-training course - valid for 2 participants.**

**Abiotrophia** defectiva
**Acetobacter** aceti
Acetobacter pasteurianus
**Acholeplasma** laidlawii
**Achromobacter** denitrificans
Achromobacter insolitus
Achromobacter piechaudii
Achromobacter ruhlandii
Achromobacter sp
Achromobacter spanius
Achromobacter xylosoxidans
**Acidaminococcus** fermentans
Acidaminococcus intestini
**Acidiphilium** acidophilum
**Acidovorax** avenae
Acidovorax defluvii
Acidovorax delafieldii
Acidovorax facilis
Acidovorax konjaci
Acidovorax temperans
**Acinetobacter** baumannii
Acinetobacter baylyi
Acinetobacter bouvetii
Acinetobacter calcoaceticus
Acinetobacter gerneri
Acinetobacter guillouiae
Acinetobacter haemolyticus
Acinetobacter johnsonii
Acinetobacter junii
Acinetobacter lwoffii
Acinetobacter nosocomialis
Acinetobacter parvus
Acinetobacter pittii
Acinetobacter radioresistens
Acinetobacter schindleri
Acinetobacter sp
Acinetobacter tandoii
Acinetobacter tjernbergiae
Acinetobacter towneri
Acinetobacter ursingii
**Actinobacillus** delphinicola
Actinobacillus equuli
Actinobacillus lignieresii
Actinobacillus pleuropneumoniae
Actinobacillus rossii
Actinobacillus suis
Actinobacillus ureae
**Actinobaculum** schaalii
Actinobaculum suis
Actinobaculum urinale
**Actinocorallia** libanotica
**Actinomyces** bovis
Actinomyces bowdenii
Actinomyces canis
Actinomyces cardiffensis
Actinomyces catuli
Actinomyces coleocanis
Actinomyces dentalis
Actinomyces denticolens
Actinomyces europaeus
Actinomyces funkei
Actinomyces gerencseriae
Actinomyces graevenitzii
Actinomyces hordeovulneris
Actinomyces hyovaginalis
Actinomyces israelii
Actinomyces marimammalium
Actinomyces meyeri
Actinomyces naeslundii
Actinomyces nasicola
Actinomyces neuii
Actinomyces odontolyticus

Actinomyces oris
Actinomyces radicidentis
Actinomyces radingae
Actinomyces ruminicola
Actinomyces sp
Actinomyces suimastitidis
Actinomyces turicensis
Actinomyces urogenitalis
Actinomyces vaccimaxillae
Actinomyces viscosus
**Adlercreutzia** equolifaciens
**Aerococcus** christensenii
Aerococcus sanguinicola
Aerococcus urinae
Aerococcus urinaehominis
Aerococcus viridans
**Aeromicrobium** flavum
**Aeromonas** bestiarum
Aeromonas caviae
Aeromonas encheleia
Aeromonas enteropelogenes
Aeromonas eucrenophila
Aeromonas hydrophila
Aeromonas ichthiosmia
Aeromonas jandaei
Aeromonas media
Aeromonas molluscorum
Aeromonas popoffii
Aeromonas punctata
Aeromonas salmonicida
Aeromonas schubertii
Aeromonas simiae
Aeromonas sobria
Aeromonas sp[2]
Aeromonas veronii
**Afipia** broomeae
Afipia felis
Afipia massiliensis
**Aggregatibacter** actinomycetemcomitans
Aggregatibacter aphrophilus
Aggregatibacter segnis
**Agrococcus** jenensis
**Agromyces** bracchium
Agromyces cerinus
Agromyces fucosus
Agromyces hippuratus
Agromyces humatus
Agromyces italicus
Agromyces lapidis
Agromyces mediolanus
Agromyces neolithicus
Agromyces rhizospherae
Agromyces salentinus
Agromyces subbeticus
**Alcaligenes** faecalis
Alcaligenes sp
**Alicyclobacillus** acidocaldarius
Alicyclobacillus acidoterrestris
Alicyclobacillus cycloheptanicus
**Aliivibrio** fischeri
**Alishewanella** fetalis
**Alistipes** finegoldii
Alistipes onderdonkii
Alistipes shahii
**Alkalibacillus** haloalkaliphilus
**Alloiococcus** otitis
**Alloscardovia** omnicolens
**Alternaria** alternata
**Amycolatopsis** alba
Amycolatopsis azurea
Amycolatopsis balhimycina
Amycolatopsis coloradensis

Amycolatopsis fastidiosa
Amycolatopsis japonica
Amycolatopsis kentuckyensis
Amycolatopsis keratiniphila
Amycolatopsis lexingtonensis
Amycolatopsis lurida
Amycolatopsis mediterranei
Amycolatopsis minnesotensis
Amycolatopsis pretoriensis
Amycolatopsis sulphurea
Amycolatopsis tolypomycina
**Anaerococcus** hydrogenalis
Anaerococcus lactolyticus
Anaerococcus murdochii
Anaerococcus octavius
Anaerococcus prevotii
Anaerococcus sp
Anaerococcus tetradius
Anaerococcus vaginalis
**Anaerotruncus** colihominis
**Aneurinibacillus** aneurinilyticus
Aneurinibacillus migulanus
**Aquincola** tertiaricarbonis
**Arcanobacterium** haemolyticum
Arcanobacterium hippocoleae
Arcanobacterium phocae
Arcanobacterium pluranimalium
**Arcobacter** butzleri
Arcobacter cibarius
Arcobacter cryaerophilus
Arcobacter halophilus
Arcobacter nitrofigilis
Arcobacter skirrowii
**Aromatoleum** alkani
Aromatoleum anaerobicus
Aromatoleum aromaticum
Aromatoleum bremensis
Aromatoleum buckelii
Aromatoleum diolicum
Aromatoleum evansii
Aromatoleum pretroleum
Aromatoleum terpenicum
Aromatoleum tolulyticus
Aromatoleum toluolicum
Aromatoleum toluvorans
**Arsenophonus** nasoniae
**Arthroascus** schoenii
**Arthrobacter** ardleyensis
Arthrobacter arilaitensis
Arthrobacter aurescens
Arthrobacter bergerei
Arthrobacter castelli
Arthrobacter chlorophenolicus
Arthrobacter citreus
Arthrobacter creatinolyticus
Arthrobacter crystallopoietes
Arthrobacter cumminsii
Arthrobacter flavus
Arthrobacter gandavensis
Arthrobacter gangotriensis
Arthrobacter globiformis
Arthrobacter histidinolovorans
Arthrobacter ilicis
Arthrobacter kerguelensis
Arthrobacter koreensis
Arthrobacter luteolus
Arthrobacter monumenti
Arthrobacter mysorens
Arthrobacter nasiphocae
Arthrobacter nicotianae
Arthrobacter nicotinovorans
Arthrobacter nitroguajacolicus

Arthrobacter oxydans
Arthrobacter parietis
Arthrobacter pascens
Arthrobacter pigmenti
Arthrobacter polychromogenes
Arthrobacter protophormiae
Arthrobacter psychrolactophilus
Arthrobacter psychrophenolicus
Arthrobacter pyridinolis
Arthrobacter ramosus
Arthrobacter roseus
Arthrobacter russicus
Arthrobacter scleromae
Arthrobacter sp
Arthrobacter stackebrandtii
Arthrobacter sulfonivorans
Arthrobacter sulfureus
Arthrobacter tecti
Arthrobacter tumbae
Arthrobacter uratoxydans
Arthrobacter ureafaciens
Arthrobacter woluwensis
**Arthroderma** benhamiae
**Arthrographis**_kalrae[ana] (Eremomyces_langeronii[teleo])
**Aspergillus** brasiliensis
Aspergillus flavus
Aspergillus fumigatus
Aspergillus niger
Aspergillus terreus
Aspergillus versicolor
Aspergillus_thermomutatus[ana] (Neosartorya_pseudofischeri[teleo])
**Atopobium** minutum
Atopobium parvulum
Atopobium rimae
Atopobium sp
Atopobium vaginae
**Aureimonas** altamirensis
**Aureobasidium** pullulans
**Austwickia** chelonae
**Avibacterium** avium
Avibacterium endocarditidis
Avibacterium gallinarum
Avibacterium volantium
**Azoarcus** communis
Azoarcus indigens
Azoarcus sp
**Azohydromonas** lata
**Bacillus** acidicola
Bacillus agaradhaerens
Bacillus akibai
Bacillus alcalophilus
Bacillus algicola
Bacillus altitudinis
Bacillus alveayuensis
Bacillus amyloliquefaciens
Bacillus aquimaris
Bacillus arsenicus
Bacillus asahii
Bacillus atrophaeus
Bacillus azotoformans
Bacillus badius
Bacillus barbaricus
Bacillus bataviensis
Bacillus benzoevorans
Bacillus carboniphilus
Bacillus cellulosilyticus
Bacillus cereus
Bacillus chagannorensis
Bacillus cibi
Bacillus circulans
Bacillus clarkii
Bacillus clausii

Bacillus coagulans
Bacillus cohnii
Bacillus decolorationis
Bacillus drentensis
Bacillus endophyticus
Bacillus farraginis
Bacillus fastidiosus
Bacillus firmus
Bacillus flexus
Bacillus fordii
Bacillus fortis
Bacillus funiculus
Bacillus galactosidilyticus
Bacillus gibsonii
Bacillus halmapalus
Bacillus halodurans
Bacillus hemicellulosilyticus
Bacillus horikoshii
Bacillus horneckiae
Bacillus horti
Bacillus humi
Bacillus hwajinpoensis
Bacillus idriensis
Bacillus indicus
Bacillus infantis
Bacillus jeotgali
Bacillus koreensis
Bacillus krulwichiae
Bacillus lentus
Bacillus licheniformis
Bacillus litoralis
Bacillus luciferensis
Bacillus macauensis
Bacillus mannanilyticus
Bacillus marisflavi
Bacillus massiliensis
Bacillus megaterium
Bacillus mojavensis
Bacillus muralis
Bacillus mycoides
Bacillus nealsonii
Bacillus niacini
Bacillus novalis
Bacillus odysseyi
Bacillus okhensis
Bacillus okuhidensis
Bacillus oleronius
Bacillus oshimensis
Bacillus patagoniensis
Bacillus pseudalcaliphilus
Bacillus pseudofirmus
Bacillus pseudomycoides
Bacillus psychrosaccharolyticus
Bacillus pumilus
Bacillus ruris
Bacillus safensis
Bacillus salarius
Bacillus seohaeanensis
Bacillus shackletonii
Bacillus simplex
Bacillus siralis
Bacillus smithii
Bacillus soli
Bacillus sonorensis
Bacillus sp
Bacillus sporothermodurans
Bacillus subterraneus
Bacillus subtilis
Bacillus thermoamylovorans
Bacillus thioparans
Bacillus thuringiensis
Bacillus vallismortis

Bacillus vedderi
Bacillus vietnamensis
Bacillus vireti
Bacillus wakoensis
Bacillus weihenstephanensis
**Bacteroides** caccae
Bacteroides coagulans
Bacteroides eggerthii
Bacteroides finegoldii
Bacteroides fragilis
Bacteroides gallinarum
Bacteroides intestinalis
Bacteroides massiliensis
Bacteroides nordii
Bacteroides ovatus
Bacteroides pyogenes
Bacteroides salyersiae
Bacteroides stercoris
Bacteroides thetaiotaomicron
Bacteroides uniformis
Bacteroides vulgatus
**Balneatrix** alpica
**Bartonella** japonica
**Beauveria** bassiana
**Bergeyella** zoohelcum
**Bibersteinia** trehalosi
**Bifidobacterium** adolescentis
Bifidobacterium angulatum
Bifidobacterium animalis
Bifidobacterium asteroides
Bifidobacterium bifidum
Bifidobacterium boum
Bifidobacterium breve
Bifidobacterium catenulatum
Bifidobacterium choerinum
Bifidobacterium coryneforme
Bifidobacterium dentium
Bifidobacterium gallicum
Bifidobacterium gallinarum
Bifidobacterium longum
Bifidobacterium magnum
Bifidobacterium merycicum
Bifidobacterium minimum
Bifidobacterium pseudocatenulatum
Bifidobacterium pseudolongum
Bifidobacterium pullorum
Bifidobacterium ruminantium
Bifidobacterium saeculare
Bifidobacterium scardovii
Bifidobacterium thermacidophilum
Bifidobacterium thermophilum
**Bilophila** sp
**Blastomonas** natatoria
Blastomonas ursincola
**Blautia** coccoides
**Bordetella** avium
Bordetella bronchiseptica
Bordetella hinzii
Bordetella holmesii
Bordetella parapertussis
Bordetella pertussis
Bordetella petrii
Bordetella sp
Bordetella trematum
**Borrelia** burgdorferi
Borrelia garinii
Borrelia spielmanii
**Brachybacterium** faecium
Brachybacterium muris
**Brachyspira** murdochii
Brachyspira pilosicoli
**Bradyrhizobium** betae

Bradyrhizobium denitrificans
**Brenneria** alni
Brenneria nigrifluens
Brenneria quercina
Brenneria rubrifaciens
Brenneria salicis
**Brevibacillus** agri
Brevibacillus borstelensis
Brevibacillus brevis
Brevibacillus centrosporus
Brevibacillus choshinensis
Brevibacillus formosus
Brevibacillus invocatus
Brevibacillus laterosporus
Brevibacillus parabrevis
Brevibacillus reuszeri
**Brevibacterium** aurantiacum
Brevibacterium casei
Brevibacterium celere
Brevibacterium iodinum
Brevibacterium linens
Brevibacterium marinum
Brevibacterium paucivorans
Brevibacterium picturae
Brevibacterium ravenspurgense
Brevibacterium sanguinis
**Brevundimonas** aurantiaca
Brevundimonas diminuta
Brevundimonas intermedia
Brevundimonas nasdae
Brevundimonas sp
Brevundimonas subvibrioides
Brevundimonas vesicularis
**Brochothrix** thermosphacta
**Budvicia** aquatica
**Bulleidia** extructa
**Burkholderia** ambifaria
Burkholderia andropogonis
Burkholderia anthina
Burkholderia caledonica
Burkholderia caribensis
Burkholderia cenocepacia
Burkholderia cepacia
Burkholderia diffusa
Burkholderia dolosa
Burkholderia fungorum
Burkholderia gladioli
Burkholderia glathei
Burkholderia glumae
Burkholderia lata
Burkholderia latens
Burkholderia metallica
Burkholderia multivorans
Burkholderia phenazinium
Burkholderia phymatum
Burkholderia plantarii
Burkholderia pyrrocinia
Burkholderia sacchari
Burkholderia seminalis
Burkholderia stabilis
Burkholderia terricola
Burkholderia thailandensis
Burkholderia tropica
Burkholderia tuberum
Burkholderia vietnamiensis
Burkholderia xenovorans
**Buttiauxella** agrestis
Buttiauxella brennerae
Buttiauxella ferragutiae
Buttiauxella gaviniae
Buttiauxella izardii
Buttiauxella noackiae

Buttiauxella warmboldiae
**Butyricimonas** virosa
**Campylobacter** avium
Campylobacter canadensis
Campylobacter coli
Campylobacter concisus
Campylobacter curvus
Campylobacter fetus
Campylobacter gracilis
Campylobacter helveticus
Campylobacter hominis
Campylobacter hyointestinalis
Campylobacter jejuni
Campylobacter lanienae
Campylobacter lari
Campylobacter peloridis
Campylobacter rectus
Campylobacter showae
Campylobacter sputorum
Campylobacter upsaliensis
Campylobacter ureolyticus
**Candida** alai
Candida albicans
Candida allociferrii
Candida ambrosiae
Candida auris
Candida blattae
Candida bohiensis
Candida boidinii
Candida bracarensis
Candida buenavistaensis
Candida carpophila
Candida castellii
Candida catenulata
Candida cylindracea
Candida dubliniensis
Candida duobushaemulonii
Candida ernobii
Candida freyschussii
Candida friedrichii
Candida frijolesensis
Candida glabrata
Candida haemulonii
Candida inconspicua
Candida infanticola
Candida intermedia
Candida labiduridarum
Candida lactiscondensi
Candida magnoliae
Candida maltosa
Candida membranifaciens
Candida mesenterica
Candida metapsilosis
Candida multigemmis
Candida nemodendra
Candida nitratophila
Candida nivariensis
Candida norvegica
Candida orthopsilosis
Candida palmioleophila
Candida parapsilosis
Candida pararugosa
Candida peltata
Candida pini
Candida pseudohaemulonii
Candida rugosa
Candida saitoana
Candida sake
Candida shehatae
Candida sojae
Candida solani
Candida spandovensis

Candida succiphila

Candida tropicalis

Candida versatilis

Candida vini

Candida viswanathii

Candida zeylanoides

Candida_cacaoi[ana] (Pichia_farinosa[teleo])

Candida_chodatii[ana] (Hyphopichia_burtonii[teleo])

Candida_ciferrii[ana] (Stephanoascus_ciferrii[teleo])

Candida_citrea[ana] (Pichia_nakasei[teleo])

Candida_colliculosa[ana] (Torulaspora_delbrueckii[teleo])

Candida_fabianii[ana] (Pichia_fabianii[teleo])

Candida_guilliermondii[ana] (Pichia_guilliermondii[teleo])

Candida_guilliermondii_var_membranaefaciens[ana] (Pichia_ohmeri[teleo])

Candida_holmii[ana] (Kazachstania_exigua[teleo])

Candida_kefyr[ana] (Kluyveromyces_marxianus[teleo])

Candida_krusei[ana] (Issatchenkia_orientalis[teleo])

Candida_lambica[ana] (Pichia_fermentans[teleo])

Candida_lipolytica[ana] (Yarrowia_lipolytica[teleo])

Candida_lusitaniae[ana] (Clavispora_lusitaniae[teleo])

Candida_norvegensis[ana] (Pichia_norvegensis[teleo])

Candida_pelliculosa[ana] (Pichia_anomala[teleo])

Candida_pintolopesii[ana] (Kazachstania_pintolopesii[teleo])

Candida_pulcherrima[ana] (Metschnikowia_pulcherrima[teleo])

Candida_reukaufii[ana] (Metschnikowia_reukaufii[teleo])

Candida_slooffiae[ana] (Kazachstania_slooffiae[teleo])

Candida_sorbosa[ana] (Issatchenkia_occidentalis[teleo])

Candida_sphaerica[ana] (Kluyveromyces_lactis[teleo])

Candida_thermophila[ana] (Ogataea_thermophila[teleo])

Candida_utilis[ana] (Pichia_jandinii[teleo])

Candida_valida[ana] (Pichia_membranifaciens[teleo]#)

**Candidatus Reyranella** massiliensis

**Capnocytophaga** canimorsus

Capnocytophaga cynodegmi

Capnocytophaga gingivalis

Capnocytophaga granulosa

Capnocytophaga haemolytica

Capnocytophaga ochracea

Capnocytophaga sp

Capnocytophaga sputigena

**Cardiobacterium** hominis

Cardiobacterium sp

Cardiobacterium valvarum

**Carnobacterium** maltaromaticum

**Castellaniella** defragrans

**Caulobacter** sp[2]

Caulobacter vibrioides

**Cedecea** davisae

Cedecea lapagei

Cedecea neteri

**Cellulomonas** fimi

Cellulomonas flavigena

Cellulomonas gelida

Cellulomonas uda

**Cellulosimicrobium** cellulans

**Chaetomium** globosum

**Chromobacterium** subtsugae

Chromobacterium violaceum

**Chromohalobacter** salexigens

**Chryseobacterium** ginsenosidimutans

Chryseobacterium gleum

Chryseobacterium hagamense

Chryseobacterium hominis

Chryseobacterium indologenes

Chryseobacterium joostei

Chryseobacterium oranimense

Chryseobacterium scophthalmum

Chryseobacterium sp
**Citrobacter** amalonaticus
Citrobacter braakii
Citrobacter farmeri
Citrobacter freundii
Citrobacter gillenii
Citrobacter koseri
Citrobacter murliniae
Citrobacter rodentium
Citrobacter sedlakii
Citrobacter youngae
**Clavibacter** michiganensis
**Clostridium** acetobutylicum
Clostridium aciditolerans
Clostridium aerotolerans
Clostridium aldenense
Clostridium algidicarnis
Clostridium algidixylanolyticum
Clostridium aminophilum
Clostridium baratii
Clostridium bartlettii
Clostridium beijerinckii
Clostridium bifermentans
Clostridium bolteae
Clostridium butyricum
Clostridium cadaveris
Clostridium carboxidivorans
Clostridium carnis
Clostridium celerecrescens
Clostridium cellobioparum
Clostridium chauvoei
Clostridium citroniae
Clostridium clostridioforme
Clostridium cochlearium
Clostridium colicanis
Clostridium colinum
Clostridium collagenovorans
Clostridium difficile
Clostridium diolis
Clostridium disporicum
Clostridium drakei
Clostridium fallax
Clostridium formicaceticum
Clostridium frigoris
Clostridium ghonii
Clostridium glycolicum
Clostridium glycyrrhizinilyticum
Clostridium haemolyticum
Clostridium halophilum
Clostridium hathewayi
Clostridium hiranonis
Clostridium histolyticum
Clostridium homopropionicum
Clostridium hylemonae
Clostridium indolis
Clostridium innocuum
Clostridium intestinale
Clostridium irregulare
Clostridium isatidis
Clostridium jejuense
Clostridium lactatifermentans
Clostridium lentocellum
Clostridium limosum
Clostridium lundense
Clostridium magnum
Clostridium malenominatum
Clostridium mayombei
Clostridium novyi
Clostridium papyrosolvens
Clostridium paraputrificum
Clostridium perfringens
Clostridium phytofermentans

Clostridium propionicum
Clostridium ramosum
Clostridium saccharobutylicum
Clostridium saccharogumia
Clostridium sardiniense
Clostridium sartagoforme
Clostridium schirmacherense
Clostridium scindens
Clostridium septicum
Clostridium sordellii
Clostridium sp
Clostridium sphenoides
Clostridium spiroforme
Clostridium sporogenes
Clostridium sporosphaeroides
Clostridium subterminale
Clostridium symbiosum
Clostridium tertium
Clostridium tetani
Clostridium thermopalmarium
Clostridium tunisiense
Clostridium xylanovorans
**Cohnella** fontinalis
Cohnella hongkongensis
**Colletotrichum** gloeosporioides
**Collinsella** aerofaciens
**Comamonas** aquatica
Comamonas kerstersii
Comamonas nitrativorans
Comamonas terrigena
Comamonas testosteroni
**Coprobacillus** cateniformis
**Corynebacterium** accolens
Corynebacterium afermentans
Corynebacterium ammoniagenes
Corynebacterium amycolatum
Corynebacterium appendicis
Corynebacterium aquilae
Corynebacterium argentoratense
Corynebacterium aurimucosum
Corynebacterium auris
Corynebacterium auriscanis
Corynebacterium bovis
Corynebacterium callunae
Corynebacterium camporealensis
Corynebacterium capitovis
Corynebacterium casei
Corynebacterium ciconiae
Corynebacterium confusum
Corynebacterium coyleae
Corynebacterium cystitidis
Corynebacterium diphtheriae
Corynebacterium durum
Corynebacterium efficiens
Corynebacterium falsenii
Corynebacterium felinum
Corynebacterium flavescens
Corynebacterium freneyi
Corynebacterium glaucum
Corynebacterium glucuronolyticum
Corynebacterium glutamicum
Corynebacterium halotolerans
Corynebacterium hansenii
Corynebacterium imitans
Corynebacterium jeikeium
Corynebacterium kroppenstedtii
Corynebacterium kutscheri
Corynebacterium lipophile_group_F1
Corynebacterium lipophiloflavum
Corynebacterium macginleyi
Corynebacterium mastitidis
Corynebacterium matruchotii

Corynebacterium minutissimum
Corynebacterium mucifaciens
Corynebacterium mycetoides
Corynebacterium phocae
Corynebacterium pilosum
Corynebacterium propinquum
Corynebacterium pseudodiphtheriticum
Corynebacterium pseudotuberculosis
Corynebacterium renale
Corynebacterium resistens
Corynebacterium riegelii
Corynebacterium simulans
Corynebacterium singulare
Corynebacterium sp
Corynebacterium sphenisci
Corynebacterium spheniscorum
Corynebacterium stationis
Corynebacterium striatum
Corynebacterium suicordis
Corynebacterium sundsvallense
Corynebacterium terpenotabidum
Corynebacterium testudinoris
Corynebacterium thomssenii
Corynebacterium tuberculostearicum
Corynebacterium tuscaniense
Corynebacterium ulcerans
Corynebacterium urealyticum
Corynebacterium ureicelerivorans
Corynebacterium variabile
Corynebacterium vitaeruminis
Corynebacterium xerosis
**Cronobacter** sakazakii
**Cryptococcus** albidosimilis
Cryptococcus curvatus
Cryptococcus diffluens
Cryptococcus flavescens
Cryptococcus flavus
Cryptococcus gastricus
Cryptococcus humicola
Cryptococcus laurentii
Cryptococcus liquefaciens
Cryptococcus macerans
Cryptococcus magnus
Cryptococcus neoformans
Cryptococcus saitoi
Cryptococcus terreus
Cryptococcus uzbekistanensis
Cryptococcus vishniacii
Cryptococcus_albidus[ana]
Filobasidium_floriforme[teleo])
Cryptococcus_gattii[ana]
(Filobasidiella_bacillispora[teleo])
Cryptococcus_uniguttulatus[ana]
(Filobasidium_uniguttulatum[teleo])
**Cryptotrichosporon** anacardii
**Cupriavidus** campinensis
Cupriavidus gilardii
Cupriavidus metallidurans
Cupriavidus necator
Cupriavidus oxalaticus
Cupriavidus pauculus
Cupriavidus respiraculi
Cupriavidus sp[1]
**Curtobacterium** albidum
Curtobacterium flaccumfaciens
Curtobacterium luteum
Curtobacterium sp
**Cyberlindnera** mississippiensis
**Debaryomyces** etchellsii
Debaryomyces hansenii
**Deinococcus** geothermalis
**Delftia** acidovorans
**Dermabacter** hominis
**Dermacoccus** nishinomiyaensis
**Dermatophilus** congolensis

**Devosia** riboflavina
**Dialister** micraerophilus
Dialister pneumosintes
**Dichelobacter** nodosus
**Dickeya** chrysanthemi
Dickeya dadantii
Dickeya dianthicola
Dickeya paradisiaca
Dickeya zeae
**Dietzia** cinnamea
Dietzia maris
Dietzia natronolimnaea
**Dysgonomonas** gadei
**Edwardsiella** hoshinae
Edwardsiella ictaluri
Edwardsiella tarda
**Eggerthella** lenta
**Eggerthia** catenaformis
**Eikenella** corrodens
**Elizabethkingia** meningoseptica
Elizabethkingia miricola
**Emericella** nidulans
**Empedobacter** brevis
**Enterobacter** aerogenes
Enterobacter amnigenus
Enterobacter asburiae
Enterobacter cancerogenus
Enterobacter cloacae
Enterobacter cowanii
Enterobacter gergoviae
Enterobacter hormaechei
Enterobacter kobei
Enterobacter ludwigii
Enterobacter pyrinus
Enterobacter radicincitans
**Enterococcus** aquimarinus
Enterococcus asini
Enterococcus avium
Enterococcus caccae
Enterococcus canintestini
Enterococcus canis
Enterococcus casseliflavus
Enterococcus cecorum
Enterococcus columbae
Enterococcus devriesei
Enterococcus dispar
Enterococcus durans
Enterococcus faecalis
Enterococcus faecium
Enterococcus gallinarum
Enterococcus gilvus
Enterococcus haemoperoxidus
Enterococcus hermanniensis
Enterococcus hirae
Enterococcus italicus
Enterococcus malodoratus
Enterococcus moraviensis
Enterococcus mundtii
Enterococcus pallens
Enterococcus phoeniculicola
Enterococcus pseudoavium
Enterococcus raffinosus
Enterococcus ratti
Enterococcus saccharolyticus
Enterococcus silesiacus
Enterococcus sulfureus
Enterococcus termitis
Enterococcus thailandicus
Enterococcus villorum
**Epidermophyton** floccosum
**Erwinia** amylovora
Erwinia billinigiae

Erwinia mallotivora
Erwinia papayae
Erwinia persicina
Erwinia psidii
Erwinia pyrifoliae
Erwinia rhapontici
Erwinia sp
Erwinia tasmaniensis
Erwinia tracheiphila
**Erysipelothrix** inopinata
Erysipelothrix rhusiopathiae
Erysipelothrix tonsillarum
**Escherichia** albertii
Escherichia coli
Escherichia fergusonii
Escherichia hermannii
Escherichia vulneris
**Eubacterium** brachy
Eubacterium callanderi
Eubacterium limosum
Eubacterium sp[2]
Eubacterium yurii
**Ewingella** americana
**Exiguobacterium** aurantiacum
Exiguobacterium sp[4]
**Exophiala** dermatitidis
**Facklamia** hominis
Facklamia languida
**Filifactor** villosus
**Filobasidium** capsuligenum
**Finegoldia** magna
**Flavobacterium** flevense
Flavobacterium gelidilacus
Flavobacterium hibernum
Flavobacterium hydatis
Flavobacterium johnsoniae
Flavobacterium lindanitolerans
Flavobacterium pectinovorum
Flavobacterium saccharophilum
**Flavonifractor** plautii
**Francisella** philomiragia
**Fusarium** poae
Fusarium proliferatum
**Fusobacterium** canifelinum
Fusobacterium equinum
Fusobacterium gonidiaformans
Fusobacterium mortiferum
Fusobacterium naviforme
Fusobacterium necrophorum
Fusobacterium nucleatum
Fusobacterium periodonticum
Fusobacterium sp
Fusobacterium ulcerans
Fusobacterium varium
**Gallibacterium** anatis
**Gardnerella** sp
Gardnerella vaginalis
**Gemella** bergeri
Gemella haemolysans
Gemella morbillorum
Gemella sanguinis
**Geobacillus** kaustophilus
Geobacillus stearothermophilus
Geobacillus thermodenitrificans
Geobacillus thermoglucosidasius
**Geotrichum** silvicola
Geotrichum sp
Geotrichum_candidum[ana] (Galactomyces_geotrichum[teleo])
Geotrichum_ingens[ana] (Dipodascus_ingens[teleo])
**Globicatella** sulfidifaciens
**Gluconacetobacter** intermedius
Gluconacetobacter liquefaciens

**Gluconobacter** cerinus
Gluconobacter oxydans
**Gordonia** aichiensis
Gordonia alkanivorans
Gordonia australis
Gordonia bronchialis
Gordonia rubripertincta
Gordonia sputi
Gordonia terrae
**Gracilibacillus** dipsosauri
**Granulicatella** adiacens
Granulicatella balaenopterae
Granulicatella elegans
**Grimontia** hollisae
**Guehomyces** pullulans
**Haemophilus** ducreyi
Haemophilus haemoglobinophilus
Haemophilus haemolyticus
Haemophilus influenzae
Haemophilus parahaemolyticus
Haemophilus parainfluenzae
Haemophilus paraphrohaemolyticus
Haemophilus parasuis
Haemophilus pittmaniae
**Hafnia** alvei
**Haloarcula** vallismortis
**Halobacterium** salinarum
Halobacterium sp
**Halococcus** morrhuae
**Halomonas** aquamarina
Halomonas cupida
Halomonas elongata
Halomonas halmophila
Halomonas halodenitrificans
Halomonas pacifica
Halomonas venusta
**Halotalea** alkalilenta
**Hannaella** luteola
**Hanseniaspora** lachancei
Hanseniaspora opuntiae
**Helcococcus** kunzii
Helcococcus ovis
Helcococcus sueciensis
**Helicobacter** canadensis
Helicobacter canis
Helicobacter cholecystus
Helicobacter cinaedi
Helicobacter fennelliae
Helicobacter mustelae
Helicobacter pullorum
Helicobacter pylori
**Herbaspirillum** aquaticum
Herbaspirillum autotrophicum
Herbaspirillum chlorophenolicum
Herbaspirillum frisingense
Herbaspirillum hiltneri
Herbaspirillum huttiense
Herbaspirillum lusitanum
Herbaspirillum rhizosphaerae
Herbaspirillum rubrisubalbicans
Herbaspirillum seropedicae
Herbaspirillum sp
**Herminiimonas** arsenicoxydans
Herminiimonas fonticola
**Histophilus** somni
**Hydrogenibacillus** schlegelii
**Hydrogenophaga** flava
Hydrogenophaga pseudoflava
**Hyphomicrobium** sp
**Ideonella** dechloratans
**Inquilinus** limosus
**Iodobacter** fluviatilis

**Issatchenkia** terricola
**Janthinobacterium** lividum
**Jeotgalicoccus** halotolerans
**Jonesia** denitrificans
**Kandleria** vitulina
**Kazachstania** bovina
Kazachstania telluris
**Kerstersia** gyiorum
**Kingella** denitrificans
Kingella kingae
Kingella oralis
Kingella potus
**Kitasatospora** phosalacinea
**Klebsiella** oxytoca
Klebsiella pneumoniae
Klebsiella variicola
**Kloeckera**_apiculata[ana] (Hanseniaspora_uvarum[teleo])
**Kluyvera** ascorbata
Kluyvera cryocrescens
Kluyvera georgiana
Kluyvera intermedia
**Kocuria** aegyptia
Kocuria carniphila
Kocuria himachalensis
Kocuria kristinae
Kocuria marina
Kocuria palustris
Kocuria polaris
Kocuria rhizophila
Kocuria rosea
Kocuria sp
Kocuria varians
**Kytococcus** schroeteri
Kytococcus sedentarius
**Lachancea** fermentati
**Lachnoanaerobaculum** orale
Lachnoanaerobaculum saburreum
Lachnoanaerobaculum umeaense
**Lactobacillus** acidifarinae
Lactobacillus acidipiscis
Lactobacillus acidophilus
Lactobacillus agilis
Lactobacillus algidus
Lactobacillus alimentarius
Lactobacillus amylolyticus
Lactobacillus amylophilus
Lactobacillus amylotrophicus
Lactobacillus amylovorus
Lactobacillus antri
Lactobacillus apodemi
Lactobacillus aviarius
Lactobacillus bifermentans
Lactobacillus brevis
Lactobacillus buchneri
Lactobacillus casei
Lactobacillus coleohominis
Lactobacillus collinoides
Lactobacillus concavus
Lactobacillus coryniformis
Lactobacillus crispatus
Lactobacillus curvatus
Lactobacillus delbrueckii
Lactobacillus diolivorans
Lactobacillus equi
Lactobacillus farciminis
Lactobacillus fermentum
Lactobacillus fructivorans
Lactobacillus frumenti
Lactobacillus fuchuensis
Lactobacillus gallinarum
Lactobacillus gasseri
Lactobacillus gastricus

Lactobacillus graminis
Lactobacillus hammesii
Lactobacillus hamsteri
Lactobacillus harbinensis
Lactobacillus helveticus
Lactobacillus hilgardii
Lactobacillus homohiochii
Lactobacillus iners
Lactobacillus ingluviei
Lactobacillus intestinalis
Lactobacillus jensenii
Lactobacillus johnsonii
Lactobacillus kalixensis
Lactobacillus kefiranofaciens
Lactobacillus kefiri
Lactobacillus kimchii
Lactobacillus kitasatonis
Lactobacillus kunkeei
Lactobacillus lindneri
Lactobacillus malefermentans
Lactobacillus mali
Lactobacillus manihotivorans
Lactobacillus mindensis
Lactobacillus mucosae
Lactobacillus murinus
Lactobacillus nagelii
Lactobacillus nantensis
Lactobacillus oligofermentans
Lactobacillus oris
Lactobacillus panis
Lactobacillus pantheris
Lactobacillus parabuchneri
Lactobacillus paracasei
Lactobacillus paracollinoides
Lactobacillus parakefiri
Lactobacillus paralimentarius
Lactobacillus paraplantarum
Lactobacillus pentosus
Lactobacillus perolens
Lactobacillus plantarum
Lactobacillus pontis
Lactobacillus psittaci
Lactobacillus rennini
Lactobacillus reuteri
Lactobacillus rhamnosus
Lactobacillus rossiae
Lactobacillus ruminis
Lactobacillus saerimneri
Lactobacillus sakei
Lactobacillus salivarius
Lactobacillus sanfranciscensis
Lactobacillus satsumensis
Lactobacillus sharpeae
Lactobacillus sp
Lactobacillus spicheri
Lactobacillus suebicus
Lactobacillus ultunensis
Lactobacillus vaccinostercus
Lactobacillus vaginalis
Lactobacillus versmoldensis
Lactobacillus vini
Lactobacillus zeae
Lactobacillus zymae
**Lactococcus** garvieae
Lactococcus lactis
Lactococcus piscium
Lactococcus plantarum
Lactococcus raffinolactis
**Laribacter** hongkongensis
**Lechevalieria** flava
**Leclercia** adecarboxylata
**Lecythophora** hoffmannii

**Legionella** anisa
Legionella beliardensis
Legionella birminghamensis
Legionella bozemanii
Legionella brunensis
Legionella cherrii
Legionella cincinnatiensis
Legionella dresdenensis
Legionella dumoffii
Legionella erythra
Legionella feeleii
Legionella geestiana
Legionella gormanii
Legionella gratiana
Legionella hackeliae
Legionella impletisoli
Legionella israelensis
Legionella jamestowniensis
Legionella jordanis
Legionella lansingensis
Legionella longbeachae
Legionella maceachernii
Legionella micdadei
Legionella moravica
Legionella oakridgensis
Legionella parisiensis
Legionella pneumophila
Legionella rubrilucens
Legionella sainthelensi
Legionella santicrucis
Legionella sp
Legionella tucsonensis
Legionella wadsworthii
Legionella waltersii
Legionella worsleiensis
Legionella yabuuchiae
**Leifsonia** aquatica
**Leminorella** grimontii
Leminorella richardii
**Leptothrix** mobilis
**Leptotrichia** sp
Leptotrichia trevisanii
Leptotrichia wadei
**Leucobacter** chironomi
Leucobacter denitrificans
**Leuconostoc** carnosum
Leuconostoc citreum
Leuconostoc gelidum
Leuconostoc holzapfelii
Leuconostoc inhae
Leuconostoc lactis
Leuconostoc mesenteroides
Leuconostoc palmae
Leuconostoc pseudomesenteroides
**Listeria** grayi
Listeria innocua
Listeria ivanovii
Listeria monocytogenes
Listeria seeligeri
Listeria welshimeri
**Lodderomyces** elongisporus
**Luteibacter** rhizovicinus
**Lysinibacillus** boronitolerans
Lysinibacillus fusiformis
Lysinibacillus sphaericus
**Macrococcus** caseolyticus
**Magnusiomyces** capitatus
**Malassezia** furfur
Malassezia pachydermatis
**Malikia** spinosa
**Mannheimia** glucosida
Mannheimia granulomatis

Mannheimia haemolytica
Mannheimia varigena
**Marinibacillus** marinus
**Marinilactibacillus** psychrotolerans
**Massilia** sp
Massilia timonae
**Megamona**s sp[2]
**Megasphaera** micronuciformis
**Mesorhizobium** loti
**Methanomonas** methylovora
**Methyloarcula** marina
Methyloarcula terricola
**Methylobacillus** glycogenes
Methylobacillus sp
**Methylobacterium** extorquens
Methylobacterium fujisawaense
Methylobacterium mesophilicum
Methylobacterium organophilum
Methylobacterium radiotolerans
Methylobacterium rhodesianum
Methylobacterium rhodinum
Methylobacterium sp
Methylobacterium zatmanii
**Microbacterium** aerolatum
Microbacterium arborescens
Microbacterium aurum
Microbacterium barkeri
Microbacterium dextranolyticum
Microbacterium flavescens
Microbacterium flavum
Microbacterium foliorum
Microbacterium halotolerans
Microbacterium hominis
Microbacterium hydrocarbonoxydans
Microbacterium imperiale
Microbacterium keratanolyticum
Microbacterium ketosireducens
Microbacterium koreense
Microbacterium lacticum
Microbacterium laevaniformans
Microbacterium liquefaciens
Microbacterium luteolum
Microbacterium maritypicum
Microbacterium mitrae
Microbacterium natoriense
Microbacterium oleivorans
Microbacterium oxydans
Microbacterium paludicola
Microbacterium phyllosphaerae
Microbacterium resistens
Microbacterium saperdae
Microbacterium schleiferi
Microbacterium sp
Microbacterium terrae
Microbacterium terregens
Microbacterium testaceum
Microbacterium thalassium
Microbacterium trichothecenolyticum
Microbacterium ulmi
**Micrococcus** flavus
Micrococcus luteus
Micrococcus lylae
Micrococcus terreus
**Micromonospora** aurantiaca
Micromonospora carbonacea
Micromonospora chalcea
Micromonospora chersina
Micromonospora citrea
Micromonospora coerulea
Micromonospora echinaurantiaca
Micromonospora echinofusca
Micromonospora echinospora

Micromonospora inyonensis
Micromonospora peucetica
Micromonospora purpureochromogenes
Micromonospora sagamiensis
Micromonospora sp
Micromonospora viridifaciens
**Microsporum** canis
Microsporum_gypseum[ana] (Arthroderma_gypseum[teleo])
**Mobiluncus** curtisii
Mobiluncus sp
**Moellerella** wisconsensis
**Moesziomyces** bullatus
**Moorella** thermoacetica
**Moraxella** sp
Moraxella_sg_Branhamella catarrhalis
Moraxella_sg_Branhamella ovis
Moraxella_sg_Moraxella atlantae
Moraxella_sg_Moraxella boevrei
Moraxella_sg_Moraxella bovis
Moraxella_sg_Moraxella bovoculi
Moraxella_sg_Moraxella canis
Moraxella_sg_Moraxella caprae
Moraxella_sg_Moraxella equi
Moraxella_sg_Moraxella lacunata
Moraxella_sg_Moraxella lincolnii
Moraxella_sg_Moraxella nonliquefaciens
Moraxella_sg_Moraxella oblonga
Moraxella_sg_Moraxella osloensis
Moraxella_sg_Moraxella pluranimalium
**Morganella** morganii
**Mucor** circinelloides
**Mycobacterium** abscessus
Mycobacterium agri
Mycobacterium asiaticum
Mycobacterium avium
Mycobacterium boenickei
Mycobacterium bovis
Mycobacterium celatum
Mycobacterium chelonae
Mycobacterium chlorophenolicum
Mycobacterium conceptionense
Mycobacterium farcinogenes
Mycobacterium fortuitum
Mycobacterium gordonae
Mycobacterium heckeshornense
Mycobacterium hiberniae
Mycobacterium hodleri
Mycobacterium kansasii
Mycobacterium kumamotonense
Mycobacterium lacus
Mycobacterium mageritense
Mycobacterium malmoense
Mycobacterium marinum
Mycobacterium montefiorense
Mycobacterium mucogenicum
Mycobacterium neoaurum
Mycobacterium palustre
Mycobacterium peregrinum
Mycobacterium phlei
Mycobacterium pseudoshottsii
Mycobacterium pulveris
Mycobacterium rhodesiae
Mycobacterium seoulense
Mycobacterium shottsii
Mycobacterium simiae
Mycobacterium smegmatis
Mycobacterium szulgai
Mycobacterium thermoresistibile
Mycobacterium tokaiense
Mycobacterium tuberculosis
Mycobacterium ulcerans
Mycobacterium xenopi

**Mycoplasma** alkalescens
Mycoplasma arginini
Mycoplasma bovirhinis
Mycoplasma bovis
Mycoplasma canis
Mycoplasma gallinaceum
Mycoplasma gallisepticum
Mycoplasma hyorhinis
Mycoplasma ovipneumoniae
Mycoplasma pullorum
**Myroides** odoratimimus
Myroides odoratus
**Neisseria** bacilliformis
Neisseria canis
Neisseria cinerea
Neisseria elongata
Neisseria flavescens
Neisseria gonorrhoeae
Neisseria lactamica
Neisseria macacae
Neisseria meningitidis
Neisseria mucosa
Neisseria perflava
Neisseria polysaccharea
Neisseria sicca
Neisseria sp[2]
Neisseria subflava
Neisseria weaveri
Neisseria zoodegmatis
**Nesterenkonia** lacusekhoensis
**Nocardia** abscessus
Nocardia africana
Nocardia anaemiae
Nocardia aobensis
Nocardia araoensis
Nocardia arthritidis
Nocardia asiatica
Nocardia asteroides
Nocardia brasiliensis
Nocardia carnea
Nocardia concava
Nocardia cyriacigeorgica
Nocardia elegans
Nocardia exalbida
Nocardia farcinica
Nocardia higoensis
Nocardia ignorata
Nocardia kruczakiae
Nocardia niigatensis
Nocardia nova
Nocardia otitidiscaviarum
Nocardia paucivorans
Nocardia pneumoniae
Nocardia salmonicida
Nocardia seriolae
Nocardia sienata
Nocardia sp
Nocardia testacea
Nocardia thailandica
Nocardia transvalensis
Nocardia vermiculata
Nocardia veterana
Nocardia yamanashiensis
**Nocardioides** jensenii
Nocardioides simplex
**Nocardiopsis** alba
**Novosphingobium** aromaticivorum
Novosphingobium hassiacum
Novosphingobium lentum
Novosphingobium naphthalenivorans
Novosphingobium nitrogenifigens
Novosphingobium pentaromativorans

Novosphingobium resinovorum
Novosphingobium rosa
Novosphingobium stygium
Novosphingobium subterraneum
Novosphingobium taihuense
Novosphingobium tardaugens
**Ochrobactrum** anthropi
Ochrobactrum gallinifaecis
Ochrobactrum grignonense
Ochrobactrum intermedium
Ochrobactrum sp[3]
Ochrobactrum tritici
**Odoribacter** splanchnicus
**Oerskovia** turbata
**Ogataea** polymorpha
**Oligella** ureolytica
Oligella urethralis
**Olsenella** profusa
Olsenella uli
**Ornithobacterium** rhinotracheale
**Paecilomyces** lilanicus
Paecilomyces variotii
**Paenibacillus** agarexedens
Paenibacillus agaridevorans
Paenibacillus alginolyticus
Paenibacillus alvei
Paenibacillus amylolyticus
Paenibacillus anaericanus
Paenibacillus apiarius
Paenibacillus assamensis
Paenibacillus azoreducens
Paenibacillus barcinonensis
Paenibacillus barengoltzii
Paenibacillus borealis
Paenibacillus brasilensis
Paenibacillus chibensis
Paenibacillus chinjuensis
Paenibacillus chitinolyticus
Paenibacillus chondroitinus
Paenibacillus cineris
Paenibacillus cookii
Paenibacillus curdlanolyticus
Paenibacillus daejeonensis
Paenibacillus dendritiformis
Paenibacillus durus
Paenibacillus edaphicus
Paenibacillus ehimensis
Paenibacillus favisporus
Paenibacillus gansuensis
Paenibacillus glucanolyticus
Paenibacillus glycanilyticus
Paenibacillus graminis
Paenibacillus illinoisensis
Paenibacillus jamilae
Paenibacillus kobensis
Paenibacillus lactis
Paenibacillus larvae
Paenibacillus lautus
Paenibacillus macerans
Paenibacillus macquariensis
Paenibacillus massiliensis
Paenibacillus mendelii
Paenibacillus motobuensis
Paenibacillus naphthalenovorans
Paenibacillus nematophilus
Paenibacillus odorifer
Paenibacillus pabuli
Paenibacillus pasadenensis
Paenibacillus peoriae
Paenibacillus phyllosphaerae
Paenibacillus polymyxa
Paenibacillus rhizosphaerae

Paenibacillus sabinae
Paenibacillus sp
Paenibacillus stellifer
Paenibacillus taiwanensis
Paenibacillus terrae
Paenibacillus thiaminolyticus
Paenibacillus timonensis
Paenibacillus turicensis
Paenibacillus urinalis
Paenibacillus validus
Paenibacillus wynnii
Paenibacillus xinjiangensis
Paenibacillus xylanilyticus
Paenibacillus zanthoxyli
**Pandoraea** apista
Pandoraea norimbergensis
Pandoraea pnomenusa
Pandoraea pulmonicola
Pandoraea sp[2]
Pandoraea sputorum
**Pannonibacter** phragmitetus
**Pantoea** agglomerans
Pantoea ananatis
Pantoea calida
Pantoea dispersa
Pantoea gaviniae
Pantoea septica
Pantoea sp
Pantoea stewartii
**Parabacteroides** distasonis
Parabacteroides goldsteinii
Parabacteroides johnsonii
**Paracoccus** denitrificans
Paracoccus versutus
Paracoccus yeei
**Parascardovia** denticolens
**Parvimonas** micra
**Pasteurella** aerogenes
Pasteurella bettyae
Pasteurella canis
Pasteurella dagmatis
Pasteurella mairii
Pasteurella multocida
Pasteurella pneumotropica
Pasteurella stomatis
**Pectobacterium** atrosepticum
Pectobacterium betavasculorum
Pectobacterium cacticida
Pectobacterium carotovorum
Pectobacterium cypripedii
Pectobacterium wasabiae
**Pediococcus** acidilactici
Pediococcus pentosaceus
**Pelomonas** saccharophila
Pelomonas sp[3]
**Penicillium** camemberti
Penicilium chrysogenum
Penicillium sp
**Peptococcus** niger
**Peptoniphilus** asaccharolyticus
Peptoniphilus gorbachii
Peptoniphilus harei
Peptoniphilus indolicus
Peptoniphilus ivorii
Peptoniphilus sp
**Peptostreptococcus** anaerobius
Peptostreptococcus sp
**Phenylobacterium** koreense
**Phoma** exigua
Phoma glomerata
Phoma herbarum
**Photobacterium** damselae

Photobacterium iliopiscarium
**Photorhabdus** asymbiotica
Photorhabdus luminescens
Photorhabdus temperata
**Pichia** cactophila
Pichia farinosa
Pichia holstii
Pichia kluyveri
Pichia manshurica
Pichia methylivora
Pichia pseudocactophila
**Pigmentiphaga** daeguensis
**Plesiomonas** shigelloides
**Porphyromonas** asaccharolytica
Porphyromonas gingivalis
Porphyromonas gulae
Porphyromonas levii
Porphyromonas macacae
Porphyromonas sp
**Pragia** fontium
**Prevotella** amnii
Prevotella baroniae
Prevotella bergensis
Prevotella bivia
Prevotella buccae
Prevotella buccalis
Prevotella corporis
Prevotella denticola
Prevotella disiens
Prevotella histicola
Prevotella intermedia
Prevotella maculosa
Prevotella melaninogenica
Prevotella multisaccharivorax
Prevotella nanceiensis
Prevotella nigrescens
Prevotella oralis
Prevotella oris
Prevotella oulorum
Prevotella pallens
Prevotella salivae
Prevotella shahii
Prevotella sp
Prevotella stercorea
**Propionibacterium** acidifaciens
Propionibacterium acidipropionici
Propionibacterium acnes
Propionibacterium australiense
Propionibacterium avidum
Propionibacterium cyclohexanicum
Propionibacterium freudenreichii
Propionibacterium granulosum
Propionibacterium jensenii
Propionibacterium microaerophilum
Propionibacterium propionicum
Propionibacterium sp
Propionibacterium thoenii
**Propioniferax** innocua
**Propionimicrobium** lymphophilum
**Proteus** hauseri
Proteus mirabilis
Proteus myxofaciens
Proteus penneri
Proteus vulgaris
**Prototheca** wickerhamii
**Providencia** alcalifaciens
Providencia heimbachae
Providencia rettgeri
Providencia rustigianii
Providencia stuartii
Providencia vermicola
**Pseudacidovorax** intermedius

**Pseudochrobactrum** asaccharolyticum
**Pseudoclavibacter** helvolus
Pseudoclavibacter sp
**Pseudomonas** abietaniphila
Pseudomonas aeruginosa
Pseudomonas agarici
Pseudomonas alcaligenes
Pseudomonas alcaliphila
Pseudomonas anguilliseptica
Pseudomonas antarctica
Pseudomonas asplenii
Pseudomonas avellanae
Pseudomonas azotifigens
Pseudomonas azotoformans
Pseudomonas balearica
Pseudomonas boreopolis
Pseudomonas brassicacearum
Pseudomonas brenneri
Pseudomonas caricapapayae
Pseudomonas cedrina
Pseudomonas chlororaphis
Pseudomonas cichorii
Pseudomonas citronellolis
Pseudomonas congelans
Pseudomonas corrugata
Pseudomonas extremorientalis
Pseudomonas flavescens
Pseudomonas fluorescens
Pseudomonas fragi
Pseudomonas frederiksbergensis
Pseudomonas fulva
Pseudomonas fuscovaginae
Pseudomonas gessardii
Pseudomonas graminis
Pseudomonas grimontii
Pseudomonas indica
Pseudomonas jessenii
Pseudomonas jinjuensis
Pseudomonas kilonensis
Pseudomonas koreensis
Pseudomonas libanensis
Pseudomonas lundensis
Pseudomonas lutea
Pseudomonas luteola
Pseudomonas mandelii
Pseudomonas marginalis
Pseudomonas mendocina
Pseudomonas migulae
Pseudomonas monteilii
Pseudomonas mosselii
Pseudomonas mucidolens
Pseudomonas nitroreducens
Pseudomonas oleovorans
Pseudomonas orientalis
Pseudomonas oryzihabitans
Pseudomonas otitidis
Pseudomonas panipatensis
Pseudomonas pertucinogena
Pseudomonas pictorum
Pseudomonas plecoglossicida
Pseudomonas poae
Pseudomonas pohangensis
Pseudomonas proteolytica
Pseudomonas pseudoalcaligenes
Pseudomonas putida
Pseudomonas resinovorans
Pseudomonas rhizosphaerae
Pseudomonas rhodesiae
Pseudomonas savastanoi
Pseudomonas segetis
Pseudomonas sp
Pseudomonas straminea

Pseudomonas stutzeri
Pseudomonas synxantha
Pseudomonas syringae
Pseudomonas taetrolens
Pseudomonas thermotolerans
Pseudomonas thivervalensis
Pseudomonas tolaasii
Pseudomonas trivialis
Pseudomonas umsongensis
Pseudomonas vancouverensis
Pseudomonas veronii
Pseudomonas viridiflava
Pseudomonas xanthomarina
**Pseudonocardia** hydrocarbonoxydans
**Pseudoxanthomonas** kaohsiungensis
Pseudoxanthomonas spadix
**Pseudozyma** aphidis
**Psychrobacillus** insolitus
Psychrobacillus psychrodurans
Psychrobacillus psychrotolerans
**Psychrobacter** lutiphocae
Psychrobacter sp
**Pullulanibacillus** naganoensis
**Rahnella** aquatilis
**Ralstonia** insidiosa
Ralstonia mannitolilytica
Ralstonia picketii
Ralstonia sp
Ralstonia syzygii
**Raoultella** ornithinolytica
Raoultella planticola
Raoultella terrigena
**Rathayibacter** rathayi
**Rheinheimera** soli
**Rhizobium** radiobacter
Rhizobium rubi
Rhizobium tropici
**Rhizopus** microsporus
**Rhodobacter** aestuarii
Rhodobacter veldkampii
**Rhodococcus** aetherivorans
Rhodococcus baikonurensis
Rhodococcus coprophilus
Rhodococcus corynebacterioides
Rhodococcus equi
Rhodococcus erythropolis
Rhodococcus fascians
Rhodococcus globerulus
Rhodococcus gordoniae
Rhodococcus imtechensis
Rhodococcus jostii
Rhodococcus koreensis
Rhodococcus kroppenstedtii
Rhodococcus kunmingensis
Rhodococcus maanshanensis
Rhodococcus marinonascens
Rhodococcus opacus
Rhodococcus percolatus
Rhodococcus phenolicus
Rhodococcus pyridinivorans
Rhodococcus rhodnii
Rhodococcus rhodochrous
Rhodococcus ruber
Rhodococcus triatomae
Rhodococcus wratislaviensis
Rhodococcus yunnanensis
Rhodococcus zopfii
**Rhodospiridium** sp
**Rhodotorula** acheniorum
Rhodotorula bacarum
Rhodotorula bogoriensis
Rhodotorula glutinis

Rhodotorula minuta
Rhodotorula mucilaginosa
Rhodotorula pustula
**Riemerella** anatipestifer
Riemerella columbina
**Roseomonas** mucosa
**Rothia** aeria
Rothia amarae
Rothia dentocariosa
Rothia mucilaginosa
Rothia nasimurium
**Rubrivivax** gelatinosus
**Ruminococcus** gnavus
**Rummeliibacillus** pycnus
**Saccharomyces** cerevisiae
**Saccharopolyspora** erythraea
Saccharopolyspora hirsuta
Saccharothrix mutabilis
**Salimicrobium** halophilum
**Salinivibrio** costicola
**Salmonella** sp (bongori)
Salmonella sp (choleraesuis)
Salmonella sp (enterica st Enterica)
Salmonella sp (enteritidis)
Salmonella sp (typhimurium)
**Samsonia** erythrinae
**Saprochaete** clavata
Saprochaete suaveolens
**Sarocladium** strictum
**Scedosporium** aurantiacum
**Schizophyllum** commune
**Schizosaccharomyces** pombe
**Scopulariopsis**_brevicaulis[ana] (Microascus_brevicaulis[teleo])
**Selenomonas** infelix
Selenomonas sputigena
**Serratia** entomophila
Serratia ficaria
Serratia fonticola
Serratia grimesii
Serratia liquefaciens
Serratia marcescens
Serratia odorifera
Serratia plymuthica
Serratia proteamaculans
Serratia quinivorans
Serratia rubidaea
Serratia ureilytica
**Shewanella** algae
Shewanella baltica
Shewanella fidelis
Shewanella frigidimarina
Shewanella profunda
Shewanella putrefaciens
**Shimwellia** blattae
**Sinomonas** atrocyanea
**Slackia** exigua
Slackia heliotrinireducens
**Sodalis** glossinidius
**Solibacillus** silvestris
**Solobacterium** moorei
**Sphingobacterium** faecium
Sphingobacterium mizutaii
Sphingobacterium multivorum
Sphingobacterium spiritivorum
Sphingobacterium thalpophilum
**Sphingobium** amiense
Sphingobium aromaticiconvertens
Sphingobium chlorophenolicum
Sphingobium cloacae
Sphingobium fuliginis
Sphingobium herbicidovorans
Sphingobium indicum

Sphingobium japonicum
Sphingobium olei
Sphingobium xenophagum
**Sphingomonas** abaci
Sphingomonas adhaesiva
Sphingomonas aerolata
Sphingomonas aquatilis
Sphingomonas asaccharolytica
Sphingomonas aurantiaca
Sphingomonas azotifigens
Sphingomonas desiccabilis
Sphingomonas faeni
Sphingomonas haloaromaticamans
Sphingomonas koreensis
Sphingomonas mali
Sphingomonas melonis
Sphingomonas molluscorum
Sphingomonas mucosissima
Sphingomonas panni
Sphingomonas parapaucimobilis
Sphingomonas paucimobilis
Sphingomonas phyllosphaerae
Sphingomonas pituitosa
Sphingomonas pruni
Sphingomonas pseudosanguinis
Sphingomonas sanguinis
Sphingomonas soli
Sphingomonas sp
Sphingomonas trueperi
Sphingomonas wittichii
Sphingomonas yabuuchiae
Sphingomonas yunnanensis
**Sphingopyxis** baekryungensis
Sphingopyxis chilensis
Sphingopyxis macrogoltabida
Sphingopyxis terrae
Sphingopyxis witflariensis
**Sporobolomyces** roseus
Sporobolomyces_salmonicolor[ana] (Sporidiobolus_salmonicolor[teleo])
**Sporolactobacillus** laevolacticus
**Sporopachydermia** cereana
**Sporosarcina** globispora
Sporosarcina psychrophila
**Sporothrix** schenckii
**Staphylococcus** arlettae
Staphylococcus aureus
Staphylococcus auricularis
Staphylococcus capitis
Staphylococcus caprae
Staphylococcus carnosus
Staphylococcus chromogenes
Staphylococcus cohnii
Staphylococcus condimenti
Staphylococcus delphini
Staphylococcus epidermidis
Staphylococcus equorum
Staphylococcus felis
Staphylococcus fleurettii
Staphylococcus haemolyticus
Staphylococcus hominis
Staphylococcus hyicus
Staphylococcus intermedius
Staphylococcus kloosii
Staphylococcus lentus
Staphylococcus lugdunensis
Staphylococcus lutrae
Staphylococcus muscae
Staphylococcus nepalensis
Staphylococcus pasteuri
Staphylococcus pettenkoferi
Staphylococcus piscifermentans
Staphylococcus pseudintermedius

Staphylococcus saccharolyticus
Staphylococcus saprophyticus
Staphylococcus schleiferi
Staphylococcus sciuri ssp sciuri
Staphylococcus simiae
Staphylococcus simulans
Staphylococcus sp[1]
Staphylococcus succinus
Staphylococcus vitulinus
Staphylococcus warneri
Staphylococcus xylosus
**Starkaya** novella
**Stenotrophomonas** acidaminiphila
Stenotrophomonas maltophilia
Stenotrophomonas nitritireducens
Stenotrophomonas rhizophila
Stenotrophomonas sp
Stenotrophomonas_maltophilia (Pseudomonas_beteli_#)
Stenotrophomonas_maltophilia (Pseudomonas_geniculata_#)
Stenotrophomonas_maltophilia (Pseudomonas_hibiscicola_#)
**Streptobacillus** moniliformis
**Streptococcus** acidominimus
Streptococcus agalactiae
Streptococcus alactolyticus
Streptococcus anginosus
Streptococcus australis
Streptococcus caballi
Streptococcus canis
Streptococcus castoreus
Streptococcus constellatus
Streptococcus criceti
Streptococcus cristatus
Streptococcus dentirousetti
Streptococcus devriesei
Streptococcus didelphis
Streptococcus downei
Streptococcus dysgalactiae
Streptococcus entericus
Streptococcus equi
Streptococcus equinus
Streptococcus ferus
Streptococcus gallinaceus
Streptococcus gallolyticus
Streptococcus gordonii
Streptococcus halichoeri
Streptococcus henryi
Streptococcus hyointestinalis
Streptococcus hyovaginalis
Streptococcus infantarius
Streptococcus infantis
Streptococcus intermedius
Streptococcus lutetiensis
Streptococcus macacae
Streptococcus marimammalium
Streptococcus massiliensis
Streptococcus merionis
Streptococcus minor
Streptococcus mitis
Streptococcus mutans
Streptococcus oralis
Streptococcus orisratti
Streptococcus orisuis
Streptococcus ovis
Streptococcus parasanguinis
Streptococcus parauberis
Streptococcus peroris
Streptococcus phocae
Streptococcus pleomorphus
Streptococcus pluranimalium
Streptococcus pneumoniae
Streptococcus porcinus
Streptococcus pseudopneumoniae

Streptococcus pseudoporcinus
Streptococcus pyogenes
Streptococcus ratti
Streptococcus salivarius
Streptococcus sanguinis
Streptococcus sinensis
Streptococcus sobrinus
Streptococcus sp
Streptococcus suis
Streptococcus thoraltensis
Streptococcus uberis
Streptococcus urinalis
Streptococcus vestibularis
**Streptomyces** albus
Streptomyces aureofaciens
Streptomyces avidinii
Streptomyces badius
Streptomyces chartreusis
Streptomyces galilaeus
Streptomyces griseus
Streptomyces hirsutus
Streptomyces hygroscopicus
Streptomyces lavendulae
Streptomyces phaeochromogenes
Streptomyces scabiei
Streptomyces sp
Streptomyces violaceoruber
**Streptosporangium** sibiricum
**Suttonella** indologenes
**Tatumella** citrea
Tatumella ptyseos
Tatumella punctata
Tatumella terrea
**Taylorella** asinigenitalis
Taylorella equigenitalis
**Tenacibaculum** discolor
Tenacibaculum ovolyticum
**Terrabacter** tumescens
**Terrimonas** ferruginea
Tessaracoccus flavescens
**Tetragenococcus** solitarius
**Thauera** aminoaromatica
Thauera aromatica
Thauera chlorobenzoica
Thauera linaloolentis
Thauera mechernichensis
Thauera phenylacetica
Thauera terpenica
**Thermoactinomyces** sp[2]
**Thermoanaerobacter** thermohydrosulfuricus
**Thermoanaerobacterium** thermosaccharolyticum
Thermoanaerobacterium thermosulfurigenes
**Tissierella** praeacuta
**Trabulsiella** guamensis
**Trichophyton** interdigitale
Trichophyton mentagrophytes
Trichophyton rubrum
Trichophyton tonsurans
**Trichosporon** asahii
Trichosporon coremiiforme
Trichosporon cutaneum
Trichosporon debeurmannianum
Trichosporon dohaense
Trichosporon dulcitum
Trichosporon faecale
Trichosporon gracile
Trichosporon inkin
Trichosporon japonicum
Trichosporon jirovecii
Trichosporon laibachii
Trichosporon loubieri
Trichosporon moniliiforme

Trichosporon montevideense
Trichosporon mucoides
Trichosporon mycotoxinivorans
Trichosporon ovoides
Trichosporon sp
Trichosporon terricola
**Trueperella** abortisuis
Trueperella bernardiae
Trueperella bialowiezense
Trueperella bonasi
Trueperella pyogenes
**Tsukamurella** inchonensis
Tsukamurella paurometabola
Tsukamurella sp
**Turicella** otitidis
**Udeniomyces** puniceus
**Vagococcus** fluvialis
Vagococcus lutrae
**Varibaculum** cambriense
**Variovorax** paradoxus
**Veillonella** atypica
Veillonella caviae
Veillonella criceti
Veillonella denticariosi
Veillonella dispar
Veillonella magna
Veillonella montpellierensis
Veillonella parvula
Veillonella ratti
Veillonella rogosae
Veillonella sp[3]
**Vibrio** aerogenes
Vibrio aestuarianus
Vibrio agarivorans
Vibrio albensis
Vibrio alginolyticus
Vibrio anguillarum
Vibrio brasiliensis
Vibrio campbellii
Vibrio chagasii
Vibrio cincinnatiensis
Vibrio coralliilyticus
Vibrio cyclitrophicus
Vibrio diazotrophicus
Vibrio ezurae
Vibrio fluvialis
Vibrio fortis
Vibrio furnissii
Vibrio gazogenes
Vibrio gigantis
Vibrio harveyi
Vibrio hispanicus
Vibrio ichthyoenteri
Vibrio kanaloae
Vibrio lentus
Vibrio mediterranei
Vibrio metschnikovii
Vibrio mimicus
Vibrio mytili
Vibrio natriegens
Vibrio navarrensis
Vibrio neptunius
Vibrio nereis
Vibrio nigripulchritudo
Vibrio ordalii
Vibrio orientalis
Vibrio ostreicida
Vibrio pacinii
Vibrio parahaemolyticus
Vibrio pectenicida
Vibrio pelagius
Vibrio penaeicida

Vibrio pomeroyi
Vibrio ponticus
Vibrio proteolyticus
Vibrio rotiferianus
Vibrio ruber
Vibrio rumoiensis
Vibrio scophthalmi
Vibrio shilonii
Vibrio splendidus
Vibrio superstes
Vibrio tasmaniensis
Vibrio vulnificus
Vibrio xuii
**Virgibacillus** halodenitrificans
Virgibacillus pantothenticus
Virgibacillus proomii
**Viridibacillus** arenosi
Viridibacillus arvi
Viridibacillus neidei
**Wautersiella** falsenii
**Weeksella** virosa
**Weissella** confusa
Weissella halotolerans
Weissella minor
Weissella viridescens
**Wohlfahrtiimonas** chitiniclastica
**Wolinella** succinogenes
**Xanthobacter** autotrophicus
**Xanthomonas** arboricola
Xanthomonas axonopodis
Xanthomonas bromi
Xanthomonas campestris
Xanthomonas cassavae
Xanthomonas citri
Xanthomonas codiaei
Xanthomonas cucurbitae
Xanthomonas cynarae
Xanthomonas hortorum
Xanthomonas hyacinthi
Xanthomonas melonis
Xanthomonas perforans
Xanthomonas pisi
Xanthomonas theicola
Xanthomonas translucens
Xanthomonas vasicola
**Xenorhabdus** beddingii
Xenorhabdus bovienii
Xenorhabdus budapestensis
Xenorhabdus ehlersii
Xenorhabdus innexi
Xenorhabdus japonica
Xenorhabdus nematophila
Xenorhabdus poinarii
Xenorhabdus szentirmaii
**Yersinia** aldovae
Yersinia aleksiciae
Yersinia bercovieri
Yersinia enterocolitica
Yersinia frederiksenii
Yersinia intermedia
Yersinia kristensenii
Yersinia mollaretii
Yersinia pseudotuberculosis
Yersinia rohdei
Yersinia ruckeri
**Yokenella** regensburgei
**Zygosaccharomyces** bailii
Zygosaccharomyces bisporus
Zygosaccharomyces florentinus
Zygosaccharomyces microellipsoides
Zygosaccharomyces rouxii

**~ 2290 species**

# Release Notes for MBT-BDAL-5627 MSP library

## What is new in MBT DB 5627?

The MBT database DB 4613 will be extended by **1020 newly generated reference MSP**, which cover **348 species** overall.

**21 new genera** and **113 new species** will be implemented and which will be covered by **220 new reference entries.**
**Additional 800 MSP** will improve the coverage of species already contained in the database.

## Main improvements:

- Implementation of *Haemophilus haemolyticus* strains
- Additional strains for improvement of *Streptococcus mitis/oralis/pneumonia* identification
- Many new yeast species and strains
- More *Nocardia* strains to cover the MALDI diversity

## The 21 new genera and 113 new species cover following groups:

| | New genera | New species | Aerobe species | Microaerophile species | Anaerobe species |
|---|---|---|---|---|---|
| **Gram -** | 6 | 23 | 18 | 3 | 2 |
| **Gram +** | 7 | 27 | 22 | 1 | 4 |
| **Yeast** | 8 | 63 | 63 | - | - |
| **Fil. Fungi** | 0 | 0 | - | - | - |

## Overall improvements:

| | New MSP (from 1020) | Species covered | Aerobe strains | Microaerophile strains | Anaerobe strains |
|---|---|---|---|---|---|
| **Gram -** | 328 | 113 | 265 | 54 | 9 |
| **Gram +** | 374 | 128 | 185 | 179 | 10 |
| **Yeast** | 316 | 106 | 106 | - | - |
| **Fil. Fungi** | 2 | 1 | 2 | - | - |

**Supported MALDI Biotyper versions** (installed on respective operating systems)**:**

- **MBT-3.0**
- **MBT-3.1**
- **MBT-4.0**

**Implementation of MSP entries for following 113 new species:**

| | New genus/species | | | |
|---|---|---|---|---|
| 1 | Actinomyces ruminicola | new species | gram + | anaerobic |
| 2 | Aeromicrobium flavum | new genus/species | gram + | aerobic |
| 3 | Alicyclobacillus cycloheptanicus | new species | gram + | aerobic |
| 4 | Alloiococcus otitis | new genus/species | gram + | aerobic |
| 5 | Arthroascus schoenii | new genus/species | yeast | aerobic |
| 6 | Arthrobacter flavus | new species | gram + | aerobic |
| 7 | Arthrobacter nitroguajacolicus | new species | gram + | aerobic |
| 8 | Bacillus altitudinis | new species | gram + | aerobic |
| 9 | Bacillus horneckiae | new species | gram + | aerobic |
| 10 | Bartonella japonica | new genus/species | gram - | aerobic |
| 11 | Brevibacillus invocatus | new species | gram + | aerobic |
| 12 | Candida alai | new species | yeast | aerobic |
| 13 | Candida ambrosiae | new species | yeast | aerobic |
| 14 | Candida auris | new species | yeast | aerobic |
| 15 | Candida blattae | new species | yeast | aerobic |
| 16 | Candida bohiensis | new species | yeast | aerobic |
| 17 | Candida bracarensis | new species | yeast | aerobic |
| 18 | Candida buenavistaensis | new species | yeast | aerobic |
| 19 | Candida carpophila | new species | yeast | aerobic |
| 20 | Candida castellii | new species | yeast | aerobic |
| 21 | Candida duobushaemulonii | new species | yeast | aerobic |
| 22 | Candida frijolesensis | new species | yeast | aerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 23 | Candida infanticola | new species | yeast | aerobic |
| 24 | Candida labiduridarum | new species | yeast | aerobic |
| 25 | Candida pseudohaemulonii | new species | yeast | aerobic |
| 26 | Candida saitoana | new species | yeast | aerobic |
| 27 | Candida shehatae var insectosa | new species | yeast | aerobic |
| 28 | Candida sojae | new species | yeast | aerobic |
| 29 | Candida viswanathii | new species | yeast | aerobic |
| 30 | Candida_citrea[ana] (Pichia_nakasei[teleo]#) | new species | yeast | aerobic |
| 31 | Candida_fabianii[ana] (Pichia_fabianii[teleo]) | new species | yeast | aerobic |
| 32 | Candida_holmii[ana] (Kazachstania_exigua[teleo]) | new species | yeast | aerobic |
| 33 | Candida_pintolopesii[ana] (Kazachstania_pintolopesii[teleo]) | new species | yeast | aerobic |
| 34 | Chryseobacterium ginsenosidimutans | new species | gram - | aerobic |
| 35 | Chryseobacterium hagamense | new species | gram - | aerobic |
| 36 | Cryptococcus albidosimilis | new species | yeast | aerobic |
| 37 | Cryptococcus curvatus | new species | yeast | aerobic |
| 38 | Cryptococcus diffluens | new species | yeast | aerobic |
| 39 | Cryptococcus flavescens | new species | yeast | aerobic |
| 40 | Cryptococcus gastricus | new species | yeast | aerobic |
| 41 | Cryptococcus humicola | new species | yeast | aerobic |
| 42 | Cryptococcus liquefaciens | new species | yeast | aerobic |
| 43 | Cryptococcus magnus | new species | yeast | aerobic |
| 44 | Cryptococcus saitoi | new species | yeast | aerobic |
| 45 | Cryptococcus terreus | new species | yeast | aerobic |
| 46 | Cryptococcus uzbekistanensis | new species | yeast | aerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 47 | Cryptococcus vishniacii | new species | yeast | aerobic |
| 48 | Cryptotrichosporon anacardii | new genus/species | yeast | aerobic |
| 49 | Cupriavidus campinensis | new species | gram - | aerobic |
| 50 | Cyberlindnera mississippiensis | new genus/species | yeast | aerobic |
| 51 | Deinococcus geothermalis | new genus/species | gram + | aerobic |
| 52 | Geobacillus thermodenitrificans ssp calidus | new species | gram + | aerobic |
| 53 | Geobacillus thermoglucosidasius | new species | gram + | aerobic |
| 54 | Gluconacetobacter intermedius | new genus/species | gram - | aerobic |
| 55 | Gluconacetobacter liquefaciens | new species | gram - | aerobic |
| 56 | Gluconobacter cerinus | new species | gram - | aerobic |
| 57 | Guehomyces pullulans | new genus/species | yeast | aerobic |
| 58 | Haemophilus haemoglobinophilus | new species | gram - | microaerophilic |
| 59 | Haemophilus haemolyticus | new species | gram - | microaerophilic |
| 60 | Haemophilus paraphrohaemolyticus | new species | gram - | microaerophilic |
| 61 | Halotalea alkalilenta | new genus/species | gram - | aerobic |
| 62 | Hannaella luteola | new genus/species | yeast | aerobic |
| 63 | Hanseniaspora lachancei | new species | yeast | aerobic |
| 64 | Jeotgalicoccus halotolerans | new genus/species | gram + | aerobic |
| 65 | Kazachstania bovina | new species | yeast | aerobic |
| 66 | Kytococcus schroeteri | new species | gram + | aerobic |
| 67 | Lachancea fermentati | new species | yeast | aerobic |
| 68 | Lachnoanaerobaculum orale | new genus/species | gram + | anaerobic |
| 69 | Lachnoanaerobaculum saburreum | new species | gram + | anaerobic |
| 70 | Lachnoanaerobaculum umeaense | new species | gram + | anaerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 71 | Laribacter hongkongensis | new genus/species | gram - | aerobic |
| 72 | Legionella dresdenensis | new species | gram - | aerobic |
| 73 | Legionella geestiana | new species | gram - | aerobic |
| 74 | Legionella gratiana | new species | gram - | aerobic |
| 75 | Legionella waltersii | new species | gram - | aerobic |
| 76 | Legionella worsleiensis | new species | gram - | aerobic |
| 77 | Leucobacter chironomi | new genus/species | gram + | aerobic |
| 78 | Leucobacter denitrificans | new species | gram + | aerobic |
| 79 | Lysinibacillus boronitolerans | new species | gram + | aerobic |
| 80 | Microbacterium mitrae | new species | gram + | aerobic |
| 81 | Micrococcus flavus | new species | gram + | aerobic |
| 82 | Micrococcus terreus | new species | gram + | aerobic |
| 83 | Nocardia asteroides | new species | gram + | aerobic |
| 84 | Ogataea polymorpha | new genus/species | yeast | aerobic |
| 85 | Paenibacillus barengoltzii | new species | gram + | microaerophilic |
| 86 | Pantoea septica | new species | gram - | aerobic |
| 87 | Pichia pseudocactophila | new species | yeast | aerobic |
| 88 | Porphyromonas levii | new species | gram - | anaerobic |
| 89 | Pseudoxanthomonas kaohsiungensis | new genus/species | gram - | aerobic |
| 90 | Rhodobacter aestuarii | new genus/species | gram - | aerobic |
| 91 | Rhodobacter veldkampii | new species | gram - | aerobic |
| 92 | Saprochaete clavata | new genus/species | yeast | aerobic |
| 93 | Saprochaete suaveolens | new species | yeast | aerobic |
| 94 | Sarocladium strictum | new genus/species | yeast | aerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 95 | Tessaracoccus flavescens | new genus/species | gram + | aerobic |
| 96 | Trichosporon coremiiforme | new species | yeast | aerobic |
| 97 | Trichosporon dohaense | new species | yeast | aerobic |
| 98 | Trichosporon dulcitum | new species | yeast | aerobic |
| 99 | Trichosporon faecale | new species | yeast | aerobic |
| 100 | Trichosporon gracile | new species | yeast | aerobic |
| 101 | Trichosporon japonicum | new species | yeast | aerobic |
| 102 | Trichosporon jirovecii | new species | yeast | aerobic |
| 103 | Trichosporon laibachii | new species | yeast | aerobic |
| 104 | Trichosporon loubieri | new species | yeast | aerobic |
| 105 | Trichosporon moniliiforme | new species | yeast | aerobic |
| 106 | Trichosporon montevideense | new species | yeast | aerobic |
| 107 | Trichosporon terricola | new species | yeast | aerobic |
| 108 | Veillonella magna | new species | gram - | anaerobic |
| 109 | Virgibacillus proomii | new species | gram + | aerobic |
| 110 | Zygosaccharomyces bisporus | new species | yeast | aerobic |
| 111 | Zygosaccharomyces florentinus | new species | yeast | aerobic |
| 112 | Zygosaccharomyces microellipsoides | new species | yeast | aerobic |
| 113 | Zygosaccharomyces rouxii | new species | yeast | aerobic |

## Deletion of MSP entries:

| Deletions | Justification |
|---|---|
| Arthrobacter castelli DSM 16402T DSM | Many polymers. Will be replaced by new measurement. |
| Arthrobacter chlorophenolicus DSM 12829T DSM | Many polymers. Will be replaced by new measurement. |
| Arthrobacter pigmenti DSM 16403T DSM | Many polymers. Will be replaced by new measurement. |
| Mycobacterium avium ssp avium 8671 VAR | match with M. scrofulaceum |
| Mycobacterium manitobense DSM 44615 DSM | no valid name; match with M. saskatchewanense |
| Delftia sp[2] 911600013 LBK | Mixed culture with Saccharomyces servazzii. Saccharomyces servazzii is not in the database so far.<br>The mixed culture was detected during project work with Saccharomyces servazzii. |

## Renaming of MSP entries:

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Anaerococcus vaginalis DSM 7457T DSM | | Anaerococcus hydrogenalis DSM 7454T DSM | DB4613 strains A. hydrogenalis and vaginalis are mixed up. Confirmed by new cultivation, measuring and sequencing. Re-naming of old entry necessary. |
| Anaerococcus hydrogenalis DSM 7454T DSM | | Anaerococcus vaginalis DSM 7457T DSM | DB4613 strains A. hydrogenalis and vaginalis are mixed up. Confirmed by new cultivation, measuring and sequencing. Re-naming of old entry necessary. |
| Aurantimonas altamirensis 284 RLT | | Aureimonas altamirensis 284 RLT | Nomenclature change according DSMZ/IJSEM - changes 11/2011:<br>Aurantimonas altamirensis -> Aureimonas |
| Candida haemulonii MY916_09 ERL | | Candida duobushaemulonii MY916_09 ERL | Species was divided into two separate species |
| Lactobacillus sp M23 101342 CIP | | Carnobacterium maltaromaticum CIP 101342 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp CIP 102035 CIP | | Carnobacterium maltaromaticum CIP 102035 CIP | More precise identification of strain by CIP - adaptation of name |
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) 29 PSB | | Cryptococcus neoformans 29 PSB | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) ATCC 14116 THL | | Cryptococcus neoformans ATCC 14116 THL | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) CCM 8312 CCM | | Cryptococcus neoformans CCM 8312 CCM | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) RV07_02 18 VML | | Cryptococcus neoformans RV07_02 18 VML | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |
| Dickeya dieffenbachiae DSM 18013T HAM | | Dickeya dadantii ssp dieffenbachiae DSM 18013T HAM | Nomenclature change according DSMZ/IJSEM - changes 07/2012:<br>Dickeya dieffenbachiae -> D. dadantii subsp.dieffenbachiae |
| Lactobacillus catenaformis 07_085 ANA IBS | | Eggerthia catenaformis 07_085 ANA IBS | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Lactobacillus catenaformis CIP 104817T B CIP | | Eggerthia catenaformis CIP 104817T B CIP | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Lactobacillus catenaformis IBS_MS_39 IBS | | Eggerthia catenaformis IBS_MS_39 IBS | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Lactobacillus catenaformis VA12065_1_11 ERL | | Eggerthia catenaformis VA12065_1_11 ERL | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Bacillus schlegelii CIP 106933T CIP | | Hydrogenibacillus schlegelii CIP 106933T CIP | Bacillus schlegelii 31:215 (basonym) ≡ Hydrogenibacillus schlegelii |
| Lactobacillus vitulinus DSM 20405T DSM | | Kandleria vitulina DSM 20405T DSM | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus vitulinus -> Kandleria vitulina |
| Lactobacillus sp 101810 CIP | | Lactobacillus delbrueckii ssp lactis CIP 101810 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp 102006 CIP | | Lactobacillus fermentum CIP 102006 CIP | More precise identification of strain by CIP - adaptation of name |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Lactobacillus sp 101909 CIP | | Lactobacillus gasseri CIP 101909 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp CIP 102309 CIP | | Lactobacillus paracasei ssp paracasei CIP 102309 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp CIP 102623 CIP | | Lactobacillus rhamnosus CIP 102623 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus zymae 108703 CIP | | Lactobacillus zymae CIP 108703T CIP | Type Strain T was missing - Typo |
| Tatlockia maceachernii 28 RLT | | Legionella maceachernii 28 RLT | New nomenclature not very accepted -> http://www.bacterio.net/t/tatlockia.html#maceachernii |
| Lactobacillus sp CIP 102166 CIP | | Marinilactibacillus psychrotolerans CIP 102166 CIP | more precise identification of strain by CIP - adaptation of name |
| Mycoplasma argini 7SR10 VLW | | Mycoplasma arginini 7SR10 VLW | Typo within species name will be corrected. |
| Mycoplasma argini NCTC 10129T VLW | | Mycoplasma arginini NCTC 10129T VLW | Typo within species name will be corrected. |
| Mycoplasma ovipneumoniae NCTC 10151T VLW | | Mycoplasma gallisepticum NCTC 10115T VLW | DB4613 strains Mycoplasma gallisepticum NCTC 10115T VLW and Mycoplasma ovipneumoniae NCTC 10151T VLW are mixed up. Confirmed by new, measuring and sequencing. Re-naming of old entry necessary. |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Mycoplasma gallisepticum NCTC 10115T VLW | | Mycoplasma ovipneumoniae NCTC 10151T VLW | DB4613 strains Mycoplasma gallisepticum NCTC 10115T VLW and Mycoplasma ovipneumoniae NCTC 10151T VLW are mixed up. Confirmed by new, measuring and sequencing. Re-naming of old entry necessary. |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) 991400574 LBK | | Saccharomyces cerevisiae 991400574 LBK | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) BJ2168 BRL | | Saccharomyces cerevisiae BJ2168 BRL | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) DTY3 BRL | | Saccharomyces cerevisiae DTY3 BRL | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) INVSc1 BRL | | Saccharomyces cerevisiae INVSc1 BRL | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) Isolat LGL Muenchen | | Saccharomyces cerevisiae Isolat LGL Muenchen | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) Kontrollstamm Humanmedizin VML | | Saccharomyces cerevisiae Kontrollstamm Humanmedizin VML | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) WS LLH | | Saccharomyces cerevisiae WS LLH | adaptation to more common nomenclature |
| Streptococcus thermophilus 37 RLT | | Streptococcus salivarius_ssp_thermophilus 37 RLT | adaptation to current nomenclature |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Streptococcus thermophilus 38 RLT | | Streptococcus salivarius_ssp_thermophilus 38 RLT | adaptation to current nomenclature |
| Streptococcus thermophilus 39 RLT | | Streptococcus salivarius_ssp_thermophilus 39 RLT | adaptation to current nomenclature |
| Streptococcus thermophilus DSM 20259 DSM | | Streptococcus salivarius_ssp_thermophilus DSM 20259 DSM | adaptation to current nomenclature |
| Streptococcus thermophilus DSM 20479 DSM | | Streptococcus salivarius_ssp_thermophilus DSM 20479 DSM | adaptation to current nomenclature |
| Streptococcus thermophilus DSM 8713 DSM | | Streptococcus salivarius_ssp_thermophilus DSM 8713 DSM | adaptation to current nomenclature |
| Listonella anguillarum 02 EGS | | Vibrio anguillarum 02 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum 03 EGS | | Vibrio anguillarum 03 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum DSM 11323 DSM | | Vibrio anguillarum DSM 11323 DSM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum DSM 21597T DSM | | Vibrio anguillarum DSM 21597T DSM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum LMG 4437T HAM | | Vibrio anguillarum LMG 4437T HAM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Listonella anguillarum serotype 02 EGS | | Vibrio anguillarum serotype 02 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum serotype 03 EGS | | Vibrio anguillarum serotype 03 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella pelagia DSM 21205T DSM | | Vibrio pelagius DSM 21205T DSM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |

## Matching Hints Changes:

| | | | Justification |
|---|---|---|---|
| Species alkalescens / argini of the genus Mycoplasma have very similar pattern: Therefore distinguishing their species is difficult. | changed to | Species alkalescens / arginini of the genus Mycoplasma have very similar pattern: Therefore distinguishing their species is difficult. | Correction of typo within the species name "arginini" |
| Corynebacterium amycolatum<br>Corynebacterium durum<br>Corynebacterium minutissimum | deletion of matching hint link | Species of this genus have very similar patterns: Therefore distinguishing their species is difficult. | Matching hint is not necessary for this species, because MALDI can separate this species from others |
| Acinetobacter baumannii<br>Acinetobacter calcoaceticus<br>Acinetobacter pittii | change to new matching hint | Member of the Acinetobacter baumanii/calcoaceticus complex. Extraction must be performed to permit reliable species identification. | For clarification change from general matching hint (Species of this genus have very similar patterns: Therefore distinguishing their species is difficult.) to this more precise one. |
| Arthrobacter castelli<br>Arthrobacter chlorophenolicus<br>Arthrobacter pigmenti | link with new matching hint | Species tend to produce polymers which can interfere with the identification. | For clarification the matching hint will inform about the production of possibly interfering polymers. |
| Burkholderia ambifaria, anthina, cenocepacia, cepacia, diffusa, dolosa, lata, latens, metallica, multivorans, pyrrocina, seminalis, stabilis, vietnamensis | link with new matching hint | Is a member of Burkholderia cepacia complex | Additional information. This will help the user to recognize members of the Burkholderia cepacia complex. |

# Release Notes for MBT-BDAL-5627 MSP library

## What is new in MBT DB 5627?

The MBT database DB 4613 will be extended by **1020 newly generated reference MSP**, which cover **348 species** overall.

**21 new genera** and **113 new species** will be implemented and which will be covered by **220 new reference entries.**
**Additional 800 MSP** will improve the coverage of species already contained in the database.

## Main improvements:

- Implementation of *Haemophilus haemolyticus* strains
- Additional strains for improvement of *Streptococcus mitis/oralis/pneumonia* identification
- Many new yeast species and strains
- More *Nocardia* strains to cover the MALDI diversity

## The 21 new genera and 113 new species cover following groups:

| | New genera | New species | Aerobe species | Microaerophile species | Anaerobe species |
|---|---|---|---|---|---|
| **Gram -** | 6 | 23 | 18 | 3 | 2 |
| **Gram +** | 7 | 27 | 22 | 1 | 4 |
| **Yeast** | 8 | 63 | 63 | - | - |
| **Fil. Fungi** | 0 | 0 | - | - | - |

## Overall improvements:

| | New MSP (from 1020) | Species covered | Aerobe strains | Microaerophile strains | Anaerobe strains |
|---|---|---|---|---|---|
| **Gram -** | 328 | 113 | 265 | 54 | 9 |
| **Gram +** | 374 | 128 | 185 | 179 | 10 |
| **Yeast** | 316 | 106 | 106 | - | - |
| **Fil. Fungi** | 2 | 1 | 2 | - | - |

**Supported MALDI Biotyper versions** (installed on respective operating systems)**:**

- **MBT-3.0**
- **MBT-3.1**
- **MBT-4.0**

**Implementation of MSP entries for following 113 new species:**

| | New genus/species | | | |
|---|---|---|---|---|
| 1 | Actinomyces ruminicola | new species | gram + | anaerobic |
| 2 | Aeromicrobium flavum | new genus/species | gram + | aerobic |
| 3 | Alicyclobacillus cycloheptanicus | new species | gram + | aerobic |
| 4 | Alloiococcus otitis | new genus/species | gram + | aerobic |
| 5 | Arthroascus schoenii | new genus/species | yeast | aerobic |
| 6 | Arthrobacter flavus | new species | gram + | aerobic |
| 7 | Arthrobacter nitroguajacolicus | new species | gram + | aerobic |
| 8 | Bacillus altitudinis | new species | gram + | aerobic |
| 9 | Bacillus horneckiae | new species | gram + | aerobic |
| 10 | Bartonella japonica | new genus/species | gram - | aerobic |
| 11 | Brevibacillus invocatus | new species | gram + | aerobic |
| 12 | Candida alai | new species | yeast | aerobic |
| 13 | Candida ambrosiae | new species | yeast | aerobic |
| 14 | Candida auris | new species | yeast | aerobic |
| 15 | Candida blattae | new species | yeast | aerobic |
| 16 | Candida bohiensis | new species | yeast | aerobic |
| 17 | Candida bracarensis | new species | yeast | aerobic |
| 18 | Candida buenavistaensis | new species | yeast | aerobic |
| 19 | Candida carpophila | new species | yeast | aerobic |
| 20 | Candida castellii | new species | yeast | aerobic |
| 21 | Candida duobushaemulonii | new species | yeast | aerobic |
| 22 | Candida frijolesensis | new species | yeast | aerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 23 | Candida infanticola | new species | yeast | aerobic |
| 24 | Candida labiduridarum | new species | yeast | aerobic |
| 25 | Candida pseudohaemulonii | new species | yeast | aerobic |
| 26 | Candida saitoana | new species | yeast | aerobic |
| 27 | Candida shehatae var insectosa | new species | yeast | aerobic |
| 28 | Candida sojae | new species | yeast | aerobic |
| 29 | Candida viswanathii | new species | yeast | aerobic |
| 30 | Candida_citrea[ana] (Pichia_nakasei[teleo]#) | new species | yeast | aerobic |
| 31 | Candida_fabianii[ana] (Pichia_fabianii[teleo]) | new species | yeast | aerobic |
| 32 | Candida_holmii[ana] (Kazachstania_exigua[teleo]) | new species | yeast | aerobic |
| 33 | Candida_pintolopesii[ana] (Kazachstania_pintolopesii[teleo]) | new species | yeast | aerobic |
| 34 | Chryseobacterium ginsenosidimutans | new species | gram - | aerobic |
| 35 | Chryseobacterium hagamense | new species | gram - | aerobic |
| 36 | Cryptococcus albidosimilis | new species | yeast | aerobic |
| 37 | Cryptococcus curvatus | new species | yeast | aerobic |
| 38 | Cryptococcus diffluens | new species | yeast | aerobic |
| 39 | Cryptococcus flavescens | new species | yeast | aerobic |
| 40 | Cryptococcus gastricus | new species | yeast | aerobic |
| 41 | Cryptococcus humicola | new species | yeast | aerobic |
| 42 | Cryptococcus liquefaciens | new species | yeast | aerobic |
| 43 | Cryptococcus magnus | new species | yeast | aerobic |
| 44 | Cryptococcus saitoi | new species | yeast | aerobic |
| 45 | Cryptococcus terreus | new species | yeast | aerobic |
| 46 | Cryptococcus uzbekistanensis | new species | yeast | aerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 47 | Cryptococcus vishniacii | new species | yeast | aerobic |
| 48 | Cryptotrichosporon anacardii | new genus/species | yeast | aerobic |
| 49 | Cupriavidus campinensis | new species | gram - | aerobic |
| 50 | Cyberlindnera mississippiensis | new genus/species | yeast | aerobic |
| 51 | Deinococcus geothermalis | new genus/species | gram + | aerobic |
| 52 | Geobacillus thermodenitrificans ssp calidus | new species | gram + | aerobic |
| 53 | Geobacillus thermoglucosidasius | new species | gram + | aerobic |
| 54 | Gluconacetobacter intermedius | new genus/species | gram - | aerobic |
| 55 | Gluconacetobacter liquefaciens | new species | gram - | aerobic |
| 56 | Gluconobacter cerinus | new species | gram - | aerobic |
| 57 | Guehomyces pullulans | new genus/species | yeast | aerobic |
| 58 | Haemophilus haemoglobinophilus | new species | gram - | microaerophilic |
| 59 | Haemophilus haemolyticus | new species | gram - | microaerophilic |
| 60 | Haemophilus paraphrohaemolyticus | new species | gram - | microaerophilic |
| 61 | Halotalea alkalilenta | new genus/species | gram - | aerobic |
| 62 | Hannaella luteola | new genus/species | yeast | aerobic |
| 63 | Hanseniaspora lachancei | new species | yeast | aerobic |
| 64 | Jeotgalicoccus halotolerans | new genus/species | gram + | aerobic |
| 65 | Kazachstania bovina | new species | yeast | aerobic |
| 66 | Kytococcus schroeteri | new species | gram + | aerobic |
| 67 | Lachancea fermentati | new species | yeast | aerobic |
| 68 | Lachnoanaerobaculum orale | new genus/species | gram + | anaerobic |
| 69 | Lachnoanaerobaculum saburreum | new species | gram + | anaerobic |
| 70 | Lachnoanaerobaculum umeaense | new species | gram + | anaerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 71 | Laribacter hongkongensis | new genus/species | gram - | aerobic |
| 72 | Legionella dresdenensis | new species | gram - | aerobic |
| 73 | Legionella geestiana | new species | gram - | aerobic |
| 74 | Legionella gratiana | new species | gram - | aerobic |
| 75 | Legionella waltersii | new species | gram - | aerobic |
| 76 | Legionella worsleiensis | new species | gram - | aerobic |
| 77 | Leucobacter chironomi | new genus/species | gram + | aerobic |
| 78 | Leucobacter denitrificans | new species | gram + | aerobic |
| 79 | Lysinibacillus boronitolerans | new species | gram + | aerobic |
| 80 | Microbacterium mitrae | new species | gram + | aerobic |
| 81 | Micrococcus flavus | new species | gram + | aerobic |
| 82 | Micrococcus terreus | new species | gram + | aerobic |
| 83 | Nocardia asteroides | new species | gram + | aerobic |
| 84 | Ogataea polymorpha | new genus/species | yeast | aerobic |
| 85 | Paenibacillus barengoltzii | new species | gram + | microaerophilic |
| 86 | Pantoea septica | new species | gram - | aerobic |
| 87 | Pichia pseudocactophila | new species | yeast | aerobic |
| 88 | Porphyromonas levii | new species | gram - | anaerobic |
| 89 | Pseudoxanthomonas kaohsiungensis | new genus/species | gram - | aerobic |
| 90 | Rhodobacter aestuarii | new genus/species | gram - | aerobic |
| 91 | Rhodobacter veldkampii | new species | gram - | aerobic |
| 92 | Saprochaete clavata | new genus/species | yeast | aerobic |
| 93 | Saprochaete suaveolens | new species | yeast | aerobic |
| 94 | Sarocladium strictum | new genus/species | yeast | aerobic |

| | New genus/species | | | |
|---|---|---|---|---|
| 95 | Tessaracoccus flavescens | new genus/species | gram + | aerobic |
| 96 | Trichosporon coremiiforme | new species | yeast | aerobic |
| 97 | Trichosporon dohaense | new species | yeast | aerobic |
| 98 | Trichosporon dulcitum | new species | yeast | aerobic |
| 99 | Trichosporon faecale | new species | yeast | aerobic |
| 100 | Trichosporon gracile | new species | yeast | aerobic |
| 101 | Trichosporon japonicum | new species | yeast | aerobic |
| 102 | Trichosporon jirovecii | new species | yeast | aerobic |
| 103 | Trichosporon laibachii | new species | yeast | aerobic |
| 104 | Trichosporon loubieri | new species | yeast | aerobic |
| 105 | Trichosporon moniliiforme | new species | yeast | aerobic |
| 106 | Trichosporon montevideense | new species | yeast | aerobic |
| 107 | Trichosporon terricola | new species | yeast | aerobic |
| 108 | Veillonella magna | new species | gram - | anaerobic |
| 109 | Virgibacillus proomii | new species | gram + | aerobic |
| 110 | Zygosaccharomyces bisporus | new species | yeast | aerobic |
| 111 | Zygosaccharomyces florentinus | new species | yeast | aerobic |
| 112 | Zygosaccharomyces microellipsoides | new species | yeast | aerobic |
| 113 | Zygosaccharomyces rouxii | new species | yeast | aerobic |

## Deletion of MSP entries:

| Deletions | Justification |
|---|---|
| Arthrobacter castelli DSM 16402T DSM | Many polymers. Will be replaced by new measurement. |
| Arthrobacter chlorophenolicus DSM 12829T DSM | Many polymers. Will be replaced by new measurement. |
| Arthrobacter pigmenti DSM 16403T DSM | Many polymers. Will be replaced by new measurement. |
| Mycobacterium avium ssp avium 8671 VAR | match with M. scrofulaceum |
| Mycobacterium manitobense DSM 44615 DSM | no valid name; match with M. saskatchewanense |
| Delftia sp[2] 911600013 LBK | Mixed culture with Saccharomyces servazzii. Saccharomyces servazzii is not in the database so far.<br>The mixed culture was detected during project work with Saccharomyces servazzii. |

## Renaming of MSP entries:

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Anaerococcus vaginalis DSM 7457T DSM | | Anaerococcus hydrogenalis DSM 7454T DSM | DB4613 strains A. hydrogenalis and vaginalis are mixed up. Confirmed by new cultivation, measuring and sequencing. Re-naming of old entry necessary. |
| Anaerococcus hydrogenalis DSM 7454T DSM | | Anaerococcus vaginalis DSM 7457T DSM | DB4613 strains A. hydrogenalis and vaginalis are mixed up. Confirmed by new cultivation, measuring and sequencing. Re-naming of old entry necessary. |
| Aurantimonas altamirensis 284 RLT | | Aureimonas altamirensis 284 RLT | Nomenclature change according DSMZ/IJSEM - changes 11/2011:<br>Aurantimonas altamirensis -> Aureimonas |
| Candida haemulonii MY916_09 ERL | | Candida duobushaemulonii MY916_09 ERL | Species was divided into two separate species |
| Lactobacillus sp M23 101342 CIP | | Carnobacterium maltaromaticum CIP 101342 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp CIP 102035 CIP | | Carnobacterium maltaromaticum CIP 102035 CIP | More precise identification of strain by CIP - adaptation of name |
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) 29 PSB | | Cryptococcus neoformans 29 PSB | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) ATCC 14116 THL | | Cryptococcus neoformans ATCC 14116 THL | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) CCM 8312 CCM | | Cryptococcus neoformans CCM 8312 CCM | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Cryptococcus_neoformans[ana]# (Filobasidiella_neoformans[teleo]) RV07_02 18 VML | | Cryptococcus neoformans RV07_02 18 VML | Anamorph/telemorph nomenclature is not very accepted - will be changed for this species |
| Dickeya dieffenbachiae DSM 18013T HAM | | Dickeya dadantii ssp dieffenbachiae DSM 18013T HAM | Nomenclature change according DSMZ/IJSEM - changes 07/2012:<br>Dickeya dieffenbachiae -> D. dadantii subsp.dieffenbachiae |
| Lactobacillus catenaformis 07_085 ANA IBS | | Eggerthia catenaformis 07_085 ANA IBS | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Lactobacillus catenaformis CIP 104817T B CIP | | Eggerthia catenaformis CIP 104817T B CIP | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Lactobacillus catenaformis IBS_MS_39 IBS | | Eggerthia catenaformis IBS_MS_39 IBS | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Lactobacillus catenaformis VA12065_1_11 ERL | | Eggerthia catenaformis VA12065_1_11 ERL | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus catenaformis (corrig.) -> Eggerthia |
| Bacillus schlegelii CIP 106933T CIP | | Hydrogenibacillus schlegelii CIP 106933T CIP | Bacillus schlegelii 31:215 (basonym) ≡ Hydrogenibacillus schlegelii |
| Lactobacillus vitulinus DSM 20405T DSM | | Kandleria vitulina DSM 20405T DSM | Nomenclature change according DSMZ/IJSEM - changes 10/2011:<br>Lactobacillus vitulinus -> Kandleria vitulina |
| Lactobacillus sp 101810 CIP | | Lactobacillus delbrueckii ssp lactis CIP 101810 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp 102006 CIP | | Lactobacillus fermentum CIP 102006 CIP | More precise identification of strain by CIP - adaptation of name |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Lactobacillus sp 101909 CIP | | Lactobacillus gasseri CIP 101909 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp CIP 102309 CIP | | Lactobacillus paracasei ssp paracasei CIP 102309 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus sp CIP 102623 CIP | | Lactobacillus rhamnosus CIP 102623 CIP | More precise identification of strain by CIP - adaptation of name |
| Lactobacillus zymae 108703 CIP | | Lactobacillus zymae CIP 108703T CIP | Type Strain T was missing - Typo |
| Tatlockia maceachernii 28 RLT | | Legionella maceachernii 28 RLT | New nomenclature not very accepted -> http://www.bacterio.net/t/tatlockia.html#maceachernii |
| Lactobacillus sp CIP 102166 CIP | | Marinilactibacillus psychrotolerans CIP 102166 CIP | more precise identification of strain by CIP - adaptation of name |
| Mycoplasma argini 7SR10 VLW | | Mycoplasma arginini 7SR10 VLW | Typo within species name will be corrected. |
| Mycoplasma argini NCTC 10129T VLW | | Mycoplasma arginini NCTC 10129T VLW | Typo within species name will be corrected. |
| Mycoplasma ovipneumoniae NCTC 10151T VLW | | Mycoplasma gallisepticum NCTC 10115T VLW | DB4613 strains Mycoplasma gallisepticum NCTC 10115T VLW and Mycoplasma ovipneumoniae NCTC 10151T VLW are mixed up. Confirmed by new, measuring and sequencing. Re-naming of old entry necessary. |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Mycoplasma gallisepticum NCTC 10115T VLW | | Mycoplasma ovipneumoniae NCTC 10151T VLW | DB4613 strains Mycoplasma gallisepticum NCTC 10115T VLW and Mycoplasma ovipneumoniae NCTC 10151T VLW are mixed up. Confirmed by new, measuring and sequencing. Re-naming of old entry necessary. |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) 991400574 LBK | | Saccharomyces cerevisiae 991400574 LBK | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) BJ2168 BRL | | Saccharomyces cerevisiae BJ2168 BRL | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) DTY3 BRL | | Saccharomyces cerevisiae DTY3 BRL | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) INVSc1 BRL | | Saccharomyces cerevisiae INVSc1 BRL | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) Isolat LGL Muenchen | | Saccharomyces cerevisiae Isolat LGL Muenchen | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) Kontrollstamm Humanmedizin VML | | Saccharomyces cerevisiae Kontrollstamm Humanmedizin VML | adaptation to more common nomenclature |
| Candida_robusta[ana]# (Saccharomyces_cerevisiae[teleo]) WS LLH | | Saccharomyces cerevisiae WS LLH | adaptation to more common nomenclature |
| Streptococcus thermophilus 37 RLT | | Streptococcus salivarius_ssp_thermophilus 37 RLT | adaptation to current nomenclature |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Streptococcus thermophilus 38 RLT | | Streptococcus salivarius_ssp_thermophilus 38 RLT | adaptation to current nomenclature |
| Streptococcus thermophilus 39 RLT | | Streptococcus salivarius_ssp_thermophilus 39 RLT | adaptation to current nomenclature |
| Streptococcus thermophilus DSM 20259 DSM | | Streptococcus salivarius_ssp_thermophilus DSM 20259 DSM | adaptation to current nomenclature |
| Streptococcus thermophilus DSM 20479 DSM | | Streptococcus salivarius_ssp_thermophilus DSM 20479 DSM | adaptation to current nomenclature |
| Streptococcus thermophilus DSM 8713 DSM | | Streptococcus salivarius_ssp_thermophilus DSM 8713 DSM | adaptation to current nomenclature |
| Listonella anguillarum 02 EGS | | Vibrio anguillarum 02 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum 03 EGS | | Vibrio anguillarum 03 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum DSM 11323 DSM | | Vibrio anguillarum DSM 11323 DSM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum DSM 21597T DSM | | Vibrio anguillarum DSM 21597T DSM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum LMG 4437T HAM | | Vibrio anguillarum LMG 4437T HAM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |

| Old MSP name | to | New MSP name | Justification |
|---|---|---|---|
| Listonella anguillarum serotype 02 EGS | | Vibrio anguillarum serotype 02 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella anguillarum serotype 03 EGS | | Vibrio anguillarum serotype 03 EGS | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |
| Listonella pelagia DSM 21205T DSM | | Vibrio pelagius DSM 21205T DSM | nomenclature change according DSMZ/IJSEM - changes 12/2011:<br>Listonella => Vibrio |

## Matching Hints Changes:

| | | | Justification |
|---|---|---|---|
| Species alkalescens / argini of the genus Mycoplasma have very similar pattern: Therefore distinguishing their species is difficult. | changed to | Species alkalescens / arginini of the genus Mycoplasma have very similar pattern: Therefore distinguishing their species is difficult. | Correction of typo within the species name "arginini" |
| Corynebacterium amycolatum<br>Corynebacterium durum<br>Corynebacterium minutissimum | deletion of matching hint link | Species of this genus have very similar patterns: Therefore distinguishing their species is difficult. | Matching hint is not necessary for this species, because MALDI can separate this species from others |
| Acinetobacter baumannii<br>Acinetobacter calcoaceticus<br>Acinetobacter pittii | change to new matching hint | Member of the Acinetobacter baumanii/calcoaceticus complex. Extraction must be performed to permit reliable species identification. | For clarification change from general matching hint (Species of this genus have very similar patterns: Therefore distinguishing their species is difficult.) to this more precise one. |
| Arthrobacter castelli<br>Arthrobacter chlorophenolicus<br>Arthrobacter pigmenti | link with new matching hint | Species tend to produce polymers which can interfere with the identification. | For clarification the matching hint will inform about the production of possibly interfering polymers. |
| Burkholderia ambifaria, anthina, cenocepacia, cepacia, diffusa, dolosa, lata, latens, metallica, multivorans, pyrrocina, seminalis, stabilis, vietnamensis | link with new matching hint | Is a member of Burkholderia cepacia complex | Additional information. This will help the user to recognize members of the Burkholderia cepacia complex. |

# Product Description

# microflex™ LRF

# MALDI Time-of-Flight Mass Spectrometer System

BDAL # 8601800

Small footprint, silently operating MALDI-TOF mass spectrometer with industrial hardened vertical design including self-diagnostics of major components.

A high performance bench-top Time-of-Flight Mass Spectrometer equipped with MALDI Ion Source, Linear/Reflectron mode, high dynamic range FlashDetector™ systems in conjunction with PAN™ wide mass range focusing for unrivaled resolution power and mass accuracy. Additional PSD-MS/MS Capability included.

- Equipped with MALDI-Ion Source
- TOF-Analyzer for Linear and Reflectron mode
- TOF-Analyzer for both positive and negative ion mode
- Resolution performance RP > 15,000 FWHM for peptides
- ppm mass accuracy (internal/external calibration) in both modes

## A. MALDI-Ion Source

- Highly sensitive microScout™ ion source; medium area target (54mm x 36mm) with exact dimensions of 1/4 microtiter plate
- 2nd generation proprietary PAN™ pulsed ion extraction technology for high mass accuracy and unmatched resolution spectra across an extended mass range
- 60 Hz N2-Cartridge-Laser including variable power attenuator and UV optics
- microScout™ Target Kit including: two MSP96 ground steel targets, one target each of MSP96 polished steel, MSP AnchorChip 600/96 and NALDI targets (5 plates)
- Manually operated sample inlet
- High resolution magnifying target observation optics with integrated display in Compass™ acquisition software

## B. High Performance Time-of-Flight Mass Analyzer

- Ultra-stable electronics for TOF analyser, detector and ion source fully enables a 1-60 Hz data acquisition rate in MS and MS/MS operation
- Integrated pumping system including vacuum measurement and control unit: 70 l/sec turbo-molecular pump including diaphragm-pump
- FlashDetector™ providing unmatched mass resolution and mass accuracy

## C. Gridless ion reflectron for increased sensitivity, resolution and accuracy:

- Gridless two stage ion reflectron for superb mass resolution
- Independent reflector power supply with high-precision control
- Includes FlashDetector™ and power supplies

## D. FAST™ (Fragmentation Analysis and Structural TOF-MS) accessory for PSD (Post-Source Decay) MS/MS-experiments:

- autoFAST™ software for calibration, pasting of segments, etc.
- FAST-FILTER Pre Cursor Ion Selector for true MS/MS of complex sample mixtures

## E. Data system:

- PC Workstation with 2.66 GHz Single-CPU-Quad-Core-Xeon-processor, 12 GB RAM, 2 TB hard disk, Ethernet connection for external networks, ≥ 2 Gs/s Digitizer
- DVD-ROM drive
- R/W DVD-ROM drive DL
- ≥ 24" flat screen colour monitor
- Windows™ WIN7 operating system
- Laser printer
- Remote Service capability via 128-bit SSL-security web connection

## F. Applications Software:

Software package Compass 1.4 for flex-series instruments including instrument control, data acquisition, post processing, and data analysis packages:

- Released for Windows™ XP and Windows™ WIN7 operating systems
- Compass / flexControl 3.4 for integrated control of the instrument
- Compass / flexAnalysis 3.4, including:
    - Advanced data processing with a high degree of automation
    - Usage of the new calibration algorithms and High-Precision-Calibration (HPC)
    - Easy export of peak list (e.g. to MS Excel)
    - Interface to bioinformatics software packages as BioTools™ and ProteinScape™
- Compass / AutoXecute™ with fuzzy-logic optimization for automated acquisition

- SW License Compass / flexControl 3.4
- SW Licence Compass / flexAnalysis 3.4
- SW Licence Compass / AutoXecute
- SW License TLC-MALDI 1.0 as an option

**G. Set of manuals and reference DVDs**

**H. Installation**

**I. Familiarization upon installation**

**J. 1 year warranty**

**K. Voucher for a factory-training course - valid for 2 participants.**

# micrOTOF-Q III

**Description**
**Part Number: # 728889**

**Benchtop easy-to-use, high-performance electrospray ionization quadrupole time-of-flight LC/MS/MS mass spectrometer designed for exact mass and true isotopic measurements**

**Small footprint system enclosure for ESI ion funnel source, quadrupole, collision cell, oa-TOF mass analyzer, electronics, and vacuum pumps, containing:**

**A. Apollo II Electrospray Ionization Source with ion funnel**

- ESI source with grounded needle for safety and easy sample introduction
- Heated counter current drying gas for gentle and efficient drying
- Pneumatic off-axis nebulization for flow rates up to 1 ml/min., with gradients from 100% aqueous to 100% organic
- Patented dual ion funnel for mass independent ion transfer
- Ion lens system including in-source collision induced dissociation control (IS-CID)
- Combined Funnel-Hexapole-Cartridge with front access for easy maintenance
- Source HV controller and drying gas controller
- Ion lens housing and vacuum system
- Flow rate with ESI-Source 1µl/min … 1ml/min
- Suitable for HPLC and CE coupling

**B. High Mass Quadrupole Mass Filter:**

- Hyperbolic quadrupole mass filter
- Ultra stable monolithic design
- RF-generator for monoisotopic precursor ion selection

**C. CID Collision cell:**

- Hyperbolic quadrupole design
- RF-Generator with fast amplitude switching
- Collision gas controller

**D. Focus™ ion optics**

- Ultra precise orthogonal ion beam focusing
- Time controlled ion extraction

**E. Orthogonal pulsed ion extraction interface**

- Interface housing and ion lens system
- In-line detector system for easy maintenance
- Ultra-stable high voltage switches with up to 20 kHz repetition rate and appropriate power supplies.



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**F. Time-of-Flight (TOF) Mass Analyzer:**

- Reflectron TOF analyzer with orthogonal mounted ion source
- High-sensitivity and fast ion detector system
- Positive and negative ion modes
- Ultra-stable high voltage power supplies for TOF analyzer and detector

**G. Electrostatic ion reflectron**

- Ion reflectron for increased mass resolution and accuracy
- Includes ion reflectron electronics

**H. Vacuum system**

- Q-q-TOF analyzer vacuum housing
- Vacuum system with 5 differential pumping stages
- One roughing pump and quadruple stage turbo-drag pumps for ESI source and Q-q-TOF analyzer
- Vacuum measurement and pump control unit

**I. Syringe pump**

**J. Modes of Operation**

- TOF Mass ranges 20-80,000 m/z
- FSR resolution 20,000 FWHM
- Internal calibration
- External calibration
- Exact mass measurements independent from sample concentration over a wide dynamic range without second sprayer.
- Dual sprayer (as an option)

**K. High-performance and accurate mass features**

- Patented ion funnel source
- Superior MS/MS sensitivity
- Long term and ultra stable mass axis stability in MS and MS/MS
- Exact mass independent from sample concentration and collision energy
- Combined calibration for both MS and MS/MS
- TIP™ technology for True-Isotopic-Pattern in MS and MS/MS
- SmartFormula 3D™ for multi-dimensional, unambiguous determination of molecular formula with sub-ppm confidence
- Wide dynamic range for quantitation
- Temperature compensated flight tube
- Max scan rate 40 spectra / sec
- Positive / negative ion operation

**L. Data system OTOF:**

- 2 GSamples/sec, 16 Gbit/sec sampling rate Digitizer
- 2,66 GHz Quad-Core Processor, 12 GB RAM, system hard-disk drive plus 2 TB hard-disk drive for data
- DVD-ROM drive
- DVD-ROM +/- R/W drive
- 24" LCD flat screen color monitor



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**Bruker Daltonics Inc.**
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- OS WinXP / Win7/32
- Laser printer
- Remote Service capability via 128-bit SSL-security web connection

**M. Applications software**

Software package Compass 1.5 for HPLC and micrOTOF-Q control, data acquisition, post processing, and data analysis:

- Operating system Windows XP / Win 7/32
- HyStar 3.2 for integrated control of most popular HPLC systems and autosamplers
- OTOFcontrol 3.2 software with smart and expert mode
  - Expert mode: extended control over instrument parameters for interactive system optimization of sophisticated exact mass methods
- Data Analysis software DA 4.1, including:
  - Advanced data processing with a high degree of automation
  - SmartFormula 3D™: Automated sum formula determination using MS and MS/MS data with both, accurate mass and isotopic fit.
  - CompoundCrawler™ for web-based searched of molecular structures
  - FragmentExplorer™ for full annotation of MS/MS spectra
  - QuantAnalysis™ quantitation package
  - LibrarySearch ™ module for search of MS, MS/MS and MSn spectra with advanced matching algorithm
  - Charge deconvolution module
  - MaxEntropy Deconvolution as an option
  - Export of spectra and ion current profiles as Windows metafiles to word-processing programs

- SW License Compass 1.5
- SW License Charge Deconvolution for DA4.1

**N. Set of manuals and reference CD-ROMs**
**O. Installation**
**P. Familiarization upon installation**
**Q. 1 year warranty**

Voucher for a factory-training course - valid for 2 participants.



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# Petrochemical Gas Chromatographs

Analyzer Solutions

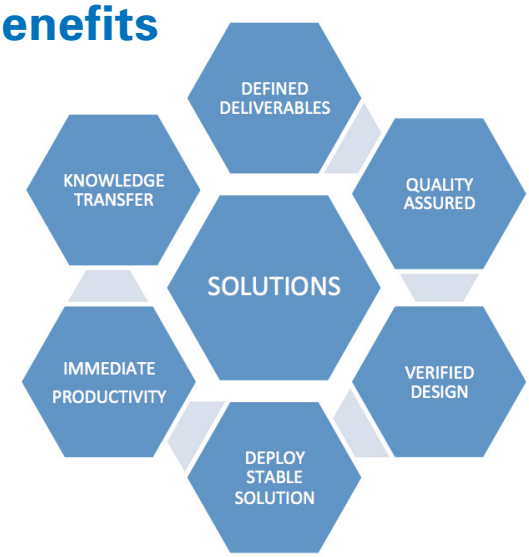
Solutions

Innovation with Integrity

**Bruker has the experience and know-how to provide pre-configured gas chromatographs that are ready at power up to handle your key applications. Our long experience in designing, configuring and manufacturing complete systems, with all their analytical benefits, ensures you get the solution that's right for you. With a host of standard solutions configured to meet the performance specifications outlined in international methods, and the capability to produce unique, tailor-made solutions, we have the answer that you seek.**

# Bruker Analyzer Solutions

## Benefits




Bruker configures and tests GC hardware and software according to widely used industry standard methods (e.g. ASTM, UOP, EN, ISO, GPA,…), to save its clients time and to ensure confidence in results. Solutions are configured to meet the performance specifications outlined in the set method itself.

## Included with all Bruker Analyzer solutions:

- All Hardware
- Software (incl. special "plug-ins" where appropriate)
- Pre-Installed methods
- Test Chromatograms
- Installation/ Validation Data
- Trouble Shooting Guide
- User documentation customized for the specific method

# Bruker Simulated Distillation Analyzers

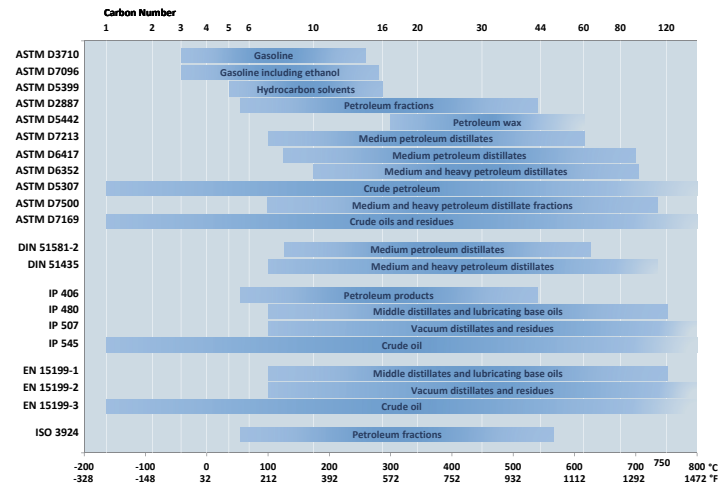



**Table 1:** Overview Simdist methods.

A gas chromatographic (GC) technique, Simulated Distillation (SimDist) reproduces the physical distillation of petroleum materials and products by determining boiling point distribution. Bruker's range of Simulated Distillation Analyzers are designed to meet all industry standard methods, Bruker's analyzer software includes both ASTM D86 and ASTM D1160 correlations. Bruker's highly automated GC, CompassCDS Chromatography Data Handling Software, and integrated SimDist software are also designed to meet worldwide industry standard test methods.


436-GC with Sampler

## Key Benefits Include:

- Accurate boiling point distribution up to 750°C
- Integrated standard test methods, applications fully comply with ASTM, IP, DIN and ISO standard test methods
- Complete, single vendor solution
- Complete control from initial setup to final report
- ASTM D86 and ASTM D1160 correlation

## Built-in Reports:

Bruker's SimDist software provides a wide variety of report options to meet specific requirements including;

- Chromatogram with merged corrected blank analysis and IBP/FBP marks versus retention time
- Boiling point versus percentage of sample
- Table and plot with retention time versus boiling point
- D86 and D1160 correlations
- DIN Noak and motor oil volatility reports
- Table with cut points and fractions plus residue analysis with recovery calculation up to C120

# Hydrocarbon Analysis by Group (PIONA+™)

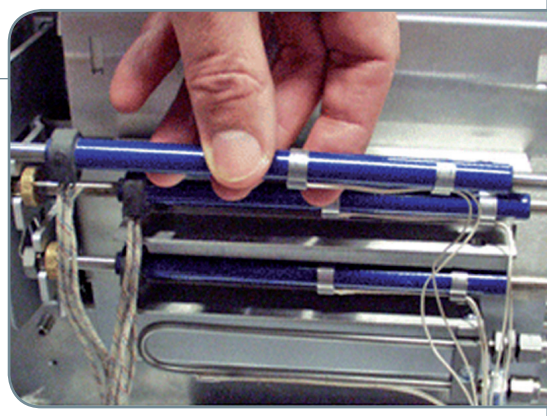


**Figure 1:** Traps are easily accessible and do not require any tools to install or replace.

## Characterization of Engine Fuels by Hydrocarbon Group Type

Bruker's PIONA+™ Analyzer is a highly flexible GC analysis platform to obtain comprehensive characterization and quantitative information, including hydrocarbon group types, oxygenates and carbon number distribution for spark ignition engine fuels.

## Key Analyzer Capabilities:

- Unparalleled operational flexibility
- Compliant with established standards
- A complete and fully integrated solution
- A powerful analyzer, easy to use, generating outstanding analysis results day after day

The PIONA+ Analyzer performs a complete analysis (as described in ASTM D6839 and similar methods) and provides unprecedented analytical flexibility and simplified operation through the use of a novel approach to column/trap heating and exchange (Figure 1).

## Reduced Analysis Time and Increased Sample Throughput Efficiency through the Use of "Concurrent" Heating

A unique aspect of the design of the Bruker PIONA+ system is the ability to independently heat the individual traps.

This has 2 major operational benefits:

- Enhanced elution integrity for wide range sample
- Significantly Reduced Analysis Time

The independent and concurrent heating design permits greater trap control and benefits in improved elution integrity of the component groups e.g napthene, iso-paraffins and n-paraffins even for a wide range sample (C4 - C11). In addition, only a single Molsieve column temperature cycle is employed thus reducing the analysis time by almost half allowing a "fast" PIONA mode of operation (see figures 2 and 3).

By employing this technique, sample throughput can be nearly doubled compared to systems that do not offer this unique capability.

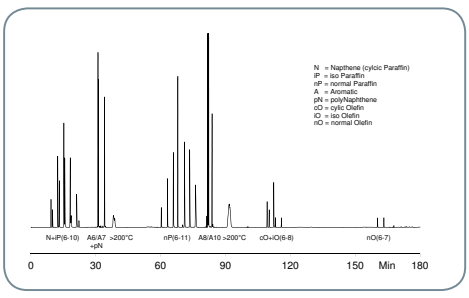



**Figure 2:** Chromatogram of a test mix in conventional PIONA mode. (Analysis Time - 180mins)

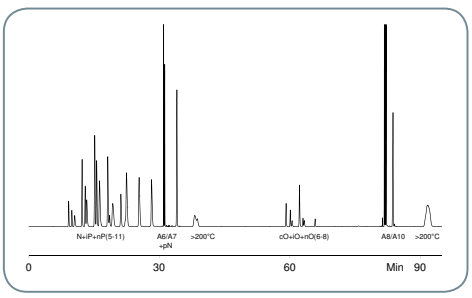



**Figure 3:** Chromatogram of a test mix using concurrent heating in "fast" PIONA mode. (Analysis Time = 95mins)

# Determining Total Olefin Content Is Now Practical

The stability, sample loading and lifetime for all of the critical chromatographic components have been improved and optimized in the Bruker PIONA+ Analyzer. Of special and particular note is the improvement in increasing the sample loading capacity of the "olefin" trap. As a result, it is now possible to analyze streams with olefin content as high as 35-40% or more. This makes it practical to employ a single analytical method to obtain total olefin content (Table 2).

**Table 2**

| | Saturates | | | Unsaturates | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Carbon | Cyclic | Iso | Normal | Cyclic | Iso | Normal | Aromatics | Oxygenates | Total |
| 3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 4 | 0.00 | 0.00 | 0.06 | 0.00 | 0.03 | 0.54 | 0.00 | 0.00 | 0.63 |
| 5 | 0.31 | 11.37 | 2.98 | 0.87 | 9.92 | 7.58 | 0.00 | 0.00 | 33.03 |
| 6 | 3.19 | 9.98 | 1.40 | 2.40 | 8.59 | 4.40 | 1.72 | 0.00 | 31.68 |
| 7 | 4.31 | 6.77 | 0.00 | 2.14 | 4.76 | 1.91 | 7.47 | 0.00 | 27.36 |
| 8 | 1.42 | 3.12 | 0.00 | 0.39 | 2.06 | 0.00 | 0.07 | 0.00 | 7.06 |
| 9 | 0.01 | 0.00 | 0.00 | 0.04 | 0.02 | 0.00 | 0.03 | 0.00 | 0.10 |
| 10 | 0.01 | 0.00 | 0.00 | 0.09 | 0.00 | 0.03 | 0.01 | 0.00 | 0.14 |
| 11 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **Total** | **9.25** | **31.24** | **4.44** | **5.93** | **25.38** | **14.46** | **9.30** | **0.00** | **100.00** |

Example weight % report for a Naphtha sample with high (46%) olefinic content; (highlighted in blue).

The analyzer design allows the operator to conduct analyses in any one of a number of different operational modes including PNA, PONA, PIONA, O-PONA and O-PIONA in standard and concurrent heating configuration. The system is compliant with established standard methods (see adjacent array).

| | PNA | PONA | PIONA | O-PONA | O-PIONA |
|---|---|---|---|---|---|
| EN 14517 | | | | | ✓ |
| EN-ISO-22854 | | | | | ✓ |
| ASTM D6839 | | | | ✓ | |
| DIN 51448-2 | | | ✓ | | |
| ASTM D1319 (FIA) | | ✓ | | | |
| DIN 51448-1 | ✓ | | | | |
| ASTM D5443 | ✓ | | | | |
| UOP 870 | ✓ | | | | |
| IP 382 | ✓ | | | | |

✓ Compliant with the method

More information generated than required for the method

# Detailed Hydrocarbon Analyzer

The DHA Analyzer is a complete high resolution GC solution for the analysis of hydrocarbons in petroleum streams. It is capable of performing all of the standard methods including ASTM D6729, D6730, D6733, D5134, D6623, IP 344/ DHA "Front End" and "Fast DHA".

Although each DHA analyzer is configured, tested and certified at the factory for a standard method specified by the customer, the DHA software permits the operator to utilize any of the other popular standard methods as well. And, because of the outstanding performance and flexibility of the Bruker GC and CompassCDS software design, Bruker is able to quickly modify the existing methods or add new ones if required as a result of the on-going dynamic industry standard processes.

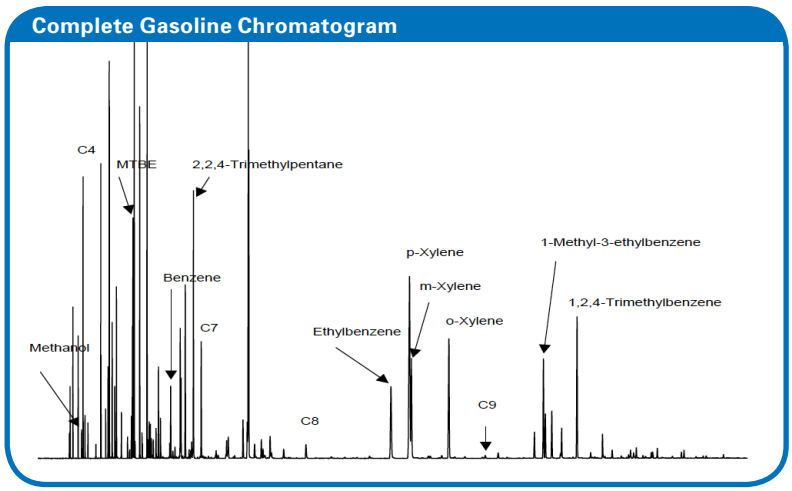



**Figure 4:** The analysis of permanent gases and hydrogen using the Rapid RGA.

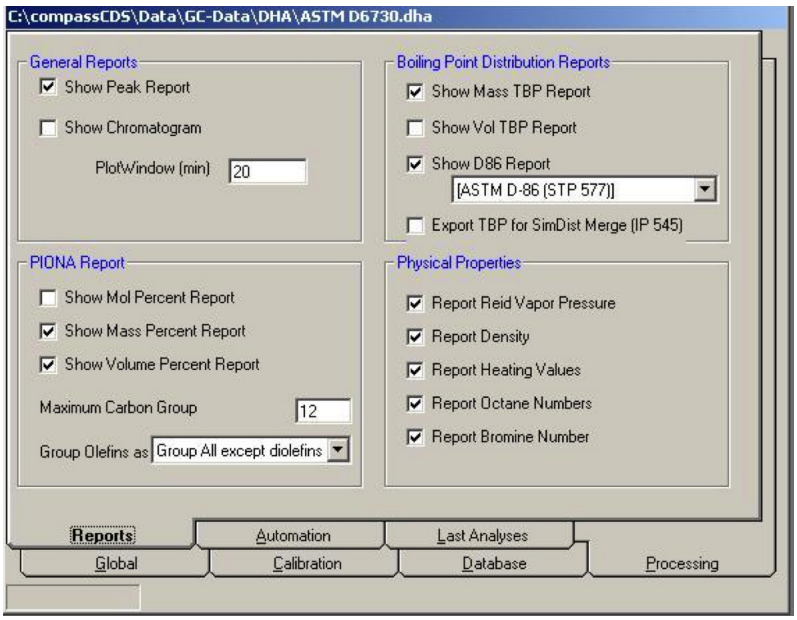



**Figure 5:** Report selection output.

# Bruker Refinery Gas Analyzers

## Peak Identification

1. Hydrogen
2. Carbon Dioxide
3. Hydrogen Sulfide
4. Oxygen
5. Nitrogen
6. Carbon Monoxide
7. Methane
8. Ethane
9. Ethylene
10. Propane
11. Cyclo Propane
12. Propylene
13. i-Butane
14. n-Butane
15. Propadiene
16. Acetylene
17. t-2-Butene
18. i-Butene
19. c-2-Butene
20. i-Pentane
21. n-Pentane
22. 1, 3-Butadiene
23. Propyne
24. Butyne
25. C6+
26. Helium

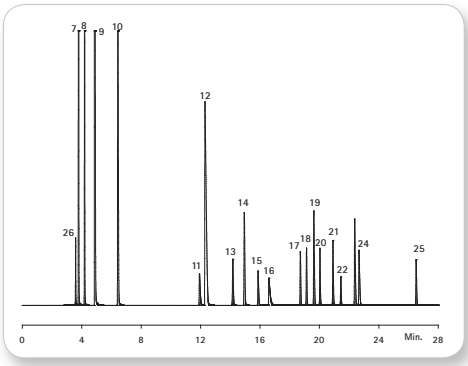



**Figure 6:** The separation of light hydrocarbons using the Standard RGA.

The source and composition of refinery gases varies considerably. Measuring gas composition precisely and accurately is a significant challenge in today's refinery operations. Bruker's Refinery Gas Analyzers (RGA) are designed to deliver superior, reliable results for a wide range of sources and analysis throughput requirements.

## Key Benefits:

- Pre-configured and tuned
- Standard methods including UOP 539, DIN-51666 and ASTM D2163
- Integrated micro-gasifier ensures complete vaporization of LPGs and high pressure samples to prevent sample discrimination (option)
- Multi-channel approach

| Characteristics | Standard RGA | Rapid RGA |
|---|---|---|
| No. of Channels/Detectors Used | 3 | 3 |
| No. of Column Ovens | 1 | 2 |
| Analysis Time | 25 min | 5 min (7 min with $H_2S$) |
| Repeatability | <1% | <1% |
| Linear Bench Space Required | 66 cm/26 in. | 66 cm/26 in. |
| Minimum Component Detection Level | 0.01% all components except $H_2S$ = 0.05% | 0.01% all components except $H_2S$ = 0.05% |
| **Suitability** | | |
| Typical Refinery Gas | Excellent | Excellent |
| Impurities in Bulk Ethylene | Excellent | Excellent |
| Impurities in Bulk Propylene | Excellent | Good |
| Impurities in Bulk C4 | Good | Good |

**Table 3:** Standard RGA vs Rapid RGA.

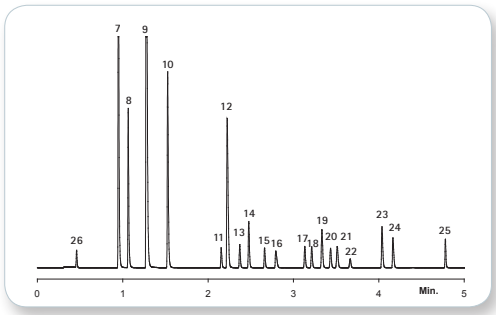



**Figure 7:** The analysis of light hydrocarbons using the Rapid RGA, with complete separation in less than five minutes.

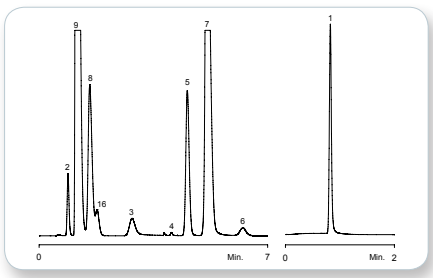



**Figure 8:** The analysis of permanent gases and hydrogen using the Rapid RGA.

## Bruker Offers Two RGA Systems to Meet the Widest Range of Analysis Requirements:

### Standard RGA:

A three channel multi-valve design using both capillary and packed columns.

Channel 1 - Analysis of permanent gases
Channel 2 - Light hydrocarbons
Channel 3 - Hydrogen.

Total analysis time for all components in 25 minutes.

### Rapid RGA:

The Standard RGA packed columns in the hydrogen and permanent gas channels are replaced by micro packed columns and installed in a separate column oven. Key benefits of this design are:

- Flexibility
- Reduced Analysis Time - 5mins (with $H_2S$ - 7mins)
- Increased Sample Throughput

# Low Level Oxygenates Analyzer

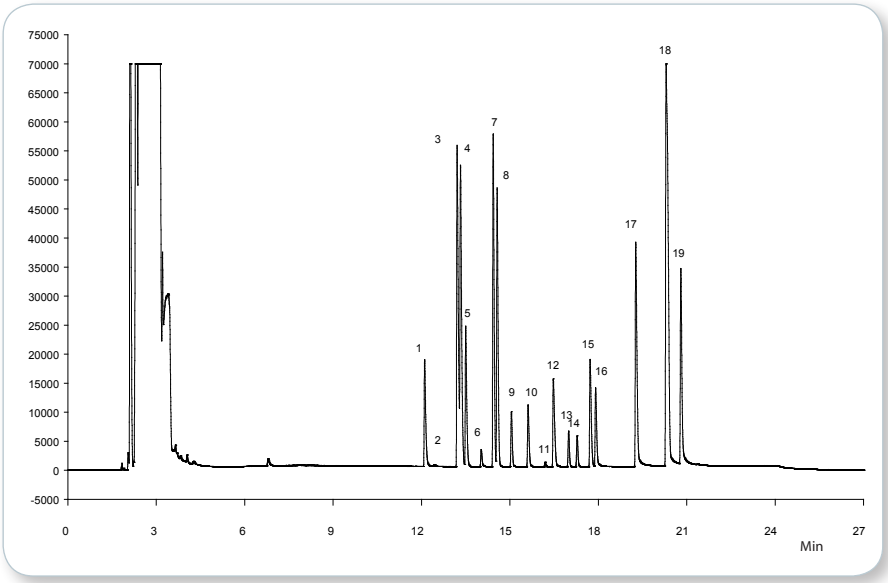



**Figure 9:** Typical chromatogram showing a wide range analysis of a liquid sample stream.

The determination of sub to high ppm levels of ethers, alcohols, aldehydes and ketones in different hydrocarbon matrices is a recurring challenge in the petroleum refining and petrochemical industry. The Bruker Low Level Oxygenates Analyzer is an easy to use solution to meet this challenge and is according ASTM D7423.

The Low Level Oxygenates Analyzer is designed and optimized to quantify ppm and sub ppm levels of ethers (e.g. DME, MTBE, ETBE, DIPE), alcohols (e.g. methanol, ethanol, propanol), ketones (e.g. acetone, MEK) and aldehydes in various hydrocarbon matrices. In general, all oxygenated components with a boiling point of up to 100°C can be analyzed and the sample can be a gas, LPG or liquid under ambient conditions with a final boiling point up to 250°C.

The system is comprised of a Bruker GC configured with gas and liquid sampling valves, two high performance capillary analysis columns, digitally controlled pneumatics including a 'fluidic' switch and Flame Ionization Detector (FID). An optional 'pressure station' can be added to eliminate the possibility of losing sample due to evaporation when analyzing LPG. The GC is controlled via the CompassCDS Chromatography Data Handling Software, which acquires data, processes it and generates analyses reports.

### Peak Identification

1. Diethylether
2. Acetaldehyde
3. Ethyl tert. Butyl ether
4. Methyl tert. Butyl ether
5. Diisopropylether
6. Propanal
7. tert amyl methyl ether
8. Propylether
9. Isobutyraldehyde
10. Butyraldehyde
11. Methanol
12. Acetone
13. Isovaleraldehyde
14. Valeraldehyde
15. 2-Butanone
16. Ethanol
17. 1-Propanol
18. tert Butyl alcohol & Isobutanol
19. 1-Butanol

# Bruker 4815 GC Oxygenates Analyzer

The Bruker 4815 GC Analyzer provides a highly cost effective solution for the analysis of oxygenates in gasoline, according to the widely used industry standard method ASTM D4815. The combination of Bruker's reliable GC hardware, powerful software and industry leading pre- and post-sales support teams make this analyzer package the most comprehensive solution available today.

Oxygenated compounds can be present in various hydrocarbon matrices either because they were purposely added (e.g. into gasoline), because they are naturally present, or formed during catalytic processes such as polymer production. In gasoline, oxygenated compounds are added as 'anti-knock' agents to increase the octane number and decrease emissions by replacing organo-lead compounds.

The type and concentration of oxygenated compounds must be measured in reformulated gasolines as part of ongoing product quality assessment, and to confirm the oxygenated components have been added in the correct amounts according to regulatory requirements (e.g. California Air Resources Board).

ASTM D4815 is frequently chosen as the standard method for the determination of oxygenated compounds. Individual ethers and alcohols are quantified in gasoline including: MTBE, ETBE, TAME, DIPE, C1-C4 alcohols and tert-amylalcohol. Individual ether components are measured from 0.1 to 20.0 mass %.The individual alcohols are measured from 0.1 to 12.0 mass %.

456-GC with Sampler

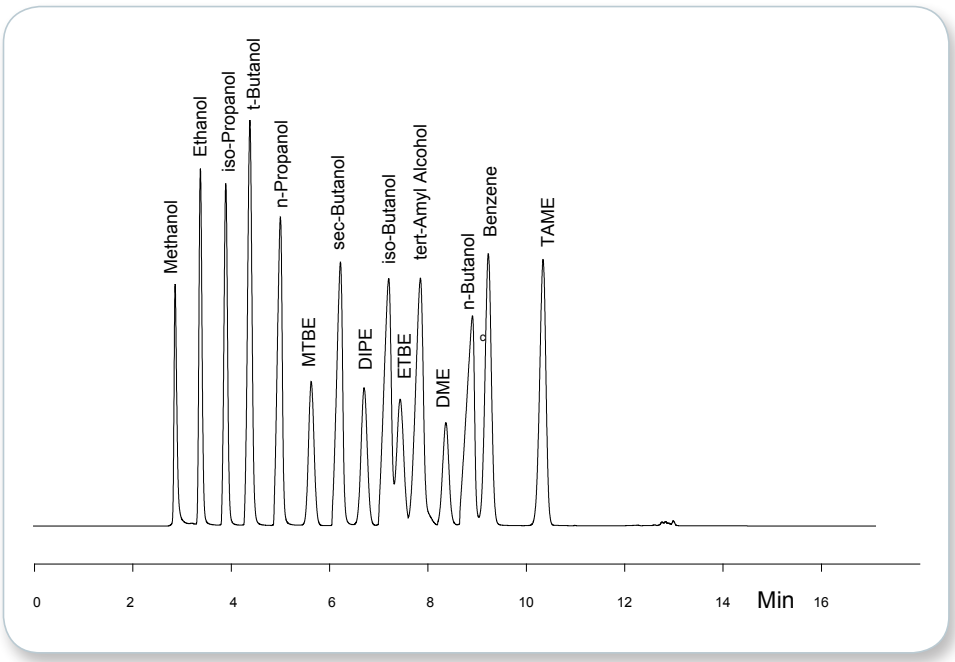



**Figure 10 :** Typical Chromatogram of the test sample.

# Trace Impurity Analyzers

## Sulfur Components in LPGs

Low level analysis of sulfur containing components such as $H_2S$, COS and mercaptanes is extremely challenging and a configured GC offers the solution.

Firstly, the system employs a micro-gasifier enabling the direct coupling of an LPG stream. Secondly, an inert steel sample path ensures a trouble free analysis of sulfur containing components at low concentrations. Finally, a two channel PFPD/ two column approach permits the analysis of all components of interest in one run whatever the LPG matrix. Two differing columns ensures quenching of PFPD signal by the matrix is overcome and full sulfur component analysis is achieved. Figures 11 and 12 show chromatograms obtained in a propane matrix and illustrates the novel benefits of the 2 channel approach.

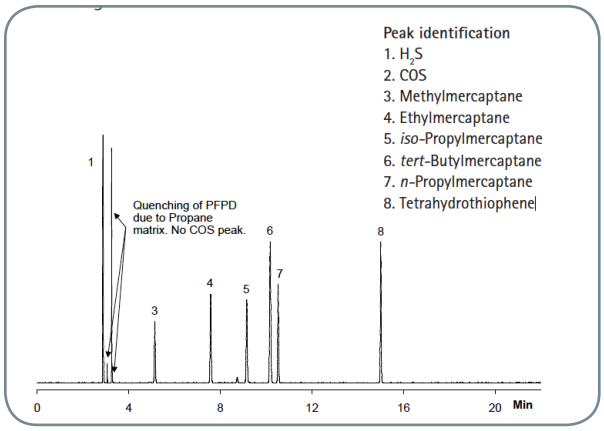



**Figure 11:** Sulfur components in propane, BR-1 column.

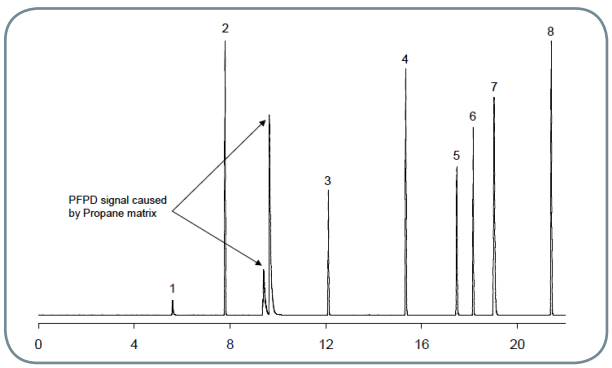



**Figure 12:** Sulfur components in propane, BR-Q PLOT.

## Permanent Gases in LPGs

Impurities such as CO, $CO_2$, $H_2$, $O_2$ and $N_2$ need to be determined at low levels in LPGs. Complete separation of these components is done using a two channel single detector (PDHID) system. The GC employs a permanent gas channel for analyzing $H_2$, $O_2$, $N_2$, $CH_4$ and CO and a specific second channel for the analysis of $CO_2$. A gasifier is used as a sample introduction device thus giving the capability of handling LPG samples C2 through C4.

Detection limits are at the ppb level (Figure 13), depending on the component of interest.

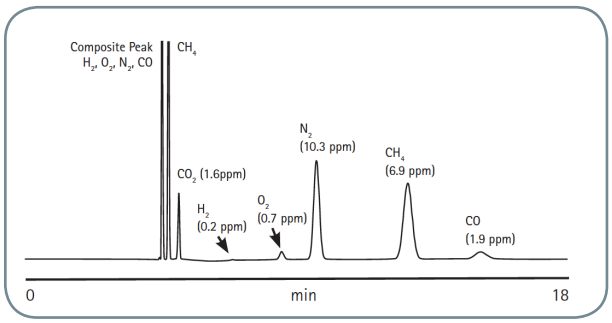



**Figure 13:** LPG sample.

# Total Characterization of Ethylene Impurities

For a total characterization of impurities in ethylene and also propylene six GC channels are required. By coupling two Bruker GCs with three channels each, a comprehensive solution is available for analyzing these components. The channels used in this analyzer are analytical tools principally developed for the determination of different gases in various hydrocarbon types of gaseous matrices.

## GC-1

- $H_2$ Channel (TCD)
- $O_2/N_2$ Channel (TCD)
- CO, $CO_2$ Channel (Methanizer/FID)

## GC-2

- Light Hydrocarbon Channel (FID)
- Oxygenates Channel (FID)
- Sulfur Channel (PFPD)

The results (see figures 14 to 19) demonstrate how this 6 channel system is perfectly suited for the total characterization of ethylene and its impurities.

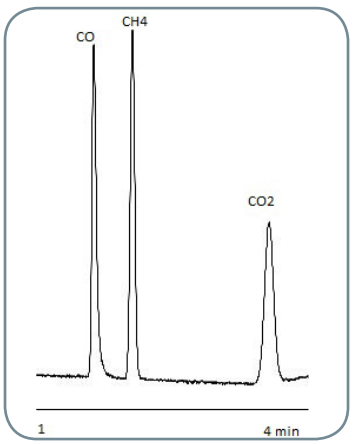



**Figure 14:** CO, $CH_4$ and $CO_2$ on GC-1.

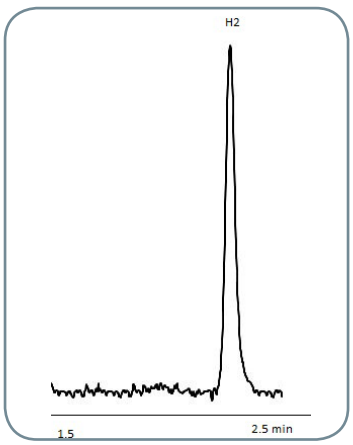



**Figure 15:** $H_2$ on GC-1.

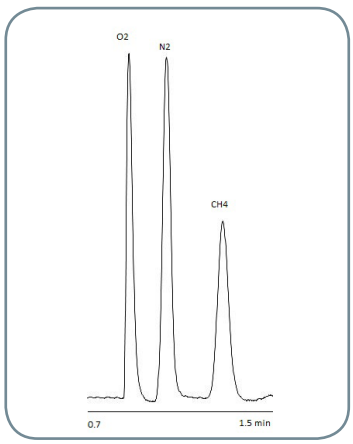



**Figure 16:** $O_2$ and $N_2$ on GC-1.

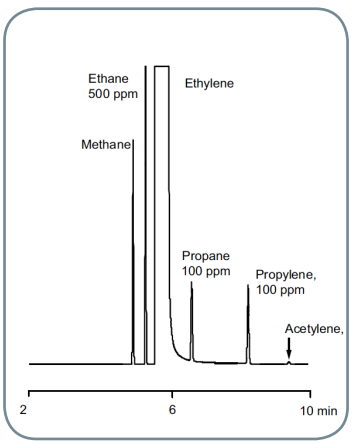



**Figure 17:** Light hydrocarbons on GC-2.

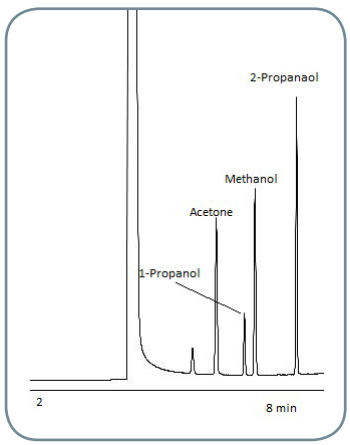



**Figure 18:** Oxygenates on GC-2.

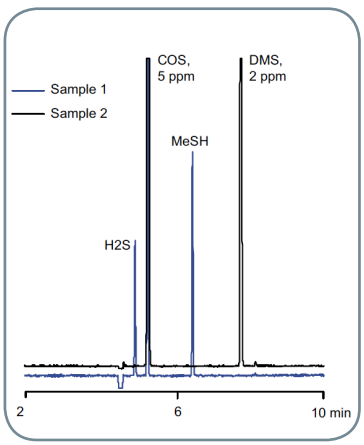
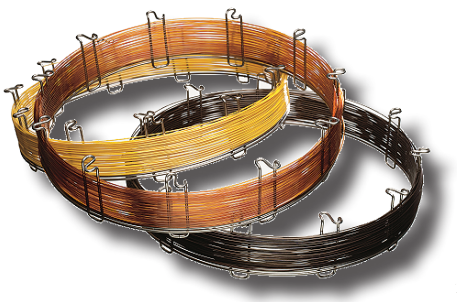



**Figure 19:** Sulfur components on GC-2.

# Bruker-Certified Consumables for Your SCION GC Series

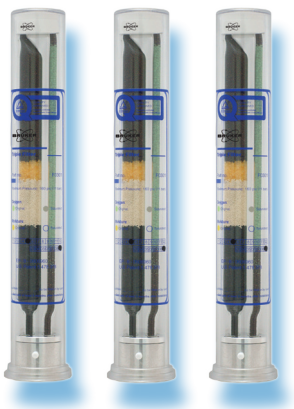
Bruker GC columns span a broad range of column diameters, stationary phases, and capillary column materials: Fused Silica (FS) and Inert Steel (IS). Ideal for either routine or research type analyses.



Bruker GC column offerings bridge across many important applications (like ASTM, UOP, ISO, GPA and EN) and include a number of offerings such as:

- Standard WCOT (Wall Coated Open Tubular)
- Solid Stationary Phase PLOT (Porous Layer Open Tubular)
- Inert Steel Micro-Packed and Packed

## Super Clean™ Gas Filters



Bruker Gas Purification Systems have the range to satisfy your needs from individual to combination filters, from Ultra purity combined with Ultra capacity, to all in one solution kits. Innovative features designed into the product yield extensive benefits to the user.

- Ultra-high capacity for long life, less change and improved productivity
- High-purity output ensures 99.9999% Pure Gas
- "Quick connect" fittings for easy, leak-tight filter changes
- Glass internals prevent diffusion; plastic externally for safety
- Easy-to-read indicators for planned maintenance and improved up-time

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

www.ScionHasArrived.com

www.GlobalEnergyTesting.com

**www.bruker.com/scion**

# Petrochemical Gas Chromatographs

Analyzer Solutions

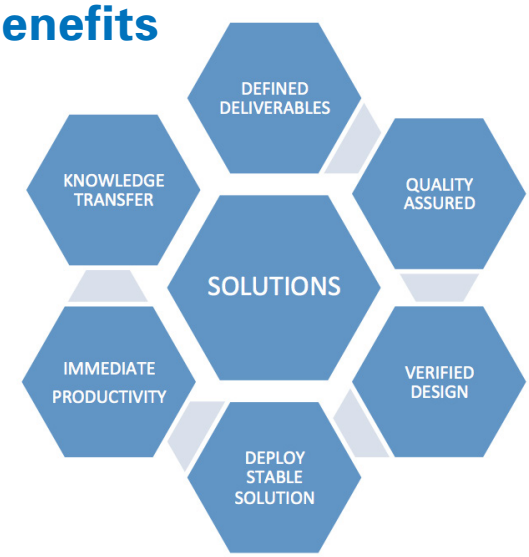
Solutions

Innovation with Integrity

**Bruker has the experience and know-how to provide pre-configured gas chromatographs that are ready at power up to handle your key applications. Our long experience in designing, configuring and manufacturing complete systems, with all their analytical benefits, ensures you get the solution that's right for you. With a host of standard solutions configured to meet the performance specifications outlined in international methods, and the capability to produce unique, tailor-made solutions, we have the answer that you seek.**

# Bruker Analyzer Solutions

## Benefits




Bruker configures and tests GC hardware and software according to widely used industry standard methods (e.g. ASTM, UOP, EN, ISO, GPA,…), to save its clients time and to ensure confidence in results. Solutions are configured to meet the performance specifications outlined in the set method itself.

## Included with all Bruker Analyzer solutions:

- All Hardware
- Software (incl. special "plug-ins" where appropriate)
- Pre-Installed methods
- Test Chromatograms
- Installation/ Validation Data
- Trouble Shooting Guide
- User documentation customized for the specific method

# Bruker Simulated Distillation Analyzers

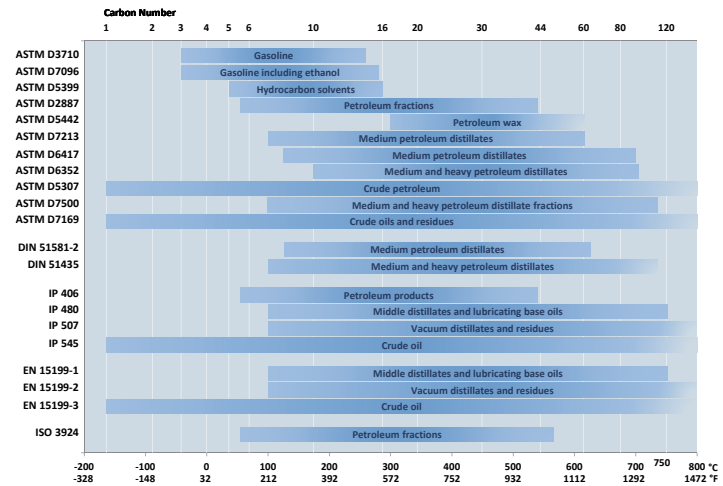



**Table 1:** Overview Simdist methods.

A gas chromatographic (GC) technique, Simulated Distillation (SimDist) reproduces the physical distillation of petroleum materials and products by determining boiling point distribution. Bruker's range of Simulated Distillation Analyzers are designed to meet all industry standard methods, Bruker's analyzer software includes both ASTM D86 and ASTM D1160 correlations. Bruker's highly automated GC, CompassCDS Chromatography Data Handling Software, and integrated SimDist software are also designed to meet worldwide industry standard test methods.


436-GC with Sampler

## Key Benefits Include:

- Accurate boiling point distribution up to 750°C
- Integrated standard test methods, applications fully comply with ASTM, IP, DIN and ISO standard test methods
- Complete, single vendor solution
- Complete control from initial setup to final report
- ASTM D86 and ASTM D1160 correlation

## Built-in Reports:

Bruker's SimDist software provides a wide variety of report options to meet specific requirements including;

- Chromatogram with merged corrected blank analysis and IBP/FBP marks versus retention time
- Boiling point versus percentage of sample
- Table and plot with retention time versus boiling point
- D86 and D1160 correlations
- DIN Noak and motor oil volatility reports
- Table with cut points and fractions plus residue analysis with recovery calculation up to C120

# Hydrocarbon Analysis by Group (PIONA+™)

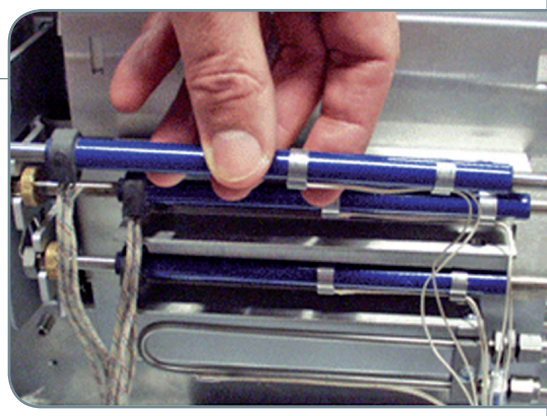


**Figure 1:** Traps are easily accessible and do not require any tools to install or replace.

## Characterization of Engine Fuels by Hydrocarbon Group Type

Bruker's PIONA+™ Analyzer is a highly flexible GC analysis platform to obtain comprehensive characterization and quantitative information, including hydrocarbon group types, oxygenates and carbon number distribution for spark ignition engine fuels.

## Key Analyzer Capabilities:

- Unparalleled operational flexibility
- Compliant with established standards
- A complete and fully integrated solution
- A powerful analyzer, easy to use, generating outstanding analysis results day after day

The PIONA+ Analyzer performs a complete analysis (as described in ASTM D6839 and similar methods) and provides unprecedented analytical flexibility and simplified operation through the use of a novel approach to column/trap heating and exchange (Figure 1).

## Reduced Analysis Time and Increased Sample Throughput Efficiency through the Use of "Concurrent" Heating

A unique aspect of the design of the Bruker PIONA+ system is the ability to independently heat the individual traps.

This has 2 major operational benefits:

- Enhanced elution integrity for wide range sample
- Significantly Reduced Analysis Time

The independent and concurrent heating design permits greater trap control and benefits in improved elution integrity of the component groups e.g napthene, iso-paraffins and n-paraffins even for a wide range sample (C4 - C11). In addition, only a single Molsieve column temperature cycle is employed thus reducing the analysis time by almost half allowing a "fast" PIONA mode of operation (see figures 2 and 3).

By employing this technique, sample throughput can be nearly doubled compared to systems that do not offer this unique capability.

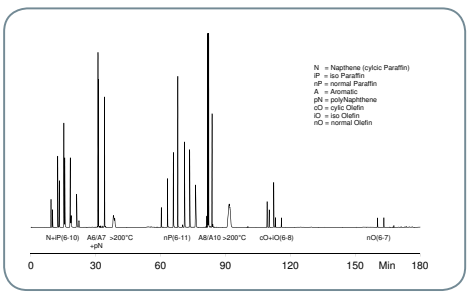



**Figure 2:** Chromatogram of a test mix in conventional PIONA mode. (Analysis Time - 180mins)

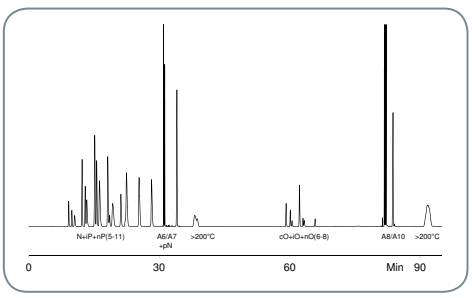



**Figure 3:** Chromatogram of a test mix using concurrent heating in "fast" PIONA mode. (Analysis Time = 95mins)

# Determining Total Olefin Content Is Now Practical

The stability, sample loading and lifetime for all of the critical chromatographic components have been improved and optimized in the Bruker PIONA+ Analyzer. Of special and particular note is the improvement in increasing the sample loading capacity of the "olefin" trap. As a result, it is now possible to analyze streams with olefin content as high as 35-40% or more. This makes it practical to employ a single analytical method to obtain total olefin content (Table 2).

**Table 2**

| | Saturates | | | Unsaturates | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Carbon | Cyclic | Iso | Normal | Cyclic | Iso | Normal | Aromatics | Oxygenates | Total |
| 3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 4 | 0.00 | 0.00 | 0.06 | 0.00 | 0.03 | 0.54 | 0.00 | 0.00 | 0.63 |
| 5 | 0.31 | 11.37 | 2.98 | 0.87 | 9.92 | 7.58 | 0.00 | 0.00 | 33.03 |
| 6 | 3.19 | 9.98 | 1.40 | 2.40 | 8.59 | 4.40 | 1.72 | 0.00 | 31.68 |
| 7 | 4.31 | 6.77 | 0.00 | 2.14 | 4.76 | 1.91 | 7.47 | 0.00 | 27.36 |
| 8 | 1.42 | 3.12 | 0.00 | 0.39 | 2.06 | 0.00 | 0.07 | 0.00 | 7.06 |
| 9 | 0.01 | 0.00 | 0.00 | 0.04 | 0.02 | 0.00 | 0.03 | 0.00 | 0.10 |
| 10 | 0.01 | 0.00 | 0.00 | 0.09 | 0.00 | 0.03 | 0.01 | 0.00 | 0.14 |
| 11 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **Total** | **9.25** | **31.24** | **4.44** | **5.93** | **25.38** | **14.46** | **9.30** | **0.00** | **100.00** |

Example weight % report for a Naphtha sample with high (46%) olefinic content; (highlighted in blue).

The analyzer design allows the operator to conduct analyses in any one of a number of different operational modes including PNA, PONA, PIONA, O-PONA and O-PIONA in standard and concurrent heating configuration. The system is compliant with established standard methods (see adjacent array).

| | PNA | PONA | PIONA | O-PONA | O-PIONA |
|---|---|---|---|---|---|
| EN 14517 | | | | | ✓ |
| EN-ISO-22854 | | | | | ✓ |
| ASTM D6839 | | | | ✓ | |
| DIN 51448-2 | | | ✓ | | |
| ASTM D1319 (FIA) | | ✓ | | | |
| DIN 51448-1 | ✓ | | | | |
| ASTM D5443 | ✓ | | | | |
| UOP 870 | ✓ | | | | |
| IP 382 | ✓ | | | | |

✓ Compliant with the method

More information generated than required for the method

# Detailed Hydrocarbon Analyzer

The DHA Analyzer is a complete high resolution GC solution for the analysis of hydrocarbons in petroleum streams. It is capable of performing all of the standard methods including ASTM D6729, D6730, D6733, D5134, D6623, IP 344/ DHA "Front End" and "Fast DHA".

Although each DHA analyzer is configured, tested and certified at the factory for a standard method specified by the customer, the DHA software permits the operator to utilize any of the other popular standard methods as well. And, because of the outstanding performance and flexibility of the Bruker GC and CompassCDS software design, Bruker is able to quickly modify the existing methods or add new ones if required as a result of the on-going dynamic industry standard processes.

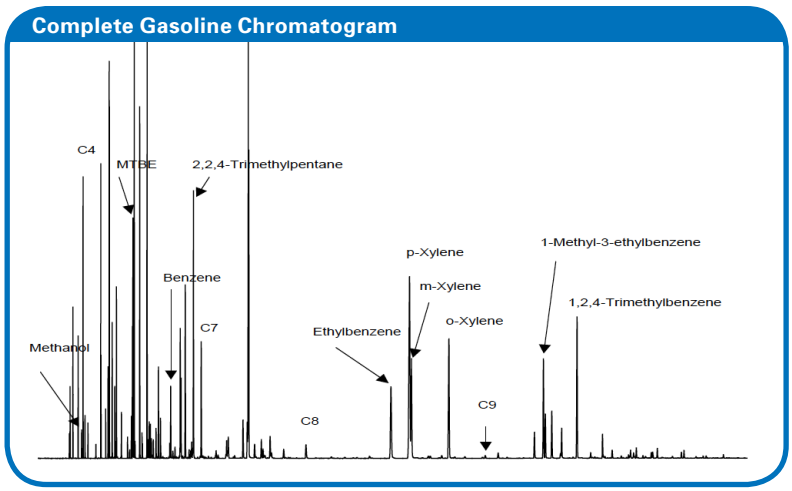



**Figure 4:** The analysis of permanent gases and hydrogen using the Rapid RGA.

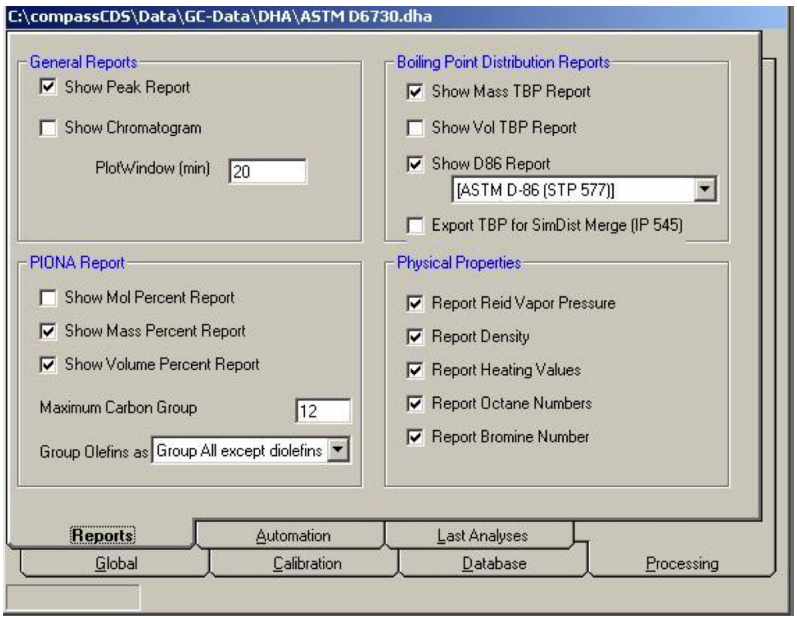



**Figure 5:** Report selection output.

# Bruker Refinery Gas Analyzers

## Peak Identification

1. Hydrogen
2. Carbon Dioxide
3. Hydrogen Sulfide
4. Oxygen
5. Nitrogen
6. Carbon Monoxide
7. Methane
8. Ethane
9. Ethylene
10. Propane
11. Cyclo Propane
12. Propylene
13. i-Butane
14. n-Butane
15. Propadiene
16. Acetylene
17. t-2-Butene
18. i-Butene
19. c-2-Butene
20. i-Pentane
21. n-Pentane
22. 1, 3-Butadiene
23. Propyne
24. Butyne
25. C6+
26. Helium

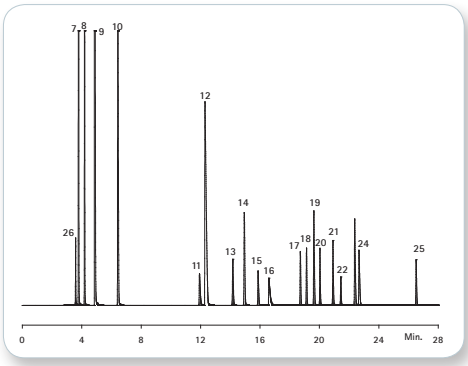



**Figure 6:** The separation of light hydrocarbons using the Standard RGA.

The source and composition of refinery gases varies considerably. Measuring gas composition precisely and accurately is a significant challenge in today's refinery operations. Bruker's Refinery Gas Analyzers (RGA) are designed to deliver superior, reliable results for a wide range of sources and analysis throughput requirements.

## Key Benefits:

- Pre-configured and tuned
- Standard methods including UOP 539, DIN-51666 and ASTM D2163
- Integrated micro-gasifier ensures complete vaporization of LPGs and high pressure samples to prevent sample discrimination (option)
- Multi-channel approach

| Characteristics | Standard RGA | Rapid RGA |
|---|---|---|
| No. of Channels/Detectors Used | 3 | 3 |
| No. of Column Ovens | 1 | 2 |
| Analysis Time | 25 min | 5 min (7 min with $H_2S$) |
| Repeatability | <1% | <1% |
| Linear Bench Space Required | 66 cm/26 in. | 66 cm/26 in. |
| Minimum Component Detection Level | 0.01% all components except $H_2S$ = 0.05% | 0.01% all components except $H_2S$ = 0.05% |
| **Suitability** | | |
| Typical Refinery Gas | Excellent | Excellent |
| Impurities in Bulk Ethylene | Excellent | Excellent |
| Impurities in Bulk Propylene | Excellent | Good |
| Impurities in Bulk C4 | Good | Good |

**Table 3:** Standard RGA vs Rapid RGA.

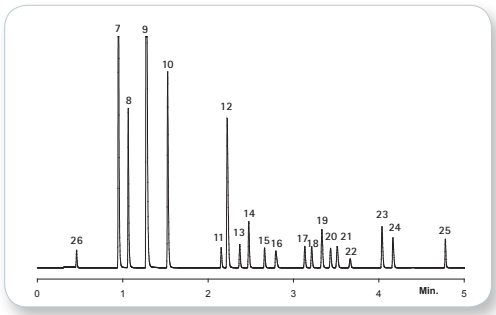



**Figure 7:** The analysis of light hydrocarbons using the Rapid RGA, with complete separation in less than five minutes.

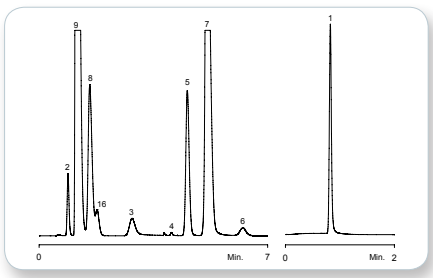



**Figure 8:** The analysis of permanent gases and hydrogen using the Rapid RGA.

## Bruker Offers Two RGA Systems to Meet the Widest Range of Analysis Requirements:

### Standard RGA:

A three channel multi-valve design using both capillary and packed columns.

Channel 1 - Analysis of permanent gases
Channel 2 - Light hydrocarbons
Channel 3 - Hydrogen.

Total analysis time for all components in 25 minutes.

### Rapid RGA:

The Standard RGA packed columns in the hydrogen and permanent gas channels are replaced by micro packed columns and installed in a separate column oven. Key benefits of this design are:

- Flexibility
- Reduced Analysis Time - 5mins (with $H_2S$ - 7mins)
- Increased Sample Throughput

# Low Level Oxygenates Analyzer

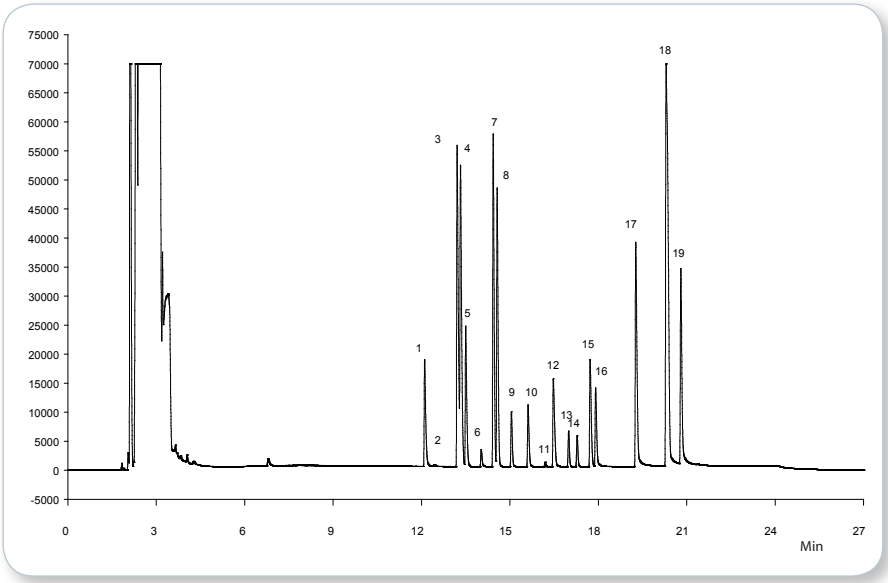



**Figure 9:** Typical chromatogram showing a wide range analysis of a liquid sample stream.

The determination of sub to high ppm levels of ethers, alcohols, aldehydes and ketones in different hydrocarbon matrices is a recurring challenge in the petroleum refining and petrochemical industry. The Bruker Low Level Oxygenates Analyzer is an easy to use solution to meet this challenge and is according ASTM D7423.

The Low Level Oxygenates Analyzer is designed and optimized to quantify ppm and sub ppm levels of ethers (e.g. DME, MTBE, ETBE, DIPE), alcohols (e.g. methanol, ethanol, propanol), ketones (e.g. acetone, MEK) and aldehydes in various hydrocarbon matrices. In general, all oxygenated components with a boiling point of up to 100°C can be analyzed and the sample can be a gas, LPG or liquid under ambient conditions with a final boiling point up to 250°C.

The system is comprised of a Bruker GC configured with gas and liquid sampling valves, two high performance capillary analysis columns, digitally controlled pneumatics including a 'fluidic' switch and Flame Ionization Detector (FID). An optional 'pressure station' can be added to eliminate the possibility of losing sample due to evaporation when analyzing LPG. The GC is controlled via the CompassCDS Chromatography Data Handling Software, which acquires data, processes it and generates analyses reports.

### Peak Identification

1. Diethylether
2. Acetaldehyde
3. Ethyl tert. Butyl ether
4. Methyl tert. Butyl ether
5. Diisopropylether
6. Propanal
7. tert amyl methyl ether
8. Propylether
9. Isobutyraldehyde
10. Butyraldehyde
11. Methanol
12. Acetone
13. Isovaleraldehyde
14. Valeraldehyde
15. 2-Butanone
16. Ethanol
17. 1-Propanol
18. tert Butyl alcohol & Isobutanol
19. 1-Butanol

# Bruker 4815 GC Oxygenates Analyzer

The Bruker 4815 GC Analyzer provides a highly cost effective solution for the analysis of oxygenates in gasoline, according to the widely used industry standard method ASTM D4815. The combination of Bruker's reliable GC hardware, powerful software and industry leading pre- and post-sales support teams make this analyzer package the most comprehensive solution available today.

Oxygenated compounds can be present in various hydrocarbon matrices either because they were purposely added (e.g. into gasoline), because they are naturally present, or formed during catalytic processes such as polymer production. In gasoline, oxygenated compounds are added as 'anti-knock' agents to increase the octane number and decrease emissions by replacing organo-lead compounds.

The type and concentration of oxygenated compounds must be measured in reformulated gasolines as part of ongoing product quality assessment, and to confirm the oxygenated components have been added in the correct amounts according to regulatory requirements (e.g. California Air Resources Board).

ASTM D4815 is frequently chosen as the standard method for the determination of oxygenated compounds. Individual ethers and alcohols are quantified in gasoline including: MTBE, ETBE, TAME, DIPE, C1-C4 alcohols and tert-amylalcohol. Individual ether components are measured from 0.1 to 20.0 mass %.The individual alcohols are measured from 0.1 to 12.0 mass %.

456-GC with Sampler

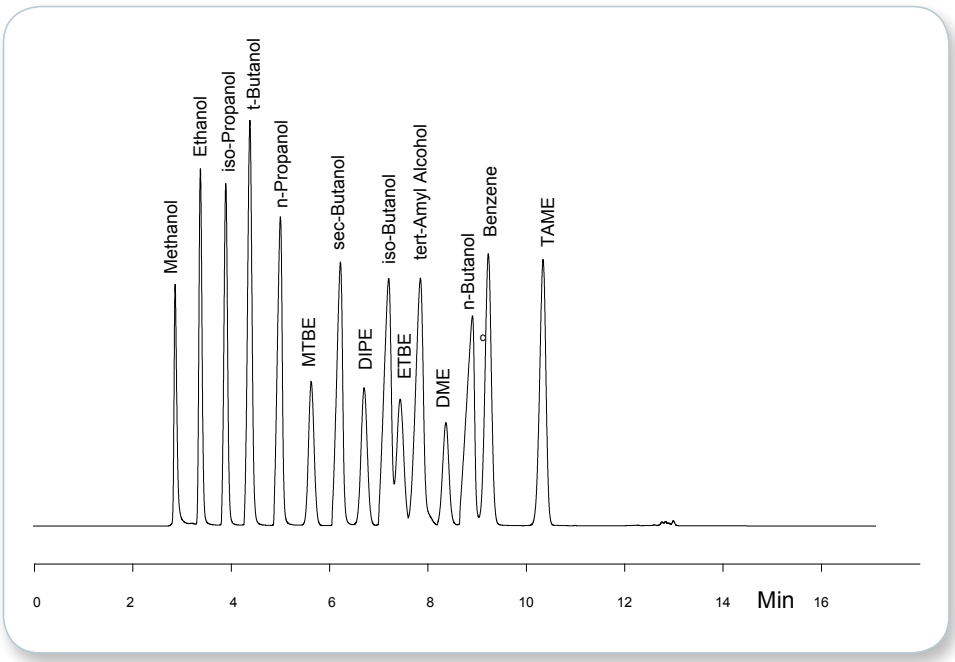



**Figure 10 :** Typical Chromatogram of the test sample.

# Trace Impurity Analyzers

## Sulfur Components in LPGs

Low level analysis of sulfur containing components such as $H_2S$, COS and mercaptanes is extremely challenging and a configured GC offers the solution.

Firstly, the system employs a micro-gasifier enabling the direct coupling of an LPG stream. Secondly, an inert steel sample path ensures a trouble free analysis of sulfur containing components at low concentrations. Finally, a two channel PFPD/ two column approach permits the analysis of all components of interest in one run whatever the LPG matrix. Two differing columns ensures quenching of PFPD signal by the matrix is overcome and full sulfur component analysis is achieved. Figures 11 and 12 show chromatograms obtained in a propane matrix and illustrates the novel benefits of the 2 channel approach.

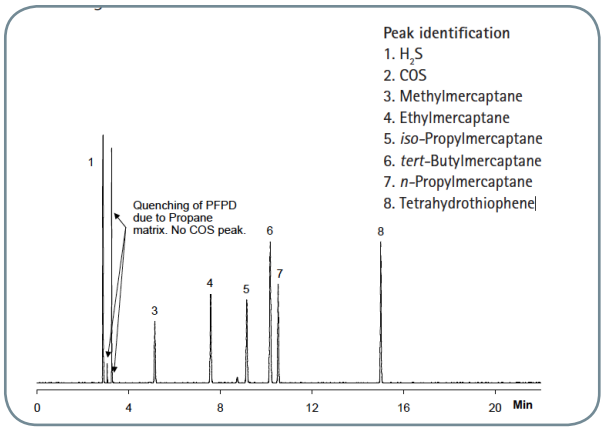



**Figure 11:** Sulfur components in propane, BR-1 column.

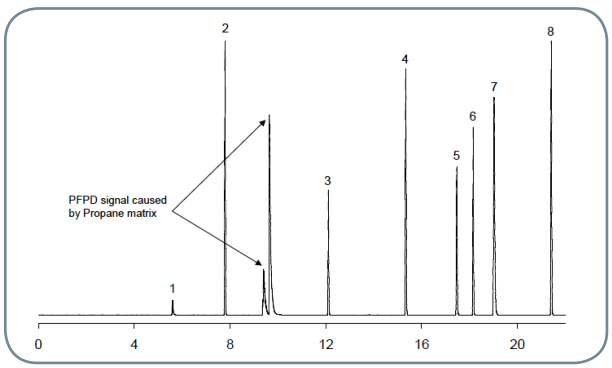



**Figure 12:** Sulfur components in propane, BR-Q PLOT.

## Permanent Gases in LPGs

Impurities such as CO, $CO_2$, $H_2$, $O_2$ and $N_2$ need to be determined at low levels in LPGs. Complete separation of these components is done using a two channel single detector (PDHID) system. The GC employs a permanent gas channel for analyzing $H_2$, $O_2$, $N_2$, $CH_4$ and CO and a specific second channel for the analysis of $CO_2$. A gasifier is used as a sample introduction device thus giving the capability of handling LPG samples C2 through C4.

Detection limits are at the ppb level (Figure 13), depending on the component of interest.

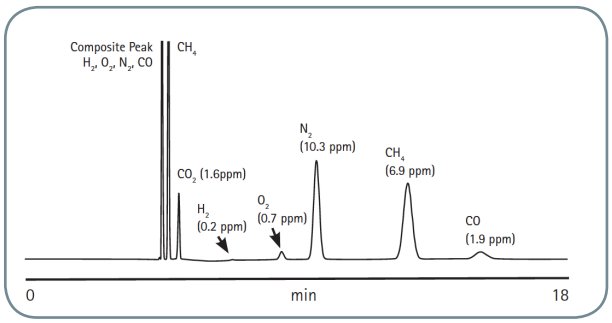



**Figure 13:** LPG sample.

# Total Characterization of Ethylene Impurities

For a total characterization of impurities in ethylene and also propylene six GC channels are required. By coupling two Bruker GCs with three channels each, a comprehensive solution is available for analyzing these components. The channels used in this analyzer are analytical tools principally developed for the determination of different gases in various hydrocarbon types of gaseous matrices.

## GC-1

- $H_2$ Channel (TCD)
- $O_2/N_2$ Channel (TCD)
- CO, $CO_2$ Channel (Methanizer/FID)

## GC-2

- Light Hydrocarbon Channel (FID)
- Oxygenates Channel (FID)
- Sulfur Channel (PFPD)

The results (see figures 14 to 19) demonstrate how this 6 channel system is perfectly suited for the total characterization of ethylene and its impurities.

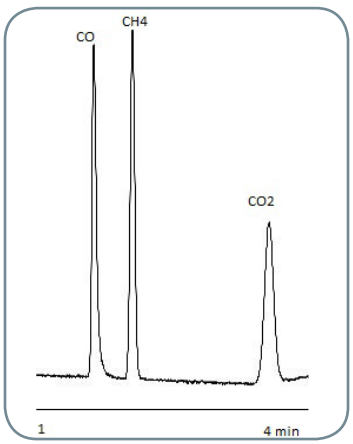



**Figure 14:** CO, $CH_4$ and $CO_2$ on GC-1.

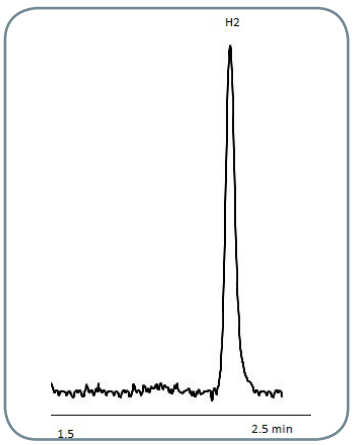



**Figure 15:** $H_2$ on GC-1.

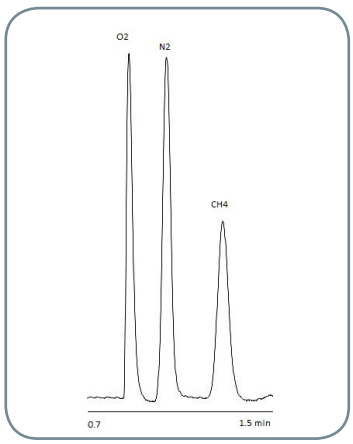



**Figure 16:** $O_2$ and $N_2$ on GC-1.

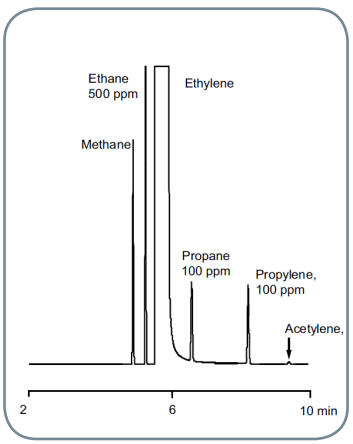



**Figure 17:** Light hydrocarbons on GC-2.

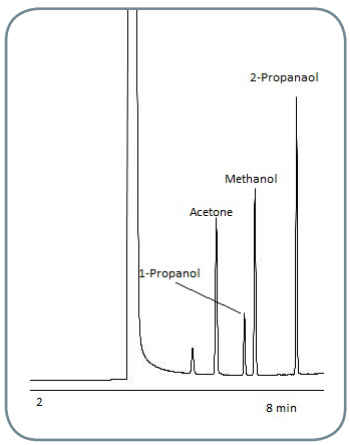



**Figure 18:** Oxygenates on GC-2.

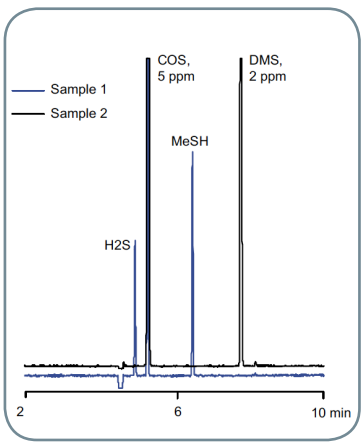
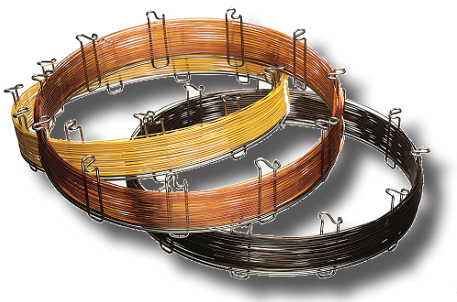



**Figure 19:** Sulfur components on GC-2.

# Bruker-Certified Consumables for Your SCION GC Series

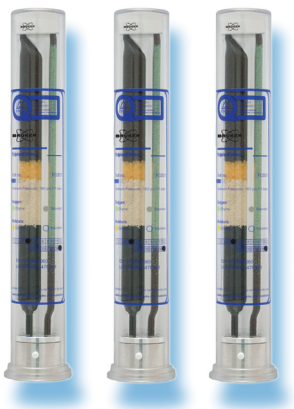
Bruker GC columns span a broad range of column diameters, stationary phases, and capillary column materials: Fused Silica (FS) and Inert Steel (IS). Ideal for either routine or research type analyses.



Bruker GC column offerings bridge across many important applications (like ASTM, UOP, ISO, GPA and EN) and include a number of offerings such as:

- Standard WCOT (Wall Coated Open Tubular)
- Solid Stationary Phase PLOT (Porous Layer Open Tubular)
- Inert Steel Micro-Packed and Packed

## Super Clean™ Gas Filters



Bruker Gas Purification Systems have the range to satisfy your needs from individual to combination filters, from Ultra purity combined with Ultra capacity, to all in one solution kits. Innovative features designed into the product yield extensive benefits to the user.

- Ultra-high capacity for long life, less change and improved productivity
- High-purity output ensures 99.9999% Pure Gas
- "Quick connect" fittings for easy, leak-tight filter changes
- Glass internals prevent diffusion; plastic externally for safety
- Easy-to-read indicators for planned maintenance and improved up-time

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

www.ScionHasArrived.com

www.GlobalEnergyTesting.com

**www.bruker.com/scion**

The New Precision Gas Generators for GC Instruments

# First we made them multi task...then we conquered space.

At Peak Scientific we understand the needs of laboratories and the people who work in them. The lab is a unique environment demanding precision, accuracy, reliability and design steeped in functionality.

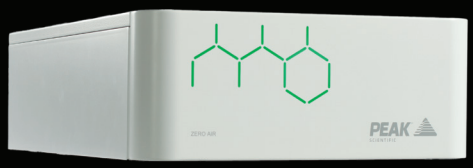
**PEAK SCIENTIFIC. GO WITH THE FLOW.**


PEAK SCIENTIFIC

# Peak expertise defined by our Precision

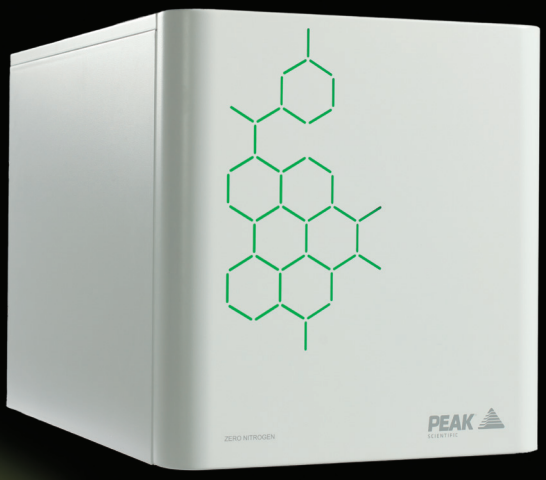
Leading the way in gas generation for over a decade, we expertly designed a new system solution that can be tailored to any GC laboratory's needs.

Our global presence allows us to support our customers quickly and effectively.  No matter where you are, you will benefit from our outstandingly fast response time and a track record of 95% first time fixes!




Zero Air


Nitrogen



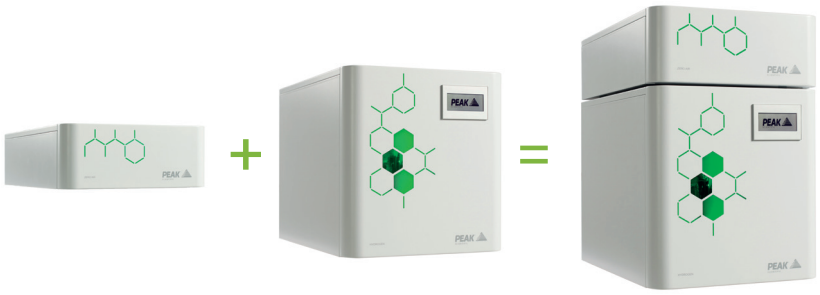

Nitrogen Trace


Hydrogen

# Why Precision?

- Modular system offering a GC gas supply solution specific to your lab
- Space saving stackable design allowing you to make the most of your lab space
- Combinations available for single GC and multiple GC applications
- Eliminates the inconvenience of gas cylinders, no more changing over, no more supply issues, no safety worries
- Very low maintenance throughout the range
- Long term cost stability
- Precision systems only utilize technology with a proven track record of safety and reliability
- Stylish lighting feature to indicate generator status

# Bespoke Combinations



Zero Air + Hydrogen

Zero Air + Nitrogen + Hydrogen Trace

Zero Air + Nitrogen Trace

# Which Precision System is right for you?

More often than not, which generator model we recommend comes down to the 'limit of detection' you are looking for in your GC results. The lower the limit of detection, the purer the gases need to be as you will be looking for the lowest possible baseline to achieve the most precise results.

This is why Peak Scientific offers a Standard Analysis Gas Generator as well as a Trace Analysis Gas Generator solution.

Gas Generator recommendation by Detection Limit:

| **Detection Limit** | **Gas Generator Purity Recommendation** |
|---|---|
| 0 - 1 ppm | Trace Analysis Purity Solution |
| 1 - 1000 ppm | Trace Analysis Purity Solution |
| 1000ppm - 1% | Standard Analysis Solution |
| 1% - 100% | Standard Analysis Solution |

Hydrogen - Trace Analysis Solution

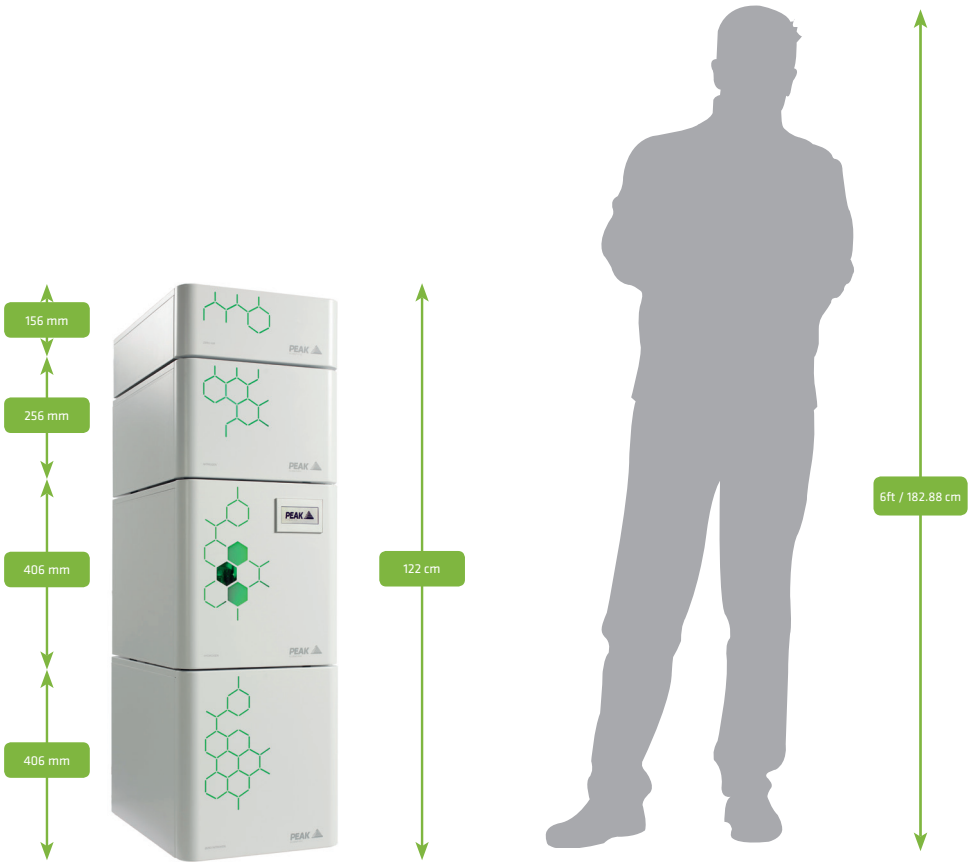
| | |
|---|---|
| Hydrogen Purity | 99.9999% |
| Moisture Content | <1ppm |
| Flow Rate Options | 500cc/min |
| Delivery Pressure | 0- 100psi/ 0- 6.9 bar |
| Water Purity Requirements | < 1.0 µS-cm Conductivity /<br>> 1.0M Ω-cm Resistivity |
| Electrical Requirements | 110-230V, 360VA |
| Dimensions | H = 406mm W = 380mm D = 539.5mm |

- Suitable for Carrier Gas and Flame Gas at trace detection limits
- Proven PEM Technology to generate Hydrogen safely and reliably
- Regenerative PSA Dryers to ensure highest level of purity
- Automatic loading pump as standard
- Maintenance limited to replacing de-ionizer cartridge
- Short and easy start-up and shutdown procedures
- Small and stackable
- Creates Hydrogen on demand, minimal storage of Hydrogen in the system
- Internal leak detection with automatic shutdown features
- Series option to combine multiple units for higher flow requirements
- Remote shutdown
- GC In Oven Hydrogen Leak Detector available as an optional extra

Hydrogen – Standard Analysis Solution

| | |
|---|---|
| Hydrogen Purity | 99.9995% |
| Flow Rate Options | 100, 200, 300, 450cc/min |
| Delivery Pressure | 0- 100psi/ 0- 6.9 bar |
| Water Purity Requirements | < 1.0 µS-cm Conductivity /<br>> 1.0M Ω-cm Resistivity |
| Electrical Requirements | 110-230V, 360VA |
| Dimensions | H = 406mm W = 380mm D = 539.5mm |

- Suitable for Carrier Gas and Flame Gas at standard detection limits
- Proven PEM Technology to generate Hydrogen safely and reliably
- Desiccant Dryers to ensure high level of purity
- Automatic loading pump as standard
- Maintenance limited to replacing de-ionizer cartridge and silica gel
- Short and easy start-up and shutdown procedures
- Small and stackable
- Creates Hydrogen on demand, minimal storage of Hydrogen in the system
- Internal leak detection with automatic shutdown features



## Nitrogen - Trace Analysis Solution

| | |
|---|---|
| Nitrogen Purity | 99.9995% |
| Hydrocarbon Content (as methane) | <0.05ppm |
| Flow Rate Options | 250, 600cc/min |
| Delivery Pressure | 0-80psi |
| Inlet Air Requirements | Minimum 35 l/min at 120-145psi |
| | Or Peak Precision Compressor |
| Electrical Requirements | 110/230V, 504VA |
| Dimensions | H = 406mm W = 380mm D = 539.5mm |

- Suitable for Carrier Gas and Make Up Gas at trace detection limits
- Generates Zero Nitrogen on demand from compressed air
- Regenerative CMS columns remove Oxygen and moisture
- Catalyst chamber to remove Hydrocarbons (as methane) to <0.05ppm
- Ultra fast start-up time
- Minimum maintenance with an annual filter change
- Small and stackable

## Nitrogen - Standard Analysis Solution

| | |
|---|---|
| Nitrogen Purity | 99.9995% |
| Flow Rate Options | 250, 600, 1,000cc/min |
| Delivery Pressure | 0-80psi |
| Inlet Air Requirements | Minimum 35 l/min at 100-120psi |
| | Or Peak Precision Compressor |
| Electrical Requirements | 110-230V, 41VA |
| Dimensions | H = 406mm W = 380mm D = 539.5mm |

- Suitable for Carrier Gas and Make Up Gas at standard detection limits
- Generates Nitrogen on demand from compressed air
- Ultra fast start-up time
- Minimum maintenance with an annual filter change
- Small and stackable

## Zero Air - Trace and Standard Analysis Solution

| | |
|---|---|
| Hydrocarbon Content (as methane) | <0.05ppm |
| Particles | <0.01µm |
| Flow Rate Options | 1,500, 3,500cc/min |
| Delivery Pressure | 0-80psi |
| Inlet Air Requirements | Minimum 1.5 or 3.5 l/min at 90-145psi |
| | Or Peak Precision Compressor |
| Electrical Requirements | 110/230V, 144VA |
| Dimensions | H = 156mm W = 380mm D = 539.5mm |

- Generates Zero Air on demand from compressed air
- Catalyst chamber to remove Hydrocarbons (as methane) to <0.05ppm
- Minimum maintenance with an annual filter change
- Small and stackable

## Compressed Air

| | |
|---|---|
| Electrical Requirements | 110/230, 564VA |
| Dimensions | H = 406mm W = 380mm D = 539.5mm |

- Suitable for a variety of Precision Generator combinations
- Minimal noise emission due to insulated compressor compartment
- Minimal vibration through especially developed compressor anti-vibration mounts
- Compressor service indication
- Serviceable compressor

| Model Description | 110v | 230v | Annual Service Kit |
|---|---|---|---|
| Precision Nitrogen Trace, 250cc | 62-0251 | 62-0250 | 08-3613 |
| Precision Nitrogen Trace, 600cc | 62-0601 | 62-0600 | 08-3613 |
| Precision Zero Air, 1.5L | 60-1501 | 60-1500 | 08-3611 |
| Precision Zero Air, 3.5L | 60-3501 | 60-3500 | 08-3611 |
| Precision Air Compressor | 65-1555 | 65-0555 | 08-8343 |

| Model Description | 110/230v | Annual Service Kit |
|---|---|---|
| Precision Nitrogen, 250cc | 61-0250 | 08-3612 |
| Precision Nitrogen, 600cc | 61-0600 | 08-3612 |
| Precision Nitrogen, 1L | 61-1000 | 08-3612 |
| Precision Hydrogen, 100cc | 63-0100 | 08-3609 |
| Precision Hydrogen, 200cc | 63-0200 | 08-3609 |
| Precision Hydrogen, 300cc | 63-0300 | 08-3609 |
| Precision Hydrogen, 450cc | 63-0450 | 08-3609 |
| Precision Hydrogen Trace, 500cc | 64-0500 | 08-3610 |

Standard Maintenance Plan 09-3110
Complete Maintenance Plan 09-3010

Website: www.peakscientific.com
Email: precision@peakscientific.com

Product Accreditation:

CE

## Our Locations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**Fax:** +1-978-608-9503


For a full list of our worldwide office locations, please visit:
www.peakscientific.com/contact


PEAK SCIENTIFIC

# SCION™ GC Series

- The Gas Chromatographers Choice for Separations

GAS CHROMATOGRAPHY

Innovation with Integrity

# Innovation in Gas Chromatography

Bruker's long tradition of innovation and product reliability have combined to create the next generation of Bruker Gas Chromatographs. By understanding and then designing to exceed the most critical performance and reliability needs of GC users, Bruker is delivering systems that are especially for, and all about, the ultimate success of the GC user. The new SCION 436-GC and SCION 456-GC have have been designed to meet the most important user specified requirements – reliable performance, ease of use and simple maintenance.

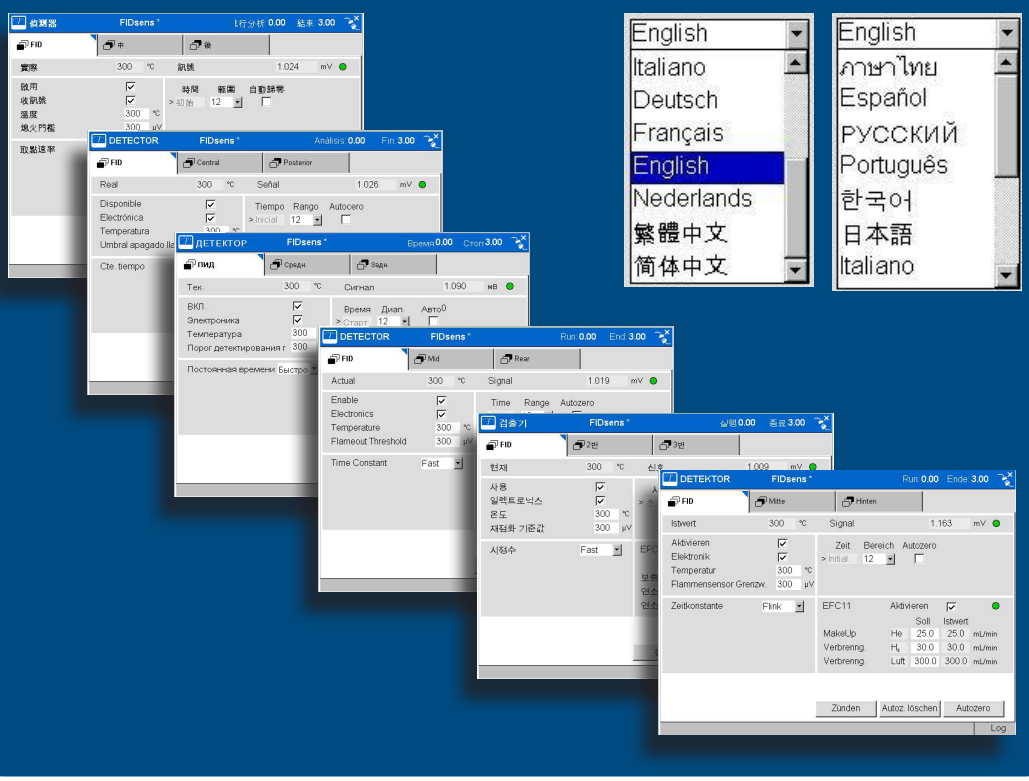
## Local User Interface

This large, high resolution display makes all GC functions accessible via touch screen control and "instant access" buttons. Easy to navigate and adapt it comes available in 13 languages for ease of local training and support.

## Fast, Flexible Detection

Bruker's comprehensive range of detectors deliver industry leading sensitivity, ease of operation and outstanding reliability. And, now all Bruker detectors feature fast sampling data rate (600Hz) for rapid separations and greater analysis throughput.

## Multi-language capability



## SCION 436-GC


## SCION 456-GC

# Enhanced Operator Benefits

Bruker offers a range SCION GCs to meet virtually all application requirements. All SCION GCs are equipped with the convenience of advanced EFC. Whatever the requirement, we have the solution.

### GC Control From Anywhere

The unique embedded control architecture incorporated into the GC enables the use of remote user interface software. This offers the user the ability to control the GC in the exact same way and with the same level of functionality as if they were standing at the GC using the User Interface but from a remote location, even from home.

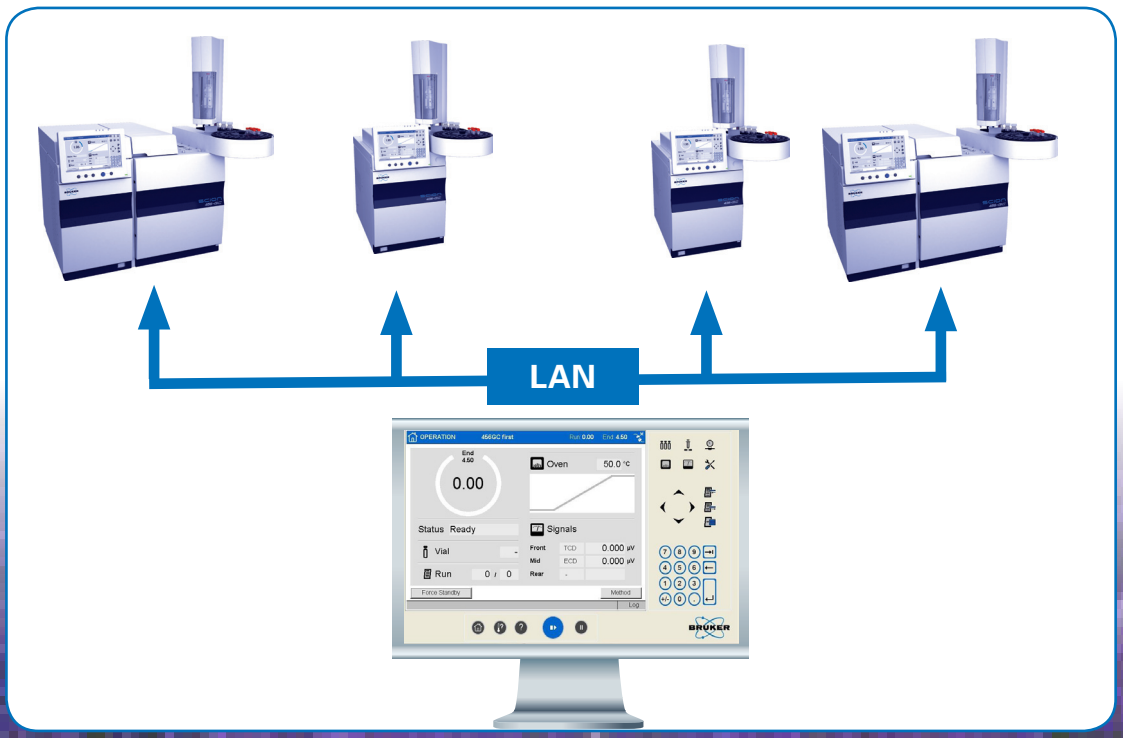
### Gas Saving Capability

Essential to any laboratory is the requirement for cost control. Gas consumption is a major source of operational cost and reduction in gas flow when not necessary is a vital function of any modern GC. Bruker GCs have the necessary functionality to save valuable gas and thus costs.

### Turnkey Analyzer Solutions

Bruker configures and tests GC hardware and software according to widely used industry standard methods (e.g. ASTM, UOP, EN, ISO, GPA), to save its clients time and to ensure confidence in results. Standard analyzers are configured to meet the performance specifications outlined in the method itself. Included in these analyzer packages:

- All hardware
- Software (including special application “plug-ins” when appropriate)
- Pre-installed methods
- Test chromatograms
- Installation/validation data
- User documentation customized to the specific method



## Targeted Solutions for Specific Markets

A series of software customization tools allow users to develop unique calculation modules, that fully integrate with CompassCDS. A large number of standard plug-ins are available that allow special reporting and other post analysis functions. Some examples include:

### Simulated Distillation

Provides automated boiling point distributions for a full range of petroleum products for applications that comply with ASTM, IP, DIN and ISO standard test methods.

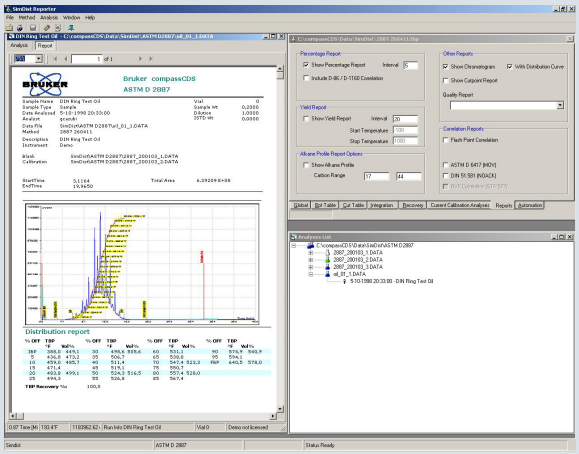
### Detailed Hydrocarbon Analysis

Reports in an automated way the physical properties of gasoline and similar products based on individual components for applications that comply with Bruker developed methods and ASTM, IP and standard test methods.

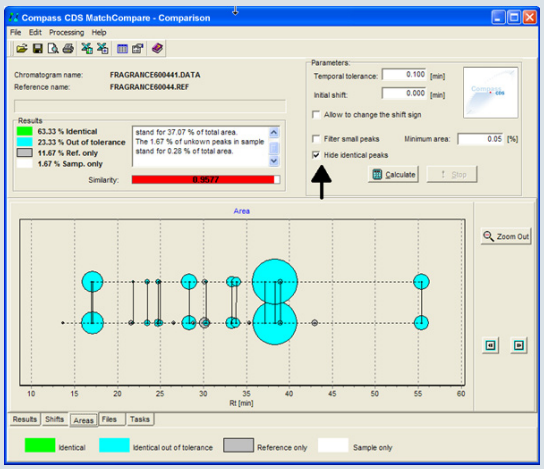
### CompassCDS PeakSynch

Provides rapid visual and quantitative comparison of complex chromatograms and is widely used in the flavor and fragrance industry.

**Simulated Distallation**




**CompassCDS PeakSynch**




OPERATION
FIDsens*
Run 1.95 End 9.50
End 9.50
1.95
Oven
68.5 °C
Status Run
Signals
Front FID 0 µV
Mid -
Rear -
Vial -
Run 0 / 0
Method
Log
Force Standby
BRUKER
SCION 456-GC

# Benefits of the SCION-GC

- Multi-language User Interface
- Full EFC Capability
- High Pressure Injection
- IntelliUpdate
- System Suitability Determination
- CompassCDS Software
- 600 Hz Data Sampling Rate On All Detectors
- Inert GC Sample Path
- Constant Linear Velocity Mode
- Fast Cycle Time

## SCION 436-GC

- Small foot print
- High performance
- Dual channel architecture

## SCION 456-GC

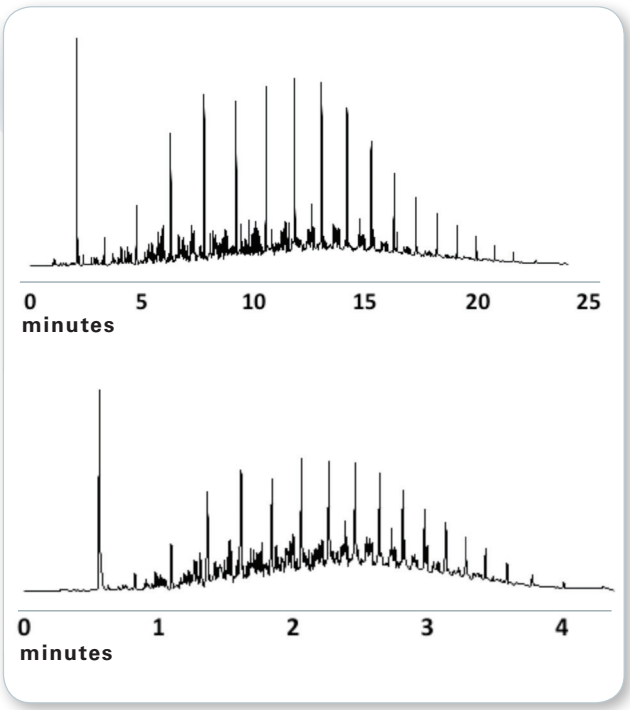
- Solutions platform
- Total flexibility
- Four channel architecture

# Increased Productivity

With over 40 years' experience in gas chromatography, we can provide unrivalled expertise, not only in building robust instruments, but also in creating solutions for ensuring productivity. With total control over design and manufacturing, Bruker ensures the quality and technological excellence of its products is complimented and combined with features that deliver the true benefits of productivity.

**Speed increased with a factor 6.5**

- Small ID from 0.25 to 0.1mm
- Short column from 15 to 4 mtr
- Increased ramp from 10 to 65 °C/min
- Data rate from 25 to 200 Hz

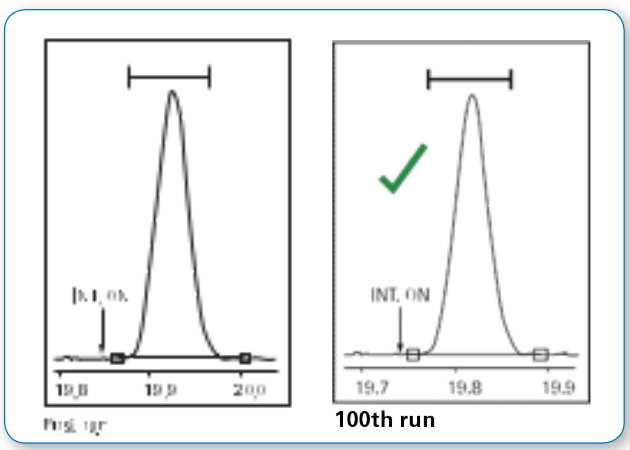



## Fast Cycle Time

The time between injections can considerably improve productivity. The high performance oven incorporating design characteristics that enhances fast heating and cooling ensures maximum productivity. This, in conjunction with high pressure injectors and ultra narrow bore columns will significantly improve and yield fast cycle times without loss of performance (see chromatograms).

## IntelliUpdate

In many cases instrument and system effects (column ageing, matrix, etc.) can cause experimental deviations e.g. retention time. CompassCDS IntelliUpdate function can be used automatically to correct and compensate for such deviations. This unique capability is also done without changing fundamental instrument parameters, maintaining accuracy of results and method continuity.

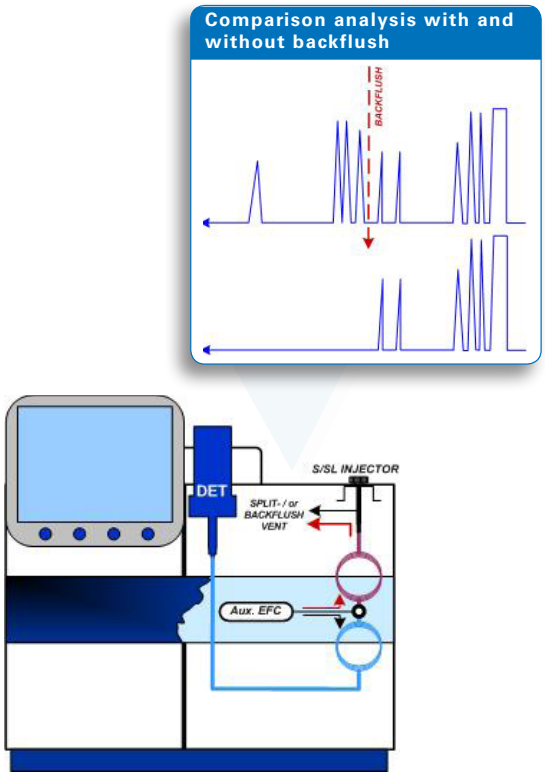


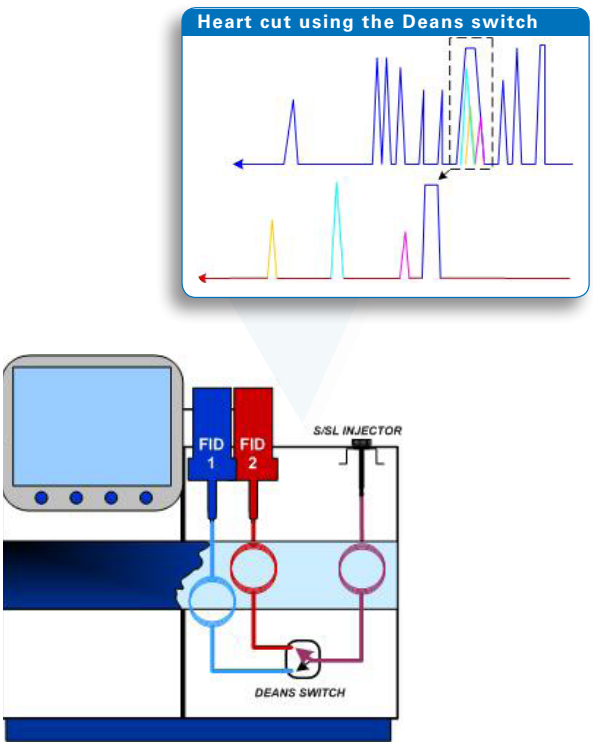
## Optimized Switching Valves

Flow splitting, backflushing and Deans switching are valuable techniques in improving cycle times, analytical performance and the robustness of GC methods. Splitting the flow of column effluent into differing detectors can enhance performance, quantitation and confirmation of targeted compounds.

Backflushing is key to reducing analysis time and column protection. It works on the basis of reversing column flow after peaks of interest have been detected. This eliminates the need for time and temperature segments to elute highly retained components injected with compounds of interest. Reversing the flow elutes these materials out through the split vent of the injector with the added benefit of protecting the column from degradation and contamination.

Backflushing capability also allows column changes and injector maintenance without loss of vacuum in the MS detector.



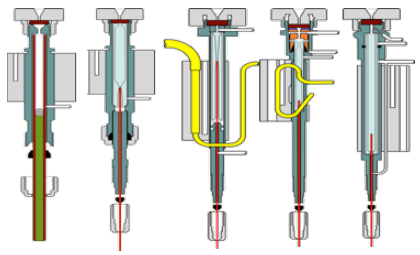

Deans switching enables the use of multiple traps and columns of differing phases in one method/analysis. It is the basis of two dimensional GC and many standard analyzers manufactured by Bruker. Use our expertize to configure the optimum system for you.

# Capability and Automation

Bruker offers an injector and detector range to meet virtually all application and market requirements. All are equipped with the convenience of advanced EFC. Whatever the requirement, be it Split/splitless, Cold-on-Column, Packed, Flash or Programmable Temperature Vapourizing injector with a universal or specific detector we have the solution.

| | Universal | | | | Specific | | |
|---|---|---|---|---|---|---|---|
| | FID | TCD | PHHID | MS | ECD | NPD (TSD) | PFPD |
| Academic | ✓ | ✓ | | ✓ | | ✓ | |
| Enviroment | | | ✓ | ✓ | ✓ | ✓ | ✓ |
| Food Beverage | ✓ | | ✓ | ✓ | ✓ | ✓ | ✓ |
| Forensics Toxicology | ✓ | | | ✓ | | | ✓ |
| Petroleum | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |

Bruker offers a range of differing injector designs for all applications, column dimensions and can be fully automated.



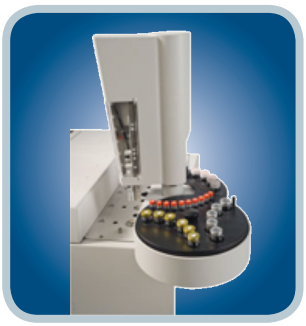
## Injector Selection Guide - Sample/Analysis Characteristics or Requirements

| Trace Analysis | Separation & Speed | Sample Capacity | Wide Range of Analytes | Preferred Column Type | 1st Choice | 2nd Choice |
|---|---|---|---|---|---|---|
| ✓ | | | | Capillary, 0.53 mm ID | Large Volume (LV) | Split/Splitless |
| | ✓ | | | Capillary, 0.1 to 0.53 mm ID | Split/Splitless | Large Volume (LV) SS Mode |
| | ✓ | ✓ | | Capillary, 0.53 mm ID | Large Volume (LV) | |
| | ✓ | | | Capillary, retention gap | Cold On-Column | Large Volume PTV Mode |
| | ✓ | | | Capillary, 0.53 mm ID | Packed | Large Volume (LV) PTV Mode |
| | | | ✓ | Capillary, 0.53 mm ID | Cold On-Column | Large Volume (LV) On-Column Mode |

Regardless of your sample throughput requirements, Bruker can provide an automated solution to meet your needs. Four samplers are available, the CP-8410, CP-8400, the SHS-40 and the PAL Combi-xt. Each is tailored to meet a differing need and workload.

## CP-8400

- High throughput
- 100 x 2ml sample capacity
- Dual/Duplicate Injection
- SPME



## CP-8410

- Flexibility
- Accommodates 2, 5, 10 ml vials
- Low cost/high performance
- Ease of use

## SHS-40

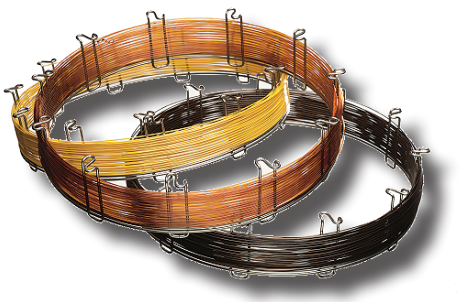
- Fully automated
- Easily Integrated
- Low maintenance
- Sample Loop or Press and Inject configuration

## PAL Combi-xt

- High throughput
- Liquid handling capability
- SPME
- ITEX

# Bruker-Certified Consumables for Your SCION GC Series

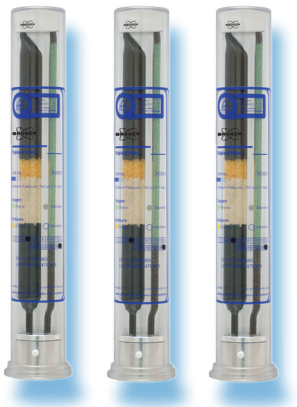
Bruker GC columns span a broad range of column diameters, stationary phases, and capillary column materials: Fused Silica (FS) and Inert Steel (IS). Ideal for either routine or research type analyses.



Bruker GC column offerings bridge across many important applications and include a number of offerings such as:

- Standard WCOT (Wall Coated Open Tubular)
- Solid Stationary Phase PLOT (Porous Layer Open Tubular)
- Inert Steel Micro-Packed and Packed

## Super Clean™ Gas Filters



Bruker Gas Purification Systems have the range to satisfy your needs from individual to combination filters, from Ultra purity combined with Ultra capacity, to all in one solution kits. Innovative features designed into the product yield extensive benefits to the user.

- Ultra-high capacity for long life, less change and improved productivity
- High-purity output ensures 99.9999% Pure Gas
- "Quick connect" fittings for easy, leak-tight filter changes
- Glass internals prevent diffusion; plastic externally for safety
- Easy-to-read indicators for planned maintenance and improved up-time

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

**www.bruker.com/scion**

# SCION™ TQ Premium GC Triple Quadrupole Mass Spectrometer

## Specification Sheet

The SCION TQ Premium is the chromatographer's choice for triple quadrupole mass detector; it is designed to match your most stringent needs for analytical performance and productivity. The SCION TQ Premium offers superior sensitivity and robustness based on the innovative ion optics, and fast and easy methods development for multi-component quantitation following the unique Compound Based Scanning (CBS) approach with MRM library. The SCION TQ Premium GC-MS/MS system defines a new standard of usability for routine analysis and has the smallest bench footprint in the industry.

**Analyzer - MS Specifications**

- Scan modes: Full Scan, Precursor, Product, Neutral Loss/Gain Monitoring, Selected Ion Monitoring (SIM), Multiple Reaction Monitoring (MRM) and Result Dependent Scanning
- Standard ionization mode: Electron Ionization (EI)
- Ion source: Auto-aligning EI source constructed of inert materials
- q0 ion guide: 90° curved RF-only entrance quadrupole with active ion beam focusing and heating at 135 °C
- Source temperature: 100 °C to 350 °C
- Filament and emission current: dual filaments; up to 200 µA
- Electron energy: adjustable from 0 to 150 eV
- Mass filters: quadrupole with pre- and post-filters; high ion transmission efficiency lens-less design
- Collision cell: 180° curved path with pre- and post-filter regions
- Collision cell gas: Argon
- Collision energy: selectable up to 75 eV
- Mass range (m/z): 1 to 1200 Da
- Scan rate: up to 14,000 Da/sec
- Minimum scan time (dwell time): 1 ms
- Maximum acquisition MRM rate: 500 MRM's/sec
- Resolution: user-adjustable from 0.7 Da (Unit) to 4 Da, also with three user-selectable settings (Unit, Standard, Open) on both Q1 and Q3.
- Mass axis stability: <±0.1 Da over 24 hours
- Transfer line temperature: up to 350 °C
- Manifold temperature: 40-50 °C
- Detector: EDR™ Electron multiplier with ±5 kV post acceleration and with on-the-fly multiplier gain optimization for Extended Dynamic Range (EDR); direct ion collection onto multiplier for negative ion detection without dynode loss
- Turbomolecular pump: dual stage, 310/400 L/sec, air-cooled for helium carrier gas flow up to 25 mL/min.
- Foreline pump: dual-stage rotary vane; voltage 120/230V
- Power requirements: 100-240 Vac, 50/60 Hz ±3 Hz, 1200 VA
- Operating environment temperature: 15 °C to 33 °C
- Operating environment humidity: 20% to 80% relative humidity (without condensation)



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**Software**

- Bruker MS Workstation equipped with the Compound Base Scanning (CBS) MRM library for data acquisition, data handling, and reporting
- Optional spectral libraries: NIST, Wiley, and Maurer/Pfleger/Weber (PMW) libraries and with user-customizable libraries and automatic searching of multiple libraries

**Gas Chromatograph (Bruker 436 and 456 Model GC)**
**For more specification on GC, refer to the GC Data Sheet**

- Injectors: Split/Splitless (SSL), Programmable Temperature Vaporization (PTV), etc. Back-flush option available for all injectors.
- Autosamplers: CP 8400; CP 8410; CTC PAL COMBI-xt
- GC Oven Temperature: Ambient+4 °C to 450 °C
- Temperature Ramps/Holds: 24/25
- Pneumatic: Electronic Flow Control (EFC) or Manual (Model 456)
- ChromatoProbe™: Direct introduction of solids, liquids or slurries (requires PTV injector)
- MS Tuning, tune-to-target, pump-down, and venting controlled by multi-language touchpad on the GC.

**Performance Specifications***

| Mode | Test (with SSL injector in hot splitless mode) | Specification† |
|---|---|---|
| EI Full Scan | 1 pg Octafluoronaphthalene (OFN) from m/z 50 to 300 for m/z 272 | S/N ≥600:1 |
| EI SIM | 25 fg OFN for m/z 272 | S/N ≥50:1 |
| EI MRM | 100 fg OFN for m/z 272>222 | S/N ≥2000:1 |
| EI MRM Precision (IDL**) | 8 replicate injections of 50 fg OFN in EI MRM mode (m/z 272>222) | Peak Area RSD ≤ 6.7% (10 fg) |
| PCI Full Scan‡ | 10 pg Benzophenone (BZP) from m/z 80 to 230 for m/z 183 | S/N ≥50:1 |
| PCI SIM‡ | 1 pg BZP for m/z 183.105 | S/N≥50:1 |
| PCI MRM‡ | 100 fg BZP for m/z 183>105 | S/N≥100:1 |
| NCI Full Scan‡ | 1 pg OFN from m/z 200 to 300 for m/z 272 | S/N ≥4000:1 |
| NCI SIM‡ | 10 fg OFN for m/z 272 | S/N ≥300:1 |

* All tests use helium as carrier gas. EI MRM sensitivity test will be used as installation checkout specifications; not all other performance tests are confirmed at installation.
† The Signal-to-Noise ratio S/N values are based on RMS
IDL**: Instrument Detection Limit, defined as IDL=t(0.99, f=7)×S, whereas t(0.99, f=7) is the one-sided student's t-distribution value of 2.998 for 99% of confidence and for degree of freedom 7 (f=n-1, n the number of injections); S is the peak area standard deviation of 8 replicate injections.
‡ CI tests use methane as reagent gas

**Dimensions (H x W x D) and Weight**

- SCION TQ: 45 cm (18 in.) x 28 cm (11 in.) x 57 cm (22.5 in.), 40 kg/88 lb
- 436 GC: 57 cm (23 in.) x 32 cm (13 in.) x 61 cm (24 in.); 27 kg/59 lb
- 456 GC: 57 cm (23 in.) x 66 cm (26 in.) x 56 cm (22 in.); 43 kg/95 lb
- CP-8400/8410 Autosamplers: 40 cm (16 in.) x 22 cm (9 in.) x 47 cm (18 in.); 7 kg/15.3 lb



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# SCION™ TQ Select GC Triple Quadrupole Mass Spectrometer

## Specification Sheet

The SCION TQ Select is the chromatographer's choice for triple quadrupole mass detector; it is designed to match your most stringent needs for analytical performance and productivity. The SCION TQ Select offers superior sensitivity and robustness based on the innovative ion optics, and fast and easy methods development for multi-component quantitation following the unique Compound Based Scanning (CBS) approach with MRM library. The SCION TQ Select GC-MS/MS system defines a new standard of usability for routine analysis and has the smallest bench footprint in the industry.

**Analyzer - MS Specifications**

- Scan modes: Full Scan, Precursor, Product, Neutral Loss/Gain Monitoring, Selected Ion Monitoring (SIM), Multiple Reaction Monitoring (MRM) and Result Dependent Scanning
- Standard ionization mode: Electron Ionization (EI)
- Ion source: Auto-aligning EI source constructed of inert materials
- q0 ion guide: 90° curved RF-only entrance quadrupole with active ion beam focusing and heating at 135 °C
- Source temperature: 100 °C to 350 °C
- Filament and emission current: dual filaments; up to 200 µA
- Electron energy: adjustable from 0 to 150 eV
- Mass filters: quadrupole with pre- and post-filters; high ion transmission efficiency lens-less design
- Collision cell: 180° curved path with pre- and post-filter regions
- Collision cell gas: Argon
- Collision energy: selectable up to 75 eV
- Mass range (m/z): 1 to 1200 Da
- Scan rate: up to 14,000 Da/sec
- Minimum scan time (dwell time): 1 ms
- Maximum acquisition MRM rate: 500 MRM's/sec
- Resolution: user-adjustable from 0.7 Da (Unit) to 4 Da, also with three user-selectable settings (Unit, Standard, Open) on both Q1 and Q3.
- Mass axis stability: <±0.1 Da over 24 hours
- Transfer line temperature: up to 350 °C
- Manifold temperature: 40-50 °C
- Detector: EDR™ Electron multiplier with ±5 kV post acceleration and with on-the-fly multiplier gain optimization for Extended Dynamic Range (EDR); direct ion collection onto multiplier for negative ion detection without dynode loss
- Turbomolecular pump: dual stage, 310/400 L/sec, air-cooled for helium carrier gas flow up to 25 mL/min.
- Foreline pump: dual-stage rotary vane; voltage 120/230V
- Power requirements: 100-240 Vac, 50/60 Hz ±3 Hz, 1200 VA
- Operating environment temperature: 15 °C to 33 °C
- Operating environment humidity: 20% to 80% relative humidity (without condensation)



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**Software**

- Bruker MS Workstation equipped with the Compound Base Scanning (CBS) MRM library for data acquisition, data handling, and reporting
- Optional spectral libraries: NIST, Wiley, and Maurer/Pfleger/Weber (PMW) libraries and with user-customizable libraries and automatic searching of multiple libraries

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- Autosamplers: CP 8400; CP 8410; CTC PAL COMBI-xt
- GC Oven Temperature: Ambient+4 °C to 450 °C
- Temperature Ramps/Holds: 24/25
- Pneumatic: Electronic Flow Control (EFC) or Manual (Model 456)
- ChromatoProbe™: Direct introduction of solids, liquids or slurries (requires PTV injector)
- MS Tuning, tune-to-target, pump-down, and venting controlled by multi-language touchpad on the GC.

**Performance Specifications***

| Mode | Test (with SSL injector in hot splitless mode) | Specification† |
|---|---|---|
| EI Full Scan | 1 pg Octafluoronaphthalene (OFN) from m/z 50 to 300 for m/z 272 | S/N ≥600:1 |
| EI SIM | 25 fg OFN for m/z 272 | S/N ≥50:1 |
| EI MRM | 100 fg OFN for m/z 272>222 | S/N ≥2000:1 |
| EI MRM Precision (IDL**) | 8 replicate injections of 50 fg OFN in EI MRM mode (m/z 272>222) | Peak Area RSD ≤ 6.7% (10 fg) |

* All tests use helium as carrier gas. EI MRM sensitivity test will be used as installation checkout specifications; not all other performance tests are confirmed at installation.
† The Signal-to-Noise ratio S/N values are based on RMS
IDL**: Instrument Detection Limit, defined as IDL=t(0.99, f=7)×S, whereas t(0.99, f=7) is the one-sided student's t-distribution value of 2.998 for 99% of confidence and for degree of freedom 7 (f=n-1, n the number of injections); S is the peak area standard deviation of 8 replicate injections.

**Dimensions (H x W x D) and Weight**

- SCION TQ: 45 cm (18 in.) x 28 cm (11 in.) x 57 cm (22.5 in.), 40 kg/88 lb
- 436 GC: 57 cm (23 in.) x 32 cm (13 in.) x 61 cm (24 in.); 27 kg/59 lb
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- CP-8400/8410 Autosamplers: 40 cm (16 in.) x 22 cm (9 in.) x 47 cm (18 in.); 7 kg/15.3 lb



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# maXis impact

**Specification Sheet**
**Part Number: # 282000**

maXis impact UHR Time-of-Flight Mass Spectrometer System


| | |
|---|---|
| Size | Bench-top:<br>(Footprint)<br>198cm (Height) |
| Weight | ~ 210 kg |
| Vacuum System | 5 stages, 28 $m^3$/h rough pump |
| Apollo II ion funnel electrospray source | Flow rate: 1 µL/min – 1 mL/min |
| Mass Range | 20 – 40,000 m/z |
| Quadrupole isolation | Up to 3,000 m/z |
| Quadrupole Mass Range | Up to 40,000 m/z |
| Mass accuracy in MS and MS/MS | With internal calibrant: better than 1ppm RMS Error<br>With external calibrant: better than 2 ppm RMS Error |
| Calibration | ONE calibration valid for MS and MS/MS analysis. Calibration is independent from charge state of calibrant mass |
| Mass resolution | 40,000 FSR (full sensitivity resolution) |
| Isotopic pattern | The true isotopic pattern is maintained due to TIP™ technology (True Isotopic Pattern) and allows three dimensional chemical characterizations of analytes via SmartFormula™3D algorithm using exact mass, TIP, and MS/MS fragment data. |
| SmartFormula™3D | Enables unambiguous formula determination at "sub-ppm" confidence level up to 1000 Da. |



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| | |
|---|---|
| Mass stability & dynamic range | hrXIC (high resolution Extracted Ion Chromatogram) technology with better than +/- 1.0 mDa stability on centroid data values over an typical LC peak. |
| Full scan sensitivity in MS | Reserpine 1 pg S/N>100:1 RMS |
| Full scan sensitivity in MS/MS | The signal height obtained from a consumption of 2.5 fmol of Glu-Fibrinopeptide B will be better than 10O counts on the most intense y' sequence ion from the MS/MS spectrum of the doubly charged precursor ion. This shall correspond to a signal to noise ratio better than 50:1. The MS/MS sensitivity specification is met while using quadrupole isolation of the precursor ion demonstrating that there is minimal transmission loss through the isolating quad. ?<br>A solution of 100 fmol/µL Glu-Fibrinopeptide B shall be introduced at a flow rate of 3 µL/min. |
| TOF repetition rate | Up to 20 kHz |
| Temperature compensation | Yes |
| Digitizer | 4Gsample/sec ADC with 32 Gbit/sec |
| Acquisition rate | up to 50 Hz MS<br>50 Hz MS/MS (profile and peak detected spectra to disk) |

## Optional accessory

| | |
|---|---|
| APCI II | Optional accessory |
| APPI II | Optional accessory |
| GC-APCI | Allows for direct GC coupling (Optional accessory) |
| Bruker CaptiveSpray | Optional accessory |
| On-/Off-Line Nanospray | Optional accessory |
| CE/MS interface | With grounded needle for easy CE-TOF set-up (Optional accessory) |
| Bruker EASY-nLC | Split-free nano-flow HPLC system |



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# micrOTOF-Q III

**Specification Sheet**
**Part Number: # 728889**

micrOTOF-Q III  ESI Quadrupole Time-of-Flight Mass Spectrometer System



| | |
|---|---|
| Size | Bench-top: 64 x 95 cm (Footprint)<br>132 cm (Height) |
| Weight | 160 kg |
| Vacuum System | 5 stages, 28 $m^3$/h rough pump |
| ESI dual ion funnel electrospray source | Flow rate: 1 µL/min – 1 mL/min |
| TOF Mass Range | 20 – 40,000 m/z |
| Quadrupole isolation | Up to 3,000 m/z |
| Quadrupole Mass Range | Up to 40,000 m/z |
| Mass accuracy in MS and MS/MS | With internal calibrant: better than 2 ppm RMS Error<br>With external calibrant: better than 5 ppm RMS Error |
| Calibration | ONE calibration valid for MS and MS/MS analysis. Calibration is independent from charge state of calibrant mass |
| Mass resolution (FSR: full sensitivity resolution) | 20,000 (FWHM) @ 922 m/z at full sensitivity |
| Isotopic pattern | The true isotopic pattern is maintained due to TIP™ technology (True Isotopic Pattern) and allows three dimensional chemical characterizations of analytes via SmartFormula™3D algorithm using exact mass, TIP, and MS/MS fragment data. |
| SmartFormula™3D | Enables unambiguous formula determination at "sub-ppm" confidence level up to 1000 Da. |
| Mass stability & dynamic range | hrEIC (high resolution Extracted Ion Chromatogram) technology with better than 2 mDa stability on centroid data values over an typical LC peak. |



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| | |
|---|---|
| ESI sensitivity in MS positive mode | Reserpine 2 pg S/N>100:1 RMS<br>200fg S/N > 100:1 RMS with IonBooster (Option) |
| Full scan sensitivity in MS/MS | The signal height obtained from a consumption of 2.5 fmol of Glu-Fibrinopeptide B will be better than 100 counts on the most intense y' sequence ion from the MS/MS spectrum of the doubly charged precursor ion. This shall correspond to a signal to noise ratio better than 50:1. The MS/MS sensitivity specification is met while using quadrupole isolation of the precursor ion demonstrating that there is minimal transmission loss through the isolating quad. ?<br>A solution of 100 fmol/µL Glu-Fibrinopeptide B shall be introduced at a flow rate of 3 µL/min. |
| TOF repetition rate | Up to 20 kHz |
| Temperature compensation | Yes |
| Digitizer | 2 GSsamples/ses sampling rate with 16Gbit/sec |
| Acquisition rate | up to 40 Hz MS<br>20 Hz MS/MS (profile and peak detected spectra to disk) |

## Optional accessory

| | |
|---|---|
| IonBooster | Optional ion source |
| APCI II | Optional ion source |
| APPI II | Optional ion source |
| GC-APCI | Allows for direct GC coupling (Optional ion source) |
| APLI | Optional ion source |
| CryoSpray | Optional ion source |
| Bruker CaptiveSpray | Optional ion source |
| On-/Off-Line Nanospray | Optional ion source |
| CE/MS interface | With grounded needle for easy CE-TOF set-up (Optional) |
| DIP | Direct Probe (Optional ion source) |





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Application Note # CA-270689

# Typical Detection Limits for the aurora M90 ICP-MS in Normal Sensitivity Mode

## Introduction

Bruker's aurora M90 is the world's first ICP-MS system with tunable gigahertz sensitivity (over $10^9$ cps per mg/L) without compromising oxide and/or doubly charged interference performance, thanks to the patented 90-degree ion mirror [1, 2]. This tunable sensitivity provides the flexibility to choose a suitable sensitivity mode for different sample types or applications, and hence, to achieve the lowest detection limits for a selected application. In this application note, typical instrument detection limits for most elements commonly monitored in environmental analyses are determined using the aurora M90 ICP-MS under normal sensitivity mode.

## Basic principles

### Limit of detection

According to the recommendation given by the International Union of Pure and Applied Chemistry (IUPAC) [3], the limit of detection expressed as the concentration $c_L$ or the quantity $q_L$ is derived from the smallest measure $X_L$ that can be detected with reasonable certainty for a given analytical procedure. The value of $X_L$ is given by the equation,

(1) $X_L = X_{bl} + k\, s_{bl}$

where $X_{bl}$ is the mean of the blank measures, $s_{bl}$ is the standard deviation of the blank measures, and k is a numerical factor chosen according to the confidence level desired. IUPAC has also recommended a value of 3 for k, which gives a confidence level of about 98%. In ICP-MS, the $X_{bl}$ is the mean cps of the blank measurements, and a typical ICP-MS calibration plot can be expressed by the following equation,

(2) $X_A = X_{bl} + m\, C_A$

where $X_A$ is the cps measured at an analyte concentration of $C_A$, and m is the sensitivity (i.e. slope of the calibration plot).

Hence in ICP-MS, the value of $X_L$ can also be given as,

(3) $X_L = X_{bl} + m\, C_L$

From equations (1) and (3), the concentration $C_L$ can be calculated by the following equation,

(4) $C_L = 3\, s_{bl} / m$

### Background Equivalent Concentration

In the Bruker ICP-MS Software, the background equivalent concentration (BEC) is calculated by the following equation,

(5) $BEC = X_{bl} / m$

Hence, the concentration $C_L$ can be calculated alternatively from the BEC and the % relative standard deviation (RSD) of the blank, that is,

(6) $C_L = 3\, RSD_{blank}\, BEC / 100$

where $RSD_{blank} = 100\, s_{bl} / X_{bl}$

## Experimental

### Instrument

Typical instrument detection limits were measured using two aurora M90 ICP-MS instruments, one located in Australia and the other in Japan. Both instruments were installed in non-clean room environment.

### Reagents and Samples

A blank solution, 1% v/v $HNO_3$, was made using high-purity nitric acid (Ultrapur®, 60%, Merck) and pure deionized water (18MΩ cm, Millipore Milli-Q, Bedford, USA). Two standards, at 1µg/L and 10µg/L levels, were prepared by diluting ICP-MS multi-element stocks with the blank. Prior to use, all labwares were thoroughly cleaned (i.e. acid washing and deionized water rinsing), and then the clean containers were left filled with 1% v/v $HNO_3$ until use.

## Results and discussion

### Sensitivity Mode

The aurora M90 ICP-MS can be operated in a number of sensitivity modes (eg. normal, high, etc.) without any hardware changes. In general, the "high" sensitivity mode is used for applications requiring highest sensitivity, such as laser ablation and analysis of semiconductor materials; while the "normal" sensitivity mode is used for general chemical analyses, including environmental, agriculture and clinical research applications. Hence the "normal" mode is recommended for most ICP-MS analyses. Typical method parameters used for tuning the instrument to a "normal" sensitivity mode are shown in Table 1.

Table 1: Typical method parameters for the aurora M90 ICP-MS tuned to "normal" mode.

| | Parameters | Settings* |
|---|---|---|
| Gas flow (L/min) | Plasma Flow<br>Auxiliary Flow<br>Nebulizer Flow<br>Sheath Flow | 16.5<br>1.65 (1.60)<br>0.95 (1.00)<br>0.28 (0.45) |
| RF | RF Power (kW) | 1.30 (0.70) |
| Sample Introduction | Sampling Depth (mm)<br>Pump Rate (rpm)<br>Stabilization Time (s)<br>Spray chamber (°C) | 5.0 (5.5)<br>3 (20)<br>30<br>3 |
| Ion Optics (volts) | 1st Extraction Lens<br>2nd Extraction Lens<br>3rd Extraction Lens<br>Corner Lens | -1<br>-140 (-20)<br>-200 (-190)<br>-180 (-110) |
| | Mirror Lens Left<br>Mirror Lens Right<br>Mirror Lens Bottom | 75 (105)<br>5 (15)<br>50 (20) |
| | Entrance Lens<br>Entrance Plate<br>Fringe Bias<br>Pole Bias | 1<br>-37 (-50)<br>-5<br>0 |
| Quadrupole Scan | Scan mode<br>Dwell Time (ms)<br>Points per Peak<br>Scans/Replicate<br>Replicates/Sample | Peak Hopping<br>100<br>1<br>30<br>10 |

* Settings in parentheses are used for "Cool Plasma" conditions.

Settings used for typical "cool" plasma are also listed in Table 1. The "cool" plasma technique is used to minimize polyatomic interferences associated with the plasma gas, such as $ArO^+$ and $Ar^+$. This technique can improve the detection limits for elements affected by such interferences, including Fe, Ca, Na, K and Mg. More discussions on the use of cool plasma and more detection limit values under cool plasma conditions can be found in other Bruker's Application Notes (from Bruker's web site www.bruker.com under the ICP-MS Application Note section).

## Better detection limits

It should be noted that tuning an ICP-MS to its highest sensitivity does not necessarily provide the lowest detection limit. To achieve the lowest possible detection limits and accurate analytical results, strict precautions must be taken to eliminate or minimize any potential contamination. Where possible, glassware including volumetric pipettes and flasks should be avoided when preparing and/or storing any solutions (with exception of Hg solutions), because some metals may be leached out from the glass or adsorbed onto the glass surface, which could result in sample contamination or loss of analyte. Prior to use, all the labwares, new or used, should be thoroughly cleaned. A typical cleaning procedure includes acid washing the labwares for at least 24 hours to remove elemental contamination, thoroughly rinsing them with high-purity deionized water, and then leaving clean containers filled with 1% v/v $HNO_3$ until use.

It is clear from the equations (4) and (6), the lower the standard deviation (or RSD) of the blank, the better the detection limits. A lower RSD can often be obtained by using a relative longer replicate reading and stabilization time. The replicate reading time is dependent on the dwell time and the number of scans per replicate. Typical stabilization and scan settings used in this work are listed in Table 1. Also, the lower the BEC, the better the detection limits. To keep BEC low, high-purity reagents and deionized water should be used in all the samples and standards preparations, and ideally the solutions should be prepared and measured in a class 100 clean room, or at least the sample preparation area should be air-conditioned and dust free. When running the aurora M90 ICP-MS under normal sensitivity mode, the counts for a blank solution should not exceed a few thousand cps per isotope for most isotopes. A higher blank count is often an indication of blank contamination. The lower the contamination (blank counts) the better the detection limits.

## Typical detection limits

Table 2 shows the typical detection limits (DLs) for the elements commonly measured in environmental samples. All DLs were calculated using equation (3), i.e. three times the standard deviation of 10 replicates of the blank (i.e. 1% v/v $HNO_3$). The instrument was tuned to "normal" sensitivity mode under either "hot" or "cool" plasma conditions. All the measurements, however, were made under routine analytical laboratory, not clean-room, conditions. This work indicates typical DL values that can be routinely achieved outside a clean-room in a clean laboratory.

## Conclusions

Detection limits are influenced by a number of factors, including the sensitivity of a given isotope, and the presence of background interferences or contamination. It is vitally important to control contamination in the laboratory to achieve the lowest possible detection limits.

Table 2: Typical IDLs for the aurora M90 ICP-MS.

| Element | Isotope (m/Z) | Measured in | | Back-ground species |
|---|---|---|---|---|
| | | Hot plasma (ng/L) | Cold plasma (ng/L) | |
| Li | 7 | 1 | 0.01 | |
| Be | 9 | 3 | | |
| B | 11 | 30 | | |
| Na | 23 | 200 | 0.5 | |
| Mg | 24<br>25 | 2<br>5 | 0.2<br>0.08 | |
| Al | 27 | 2 | 0.2 | |
| Si | 28 | 1000 | | $Co^{++}$, $N_2^+$ |
| P | 31 | 700 | | $NOH^+$ |
| S | 34 | 20000 | | $(OH)_2^+$ |
| K | 39 | 500 | 0.5 | $ArH^+$ |
| Ca | 40<br>44 | 500 | 1 | $Ar^+$, $CO_2^+$ |
| Sc | 45 | 0.8 | | $CO_2H^+$, $N_2OH^+$ |
| Ti | 47 | 3 | | |
| V | 51 | 3 | | $ArNH^+$, $ClO^+$ |
| Cr | 52<br>53 | 8<br>3 | | $ArO^+$, $ArC^+$ |
| Mn | 55 | 2 | | $ArNH^+$ |
| Fe | 56<br>57 | 4000<br>300 | 0.3<br>0.9 | $ArO^+$<br>$ArOH^+$ |

| Element | Isotope (m/Z) | Measured in | | Back-ground species |
|---|---|---|---|---|
| | | Hot plasma (ng/L) | Cold plasma (ng/L) | |
| Co | 59 | 0.2 | | $ArOH^+$ |
| Ni | 60 | 2 | | |
| Cu | 63<br>65 | 0.3<br>2 | | |
| Zn | 66<br>68 | 5<br>20 | | |
| Ga | 69<br>71 | 0.3<br>0.2 | | |
| Ge | 72 | 4 | | |
| As | 75 | 20 | | |
| Se | 77<br>78<br>82 | 30<br>400<br>300 | | |
| Rb | 85 | 1 | | $KrH^+$ |
| Sr | 88 | 0.7 | | |
| Y | 89 | 0.2 | | |
| Zr | 90 | 0.4 | | |
| Nb | 93 | 0.8 | | |
| Mo | 98 | 0.4 | | |
| Ru | 101 | 0.4 | | |
| Rh | 103 | 0.1 | | |
| Pd | 108 | 0.3 | | |
| Ag | 107 | 0.6 | | |

Table 2 (cont.): Typical IDLs for the aurora M90 ICP-MS.

| Element | Isotope (m/Z) | Measured in | | Back-ground species |
|---|---|---|---|---|
| | | Hot plasma (ng/L) | Cold plasma (ng/L) | |
| Cd | 111 | 0.2 | | |
| In | 115 | 0.1 | | |
| Sn | 118 | 7 | | |
| Sb | 121 | 0.1 | | |
| Te | 125 | 4 | | |
| Cs | 133 | 0.4 | | |
| Ba | 138 | 0.2 | | |
| La | 139 | 0.4 | | |
| Ce | 140 | 0.06 | | |
| Pr | 141 | 0.06 | | |
| Nd | 146 | 0.3 | | |
| Sm | 147 | 0.2 | | |
| Eu | 153 | 0.1 | | |
| Gd | 157 | 0.2 | | |
| Tb | 159 | 0.09 | | |
| Dy | 163 | 0.2 | | |
| Ho | 165 | 0.06 | | |
| Er | 166 | 0.18 | | |

| Element | Isotope (m/Z) | Measured in | | Back-ground species |
|---|---|---|---|---|
| | | Hot plasma (ng/L) | Cold plasma (ng/L) | |
| Tm | 169 | 0.08 | | |
| Yb | 172 | 0.3 | | |
| Lu | 175 | 0.05 | | |
| Hf | 178 | 2 | | |
| Ta | 181 | 0.2 | | |
| W | 182 | 1.3 | | |
| Re | 185 | 0.2 | | |
| Ir | 193 | 0.2 | | |
| Pt | 195 | 0.3 | | |
| Au | 197 | 0.3 | | |
| Hg | 202 | 1 | | |
| Tl | 205 | 1 | | |
| Pb | 206+ | 0.3 | | |
| Bi | 209 | 0.3 | | |
| Th | 232 | 0.04 | | |
| U | 238 | 0.06 | | |

## References


[1] I. Kalinitchenko, Ion Optical System for a Mass Spectrometer, US Patent 6,614,021 B1, 2 September 2003

[2] S. Elliott, M. Knowles and I. Kalinitchenko, "A New Direction in ICP-MS", Spectroscopy, 19(1), 30 (2004).

[3] V. Thomsen, D. Schatzlein, and David Mercuro, "Limits of Detection in Spectroscopy", Spectroscopy 18(12), 112 (2003)


## Authors


XueDong Wang and Shane Elliott



| Keywords |
|---|
| Sensitivity |
| Detection Limit |
| Interference |
| Contamination |

| Instrumentation |
|---|
| aurora M90 ICP-MS |


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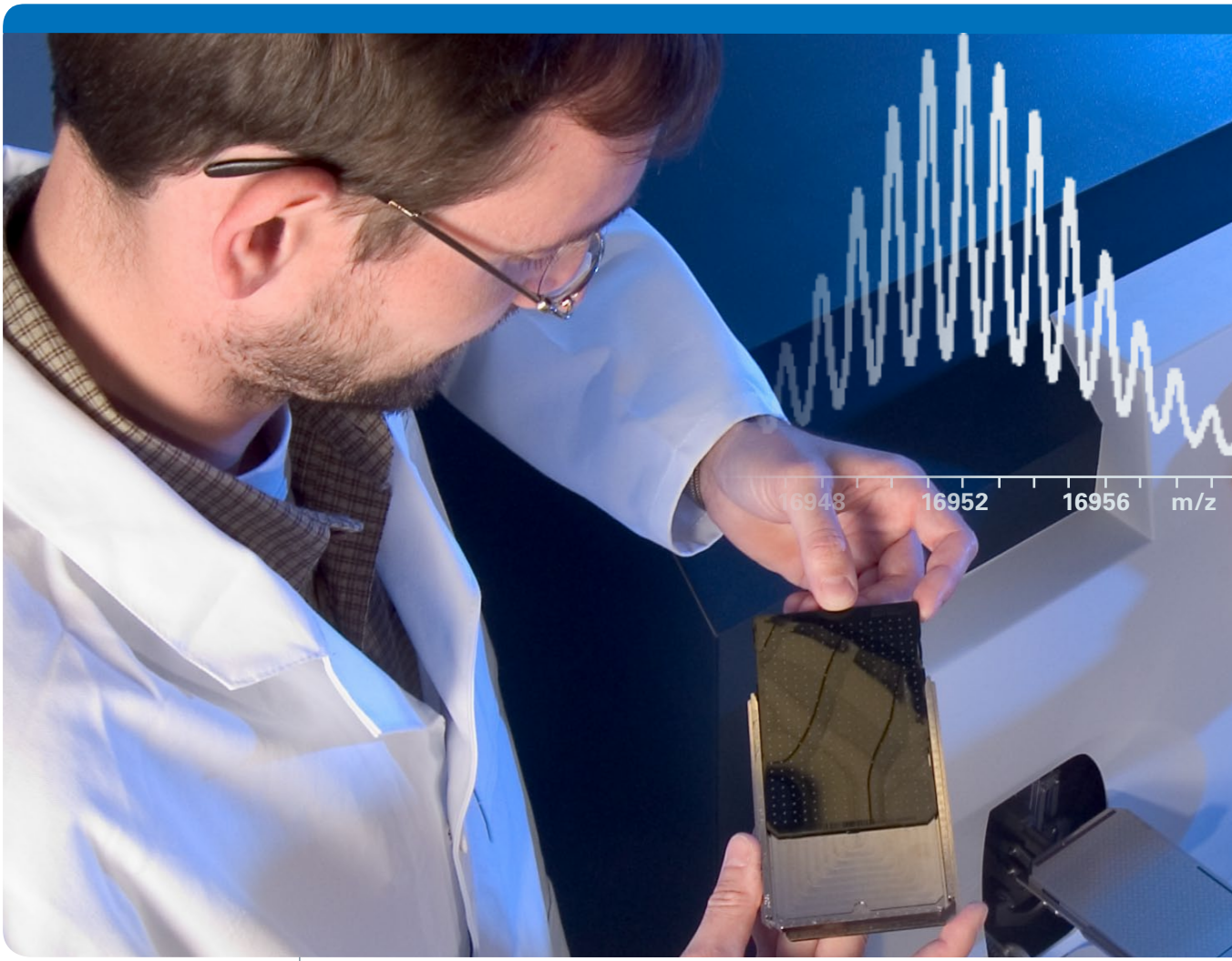


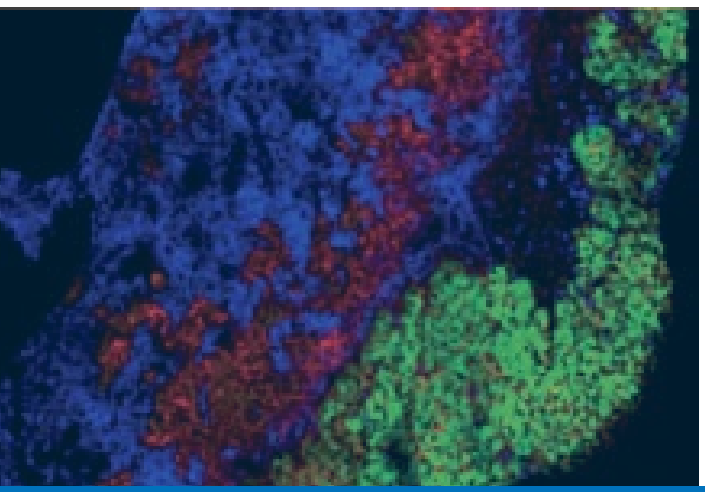

# The new ultrafleXtreme

Beyond Imagination

MALDI-TOF/TOF-MS

Innovation with Integrity

# Explore Your Applications with MALDI-TOF



The new ultrafleXtreme™ revolutionizes what you can achieve with a MALDI-TOF and opens new fields for research and industry.

Applications such as in-depth characterization of Biopharmaceuticals, high speed tissue imaging based biomarker discovery and glycoproteomics extend beyond classical proteomics utilizing a multitude of technology innovations and unique proprietary software.

### MALDI Imaging – the complete molecular histology solution from the technology leaders

- Top-Down Biomarker Discovery
- New Bottom-Up ImageID™ workflow for protein identification and localization – even suitable for FFPE tissue and large proteins
- Highly enhanced data acquisition speed and instrument robustness to perform large scale studies

### Proteomics and Glycoproteomics – additional capabilities extending your research scope

- Integrated workflows for LC-MS/MS and 2D gels
- Quantification with any label or label-free Top-Down [1] and Bottom-Up workflow
- Glycoproteomics: Integrated GlycoQuest™ search engine for automated glycan structure elucidation in proteins for high-throughput studies

### BioPharma – intact protein MW determination and direct protein sequencing as never before with MALDI-TOF

- Accurate assignment of intact protein molecular weights by novel multiple charge state analysis
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### Glycoprotein Analysis – the next life science frontier at your finger tips

- Full glycan analysis
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- Glycopeptide structure elucidation by unique MS/MS patterns in MALDI-TOF and automated glycan database search with GlycoQuest

### MALDI Biotyper – microbial identification for the 21st century

- Bacteria ID
- Yeast and fungi ID
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# More Flexible Than Ever

## Accurate Intact Protein Molecular Weight Analysis – completing the picture for biopharmaceutical characterization

- Up to 100x increase of mass accuracy down to the low ppm range for intact protein MW determination due to multiple charged ion signals
- Bruker DHAP matrix proven for Top-Down analysis producing multiple charged ions
- Greater than 30,000 resolution for intact proteins due to FlashDetector™

## Gold Standard in Top-Down Protein Sequencing

- Monoisotopic sequence readout of up to 90 residues from N- and C-termini
- Automated, rapid protein QC reports from BioPharma Compass software
- Patented $T^3$-Sequencing for direct N- or C-terminal characterization [2]

## High Definition MALDI Imaging

- Continuing innovation leadership with patented enabling technologies from sample preparation to the molecular histology workflow, advanced data treatment and automated tissue classification
- Access to FFPE tissue and large proteins: New proprietary ImageID workflow provides identities and localization of ~ 80% of observed peptides in tissue
- 2 kHz FlatTop smartbeam-II™ laser for non-destructive tissue analysis permitting seamless correlation with high resolution histopathology from the same tissue slice
- High definition MALDI Imaging by industry leading 10 µm laser focus and true edge-to-edge pixel definition
- High spatial resolution for protein images at best image brightness by patented smartbeam laser technology

## Targeted Protein Quantification with 1-2% CV [4]

- HPLC-free MALDI-TOF for highest assay speed and accuracy

## LC-MALDI – the workhorse for proteomics and glycobiology

- smartbeam-II laser for acquisition of maximum number of MS/MS spectra per fraction
- Highest sensitivity through AnchorChip™ technology – now with up to 1536 spots/plate
- Market leading mass resolution (> 40,000) and accuracy (< 1 ppm)
- ProteinScape™ software covering all proteomics and glycoproteomics workflows
- Direct analysis of glycans and glycopeptides enabled by GlycoQuest

### Read more


[1] Maltmann DJ *et al.* Proteomics. 2011;11(20):3992-4006.
[2] Suckau D, Resemann A. Anal Chem. 2003;75(21):5817-24.
[3] Resemann a *et al.* Anal Chem. 2010;82(8):3283-92.
[4] Anderson NL *et al.* J Proteome res. 2012;11(3):1868-78.


# Extreme Performance for Bottom-Up Proteomics

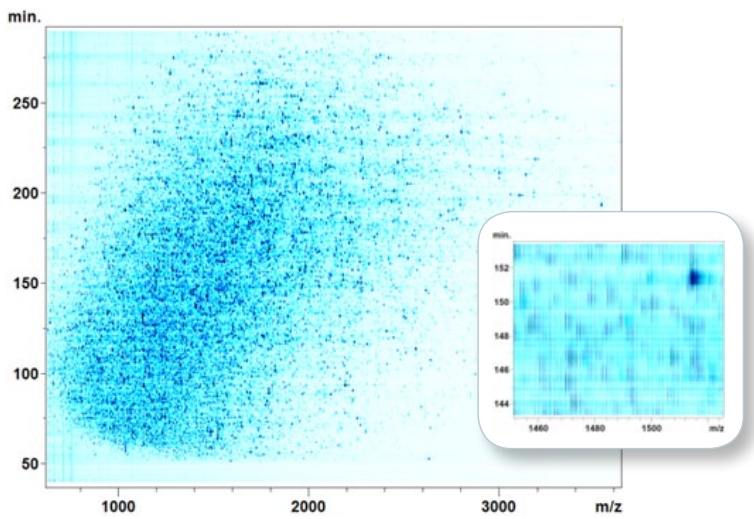
The ultrafleXtreme's next-generation MS technologies enable greater proteome coverage than ever before. The ultrafleXtreme offers unparalleled cutting-edge capabilities for Bottom-Up proteomics at your fingertips.

Bruker's 25 years Life Science experience and excellent bioinformatics compliant with HUPO/PSI publication guidelines effortlessly converts unrivalled MALDI-TOF/TOF data into published results.

## Identify, quantify and characterize – all your results in the blink of an eye

ProteinScape software makes it possible to access, process, merge, query and report all Bottom-Up proteomics data from high throughput 2D gel identification to label or label-free LC-MALDI quantification.

**First-class LC-MALDI results**




5µg HeLa Cell digest resulting in 2890 protein IDs

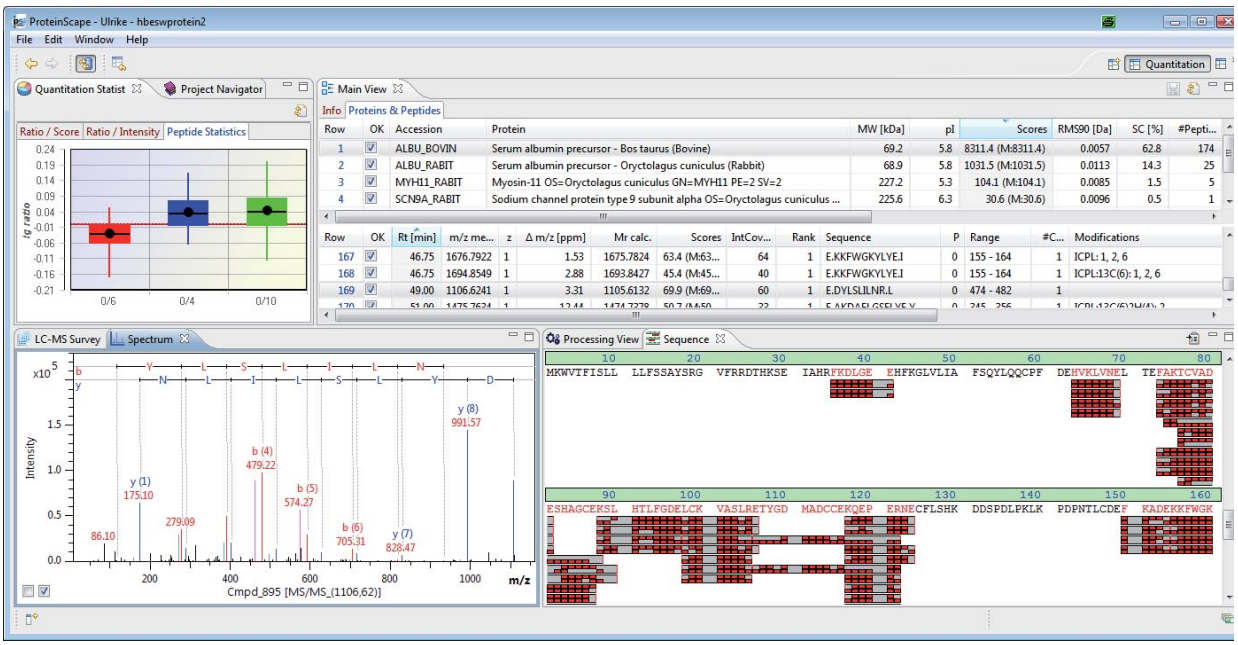
**First-Class LC-MALDI results from even the most complex Bottom-Up proteomics analysis**

5 µg HeLa Cell digest

- **2890 Protein IDs @ 1% Peptide FDR**
- 11,960 Spectrum matches
- 38% Spectrum ID rate

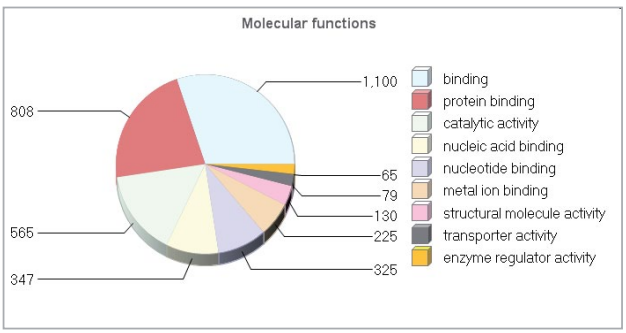
Providing a perfect complement to ESI protein ID workflows

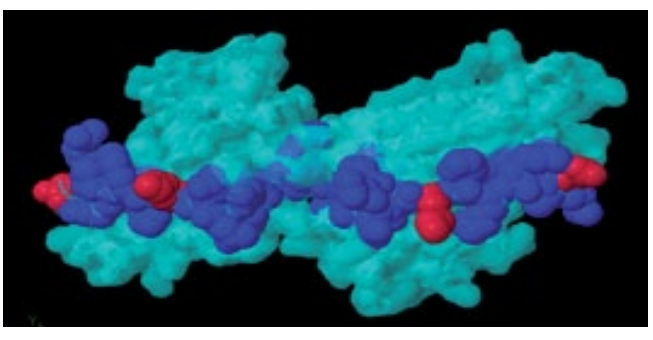
## Identification, structural characterization and quantification at a glance




## ProteinScape – From data to knowledge

- Data from various workflows (multiple digest enzymes, label or label-free quantification, ESI or MALDI) can be merged into confident, non-redundant protein information
- Just a few mouse clicks to compare results across multiple studies
- Direct access to web resources relates information such as gene ontology or mapping of PTMs on the 3D protein structure



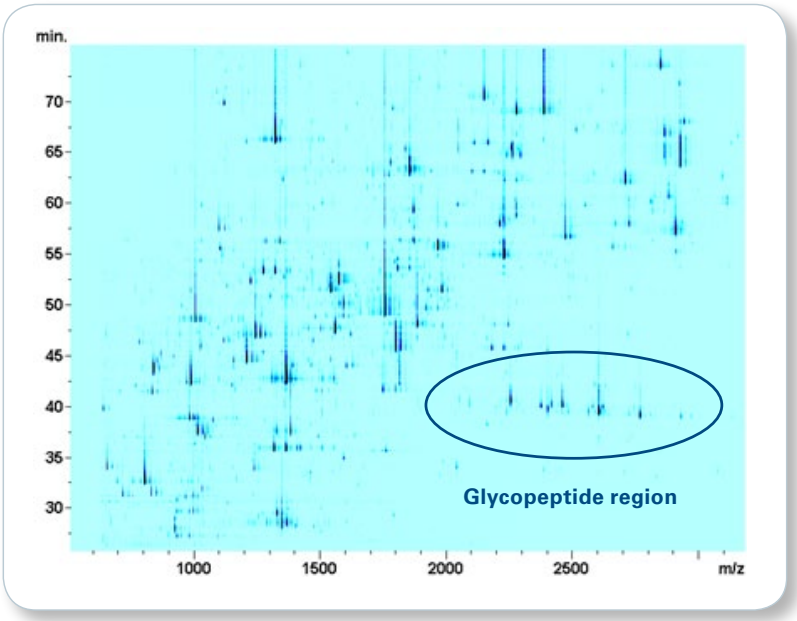



# Cross the Next Frontier – Glycoproteomics Expertise Delivered

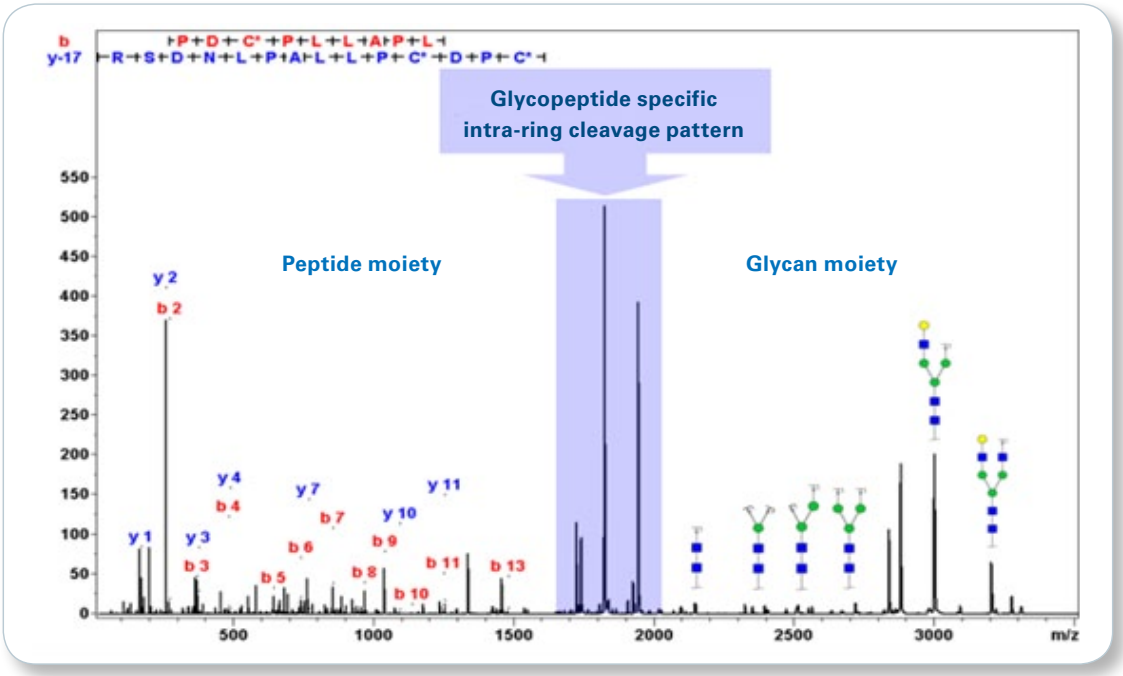
## Get the full picture

The ultrafleXtreme TOF/TOF spectra of N-glycopeptides contain both peptide and glycan information. ProteinScape uses a TOF/TOF specific signature fragmentation pattern generated by intra-ring cleavage of the peptide-binding sugar to assign the aglycone and the glycan molecular weights and triggers their identification in parallel database searches.

The specific signature enables the classification and filtering of glycopeptides from non-glycosylated ones in complex cell lysates. ProteinScape integrates the GlycoQuest search engine for glycan structure DB searches.

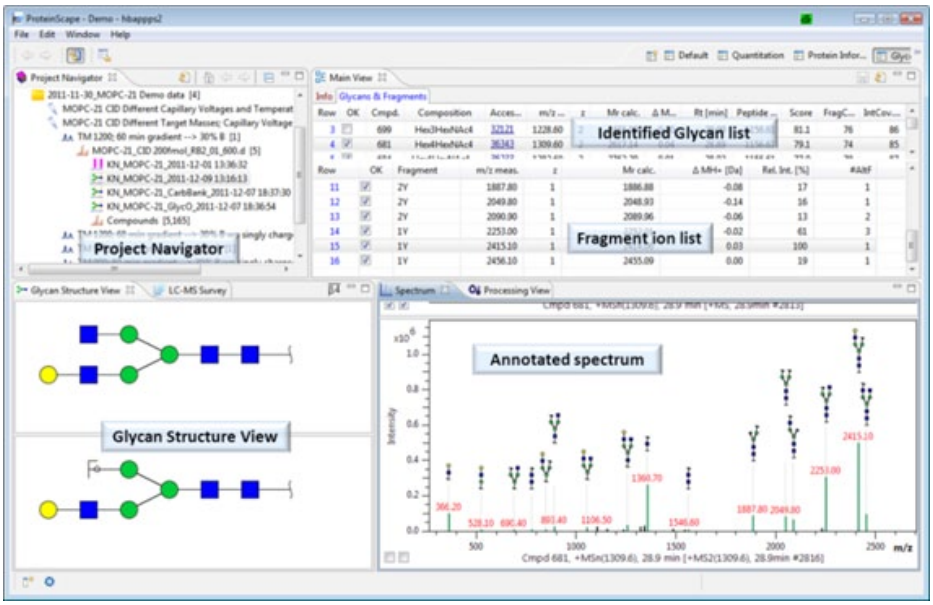



LC-MALDI analysis of a human antibody digest, shows at the first glance the separated glycopeptide region on the MS-level.




Automated glycopeptide detection by ProteinScape. Signature ion pattern provides molecular weights for both the peptide and glycan from a single glycopeptide TOF/TOF spectrum. Structures from both moieties are assigned in this spectrum.

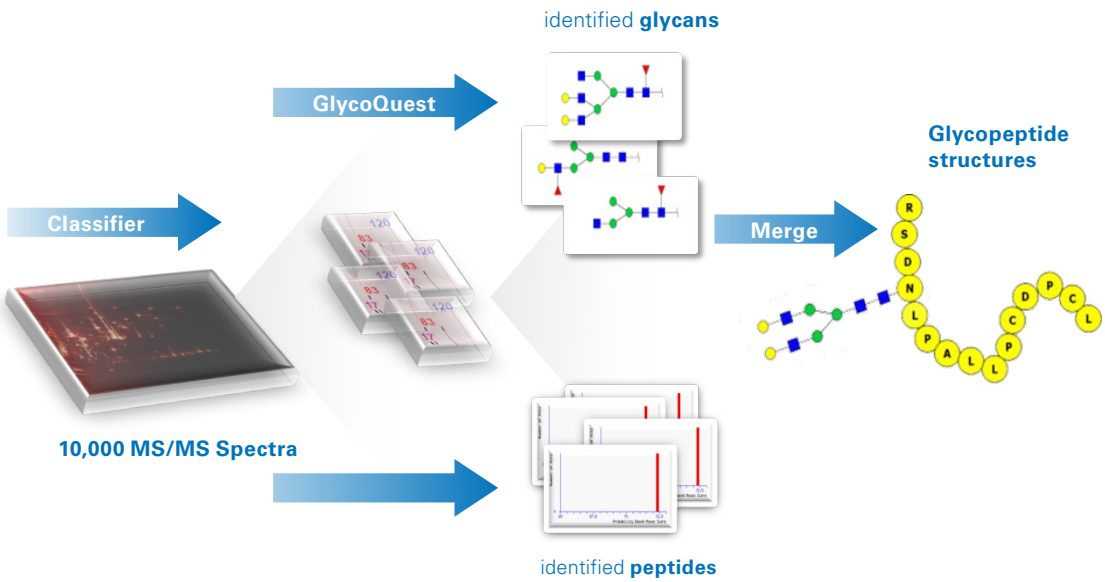
## Easily and comprehensively ID and assign glycan structures in MS/MS spectra




Representation of an ultrafleXtreme glycoprotein analysis in ProteinScape. All glycopeptides were detected in the LC-MS/MS dataset and the glycan were searched using GlycoQuest.

A structure candidate is shown as structure and its fragments annotated to a matching MALDI-TOF/TOF spectrum permitting manual inspection whenever requested.

## Analysis of N-glycosylation pattern present on antibodies




Bruker's ProteinScape software detects glycopeptide-specific fragmentation patterns in MALDI-TOF/TOF spectra that allows a separate glycane database search with GlycoQuest to ID the glycane part and a Mascot search to ID the peptide part. ProteinScape can then visualize both results to merge the information on the glycopeptide level.

# From Tissue Biomarker Discovery...

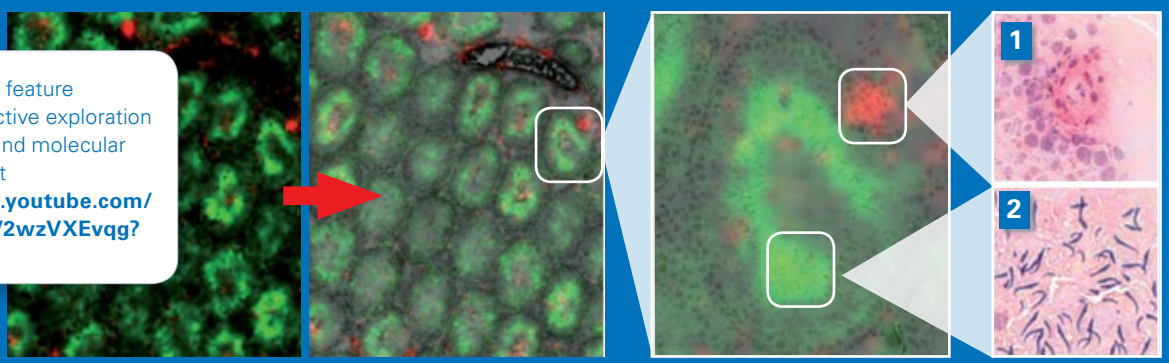
MALDI Imaging is emerging into an indispensable discovery tool for molecular tissue and histopathological research, reaching out from high resolution imaging tools to statistical cohort analysis and biomarker discovery and identification.

Brukers MALDI Molecular Imager solution enables robust and quality-controlled tissue preparations, and links the classical histopathology workflow with the molecular dimension. Unique, patented software and techniques for clinical studies enable powerful biomarker discovery.

The ultrafleXtreme is an essential element in any imaging project.

## Rat testis at 20 µm spatial resolution

See how this feature allows interactive exploration of histology and molecular information at **http://www.youtube.com/watch?v=YV2wzVXEvqg?hd=1**



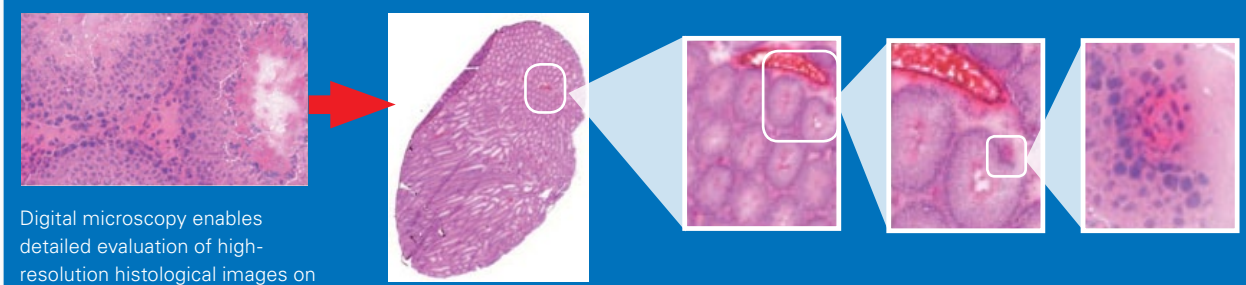

MALDI image of rat testis at 20 µm spatial resolution. Two molecular signals that highlight different features are selected.

Bruker flexImaging software allows cross-fading between the MALDI image and the superimposed virtual slide.

At higher resolution, histological features become visible in the virtual slide image.

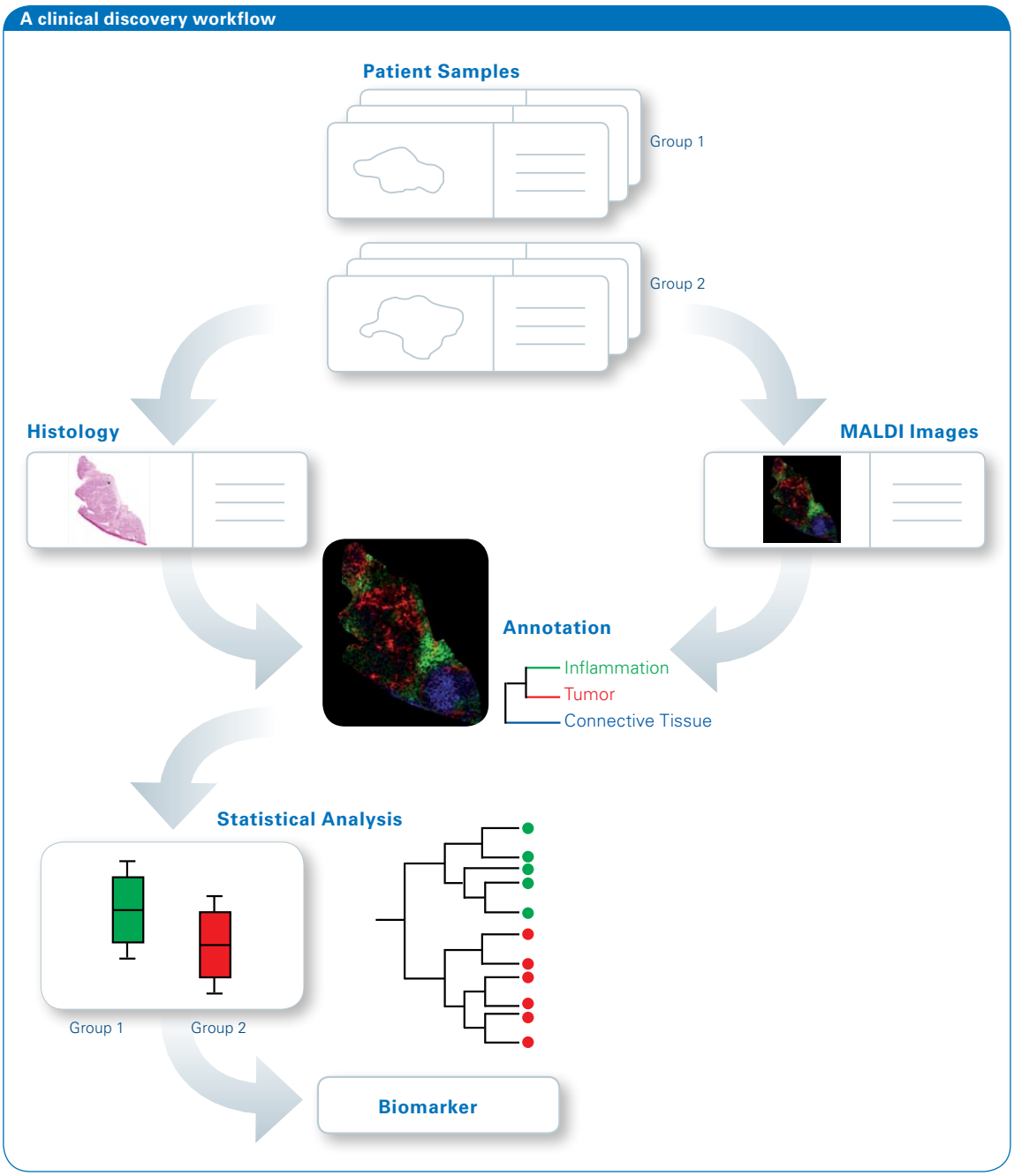
Full resolution reveals (1) a capillary vessel (2) nuclei of mature spermatids and demonstrates correlation of histological features and molecular signals.

## Virtual microscopy



Digital microscopy enables detailed evaluation of high-resolution histological images on a computer screen.

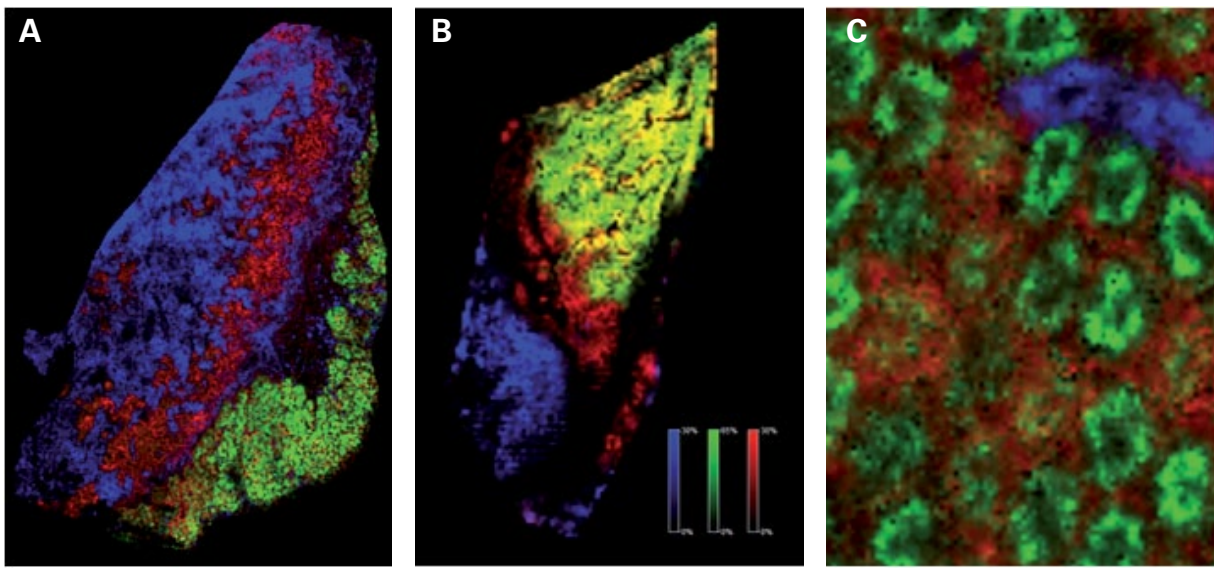
The alignment of MALDI Imaging data with other images (e.g. histological stains) is crucial for the interpretation of results. Bruker's proprietary solution for virtual microscopy allows co-registration of multiple image modalities with unparalleled ease.




From beautiful pictures to true biomarker discovery – MALDI Imaging is perfectly suited to analyze biomarkers in tissue samples. Bruker's unique suite of software tools supports the entire workflow, including statistical analysis. Comprehensive bioinformatic tools for statistical analysis of MALDI Imaging data, such as hierarchical clustering, PCA or pLSA allow researchers to mine data efficiently.

# ...To Identification and Validation

**MALDI Imaging covers a multitude of application areas ranging from clinical samples to plant material and animal tissue**

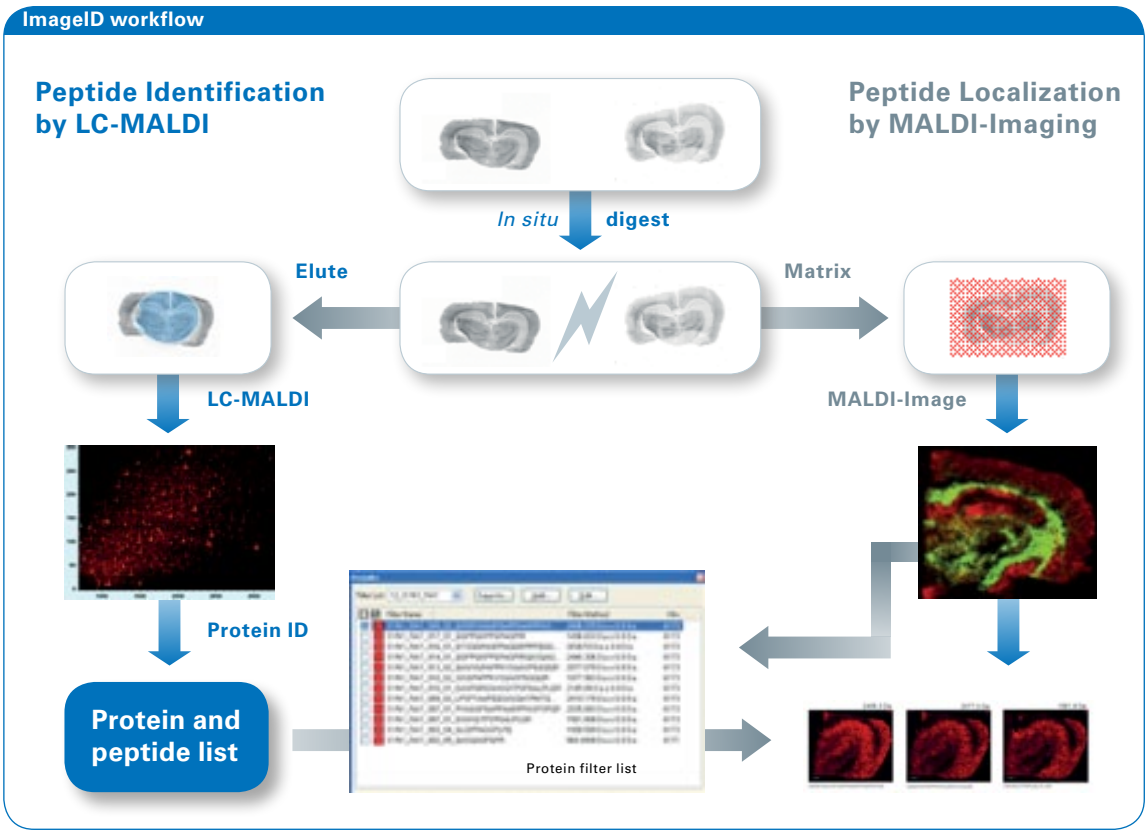



A: Human bladder cancer specimen; B: Barley seed; C: Rat testis

Identification of biomarker candidates are essential for validating results and the translation of MALDI Imaging derived biomarkers to subsequent clinical stages, such as treatment prognosis or survival prediction. Top-Down discovery and identification has been demonstrated successfully*.

As well, higher MW protein detection and analysis of formalin-fixed tissues are now enabled by the novel ImageID workflow. In this Bottom-Up workflow highly resolved images from on-tissue digests are merged with classical LC-MS/MS identification.

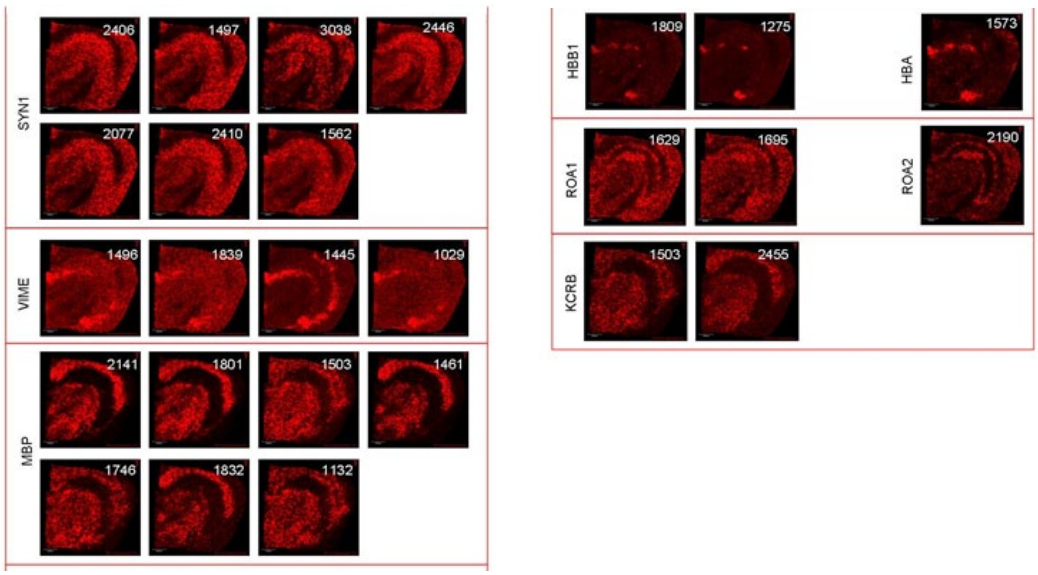
*References:
Lemaire 2007 Reg-$\alpha_2$, Hanrieder 2011 S100-A10, Hardesty 2011 S100-A6, Nipp 2011 S100-A6/10, Meistermann 2006 TrT, Rauser 2010 CRIP1, Lagarrigue 2011 Thym$\beta$, LCFA-CoA




Consecutive sections are processed in parallel to provide both protein distribution and identification simultaneously. A tryptic digest is performed maintaining the resolution of protein distributions. Peptide imaging (right) and LC-MALDI-MS/MS (left) yield protein and peptide IDs that is software merged for visualization of protein distribution. 80% of all peptides visible in the images can thus be identified and turned into protein localization of more than 100 proteins per image.

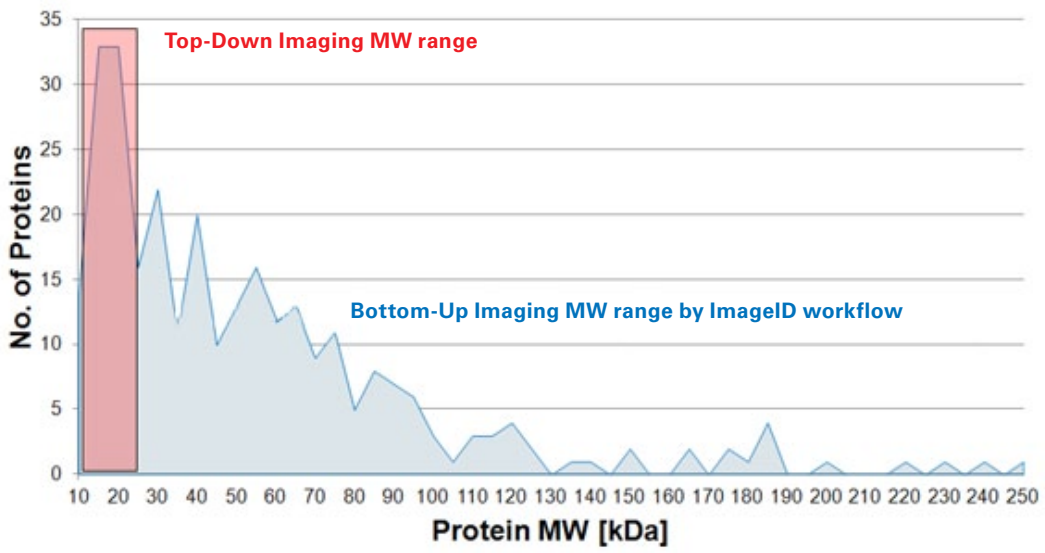
# ImageID Results

**ImageID results from mouse brain**




Increased confidence in peptide identifications: Peptides derived from the same protein show the same spatial distribution.

**Bottom-Up Imaging vs. TopDown Imaging**




Bottom-Up Imaging with the ImageID workflow extends the mass range of detectable proteins from approx. 25 kDa to greater 100 kDa and grants access to proteins cross-linked by formalin fixation.

# Biopharmaceutical Characterization

## Ultra rapid product confimation of 150 kDa (MOPC21) antibody

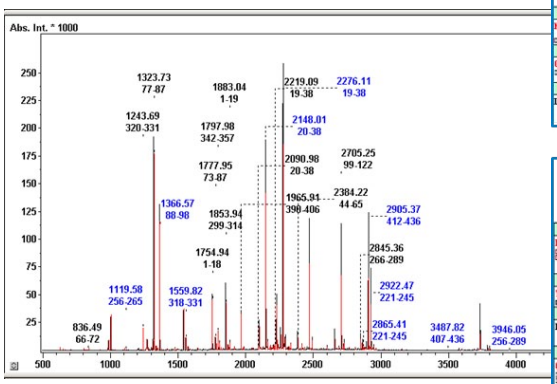
**Peptide Mass Fingerprints confirm product identity in 5 seconds without LC-separation**

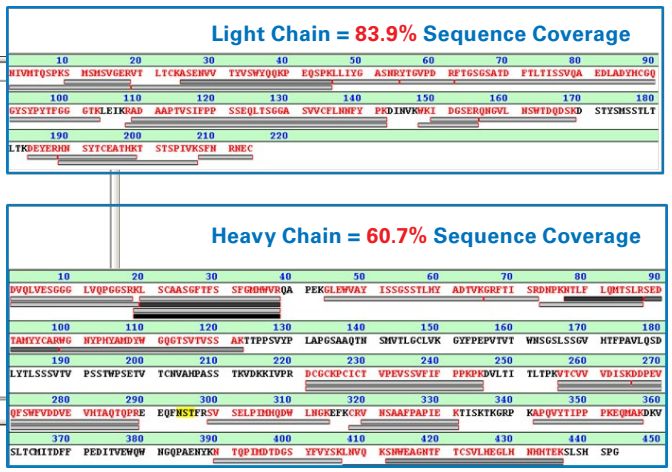
Confident characterization at 1 ppm mass accuracy

> 40,000 resolution

Immediate visualization and automated reporting

**5 second analysis**

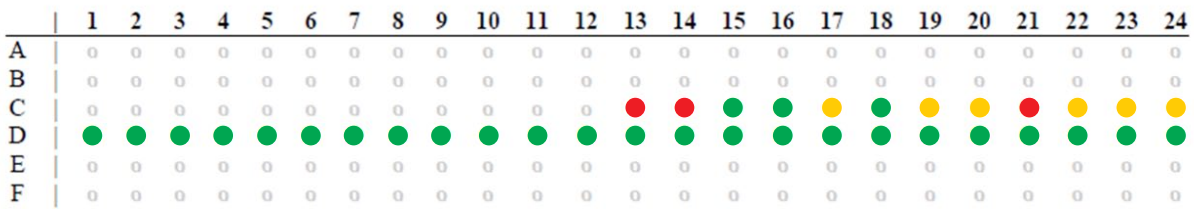



- Tryptic digest of MOPC21 IgG
- Ultra fast product confirmation

Rapid combination of data from multiple digests & instruments in 3 clicks in ProteinScape for ultimate sequence coverage. BioPharma Compass software – Fully automated acquisition, processing and reporting of data.

## Batch report view for automated QC PMF



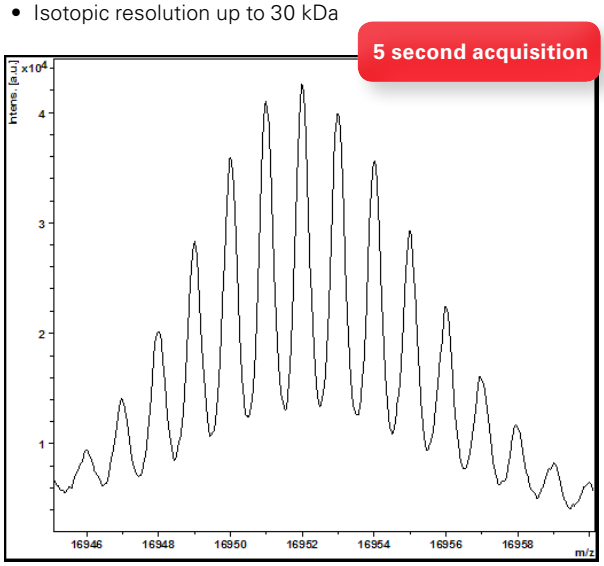

Sequence coverage acceptance criteria can be altered by user depending on desired result.

# Intact Molecular Weight Analysis

**MALDI intact molecular weight analysis**

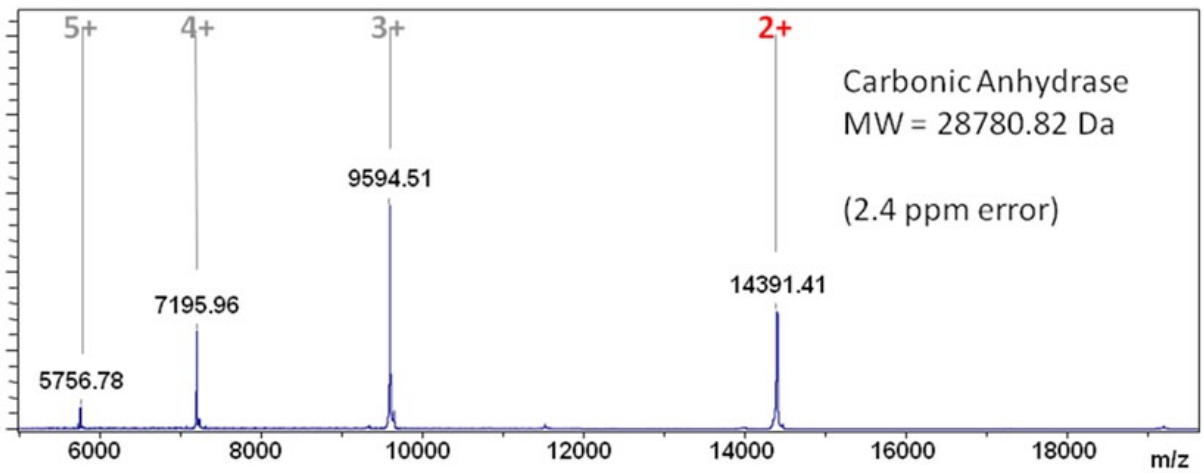
### Intact Myoglobin (17 kDa)

- Isotopic resolution up to 30 kDa




Intact molecular weight analysis confirms presence of product and/or contaminants in 5 seconds.

**High accuracy MW determination of CA based on double charged ions**




- < 15 ppm mass accuracy for intact proteins
- Using multiple charged ions
- Generated in DHAP matrix

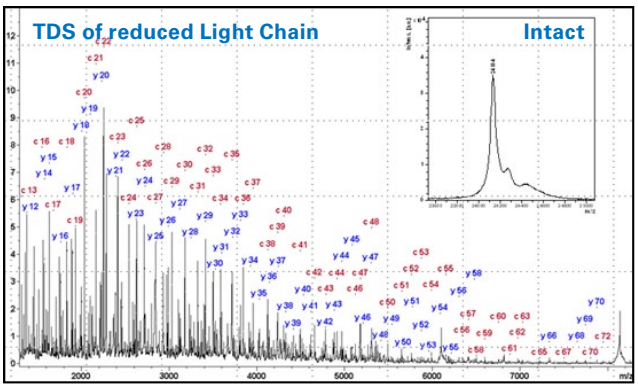
Full resolution @ full sensitivity with high mass accuracy is unique to Bruker MALDI-TOF.

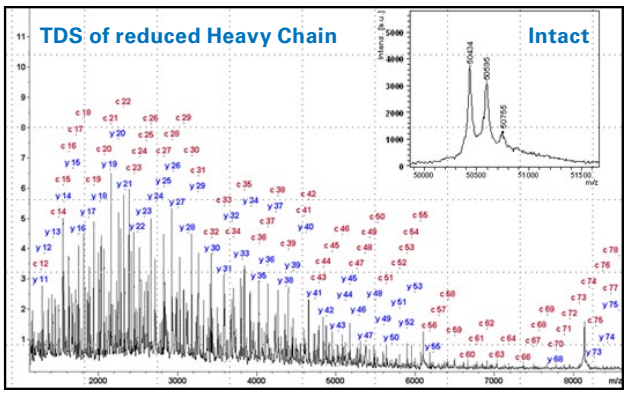
# N/C-Terminal Sequencing

## MALDI Top-Down N/C-terminal Sequencing

**1 minute acquisition**

**$ 0.10 Cost**




Top-Down sequencing delivers N/C-terminal sequence information in 1 minute without proteolytic digestion. Terminal modifications can be confirmed with an additional Bruker-patented T³-Sequencing step.

## Characterization information generated by TDS for IgG

- Glycan heterogeneity observed at intact level
- > 140 amino acid residues confirmed for light & heavy chain
- N/C-termini identified
- N-terminal pyro-Glu detected
- C-terminal Lys deletion detected
- Isotopically resolved TDS data = characterization certainty
- Automated acquisition & reporting of data

# Technical Specifications

## Redefining MALDI-TOF/TOF Performance

- 2 kHz smartbeam-II™ laser technology enables ultra-high data acquisition speed
- Laser focus diameters down to 10 µm for high spatial resolution imaging without pixel overlap
- Wide mass range resolution up to 40,000 due to proprietary PAN™ technology delivers:
    - Low ppm accuracy for protein MW determination
    - Long and reliable Top-Down sequence readout, at monoisotopic resolution
- Patented AnchorChip™ technology for unmatched consistency and sensitivity levels
- FlashDetector™ provides 1 ppm mass accuracy for highest confidence
- MALDI Perpetual™ Ion Source with entirely automated self-cleaning in < 15 minutes using a patented IR-laser process.
- Bruker DHAP matrix proven for Top-Down analysis

## Optional bioinformatics packages

- BioPharma Compass for comprehensive Biopharmaceutical characterization and QC
- flexImaging™, the leading MALDI Imaging platform – now with enhanced data compression for larger scale studies
- ProteinScape™ for the full execution of proteomics projects featuring GlycoQuest™ search engine for glycoproteomics
- Cutting-edge tools for protein analysis and Top-Down Sequencing
- PolyTools™: Interactive interpretation of MALDI polymer spectra
- Support of a wide variety of external software tools and data export functionality

## Support features

- Comprehensive self diagnostics and software update checks
- Remote on-line service and support capability
- Compass Security Pack™: Assisting in 21CFR part 11 compliance
- IQ/OQ/PV procedures for regulated environments
- Maintenance contracts available at various levels

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