

MAGNETIC RESONANCE MASS SPECTROMETRY

timsMRMS

Deciphering the world of **eXtreme** chemical complexity

Innovation with Integrity

An **eXtreme** leap in addressing high chemical complexity

Welcome to the timsMRMS, the next generation in magnetic resonance mass spectrometry (MRMS) —where trapped ion mobility meets the world's most powerful mass spectrometer. This unique combination delivers greater depth and confidence in the analysis of high complexity samples.

Many application areas remain challenging even when using advanced front-end separation techniques such as **HPLC**, and in some cases are not amenable to chromatography at all.

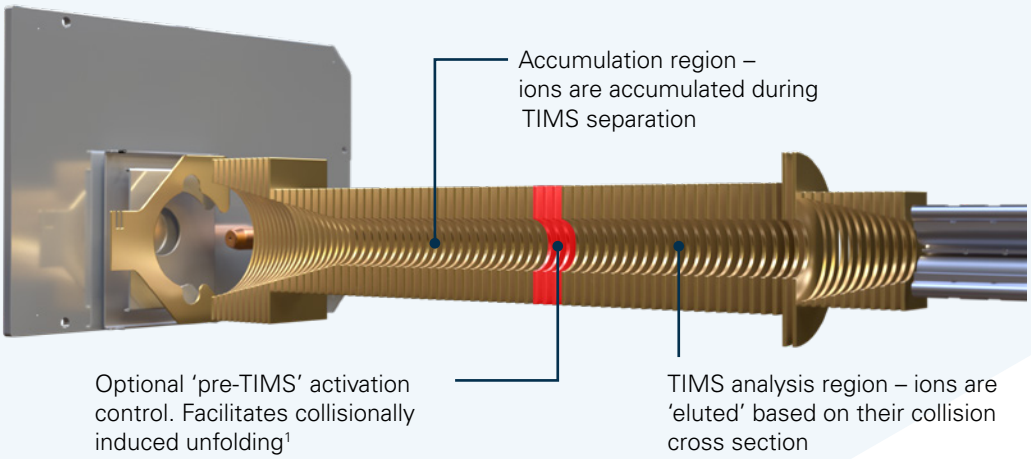
These include, for example, **MALDI** imaging of tissue (**lipids, drugs, metabolites**), direct analysis of **biofuels** and **petroleum**, **structural isomers**, **battery materials** for energy research, and environmental matrices such as dissolved organic matter **(DOM) in soil and water**, including contaminants like **PFAS**. In addition, timsMRMS supports detailed characterization of intact proteins.

The timsMRMS is ideally suited to tackle such challenging applications as it is equipped to discern and elucidate chemical features directly, all in the *m/z* domain. This is facilitated by TIMS which employs gas-phase fractionation, based on ion mobility, prior to MRMS detection. This combination delivers unmatched depth and accuracy for complex chemical mixtures.



Enhanced specificity and selectivity with TIMS

TIMS (Trapped Ion Mobility Spectrometry) simplifies complexity through gas-phase fractionation that facilitates the separation of ions, including isomeric species, based on ion mobility (**selectivity**) while offering an additional property of the collision cross section (CCS) for added **specificity**.

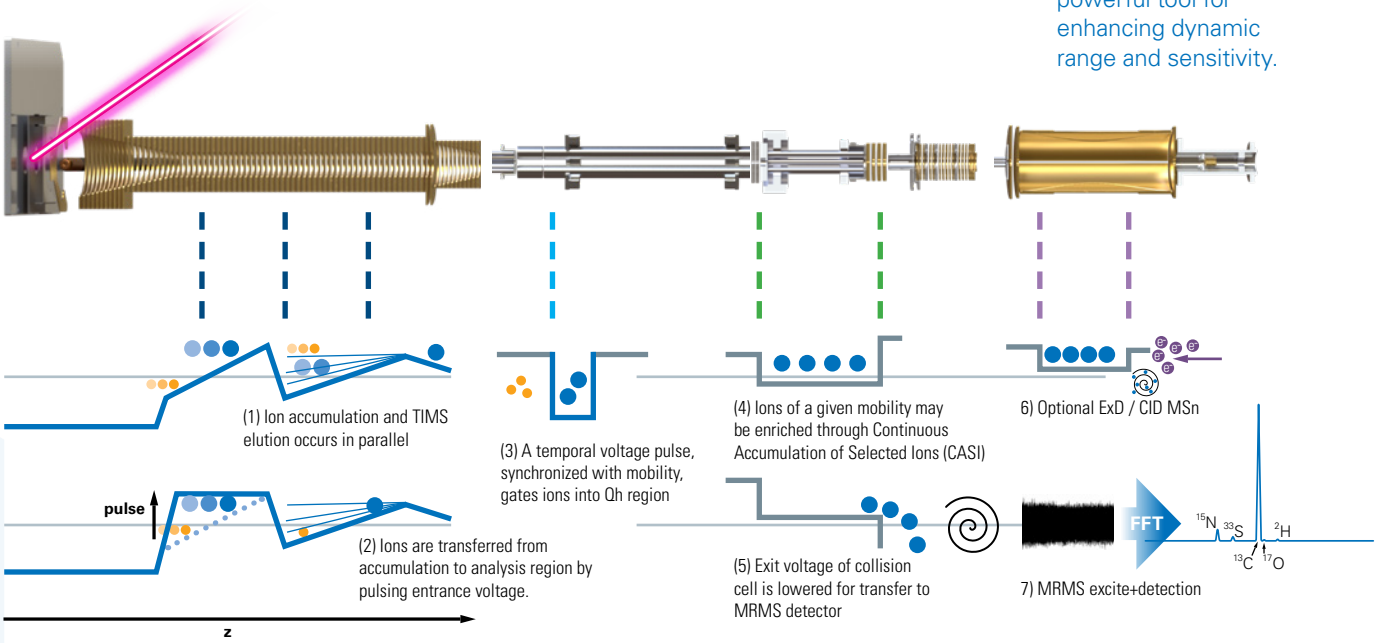


CCS-aware

Bruker's CCS-aware is supported on the timsMRMS. CCS-aware technology refers to the integration of collision cross section values, derived from TIMS, into mass spectrometry data analysis workflows to increase confidence in molecular identification.

Gated TIMS with ion enrichment

Gated TIMS is an implementation of TIMS that releases ions of a given mobility range to the MRMS system. This increases ion sampling and dynamic range while complementing the detection timeframe of MRMS. Gated TIMS can be combined with Quadrupole *m/z* selection for a 2 dimensional CASI (Continous Accumulation of Selected Ions).

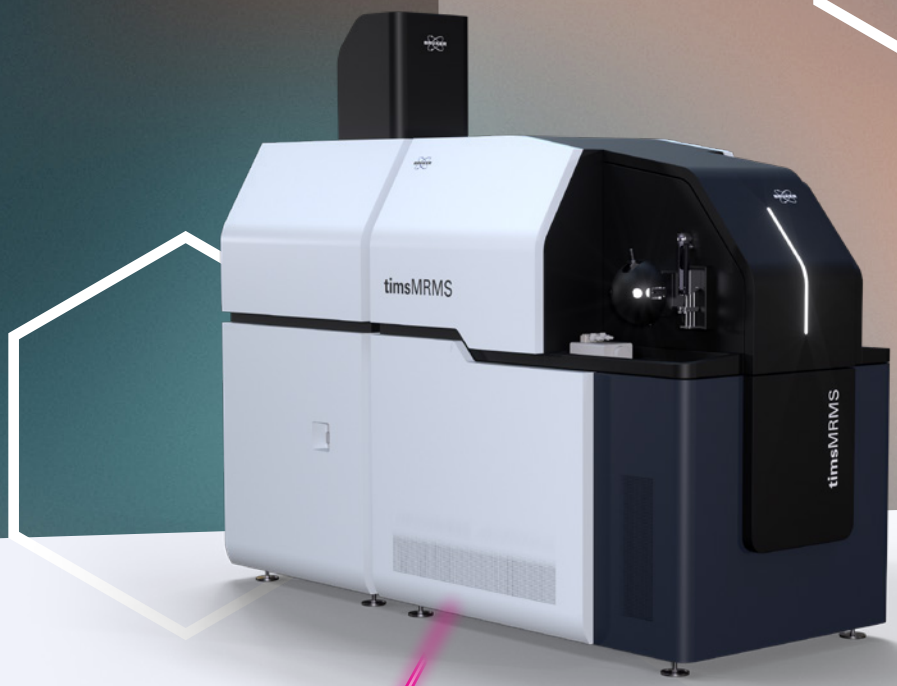


CASI Enabled

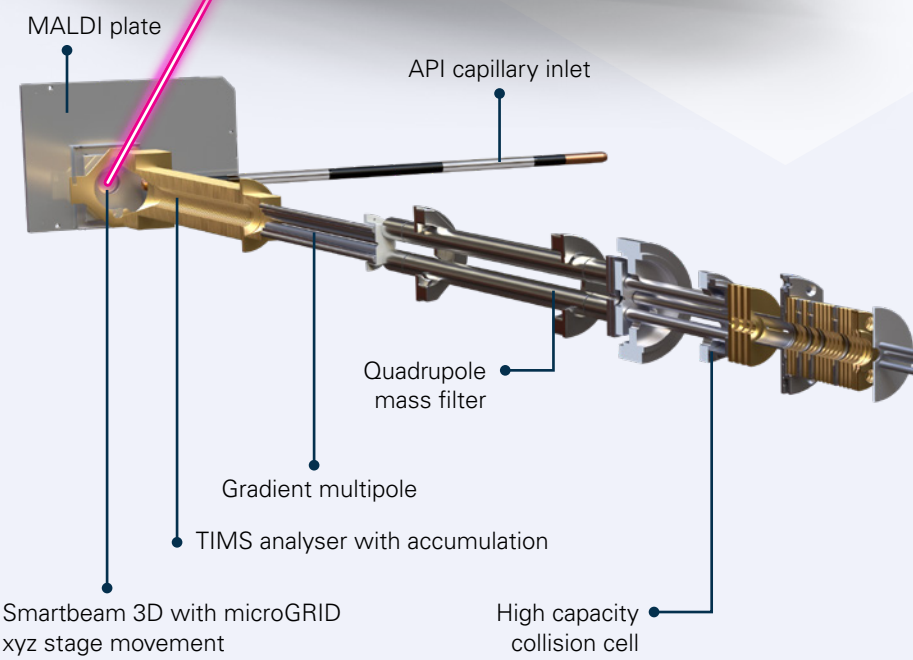
In a targeted fashion, CASI concentrates ions based on *m/z* or ion mobility for better detection of lower-abundance compounds - a powerful tool for enhancing dynamic range and sensitivity.

timsMRMS

The next-gen in magnetic resonance mass spectrometry (MRMS) – a marriage of trapped ion mobility spectrometry (TIMS) with the world's most powerful mass spectrometer

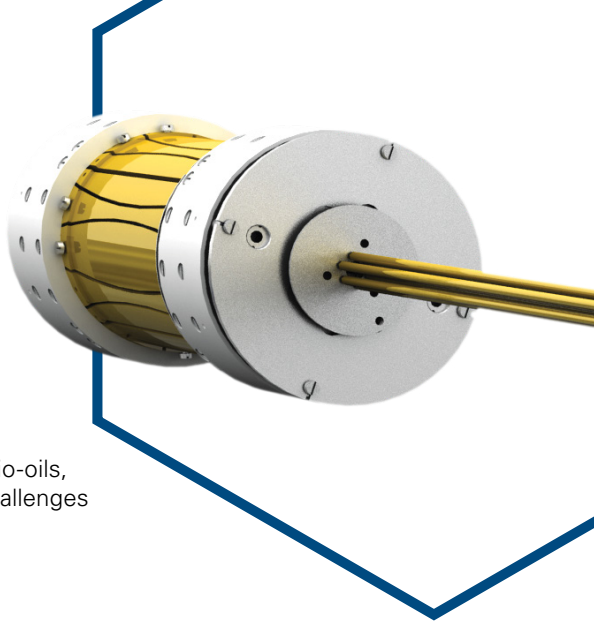


- Dual ESI/MALDI source – Fast and effortless switching between ionization modes.
- Smartbeam 3D laser and microGRID technology for high spatial resolution imaging.
- Proprietary gated TIMS for accurate CCS values and detection of isomeric diversity
- High capacity collision cell that enables continuous accumulation of selected ions (CASI) and Q-CID.
- ParaCell with 2xR capability delivering ultra-high mass resolution and accuracy.
- Heated cathode – accessibility to all modes of ExD fragmentation



Wootton *et al*, Analytical Chemistry, 2024, 96, 11343-11352

timsMRMS redefines the limits of what is achievable



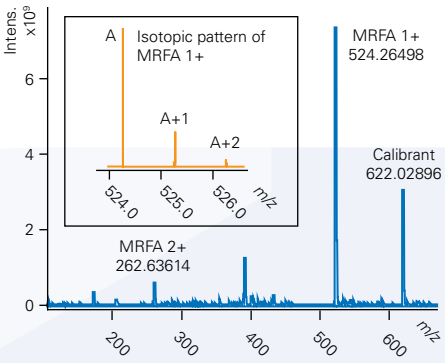
Ultra-high mass resolving power

(>10 M) that helps untangle the complexity. The benefit of high mass resolving power is profound for the analysis of complex mixtures. It increases the 'peak capacity' of your measurement for the detection of more molecular species. Bio-oils, crude oil, dissolved organic matter, and other environmental matrices are all challenges that benefit significantly from ultra-high resolving power.

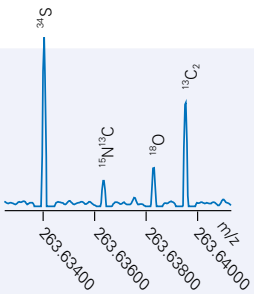
Ultra-high mass measurement accuracy

(600 ppb) that provides confidence in mass and molecular assignment. Mass measurement accuracy tracks with mass resolving power. Sub ppm mass measurement accuracy dramatically limits the number of molecular formula candidates and adds significant confidence in annotation.

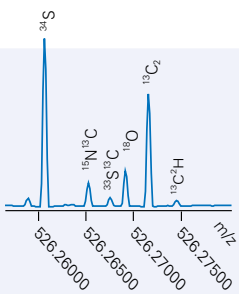
Broadband IFS of MRFA Peptide



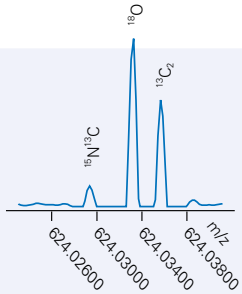
MRFA 2+
A+2 pattern
RP: 2,200,000



MRFA 1+
A+2 pattern
RP: 1,200,000

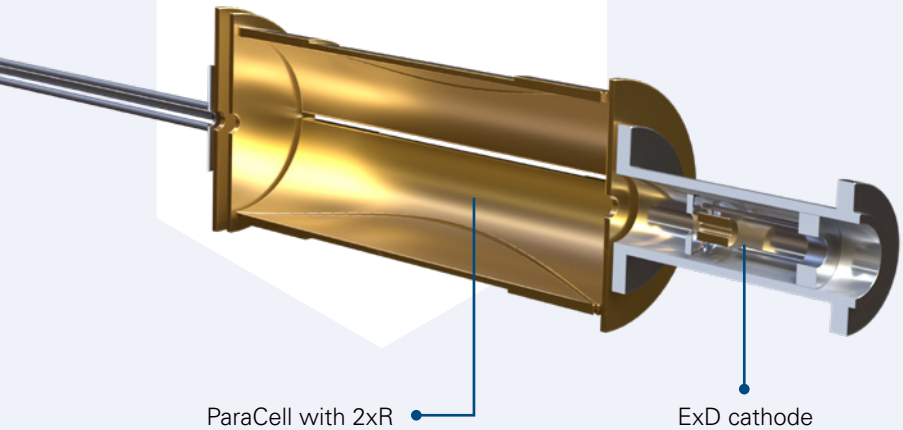


Calibrant
A+2 pattern
RP: 1,000,000



Isotopic fine structure (IFS)

Enhances specificity of molecular assignments. IFS dramatically boosts confidence in assignments that build on the power of mass measurement accuracy.



Like an elemental bar code

Only MRMS can routinely deliver this level of broadband performance!

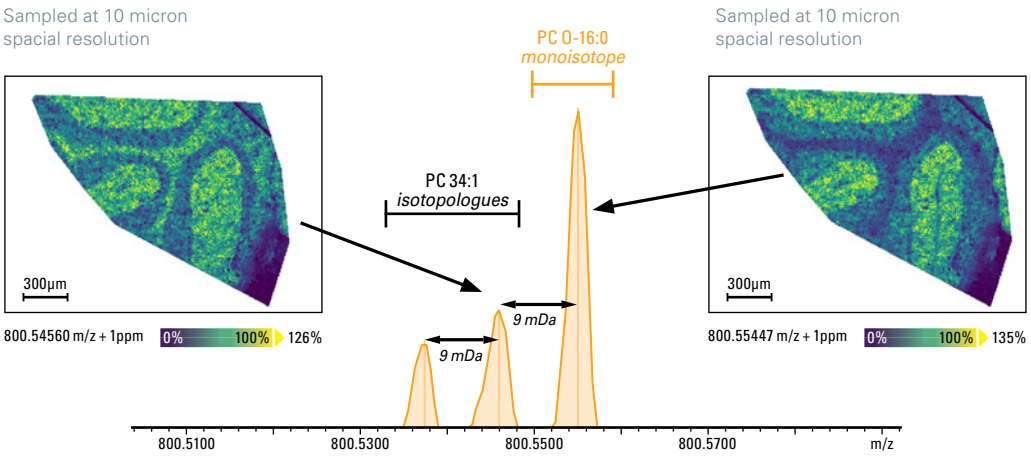


MALDI Imaging

The timsMRMS combines Bruker's smartbeam 3D MALDI laser with a microGRID stage that enables high spatial resolution measurements in MALDI Imaging.. This powerful combination brings unprecedented clarity to tissue imaging.

Biological tissue samples are extremely complex. Ultra-high resolving power is necessary to distinguish the individual molecular features and isotopologues (for IFS). By precisely resolving isotopologues, two closely related lipid species are confidently separated and identified where lower resolution fails.

When this molecular precision is fused with spatial information, distinct molecular images emerge—revealing biology with stunning specificity maintained at mDa level.



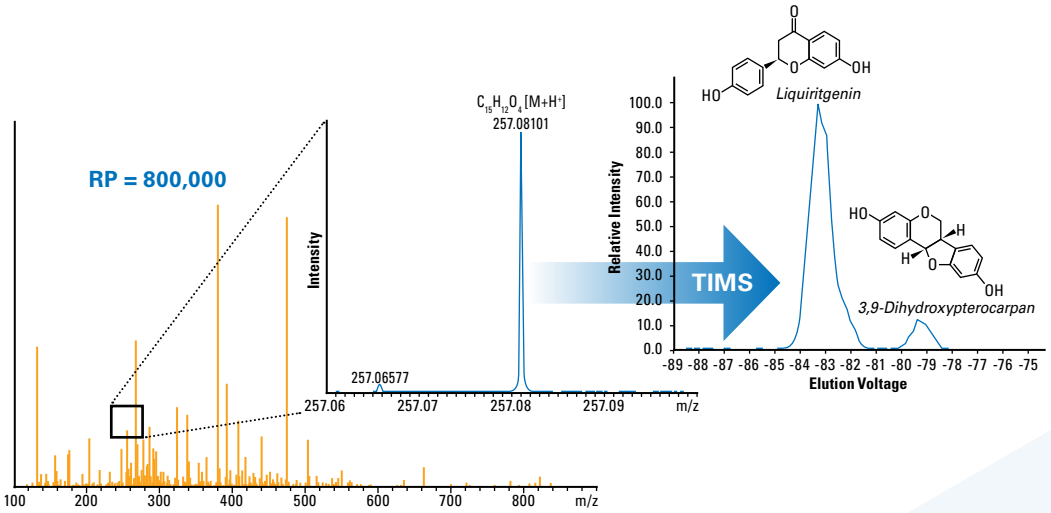
MALDI-MRMS imaging of rat brain tissue acquired using 7 T magnet, absorption mode processed (AMP).

Samples provided by Prof. Dr. Andreas Römpp, Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth.

Natural Products and Metabolites

timsMRMS delivers the ultra-high resolving power required to confidently analyze metabolite or natural product extracts directly. TIMS adds functionality to separate structural isomers providing a powerful new dimension of molecular specificity.

Sensitivity and dynamic range is further enhanced through CASI enrichment, enabling the detection of low-abundance species without compromising resolution.



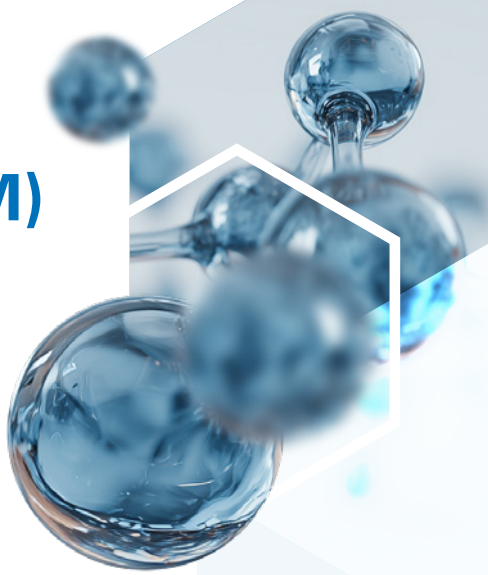
ESI-MRMS analysis of natural product mixture with TIMS separation and detection of isomeric species

Sample provided by Prof. Sunghwan Kim, Kyungpook National University College of Natural Science

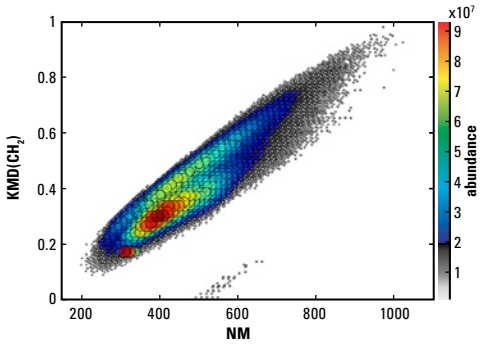
Environmental Analysis - Dissolved Organic Matter (DOM)

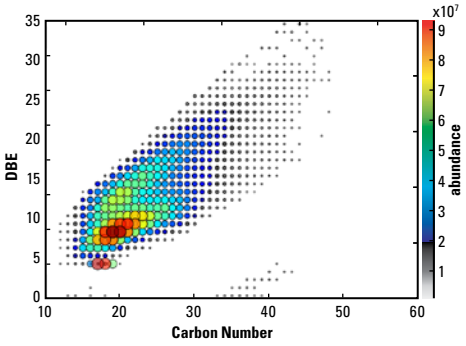
DOMs like Suwannee River Fulvic Acid (SRFA) are estimated to contain 10^5 to 10^7 individual molecular structures, including isomers.

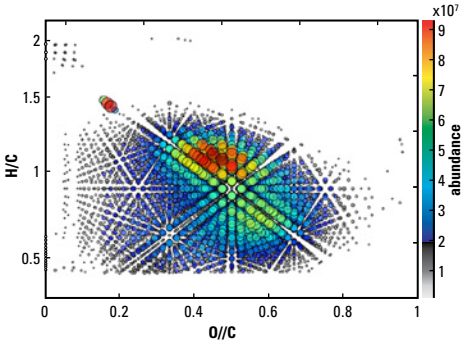
An added feature of gated TIMS is control over ion packet density transferred to the MRMS cell. Peaks previously convoluted by multiple charge states are separated by TIMS thereby enhancing ultimate dynamic range. As shown below, timsMRMS analysis provides richer data with more peaks as exemplified in the clarity of the bimodal distributions.



WITHOUT TIMS





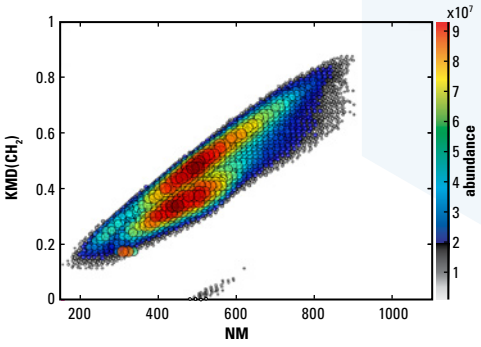


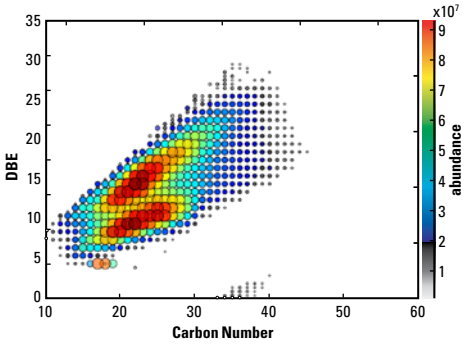
+ TIMS

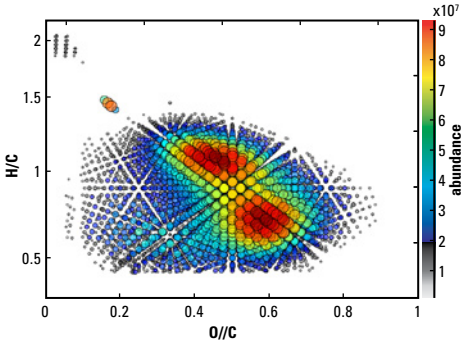
+ TIMS

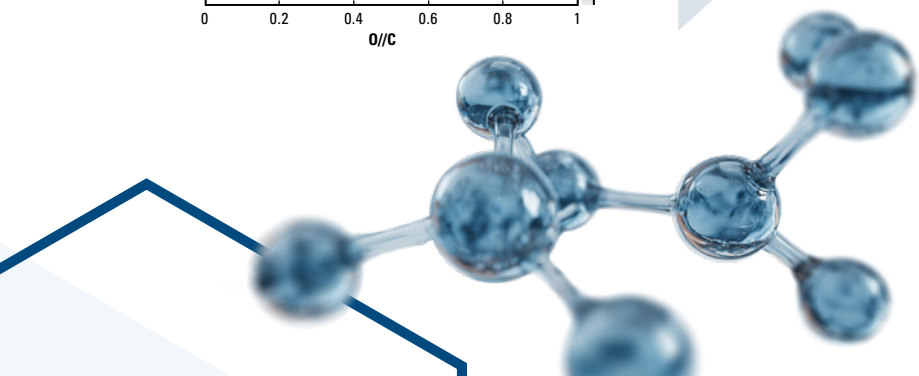
+ TIMS

WITH TIMS









Figures and analysis provided by: Dr. Christopher Rüger
Research Group Leader, Universität Rostock

Ultra-high magnetic field option – The 18 T timsMRMS magnet

The MRMS performance figures-of-merit increase with increasing magnet field strength. These include: speed, mass resolving power, mitigation of peak coalescence, mass measurement accuracy and upper mass limit. Moreover, some of these scale quadratically with field, offering exponential gains in performance.

Bruker's 18 T magnet option creates a path to exclusive and unparalleled MS technology that will enable researchers to tackle the most challenging and complex analytical problems with unsurpassed depth and confidence.



Carlos Afonso

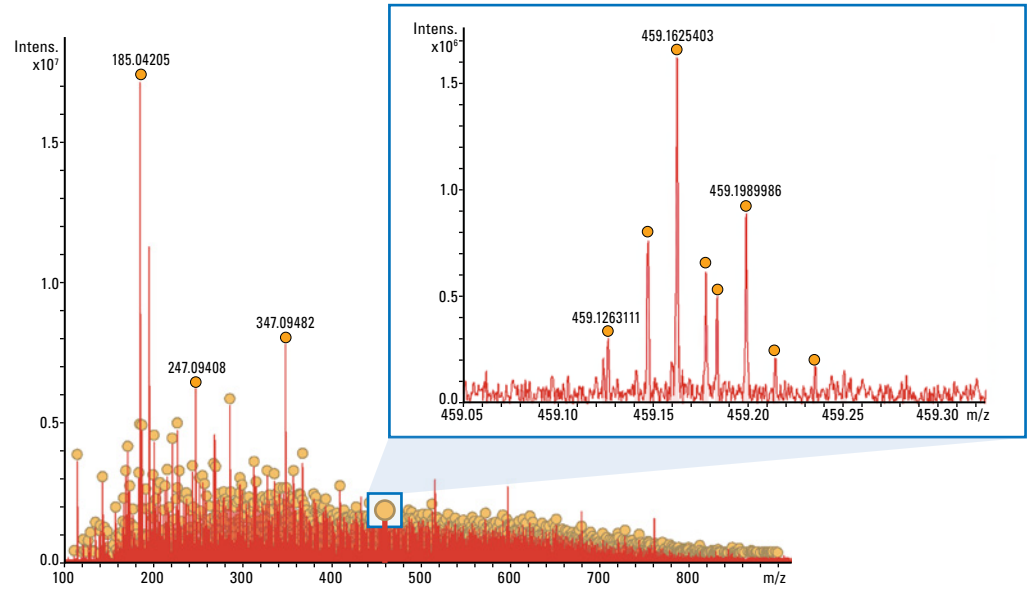
Professor of Analytical Chemistry at the University of Rouen-Normandy, France

"The next generation MRMS cart equipped with the new high-field 18 T magnet revolutionizes LC-MS, enabling routine operation while delivering unparalleled resolution, sensitivity, and throughput for complex sample analysis."

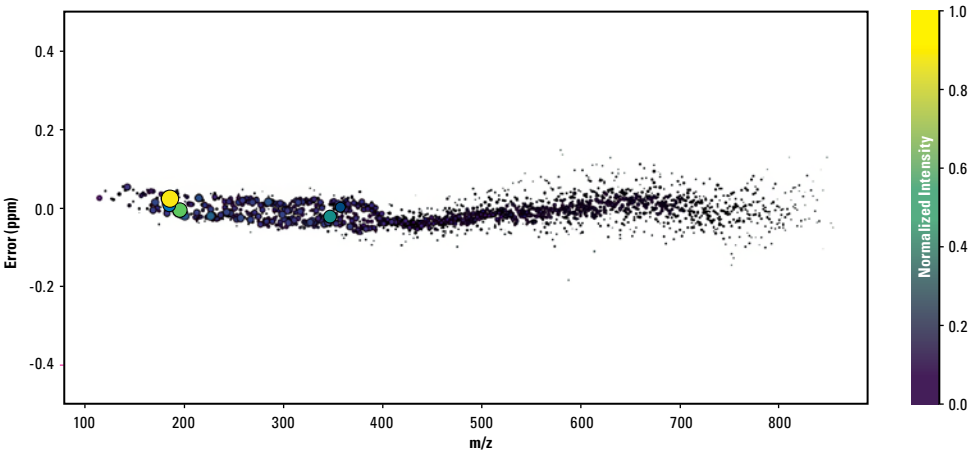


Complex bio-oil analysis using 18 T timsMRMS

Single scan, high resolution (>1.0M RP), broadband mass spectrum!



High resolution, broadband mass spectrum of bio-oil from wood pyrolysis acquired using 18 T timsMRMS. Data and figures courtesy of Prof. C. Afonso and Dr. P. Giusti acquired on the 18 T timsMRMS at the University of Rouen/ iC2MC.



Mass measurement error distribution as a function of m/z species assignments are approximately within +/- 100 ppb!

Courtesy of the University of Rouen team.



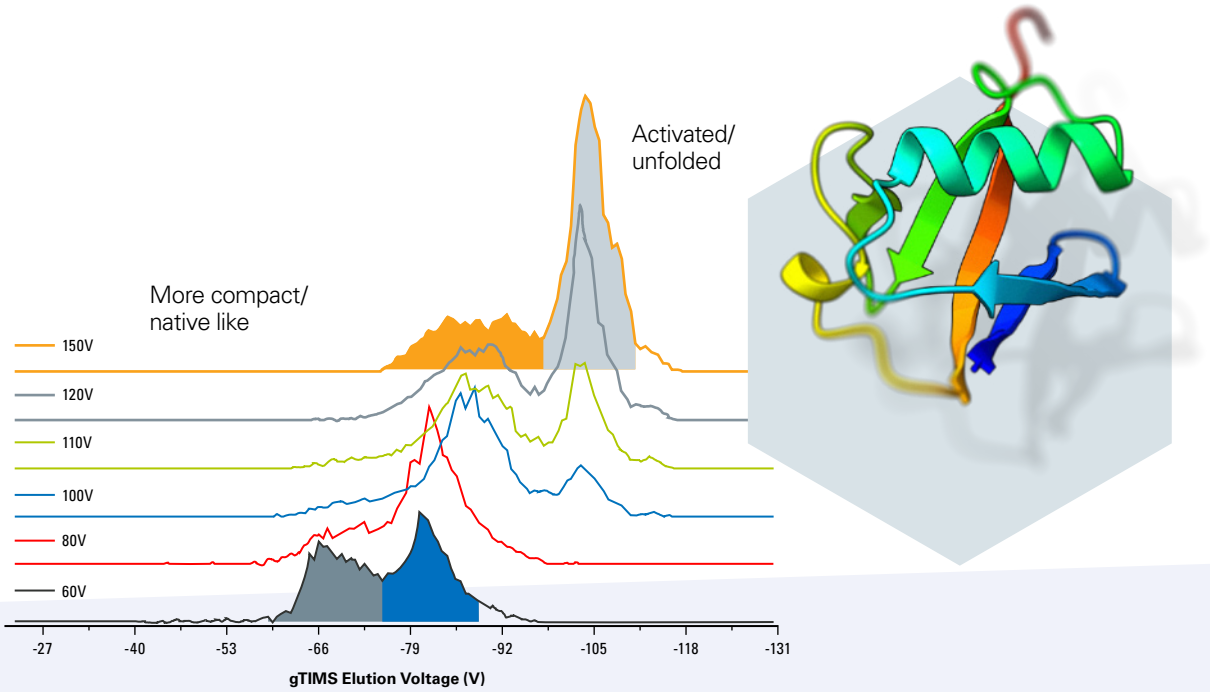
Patrick Bernard

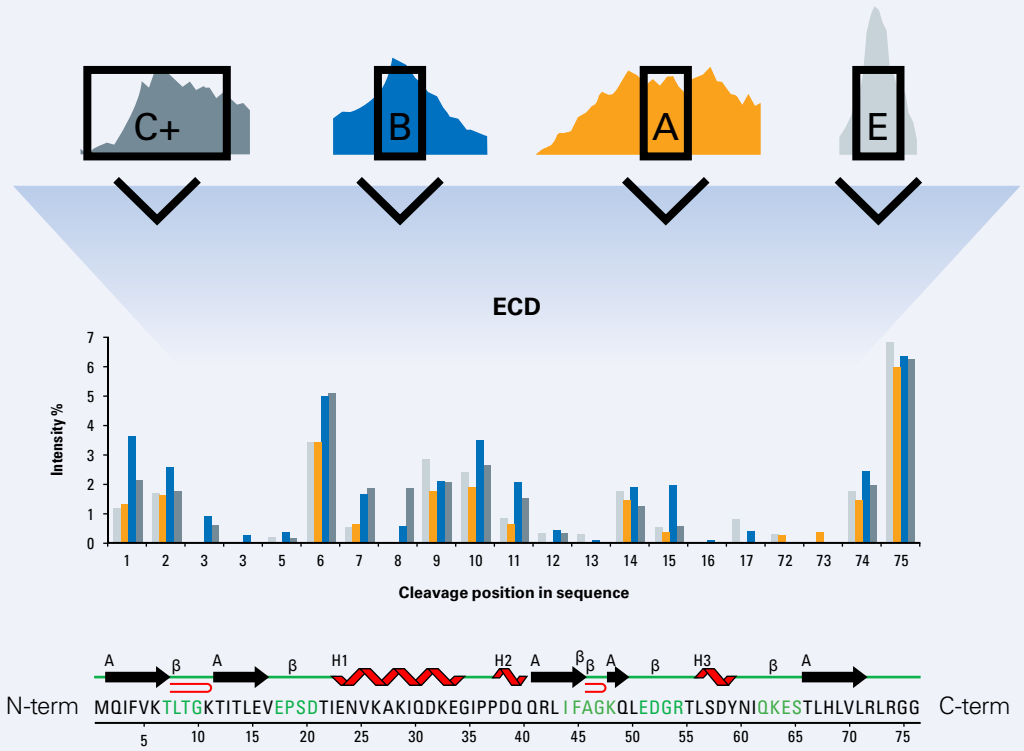
Research and Technology Director Saft (wholly-owned subsidiary of TotalEnergies)

"The first time I saw these results, I felt like Champollion in front of the Rosetta Stone! These remarkable results are incredibly valuable for improving Li-Ion batteries, deciphering the composition, and for understanding the properties of the passivation layer on the electrodes, which largely determines their performance."

Intact Protein Analysis

The gentle source and TIMS region of the timsMRMS allow compact gas-phase protein conformations to remain intact for detection. Using TIMS, specific conformations of a protein can be separated and isolated for further ExD experiments. Multiple fills of these selected conformations are possible to enhance dynamic range and depth of MS/MS sequencing without ion loss. With this approach timsMRMS is able to decipher the complexity of intact proteins.





Analytical Power that is Accessible

Maxwell magnet allows easy placement in MS labs

- **Eliminates liquid cryogen filling**
  - No liquid helium or nitrogen fills provides freedom from helium availability issues.
- **timsMRMS to match your needs**
  - 7 T Maxwell magnet is standard, with 12, 15 and 18 T magnet options available.
  - Bruker offers customized solutions to match your research needs.
- **Standard siting and maintenance for 7T Maxwell timsMRMS**
  - Smaller footprint, operated in a standard laboratory space.
  - Cryo compressor planned maintenance is only needed once every four years.

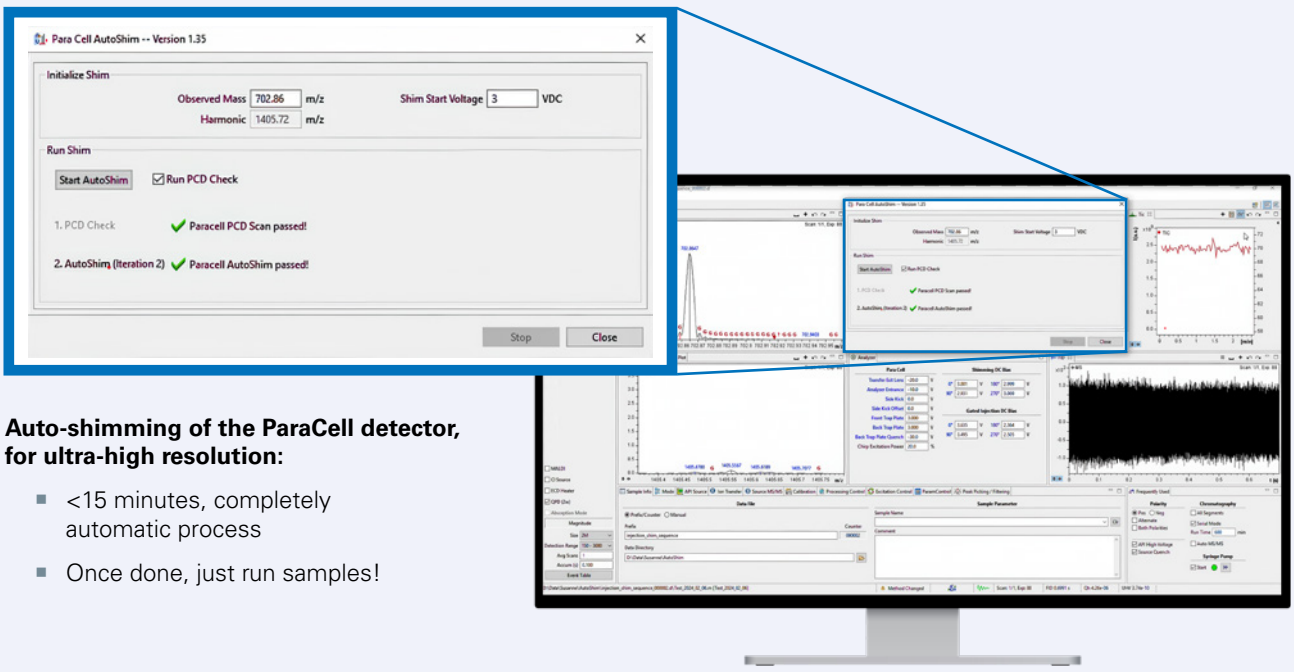


Kristina Hakansson, Ph.D.

Professor of Chemistry & Biochemistry, Florida State University. Director, Ion Cyclotron Resonance Program, National High Magnetic Field Laboratory

"A key goal for me as a new Director at the National High Magnetic Field Laboratory is to make the unrivaled performance of FT-ICR mass spectrometry available to the broader scientific community. I am thrilled to collaborate with Bruker who are focusing on accessibility and ease of use with their new MRMS instrumentation."

Auto-shim: Optimal performance for all operators

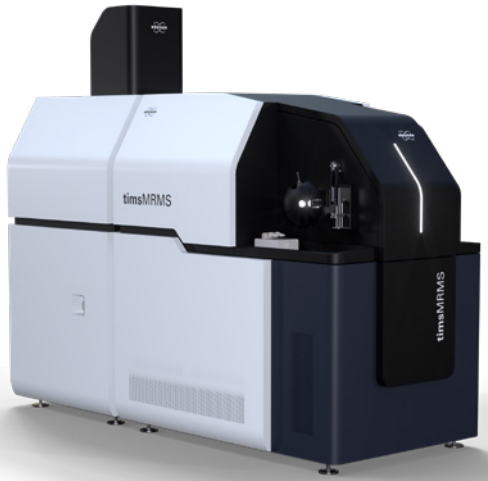


Auto-shimming of the ParaCell detector, for ultra-high resolution:

- <15 minutes, completely automatic process
- Once done, just run samples!

Untangle Complexity:
Discern and identify with confidence

- timsMRMS combines the added specificity and selectivity of TIMS with the unparalleled eXtreme resolution and mass accuracy of MRMS for ultimate **depth of analysis**.
- **Versatility** powered by a broad choice of ion sources, and fragmentation options for flexible experiment design.
- Automatic detector optimization and Maxwell magnet technology making the timsMRMS **approachable** and powerful.
- Whether Tissue Imaging or analyzing ultra complex mixtures, timsMRMS is the **ultimate solution.**





Madeline E. Colley, Ph.D.

Research Instructor (She/Her/Hers), Vanderbilt University

"The new timsMRMS system combines the high spatial resolution qualities of the timsTOF fleX and the high spectral resolving power and dynamic range of the FT-ICR for a perfect pairing of high specificity molecular imaging for capturing spatial biology at cellular resolution."

The timsMRMS cart and electronics are available as technology upgrades to existing MRMS magnets.
Contact Bruker Daltonics for more details, terms and conditions.

MRMS: *Magnetic resonance mass spectrometry.* ***TIMS****: Trapped Ion Mobility Spectrometry.* ***HPLC****: High-performance liquid chromatography.* ***MALDI****: Matrix-assisted laser desorption/ionization.* ***DOM****: Dissolved organic matter.* ***PFAS****: Per- and polyfluoroalkyl substances.* ***CCS****: collisional cross section.* ***CASI:*** *Continuous accumulation of selected ions.* ***ExD****: Electron-based dissociation.* ***(Q)-CID****: (Quadrupole)-Collision-induced dissociation.* ***API****: Atmospheric pressure ionization.* ***ESI****: Electrospray ionization.* ***MSn****: tandem mass spectrometry.* ***MRFA****: Methionine-Arginine-Phenylalanine-Alanine.* ***IFS****: Isotope fine structure.* ***PC****: Phosphatidylcholine.* ***SRFA****: Suwannee River Fulvic Acid.*

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