

NEW ULTRA-HIGH-RESOLUTION MASS SPECTROMETER RACES ALONG WITH ULTRA-PERFORMANCE LIQUID CHROMATOGRAPHY

Bruker has just announced the maXis, a revolutionary new Electrospray Ultra-High Resolution tandem Time-Of-Flight mass spectrometer. This novel mass spectrometer has been designed by Bruker to meet head-on the biggest challenge in discovery LC/MS today: to deliver ultra-high performance mass spectrometry data at speeds capable of fully exploiting modern ultra-performance liquid chromatography. The resulting innovative mass spectrometer provides scientists with a breakthrough solution for their future requirements in advanced applications like small molecule identification, metabolomics, quantitative proteomics, and biomarker panel discovery. Bruker's innovative maXis redefines scientists' expectations of what can be achieved with LC/MS.

Adding MS/MS fragment information with isotopic data to a sophisticated relational algorithm, SmartFormula 3D solves real life identification problems in record time, making **maXis** the first 'One-Shot Molecular Formula Machine'. SmartFormula 3D was jointly developed with Pfizer UK.

QUANTITATIVE PROTEOMICS NOW WITH SPEED AND FIDELITY

The astonishing stability over dynamic range of the UHR-TOF technology has given rise to entirely new selectivity criteria for analysis of trace species in complex matrices: high resolution extracted ion chromatograms (hrEIC) are the definition of an entire compound LC peak by a trace of only 1.5 millidalton width. Comparisons using such selective chromatograms permit a new rapid, high sample number and high fidelity

Mass Spectrometry Focus

The most modern discovery applications now demand definitive tandem LC/MS and MS/MS results on ever more complex samples. Pursuing maximum resolution from both LC and MS techniques is a natural response to the challenges of such complexity. This revolutionary **maXis** is the only mass spectrometer capable of providing the maximum MS performance specification at the very highest speeds delivered by modern Ultra Performance Liquid Chromatography and Capillary Electrophoresis. In an example experiment, a five-component drug mixture was separated in 30 seconds, providing LC peak widths of 1 second or less. **maXis** confidently assigned the elemental formula of each drug compound, taking advantage of subppm mass accuracy, over 40,000 resolution while acquiring some 20 spectra over each LC peak [4].

SCIENTISTS NOW HAVE A ONE-SHOT MOLECULAR FORMULA MACHINE

The exceptional accurate mass capabilities of < 1 ppm of the **maXis** UHR-TOF (Ultra High Resolution Time-of-Flight mass spectrometer) define new confidence standards in formula elucidation. The few resulting formula candidates from very precise mass measurement are further reduced to typically one single formula by Bruker's SmartFormula. This complex algorithm takes advantage of the exact measured isotopic pattern profile and excludes further candidates by comparing the isotopic pattern from the spectrum with the theoretical isotopic pattern. Species are identified without assumptions or recourse to libraries. Moreover, the sub-ppm MS/MS capabilities of the **maXis** further enhance correct formula elucidation for e.g. larger molecules.

quantitative method for quantitative proteomics and biomarker panel discovery in combination with Bruker's dedicated ProteomeQuant software.

BIOMARKER PANEL DISCOVERY WITH HIGH CONFIDENCE

In both metabolomics and proteomics, the sample complexity often is a limitation to biomarker panel evaluation. A resolution of beyond 40,000 FWHM enables the **maXis** for the discreet analysis of near-isobaric species. Peptides extremely close in mass can be clearly separated, even at relatively high mass. High precision hrEIC definition of marker peaks over large sample sets permits high confidence valid data comparisons.

OUTSTANDING RESOLUTION FOR INTACT PROTEIN ANALYSIS

Analysis of intact proteins requires outstanding resolution capabilities at high mass ranges. **maXis'** high resolution power accompanied by extended mass range and high mass accuracy allows for precise protein analysis. Casein®, for example, with a molecular weight of 24 kDa, can be analysed with isotopic resolution and a mass accuracy of $\delta m/w = 1.5$ ppm.

ENABLING TECHNOLOGY: MAKING PERFORMANCE@SPEED POSSIBLE

Modern chromatography can now deliver LC peak widths of around 1 second wide, compelling the requirement for MS technologies to work at speeds of 15 or 20 Hz to provide sufficient datapoints to characterise the LC peak. Time-of-flight technology is the natural choice for high-speed acquisition, however, for over a



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decade time-of-flight technology was believed to be limited to moderate performance in the 15,000 mass resolution range.

Technologies such as Fourier Transform Mass Spectrometry or orbital trapping designs could deliver significantly higher mass performance, but such enhanced MS performance is entirely lost when running at speeds of 10 to 20 spectra-per second required for high resolving LC.

With UHR-TOF technology embodied first in **maXis**, Bruker scientists have broken through the limitations of previous technology with an uncompromised 40,000 plus resolution and sub ppm mass accuracy on both MS and MSMS, all achievable simultaneously at full 20 spectra per second [5].

SCIENTISTS SEE SPEED, ACCURACY AND SENSITIVITY - FUNDAMENTAL FOR SCIENTISTS' APPLICATIONS

Scientists see **maXis** as a real revolution in high-resolution tandem mass spectrometry, offering a no-compromise solution for exceptional accurate mass, high resolution and high sensitivity analysis at a speed able to take full advantage of ultra-high performance chromatography:

SUMMARY


In summary, the revolutionary **maXis** mass spectrometer now provides scientists worldwide with:

- Extraction of full quantitative information from ultra performance chromatography
- High resolution analysis for the evaluation of complex samples in metabolomics and biomarker panel discovery
- Selectivity from complex mixtures with high resolution extracted ion chromatograms (hrEICs) for quantitative studies
- Certainty in identification in combination with SmartFormula 3D – unequivocal formula generation with superb mass accuracy.


REFERENCES

- [1] Brochure **maXis** – Maximum Information@Maximum Speed
- [2] Technical Note # TN-23: Certainty in Small Molecule Identification by Applying SmartFormula 3D on a UHR-TOF Mass Spectrometer
- [3] Technical Note # TN-27: ProteomeQuant – A Highly efficient Solution for Biomarker Discovery and label-free Identification of Regulated Proteins in Biological Systems
- [4] Technical Note # TN-28: **maXis** High Resolution LC/MS Makes the Most of Ultrafast LC Separations
- [5] Technical Note # TN-29: UHR-TOF: A Revolution in Time-Of-Flight Technology
- [6] www.bdal.com/maxis


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The most modern discovery applications now demand definitive tandem LC/MS and MS/MS results on ever more complex samples
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Bruker Daltonics



Maximum Performance



... at Maximum Speed

- Analytical Power and Speed for:
- Fast chromatography applications
- Trace analysis studies

- Small molecule ID
- Metabolomics
- Quantitative proteomics

++ >40.000 FWHM resolution ++ <1 ppm mass accuracy ++ 20 spectra/second ++

It's time to embrace a new concept of what is possible with a mass spectrometer. The maXis Ultra High Resolution (UHR) - TOF is the only tandem mass spectrometer able to provide maximum information at the very highest speeds delivered by latest Ultra Performance Liquid Chromatography. No other mass spectrometer is better equipped to acquire definitive data for small molecule identification, proteomics and metabolomics applications.

Contact us now and get involved with the maXis today: www.bdal.com

think forward

UHR-TOF MS