BRUKER

MRMS aXelerate

- Phenomics, Metabolomics and beyond

FIA-MRMS

Innovation with Integrity

Answers in Minutes not Hours

Flow Injection Analysis

The chemical complexity of clinical samples is traditionally measured by GC- or LC-MS. While powerful, the performance is dependent on the time invested, limiting throughput and coverage.

What if we can eliminate the time consuming LC step and still provide the answers needed in minutes? Flow injection analysis (FIA), provides an additional and unique tool to Metabolomics and Phenomics labs.

MRMS, Magnetic Resonance Mass Spectrometry, is the pinnacle of MS for both resolving power and mass accuracy. This performance provides the foundation for the utility of the FIA-MRMS workflow, or simply MRMS aXelerate.

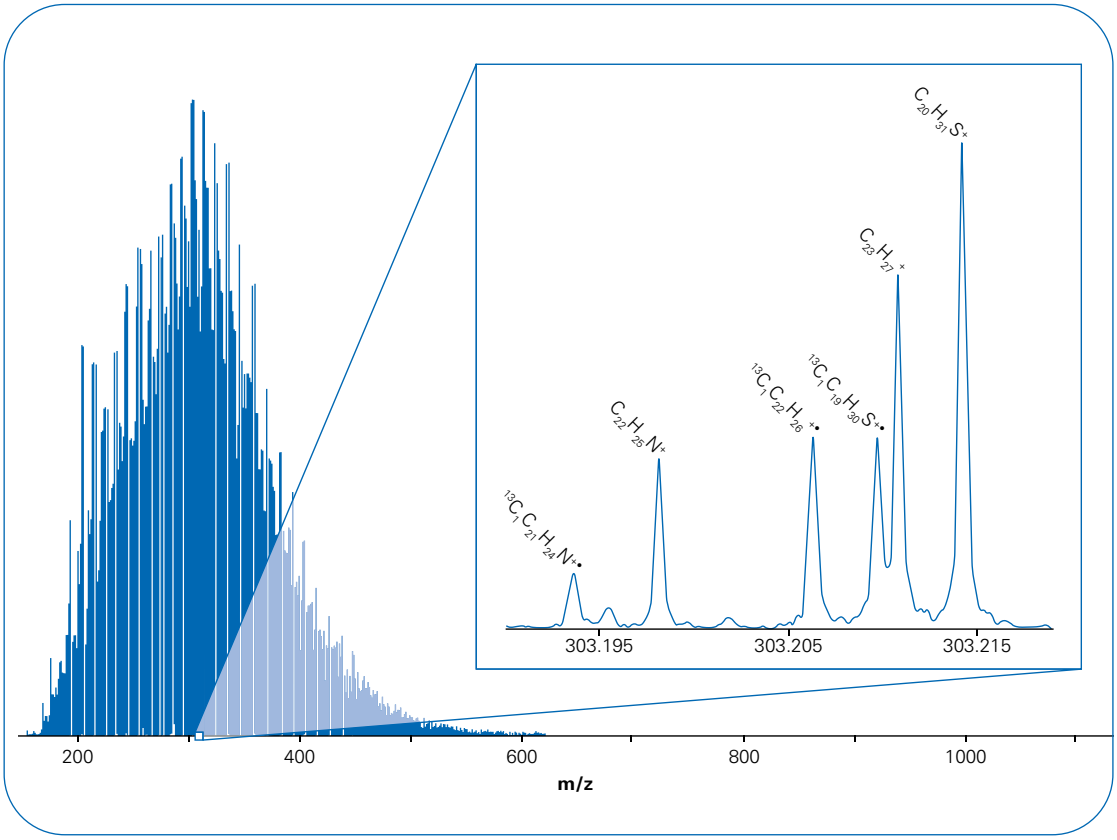
Knowing the value of the FIA-MRMS workflow allows researchers to move beyond the conventional concerns of dynamic range and ion suppression and apply this new information to solving real problems, as is being done in the oil industry. (see adjacent page)

Traditional Metabolomics and Phenomics labs are already discovering the many benefits of MRMS aXelerate.

Complex Mixture Analysis

FIA and Industry

FIA-MRMS is a proven workflow for major petrochemical companies as it provides real answers to real problems. Essentially ancient metabolites, crude oil serves as the worst case scenario for LC free analysis, especially when compared to clinical samples.



FIA
Provides Real Solutions For The Petroleum Industry

Corrosion Issues
Prevention
Asphaltene Characterization
Biodegradation
Catalyst Poisoning
Environmental Monitoring
Reservoir Characterization
Process Optimization
Emulsion Stability
Waste Water Treatment
Dissolved Organic Matter

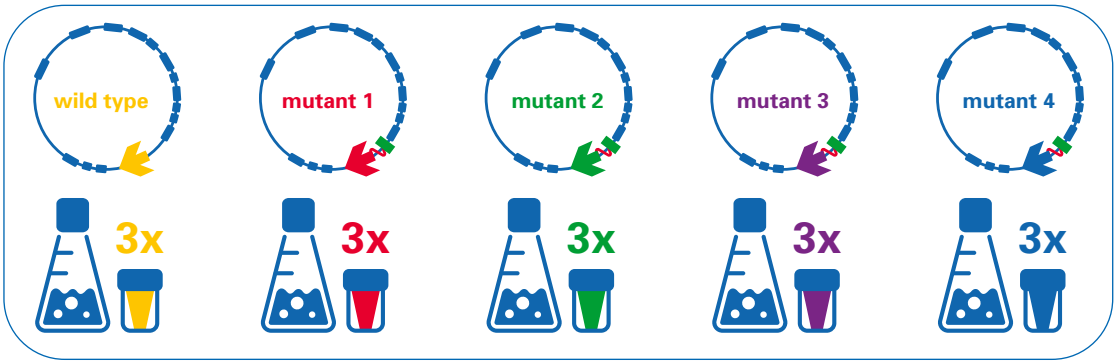
Finding a Needle in a Haystack

Rapid Statistical Analysis

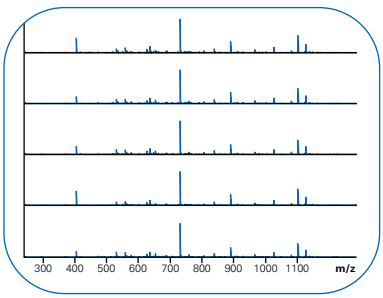
Rapid, LC-free MS followed by statistical analysis provides a sensitive, high-throughput workflow for modern phenotyping and metabotyping.

Workflow: A: Generate a series of different samples B: Rapidly measure high resolution mass spectra C: Perform rapid statistical analysis D: Discover unique biomarkers

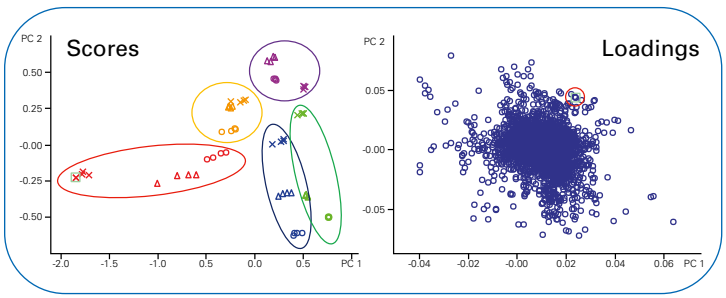
A



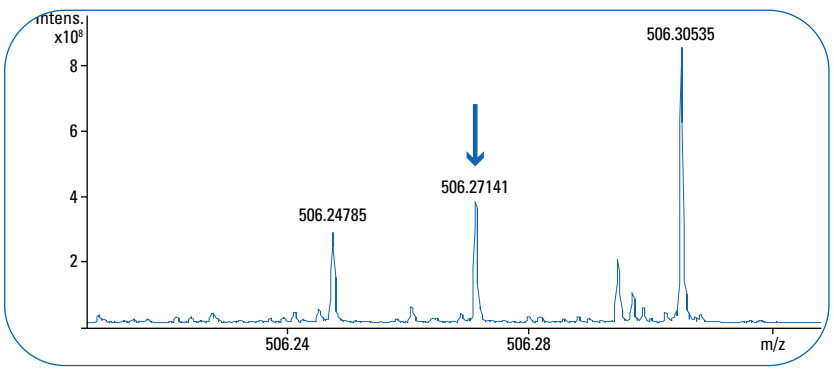
B



C



D



If required, additional analysis can be run for quantitation, MS/MS, or any further analysis.

Rolf Müller and co-workers, Ultrafast Statistical Profiling of Bacterial Metabolite Extracts, Bruker Daltonics Application Note.

Composition and Structure

Isotopic Fine Structure

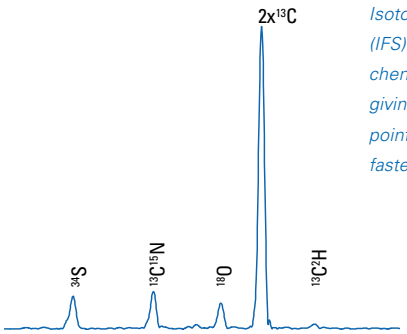
NMR is the gold standard for structural analysis and ID; however, it can be very time consuming if structural elucidation is done blindly. Providing the exact formula greatly improves the confidence in identification, and drastically increases the analysis time and overall throughput.

Fractionated samples are provided to both NMR and MRMS for analysis

MRMS analysis reveals Isotopic Fine Structure (IFS) providing an unambiguous molecular formula

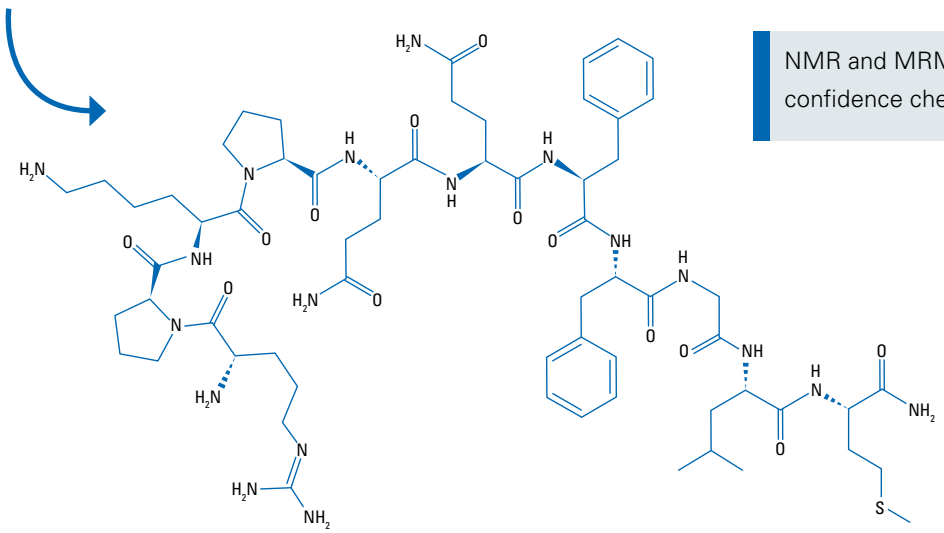
Providing NMR with the correct starting formula enables faster structural elucidation of unknowns

$C_cH_hN_nO_oP_pS_s$



A+2 isotopic fine structure

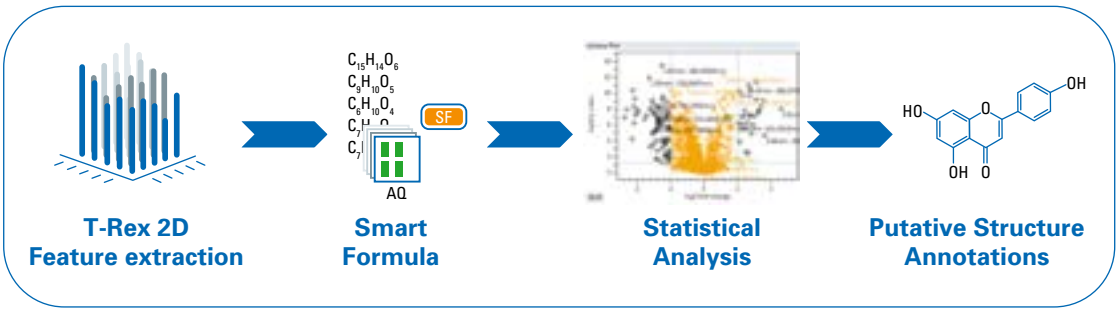
Isotopic Fine Structure (IFS) provides a definitive chemical composition giving a better starting point for NMR, enabling a faster analysis time



NMR and MRMS provide a high confidence chemical assignment

MRMS aXelerate

The Complete Solution



- Accelerate throughput (> 200 samples/day)
- Complementary to established NMR based solutions
- Simultaneous analysis of known and unknown metabolites
- Access compounds not readily detectable by LCMS analysis
- 3-tiered confidence in annotation

Prof. Philippe Schmitt-Kopplin Analytical BioGeoChemistry, Helmholtz Zentrum München, Germany

"MRMS eXtreme Resolution enables us to address next generation metabotyping, i.e. simultaneous rapid description of hundreds of known and thousands of new metabolites relevant for dynamic biological/chemical processes."

Pushing the Frontiers

of Scientific Discovery

Systematic isolation and structure elucidation of urinary metabolites optimized for the analytical-scale molecular profiling laboratory.
Matt Lewis and co-workers
Anal. Chem. 2019, 91, 14, 8873-8882
A *de novo* strategy for the structural elucidation of urinary metabolites, where MRMS provides a high-confidence starting point for NMR analysis, increasing the efficiency and reducing the time required for complete structural elucidation.

A metabolomic study based on accurate mass and isotopic fine structures by dual mode combined-FT-ICR-MS to explore the effects of *Rhodiola crenulata* extract on Alzheimer disease in rats.
Fei Han and co-workers
J Pharm Biomed Anal. Vol 166, p347-356 (2019)
A dual mode MRMS strategy (HPLC & Fractionation) is applied to profile biochemically the metabolic pathways of plasma serum of Alzheimer disease rats affected by *Rhodiola crenulata* extract.

Potential of dynamically harmonized Fourier transform ion cyclotron resonance cell for high-throughput metabolomics fingerprinting: control of data quality
Estelle Rathahao-Paris and co-workers
Anal Bioanal Chem, 410 (2), 483-490 (2018)
Details the utility and robustness of the FIA-MRMS workflow for performing large-scale high-throughput metabolomic analyses under routine condition.

Coculture of Marine Invertebrate-Associated Bacteria and Interdisciplinary Technologies Enable Biosynthesis and Discovery of a New Antibiotic, Keyicin
Tim S. Bugni and co-workers
ACS Chem. Biol., 12 (12), pp 3093–3102 (2017)
As part of a larger complete antibiotic discovery process, Isotopic Fine Structure provides the exact molecular formula to identify the novel antibiotic.

Metabolomics reveals metabolic biomarkers of Crohn's disease
Philippe Schmitt-Kopplin and co-workers
PloS one, 4 (7), e6386 (2009)
Non-targeted metabolic profiling is used to determine the contribution of metabolites produced by the gut microbiota towards disease status of the host. MRMS is used to discern the masses of thousands of metabolites.

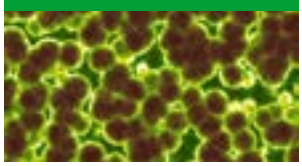
Molecular Profiling

Traditional Chinese Medicine

High Throughput

Natural Products

Biomarkers



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