

# Mass Spectrometry & Spectroscopy

## 64th ASMS Conference on Mass Spectrometry and Allied Topics Held in San Antonio from 5th to 9th June, 2016 at the Henry B. González Convention Center, San Antonio, Texas USA



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A very hot and steamy San Antonio, Texas saw the conference start early for many attendees; with one-and two-day short courses beginning on Saturday and Sunday 4th and 5th June from 9:00 am to 4:30 pm, and later on Sunday afternoon with two informative tutorial lectures from 5:00 to 6:30 pm.

The brief opening ceremony was followed by a very interesting lecture entitled 'A Molecular Toolkit for Viral Hemorrhagic Fevers' presented by Professor Erica Ollmann Saphire from the The Scripps Institute-La Jolla, California. Professor Ollmann Saphire, a leading X-Ray Crystallographer, discussed how the recent Ebola virus outbreak of 2014-2016 had 30,000 sufferers which all started from a single 2-year-old child playing in a tree. She continued by explaining how, from a genetic perspective, these viruses (Ebola filovirus has 7 genes and Lassa arenavirus has 4 genes) were simple compared to the human with 20,000 genes and then posed the question "How do these limited gene viruses create so many mutations". Professor Ollmann Saphire's work has revolved around attempting to answer this question by utilising x-ray crystallography and modelling and solving the conundrum, "that in vitro experiments do not predict in vivo results". Even though this was a mass spectrometry conference she only referenced mass spectrometry three times in her presentation, the final time being a heartfelt plea to the mass spectrometry community for "help in finding the molecular evolution that takes place in viruses, human proteins, diseases and drug targets".

This was followed by the Opening Reception, located in the poster-exhibit hall, which was an opportunity to eat, drink and meet up with colleagues and friends. Heavy hors d'oeuvres (yes, enough for dinner!), free Rye Saison and India Pale Ale beers from the Granary which is brewed in San Antonio and a cash bar for wine were all available. Technical posters were not posted until Monday morning at 10:30, making this the ideal time to connect with exhibitors at their booths.

Monday saw ASMS start in earnest at 08:30 with 128 parallel oral sessions of the scientific programme over the four days (32 sessions daily running concurrently) and culminating in the plenary lecture, 'More than the Sum of its Parts: Collective Phenomena in Living Systems, from Single Molecules to Flocks of Birds', presented by William Bialek of Princeton University, Princeton New Jersey.

This year there was a much more manageable 2982 posters (compared to 3141 in 2015) displayed during the week covering topics from antibody and antibody drug conjugates (Intact and characterisation) to imaging MS for disease markers and daily workshops ensuring that if you did not utilise a prior selection process of some sort you would miss out on many interesting topics, and have very sore feet. If you weren't exhausted by 17:00 then there were 14 Workshops running daily Monday to Wednesday from 17:45 to 19:00 leaving one hour for dinner before the Corporate Hospitality suites swung into action at 20:00; providing endless snacks, refreshments and entertainment ranging from music, line dancing, kicking some mass – with sheriff's deputies, tee-shirts and cowboy hats – all lasting until 23:00.

Attendance was up slightly (3%), compared to the ASMS 2015 conference, at 6276 (see Table 1 for recent history) with attendees from the USA, Canada, UK, Australia and Asia there in force. There were 188 (171 in 2015) exhibit booths.

Table 1. ASMS attendees by year.

Year	Location	Total Attendees
2009	Philadelphia	6,530
2010	Salt Lake City	6,096
2011	Denver	6,477
2012	Vancouver	6,277
2013	Minneapolis	6,140
2014	Baltimore	6,913
2015	St. Louis	6,100
2016	San Antonio	6,276

### ASMS Awards

#### 2016 Award for a Distinguished Contribution in Mass Spectrometry

The 2016 ASMS Award for a Distinguished Contribution in Mass Spectrometry was awarded to Dr Scott A. McLuckey, the John A. Leighty Distinguished Professor of Chemistry at Purdue University, West Lafayette, Indiana, USA.

The study of ion/ion reactions originated with J.J. Thomson and have played a central role in mass spectrometry since its inception. Gas-phase ion chemistry formed the basis for Dr McLuckey's work and pioneering contributions to the understanding of the gas-phase ion/ion reactions of polyatomic molecules and their applications in analytical mass spectrometry. Ion/ion reactions have not been utilised in mainstream mass spectrometry until relatively recently with the introduction of techniques such as electrospray and the use of electrodynamic ion traps.

Dr McLuckey and co-workers, have since 1990 followed a line of research employing electrospray and ion traps that has revealed an array of ion/ion reactions that significantly expand the scope of tandem mass spectrometry, particularly in biological mass spectrometry focusing on both understanding the dynamics of ion/ion reactions and on developing ion/ion reactions for analytical applications. He and his co-workers demonstrated that ion/ion reactions in ion traps can be both highly efficient and fast.

In recent years, McLuckey's group have expanded ion/ion chemistry to include selective metal ion insertion/removal and functional group specific covalent bond formation. Collectively, these chemistries, along with proton and electron transfer, significantly expanded the power of MS/MS in characterising peptides, proteins, oligonucleotides and lipids.

#### Biemann Medal

Dr Kristina Håkansson, professor in the Department of Chemistry, University of Michigan, Ann Arbor was awarded the 2016 Biemann Medal for her contributions related to her work on the mechanisms of electron-based activation methods, including electron capture dissociation, electron detachment dissociation, and electron induced dissociation and the utilisation of these methods to identify and characterise biological molecules such as peptides, oligonucleotides, and oligosaccharides.

The challenges and opportunities with the structural characterisation of complex biological molecules inspired the development of many new activation methods such as ones involving the attachment or detachment of an electron to an ion. Dr Håkansson's work focused on deciphering the mechanisms of electron-activated dissociation and showing

the outstanding utility of these methods for the analysis of nucleic acids, oligosaccharides, and peptides including ones with labile modifications like phosphorylation. Her group has shown that electron-activated dissociation methods are gentle enough to allow the preservation of higher order structures of nucleic acids.

### Ron A. Hites Award Outstanding Research Publication in JASMS

The Ron Hites Award, which includes \$2,000 and a certificate for each author, recognises an outstanding original research publication, based on its innovation, technical and presentation quality, likely stimulation of future research and impact on future applications. The 2016 award recognises Kevin Pagel, Max Planck Society Berlin, and co-authors Waldemar Hoffmann and Johanna Hofmann for their paper entitled, 'Energy-Resolved Ion Mobility-Mass Spectrometry: A Concept to Improve the Separation of Isomeric Carbohydrates', which was published in JASMS (2014) 25, 471-479.

## New Product Roundup

In the interests of impartiality companies introducing new instruments and products are listed in alphabetical order, we have tried to feature the majority of new products introductions for 2016.

### Agilent Technologies

Announced the launch of the **Agilent 8900 Triple Quadrupole ICP-MS system**.



Figure 1. Agilent 8900 Triple Quadrupole ICP-MS system.

According to Agilent the controlled-reaction chemistry of this inductively coupled plasma/ mass spectrometry system provides the lowest detection limits for elements which previously had been difficult, such as sulphur, silicon and phosphorus.

An innovative product released at the conference by Agilent is the first commercially available ion source that cleans itself. The **JetClean** self-cleaning ion source is designed to keep Agilent quadrupole gas chromatography/mass spectrometry systems free of matrix deposits that would otherwise build up over time and degrade instrument performance. Using a carefully controlled hydrogen flow, JetClean technology greatly reduces, or even eliminates, the need for source cleaning on Agilent single and triple quadrupole GC/MS systems.

Other products being showcased at ASMS include the application specific:

- **Arsine/Phosphine GC/MS Analyzer**, which enables polyethylene and polypropylene producers to reduce costs by moving impurity detection to an internal quality-control workflow, and the
- **Water Screener GC/MS Analyzer**, specifically designed to provide fast data review and reporting of regulated compounds and contaminants of emerging concern, as well as unknowns.

In addition to hardware, Agilent introduced updates to several software tools:

- **MassHunter BioConfirm Software** now includes a new walkup version of the drug-to-antibody calculator, which enables characterisation of antibody drug conjugates by non-expert LC/MS users.
- **MassHunter Profinder Software** speeds up recursive feature extraction and performs simultaneous analysis of multiple data files from qtof mass spectrometers used in tandem with gas or liquid chromatographs.
- **MassHunter Quant Software**, as well as support for national pharmacopoeia system suitability testing and a new metabolomics database and method for dynamic multiple reaction monitoring, enabling routine analysis of central carbon pathway metabolites.
- **MassHunter VistaFlux Software**, which enables cutting-edge, targeted, isotopologue data extraction and pathway visualisation of metabolomic flux results for greater biological understanding.

Several personal compound databases and libraries in water purity assessment, extractables and leachables, for food and pharmaceuticals, were also announced providing scientists with up-to-date references. Important additions were also made to existing PCDLs for pesticides, veterinary drugs and forensic toxicology.

### Bruker

Announced an entirely new mass spectrometry technology platform: the **timsTOF™** system that combines very high ion mobility resolution greater than 200, using proprietary **Trapped Ion Mobility Spectrometry (TIMS)**, with their ultra-high performance ESI-QTOF mass spectrometry.

The new **timsTOF** is a flexible, research-grade instrument for the separation and analysis of unresolved compounds and conformations and is supposed to 'take the stress off the LC system' according to Frank H. Laukien PhD Bruker CEO and President. The Ion Mobility Expansion (imeXTM) TIMS technology can be adjusted to research or analytical needs and has an Open Data Format that supports user-created software tools tailored to specific research questions.

Bruker also announced several mass spectrometry-based product introductions including:

The New Bruker **rapifleX™**, claimed to be the highest performance MALDI-TOF/TOF mass spectrometer, is an advanced TOF/TOF system, and was re-designed from the ground up to meet the demands for in-depth intact and top-down protein characterisation, and high-performance, high-throughput mass spectrometry imaging (MSI).

Bruker also announced the launch of the **rapifleX™ MALDI PharmaPulse™ (MPP)** solution designed to assist pharmaceutical, biotech and CRO customers to accelerate drug discovery. The rapifleX MPP can also dramatically lower the cost of ultra-high throughput screening (uHTS) with further improved results.

Ultra-high throughput screening is primarily performed by fluorescence techniques, which require labelled compounds. Mass spectrometry offers label-free screening, and inherently reduces or avoids false positives and the new rapifleX MPP offers the speed, specificity and robustness of mass spectrometry for large primary screens with a low false positive rate.

The new **Bruker HDX Solution** provides a solution that offers a complete workflow combining the LEAP H/D-X PAL autosampler with pre-defined labelling experiments, a UHPLC system, the maXis II ETD UHR-QTOF mass spectrometer, plus the Sierra Analytics HDExaminer HDX-MS interpretation software.

#### Software updates were also released, and included:

**PesticideScreener™ 2.1** With a database of over 800 pesticides and a pre-defined UHPLC method and workflow, food safety and environmental labs can quickly screen, identify and quantify hundreds of low level pesticide residues in various food or water samples. The optimised pesticides database includes accurate mass, isotopic pattern, fragment ion, adduct, isomer and retention time information, while the pre-defined UHPLC-MS/MS method can screen and quantify the entire database in less than 20 minutes.

**ToxScreener™ 2.1** is designed to allow forensic toxicology labs to easily screen, identify and quantify hundreds of low level drugs of abuse or poisons in various complex samples. Using the same pre-defined UHPLC-MS/MS method as the PesticideScreener, users can also screen and quantify the larger database of over 2,000 toxicology-relevant compounds in less than 20 minutes.

**Sciex** released new mass spectrometry solutions in launching their theme of 'It's Time to see the future differently' that will allow scientists globally to make more breakthroughs using innovative workflows to achieve intelligent outcomes that will impact peoples' lives for a healthier future.

The new solutions included the following:

#### Innovations for advanced workflows:

- **QTRAP 6500+ LC-MS/MS System for Quant** - This new system achieves improved sensitivity and selectivity over previous generation systems for small molecule quantitation and is now integrated with the BioBA Solution for large molecule quantitation, putting everything in one place for biologics bioanalysis.



Figure 3. QTRAP 6500+ LC-MS/MS System for Quant.



Figure 2. Bruker timsTOF system.

- High-throughput Omics Solutions – New advances in automation, reproducibility, robustness, and retrospective analysis allow high-throughput labs to scale-up their research. Sciex has upgraded their platforms to industrialised performance levels, adding new tools to analyse larger sample sets, faster and with more confidence.
- The Sciex Next-Generation Proteomics (NGP) platform is said to offer solutions for large-scale quantitative proteomics with technologies such as the TripleTOF® 6600 system with SWATH® 2.0 Acquisition, to perform quantitative proteomics research by solving the missing data problem, enhancing data processing and results visualisation, with retrospective analysis, and OneOmics™ cloud computing.

Additions to the Sciex NGP platform for industrialised proteomics includes:

- o New sample prep automation with the Beckman Coulter® Biomek NX, powered by Protein Preparation Kits: to automate tedious manual steps and improve reproducibility.
- o Microflow SWATH Acquisition: Offering a higher flow rate for significant time savings and improved robustness, while maintaining the high quantitative quality of SWATH acquisition.
- o SWATH Performance Kits: Facilitating a quick start-up by enabling customers to check the performance of their SWATH Acquisition and monitor performance across their sample sets.
- o OneOmics AutoUploader: Featured in CloudConnect, AutoUploader moves data files automatically to the cloud right after acquisition to further streamline the quantitative proteomics workflow.
- o SWATH to MRM Builder: This new Cloud enables researchers to easily transition from SWATH to MRM workflows, bridging the gap between discovery and targeted validation.
- New Biopharma Innovations – The revised Sciex BioPharmaView™ Software 2.0 which forms an integral part of the Sciex '360-degree innovation approach' to characterisation, a full-circle portfolio has software solutions for biopharmaceutical analyses, to simplify and accelerate both routine and complex workflows and covers solutions for CE, CESI and MS from identity, purity, and heterogeneity, to glycan monitoring and intact mass analysis

#### Innovations for routine workflows:

- The X500R QTOF System – Launched in late 2015, the X500R QTOF System is the first model of the new X-Series mass spectrometry (MS) platform, which was designed exclusively for routine food, environmental and forensic testing labs. The X500R QTOF System was developed based on customer input and key criteria, such as performance, software ease of use, and robustness, so labs can adopt high resolution MS to collect clear, confident results without making performance trade-offs.

## Shimadzu Corporation

Introduced the following new products at ASMS 2016:

The new **LCMS-8045** for routine quantitative analyses in such areas as food safety and environmental testing provides a balance of sensitivity, robustness, and cost-effectiveness operated by using Shimadzu's LabSolutions software. It features some of the components of higher performance models such as the 8040 optics and a heated source. In addition, the ion source features a cable-less, tubeless housing and the desolvation capillary can be replaced without breaking vacuum resulting in easier maintenance and a lower cost of ownership. The shipments of LCMS-8045 will start at the end of summer.



Figure 4. The Shimadzu LCMS-8045 for routine quantitative analyses

Shimadzu Scientific Instruments also released of the Clinical Laboratory Automation Module (CLAM-2000), a fully integrated sample pretreatment module for LC-MS. The system is designed to automatically perform all of the processes necessary to analyse blood and other biological samples.

The CLAM-2000 is the first integrated sample preparation system for LCMS that allows users to process samples in an instrument that is directly attached to the LCMS system, thus enabling a very simple and safe means for lab personnel to both process and analyse samples. The user only needs to place the blood collection tube or other sample in the system, and it performs all other processes automatically, including loading the sample into the autosampler for LCMS analysis. The system offers a variety of functions that help control the precision of analytical results, including reagent management, calibration curve management, control management, and system maintenance management. All of these functions, in conjunction with a user-friendly interface, help ensure a next-generation workflow that provides reliable, rapid, and high-quality results.

Shimadzu also featured three products which were released at the Pittsburgh Conference in March 2016:

ICPMS-2030 inductively coupled plasma mass spectrometer

Nexera MX ultra-high speed LCMS system for Multiplex Analysis

GCMS-QP2020 high-sensitivity gas chromatograph mass spectrometer

## Thermo Fisher Scientific

Headlining the new ThermoFisher Scientific launches was the **Q Exactive BioPharma** MS/MS Hybrid Quadrupole-Orbitrap mass spectrometer that takes full advantage of the high-resolution, accurate-mass (HRAM) capabilities of the Orbitrap mass analyser to enable key workflows for protein characterisation in a single instrument. Combined with sample preparation and analysis methods using ThermoFisher Scientific reagents, columns, UHPLC and data processing technologies, the Q Exactive BioPharma system provides a comprehensive solution for customers performing biopharmaceutical characterisation.



Figure 5. Q Exactive BioPharma MS/MS Hybrid Quadrupole-Orbitrap

Thermo Fisher Scientific also featured its new **ThermoFisher Scientific Vanquish Flex Binary UHPLC system**, an ideal mid-price point complement to its Vanquish range, for pharmaceutical and biopharmaceutical laboratories performing qualitative and quantitative LC or LC-MS analysis.

Thermo Fisher also featured the new ZipChip technology from **908 Devices**, a collaborating pioneer in purpose-built analytical devices for chemical analysis. The ZipChip provides a new and innovative inlet technology that provides fast, high resolution separations of biomolecules for MS analysis in biopharma characterisation workflows. Users can select between two chip types; **ZipChip HS** for small molecule analysis and peptide mapping or **ZipChip HR** for intact large molecules.

The following software and cloud solutions were launched at the conference by Thermo Fisher Scientific:

- **TraceFinder 4.1** - an easy-to-use, workflow-driven solution for quantitation and screening of both small and large molecules. The newly updated version offers support for peptide/protein quantitation, including a predictor tool to aid with method set up and enhanced data displays to facilitate throughput for data review. A new high-resolution accurate mass (HRAM) library and searching algorithms for targeted screening are also included.
- **Compound Discoverer 2.0 Software** for small molecule identification and characterisation using high resolution accurate mass (HRAM) Orbitrap data. Designed for a range of applications including metabolomics, drug metabolism, environmental, food research and toxicological studies, the software provides powerful untargeted and targeted workflows.
- **Proteome Discoverer 2.1 Platform** offers comprehensive data analysis for quantitative and qualitative proteomics research using a distinctive node-based processing framework. The new version of this platform incorporates additional support for analysing large data sets, an updated user interface for quantitative ratios and enhanced capabilities for TMT quantitation workflows.
- For in-depth characterisation of biopharmaceutical proteins, **Thermo Scientific BioPharma Finder 1.0 Software** provides an integrated workflow-driven interface for comprehensive and easy interpretation of biologics. This new solution automates the analysis of peptide digests and intact proteins, providing relative quantitation of proteins, sequence variants, disulphide bonds and low level modifications.
- **LipidSearch 4.1 Software** provides an automated solution for the identification and relative quantitation of lipids. This latest release includes an enhanced database, improved lipid annotation and supports HCD and CID data in the same search.

• Combining a highly curated collection of high resolution/accurate mass MS/MS and MSn spectra, the updated **mzCloud™ Advanced Mass Spectral Database\*** provides a different approach to mass spectral fragmentation libraries. The new version of the database is equipped with twice the amount of compounds as the previous version, triple the number of spectra and automatic batch search tools to offer a remarkable amount of fragmentation information.

In addition to the new products above being released at ASMS, Thermo Fisher also previewed the following applications developed to further enhance capabilities of the Thermo Fisher Cloud:

- **Pathway Over-representation** – This new cloud-based project explores the use of statistical analysis to detect biological pathways that are either over- or under-represented in a list of input proteins or genes.
- **Sample Profiler** – Using cloud-based software, this project aims to enable users to build their own 'product' profile of both known and unknown components. Having determined an 'authentic' profile, new samples can be easily compared and component outliers identified.
- **MS Instrument Connect** – This new tool enables researchers to monitor their MS instruments and lab productivity remotely. The solution provides an at-a-glance dashboard for a quick overview of the instruments' status, detailed real-time instrument viewing, sequence progress and errors, and cloud-enabled data storage for uploading raw data.

## Waters Corporation

Unveiled the new **Xevo® TQ-XS mass spectrometer**, the most sensitive benchtop tandem quadrupole instrument available. Enabled by the newly designed StepWave™ XS ion guide, this mass spectrometry system features a unique combination of ion optics, detection and ionisation technologies resulting in high levels of sensitivity. The Xevo TQ-XS is expected to be available for shipment in June 2016.



Figure 6. Xevo® TQ-XS mass spectrometer

The new levels of performance have been achieved through a number of technological advances.

- The new StepWave XS ion guide which removes neutral species and transmits ions in a more focused beam to the detector by incorporating segmented quadrupole transfer optics in the second stage. The result is a 2x to 10x increase in signal/noise over its StepWave predecessor, and it delivers excellent robustness over thousands of injections.
- The XDR Detector. First introduced on the Xevo TQ-S micro, it is a photomultiplier detection system capable of quantifying sample compounds across a concentration range of six orders of magnitude. Scientists no longer need to dilute and re-inject samples in order to stay within the limited dynamic range of the instrument they have been using.
- Also introduced was UniSpray™, a novel, proprietary ionisation source that is only available on the Xevo TQ-XS at the moment (it is expected to be released for other members of the Waters Mass Spec family later), which enables ionisation of a wider range of analytes in a single chromatographic run. The result is an increased response across a wide range of compound polarities for a broader range of compounds accompanied by a boost in signal/noise, making it possible to consolidate several analytical methods into one, or eliminate the need to change ionisation sources between analyses, saving time and increasing laboratory efficiency.

Also unveiled by Waters was an upgraded **Progenesis® QI for proteomics Version 3.0**, that enables you to quantify and identify proteins in complex samples using the advantages of label-free analysis.

With support for all common vendor data formats and a guided workflow, Progenesis QI Software helps to overcome the data analysis challenges, enabling rapid, objective and reliable protein discovery from single or fractionated samples.

The new **Metabolic Profiling CCS Library** includes more than 900 measurements of collision cross-section (CCS) values, which measure the gas phase three-dimensional shape of a molecule for an additional identification coordinate used to confirm analytical results. The library also includes more than 600 MS/MS spectra.

**Symphony™ Data Pipeline** software, a client-server application for laboratories acquiring and archiving large amounts of data was also introduced that automates the movement and transformation of large amounts of LC-MS data to speed up analytical workflows and save time, reduce human error, and reduce data file management. Being able to seamlessly and automatically copy raw files to a remote file location while a column is conditioning, maximises the time the instrument can be used for analysis, previously the mass spectrometer may stand idle for one to two hours while an operator copies data to a filestore in preparation for processing.

Symphony Data Pipeline software is compatible with Microsoft® Windows® 7 (64 bit) professional edition operating system and is available immediately worldwide from Waters

### Future ASMS Dates:

Dates and venues for the forthcoming ASMS meetings have been announced as follows:

- 65th ASMS Conference, 4 – 8 June, 2017, Indianapolis, IN
- 66th ASMS Conference, 3 – 7 June, 2018, San Diego, CA
- 67th ASMS Conference, 2 – 6 June, 2019, Atlanta, GA
- 68th ASMS Conference, 14 – 18 June, 2020, Denver, CO
- 69th ASMS Conference, 6 – 10 June, 2021, Philadelphia, PA

## Intelligent and Standardless Software for Wide Ranging Elemental Analysis

With modern XRF analysis there are two major analytical strategies: conventional calibration and standardless analysis. When working with known sample materials and when highest precision and accuracy are in demand, a standard-based calibration delivers best results. However, almost all labs are faced with unknown samples now and then or with samples for which no reference material is available. In these situations standardless analysis provides an effective tool to analyse elemental composition. This is only possible with powerful standardless software. **Bruker AXS'** new SMART-QUANT FP is offered as a fully integrated component of the S2 PUMA's Spectra Elements instrument software package and delivers reliable elemental data from C to U for solid, fused, pressed, powdery or liquid material without the need for laborious calibration.

SMART-QUANT FP uses fundamental parameters to calculate theoretical spectra based on given sample and instrument parameters and detector response. The software then compares the theoretical with the measured spectrum and minimises differences between them by adjusting the element concentrations in its model. This iterative process is continued until a perfect match between the theoretical and the measured spectrum is found. All this is carried out fully automated in the background so that the operator does not have to worry about it. However, if one wishes to do so, the process can be constrained by the input of a variety of parameters to tune the standardless calibration to the application's needs.

To start a measurement in its simplest form, place your sample into the spectrometer, enter a sample name and press 'Start'. That's it. After a few minutes you will have your results. For specific user and application needs measurement parameters can be adjusted to fit the respective analysis requirements. The software allows a wide range of customisations with regards to sample definition, measurement specifications, analysis scheduling, and result presentation. To further tailor the hardware towards your specific applications needs, the S2 PUMA can be ordered with different X-ray tubes, several detector options, and variety of sample handling options.

Nevertheless, SMART-QUANT FP is set up in a 'one fits all' standard configuration to let you start measurements immediately without lengthy adjustments. The intuitive user interface guides the operator through the process from placing the sample through result handling, be it an out-of-the-box standardless application or a more advanced analysis program. Essential results are displayed immediately after the measurement in the 'Loader' tab. More detailed analytical information is provided in the 'Results Manager' (see Figure 2). Every sample is displayed in a dedicated window where all analytical data can be viewed without scrolling. This includes detailed analytical information and measured as well as fitted spectra. The goodness of the fit can be judged on a displayed figure of merit 'R/R0'.

This system offers quick, accurate and precise analysis of unknown samples without calibration. Users will appreciate its analytical flexibility, whether they are analysing solid, fused, pressed, powdery or liquid samples, SMARTQUANT FP can handle all of them. This instrument's operator-friendly user interface guarantees a fast and straightforward measurement setup and an integrated results viewer offers quick and easy data access. Advanced analysis settings allow for customised measurement and preparation conditions to further increase analytical performance. SMARTQUANT FP performs a seamless integrated solution within the spectrometer software with no lengthy installation required.

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