



NEWS RELEASE

## Bruker Introduces Breakthrough MALDI-2 Source on timsTOF fleX, and Further Innovations in CCS-Enabled 4D Proteomics on timsTOF

5/29/2020

MALDI-2 Increases Small Molecule Sensitivity by One or Two Orders of Magnitude  
New prm-PASEF Workflow for Translational 4D Proteomics  
Large-Scale, High-Precision Peptide CCS Measurements for Deep Learning  
Short-gradient dia-PASEF Methods for High Throughput 4D Proteomics  
Unique CCS-enabled Mobility Offset Mass Aligned (MOMA) for Identification of Isobars  
'Run & Done' Novel IP2/GPU Real-Time Search Engine for High-Throughput 4D Proteomics

BILLERICA, Mass.--(BUSINESS WIRE)-- At the virtual ASMS 2020 Reboot conference, **Bruker Corporation** (Nasdaq: BRKR) today announces a major advance in matrix-assisted laser desorption ionization (MALDI) with the launch of the world's first commercial MALDI-2 post-ionization (PI) source, which is now available as an option on the timsTOF fleX™ ESI/MALDI mass spectrometer. The novel MALDI-2 technology can offer one or two orders of magnitude higher sensitivity for many small molecules and lipids. MALDI-2 increases the applications range of MALDI mass spectrometry and imaging even further.

This press release features multimedia. View the full release here:

<https://www.businesswire.com/news/home/20200529005143/en/>

(Photo: Business Wire)

Moreover, Bruker launches additional unique TIMS/PASEF-enabled 4D proteomics methods that leverage the large-scale, real-time availability of accurate collision cross sections (CCS) for tens of thousands of measured peptides per 4D nanoLC-CCS-MS/MS run. These new methods and software include prm-PASEF, short-gradient dia-PASEF, MOMA, and 'Run and Done' proteomics using a novel GPU-based real-time search engine. In

addition to further enhanced peptide, protein and PTM identification, these CCS-enabled innovations allow for sustained, ultra-high sensitivity LFQ performance, and for truly high-throughput methods for 4D proteomics, 4D lipidomics and 4D metabolomics on the exceptionally robust timsTOF Pro platform.

## A. SpatialOMx® and Translational Mass Spectrometry Imaging on timsTOF flex

The innovative MALDI-2 PI source increases both the sensitivity and range of applications of MALDI very significantly. MALDI-2 requires a second laser (266 nm) fired orthogonally into the expanding MALDI plume that is generated by Bruker's proprietary primary SmartBeam™3D (355 nm) laser. An optimized flexMatrix™ formulation is recommended for MALDI-2. The new MALDI-2 source is now available as an option on the timsTOF flex ESI/MALDI instrument.

**Professor Klaus Dreisewerd**, Leader Section for Biomedical Mass Spectrometry at the University of Muenster in Germany, and the pioneer of MALDI-2, said: "In the last 35 years, MALDI has become a unique and rapid analytical tool for a wide variety of applications. We developed MALDI-2 to significantly extend the technique by providing much higher sensitivity for small molecules, and the inclusion of chemical classes that did not ionize efficiently with MALDI. The MALDI-2 powered timsTOF flex will take MALDI to new scientific and analytical frontiers."

**Dr. Michael Easterling**, Global MS Imaging Director at Bruker Daltonics, added: "The growing value of MALDI Imaging and SpatialOMx for tissue-specific models in drug development drives demand for even higher sensitivity and versatility. With its dramatically increased sensitivity and accessible range of chemical classes, the novel MALDI-2 source option can now further enhance mass spectrometry-based, non-targeted tissue analysis."

Bruker now also offers a MALDI-2 compound reference library for its MetaboScape® metabolomics software, which was created during various academic and pharma collaborations. MetaboScape provides automatic analyte annotation within the SCiLS™ Lab MALDI imaging software, including CCS-algorithms that improve the confidence of annotation for many metabolites, glycans and lipids directly in tissue images.

## B. CCS-Enabled 4D Proteomics™ Innovations on timsTOF Platform

### prm-PASEF for Translational Quantitative 4D Proteomics

Bruker's revolutionary timsTOF™ Pro has been further enhanced by combining PASEF® with parallel reaction monitoring (PRM) for label-free quantitative proteomics. This unique mode of prm-PASEF takes advantage of the 4th dimension of separation using TIMS to improve selectivity and sensitivity, combined with the speed of PASEF to increase the number of precursor targets. Working closely with the Skyline team to enable prm-PASEF methods, Skyline software can now analyze the prm-PASEF data and produce quantitative reports.

The group of **Prof. Gunnar Dittmar** from the Luxembourg Institute of Health and **Prof. Antoin Lesur**, who both worked on the prm-PASEF workflow development, commented: “We have been extremely impressed by the early results from prm-PASEF on the timsTOF Pro in our lab. The sensitivity and speed of prm-PASEF already rivals that of PRM methods that have been developed over many years on other platforms.”

**Dr. Jarrod Marto**, Associate Professor at the Dana-Farber Cancer Institute, Harvard Medical School, and Brigham and Women’s Hospital added: “We have made tremendous progress since initiating co-development of prm-PASEF with the Bruker Team. The unique combination of acquisition speed and integrated ion mobility on the timsTOF Pro enable us to robustly quantify potential biomarker candidates across clinical cohorts. Moreover, real-time adjustment of acquisition parameters with prm-PASEF LIVE will push usability and throughput even further.”

## Large-Scale, High-Precision Peptide CCS Measurements for Deep Learning

Peptide collisional cross sections (CCS) measured at large scale and with high precision by the unique TIMS technology deliver added dimensionality for increased confidence of identification in 4D proteomics. A new study by Florian Meier et. al., entitled ‘Deep learning the collisional cross sections of the peptide universe from a million training samples’, and submitted to bioRxiv, (2020.05.19.102285; doi: <https://doi.org/10.1101/2020.05.19.102285>), uses a deep learning training set of 570,000 CCS values measured in 360 LC/MS runs of fractionated digests of five organisms, run on a timsTOF Pro system.

**Professor Matthias Mann**, Director at the Max Planck Institute of Biochemistry, Germany, commented: “The size and shape of peptide ions in the gas phase are an under-explored dimension for mass spectrometry-based proteomics. CCS values can now be predicted for any peptide and organism, forming a basis for advanced proteomics workflows that make full use of the additional information.”

## Short-gradient dia-PASEF and Mobility Offset Mass Aligned (MOMA) for 4D Proteomics

New short-gradient methods have been developed using the **dia-PASEF workflow**, which is finding increasing use in many timsTOF Pro labs. Dia-PASEF can provide a meaningful advance in data completeness, and the dia-PASEF workflow is now supported by Bioinformatics Solutions Inc. PEAKS and Biognosys Spectronaut software.

**Dr. Lukas Reiter**, Chief Technology Officer of Biognosys commented: “With the Spectronaut 14 launch, we have complete support for the timsTOF Pro: Fast library generation from PASEF and ion mobility calibration for a more specific targeted extraction in Spectronaut. Furthermore, we have added directDIA support for the timsTOF Pro. We are also excited to have a timsTOF Pro in our lab to further speed up our software development for this new and exciting platform.”

**Dr. Gary Kruppa**, Vice President for Proteomics at Bruker Daltonics, added: "With the launch of prm-PASEF, the growing success of dia-PASEF, and the trend towards shorter gradients that take advantage of the robustness, sensitivity and unmatched duty-cycle of PASEF, the timsTOF Pro provides the capabilities to make 4D-proteomics 'translational reality'. Furthermore, the unique MOMA feature of TIMS allows for targeting isobaric precursors at similar retention times for MS/MS acquisition. Having MOMA capability helps improve the depth of coverage using short gradients, and this is important to our translational research proteomics users who are running >50 samples per day per timsTOF Pro."

## 'Run & Done' Real-Time Search Developed by Yates Lab for High-Throughput 4D Proteomics

Bruker announces the availability of the proteomic pipeline (IP2) with a GPU-based search engine incorporating the ProLuCID database search tool from the laboratory of Professor John Yates at The Scripps Research Institute based in La Jolla, CA. This unique GPU-based IP2 software has been developed by Dr. Robin Park and allows timsTOF Pro 4D data to be searched in real-time during acquisition, with search results available at the end of the run.

**Prof. John Yates III and Dr. Robin Park** said: "The co-evolution of computational advances with mass spectrometry sensitivity and scan speed have enabled more accurate, large-scale data analysis approaches that help answer many biological questions. GPU-based search engines designed to simultaneously execute many parallel instruction threads can reduce search times to the point where the search results can be converted into real-time input to drive tandem MS acquisition. This becomes an exciting part in our partnership with Bruker, as it will utilize the timsTOF Pro even more intelligently."

**Dr. Rohan Thakur**, Executive Vice President of Life Sciences Mass Spectrometry at Bruker Daltonics, added: "The IP2/GPU solution provides a software infrastructure that's amenable to supporting 'plug-in applications' from our third-party software partners that take advantage of high-performance cluster or cloud capabilities. We are committed to our strategy of open data file formats to facilitate community-driven software development, including our third-party partners through API access for the benefit of the timsTOF user community."

Featured speakers at our eXceed symposia and breakfast events. For more detailed information on our eXceed Symposia and Breakfast Workshops please visit [www.bruker.com/events/2020/asms-2020-reboot](http://www.bruker.com/events/2020/asms-2020-reboot).

- The Synergies of Mass Spectrometry and Informatics  
Prof. John Yates, The Scripps Research Institute, La Jolla, CA, USA
- Next level imaging Mass Spectrometry: Single cells in focus with SpatialOMx  
Prof. RonHeeren, Maastricht University, Maastricht, Netherlands
- Clinical Proteomics in interesting times

Roman Fischer, University of Oxford, Oxford, United Kingdom

- Developing PRM on the timsTOF Pro for biomarker studies in cerebrospinal fluid

Jarrold Marto, Dana-Farber Cancer Institute, Harvard Medical School, Boston, MA, USA

- High-speed MALDI-2 on a timsTOF fleX: An overview of applications

Dr. Bram Heijs, Leiden University Medical Center, Leiden, The Netherlands

- Affinity-Bead Assisted Mass Spectrometry (Affi-BAMS): A Multiplexed Microarray Platform for Targeted Proteomics

Ghaith Hamza, Astra Zeneca, Discovery Science, MA, USA

- Kinase-substrate analysis via diaPASEF phosphoproteomics

Danielle Swaney, School of Medicine, University of California, San Francisco, CA, USA

- PASER: Parallel Database Search Engine in Real-Time and beyond

Robin Park, The Scripps Research Institute and CEO Integrated Proteomics Applications, La Jolla, CA, USA

- Introducing the Novel timsTOF fleX MALDI-2 a powerful tool to enhance sensitivity and dimensionality for SpatialOMx

Prof. Klaus Dreisewerd, University of Münster, Münster, Germany

- Trapped Ion Mobility Spectrometry (TIMS) and Parallel Accumulation Serial Fragmentation (PASEF) for Urine Metabolomic Profiling

Christina Di Poto, AstraZeneca, Gaithersburg, MD, USA

Bruker will host a virtual scientific and trade press conference on Monday, June 1st, 2020, at 8:00 am CDT, including Bruker management and guest speaker Professor John Yates.

Customers are invited to visit **Bruker's ASMS 2020 Reboot virtual hospitality suite** throughout the conference.

## About Bruker Corporation (Nasdaq: BRKR)

Bruker is enabling scientists to make breakthrough discoveries and develop new applications that improve the quality of human life. Bruker's high-performance scientific instruments and high-value analytical and diagnostic solutions enable scientists to explore life and materials at molecular, cellular and microscopic levels.

In close cooperation with our customers, Bruker is enabling innovation, improved productivity and customer success in life science molecular research, in applied and pharma applications, in microscopy and nanoanalysis, and in industrial applications, as well as in cell biology, preclinical imaging, clinical phenomics and proteomics research and clinical microbiology. For more information, please visit: [www.bruker.com](http://www.bruker.com).

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