NEWS RELEASE

Bruker Announces Further Progress in 4D Proteomics and Additional Novel timsTOF Pro™ Workflows at EuPA 2019

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New capabilities of timsTOF Pro introduced at EuPA 2019:
- DIA-PASEF work-in-progress with excellent peptide and protein ID performance
- New workflows for intact protein analysis in biopharma on timsTOF Pro
- New workflows for next-generation 4D metabolomics, leveraging routine, accurate and large-scale collision cross section (CCS) determinations on timsTOF Pro

POTSDAM, Germany, March 25, 2019 /PRNewswire/ -- At the XIIIth Annual Congress of the European Proteomics Association (**www.eupa.org**), Bruker announces further progress in ultra-high sensitivity, high-throughput 4D proteomics using the timsTOF Pro mass spectrometer. Moreover, new intact protein analysis and next-generation 4D metabolomics workflows are being introduced, which all are available on the same, remarkably flexible timsTOF Pro platform.

The extraordinary advances in speed, sensitivity and robustness provided by the timsTOF Pro have generated tremendous interest in the proteomics community. All work performed to date has been done using Data Dependent Analysis (DDA) and the innovative parallel accumulation serial fragmentation (PASEF) method developed in collaboration with Professor Matthias Mann at the Max Planck Institute of Biochemistry in Martinsried, Germany.

In ddaPASEF, individual multiply-charged peptides are selected in real-time for MS/MS, based on the acquired 'mobility-mass heat map'. Even with the high >100 Hz MS/MS speed of the timsTOF Pro, not all peptides can be targeted for MS/MS identification. Due to biological variation in the data from sample to sample, the same peptides may not be targeted in all runs, leading to the so-called "missing value problem" when performing quantitative proteomics.

Data Independent Analysis (DIA) is an alternative approach to fragment most of the peptides using wide selection windows, rather than selecting individual peptides in DDA. For many years, Bruker has been collaborating with the laboratories of Professor Matthias Mann to develop the timsTOF Pro for proteomics. More recently, they have teamed up with Professor Ruedi Aebersold and Dr. Ben Collins at the ETH in Zuerich, and Professor Hannes Roest at the University of Toronto, to develop a novel DIA technique on the timsTOF Pro, called diaPASEF. The speed and sensitivity of the timsTOF Pro have been shown to lead to improved throughput and better results for DIA library generation, and promise even more comprehensive proteome coverage in DIA experiments. Further progress on diaPASEF will be presented at EuPA 2019.

Professor Matthias Mann stated: "The timsTOF Pro offers very high MS/MS speed, dynamic range and an additional 4th dimension of separation by ion mobility. Due to its dual-TIMS front end, when operated with our PASEF method, the timsTOF Pro also uses ions very efficiently with nearly 100% duty cycle for highest sensitivity. The ion mobility separation provides accurate and highly reproducible collision cross section (CCS) values that allow for an additional dimension for alignment and feature matching in data processing and analysis software. The new diaPASEF method with the OpenSwath analysis software takes advantage of these attributes to provide a next-generation DIA method with superior coverage of proteins in biological samples, and with excellent quantitative performance. We are very excited about the diaPASEF work, and we look forward to continuing the collaboration with our academic collaborators and Bruker."

Rohan Thakur, Ph.D., and Bruker Executive Vice President for Life-Science Mass Spectrometry, commented further: "With both ddaPASEF and soon also diaPASEF workflows, the timsTOF Pro represents a major advance in robust, ultra-high sensitivity and high-throughput quantitative proteomics. Its unique 4D nanoLC-TIMS-MS-MS analysis capabilities deliver ultra-high sensitivity and speed due to its unique time-focusing advantages inherent in the combination of dual TIMS technology and the breakthrough PASEF method. In addition, we have recently demonstrated that the timsTOF Pro is also an excellent system for intact protein analysis for biopharma applications, using appropriate LC separations, but all on the exact same mass spectrometer."

Dr. Thakur continued: "Beyond 4D proteomics, we have now also introduced novel 4D workflows that could revolutionize next-generation lipidomics and metabolomics. Both of these phenomics methods greatly benefit from the additional, large-scale and accurate CCS information for every known and unknown compound measured. We are very pleased that Professor Jeremy Nicholson will explore and further develop novel 4D phenomics methods on the timsTOF Pro platform at his new, world-class phenomics laboratories at Murdoch University and at the Australian National Phenome Center."

Bruker had previously introduced the timsTOF Pro for 4D lipidomics with MetaboScape software at HUPO

2018. This combination enables molecule-specific and accurate collision cross section prediction for most classes of lipids using machine learning with the CCSPredict™ algorithm.

The additional innovations introduced at EuPA 2019 follow just three weeks after Bruker announced the following new timsTOF® Pro-based solutions and capabilities at US HUPO 2019 (see separate press release, dated March 4, 2019):

- High-throughput clinical plasmaproteomics research: 192 depleted plasma samples from septic shock patients measured in 2 days, with 11.5 minute gradients using the Evosep One HPLC system with only 100 ng/run
- Enhanced proteomics data completeness: MaxQuant 'match-between-runs' with large-scale CCS values for dramatic improvements in peptide and protein data completeness
- Host cell protein (HCP) analysis for biologics: Protein Metrics adds large-scale, accurate CCS to Byonic 4D database search engine for biopharmaceutical companies

About the timsTOF PRO with PASEF

The proprietary timsTOF Pro system uses PASEF, enabled by Trapped Ion Mobility Spectrometry (TIMS) to provide industry-leading data acquisition speed for shotgun proteomics. The unique dual TIMS geometry of the timsTOF Pro, combined with the time focusing of the ion packets in the TIMS device, means that the speed advantage provided by PASEF comes along with simultaneous improvements in sensitivity and quantitation. All of these gains in speed, sensitivity and quantitation maintain the advantages of Bruker's high-performance QTOF mass spectrometers, including high mass resolution (resolving power of 50,000 FWHM even at highest data acquisition rates) in MS and MS/MS mode, ppm accurate mass, and high isotopic fidelity (True Isotopic Pattern, or TIP™). The robust timsTOF Pro with PASEF gives scientists the tools to dig deeper into the complex cellular machinery with the potential to discover low-level, biologically significant peptides or proteins, or validate them in translational proteomics research.

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