NEWS RELEASE

Bruker Announces Breakthrough Proteomics and Lipidomics Workflow Advances for the timsTOF™ Pro at HUPO 2018

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- First Large-Scale Use of Peptide CCS Values to Enhance Search Specificity
- Machine-Learning CCSPredictTM for Advanced Annotation in Lipidomics

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ORLANDO, Fla., Oct. 1, 2018 /PRNewswire/ -- At the 17th Annual World Congress of the Human Proteome Organization (**www.hupo.org**), Bruker announces next-generation workflows for the timsTOF Pro mass spectrometer. Introduced a year ago at the HUPO conference in Dublin, this revolutionary mass spectrometry platform is a new enabling technology for ultra-high sensitivity proteomics and large-cohort clinical validation. The exclusive PASEF (parallel acquisition serial fragmentation) method results in high duty-cycle due to the proprietary trapped ion mobility spectrometry (TIMS) technology. In addition to highest throughput and highest sensitivity, this unique TIMS-PASEF combination delivers outstanding peptide and protein identifications (ID), excellent quantitation performance, and exceptional robustness.

Novel advances on the timsTOF Pro introduced at HUPO 2018 include:

1. Large-scale, reproducible, accurate collision cross section (CCS) values for tryptic peptides to further reduce proteomics FDRs and to enhance the performance of label-free quantitation

2. FastPro™ method for even higher peptide and protein group ID rates with better sequence coverage and enhanced detection of post-translational modifications (PTMs)

3. A breakthrough CCS-based lipidomics workflow that includes CCS prediction using machine learning

for reliable lipid ID and reduced reliance on retention time matching

The ability to harness the potential of accurate CCS values at a large scale is a unique timsTOF Pro feature. The CCS values are intrinsic and universal properties of the peptides, and tens of thousands of CCS values are determined with every LC-CCS-MS/MS run, with CCS reproducibility of better than 0.3% between runs. The large-scale use of accurate CCS values is a novel molecular parameter to confirm peptide ID, in addition to mass-to-charge and MS/MS fragmentation, resutling in much better lab-to-lab and system-to-system reproducibility than LC retention times.

The first large-scale use of peptide CCS values is new in the "match between runs" feature in MaxQuant, in addition to using mass-to-charge and retention time to search for peptides in runs where they were not fragmented. Using TIMS for molecule-specific CCS values as additional search parameters makes 'match between runs' even more specific. Bruker has expanded its collaboration with the group of Professor Juergen Cox, the developer of MaxQuant at the Max Planck Institute for Biochemistry in Martinsried, Germany.

Dr. Cox commented: "We are very pleased to have established a close working collaboration with Bruker to develop features in MaxQuant for the processing of the 4-dimensional data produced by the timsTOF Pro. The collision cross sections obtained are proving to be very valuable in reducing false positives in the 'match between runs' analysis used in label-free quantitation. We are looking forward to many other exciting developments using MaxQuant with timsTOF Pro CCS data to advance the field of proteomics."

To address the trend towards single-cell proteomics, optimization of PASEF collision energy switching has resulted in a new method termed FastPro. The timsTOF Pro with PASEF and FastPro requires only 200 ng of HeLa using a 90 min LC gradient to deliver ~6000 protein IDs and another ~10% increase in peptide spectrum matches (PSMs) with ~60,000 unique PSMs. This provides better sequence coverage of identified proteins, more confident quantitation, and deeper coverage of post-translational modifications and sequence variants.

Bruker has expanded its relationship with Bioinformatics Solutions Inc., the developer of PEAKS software, to include re-selling. PEAKS can efficiently analyze timsTOF Pro data for ID, label-free quantitation (LFQ), and quantitation with isotopic labeling such as TMT, iTRAQ and SILAC. PEAKS can now also use all four dimensions of timsTOF Pro data to deconvolute spectra from species that overlap in two or more dimensions. These overlaps result in MS/MS spectra containing peaks from multiple precursors, which may not provide reliable ID of the precursors. The novel ability to correlate MS/MS peak intensities with TIMS elution profiles represents another unique use of the timsTOF Pro to obtain highly reliable peptide identifications.

Bruker also has enhanced its collaboration with Evosep, which provides a robust, high-throughput liquid chromatography system for clinical research proteomics that allows users to fully utilize the ultra-high scan-speed

advantages of the timsTOF Pro with PASEF. With the release of a Bruker plug-in to control the Evosep One LC system, Bruker and Evosep now announce a co-selling agreement, which enables Bruker to sell, support and service a complete solution for proteomics labs requiring extreme throughput, sensitivity and robustness. Moreover, the companies have developed a high-throughput method for the analysis of host cell proteins (HCPs) in biopharmaceutical applications with excellent sensitivity and robustness.

Michael Barrett Andersen, Head of Product Management at Evosep, said: "We are very pleased to have Bruker as a partner for distribution and support of the Evosep One. The speed, sensitivity and robustness of the timsTOF Pro are highly complementary to the robustness and high-throughput of the Evosep One. We have a high degree of interest from our prospective customers in proteomics for this combination, and we look forward to working with Bruker to promote our joint solution for high-throughput proteomics."

Gary Kruppa, Vice President for Proteomics at Bruker Daltonics, added: "The timsTOF Pro is an exciting new platform in proteomics. The large-scale use of accurate CCS values will enable next-generation methods and workflows in proteomics and lipidomics. We are introducing the machine-learning based CCSPredict capability for lipidomics in a revolutionary new LC-CCS-MS workflow for the timsTOF Pro. The CCSPredict algorithm automatically assigns CCS values which can significantly increase confidence in lipids annotations, in addition to accurate mass, true isotopic pattern (TIP™), MS/MS and retention time."

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 TIPTM). 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.

About the MaxQuant and Perseus software platforms

MaxQuant is the industry standard in shotgun proteomics data analysis. Developed over the last decade by Juergen Cox, it has become the most used package for the identification and quantification of peptides, proteins and

posttranslational modifications. Recently, MaxQuant has been adapted to the analysis of timsTOF data, managing 4D features in the space spanned by retention time, ion mobility, mass and signal intensity. The Perseus software for multi-omics data analysis supports biological and biomedical researchers in interpreting molecular quantification, interaction and protein post-translational modification data. Perseus contains a comprehensive portfolio of statistical tools for high-dimensional data analysis covering normalization, pattern recognition, time-series analysis, cross-omics comparisons and multiple-hypothesis testing. For more information: **http://www.biochem.mpg.de/5111795/maxquant**.

About PEAKS Studio

PEAKS Studio, the flagship software of Bioinformatics Solutions, Inc., offers an innovative mass spectrometry data analysis workflow to the proteomics community. Since its debut in the early 2000s, PEAKS Studio has been highly recognized for its benchmarking de novo sequencing algorithm, which was integrated in all other software modules for shotgun proteomics. The combination of de novo sequencing with traditional database searches ensures a complete interpretation of raw spectral data to embrace the complexity and sensitivity of mass spectrometry, and offers advanced solutions for proteomic and therapeutic protein discovery as provided through peptide/protein identification and quantification, peptide mapping, post-translational modifications and sequence variants. The unique workflow offered by PEAKS Studio together with the compelling data quality derived by 4D ion mobility of the timTOF Pro has sparked Bioinformatics Solutions and Bruker to expand collaborative work. For more information: **www.bioinfor.com**

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: **www.bruker.com**.

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