Software Solutions

Compass and Bioinformatics

Bruker Daltonics software solutions provide maximum information via streamlined, easy to use processes

BioPharma Compass® Field of Application: BioPharma	BioPharma Compass provides integrated workflows for biopharmaceutical industry supporting 21 CFR Part 11 requirements. Workflows comprise all aspects from data acquisition to report generation, characterization and comparative quantitative assessments in multiple attribute monitoring (MAM) analyses. MAM peptide analysis as well as host cell protein (HCP) analyses can benefit from the use of CCS-enabled data analysis in terms of sequence coverage and dynamic range. Multi-Target-Screening workflows enable batchwise processing multiple samples.
PaSER Field of Application: Proteomics	PaSER is a Hardware and Software solution, enabling fully integrated real-time database searches with sample queue management. With GPU based searches, PaSER delivers the same results in real-time mode or offline mode. The search speed of PaSER provides results seconds after the acquisition ends, Run & Done! PaSER removes the data analysis bottleneck introduced by large sample cohorts and greater throughput. Real-time LFQ quant can also be performed across pre-acquired datasets making the transition into quantitative proteomics instantaneous. Visualization of mobility offset mass aligned (MOMA) features using TIMS Viz visualizes isobaric peptides only capable by 4D-Omics.
PEAKS® Studio Field of Application: Proteomics	For a complete proteomics data processing and analysis pipeline for the timsTOF Pro, we teamed up with Bioinformatics Solutions Inc. Their PEAKS Studio and PEAKS Online platforms perform LC-MS/MS-based protein identification and statistics for LFQ, TMT, iTRAQ, SILAC and dia-PASEF workflows using CCS-enabled algorithms. PEAKS Online is the solution for high-throughput applications, such as large cohort studies. They also continue to support data from other Bruker instruments as well as from other vendors.
Other solutions Field of Application: Proteomics	Bruker's data formats are open to all, including third-party software vendors. We collaborate intensively with various partners, including the Max-Planck-Institute for Biochemistry on MaxQuant, the University of Michigan on the FragPipe suite, and the University of Washington on Skyline. We work closely with Protein Metrics on Byos® for biopharma-related workflows, and Biognosys on Spectronaut™ for dia-PASEF.

MetaboScape® Field of Application: Metabolomics	MetaboScape is the software for discovery metabolomics and phenomics. Main purpose is to pinpoint and identify compounds that change because of perturbation or disease. Using pathway mapping, data can be visualized in a biological context. For 4D-Metabolomics™, T-ReX 4D uses CCS values as additional criterion for the Annotation Quality Scoring (exact mass, retention time, isotopic pattern, MS/MS spectrum, CCS value). MetaboScape supports spectral libraries like MetaboBASE®, HMDB, MetaboBASE Plant, as well as custom libraries.
MetaboScape® Field of Application: Lipidomics	The 4D-Lipidomics™ workflows integrated in MetaboScape uses rule-based annotation routines for identification of lipids. For timsTOF, timsTOF Pro and timsTOF fleX PASEF data, MetaboScape offers the CCSPredict lipid confirmation tool. Based on machine learning, it predicts CCS values for lipid structures, which further increases the confidence in annotations. CCS and retention time aware Kendrick mass defect plots offer an intuitive 4D visualization tool for investigation of assignments and detection of novel species.
TASQ Field of Application: Screening, Quantitation	TASQ (Target Analysis for Screening and Quantitation) is Bruker's solution for screening, confirmation and quantitation of large sample batches, including hundreds of compounds per analysis. CCS-enabled TASQ allows exploiting the ion mobility separation on timsTOF instruments for further confidence. TASQ takes advantage of both nominal and high resolution, accurate-mass data generated by Bruker's triple quadrupole and OTOF mass spectrometers. TargetScreener HR – driven by TASQ – allows report generation from 'vial to report' in seven clicks.
SCiLS Lab Field of Application: Imaging	SCiLS Lab is the worldwide leading software for analysis of mass spectrometry imaging (MSI) data from all major mass spectrometry vendors. Comparative analysis of multiple samples can be visualized in both 2D and 3D, enabling a multitude of applications in pharmaceutical drug development, in biomarker research, as well as in translational pathology research. The quantitation workflow enables to easily quantify target molecules directly from tissue. SCiLS Lab integrates with the SpatialOMx workflow from MetaboScape.
PolyTools 2.0 Field of Application: Polymer Analysis	PolyTools interprets homopolymer spectra in any mass range. Equidistant signals are automatically found and interpreted as individual polymer distribution. Based on user-defined tables of monomer units and end-groups PolyTools suggests interpretations of the ion series. For each single distribution average molecular weights, dispersity, degree of polymerization and percentage of the individual ion series in the spectrum can be calculated. Results are displayed in the form of several Kendrick mass defect (KMD) plots and in a table format.
Polymerix Field of Application: Polymer Analysis	For interpretation of isotopically resolved homo- and copolymer spectra and polymer distributions separated by liquid chromatography Polymerix calculates characteristic values, corresponding dispersity, and percentage of the individual ion series in the homopolymer spectrum. Additionally, the average values for the complete spectrum are computed. Copolymers are visualized as AB distribution plots. Beside graphical spectrum interpretation detailed numerical data interpretation is available.
MALDI PharmaPulse (MPP) Field of Application: High-Throughput Screening (HTS)	MPP is integrated part of Bruker´s rapifleX MALDI PharmaPulse enabling fully automated MALDI-TOF based label-free screening campaigns allowing for ultrafast primary screening of millions of compounds. It features a method development module supporting assay development. The actual screening software module provides the tools required for seamless setup, execution and result visualization of HTS screens. The new synthesis screening module allows flexible screening of many different target compounds per individual well.