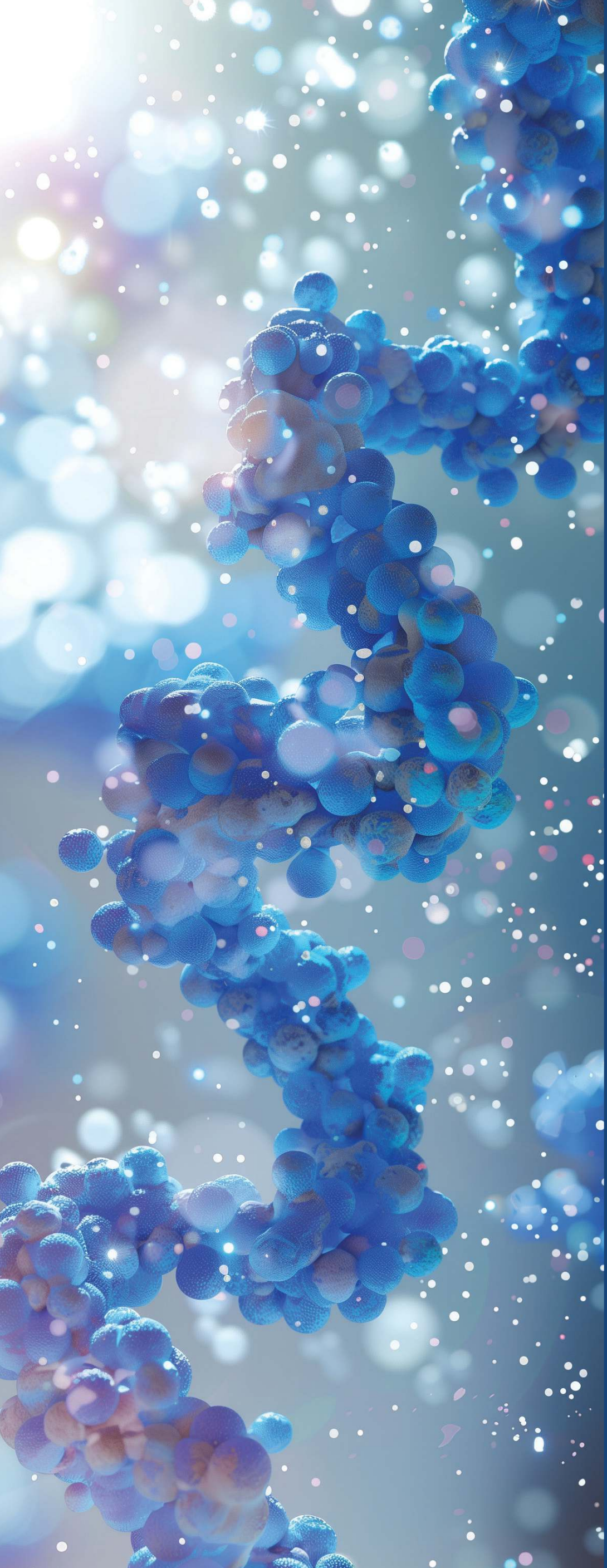
Bioinformatics Solutions Inc.

PEAKS® Studio 13

A Complete Solution to Proteomics



PEAKS® Studio 13

BROCHURE

For more information on each of these offerings, visit our website at:

www.bioinfor.com

YOUR PROTEOMICS SOLUTIONS

At Bioinformatics Solutions Inc, our mission is to empower researchers and industry leaders with innovative tools and services that drive discovery and innovation in proteomics. Guided by values of precision, reliability, and collaboration, we combine cutting-edge technology with expert support to deliver transformative solutions. Our flagship software, including **PEAKS Studio**, **PEAKS Online**, **PEAKS GlycanFinder**, and **PEAKS AB**, leverage advanced algorithms and deep learning to set new standards in protein identification and quantification, *de novo* sequencing, and glycan profiling.

Complementing these tools, our specialized lab services provide dependable, cost-effective results, ensuring our partners achieve their research and development goals efficiently. At BSI, we are committed to advancing science and building lasting partnerships that fuel breakthroughs in biological research, drug development, and beyond.

UNLOCK PRECISION PROTEOMICS

with Cutting-Edge Deep Learning Strategies

PEAKS® Studio 13 continues to harness the latest deep learning technology to improve identification accuracy and sensitivity, by using algorithms to predict retention time, fragment ion intensity, mass-to-charge ratios, and ion mobility.

FACILITATE DRUG DISCOVERY AND ADVANCE THE FRONTIER OF BIOLOGICAL RESEARCH THROUGH AI-DRIVEN SOFTWARE SOLUTIONS

Peptide *de novo* sequencing: PEAKS® has been known as the gold standard for automated peptide *de novo* sequencing for over 20 years! The latest GPU enabled deep learning based *de novo* sequencing, "DeepNovo", will bring your accuracy and confidence to the next level, including PEAKS exclusive unbiased FDR control. Use peptide sequencing algorithms as standalone for non-model organisms or assisting classical proteomics and immunopeptidomics searches.

DIA Analysis: PEAKS® 13 latest algorithm innovations offer highly competitive DIA speeds, both CPU and GPU powered, and exceptional accuracies. Take advantage of flexible and streamlined workflows using Spectral library or/and Database searches now with Sequence Variants, *de novo* peptides, as well as enhanced algorithm for DIA Phosphoproteome. PEAKS® database relies on in silico spectral library generated from the protein sequence database using internal deep learning models, and includes prediction details on the fragment ion pattern, indexed retention time, and ion mobility.

DeepNovo Peptidome: This workflow supports both DDA and DIA data analysis and is a specialized workflow for immunopeptidomics. The latest high-accuracy DeepNovo algorithm is integrated with peptide identifications including a variety of modifications, sequence variants, and/or splice sites in one comprehensive analysis. Users can link the peptides to genes and bridge the gap between proteomics and genomics to help identify and validate peptides potentially originating from rare sequence variants and non-coding regions. Complex Peptidome algorithm allows for high confidence multi-round searches with label-free quantification.

PEAKS® DB: PEAKS® provides a unique *de novo*-assisted database search to improve both sensitivity and accuracy with the deep learning boost for peptide confidence re-scoring. PEAKS® 13 brings back Labelled and Label-Free Quantification following PEAKS PTM and SPIDER.

PEAKS® DDA

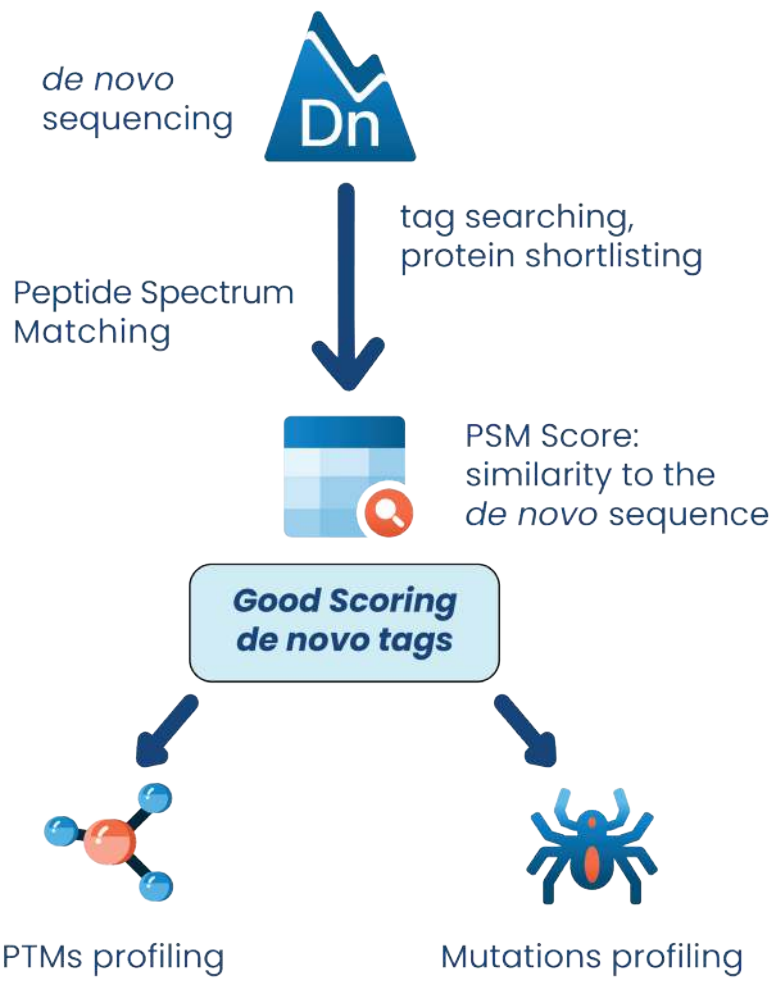
de novo Assisted Database Search

De novo Sequencing

In the first step of the workflow, all MS2 spectra are *de novo* sequenced. The *de novo* sequencing results are used to create a shortlist of database proteins to search.

Database Search

Each spectrum is searched against a protein database to find the best peptide-spectrum match. PEAKS® provides enhanced separation of true and false hits by incorporating the *de novo* sequencing results into the scoring algorithm. This unique *de novo*-assisted approach will allow you to identify more peptides and proteins with greater confidence.



PEAKS® PTM

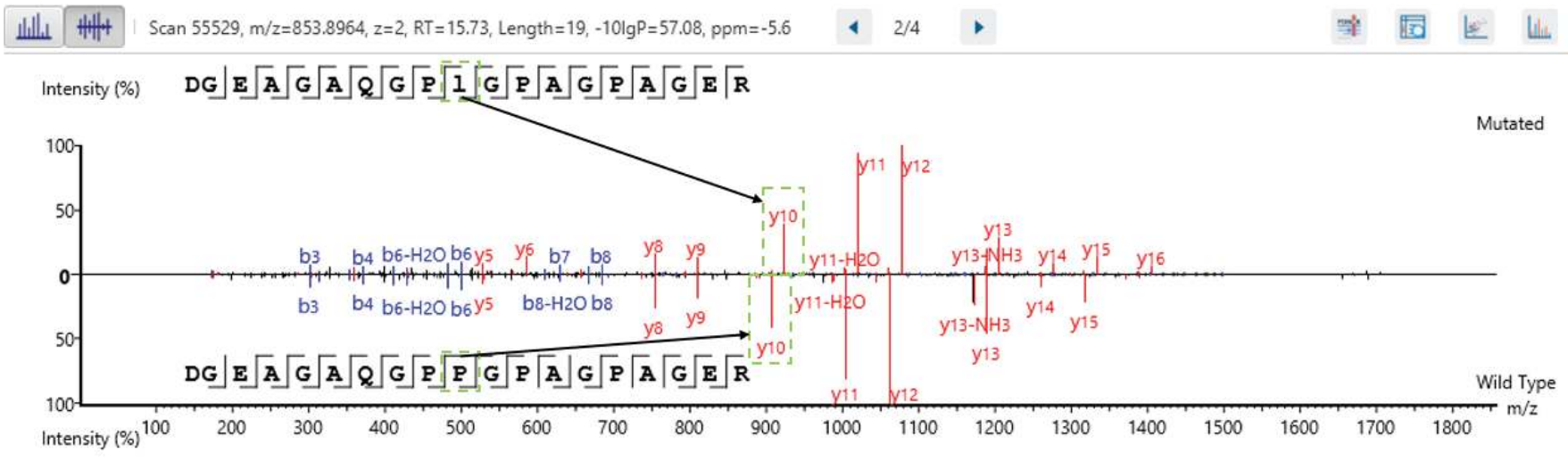
Specify the PTMs of interest or search all 313 naturally occurring biological modifications from the Unimod database in your PEAKS® PTM search.

SPIDER

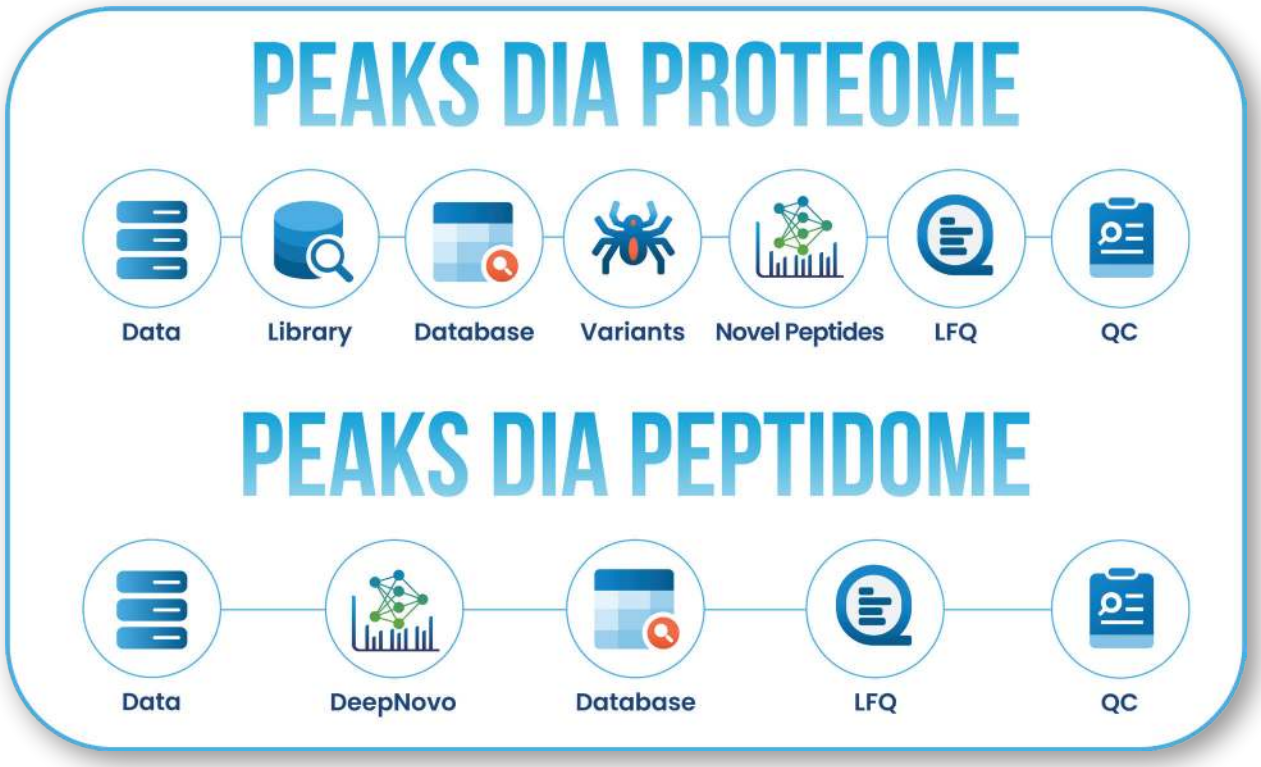
Homology search with *de novo* tags identifies amino acid mismatches between *de novo* and database sequences. Confident mutations are determined by the number of consecutive fragment ions at the mutation site with relative ion intensities above a threshold, each of which is user-defined.

Discover Hidden Modifications

In PEAKS® PTM and SPIDER, fragment spectra with a good *de novo* scores are reanalyzed to assess any unknown PTMs or sequence variants. Additional confident modification and mutation algorithms with the use of Potential Signature Ions for modified peptides' re-scoring, allow for enhanced accuracy in PTM and sequence variant identification. Finally, unified scoring using -10logP logic allows for easy result interpretation.



PEAKS® DIA WORKFLOWS



PEAKS offers a comprehensive and flexible solution for DIA data analysis while ensuring high accuracy identifications, for both proteome and peptidome insights.

The user can pick the steps that suit their specific research need.

Spectral Library Search

If peptide spectral library is available, PEAKS will provide the library peptide matches that pass the false discovery rate control and report as “Found by Library”.

Database Search

MS/MS spectra, including those that did not match a spectral library entry if spectral library was used in prior step, are searched against an in silico digested and predicted protein sequence database.

Novel Peptides

DIA *de novo* Sequencing is available to find a peptide when a database may be inadequate.

Sequence Variants New in PEAKS Studio 13!

Amino acid mutations against the reference database will be reported with Ion Intensity filter available.

Label-free quantification (LFQ)

LFQ can be performed on identified library and database peptides to investigate changes in relative protein/peptide abundance across multiple conditions.

ADVANTAGES OF A DIA WORKFLOW

- Decreased bias by including all peptides in analysis
- Reproducible peptide detection and quantification across MS runs
- Proteins quantified in complex mixtures over a dynamic range
- Eliminated under sampling
- Increased sensitivity and depth of proteome coverage

DID YOU KNOW

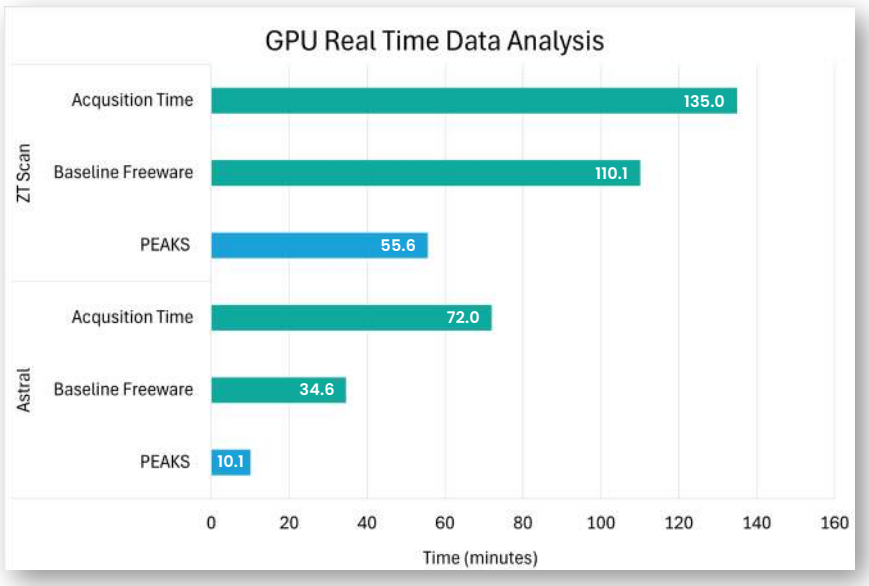
PEAKS® offers hybrid-PRM/DIA that combines targeted and discovery proteomics?

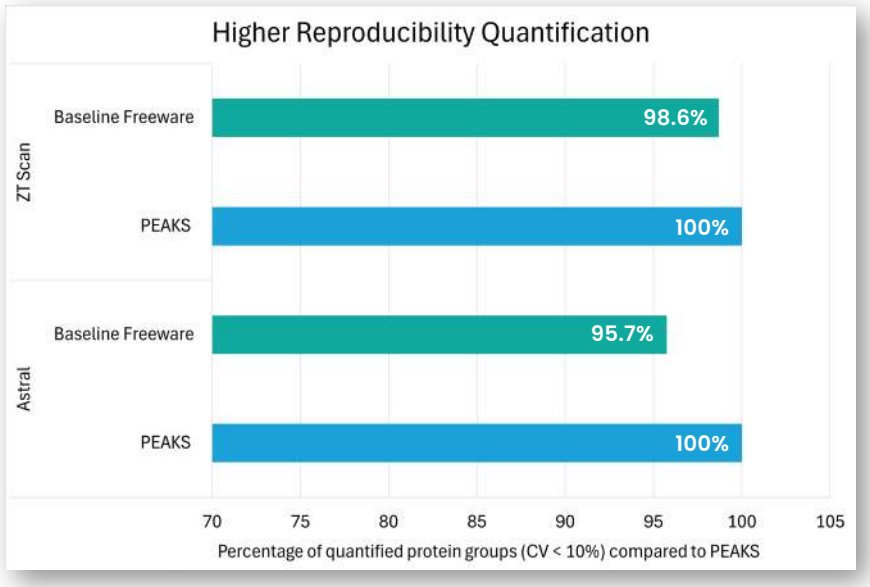
NEW IN PEAKS 13
FOR DIA WORKFLOWS

Our enhanced DIA solution will accelerate your discovery ensuring accurate and comprehensive result to provide complex biological insights!

Enhanced Speed and Performance

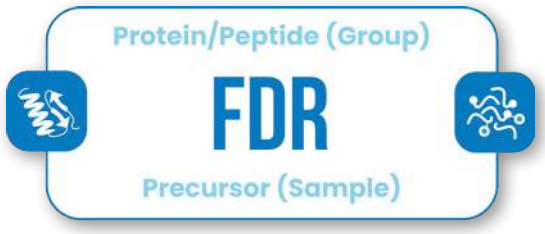
Improved CPU and GPU based analysis times while ensuring high sensitivity and accuracy.





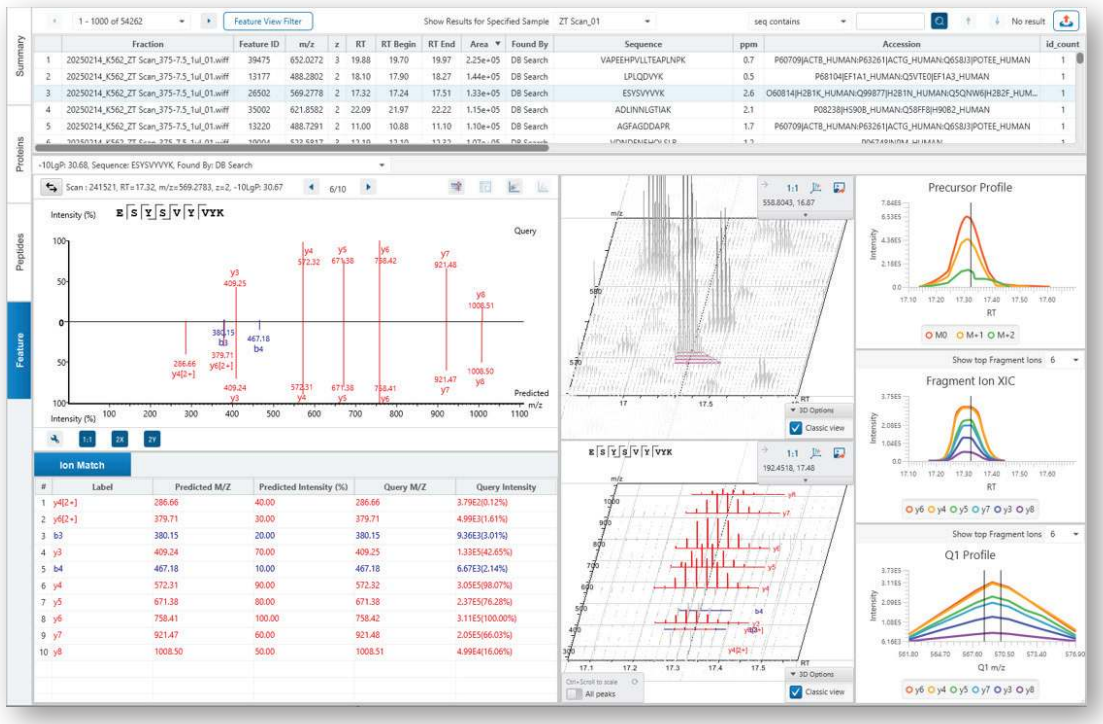
Streamlined Workflows

Seamlessly select steps and versatile report filters at both sample and group levels to gear your research need and ensure a confident result.



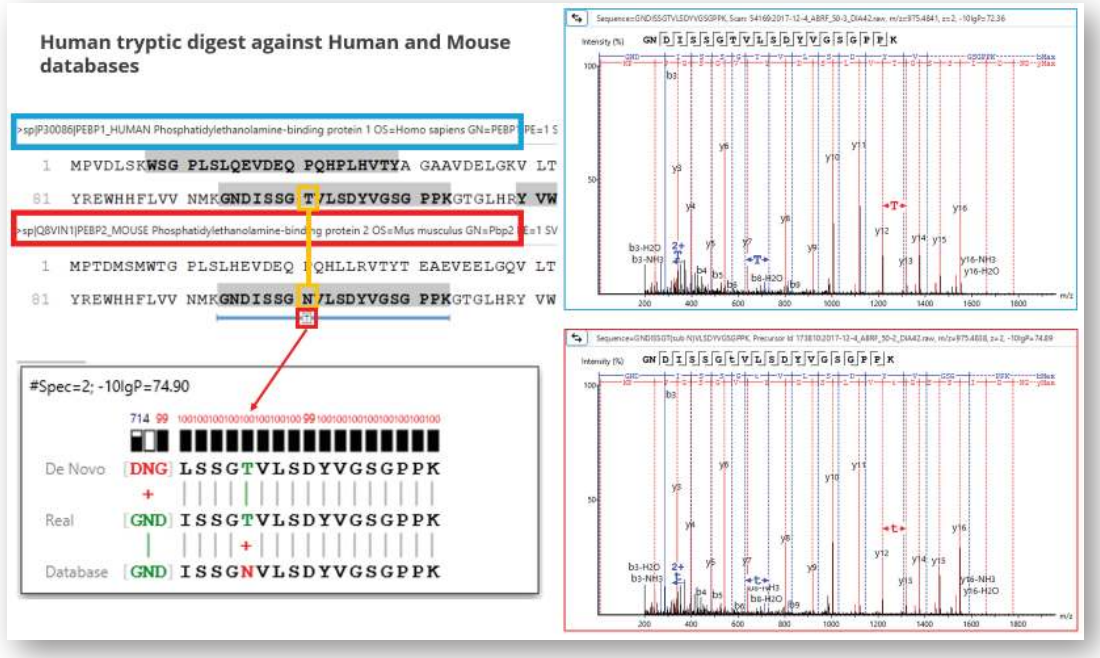
Full Result Transparency

Newly added feature tab gives an overview of feature associations with each DIA identification step.



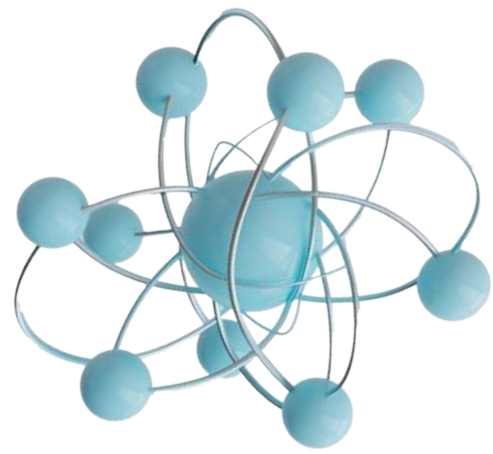
Deeper Insight

Sequence Variants search to find mutations in DIA Proteome and Peptidome.



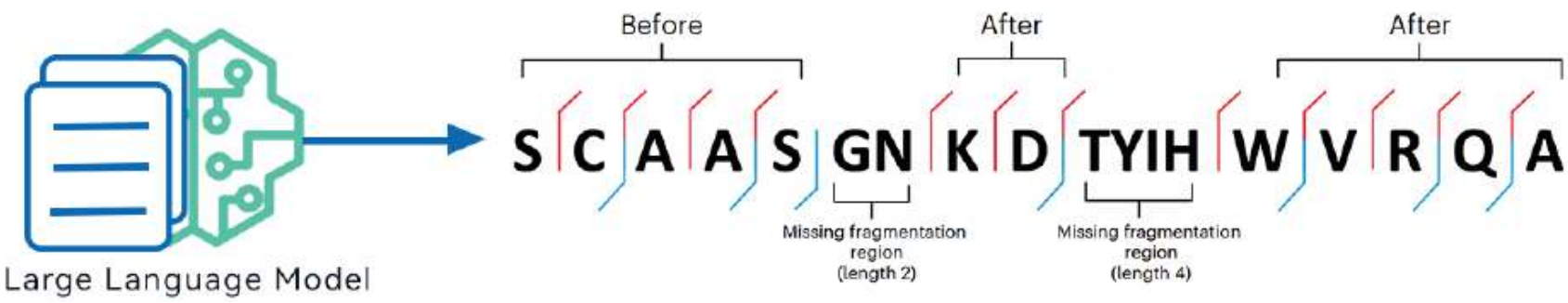
The gold standard for peptide *de novo* sequencing just got even better

NEXT GENERATION PEAKS® DEEPNOVO



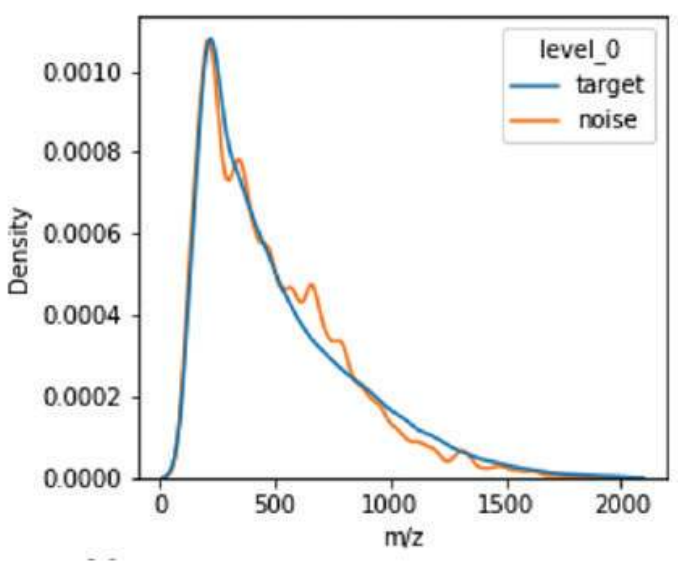
In mass spectrometry, *de novo* sequencing derives an amino acid sequence from a mass spectrum without the need of a sequence database. In contrast to the popular 'database search' peptide identification approach, *de novo* sequencing is the only choice when the sequence database is not available. This makes PEAKS® the preferred method for identifying novel peptides and proteins from or from incomplete databases.

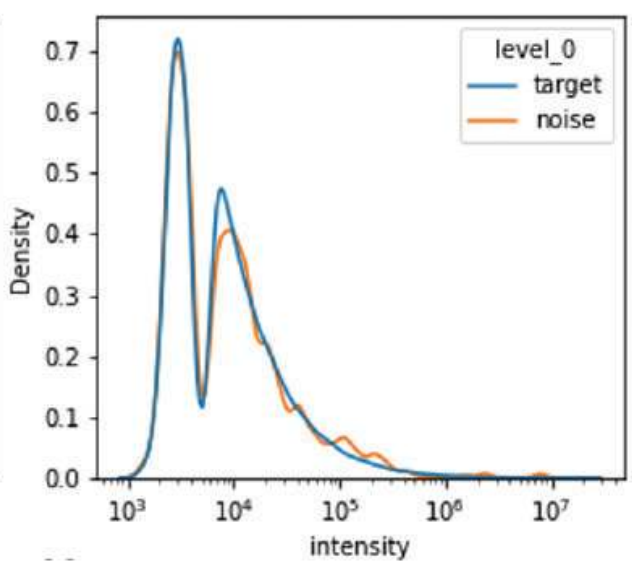
Empowered by the latest GraphNovo algorithm, the new DeepNovo has resolved the issue of accumulated prediction errors due to missing fragment ions by finding the optimal path in the first stage to guide sequence prediction in the second stage.

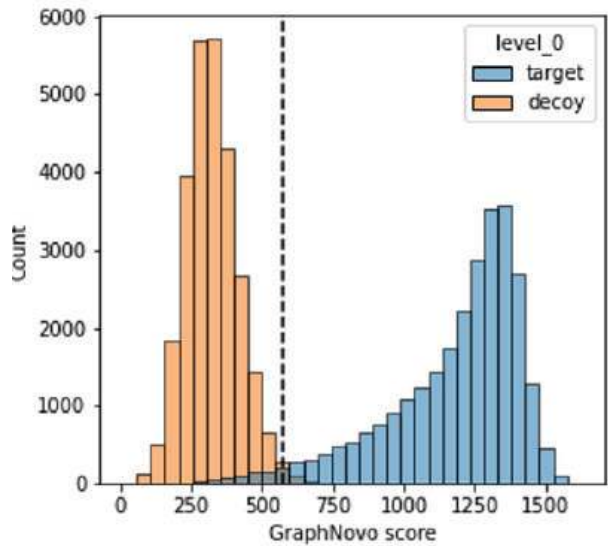


As a key technology for finding novel peptides from MS data, DeepNovo provides an advanced solution and will push research such as antibody sequencing and neoantigen discovery further.

In PEAKS® decoy spectra are used in DeepNovo to estimate an FDR for *de novo* peptide sequencing. The decoy generation process ensures decoy spectra have the same fragment ion distribution as target spectra. Furthermore, DeepNovo scoring function efficiently separates target and decoy. An FDR curve of *de novo* sequencing is now available in DeepNovo.







As a deep learning based solution, DeepNovo harnessed the computation power of NVIDIA GPUs for speed. NVIDIA A100 enabled *de novo* sequencing 1200 + spectra/s.

Enhanced PEAKS® DeepNovo
PEPTIDOME WORKFLOW

New! DIA Peptidome 13 uses the latest GraphNovo deep learning sequencing

New! DIA Peptidome now offers insight into Sequence Variants

New! DIA Peptidome LFQ includes Database found peptides and Sequence Variants

DDA Peptidome embraces comprehensive multi-round Canonical and Noncanonical database searches

	Peptide	-10lgP	CAA(%)	Accession	Gene	Database	PTM	Found By	Ion Intensity	Length	Mass
21	M(+15.99)VAGA(sub S)E(sub Q)GKAE	40.45	50.0	Q8WY91|THAP4_HUMAN	THAP4	TARGET	O A E	Sequence Variants	O1:2.3162,S5:1.2409,G6:2.1255	10	977.4488
22	TA(sub V)ASSSSLEK	40.45	80.0	A5A3E0|POTEF_HUMAN	POTEF	TARGET	A	Sequence Variants	V2:10.9047	10	979.4822
23	TTIQV(sub M)SSQLSGR	40.45	33.3	P80217|IN35_HUMAN	IFI35	TARGET	V	Sequence Variants	M5:9.9683	12	1275.6783
24	LSQDT(sub S)TGRV	40.42	66.7	P52788|SPSY_HUMAN	SMS	TARGET	T	Sequence Variants	S5:5.0107	9	975.4985

Bridge Proteome and Genome

A Gene tab is included in the workflow to show where each peptide is expressed in the genome. This feature helps in understanding non-canonical peptide biosynthesis.

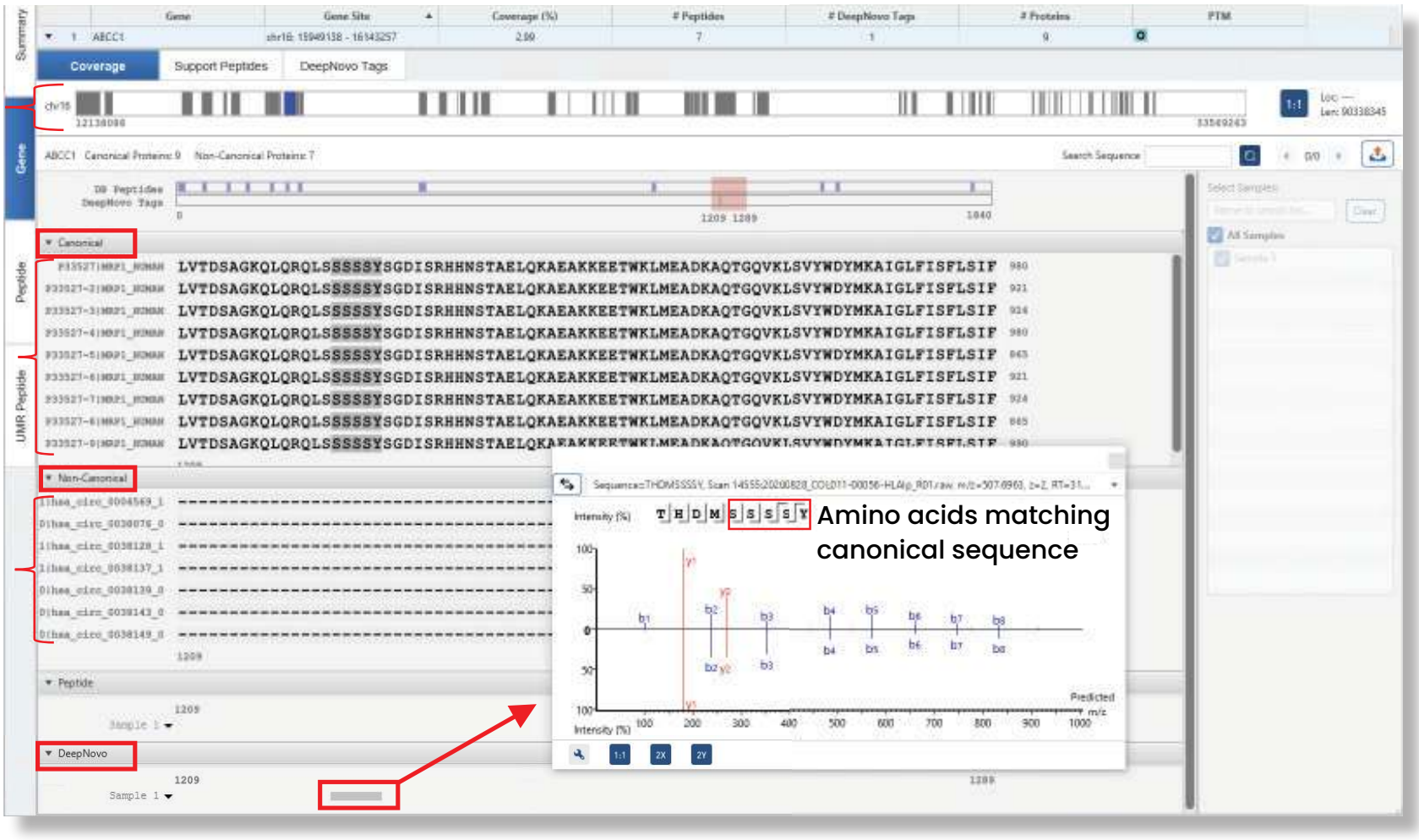
DeepNovo Peptide Mapping

The Gene tab also shows DeepNovo peptides, where part of the peptide sequence matches canonical or non-canonical databases. This helps identify post-translationally spliced peptides.

Chromosome loci
(selected gene in blue)

Protein isoforms
from Target DB

Entries from
non-canonical DB



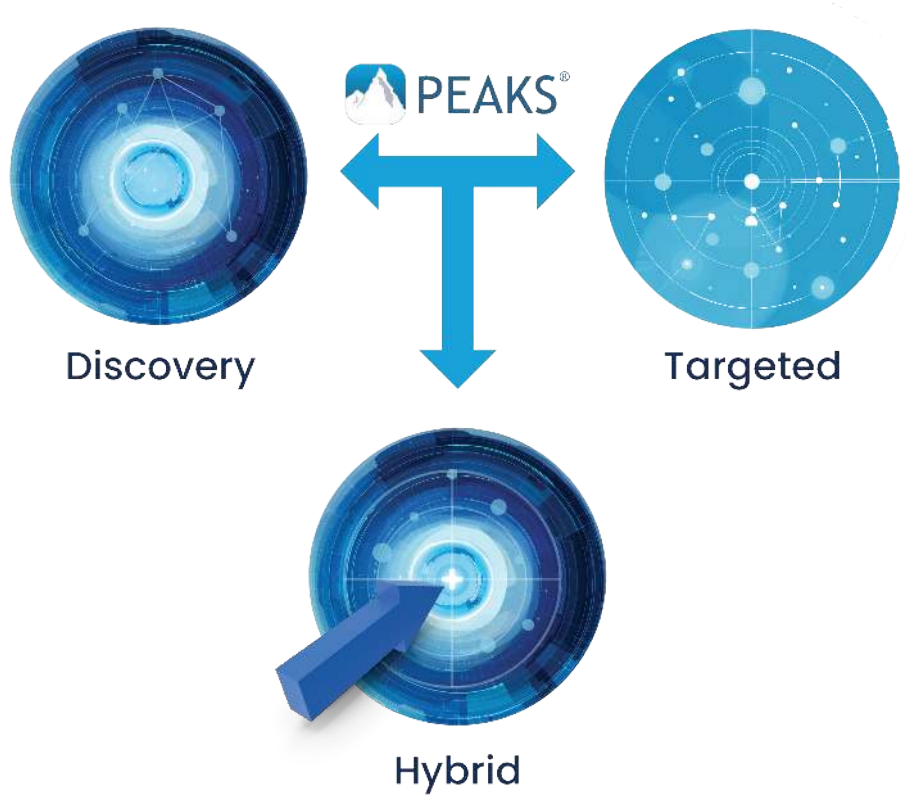
Targeted and Discovery-Driven

CLINICAL PROTEOMICS

Hybrid-PRM/DIA Analysis

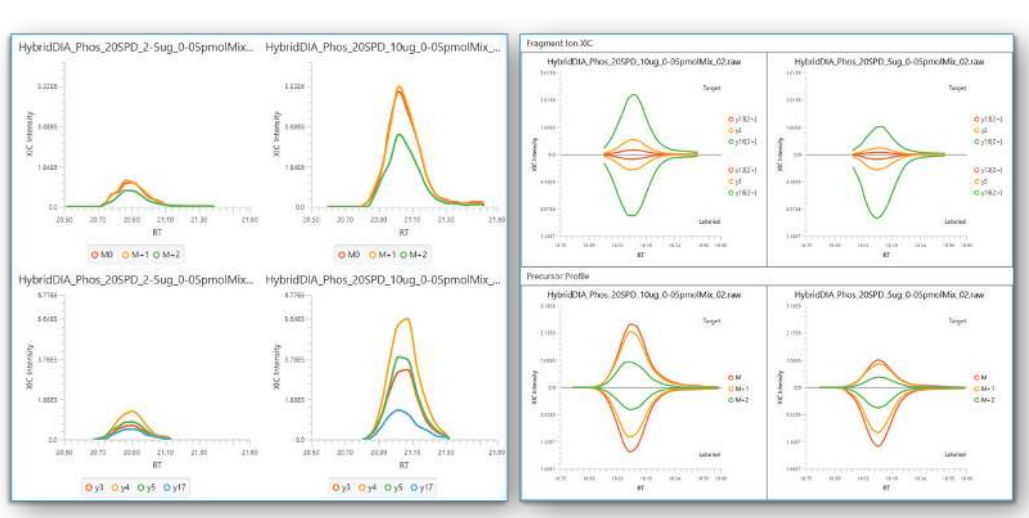
Hybrid PRM/DIA technology is a new intuitive data acquisition strategy combining enhanced sensitivity for target via intelligent triggering of multiplexed parallel reaction monitoring (PRM) and depth of the DIA discovery driven digitization of the clinical biospecimen.

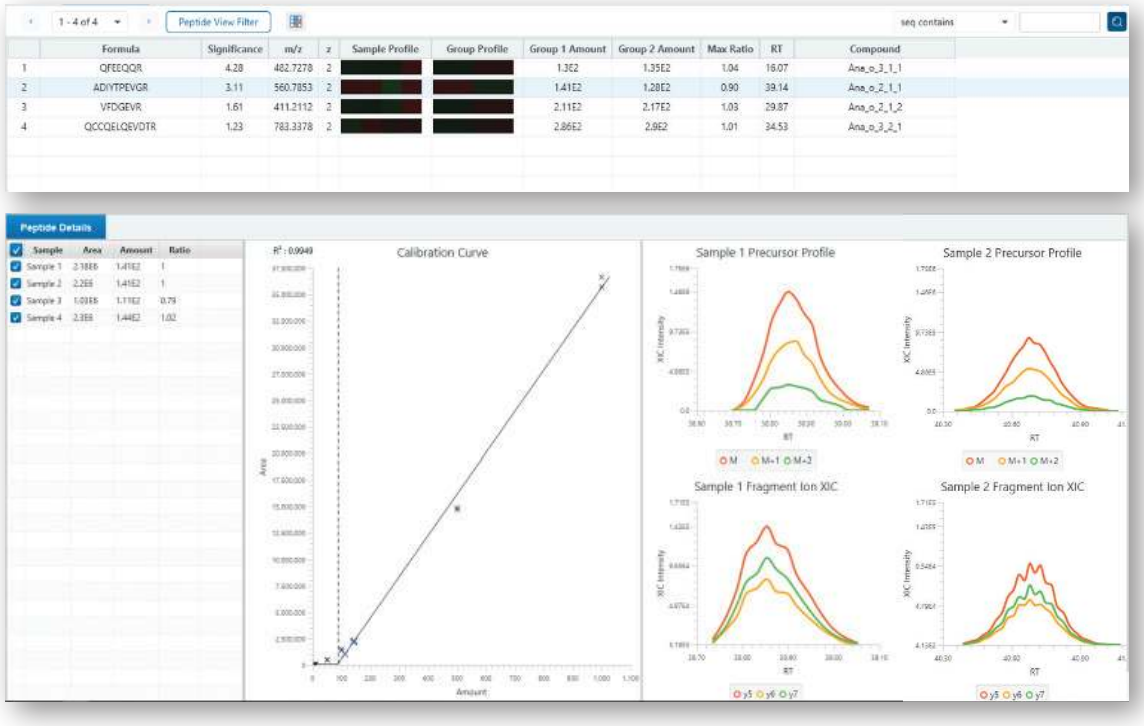
New! Enhanced algorithm for quantifying endogenous peptides against the heavy labelled reference counterparts.



DID YOU KNOW

PEAKS PRM enables the absolute quantification of target proteins through calibration data input?





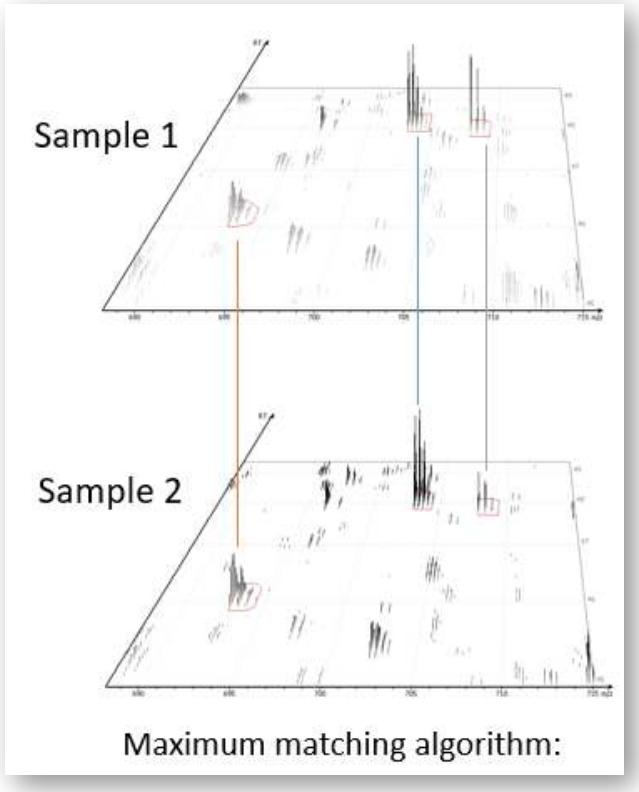
PRM Analysis

PRM provides high selectivity, high sensitivity, and high-throughput quantification with confident targeted peptide confirmation.

New! PEAKS Labelled PRM supports SILAC and other metabolic labelling for improved accuracy.

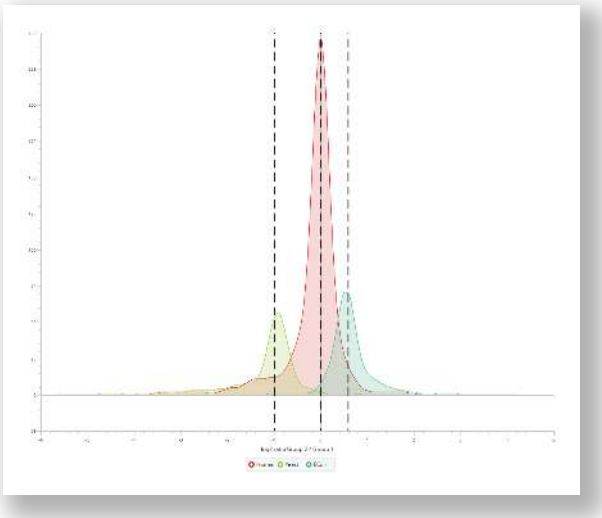
New! PEAKS PRM now supports timsTOF technologies.

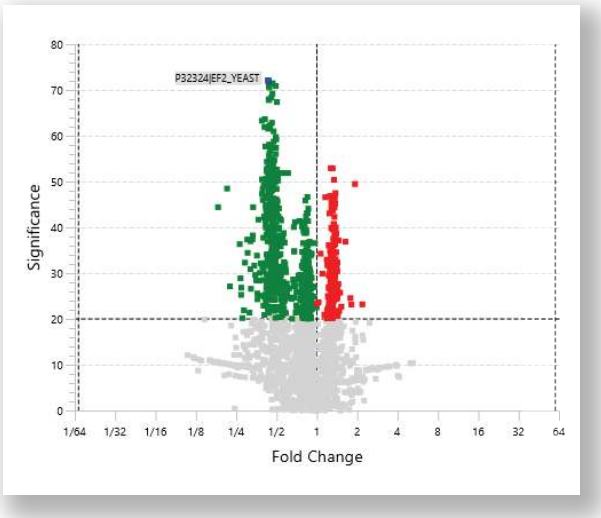
PEAKS® Q
For Quantitative Proteomics



Label-Free Quantification (LFQ):

LFQ offers an efficient, cost-effective strategy to assess significance of biological changes in peptide and protein expression levels. PEAKS® Q 's LFQ function allows researchers a detailed investigation of differences in identified peptide/protein abundances as well as unidentified features between samples with high accuracy, sensitivity, and precision.

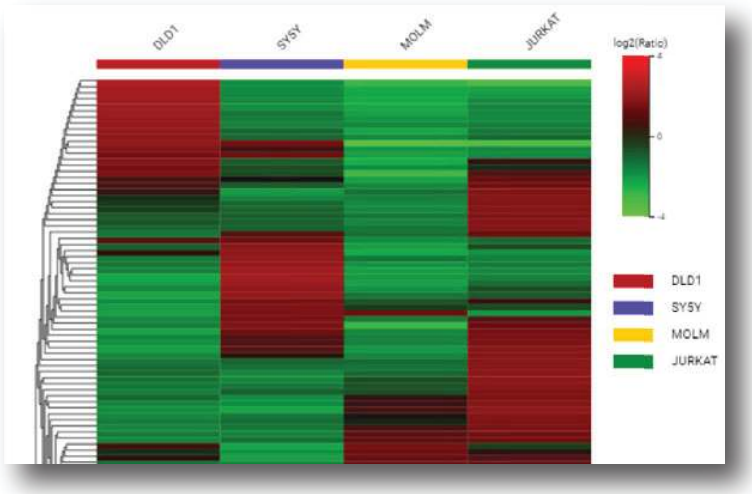




LFQ for DIA

New! Flexible protein quantification using Top 3 unique peptides or all unique peptides with MaxLFQ.

New! Improved Sensitivity and Accuracy for benchmarking.

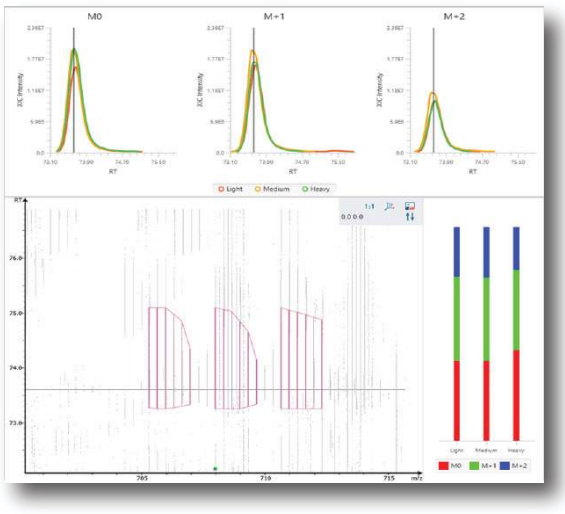


Reporter Ion Quantification

Isobaric tags (e.g. TMT/iTRAQ) allow for multi-conditions quantification taking advantage of isobaric chemical labelling with the use of Reporter ion abundance at MS2 or MS3 levels. Ideal for large-scale protein quantification studies offering both intra- and inter-experiment normalizations.

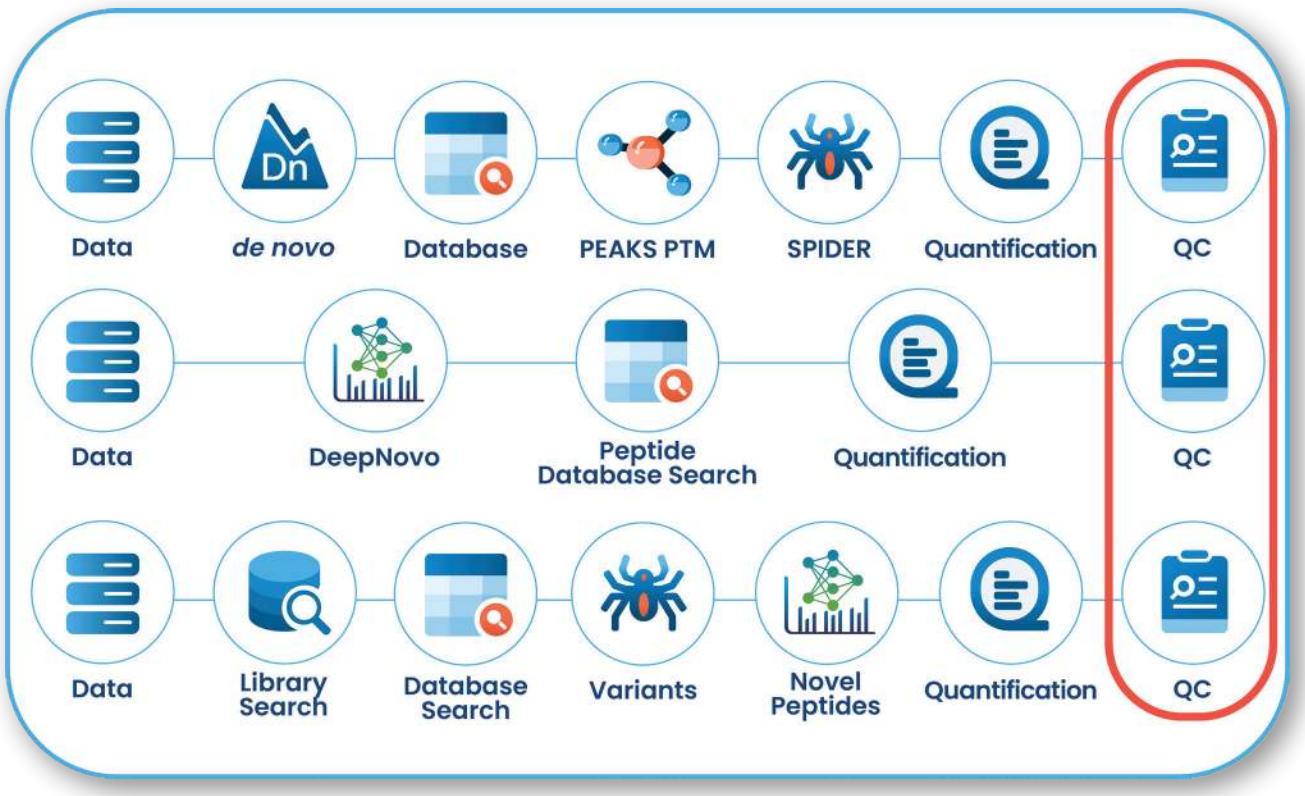
Precursor Ion Quantification

Stable Isotope Labelling by Amino Acids in Cell Culture (SILAC) is a powerful approach for MS1-based quantitative proteomics. PEAKS® Q's enables unsurpassed sensitivity of peptide feature pair detection through a state-of-the-art algorithm.

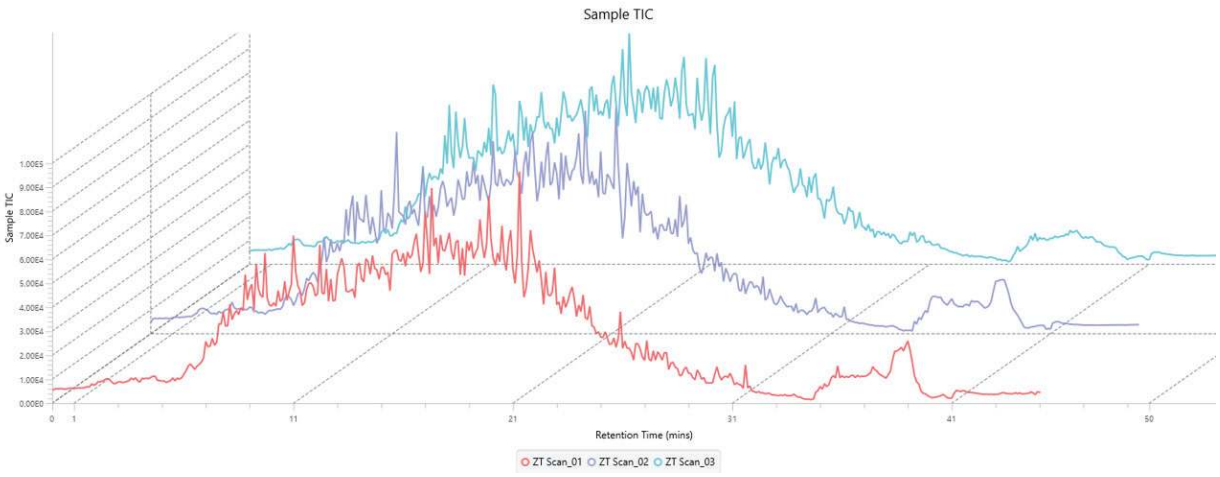


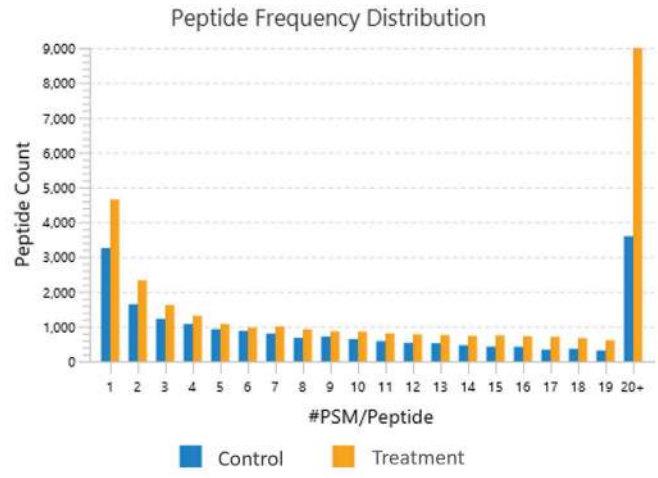
PEAKS Automated
QUALITY CONTROL (QC) TOOL

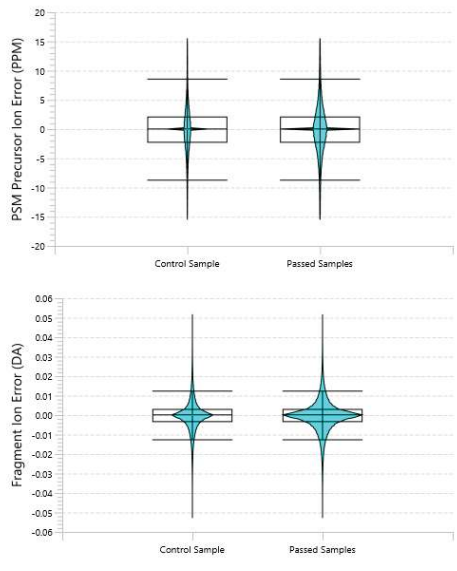
PEAKS® Studio provides a specialized QC tool designed to validate the reproducibility of peptide and protein identification and quantification. It is available for all DDA and DIA workflows.

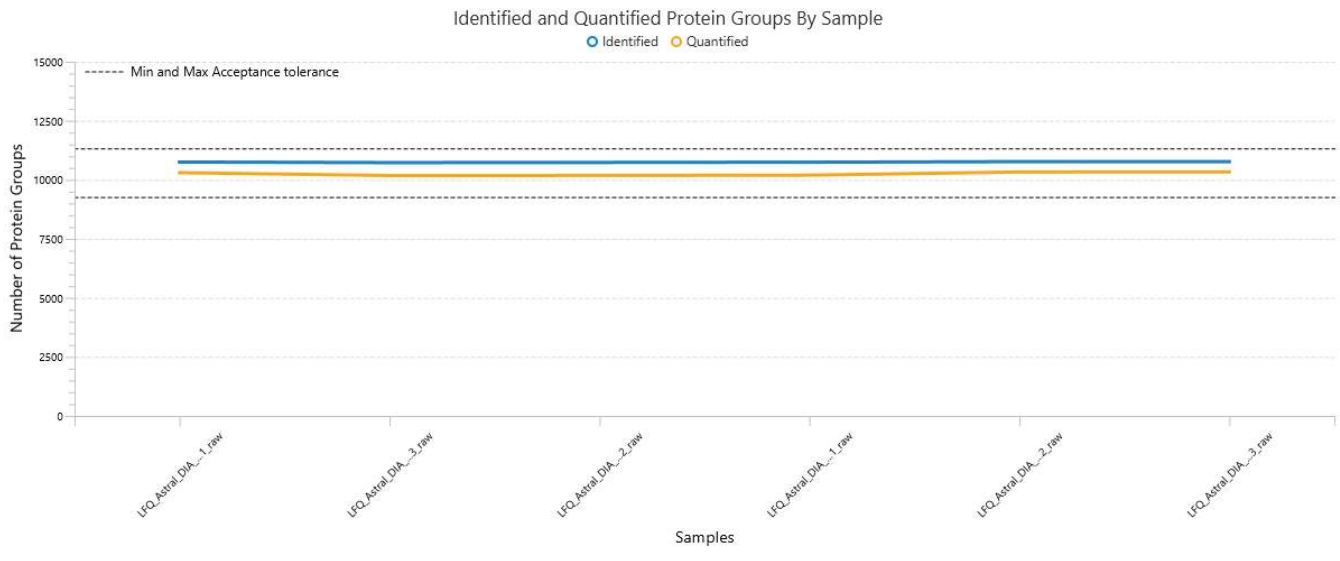


PEAKS QC delivers detailed information in an automated, systematic, and customizable manner, aiding instrumentation and data processing troubleshooting . By seamlessly integrating QC analysis into a single workflow, followed by consolidating statistical analyses into a comprehensive report, users can freely export data and figures as needed.







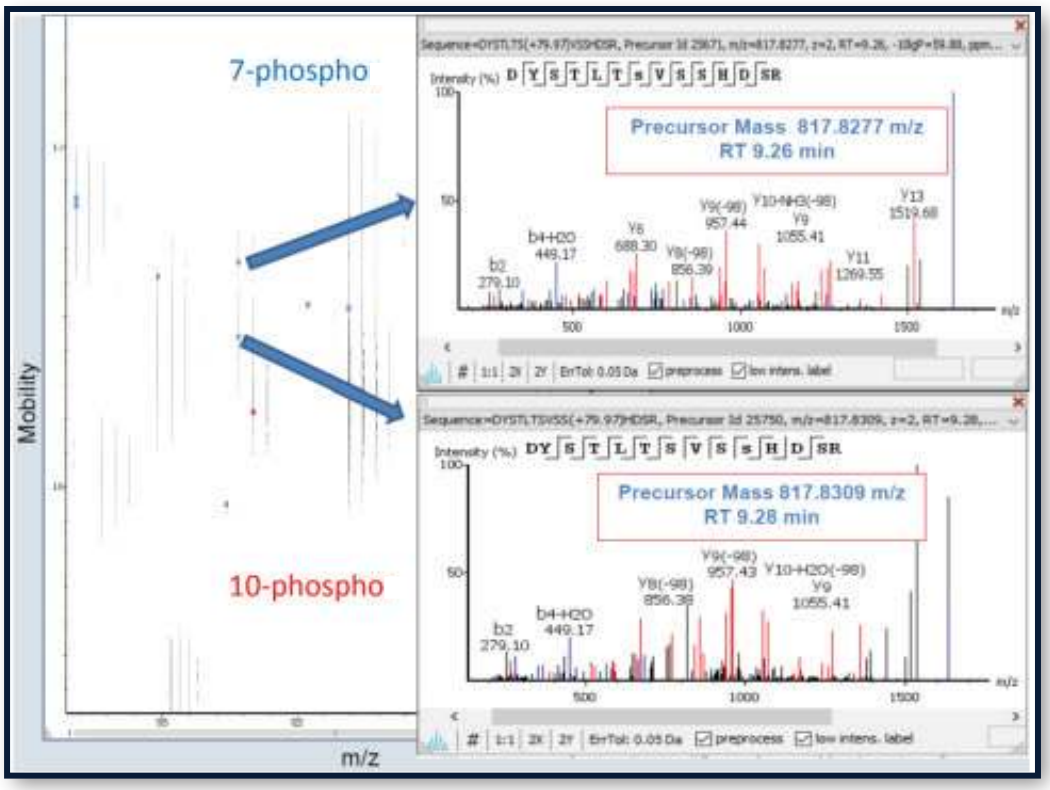


ION MOBILITY SPECTROMETRY – MASS SPECTROMETRY (IMS-MS)

IMS-MS provides a compelling analytical workflow for complex biological and chemical mixtures by adding a 4th-dimension of ion separation; ion mobility. With IMS-MS, ions are separated based on their mobility through a buffer gas, which provides the capability to differentiate ions based on their size, shape, charge, and mass mobilities. Thus, it is possible to resolve ions that may be indistinguishable by traditional mass spectrometry.

Using PEAKS®, the ion mobility data can be viewed in the Mobility-LC-MS 4th-Dimension. The additional dimension enables increased identification sensitivity with smaller sample amounts.

- Analyze IMS-MS data using PEAKS® *de novo*, identification and quantification workflows.
- Interactive data visualization tools to view data projected on m/z-rt or m/z-1/k0 dimensions.
- Vendor neutral; PEAKS® is able to support IMS data from any instrument
- Enable accurate and sensitive quantification analyses for IMS-based proteomics studies (Ex. label-free, SILAC, TMT/iTRAQ)

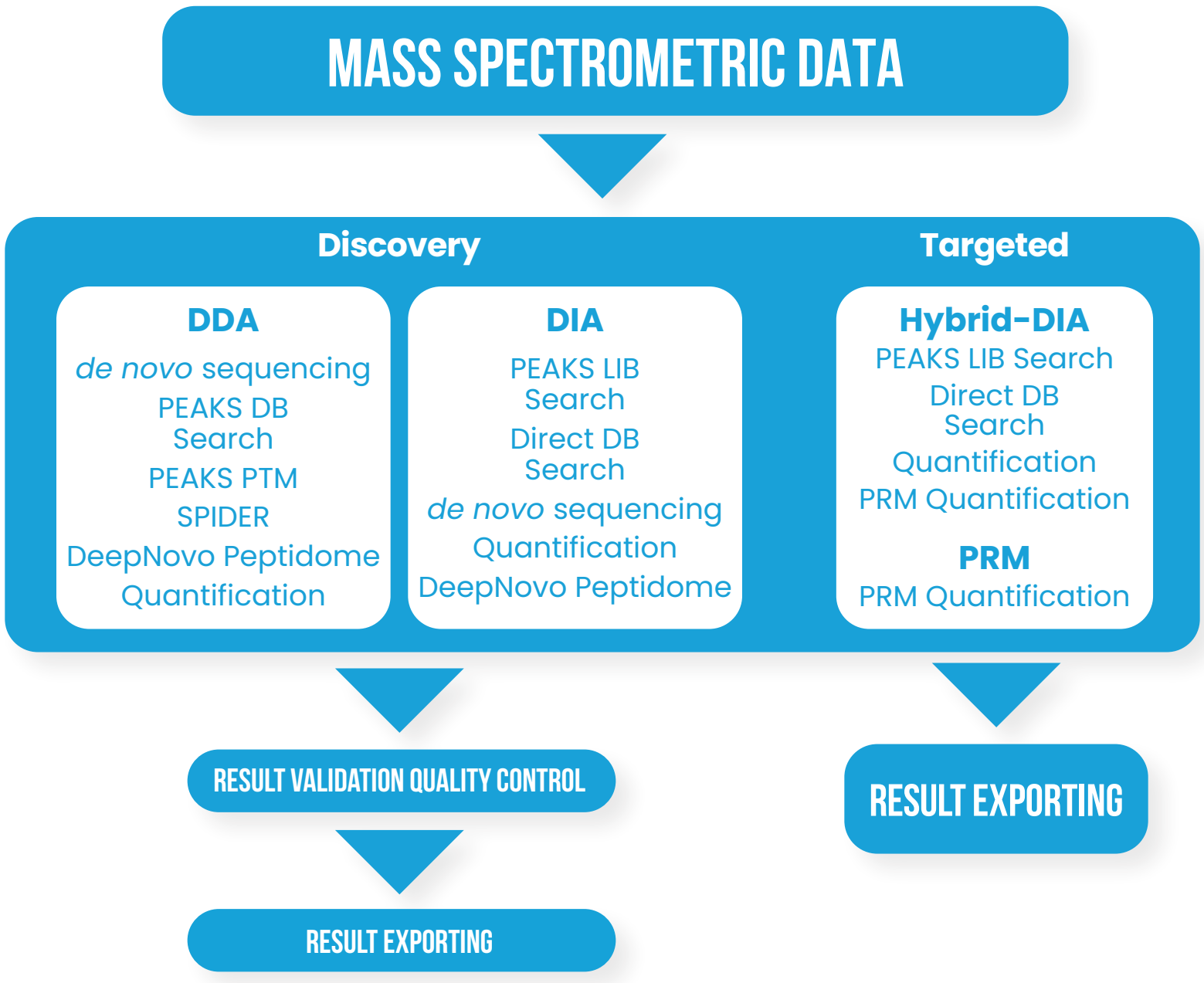


PEAKS® was used to analyze an extract of a HEK cell digest after a PASEF acquisition. The two co-eluting parent ions were separated in the ion mobility dimension, revealing two isobaric peptides differing only in the position of phosphorylation.

DEEP INSIGHT AND CONFIDENT DISCOVERY

Advancing proteomics research relies on innovative software and AI-driven technology to enable faster, more accurate, and sensitive data identification and quantification. Together the latest mass spectrometry technology combined with PEAKS® will advance the frontier of biological research.

Updated workflows for a variety of applications, such as in depth canonical and non-canonical peptide and protein identifications, make PEAKS® a unique solution. From DDA to DIA data support, PEAKS® provides a comprehensive solution to bring your research to new heights!



KEY HIGHLIGHTS

- One stop solution for discovery and targeted proteomics
- Powered by world leading *de novo* sequencing technology
- Vendor neutral
- Detailed and easy-to-use graphical user interface (GUI) to view, filter and validate results.

FULL BSI SOFTWARE AND SERVICE SUITE

PEAKS®

PEAKS® Studio

PEAKS® Online

PEAKS® AB

PEAKS® GlycanFinder

DeepSuite

Deep AB

Deep Immu

Deep Proteo

Deep Glycan

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