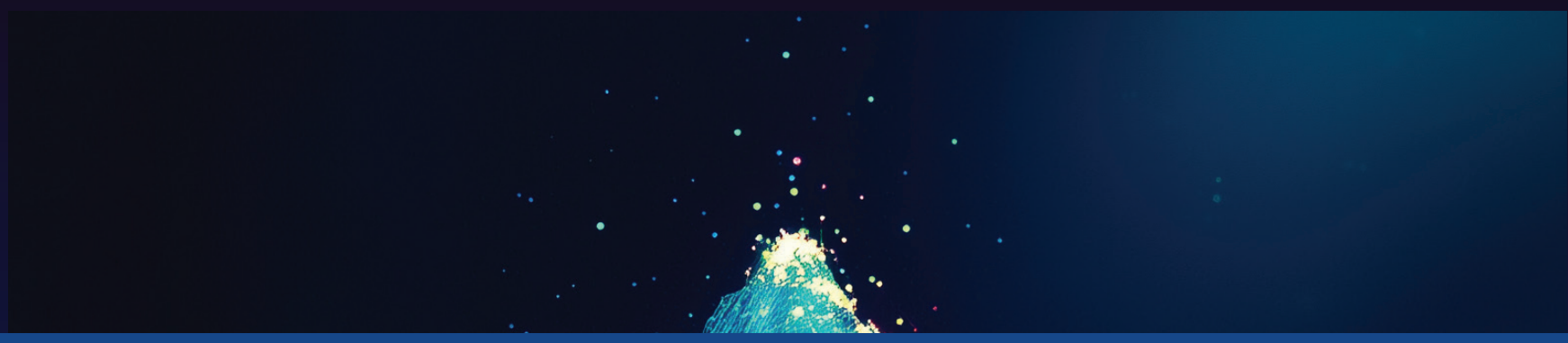
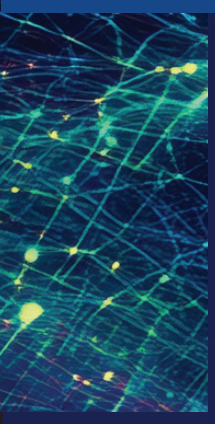
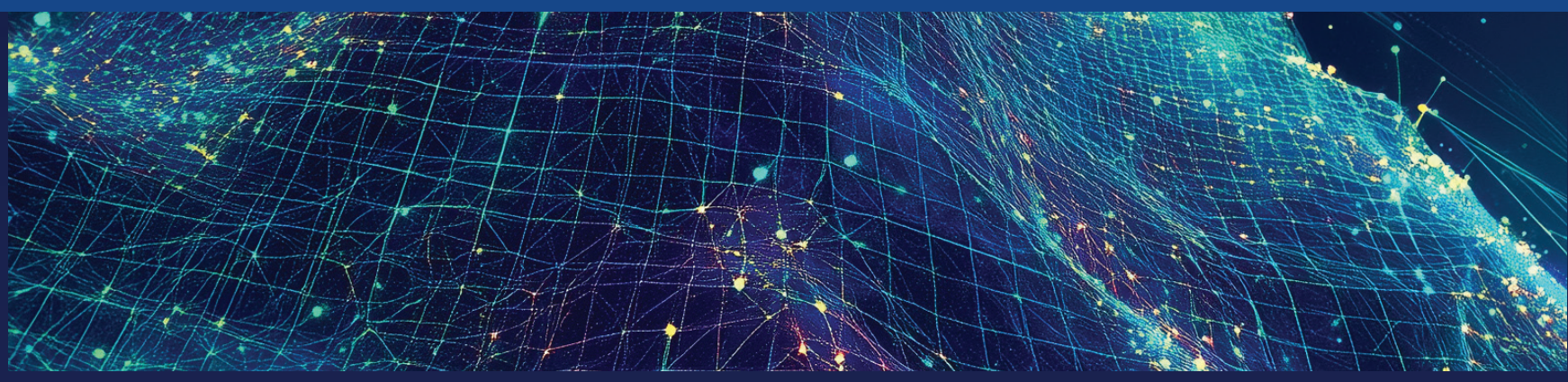


PEAKS® Studio 12.5

A Complete Solution for Proteomics





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Bioinformatics Solutions Inc

PEAKS® Studio 12.5

ASCEND TO NEW HEIGHTS WITH

DEEP PROTEOMICS SOLUTIONS

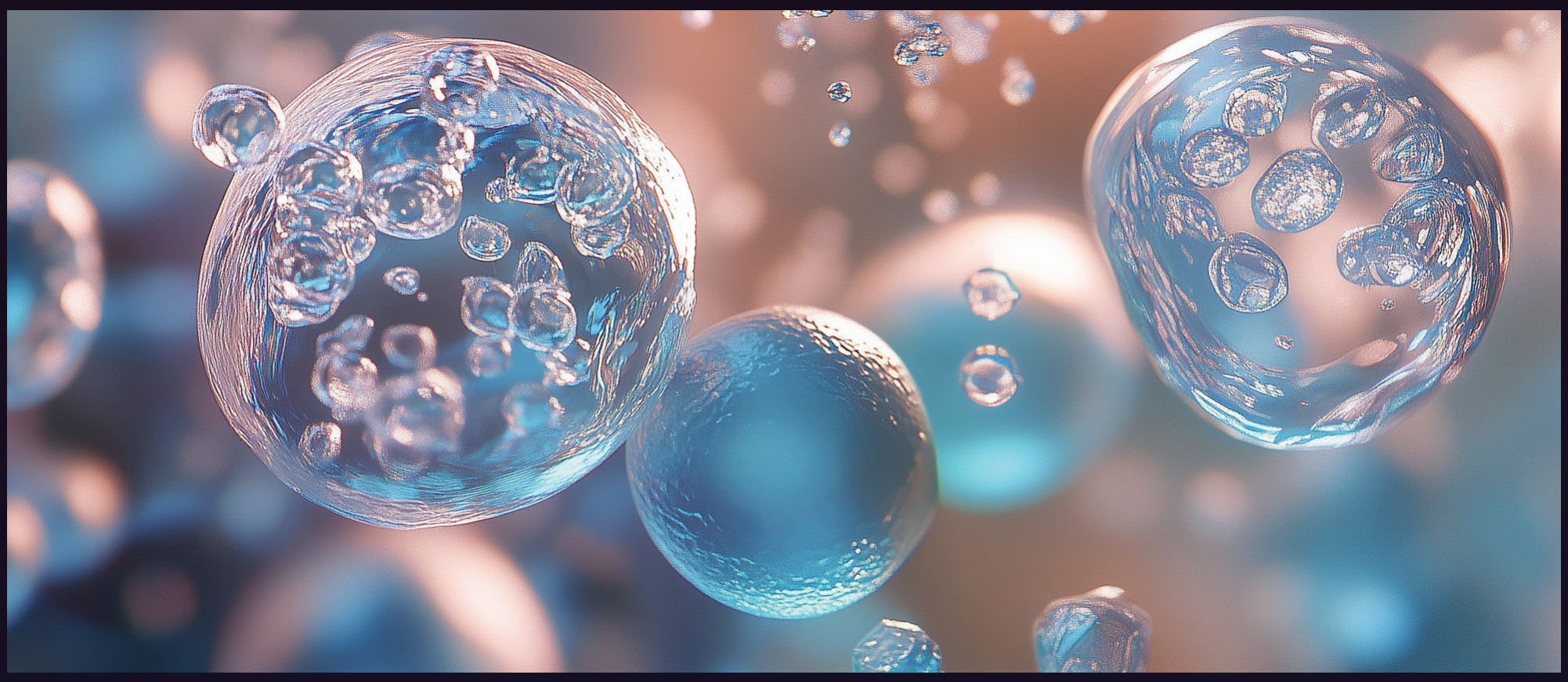
Mass spectrometers and other related analytical techniques have continued to improve at a rapid pace over the past few decades. It is important for researchers to have software that is up to date and can handle the continuously improving data outputs.

Developing innovative software and applying AI-driven technology to advance proteomics data analysis is vital to advance research by providing faster, more accurate and sensitive identification and quantification. Together the latest mass spectrometry technology combined with PEAKS® Studio will advance the frontier of biological research and facilitate drug discovery.

NEXT GENERATION OF PEAKS®

PEAKS® Studio 12.5 is the next generation of the studio platform and features an architecture to provide increased speed and stability. With the updated Graphical User Interface, users still get the intuitive data visualization that PEAKS® is known for, but with deep learning based optimized workflows to streamline your data analysis. From DDA to DIA data support, PEAKS® Studio 12.5 provides a complete solution to bring your research to new heights!

PEAKS® Studio 12.5



PEAKS® Studio is a powerful and comprehensive software suite designed for the analysis of mass spectrometry proteomics data. PEAKS® Studio is a versatile and powerful tool that supports a wide range of proteomics applications, from basic protein identification to advanced functional and clinical proteomics studies.

TABLE OF CONTENTS

EXTENDING THE DISCOVERY PROTEOMICS DEEP LEARNING REVOLUTION

PEAKS® Studio 12.5 harnesses 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

In **PEAKS® Studio** we have integrated AI to advance the following workflows:

Peptide *de novo* sequencing: Users will experience the most accurate and fastest peptide *de novo* sequencing available in any PEAKS® product. PEAKS® has been known as the gold standard for automated peptide *de novo* sequencing for many years but with the new GPU-enabled "DeepNovo", *de novo* sequencing in PEAKS® is the best it has ever been. In PEAKS® 12.5, users can take advantage of the first *de novo* sequencing with FDR estimation.

DIA Workflow: Deep learning has been integrated into our DIA workflow for spectral library search, database search, and *de novo* sequencing. PEAKS® database search examines the dataset with an *in silico* spectral library generated from the protein sequence database. *In silico* peptide details including the fragment ion pattern, indexed retention time, and ion mobility are predicted using deep learning. In PEAKS® 12.5 users will experience faster CPU/GPU analysis speeds.

DeepNovo Peptidome: This workflow supports both DDA and DIA data analysis and is a specialized workflow for immunopeptidomics. We have integrated the latest DeepNovo algorithm to improve processing speed and identify peptides with a variety of modifications, sequence variants, and/or splice sites. 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.

PEAKS® DB: PEAKS® provides a unique *de novo*-assisted database search to improve both sensitivity and accuracy. The users have the option to include the deep learning boost for MS2 rescoring and improving the number of identifications by ~10%.

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

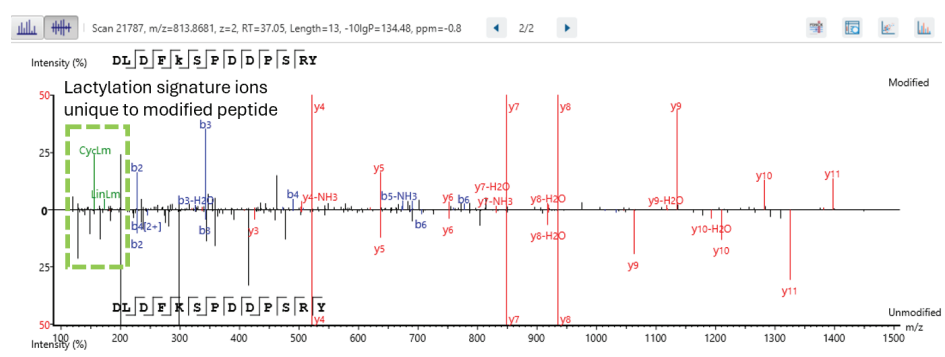
Each spectrum is searched against a protein database to find the best peptide-spectrum match. PEAKS® provides enhanced separation of true and false hits by incorporating the *de novo* sequencing results into the scoring algorithm. This unique *de novo*-assisted approach will allow you to identify more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

Discover Hidden Modifications

In PEAKS® PTM and SPIDER, the highly confident spectra with a good *de novo* score are reanalyzed to assess any unknown PTMs or sequence variants. Additional confident modification algorithm and the use of Potential Signature Ions are implemented for modified peptide re-scoring and enhance accuracy in PTM and sequence variant identification.

PEAKS® PTM

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

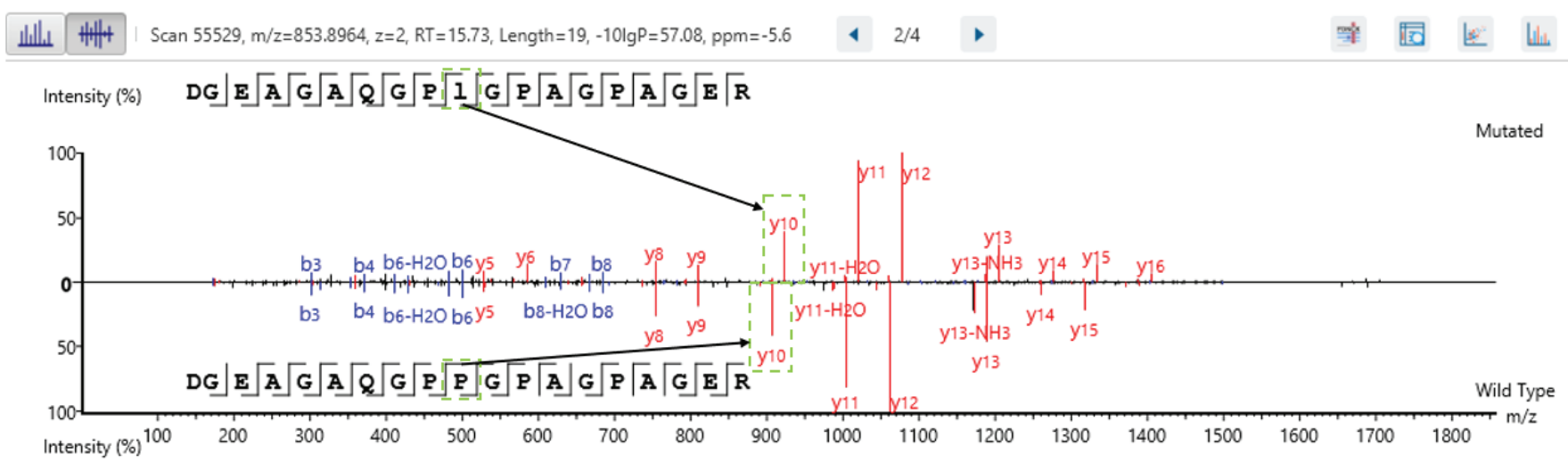


SPIDER

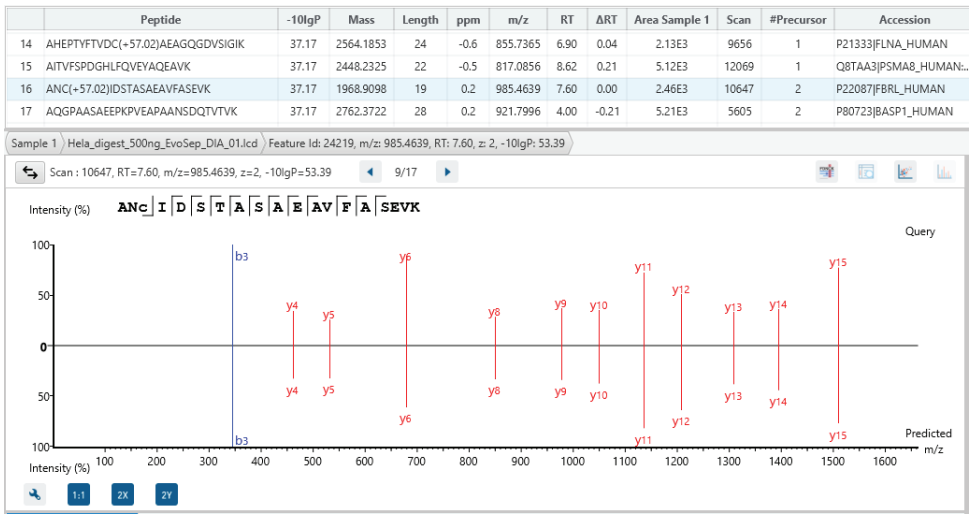
Homology search with *de novo* tags identifies amino acid mismatches between *de novo* and database sequences. Confident mutations are determined by the number of consecutive fragment ions at the mutation site with relative ion intensities above a threshold, each of which are user-defined.

Unified Scoring for Easy Interpretation

PEAKS DB, PEAKS PTM, and SPIDER results are all scored using -10lgP. So, results from the three algorithms can be displayed together on the same scale.



PEAKS® DIA WORKFLOWS



PEAKS offers a robust solution for DIA data analysis. It incorporates three methods of peptide identification: spectral library search, database search, and *de novo* sequencing. Each of these methods can be performed individually or in combination with an with an improved search space.

Spectral Library Search

First, a search is performed against a library of previously identified spectra. By estimating the false discovery rate, peptides that pass the filter are saved and reported as library peptides.

Database Search

MS/MS spectra that don't match a spectral library entry within the false discovery rate are brought forward to a direct database search against an *in silico* protein sequence database. Confident database matches are added to the result.

De Novo Sequencing

Then, using the same FDR approach, unmatched spectra from the database search are analysed using *de novo* sequencing to find a peptide with the best match to the spectrum.

Label-free quantification (LFQ)

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

Quality Control

The automated Quality Control (QC) tool can be used in this workflow to provide sophisticated and systematic QC analysis of raw data, identification, and quantification result.

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 12.5
FOR DIA WORKFLOWS

Faster Processing Times for DIA with or without a GPU.

PEAKS 12.5 processes DIA data 10-20% faster compared to PEAKS 12.0 when a GPU is utilized.

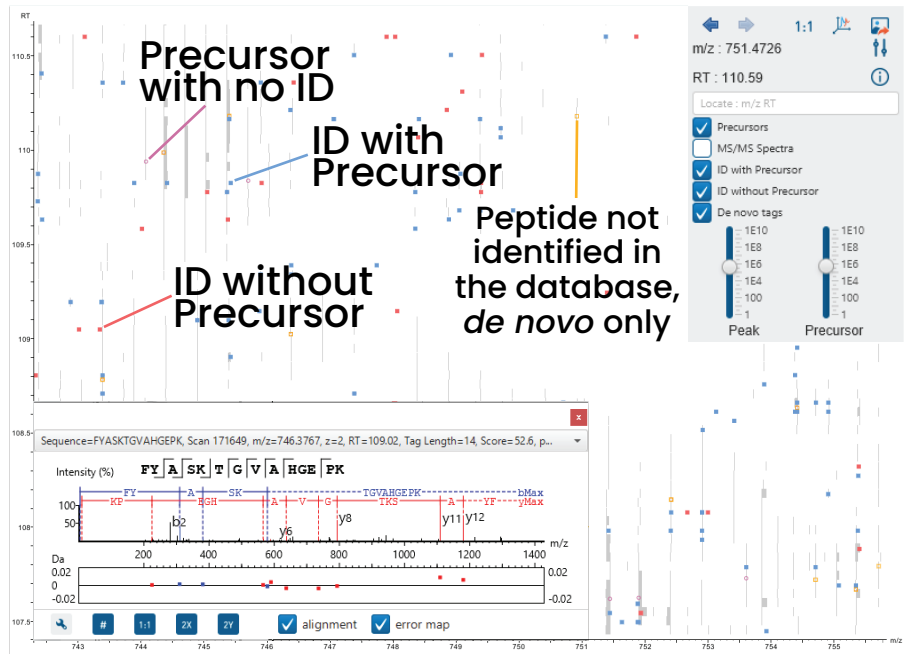
The DIA algorithm in PEAKS 12.5 has been updated to take better advantage of CPU resources.

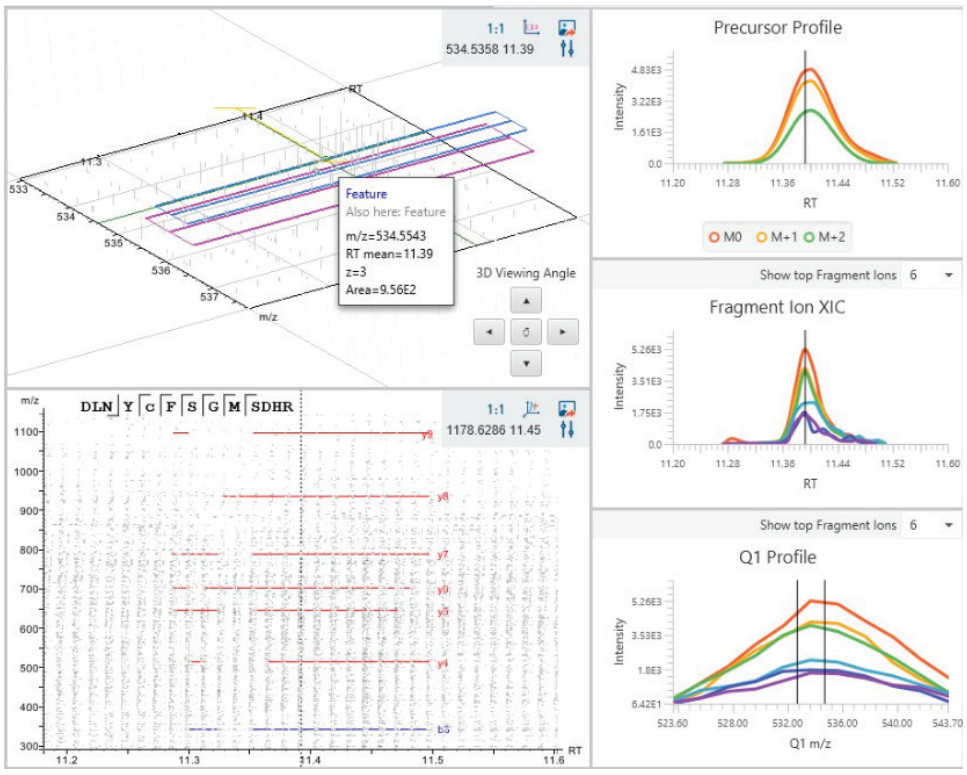
Now, data processing times are much faster, even without a GPU.

Improved DIA Data and Result View

In the Data Refine LCMS view, there are now more options for visualizing precursors, MS/MS windows, identifications, and *de novo* tags.

It is now easy to distinguish between identifications with and without a precursor. Identifications with a precursor are coloured in blue and identifications without a precursor are coloured in red.



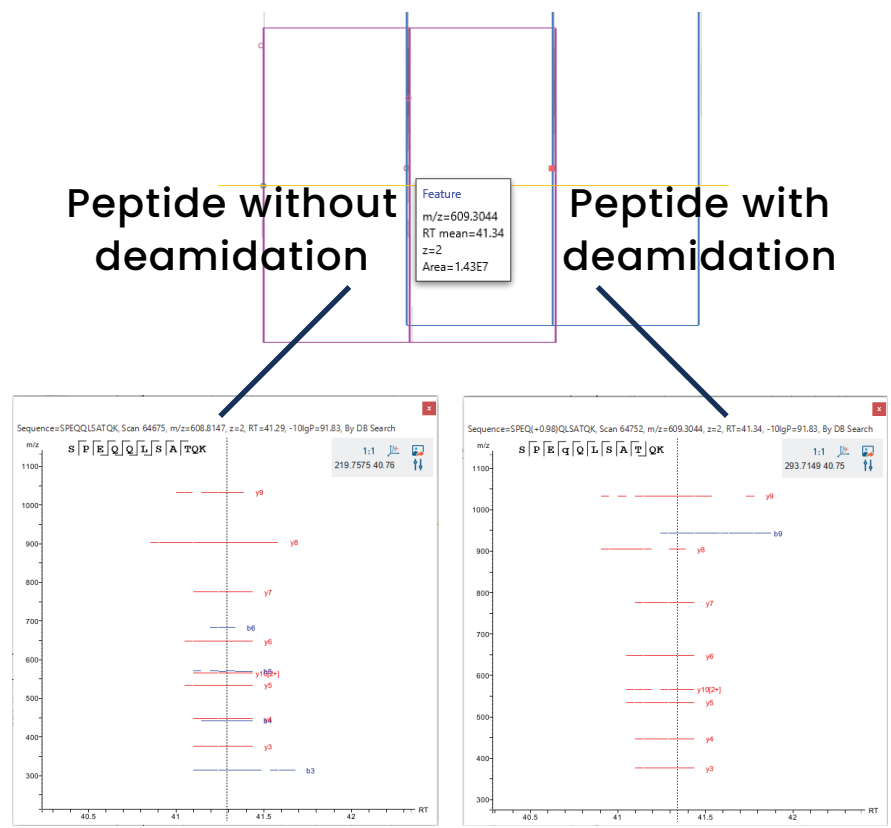


Seamlessly move between the Peptides tab and LCMS map for a given peptide.

Visualize overlapping precursors on the LCMS map with associated identifications. Click on an identification in the LCMS map to show each fragment ion as a function of retention time.

ZT Scan DIA

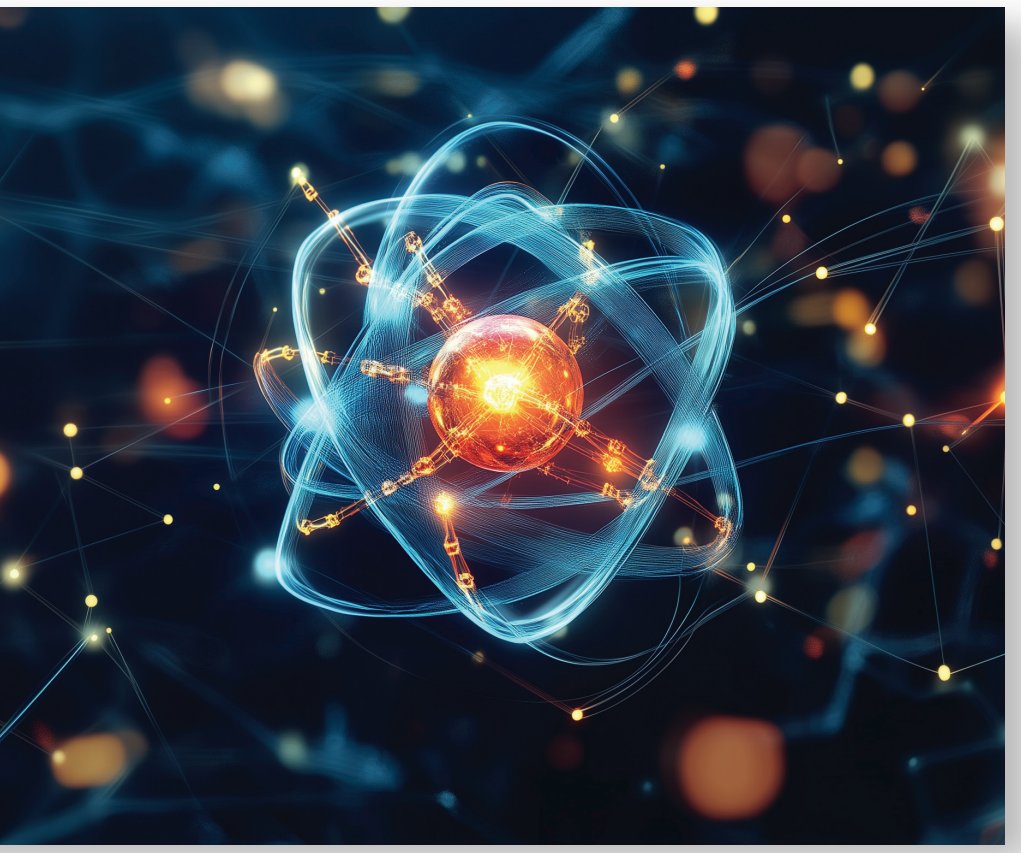
PEAKS 12.5 introduces the support for the latest **ZT Scan DIA** technology from SCIEX. PEAKS uses the **Q1 dimension** from ZT Scan DIA for improved identification sensitivity, reproducibility, and quantitative precision.



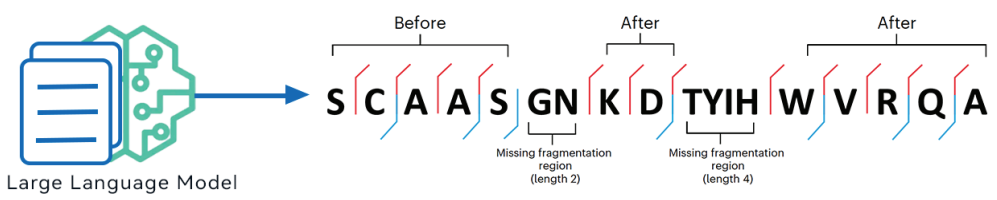
The gold standard for peptide *de novo* sequencing just got even better

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.

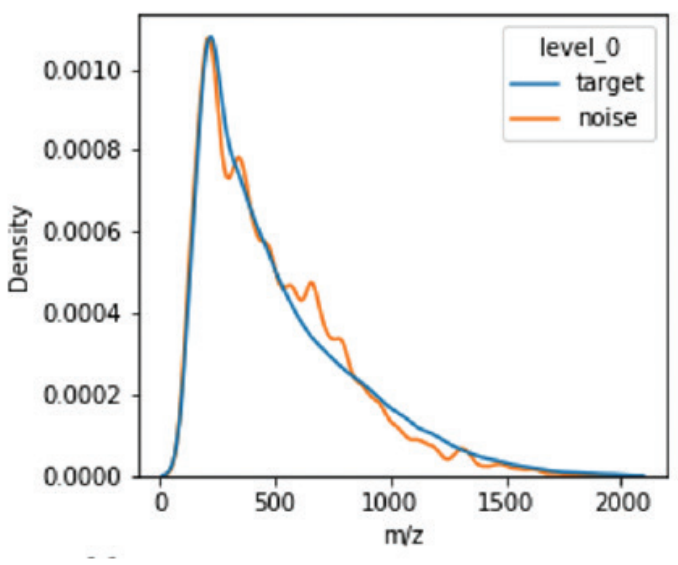


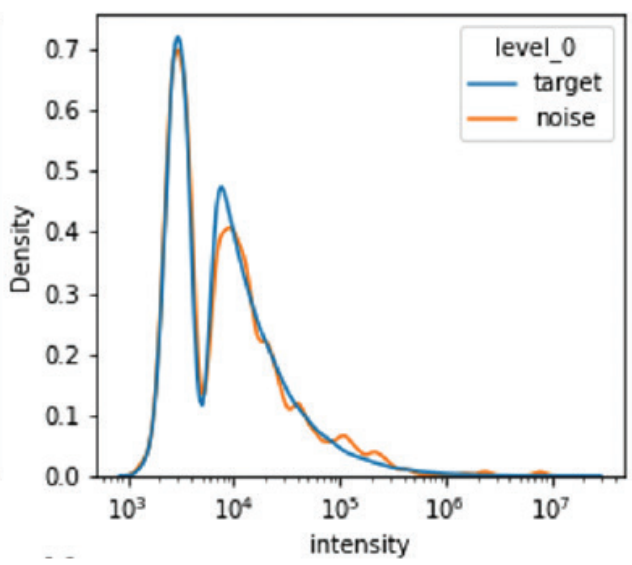
Empowered by the latest GraphNovo algorithm, the new DeepNovo resolved the issue of accumulated prediction errors due to missing fragment ions by finding the optimal path in the first stage to guide sequence prediction in the second stage.

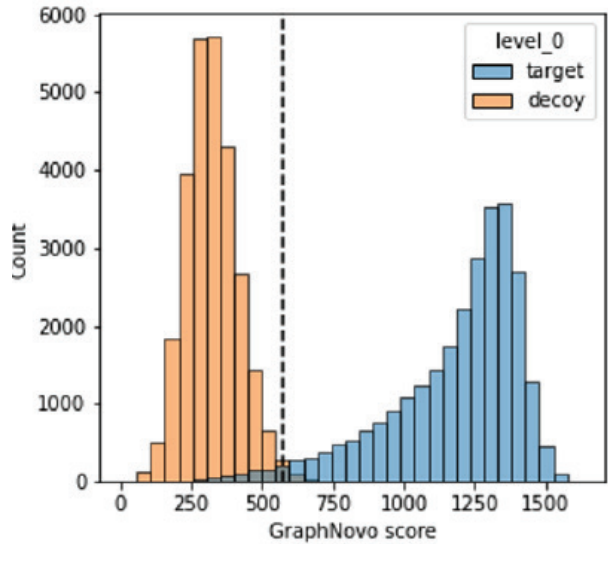


As a key technology for finding novel peptides from MS data, DeepNovo provides an advanced solution and will push research such as antibody sequencing and neoantigen discovery further.

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.



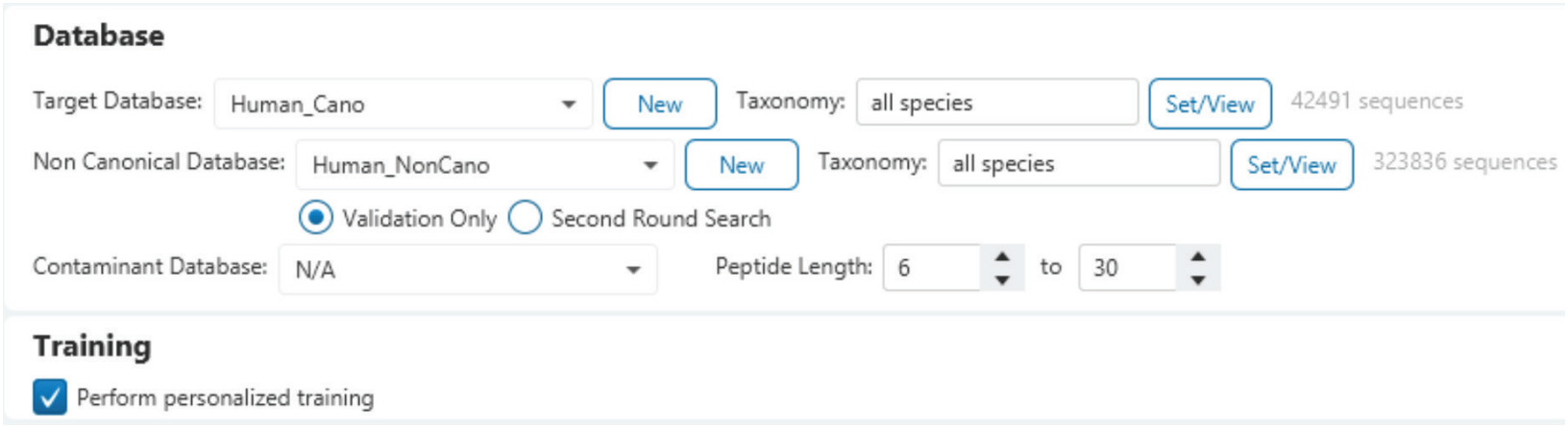




As a deep learning based solution, DeepNovo harnessed the computation power of NVIDIA GPUs for speed. NVIDIA A100 enabled *de novo* sequencing 1200 + spectra/s.

ENHANCED PEAKS® DEEPNOVO PEPTIDOME WORKFLOW

- **NEW:** DeepNovo peptide sequencing using Graphnovo, our latest deep learning algorithm
- Database and mutated peptides identifications from canonical and non-canonical databases
- Group specific FDR search allows for improved search space control and higher accuracy
- **NEW:** New On-the-fly training allows for allele specific personalized training



Gene Tab Integration

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)

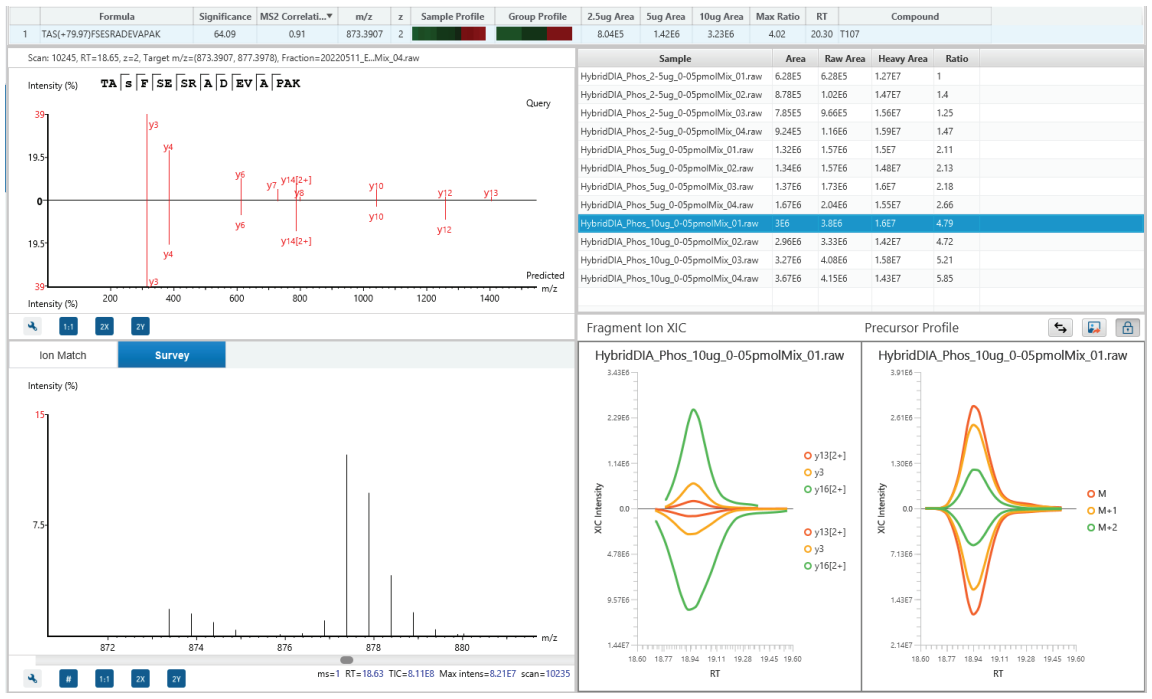
Protein isoforms from Target DB

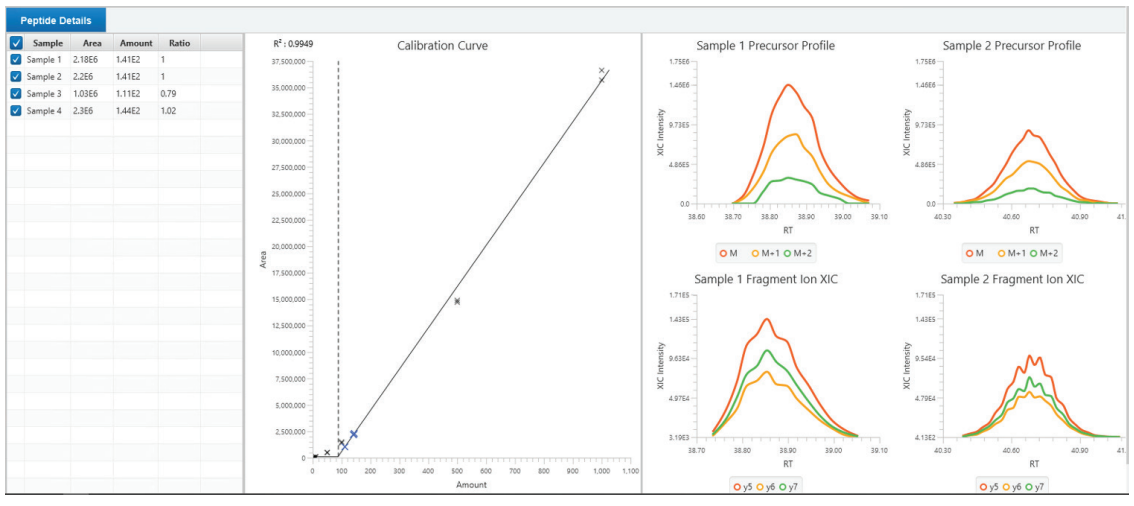
Entries from non-canonical DB

Targeted and discovery- driven clinical proteomics using HYBRID-PRM/DIA

Hybrid-PRM/DIA Analysis

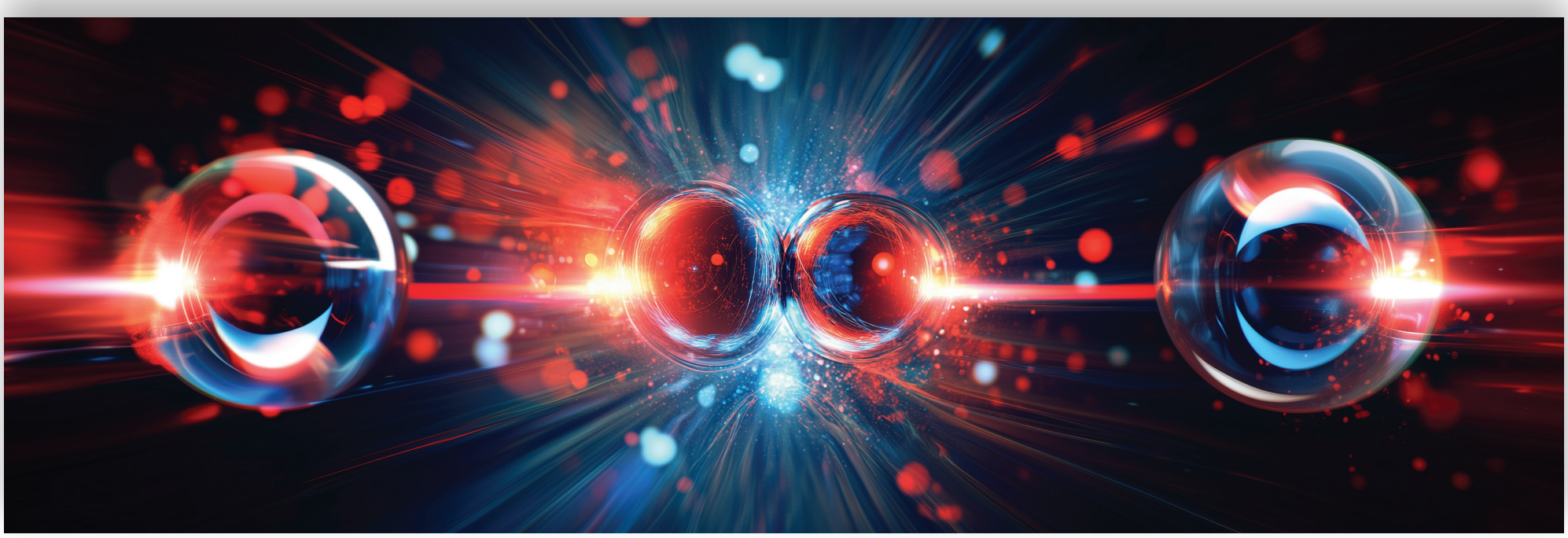
Hybrid-PRM/DIA technology as a new intuitive data acquisition strategy enables enhanced sensitivity for a specific set of analytes by the intelligent triggering of multiplexed parallel reaction monitoring (PRM) in combination with the discovery-driven digitization of the clinical biospecimen using DIA. Heavy-labeled reference peptides are utilized as triggers for PRM and monitoring of endogenous peptides.





PRM Analysis

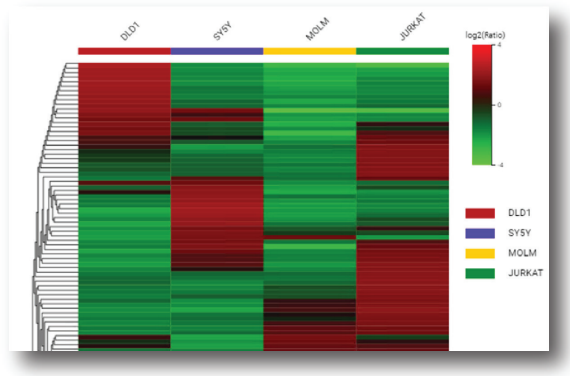
PRM provides high selectivity, high sensitivity, and high-throughput quantification with confident targeted peptide confirmation. A DIA / PRM workflow is suitable for discovery of biomarkers. PEAKS supports MS data analysis with DDA, DIA, and PRM.



PEAKS® Q
FOR QUANTITATIVE PROTEOMICS

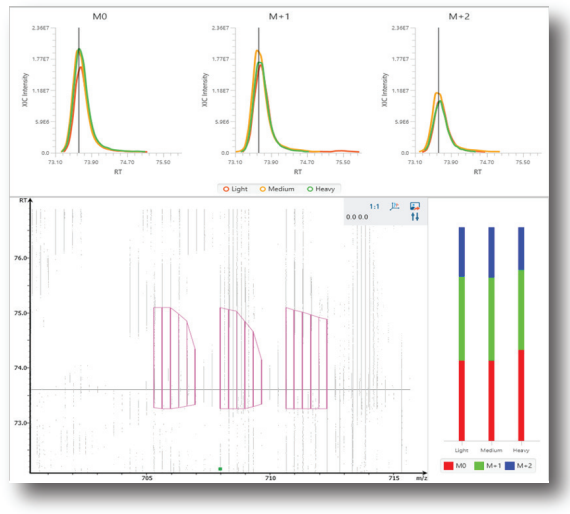
Reporter Ion Quantification

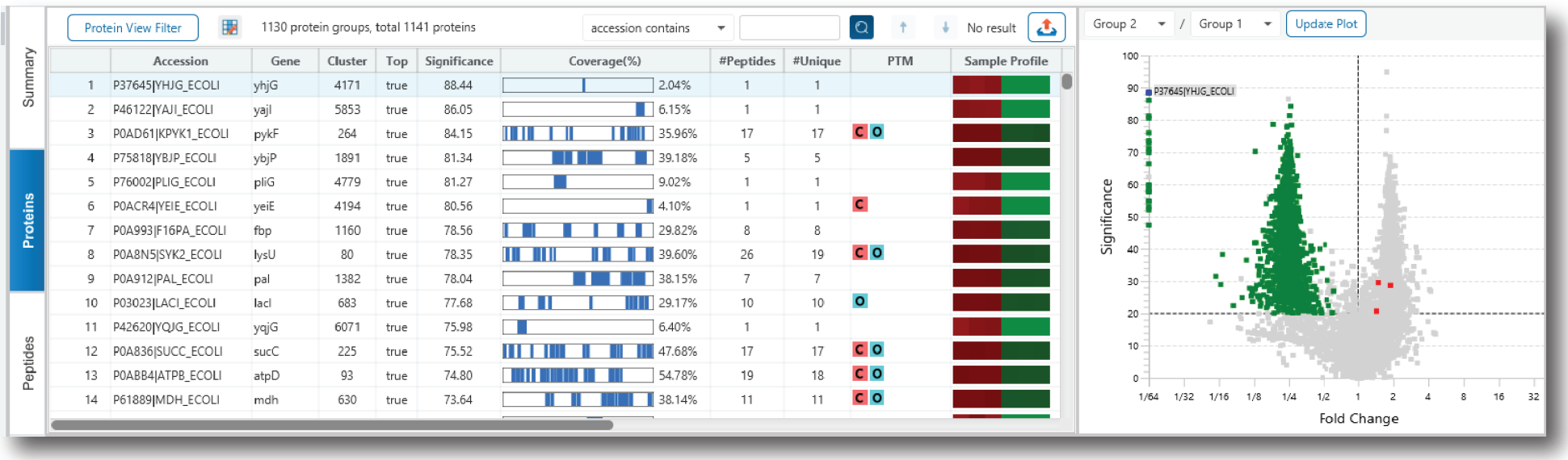
Isobaric tags (ex. TMT/iTRAQ) have identical masses and chemical properties that allow heavy and light isotopologues to co-elute. The tags are then cleaved from the peptide by collision-induced dissociation during MS/MS, which is used for quantification. For large-scale protein quantification studies, researchers can use PEAKS® Q to expand the sample size with reference channels to enhance the accuracy of quantification.



Precursor Ion Quantification

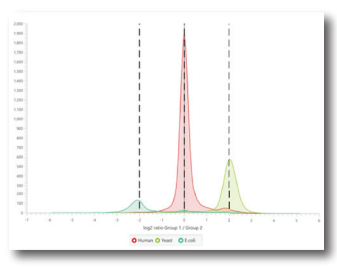
Stable Isotope Labelling by Amino Acids in Cell Culture (SILAC) is a powerful and popular approach for mass spectrometry (MS)-based quantitative proteomics. PEAKS® Q's SILAC quantification enables unsurpassed sensitivity of peptide feature detection through a novel algorithm to find peptide feature pairs. Researchers can take advantage of the intuitive interface showing paired features at first glance and minimize the biases from missing values.

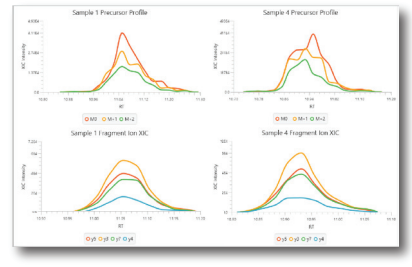




Label-Free Quantification (LFQ):

The ability to quantify the levels of proteins present in the samples by LFQ offers an efficient, cost-effective workflow to further understand the biological significance. PEAKS® Q 's LFQ function provides researchers with the option to calculate protein abundance and thoroughly investigate differences in peptide/protein abundance between samples with confident and accurate results. Use PEAKS® Q to uncover subtle changes in protein expression with high acuracy, sensitivity and specificity in your experiments.



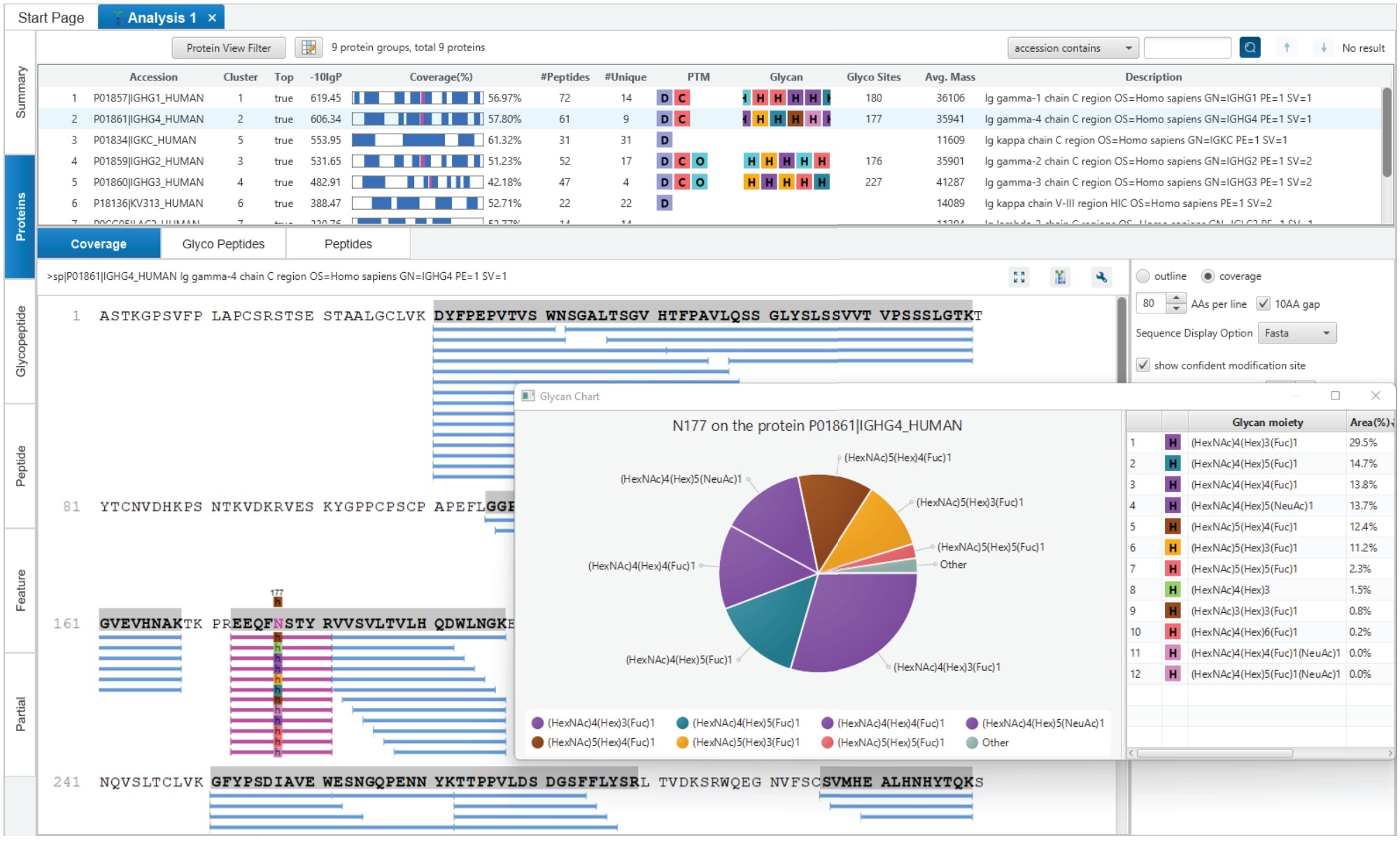


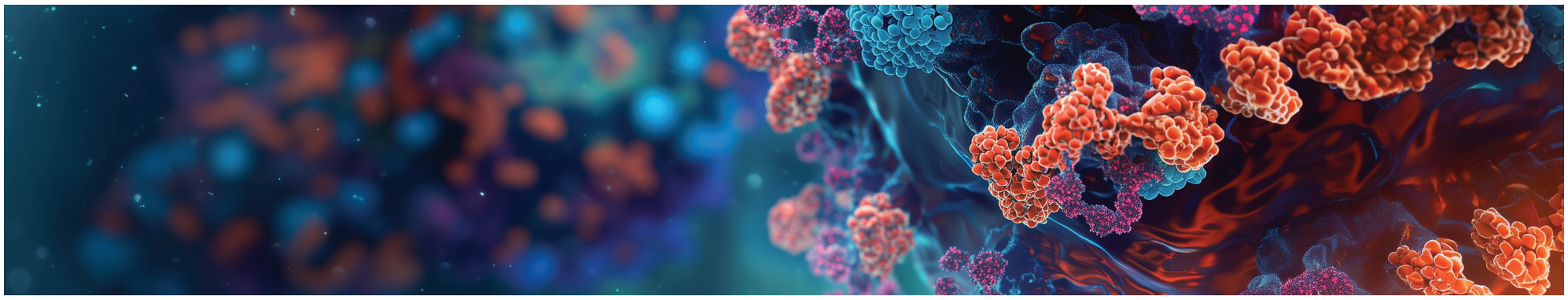
PEAKS® GLYCAN

provides in-depth glycoproteomic analysis

Protein glycosylation is one of the most common post-translational modifications and plays a crucial role in important biological processes but is drastically understudied and deserves a specialized tool for both N- and O-linked glycan analysis!

PEAKS® Glycan is a comprehensive data analysis tool that provides a highly sensitive and accurate glycoproteomics software solution to advance our understanding of the glycoproteome. PEAKS® Glycan search enables scientists to determine glycan site localization and glycan structures.



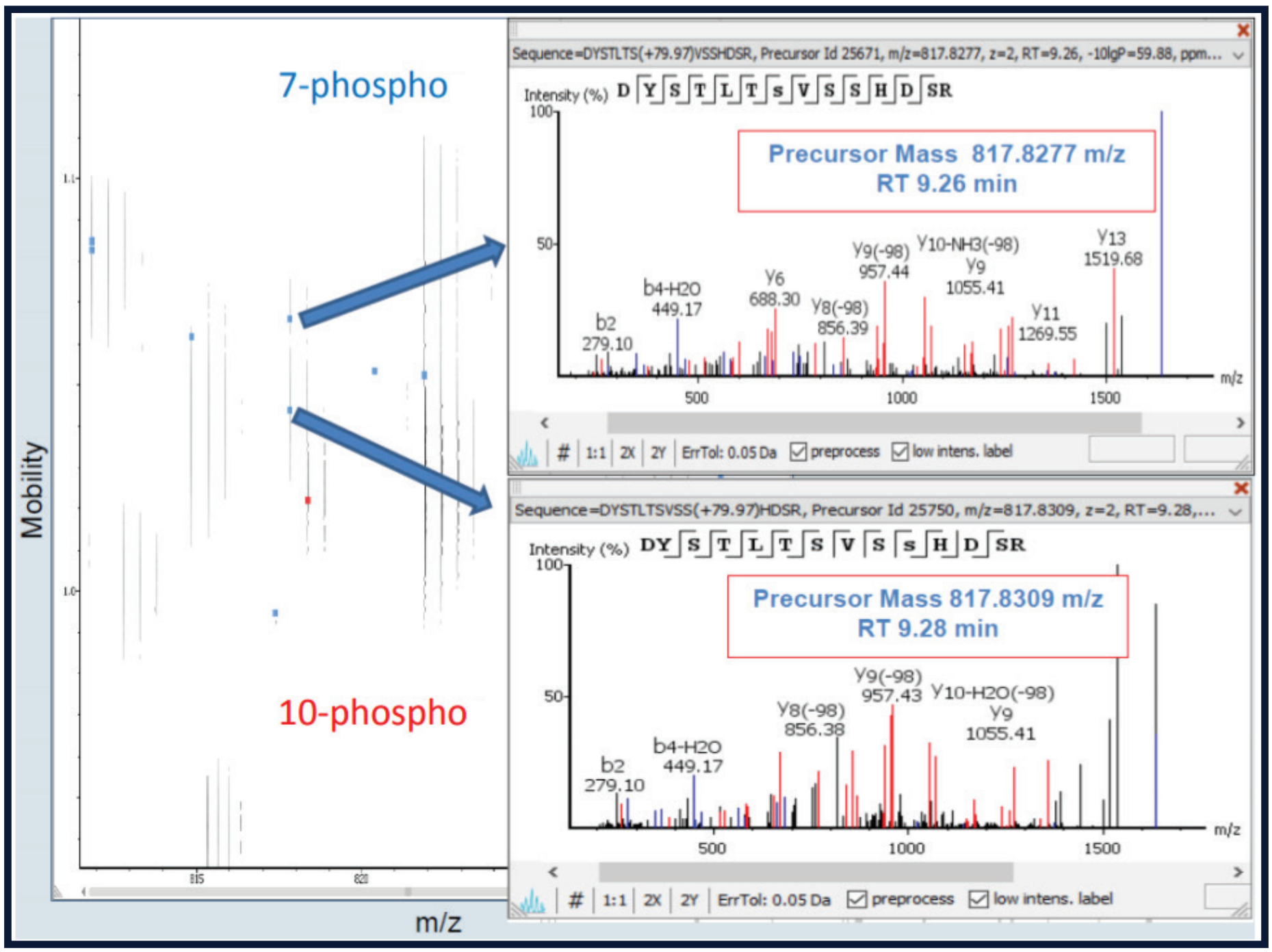


Ion Mobility Spectrometry - Mass Spectrometry (IMS-MS)

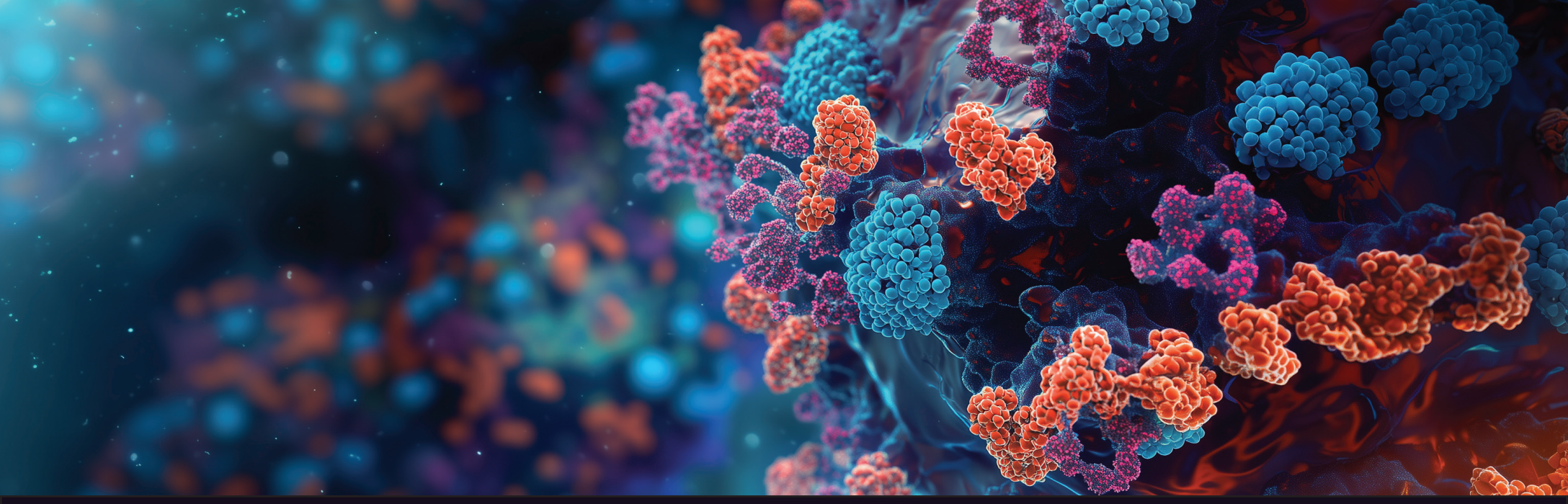
provides a compelling analytical workflow for complex biological and chemical mixtures by adding a 4th-dimension of ion separation; ion mobility. With IMS-MS, ions are separated based on their mobility through a buffer gas, which provides the capability to differentiate ions based on their size, shape, 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)

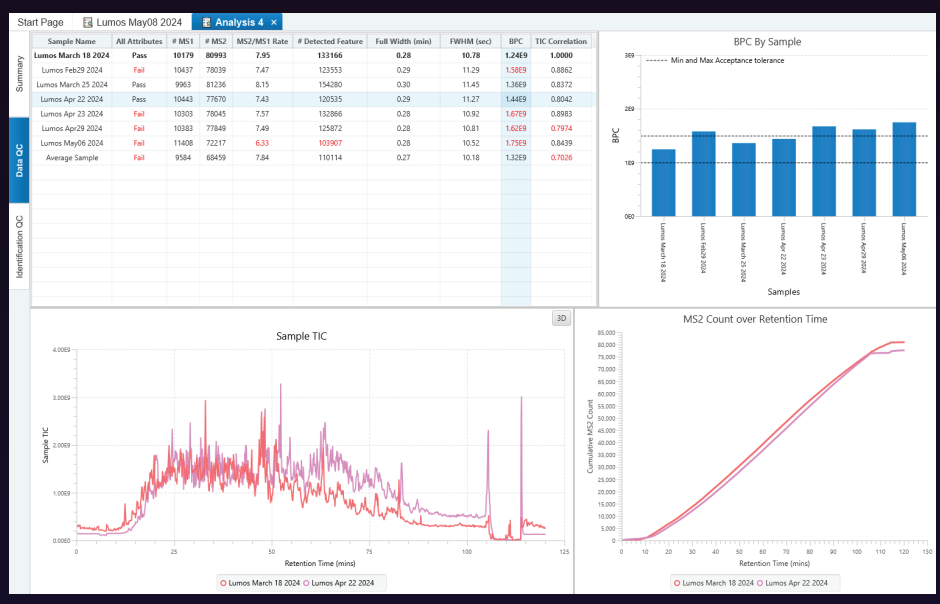


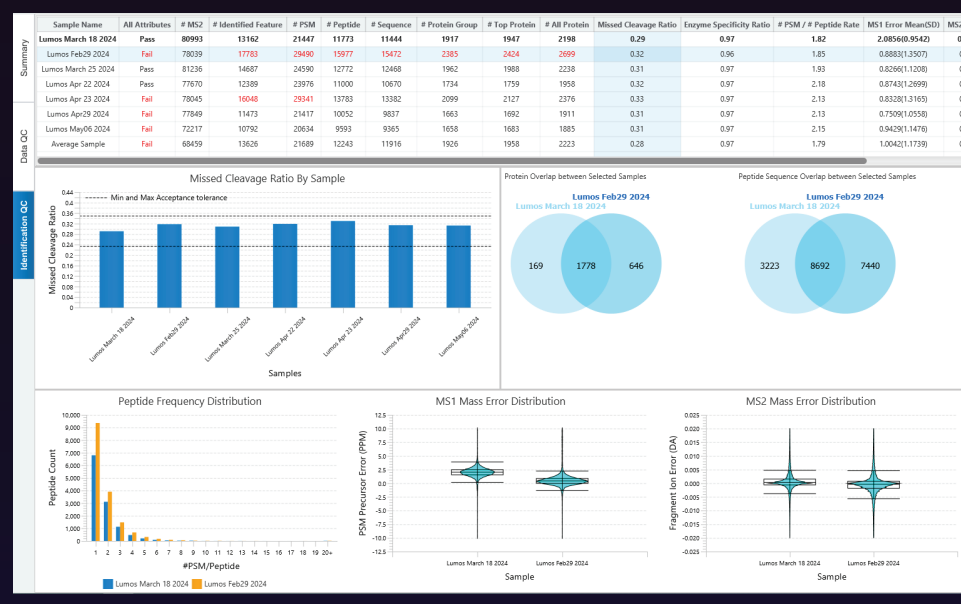
PEAKS® was used to analyze an extract of a HEK cell digest after a PASEF acquisition. The two co-eluting parent ions were separated in the ion mobility dimension, revealing two isobaric peptides differing only in the position of phosphorylation.



Automated Quality Control (QC) Tool

PEAKS® Studio presents a specialized QC tool designed to validate the reproducibility of peptide and protein identification and quantification. This tool delivers detailed QC analysis, presenting complex information in an organized and user-friendly manner, which aids in troubleshooting instrumentation and data processing issues. By seamlessly integrating database searching, quantification, and QC analysis into a single workflow, and consolidating statistical analyses into a comprehensive report, users can freely export data and figures as needed. The entire process is automated, systematic, and customizable.





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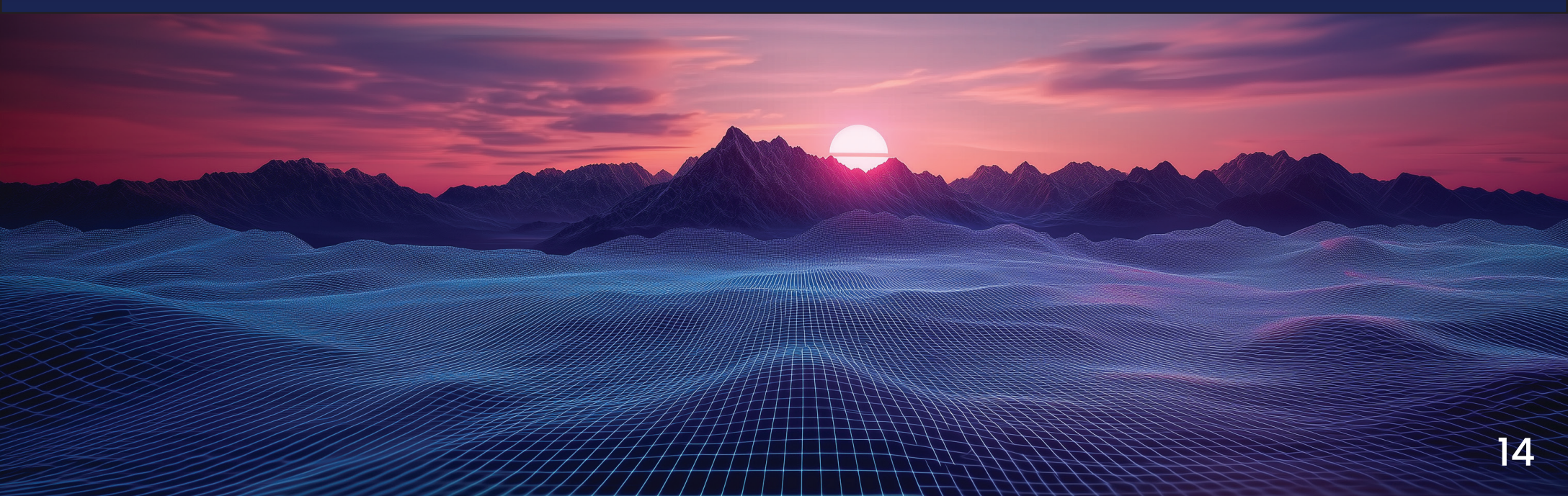
Complete Multi-User Proteomics Solution

PEAKS® AB

Antibody *de novo* Sequencing Software

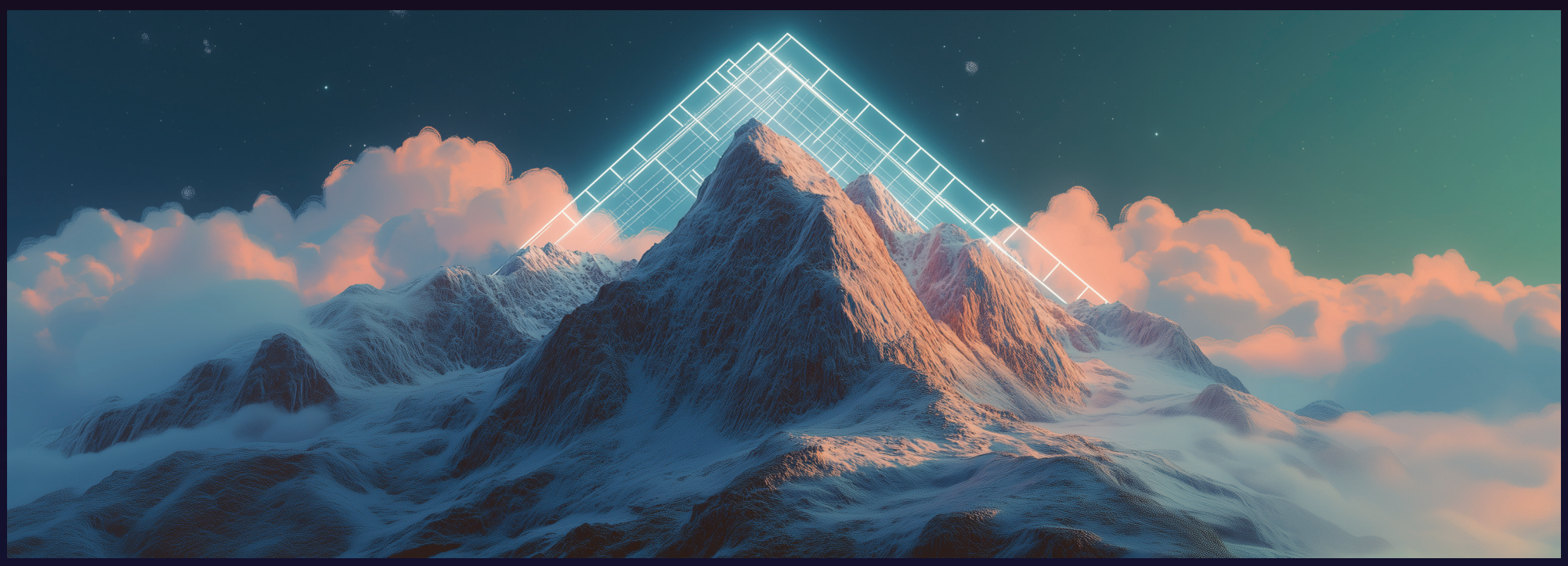
PEAKS® GlycanFinder

A Software Solution for In-Depth Glycoproteomic Analysis



NEXT GENERATION PEAKS® STUDIO 12.5

Next generation PEAKS® Studio with Enhanced speed and stability
Accurate and sensitive identification for both DDA and DIA Analyses
Robust label-free , labelled , and PRM quantification support
AI technology integrated to advance *de novo*, DDA-DB, DIA-DB, and Quant
Automated QC Tool for in-depth analysis from raw data to results



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