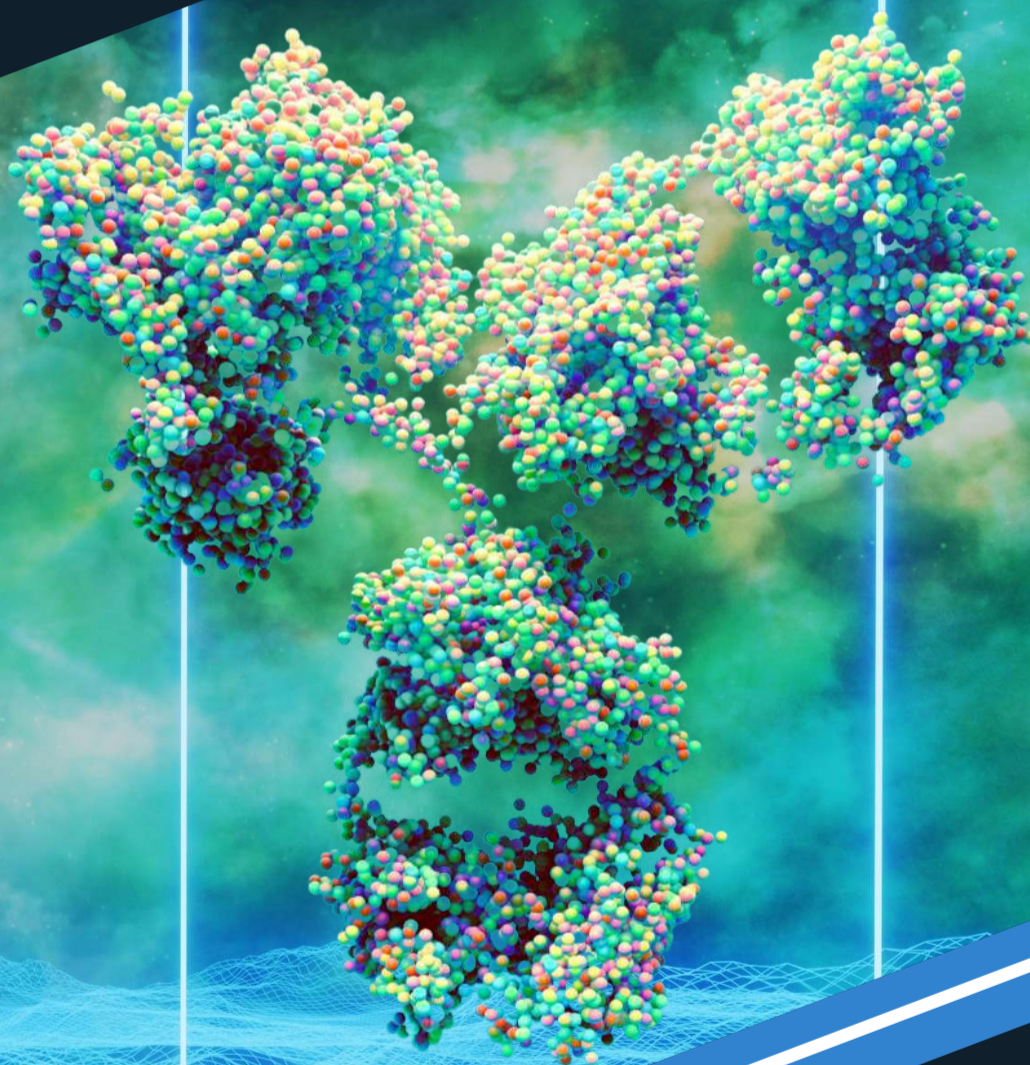




PEAKS[®] AB

Protein *de novo* Sequencing Software



AUTOMATED PROTEIN DE NOVO SEQUENCING WITH INDUSTRY LEADING ACCURACY

COMPREHENSIVE SOLUTION FOR CHARACTERIZING GLYCOSYLATION STATES OF ANTIBODIES

IN-DEPTH IDENTIFICATION AND QUANTIFICATION OF PTMS AND SEQUENCE VARIANTS

ADVANCED DECONVOLUTION ALGORITHM FOR ACCURATE INTACT MASS ANALYSIS



BIOINFORMATICS SOLUTIONS INC.

Bottom-Up MS for

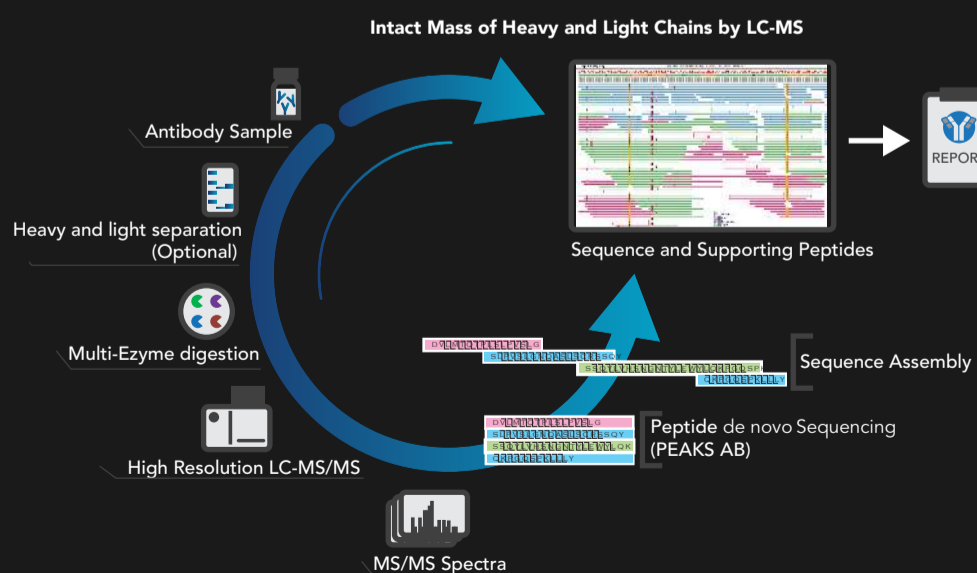
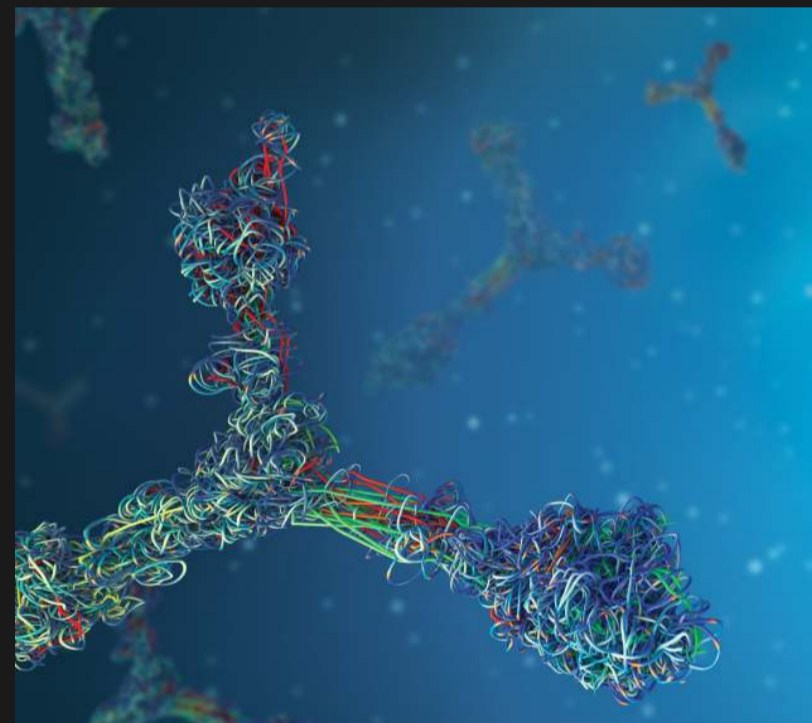
PROTEIN SEQUENCING

PEAKS AB software directly sequences the protein using high-resolution LC-MS/MS datasets from orthogonal enzyme digests. It performs de novo peptide sequencing first, then assembles the confident sequence tags into a complete protein sequence.

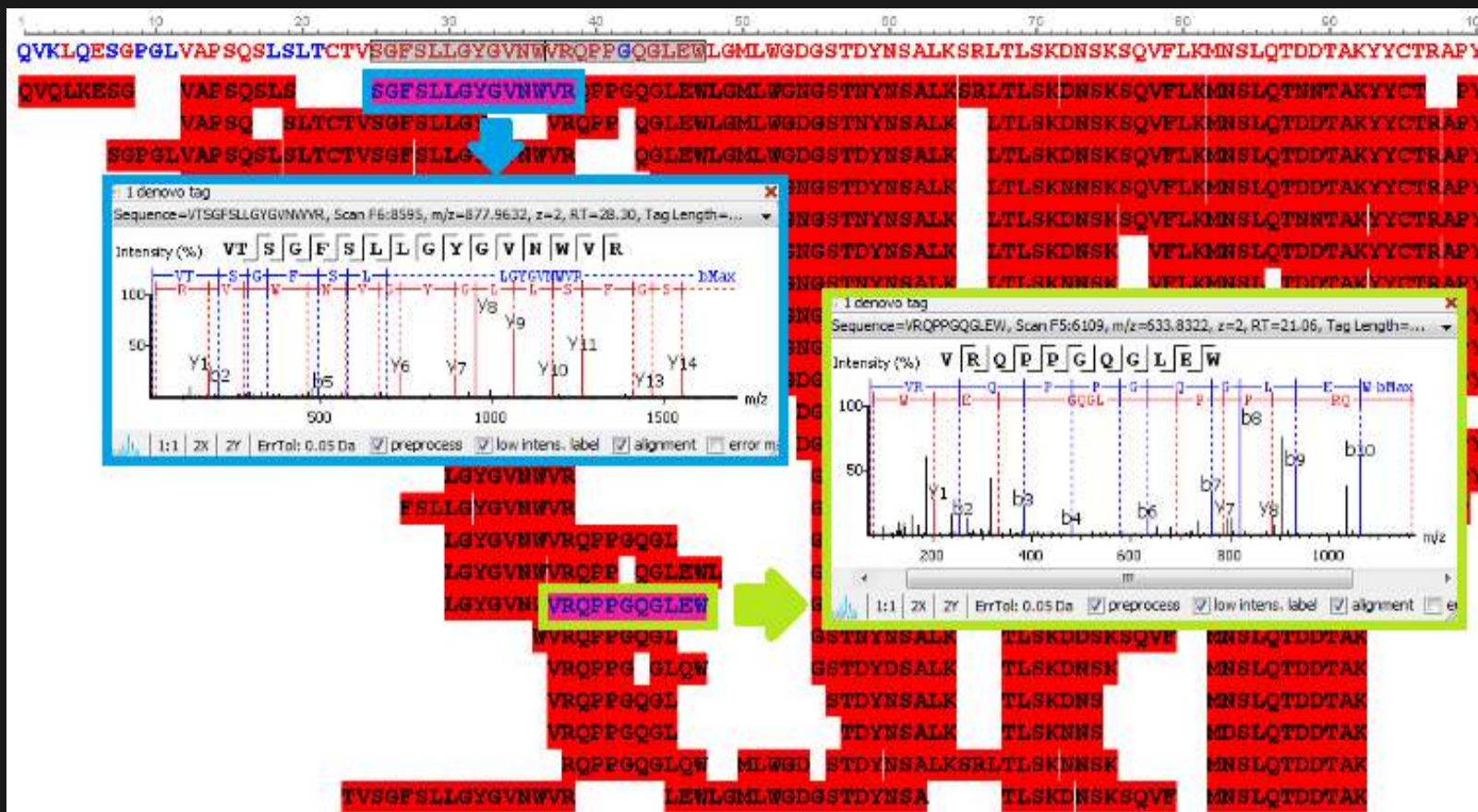
The newest release of PEAKS AB Software, version 3.0, is equipped with multiple tools to guarantee accurate sequencing and protein characterization.

What PEAKS AB 3.0 Provides?

- Intact mass analysis and multi-enzyme LC-MS/MS analysis
- Ile/Leu differentiation by the signature w-ions with EThcD fragmentation
- Peptide de novo sequencing for combined fragmentation (CID/HCD/ETD)
- In-depth glycan profiling
- Sequence assembly of non-antibody proteins
- Customized annotation and report generation
- Vendor-neutral mass spectrometry data analysis including ZenoTOF support



Combine bottom-up and top-down MS with PEAKS AB 3.0 software platform to guarantee accuracy at the amino acid level



Protein de novo Sequencing

PEAKS AB provides a powerful, automated solution for the complete de novo sequencing of proteins from high-resolution LC-MS/MS datasets.

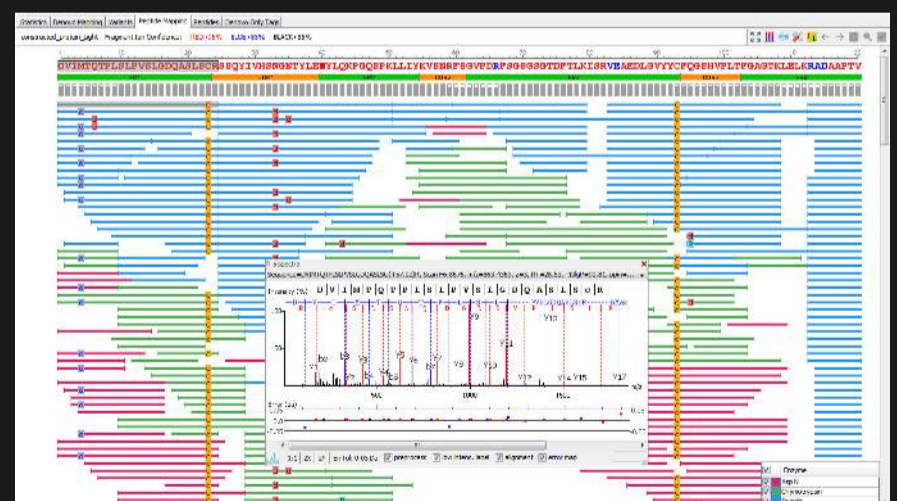
From the raw spectral data, PEAKS AB first performs de novo peptide sequencing, and then assembles confident sequence tags to construct a full protein sequence.

State-of-the-art research tool for sequencing the unknown

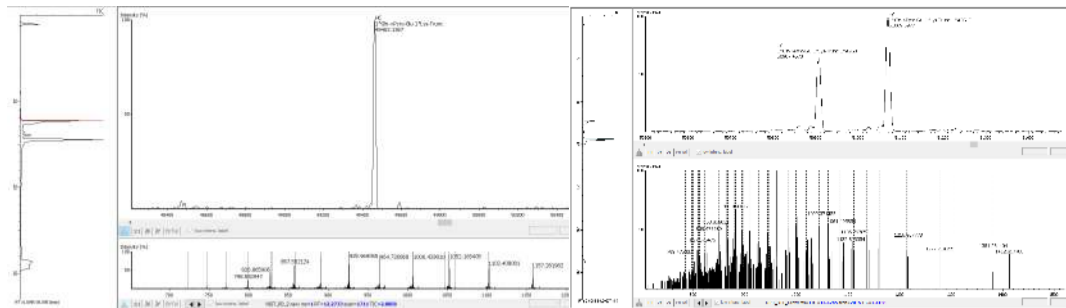
Powerful de novo sequencing and protein assembly algorithms enable more accurate protein sequencing.

Users can benefit from advanced mass spectrometers equipped with multiple fragmentation approaches, including CID, HCD, ETD, EThcD, and EAD.

Confident de novo sequence tags from each spectrum are used to construct the optimal peptide sequence.



Enhanced tools for Protein de novo Sequence Validation

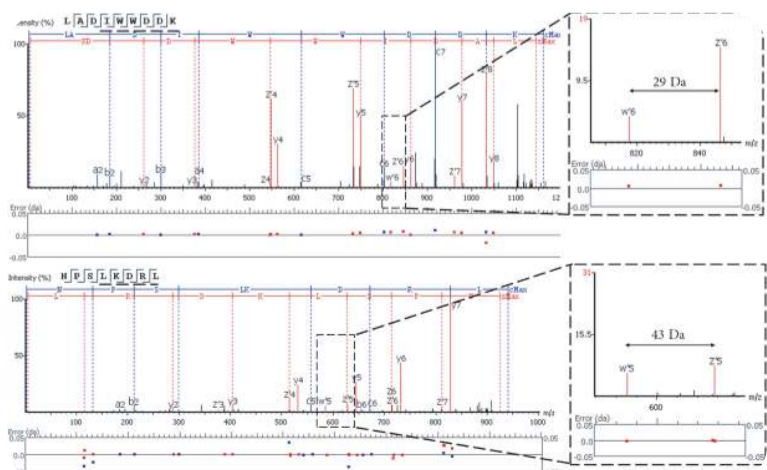


Advanced Intact Mass Analysis

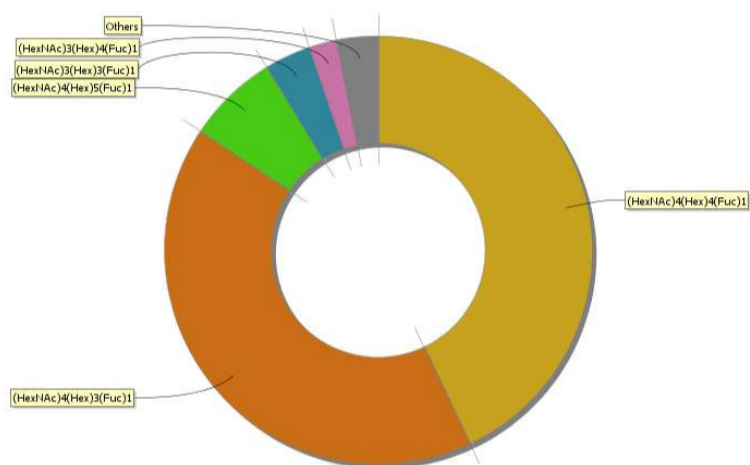
The advanced deconvolution algorithm enabled automated, efficient, and accurate intact mass spectral data analysis. Intact mass measurements of heavy and light chains are performed to validate the assembled sequence and presence of any modifications such as N-terminal pyro-glutamate, heavy chain C-terminal lysine truncation, and N-linked glycosylation.

In-Depth Glycan Profiling

A new feature introduced in PEAKS AB 3.0 is the Glycan Profiling tool. This tool performs in-depth glycan profiling for N-linked sites identified in the heavy and/or light chains of the antibody. In addition to accurate glycopeptides mapping to the assembled antibody sequence, enzyme-based glycan profiling displays the composition and relative abundance of each glycan at a selected glycosylation site. Glycan composition and structure annotation are provided within each glycopeptide spectrum and are based on glycan fragment ions that match to an N-linked glycan database. Accurate localization of the glycan at each N-linked site is achieved by identifying fragment ions of glycan moieties associated with the peptide backbone.



constructed_protein_Heavy_N300_Trypsin



● (HexNAc)4(Hex)4(Fuc)1 ● (HexNAc)4(Hex)3(Fuc)1 ● (HexNAc)4(Hex)5(Fuc)1 ● (HexNAc)3(Hex)3(Fuc)1 ● (HexNAc)3(Hex)4(Fuc)1 ● Others

		Glycan moiety	Area (%) ↓	#Feature
1	h	(HexNAc)4(Hex)4(Fuc)1	42.93%	8
2	h	(HexNAc)4(Hex)3(Fuc)1	41.47%	5
3	h	(HexNAc)4(Hex)5(Fuc)1	6.88%	3
4	h	(HexNAc)3(Hex)3(Fuc)1	3.49%	3
5	h	(HexNAc)3(Hex)4(Fuc)1	2.07%	3
6	h	(HexNAc)5(Hex)3	0.84%	2
7	h	(HexNAc)5(Hex)3(Fuc)1	0.63%	2
8	h	(HexNAc)3(Hex)5(Fuc)1	0.52%	2
9	h	(HexNAc)5(Hex)4	0.46%	2
10	h	(HexNAc)2(Hex)3(Fuc)1	0.25%	1
11	h	(HexNAc)3(Hex)3	0.2%	1
12	h	(HexNAc)2(Hex)5	0.13%	1
13	h	(HexNAc)3(Hex)4	0.08%	1
14	h	(HexNAc)7(Hex)5	0.05%	1
15	h	(HexNAc)3(Hex)6	0.02%	1
16	h	(HexNAc)5(Hex)4(Fuc)1	0.0%	0

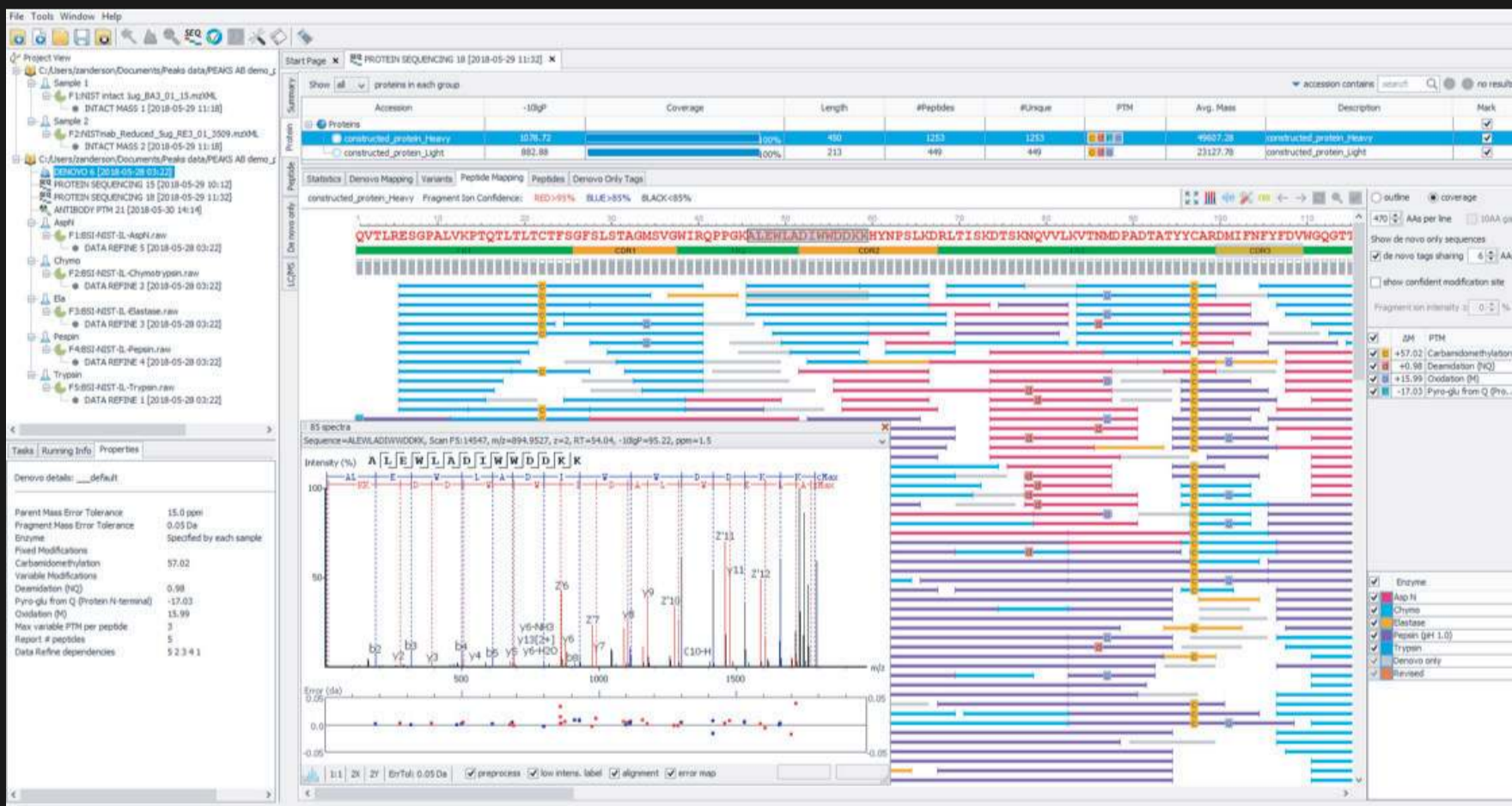
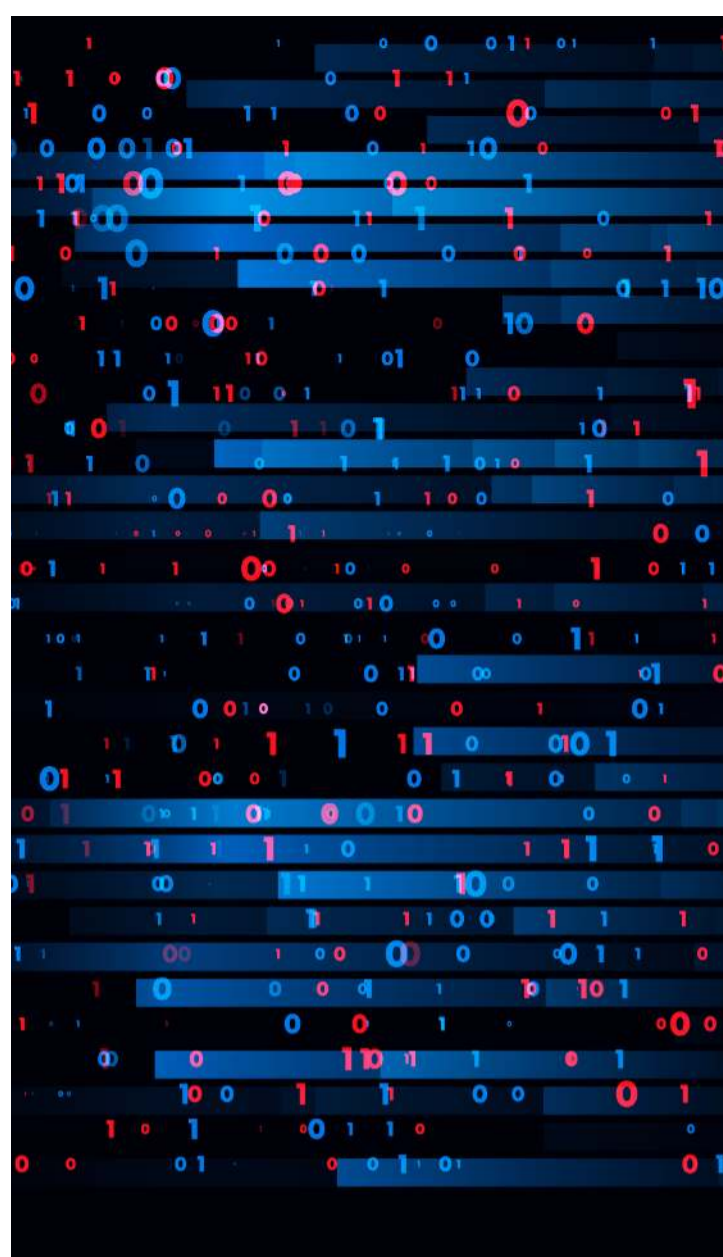
Enhanced Ile/Leu Differentiation

Electron dissociated fragmentation methods produces signature w-ions for isoleucine and leucine from the characteristic loss of C₂H₅ (-29 Da) or C₃H₇ (-43 Da), respectively.

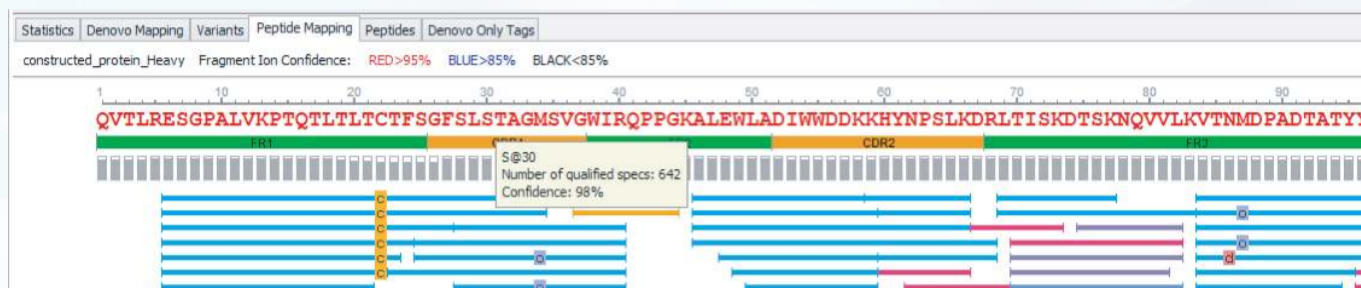
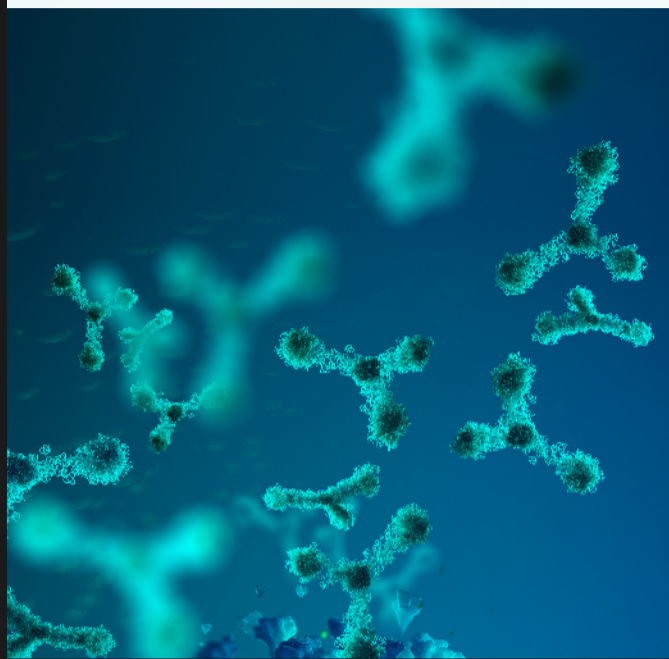
PEAKS AB 3.0 uses this information, plus enzyme digestion specificity and homolog database analysis in the improved Ile/Leu discrimination feature.

PEAKS AB 3.0 provides a convenient workflow for protein sequencing

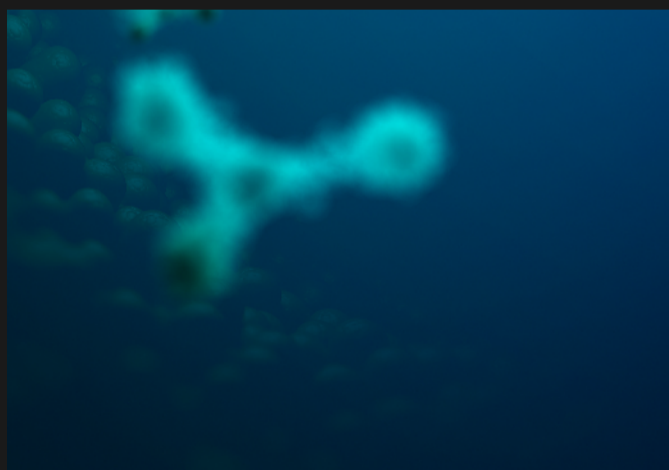
The protein sequence of a target protein encodes critical information for its structure and function. The superior result validation of PEAKS AB is designed to be user friendly, and ultimately reduces the manual work of strategically organizing the sequencing results. Accessing the results visually provides additional advantages and allows researchers to examine their sequencing results with precision. The user can expect visualization that PEAKS is known for but with a new look and optimised workflows to streamline your data analysis.



Robust analytical tools for comprehensive ANTIBODY CHARACTERIZATION

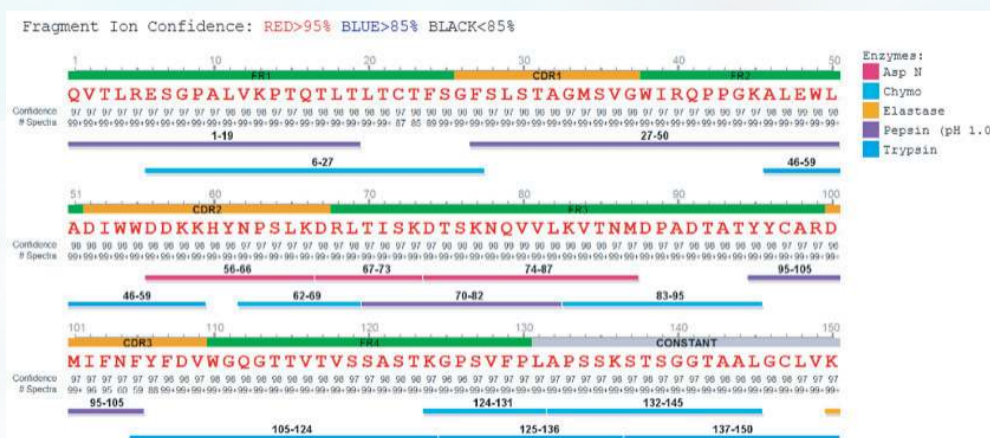
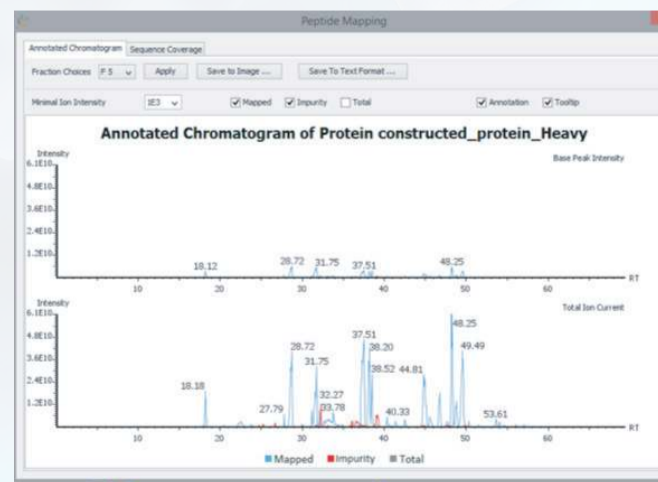


With the Peptide Mapping function, PEAKS AB can compare annotated chromatograms between different samples. Possible sequence variants will be highlighted to facilitate the product quality control



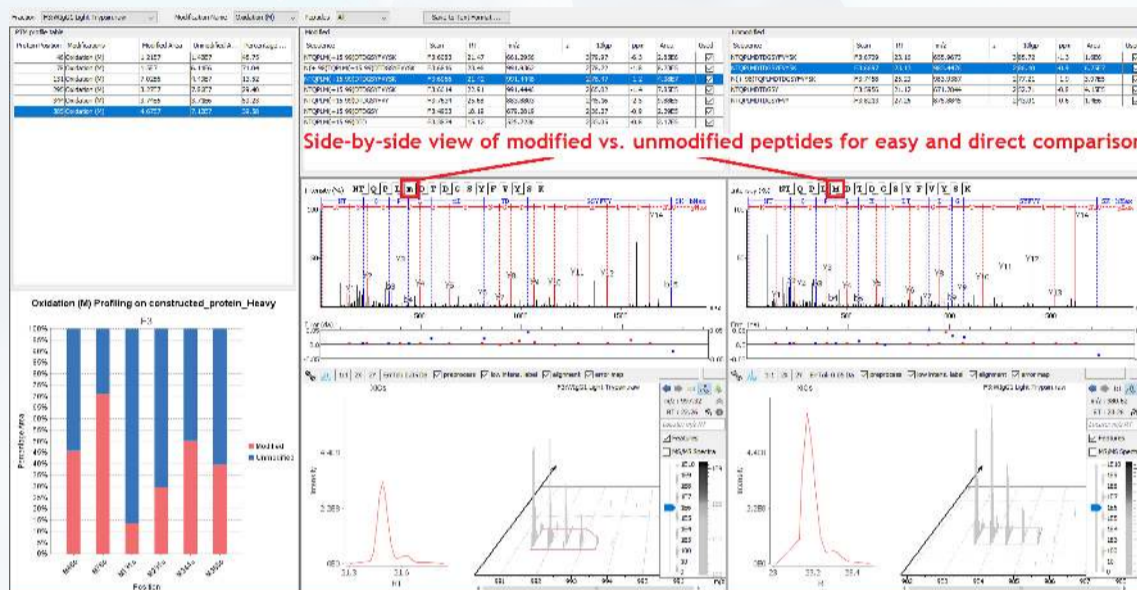
Comprehensive amino acid scoring

With PEAKS AB, users are given two levels of scoring to fully evaluate the confidence of the constructed antibody sequence. PEAKS AB provides fragment ion confidence and precursor ion coverage for enhanced sequencing accuracy, and supplies the tools to assess each amino acid assignment.



PTM and Variant Analysis

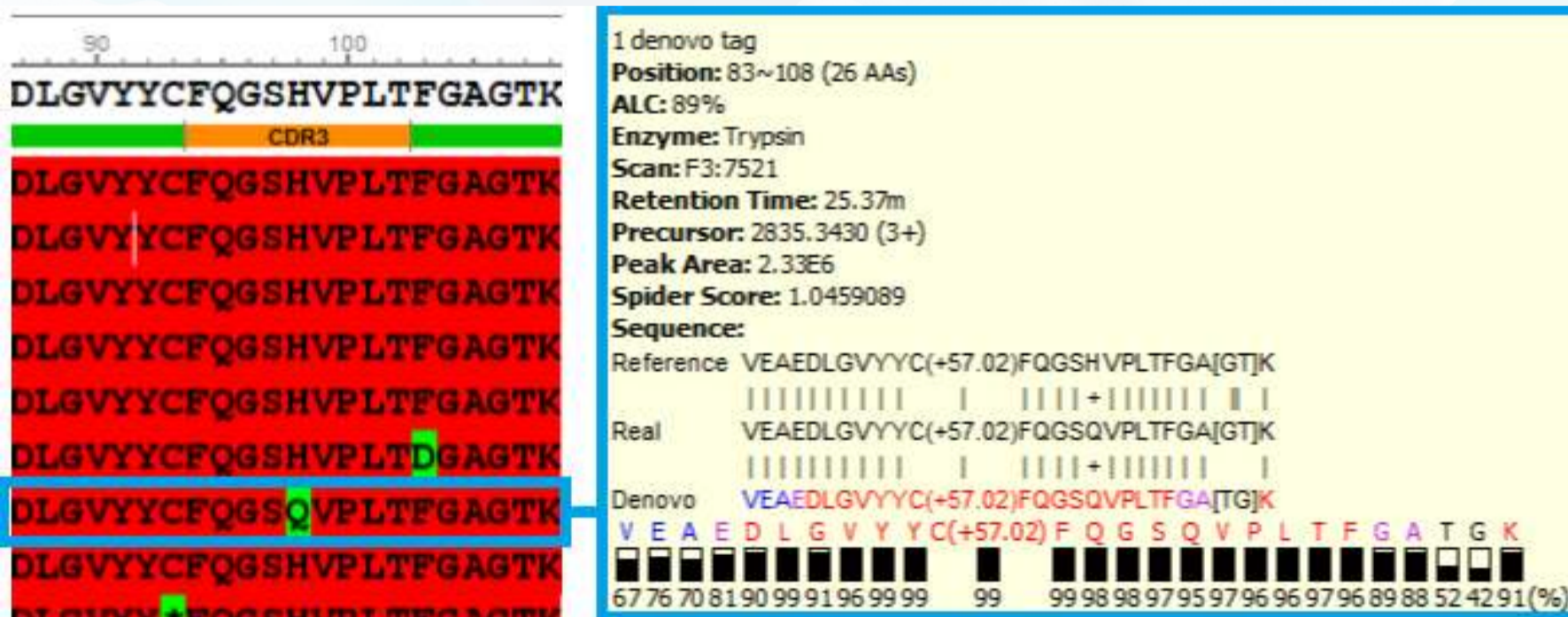
Achieve thorough quantitative analyses for post-translational modifications (PTMs) using PEAKS AB PTM Profiling tool. The PTM Profiling tool is presented through a single interactive interface which displays all quantitative information regarding identified PTMs. Easily compare the supporting peptide-spectrum matches (PSMs), precursor profiles, peptide features, and the ratios between the modified and unmodified peptides within each sample.



For each sequence position with modifications, the modified and native peptide forms, along with their corresponding chromatograms, are listed for quantitative comparison.

Sequence Variant View

The Sequence Variant View highlights amino acid substitutions, deletions, or insertions, which may result from errors in protein translation, or from contamination of other antibodies having peptide sequence homology.



Protein de novo sequencing and glycan profiling software

Protein de novo Sequencing

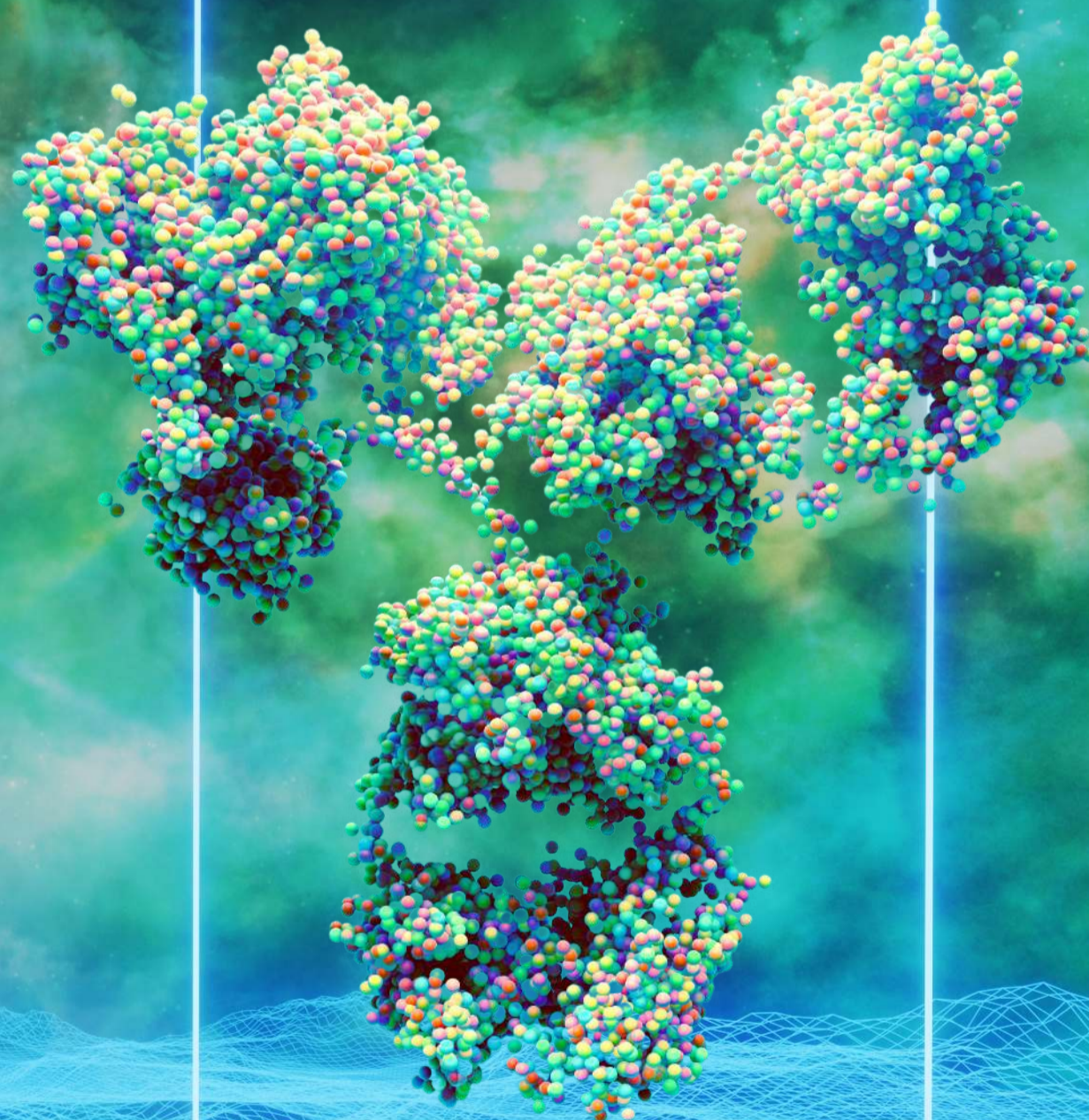
PEAKS AB Software automatically sequences a protein using LC-MS/MS data sets from orthogonal enzyme digests. It performs de novo peptide sequencing first, and assembles the confident sequences tags into a full length protein sequence.

In-depth Glycan Profiling

A glycopeptide-based approach is utilized to profile glycans in your sample using LC-MS/MS. This new tool performs in-depth glycan profiling for N-linked sites identified in the heavy and light chains of the antibody.

PTM and Variant Quantification

Achieve thorough quantitative analyses for post-translational modifications (PTMs) using PEAKS AB PTM Profiling tool. For each sequence position with modifications, the modified and native peptide forms, along with their chromatogram are listed for quantitative viewing.



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