PEAKS® GlycanFinder

A Software solution for in-depth Glycoproteomic analysis

BOTH N-LINKED AND O-LINKED GLYCAN PROFILING WITH STRUCTURAL RESOLUTION

PANORAMIC PROFILING OF GLYCOSYLATION SITES WITH MULTIPLE ENZYME DIGESTS

GLYCOPEPTIDE QUANTITATIVE ANALYSIS WITH LABEL-FREE AND LABELLING METHODS

GLYCAN DE NOVO SEQUENCING FOR FINDING UNKNOWN GLYCANS

INTUITIVE GUI FOR VISUALIZATION, EASY VALIDATION AND REPORTING

BIOINFORMATICS SOLUTIONS INC.

New Era of

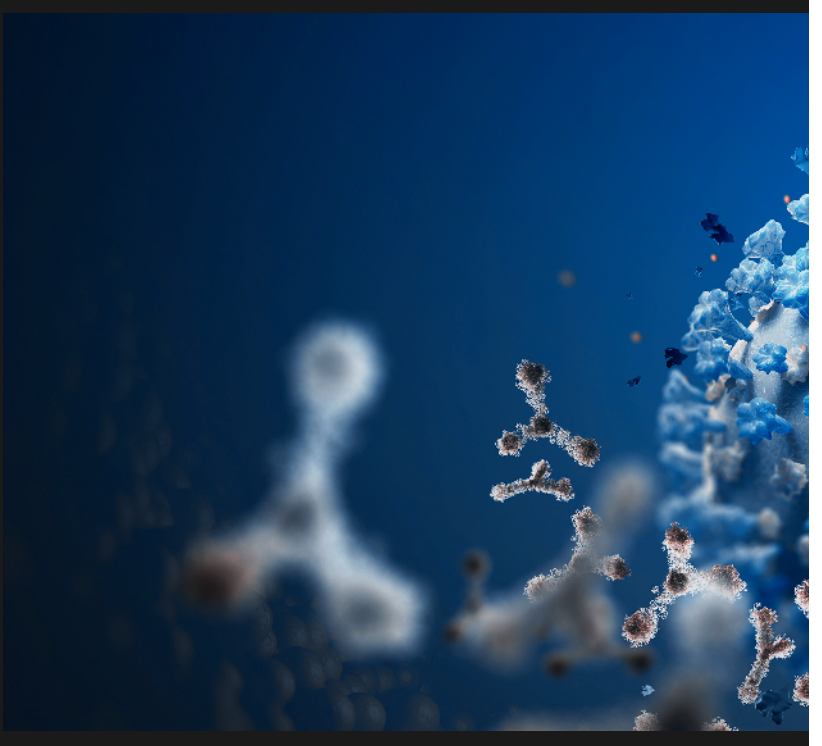
Glycoproteomic Analysis

PEAKS GlycanFinder is a comprehensive software for in-depth glycoproteomic analysis with glycan structural resolution.

This standalone software solution utilises a glycopeptide-based approach to profile the glycoproteins from LC-MS/MS data and harnesses deep learning-enabled algorithms to resolve the ambiguity of glycosylation sites and glycan structures. PEAKS GlycanFinder integrates glycan database search and glycan *de novo* sequencing to facilitate the identification and quantification of N- and O-linked glycans.

PEAKS GlycanFinder Highlights:

- Both N-linked and O-linked glycan identification with structural resolution.
- In-depth glycan site profiling with multiple enzyme digests.
- Glycopeptide quantitative analysis with label free and labelling methods.
- Glycan *de novo* sequencing for finding unknown glycans.
- Intuitive Graphical User Interface (GUI) for visualization, easy validation and reporting.
- Support of Orbitrap, timsTOF and ZenoTOF data.

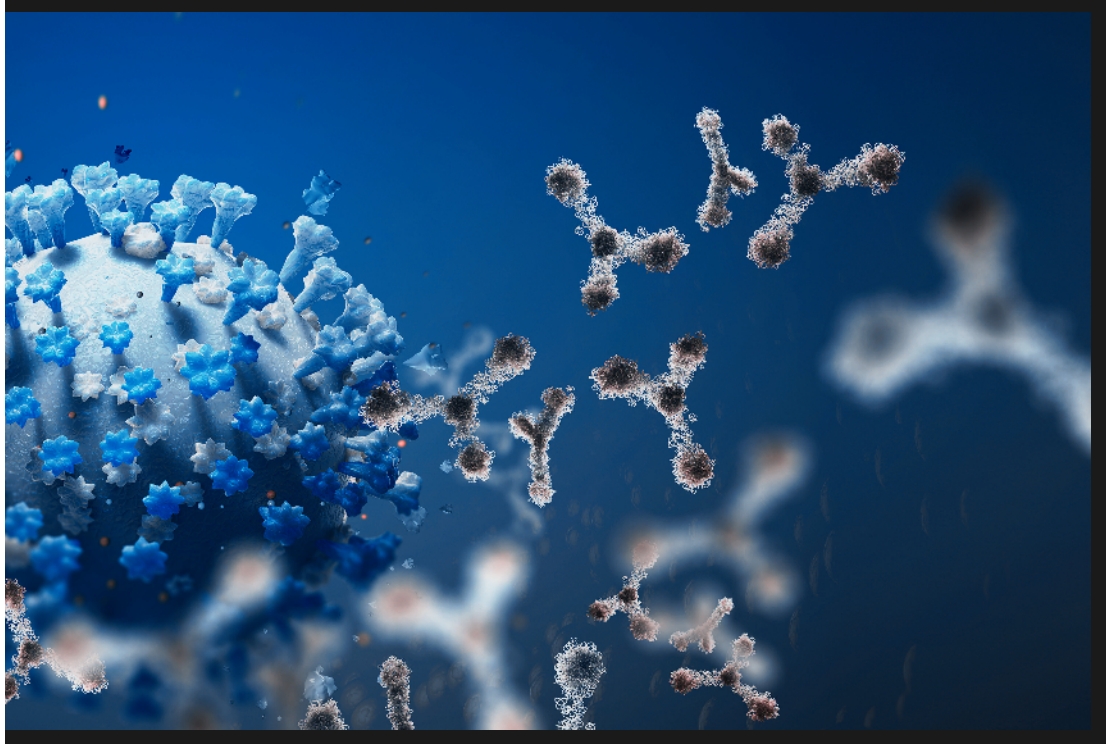


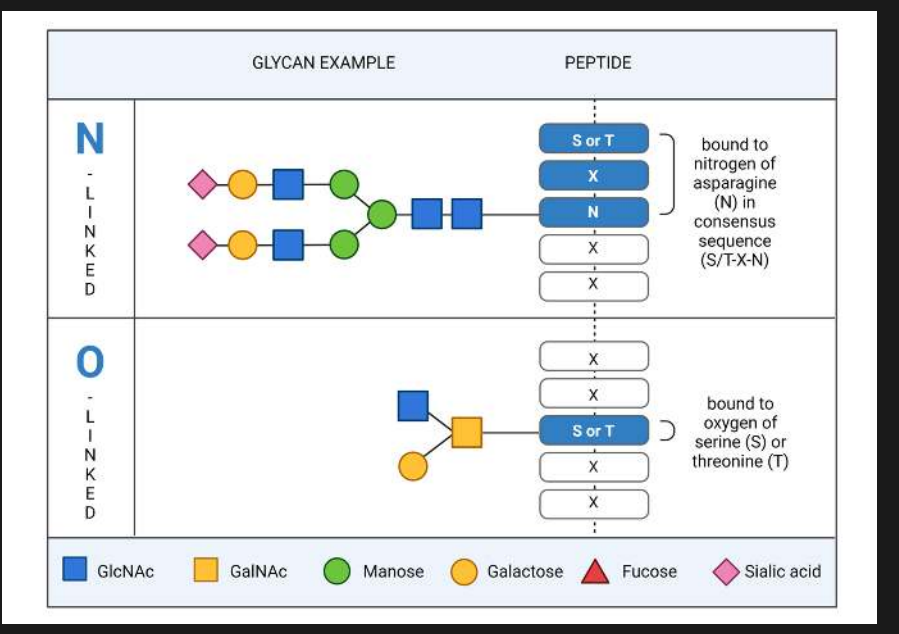
Deep learning-based algorithms are developed to resolve the ambiguity of glycosylation sites and glycan structures

Protein Glycosylation

Protein glycosylation, the attachment of sugar moieties or glycans to organic molecules, is one of the most important post-translational modifications that plays a critical function in a wide range of biological processes including protein's structure, stability, and function.

Glycans are a heterogenous group of carbohydrate-based structures that can be linear or branched and are attached to the side chain of amino acids within glycoproteins. The glycans in glycoproteins can be categorised as being N-linked, glycans bound to nitrogen atom of asparagine (N), or O-linked, glycans bound to the oxygen of serine (S) or threonine (T) side chains.



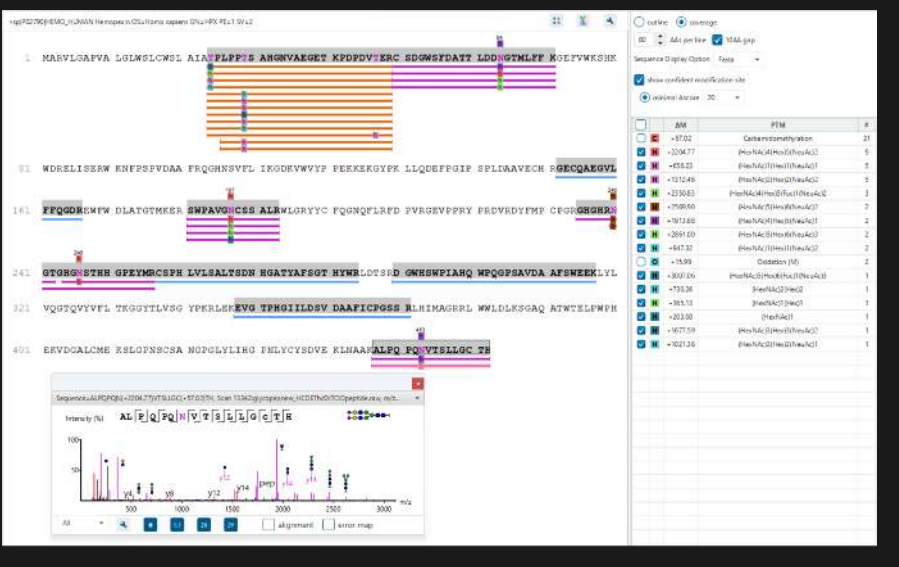


Glycoproteomics and Mass Spectrometry

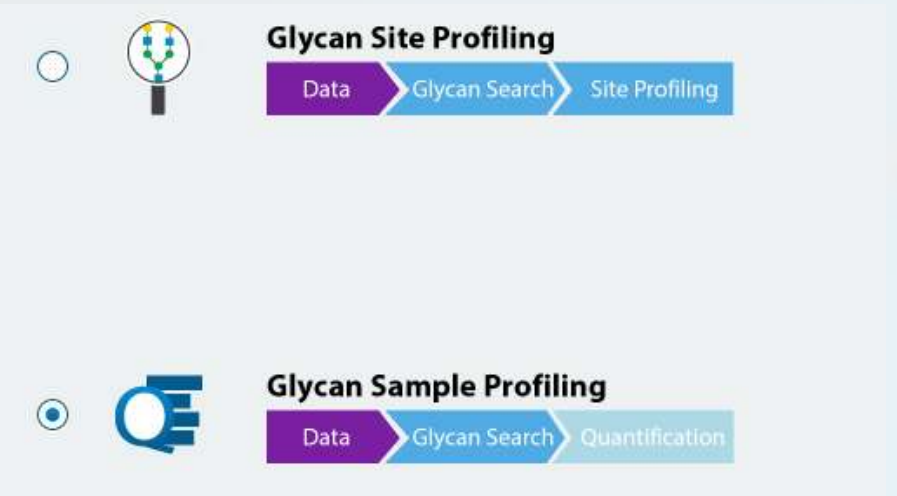
Glycoproteomics involves identifying glycans and the associated glycosylation sites within proteins across the proteome of a given cell or tissue. Fragmentation data from MS/MS spectra are used to identify glycosylation sites and the attached N- or O-linked glycan structures. In the past, LC-MS/MS-based glycoproteomics has been challenged by the super heterogeneity that there may be multiple glycosylation sites per peptide and multiple structures with the same glycan composition.

PEAKS GlycanFinder: Advancing our understanding of the glycoproteome

PEAKS GlycanFinder was designed to handle the challenges of mass spectrometry-based glycoproteomics. Consensus results from all peptide spectrum matches (PSMs) are used to determine glycosylation sites. With multiple enzyme digestion, PEAKS GlycanFinder provides very accurate profiling of glycosylation sites. In cases where multiple glycan candidates match a given glycopeptide spectrum, S-Score is assigned to each candidate for structural resolution. In addition, glycan *de novo* sequencing alleviates the limitations of the incompleteness of the glycan database.



Advanced software solution for in-depth glycoproteomic analysis

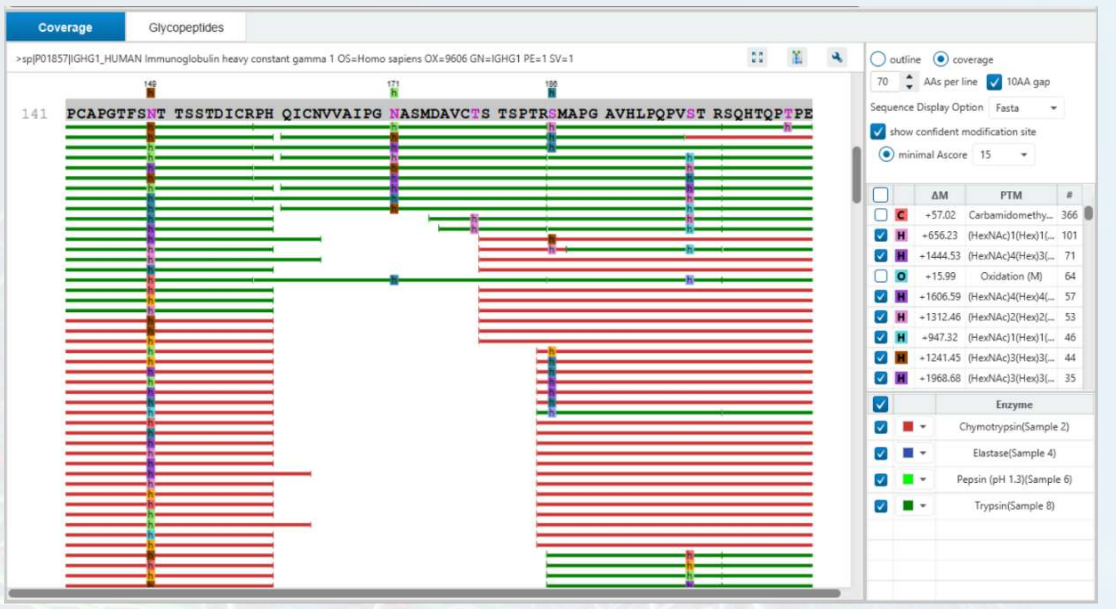


Multi-Level In-Depth Glycan Profiling

PEAKS GlycanFinder provides two kinds of workflows to analyse glycoproteomics. There are identification and quantification workflows available including, Glycan Site Profiling and Glycan Sample Profiling.

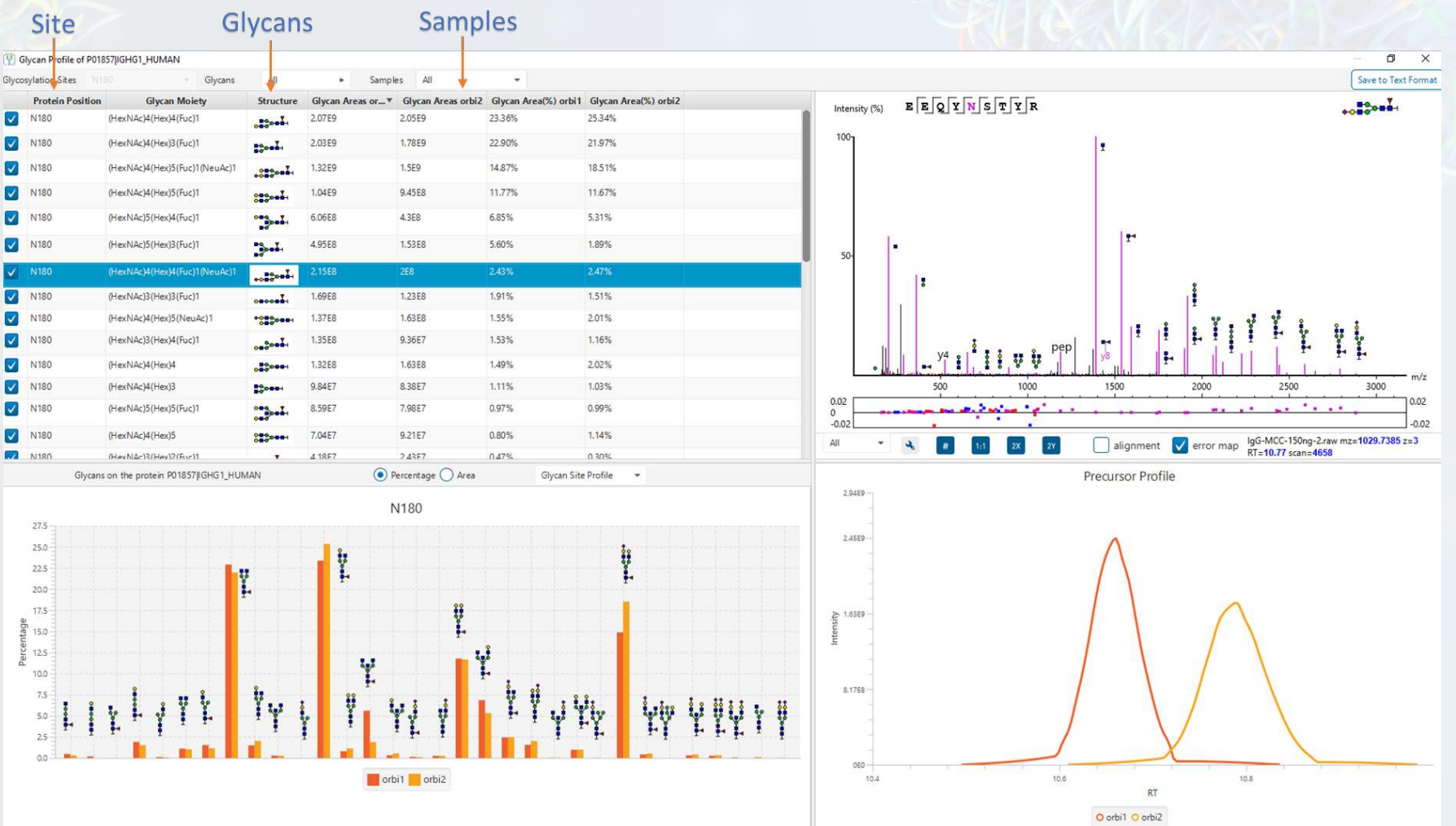
Site Profiling Workflow

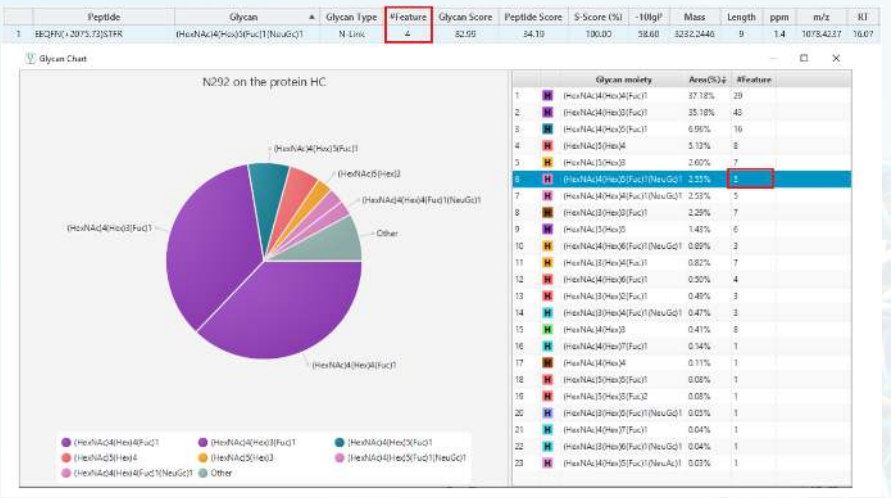
Multiple enzyme digests reveal the details of glycan profiling in each glycosylation site. For each site, PEAKS GlycanFinder will 1) determine glycosylation sites with the consensus identification of glycopeptides from all enzymes; 2) present glycan profiling of each site with best suitable enzyme.



Sample Profiling Workflow

Using sample profiling workflow obtains positional profiling of a protein and compares glycopeptide abundances across samples by label-free and labelled quantification.



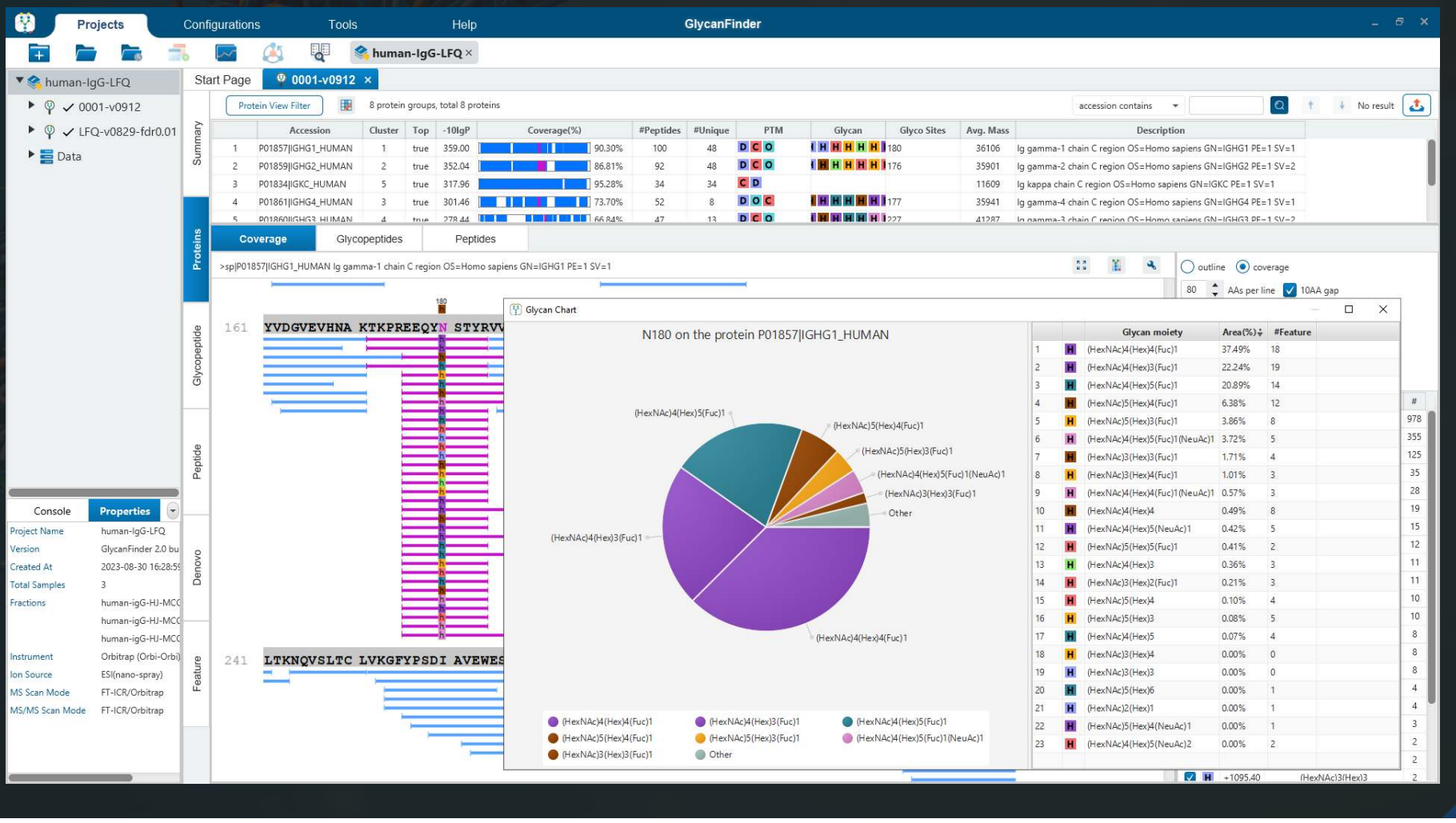


Charge Lookup

A peptide often produces several precursors with different charges, and not all the precursors could be identified. Normally, a peptide area is the sum of all identified feature areas. This will affect glycan profiling based on glycopeptide feature areas. To calculate the peptide feature area more accurately, a charge lookup is applied to find the precursors of the same peptide without identification. Then, the sum of all precursor feature areas is used for glycan profiling.

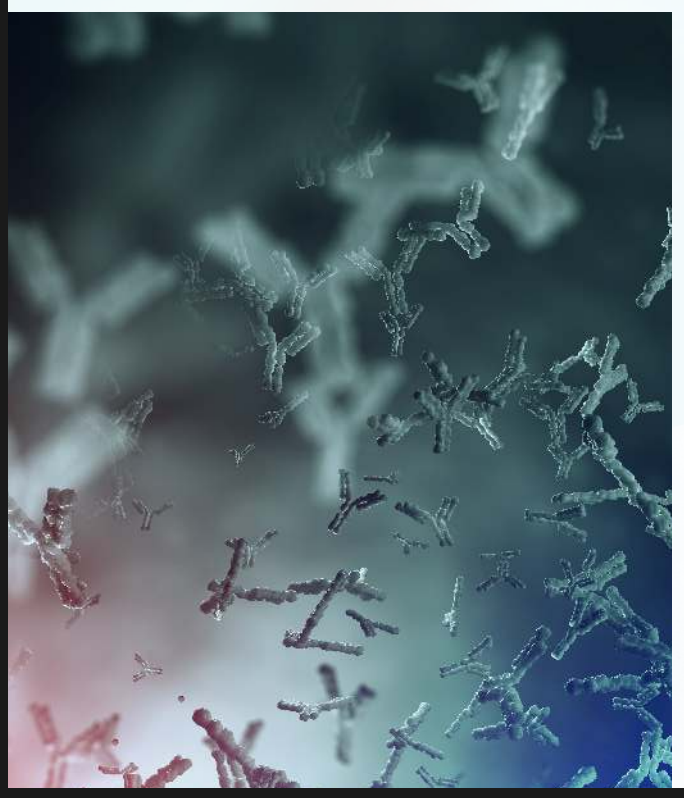
Interactive Protein View

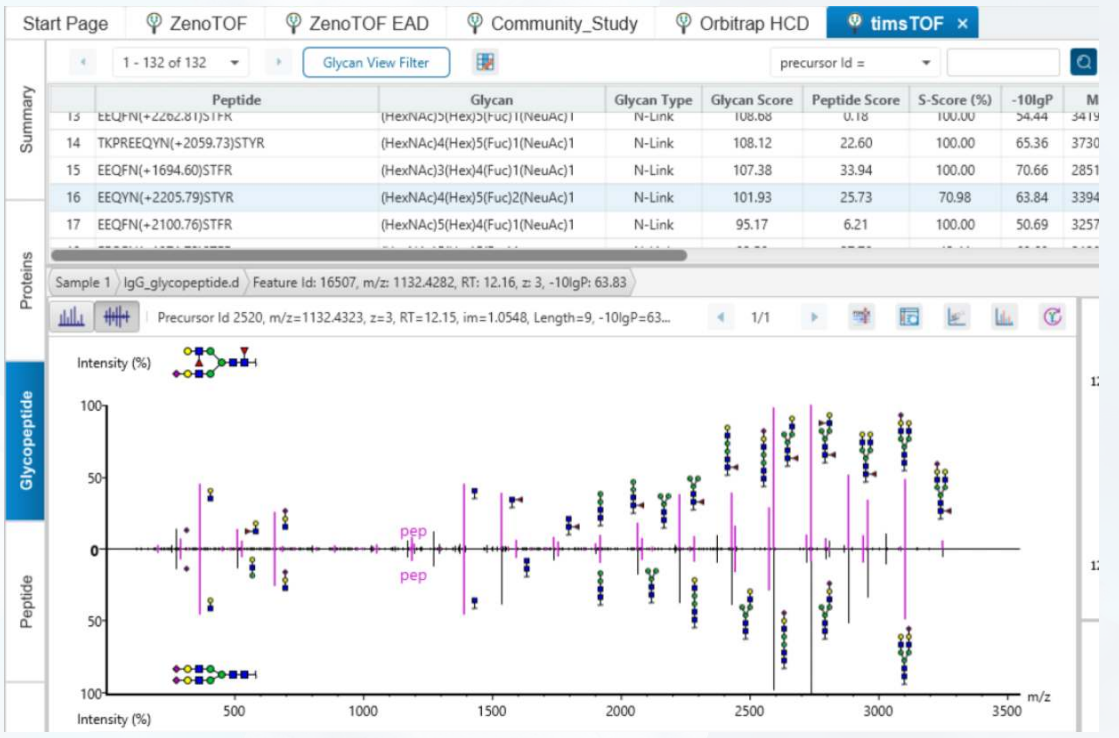
The Protein View presents proteins identified across complex biological samples. For each protein, the sequence coverage view displays the peptide mapping to each protein and is interactive so the user can view each peptide spectrum. Simply by clicking on a protein Glycosylation site (N in purple) a Glycan chart with distribution of glycans in a table format and pie chart will be displayed.



Specialized software tool dedicated to

PUSH NEW BOUNDARIES IN THE FIELD OF GLYCOPROTEOMICS





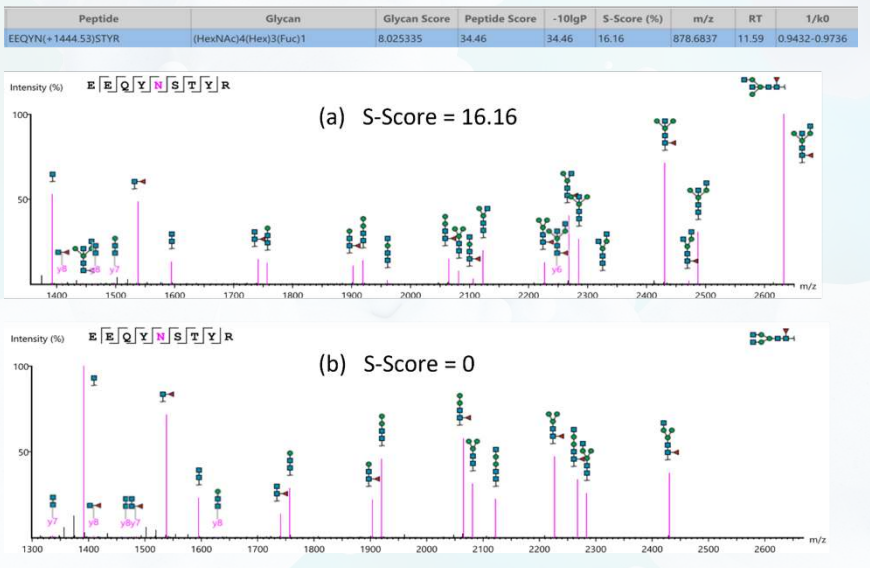
Glycopeptide View

The Peptide View provides a list of identified glycopeptides and critical information to assess each identification. The spectrum annotation mirror plot view can be used to validate the glycan structure.

Intuitive Graphical User Interface (GUI) strategically designed to advance glycoproteomic data analysis from identification and quantification to glycan structure validation

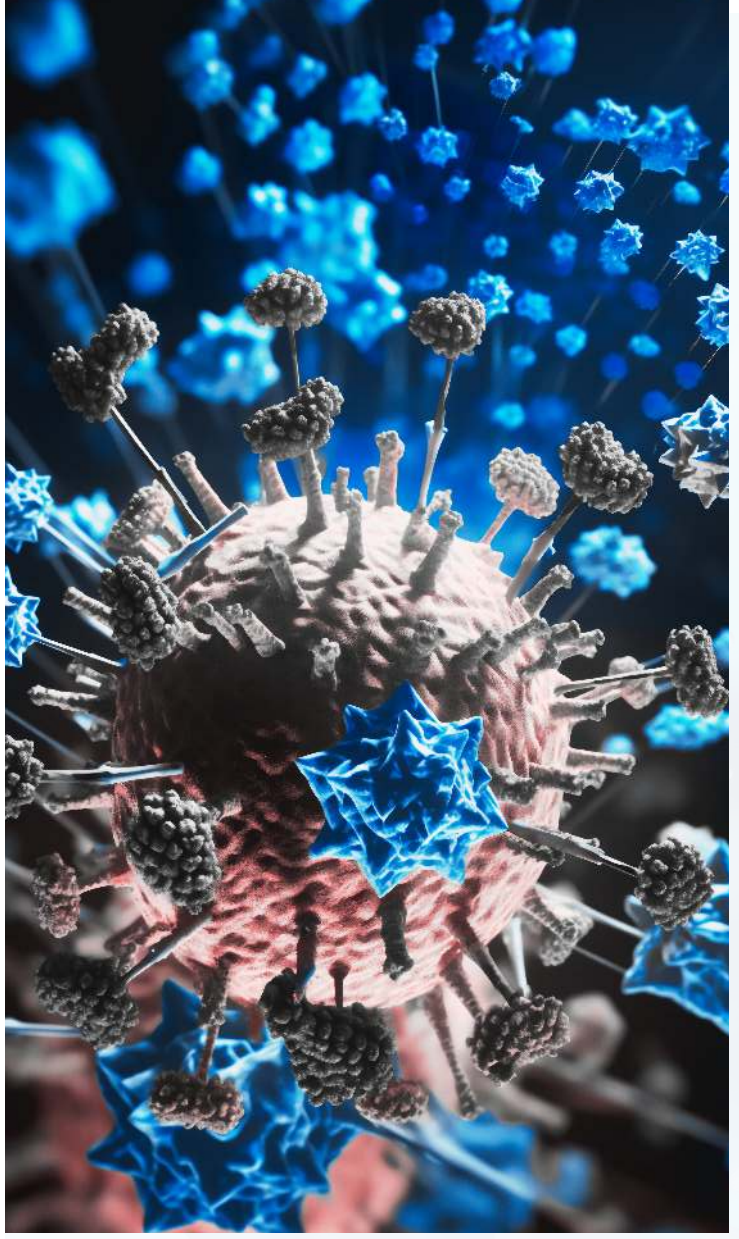
Glycosylation Site-Specific Accuracy (A-Score)

To accurately identify the glycosylation site at the MS/MS level A-score is used. An A-score calculates an ambiguity score as -10×log10(P). The p value indicates the likelihood that the glycan site is assigned by chance. Thus, a higher A-score indicates more confidence in the glycan site assignment within a peptide.



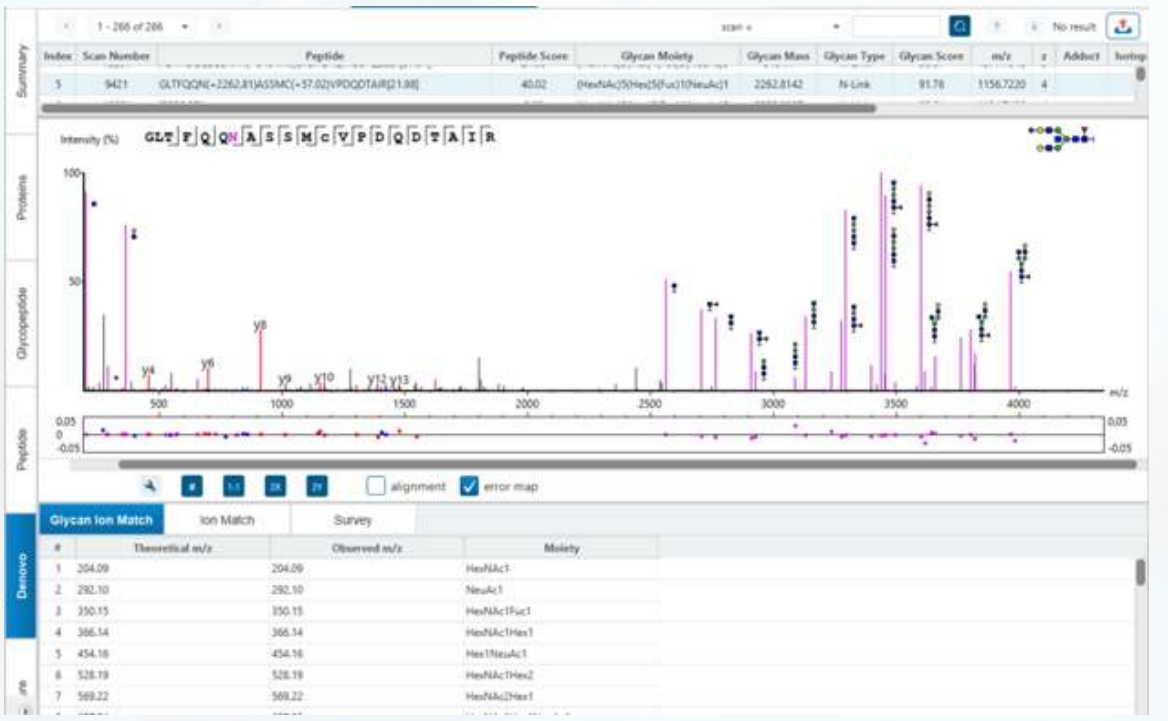
Glycan Structure Specificity Matching (S-Score)

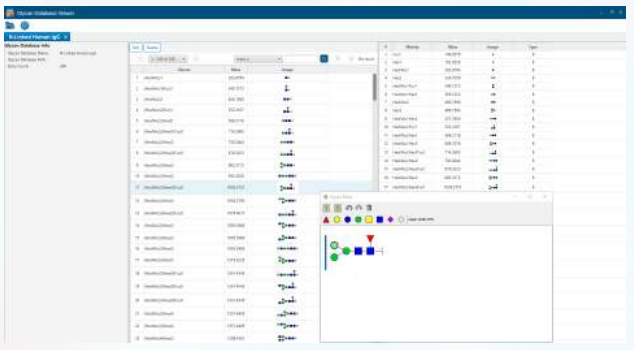
The associated glycan on the glycopeptide is given a S-score (%), which indicates the confidence in the matched glycan structure in the glycan database. For glycan candidates in the database with the same composition, the candidate is sorted by matched glycan Y-ion count. S-Score = (most Y-ion count - 2nd most Y-ion count)/(most Y-ion count). The higher the score the better. 100% indicates only 1 result, and it is the best match. 0% indicates that the top1 and top2 results are very similar, and we cannot confidently say the result is the best match.



Glycan de novo

When the glycan database is incomplete, or there are some unexpected modifications, PEAKS GlycanFinder de novo algorithm will provide extra glycopeptide identifications.



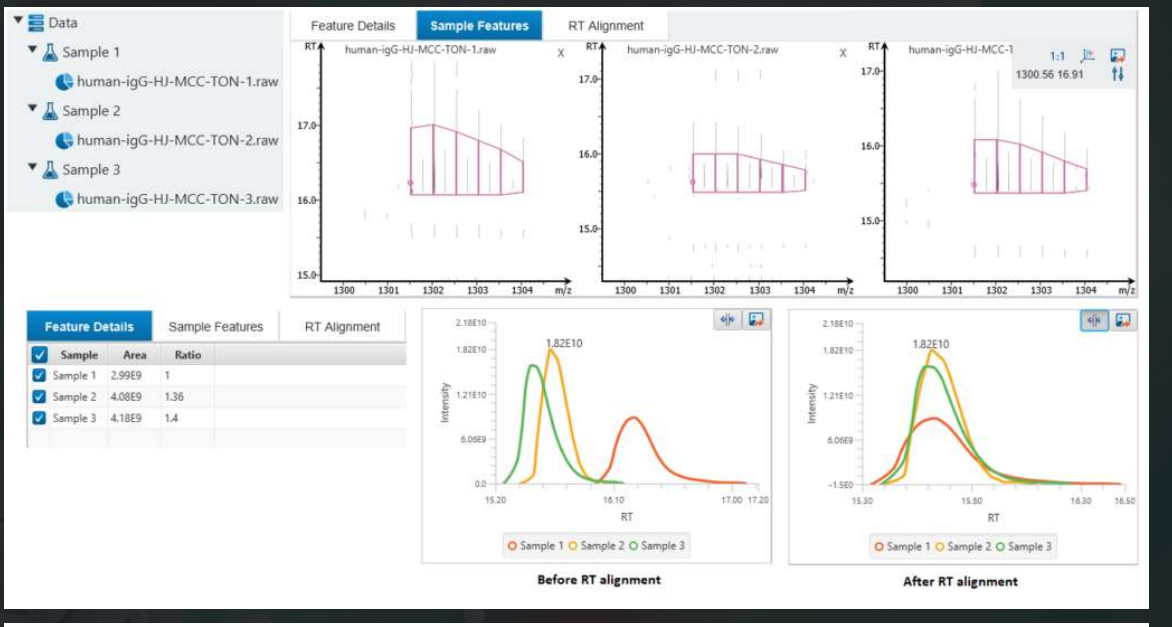


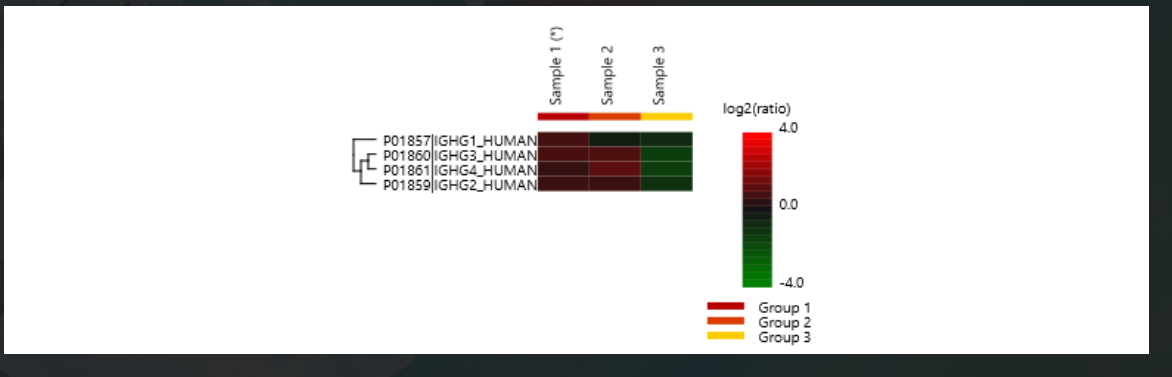
Glycan Database Editor

Glycan database editor tool helps to build your own glycan database, users can edit and modify the glycan database through a drawing board, and easily configure it into the software. It also provides the fragment ion information of glycans.

Glycoprotemics Quantification with Label Free (LFQ) and Labelled Methods

It is essential to know the change of the glycosylation levels across the glycoproteome, as it helps us to understand the biological processing regulated by glycoproteins. PEAKS GlycanFinder currently supports label free quantification and labelled quantification methods including user-defined and commercial labels (i.e. iTRAQ and TMT) .





COMPREHENSIVE SOFTWARE FOR IN-DEPTH GLYCOPROTEOMIC ANALYSIS

In-depth glycoproteomic analysis with glycan structural resolution

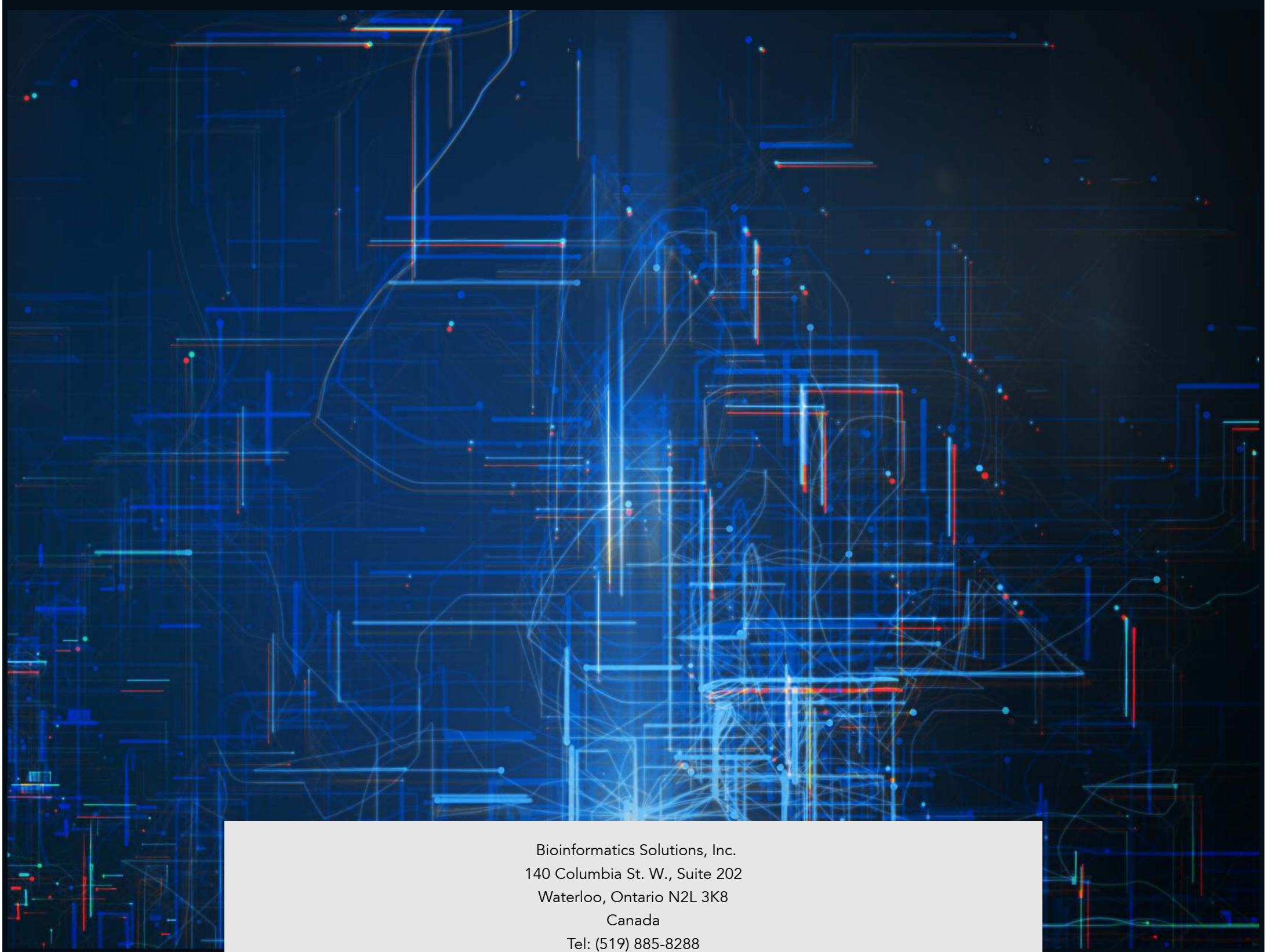
PEAKS GlycanFinder integrates glycan database search and glycan de novo sequencing to facilitate the identification and quantification of both, N- and O-linked glycans. Deep learning-based technologies are harnessed to resolve the ambiguity of glycosylation sites and glycan structures.

Panoramic profiling of glycosylation sites with multiple enzyme digests

PEAKS GlycanFinder was designed to handle challenges of glycan microheterogeneity. With multiple enzyme digestion, PEAKS GlycanFinder provides very accurate profiling of glycosylation sites. Consensus results from all peptide spectrum matches (PSMs) are used to determine glycosylation sites.

Superior Glycoproteomics Quantification with labelled and label-free support

Achieve thorough quantitative analyses for glycosylation levels across glycoproteomes using PEAKS GlycanFinder. With labelled and label-free quantification support, essential quantitative information can be obtained to further our understanding of biological processes regulated by glycoproteins.



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