

Mass spectrometry

Proteome Discoverer 3.0 software with the CHIMERYs intelligent search algorithm

Current generation proteomics data analysis tools are unable to fully interpret data generated by Thermo Scientific™ Orbitrap™ mass spectrometers. Tandem mass spectra often contain fragments from multiple co-isolated peptides and existing algorithms cannot identify them all. We've teamed up with the leader in proteomics artificial intelligence, MSAID®, to overcome this barrier and get the most out of your proteomics data sets.

Artificial intelligence for chimeric spectra

The CHIMERYs™ intelligent search algorithm by MSAID uses artificial intelligence and reimagines the analysis of tandem mass spectra to decipher chimeric spectra from the ground up to overcome current limitations in proteomics data analysis. This revolutionary new approach leads to a deeper mining of data and substantially increases the number of peptide-spectrum matches (PSMs) found in data-dependent acquisition data (Figure 1). In

comparison to previous strategies, CHIMERYs finds more PSMs per tandem mass spectrum and markedly improves the identification rate, with fewer spectra returning no PSMs and many spectra returning three or more PSMs (Figure 2).

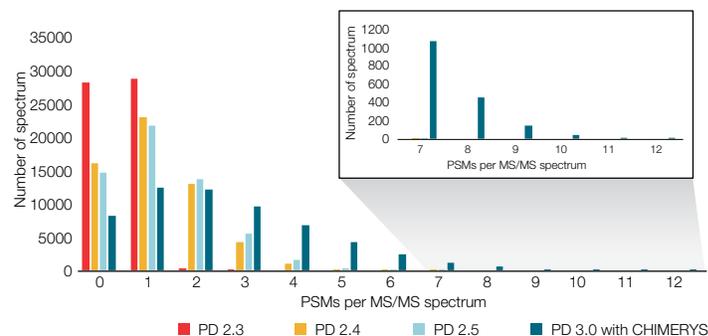


Figure 2. Analysis of PSMs in tandem mass spectra using Thermo Scientific™ Proteome Discoverer™ software with CHIMERYs versus previous versions.

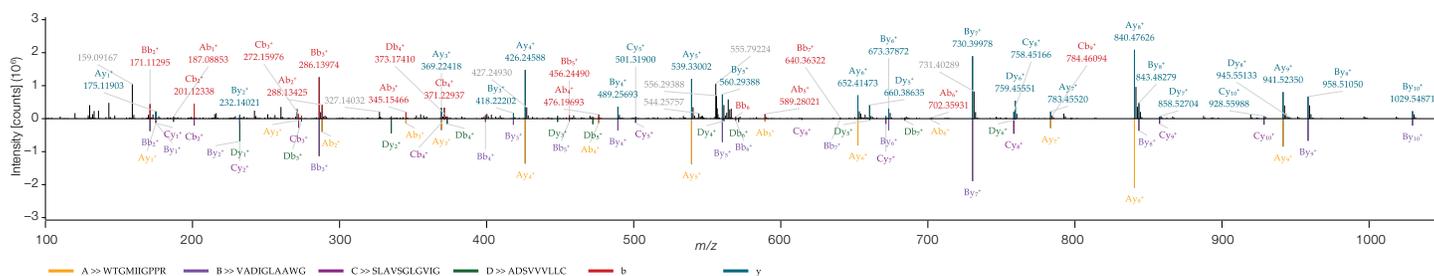
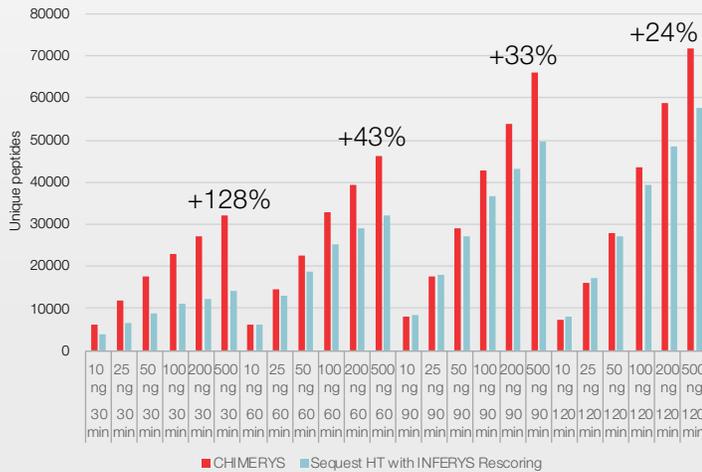


Figure 1. Mirror plot showing the annotation of a chimeric spectrum containing four PSMs by CHIMERYs.

Improved peptide and protein coverage

The addition of CHIMERYYS allows for a more complete analysis of both new and existing proteomics data sets by uncovering more unique peptide identifications, improving protein coverage and quantitation capabilities, and unlocking more efficient data acquisition schemes. CHIMERYYS provides substantial increases in unique peptides and proteins for improved quantitative



performance across different protein loads and run times (Figure 3). In particular, CHIMERYYS enables considerable improvements over traditional search algorithms for shorter gradients and higher protein loads. This enhancement enables more efficient data acquisition schemes for increased sample throughput and instrument utilization.

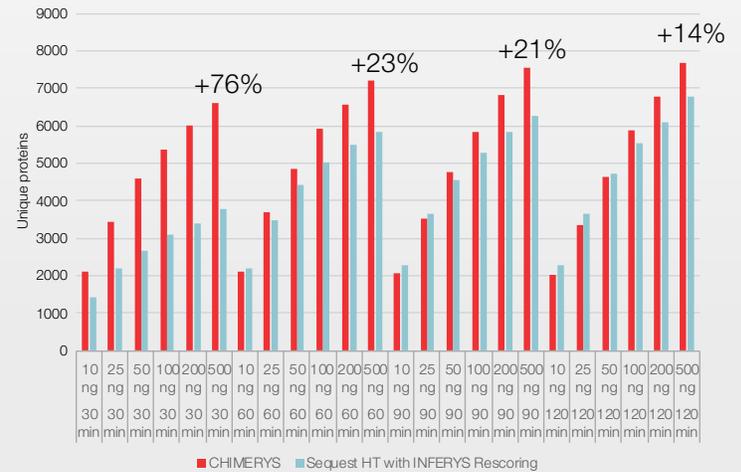


Figure 3. Improvement in unique peptides and proteins across various protein loads and run times for CHIMERYYS versus SEQUEST™ HT with INFERYYS™ Rescoring.

Increased biological insights

The increase in identification of unique peptides and proteins provided by CHIMERYYS enables scientists to generate more biological insights for any proteome from their existing and newly acquired data. These extra quantified proteins can fill in previously missing information in pathway analyses to provide a more comprehensive illustration of biological processes.

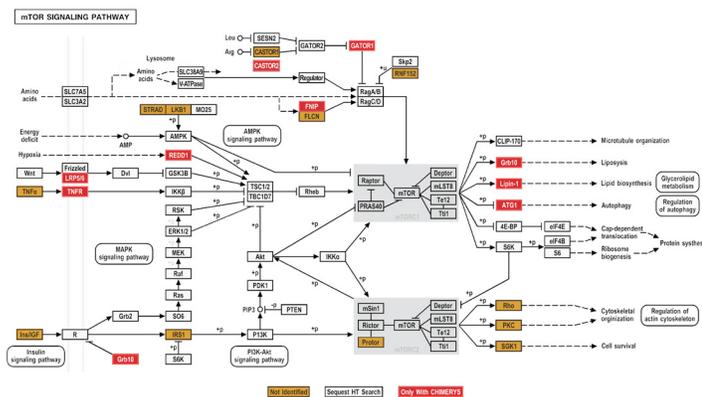


Figure 4. Improved signaling pathway coverage with proteins only identified by the CHIMERYYS intelligent search algorithm (red) or both the SEQUEST HT search and CHIMERYYS intelligent search algorithm (gray).

HLA immunopeptidomics

Proteome Discoverer 3.0 software integrates INFERYYS 2.0, which also improves support for HLA peptides. The addition of INFERYYS Rescoring provides a substantial increase in identifications at 1% and 0.1% false discovery rates (FDRs) for this very large search space containing very similar peptides. For a publicly available HLA Class I data set from a patient derived melanoma cell line (Chong et al., Nat. Com. 2020), this translates to a 55% increase in identifications at the peptide level.

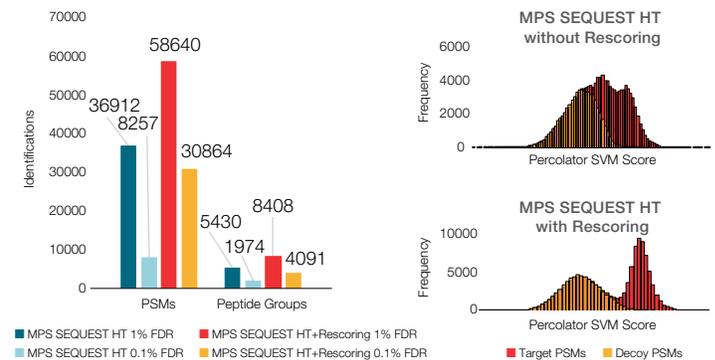


Figure 5. Impact of INFERYYS Rescoring on HLA Class I peptide identification.

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