From Data Sets to Meaningful Biology
Proteomics studies generate large amounts of data that, even after preliminary identification and validation, leave scientists with the time-consuming, yet critical, task of data interpretation. Using Thermo Scientific ProteinCenter software, scientists confidently interpret complex data sets and extract meaningful biological information within minutes – an analysis that could take months to finalize using conventional bioinformatics software tools.

Drawing from a biologically-annotated sequence database, regularly updated from all major protein sequence and annotation databases, ProteinCenter™ software enables single and combined data sets to be filtered, clustered, compared and analyzed statistically while, at the same time, overcoming the hurdle of proteins existing under different names and accession keys in different databases.

"We have used ProteinCenter to quickly compare and interpret our proteomics data sets. ...we have overcome the hurdle of proteins existing under different names and accession keys in the protein databases and are confident in our protein characterization results."

Dr. Thomas Neubert, Associate Professor, New York University Langone Medical Center

"Most notably, we found generic problems in databases to be the major hurdle for the correct characterization of proteins in the test sample."

Solutions to Facilitate Data Analysis and Interpretation in Proteomic Workflows

A full range of Thermo Scientific software solutions enable comprehensive, accurate data analysis for proteomic workflows. ProteinCenter serves as a bioinformatics tool, which supports the critical final step involving data interpretation, while the following software packages serve as tools for the remaining steps along the proteomic workflow.

- **Thermo Scientific Proteome Discoverer Software** is a comprehensive data analysis platform for qualitative and quantitative proteomics research, providing confident, comprehensive protein identification and characterization.

- **Thermo Scientific ProSightPC Software** supports top-down, middle-down and bottom-up experiments to provide an all-around tool for identification and characterization of intact proteins and peptides.

- **Thermo Scientific SIEVE Software** is an automated, label-free differential analysis platform for proteomics and metabolomics biomarker discovery that enables comparison of LC/MS^n spectra from healthy and diseased (or control and treated) samples.

- **Thermo Scientific Pinpoint Software** supports targeted protein quantification assays and facilitates the transition from identifying biomarker candidates to targeted validation of those candidates.

---

**Supporting Proteomics Workflows**

Leading in the development of innovative, comprehensive solutions for proteomics research, Thermo Scientific technology addresses the most challenging analyses faced by proteomics researchers at every step in their workflow.

Best-in-class instruments, consumables, reagents, software and services combine to provide the highest analytical performance and productivity, from sample handling through sample preparation, separation, detection and data analysis.
Access the Latest Data and >10 Million Non-redundant Proteins

ProteinCenter database updates bi-weekly, distilling over 83 million accession codes from past and present versions of public databases. A sequence of computational enrichments, including protein-protein similarity, signal peptide and domain predictions, is performed after each update.

- Access a single database consolidated from >20 public databases and including all historical data
- Compare data sets with the latest, as well as outdated, protein sequences and annotations

ProteinCenter database updates bi-weekly from major public databases.

Produce Meaningful Results

ProteinCenter tracks the frequent changes that occur during updating of protein sequence databases. This ensures that the same protein is followed despite changes in accession key or exclusion from a sequence database.

- Remove redundancy*
- Seamlessly compare data sets identified at different times and in different databases
- Cluster proteins by protein sequence, shared peptides or peptide-indistinguishable protein groups

* same protein with different accession key or alleles and fragments

Example of a protein’s history from Ensembl™. The same protein has been known under seven different accession keys during its lifetime.

“ProteinCenter enabled us to jump three months ahead of plan on our project.”
Dr. Christoph Rösli, Department of Chemistry and Applied Biosciences, ETH Zurich
ProteinCenter frees scientists from time-consuming work by eliminating redundancy, correcting for alternative splicing and poor annotation, as well as handling the dynamic nature of protein lists from different labs, sources and databases.

- Compare imported data sets in terms of proteins or peptides independent of input format, protein database and its version
- Compare 20 or more samples simultaneously – independent of the searched database and its version
- Compare protein lists from different databases against each other or international studies
- Reduce complexity – group proteins based on peptides or sequence homology
- Create exclusion lists and remove protein contamination

"ProteinCenter has really been a huge part of streamlining the data analysis process, and the ability for comparisons is really essential."

Rebekah L. Gundry, PhD, Bayview Proteomics Research Center, Johns Hopkins University
Reveal the Biological Context of each Data Set

ProteinCenter reveals all relevant biological annotations for newly-identified proteins and determines the most significant annotations.

- See differences in expression levels of healthy and diseased samples
- Reveal the results of chemical perturbation or genetic modification
- Compare each data set against complete proteomes of any species from any database

View which proteins were identified for relevant pathways

ProteinCenter calculates which annotations are statistically enriched or depleted

Gene Ontology distribution of a data set as a pie chart

"ProteinCenter is a great bioinformatics tool to analyze results (such as sorting, comparing, categorizing and presenting) of large scale proteomics studies."

Dr. Hua Liao, Millennium Pharmaceuticals
“All in all, ProteinCenter is a one-stop-shop for detailed bioinformatics mining of extensive proteomics data in a highly efficient and streamlined manner. I can highly recommend this tool to both the experienced proteomics laboratory and the first timer trying to make sense of their first proteomics experiments.”

Dr. Thomas Kislinger, Division of Cancer Genomics and Proteomics

ProteinCenter helps overcome the additional complexity of data interpretation when using labeled or label-free methods to produce quantitative proteomics data.

Group proteins based on their quantitative profile at the protein or peptide level (e.g. iTRAQ®, TMT®, SILAC or ICAT®) or merge label-free studies to create profiles for proteins found in multiple data sets.

Heat maps enable data to be visualized in two dimensions.
ProteinCenter gathers all information about a single protein on a single page for easy reviewing.

ProteinCenter provides external links to the protein annotation source. e.g. a single click enables a search of PubMed® using all the protein's aliases.

**Reveal the Biological Context for a Single Protein**

View domains, potential signal peptide and known post-translational modifications in graphics ready to use for presentations or papers.

View which peptides were identified for a protein found in multiple data sets in a comparison between data sets.

*“ProteinCenter helped me to quickly verify a sample preparation method via its comprehensive biological annotations.”*

K. Poulsen, Statens Serum Institut, Denmark
**Answer Complex Biological Questions**

Drill down to the most relevant proteins based on up-to-date annotations and predictions from all major sources. Use predefined filters to sort out the most relevant proteins.

<table>
<thead>
<tr>
<th>Filter proteins based on experimental parameters</th>
<th>Filter proteins based on biological annotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Modifications identified by a search engine</td>
<td>• Gene Ontology (both slim and full ontology)</td>
</tr>
<tr>
<td>• Number of unique peptides</td>
<td>• KEGG and UniProt pathways</td>
</tr>
<tr>
<td>• Peptide length</td>
<td>• PFAM and Interpro protein domains</td>
</tr>
<tr>
<td>• Quantification ratios</td>
<td>• Diseases</td>
</tr>
<tr>
<td>• Protein and peptide sequence (motifs)</td>
<td>• Interacting proteins</td>
</tr>
<tr>
<td>• Protein and peptide score from search engine</td>
<td>• PTMs</td>
</tr>
</tbody>
</table>

“ProteinCenter optimized my workflow from analyzing 4 samples per week to 20 samples per week.”

Dr. J. S. Rees, Cambridge Centre for Proteomics, UK

---

**Share Data Sets and Results Around the World**

- **Import data sets**
- **Interpret results**
- **Email**

No need to email large files or struggle with inconsistent formats – simply upload new data and share online through ProteinCenter.

Review the same data set at the same time.
Integrate Data Sets from Multiple Search Engines

- Overcome the challenges of entering data sets from multiple sources and filtering out redundant data – no more spreadsheet comparisons
- Easily import data sets from different vendors and open source search engines
- Import conventional data sets or supplementary data from papers in Microsoft® Excel® spreadsheets

<table>
<thead>
<tr>
<th>Source</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermo Scientific Bioworks / Proteome Discoverer</td>
<td>XML-file / csv-based file</td>
</tr>
<tr>
<td>EBI’s repository PRIDE</td>
<td>XML-file</td>
</tr>
<tr>
<td>iProphet</td>
<td>XML-based</td>
</tr>
<tr>
<td>Mascot™</td>
<td>XML-file exported directly from the search result html view</td>
</tr>
<tr>
<td>Mascot Distiller</td>
<td>XML-file</td>
</tr>
<tr>
<td>MaxQuant</td>
<td>Text-based report for either proteins or peptides containing quantitative SILAC information</td>
</tr>
<tr>
<td>MSQuant</td>
<td>Excel-based report containing proteins, peptides, modifications and quantifications</td>
</tr>
<tr>
<td>Phenyx™ (<a href="http://www.genebio.com">www.genebio.com</a>)</td>
<td>Integrated directly with ProteinCenter to enhance efficiency</td>
</tr>
<tr>
<td>ProteinPilot™</td>
<td>Protein and peptide summaries exported from ProteinPilot</td>
</tr>
<tr>
<td>ProteinProphet</td>
<td>CSV-file or protXML file</td>
</tr>
<tr>
<td>Scaffold</td>
<td>XML-file</td>
</tr>
<tr>
<td>SpectrumMill</td>
<td>CSV-based file</td>
</tr>
<tr>
<td>Spreadsheets</td>
<td>Any CSV-file containing protein IDs, peptides, modifications, quantification, etc.</td>
</tr>
<tr>
<td>ProteinLynx Global SERVER™ (PLGS)</td>
<td>Database search result</td>
</tr>
<tr>
<td>X!Tandem</td>
<td>XML-file exported directly from the search result html view</td>
</tr>
</tbody>
</table>

More Information about ProteinCenter

Visit [www.thermoscientific.com/proteincenter](http://www.thermoscientific.com/proteincenter) to listen to recent web seminars from users, see the latest publications or request an appointment with a ProteinCenter specialist to interpret your data online.

If you are interested in the possibility of developing an enterprise-wide solution for your institute or company, please contact your local representative.
Laboratory Solutions Backed by Worldwide Service and Support

Tap our expertise throughout the life of your instrument. Thermo Scientific Services extends its support throughout our worldwide network of highly trained and certified engineers who are experts in laboratory technologies and applications. Put our team of experts to work for you in a range of disciplines – from system installation, training and technical support, to complete asset management and regulatory compliance consulting. Improve your productivity and lower the cost of instrument ownership through our product support services. Maximize uptime while eliminating the uncontrollable cost of unplanned maintenance and repairs. When it’s time to enhance your system, we also offer certified parts and a range of accessories and consumables suited to your application.

To learn more about our products and comprehensive service offerings, visit us at www.thermoscientific.com.