

Proteomics

Exploring your proteomics universe with the Thermo Fisher Scientific proteomics solution

The field of proteomics has always held its own set of unexpected challenges. Not only are we dealing with a large number of targets in a vast field of other background molecules, but sometimes we are hunting for low abundance features that would mirror identifying planets in a galaxy of stars.

Discover our proteomics solution that combines our Thermo Scientific™ Orbitrap™ mass spectrometers with our Thermo Scientific™ Proteome Discoverer™ software using the MSAID™ CHIMERY™ intelligent search algorithm empowered by deep learning for automated data processing, all powered by the Thermo Scientific™ Ardia™ Platform on a server that supports multitasking, centralizes large data files, and expands collaboration on this traditionally siloed data type into a global universe.

Seeing the stars

Maximize your identification and maintain precise quantitation without needing to compromise on your resolution with our market leading Orbitrap technology which includes the Thermo Scientific™ Exploris™ 480 Mass Spectrometer and the Thermo Scientific™ Orbitrap Astral™ Mass Spectrometer.

Rethink what is possible to see, identify, and quantitate with faster throughput, deeper coverage, and higher sensitivity.



Figure 1. The Orbitrap Astral mass spectrometer

Counting the stars (DDA) and finding new planets (DIA)

Omics sample analyses is complex, especially in the discovery phase when maximizing information is imperative. This mode can lead us to generate data with multiple fragmentation levels, acquisition schemes, and activation types, and can result in a complex experimental design with multiple biological groups.

Proteome Discoverer software can map sample types, study factors, and quantitation channels to simplify study management and create comparative statistical analysis for label-free, isotope-labeled, and tandem-mass tag™ (TMT™) studies, supporting all data-independent (DIA), data-dependent (DDA), wide-window acquisitions (WWA), and limited parallel reaction monitoring (PRM) data support.

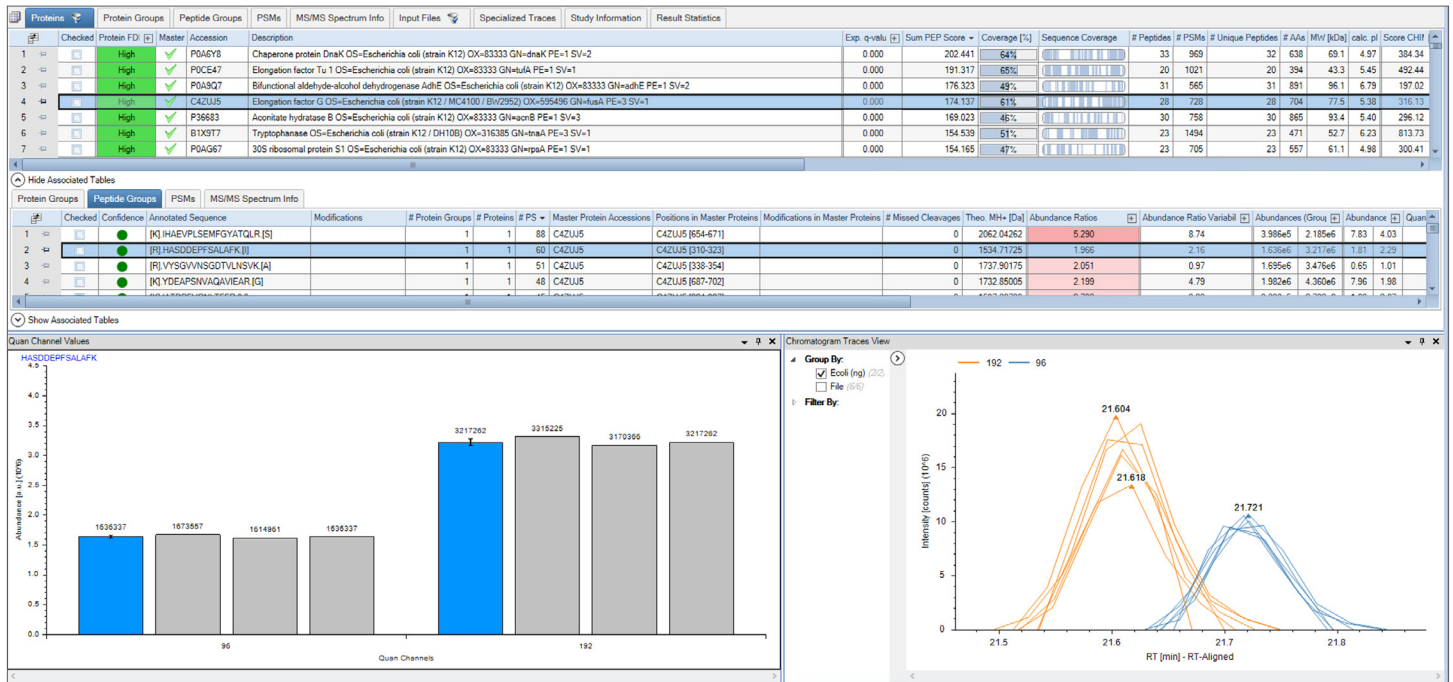


Figure 2. LFQ DIA results can be visualized with chromatograms, principal components analysis plots, heat maps, quantitation channel charts, and more within the Proteome Discoverer software framework, allowing for quick and easy interpretation of results. The ability to perform match-between-runs for DIA data ensures reproducible quantitative coverage.

The powerful workflow system allows user-friendly customization, including multiple peptide identification approaches, biological annotation, and quantitation to support accurate annotation and confident identification while also providing automated processing capabilities.

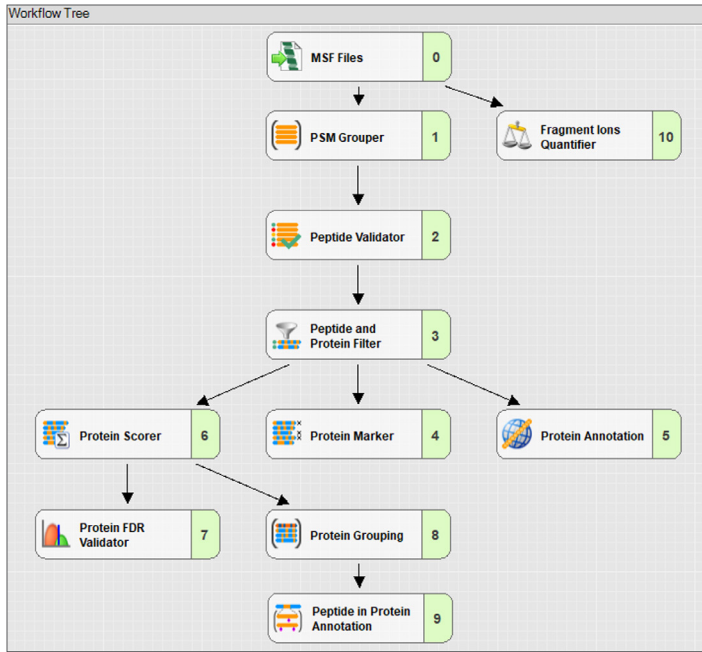


Figure 3. Spectra are streamed from the top of the workflow and pass through nodes that perform filtering, peptide ID, quantification, FDR calculation, grouping, and more.

Data interpretation tools include hierarchal views with links between proteins, peptides, and protein spectrum matches with interactive graphical views to help decipher the links. Easily position the CHIMERYYS node in the workflow tree which supports analysis of both DDA and DIA data, including TMT and added support for phosphopeptide identification. On top of these features, users can mirror-plot the experimental spectrum against the accurately predicted spectra from the deep-learning algorithm of INFERYYS™ rescoring model 3.0 from MSAID which also includes support for phosphorylation, heavy label K/R, and neutral loss annotation.

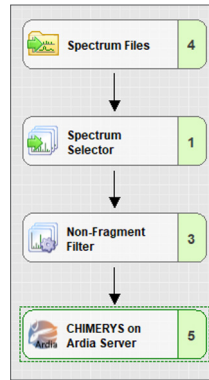


Figure 4. The highly customizable workflow system is composed of nodes that can connect in linear and branched modes with included pre-defined workflows such as TMT, LFQ, post-translation modification (PTM), ID, and cross-linked peptide ID.

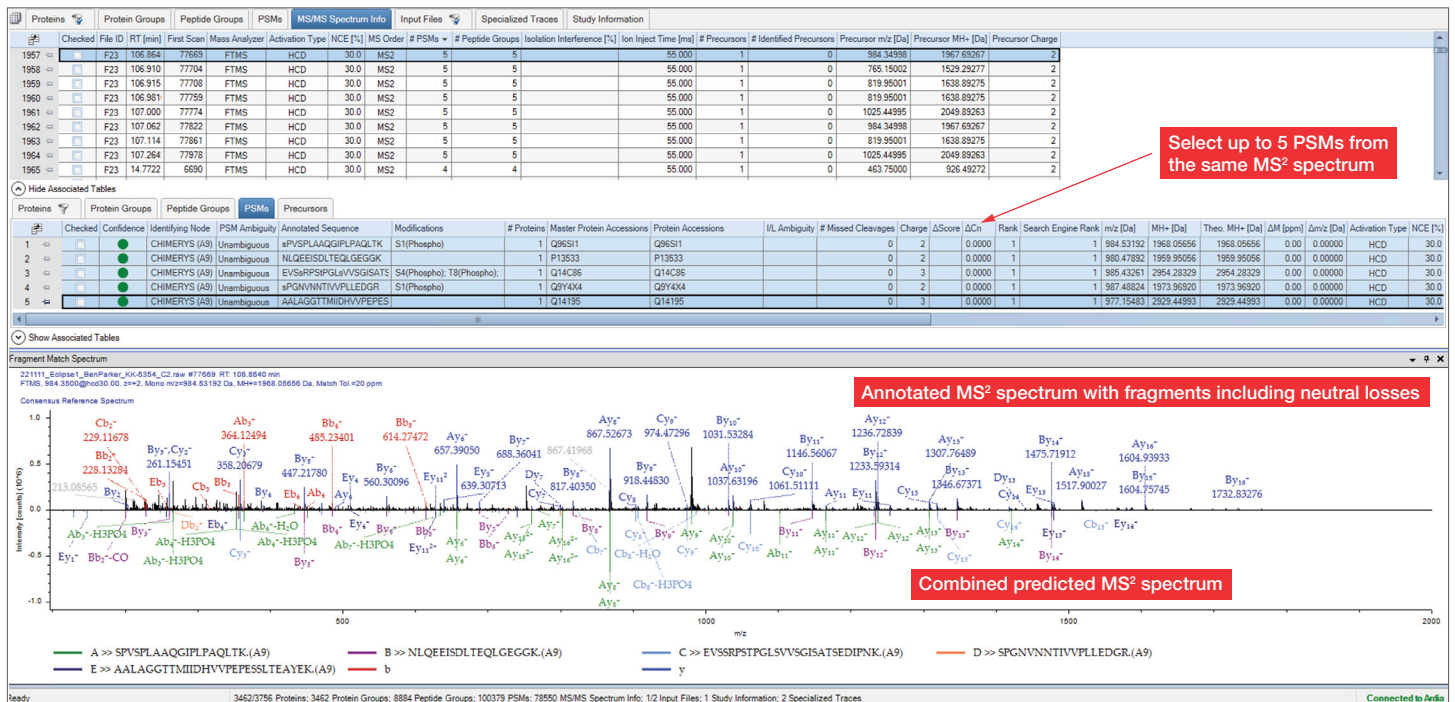


Figure 5. Deconvolution and visualization of chimeric spectra. The experimental and predicted spectrum can be visualized by selecting up to five PSMs at a time to display a mirror plot.

The telescope versus the spaceship

The expansive data acquired from mass spectrometers can fill hard drives, spill over into external drives, and require users to spend time on just managing and tracking data across different locations.

With the Ardia Platform, users have the ability to set up automated background processing, intuitively interface with shared files and results, and ultimately connect our hardware and software technology to help them speed through manual tasks that slow discovery.

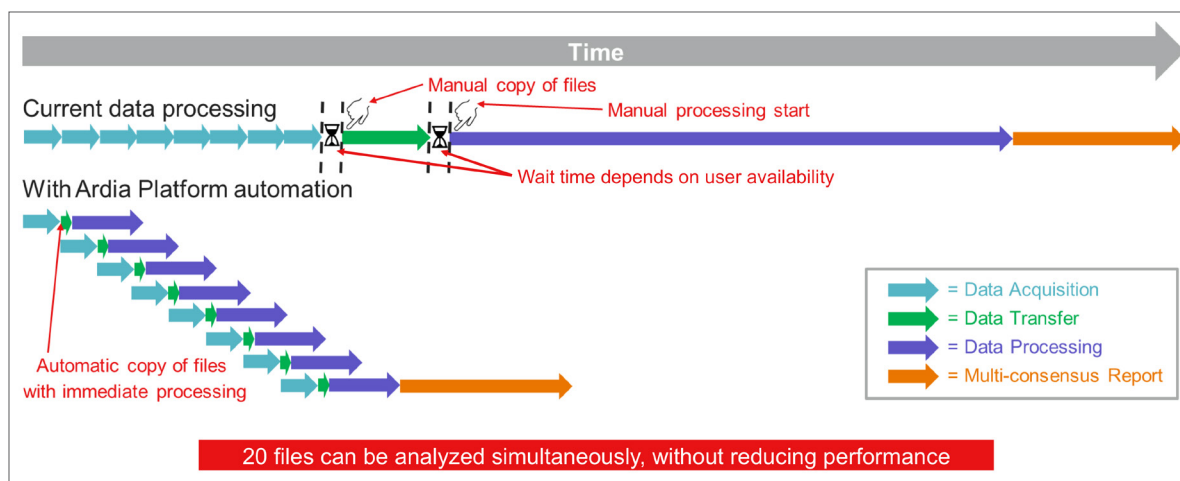


Figure 6. Visual representation of containerized software design demonstrates how multi-stream multitasking of processes enhanced with automated functions reduce wait time.

Exploring the universe

With the Ardia Platform on the Ardia Advanced Tower Server that includes the installation of CHIMERY'S intelligent search algorithm, you can power your proteomics experiments and take advantage of an environment capable of organizing, managing and processing large data files. Connect our suite of hardware including our newest Orbitrap Astral mass spectrometer, centralize data files from Thermo Scientific™ Xcalibur™ software, and achieve deep processing and exploration with the built-in enhancements made to connect Proteome Discoverer software to this new universe.

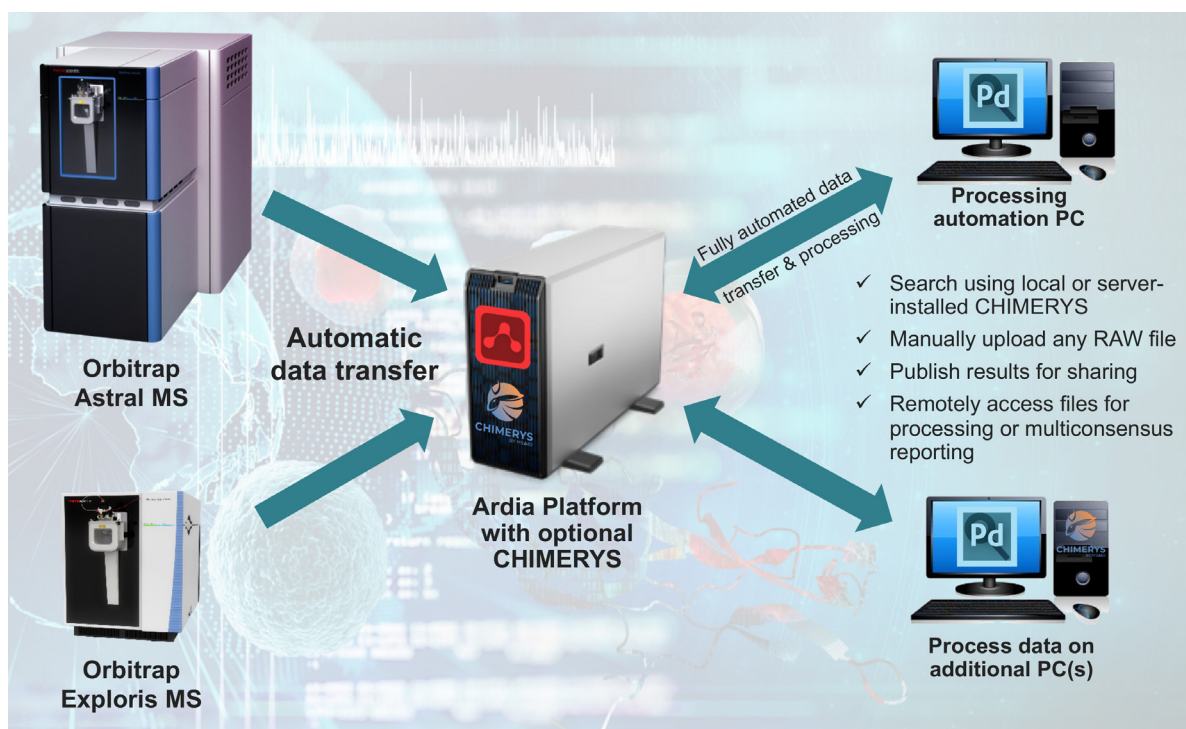


Figure 7. Leverage software architecture to work cooperatively, remotely, and efficiently.

Work cooperatively inside that universe with study management grouping. Select to add local and remote files that retain the link to raw or processed data on the Ardia Platform server for quick and easy access.

The screenshot shows the Ardia Platform interface. At the top, there are buttons for 'Add Files', 'Remove Files', 'Open Containing Folder', 'New Analysis', and 'Open Analysis Template'. Below these is a menu with options: 'Add Local Files', 'Add Local Fractions', 'Add Remote Files', and 'Add Remote Fractions'. The main area is a table with columns: 'Local Status', 'Remote Status', 'ID', 'Name', 'File Type', and 'Sample Information'. The table contains 15 rows of file entries, each with a green checkmark in the 'Local Status' column. The file names are long alphanumeric strings ending in '.raw'. The 'Sample Information' column contains details like 'Sample Type: [Sample], Ecoli (ng): [24]'.

Figure 8. Select files, indicated as remote or local, to add to a study for processing or creating multi-consensus reports.

Utilize the power of the Ardia Platform universe to program automated background processing as soon as the MS analysis is concluded while still retaining the ability to operate in the foreground.

The screenshot shows the Proteome Discoverer software interface. At the top, there are two red callout boxes: 'Connect to Ardia Platform' pointing to the 'Ardia Platform' radio button, and 'Configure automated processing' pointing to the 'Ardia Platform processing with Proteome Discoverer software' checkbox. Below these is a table with columns: 'File Name', 'Path', 'Inst Meth', 'Position', 'Inj Vol', 'Processing Method', 'Quantification Method', and 'Results Path'. The table contains three rows of sample data. A dropdown menu is open for the 'Processing Method' column, showing a list of methods. A red callout box 'Select from published analysis methods' points to this dropdown menu. The methods listed include iTRAQ 4plex, iTRAQ 8plex, TMT 2plex, TMTe 6plex, Low Resolution TMTe 6plex, TMTe 6plex (ETD), iodo TMT 6plex, Low Resolution iodo TMT 6plex, TMT 10plex, TMT 11plex, TMTpro 16plex, TMTpro 18plex, Full 18O Labeling (O2 | 18O2), Incomplete 18O Labeling (O2 | O18O + 18O2), and SILAC 2plex (Arg10, Lys6).

Figure 9. From Proteome Discoverer software, select from the published analysis methods to apply to files on the Local Drive or Ardia Platform and further configure to automate processing with the Ardia Advanced Tower Server.

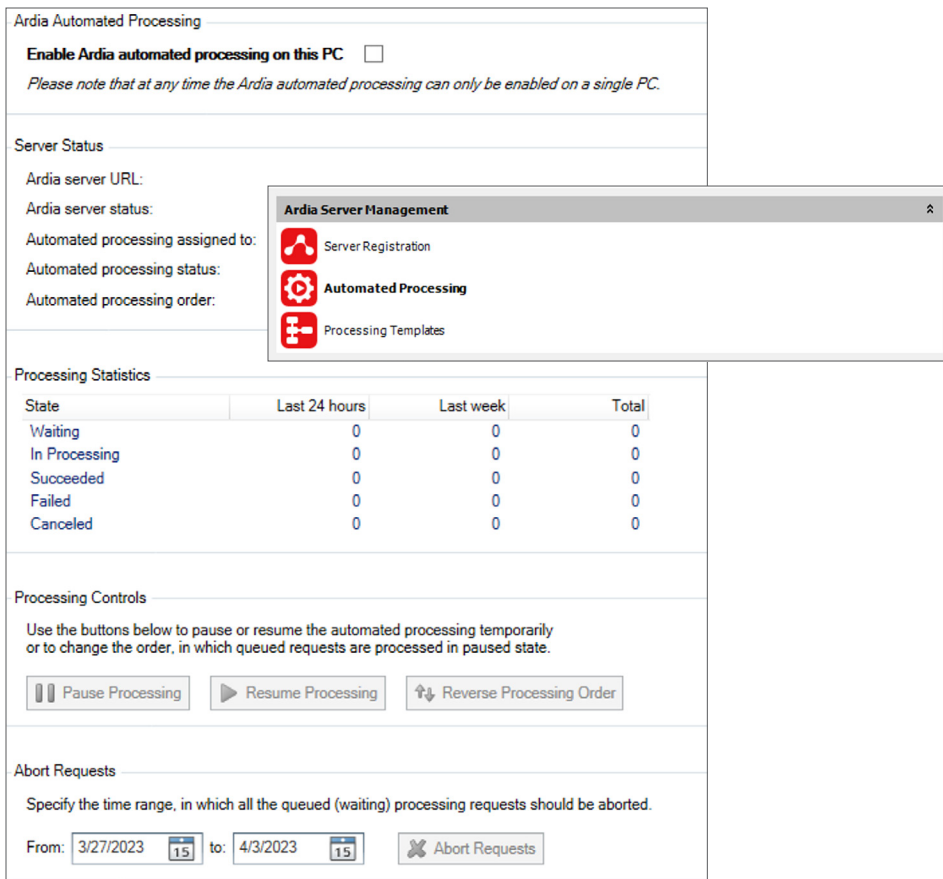


Figure 10. Initiate, pause, modify, or discontinue background automated processing with the ability to monitor completion progress from the user interface.

Then, choose to publish results back to the shared universe for retrieval from any web-connected access point.

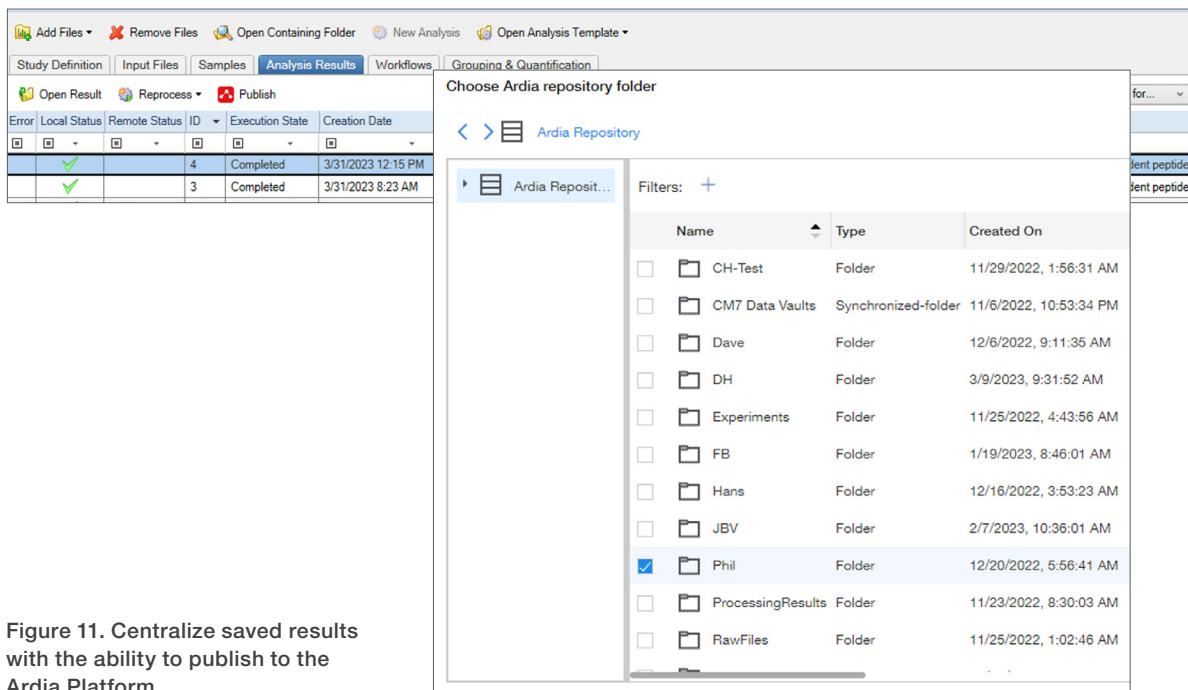


Figure 11. Centralize saved results with the ability to publish to the Ardia Platform.

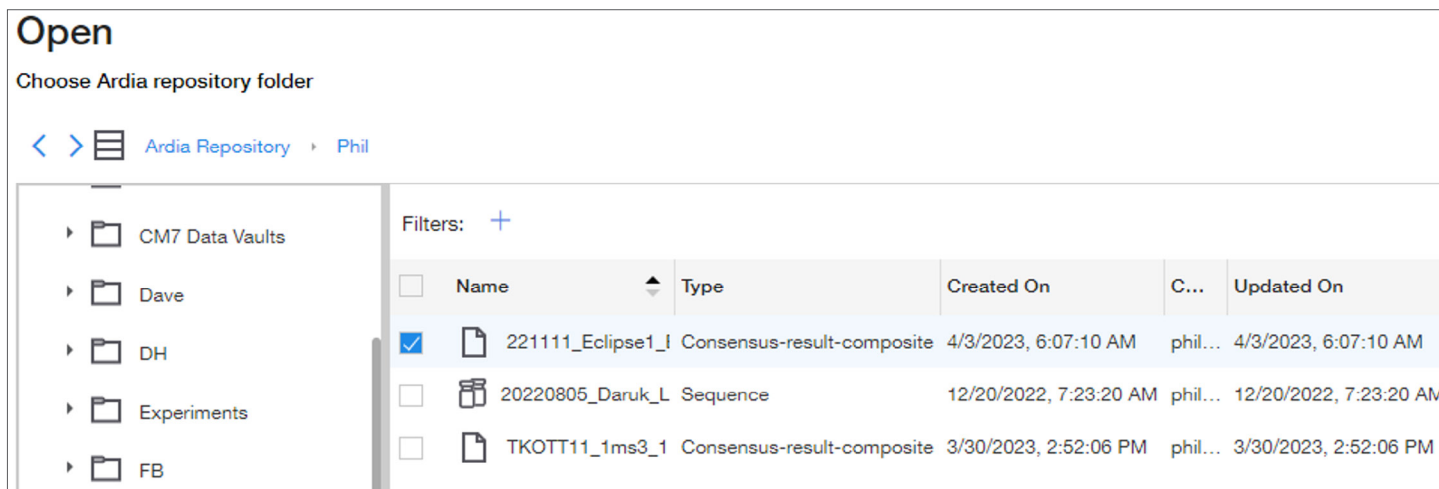


Figure 12. Retrieve results or raw files from the Ardia Platform file repository on a connected interface from anywhere.

Join us on our journey to revolutionize proteomics data from ground-breaking acquisition to futuristic processing. Build your capabilities and break down data silos with combined solutions from Thermo Fisher Scientific and get closer to the truth.

Learn more at www.thermofisher.com/ardiaproteomics

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