

## 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 AI-empowered CHIMERYS™ algorithm 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

Thermo Fisher Scientific understands the typical balancing act between discovery, with the goal to maximize protein identification over a broad range, and targeted, where increased throughput drives narrower data focus, but we share in the desire to always push the boundaries and somehow achieve both.

In our hunt to discover significantly measurable changes and identify the finest new data details, we continue to innovate with novel technology to propel new levels of data collections. The Thermo Scientific™ Orbitrap™ Astral™ mass spectrometer delivers faster throughput, deeper coverage, and higher sensitivity with accurate and precise quantitation to rethink what is possible for proteomics.



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), and wide-window (WWA) acquisitions.

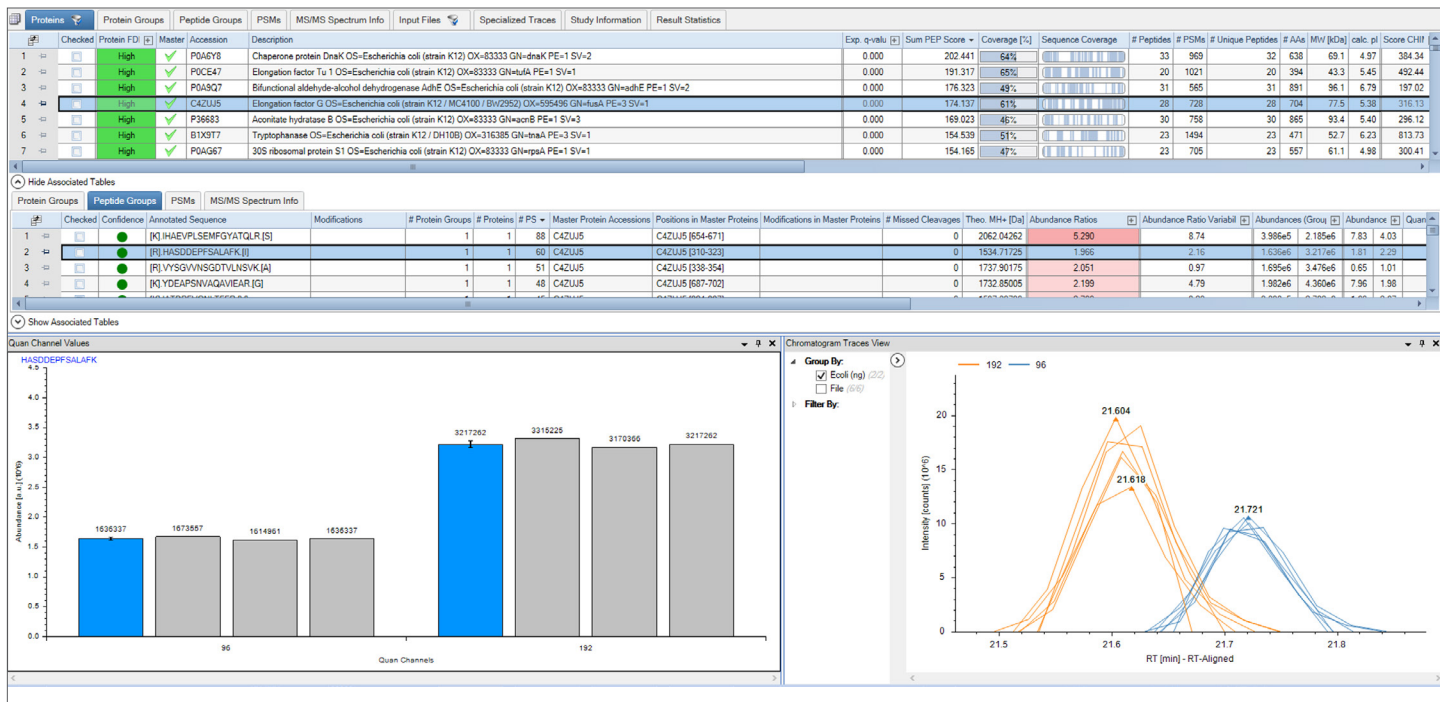


Figure 2. LFQ DIA results can be visualized with chromatograms, principal components analysis plots, heat maps, quantitation channel charts, and more within the Proteome Discoverer software framework, allowing for quick and easy interpretation of results. The ability to perform match-between-runs for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

Data interpretation tools include hierarchal views with links between proteins, peptides, and protein spectrum matches with interactive graphical views to help decipher the links. On top of these features, users can mirror-plot the experimental spectrum against the accurately predicted spectra from the deep-learning algorithm of INFERYYS™.

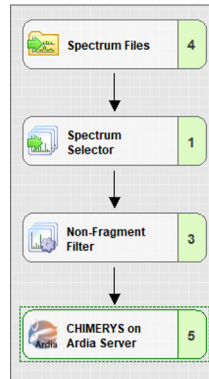
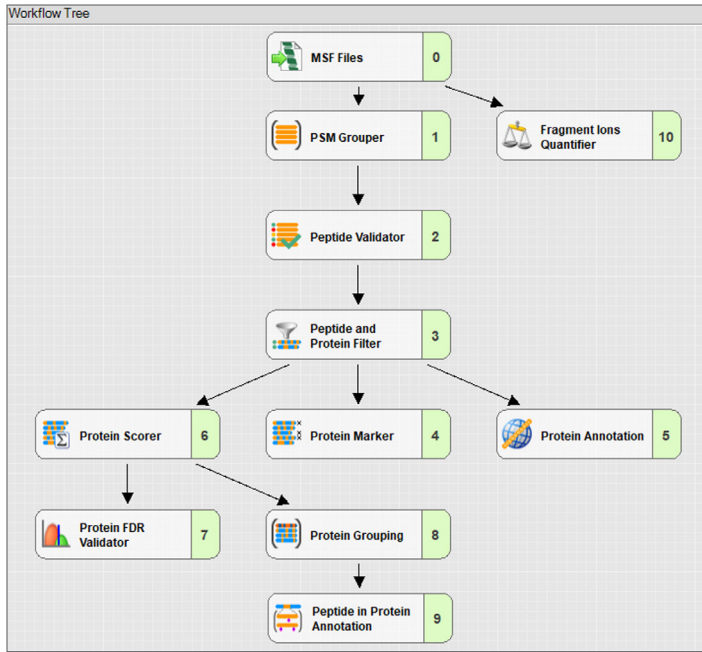


Figure 4. The highly customizable workflow system is composed of nodes that can connect in linear and branched modes with included pre-defined workflows such as TMT, LFQ, post-translation modification (PTM), ID, and cross-linked peptide ID.

Figure 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. The CHIMERYs node supports analysis of both DDA and DIA data, including TMT and added support for phosphopeptide identification.

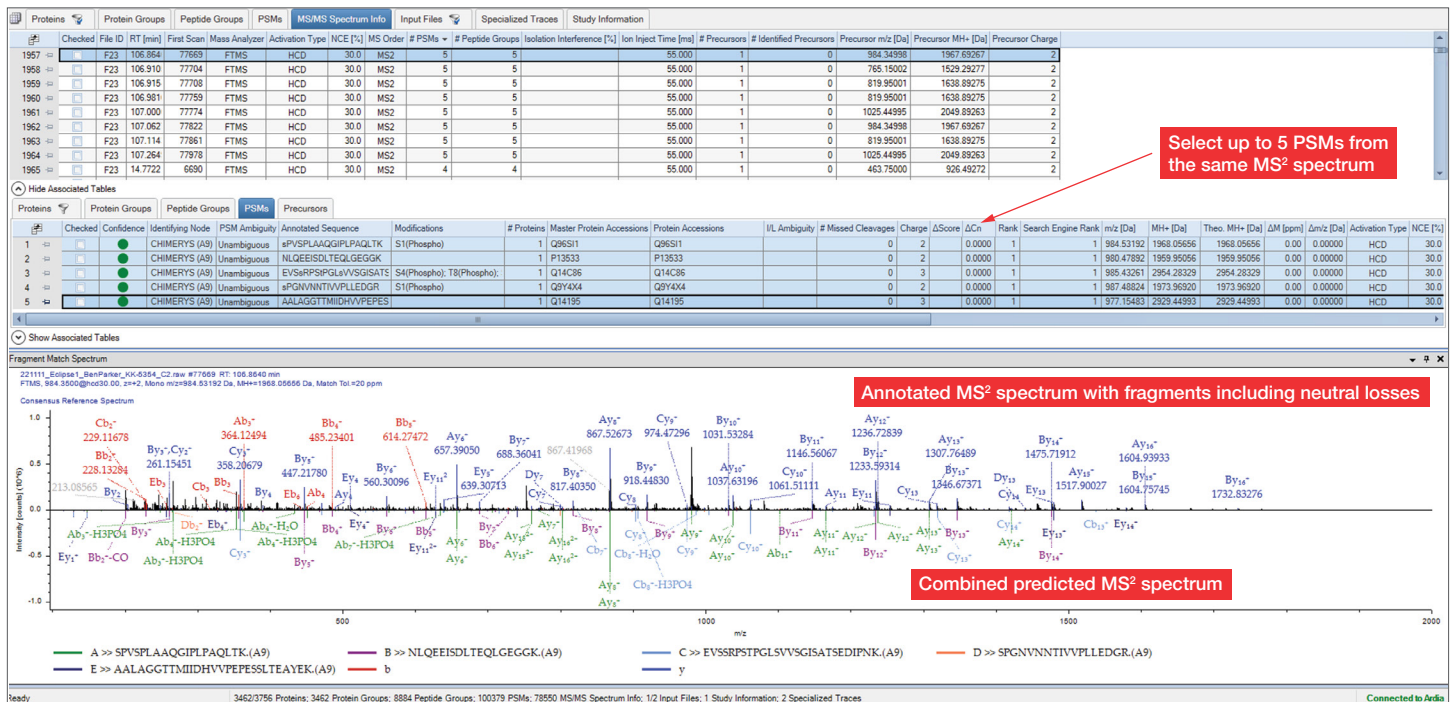


Figure 5. Deconvolution and visualization of chimeric spectra. The experimental and predicted spectrum can be visualized by selecting up to five PSMs at a time to display a mirror plot.

## 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.

Depending on complexity, processing mass spectrometry data on workstations can take hours or days. Even where processing and data storage are handled by separate workstations to manage the size and performance requirements, transferring files externally or through networks can test the limits of the most patient of us.

We, at Thermo Fisher, are thinking about file management and data processing. We see and develop these tools, and we recognize that exploring these kinds of experiments deserves a flexible ecosystem built in a future-proof architecture that can power new discovery.

We developed the Ardia Platform to minimize large-file transfers by centralizing them and maximizing the processing power

that supports sophisticated algorithms with server-level resources. 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 explore data in a new way.

## Exploring the universe

With the Ardia Platform on the Ardia Advanced Tower Server that includes the installation of CHIMERYS™ from MSAID™, 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.

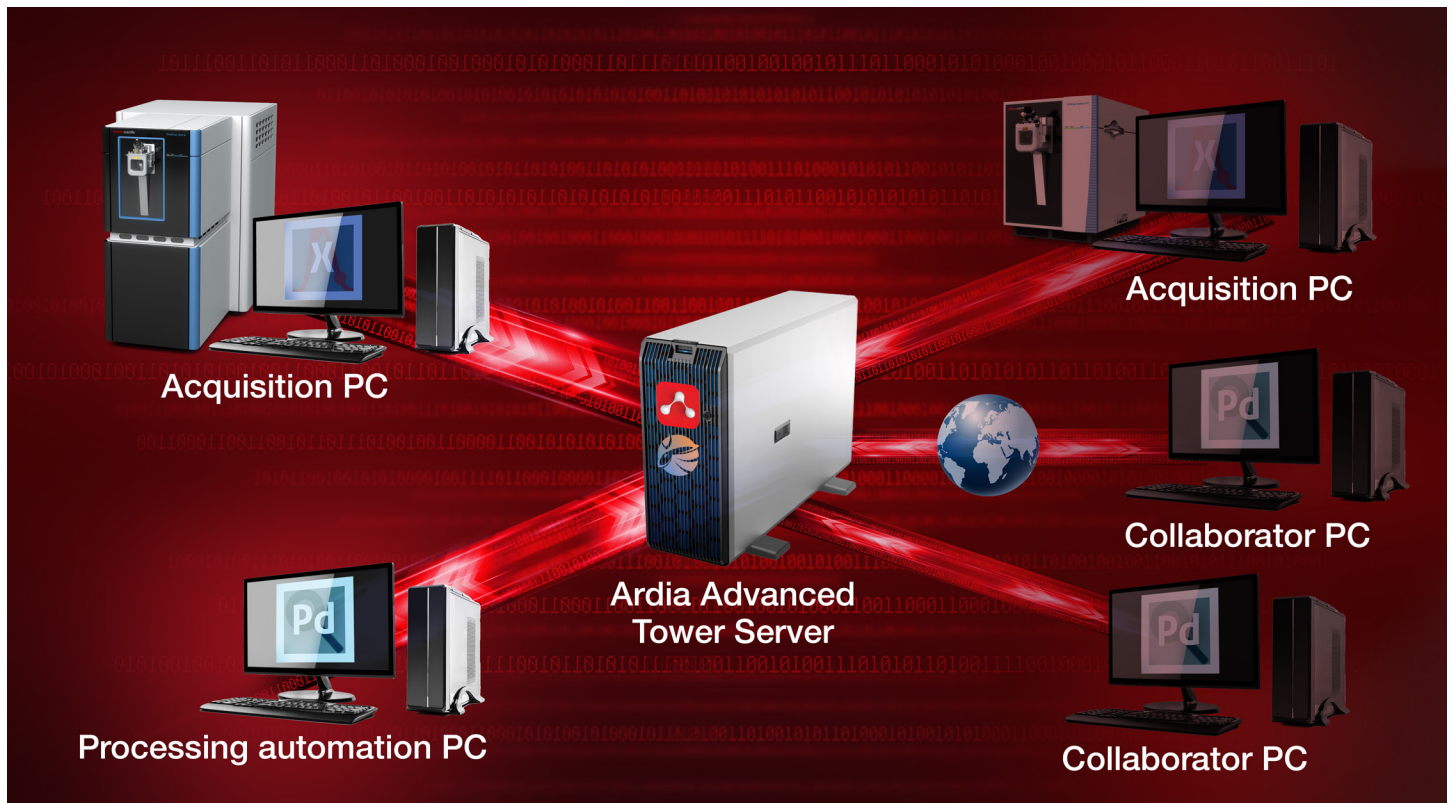


Figure 6. Leverage software architecture to work cooperatively, remotely, and efficiently.



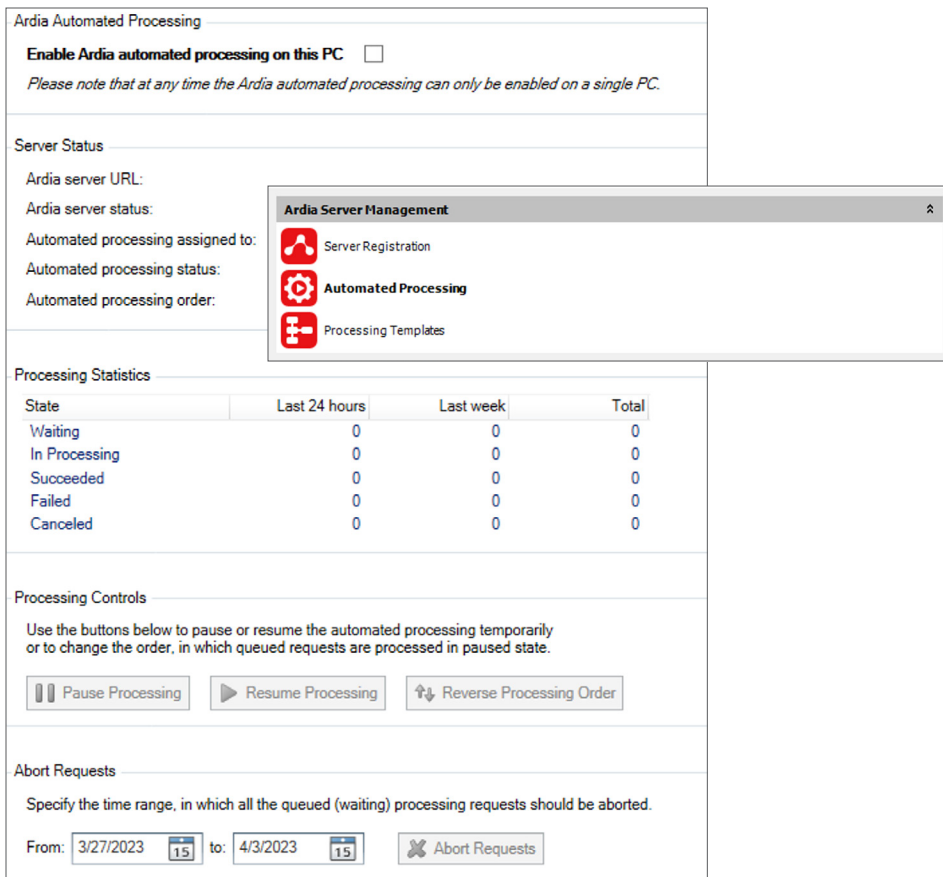


Figure 9. Initiate, pause, modify, or discontinue background automated processing with the ability to monitor completion progress from the user interface.

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

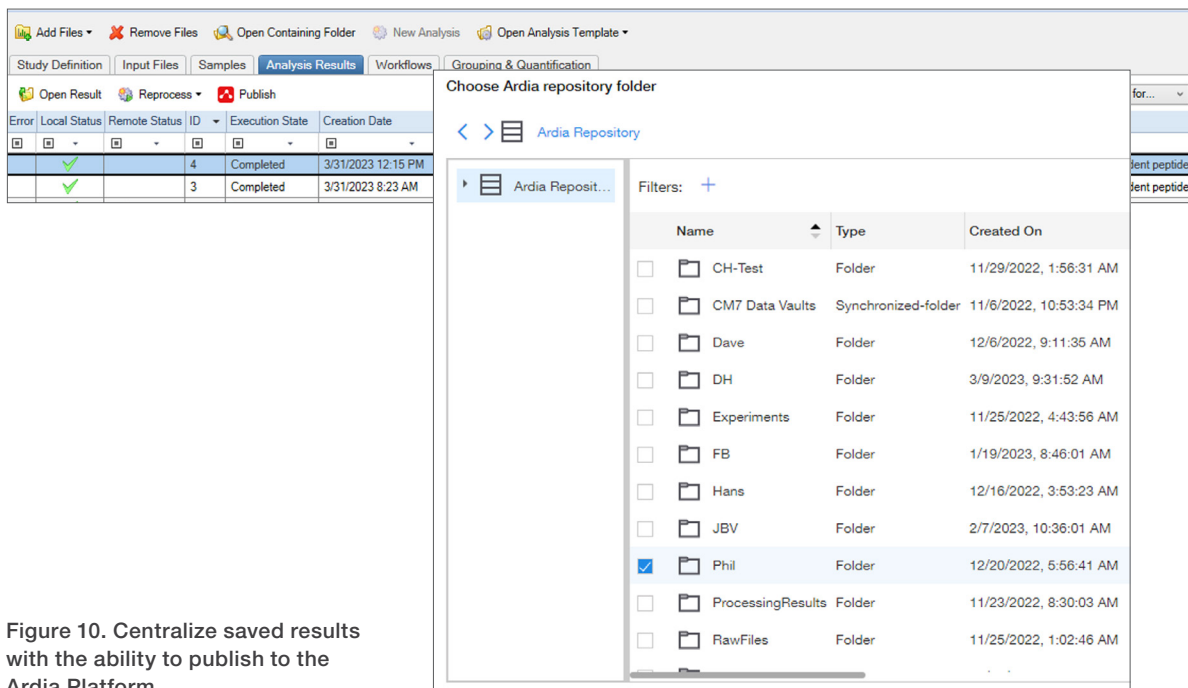


Figure 10. Centralize saved results with the ability to publish to the Ardia Platform.

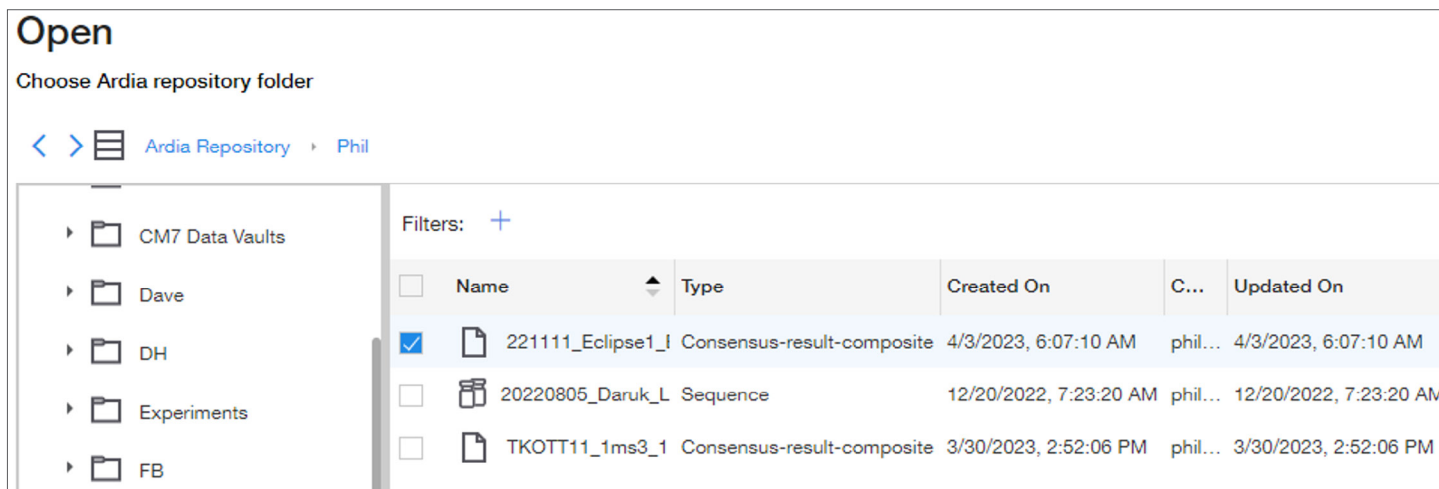


Figure 11. Retrieve results or raw files from the Ardia Platform file repository on a connected interface from anywhere.

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](http://www.thermofisher.com/ardiaproteomics)

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