



**Spectronaut<sup>®</sup>**  
*powered by Pulsar*

## **Spectronaut<sup>®</sup> 19**

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## 1 Major improvements in directDIA

- Improved scoring: 10% more proteins groups and 13% more precursors on average based on a large and diverse set of DIA datasets
- Improved quantification: 11% more true candidates based on a large and diverse set of controlled quantitative experiments.

## 2 Powered by AI

- Up to 40% improvement in key performance metrics of deep learning models
- Option for using deepQuant, a deep learning-based interference correction algorithm
- Improved inference for an extended list of modifications and labels such as dimethylation, ubiquitination, mTRAQ, etc.

## 3 Significant computational performance

- 40% faster directDIA on timsTOF and Astral data in comparison to Spectronaut 18.0
- Reduced directDIA RAM usage: 90% reduction in memory growth. 10,000 samples can be theoretically processed with 512 GB of RAM using directDIA plus SNECombine workflow.
- Spectronaut saved experiment (.SNE) file size reduced by up to 80%
- Temporary hard drive requirements are lower by up to 86% (directDIA from HTRMS)
- Temporary hard drive requirements are lower by up to 50% (directDIA from raw Vendor formats)

## 4 New acquisition method support

- diagonal-PASEF on Bruker's timsTOF platform is supported with directDIA and library based analysis
- New visualizations for diagonal-PASEF in the analysis perspective

## 5 Improved support for labeled DIA workflows

- Added support for run level channel q-values
- Annotate biological conditions at the channel level



## 6 New features for analyzing post translational modifications

- Input normalization by linking enriched experiment with non-enriched
- Support for site occupancy rate calculation
- New visualizations in the analysis and post-analysis perspective

## 7 Improved command line interface

- New SNEmerge option facilitates batchwise or parallel processing: Merge multiple SNE files into a single SNE file
- New option for input normalization
- Graceful and immediate exit if a command has errors
- Separate commands for every pipeline with a clear options scope
- Increased POSIX compatibility

## 8 New Visualizations and Reportables

- Elution Group Level → EG.InputNormalizationFactor
- Elution Group Level → EG.QuantityPerProtein
- PTM Site Report → PTM.QuantityPerProtein
- PTM Site Report → PTM.InputNormalizationFactor
- PTM Site Report → PTM.Stoichiometry
- New R.PTMSites category lists all identified sites per PTM
- Peptide vs Protein Quantity plot
- Post-analysis analysis overview Average PTMs localized
- Sample linking page in Experiment setup

## 9 New and Changed Analysis Settings

- [New] DIA Analysis → PTM Workflow → Input Normalization Strategy
- [New] DIA Analysis → PTM Workflow → PTM Localization → Stoichiometry Calculation Strategy
- [New] DIA Analysis → Quantification → DeepQuant Correction [Beta]
- [New] DIA Analysis → Workflow → Hybrid (DDA + DIA) Library
- [New] directDIA → Pulsar Search → Speed-up → diaPASEF Processing → Fast
- [New] directDIA → Pulsar Search → Identification → directDIA Workflow → RT Sampling Reduction
- [Change] Spectronaut 19 uses only MS2 quantification for differential abundance. Previously, the default was to use both MS1 and MS2