



Spectronaut™
powered by Pulsar

Spectronaut™ 15

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1 More Identifications

- Improved identification with new scores, especially for short gradients
- Up to 35% more precursor identifications for directDIA with diaPASEF
- Up to 10% more precursor identifications for directDIA in general
- Up to 30% more precursor identifications for short gradient DIA analysis with library
- Up to 10% more precursor identifications for DIA analysis with library in general

2 Accurate Quantification

- Improved default settings for quantification
- New MaxLFQ based protein quantification
- Up to 15% more protein identifications with CVs below 10% in controlled quantitative experiments

3 Improved Ion Mobility Support

- Ion Mobilogram visualization for dia-PASEF
- Ion Mobilogram based manual peak refinement
- Up to 30% faster processing of dia-PASEF data
- Added optimal support for high-sensitive py5 dia-PASEF method

4 General DIA Analysis

- New Run-wise protein FDR calculation and filtering
- New peptide posterior error probability (PEP) filtering
- Improved flexibility for directDIA search settings
- Improved multi-channel quantity summarization
- Command line support for SNECombine workflow
- New “Method Evaluation” workflow with directDIA

5 Comprehensive PTM Analysis

- Site collapse calculation
- Site regulation analysis
- Modification specific normalization filter for enrichment workflows
- New PTM site report



6 Pulsar Database Search Engine

- Improved performance for large protein databases (> 2 GB) with Pulsar
- Improved identification and performance for unspecific searches

7 Deep-learning Augmented Improvements

- Prediction for ion mobility (1/K0) during library generation
- Improved fragment prediction for unspecific peptides

8 New Post Analysis Features

- Added PCA analysis
- Added custom selection for protein rank plot
- Added custom selection for volcano plots
- New PTM Analysis node

9 Improved User Experience and Visualization

- Improved Protein Coverage plot
 - PTM support
 - Peptide tooltip and highlighting
- New sub-perspective “Protein Grid View” in the analysis perspective
- Improved XIC Alignment plots with support for unlimited number of runs
- Detachable perspective and plots for side-by-side visualization
- Improved XIC grid overview plots
- One-Click tree navigation in plots
- Improved plot and tree filter selection
- Quick-Action bar for analysis perspective
- Improved warning messages with actionable links
- Improved UI for analysis log
- Updated Analysis Summary plot for easier access

10 Other Changes

10.1.1 Report Perspective Changes

- New PTM site level report when performing PTM localization



10.1.2 DIA Analysis Settings Changes

- Default row filtering for quantification changed from *Q-value* to *Q-value Sparse*
- Default quantification strategy changed from *Quant 2.0* to *Auto*, where it will use MaxLFQ if analyzing less than 500 runs
- Default normalization strategy changed from *Global Normalization* to *Auto*, where it will use *Local Normalization* if analyzing less than 500 runs
- New *PTM workflow* node in the settings

10.1.3 directDIA Analysis Settings Changes:

- New Method Evaluation setting in directDIA settings → Workflow → Method Evaluation
- Distinguish between Pulsar and DIA analysis settings for directDIA for more flexibility