



Spectronaut[®]
powered by Pulsar

Spectronaut[®] 21

Release Notes

1. Powered by advanced ML scoring and AI models

- 10% more protein groups on average
- 11% more immunopeptides on average
- Next gen AI models can accurately predict unseen PTMs
- Improved AI predictions for both tryptic and unspecific peptides

2. Improved Computational Performance

- Up to 30% faster merging steps when parallelizing
- 10% faster directDIA for immunopeptidomics (class I and II)
- 15% faster directDIA for timsTOF on average
- 50% smaller SNE file size when saving with XIC
- New directDIA workflow that randomly sub-selects samples for library gen

3. Improved PTM processes and reporting

- Improved PTM site localization leads to higher quality data
- Added option to collapse PTM site report by protein group
- Further improvements in site stoichiometry calculations
- New PTM site specific statistics and visualizations in post-analysis

4. Changes in Analysis Settings and Reporting

- Simplified identification settings for directDIA; default behavior remains same
- Simplified mass tolerance settings for directDIA and library generation
- New option to group peptides by In-Source Fragmentation events in the tree view
- Added summary for identifications per channel (e.g. SILAC experiment)
- Added option to automatically sub-sample runs during directDIA to increase analysis throughput
- Reorganized some global settings into more appropriate categories
- Added “Calibration Carry-over” and “Profile Strategy” options to directDIA settings

5. Bug fixes and other improvements

- Fixed issue where some peptides were incorrectly labelled with UNKNOWN proteotypicity assignment
- Fixed issue where the reference condition in the condition setup could not be unselected
- Fixed issue where library export to text based format, from the library perspective, could stall the software
- Fixed issue where using R.Attributes report column could cause an incorrect cell alignment in the resulting export table
- Fixed issue with “diagonalPASEF reprocessing” warning message in the UI would never disappear
- Fixed issue with manual peak integration sometimes not re-scoring the peak properly
- Fixed issue where changing temporary storage path while an analysis is running would break that analysis
- Fixed several issues related to Spectronaut Uninstaller
- Fixed issue where the user could trigger a experiment post-analysis refresh while a report export process was running
- Fixed an issue where 2 variable modifications with a combined delta-mass of 0 would cause a peptide to be treated as non-modified
- Improved error handling for experiments with individual runs that have 0 identifications