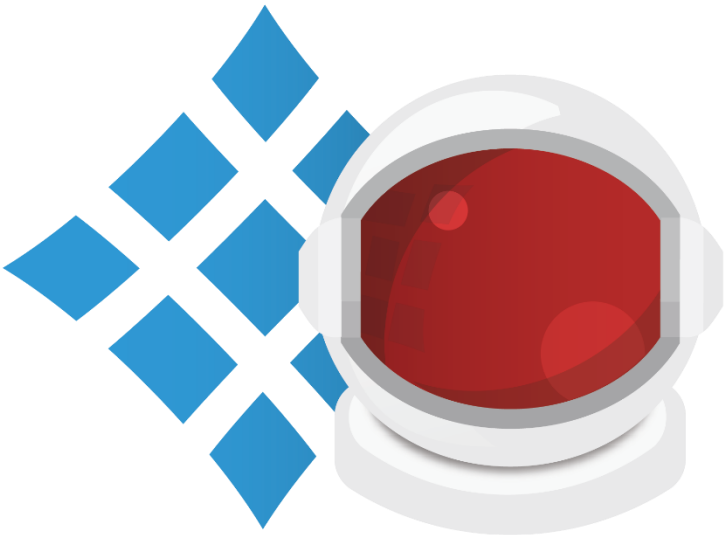

Spectronaut® 20

Release Notes

1 Powered by Kuiper

- Kuiper, a new search engine, boosts Pulsar for state-of-the-art unspecific directDIA analysis
- Introducing “PTM probing” open search mode for fast querying of potential PTMs
- Up to 85% faster unspecific (and semi-specific) directDIA search; independent of peptide length constraint
- Up to 80% more identifications for MHC Class I immunopeptides
- Up to 30% more identifications for MHC Class II immunopeptides and other unspecific searches
- Unparalleled speed without sacrificing scalability

2 Features for high data quality

- Improved FDR processes for higher confidence in protein identifications
- Added global precursor FDR, especially relevant for peptidomics study
- Added beta feature to improve confidence in identification from non-canonical protein database by calculating precursor FDR per group

3 Improved AI for unspecific peptides

- Up to 50% improvement in key performance metrics of deep learning models for unspecific peptides
- Novel scores improve identifications in unspecific searches

4 Improved quantification

- Improved processing of ion mobility dimension boosts quantitative accuracy for timsTOF

5 New visualizations for QC and biological insights

- New peptide motif plot based on Shannon entropy in post analysis
- New peptide length plot, per and across samples, in post analysis
- New precursor charge plot in post analysis
- Overlay identifications per charge in “IM overview plot” in the analysis perspective

6 Improved command line options

- Support for Apache Parquet format for exporting reports
- Support for providing settings for library generation step of directDIA via JSON filesSupport for explicitly specifying modification repository per analysis job
- Improved scalability and functionality for SNE combine pipeline
- Support for reading raw and fasta files directly from Azure object storage

7 New and Changed Analysis Settings

- [New default] DIA Analysis → Identification → Precursor Qvalue Cutoff (Experiment) → 0.01
- [New default] DIA Analysis → Identification → Single Hit Protein Rule → Stratified Single Hit Protein FDR
- [New default] DIA Analysis → Identification → Run level protein scoring → All Expected Observations
- [New default] DIA Analysis → Quantification → Perform Background Noise Removal
- [New default] DIA Analysis → Quantification → Perform IM Peak Picking for Quantification
- [New Option] Pulsar Search → Modifications → Search Mode → PTM Probing Search
- [Removed Option] DeepQuant Correction [Beta] feature