Spectronaut™

powered by Pulsar

Spectronaut® 16

Release Notes

1 More Identifications

- Improved identifications with new machine learning framework
- Improved identifications with new DeepLearning score models
- Up to 17% more precursor and 10% more protein groups identifications for directDIA
- Up to 25% more precursor and 15% more protein groups identifications for library based DIA analysis
- New "1-step" hybrid library workflow via directDIA enrichment

2 Pulsar Database Search Engine

- 30% faster directDIA and DDA searches
- Improved machine learning and scoring

3 Deep-learning Augmented Improvements

- Added DeepXIC scoring model for improved identifications
- Novel Deep PSM scoring model for spectrum centric analysis

4 New Post Analysis Features

- Ranked protein groups in post analysis perspective now reflects quantity IQR per protein
- Added principal component contribution bar plot to PCA plot

5 Improved User Experience and Visualization

- Streamlined settings for clarity with new advanced category
- Streamlined quantification settings by replacing q-value sparse with new imputation strategy "Use Background Signal"
- Added condition box plot in the protein grid view
- Added mass error histogram at run level in analysis perspective
- Added DIA acquisition method overview at run level in analysis perspective
- Improved data completeness plot to easily tell how many proteins, precursors were identified in x% of samples
- Library ion mobility 1/k0 distribution plot in library perspective
- Export peptide precursor list from library via right-click option
- Switched to 2-color (Green and Red) system for identification status annotation
- Swapped heatmap colors in analysis protein grid view (red = high, blue = low) based on user feedback
- Added condition box plot in analysis protein grid view

6   Other Changes

6.1.1   DIA Analysis Settings Changes

- JSON settings override for more flexible pipeline integration
- Changed default quantification setting back to q-value without imputation based on user feedback

6.1.2   directDIA Analysis Settings Changes:

- Improved flexibility for directDIA analysis settings
- Added option to disable MS2 Index filtering

7   New Downloadable Content

- Added a high-quality Hela search archive as a resource for Hela DIA analysis
- Added search archive from our new plasma publication (Tognetti et al., 2022, JPR)
- Added Uniprot protein databases from January 2022