

SpectroMine 2 Release Notes

Improved Identifications

- Machine Learning
- Prediction of retention time and fragmentation with deep learning

Improved Performance

- MS2 index to speed up searches with many modifications
- Improved management of the temporary folder

Improved ILQ Support

- Missing value imputation for ILQ experiments
- Improved EASI-tag quantification
- Peak-to-threshold and signal-to-interference filters for ILQ with Thermo
- Option to exclude single hit proteins from quantification

New Workflows

- Searching from a library instead of a FASTA file
- Support for EThcD fragmentation
- Improved ion mobility support
- Improved support for MaxQuant.Live data

Visualizations

- Added to Analysis Perspective: quantity bar plots, fragment intensity prediction
- Added to Post Analysis Perspective: digestion efficiency, LFQBench
- Improvements to plots in Analysis and Post Analysis Perspective
- “Many Run Visualization” option for plots in Post Analysis Perspective

Other Features

- SpectroMine Viewer is available now for browsing of already analyzed experiments
- Unpaired t-test for differential abundance