SpectroMine™ 5

Release Notes

1 Powered by Kuiper

- Kuiper, a new search engine, boosts Pulsar for state-of-the-art unspecific analysis
- Introducing “PTM probing” open search mode for querying unknown PTMs
- On average 84% faster unspecific search; independent of peptide length constraint
- On average 23% more peptide identifications for immunopeptidomics class I data
- Unparalleled speed without sacrificing scalability

2 Pulsar Improvements

- Uses the latest version of Pulsar search engine
- Fixed issue with modifications using "terminus specificity" during Pulsar search
- Fixed incorrect composition of Hex(1)HexNAc(1) in modifications database

3 Linux

- Linux support via command line (Bruker and Thermo)
- Cloud readiness thanks to linux support
- Added possibility to import and export custom digestion rules for SpectroMine Linux

4 Deep Learning

- Up to 50% improvement in key performance metrics of deep learning models for unspecific peptides
- Improved property prediction models for unspecific searches

5 Library Generation Improvements

- Improved memory management during library generation
- Fixed crash when trying to analyze timsTOF DDA data for library generation
- Fixed issue during library generation when using variable modifications containing heavy isotopes
- Fixed issue with parsing .d raw files in library generation workflow

- Fixed issue with modification parsing in library generation from external search engines

6 User Experience Improvements

- Added violin plot option for all box plots
- Added option for providing settings in a JSON file in command line mode
- Added feature of exporting reports in Apache Parquet
- Added peptide length plot, per and across samples, in post analysis
- Added precursor charge plot in post analysis
- Improved motif plot on run level based on Shannon entropy in post analysis
- Changed all files exported as .XLS to .TSV
- Fixed issue with non-ascii characters in file path for timsTOF API

7 Security

- Updated to .NET 8 (current long term support version of .NET)
- Patched known vulnerabilities in 3rd party libraries

8 New and Changed Settings

- [New] Search → Labeling → Channels → added 2 more channels
- [New] Search → Modifications → Search Mode
- [New] Experiment → Experiment-Wide Parameters\Post-Analysis → Log2 Ratio Candidate Filter
- [New] Experiment → Experiment-Wide Parameters\Post-Analysis → Confidence Candidate Filter
- [New] Experiment → Experiment-Wide Parameters\Post-Analysis → Confidence
- [New] Experiment → Library Generation\Identification → Use Source Specific iRT
- [New] Experiment → Library Generation\Spectral Library Filters → Overlapping between Channels