

Progenesis LC-MS v4.1 – benefits and features of the current release

Benefits

- **Reduce the time spent at your computer** by applying key data processing steps to all your runs automatically and objectively as they load
- **Be confident that your analysis will deliver reliable results** and data variance is minimised with objective measures of your LC-MS run alignment

Features

Version 4.1 includes automation of key analysis steps to **increase objectivity** and **free-up your research time** as well as other features added in response customer feedback:

- Reference run selection and alignment can be started and left to process the runs automatically as they load
- Automatic reference run selection increases objectivity and reproducibility of analysis results
- Report the quality of automated alignment, giving you confidence that downstream analysis steps will deliver the most reliable results

Automated data processing summarised in Progenesis LC-MS v4.1



1 Choose the runs to import, apply automatic reference run selection and alignment - then walk away!

2 Review alignment quality metrics (and edit if needed) to ensure consistent and reliable results are generated downstream

3 Automatic peak picking and normalisation to directly compare peptide abundance across the groups you set

Review Alignment
Align peptide ions to compensate for drifts in retention time by dragging them up or down in the Vector Editing window.

| Run | Include? | Vectors | Score |
|-----|-------------------------------------|---------|-------|
| A1 | <input checked="" type="checkbox"/> | 206 | 83.4% |
| A2 | <input checked="" type="checkbox"/> | 255 | 84.4% |
| A3 | <input checked="" type="checkbox"/> | 241 | 85.4% |
| C1 | <input checked="" type="checkbox"/> | 388 | 98.9% |
| C2 | <input checked="" type="checkbox"/> | Ref | |
| C3 | <input type="checkbox"/> | 0 | 54.7% |

Alignment quality: ● Good ● OK ● Needs review

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The new data processing workflow

- Check the quality of your LC-MS system with each run displayed as an ion intensity map once they are loaded
- Walk away as reference run selection and alignment are applied as your runs are loaded
- Automated reference run selection as the software chooses the one that gives the best alignment scores (see below) for all your runs
- Reviewing alignment quality scores means you can be confident that applying the next automatic step, peak picking and normalisation, will achieve the best analysis results possible
- Visualise alignment quality with a simple red/orange/green colour-coded grid overlaid across each run
- Immediately see the effect adding manual alignment vectors has on the alignment scores, should editing be required
- Reduce automated processing time by selecting a single run or a limited set of runs, which routinely produce the best alignment scores, for the software to choose a reference from

Additional new features and enhancements

Experiment design set-up from files

Experiment design files, your run file names organised into the groups that you would like to compare for relative protein expression, can be imported and applied from a CSV file or Waters MassLynx .SPL file.

Faster review of any step in a completed analysis

Once peak picking and normalisation are completed you can navigate straight to any analysis screen without having to move backwards or forward while saving or re-analysing at each step.

Progenesis Improvement Program

You can opt-in to this as you start the program or at any time via the file menu at the front screen. This provides information, including usability of each screen, to our software development team. This information will help us improve software updates available to you.

Clip Gallery

This has been added to some of most important data display screens so you can select and save a catalogue of print-quality images for sharing your results as you review your completed analysis.

User interface changes and bug fixes

- Bruker file loading, including Maxis data, is faster and more reliable
- mzML file loading option is included as standard
- View your experiment properties by selecting from the file menu
- Selecting retention time limits is an added option for peak picking parameters
- The list of runs to include in peak picking has a "select all" function to help choose which ones influence co-detection before peptide ion detection is applied consistently across all runs