Progenesis LC-MS v2.6 – new features in the latest release

Version 2.6 of Progenesis LC-MS is now available with a wide range of new features developed in response to feedback from our customer base. Highlights in the new release include the addition of detection parameters, a new experiment design set-up and the option to visualise the results of normalisation. Progenesis LC-MS v2.6 also works on Microsoft Windows 7.

Feature highlights include:

Full control over detection parameters
There are several new options which allow you full control over the feature detection process.

Sensitivity
You now have the option to adjust the sensitivity of the detection algorithm, with a choice of methods. Each method examines the intensities of groups of MS peaks to judge if they are likely to form part of a peptide ion or whether they represent noise and so should be ignored.

Automatic
- Uses a noise estimation algorithm to determine the noise levels in the data and sets a default sensitivity which is adjustable so you can fine tune the level

Absolute ion intensity
- Groups of peaks with an intensity less than the value you define are regarded as noise and therefore ignored

% Base Peak
- Peaks with an intensity less than a given percentage of the most intense peak are ignored
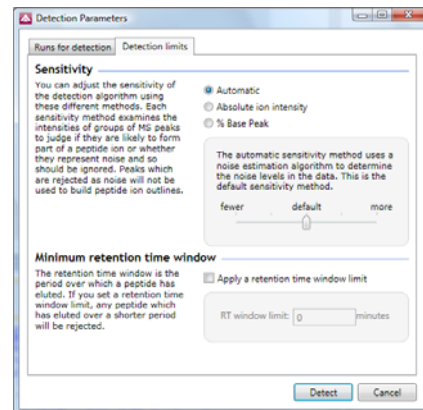
Minimum retention time window
There is the option to set a minimum retention time window. The retention time window is the period over which a peptide has eluted. If you set a retention time window limit, any peptide which has eluted over a shorter period will be rejected.

Runs for detection
You can select which runs you want the feature detection algorithm to use when generating the detected features outline map. All of the runs still have the final outlines passed to them and are measured as part of the experiment.

Further developments to feature detection
We have invested significant time and effort on improvements to the peptide detection algorithm. These new developments mean less fragmentation in the time dimension and noticeable improvements in the algorithm's ability to distinguish between streaks and real peptide ions. The end result is more accurate detection of peptide ions which saves time further down the workflow.

Additional Features for Data Quality Control

Normalisation

You can now visualise the results of normalisation on a scatter plot and the normalisation factor for each run. You can then take corrective action to ensure experimental quality is maintained.

You now have the option to choose whether to use raw abundances or normalised abundances in your experiment. For example, if the assumption that a significant number of features are not changing is invalid, you can turn off normalisation.
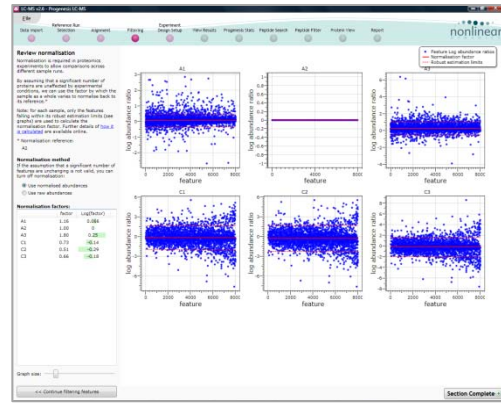

Calculation of CVs

Coefficient of Variation or CV is a useful measure to show peptide ions with a high variance in measurement between runs. The CVs are calculated at the experimental condition level so a low variance is expected. You can export the values and produce a plot of the CV data to help you determine whether there is too much variance within the experimental condition. This gives you added confidence that your results are showing real changes.

Increased flexibility in the type of experiment design you can analyse

The addition of a second experiment design option allows the comparison of different samples from the same subjects, under different conditions. The software then performs a repeated measures ANOVA – the appropriate statistical test for this type of experiment. An example of where you would use this is for the analysis of a time-course experiment.
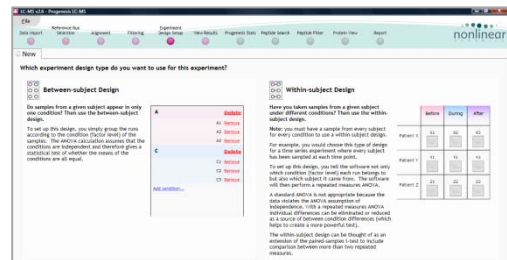
Improved data import from external statistical analysis packages

You can export your data out of Progenesis LC-MS if you wish to perform some statistical analysis using external stats software. You can then import your set of interesting peptide ions back into Progenesis LC-MS, applying a tag to identify them. This means you can apply statistical tests using third party software that are specific for your research needs.

Additional New Features

- Works on Microsoft Windows 7
- Can handle Waters' lock mass correction for .RAW format data which is used to calibrate the *m/z* values in the sample data
- There is a new file handler, available separately, which allows you to import peptide identification results from Waters MS^E data generated by ProteinLynx Global SERVER™ (PLGS)
- Has more robust handling of chemical noise so it does not affect peptide detection
- Independent contrast setting for alignment target and run being aligned in alignment step
- All of the alignment views can be expanded so you can get a more detailed view of the runs being aligned
- Data table in View Results expands to reveal additional fields:
    - Max CV (%)
    - Highest Mean
    - Lowest Mean