

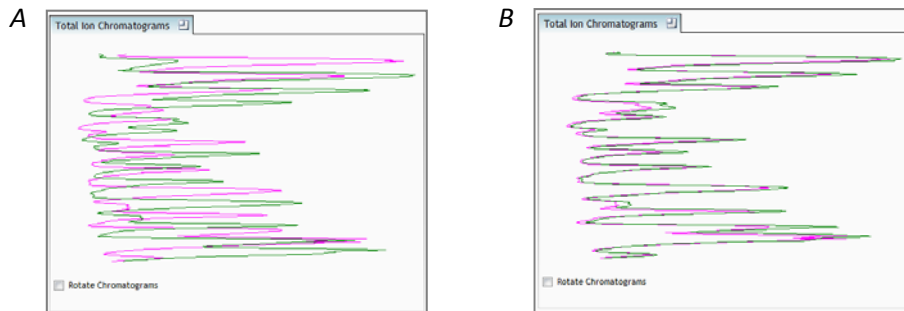
Progenesis LC-MS v2.5 – new features in the current release

The new version of Progenesis LC-MS is now available with further improvements and refinements to ensure that it remains at the forefront of label-free LC-MS data analysis. Particular attention has been focussed on the filtering and management of MS/MS data and peptide search results to further streamline the workflow.

Here is a summary of the new features:

Total ion chromatogram (TIC) view to aid alignment verification

The new TIC view in the alignment step allows you to easily verify the accuracy of alignment providing an additional quality check and increased confidence in your results.



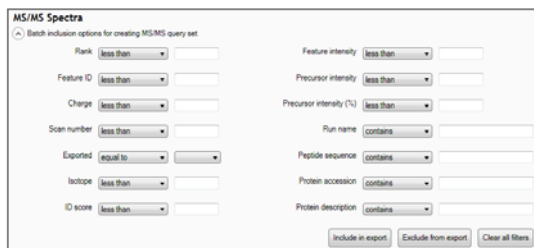
TIC view – before (A) and after (B) alignment. Magenta line shows the alignment target and the green line shows the run being aligned.

Manually added alignment vectors override automatically generated vectors

The addition of a manual vector will now override any automatically generated vectors in close proximity. This increased weighting on manual vectors gives you more control over the alignment process and makes it easier to accurately align difficult data.

Filtering of MS/MS spectra prior to export

Often MS/MS can generate many thousands of spectra which some search engines cannot handle. New filter options enable the removal of spectra from your search before they are exported for identification, reducing the amount of data sent to the search engine. This makes a significant difference to the time taken to perform searches.



Wide range of easy-to-use filter options to remove spectra from your peptide search

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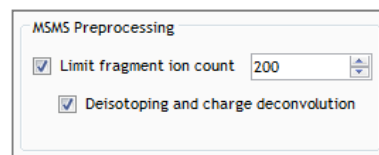
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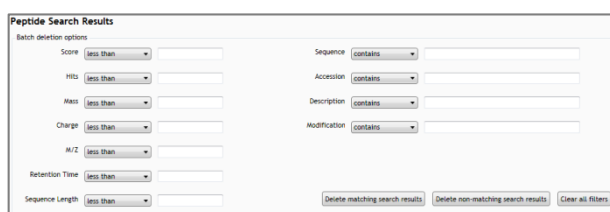
The new MS/MS peak processing reduces the size of the spectra by removing the noisy peaks and retaining only the essential data required by the peptide search engines. This reduces the data file size, improves the quality of search results obtained and also reduces the number of false positives.



MS/MS pre-processing reduces the size of each spectra

New Peptide Filter step

When you have imported the peptide identifications back into Progenesis LC-MS, the new Peptide Filter step allows you to filter out identification results, rapidly reducing the number of incorrect assignments. Examples of identifications you may want to remove could be those associated with hypothetical proteins, those with a low score, or those with an incorrect taxonomy. As a result you can save time in reviewing the search results and quickly focus on the relevant data.



Range of filter options to reduce number of peptide identifications for review which dramatically speeds up the workflow

Additions to the Protein View

If you applied tag filters to peptides in the earlier steps of the analysis, they are now shown at the protein level so you can filter the displays by their tags. This allows you to highlight the interesting proteins based on significant measurements made at the peptide level.

The protein list has a new “conflicts” field. This allows you to order and target your conflict resolution using the data displays and views to confirm your findings.

Accession	Peptides	Conflicts	Score	Anova (p)*	Fo ^
gi1126701091	1	6	87.5	0.00151	2.9
gi16652833	1	6	87.5	0.00151	2.9
gi1224477091	1	6	87.5	0.00151	2.9
gi115674808	1	6	87.5	0.00151	2.9
gi123100430	1	6	87.5	0.00151	2.9
gi1150388193	1	6	87.5	0.00151	2.9
gi152082213	1	6	87.5	0.00151	2.9
gi1153953101	1	3	58.8	0.0119	3.2
gi1218288237	1	3	58.8	0.0119	3.2
gi138327294	1	3	50	0.0119	3.2

Protein table ordered by number of conflicts

Additional Improvements:

- It is now possible to import and analyse a single data file
- There is a new option to import and analyse low noise FTMS data
- In View Results there are additional data fields in the Feature Details table:
 - Retention time window – shows the length of time over which the feature was eluted
 - Maximum group mean intensity – allows you to select more reliable features for targeted MS/MS
- In View Results you can now delete multiple features in bulk
- There is a new, interactive HTML protein report containing protein and peptide information
- We offer increased flexibility in exporting inclusion lists
- We also offer increased flexibility in importing peptide identifications