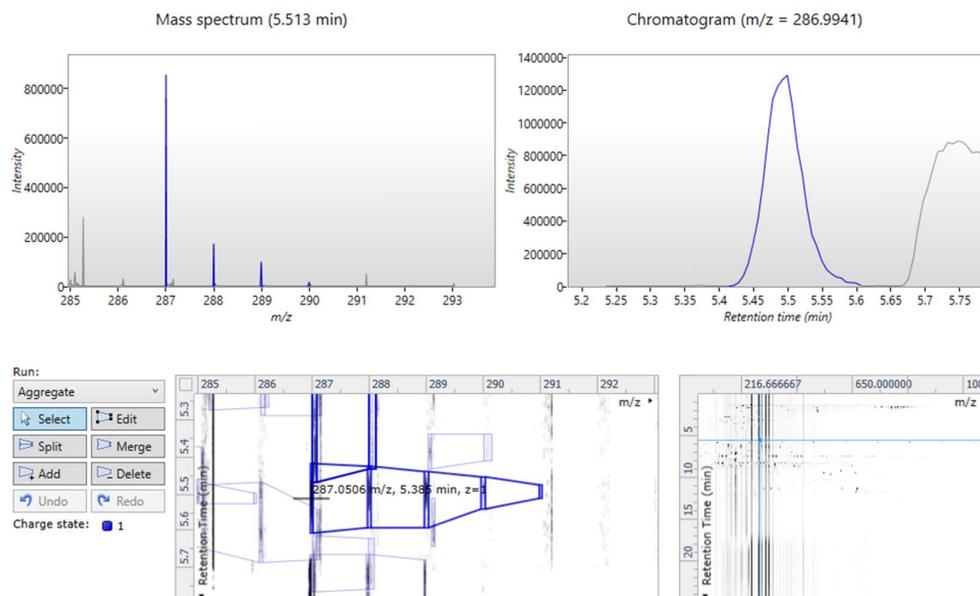


## What's new in Progenesis Q1 v3.0?

The latest release of Progenesis Q1 helps scientists to overcome challenges in their research by offering some significant new developments. At the same time, attention has been paid to the usability of Progenesis Q1, making it even more enjoyable to use.

### Peak Editing

Peak Editing functionality has been added to Peak Picking View allowing the ability to review and then manually re-integrate, delete, split, merge and add new peak selections. This includes the ability to multi-delete peaks.



### Support for Waters METLIN LC/MS/MS library 2019

Progenesis Q1 version 3 adds support for the forthcoming Waters METLIN LC/MS/MS library 2019.

With this second version of the industry leading metabolomic resource, all MS/MS data are now experimentally derived. We have also included support to integrate Waters CCS measurements which have been generated using a research version of our new CCS prediction algorithms which utilize machine learning approaches. With Waters ion mobility data, you will now be able to filter the Waters METLIN search results that match a CCS tolerance.

### Identify Compounds

Select your identification method:

[About this method](#) | [Download others](#)

- Filter the compounds**  
Using the list below, [filter the compounds](#) to show only those you want to identify.
- Choose search parameters**  
Select your METLIN search parameters or create a new parameter set:
- Search for identifications**  
After searching, identifications will be assigned to the relevant compounds automatically.

### METLIN search parameters

Define a set of METLIN parameters that can be saved for later reuse. [Learn more in the online reference.](#)

Name:

Search tolerances

Precursor tolerance:  ppm

Fragment tolerance:  ppm

Composition filters

Elemental composition:

C: 0-100 H: 0-150 N: 0-10 O: 0-30 P: 0-2 S: 0-2

Include CCS predictions in the output table

CCS predictions were generated using a machine learning approach as part of a Waters research project (CCSondemand). These predictions may change in the future as the Waters model is improved and enhanced. [Learn more in the CCSondemand online reference.](#)

Use CCS difference to limit matches:  %

### Adduct measurement export

We have improved the export functionality so you can now export individual adduct measurements to a CSV file.

### Peak picking performance improvements

We have made some changes in the peak picking algorithm to improve the detection of peaks with long fronting or long tailing.

### Improved data compatibility

- Updated Agilent plugin to support recent data format changes
- Support for importing Waters RDa data with dynamic lockmass correction from UEP files

### More pathway analysis options

We have added a new plugin to export metabolite identifications to MetaCore, a Cortellis solution, which allows for comprehensive pathway analysis to be conducted for multi-omic datasets. Metabolite IDs need to be KEGG identifiers. Now matching the capabilities of Progenesis QI for proteomics.

You are entitled to the latest version of Progenesis QI if you have an [active maintenance plan](#). Please [contact us](#) if you would like to review your maintenance plan.