# Progenesis CoMet v2.0 – benefits and features of the current release

## Benefits:

- **One streamlined package** to quantify-then-identify the significantly changing compounds in a complex mixture
- **An objective approach to analysis** using a complete matrix of data, with no missing values, for reliable multivariate statistics
- **Automatic deconvolution of ions** to generate a list of experimentally-significant compounds, including chemical structures, which you can easily share or validate
- **MetaScope, our search tool, is included** so you can search your databases and combine compound identifications, including chemical structures, with quantification data

## Key features of the current release

The latest version was developed based on feedback to previous versions by metabolomics researchers. As a result new data visualisation screens and analysis steps have been created and added specifically for measuring relative compound abundance and providing identification of compounds. A summary of the new features and workflows compared to version 1.0 are below: (*features added to current version compared to version 2.0 *beta*).

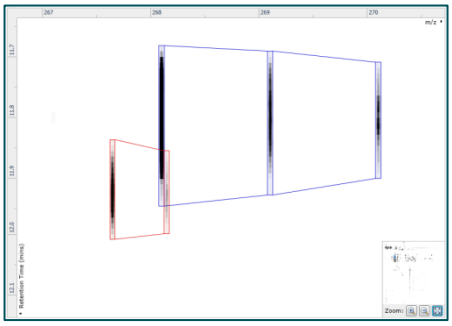
## Data import

At the start of the workflow you select a list of possible adducts present in your samples, which allows for automatic deconvolution of compound ions. A standard list of adducts is provided with the option to add your own specific adduct ions.

## Data analysis

### Peak picking

Improvements to the **automatic peak picking** algorithm have made it more sensitive to detect single isotope peaks and measure overlapping compound ions.



A new screen in the peak picking step, displaying an ion intensity map of the results, allows you to review and optimise peak picking before comparing relative compound abundances between samples. Options have been added to edit peak picking parameters to optimise detection of ions within your own samples if required.

### Normalisation

A total of **five methods** are now included to support commonly requested normalisation strategies:

- Normalise to all compounds
- Normalise to a set of known compounds native to your sample
- Normalise using total ion intensity*
- Normalise to external standard*
- No normalisation applied

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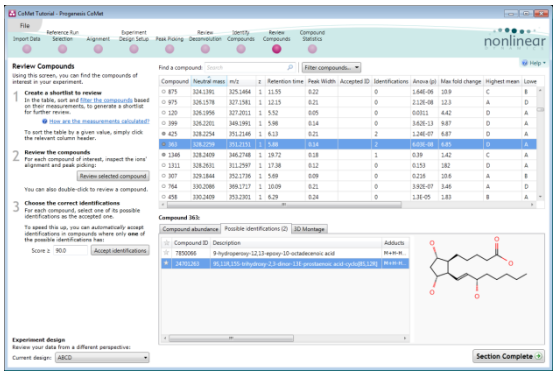
## Compound Identification

**MetaScope**, our our own compound identification tool, is included so you can directly search your own compound data based on neutral-mass or m/z and, if it is available, RT with tolerances as well.

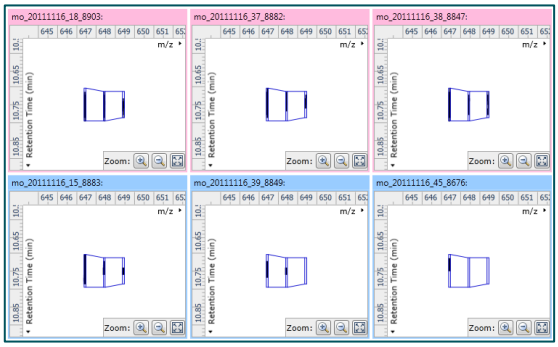


MetaScope search results, with a **compound identification score** applied, are automatically associated with the quantified compound ions so quantitative and qualititative data are bought together within the software. MetaScope also supports **SDF database searches** to display chemical structures alongside compound identification and quantification results *

## Reviewing analysis

### Review compounds

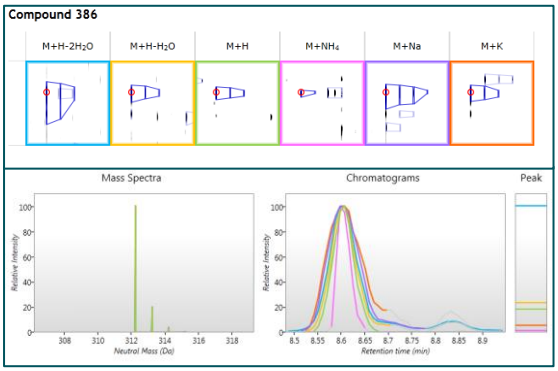
**Ion intensity maps, 3D views, mass spectra and chromatograms** are now displayed for each compound ion on all runs to provide quality assurance of peak picking and alignment*. You can **edit peak picking** on any ion by adding or subtracting isotopes*. Our unique analysis approach means that an edit on one run is applied instantly and consistently to the same ion across all runs.



Compounds with more than one possible identification can be reviewed and **one can be selected as the correct one** based on your understanding of the samples and experiment. Alternatively, you can simply export a final list of all possible compound identifications to review or provide the basis for targeted compound analysis.

### Review deconvolution

A new-step to **review all the compound ions used to quantify and identify a compound**. Mass spectra and extracted ion chromatograms are also displayed for each compound ion, showing how similar they are. This is useful in checking the quality of data underlying each quantified compound.




If any compounds ion appears as an outlier in terms of its m/z and RT characteristics, within expected limits, it can be removed. Likewise, you have the opportunity to look if a compound ion appears at an expected position on the ion intensity map and, if it is present, add it to the compound quantification.

## Additional new features and enhancements

- **Import experiment design files** to automatically set up the groups you need for relative quantification of compounds across hundreds of runs.*
- **Ability to export the raw abundance** of every isotope peak for every adduct.* This is in addition to the two main data export option already included (compound measurements and compound identifications).
- **Normalised adduct abundance displayed** for each run and each adduct to show trends within an experiment and highlight any inconsistencies.