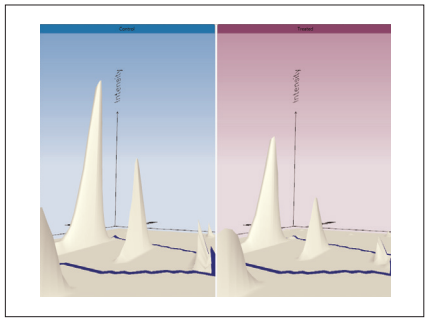
[PRODUCT SOLUTION]

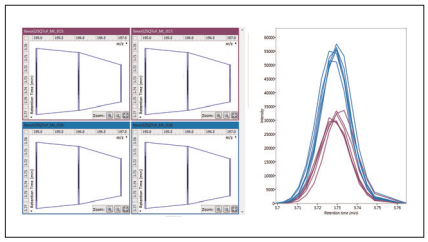
nonlinear DYNAMICS
A Waters Company

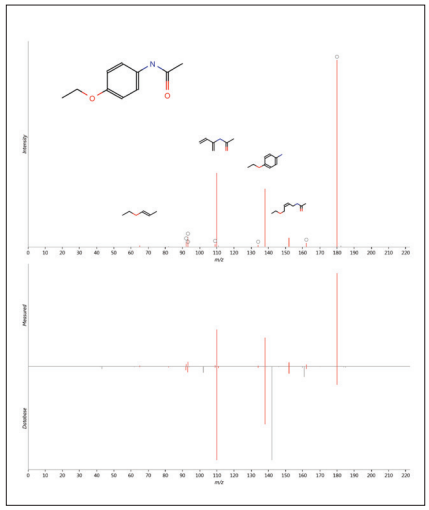
The next generation in LC-MS data analysis software.

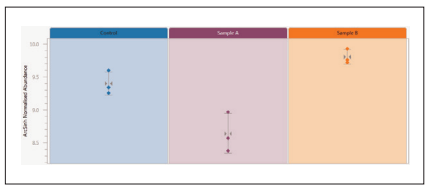
Discover the significantly changing compounds in your samples.

Progenesis® QI enables you to accurately quantify and then identify the compounds in your samples that are significantly changing. With support for all common vendor data formats and a guided workflow, Progenesis QI software helps to overcome your data analysis challenges, enabling you to rapidly, objectively and reliably discover compounds of interest and export results for 'omics research applications.









Solving your analysis challenges

- Consistent peak picking across all runs, vital for accurate and precise quantification, using our unique approach to co-detection of compound ions.
- Flexible compound search methods with LipidBlast, ChemSpider, Elemental Composition, METLIN, and our own search tool, MetaScope.
- Compound identification using exact mass, MS/MS fragments, isotope distribution, retention time (RT) and collisional cross-sectional area (CCS).
- Complete data matrix and no missing values, for reliable multivariate statistics.
- Comprehensive data export options that allow you to combine results with other informatics data streams and create publication quality reports.
- Powerful data visualization and guided-workflow for DIA and DDA analyses of large numbers of samples in one package.

"Progenesis QI has become the standard software for processing our metabolic profiling data, it has increased our processing speed, from aligning chromatograms up to identifications of significantly changed metabolites, with at least a factor of 10!"

GEERT GOEMINNE
VIB Department of Plant Systems Biology, Ghent University, Belgium

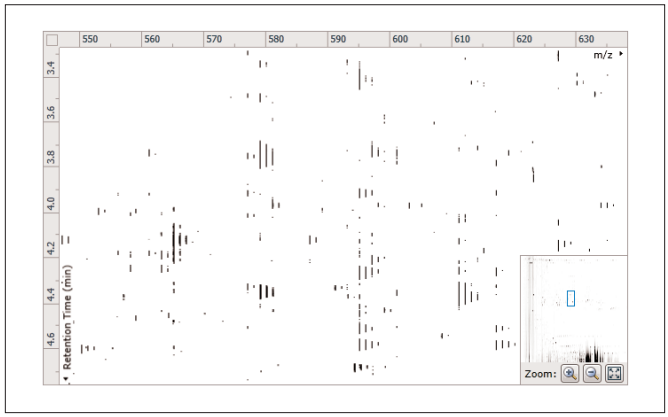
Progenesis® QI

PROGENESIS QI – KEY STEPS IN LC-MS DATA ANALYSIS

Quantify

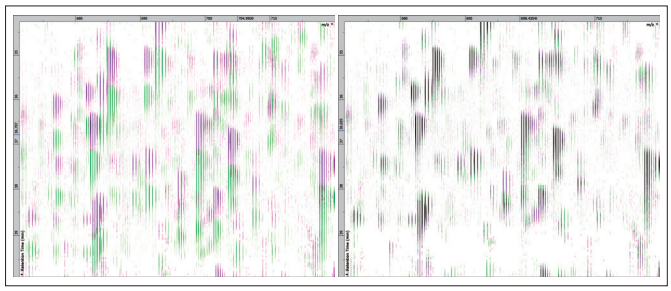
Raw data import and quality control

- Define multimers and adducts present in your samples for automatic compound ion deconvolution
- Supports positive or negative ionization mode data as well as polarity switching
- Highlight raw data quality before you proceed with analysis with ion intensity maps representing RT vs. m/z vs. ion intensity
- Optional auto processing wizard to move from Data Import to Compound ID and free up your research time



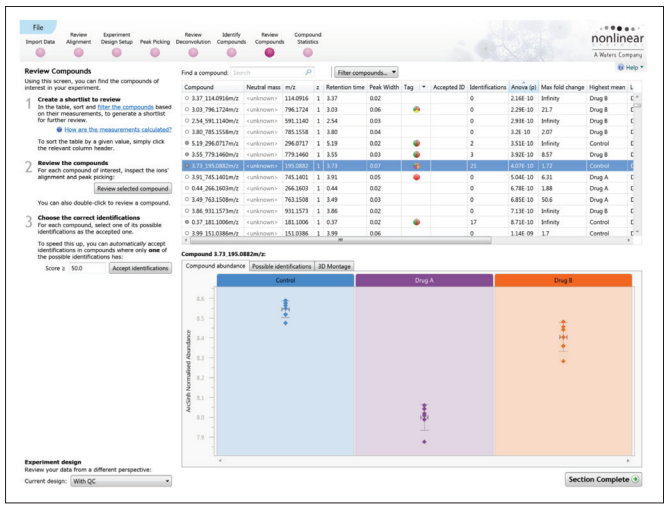
Retention time alignment

- Correct RT differences in complex datasets containing multiple spectra
- Measure the quality of your automated alignment to give you confidence that downstream analysis steps will deliver the most reliable results
- Create a single “aggregate run” containing all the compound ions from your sample runs, to confidently peak pick and compare the same compound ion across all samples



Peak picking, normalization and quantification of compound ions

- Minimize data variance and increase sensitivity with alignment and co-detection of ions across all replicates
- No missing values, no matter how many replicates you run
- Optimize analysis with user control of peak picking parameters and normalization methods
- Quantify across any number of groups and high numbers of runs in one experiment
- Uniquely take advantage of ion mobility separated isobaric peaks for accurate quantification
- Visualize LC-MS analysis data to easily interrogate and verify your results



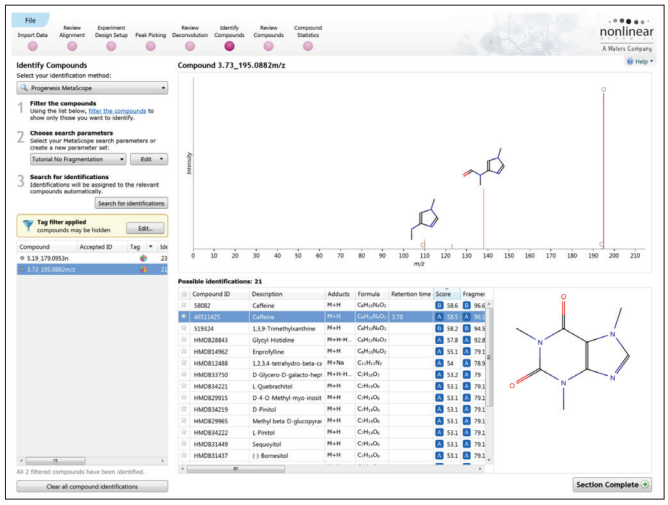
Identify

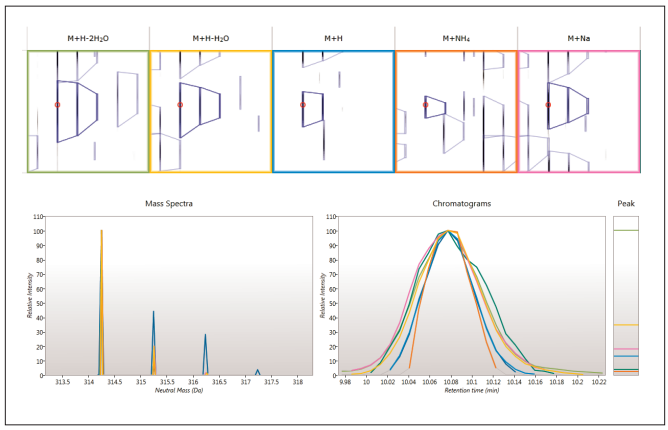
Identify and review compounds

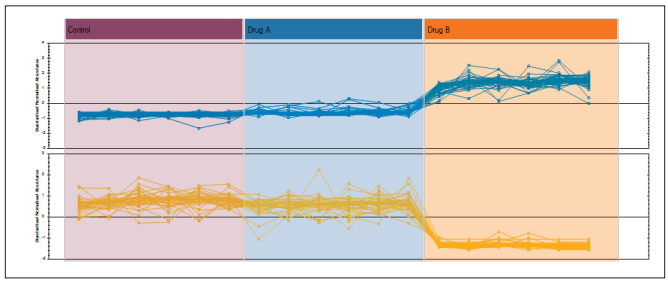
- Flexibly search compound data using LipidBlast, ChemSpider, Elemental Composition, METLIN, or our own search method MetaScope
- Reduce false positive IDs by using multiple search parameters: exact mass, MS/MS fragments, isotope distribution, RT and CCS
- Import identification results, including chemical structures from SDF databases and embedded web-links to compound details
- Quickly find significantly changing compounds (e.g. Anova p-value, fold-change, power)
- Visualize relative compound abundance using compound abundance profile graphs
- Comprehensive data export options to easily integrate results with other bioinformatics platforms
- Review and edit the compound adduct deconvolution used to quantify and identify a compound

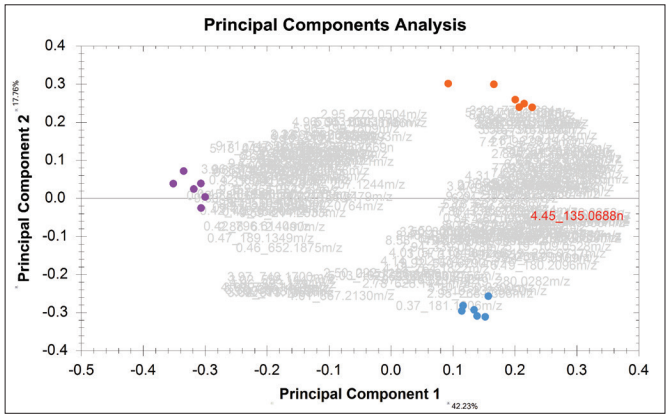
Statistics

- Discover the compounds that define the biological differences between your samples with easy-to-use multivariate statistics, including Principal Component Analysis (PCA) and Correlation Analysis
- Determine false discovery rate using q-values to control false positives (Type 1 error) and Power Analysis to control false negatives (Type II error)
- Utilize streamlined two-way integration with Umetrics EZinfo statistical analysis software









Find out how you can quickly and confidently generate results with our powerful, easy-to-use software, with the benefit of full-technical support: www.nonlinear.com/ProgenesisQI

"Progenesis QI gives an accurate and fast data processing experience using a user friendly workflow approach. Within the same data set you can switch between different experimental designs with the statistics updating in seconds, a key tool for complex metabolomics experiments involving many different groups."

MIKE DICKINSON
The Food and Environment Research Agency (FERA), York, United Kingdom

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