Progenesis® QI - benefits and features of the current release

Version 1.0

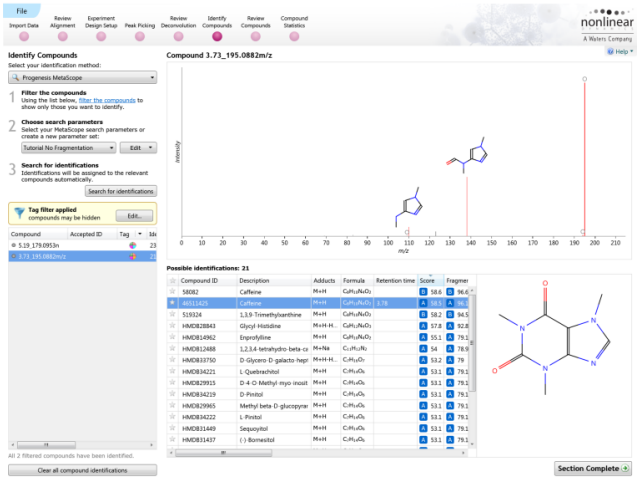
Progenesis QI enables you to accurately quantify and then identify the compounds that are significantly changing in your samples. With support for all common vendor data formats and a guided workflow, Progenesis QI software enables you to rapidly, objectively and reliably discover compounds of interest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

Why the new branding?
Nonlinear Dynamics was acquired by Waters Corporation in August 2013 after a successful partnership where Nonlinear supplied a customised version of Progenesis LC-MS under the TransOmics™ Informatics name to support analysis using the enhanced and unique functionality available with Synapt G2, G2-S and G2-Si high definition mass spectrometers. With this latest release we have combined the functionality of the two separately branded software products, Progenesis CoMet and TransOmics Informatics, into one offering. Progenesis QI maintains the Progenesis heritage and focusses our resources in delivering a single world-leading informatics platform or omics data analysis. It is appreciated that modern laboratories often have instruments from multiple vendors and thus, the software will continue to support LC-MS data from the majority of sources.

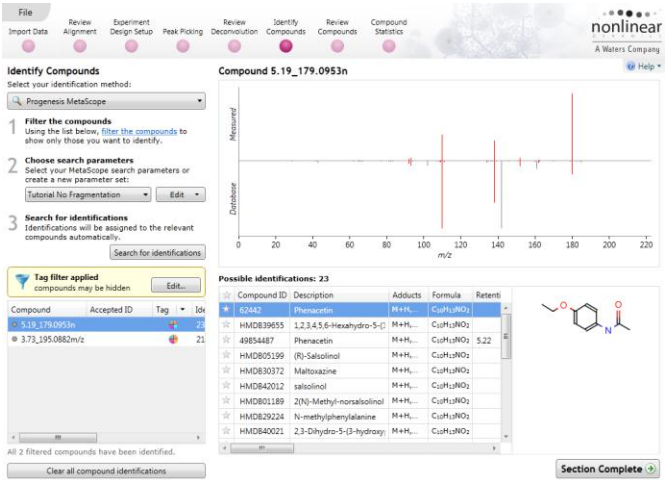
New features

Compound identification using fragmentation data with MetaScope
Progenesis QI now allows you to search for compound identifications based not only on neutral mass, isotope distribution and retention time (if data was available) but also using MS/MS fragments and collisional cross-sectional area (CCS). These additional parameters greatly improve the specificity of your database search and the likelihood of a correct compound identification.

- **Perform theoretical fragmentation:** Your experimental fragmentation data is compared to theoretical fragmentation patterns generated by the simulated breaking of bonds in the structures of possible identifications. The resultant data is scored to provide convenient guidance for acceptance of identifications.
- **Perform fragment-ion database search:** Your experimental fragmentation data is compared to known fragmentation patterns of a library of compounds, which are stored in a fragment database you have created or accessed on-line. The resultant data is scored to provide convenient guidance for acceptance of identifications.
- **Create your own fragment-ion databases.** This feature allows you to export MS/MS spectra and create your own databases of accepted identifications for use in future ID searches.



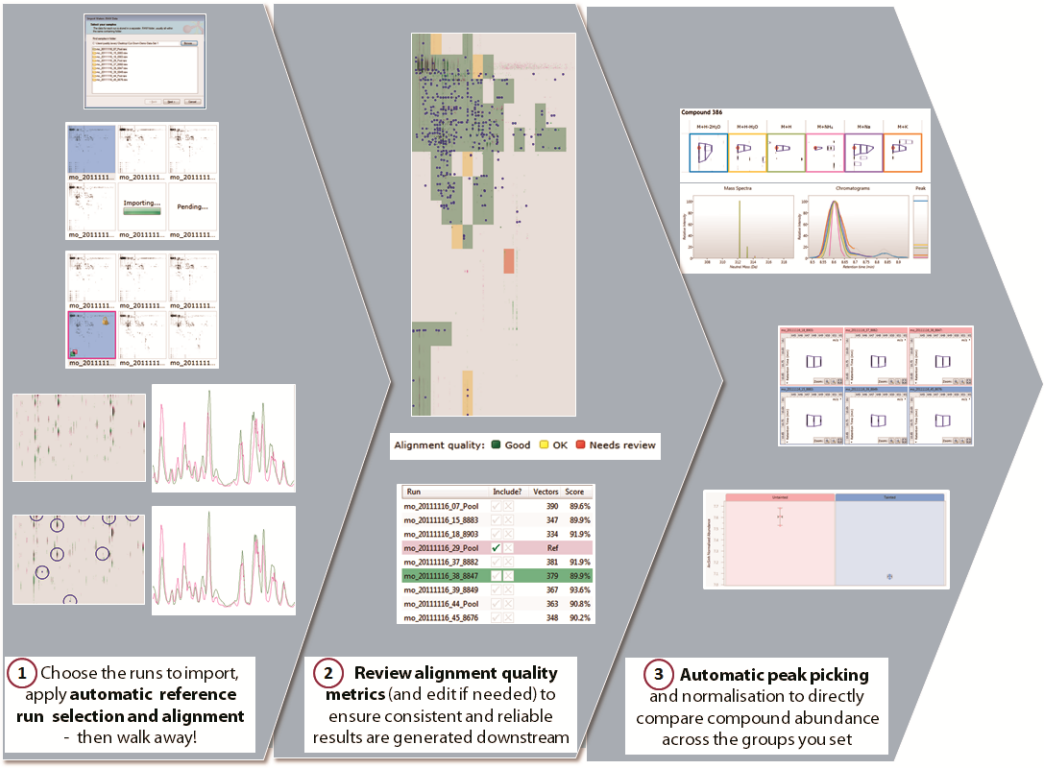
Theoretical fragment ion prediction and comparison with experimental



Comparison of experimental data with empirically derived fragment ion databases

Nonlinear Dynamics Ltd.
Keel House, Garth Heads, Newcastle upon Tyne, NE1 2JE, UK **[T]** +44 (0) 191.230.2121 **[F]** +44 (0) 191.230.2131
Americas Sales Office.
2530 Meridian Parkway, 3rd Floor, Durham, NC 27713 U.S.A.
[T] +1 919.806.4401 **[TOLL FREE]** +1 866.435.7872 **[F]** +1 919.806.4301 **[E]** info@nonlinear.com **[W]** www.nonlinear.com

Automated data processing workflow
Decreases user hands-on time and speeds up data processing between data import and peak picking stages.



- Visually check the quality of your LC-MS acquisition with each data file displayed as an ion-intensity map once they are imported into the software
- Walk away as the software automatically selects a reference data file which produces the optimal alignment performance and scoring
- Review alignment quality scores to be confident that the next automatics steps (peak picking and normalisation) will produce the best possible results
- Visualise alignment quality with a simple red/orange/green colour-coded grid overlaid across each run
- If manual editing is required, immediately see the effect adding manual alignment vectors has on the alignment scores
- Throughout, processing times can be minimised by selecting a single or limited set of data files for consideration for reference selection. This is often useful when many replicates of very similar samples are being investigated.

Utilise Ion mobility data
Ion mobility MS separations are commercially unique to the Waters Synapt range of mass spectrometers and enable the separation of co-eluting isobaric analytes. Progenesis QI for proteomics uniquely takes advantage of this additional dimension of resolution to give improvements in accuracy and precision of identification and quantification. The highly visual nature of the software enables the user to view the full benefit of ion mobility separations for the analysis of the highly complex samples typically found in a bottom-up proteomics experiment.

Support for MS^E and $HDMS^E$ data-independent (DIA) analysis
As well as conventional data-dependent analysis (DDA), Progenesis QI for proteomics now supports the analysis of Waters MS^E and $HDMS^E$ data. Split-screen views show low-energy (parent ion) and high-energy (fragment ion) data functions as you import your data.

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Noise-reduction filter

As MS instrument performance continues to improve, we have introduced a new feature to allow user-control of the peak-modelling applied during import of raw data from high-resolution instruments. The new import filter strength tool provides more flexible control on the levels of background noise detected in your samples, which delivers faster analysis times per run and provides more reliable quantification of smaller but real features within each experiment.

Additional new features

- Support for direct import of AB SCIEX WIFF files
- Define multimers present in your samples for automatic compound ion deconvolution
- Additional quick-tags to help review the results of new identification features
- Compatible with existing experiments analysed by Progenesis CoMet and TransOmics for Metabolomics and Lipidomics
- MetaScope search parameters indicated for each compound identification, to avoid inappropriate comparison of score
- Performance and responsiveness improvements

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