TechnicalNOTE

Waters

QUANLYNX™ APPLICATION MANAGER

OVERVIEW

QuanLynx™, an Application Manager included with Waters® MassLynx™ Software, is designed for quantitative analysis. Simply acquiring mass spectrometry data is not enough. The ability to rapidly process LC/MS or GC/MS data to provide accurate quantitative information on sample batches is as important to today's analysts as the method and speed of acquisition.

QuanLynx automates data acquisition, processing and reporting; a diagram of this workflow is shown in Figure 1. The software incorporates a wide range of interactive reviewing tools that improve productivity, confidence and security when reporting quantitative results.

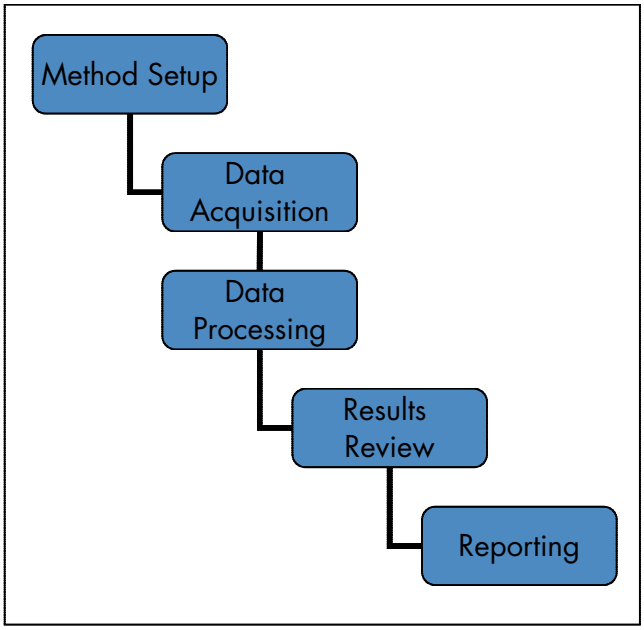

Figure 1. QuanLynx Application Manager workflow.

INTRODUCTION

The ability to accurately and rapidly reduce raw data to useful information is as important as the analytical technology employed. Waters MassLynx Software is available with a range of application-specific data processing tools to simplify raw data analysis.

The QuanLynx Application Manager provides accurate quantitative results from LC/MS and GC/MS data. The program operates on groups of data files to generate quantitative results sets. Results sets may be reviewed electronically, exported to LIMS or printed.

QuanLynx operates with all Waters mass spectrometers. The software is designed to simplify quantification from both routine screening and trace analysis. The application quickly generates results from acquired data sets permitting accurate quantification and review of results. Any required reprocessing is accomplished within the standalone results file.

The MassLynx data security model extends to QuanLynx. The electronic QuanLynx results file includes an internal audit trail, and allows the use of electronic signatures.

HOW QUANLYNX WORKS

QuanLynx methods define the processing parameters necessary to create a results set from the samples included in a MassLynx Sample List. Quantification methods may be applied to GC/MS, LC/MS or LC/MS/MS data in any acquisition mode (e.g. full scan or selected ion recording).
Data may be processed automatically when acquired or at a later time. The method editor is used to create a quantification method for all compounds assayed in a sample set. Results are then presented in a browser, which enables on-line review and re-processing of calculated results. It is a standalone file that may be viewed independently of MassLynx.

CREATING A QUANLYNX METHOD

The QuanLynx Method Editor (Figure 2) has a range of user-settable parameters to optimize integration, calibration, quantification, reporting and data export to other systems such as LIMS.

Configurable views optimize the functionality of the editor for particular applications. The views include:

- **All Parameters** – customizable to allow all parameters of interest to be viewed in a single pane
- **Compound Properties** – includes compound name, retention time, quantitation trace and concentration reporting limits
- **Calibration Properties** – includes calibration reference (internal standard), polynomial type and linearity threshold
- **Integration Properties** – includes smoothing parameters, peak detection and thresholding
- **Calculation Factors** – signal to noise measurement and detection limits

Method editor parameters can be stored for each compound of interest to build up a 'compound library' of parameters which aids creation of methods that are a subset or combination of those previously used.

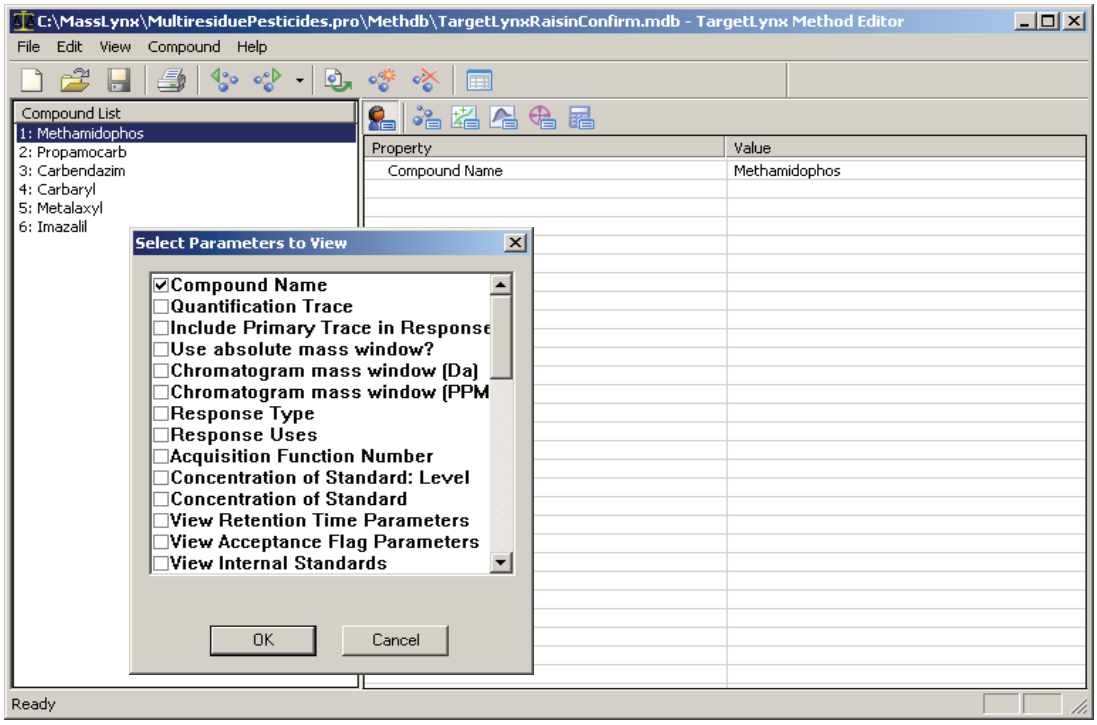

Figure 2. QuanLynx Method Editor showing parameter selection box.

QUANTIFYING SAMPLES

When processing from the MassLynx Sample List (Figure 3) settable processing options include:

- Acquire data
- Integrate samples
- Calibrate standards
- Quantify samples
- Report results
- Export results

Peak integration is accomplished with ApexTrack™, an advanced peak detection algorithm. The ApexTrack algorithm automates chromatographic peak detection and baseline determination (including tailing, skew, shoulders) and avoids manual optimisation of integration for individual peaks where chromatography is not ideal.

After integration, QuanLynx develops calibration curves for sample components from samples defined as standards in the sample list. A variety of polynomial curve fitting routines with or without internal standards and with or without sample weighting are available.

Following calibration, samples with unknown concentrations are quantified from the fitted calibration curves and the integrated responses in the unknown samples.

During results review it is possible to manually adjust integration of peaks as necessary and recalculate the results.

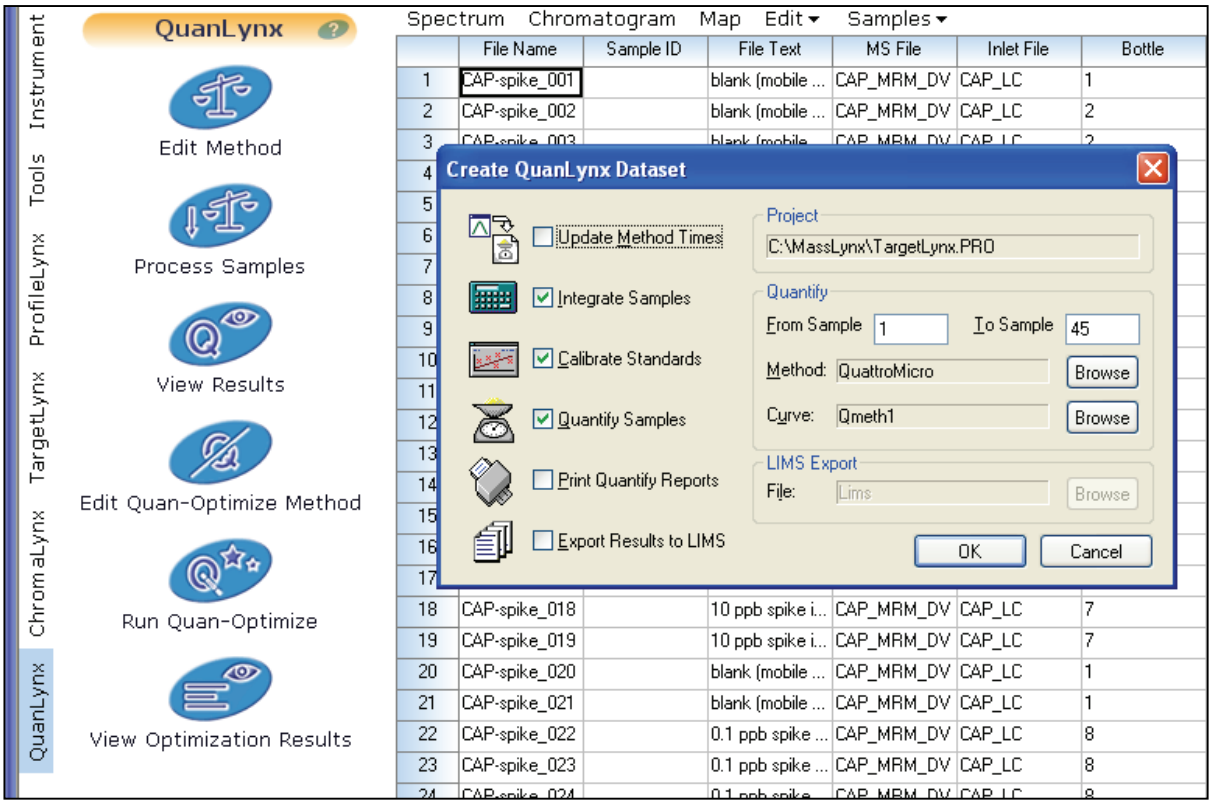

Figure 3. MassLynx Sample List showing processing options.

REVIEWING RESULTS

Processed results are presented in the QuanLynx Browser (Figure 4). The browser consists of several configurable panes to display information related to particular samples or compounds. The panes are:

- Sample summary table
- Calibration curve
- Residuals plot
- Chromatogram display
- Data security record (where required)

The summary table presents information from the acquisition Sample List plus the related quantification results. The display can be filtered by sample, or by compound. Data reported includes:

- Calculated concentration (in user defined units)
- Peak area/height
- Response
- Internal standard area
- Retention time
- Detection flags (eg concentration out of tolerance)
- % Deviation

Additional results fields may be added to the table as necessary.

Because the results file is viewed in the QuanLynx Browser, a standalone application, data can be reviewed and reprocessed without needing access to the raw data. This allows QuanLynx results to be distributed for review offline.

The file contains all method parameters, which can be changed and saved locally, and results recalculated.

Selecting a sample of interest displays related data in the chromatogram pane (for analytes and/or internal standards). The chromatogram and calibration panes are interactive, allowing users to manually optimize peak integration and exclude inappropriate calibration points.

To speed up the peak integration review, an automated slideshow presents each sample in sample list order. The show may be paused as necessary to allow manual integration and recalculation of results.

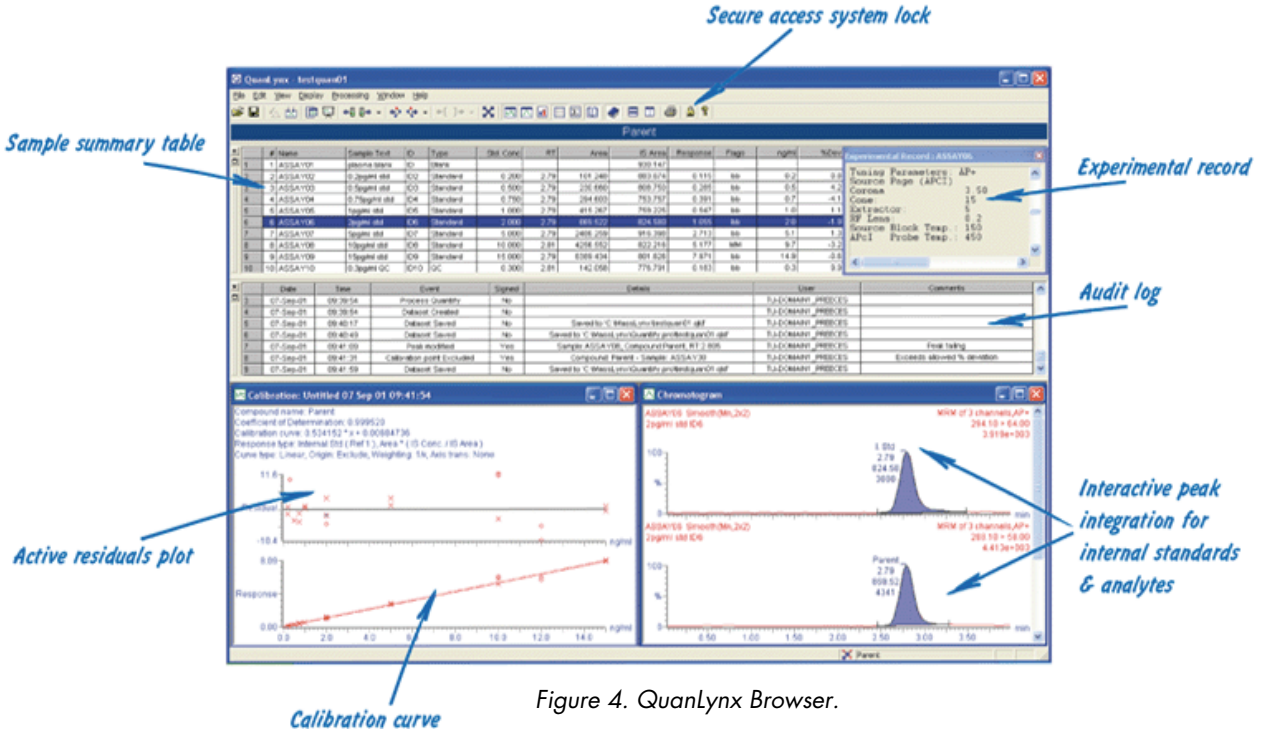

Figure 4. QuanLynx Browser.

DATA INTEGRITY

Regulations applicable to many quantitative assays require extra measures to ensure data integrity, including documented evidence of changes to results. The QuanLynx Browser documents the creation of a results file and all changes to the file in a secure audit trail. The audit trail includes the who, what , when, and why of changes. Changes are permitted based on permissions defined in the MassLynx Security Manager, supporting GxP and other regulatory requirements. Electronic signature capability is available whenever necessary. It is implemented according to local Standard Operating Procedures.

REPORTING

With the secure, independent results file, QuanLynx results are stored in their native file format. Configurable electronic and printed report formats permit output to paper and to files that may be transferred to other software applications (*.txt, *.CSV, *.XML, etc.). Direct export to LIMS is also available for immediate results transfer and distribution.

PRODUCTIVITY THROUGH QUANLYNX

QuanOptimize

Coupling QuanLynx and QuanOptimize™ permits fully automated method development of complete quantitative assays for LC/MS or LC/MS/MS methods. QuanOptimize automatically optimises instrument parameters for each compound required in a sample set by injecting a series of standards. The resulting method files may be used to acquire and quantify a data set. The result is an automated workflow from sample submission, to method development, data acquisition and data processing. The final output is the QuanLynx results file.

Open Access Quantification

For non-expert users that require access to quantitative analysis, QuanLynx can be coupled with OpenLynx™ to create a "walk-up" system. Employing either pre-defined LC/MS/MS methods for known compounds, or utilising QuanOptimize for unknowns, the system allows users to submit samples via a login PC, without having to interact with MassLynx. The result is a simple interface that allows chemists to submit a sample and later receive the results as the QuanLynx Browser report via email, or as a printed report.

SUMMARY

Coupling QuanLynx to MassLynx Software automates data acquisition, processing and reporting of quantitative results.

The embedded ApexTrack algorithm significantly improves the accuracy of peak detection, saving time in data review and giving greater confidence in the results.

QuanLynx provides an easy to use and flexible solution to increase laboratory productivity, including automated LC/MS(/MS) method development using QuanOptimize or walk-up quantitation with Open Access Quan.

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