# ACD/LABS [ADVANCED CHEMISTRY DEVELOPMENT, INC.]

# Accurate and Reproducible Quantitation of xC/UV/MS Data from Any Instrument

Anne Marie Smith
Baljit Bains

## How Much Analyte is in the Sample?

Quantitative analysis addresses scientific challenges across various industries such as food, environment, pharmaceutical, and more. It is crucial to ensure a product's safety, efficacy, and quality by answering "*How much*?" This question is answered using quantitation xC/UV/MS workflows.

To meet different needs in terms of sensitivity, resolution, etc., it is common for laboratories to have instruments from multiple vendors. With multi-vendor laboratories, there are challenges in learning and navigating multiple applications with different interfaces and difficulty in standardizing data. Using software compatible with most leading vendor data formats eases the workload on the analyst, allowing them to learn one software for quantitation—enabling consistency and standardization of quantitative analysis.

MS Workbook Suite offers a fully integrated quantitative workflow where all xC/UV/MS data can be processed and quantitated in a single interface—ensuring consistently reliable and accurate results.

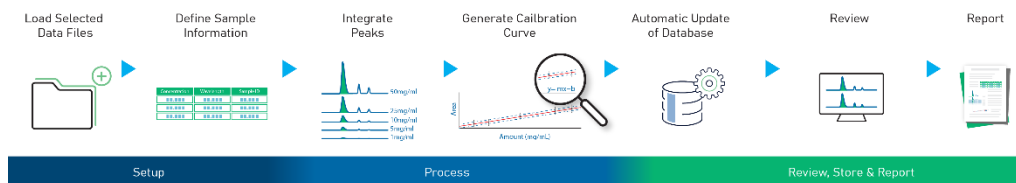# An Example Quantitation Workflow in MS Workbook Suite



*Figure 1. The intuitive calibration and quantitation workflow in MS Workbook Suite.*

Quantitation studies were designed within the software post-acquisition for a mixture of 4 compounds prepared in triplicate at 7 concentrations. The quantitation workflow creates a calibration curve to determine the amount of analyte present in a sample. Here, the quantitation workflow was implemented to quantify 24 unknown samples against the set of standards. The steps include:

## SET UP

Acquired calibration data is added and sample information is defined as:

→ *Sample type*—calibration, standard, blank, unknown sample

→ *Type of trace*—extracted ion chromatogram (XIC, user-specified mass during calibration), flat chromatogram (specified wavelength pre-acquisition), or DAD (user-specified wavelength during calibration)

→ *Compound(s) for quantitation*—material A, B, C, and D

Samples set as "standards" will be incorporated into the calibration curve.

Automatic background subtraction can be performed on samples with their type set as "blank", to provide more accurate analyte concentrations.

## PROCESS

To determine the amount of analyte present, the unknown samples must be quantified against the set of standards.

It is important to know the retention time of the analyte(s) as this is used to identify the peaks for quantitation. Once the processing parameters are defined, the peak detection and integration parameters are applied to create a calibration curve. To generate the calibration curve, the following must be provided:

1    Appropriate traces to import into the calibration project

2    Concentration of standards (expedited entry by copy/paste from existing tables and keyboard shortcuts)

Once the curve has been generated, it is represented in tabular and graphical form along with a residual plot. Here you have options to force the curve through zero, change the polynomial degree of the curve, and further optimize the processing parameters. Any adjustments made to optimize the integration of the peaks result in automatic updates within the calibration curve.

Once the sample is added, the analyte(s) in the sample will be quantitated against the calibration curve and the results can be viewed in the calibration window. The linear regression, standard deviation, and $r^2$ are calculated from the calibration curve. The Residual analysis (ANOVA table) is provided to determine the validity of the regression model. The software enables the standardization of repeat measurements by normalizing data to internal standards.
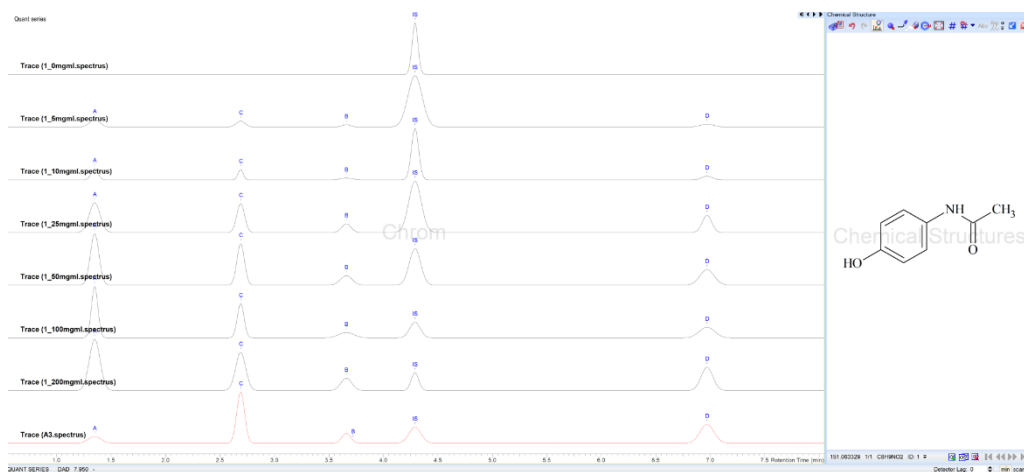


*Figure 2. A series of chromatograms showing the associated structure, peaks of 4 components, and the internal standard across various concentrations of standards and unknown samples.*
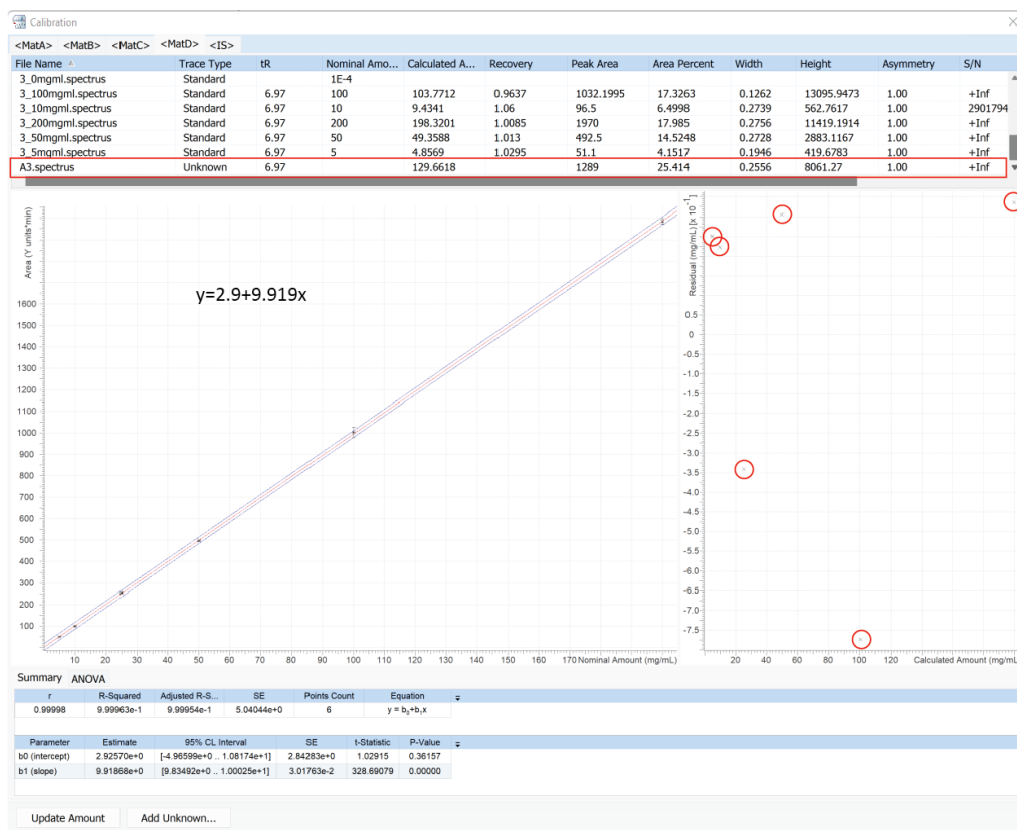
*Figure 3. Calibration curve for Material D, showing the regression line, standard deviation, residuals plot, amount of unknown (A3), and summary table (including r, r², equation, etc.).*

## REVIEW, STORE & REPORT

The full data set (raw and processed) is automatically saved to a database. It is possible to store data in a remote database, leveraging knowledge across organizations. You can visualize the data with its chemical context including chromatograms, calibration curves, and tabulated results. You can view or modify the results (i.e., alteration of processing parameters, or the addition of unknowns to be quantified) and track any changes made in the processing interface for data integrity. Finally, you can create and share customized reports.

Processing and quantitating all xC/UV/MS data in MS Workbook Suite ensures connectivity between data and numerical results. Reproducible and accurate quantitative analysis allows confident determination of "how much" is in the sample, guaranteeing the quality of final products whether food, water, or drugs.