APPLICATION NOTE

ACD/LABS [ADVANCED CHEMISTRY DEVELOPMENT, INC.]

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

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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 the quality of a product by answering "*How much*?" This question is answered using essential quantitation xC/UV/MS workflows. Using MS in tandem with gas chromatography (GC) or liquid chromatography (LC) detects and quantitates analytes of interest in highly complex mixtures and allows for an efficient, selective, and sensitive separation.

In present-day 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 minimizes limitations in instrument suitability and selection—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.

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An Example Quantitation Workflow in MS Workbook Suite

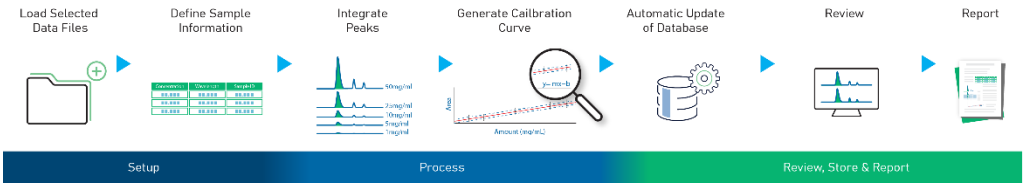


Figure 1: The intuitive calibration and quantitation workflow in MS Workbook Suite.

Quantitation studies were designed within the software post-acquisition for a mixture prepared in triplicate (containing 4 compounds and 7 standards). Using the quantitation workflow to determine the amount of analyte present, 24 unknowns were quantified against the set of standards. The workflow consists of:

SET UP

Define sample information:

- *Sample type*—calibration, standard, blank, unknown sample
- *Type of trace*—extracted ion chromatogram (XIC), flat chromatogram (specified wavelength pre-acquisition), or DAD (user-specified wavelength during calibration)
- *Compound(s) for quantitation*—material A, B, C, or D

PROCESS

To determine the amount of analyte present, quantify the unknown samples against the set of standards. Define the processing parameters and identify the peaks for quantitation via retention time. Apply the peak detection and integration parameters to create a calibration curve and calculate the linear regression, standard deviation, and r^2. Determine the suitability and validity of the statistical regression model by using the analysis of residuals (ANOVA table).

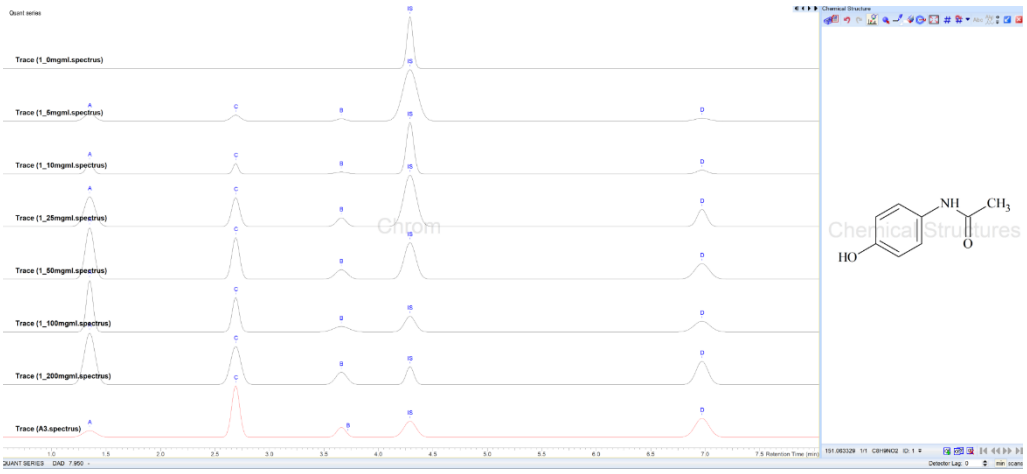
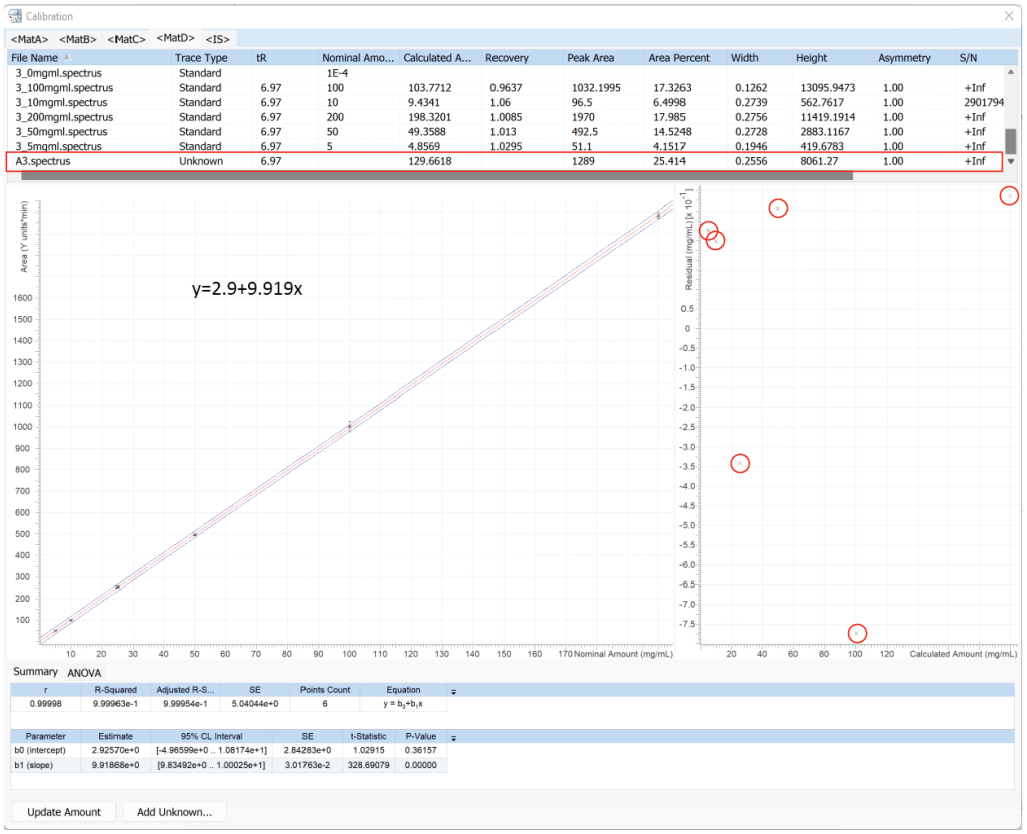


Figure 2. Chromatograms in MS Workbook Suite showing the associated structure and peaks for all 4 components, the internal standard, and the unknown at various concentrations.



File Name	Trace Type	tR	Nominal Amo...	Calculated A...	Recovery	Peak Area	Area Percent	Width	Height	Asymmetry	S/N
3_0mgml.spectrus	Standard		1E-4								
3_100mgml.spectrus	Standard	6.97	100	103.7712	0.9637	1032.1995	17.3263	0.1262	13095.9473	1.00	+Inf
3_10mgml.spectrus	Standard	6.97	10	9.4341	1.06	96.5	6.4998	0.2739	562.7617	1.00	2901794
3_200mgml.spectrus	Standard	6.97	200	198.3201	1.0085	1970	17.985	0.2756	11419.1914	1.00	+Inf
3_50mgml.spectrus	Standard	6.97	50	49.3588	1.013	492.5	14.5248	0.2728	2883.1167	1.00	+Inf
3_5mgml.spectrus	Standard	6.97	5	4.8569	1.0295	51.1	4.1517	0.1946	419.6783	1.00	+Inf
A3.spectrus	Unknown	6.97		129.6618		1289	25.414	0.2556	8061.27	1.00	+Inf

r	R-Squared	Adjusted R-S...	SE	Points Count	Equation
0.99998	9.99963e-1	9.99954e-1	5.04044e+0	6	$y = b_0+b_1x$

Parameter	Estimate	95% CL Interval	SE	t-Statistic	P-Value
b0 (intercept)	2.92570e+0	[-4.96599e+0 .. 1.08174e+1]	2.84283e+0	1.02915	0.36157
b1 (slope)	9.91868e+0	[9.83492e+0 .. 1.00025e+1]	3.01763e-2	328.69079	0.00000

Figure 3. Calibration curve for Material D in MS Workbook Suite, showing the regression line, standard deviation, residuals plot, amount of unknown (A3), and summary table (including r, r^2, equation, etc.)

REVIEW, STORE & REPORT

Automatically save the full set of data (raw and processed) to a database. It is possible to store and visualize data with its chemical context including chromatograms, calibration curves, and tabulated results. 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 purposes. 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 ensuring the quality of final products whether food, water, or drugs.