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Quantitation Workflow Using KnowItAll 2024

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Introduction

Chemical quantification analysis can vary across multiple software packages, many varying in compatibility, compliance, and efficiency – however, mastering multiple software tools to the same level of expertise and reproducibility is a source of laboratory inefficiency and a pain point for researchers. They may have to switch tools, depending on the type of analytical technique or data format, or may not have access at all. Ideally laboratory staff should have access to one tool the provides compatibility, compliance, and efficiency to do quantitation consistently.

KnowItAll 2024 introduces a comprehensive quantitation application for multiple analytical instrumental methods, including IR, Raman, GC-MS, and UV-Vis. Quantitation methods include external calibration, internal calibration, and standard addition analysis using data from all spectral formats supported by KnowItAll.[1]

Method

The process of using the Quantitation tool in KnowItAll 2024 is outlined in Figure 1. The software's widgets guide users through the process of analyte calibration, then quantitation. This flow is especially beneficial for GC-MS data, where the appropriate sample file, analyte ion(s), and internal standard ion(s) have to be selected carefully.

Figure 1: KnowItAll Quantitation workflow.

Results

Figure 2 shows the result of an IR analysis. Region 1 is the spectral pane, displaying the analyte spectra and selected peak region. Region 2 is the table of calibrants' concentrations as well as calculated area under curve or peak height values for picked peaks. Region 3 displays the calculated concentration(s) for the unknown sample(s). Region 4 displays the calibrations' curve fitting and necessary statistics.

Figure 2: Example IR quantitation result, using External Calibration method.

The GC-MS example[2] follows the same procedure, where the ratios of analyte vs internal standard are used. As one can see, multiple unknown concentration samples can be processed with a one-button click (Figure 3).

Figure 3: Example GC-MS quantitation result, using Internal Calibration method.

Summary

This new system is streamlined and comprehensive. Coupled with the qualitative analysis for which KnowItAll has been traditionally renowned, Wiley Science Solutions is there to help analytical chemistry research at a new level.

References

1. KnowItAll Analytical Edition (Version 24.0.59.0); John Wiley & Sons, Inc.: Hoboken, NJ, 2023. https://sciencesolutions.wiley.com/software/ https://sciencesolutions.wiley.com/software/

2. This dataset can be downloaded from https://arts-sciences.und.edu/academics/chemistry/kubatova-research-group/chrom_ms02.html