KnowItAll Quantitative Software for EI GC-MS

Version 2024

J. Little, MS Interpretation Services

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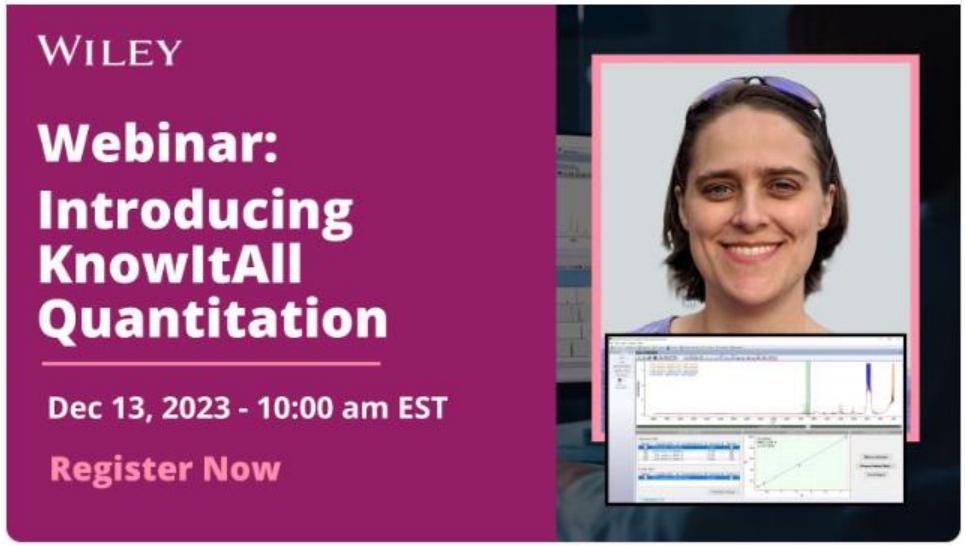
- Full videos including this one found on demand at the following link
- https://sciencesolutions.wiley.com/webinars/
- My excerpt ***only*** shows Introduction and EI GC-MS software demonstration part of the webinar

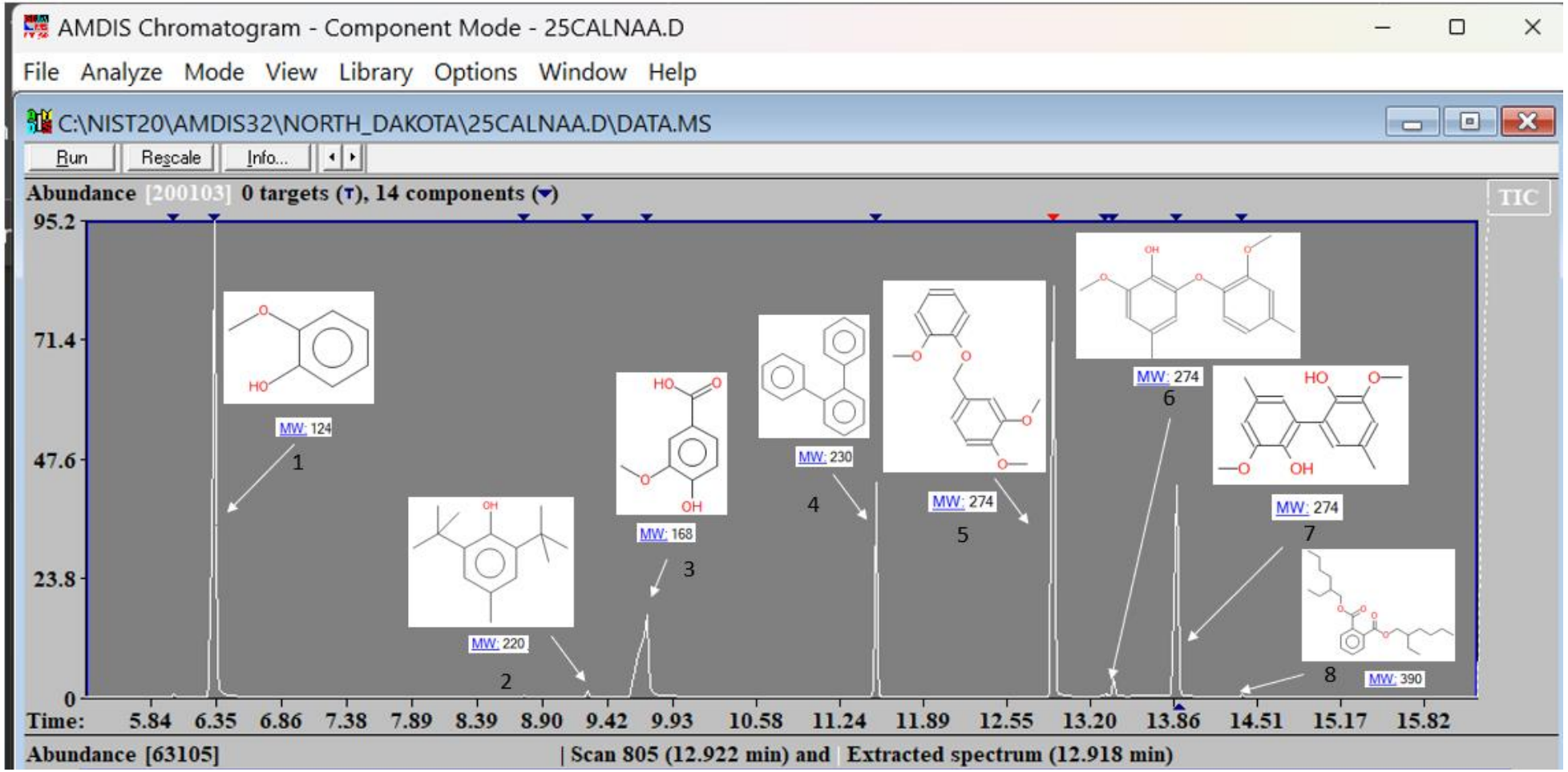


Speaker: Dr. Leanna Ergin

Dr. Leanna Ergin is an Assistant Editor for Wiley Science Solutions, for which she helps create tools for spectroscopy, structural, and scientific standard reference data and helps create innovative software applications. Leanna completed her PhD in Clinical-Bioanalytical Chemistry from Cleveland State University, where she developed a protocol for processing hyperspectral image data that distinguishes the spectra, removes degeneracies caused by symmetry, and is generalized to work with any number of wavelength dimensions and spectra. The results are mapped to the full RGB colorspace of modern computer displays. Leanna joined Wiley in 2022.

Files Used for Demonstration

- Files used for demo are found on my website in a zip file
- Obtained from University of North Dakota website and file names modified to match Wiley Webinar examples
- https://arts-sciences.und.edu/academics/chemistry/kubatova-research-group/chrom_ms02.html
- North Dakota website does not totally show the identity of the species in file, my interpretation shown below



More Information on Files from North Dakota Website

- Wiley used the files shown in the first screen capture shown below with concentrations in ug/mL added to end of file name
- Selected *m/z* 124 for Compound 1 and *m/z* 230 for internal standard, Compound 4
- Lower screen capture shows information for other files and species on their website
- Some of their species are *NOT found* in either the Wiley or NIST libraries

11CALNAB_unknown.D

22CALNAD_1_60.D

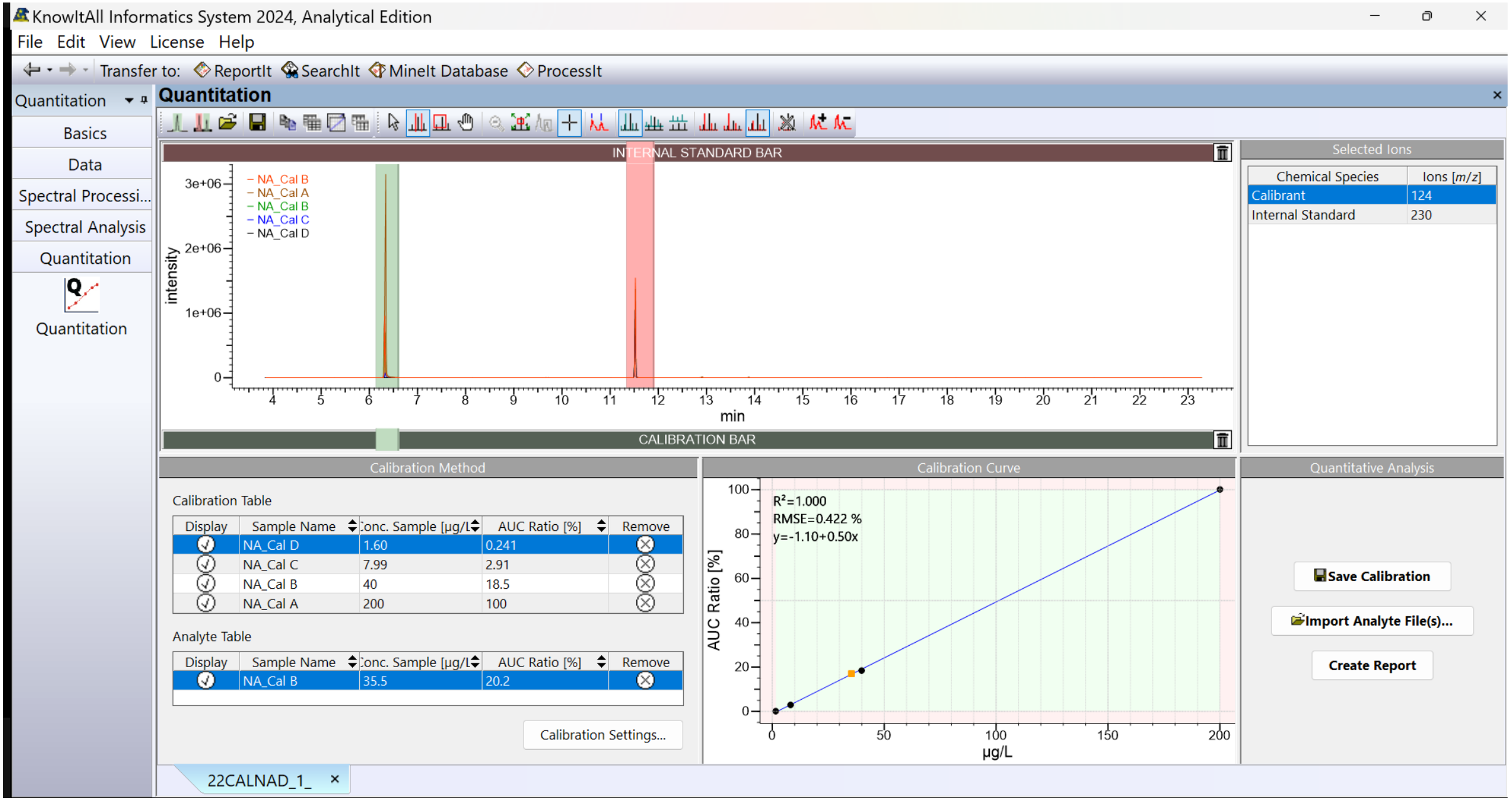
23CALNAC_7_99.D

24CALNAB_40.D

25CALNAA_200.D

Species		Formula	Mix F NA2-74-F	Mix E NA2-74-E	Mix D NA2-74-D	Mix C NA2-74-C	Mix B NA2-74-B	Mix A NA2-74-A
1	Guaiacol	$C_7H_8O_2$	0.064	0.320	1.60	7.99	40.0	200
3	Vanillic acid	$C_8H_8O_4$	0.064	0.319	1.60	7.99	39.9	200
5	1,2-Dimethoxy-4-[(2-methoxyphenoxy) methyl]benzene	$C_{16}H_{18}O_4$	0.064	0.320	1.60	8.00	40.0	200
7	Bicreosol	$C_{16}H_{18}O_4$	0.064	0.320	1.60	8.00	40.0	200
4	o-Terphenyl (IS)	$C_{18}H_{14}$	62.0	62.0	62.0	62.0	62.0	62.0

Final Result Page from Demonstration



Excerpt *(13 Pages)* of EI GC-MS Quantitation from Wiley Self-Guided Training Course

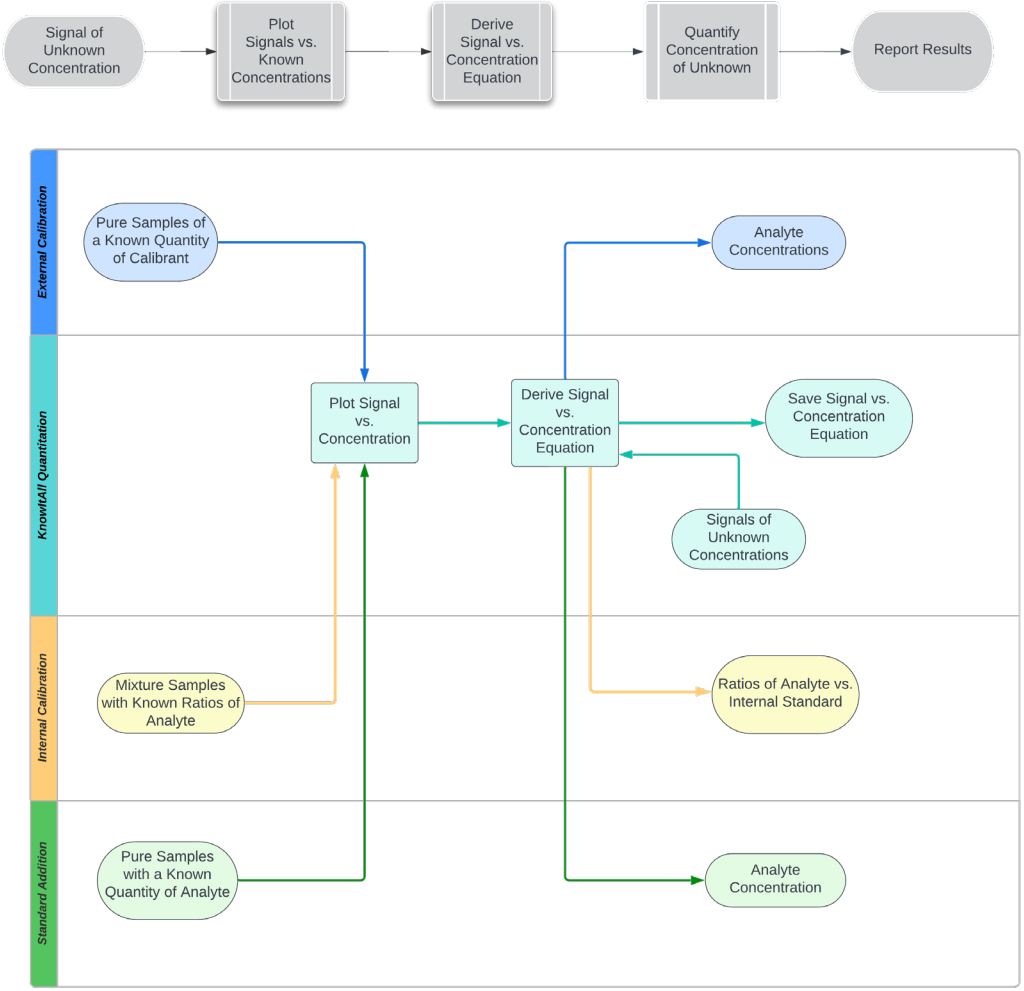
Original Document Links:

https://sciencesolutions.wiley.com/knowitall-software-training-course/

16_Training-Quantitation.pdf (wiley.com)

EI GC-MS Quantitation Excerpts Found on *Following* 13 Pages:

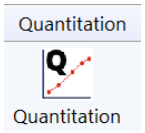
Quantitation Workflow

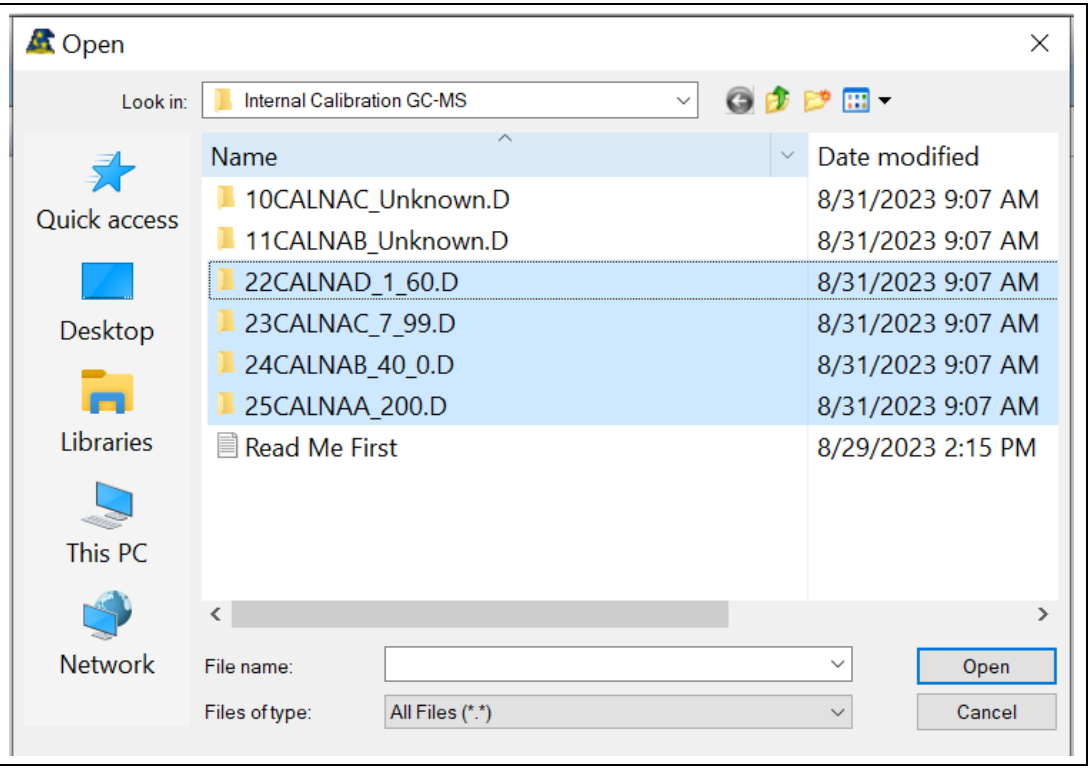


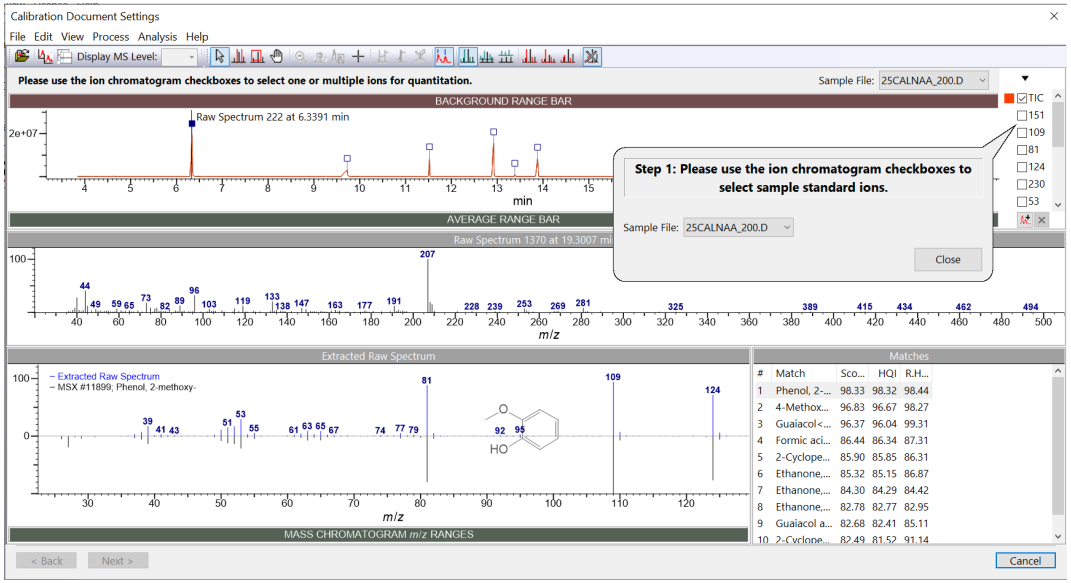
GC-MS

This exercise requires user to download sample datasets from https://arts-sciences.und.edu/academics/chemistry/kubatova-research-group/chrom_ms02.html. It is helpful to rename files so that analyte (Guaiacol) concentrations are reflected in the names.

Internal stanard: *o-Terphenyl (IS) RT 11.5192 62.0 ug/ml*
Analyte: *Guaiacol RT 6.3368 min*

	Action	Result
1	Open the **Quantitation** application by clicking its icon, typically found in the **Quantitation** group.	
2	Click **New Internal Calibration** button.	KnowItAll prompts user to open calibrant files.

3	Navigate to the downloaded GC-MS file folder. Select folders as shown in the right screenshot. Click **Open.**	

4	In the drop-down list, select the calibrant file where analyte concentration is the largest, in this example, it is the **25CALNAA_200.D**	

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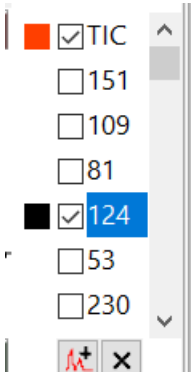
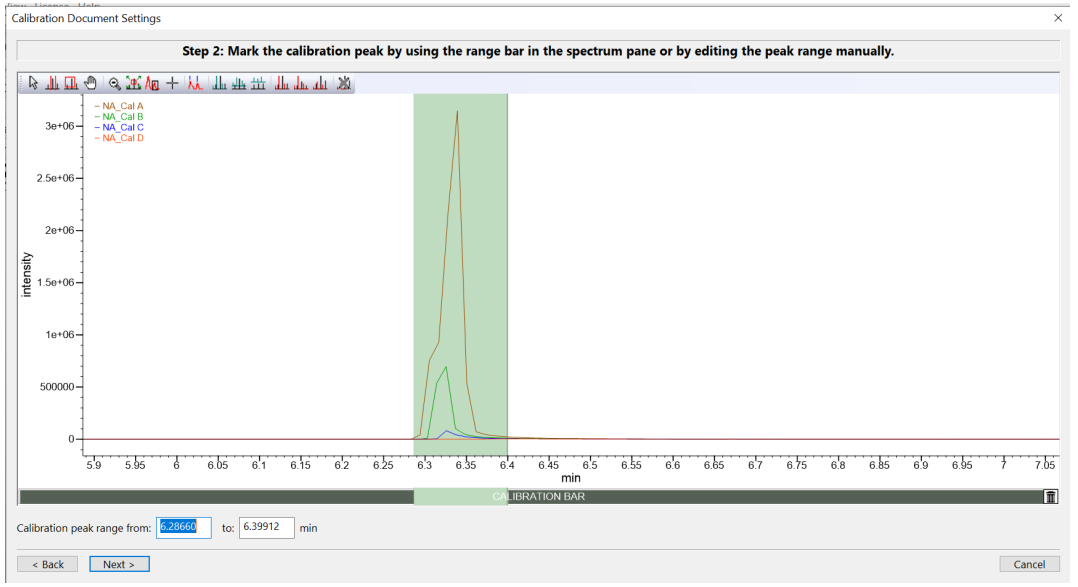
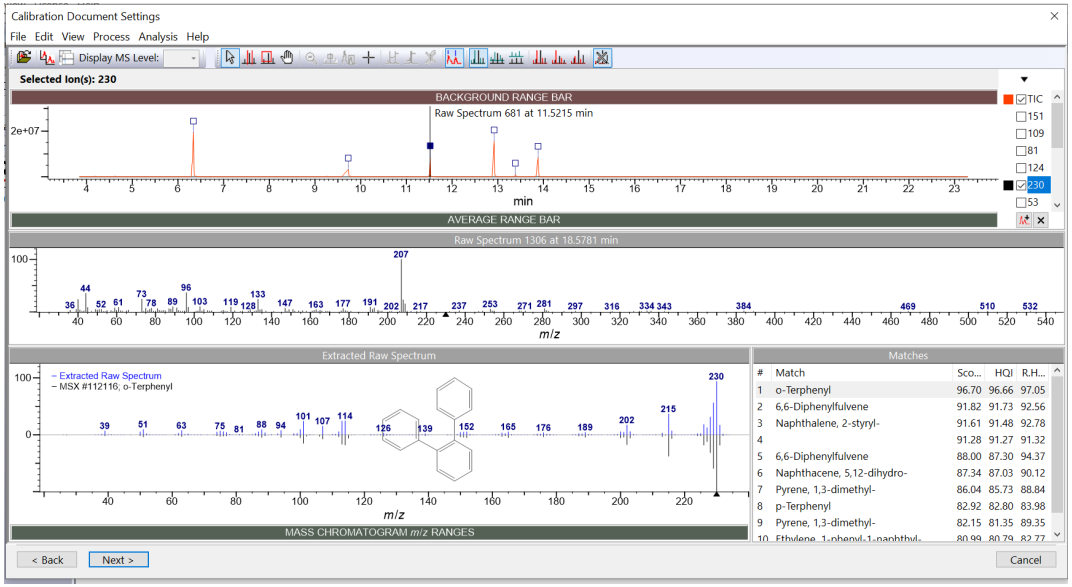
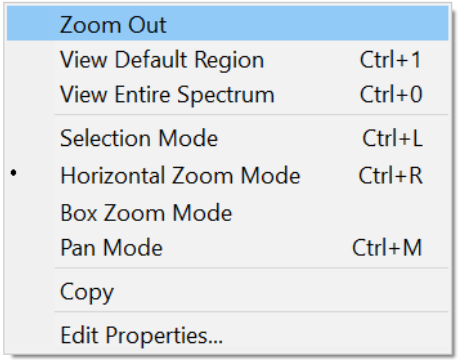
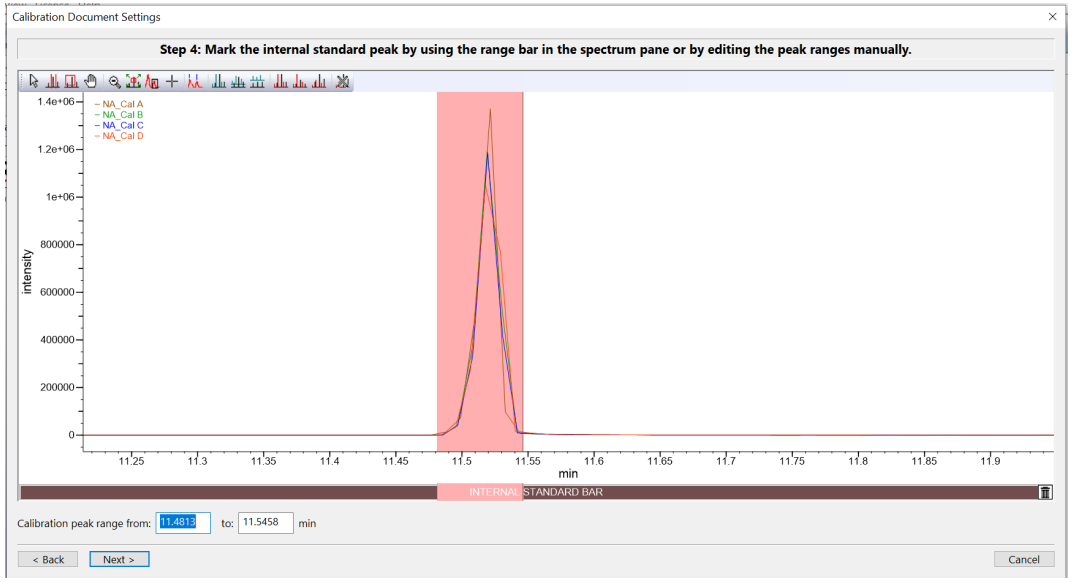
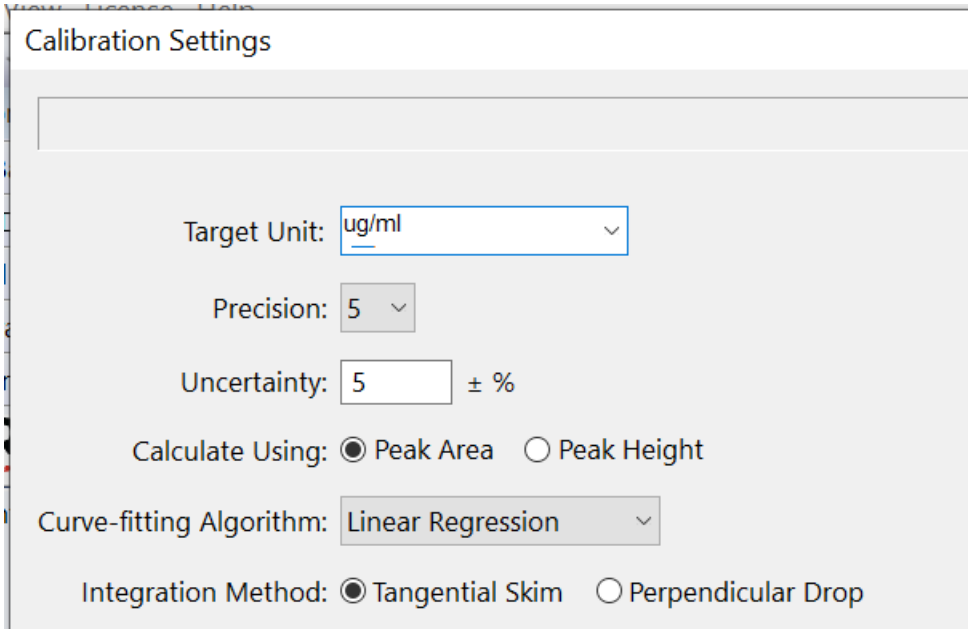
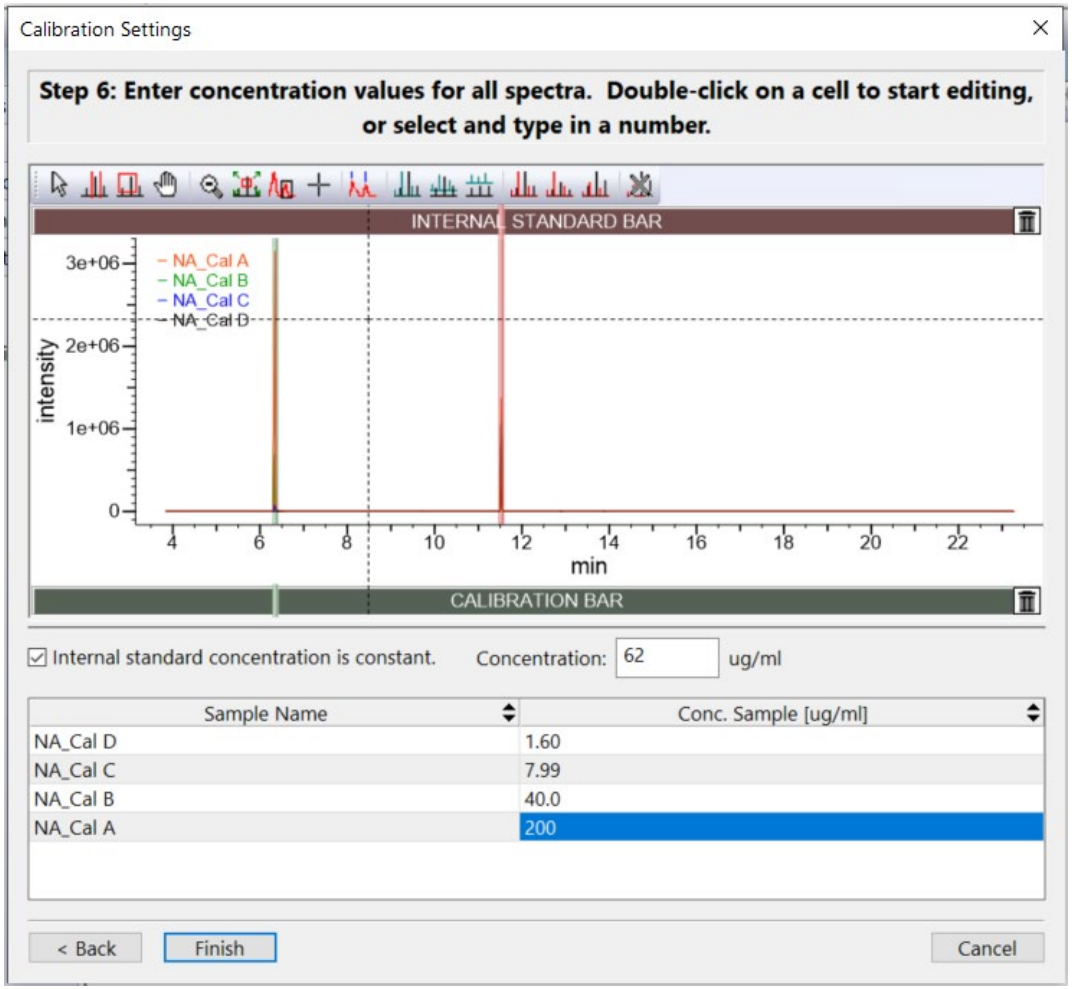
5	Select a component from the **Raw Spectrum** pane, in our example, the interested component has a TIC peak at **6.45** min. Select an ion, in this case, we select its **molecular m/z 124.** Click **Next >** (bottom left corner)	

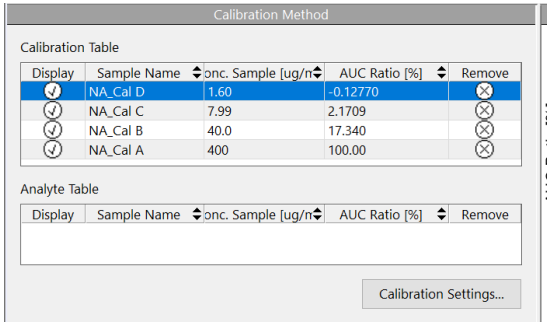
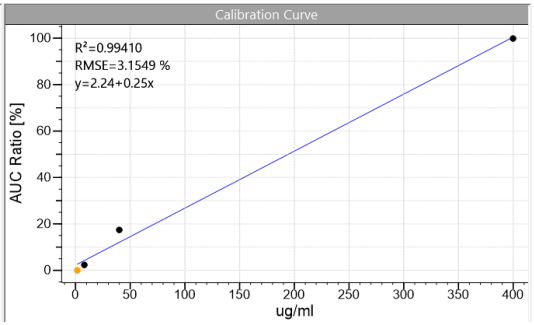
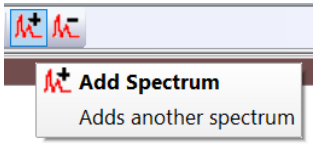
6	Click the **Spectrum** pane, drag and drop mouse to zoom into region 6 – 6.5 min. Select peak region by clicking down the CALIBRATION BAR (drag and drop). Click button **Next >.**	

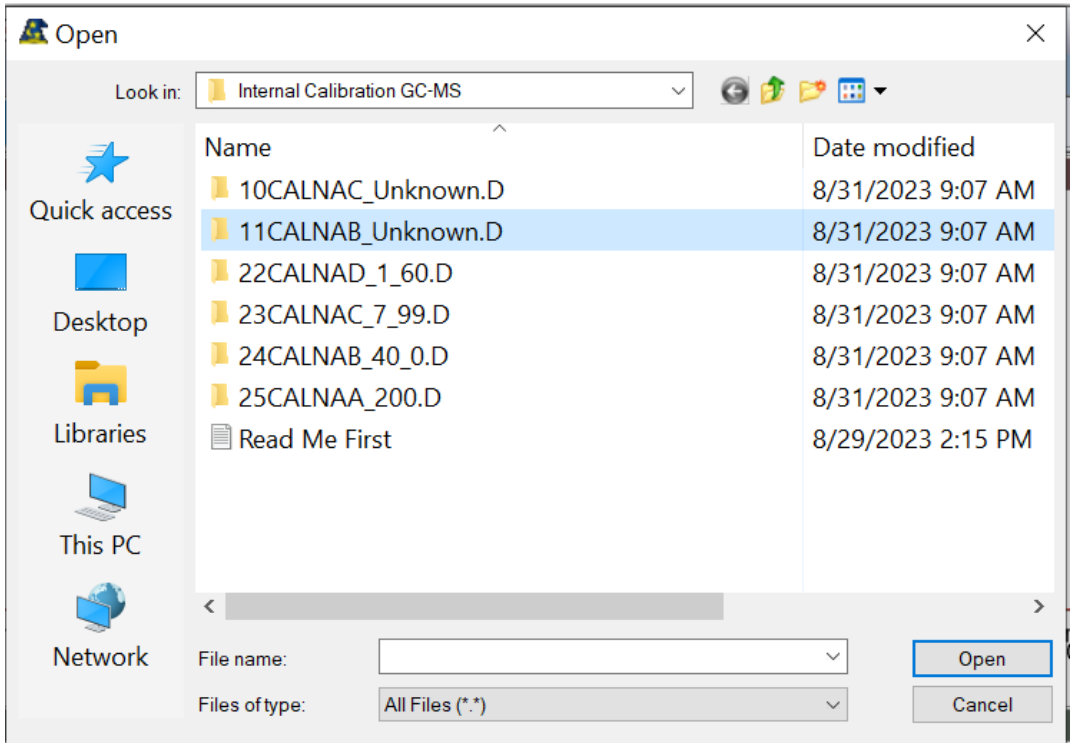
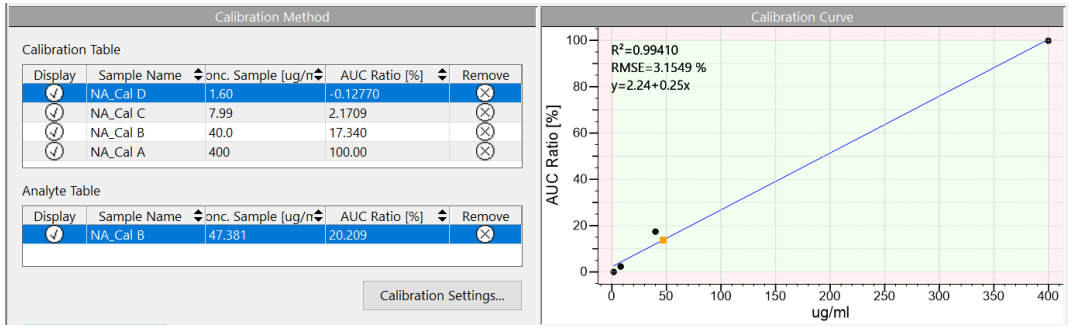
7	Select a component from the **Raw Spectrum** pane, in our example, the interested component has a TIC peak at **11.5** min. Select an ion, in this case, we select its **molecular m/z 230.** Click **Next >** (bottom left corner)	
8	Right mouse click the spectrum pane. Select **Zoom out.**	

10	Click the **Spectrum** pane, drag and drop mouse to zoom into region 10.5 – 12 min region. Select peak region by clicking down the INTERNAL STANDARD BAR (drag and drop). Click button **Next >.**	

9	In the following window, define calibration settings. Target Unit: **ug/ml** (you have to type in) Calculate Using: **Peak Area** Click button **Next >.**	

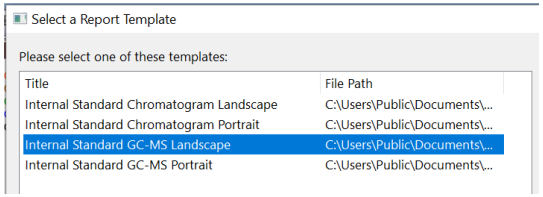
10	Enter concentration and ratio values in the pop-up window. Concentration (internal standard) 62 **ug/ml** Calibrant File Concentration [**ug/ml**] NA_Cal D 1.60 NA_Cal C 7.99 NA_Cal B 40.0 NA_Cal A 200 Click **Finish** button.	

11		  Statistics are reported in the calibration curve. The lower the **RMSE** (**root mean squared error)**, the better the curve is fitting. The closer the **R^2** (**coefficient of determination**) is to 1**,** the better the curve is fitting. One can use ⊗ in the **Remove** cell to remove samples from calibration; and use **Add Spectrum**  to add new calibrants, One can reset parameters using the **Calibration Settings** button. One can save this calibration for future use or sharing by clicking the **Save Calibration** button.

12	Click the **Import Analyte File(s)** button. Select unknown file folder **11_CLANAB_Unknown.D** to calculate the concentrations. Click **Open.**	
13		 The concentration ratio of analyte to internal standard is shown in the **Analyte Table** and as a sqaure spot in the **Calibration Curve**.

14 Click **Transfer to**: Report

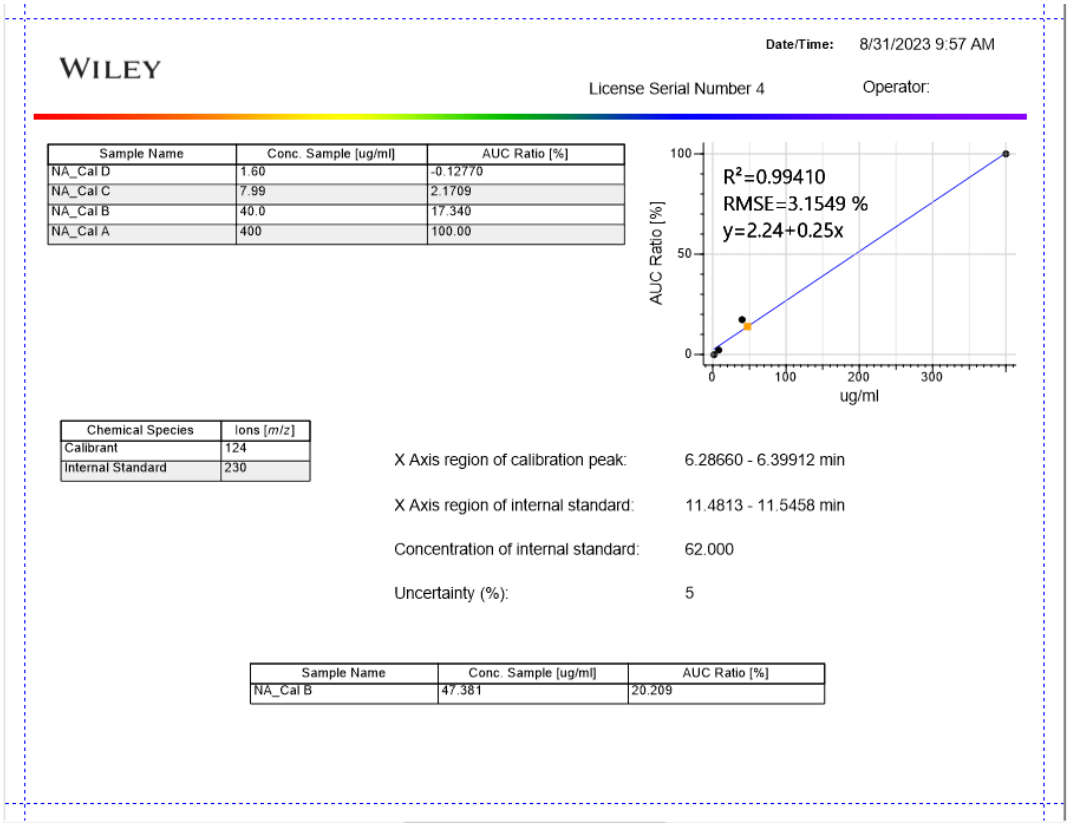
Select the **Internal Standard GC-MS Landscape** template



Click **OK**

Note: if a template is used for the first time, user has to do the following before transfer data to ReportIt application:

File > Edit Report Templates
Click Add button
Navigate to the template file
Open



This is a basic report, one can select these objects and copy/paste to other applications.

Wiley KnowItAll Training Resources (1 of 2)

https://sciencesolutions.wiley.com/knowitall-software-training-course/

This self-guided training course will familiarize you with the KnowItAll software through a series of lessons.

- This series is designed for you to follow along with in the KnowItAll software.
- The lessons are organized by category, each containing a series of short, easy to follow tutorials.

Wiley KnowItAll Training Resources (2 of 2)
Quantitation Training Link:
16_Training-Quantitation.pdf

#	Lesson	Lesson PDF
1	General Features: Introduction to the Basic Applications in the KnowItAll Informatics System	Download
2	Simple Spectral Search/Identification with KnowItAll ID Expert	Download
3	Searching: IR & Raman	Download
4	Mixture Analysis: IR & Raman	Download
5	Functional Group Analysis: IR, Raman, & Polymer	Download
6	Mass Spectrometry Search	Download
7	GC-MS Analysis Using KnowItAll MS Expert, ProcessIt and SearchIt	Download
8	Create Databases	Download
9	Drawing Structures & Reactions	Download Hotkeys/Shortcuts
10	Creating Reports	Download
11	Data Mining & Analysis	Download
12	Quality Control Analysis with QC Expert	Download
13	NMR Processing Tools	Download
14	NMR Analysis Tools	Download
15	NMR Prediction	Download
16	Quantitation	Download
17	LC-MS Databases using Processing and MineIt	Download
18	Using Predicted IR Spectra in KnowItAll	Download