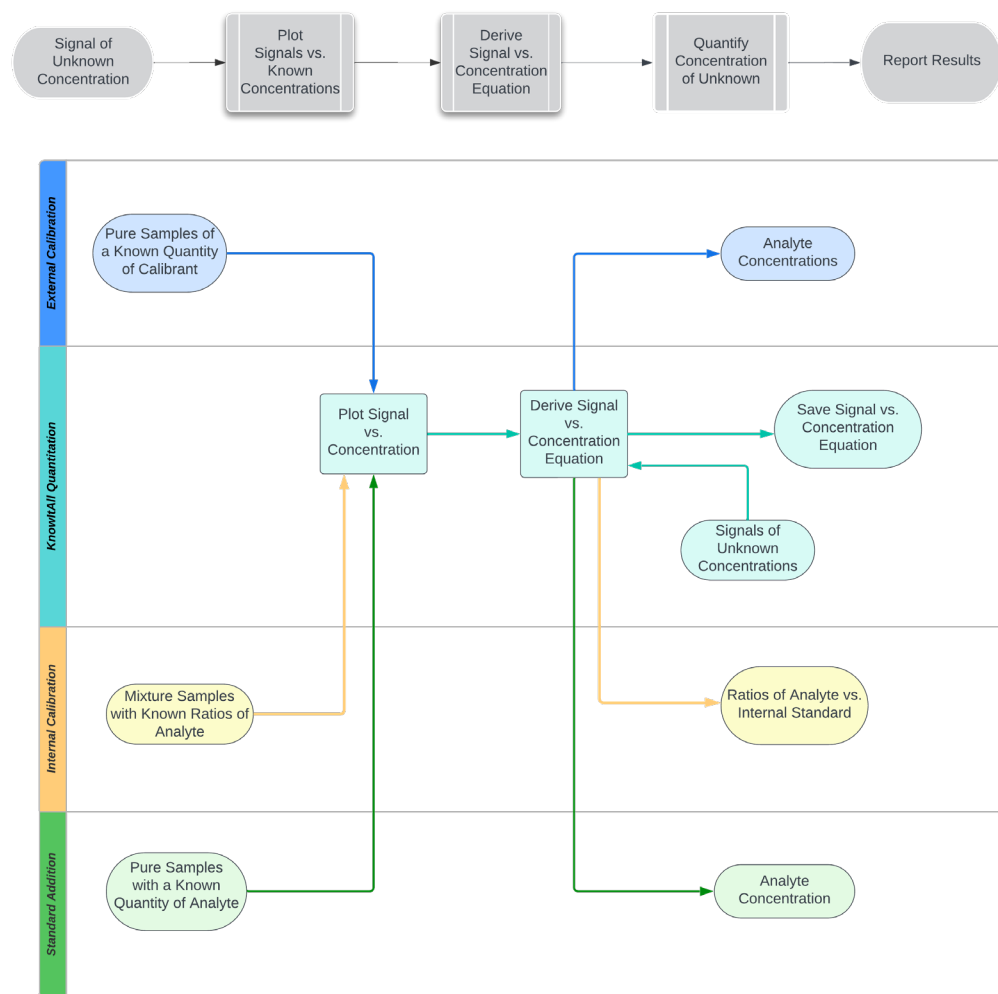


# **KnowItAll Informatics Training**

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## Quantitation

# Quantitation Workflow



# External Calibration Quantitation

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## Perform External Calibration Quantitation

### Purpose

These exercises demonstrate how to perform external calibration quantitation using KnowItAll Quantitation software.

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### Objectives

This exercise will teach you:

- How to create external calibration
  - How to perform quantitation
- 

### Background

Wiley's KnowItAll Quantitation application performs accurate quantitation over comprehensive types of analytical data.

#### *Training Files Used in This Lesson*

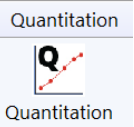
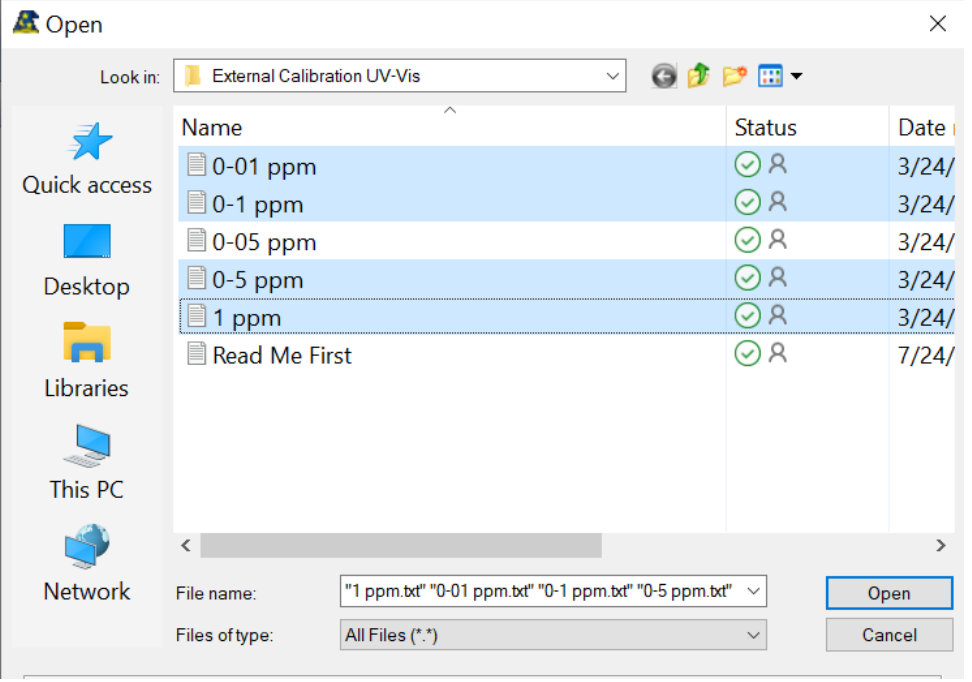
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Quantitation folder

- External Calibration UV-Vis
- External Calibration IR

#### *KnowItAll Applications Used*

- Quantitation

### UV-Vis

	Action	Result																					
1	Open the <b>Quantitation</b> application by clicking its icon, typically found in the <b>Quantitation</b> group.	 <p>The image shows the 'Quantitation' application icon, which features a stylized 'Q' with a red line graph and the word 'Quantitation' below it.</p>																					
2	Click <b>New External Calibration</b> button	KnowItAll prompts user to open calibrant files.																					
3	<p>Navigate to the <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Quantitation\External Calibration UV-Vis</b> folder.</p> <p>Select sample files and leave one out as the "unknown."</p> <p>Click <b>Open</b>.</p>	 <p>The image is a screenshot of a Windows File Explorer window titled 'Open'. The 'Look in:' path is 'External Calibration UV-Vis'. The file list contains the following items:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Status</th> <th>Date</th> </tr> </thead> <tbody> <tr> <td>0-01 ppm</td> <td>✓</td> <td>3/24/</td> </tr> <tr> <td>0-1 ppm</td> <td>✓</td> <td>3/24/</td> </tr> <tr> <td>0-05 ppm</td> <td>✓</td> <td>3/24/</td> </tr> <tr> <td>0-5 ppm</td> <td>✓</td> <td>3/24/</td> </tr> <tr> <td>1 ppm</td> <td>✓</td> <td>3/24/</td> </tr> <tr> <td>Read Me First</td> <td>✓</td> <td>7/24/</td> </tr> </tbody> </table> <p>The '1 ppm' file is selected. The 'File name:' field at the bottom contains '"1 ppm.txt" "0-01 ppm.txt" "0-1 ppm.txt" "0-5 ppm.txt"'. The 'Files of type:' is set to 'All Files (*.*)'. 'Open' and 'Cancel' buttons are visible.</p>	Name	Status	Date	0-01 ppm	✓	3/24/	0-1 ppm	✓	3/24/	0-05 ppm	✓	3/24/	0-5 ppm	✓	3/24/	1 ppm	✓	3/24/	Read Me First	✓	7/24/
Name	Status	Date																					
0-01 ppm	✓	3/24/																					
0-1 ppm	✓	3/24/																					
0-05 ppm	✓	3/24/																					
0-5 ppm	✓	3/24/																					
1 ppm	✓	3/24/																					
Read Me First	✓	7/24/																					

- 4 In **Technique Parameters** prompt window:
- define file type **UV-Vis**
  - check **Apply Parameters to All Files**
  - click **OK**

**Technique Parameters**

Data Type: IR

X Axis Unit: Vapor Phase IR

Y Axis Unit: Raman

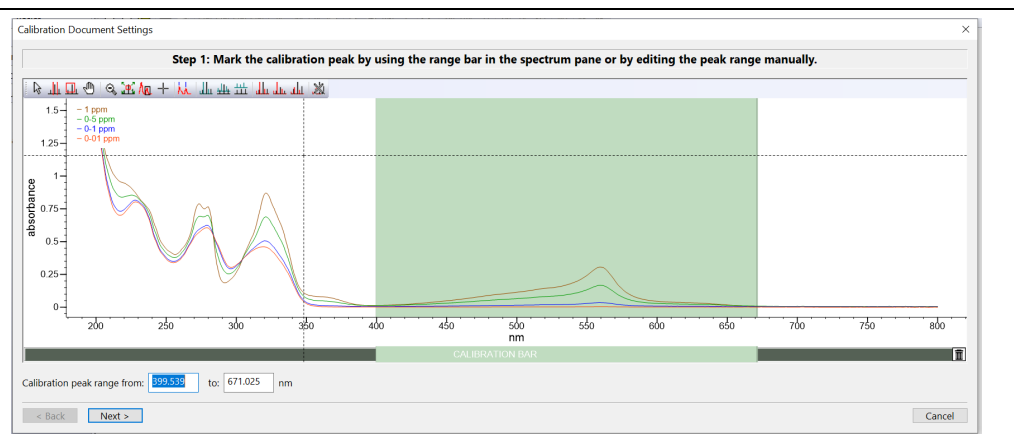
Data is spectral  Data is table

X	Y
800.0401	
798.9311	
797.9603	0.0007610
796.9891	0.0008650
796.0175	-2.15e-05
795.0456	0.000640
793.9344	0.0003440
792.9616	-0.0001240
791.9885	0.0001950
791.0150	0.001140

Apply Parameters to All Files

Buttons: OK, Cancel

5 Select peak region around 560 nm by clicking down the CALIBRATION BAR (drag and drop).  
  
Click button **Next >**



6 In the following window, define calibration settings as shown in the image to the right.  
  
Target Unit: **ppm**  
Calculate Using: **Peak Height**  
  
Click button **Next >**.

Calibration Settings

**Step 2: Define the calibration settings.**

Target Unit:

Precision:

Uncertainty:  ± %

Calculate Using:  Peak Area  Peak Height

Curve-fitting Algorithm:

Integration Method:  Tangential Skim  Perpendicular Drop

7 Enter concentrations in the right column based on the file names.

(Note that in the sample files, dashes were used instead of decimals in the sample name. The file “0-01 ppm” has a concentration of 0.01 ppm.)

Click **Finish** button.

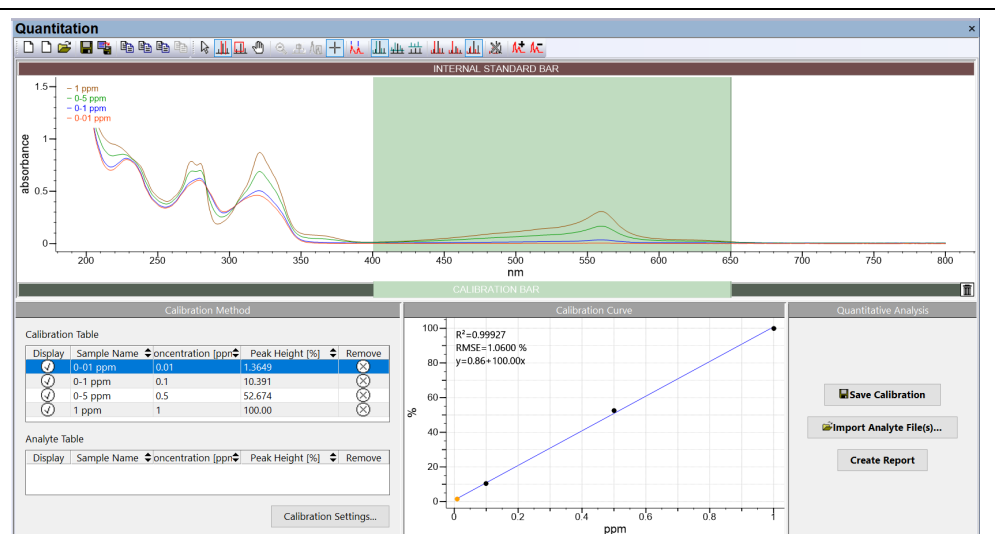
Calibration Settings

Step 3: Enter concentration values for all spectra. Double-click on a cell to start editing, or select and type in

Sample Name	Concentration [ppm]
0-01 ppm	0.01
0-1 ppm	0.1
0-5 ppm	0.5
1 ppm	1

< Back Finish

8



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<sup>2</sup> (coefficient of determination)** is to 1, the better the curve is fitting.

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.



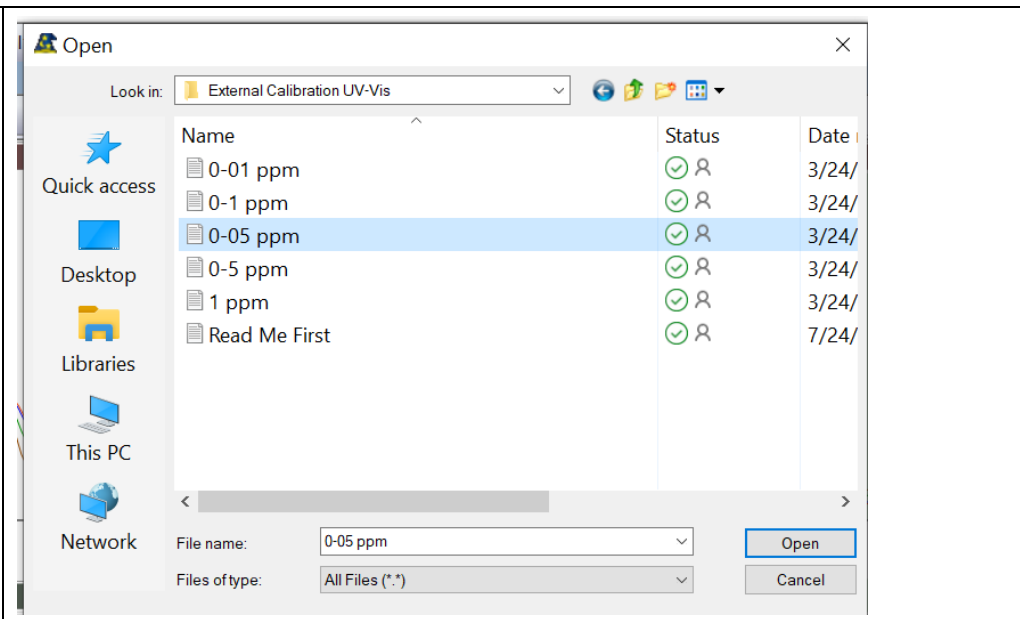
9 Click the **Import Analyte File(s)** button.

Select the file that was left out (0-05 ppm).

Click **Open**.

Select file type to be **UV-Vis** at the prompt.

Click **OK**.



10

The concentration of the unknown is calculated and marked.

Display	Sample Name	Concentration [ppm]	Peak Height [%]	Remove
✓	0-01 ppm	0.01	1.3649	✕
✓	0-1 ppm	0.1	10.391	✕
✓	0-5 ppm	0.5	52.674	✕
✓	1 ppm	1	100.00	✕

Display	Sample Name	Concentration [ppm]	Peak Height [%]	Remove
✓	0-05 ppm	0.042183	5.0764	✕

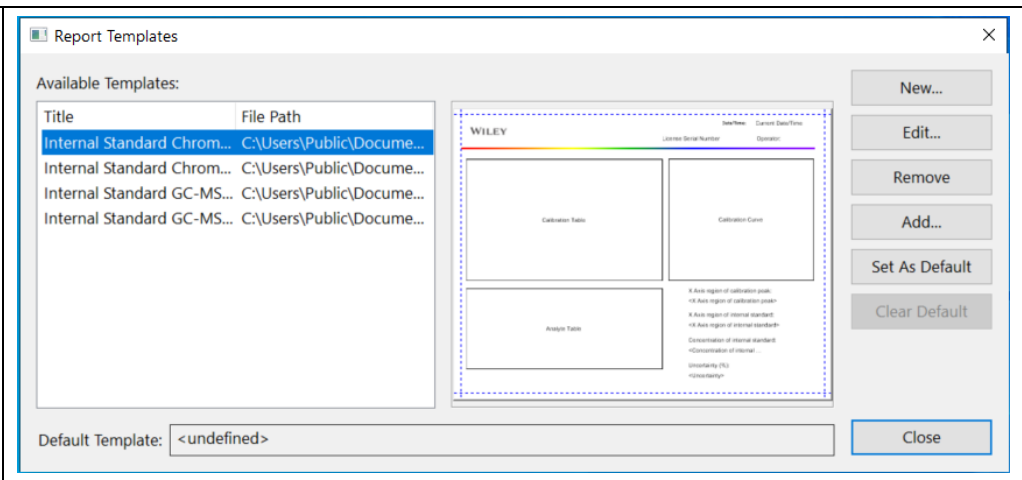
Calibration Curve

$R^2=0.99927$   
 $RMSE=1.0600\%$   
 $y=0.86+100.00x$

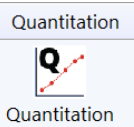
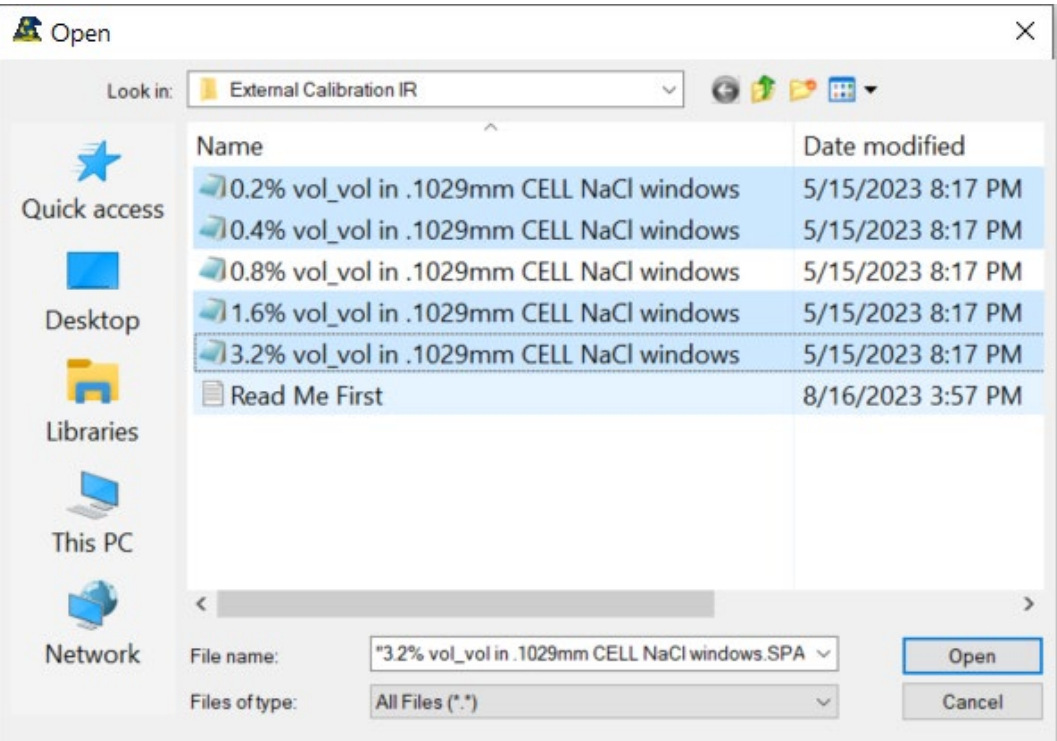
11 Click the **Create Report** button or use **Transfer to: ReportIt** to can generate a report in which objects can be copied/pasted into other desktop tools.

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**



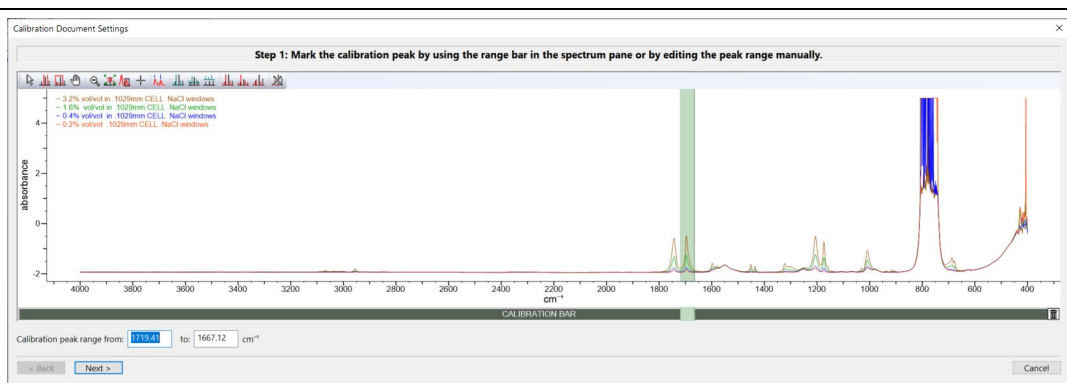
## IR

	Action	Result														
1	Open the <b>Quantitation</b> application by clicking its icon, typically found in the <b>Quantitation</b> group.	 <p>Quantitation</p>														
2	Click <b>New External Calibration</b> button.	KnowItAll prompts user to open calibrant files.														
3	<p>Navigate to the <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Quantitation\External Calibration IR</b> folder.</p> <p>Select sample files and leave one (<b>0.8%</b>) out as the “unknown.”</p> <p>Click <b>Open</b>.</p>	 <p>The screenshot shows a Windows File Explorer window titled 'Open' with the address bar set to 'External Calibration IR'. The file list contains the following items:</p> <table border="1"> <thead> <tr> <th>Name</th> <th>Date modified</th> </tr> </thead> <tbody> <tr> <td>0.2% vol_vol in .1029mm CELL NaCl windows</td> <td>5/15/2023 8:17 PM</td> </tr> <tr> <td>0.4% vol_vol in .1029mm CELL NaCl windows</td> <td>5/15/2023 8:17 PM</td> </tr> <tr> <td>0.8% vol_vol in .1029mm CELL NaCl windows</td> <td>5/15/2023 8:17 PM</td> </tr> <tr> <td>1.6% vol_vol in .1029mm CELL NaCl windows</td> <td>5/15/2023 8:17 PM</td> </tr> <tr> <td>3.2% vol_vol in .1029mm CELL NaCl windows</td> <td>5/15/2023 8:17 PM</td> </tr> <tr> <td>Read Me First</td> <td>8/16/2023 3:57 PM</td> </tr> </tbody> </table> <p>The file '3.2% vol_vol in .1029mm CELL NaCl windows.SPA' is selected in the 'File name' field, and 'All Files (*.*)' is selected in the 'Files of type' dropdown. The 'Open' button is highlighted.</p>	Name	Date modified	0.2% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM	0.4% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM	0.8% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM	1.6% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM	3.2% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM	Read Me First	8/16/2023 3:57 PM
Name	Date modified															
0.2% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM															
0.4% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM															
0.8% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM															
1.6% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM															
3.2% vol_vol in .1029mm CELL NaCl windows	5/15/2023 8:17 PM															
Read Me First	8/16/2023 3:57 PM															

4 Select peak region around 1696  $\text{cm}^{-1}$  by clicking down the **CALIBRATION BAR** (drag and drop).

**Note:** In IR quantitation, one should avoid using the strongest peak.

Click button **Next >**.



6 In the following window, define calibration settings:

(Target Unit: %  
Calculate Using: **Peak Area**)

Click button **Next >**.

Calibration Settings

Step 2: Define the calibration settings.

Target Unit: %

Precision: 5

Uncertainty: 5 ± %

Calculate Using:  Peak Area  Peak Height

Curve-fitting Algorithm: Linear Regression

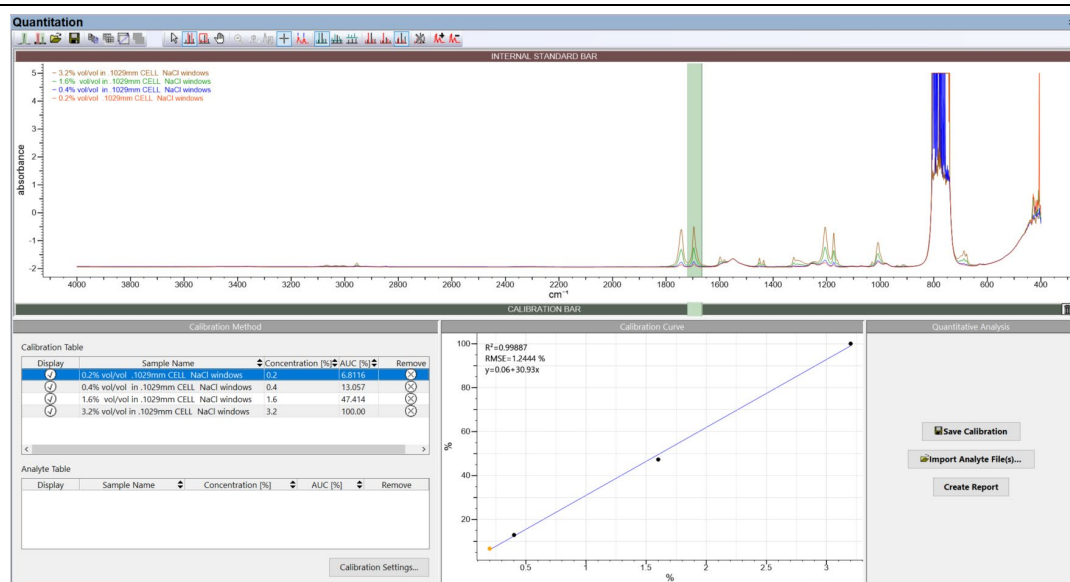
Integration Method:  Tangential Skim  Perpendicular Drop

7 Enter concentrations in the pop-up window based on the numbers in the sample names.

Click **Finish** button.

Sample Name	Concentration [%]
0.2% vol/vol .1029mm CELL NaCl windows	0.2
0.4% vol/vol in .1029mm CELL NaCl windows	0.4
1.6% vol/vol in .1029mm CELL NaCl windows	1.6
3.2% vol/vol in .1029mm CELL NaCl windows	3.2

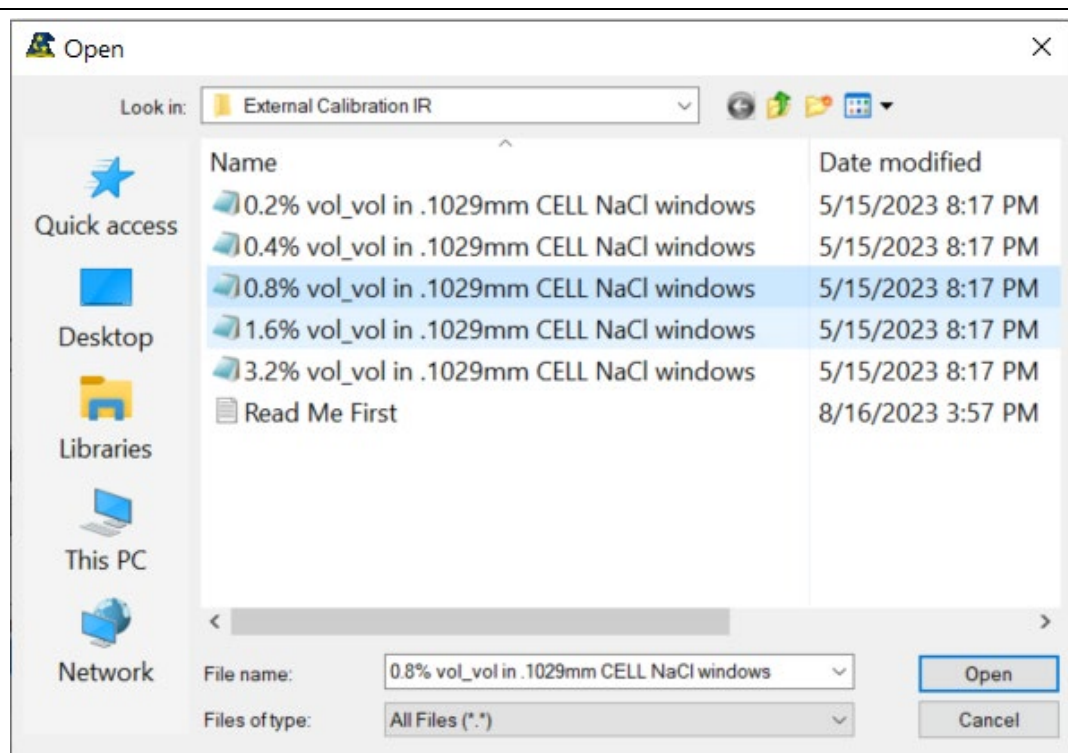
8



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<sup>2</sup> (coefficient of determination)** is to 1, the better the curve is fitting.

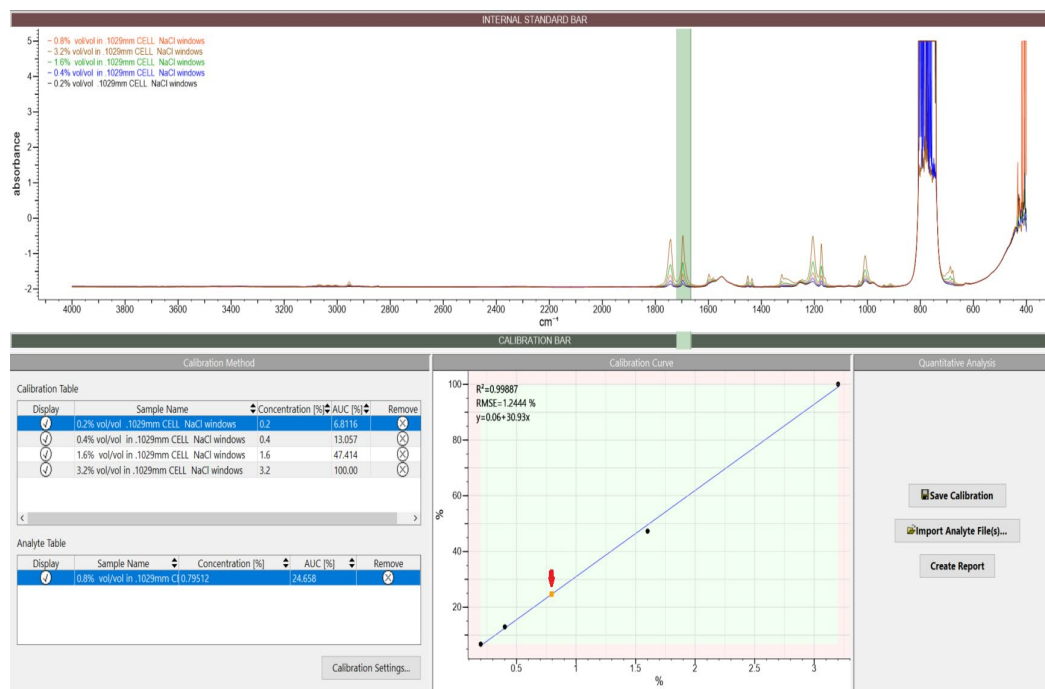
One can reset parameters using the **Calibration Settings** button. One can save this calibration for future use or sharing by clicking the **Save Calibration** button.

- 9 Click the **Import Analyte File(s)** button.
- Select the file that was left out (**0.8%**).
- Click **Open**.



10

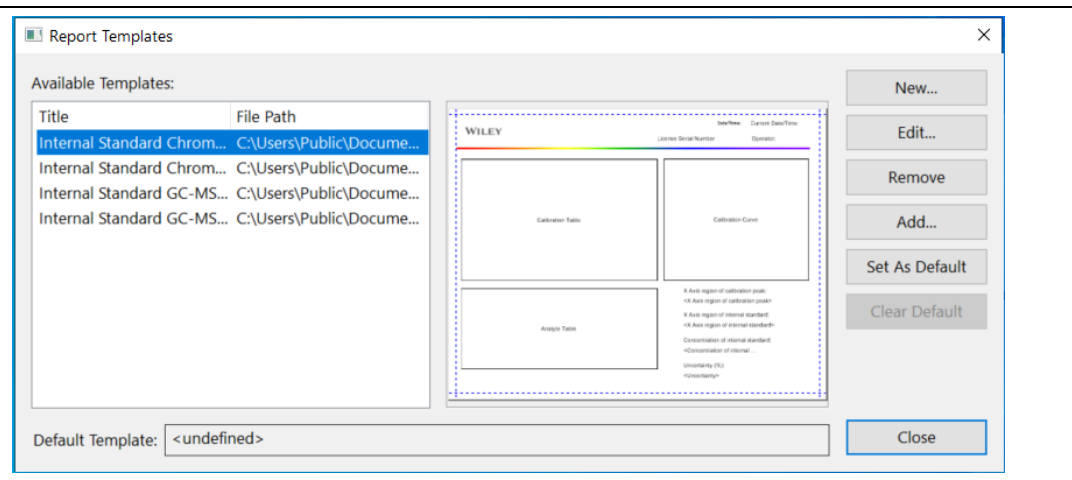
The concentration of the unknown is calculated and marked.



11 Click the **Create Report** button or use **Transfer to: ReportIt** to can generate a report in which objects can be copied/pasted into other desktop tools.

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**

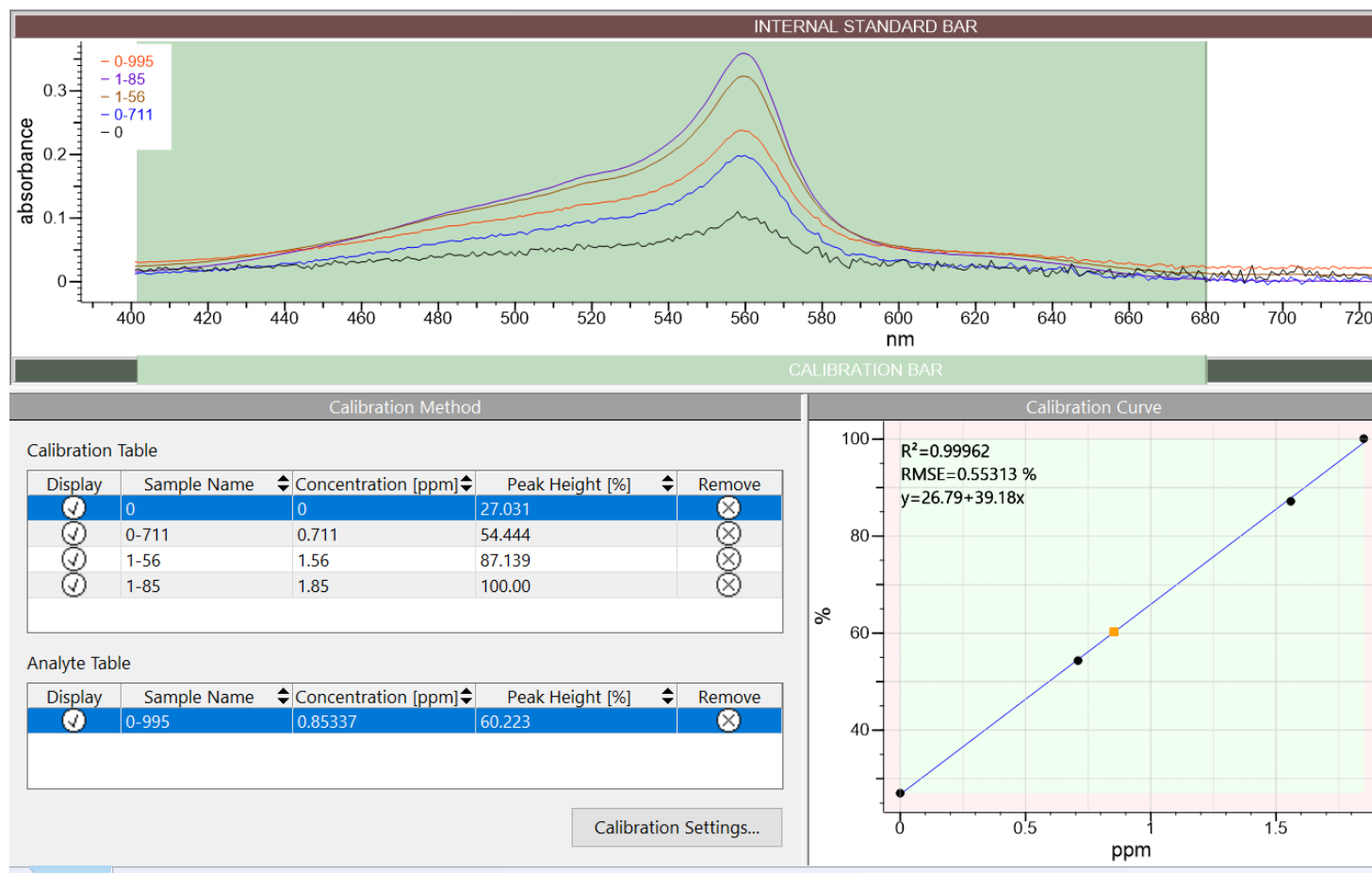




# Standard Addition Quantitation

## Perform Standard Addition Quantitation

This screenshot shows a Standard Addition result, where when the added concentration is 0, the Y-axis value of 26.79 is the signal (due to iron in this case) in the original unknown sample:



# Internal Standard Calibration Quantitation

---

## Perform Internal Standard Calibration Quantitation

### Purpose

These exercises demonstrate how to perform internal standard calibration quantitation using KnowItAll Quantitation software.

---

### Objectives

This exercise will teach you:

- How to create internal standard calibration
  - How to perform quantitation
- 

### Background

Wiley's KnowItAll Quantitation application performs accurate quantitation over comprehensive types of analytical data.

#### ***Training Files Used in This Lesson***

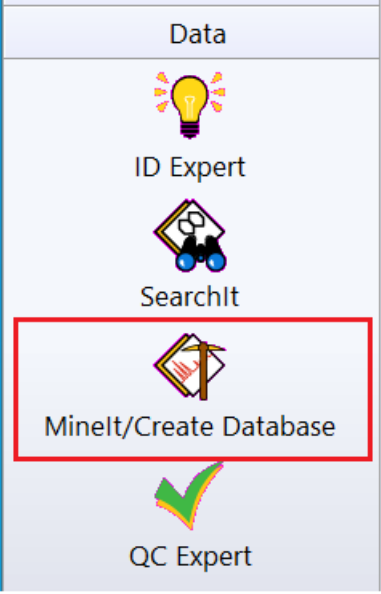
C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Quantitation folder

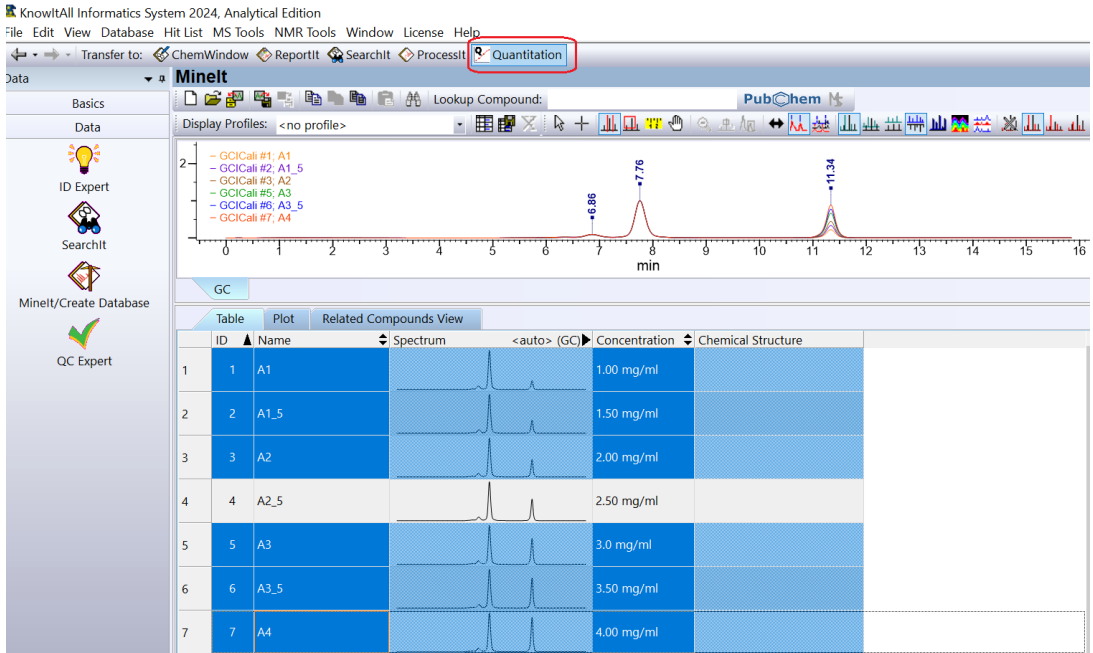
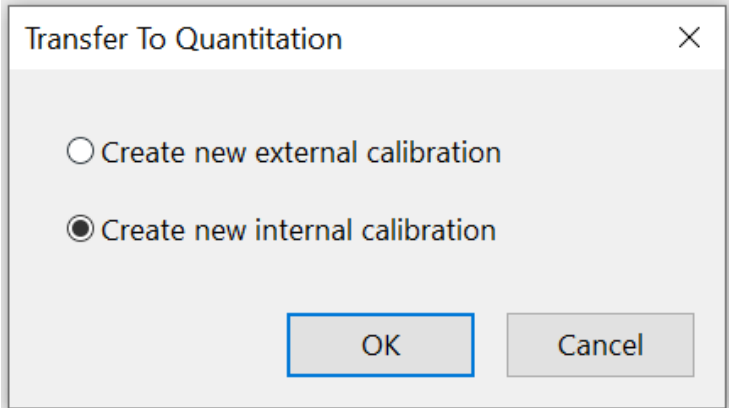
- Internal Calibration Chromatogram

#### ***KnowItAll Applications Used***

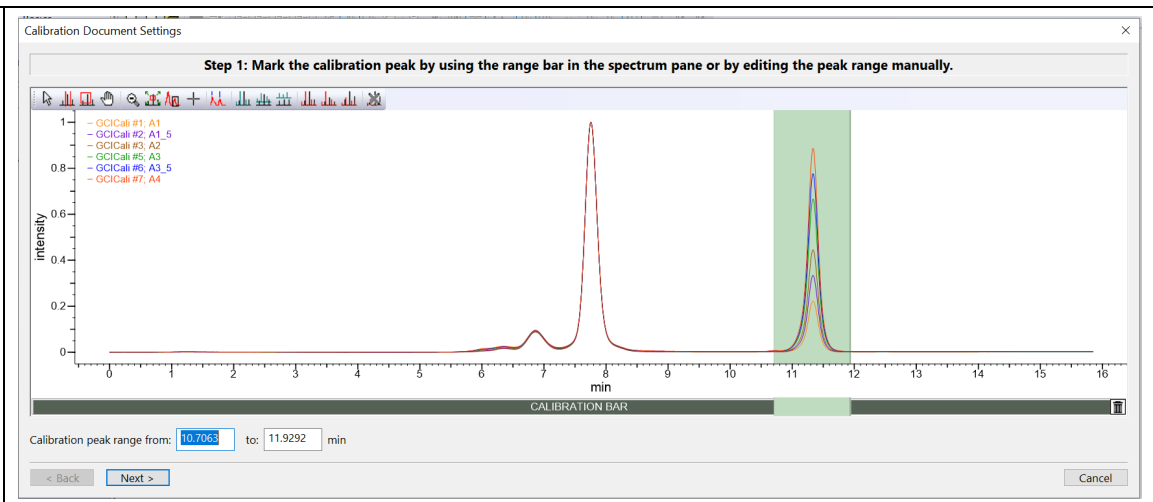
- Quantitation

## Chromatogram

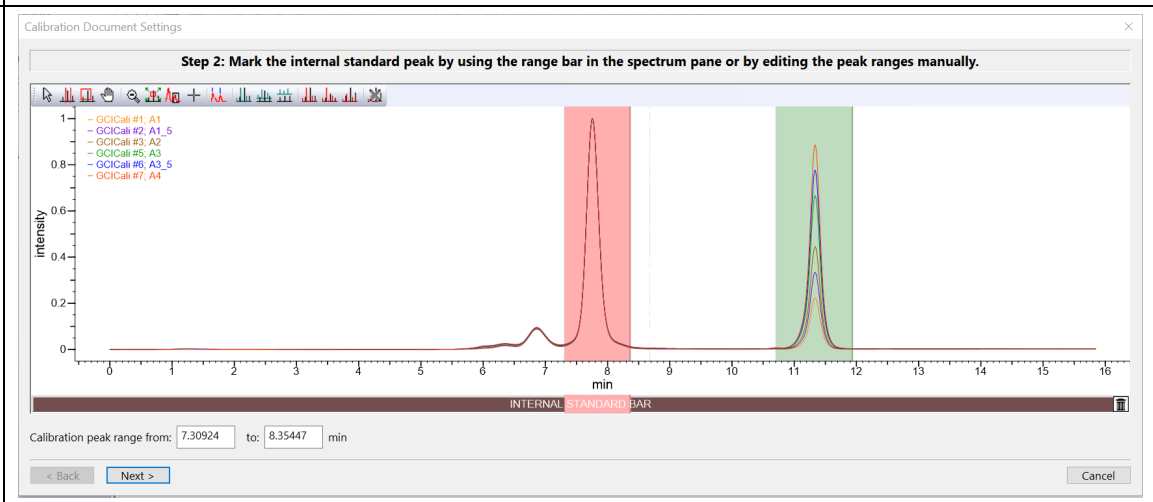
	Action	Result
1	<p>Open the <b>Minelt</b> application by clicking its icon, typically found in the <b>Data</b> group.</p> <p>Choose <b>Database &gt; Open</b>.</p> <p>Click the button <b>Open By Browsing</b>.</p>	 <p>The screenshot shows a vertical menu with the following items from top to bottom: 'Data' (with a light blue header), 'ID Expert' (with a lightbulb icon), 'SearchIt' (with a magnifying glass icon), 'Minelt/Create Database' (with a document and pencil icon, highlighted by a red rectangular box), and 'QC Expert' (with a green checkmark icon).</p>

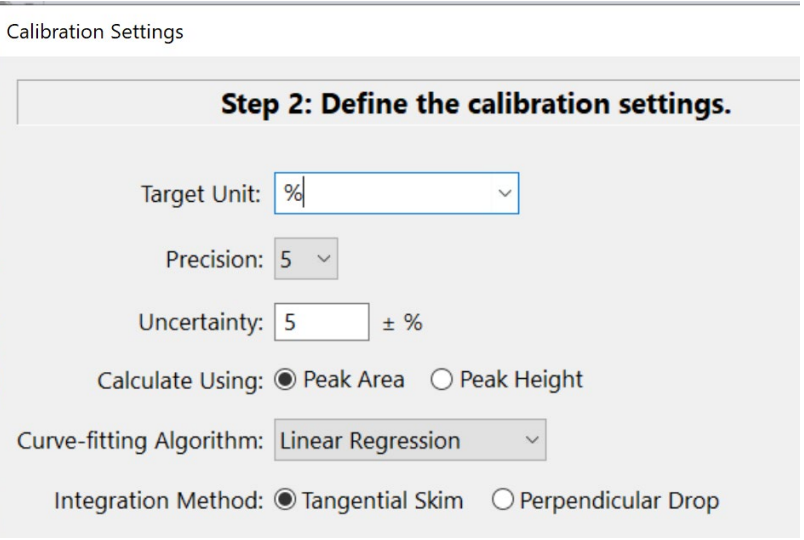
<p>2</p> <p>Navigate to the <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Quantitation\Internal Calibration Chromatogram</b> folder.</p> <p>Select the <b>Chromatograms For Internal Calibration Demo</b>.</p> <p>Click <b>Open</b>.</p> <p>Select a set of records (leave one out to be the unknown), and then select <b>Transfer to: Quantitation</b>.</p>	 <p>The screenshot shows the Minelt software interface. The top menu bar includes File, Edit, View, Database, Hit List, MS Tools, NMR Tools, Window, License, and Help. The 'Transfer to:' dropdown menu is set to 'Quantitation'. The main window displays a chromatogram with peaks labeled at 6.86, 7.76, and 11.34 minutes. Below the chromatogram is a table with the following data:</p> <table border="1"><thead><tr><th>ID</th><th>Name</th><th>Spectrum</th><th>&lt;auto&gt; (GC)</th><th>Concentration</th><th>Chemical Structure</th></tr></thead><tbody><tr><td>1</td><td>A1</td><td></td><td></td><td>1.00 mg/ml</td><td></td></tr><tr><td>2</td><td>A1_5</td><td></td><td></td><td>1.50 mg/ml</td><td></td></tr><tr><td>3</td><td>A2</td><td></td><td></td><td>2.00 mg/ml</td><td></td></tr><tr><td>4</td><td>A2_5</td><td></td><td></td><td>2.50 mg/ml</td><td></td></tr><tr><td>5</td><td>A3</td><td></td><td></td><td>3.0 mg/ml</td><td></td></tr><tr><td>6</td><td>A3_5</td><td></td><td></td><td>3.50 mg/ml</td><td></td></tr><tr><td>7</td><td>A4</td><td></td><td></td><td>4.00 mg/ml</td><td></td></tr></tbody></table>	ID	Name	Spectrum	<auto> (GC)	Concentration	Chemical Structure	1	A1			1.00 mg/ml		2	A1_5			1.50 mg/ml		3	A2			2.00 mg/ml		4	A2_5			2.50 mg/ml		5	A3			3.0 mg/ml		6	A3_5			3.50 mg/ml		7	A4			4.00 mg/ml	
ID	Name	Spectrum	<auto> (GC)	Concentration	Chemical Structure																																												
1	A1			1.00 mg/ml																																													
2	A1_5			1.50 mg/ml																																													
3	A2			2.00 mg/ml																																													
4	A2_5			2.50 mg/ml																																													
5	A3			3.0 mg/ml																																													
6	A3_5			3.50 mg/ml																																													
7	A4			4.00 mg/ml																																													
<p>3</p> <p>Choose <b>Create new internal calibration</b> at the prompt window.</p> <p>Click <b>OK</b>.</p>	 <p>The screenshot shows a dialog box titled 'Transfer To Quantitation'. It contains two radio button options: 'Create new external calibration' (unselected) and 'Create new internal calibration' (selected). At the bottom, there are 'OK' and 'Cancel' buttons.</p>																																																

4 Select peak region around 11.3 as the calibrant peak by clicking down the CALIBRATION BAR (drag and drop).  
  
Click button **Next >**.



5 Select peak region around 7.8 as internal standard peak by clicking down the CALIBRATION BAR (drag and drop).  
  
Click button **Next >**.



<p>6 In the following window, define calibration the settings as shown: (Target Unit: %)</p> <p>Click button <b>Next &gt;</b>.</p>	 <p>The screenshot shows a software window titled "Calibration Settings". At the top, it says "Step 2: Define the calibration settings." Below this, there are several settings:</p> <ul style="list-style-type: none"><li>Target Unit: A dropdown menu showing "%".</li><li>Precision: A dropdown menu showing "5".</li><li>Uncertainty: A text input field containing "5" followed by "± %".</li><li>Calculate Using: Two radio buttons, "Peak Area" (which is selected) and "Peak Height".</li><li>Curve-fitting Algorithm: A dropdown menu showing "Linear Regression".</li><li>Integration Method: Two radio buttons, "Tangential Skim" (which is selected) and "Perpendicular Drop".</li></ul>
--	--

7 Enter concentration ratios in the pop-up window.  
 (Note that the sample names are based on concentrations but decimals have been replaced with underscores. The sample name GCICali #6; A3\_5 has a sample concentration of 3.5%.)  
 Click the **Finish** button.

Calibration Settings

Step 4: Enter concentration values for all spectra. Double-click on a cell to start editing, or select and type in a

INTERNAL STANDARD BAR

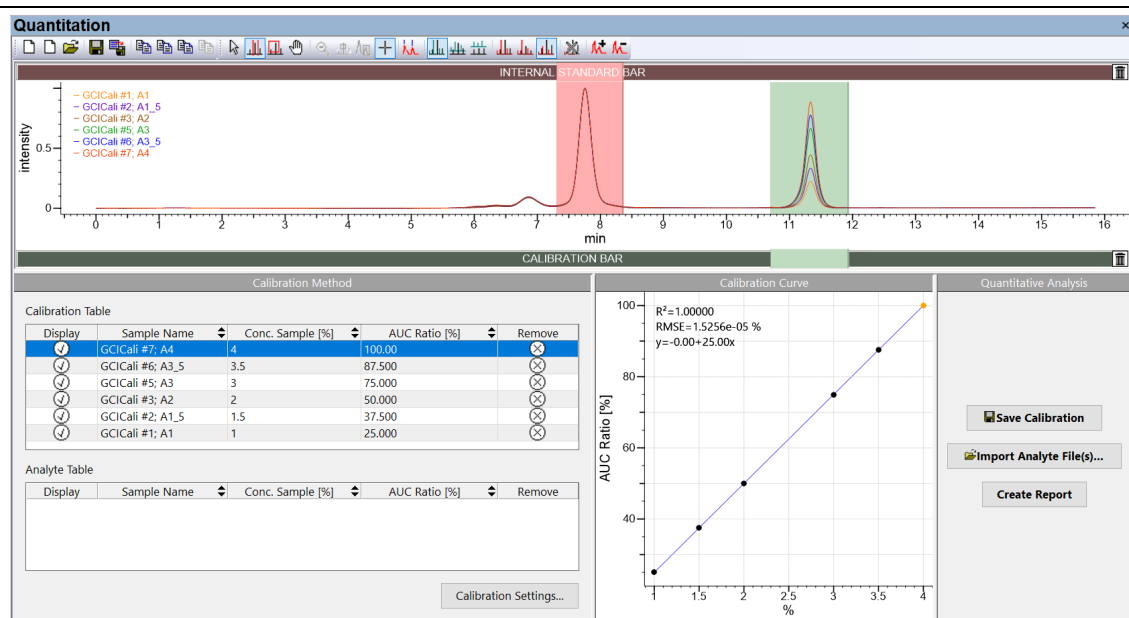
CALIBRATION BAR

Internal standard concentration is constant. Concentration:  %

Sample Name	Conc. Sample [%]
GCICali #7; A4	4
GCICali #6; A3_5	3.5
GCICali #5; A3	3
GCICali #3; A2	2
GCICali #2; A1_5	1.5
GCICali #1; A1	1

< Back Finish

8



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<sup>2</sup> (coefficient of determination)** is to 1, the better the curve is fitting.

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.



- 9 Go back to the **Minelt** database.
- Select the file we have left out, **A2\_5**.
- Select **Transfer to: Quantitation**.
- At the prompt, select **Calculate concentration**.
- Click **OK**.

KnowItAll Informatics System 2024, Analytical Edition

File Edit View Database Hit List MS Tools NMR Tools Window License Help

Transfer to: ChemWindow ReportIt SearchIt ProcessIt **Quantitation**

Data

Basics

Data

Lookup Compound: PubChem

Display Profiles: <no profile>

GC1Cali #4; A2\_5

min

6.86 7.76 11.34

GC

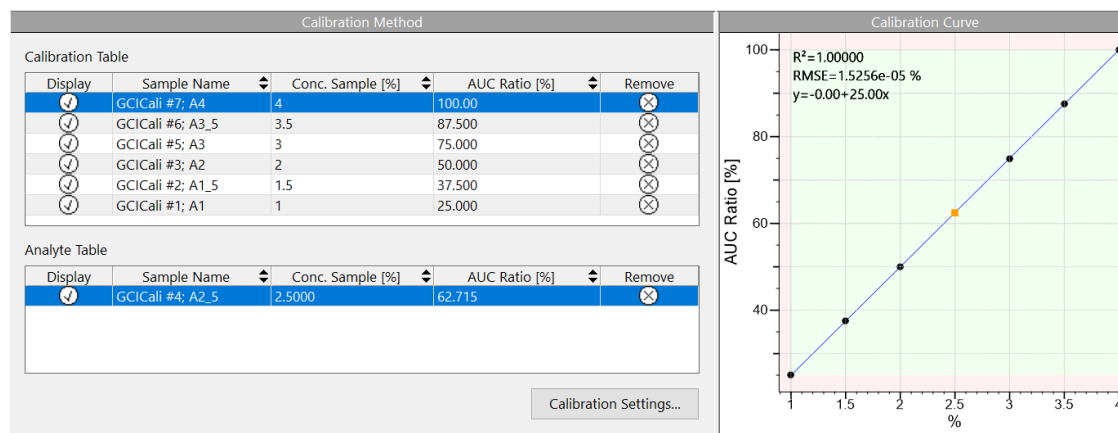
Table Plot Related Compounds View

ID	Name	Spectrum	<auto> (GC)	Concentration	Chemical Structure
1	1 A1			1.00 mg/ml	
2	2 A1_5			1.50 mg/ml	
3	3 A2			2.00 mg/ml	
4	4 A2_5			2.50 mg/ml	
5	5 A3			3.0 mg/ml	
6	6 A3_5			3.50 mg/ml	
7	7 A4			4.00 mg/ml	

Spectral Processing

10

The concentration of the unknown is calculated and marked

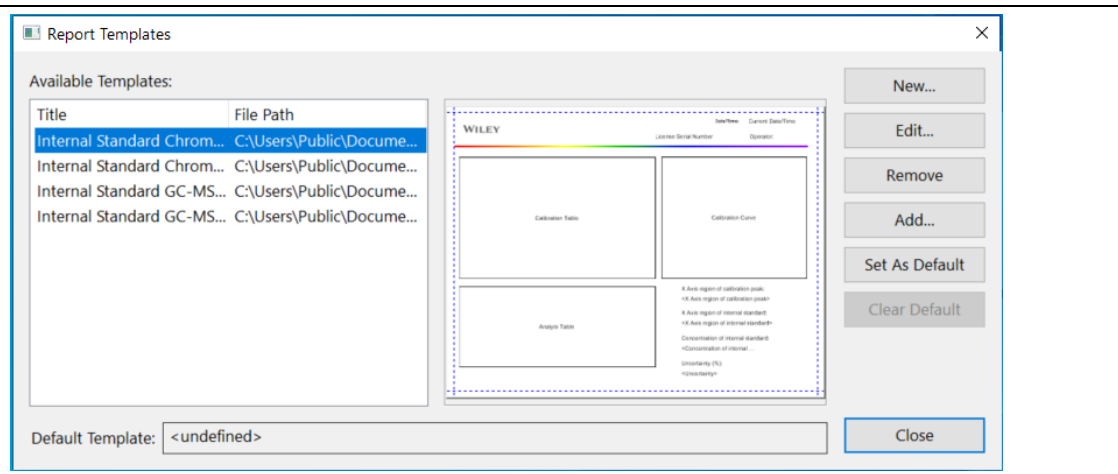


11

Click the **Create Report** button or use **Transfer to: ReportIt** to can generate a report in which objects can be copied/pasted into other desktop tools.

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**

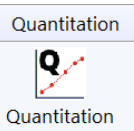


## GC-MS

This exercise requires user to download sample datasets from [https://arts-sciences.und.edu/academics/chemistry/kubatova-research-group/chrom\\_ms02.html](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 standard: *o*-Terphenyl (IS) RT 11.5192 62.0 ug/ml

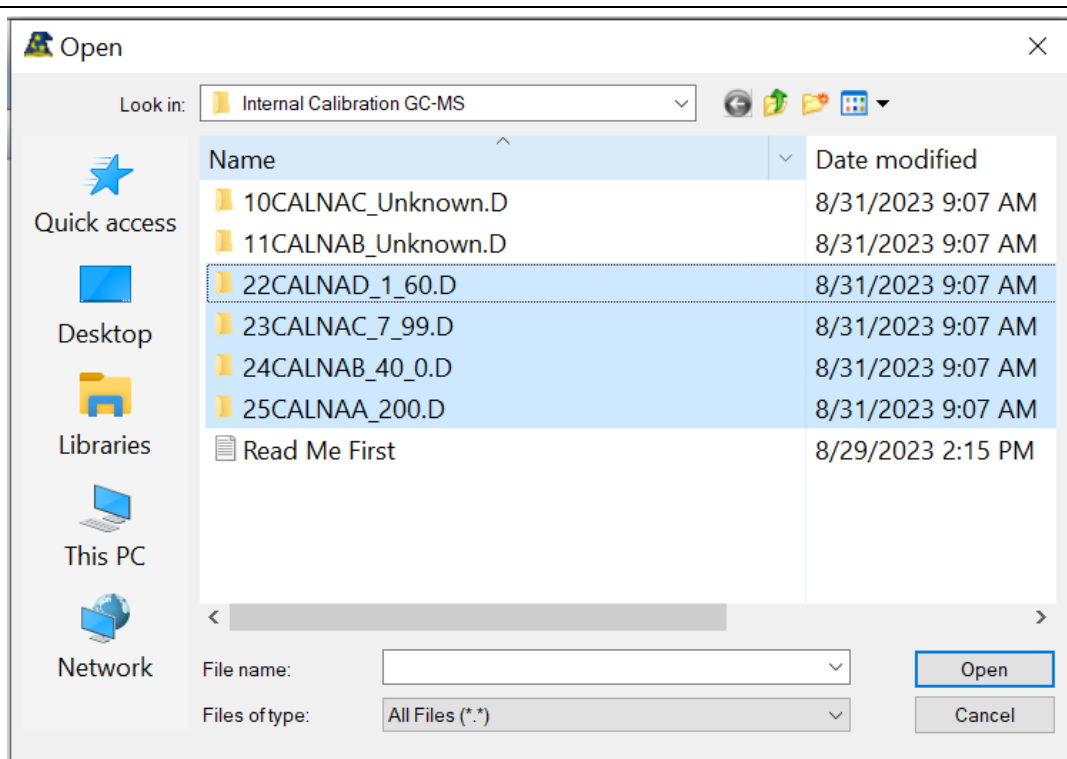
Analyte: Guaiacol RT 6.3368 min

	Action	Result
1	Open the <b>Quantitation</b> application by clicking its icon, typically found in the <b>Quantitation</b> group.	 The image shows the Quantitation application icon, which consists of a blue square with the word "Quantitation" at the top, a white circle containing a red 'Q' and a red dashed line graph, and the word "Quantitation" at the bottom.
2	Click <b>New Internal Calibration</b> 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.

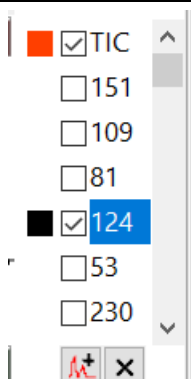
Click **Open**.



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**

The screenshot displays the 'Calibration Document Settings' window. At the top, the 'Sample File' is set to '25CALNAA\_200.D'. A callout box with the text 'Step 1: Please use the ion chromatogram checkboxes to select sample standard ions.' points to a list of checkboxes on the right side of the window. The list includes TIC (checked), 151, 109, 81, 124, 230, and 53. Below the callout, the 'Raw Spectrum 222 at 6.3391 min' is shown in the 'BACKGROUND RANGE BAR'. The 'AVERAGE RANGE BAR' shows 'Raw Spectrum 1370 at 19.3007 min'. The 'Extracted Raw Spectrum' plot shows peaks at m/z 81, 109, and 124, with a chemical structure of 2-methoxyphenol (guaiacol) overlaid. A 'Matches' table is visible on the right side of the interface.

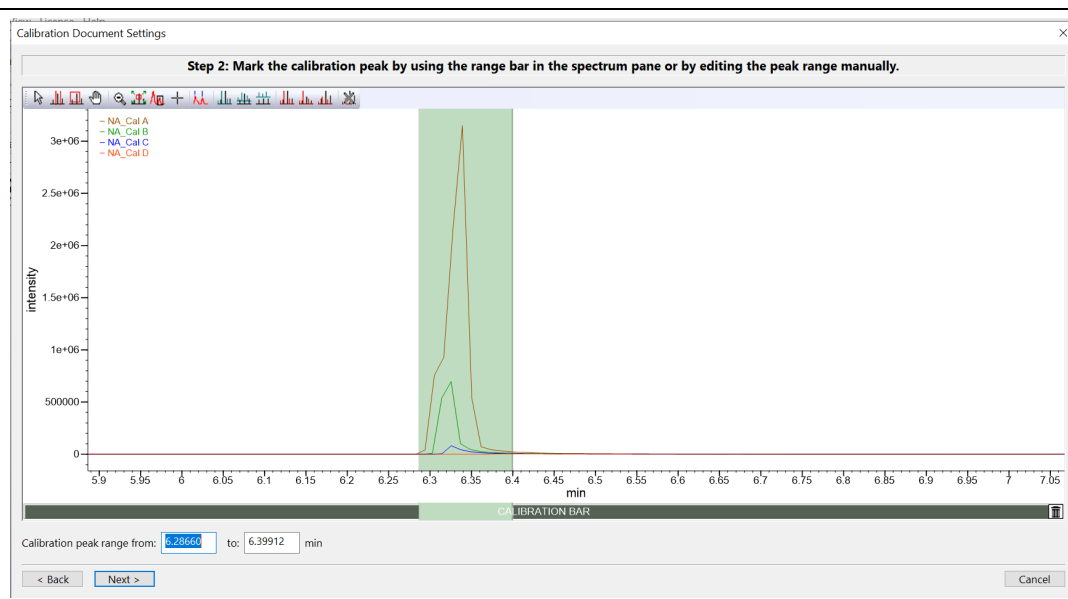
#	Match	Score	HQI	R.H.
1	Phenol, 2-...	98.33	98.32	98.44
2	4-Methox...	96.83	96.67	98.27
3	Guaiacol<...	96.37	96.04	99.31
4	Formic aci...	86.44	86.34	87.31
5	2-Cyclope...	85.90	85.85	86.31
6	Ethanone...	85.32	85.15	86.87
7	Ethanone...	84.30	84.29	84.42
8	Ethanone...	82.78	82.77	82.95
9	Guaiacol a...	82.68	82.41	85.11
10	2-Cyclope...	82.49	81.52	91.14

5	<p>Select a component from the <b>Raw Spectrum</b> pane, in our example, the interested component has a TIC peak at <b>6.45</b> min.</p> <p>Select an ion, in this case, we select its <b>molecular m/z 124</b>.</p> <p>Click <b>Next &gt;</b> (bottom left corner)</p>	 <p><input checked="" type="checkbox"/> TIC <input type="checkbox"/> 151 <input type="checkbox"/> 109 <input type="checkbox"/> 81 <input checked="" type="checkbox"/> 124 <input type="checkbox"/> 53 <input type="checkbox"/> 230</p> <p>⏪ ⏩ ✕</p>
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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).

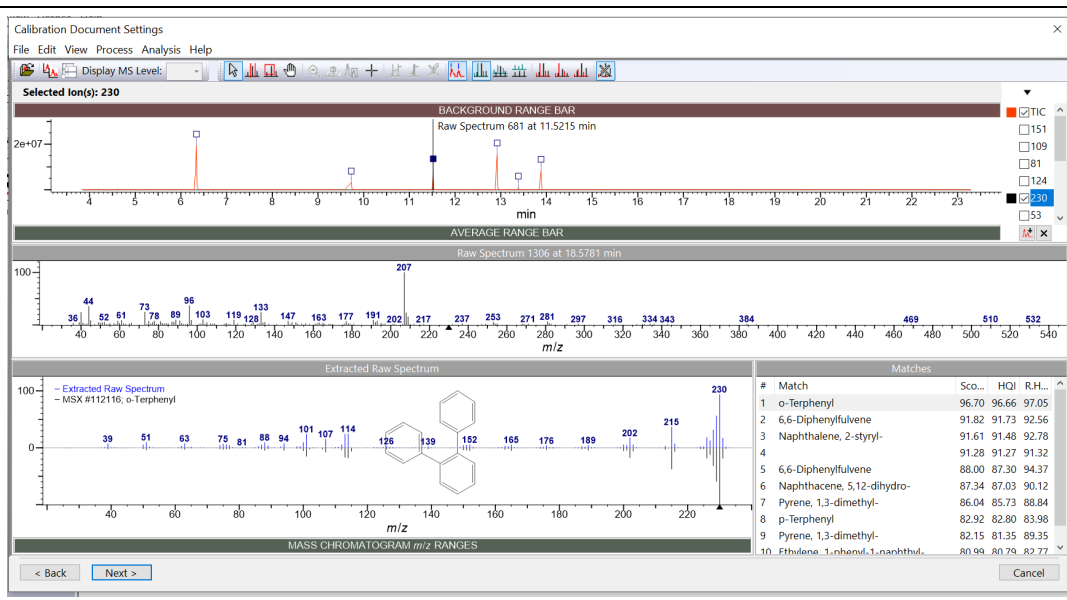
Click button **Next >**.



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)



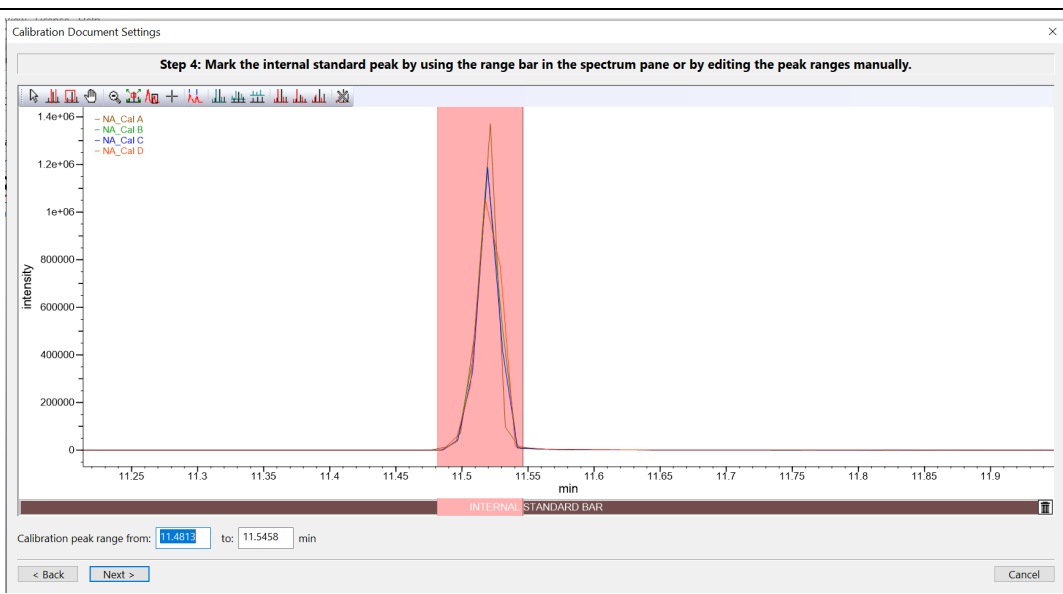
8 Right mouse click the spectrum pane.

Select **Zoom out**.

- Zoom Out
- View Default Region      Ctrl+1
- View Entire Spectrum      Ctrl+0
- Selection Mode      Ctrl+L
- Horizontal Zoom Mode      Ctrl+R
- Box Zoom Mode
- Pan Mode      Ctrl+M
- Copy
- Edit Properties...



- 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 >**.

Calibration Settings

Target Unit:

Precision:

Uncertainty:  ± %

Calculate Using:  Peak Area  Peak Height

Curve-fitting Algorithm:

Integration Method:  Tangential Skim  Perpendicular Drop

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.

Calibration Settings

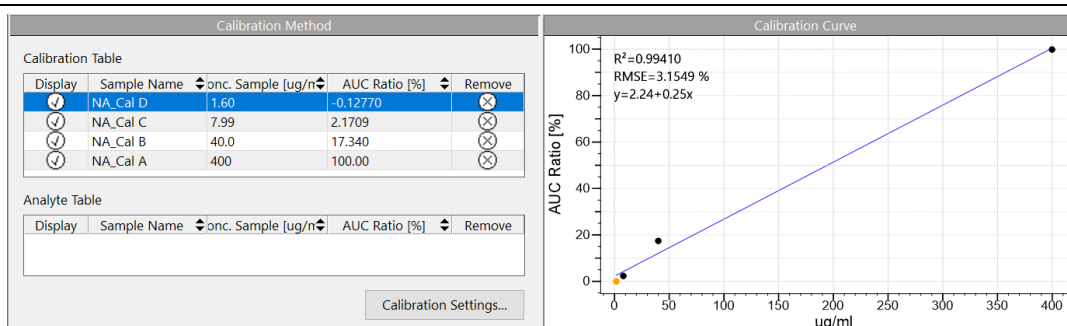
**Step 6: Enter concentration values for all spectra. Double-click on a cell to start editing, or select and type in a number.**

Internal standard concentration is constant. Concentration:  ug/ml


Sample Name	Conc. Sample [ug/ml]
NA_Cal D	1.60
NA_Cal C	7.99
NA_Cal B	40.0
NA_Cal A	200

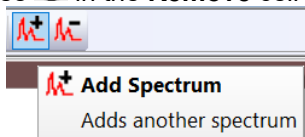
< Back Finish Cancel

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<sup>2</sup> (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**



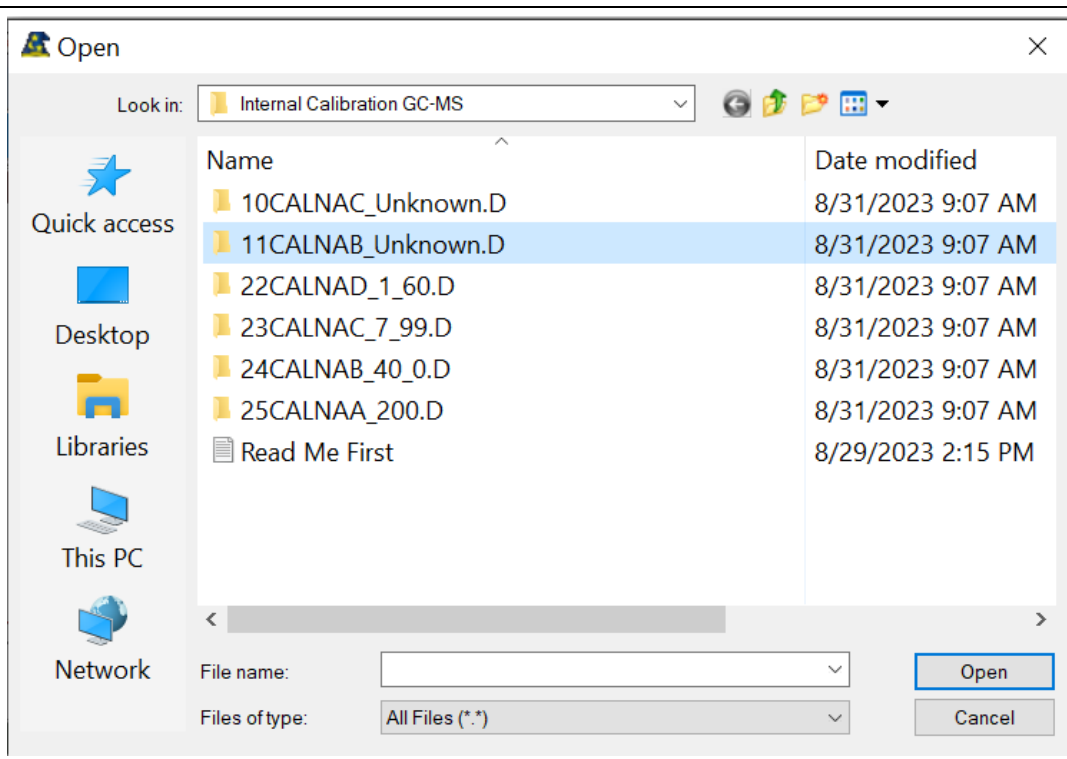
**Spectrum** to add new calibrants,

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.

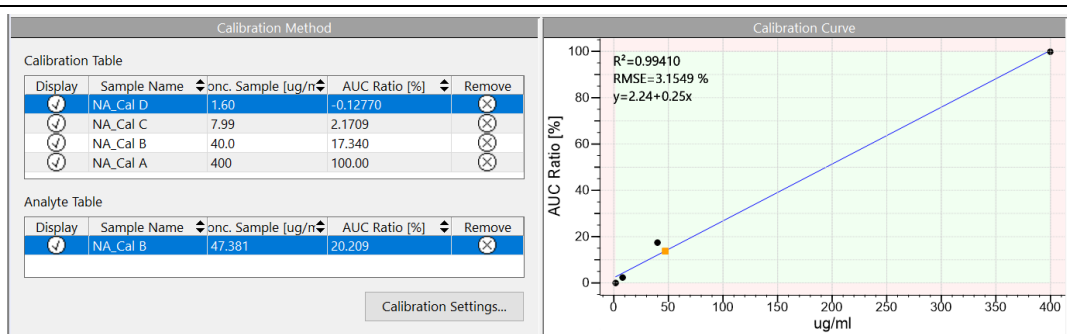
12 Click the **Import Analyte File(s)** button.

Select unknown file folder **11\_CLANAB\_Unknown.D** to calculate the concentrations.

Click **Open**.



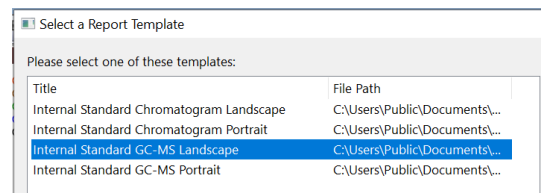
13



The concentration ratio of analyte to internal standard is shown in the **Analyte Table** and as a square spot in the **Calibration Curve**.

14 Click **Transfer to: Report**

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



Click **OK**

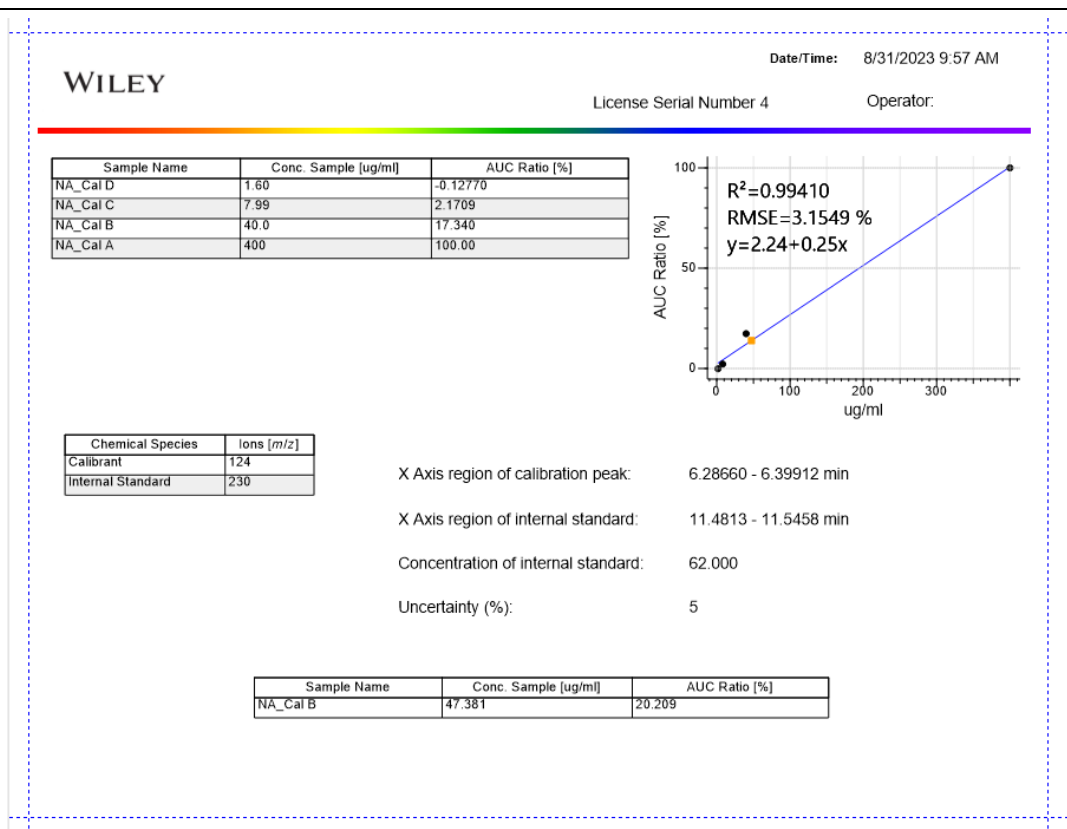
Note: if a template is used for the first time, user has to do the following before transfer data to ReportIt application:

**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.