

Moisture Analysis Toolkit 3

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1.1 Installation

To begin, download and install the latest version of the Moisture Analysis Toolkit (MAT) 3 from the AQUALAB website at aqualab.com/en/get-started.

Upon launching the application for the first time, a prompt will appear requesting a valid software license key. This license key is delivered as a PDF document and sent via email upon confirmation of purchase. Once the License has been successfully verified, the application proceeds to the MAT 3 Home screen.

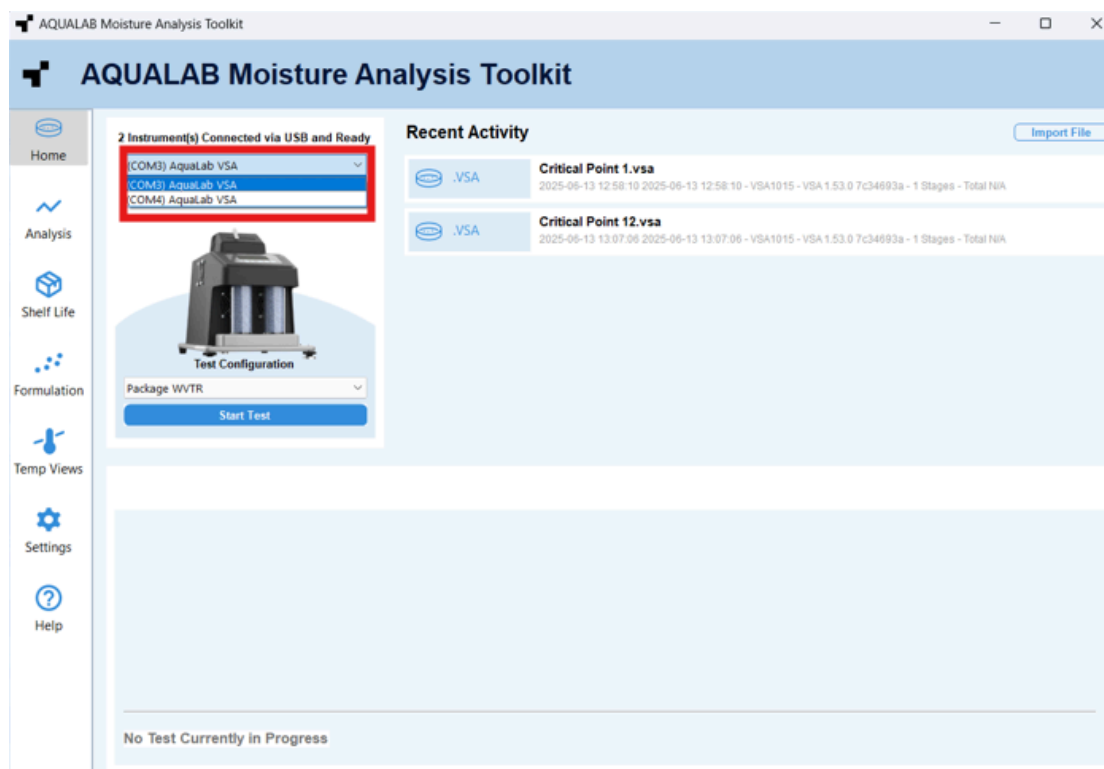
1.2 Operation

1.2.1 Conducting a test

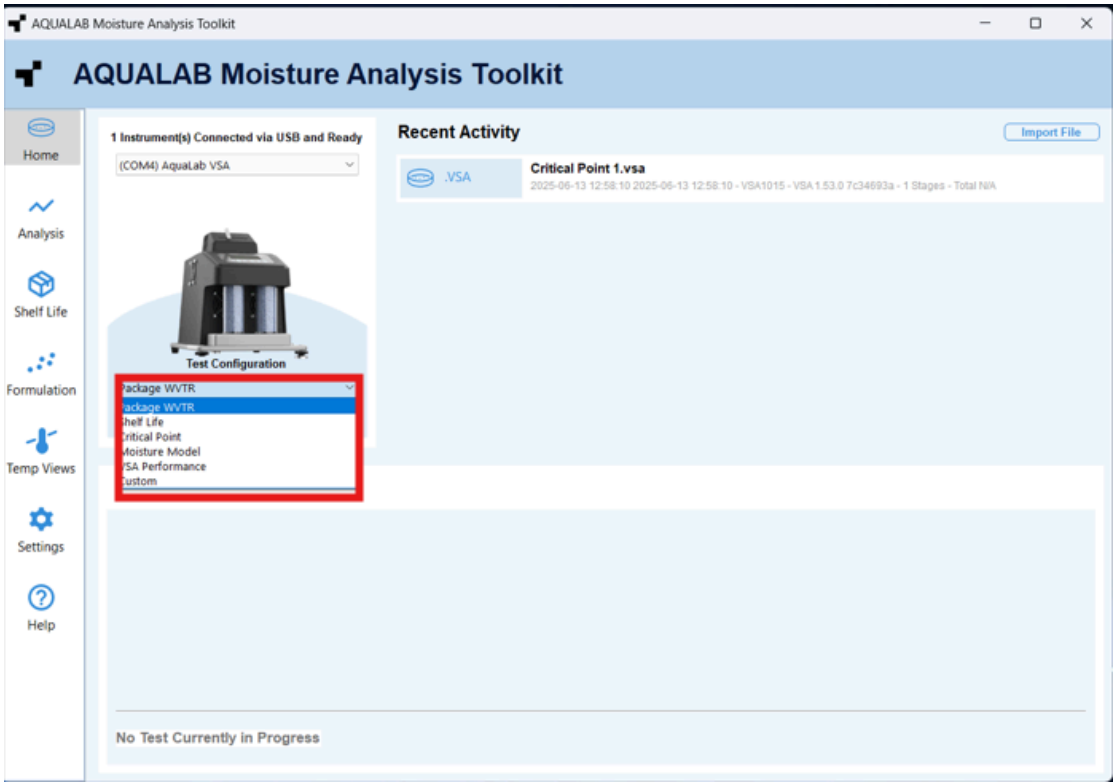
Note: It is important to verify the AQUALAB VSA water activity calibration against known standards to guarantee optimal performance and accuracy. Addium recommends verification before performing each isotherm test.

Addium also recommends annual factory calibration to maintain optimal performance.

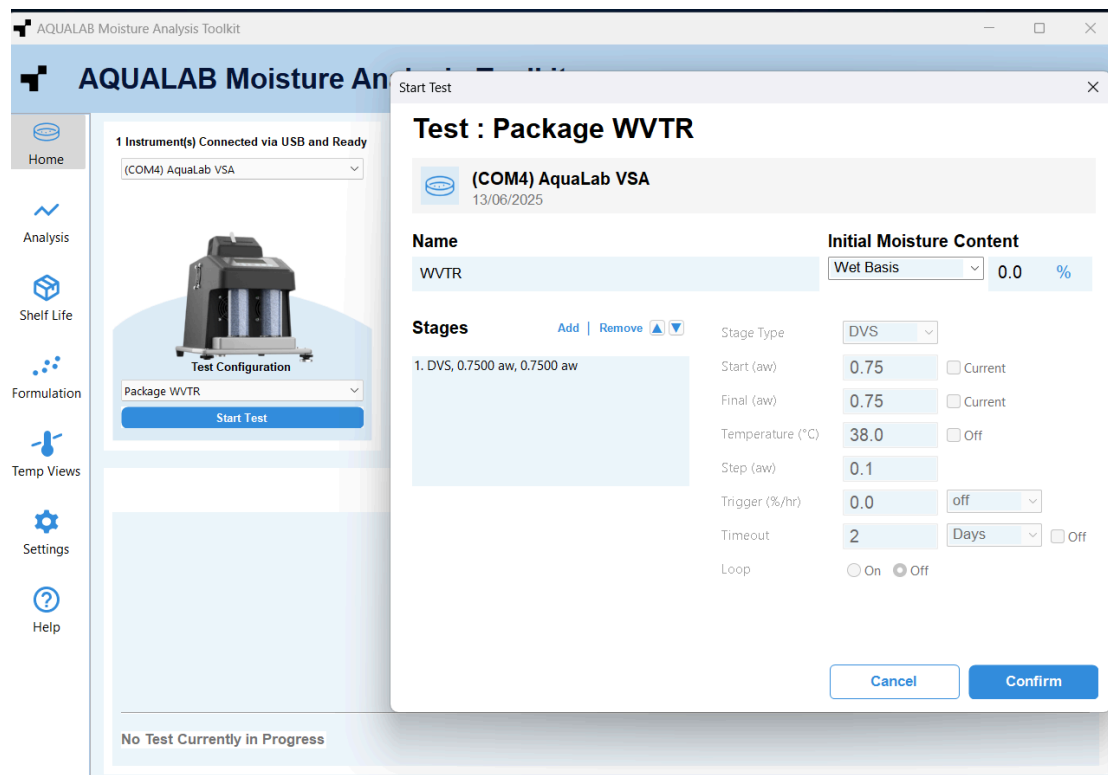
To conduct a test using MAT, begin by connecting the VSA to the computer via USB. Within the MAT software, select the VSA from the instrument drop-down menu.



Next, choose the desired test configuration from the test configuration drop-down list.

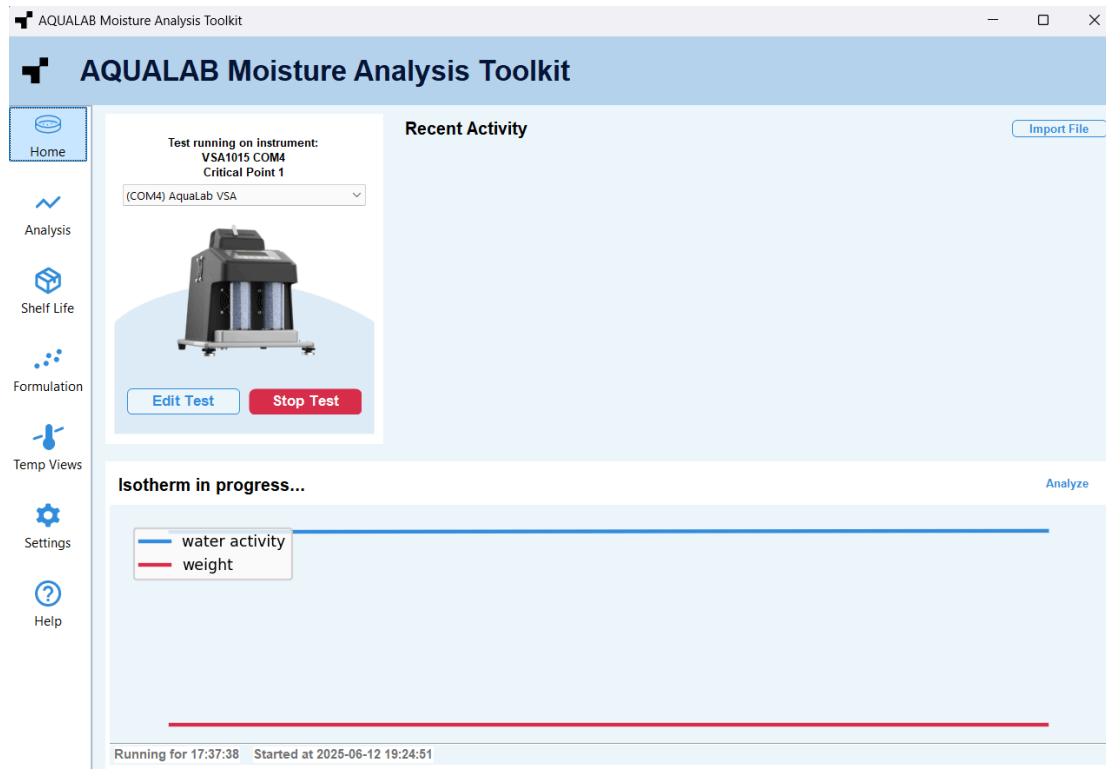


Upon selection, a configuration dialog will appear. Fields in blue are editable. The configuration parameters can be changed by first clicking on the Stage, then selecting the parameter to be adjusted. Once all changes have been made, select 'Confirm' to proceed.

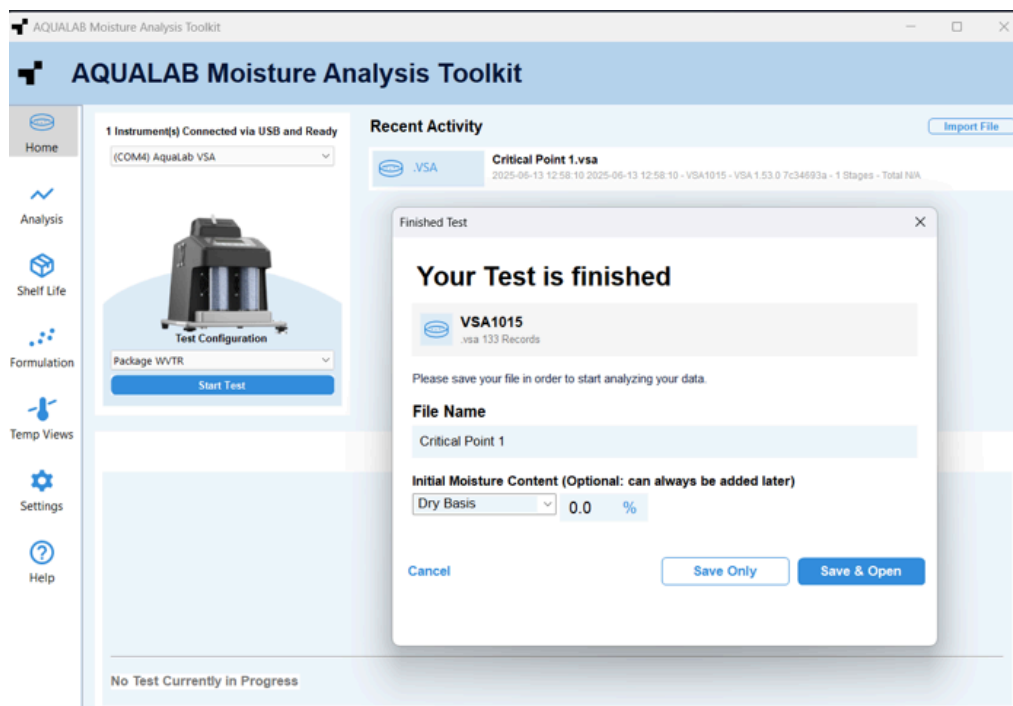


Follow the Test Instructions and press Start Now when ready. Complete test set-up at VSA. The test will begin automatically once VSA prompts have been completed. Follow the message on the VSA screen to place the sample in the cup and press the next button to weigh the sample.

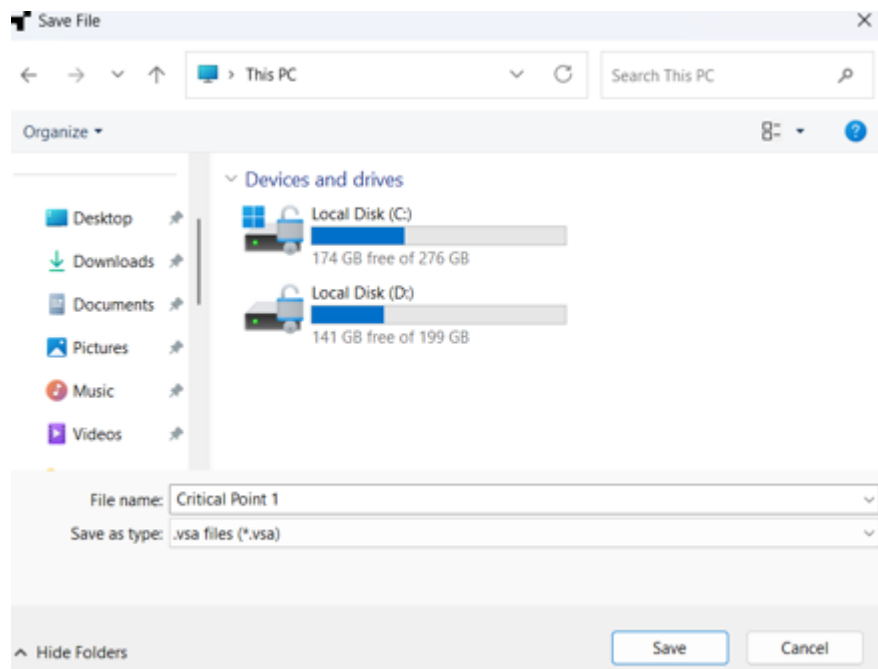
1. Test in progress



2. Once the test is completed a dialog box opens up automatically



3. You can edit the test name to name your file and enter the initial moisture content needed for analysis. Click on Save Only or Save & Open to save the results of the test. upon clicking the windows export save wizard opens up.



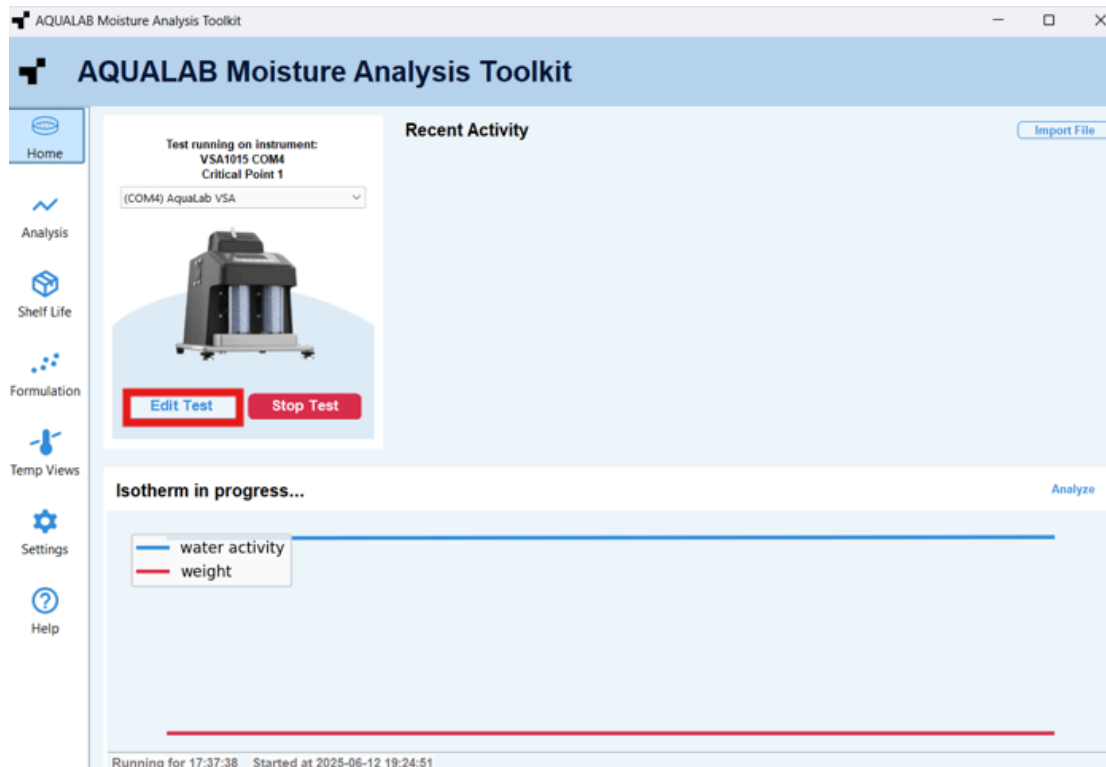
4. If Save & Open is clicked the test results are open for analysis in the analysis page.

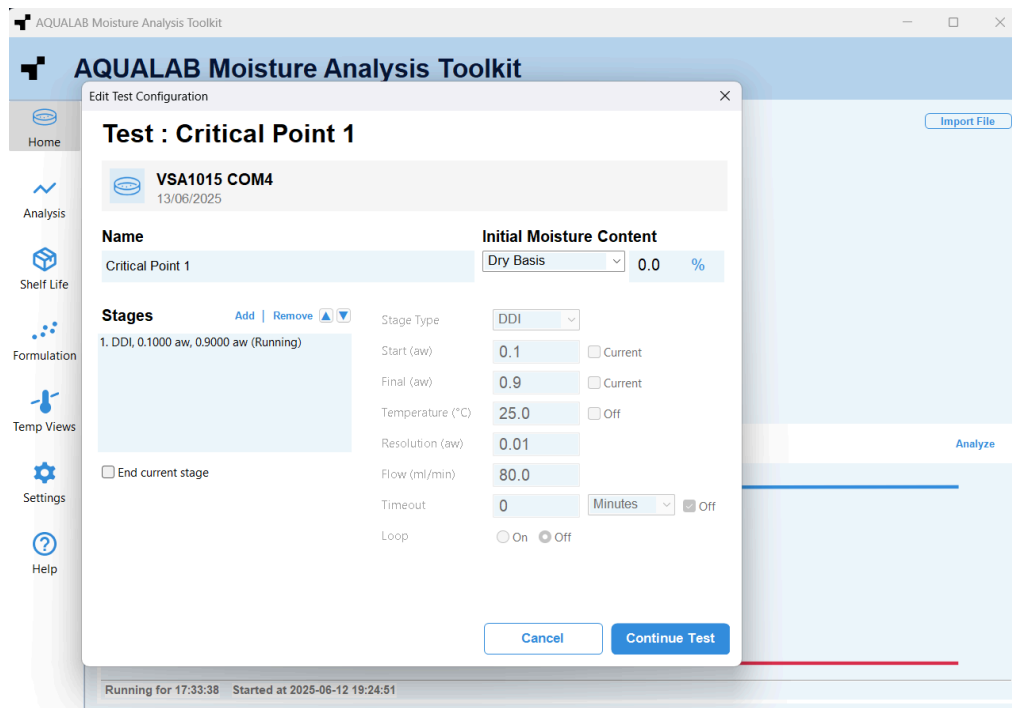
1.2.1.1 Edit configuration of an ongoing test

A test that is already running can be edited and additional stages can be added to a running test (inserted after the current running stage) at any time using the edit test function. To edit the test follow these steps.

Steps

1. Click on the Edit Test button in the Home screen. The test configuration dialog box will open.

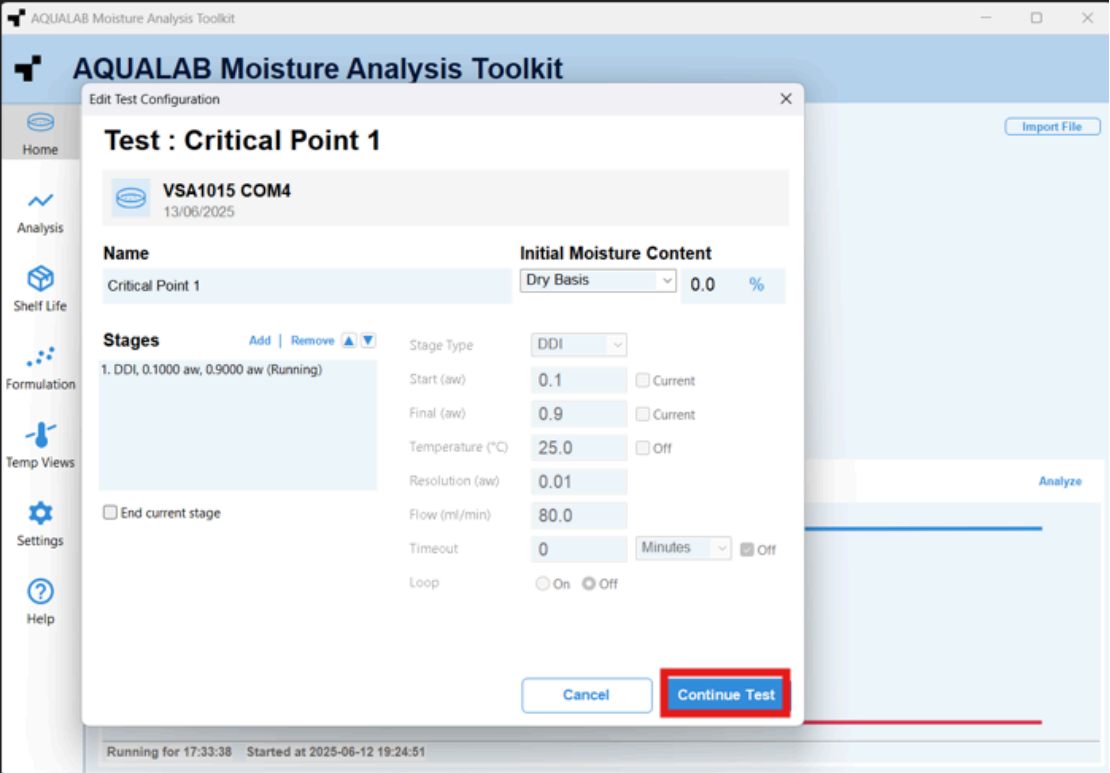




2. Make changes to the configuration.

- The current running stage and any completed stages cannot be edited. To add additional stages, select the "Add" button. Then set up each new stage. To edit an existing stage that is not currently running and is not complete. Select the stage and adjust the settings accordingly.
- To alter a currently running stage, insert a new stage after the currently running stage. Make sure to set the starting aw to "Current" if you want the new stage to resume where the previous stage left off. Then select "End current stage" and click OK. The current stage will end and the newly created stage will start.

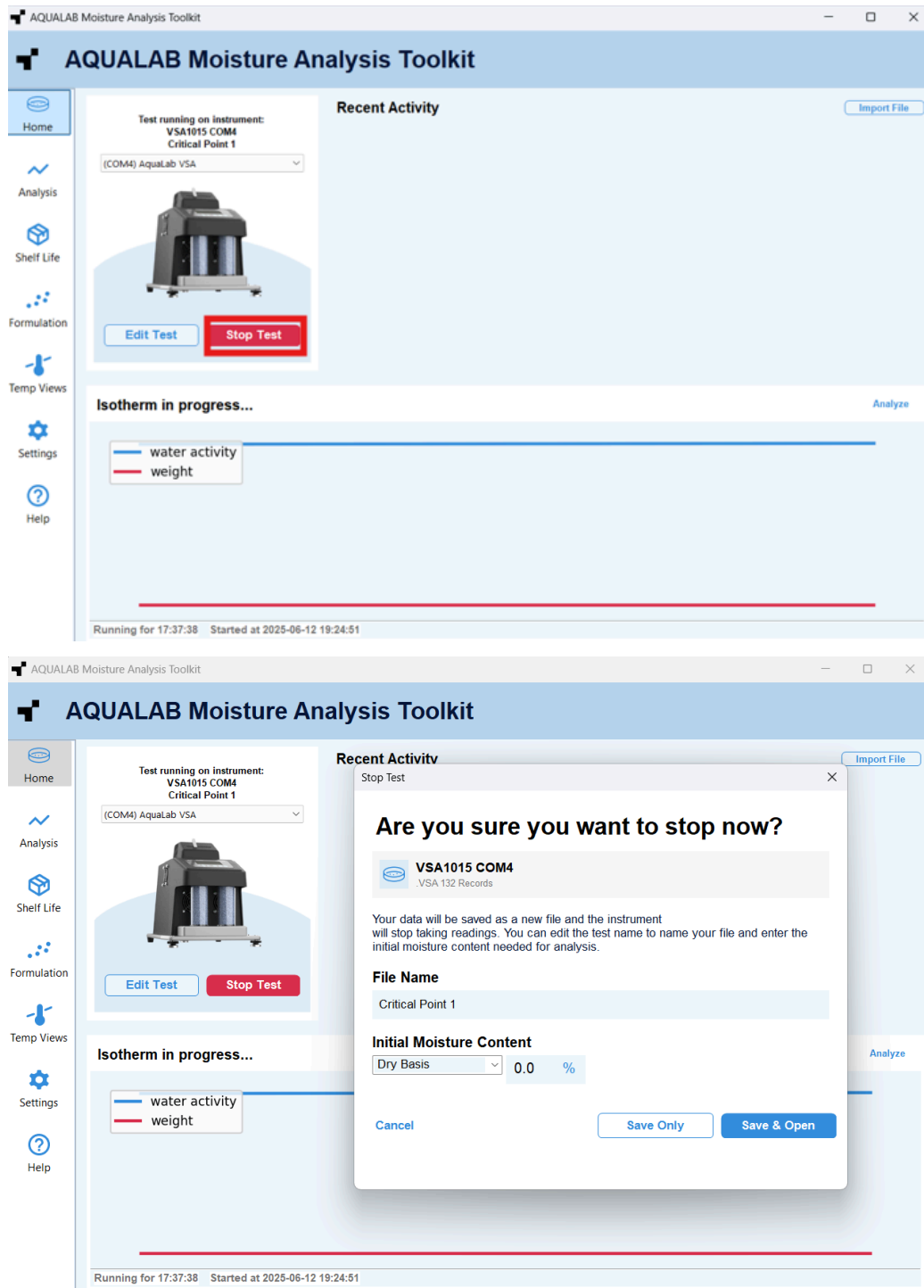
3. Once changes have been made, click Continue Test to save changes to the configuration and the test shall continue with the updated configurations.



1.2.1.2 Stop test

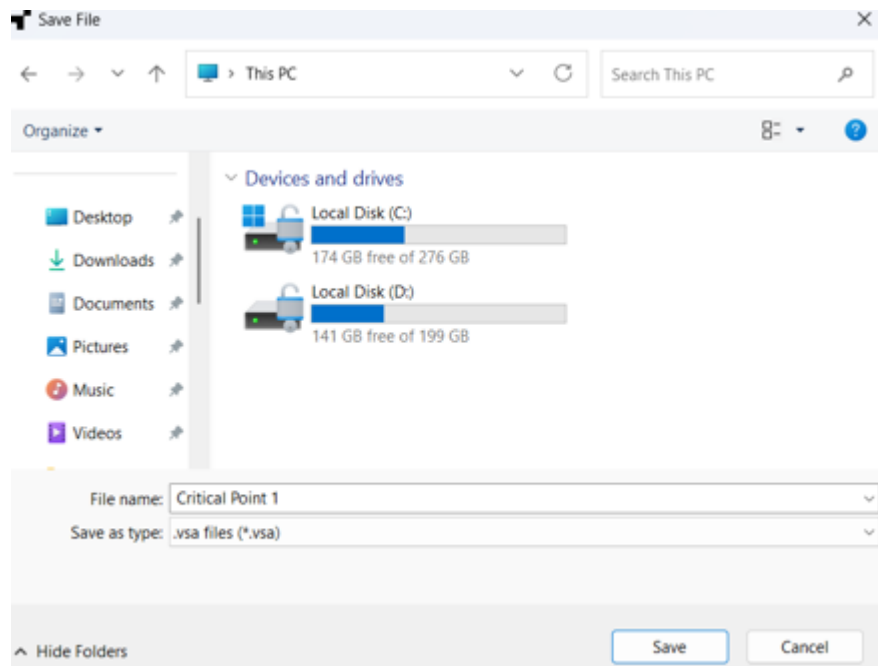
Steps

1. Click the Stop Test button to stop the test, upon clicking a confirmation dialog opens up.



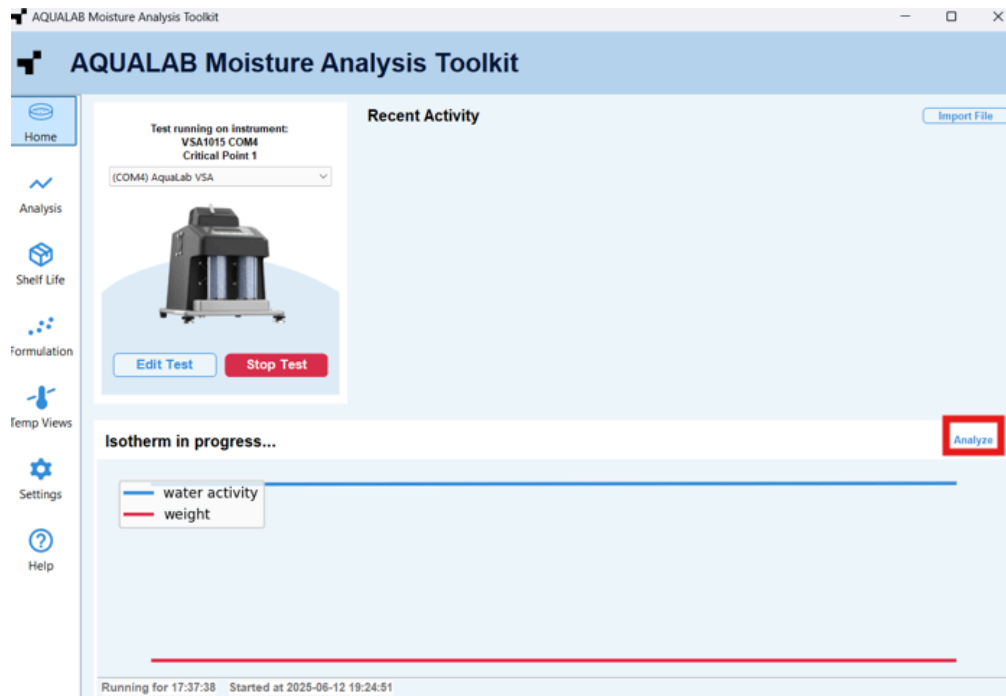
2. Click Save Only to save the test results in the local machine or click Save & Open to save the file and open the file in the Analysis page. You can edit the test name to name your file and enter the entail moisture content needed for analysis.

3. Once one of the save options is clicked the export wizard opens up. Provide the folder location to save the results. Then click Save



1.2.1.3 Analyze an ongoing test

Step 1: Users will be able to analyze an ongoing test by clicking the Analyze button on the top right corner of the progression graph.

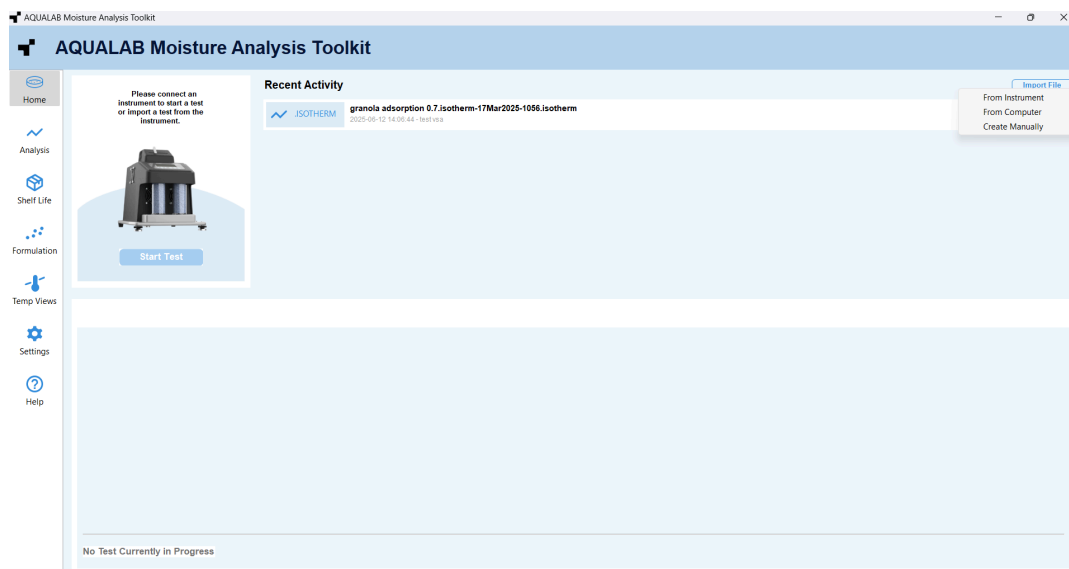
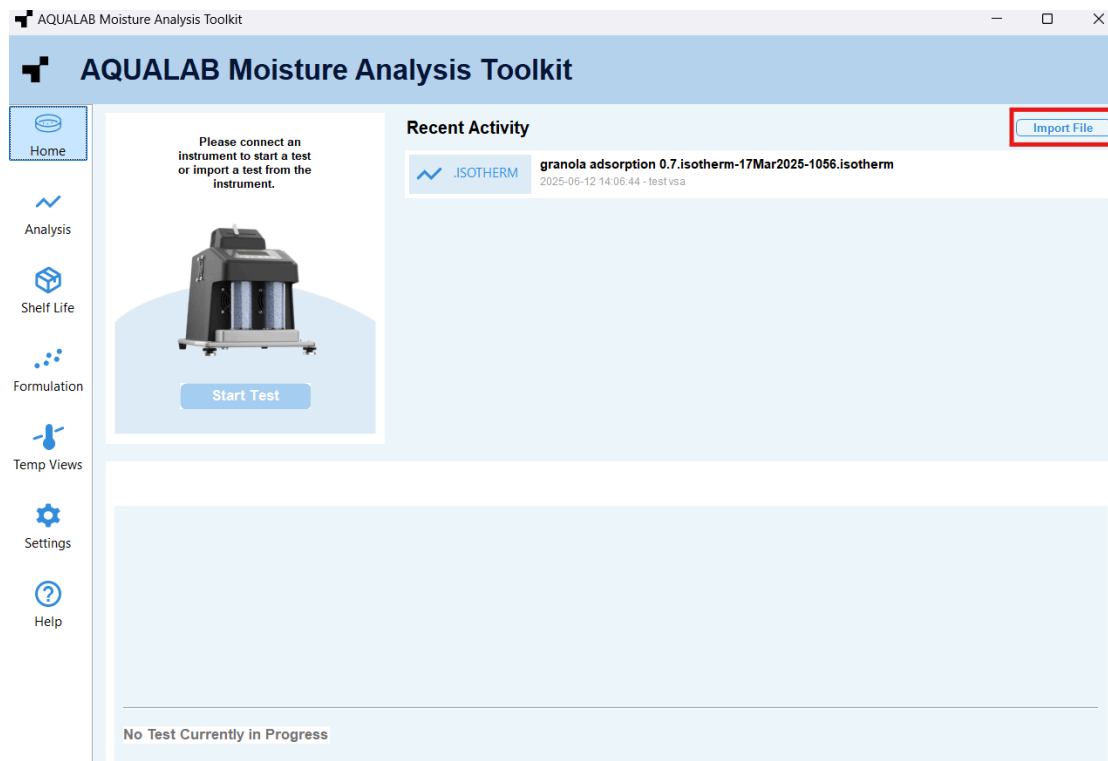


Step 2: Once selected users will be directed to the Analysis page which will show the analysis of the data points calculated up until that point.

1.2.1.4 Import Files

Steps to import files:

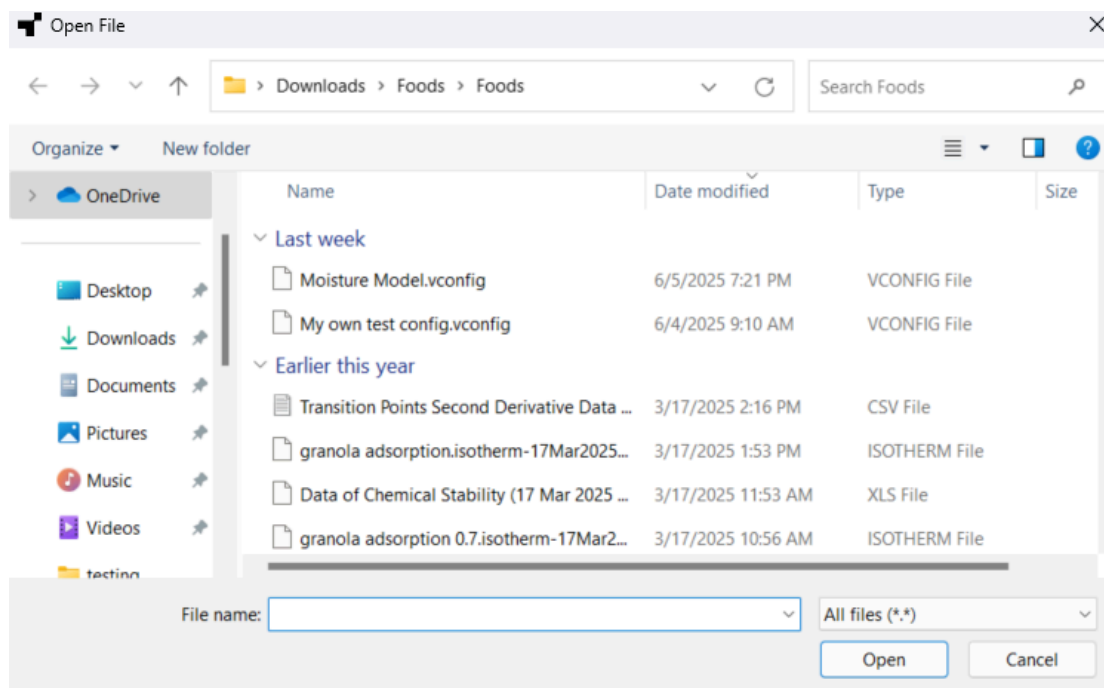
1. Click on Import File, then a dropdown shall appear where you can select from where you need to import the file options include your computer, an instrument or to create manually.



2. Select the suitable option as needed

(i) From Computer

When the from computer option is selected, the windows default import wizard opens up, you will be able to browse files available in the local machine. This option supports .vsa and .isotherm files to be imported.



Once the file to be imported is selected. Click Open.

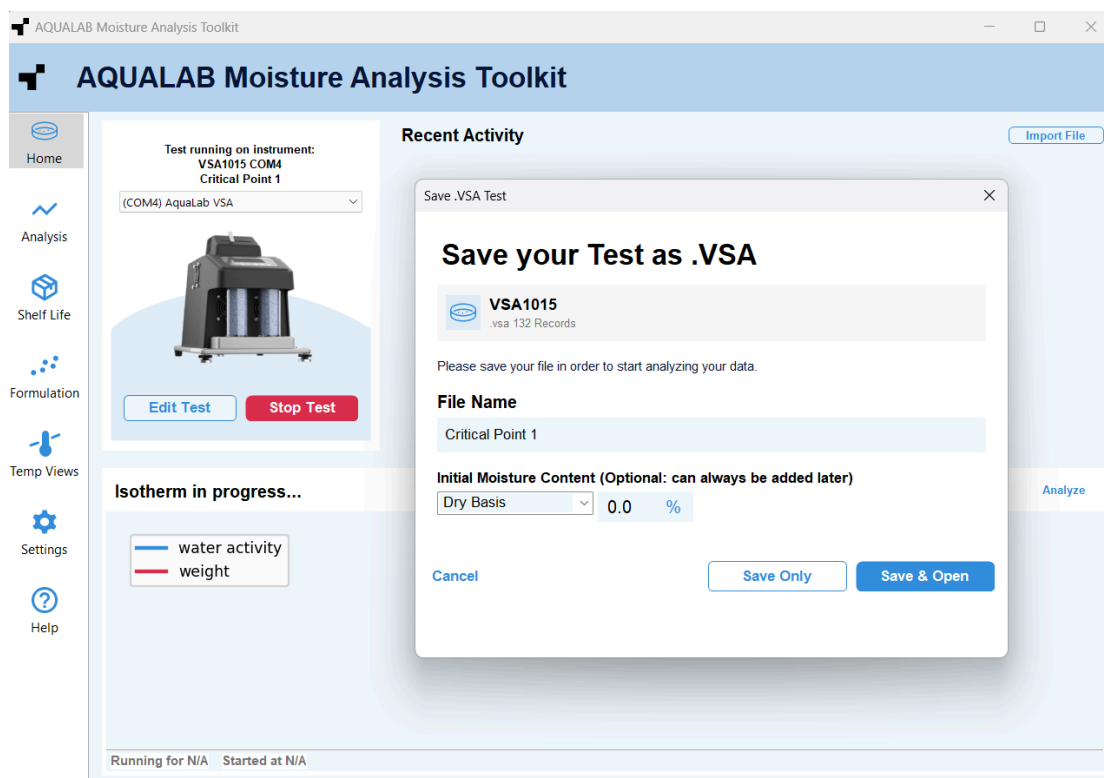
(ii) From Instrument

If an instrument is connected to the application and selected in the instrument dropdown.

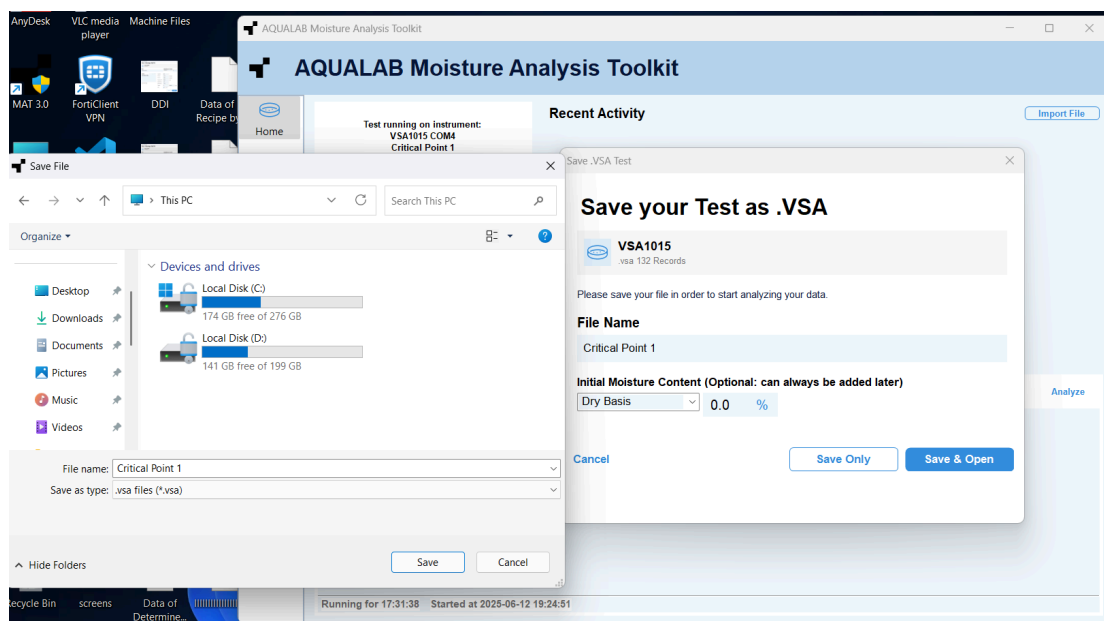
Once you click the from instrument option

- If a test is ongoing it will import the data of records available up until the time it was clicked
- If no test is ongoing it will import the results of the last test conducted by the selected device.

You will be able to save the retrieved results by clicking with Save Only or Save & Open.



Upon selecting one of the save options the windows save wizard opens up where you can specify the location to save the results and click on Save.



(iii) Create Manually

When selected a dialog box to create isotherm manually pops up, you will be able to enter the relevant details. The data can either be manually typed, copy and paste or import an excel file with the data. Time and Weight data is optional, but you must either provide it for every point, or for no points at all. You may also select an isotherm method (DDI or DVS)

and a sorption direction. A temperature is required and will be applied to all the data points entered. Please note: When selecting the DVS method, all data points will be treated as equilibration points.

Then click on Analyze the created file will open up in the Analysis page.

Create Isotherm Manually

X

Create Isotherm

Manually input data or import from Excel with columns in the same order as shown. Save as a .isotherm file for subsequent analysis.

Isotherm Method

DDI

Adsorption/Desorption

Adsorption

Temperature

25

°C

Enter data for modelling

[Import Excel](#)

Water Activity	Moisture Content	Time (min, optional)	Weight (mg, optional)
0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000

+ Row

Test File

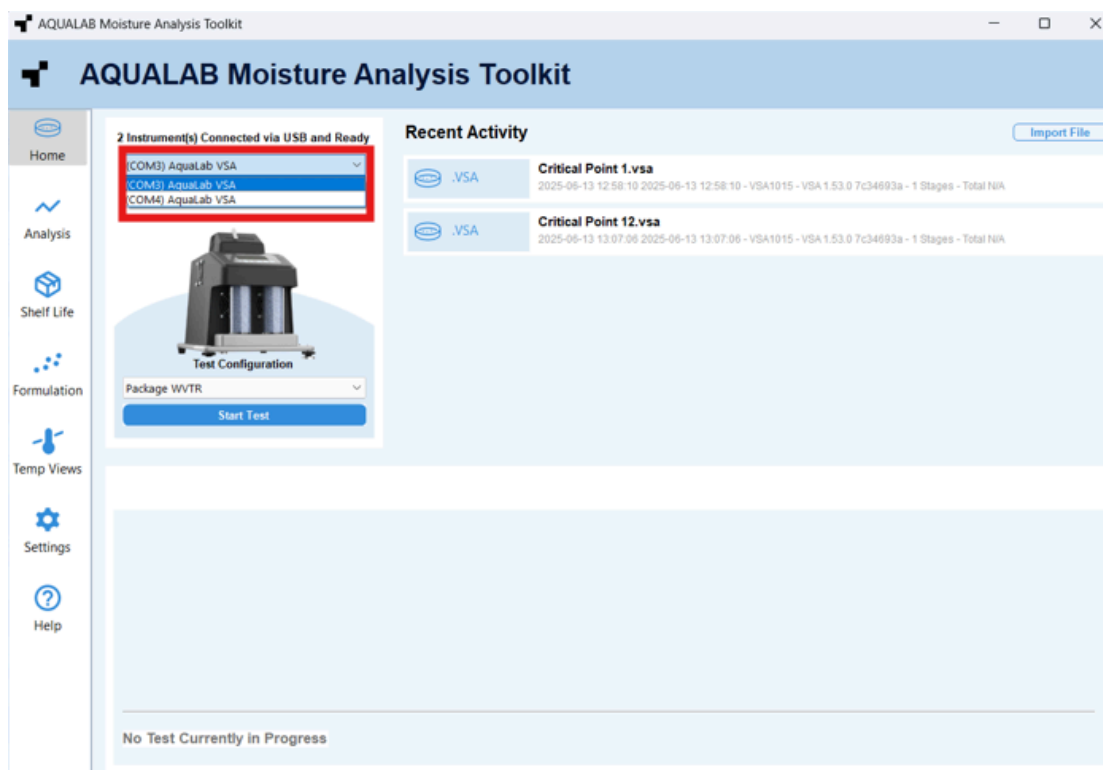
test.xlsx

Cancel

Analyze

1.2.1.5 Multiple Device Connectivity

You will be able to connect multiple VSA devices to MAT 3 via the USB ports. The connected devices will be shown in the device dropdown



Switching between instruments while a test is ongoing.

The application allows you to switch between connected devices using the device dropdown on the Home page, even while a test is running. Depending on the test status of the newly selected device, the interface updates accordingly.

1. Switching to a Device with No Ongoing Test

- The Home page displays that a test is currently running on the initially selected device.
- The user opens the Device dropdown and selects a different device.
Note: The test shall continue in the initially selected device without interruption only the toolkit interface is switched to reflect the progress of an alternative device
- The newly selected device does not have a test in progress.
 - The Home page updates to reflect no test is running.
 - The Device dropdown continues to show the selected device name along with its port ID.

2. Switching to a Device with a Running Test

- The Home page shows a test is currently running on the current device.
- The user selects a different device from the Device dropdown.
Note: The test shall continue in the initially selected device without interruption only the toolkit interface is switched to reflect the progress of an alternative device
- The newly selected device also has an ongoing test.

- The Home page updates to reflect the status of the new device's running test.
- The Device dropdown updates to show the newly selected device and its port ID.

1.2.2 Analysis

This is the component users will mostly interact with to analyse test results, it enables users to view, manipulate, compare, and export data both raw and modeled data for deeper insight.

Accessing the Analysis Page

There are multiple ways a user can reach the Analysis page in Addium MAT 3, depending on where they are in the workflow. The system automatically opens the file in the appropriate analysis view.

Ways to Enter Analysis:

1. Import from Computer (Follow [these](#) steps to import data from computer)

- After importing a file from the computer on the Home Page , the file opens automatically in the Raw Data tab of the Analysis page.

2.Import from Instrument(Follow [these](#) steps to import data from Instrument)

- After importing data from a connected instrument on the Home Page and selecting Save & Open, the created .vsa file is immediately opened in Raw Data Analysis.

3.Create Manually → Analyze (Follow [these](#) steps to manually create data)

- After manually creating data and selecting Analyze, a new .isotherm file is created and opened directly in the Raw Data tab of the Analysis page.

4.Click Analyze During Ongoing Test (Follow [these](#) steps to analyze data of an ongoing test)

- Clicking the Analyze button during an ongoing test opens the current test progress as a .vsa file in Raw Data Analysis.

5. Stop Test → Save & Open (Follow [these](#) steps to stop a test)

- When stopping an active test and selecting Save & Open in the proceeding pop up, the test data is saved as a .vsa file and opened immediately in Raw Data Analysis.

6. Test Completed → Save & Open Prompt

- After a test finishes, a Save & Open prompt appears. Confirming this allows the user to access the saved file via the Analysis page.

7. Manual Navigation → Import or Create Isotherm

Users can also access analysis features by navigating directly to the Analysis page using the left-hand menu. From there, isotherm files can be loaded or created without using the Home screen.

Steps:

1. Click on Analysis from the main navigation panel on the left.
2. At the top of the page, use the dropdown menu.
3. Choose one of the following:
 - Import Isotherm – Upload an existing .isotherm file from your computer.
 - Create Isotherm Manually – Open a form to input data and generate a new isotherm file.
4. Once the file is selected or created, the system will automatically open the .isotherm file.

8. Select from Recent Activity

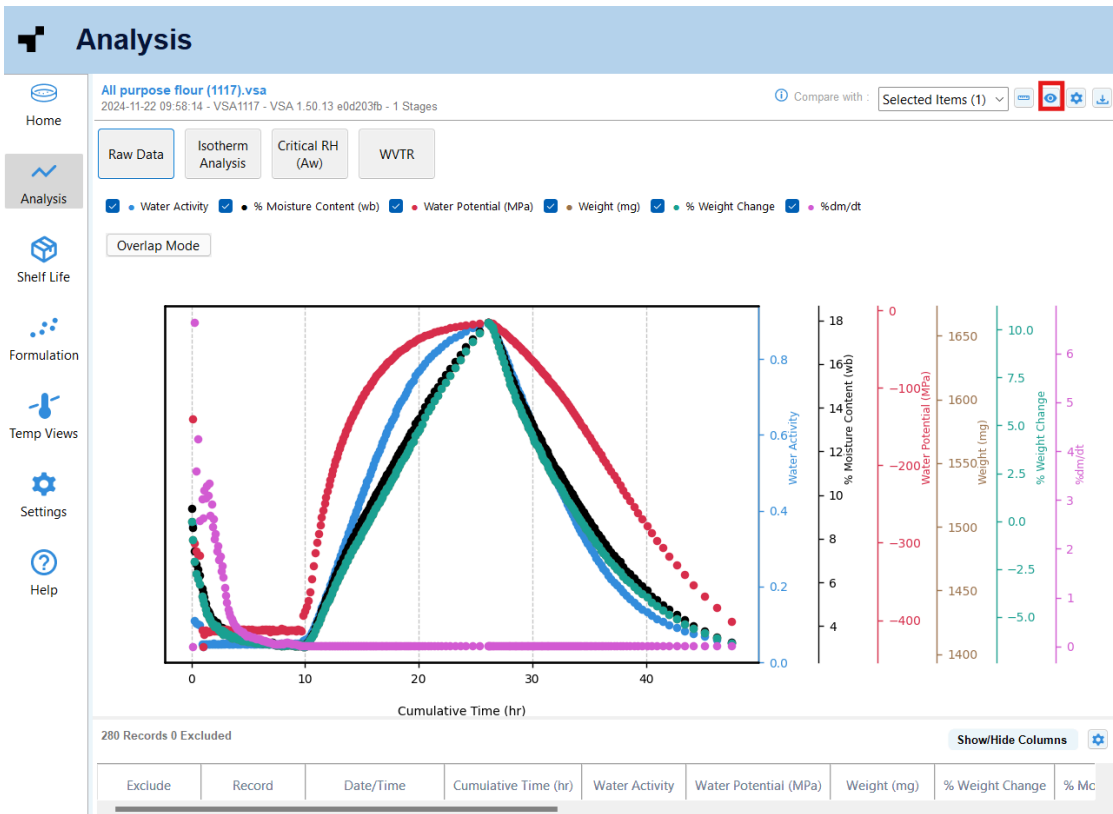
- On the Home page, selecting a file from the Recent Activity list directly opens that file in its corresponding analysis view.

View Test Configuration

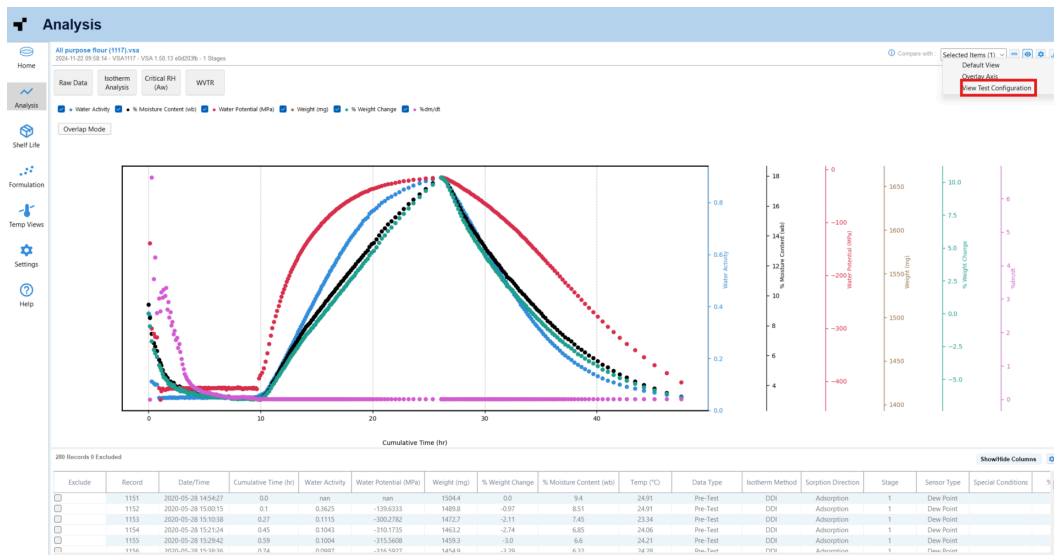
This feature will be available only if the file used for analysis is a .vsa file and the file contains stages. Follow these directions to view test configurations of a .vsa file that contains stages.

Steps:

1. Click on the Eye icon.



- On click a dropdown will appear, Select the View Test Configuration option on the dropdown.



- On selection of the View Test Configuration option a pop up shall appear with the test configurations.

The screenshot shows the 'Analysis' window of the AQUALAB Moisture Analysis ToolKit with the 'View Test Configuration' dialog box open. The dialog box displays the following information:

- Test: Flour**
- VSA1117**
- 2025-06-26**
- Name:** Flour
- Initial Moisture Content:** Wet Basis, 9.4 %
- Stages:** 1. DDI, 0.0500 aw, 0.9000 aw
- Stage Type:** DDI
- Start (aw):** 0.05
- Final (aw):** 0.9
- Temperature (°C):** 25.0
- Resolution (aw):** 0.01
- Flow (ml/min):** 80.0
- Timeout:** 0
- Loop:** On

The dialog box has 'Cancel' and 'Save' buttons. The background window shows the same data table as the previous screenshot.

Change Test Configuration

The configuration can be changed only for those files that the configuration can be viewed.

Editable Fields:

Within the configuration pop-up, only the following fields can be changed:

- Initial Moisture Content (used for generating isotherms or applying models)
- File Name

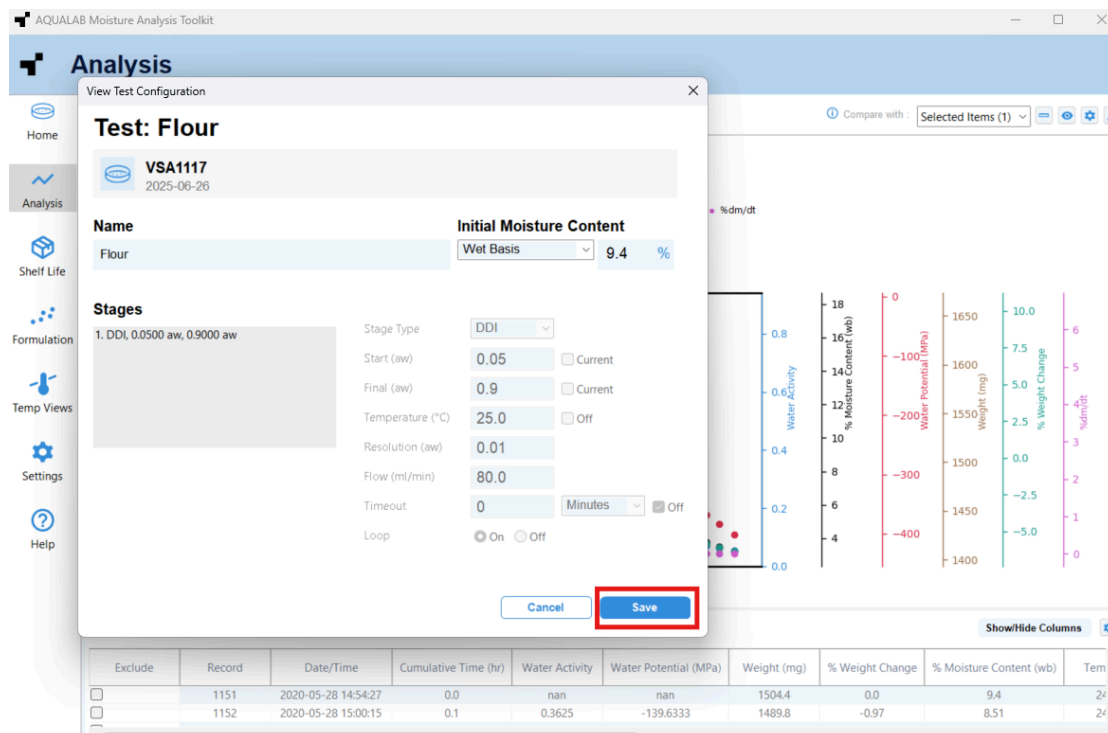
Steps:

1. Access the test configuration (Follow [these](#) steps to access the test configuration)
2. Change the values of the editable fields as required.

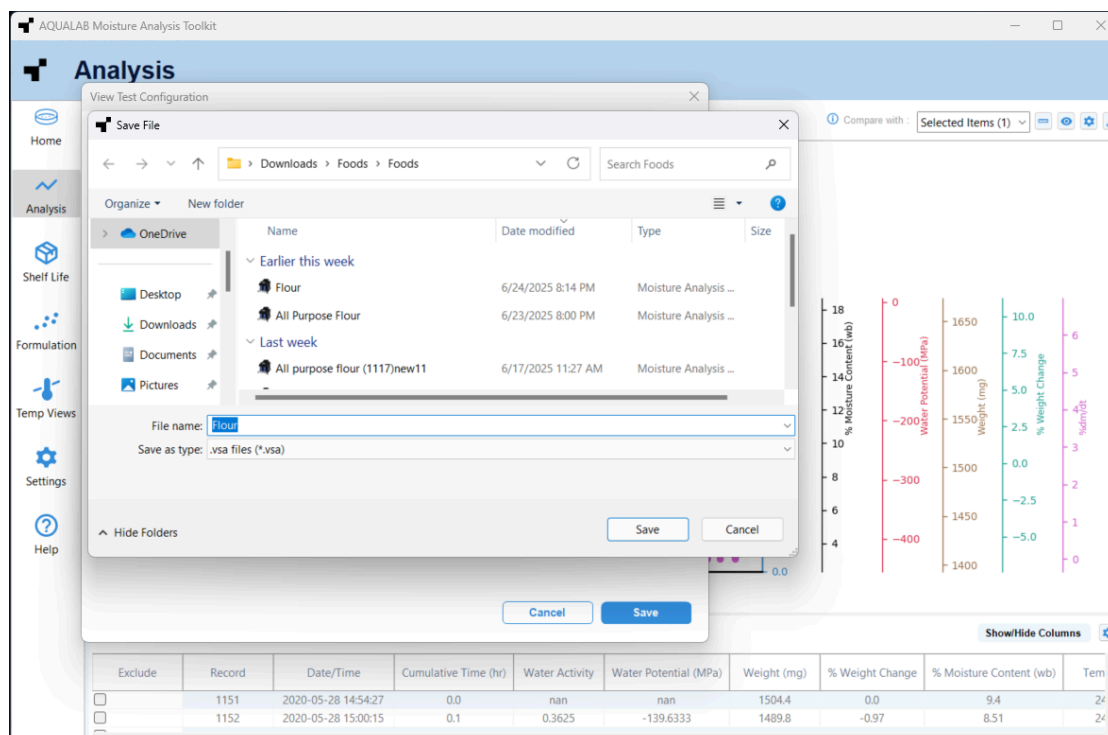
The screenshot displays the AQUALAB Moisture Analysis Toolkit interface. A 'View Test Configuration' dialog box is open, showing the configuration for 'Test: Flour' (VSA1117, 2025-06-26). The dialog box has a red border around the 'Name' and 'Initial Moisture Content' fields. The 'Name' field is set to 'Flour'. The 'Initial Moisture Content' field is set to 'Wet Basis' and '9.4 %'. Below these fields, the 'Stages' section shows a single stage: '1. DDI, 0.0500 aw, 0.9000 aw'. The 'Stage Type' is 'DDI'. The 'Start (aw)' is '0.05', 'Final (aw)' is '0.9', 'Temperature (°C)' is '25.0', 'Resolution (aw)' is '0.01', 'Flow (ml/min)' is '80.0', 'Timeout' is '0' (Minutes), and 'Loop' is 'On'. The background shows a graph of 'Water Activity' vs. 'Weight (mg)' and a table of test results.

Exclude	Record	Date/Time	Cumulative Time (hr)	Water Activity	Water Potential (MPa)	Weight (mg)	% Weight Change	% Moisture Content (wb)	Tem
<input type="checkbox"/>	1151	2020-05-28 14:54:27	0.0	nan	nan	1504.4	0.0	9.4	24
<input type="checkbox"/>	1152	2020-05-28 15:00:15	0.1	0.3625	-139.6333	1489.8	-0.97	8.51	24

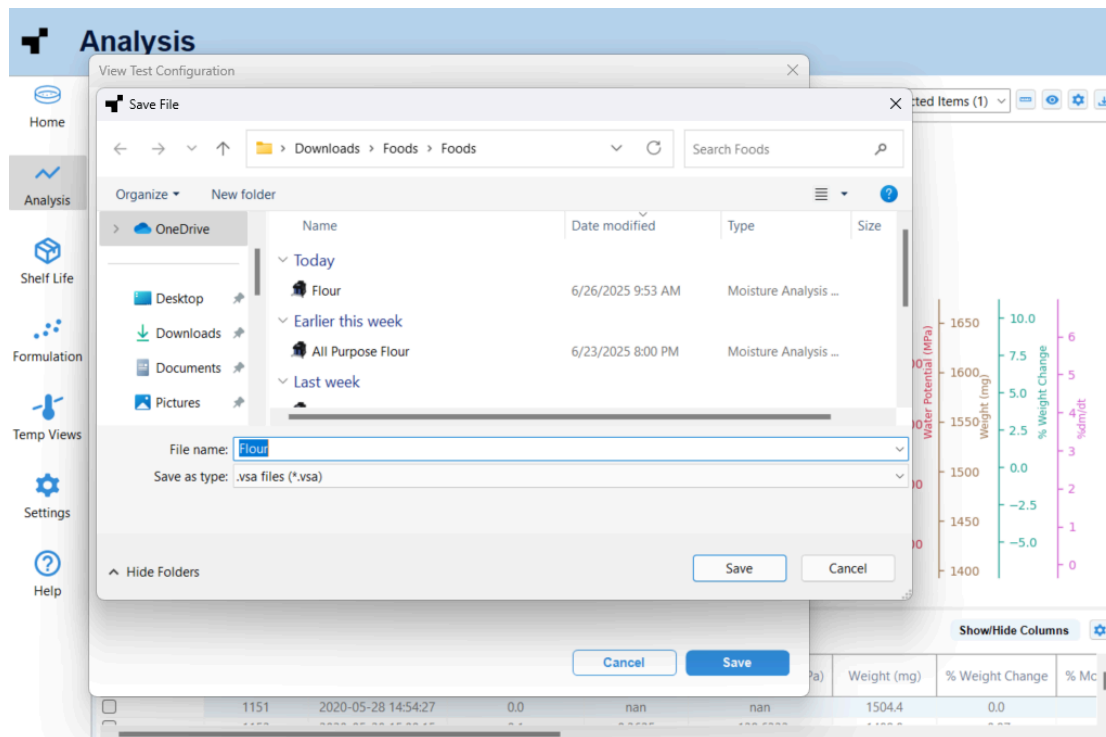
3. After updating the editable fields, click Save.



4. The file save wizard will open.



5. Click Save on the file save wizard. A new .vsa file will be created containing the same raw data but with the updated test configuration



Note:

- Changing the configuration does not modify the currently loaded file. Instead, it saves a completely new file with the updates.
- To analyze the new file, import the saved file and continue analysis. (Follow [these](#) steps to import the saved .vsa file)

Exporting Data

Data can be exported in three ways

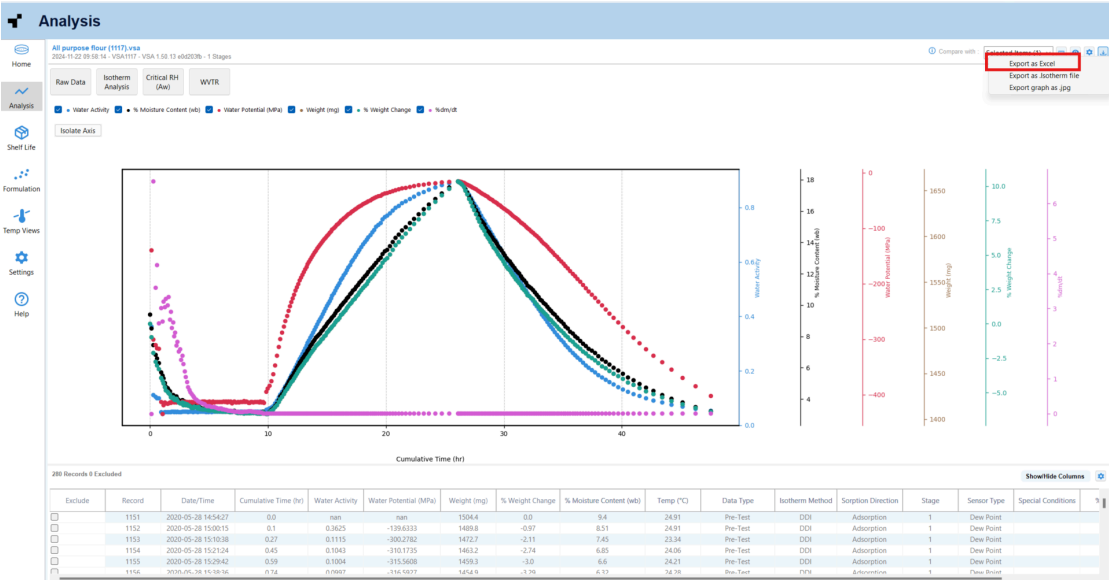
1. Export as Excel

The export as excel option will enable you to save the table of data available in the page to an excel file. This feature is available throughout all analysis tabs. To do export as excel follow these steps

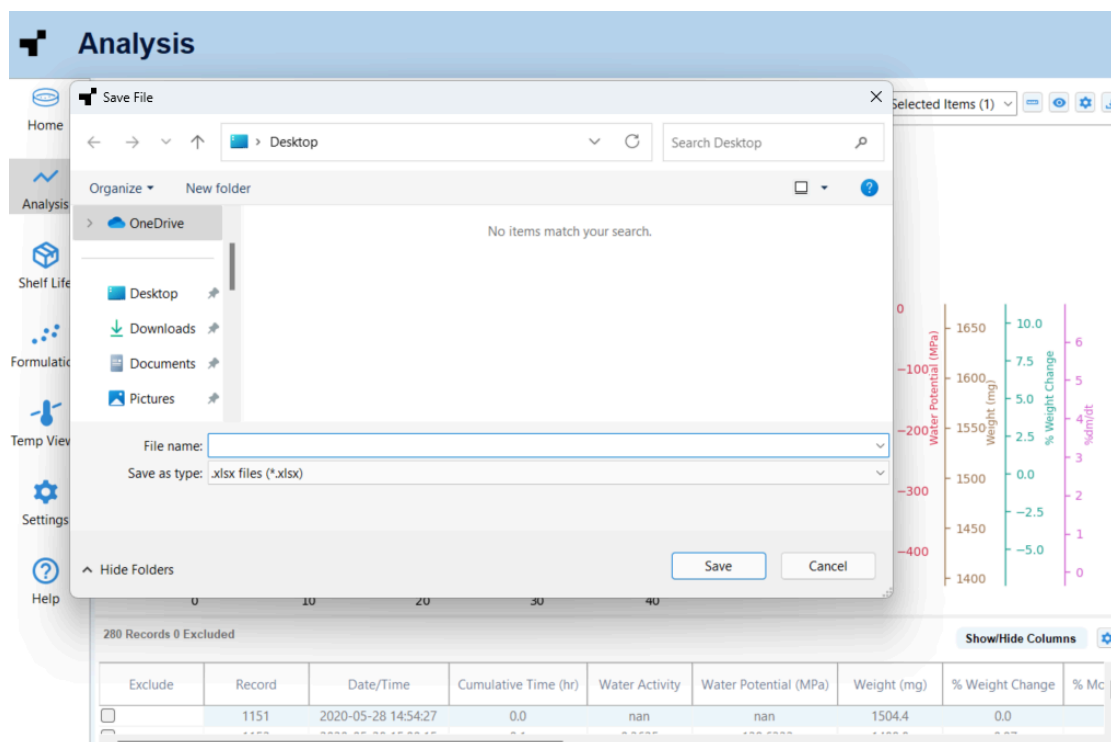
1. Click the download icon on the top right corner of the page.



2. On click a dropdown menu will appear, select the Export as Excel option on the dropdown.



3. On selection the save file wizard will pop up, choose the preferred location.



4. Click on Save. When you click Save, the system will download the exact table as it appears on the screen at that moment in the .xlsx file format.
 - The visible columns and rows only will be included in the exported Excel file.
 - If you have hidden or reduced columns using the show/hide column feature, those will not appear in the export.
 - The column order, names, and formatting will match what's currently displayed in the UI.

2. Export as .Isotherm file

The Export as .isotherm feature allows you to save a test's isotherm data in a proprietary file format (.isotherm) that can be later reimported into the platform for further viewing, comparison, or analysis.

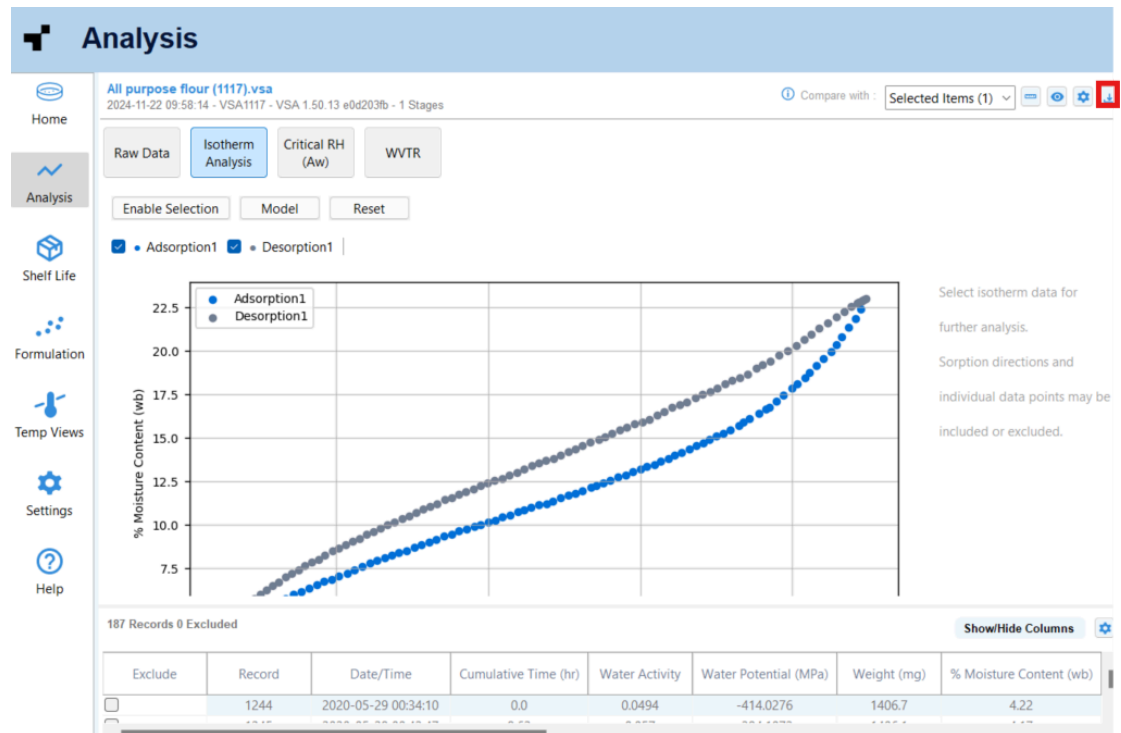
The functionality of this feature depends on the file type:

- If the file is already a .isotherm file:
 - You can export it from any tab in the analysis page.
- If the file is a .vsa file:
 - You must first navigate to the Isotherm Analysis tab.

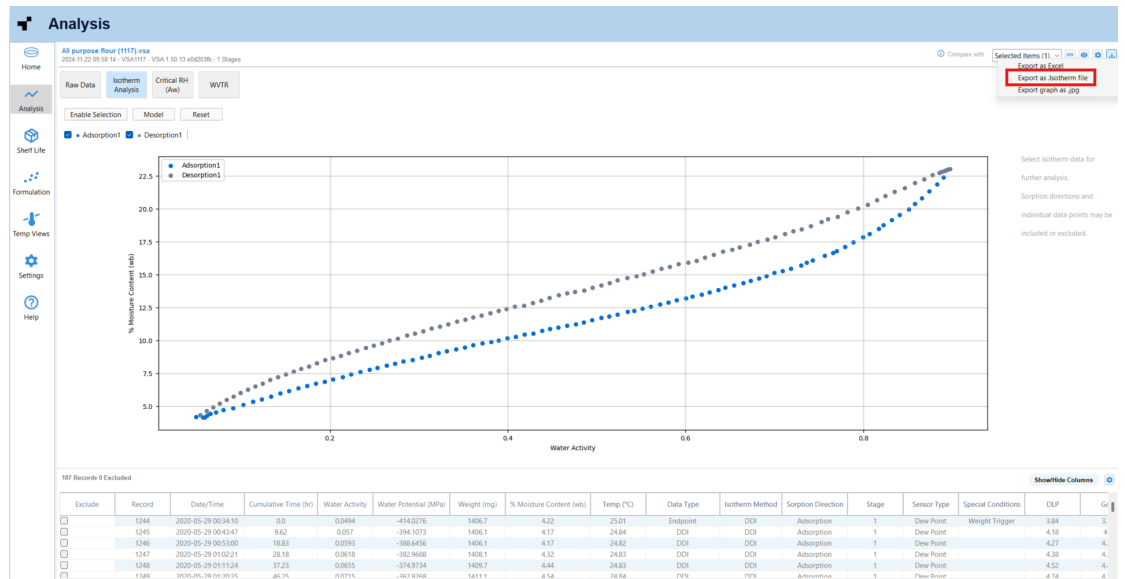
- This triggers the conversion of the raw .vsa data into a processed .isotherm file.
- Once the conversion is complete, you will be able to export it as a .isotherm from that point onward.

To export as .isotherm file follow these steps:

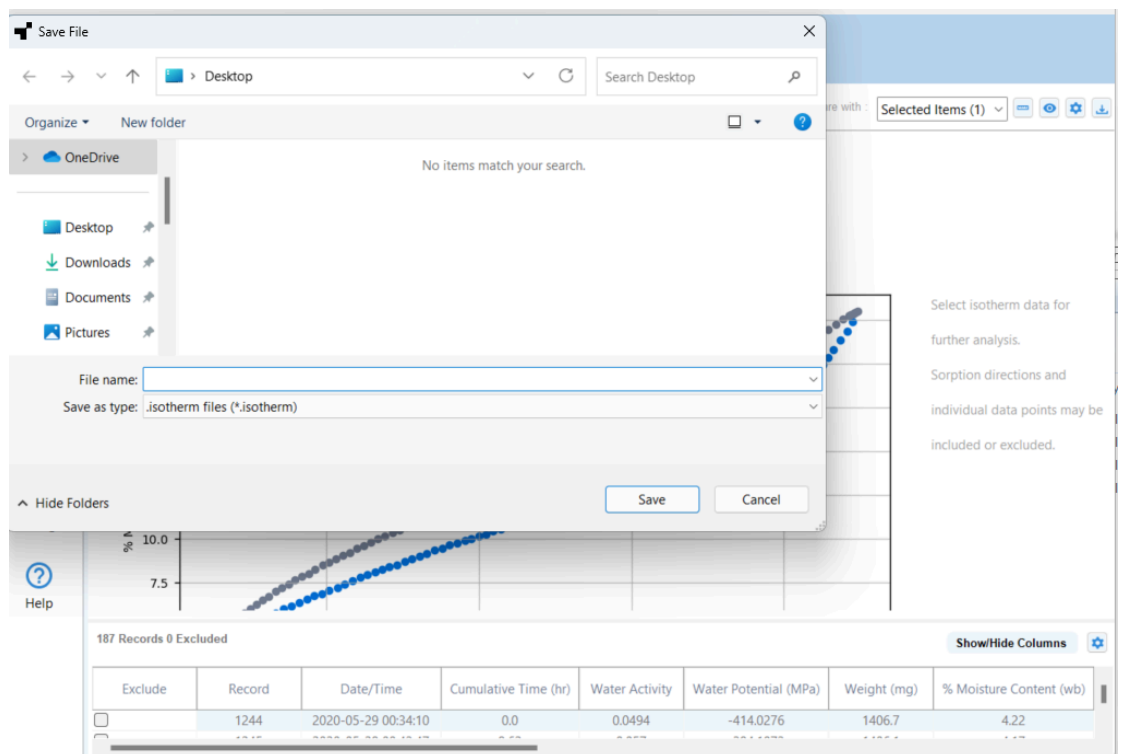
1. Click the download icon on the top right corner of the page.



2. On click a dropdown menu will appear, select the Export as.Isotherm file option on the dropdown.



3. On selection the save file wizard will pop up, choose the preferred location.

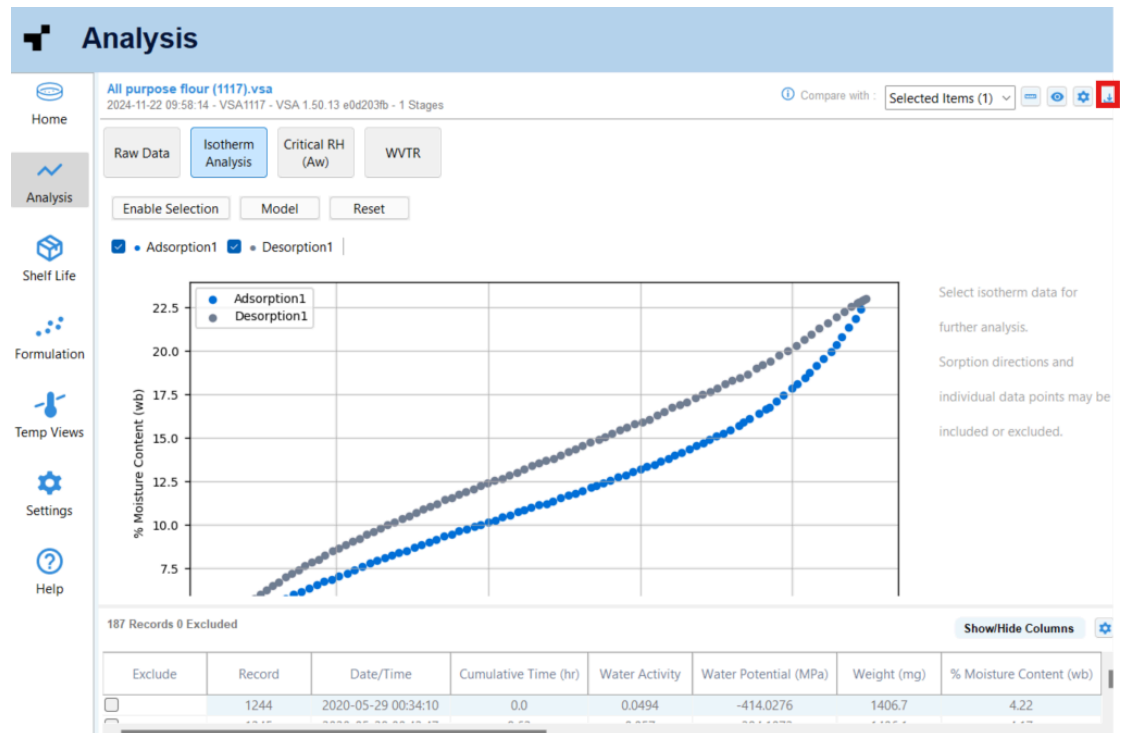


4. Click on Save.

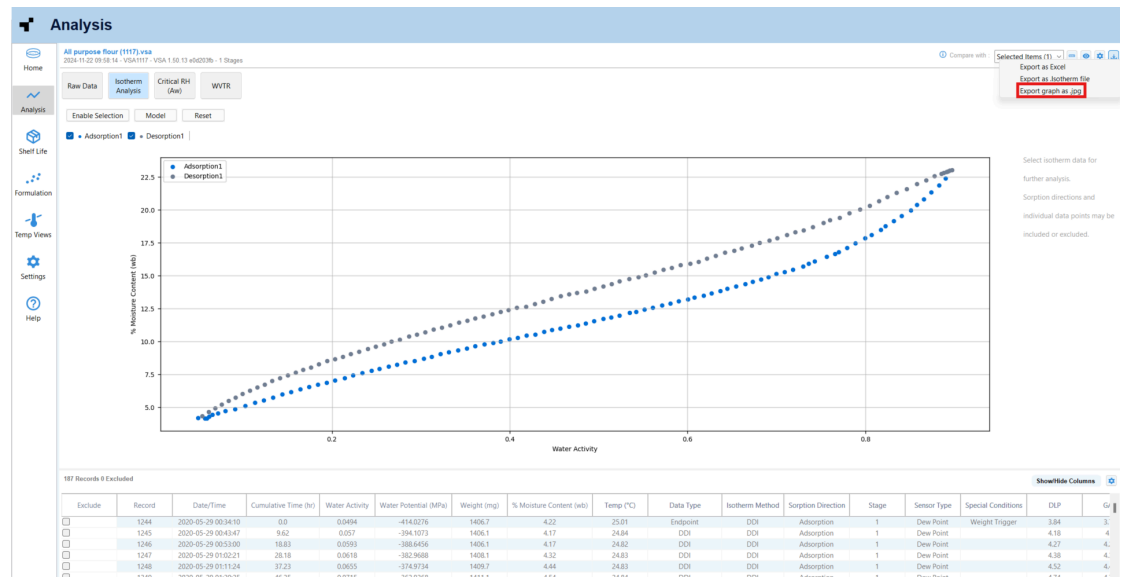
3. Export graph as .jpg

The Export Graph as .jpg option allows you to save a snapshot of the currently visible graph as an image file. To do this follow these steps.

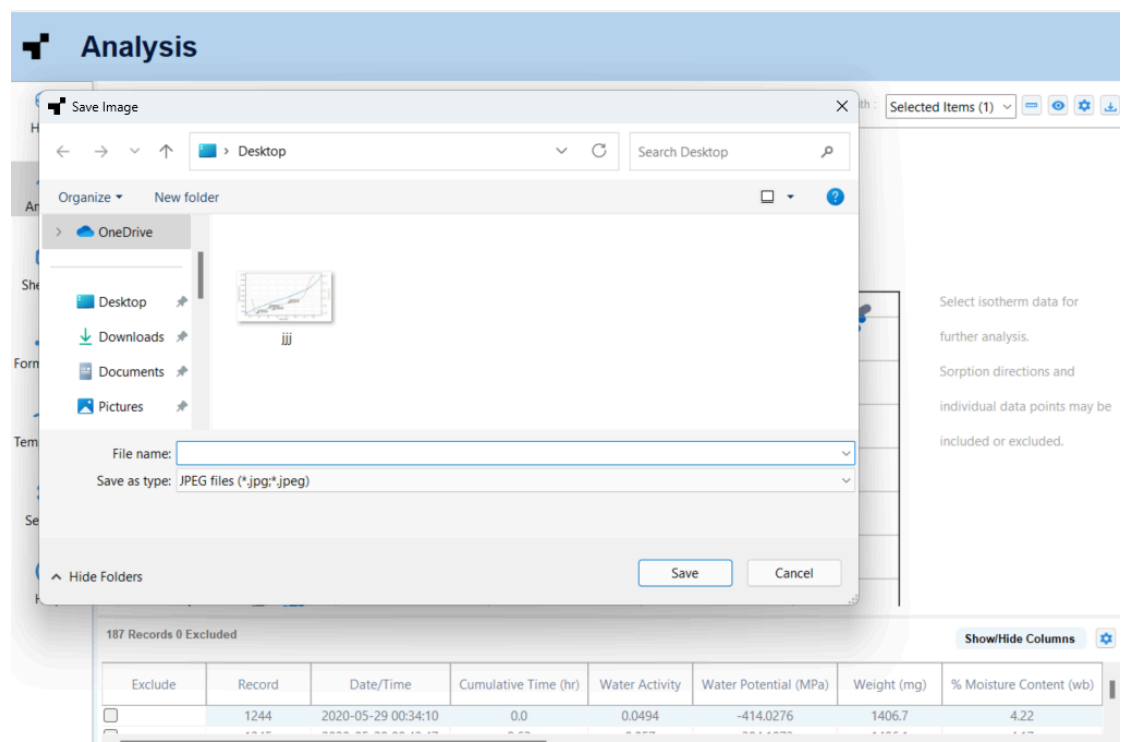
1. Click the download icon on the top right corner of the page.



2. On click a dropdown menu will appear, select the Export as Isotherm file option on the dropdown.



3. On selection the save file wizard will pop up, choose the preferred location.



4. Click on Save.

1.2.2.1 Raw Data

This is the starting point in the Analysis section, where users view and interact with raw test results collected.

Graph View

Zoom In / Out

Use your mouse scroll wheel or two-finger scroll on a touchpad to zoom in or out of the graph.

Pan

Click and hold anywhere on the graph., drag with your mouse or touchpad. Move in any direction (left, right, up, down).

Hover Tooltips

Hover over a data point to see its exact value and corresponding X/Y data.

Isolate y-axis

To move a single y-axis up and down while the other axis stays constant this feature can be used. To isolate an axis follow these steps.

Steps:

1. Click on the Isolate Axis button.



2. On click a the y-axis values shall be shown as radio buttons.



3. Select the radio button of y-axis you wish to isolate

4. Move the touchpad or mouse scroll up and down to move the selected y-axis curve up and down.

To exit the isolate axis mode click back on the Isolate Axis button or direct to [default view](#).

Change visible y-axis values

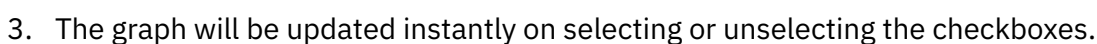
For .vsa files there will be 6 y-axis values that are:

- For .isotherm files there will be 4 y-axis values that are:

- To change the visible y-axis selection follow the below steps:

Steps:

1. Access the graph view
2. Select/Unselect the check box of y-axis values on top of the graph as required.

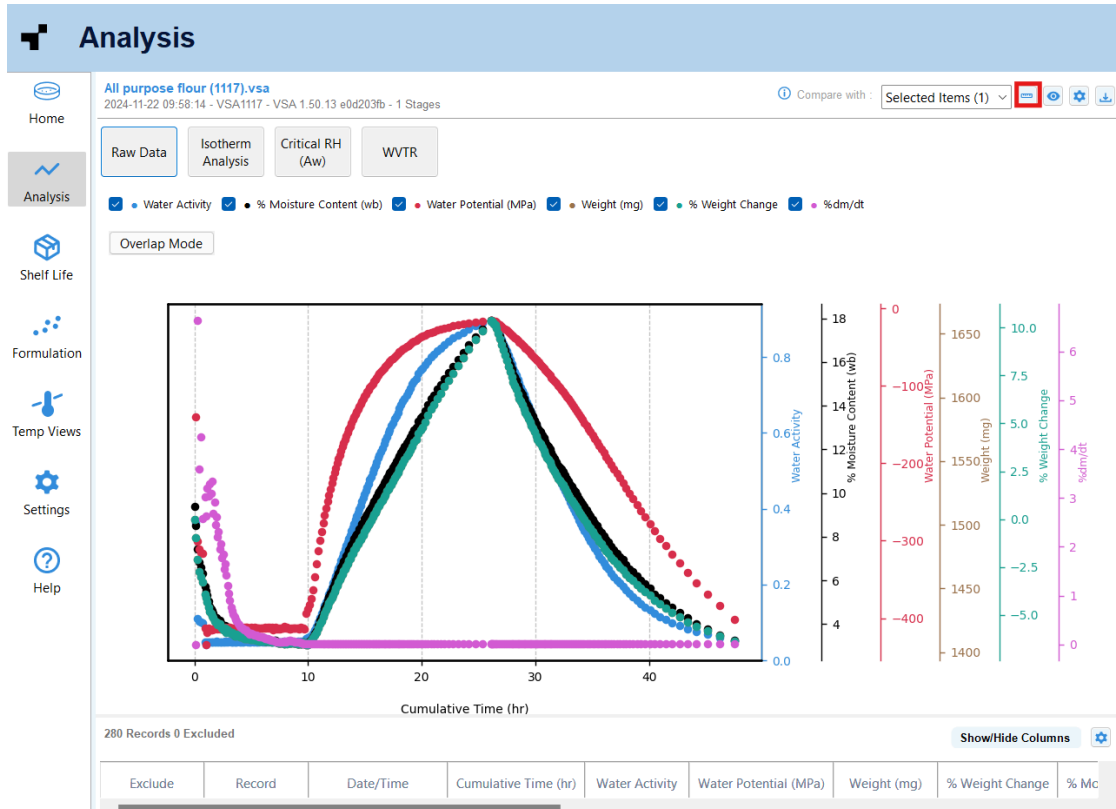


Change Principal Axis (x-axis)

The default value of the x-axis will be cumulative time, in order to change the value of the x-axis follow the following steps.

Steps:

1. Click on the Ruler Icon on the top of the page.



2. Once selected a pop-up window will appear for the selection of the principal axis.



3. Select the preferred value for the x-axis from the options available.

Change graph default axis

This feature allows users to customize which parameters appear on the X-axis and Y-axis in the graph view of the Raw Data Analysis tab. Follow the following steps to change the default axis of the graph.

Steps:

1. Click on the gear icon on the top of the page.



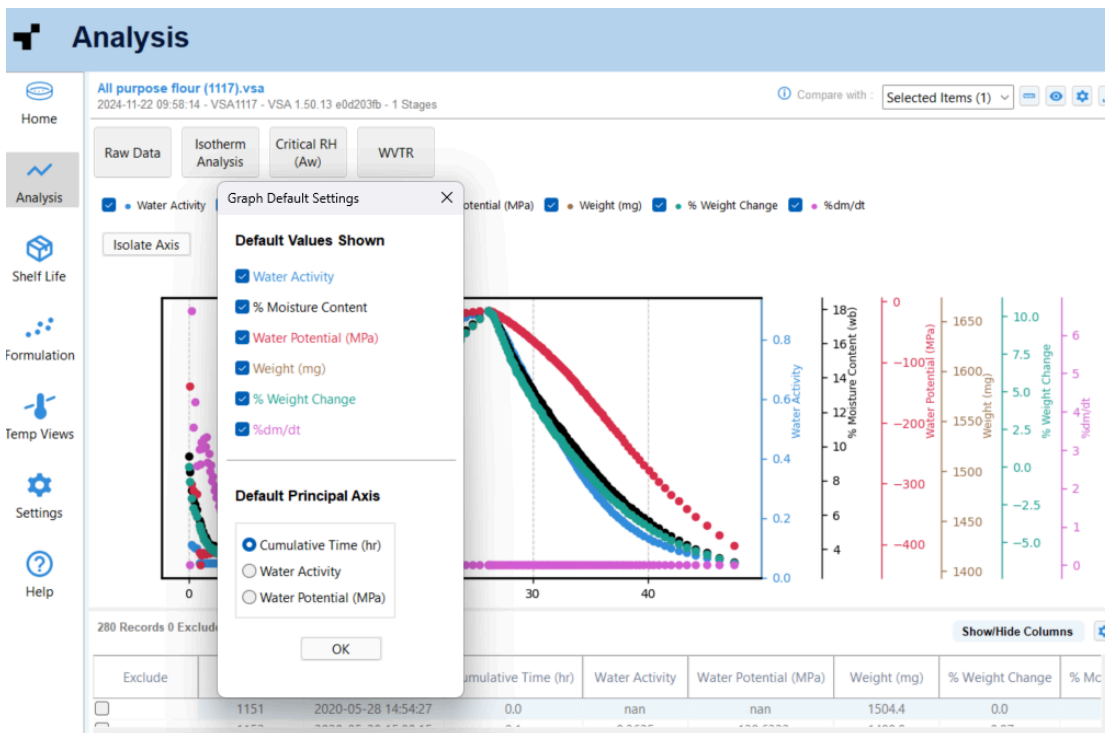
2. A configuration pop-up of the graph default settings will appear with two sections:

A. Default Values Shown (Y-axis)

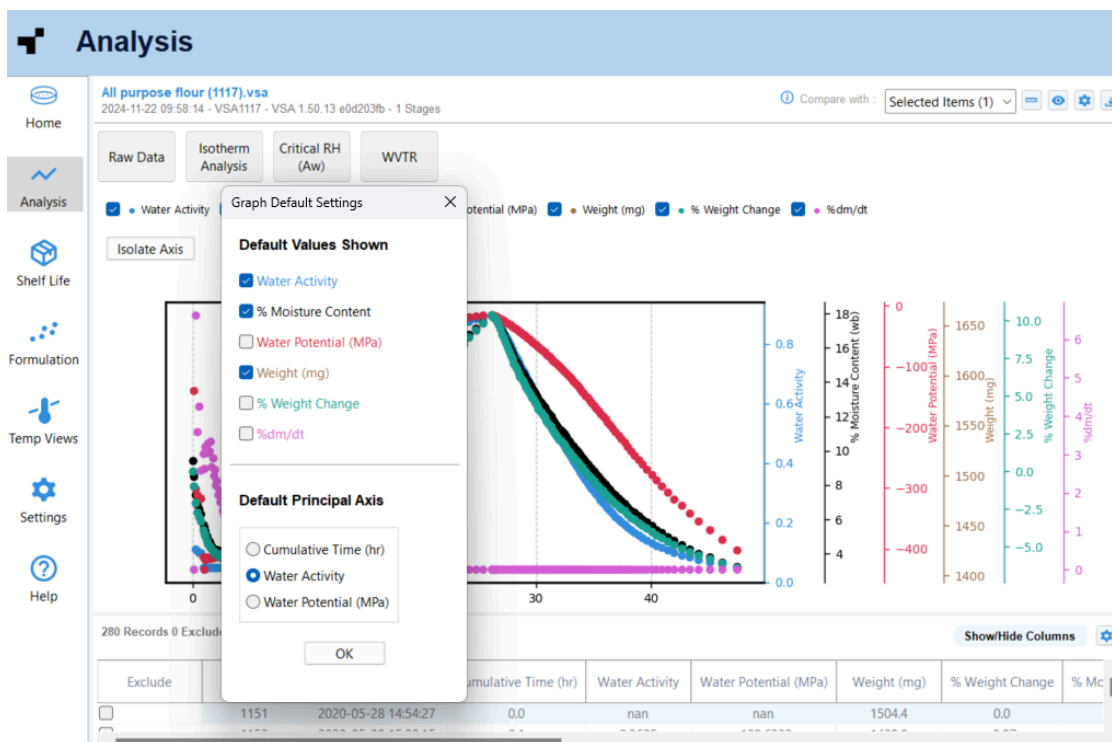
- You'll see a list of available parameters (e.g., Moisture Content, Weight, Temperature).
- Use the checkboxes to select one or more Y-axis values to display on the graph.

B. Default Principal Axis (X-axis)

- Below the Y-axis section, you'll see a list of radio buttons.
- Choose one option to set it as the X-axis (e.g., Time, Water Activity).



3. Once you've made your selections, click OK at the bottom of the pop-up.



4. The graph will refresh and display data according to your updated axis settings.

Default View

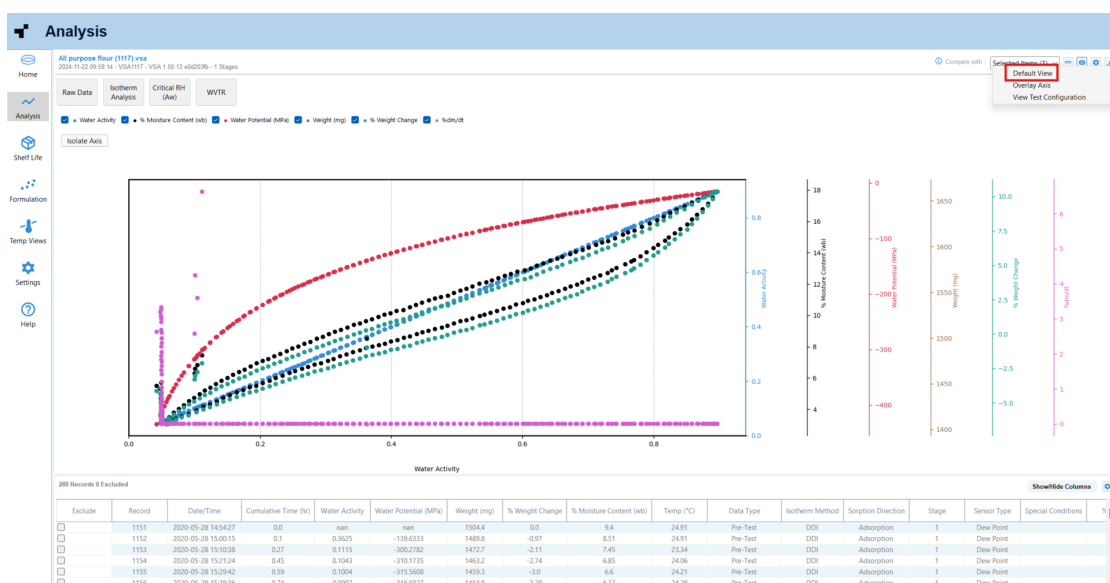
To access the default view of the Raw Data. Follow the following steps.

Steps:

1. Click on the Eye icon.



2. On click a dropdown will appear, Select the Default View option on the dropdown.



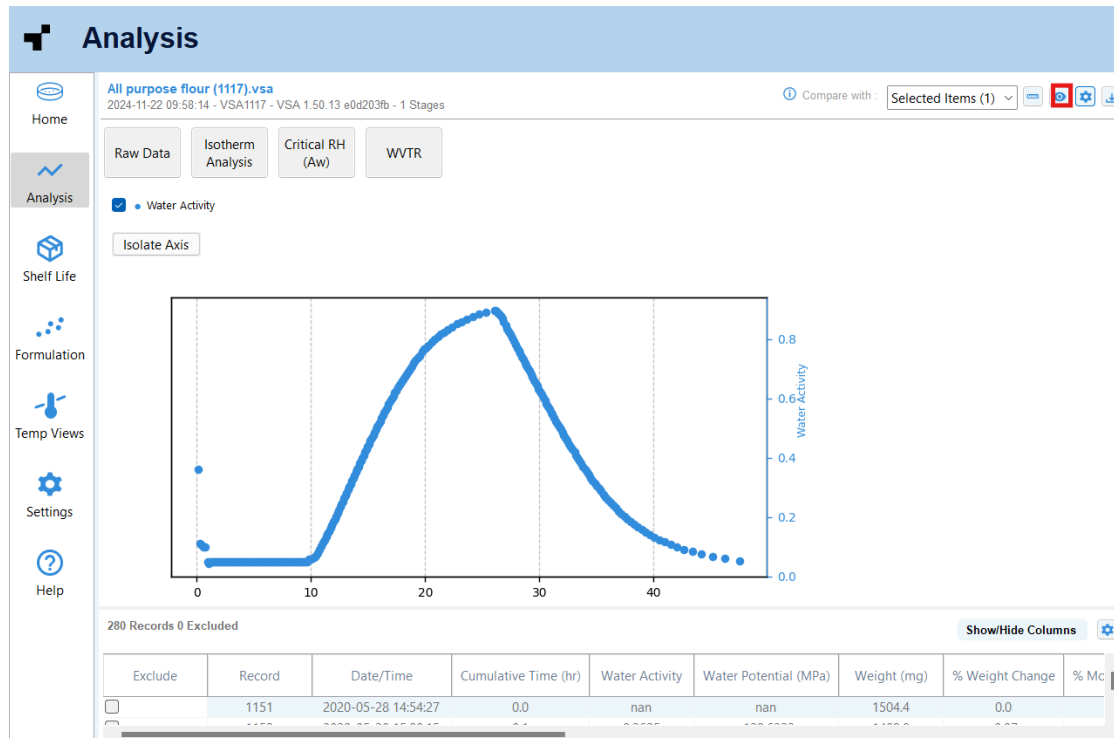
3. On selection the graph will be reset to the default view of raw data, with x-axis showing cumulative time and default y-axes (Will display 4 y-axis if the file is .isotherm and will display 6 y-axis if the file is .vsa)

View Sorption Direction

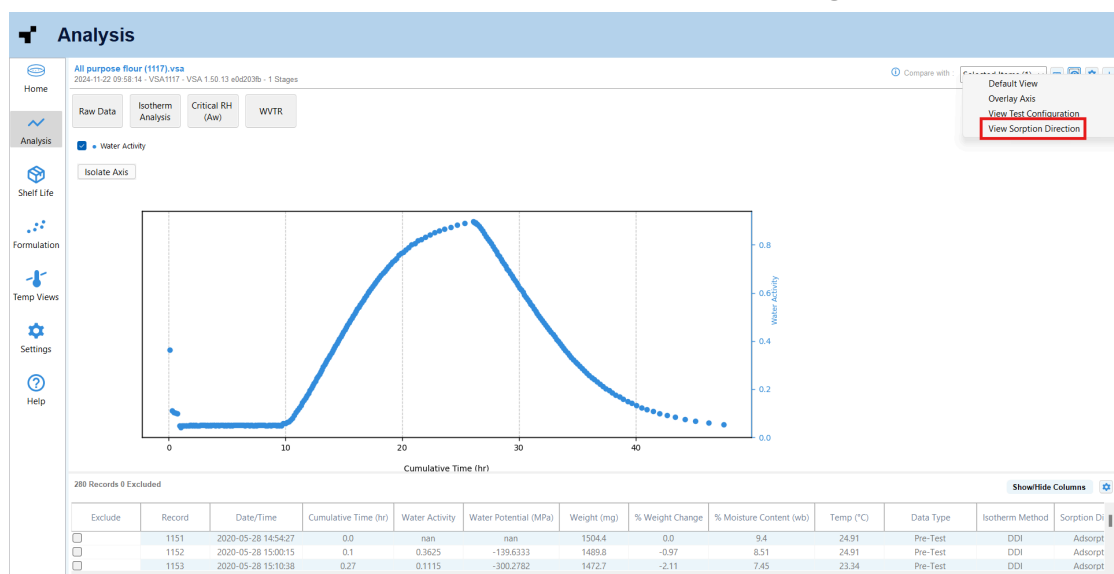
In order to view sorption direction only a single default y-axis should be available. To view sorption direction follow the following steps:

Steps:

1. Ensure only one default y-axis value is available. In order to have one default y-axis value follow [these](#) steps.
2. Click on the Eye icon.



3. On click a dropdown will appear. On the dropdown select View Sorption Direction
Note : The View Sorption Direction will be available only if a single y- axis is available



- On selecting View Sorption Direction the graph will be updated to show the sorption direction based on the available stages. The graph will reflect the sorption direction relative to the chosen y-axis and relative to moisture content.



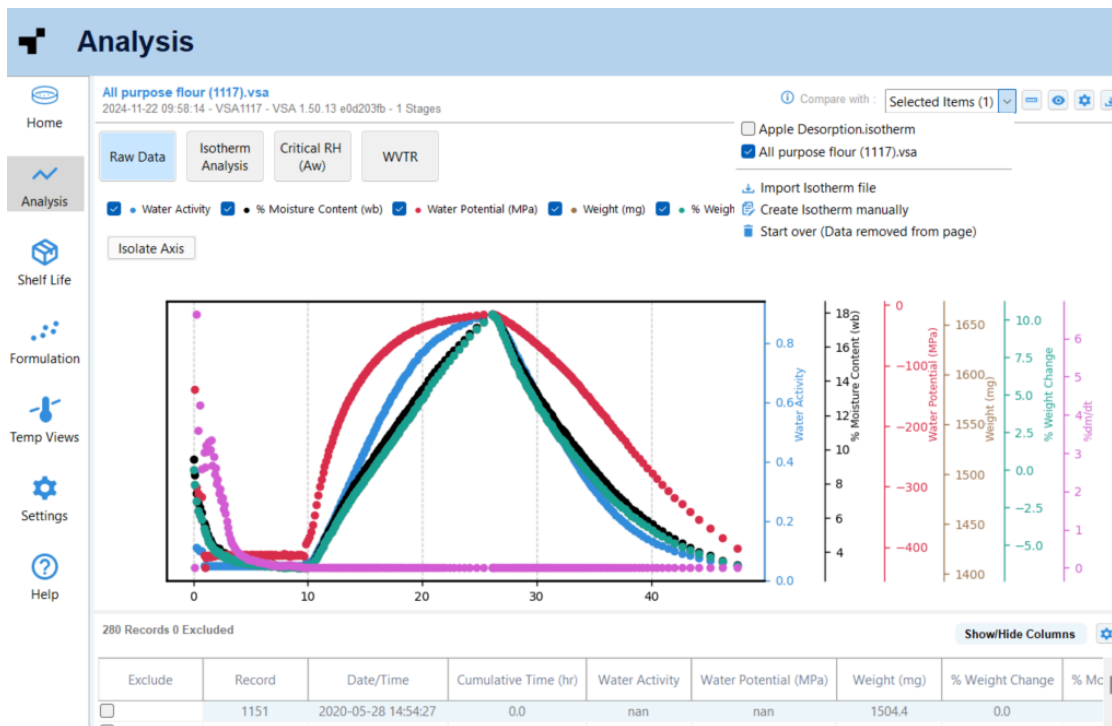
To exit the sorption direction mode, direct to the default view by following [these](#) steps.

Compare Raw Data

The Raw Data Compare Mode allows users to view and analyze the raw experimental data from multiple tests side by side in a single graph.

Steps

- Ensure a primary file is loaded.
- Click the “Compare With” dropdown near the top of the page.
- Select one or more test files (up to 10) for comparison (Import files if needed).



- Following the selection of the files you will move to the comparison mode.



- You can check and uncheck files on the list of files shown alongside the graph to change the visibility on the graph and select the various radio buttons to change across the y-axis.

Table View

The Table View displays your data in a spreadsheet format.

Copy

Select the data points to be copied, then use the keyboard shortcut CTRL + C to copy the values.

Show/Hide Columns

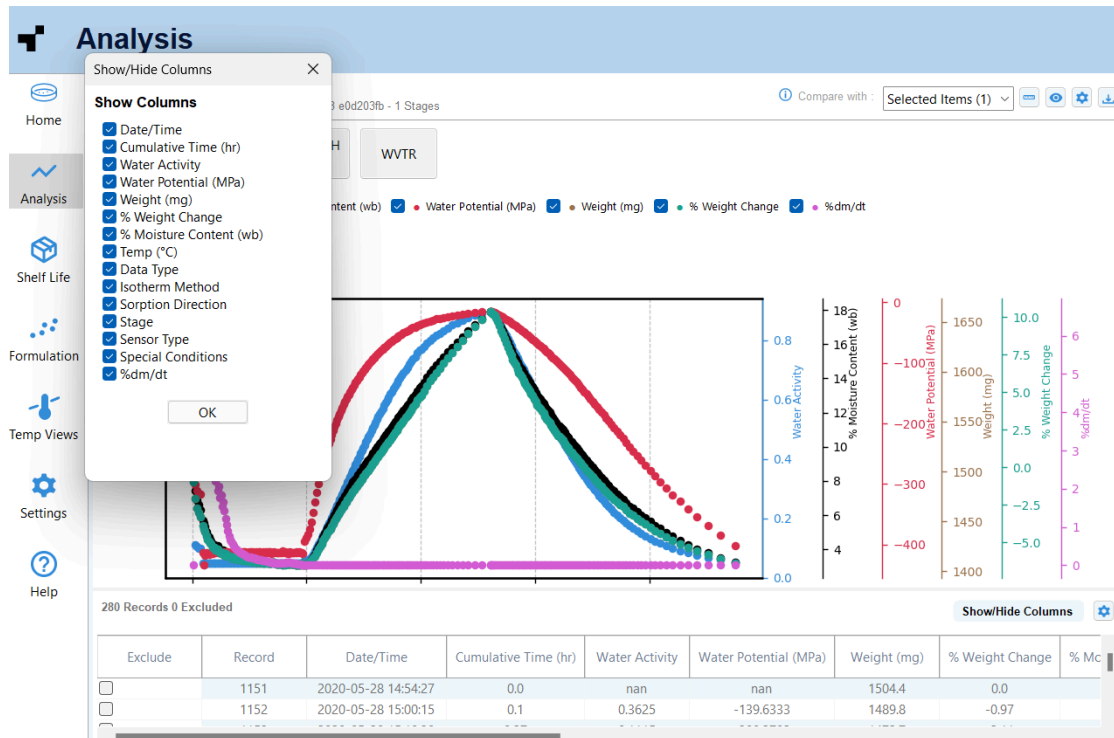
Control the columns visible on the table. Follow these steps to show/hide columns.

Steps:

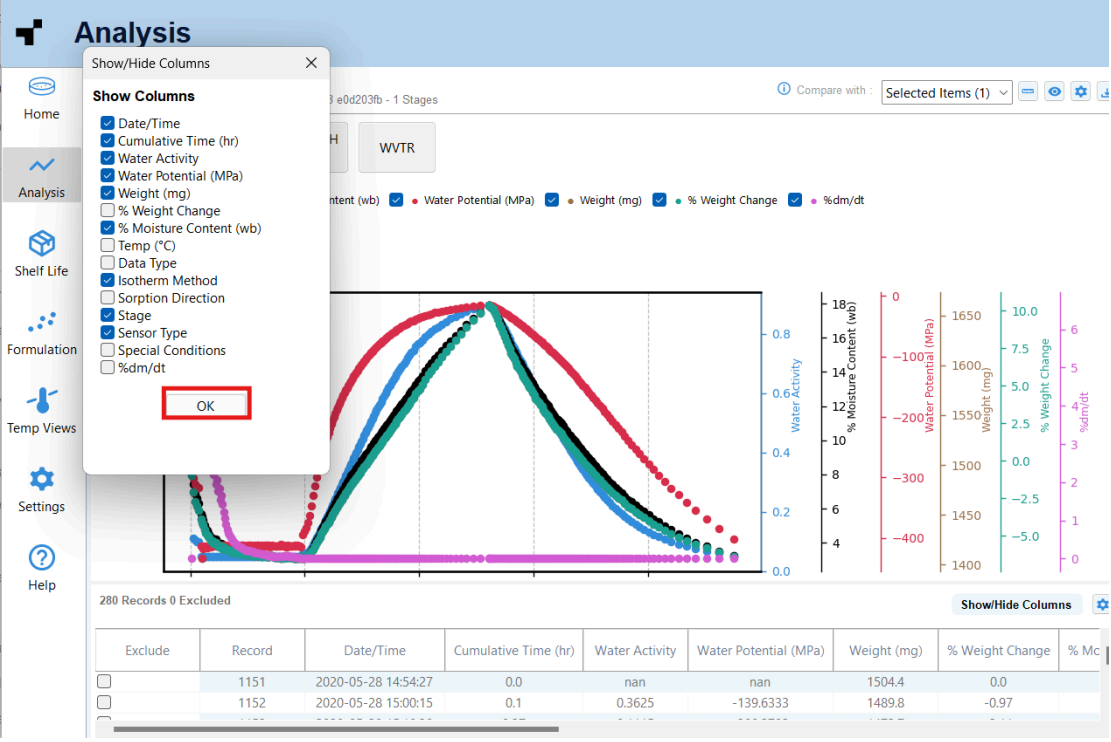
1. Click the Show/Hide Columns button at the top of the table.



2. On click a pop up with the list of all available columns will appear.



3. Each column has a checkbox:
 - a. Checked = visible in the table
 - b. Unchecked = hidden from view
4. Use this to declutter the table and focus on only the columns you need.
5. Once the needed columns have been checked, Click OK to update the table with the changes.



Note : Changes affect only the current table— the original data remains unchanged.

Change Table Setting

Changing Temperature units

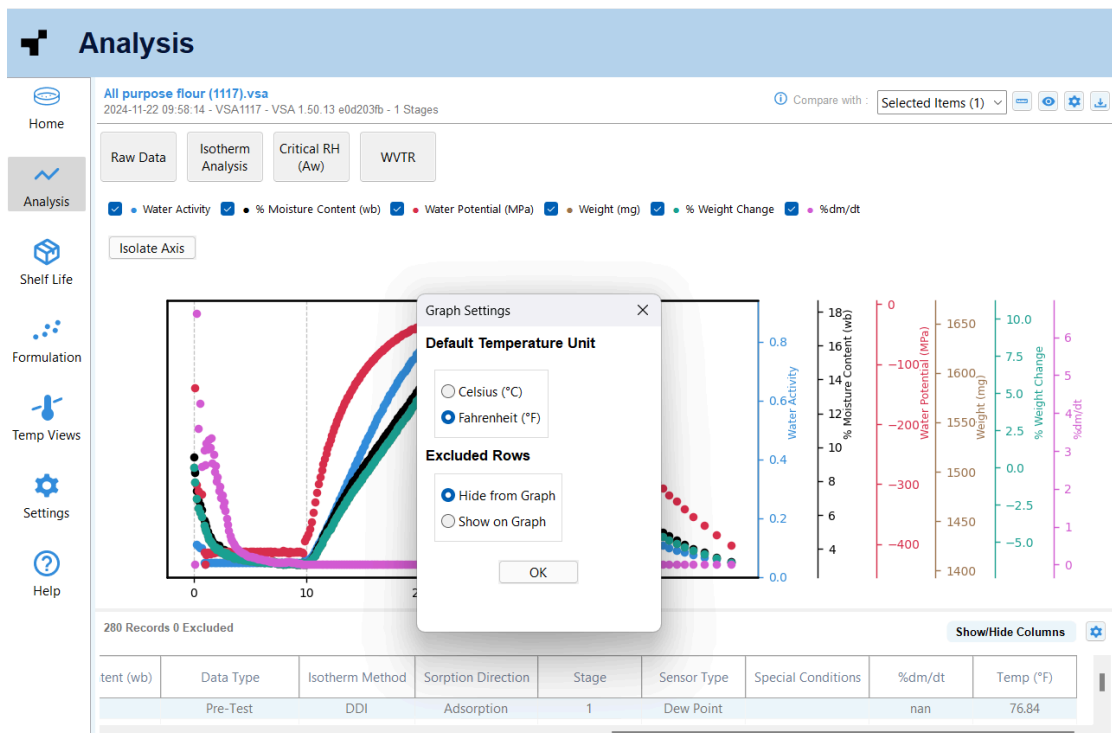
To change the units of temperature between celsius and fahrenheit follow these steps.

Steps:

1. Click on the gear icon at the top right corner of the table.



2. A pop up will appear with the settings.



3. Select the default temperature as required.
4. Click on OK. The table will be updated with the new temperature unit.

1.2.2.2 Isotherm Analysis

This is the component that is used to visualize and interpret sorption curves, either from a test or imported isotherm file.

To use Isotherm Analysis, follow these steps.

Steps:

1. Click the Isotherm Analysis tab in the Analysis page.
 - Moving to the Isotherm Analysis tab will filter the relevant data points from the raw data.
2. A dialog box opens up if Initial moisture content is undefined where the user is prompted to enter initial moisture content to proceed with isotherm analysis.

Missing Moisture Content Entries

×

The test file has missing info

To perform an isotherm analysis, Initial Moisture Content needs to be added. You can enter it below or open the full configuration to complete.

Initial Moisture Content

Select

▼

%

Stage Type

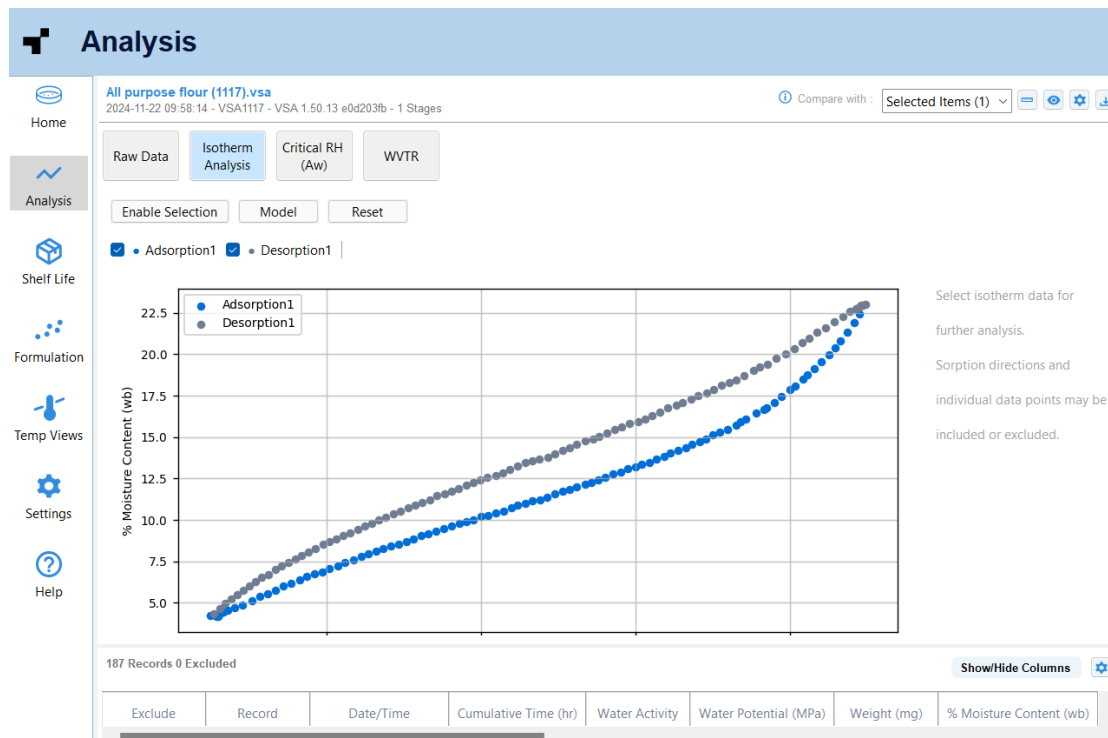
Select

▼

Go Back

Save and Continue

3. View the sorption curves based on stages on the graph.



Graph View

Zoom In / Out

Use your mouse scroll wheel or two-finger scroll on a touchpad to zoom in or out of the graph.

Pan

Click and hold anywhere on the graph., drag with your mouse or touchpad. Move in any direction (left, right, up, down).

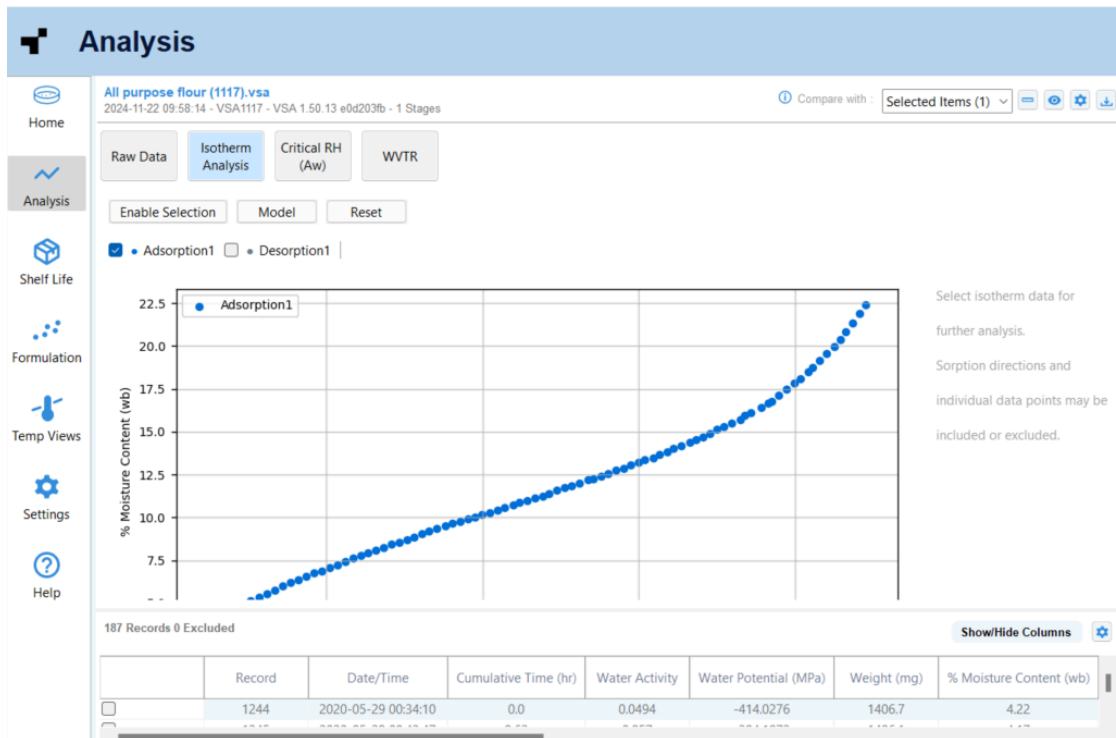
Fitting a Model to a Sorption Curve

The model fitting feature in Isotherm Analysis allows users to apply standard models (DLP, GAB, BET, Linear.) to a selected curve or a specific region of a curve. This helps in interpreting the data and estimating sorption parameters.

In order to fit a model only a single sorption curve must be selected and there must be at least 2 datapoints selected to model. To fit isotherm stages to models follow these steps.

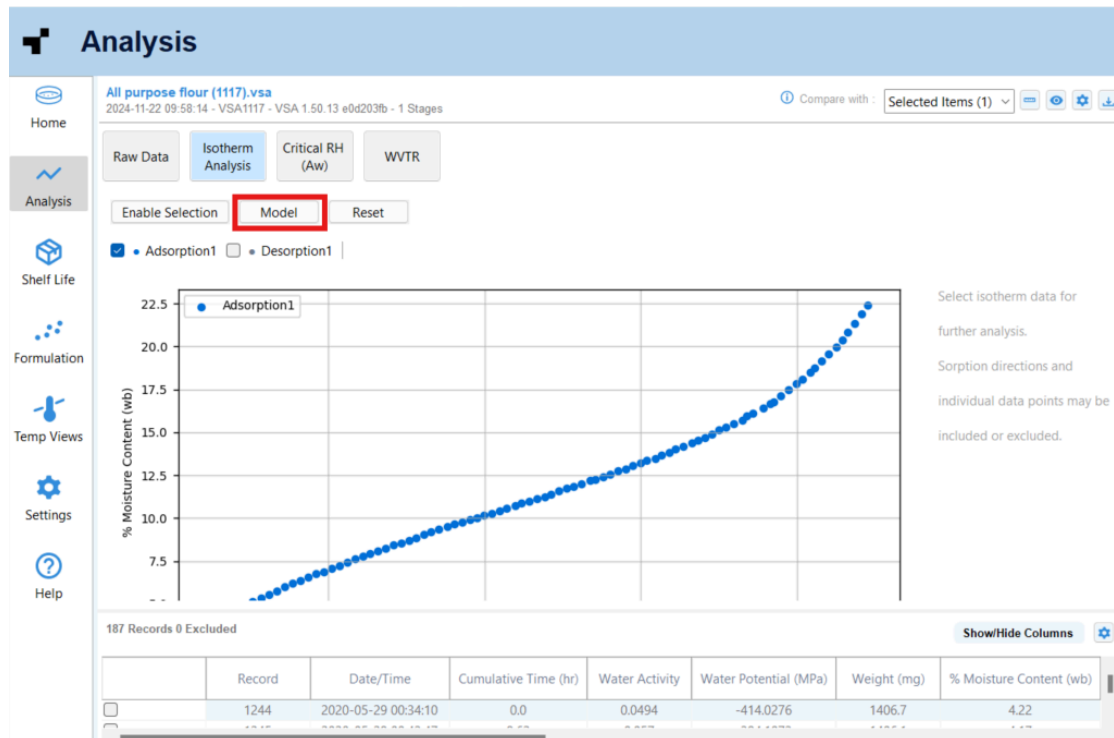
Steps

1. Select a Single Sorption Curve



2. Once a curve is selected and you are ready to model, you have multiple options for defining which part of the curve the model will apply to:
 - Model the entire curve
 - Enable selection for a specific portion of the curve (follow [these](#) steps to enable selection)
 - Exclude data points manually using the table (follow [these](#) steps to exclude datapoints)

- After selecting your modeling region (full, partial, or filtered), click the Model button.

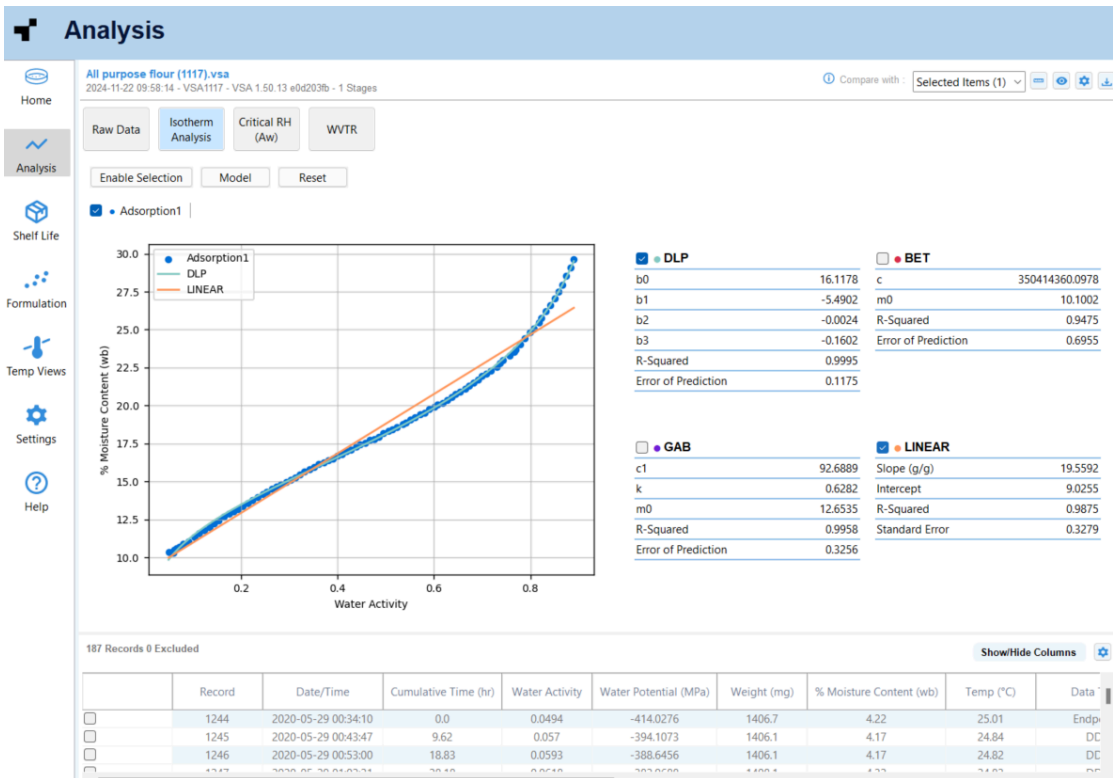


- Upon selecting the model button, you will be able to view all the models you can fit to the selected curve.

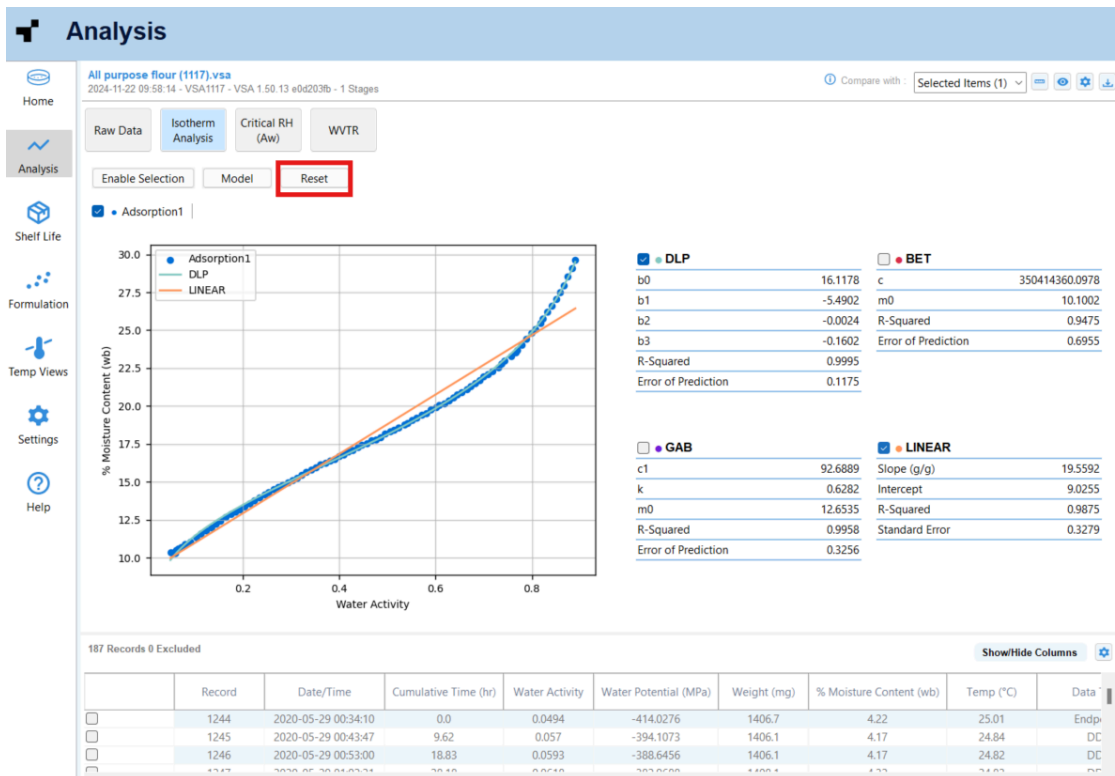


The system automatically calculates model parameters for all available models and displays each model's result card on the right side of the screen under each model's name.

5. Check the boxes next to the models you want to fit to the curve.



6. Click the Reset button to return to the original isotherm screen. (See [here](#) to see what reset does)

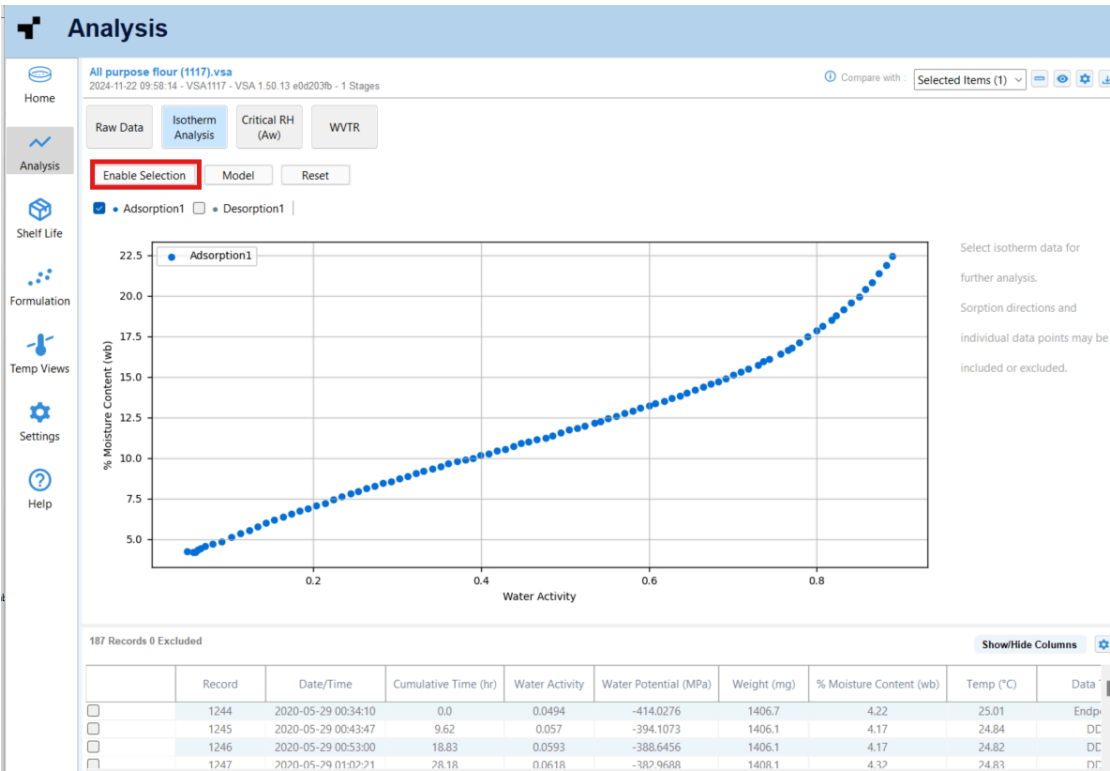


Enable Selection (Modeling a Curve Segment)

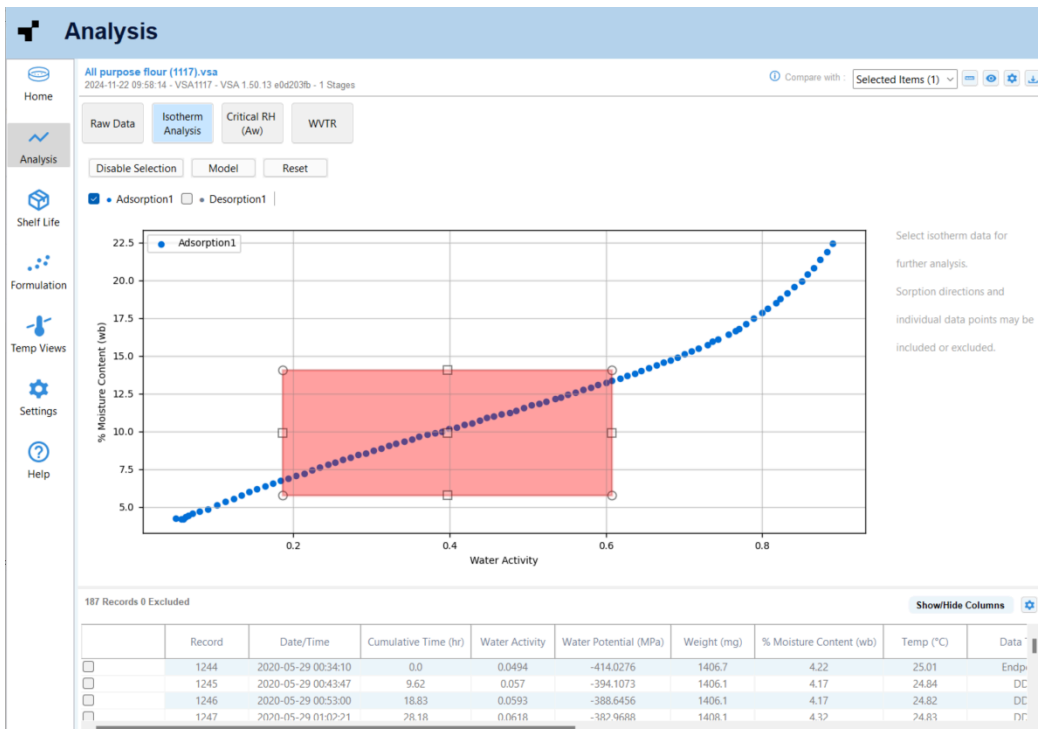
The Enable Selection feature allows you to apply modeling only to a specific portion of the curve. To do so follow these steps.

Steps.

1. Click Enable Selection.

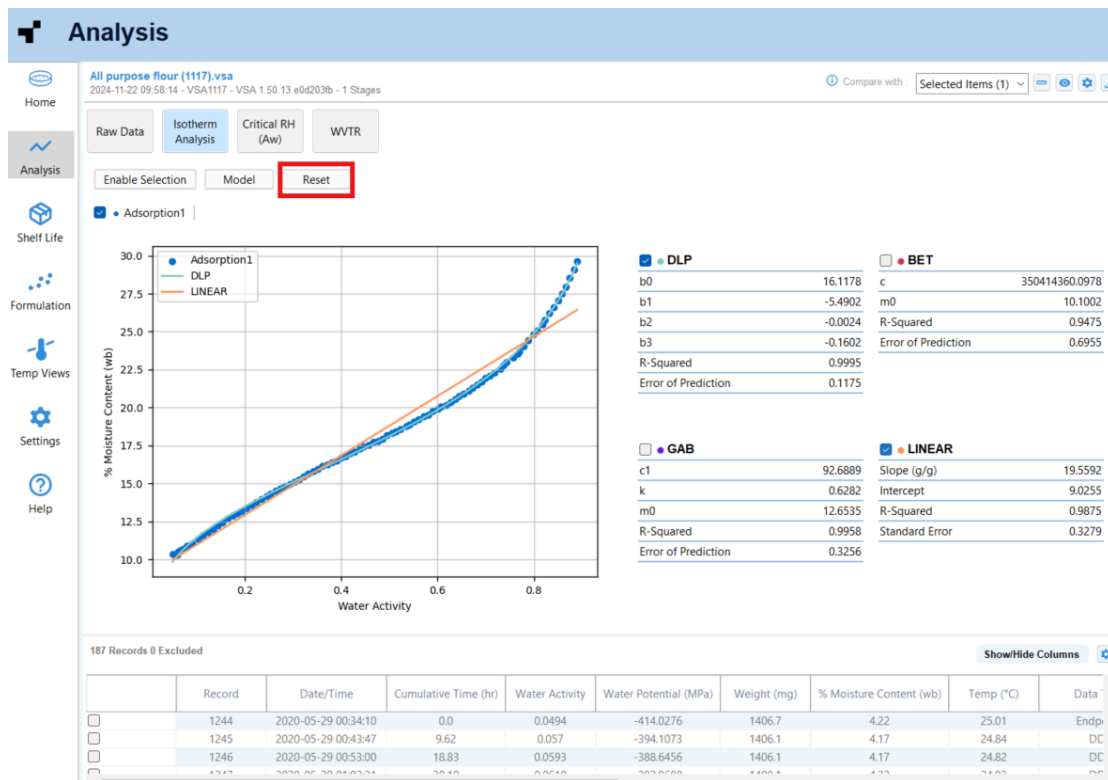


2. Drag across the graph to highlight a region of the curve.



Using the Reset Button

The Reset button in the Isotherm Analysis tab allows users to return to the initial isotherm view, clearing any modeling or selection activity.



What Reset Does:

- Deselects any models you selected for graph overlay.
- Clears any selected portion of the curve (from Enable Selection).
- Restores any previously excluded data points.
- Returns the view to show all sorption curves (e.g., both Adsorption and Desorption if available).
- Collapses the model cards on the right.
- Effectively takes you back to the default isotherm view, as it appeared when you first opened the file.

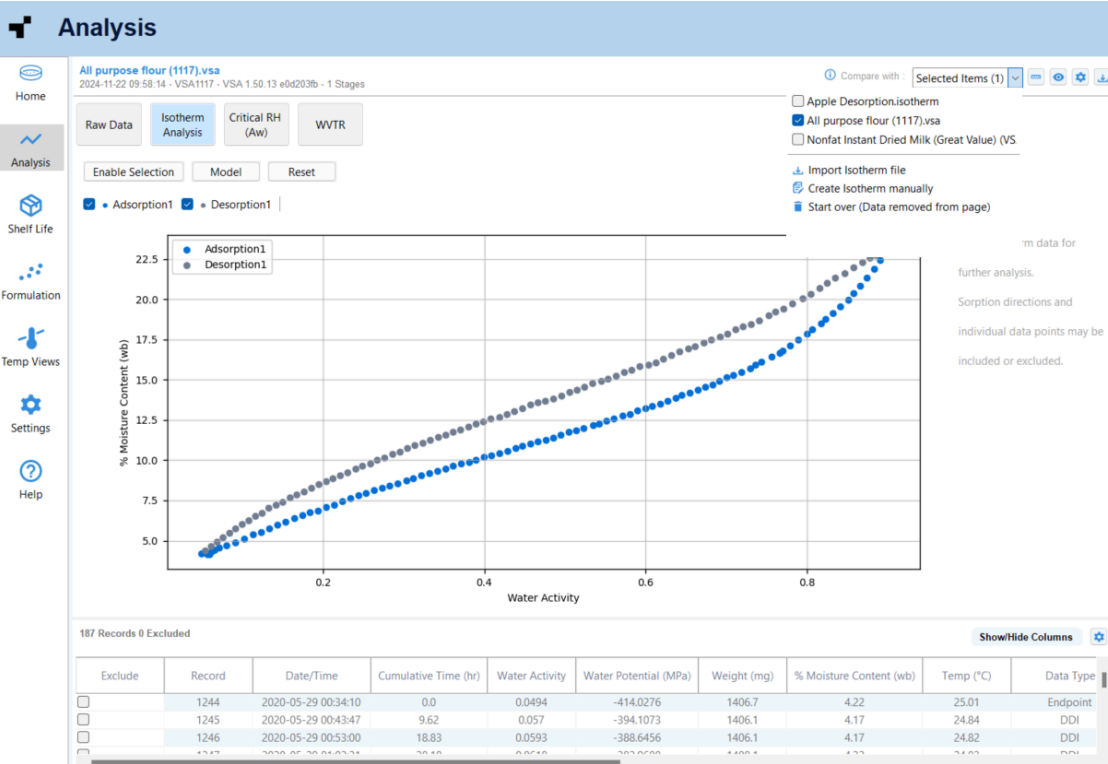
Compare Isotherms

This tool allows you to visually compare multiple isotherms graphs. You can choose between multiple parameters for both the x and y axes. To compare isotherms follow these steps.

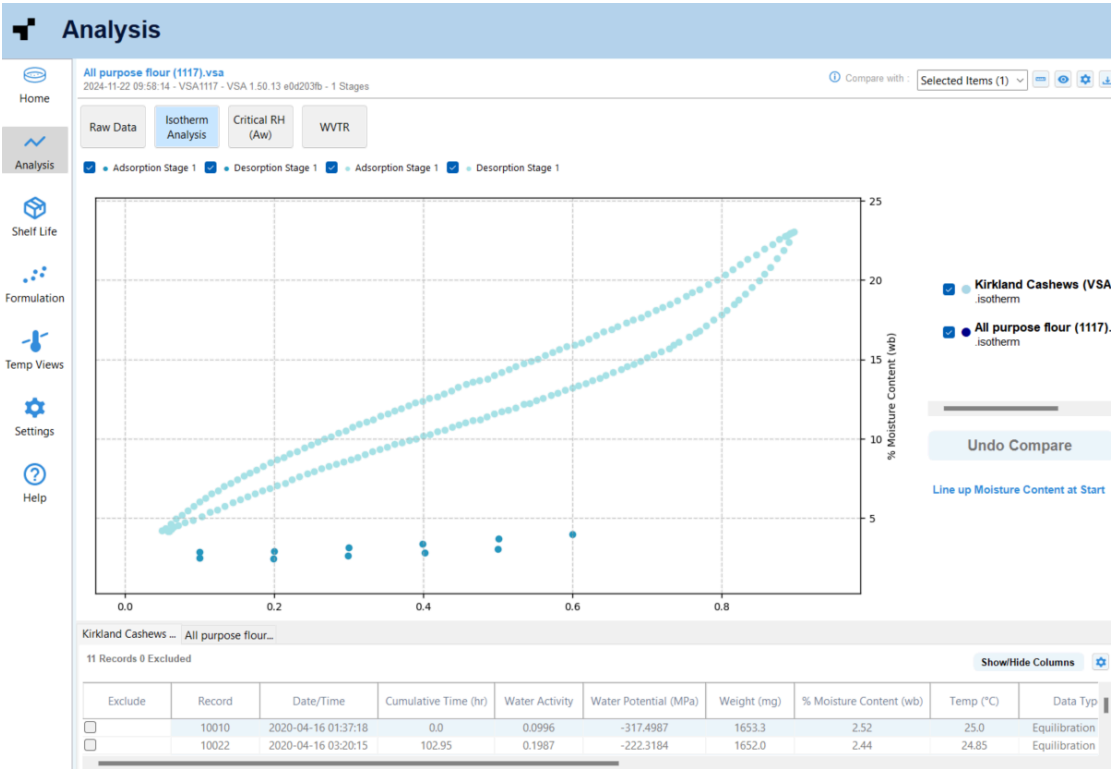
Steps

6. Navigate to the Isotherm Analysis section (follow [these](#) steps).
7. Ensure a primary file is loaded.

- Click the “Compare With” dropdown near the top of the page.
- Select one or more test files (up to 10) for comparison (Import files if needed).



10. Following the selection of the files you will move to the comparison mode.



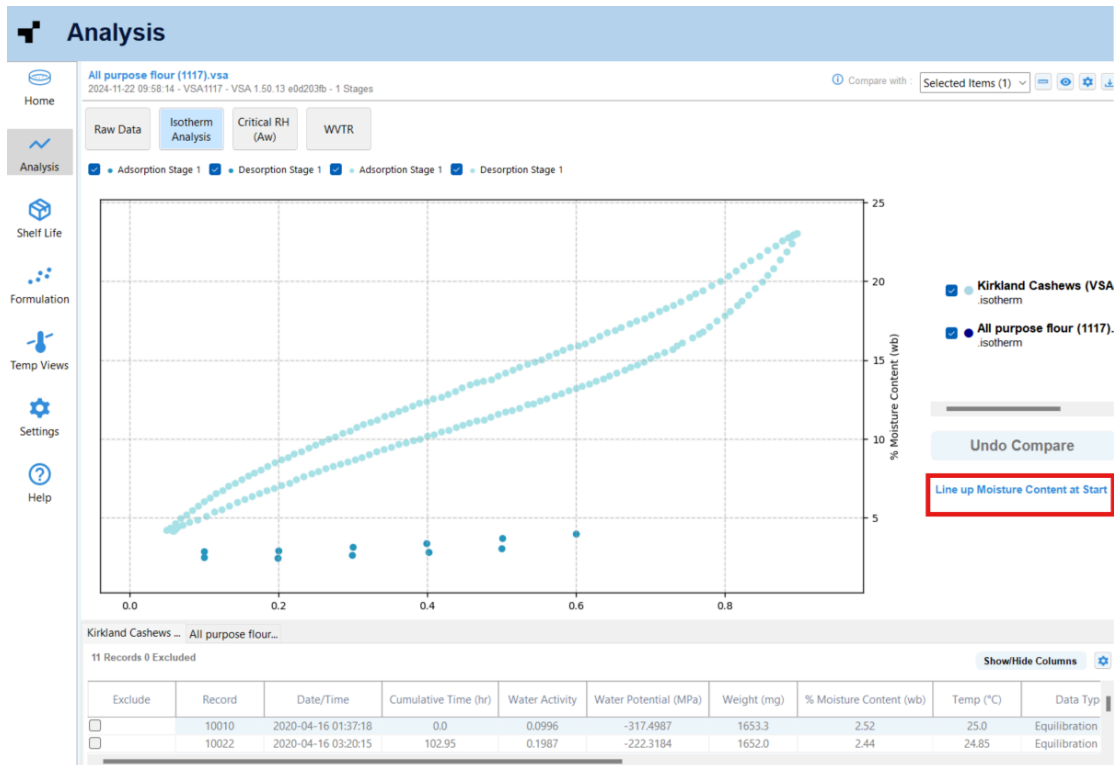
11. You can check an uncheck files alongside the graph to change the visibility on graph

Line up moisture content at start

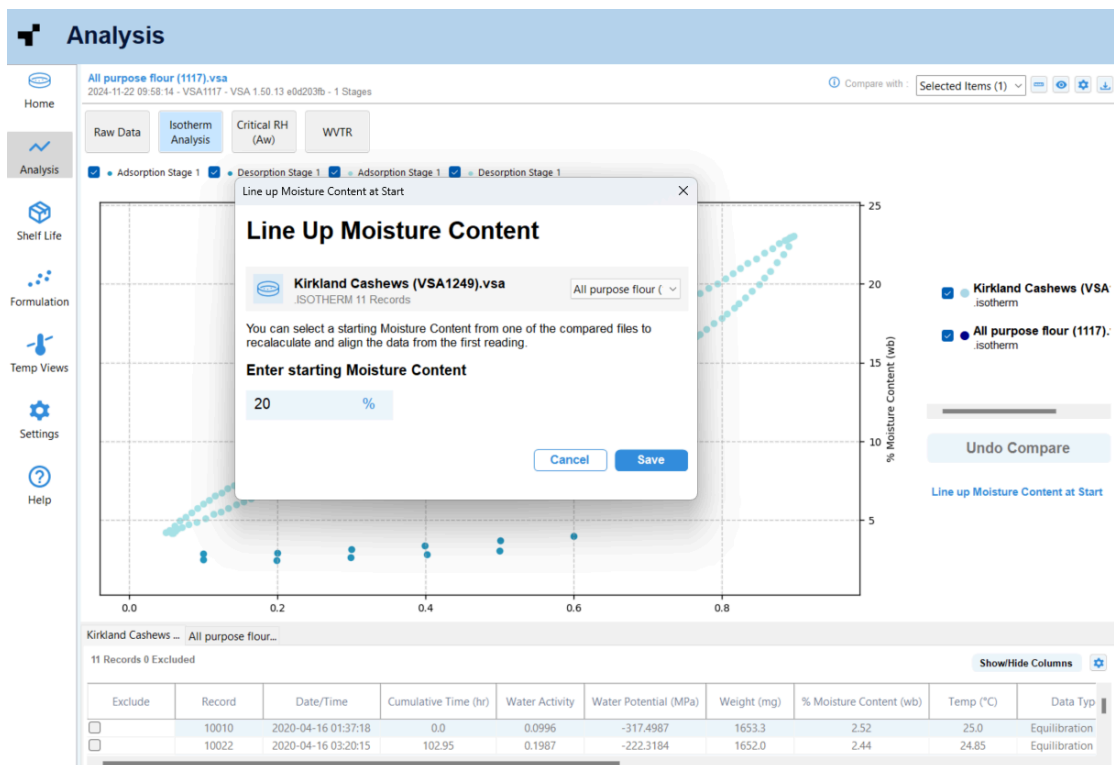
Line up moisture content at start will allow you to select a starting moisture content from one of the compared files to recalculate and align the data from the first reading. To do this follow these steps

Steps:

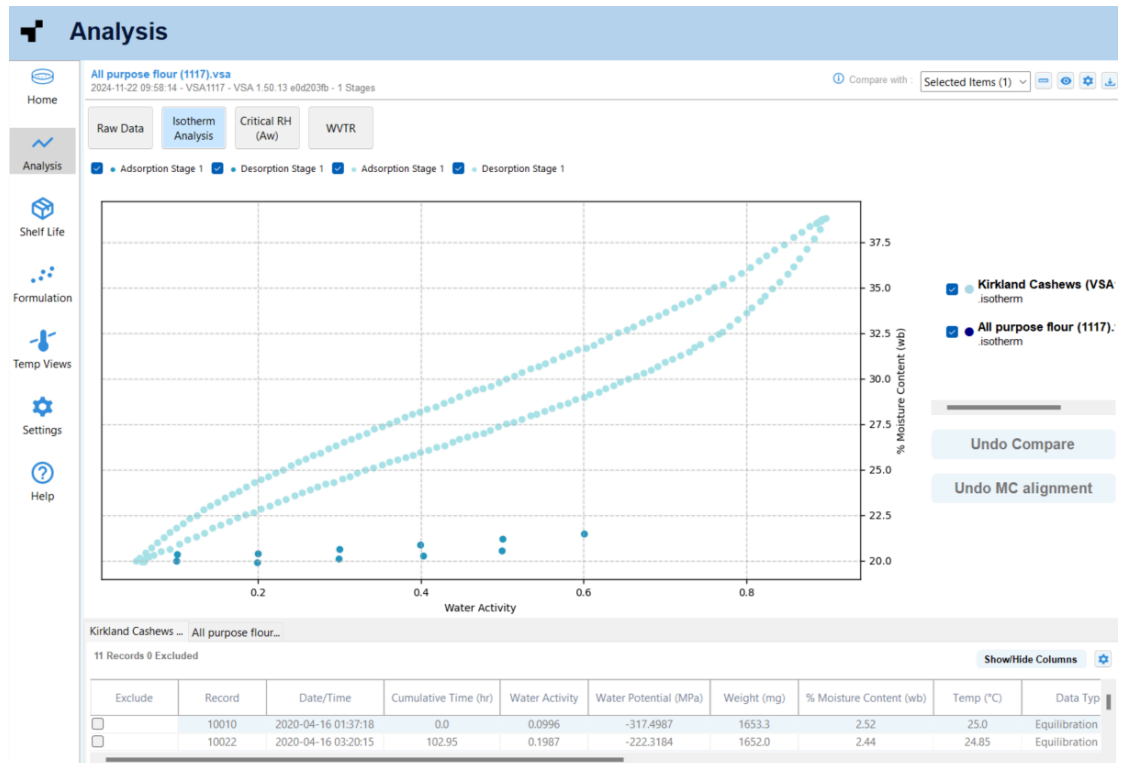
1. Click the Line up moisture content at start button.



2. On click a pop up shall appear, configure the file to be compared with using the files available in the drop down and enter the starting moisture content.



- Click Save. This will line up the moisture content accordingly.



- In order to undo the moisture content alignment to how it was by default. Click on Undo MC alignment

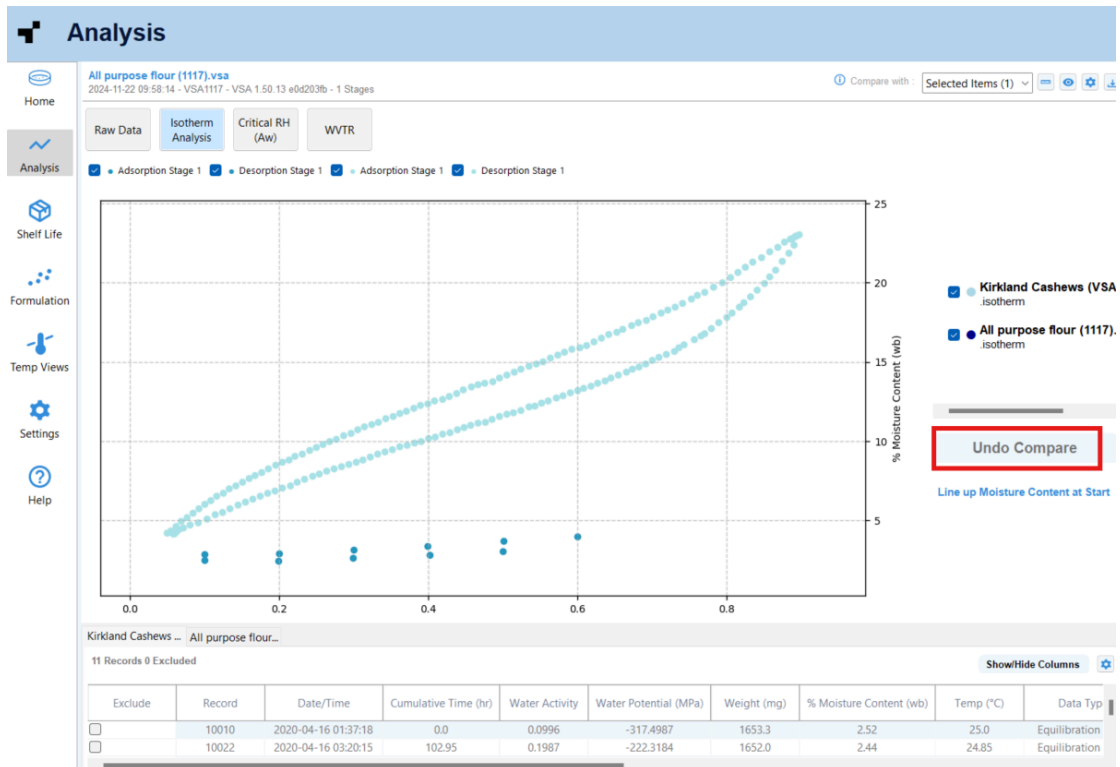
Undo Compare

If you've entered Comparison Mode and wish to return to the standard single-test view, use the Undo Compare option.

Steps to undo compare

How to Undo a Comparison:

- In the comparison mode, locate and click the “Undo Compare” button.



2. The system will exit Comparison Mode and return you to the main isotherm view.

View Data points of compared files

The data points of the compared files will be available in the table below the graph. You will be able to toggle between the multiple files to view their respective data points.

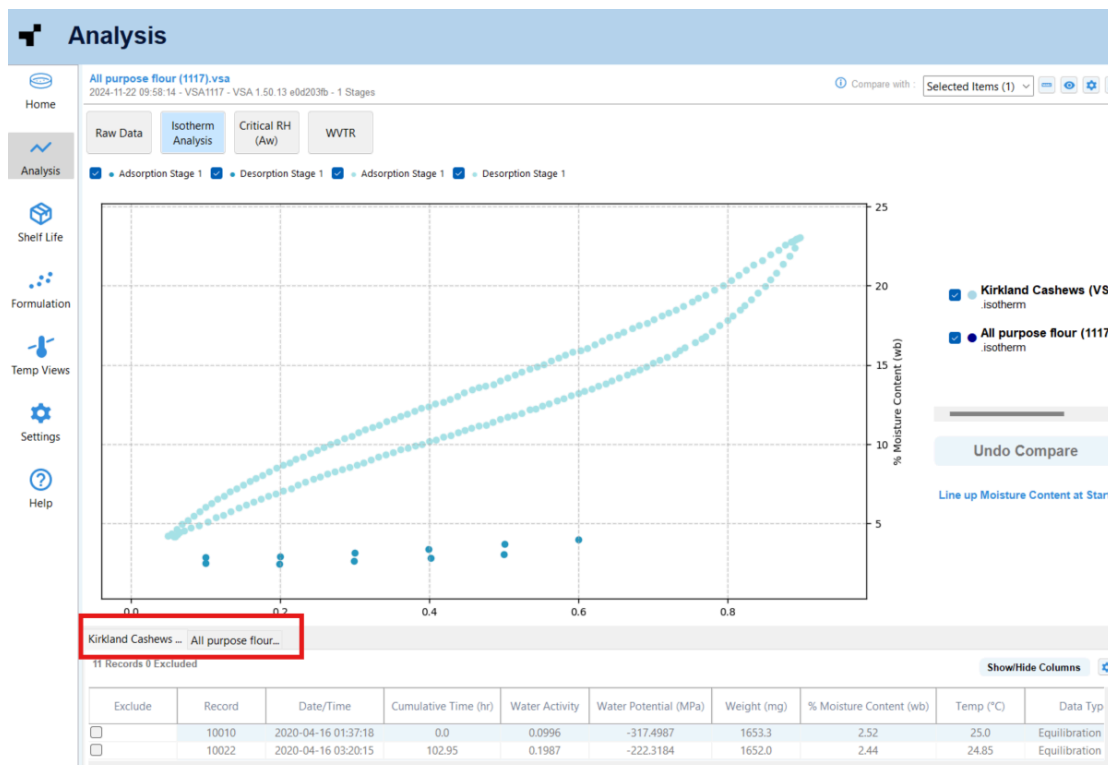


Table View

The Table View displays your data in a spreadsheet format.

Copy

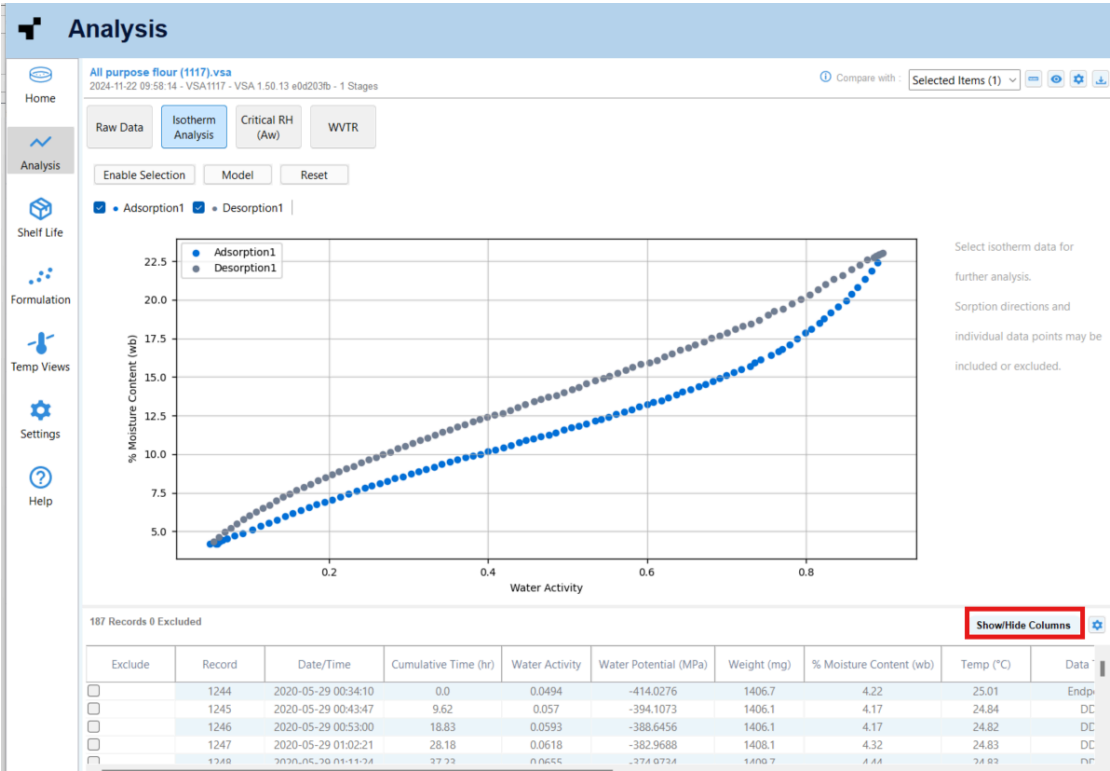
Select the data points to be copied, then use the keyboard shortcut CTRL + C to copy the values.

Show/Hide Columns

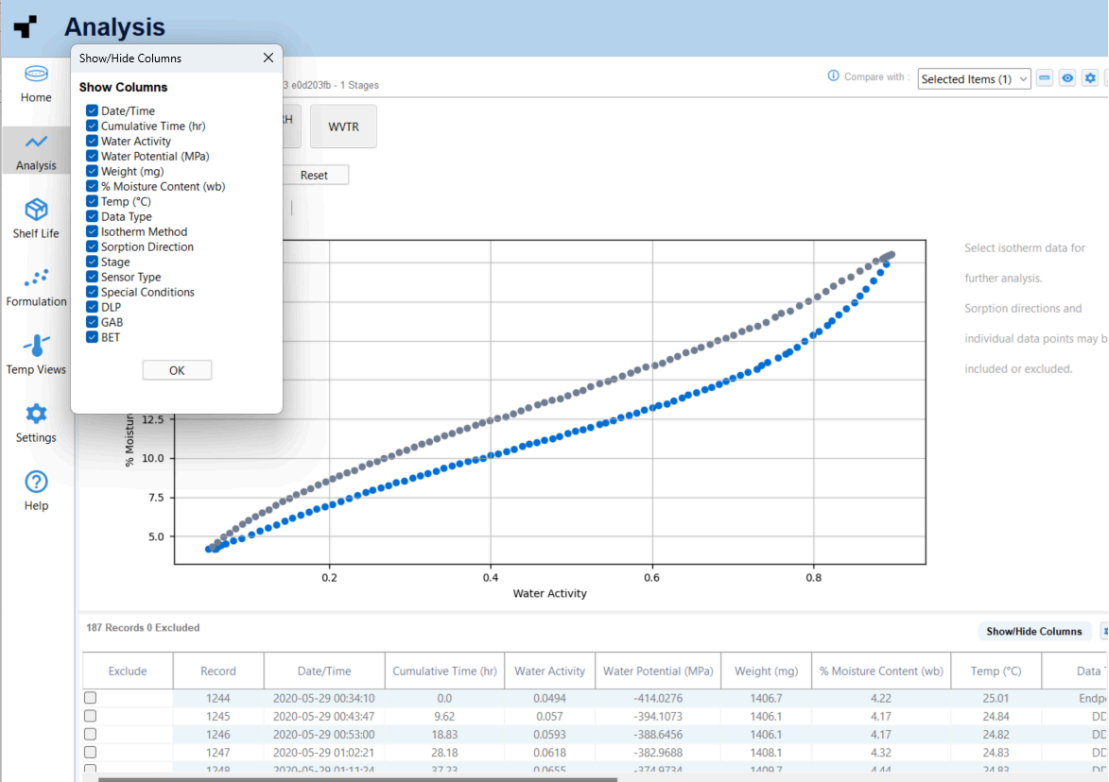
Control the columns visible on the table. Follow these steps to show/hide columns.

Steps:

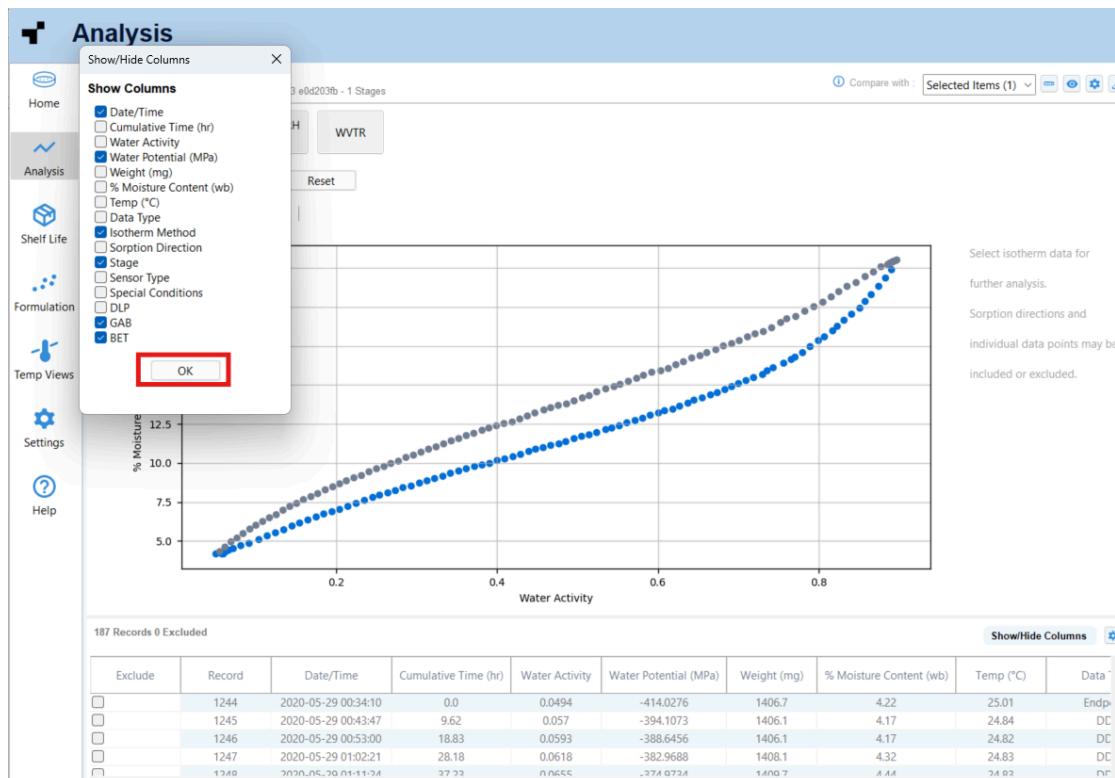
- 6. Click the Show/Hide Columns button at the top of the table.



- 7. On click a pop up with the list of all available columns will appear.



8. Each column has a checkbox:
 - a. Checked = visible in the table
 - b. Unchecked = hidden from view
9. Use this to declutter the table and focus on only the columns you need.
10. Once the needed columns have been checked, Click OK to update the table with the changes.



Note : Changes affect only the current table— the original data remains unchanged.

Change Table Setting

Changing Temperature units

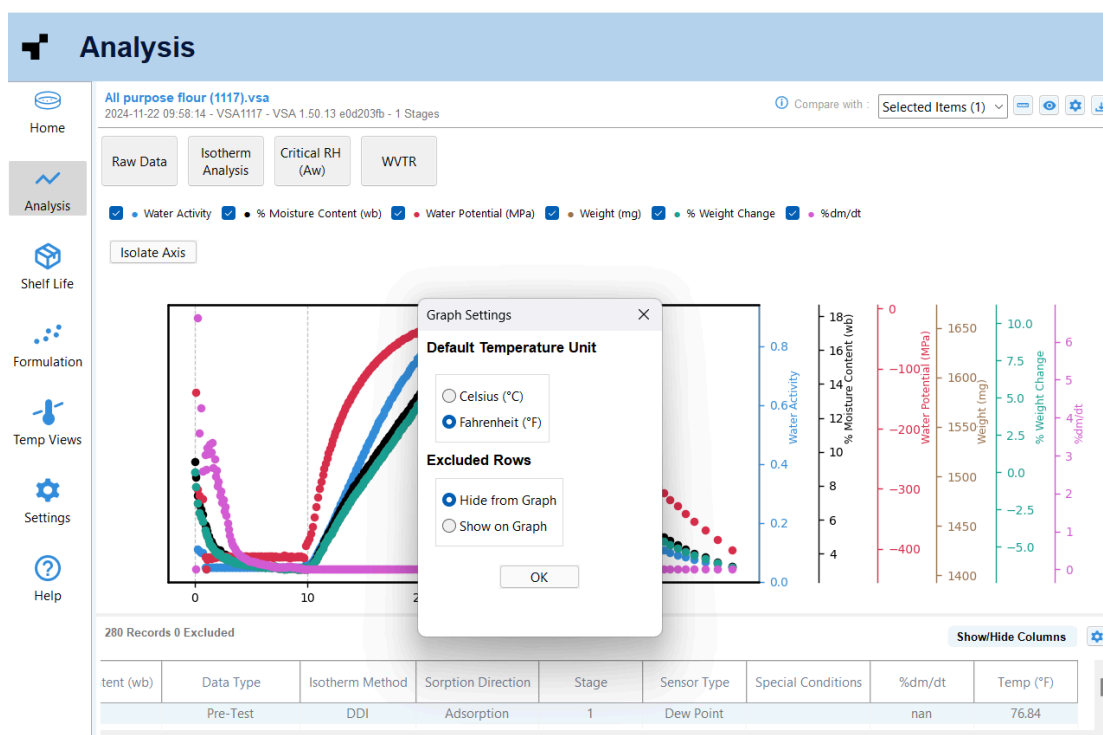
To change the units of temperature between celsius and fahrenheit follow these steps.

Steps:

5. Click on the gear icon at the top right corner of the table.



6. A pop up will appear with the settings.



7. Select the default temperature as required.

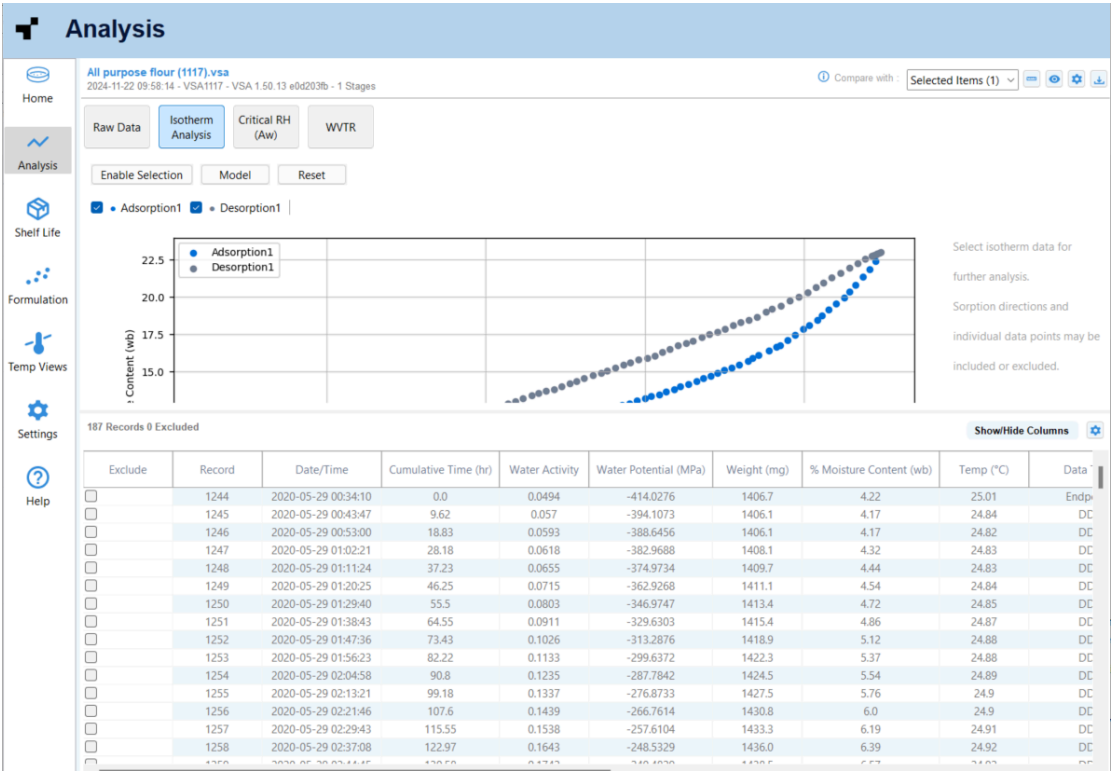
8. Click on OK. The table will be updated with the new temperature unit.

Excluding Data Points from the Graph

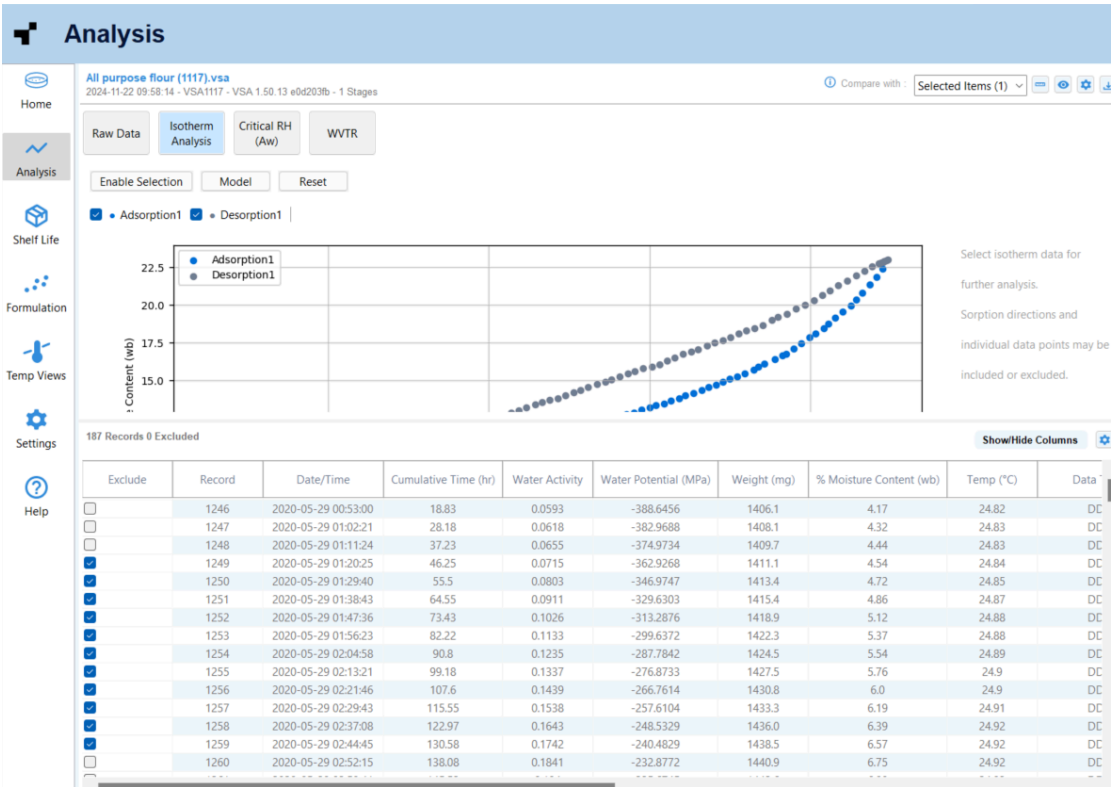
To exclude specific data points from being reflected in the graph, follow these steps.

Steps:

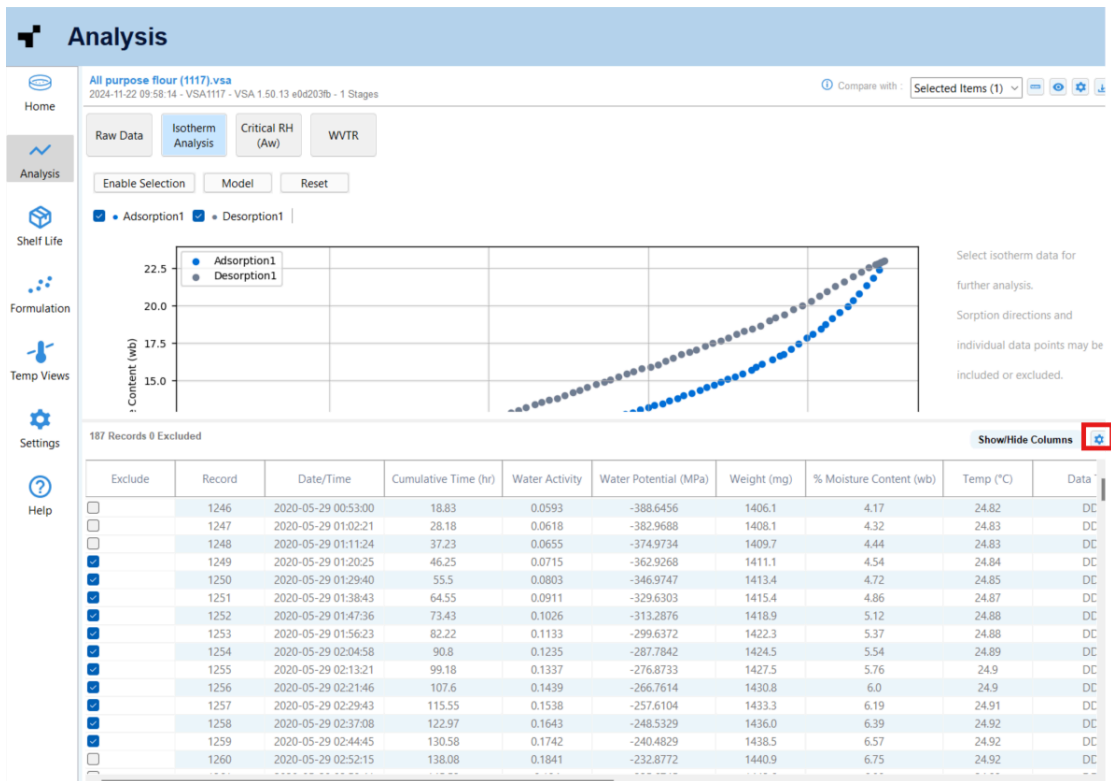
1. Go to the Table displayed below the graph.



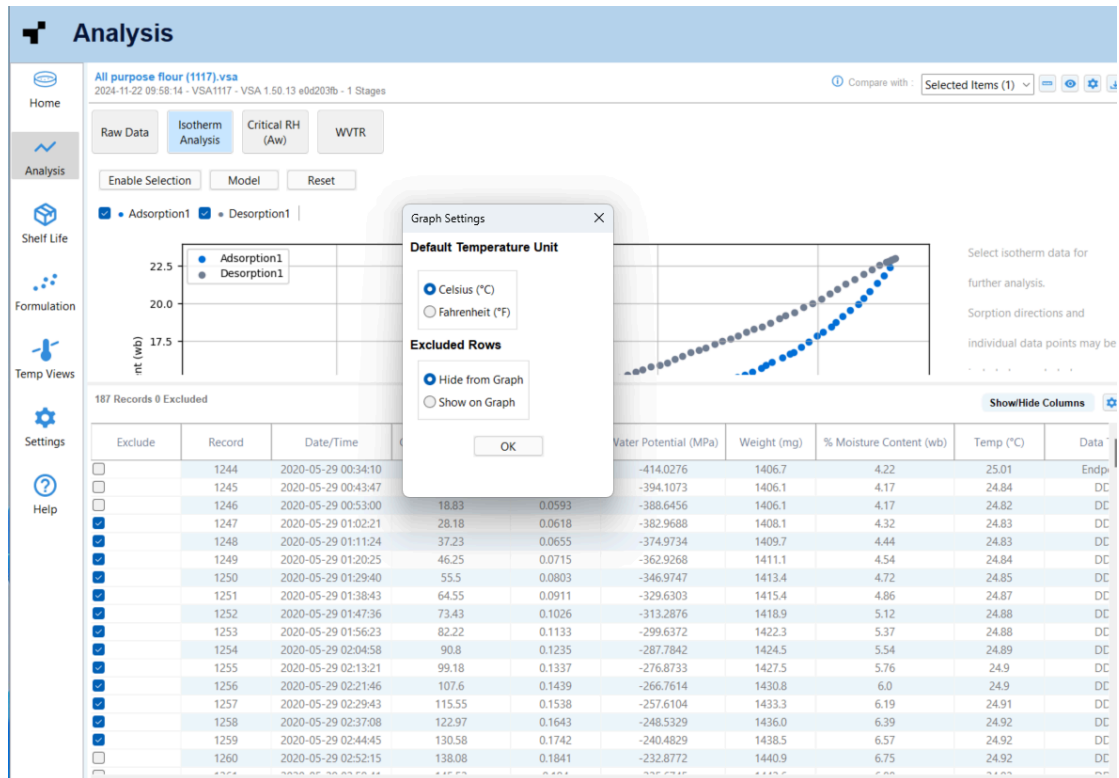
2. Uncheck the checkbox beside the data point(s) you wish to exclude.



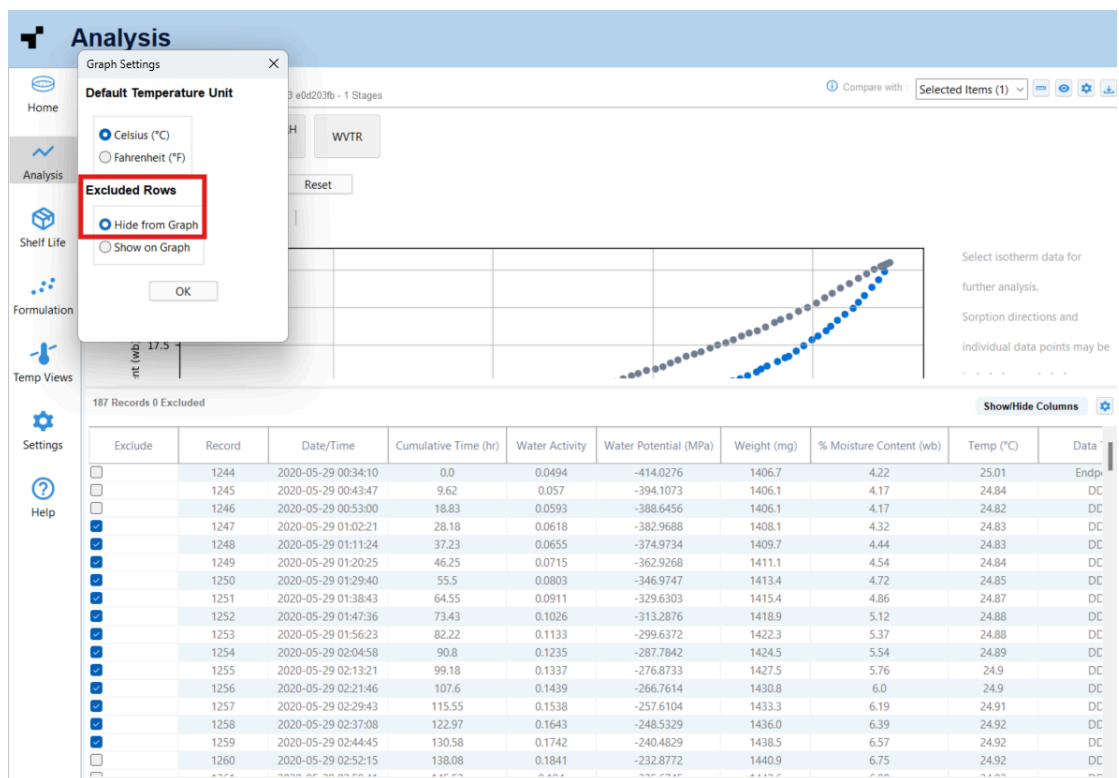
3. Click on the gear icon at the top right corner of the table.



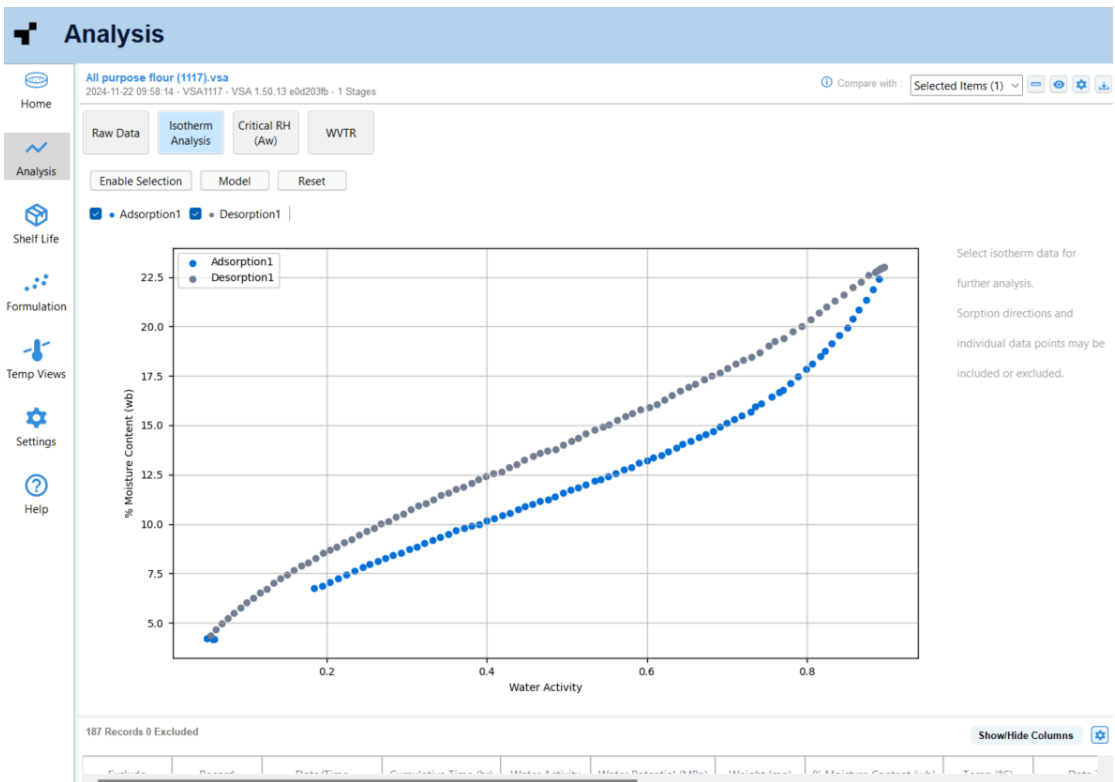
4. Upon clicking a pop up will appear with the settings.



5. In the pop up select Hide from Graph under the Excluded Rows section.



6. Click on OK. The graph will be updated with the excluded points.



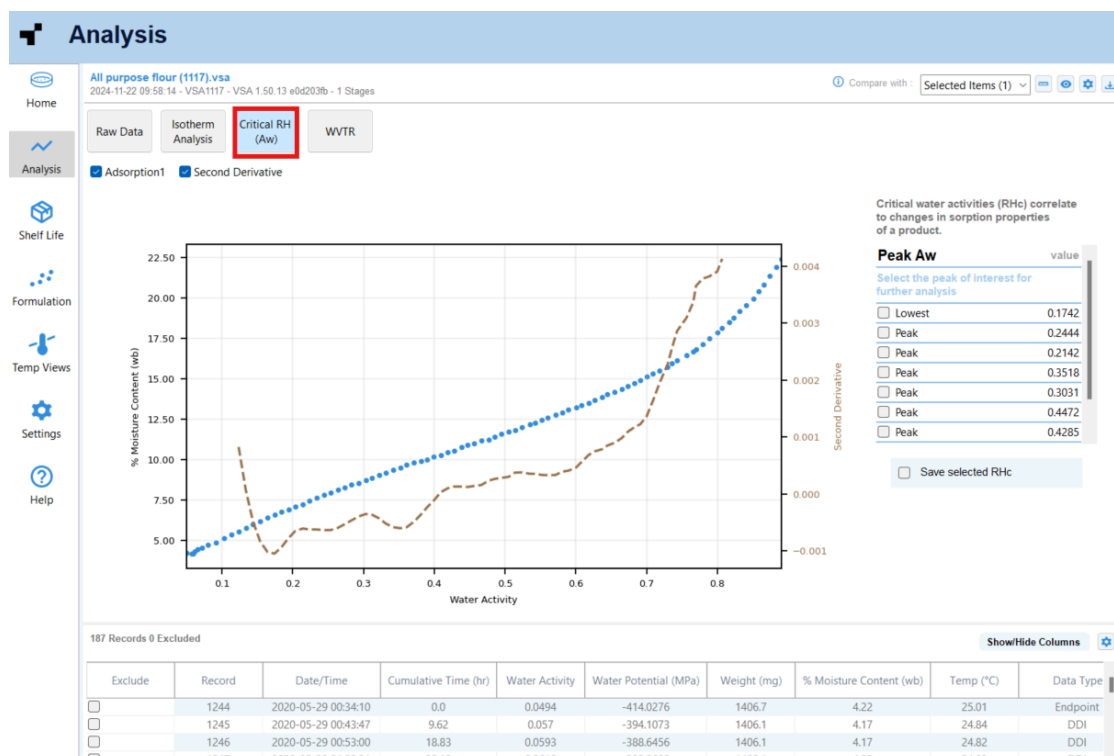
Note: Excluding a data point from the graph will also remove its contribution from any model fits or parameter estimations.

1.2.2.3 Critical RH (Aw)

Critical RH shall be enabled only when a single isotherm stage is selected from the Isotherm Analysis tab.

To use Critical RH(Aw), follow these steps:

1. Go to the Analysis section.
2. Select the Critical RH tab (visible when a valid isotherm and a single isotherm stage is selected from the isotherm analysis tab).



3. The system generates a graph based on the input data.

Graph View

Zoom In / Out

Use your mouse scroll wheel or two-finger scroll on a touchpad to zoom in or out of the graph.

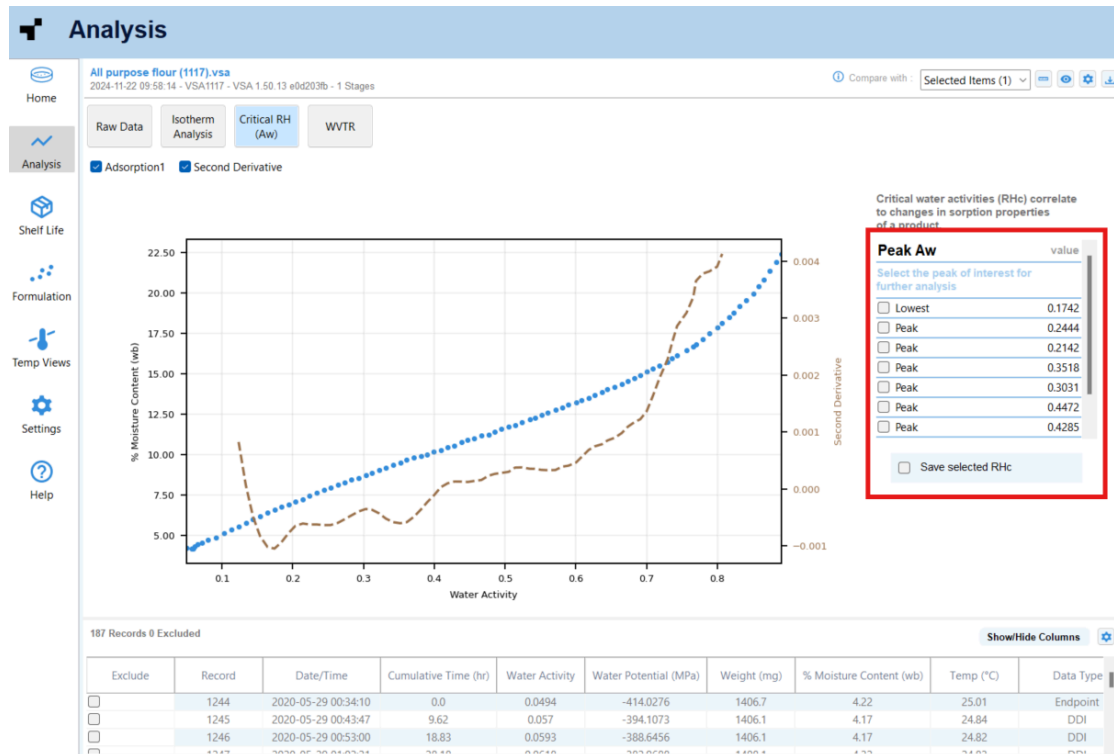
Pan

Click and hold anywhere on the graph., drag with your mouse or touchpad. Move in any direction (left, right, up, down).

View peak water activity

Critical water activity correlates to changes in the sorption properties of a product. You shall be able to identify peak values of water activity for further analysis. In order to view the critical water activity points follow these steps

1. Check the checkbox of the peak of interest on the Peak Aw list alongside the critical RH graph.



2. When the values are checked these points will be reflected on the graph.



Save selected RHc

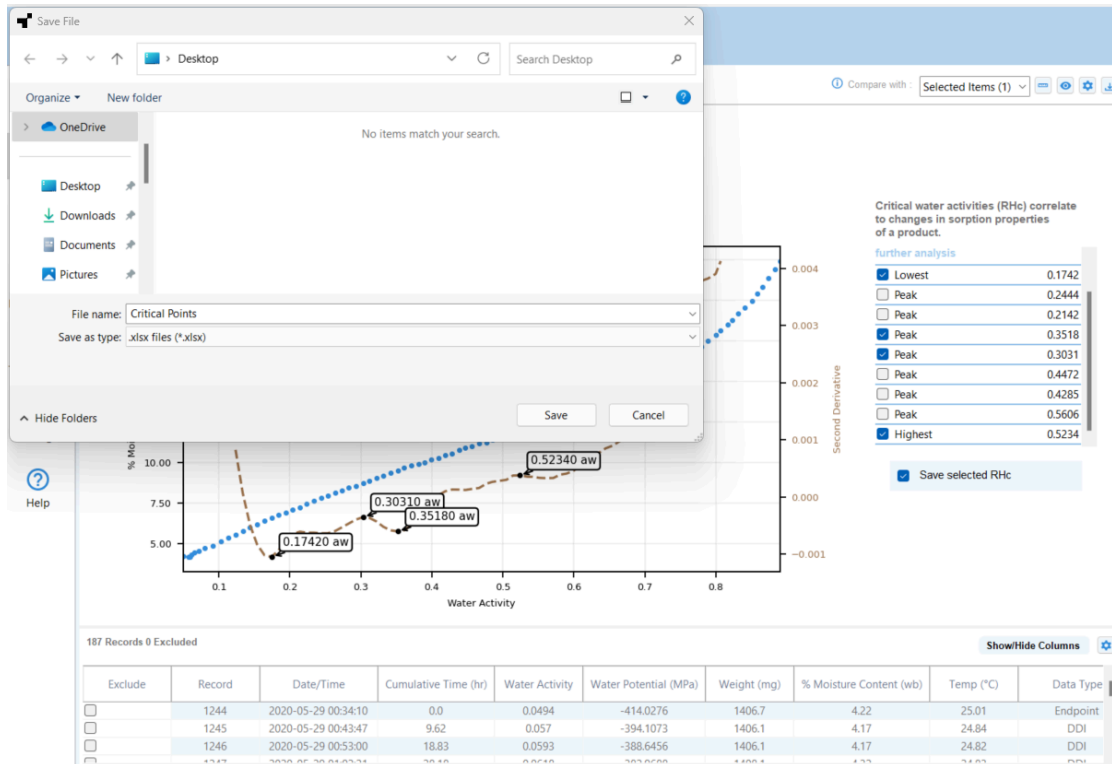
The Save Selected RHC feature allows users to store and export specific RHc points. To do this follow these steps.

Steps

1. Check the checkbox of critical water activities of interest from the list available.



2. Check the checkbox of Save Selected RHC.
3. On check the save file wizard will open



4. Select the preferred location and click Save

Table View

The Table View displays your data in a spreadsheet format.

Copy

Select the data points to be copied, then use the keyboard shortcut CTRL + C to copy the values.

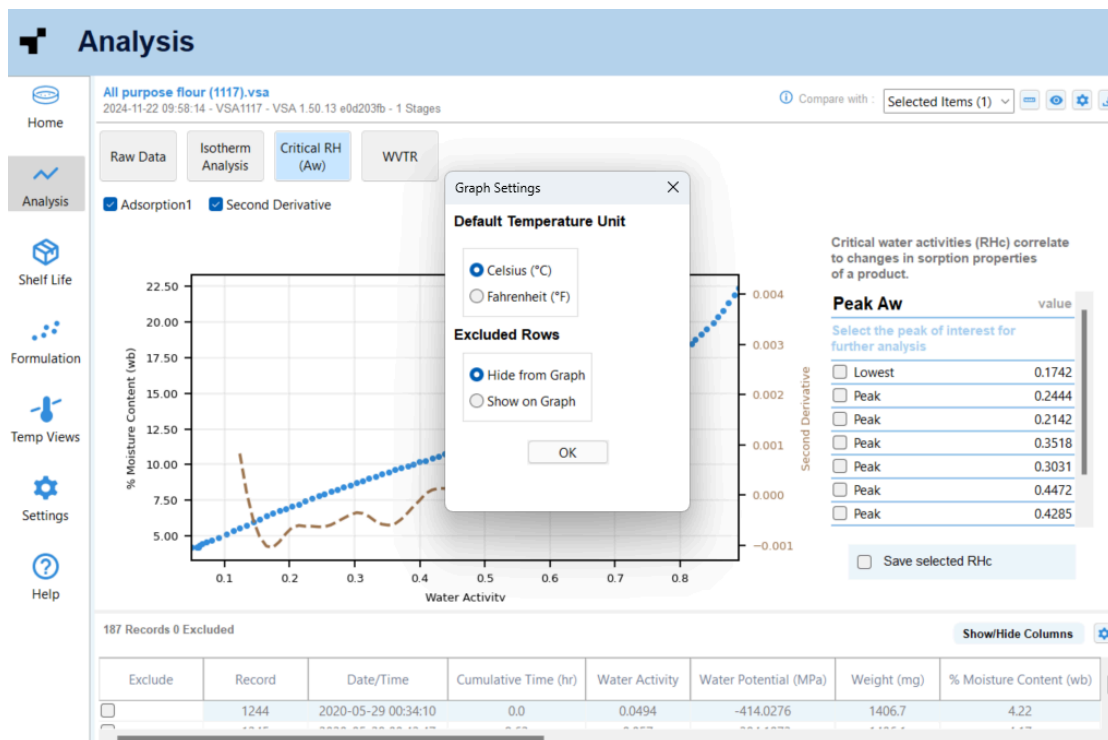
Change Table Setting

Changing Temperature units

To change the units of temperature between celsius and fahrenheit follow these steps.

Steps:

1. Click on the gear icon at the top right corner of the table.
2. A pop up will appear with the settings.



3. Select the default temperature as required.
4. Click on OK. The table will be updated with the new temperature unit.

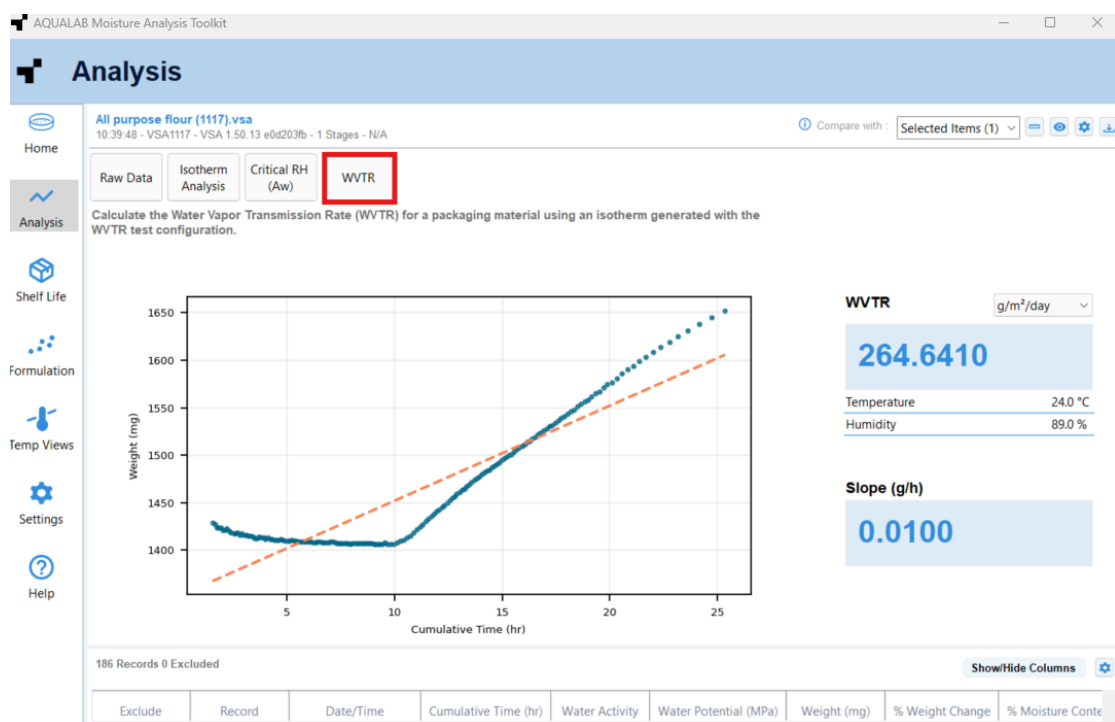
1.2.2.4 WVTR

This is the component users will interact with to calculate and visualize Water Vapor Transmission Rate (WVTR) for a packaging based on isotherm generated with the WVTR test configuration.

To use WVTR:

Steps

1. Go to the Analysis section.
2. Select the WVTR tab (visible when a valid isotherm with a minimum of 12 data points is available).



3. The system uses available data to generate WVTR calculations and curves.

Available features:

- View WVTR curve plotted based on input data.
- View slope value
- Change WVTR units (e.g., g/in²/day, g/m²/day) using the unit selector.

1.2.3 Shelf Life

1.2.3.1 Shelf Life Calculation

This section enables users to predict shelf life based on packaging, the expected storage conditions and the unique moisture properties of a product.

Predict Shelf Life

This tool is used to predict the shelf life of a product based on a critical water activity and the moisture barrier properties, typically reported as Water Vapor Transmission Rate (WVTR). Using this tool, the shelf life can be predicted under any potential storage conditions.

To use this tool, follow these steps:

Steps:

1. Navigate to the shelf life page by selecting the Shelf Life option in the side panel

AQUALAB Moisture Analysis Toolkit

Shelf Life

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☒ Predict Shelf Life ☐ Determine Water Activity ☐ Determine WVTR for desired Shelf Life

Please fill in below fields

WVTR (g/m ² /days)	00
WVTR Testing Temp (°C)	00
WVTR Testing Humidity (%)	00
Humidity of Air (%)	00
Ambient Temperature (°C)	00
Atmospheric Pressure (kPa)	00
Surface Area of Packaging (m ²)	00
Total Mass (g)	00
Initial Aw	00
Critical Aw that ends Self Life	00

[Import Excel](#) [Add slope, DLP coefficients or .isotherm file](#)

Slope from Isotherm in g/g

[Save to Excel](#)

[Start Over](#) [Calculate](#)

Results

Predicted Shelf Life Days

0.00

Convert WVTR Units

g/100in ² /days	----
g/m ² /days	----

2. Click on the Shelf Life Calculation tab.

AQUALAB Moisture Analysis Toolkit

Shelf Life

Home | **Shelf Life Calculations** | Multiple Package WVTR | Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☐ Predict Shelf Life
 ☐ Determine Water Activity
 ☒ Determine WVTR for desired Shelf Life

Please fill in below fields [Import Excel](#)

Desired Shelf Life (days)	00
WVTR Testing Temp (°C)	00
WVTR Testing Humidity (%)	00
Storage Humidity (%)	00
Ambient Temperature (°C)	00
Atmospheric Pressure (kPa)	00
Surface Area of Packaging (m²)	00
Total Mass (g)	00
Initial Aw	00
Critical Aw that Ends Shelf Life	00

[Save to Excel](#)

Add slope, DLP coefficients or .isotherm file

Import Isotherm

Results

WVTR

0.00

Permeance

0.00

Convert WVTR Units

g/100in²/days	----
g/m²/days	----

[Start Over](#) [Calculate](#)

- Choose Predict Shelf Life from the available radio buttons.

Shelf Life

Home | **Shelf Life Calculations** | Multiple Package WVTR | Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☒ **Predict Shelf Life**
☐ Determine Water Activity
 ☐ Determine WVTR for desired Shelf Life

Please fill in below fields [Import Excel](#)

WVTR (g/m²/days)	00
WVTR Testing Temp (°C)	00
WVTR Testing Humidity (%)	00
Humidity of Air (%)	00
Ambient Temperature (°C)	00
Atmospheric Pressure (kPa)	00
Surface Area of Packaging (m²)	00
Total Mass (g)	00
Initial Aw	00
Critical Aw that ends Self Life	00

[Save to Excel](#)

Add slope, DLP coefficients or .isotherm file

Slope from Isotherm in g/g

Results

Predicted Shelf Life Days

0.00

Convert WVTR Units

g/100in²/days	----
g/m²/days	----

[Start Over](#) [Calculate](#)

- In order to obtain the shelf life, do the following:
 - Enter the package Water Vapor Transmission Rate (WVTR), the WVTR Testing Temperature, and the WVTR Testing Humidity. The WVTR testing temperature and

humidity are needed to convert WVTR, which is not a fundamental value, to Permeance, which can be used in first principles models. If you already know the Permeance, you can simply enter its value without providing WVTR information.

- You must enter the data for each of the data fields on this screen
 - Atmospheric Pressure - typically assume 100 kPa
 - Total Dry mass of sample in the package in grams
 - Ambient Temperature or storage temperature (oC)
 - Surface Area of packaging (total of all exposure sides) (m²)
 - Humidity of Air - storage relative humidity
 - Initial aw of sample when placed in the package
 - Critical Water Activity that Ends Shelf Life - the critical water activity will have been determined using other experimentation.
 - The isotherm slope is needed for the calculations. You may choose whether to manually enter the slope, DLP coefficients, or load an isotherm containing that data. A manual slope may be obtained from simple linear regression on existing isotherm data and entered as g/g. A more accurate slope can be determined using the DLP isotherm model. The DLP coefficients can either be entered manually or provided by an .isotherm file. To choose an isotherm option, simply click the appropriate radio button on the left. The selected field will no longer be greyed out, and you will be able to enter data or load an .isotherm file.
5. After you have finished entering all the required data, click the Calculate button at the bottom.
 6. The resulting Shelf Life will be displayed in the "Predicted Shelf Life" field at the right. You may select to report the shelf life in "Days," "Weeks," or "Years" using the drop down box to the right of the predicted shelf life field.

Determine Water Activity

This tool allows you to determine the water activity of an ingredient in a package when stored under specific conditions based on the permeability properties of the packaging.

To use this tool, follow these steps:

Steps:

1. Navigate to the shelf life page by selecting the Shelf Life option in the side panel

AQUALAB Moisture Analysis Toolkit

Shelf Life

Home

Analysis

Shelf Life

Formulation

Temp Views

Settings

Help

Shelf Life Calculations

Multiple Package WVTR

Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

Predict Shelf Life

Determine Water Activity

Determine WVTR for desired Shelf Life

Please fill in below fields

WVTR (g/m²/days)

00

WVTR Testing Temp (°C)

00

WVTR Testing Humidity (%)

00

Humidity of Air (%)

00

Ambient Temperature (°C)

00

Atmospheric Pressure (kPa)

00

Surface Area of Packaging (m²)

00

Total Mass (g)

00

Initial Aw

00

Critical Aw that ends Self Life

00

Import Excel

Add slope, DLP coefficients or .isotherm file

Slope from Isotherm in g/g

Save to Excel

Results

Predicted Shelf Life

Days

0.00

Convert WVTR Units

g/100in²/days

g/m²/days

Start Over

Calculate

2. Click on the Shelf Life Calculation tab.

AQUALAB Moisture Analysis Toolkit

Shelf Life

Home

Analysis

Shelf Life

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Help

Shelf Life Calculations

Multiple Package WVTR

Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

Predict Shelf Life

Determine Water Activity

Determine WVTR for desired Shelf Life

Please fill in below fields

Desired Shelf Life (days)

00

WVTR Testing Temp (°C)

00

WVTR Testing Humidity (%)

00

Storage Humidity (%)

00

Ambient Temperature (°C)

00

Atmospheric Pressure (kPa)

00

Surface Area of Packaging (m²)

00

Total Mass (g)

00

Initial Aw

00

Critical Aw that Ends Shelf Life

00

Import Excel

Add slope, DLP coefficients or .isotherm file

Import Isotherm

Save to Excel

Results

WVTR

0.00

Permeance

0.00

Convert WVTR Units

g/100in²/days

g/m²/days

Start Over

Calculate

3. Choose Determine Water Activity from the available radio buttons

Shelf Life

Home

Analysis

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Shelf Life Calculations Multiple Package WVTR Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☐ Predict Shelf Life ☒ Determine Water Activity ☐ Determine WVTR for desired Shelf Life

Please fill in below fields

Import Excel

Add slope, DLP coefficients or .isotherm file

Import Isotherm

Results

Water Activity

0.00

Convert WVTR Units

g/100in ² /days	----
g/m ² /days	----

Start Over Calculate

4. Enter the required details.

- You will need to enter information about your packaging, including the testing Water Vapor Transmission Rate (WVTR), the WVTR testing temperature, and the WVTR testing humidity.

Note: if you do not have this information, contact the packaging manufacturer.

Packages tested under the ASTM standard are tested at 37.7#176;C and 90% humidity, but do not assume this to be the case unless it is specified.

- You must enter the data for each of the data fields on this screen:
 - Atmospheric Pressure - typically assume 100 atm
 - Total Mass of sample in the package in grams
 - Ambient temperature or storage temperature- The highest temperature at which the product will be stored.
 - Surface Area of packaging - Total of all exposure sides)
 - Humidity of air - Storage relative humidity in percent (0-100), not decimal (.01-1.0), form (the highest humidity at which the product will be stored)
 - Initial Aw - Aw of sample when placed in the package
 - Time in package - Time the sample has been stored.
- The isotherm slope is needed for the calculations. You may choose whether to manually enter the slope or DLP coefficients, or load an isotherm containing that data. A manual slope may be obtained from simple linear regression on existing isotherm data and entered as g/g. A more accurate slope can be determined using the DLP isotherm model. The DLP coefficients can either be entered manually or

provided by a .isotherm file. To choose an isotherm option, simply select import an isotherm from the dropdown on the left, then the import wizard will be generated, select the relevant file and import it.

5. After you have finished entering all the required data, click the Calculate button at the bottom.

6. The resulting water activity will be displayed in the Water ACTivity field available on the right side of the page.

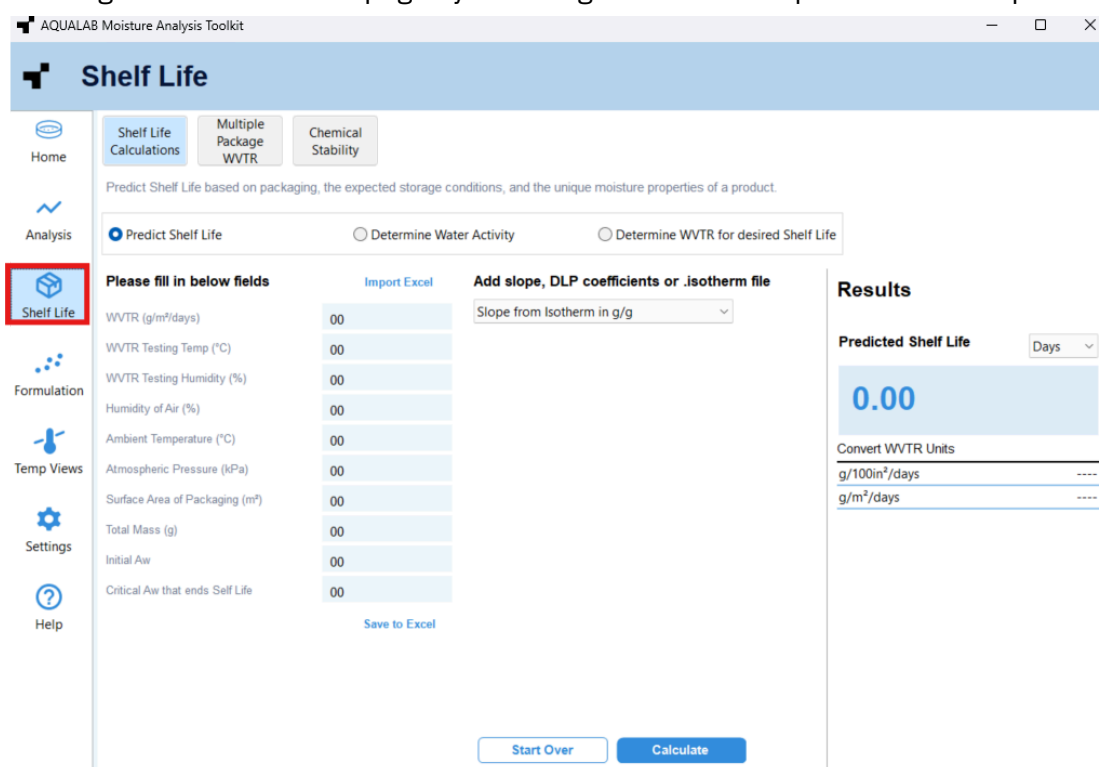
Determine WVTR for desired Shelf Life

This tool helps you to determine the moisture barrier requirements, typically reported as Water Vapor Transmission Rate (WVTR), for packaging to achieve a desired shelf life based on a critical water activity.

To use this tool, follow these steps:

Steps:

1. Navigate to the shelf life page by selecting the Shelf Life option in the side panel



AQUALAB Moisture Analysis Toolkit

Shelf Life

Home | Shelf Life Calculations | Multiple Package WVTR | Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☒ Predict Shelf Life ☐ Determine Water Activity ☐ Determine WVTR for desired Shelf Life

Please fill in below fields

	Import Excel
WVTR (g/m ² /days)	00
WVTR Testing Temp (°C)	00
WVTR Testing Humidity (%)	00
Humidity of Air (%)	00
Ambient Temperature (°C)	00
Atmospheric Pressure (kPa)	00
Surface Area of Packaging (m ²)	00
Total Mass (g)	00
Initial Aw	00
Critical Aw that ends Self Life	00

Save to Excel

Add slope, DLP coefficients or .isotherm file

Slope from Isotherm in g/g

Results

Predicted Shelf Life Days

0.00

Convert WVTR Units

g/100in ² /days	----
g/m ² /days	----

Start Over Calculate

2. Click on the Shelf Life Calculation tab.

3. Choose Determine WVTR for desired shelf life from the available radio buttons

Shelf Life

Home | Shelf Life Calculations | Multiple Package WVTR | Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☐ Predict Shelf Life ☐ Determine Water Activity ☒ Determine WVTR for desired Shelf Life

Please fill in below fields [Import Excel](#) **Add slope, DLP coefficients or .isotherm file**

Desired Shelf Life (days) 00
WVTR Testing Temp (°C) 00
WVTR Testing Humidity (%) 00
Storage Humidity (%) 00
Ambient Temperature (°C) 00
Atmospheric Pressure (kPa) 00
Surface Area of Packaging (m²) 00
Total Mass (g) 00
Initial Aw 00
Critical Aw that Ends Shelf Life 00

[Save to Excel](#)

[Start Over](#) [Calculate](#)

Results

WVTR

0.00

Permeance

0.00

Convert WVTR Units

g/100in²/days	----
g/m²/days	----

4. Enter the required values in order to determine WVTR.

- Enter the temperature and relative humidity you expect would be used to determine WVTR of your packaging. This value should be obtainable from any packaging manufacturer, but typical conditions are 37.7°C and 90% Relative Humidity. The WVTR testing temperature and humidity are needed to convert Permeance, which is calculated using first principles models, into WVTR, which is not a fundamental value.
- You must enter the data for each of the data fields on this screen
 - Desired Shelf Life, enter the number of days of shelf life desired
 - Atmospheric Pressure - typically assume 100 kPa
 - Total Mass of sample in the package in grams
 - Ambient temperature or storage temperature- (the highest temperature at which the product will be stored)
 - Surface Area of packaging (total of all exposure sides) (m²)
 - Storage Humidity - storage relative humidity in percent (0-100), not decimal (.01-1.0), form (the highest humidity at which the product will be stored)
 - Initial aw of sample when placed in the package
 - Critical Water Activity that Ends Shelf Life - The critical water activity will have been determined using other experimentation.
- The isotherm slope is needed for the calculations. You may choose whether to manually enter the slope or DLP coefficients, or load an isotherm containing that data. A manual slope may be obtained from simple linear regression on existing isotherm data and entered as g/g. A more accurate slope can be determined using

the DLP isotherm model. The DLP coefficients can either be entered manually or provided by a .isotherm file. To choose an isotherm option, simply select import an isotherm from the dropdown on the left, then the import wizard will be generated, select the relevant file and import it.

4. After you have finished entering all the required data, click the Calculate button at the bottom. The resulting WVTR and Permeance will display in the "WVTR" and "Permeance" fields at the right under the "Results" section.

1.2.3.2 Multiple Package WVTR

This section allows users to calculate the cumulative WVTR for multiple layers of packaging. To access this tool follow these steps.

Steps

1. Navigate to the shelf life page by selecting the Shelf Life option in the side panel

AQUALAB Moisture Analysis Toolkit

Shelf Life

Home | Shelf Life Calculations | Multiple Package WVTR | Chemical Stability

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☒ Predict Shelf Life ☐ Determine Water Activity ☐ Determine WVTR for desired Shelf Life

Please fill in below fields [Import Excel](#) **Add slope, DLP coefficients or .isotherm file**

WVTR (g/m²/days) 00 Slope from Isotherm in g/g

WVTR Testing Temp (°C) 00

WVTR Testing Humidity (%) 00

Humidity of Air (%) 00

Ambient Temperature (°C) 00

Atmospheric Pressure (kPa) 00

Surface Area of Packaging (m²) 00

Total Mass (g) 00

Initial Aw 00

Critical Aw that ends Self Life 00

[Save to Excel](#)

[Start Over](#) [Calculate](#)

Results

Predicted Shelf Life Days

0.00

Convert WVTR Units

g/100in²/days	----
g/m²/days	----

2. Select the Multiple package WVTR tab in the page.

The screenshot shows the AQUALAB Moisture Analysis Toolkit interface. The main header is "Shelf Life". On the left is a sidebar with icons for Home, Analysis, Shelf Life (selected), Formulation, Temp Views, Settings, and Help. At the top of the main area are three tabs: "Shelf Life Calculations", "Multiple Package WVTR" (highlighted with a red box), and "Chemical Stability". Below the tabs is a description: "Calculate the cumulative Water Vapor Transmission Rate (WVTR) for multiple layers of packaging." The "Packages" section contains a table with 10 rows, each with an "Enter Name" field and a "WVTR (g/m²/days)" field. Above the table are "Import Excel" and "Save to Excel" buttons. On the right, the "Results" section shows "Cumulative WVTR (g/m²/day)" as 0.00. Below this is a "Convert WVTR Units" section with two rows: "g/100in²/days" and "g/m²/days", both with "----" in the adjacent field.

3. Enter the name and WVTR of the packages, as the details are entered the cumulative WVTR is calculated in real time.

1.2.3.3 Chemical Stability

This component calculates shelf life from a chemical change based on water activity and temperature using the arrhenius equation. To use this tool follow these steps.

Steps

1. Navigate to the shelf life page by selecting the Shelf Life option in the side panel

AQUALAB Moisture Analysis Toolkit

Shelf Life

Home | Analysis | **Shelf Life** | Formulation | Temp Views | Settings | Help

Predict Shelf Life based on packaging, the expected storage conditions, and the unique moisture properties of a product.

☒ Predict Shelf Life ☐ Determine Water Activity ☐ Determine WVTR for desired Shelf Life

Please fill in below fields [Import Excel](#)

WVTR (g/m ² /days)	00
WVTR Testing Temp (°C)	00
WVTR Testing Humidity (%)	00
Humidity of Air (%)	00
Ambient Temperature (°C)	00
Atmospheric Pressure (kPa)	00
Surface Area of Packaging (m ²)	00
Total Mass (g)	00
Initial Aw	00
Critical Aw that ends Self Life	00

[Save to Excel](#)

Add slope, DLP coefficients or .isotherm file

Slope from Isotherm in g/g

Results

Predicted Shelf Life Days

0.00

Convert WVTR Units

g/100in ² /days	----
g/m ² /days	----

[Start Over](#) [Calculate](#)

2.

Select the Chemical Stability tab in the page.

AQUALAB Moisture Analysis Toolkit

Shelf Life

Home | Analysis | Shelf Life | Formulation | Temp Views | Settings | Help

Calculate a shelf life from a chemical change based on water activity and temperature using the Arrhenius equation.
Input independent study results for a minimum of 4 conditions (2 water activities and 2 temperatures).
Select the correct Kinetic Model to produce the best linear regression fit to the experimental data. Q10 is the factor to adjust the shelf life for every 10°C change in temperature.
Qa is the factor to adjust the shelf life for every 0.10 change in water activity.

Enter collected data [Import Excel](#) [Save to Excel](#)

Aw	Temp	Action

Temp. of Interest: 00 °C Aw of Interest: 00 Amount left at End of Shelf Life: 00

[Start Over](#) [Calculate](#)

Calculated Results Kinetic Model: Zero Order

Shelf Life (Days) Q10 Qa

0 0.0 0.0

In (Amount)

Time (days)

Exclude AW Temperature Regression

<input type="checkbox"/>			
<input type="checkbox"/>			
<input type="checkbox"/>			
<input type="checkbox"/>			

3. Input independent study results for a minimum of 4 conditions (2 water activities and 2 temperatures)

4. After you have finished entering all the required data, click the Calculate button at the bottom.

5. Select the correct kinetic model to produce the best linear regression fit to the experiment data.

The results shall contain:

- Shelf Life in Days
- Q10 - The factor to adjust the shelf life for every 10°C change in temperature
- Qa - The factor to adjust the shelf life for every 0.10 change in water activity.
- Graph of the regression lines for each corresponding pair of Aw and temperature.
- Table of details
 - Aw - Water Activity (input data)
 - Temperature (input data)
 - Regression
 - R-Squared - An indication of the goodness of fit of time and Amount under a given Aw and temperature condition.

1.2.4 Formulation

1.2.4.1 Water Activity Prediction

This is the component the user will mostly interact with when estimating the water activity (A_w) of a formulation. It is used to calculate the water activity or the necessary amount of humectant for desired water activity. To use this tool follow these steps.

Steps

1. Navigate to the formulation page by selecting the Formulation option in the side panel.

AQUALAB Moisture Analysis Toolkit

Formulation

Home

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Water Activity Prediction **Ingredient Mixing**

Calculate the effect on the water activity or the necessary amount of a humectant for a desired water activity.
By Humectant (Norrish) uses the Norrish equation to model the water activity from the interaction of water and a humectant in a system.
By Ingredient (Grover) uses ingredient classifications to determine the effect on water activity.
By Recipe can be performed for multicomponent systems using Ross or Grover equations.

☒ By Humectant (Norrish) ☐ By Ingredient (Grover) ☐ By Recipe

Name of Humectant
Alanine

Predict Water Activity

Amount of Solid: 0 g Amount of Water: 0 g **Calculate**

Calculate Humectant to Add

Amount of Water: 0 g Current: 0 Desired Aw: 0 **Calculate**

Results

Water Activity
0.00

Humectant to Add g
0.00

2. Select the Water Activity Prediction tab on the page.

AQUALAB Moisture Analysis Toolkit

Formulation

Home

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Water Activity Prediction

Ingredient Mixing

Calculate the effect on the water activity or the necessary amount of a humectant for a desired water activity.
By Humectant (Norrish) uses the Norrish equation to model the water activity from the interaction of water and a humectant in a system.
By Ingredient (Grover) uses ingredient classifications to determine the effect on water activity.
By Recipe can be performed for multicomponent systems using Ross or Grover equations.

☒ By Humectant (Norrish)

☐ By Ingredient (Grover)

☐ By Recipe

Name of Humectant

Alanine

Predict Water Activity

Amount of Solid

0g

Amount of Water

0g

Calculate

Calculate Humectant to Add

Amount of Water

0g

Current

0

Desired Aw

0

Calculate

Results

Water Activity

0.00

Humectant to Add

g

0.00

3. Choose one of the available prediction methods by selecting the relevant radio button.

The screenshot shows the 'Formulation' tab of the AQUALAB Moisture Analysis Toolkit. The interface includes a sidebar with navigation links: Home, Analysis, Shelf Life, Formulation (active), Temp Views, Settings, and Help. The main content area has two tabs: 'Water Activity Prediction' (selected) and 'Ingredient Mixing'. Below the tabs, a red box highlights three radio buttons: 'By Humectant (Norrish)' (selected), 'By Ingredient (Grover)', and 'By Recipe'. Below these, there is a dropdown for 'Name of Humectant' set to 'Alanine'. The 'Predict Water Activity' section has input fields for 'Amount of Solid' (0 g) and 'Amount of Water' (0 g), with a 'Calculate' button. The 'Calculate Humectant to Add' section has input fields for 'Amount of Water' (0 g), 'Current' (0), and 'Desired Aw' (0), with a 'Calculate' button. On the right, the 'Results' section displays 'Water Activity' as 0.00 and 'Humectant to Add' as 0.00 g.

Water Activity Prediction Methods

The Water Activity Prediction tool allows you to use three different methods:

- By Humectant (Norrish)
- By Ingredient
- The amount of a humectant to add to an existing formulation to lower water activity to a desired point.

By Humectant (Norrish)

Home

Analysis

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Formulation

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Water Activity Prediction

Ingredient Mixing

Calculate the effect on the water activity or the necessary amount of a humectant for a desired water activity.
 By Humectant (Norrish) uses the Norrish equation to model the water activity from the interaction of water and a humectant in a system.
 By Ingredient (Grover) uses ingredient classifications to determine the effect on water activity.
 By Recipe can be performed for multicomponent systems using Ross or Grover equations.

☒ By Humectant (Norrish)
 ☐ By Ingredient (Grover)
 ☐ By Recipe

Name of Humectant
 Alanine

Predict Water Activity

Amount of Solid
 0 g

Amount of Water
 0 g

Calculate

Calculate Humectant to Add

Amount of Water
 0 g

Current
 0

Desired Aw
 0

Calculate

Results

Water Activity

0.00

Humectant to Add

0.00 g

This method uses the Norrish equation to model the water activity from the interaction of water and a humectant in a system. The Norrish equation (Norrish, 1966) is the most common prediction equation used to calculate the water activity of the individual ingredients for use in the Ross Equation. This equation uses the Hildebrand and Scott assumptions and shows that

$$a_w = X_w [e^{(KX_s^2)}]$$

Where X_w = mole fraction of water, X_s = mole fraction of solute, and K is the empirical constant for the solute. The mole fraction of water and solute are determined based on the assumption that the solute is dissolved in all of the water in the product. The advantage of the Norrish equation is the wide availability of k values for common humectants, but it is limited to just binary solutions

1. Predict Water Activity

Using the By humectant (Norrish) option to predict water activity you may calculate the water activity of a binary solute in water solution based on the amount of solid and water present. To do this:

1. Select the humectant you would like to use from the drop down list.
2. Enter the amount of solute (in pounds, or grams)
3. Enter the amount of water (in pounds, or grams)
4. Click "Calculate" to display the resulting water activity.


2. Calculate Humectant to Add


Using the By Humectant (Norrish) option to calculate the humectant to add you may calculate the amount of humectant needed to lower water activity to a desired point. To use this tool, do the following:


1. Select a humectant you would like to use by selecting it in the dropdown menu (default: Alaine)
2. Enter the amount of water (pounds or grams) total in your product.
3. Enter the Current water activity of your product.
4. Enter the Desired water activity of your product.
5. Click "Calculate."


The amount of Humectant to add in order to reach the desired water activity will be displayed. You may select this value in grams or pounds.


By Ingredient (Grover)


 Home


 Analysis

 Shelf Life

 Formulation

 Temp Views

 Settings

 Help

Water Activity Prediction

Ingredient Mixing

Calculate the effect on the water activity or the necessary amount of a humectant for a desired water activity.
By Humectant (Norrish) uses the Norrish equation to model the water activity from the interaction of water and a humectant in a system.
By Ingredient (Grover) uses ingredient classifications to determine the effect on water activity.
By Recipe can be performed for multicomponent systems using Ross or Grover equations.

☐ By Humectant (Norrish) ☒ By Ingredient (Grover) ☐ By Recipe

Name of Ingredient (type)
Acids

Predict Water Activity

Amount of Solid
0 g

Amount of Water
0 g

Calculate

Calculate Humectant to Add

Amount of Water
0 g

Current
0

Desired Aw
0

Calculate

Results

Water Activity
0.00

Humectant to Add
g
0.00

This method uses ingredient classification to determine effect on water activity based on the Grover equation. The Grover equation (1947) was empirically derived using data from studies on confectionaries. It takes the form

$$a_w = 1.04 - 0.1(E^\circ) + 0.0045(E^\circ)^2$$

where $E^\circ = \sum (E_i / W_i)$, E_i is a constant for the solute and W_i is the total moisture content in grams of water per gram of ingredient i (Grover, 1947). Its value lies in being able to calculate the water activity of both binary and more complex solutions. It also can be used to estimate the amount of solute to add to achieve a desired water activity. Its limitations are that it can only be used for a limited number of ingredients specific to the confection market. To use the Grover equation, simply choose the desired tool.

1. Predict Water Activity

The screenshot shows the 'Formulation' software interface. On the left is a sidebar with navigation icons for Home, Analysis, Shelf Life, Formulation (highlighted), Temp Views, Settings, and Help. The main area has a header 'Formulation' and two tabs: 'Water Activity Prediction' (active) and 'Ingredient Mixing'. Below the tabs, there is explanatory text about the calculation methods and three radio buttons: 'By Humectant (Norrish)', 'By Ingredient (Grover)' (selected), and 'By Recipe'. A red rectangle highlights the 'Predict Water Activity' section, which includes a dropdown for 'Name of Ingredient (type)' set to 'Acids', input fields for 'Amount of Solid' and 'Amount of Water' (both set to 0 g), and a 'Calculate' button. Below this is the 'Calculate Humectant to Add' section with input fields for 'Amount of Water' (0 g), 'Current' (0), and 'Desired Aw' (0), and another 'Calculate' button. On the right, a 'Results' panel displays 'Water Activity' as 0.00 and 'Humectant to Add' as 0.00 g.

Selecting the By Ingredient (Grover) radio button will open up this tool where you may calculate the water activity of a binary solute in water solution based on the amount of solid and water present. To do this :

1. Select the ingredient you would like to use from the drop down list.
2. Enter the amount of solute (in pounds, or grams)
3. Enter the amount of water (in pounds, or grams)
4. Click "Calculate" to display the resulting water activity.

2. Prediction of Added Solute to Lower Water Activity

The screenshot shows the 'Formulation' software interface. On the left is a sidebar with icons for Home, Analysis, Shelf Life, Formulation, Temp Views, Settings, and Help. The main area has two tabs: 'Water Activity Prediction' (selected) and 'Ingredient Mixing'. Below the tabs, there is explanatory text about the calculation methods. Three radio buttons are present: 'By Humectant (Norrish)', 'By Ingredient (Grover)' (selected), and 'By Recipe'. Below these, a dropdown menu for 'Name of Ingredient (type)' is set to 'Acids'. The 'Predict Water Activity' section has input fields for 'Amount of Solid' and 'Amount of Water', both set to 0, with a 'Calculate' button. The 'Calculate Humectant to Add' section has input fields for 'Amount of Water' (0), 'Current' (0), and 'Desired Aw' (0), with a 'Calculate' button. On the right, the 'Results' section displays 'Water Activity' as 0.00 and 'Humectant to Add' as 0.00.

Selecting the By Ingredient(grover) radio button will open up the page to use this tool where you may calculate the amount of humectant needed to lower water activity to a desired point. To use this tool, do the following:

1. Select an ingredient you would like to use by selecting it in the dropdown menu (default: Acids)
2. Enter the amount of water (pounds or grams) total in your product.
3. Enter the Current water activity of your product.
4. Enter the Desired water activity of your product.
5. Click "Calculate."

The amount of Humectant to add in order to reach the desired water activity will be displayed. You may select this value in grams or pounds.

By Recipe

Calculation Method - Grover

This can be performed on multicomponent systems and uses the Grover equation. The Grover equation (1947) was empirically derived using data from studies on confectionaries. It takes the form

$$a_w = 1.04 - 0.1(E^o) + 0.0045(E^o)^2$$

where $E^o = \sum (E_i / W_i)$, E_i is a constant for the solute and W_i is the total moisture content in grams of water per gram of ingredient i (Grover, 1947). Its value lies in being able to calculate the water activity of both binary and more complex solutions. It also can be used to estimate the amount of solute to add to achieve a desired water activity. Its limitations are that it can only be used for a limited number of ingredients specific to the confection market.

Water Activity Prediction recipe

Selecting the By Recipe radio button and Grover in the proceeding calculation method dropdown will open up this page.

In order to use this tool, do the following:

1. Choose an ingredient from the "Add Ingredient (type)" dropdown on the right bottom. This will allow you to choose an ingredient (remember that the ingredient options available are limited to those commonly found in confectionery products). Then enter the amount of the ingredient (solid) and the amount of water in the recipe. The other values are automatically calculated based on the entered solid and the water.
2. Continue adding ingredients as desired.
3. When you are done adding ingredients, click "Calculate" to display the totals.

Should you wish to edit an ingredient, simply select the value of the ingredient to be changed and change as needed, and if you wish to delete an ingredient press the "Delete" icon under the action tab of the relevant ingredient record.

Calculation Method - Ross

The best equation for predicting the water activity of a multi-component product is the Ross equation (Ross, 1975). This equation assumes that each solute (or ingredient) behaves independently and dissolves or interact with all of the water in the system. The relationship is based on the Gibbs-Duhem relationship and shows that:

$$a_w = a_w \text{ initial} \times a_{w1} \times a_{w2} \times \dots a_{wi}$$

Where a_w is the final water activity, $a_w \text{ initial}$ is the initial a_w before adding solute i , and a_{wi} is the a_w the solute would have if it dissolved in all the water. The advantage of this equation is its ease of use and ability to handle multiple ingredients. Its disadvantage is that it requires determination of the a_w of each component separately using another a_w prediction equation or using the components' sorption isotherm data if available. The only tool for the Ross equation is the prediction of the water activity of a recipe, but it is also used in

conjunction with the other 2 equations to determine how much humectant to add to lower water activity:

Water Activity Prediction Recipe

The screenshot shows the 'Formulation' software interface. The left sidebar contains navigation icons for Home, Analysis, Shelf Life, Formulation (highlighted), Temp Views, Settings, and Help. The main area is titled 'Formulation' and has two tabs: 'Water Activity Prediction' (selected) and 'Ingredient Mixing'. Below the tabs, there is a descriptive text block and three radio buttons: 'By Humectant (Norrish)', 'By Ingredient (Grover)', and 'By Recipe' (selected). A 'Calculation Method' dropdown menu is set to 'Ross'. Below this is a table titled 'Enter all ingredient data by Ingredient type' with columns: Name Ingredient, Solid (g), Water (g), Water/Solid (g/g), Aw, Source, and Action. An 'Import Excel' link is to the right of the table. At the bottom of the main area are buttons for 'Enter Ingredient', 'Start Over', and 'Calculate'. On the right side, there is a 'Results' section with a 'Water Activity' label and a blue bar representing the calculated value.

Formulation

Home Analysis Shelf Life **Formulation** Temp Views Settings Help

Water Activity Prediction Ingredient Mixing

Calculate the effect on the water activity or the necessary amount of a humectant for a desired water activity.
By Humectant (Norrish) uses the Norrish equation to model the water activity from the interaction of water and a humectant in a system.
By Ingredient (Grover) uses ingredient classifications to determine the effect on water activity.
By Recipe can be performed for multicomponent systems using Ross or Grover equations.

☐ By Humectant (Norrish) ☐ By Ingredient (Grover) ☒ By Recipe

Calculation Method
Ross

Enter all ingredient data by Ingredient type [Import Excel](#)

Name Ingredient	Solid (g)	Water (g)	Water/Solid (g/g)	Aw	Source	Action

[Enter Ingredient](#) [Save to Excel](#)

[Start Over](#) [Calculate](#)

Results

Water Activity

Selecting the By Recipe radio button and Ross in the proceeding calculation method dropdown will open up this page.

In order to use this tool, do the following:

1. Click the "Enter Ingredient" button on the right. This will create a new record on the table. Then enter the name of the ingredient, the amount of solid and water in the recipe, the water activity of the ingredient as determined using the other equations or an isotherm, and indicate the source as Norrish, Grover, Isotherm, or other. The Water/Solid will be automatically calculated based on the entered solid and water
2. Continue adding ingredients as desired.
3. click "Calculate." The total water activity will be displayed for you.

Should you wish to edit an ingredient, simply select the value of the ingredient to be changed and change as needed, and if you wish to delete an ingredient press the "Delete" icon under the action tab of the relevant ingredient record.

1.2.4.2 Ingredient Mixing

This is the component the user will interact with when blending multiple ingredients to final water activity, isotherm model and final moisture content

It allows the user to calculate the resulting Aw when two or more ingredients are blended.

To use this feature follow these steps:

Steps

1. Navigate to the formulation page by selecting the Formulation option in the side panel

AQUALAB Moisture Analysis Toolkit

Home

Analysis

Shelf Life

Formulation

Temp Views

Settings

Help

Water Activity Prediction

Ingredient Mixing

Calculate the effect on the water activity or the necessary amount of a humectant for a desired water activity.
By Humectant (Norrish) uses the Norrish equation to model the water activity from the interaction of water and a humectant in a system.
By Ingredient (Grover) uses ingredient classifications to determine the effect on water activity.
By Recipe can be performed for multicomponent systems using Ross or Grover equations.

☒ By Humectant (Norrish) ☐ By Ingredient (Grover) ☐ By Recipe

Name of Humectant

Alanine

Predict Water Activity

Amount of Solid

0

g

Amount of Water

0

g

Calculate

Calculate Humectant to Add

Amount of Water

0

g

Current

0

Desired Aw

0

Calculate

Results

Water Activity

0.00

Humectant to Add

g

0.00

2. Select the Ingredient Mixing tab in the page.

AQUALAB Moisture Analysis Toolkit

Formulation

Water Activity Prediction | **Ingredient Mixing**

Mathematically blend ingredients to predict the final water activity, isotherm model, and final moisture content. Add information for the main ingredients in a prospective blend to calculate their combined moisture sorption properties.

Import Excel

Name Ingredient	File	Initial Aw	Mass(g)	Initial MC(%)	Action
Enter Ingredient					

Start Over | Calculate

Save to Excel

Calculated Results

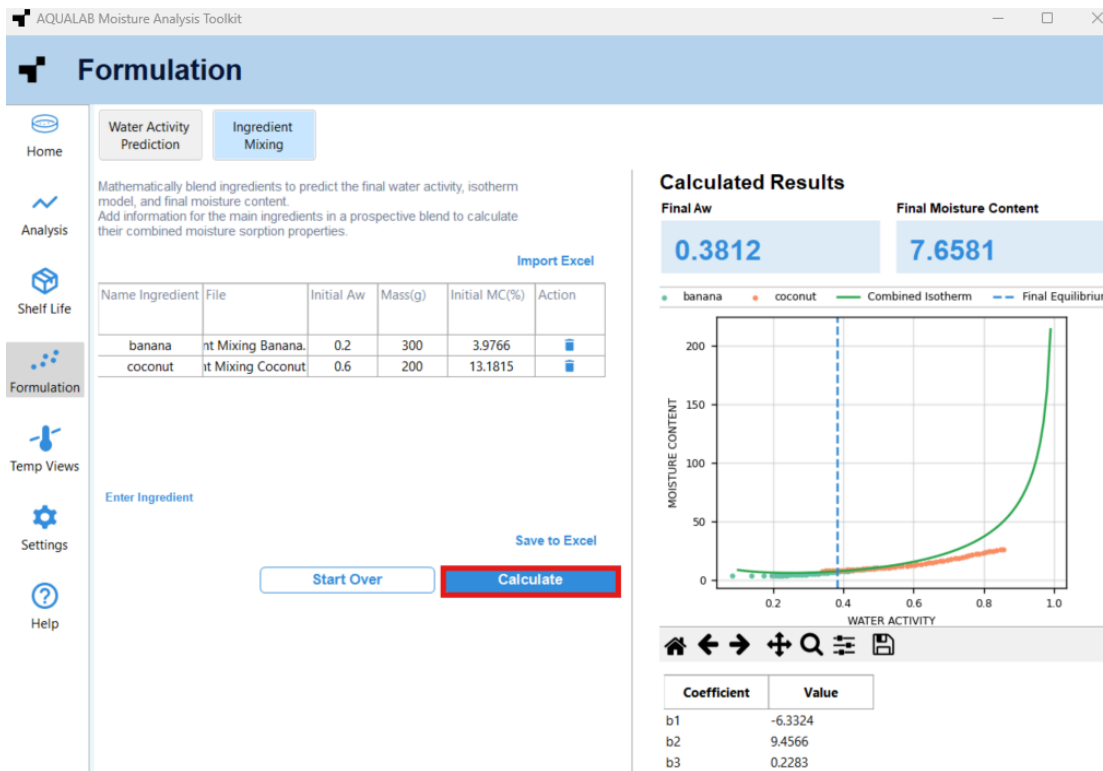
Final Aw: **0.00** | Final Moisture Content: **0.00**

Graph: A plot of Final Aw (0.0 to 1.0) vs Final Moisture Content (0.0 to 1.0).

Chart Tools: Home, Left, Right, Zoom, Pan, Save

Coefficient	Value
b1	
b2	
b3	

3. Input the necessary values or import an excel with relevant data
 - Click the Enter Ingredient button on the bottom. This will add a new record to the table.
 - In this new record, enter an ingredient name.
 - Click on the Select .isotherm button under the file dropdown to load the isotherm of this ingredient. Note that if the ingredient will gain moisture when added to the mixture, you should use an adsorption curve. If the ingredient will lose moisture, use a desorption curve.
 - Enter the "Initial Aw" -the water activity the ingredient will have when first added to the mixture.
 - Enter the Initial Moisture content in the "Initial MC (%)" field.
 - Enter the mass (in grams) that will be added to the mixture in the "Mass (g)" field.
 - Repeat the previous steps to add more ingredients.
4. Once you have finished adding ingredients, click Calculate



The graph will now display your ingredients, combined isotherm, and equilibrium water activity. The final water activity will also be displayed in the "Final Aw" field on the left, along with the ingredients final moisture content.

1.2.5 Temperature Views

1.2.5.1 RHC by Temperature

This is the component the user will interact with to estimate the critical water activity at a new temperature based on the linear relationship of temperature vs critical water activity (RHc).

To use this feature follow these steps:

1. Navigate to the temperature view page by selecting the Temp Views option in the side panel

AQUALAB Moisture Analysis Toolkit

Temperature Views

Home Analysis Shelf Life Formulation **Temp Views** Settings Help

RHc by Temperature Heat of Sorption

Estimate the critical water activity at a new temperature based on the linear relationship of temperature vs. critical water activity (RHc). Select at least two isotherm files run at different temperatures that have a critical point identified in the Analysis Tab and click Calculate.

Import Excel

Entry	Temp (°C)	RHc	Action

Add Entry

Save to Excel

Temperature to Use:

Temperature (°C) 00

Start Over Calculate

Calculated Results

RHc

0.0000

Home < > + - 🔍 📄

Temp	Est.Aw
10	
20	
30	
40	
50	

2. Select the RHc by Temperature tab on the page.

AQUALAB Moisture Analysis Toolkit

Temperature Views

Home **RHc by Temperature** Heat of Sorption

Analysis Shelf Life Formulation Temp Views Settings Help

Estimate the critical water activity at a new temperature based on the linear relationship of temperature vs. critical water activity (RHc). Select at least two isotherm files run at different temperatures that have a critical point identified in the Analysis Tab and click Calculate.

Import Excel

Entry	Temp (°C)	RHc	Action

Add Entry

Save to Excel

Temperature to Use:

Temperature (°C) 00

Start Over Calculate

Calculated Results

RHc

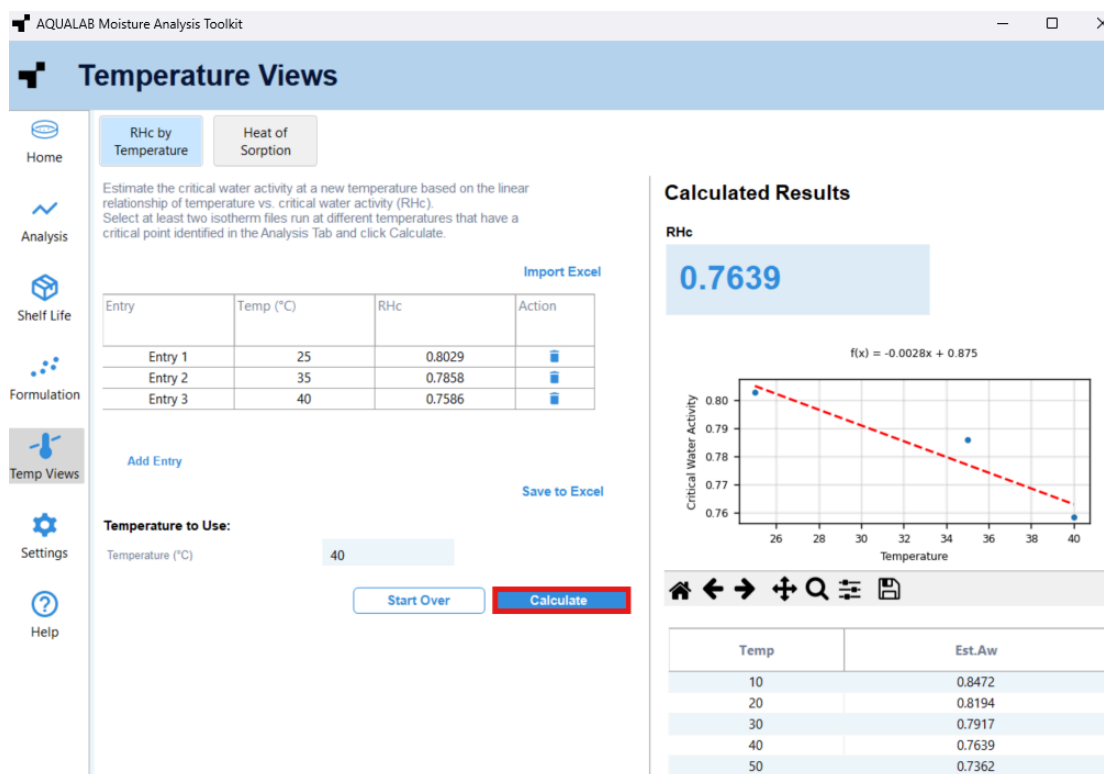
0.0000

Home < > + - 🔍 📄

Temp	Est.Aw
10	
20	
30	
40	
50	

3. Enter the temperature values and related parameters or import an excel file with required data.

4. Click Calculate to get the RHc at the specified temperature.



1.2.5.2 Heat of Sorption

This tool is used to investigate the effect of temperature on water activity at a given moisture content. This is accomplished through the Clausius-Clapeyron relationship, which is

$$\ln \frac{a_{w2}}{a_{w1}} = \frac{\Delta H}{R} \left[\frac{1}{T_1} - \frac{1}{T_2} \right]$$

where a_{w2} and a_{w1} are water activities at temperatures (K) T_2 and T_1 , respectively; ΔH is the heat of sorption in J/mol (as a function of moisture content); and R equals 8.314 J mol⁻¹ K⁻¹. The heat of sorption (ΔH) is the only unknown and must be determined empirically by regression analysis. Plotting $\ln(a_w)$ vs $1/T$ (K), the slope of the line is equal to $\Delta H / R$. Once ΔH is known, the water activity at any temperature can be determined using this equation. Determining ΔH requires a minimum of 2 water activity values recorded at 2 different temperatures on samples of common moisture content. The heat of sorption is specific to the moisture content, investigations into temperature effect must be at a common moisture content. This data can be provided by either an isotherm(s) with data collected at 2 different temperatures, or by manually entering water activity/temperature data collected on samples with equivalent moisture contents

In order to use this tool, follow these steps:

Steps

1. Navigate to the temperature view page by selecting the Temp Views option in the side panel

The screenshot shows the 'Temperature Views' page of the AQUALAB Moisture Analysis Toolkit. The interface includes a sidebar with navigation options: Home, Analysis, Shelf Life, Formulation, Temp Views (highlighted with a red box), Settings, and Help. The main content area is titled 'Temperature Views' and features two tabs: 'RHc by Temperature' (selected) and 'Heat of Sorption'. Below the tabs, a text box explains the purpose: 'Estimate the critical water activity at a new temperature based on the linear relationship of temperature vs. critical water activity (RHc). Select at least two isotherm files run at different temperatures that have a critical point identified in the Analysis Tab and click Calculate.' A table with columns 'Entry', 'Temp (°C)', 'RHc', and 'Action' is present, with an 'Import Excel' link above it. Below the table is an 'Add Entry' link. A 'Temperature to Use:' section shows a text input field with '00' and a 'Save to Excel' link. At the bottom are 'Start Over' and 'Calculate' buttons. On the right, the 'Calculated Results' section displays 'RHc' as '0.0000' and a graph of 'Critical Water Activity' vs 'Temperature'. Below the graph is a table with 'Temp' and 'Est.Aw' columns, showing values for 10, 20, 30, 40, and 50.

AQUALAB Moisture Analysis Toolkit

Temperature Views

Home Analysis Shelf Life Formulation **Temp Views** Settings Help

RHc by Temperature Heat of Sorption

Estimate the critical water activity at a new temperature based on the linear relationship of temperature vs. critical water activity (RHc). Select at least two isotherm files run at different temperatures that have a critical point identified in the Analysis Tab and click Calculate.

Import Excel

Entry	Temp (°C)	RHc	Action
-------	-----------	-----	--------

Add Entry

Save to Excel

Temperature to Use:

Temperature (°C) 00

Start Over Calculate

Calculated Results

RHc

0.0000

Critical Water Activity

Temperature

Temp	Est.Aw
10	
20	
30	
40	
50	

2. Select the Heat of Sorption tab on the page.

The screenshot shows the AQUALAB Moisture Analysis Toolkit interface. The title bar reads "AQUALAB Moisture Analysis Toolkit". The main header is "Temperature Views". On the left sidebar, there are icons for Home, Analysis, Shelf Life, Formulation, Temp Views (selected), Settings, and Help. The main content area has two tabs: "RHc by Temperature" and "Heat of Sorption" (which is highlighted with a red box). Below the tabs, there is a description: "Investigate the effect of temperature on water activity at a given moisture content by using the Clausius-Clapeyron equation. Select at least two isotherm files or two manual water activity readings at different temperatures. Once the necessary fields have inputs, press Calculate to determine the Heat of Sorption and corresponding water activity for the temperature of interest." There are two radio buttons: "Using .Isotherm files" (selected) and "Manual Temperature and Aw values". Below this is a table with columns: File, Temp (°C), Peak 1, and Action. There is an "Import Excel" button above the table. Below the table is a "Select .Isotherm" dropdown menu. To the right of the dropdown is a "Save to Excel" button. Below these are "Additional Specifications" with input fields for "Temperature (°C) of interest" (00), "Moisture Content" (00), and a dropdown for "Sorption Direction" (Adsorption). There are "Start Over" and "Calculate" buttons at the bottom. On the right side, there is a "Calculated Results" section with two boxes: "Result Heat Sorption" (0.0000) and "Predicted Water Activity" (0.0000). Below these is a graph with "Critical Water Activity" on the y-axis (0.0 to 1.0) and "Temperature" on the x-axis (0.0 to 1.0). At the bottom right, there is a toolbar with icons for home, back, forward, zoom in, zoom out, and save.

3. Choose your simulation method:

- Using .Isotherm Files — load two or more isotherm files with different temperatures.
- Manual Temperature and Aw values— enter multiple sets of Aw and temperature values manually.

AQUALAB Moisture Analysis Toolkit

Temperature Views

Home | Analysis | Shelf Life | Formulation | Temp Views | Settings | Help

RHc by Temperature | **Heat of Sorption**

Investigate the effect of temperature on water activity at a given moisture content by using the Clausius-Clapeyron equation. Select at least two isotherm files or two manual water activity readings at different temperatures. Once the necessary fields have inputs, press Calculate to determine the Heat of Sorption and corresponding water activity for the temperature of interest.

☒ Using .Isotherm files | ☐ Manual Temperature and Aw values

[Import Excel](#)

File	Temp (°C)	Peak 1	Action

Select .Isotherm

[Save to Excel](#)

Additional Specifications

Temperature (°C) of interest: 00

Moisture Content: 00

Sorption Direction: Adsorption

[Start Over](#) [Calculate](#)

Calculated Results

Result Heat Sorption 0.0000

Predicted Water Activity 0.0000

Navigation icons: Home, Back, Forward, Zoom In, Zoom Out, Print, Save

4. From there do the following based on the simulation method you choose.

Using .isotherm

AQUALAB Moisture Analysis Toolkit

Temperature Views

Home | Analysis | Shelf Life | Formulation | Temp Views | Settings | Help

RHc by Temperature | **Heat of Sorption**

Investigate the effect of temperature on water activity at a given moisture content by using the Clausius-Clapeyron equation. Select at least two isotherm files or two manual water activity readings at different temperatures. Once the necessary fields have inputs, press Calculate to determine the Heat of Sorption and corresponding water activity for the temperature of interest.

☒ Using .Isotherm files | ☐ Manual Temperature and Aw values

[Import Excel](#)

File	Temp (°C)	Peak 1	Action

Select .Isotherm

[Save to Excel](#)

Additional Specifications

Temperature (°C) of interest: 00

Moisture Content: 00

Sorption Direction: Adsorption

[Start Over](#) [Calculate](#)

Calculated Results

Result Heat Sorption 0.0000

Predicted Water Activity 0.0000

Navigation icons: Home, Back, Forward, Zoom In, Zoom Out, Print, Save

- Select the Select .isotherm dropdown and on the dropdown click select .isotherm and then select the isotherm you wish to load. This will create a record on the table. Remember that you must have isotherm data collected

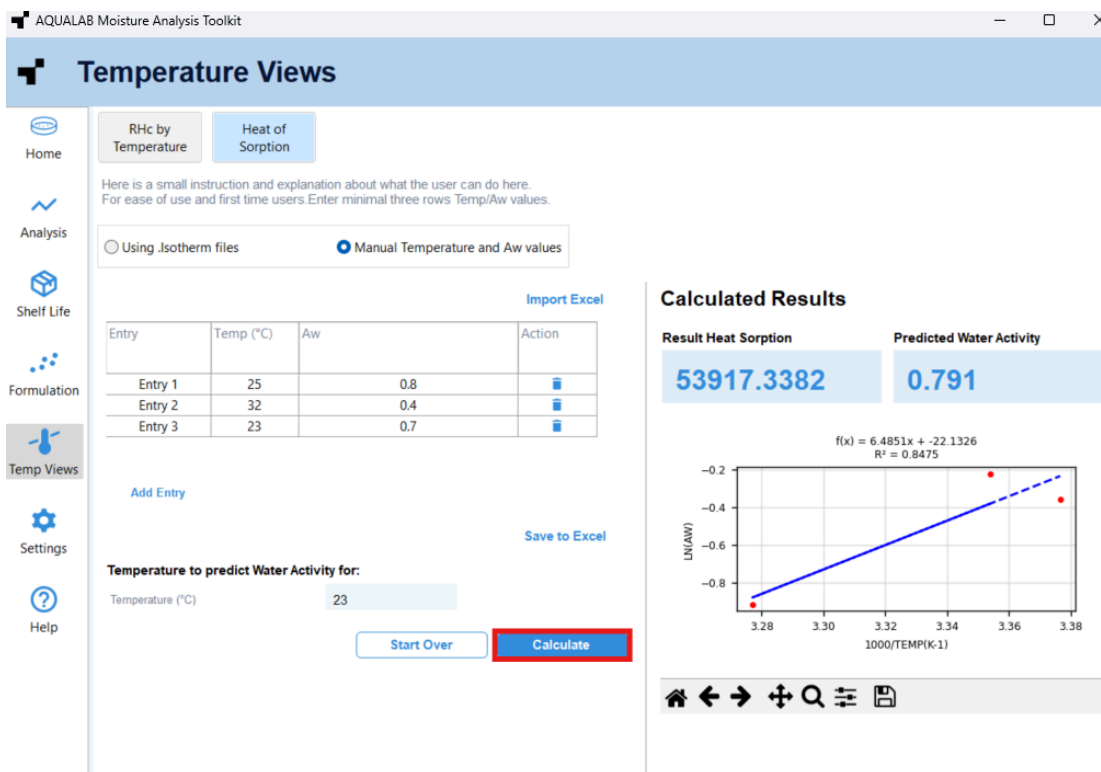
for a minimum of three temperatures. This data may be found in a single isotherm file containing isotherms conducted at different temperatures, or in different isotherm files, each conducted at different temperatures. If you need to change or delete one of the isotherms you load, you can edit or click the Delete button accordingly.

- Enter the Temperature for the corresponding file.
- Repeat the previous steps for the desired number of isotherm files
- Under the additional specification specifications section, enter the Temperature of Interest, moisture content value you wish to use and select whether you will be using Adsorption or Desorption points since the relationship will depend on the sorption direction.

Manual Temperature and Aw values

- Click the Add Entry button to the right. This will create a new record on the table.
- Type the temperature you wish to use and its associated water activity.
- Repeat the previous step, using different temperatures, until you have entered at least two temperatures. If you wish to edit, simply change the data on the record or if you wish to delete any of the temperatures, click on the delete icon under the action tab of the relevant record.
- Enter the temperature to predict water activity for.

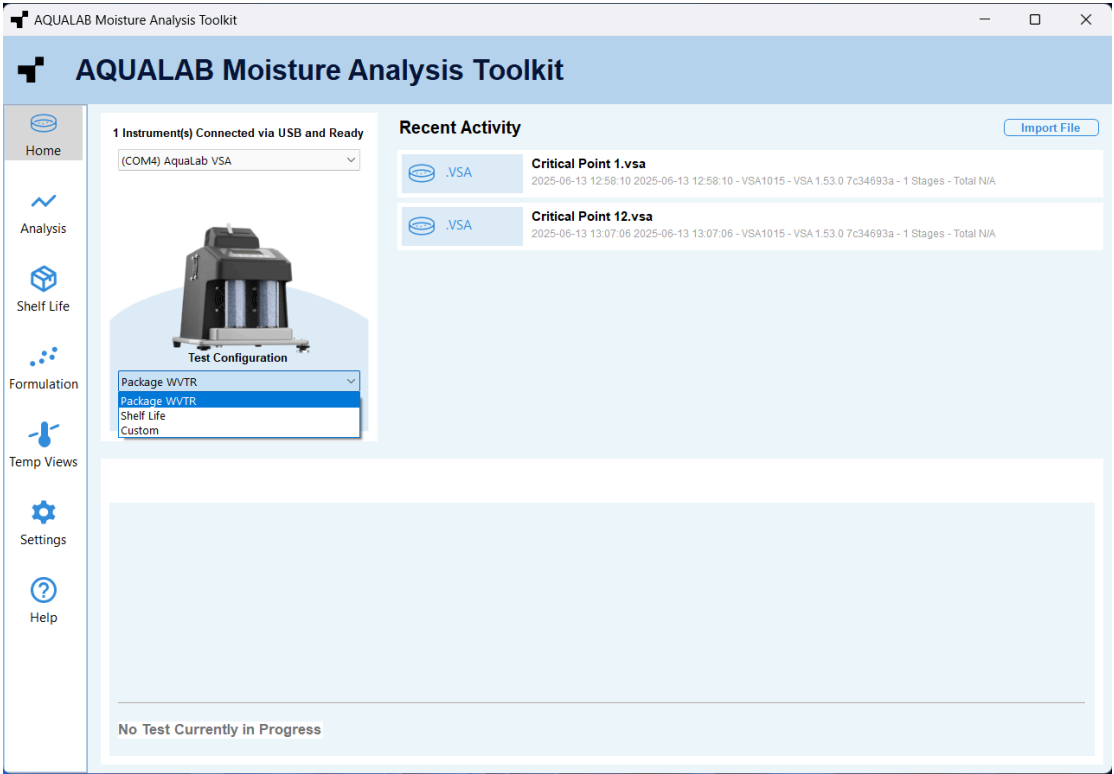
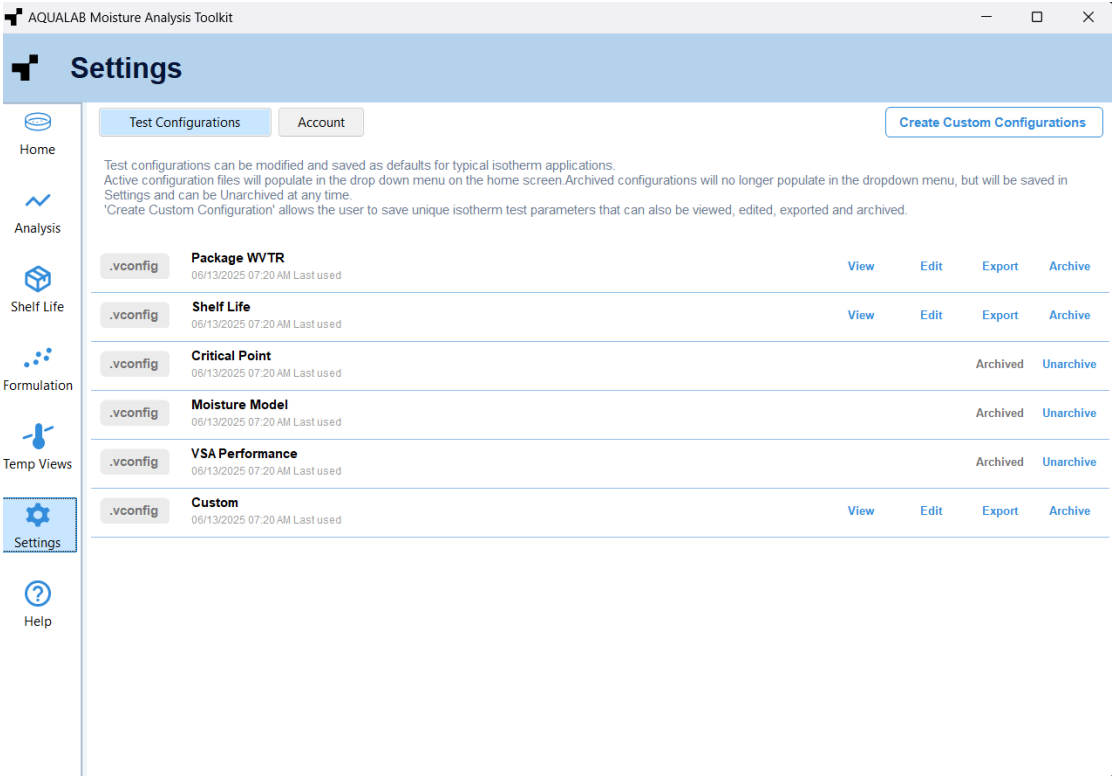
5. After you have entered the data to use, press the Calculate button, at the bottom of the screen. The resulting points will be graphed based off of the data you have entered, and the heat of Sorption and the predicted water activity for temperature of interest will be calculated and displayed under the “Results” on the left..



1.2.6 Settings

1.2.6.1 Test Configuration

This section will contain 6 test configurations by default which can be modified and saved. Active configurations files will be populated in the dropdown menu of the home screen. Archived configurations will no longer populate in the dropdown menu but will be available in the settings and can be unarchived at any time.



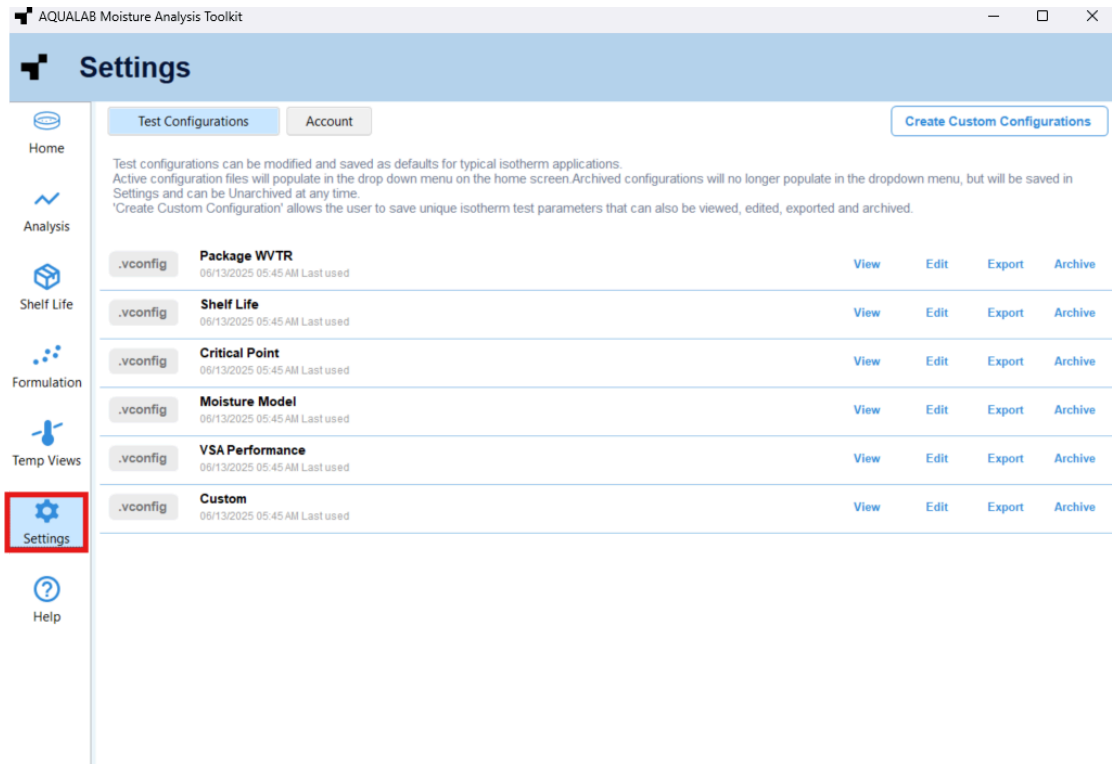
Create Custom Configurations

This feature allows the user to save unique isotherm test parameters that can be viewed, edited, exported and archived.

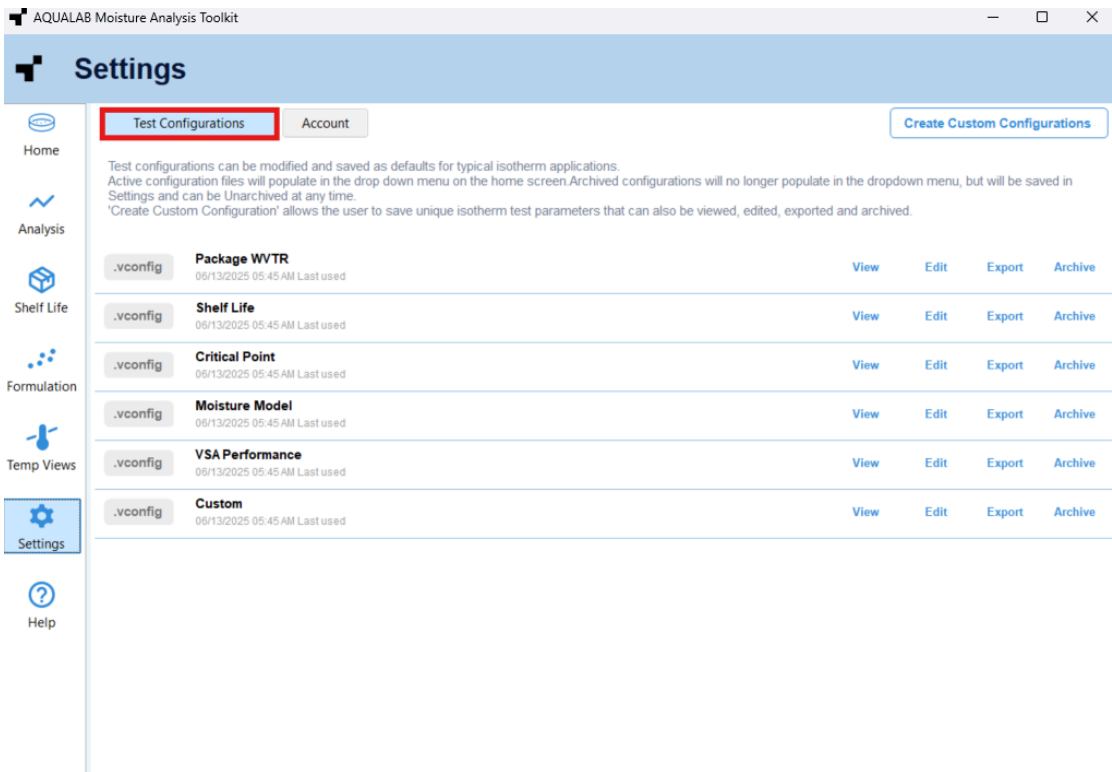
To create custom configurations:

Steps

1. Navigate to the settings page by selecting the Settings option in the side panel



2. Select the Test Configurations tab on the page.



3. Click on the Create Custom Configuration button on the top right corner of the page, then a dialog box will open up.

AQUALAB Moisture Analysis Toolkit

Settings

Home

Analysis

Shelf Life

Formulation

Temp Views

Settings

Help

Test Configurations

Account

Create Custom Configurations

Test configurations can be modified and saved as defaults for typical isotherm applications. Active configuration files will populate in the drop down menu on the home screen. Archived configurations will no longer populate in the dropdown menu, but will be saved in Settings and can be Unarchived at any time. 'Create Custom Configuration' allows the user to save unique isotherm test parameters that can also be viewed, edited, exported and archived.

.vconfig	Package WVTR	06/12/2025 09:34 AM Last used	View	Edit	Export	Archive
.vconfig	Shelf Life	06/12/2025 09:34 AM Last used	View	Edit	Export	Archive
.vconfig	Critical Point	06/12/2025 09:34 AM Last used	View	Edit	Export	Archive
.vconfig	Moisture Model	06/12/2025 09:34 AM Last used	View	Edit	Export	Archive
.vconfig	VSA Performance	06/12/2025 09:34 AM Last used	View	Edit	Export	Archive
.vconfig	Custom	06/12/2025 09:34 AM Last used	View	Edit	Export	Archive

Create Custom Configuration

New Test Configuration

Title

My own test config

Stages

Add | Remove

1. DDI, 0.1000 aw, 0.9000 aw

Stage Type

DDI

Start (aw)

0.1

Final (aw)

0.9

Temperature (°C)

25.0

Resolution (aw)

0.01

Flow (ml/min)

100.0

Timeout

0

Loop

On

Current

Current

Off

Off

Minutes

Off

Off

Cancel

Save Configuration

4. Define configuration and stages with required values and add stages as needed.

- A name for the test can be provided by changing the default name, a default name will be automatically populated in the space.
- Use the stage section to setup each stage of the isotherm test. A stage is used to adjust the isotherm settings for an individual sample (up to 20 stages). Each stage is setup with the isotherm method (DDI or DVS) and the settings for that portion of the isotherm. Once a stage is created, it can be modified or deleted anytime. (A default stage is available on creating of the configuration)
- To edit any stage, simply select it from the list. To change the order of stages, select the stage to move and use the up and down arrows to change the order of that stage. Use the Add button to add an additional stage and the Remove button to remove a stage.
- A group of settings for each stage type are available. Select the stage type as either Dynamic Dewpoint Isotherm (DDI) or Dynamic Vapor Sorption (DVS). DDI will create a dynamic isotherm and DVS will create a static or equilibrium isotherm. The other choices will adjust based on which method is selected.
- The settings shall differ based on the selected stage type
 - For DDI method

Create Custom Configuration

×

New Test Configuration

Title

My own test config

Stages

Add

Remove

▲

▼

1. DDI, 0.1000 aw, 0.9000 aw

Stage Type

DDI

▼

Start (aw)

0.1

☐ Current

Final (aw)

0.90

☐ Current

Temperature (°C)

25.00

☐ Off

Resolution (aw)

0.01

Flow (ml/min)

100.0

Timeout

Minutes

▼

☒ Off

Loop

☒ On

☐ Off

Cancel

Save Configuration

- For the initial water activity (Start (aw)), enter the desired starting water activity. Any value between 0.03 and 0.95 aw can be chosen including "current". Choosing "current" means that the stage will start at the as-is aw of the sample.

- Enter the desired final water activity (Final (aw)). Any value between 0.03 and 0.95 aw can be chosen including current (see "current" definition above). Selecting a final aw that is lower than the starting aw will result in desorption, while selecting a final aw higher than the starting aw will result in adsorption.
 - Enter the desired testing temperature in the space labeled temperature. Any temperature between 10-60° C can be chosen. Each stage can run at a unique temperature.
 - Enter the desired aw resolution. Any value between 0.001 and 1.0 aw can be chosen. The resolution for DDI determines the target aw resolution. Setting a larger resolution will make the test faster, but will decrease the test resolution. A DDI step of 0.01 aw is recommended.
 - Enter the desired flow rate in the space provided. Any value between 10-163 ml/min can be selected. Higher flow rates will speed up the test, but may result in lower data resolution and non-equilibrium conditions. The default value of 100 ml/min is suitable for most products.
 - To place a time limit on the test length, enter a value in the timeout space provided. Any value between 5.0 min to 30 days can be selected. The timeout determines the maximum time allotted to move from the starting aw to the final aw (DDI only) and is optional. The default value is off, which means there is no timeout value.
 - Choose "Loop On" to have the isotherm automatically return to the start aw (with the same settings) once the final aw has been achieved. This would create both an adsorption and desorption curve (or vice versa depending on the starting direction).
- For DVS Method

New Test Configuration

Title

My own test config

Stages

Add | Remove ▲ ▼

1. DDI, 0.1000 aw, 0.9000 aw

2. DVS, 0.1000 aw, current aw

Stage Type

DVS ▼

Start (aw)

0.1

☐ Current

Final (aw)

☒ Current

Temperature (°C)

25.0

☐ Off

Step (aw)

0.0

Trigger (%/hr)

0.0

1 event ▼

Timeout

Minutes ▼

☒ Off

Loop

☒ On ☐ Off

Cancel

Save Configuration

- For the initial water activity (start (aw)), enter the desired starting water activity. Any value between 0.03 and 0.95 aw can be chosen including "current". Choosing "current" means that the stage will start at the as-is aw of the sample.
- Enter the desired final water activity(final(aw)). Again, any value between 0.03 and 0.95 aw can be chosen including current (see "current" definition above). Selecting a final aw that is lower than the starting aw will result in desorption, while selecting a final aw higher than the starting aw will result in adsorption.
- Enter the desired testing temperature in the space labeled temperature. Any temperature between 10-60°C can be chosen. Each stage can run at a unique temperature.
- Enter the step (aw) this indicates that after the weight is equilibrated, the current humidity is incremented/ decremented by this step. This value can be between the range of 0.003 to 1.000 aw
- To set a trigger value that indicates equilibrium, enter a value in the space provided. The trigger can be shut off or be any value between 0.001-1% Δ wt/hr. The trigger value represents an acceptable change in mass per change in time to indicate equilibrium for a given step.

You can also choose the number of readings or events that must meet the trigger value to achieve equilibration. For example, choosing 3 means that in order for a step to have reached equilibrium, 3 weight change readings in row must be less than the set trigger value. Any value between 1 to 10 can be chosen. Setting a higher trigger value and a lower number of events will make the test faster, but may not result in complete equilibrium. If the trigger is turned off, the sample will be held at each step for the time indicated by the timeout setting.

- To place a time limit on the test length (timeout), enter a value in the space provided. Any value between 5.0 min to 30 days can be selected. The timeout determines the maximum time allotted for each aw step NOT the time from starting aw to final aw. The default value is off, which means there is no timeout value and only the trigger value will determine the end of step. If both a trigger value and timeout value are set, whichever is reached first will determine the end of the step.
- Choose "Loop On" to have the isotherm automatically return to the start aw (with the same settings) once the final aw has been achieved. This would create both an adsorption and desorption curve (or vice versa depending on the starting direction).

5. Click Save Configuration

Create Custom Configuration ×

New Test Configuration

Title

My own test config

Stages Add | Remove ▲ ▼

1. DDI, 0.1000 aw, 0.9000 aw
2. DVS, 0.1000 aw, current aw

Stage Type DDI ▼

Start (aw) 0.1 ☐ Current

Final (aw) 0.90 ☐ Current

Temperature (°C) 25.00 ☐ Off

Resolution (aw) 0.01

Flow (ml/min) 100.0

Timeout 0 Minutes ▼ ☒ Off

Loop ☒ On ☐ Off

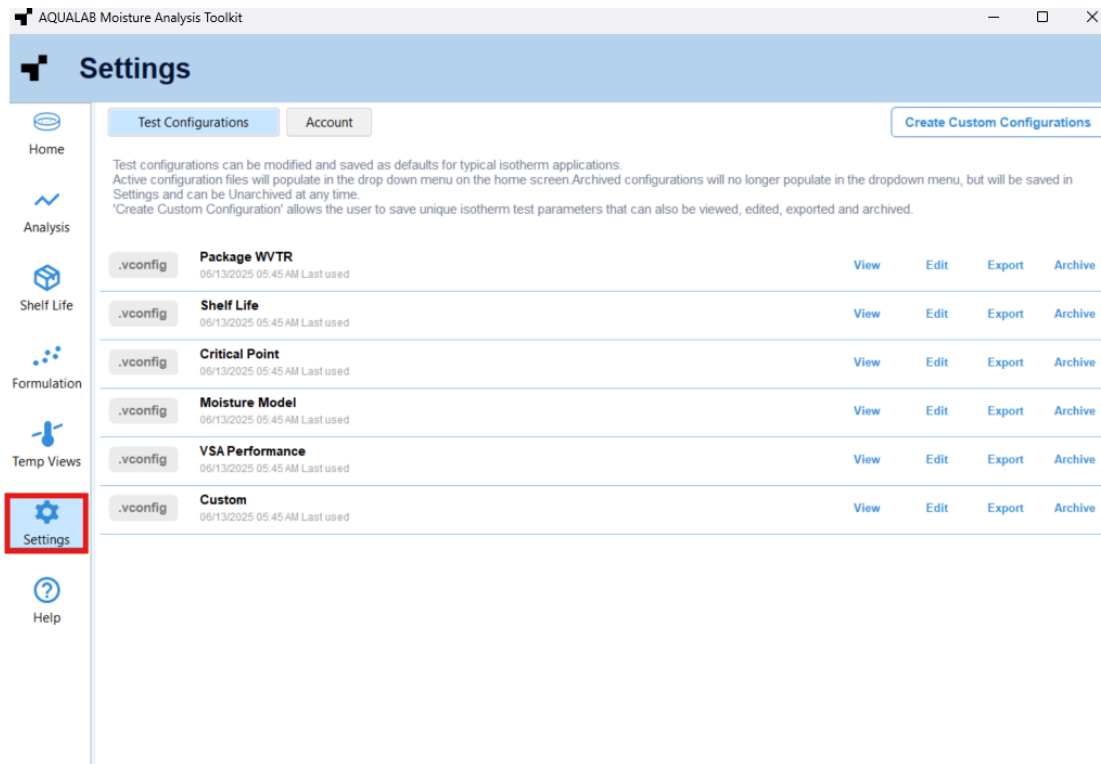
Cancel Save Configuration

1.2.6.2 Account

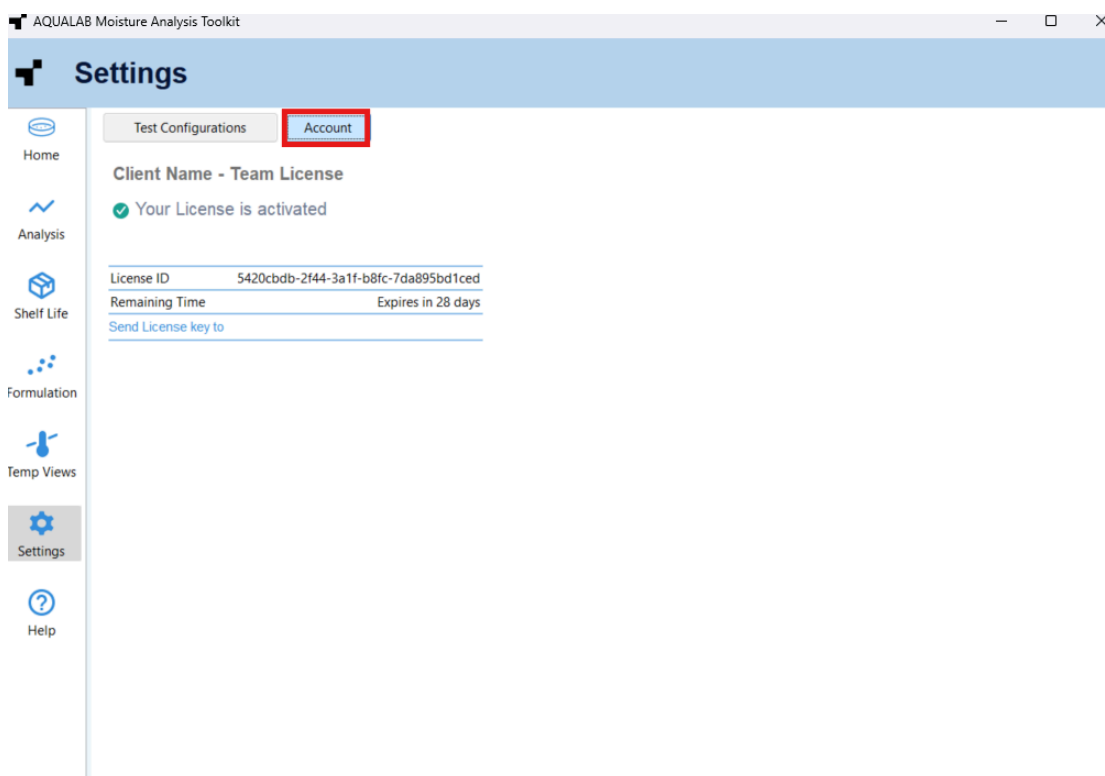
This component enables users to view their account details including the account status, License ID and license expiration time.

To view account details:

1. Navigate to the settings page by selecting the Settings option in the side panel



2. Select the Account tab



3. View details such as licence ID and remaining time to license expiry.

1.2.6.3 License Expiry and Renewal

At the end of the validity period the license will expire. When the license has expired you will not be able to access the application anymore.

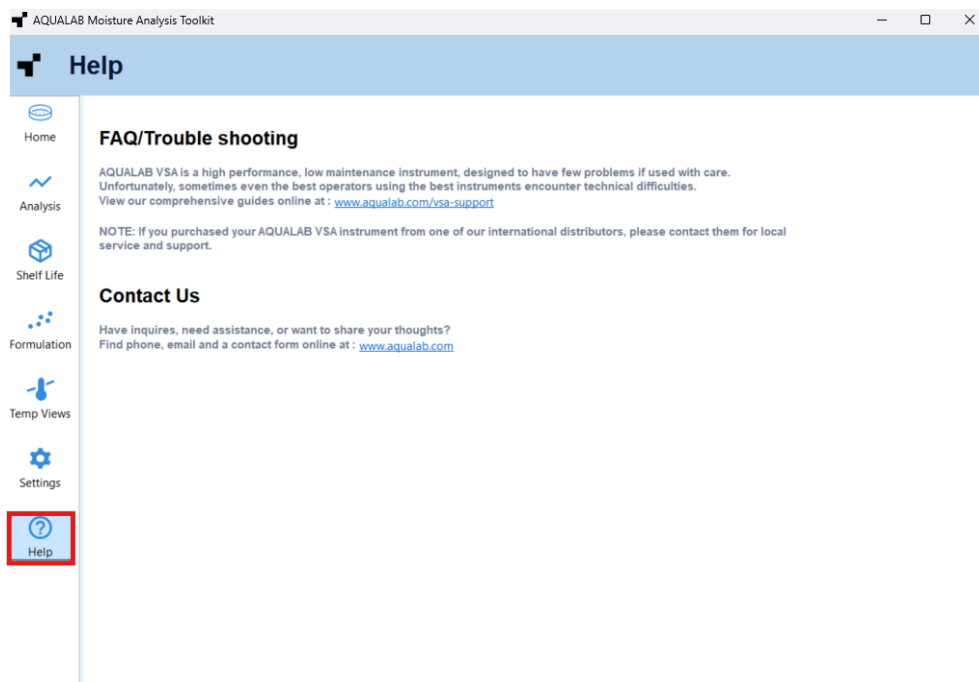
You can request for a license renewal from Addium. Once you receive a new license key follow the instruction given in section [3.2](#).

1.2.7 Help

This is the section users will interact with when they need support or encounter issues while using the Addium MAT application.

It includes quick access to FAQs, troubleshooting steps, and support contact information. To access the help section.

1. Navigate to the help page by selecting Help in the side panel.

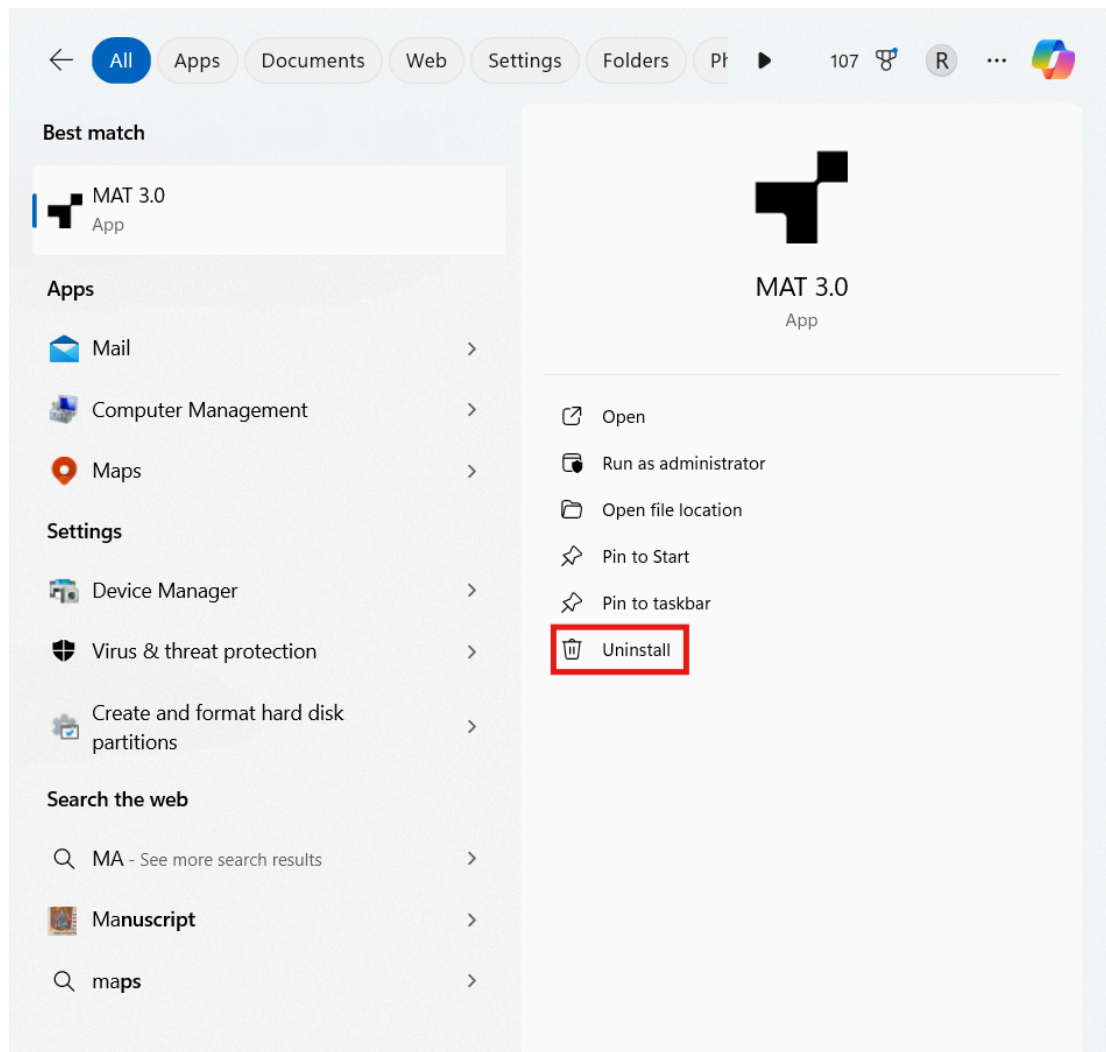


1.3 Uninstalling MAT 3

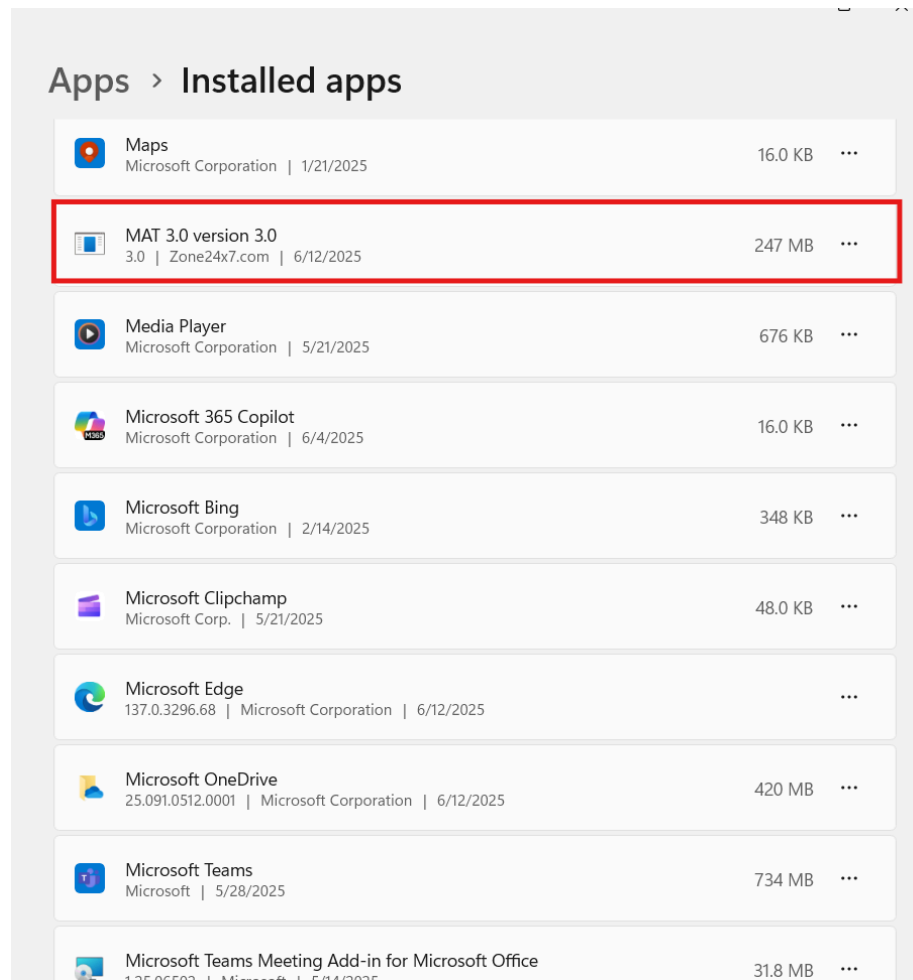
If you need to uninstall the MAT 3 application you can follow these steps (The steps may differ based on the windows operating system)

Steps to uninstall MAT 3 on windows 11

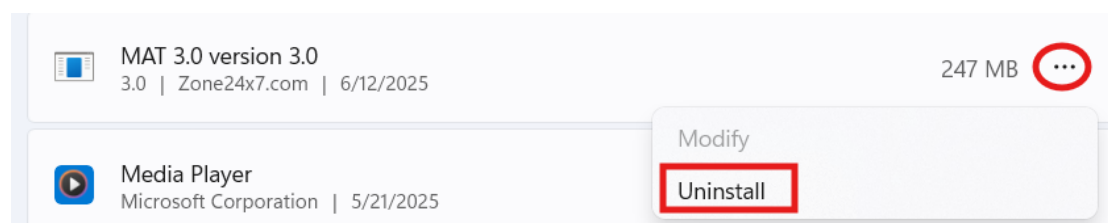
1. Search MAT 3 on the windows search bar on the search bar of the desktop.



2. Click on the Uninstall option on the right side of the menu. This will take you to the Installed Apps section in window settings. Here find MAT 3 application



3. Click on the ellipsis button, A dropdown menu will appear. Click on the Uninstall option on it.



4. Select Yes on the following pop-up message that appears. This will run the uninstaller and the MAT 3 application will be removed from your pc.

1.4 Support

1.5 North America

Customer service representatives are available for questions, problems, or feedback Monday through Friday, 7:00 am to 5:00 pm Pacific time.

Email: support@aqualab.com
sales@aqualab.com
Phone: +1.509.332.5601
Website: aqualab.com

1.6 Europe

Customer service representatives are available for questions, problems, or feedback Monday through Friday, 8:00 to 17:00 Central European time.

Email: sales.europe@aqualab.com
Phone: +49 89 20 80 49 202
Website: aqualab.com/de