KEIT INDUSTRIAL ANALYTICS

IRmadillo™

DOC0893 KeitSpec Software User Manual – Version 5.2.1

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1. GETTING STARTED

1.1. Pre-requisites

It is assumed the instrument is correctly set up according to the relevant User Manual.

The controller operates on Windows 10 IoT Enterprise LTSC. To ensure stability, it does not install Windows updates automatically. Keit recommends running Windows updates before setting up the IRmadillo.

KeitSpec should only be run in the Spectrometer User account. The IRmadillo can connect to only one instance of KeitSpec. If KeitSpec is opened in another user account, it will not connect to the spectrometer.

1.2. The Spectrometer tab: an overview

When the controller powers on, KeitSpec automatically loads with the Spectrometer tab open. It will connect to the IRmadillo and open the last used project file. The IRmadillo comes with a factory background scan that loads automatically.

Before you start taking spectral measurements, it is important to ensure that the spectrometer is connected, is stable and is purged. Look for the following indicators:

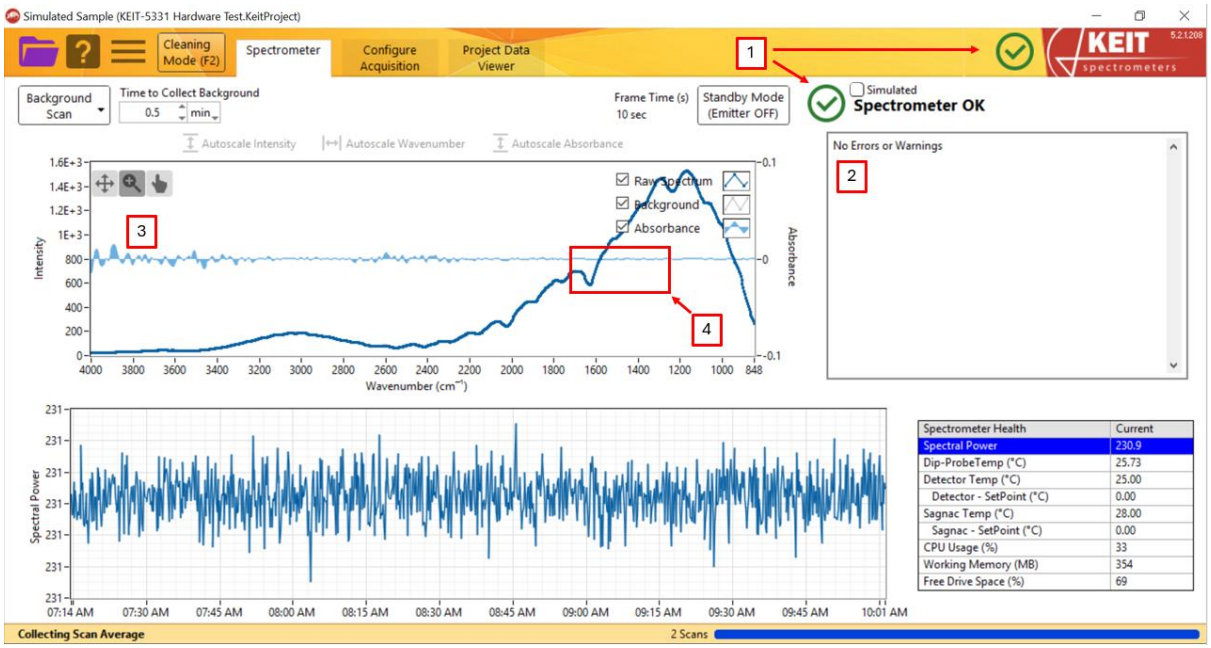


Figure 1: The Spectrometer tab

1. Spectrometer Status indicators

The following indicators may be shown:

Green tick: IRmadillo is connected and is thermally stable.

Red thermometer icon: IRmadillo is connected but is not yet thermally stable. Wait for the IRmadillo to stabilise before taking any measurements.

 Red cross: IRmadillo an error. Refer to the troubleshooting section of the IRmadillo User Manual.

 Black arrows: IRmadillo is not connected

 Not saving icon: IRmadillo is not autosaving data

Before collecting data, ensure that the green tick is showing, and that the status is ‘Spectrometer OK’.

2. Errors and Warnings pane

Displays any errors or warnings on the IRmadillo. It should read "No Errors or Warnings." If not, refer to the troubleshooting section of the IRmadillo User Manual.

3. Spectrum view

Displays the live spectrum from the IRmadillo, updating every ten seconds.

4. Water vapour absorbance region

Water vapor peaks appear between 1350 cm^{-1} and 1700 cm^{-1}. Broad peaks in this region suggest a poor air purge; check the IRmadillo User Manual. Narrow peaks elsewhere indicate the probe's sensing ATR element needs cleaning and drying. Refer to DOC0935 for guidance.

1.3. Collecting spectra in a continuous process

These steps guide you in creating a new continuous collection project, collecting a background spectrum, and selecting settings. For measuring individual spectra of discrete samples, see Section 1.9 Manual sampling.

1. Create a new continuous project by clicking the purple folder icon in the top left, then choose **Create New Empty Project > Continuous Collection…**

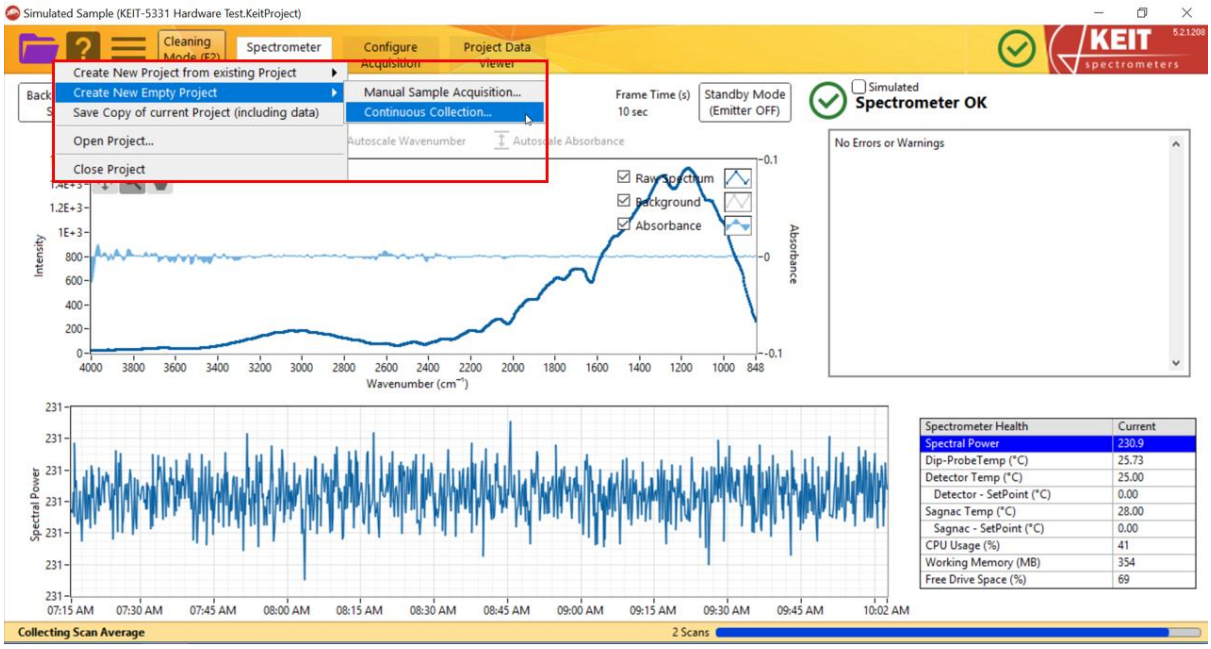


Figure 2: Creating a new Empty Continuous Collection project

2. In In the window that opens, navigate to the desired location, enter a project name, and click OK.

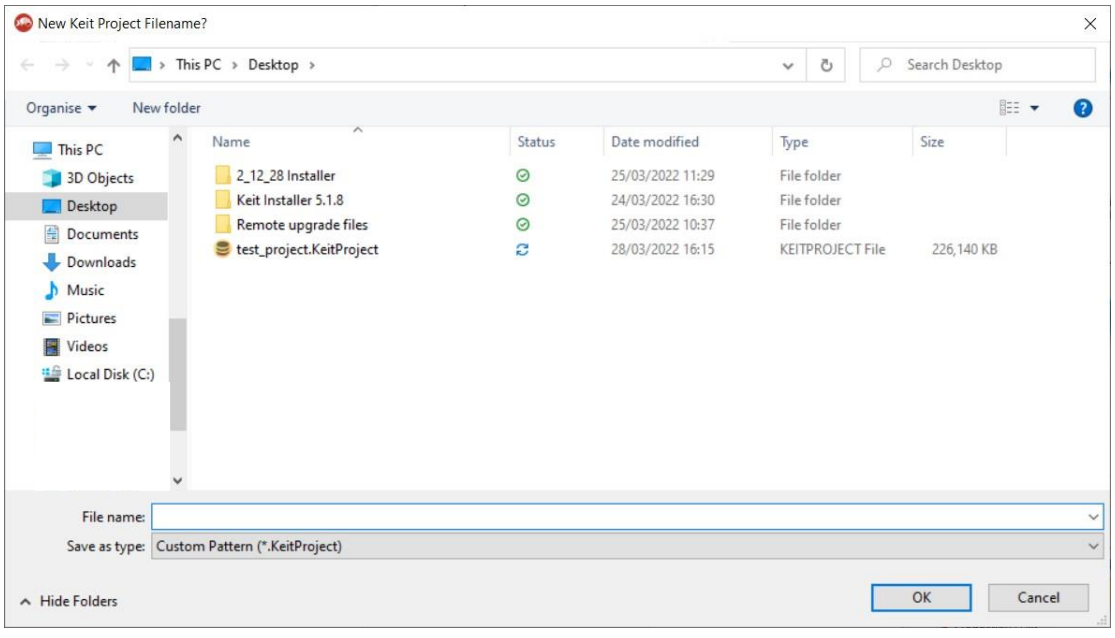


Figure 3: Creating a new Continuous Collection project

3. Record a background spectrum. Keit recommends a 30-minute air scan. Ensure the probe ATR element is clean. Adjust the scan duration using the Time to Collect Background inputs.

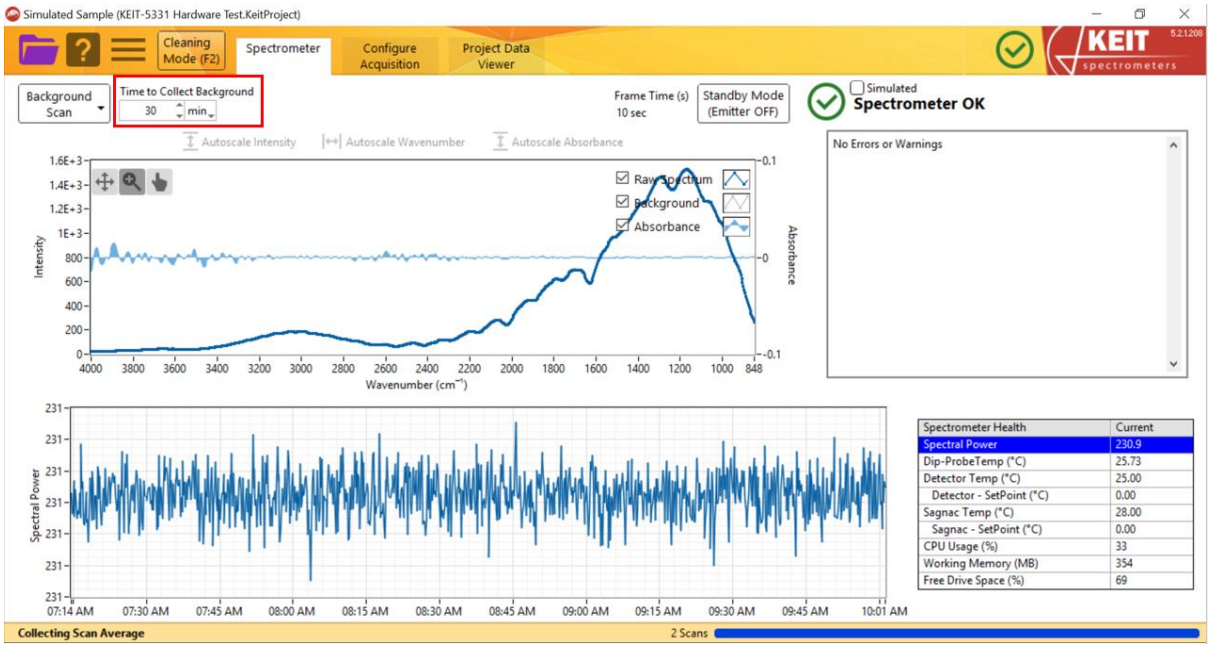


Figure 4: Changing background spectrum collection settings

Next, click **Background Scan > Collect New Background**.

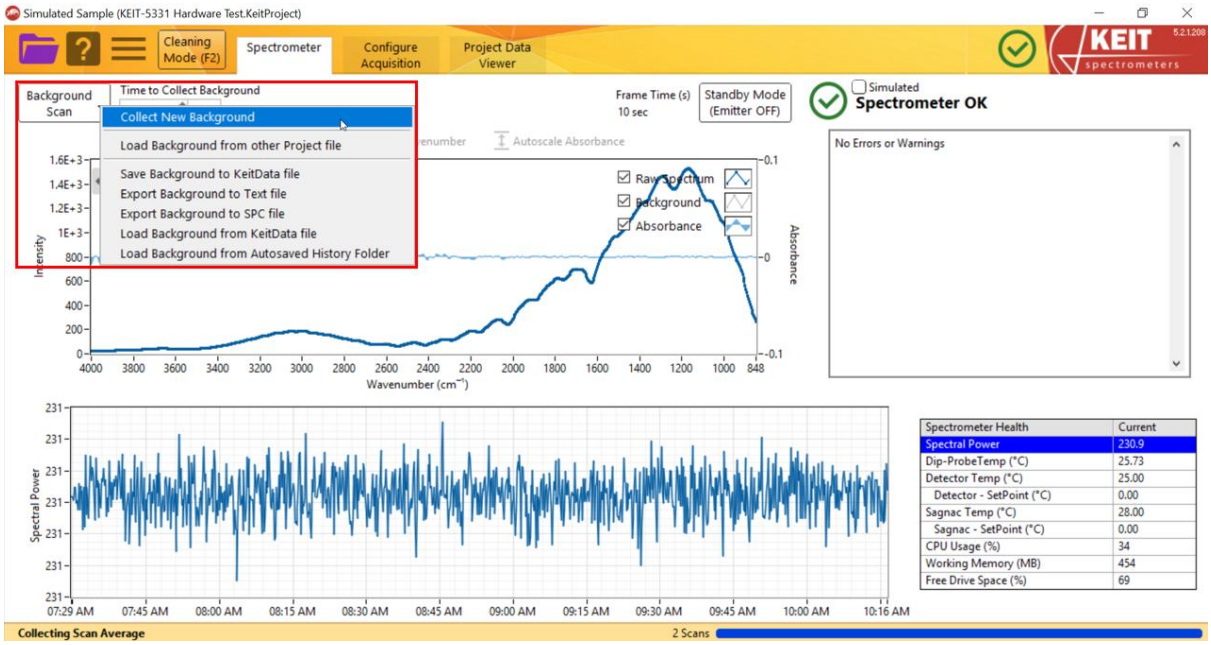


Figure 5: Recording a new background spectrum

The Background Scan button turns green, and a progress bar at the bottom right shows the scan's progress. Once completed, the button returns to white. Note: background scan collection cannot be cancelled once started.

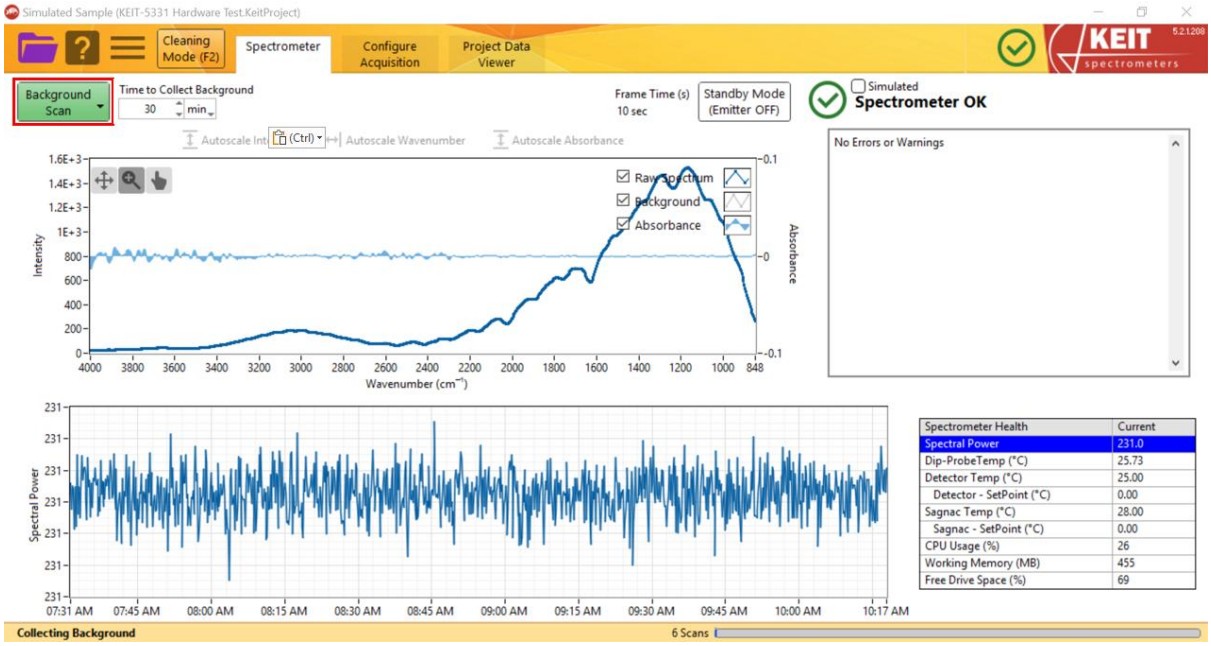


Figure 6: Recording of a new background spectrum in progress

4. You're now ready to collect spectra. On the Configure Acquisition tab, set the Scan Averaging Duration (default is 120 seconds).

   For details on the **Data Communications Methods** panel, see Section 1.8.

   The instrument will start recording spectra automatically once a valid background is detected.

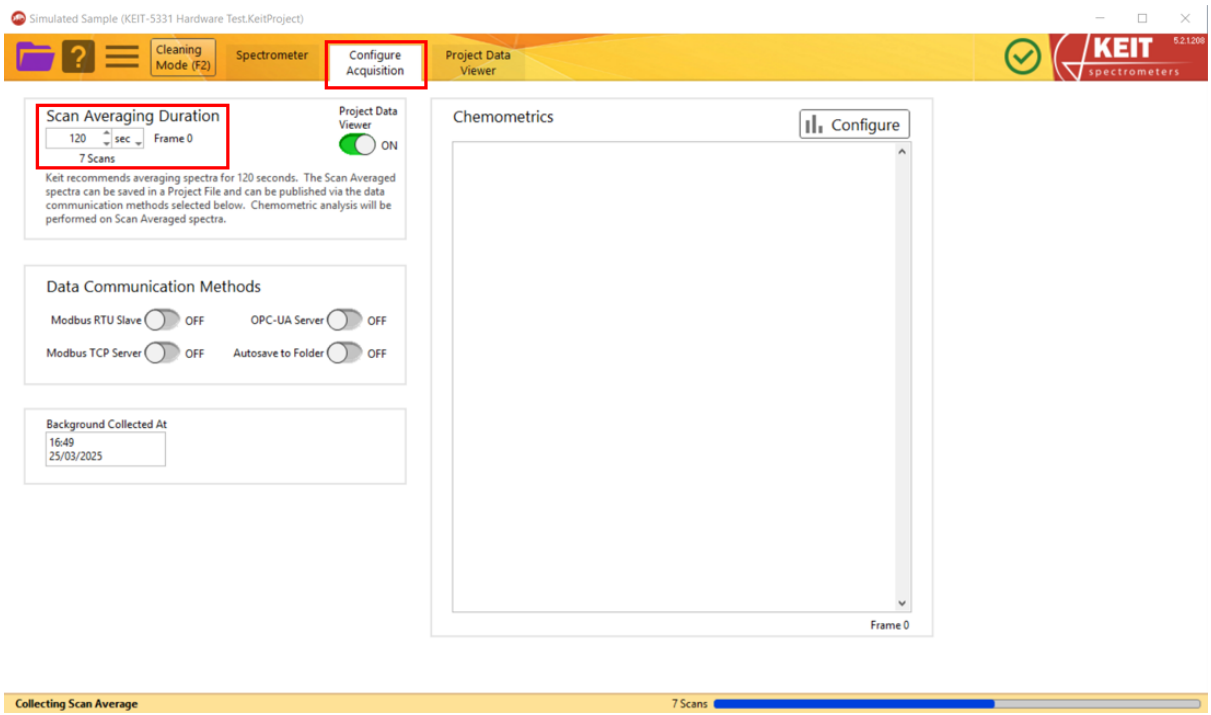


Figure 7: The Configure Acquisition tab

5. View spectra in real time on the **Spectrometer tab**. Interactive graphs display changes in absorbance and spectral power over time. A table in the bottom right corner provides the spectrometer's status.

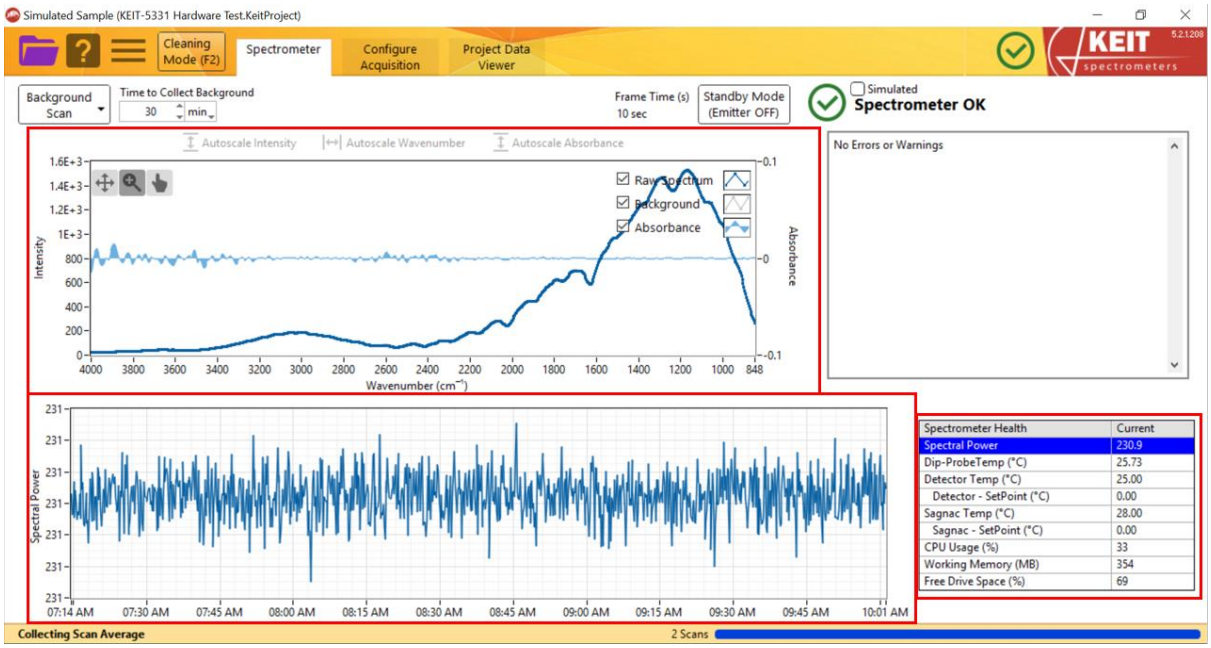


Figure 8**: Viewing of incoming spectra**

1.4. Loading a univariate model

Loading a univariate model allows you to see how a spectral region evolves over time. It is simpler and less informative than the chemometric models described in Section 1.5 but can be useful for some applications.

1. On the **Configure Acquisition** tab, click the **Configure** button.

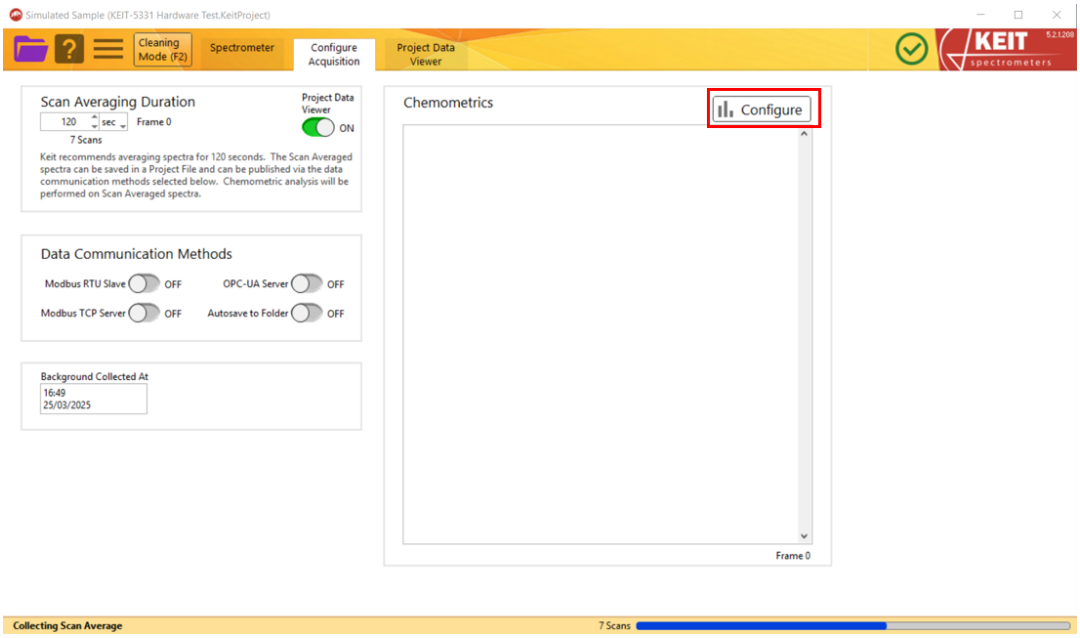


Figure 9: Loading a chemometric model

2. A **Chemometrics Editor** window will open. Click the **+** icon on the left of the screen to open a menu of model types and select **Add New Model>> Univariate**. This will open an **Edit Univariate** window.

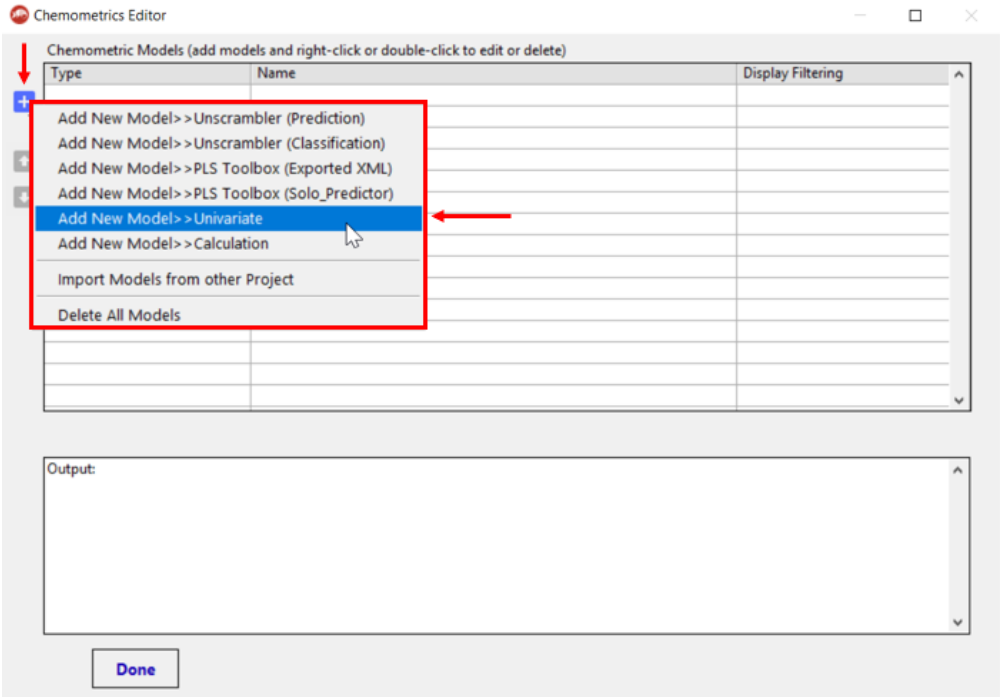


Figure 10: The Chemometrics Editor

3. In the **Edit Univariate** window, use the **Min** and **Max** inputs to set the wavenumber range. Checkboxes allow you to toggle whether the **Maximum**, the **Average** and the **Minimum** are reported. When you have made your selection, click **OK** to load the model.

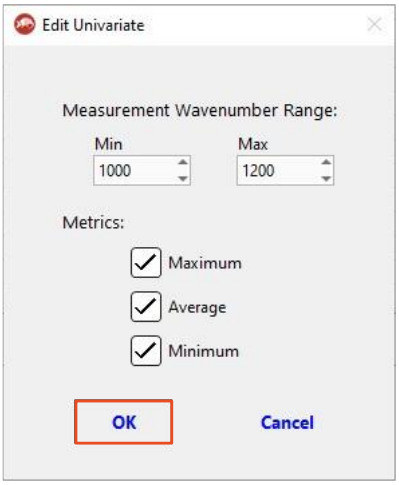


Figure 11: Editing a Univariate model

4. A model of type **Univariate** should now be loaded into the **Chemometrics Editor** window. When this model is selected, its details will be shown in the bottom panel.

   Additional models can be added using the **+** button as before. Models can also be deleted by right-clicking on a model and selecting **Delete this Model**. When you have added all your models, click **Done** to close this window.

   Click **Done** to finish.

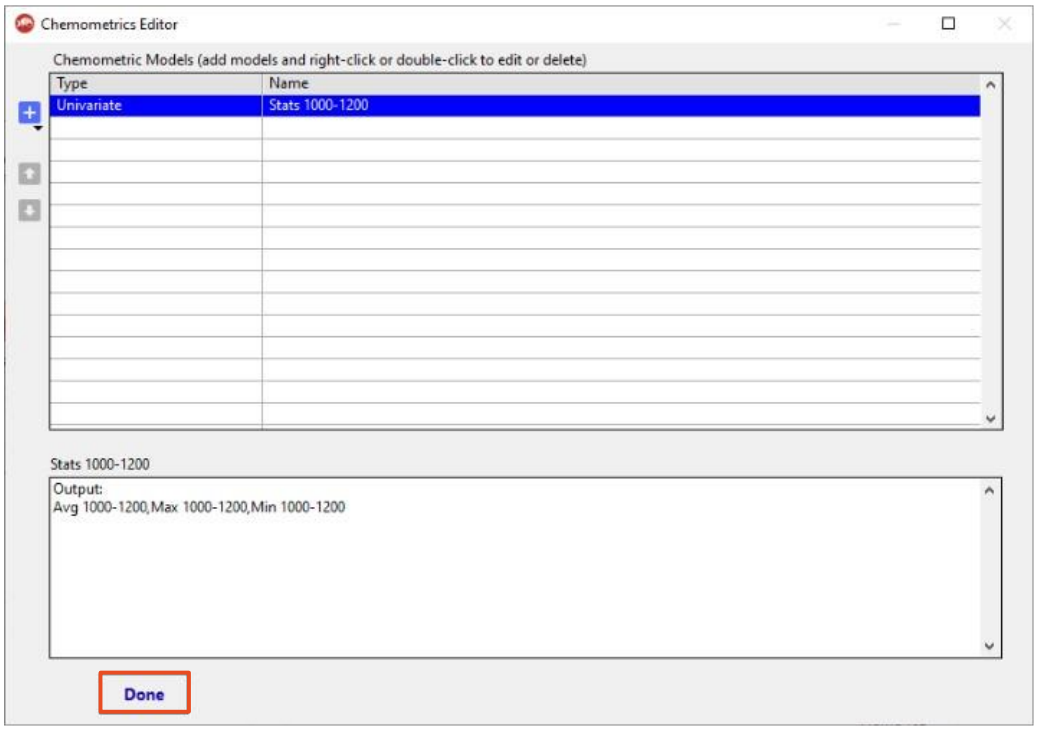


Figure 12: Applying a Univariate model

1.5. Loading a chemometric model

Chemometric models allow you to view an interpretation of the spectra in terms of concentrations of chemical species, or diagnostic statistics of the collected spectra, in real time.

1. On the **Configure Acquisition** tab, click the **Configure** button.

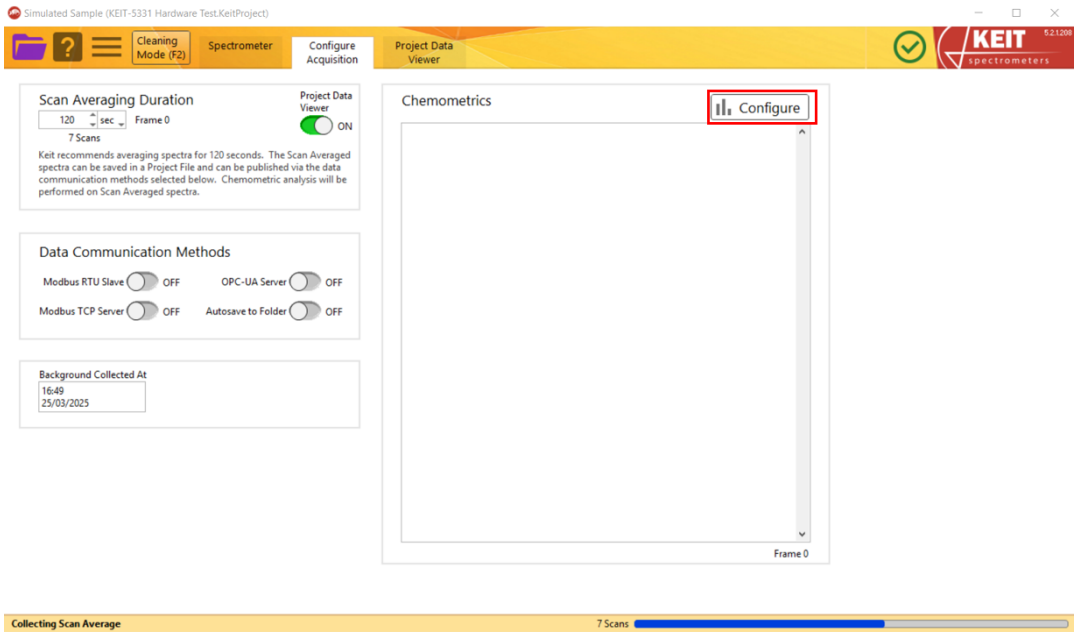


Figure 13: Loading a chemometric model

2. A **Chemometrics Editor** window will open. Click the **+** icon on the left of the screen to open a menu of model types and select the type of chemometric model to add. In this example we will use a **PLS Toolbox (Solo_Predictor)** model (see Section 3.1 Configure Chemometrics for more information about available model types). Click the model type and, when the file explorer window opens, navigate to the model you want to load and click **OK**.

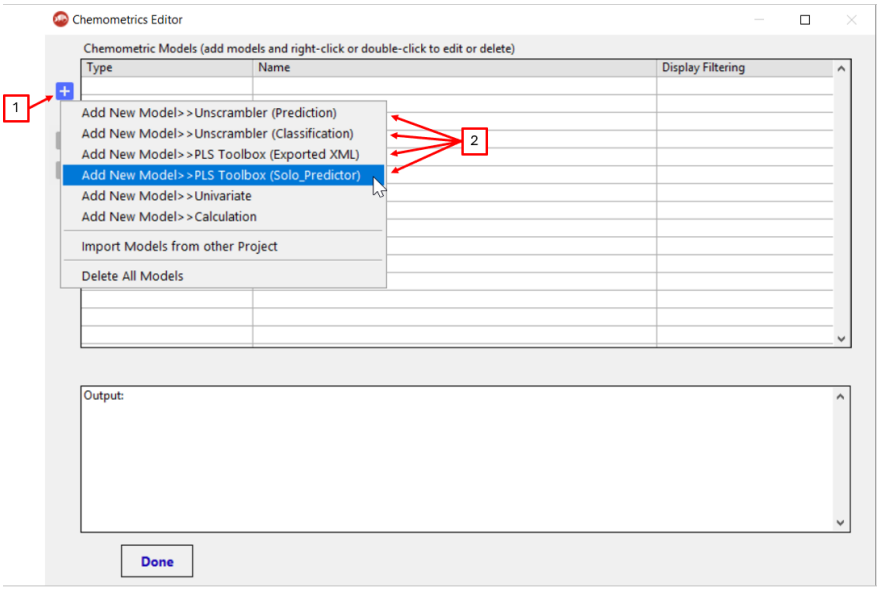


Figure 14: The Chemometrics Editor window

3. A model can report several features of the spectra. In this example, the features are the DP3+ measurement, the Hotelling's T^2, and the Q residuals. Select the features to report by checking or unchecking the boxes. Check that the desired outputs are listed in the description window, then click **OK** when done. This will close the window.

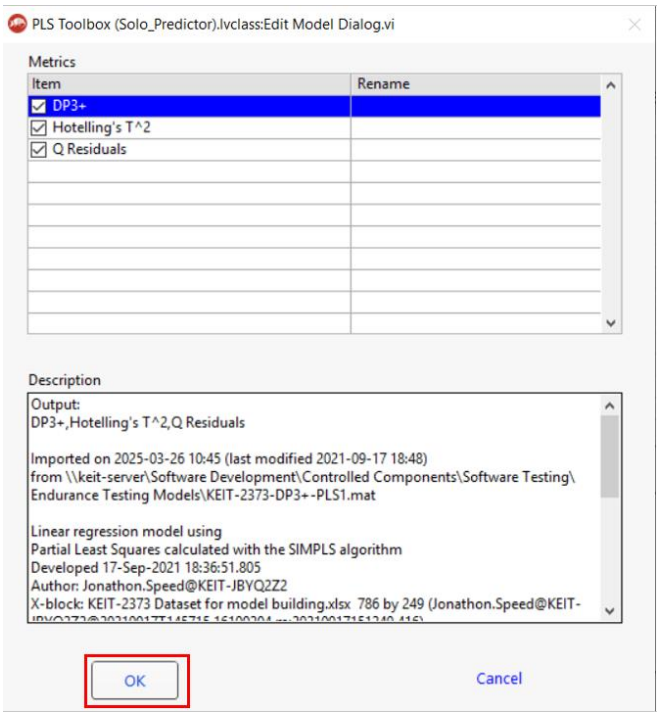


Figure 15**: Adding a Solo_Predictor model**

4. Additional models can be added using the **+** button as before. Models can also be deleted by right-clicking on a model and selecting **Delete this Model**. When you have added all your models, click **Done** to close this window.

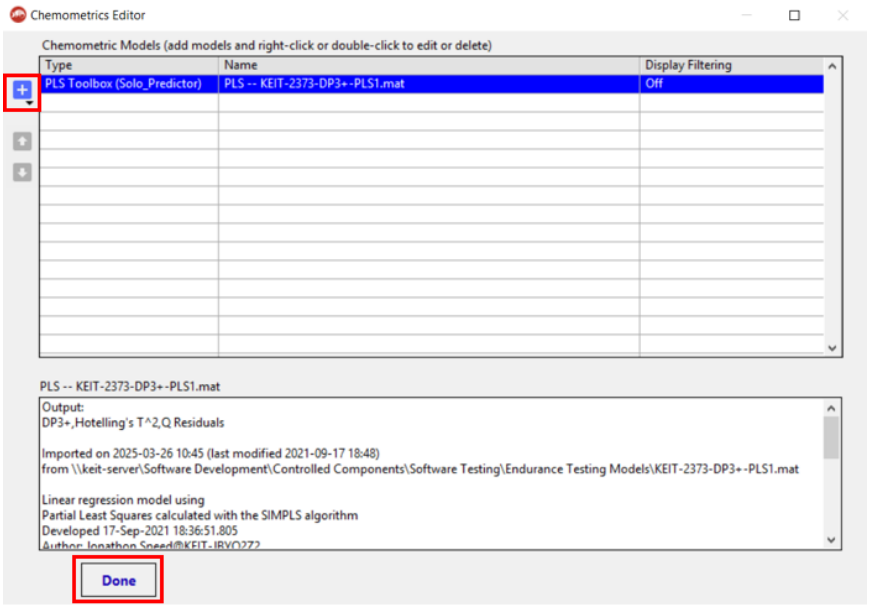


Figure 16: Adding an additional chemometric model

5. The outputs of the model are now displayed in the **Chemometrics** panel. These values update in real time as spectra are collected.

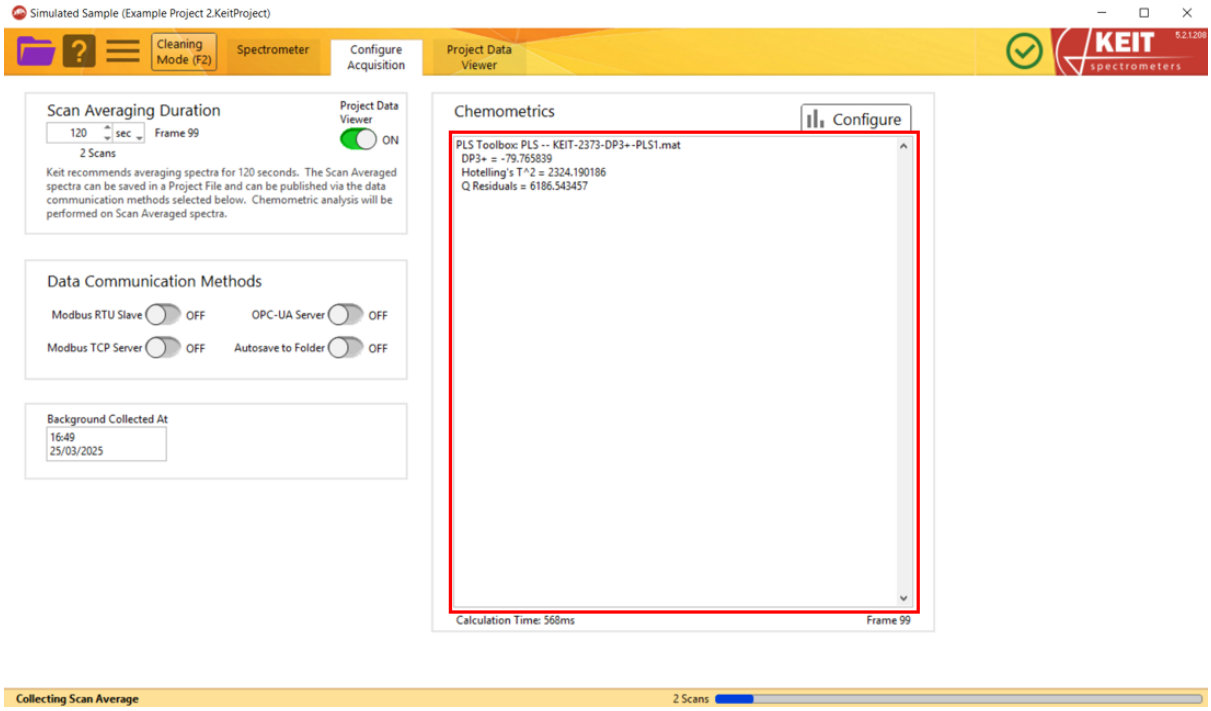


Figure 17: The Chemometrics panel

1.6. Filtering

To reduce noise, consider applying an exponential filter to the IRmadillo's predictions, depending on your process dynamics and chemistry changes.

1. Open the **Chemometrics Editor**. This window shows all models currently loaded on your system and includes the **Display Filtering** column.

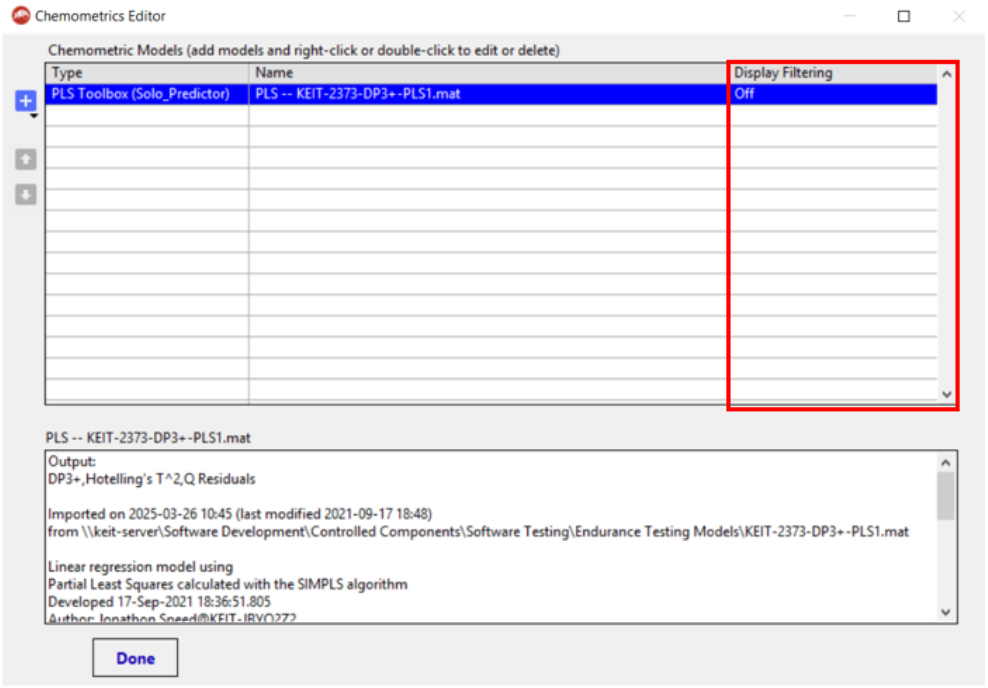


Figure 18 Display Filtering Column

2. Double-click the model in the Display Filtering column to edit the Display Filtering Times. This opens the Edit Display Filtering Times window:

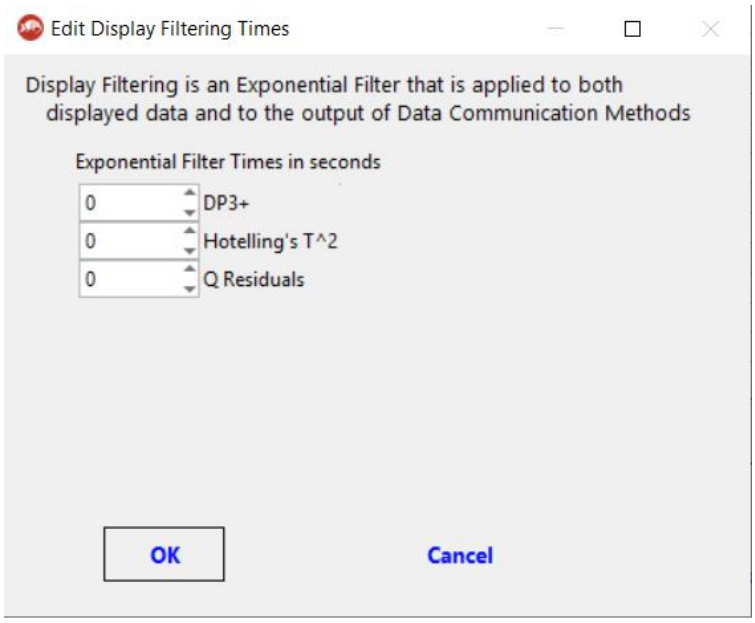
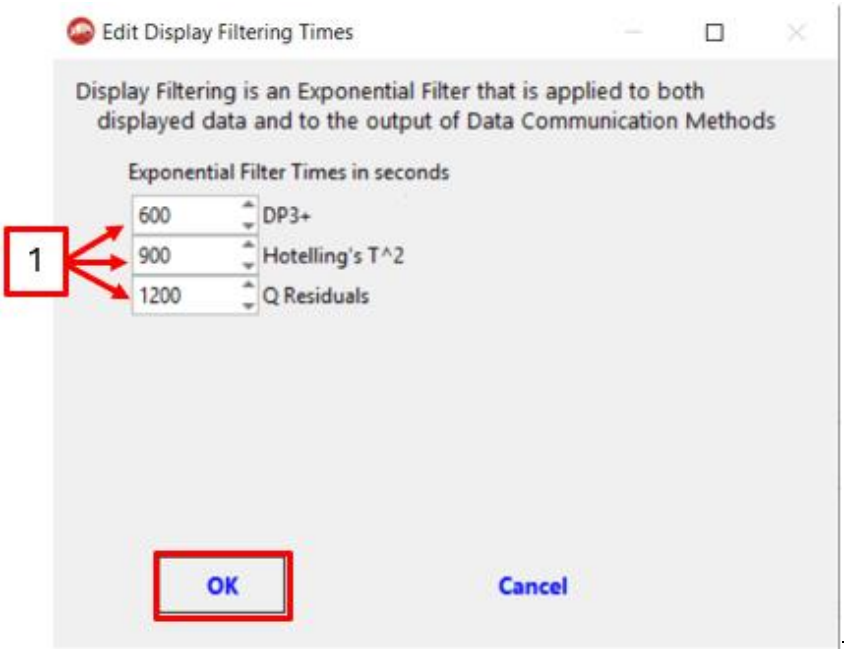
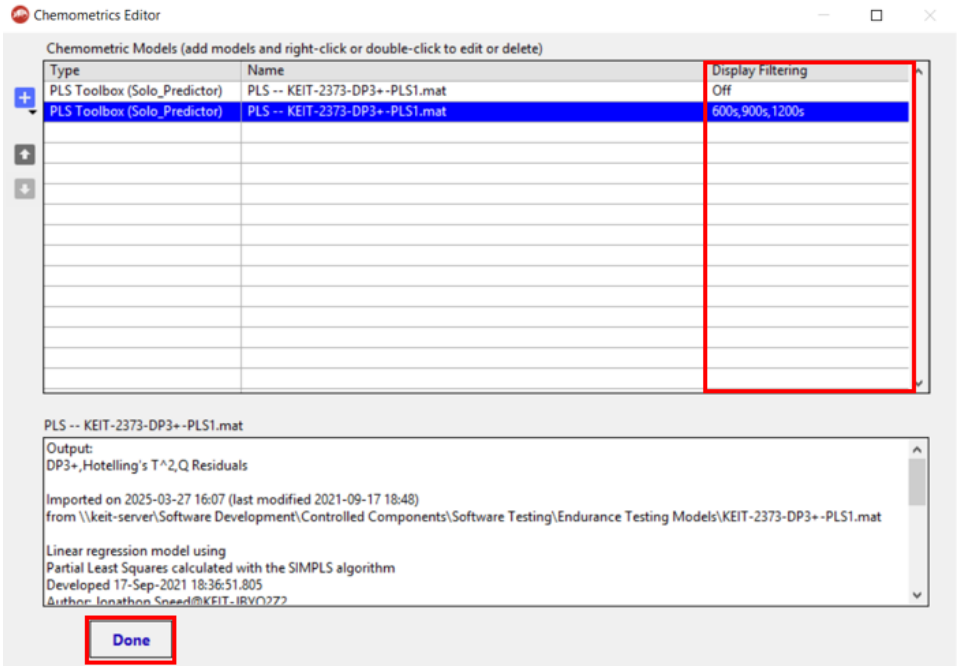


Figure 19 Edit Display Filtering Times

3. In the **Edit Display Filtering Times** window, enter the filter time constant in seconds. The example shows 10, 15, and 20 minutes. Press OK when done**.**



4. The filtering time constant will appear in the Display Filtering column. Click Done to apply the filters.



1.7. Exporting data

Data recorded by the spectrometer and processed by the models can be exported as a text file.

1. Open the **Project Data Viewer** tab. The model outputs are shown in an interactive graph (top panel), which you can explore using the buttons in the top left corner. The spectra are displayed in the bottom panel.

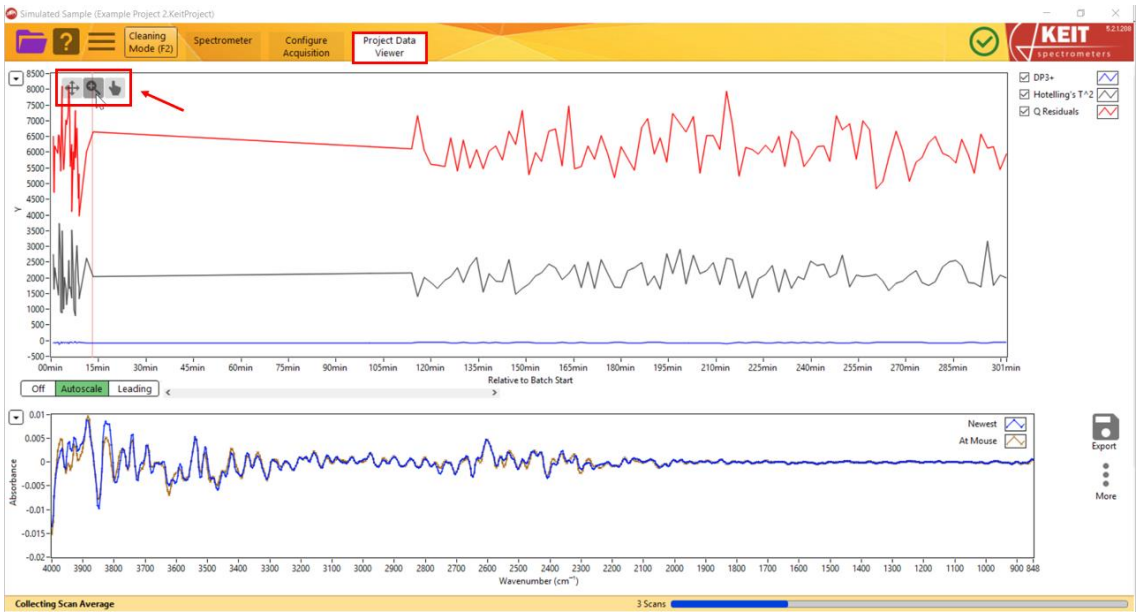


Figure 20: The Project Data Viewer tab

2. You may wish to mark time points in an experiment. To do this, right click the interactive graph in the top panel at the point you wish to mark. A menu will open allowing you to

Set Marker Here. Clicking this will open a new window prompting you to name the time point.

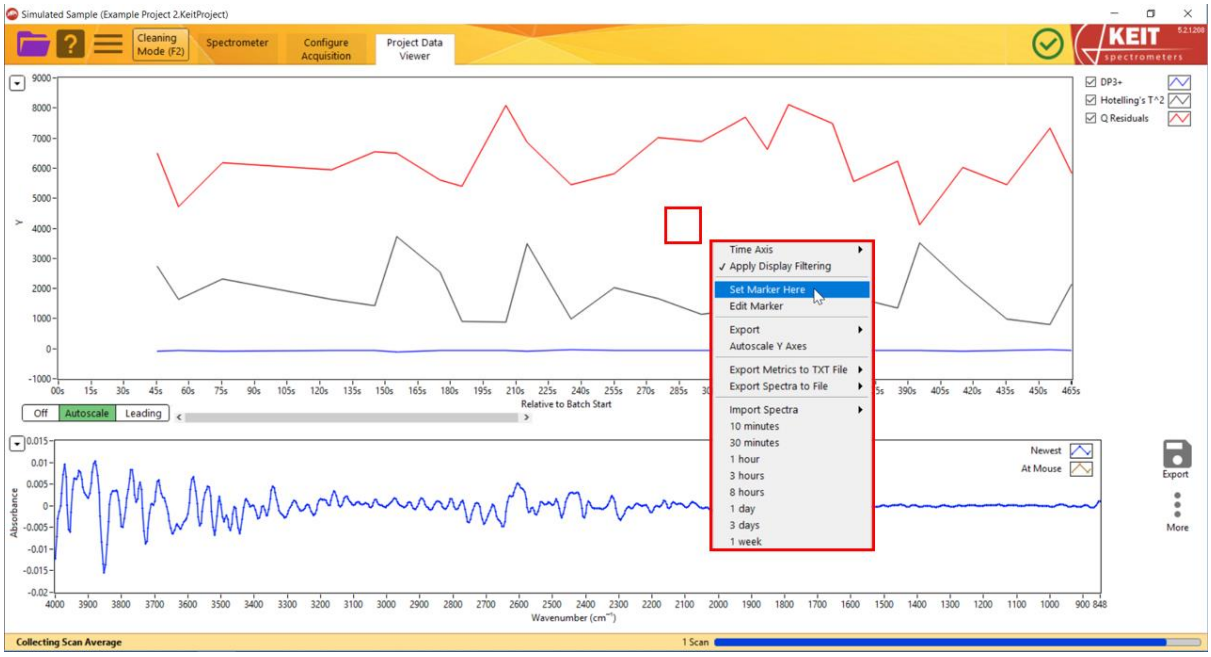


Figure 21: Adding a Marker

3. To export the data, click the **Export** button on the right of the screen.

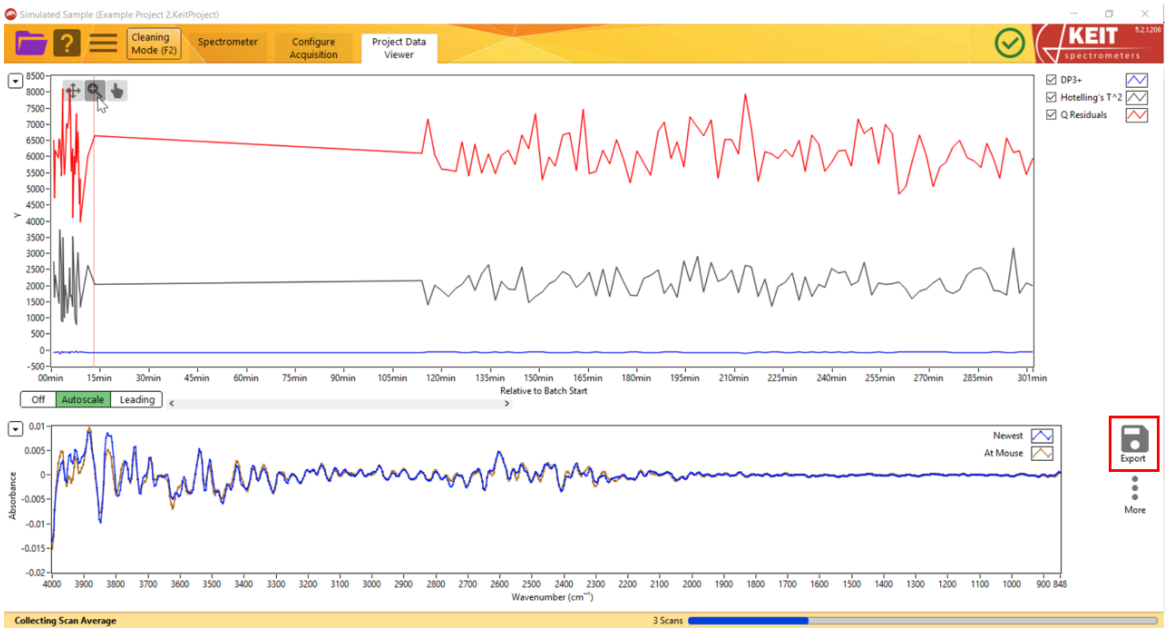


Figure 22: Exporting data

4. Selecting **Export Metrics to TXT File** will open a second menu allowing you to export either the model outputs currently displayed in the graph (**As Viewed**) or the entire dataset (**All Data**). Click your preference and a window will open, allowing you to navigate to the desired location to save your file.

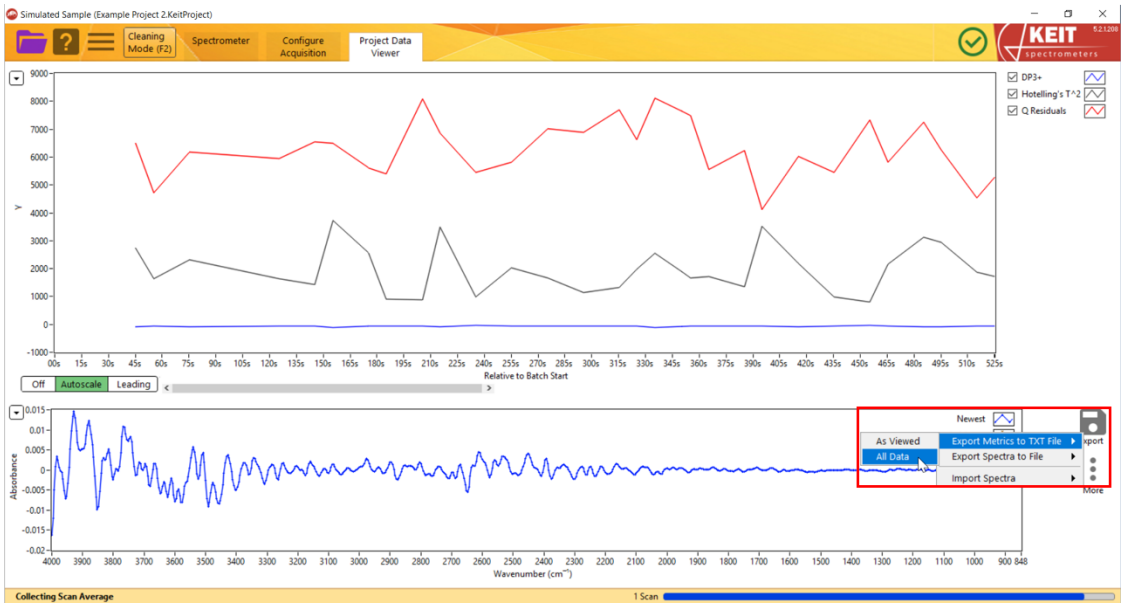


Figure 23: Exporting chemometric predictions

5. Similarly, selecting **Export Spectra to File** will open a menu to export only **Spectra in View Range**, **All Spectra**, or only **Marked Spectra**.

1.8. Connecting to control system (DCS or PLC)

KeitSpec provides four methods for data to be exported in real time:

- Modbus RTU Slave (models ASM0627-xx-x-x-**O**-x-x only)
- Modbus TCP Server
- OPC-UA Server
- Autosave to Folder

These can be activated configured on the **Configure Acquisition** tab in the **Data Communication Methods** panel. Toggling the switches from OFF to ON adds new tabs to the main window.

1.8.1. Modbus RTU Slave

1. To enable Modbus RTU Slave, toggle the **Modbus RTU Slave** switch. This will create a new tab at the top of the window.

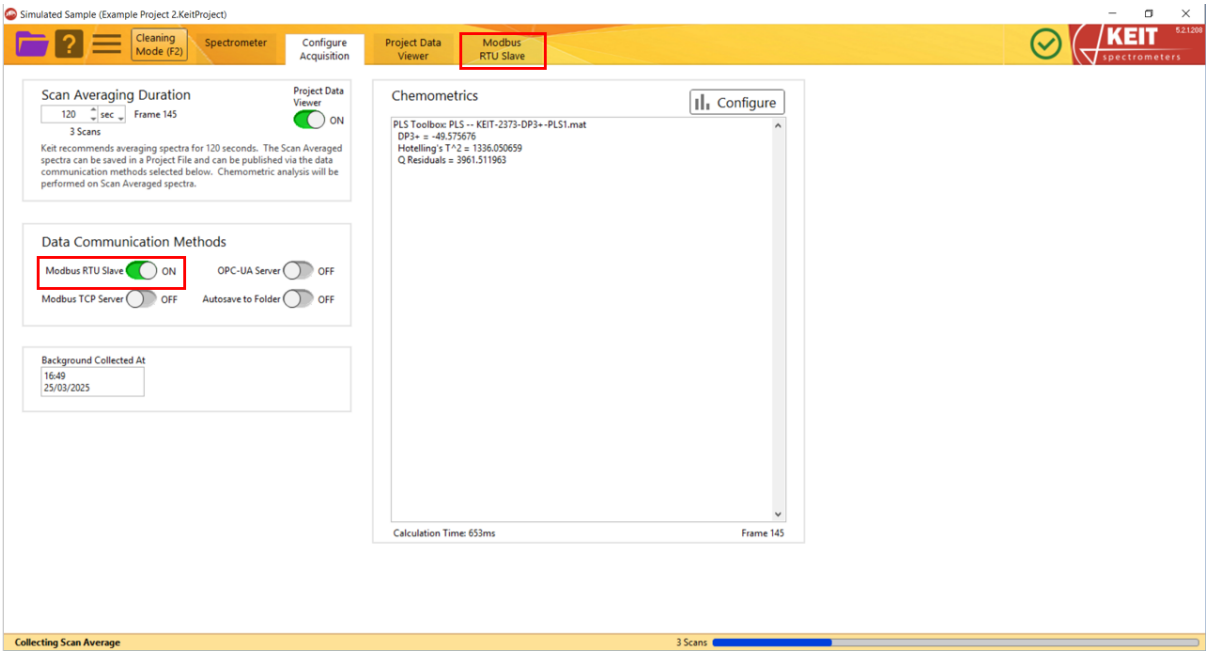


Figure 24: Enabling Modbus RTU Slave

2. Open the **Modbus RTU Slave** tab. A list of Input and Holding Registers is given on the panel on the right-hand side, showing the various outputs and their addresses. To enable the connection, toggle the **Enable Slave** switch to the **ON** position. The text below will show **Connected** when the connection has been made.

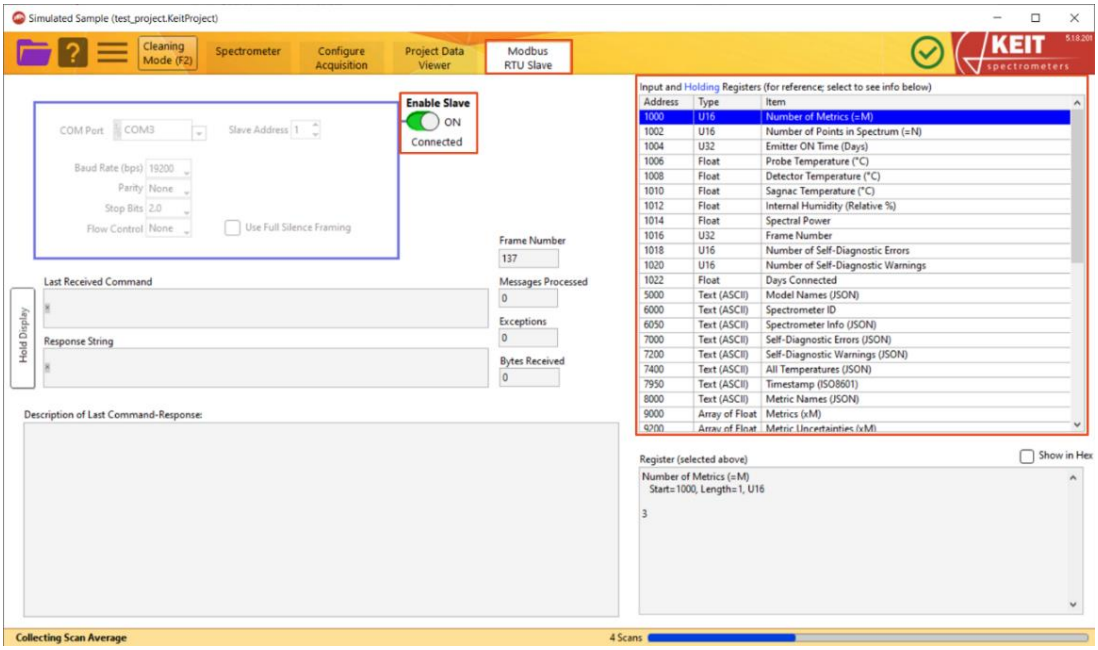


Figure 25: The Modbus RTU Slave tab

3. For further details on connecting via Modbus RTU, refer to DOC0871 Commissioning Guide - data communication - Modbus RTU.

1.8.2. Modbus TCP Server

1. To enable Modbus TCP Server, toggle the **Modbus TCP Server** switch. This will create a new tab at the top of the window.

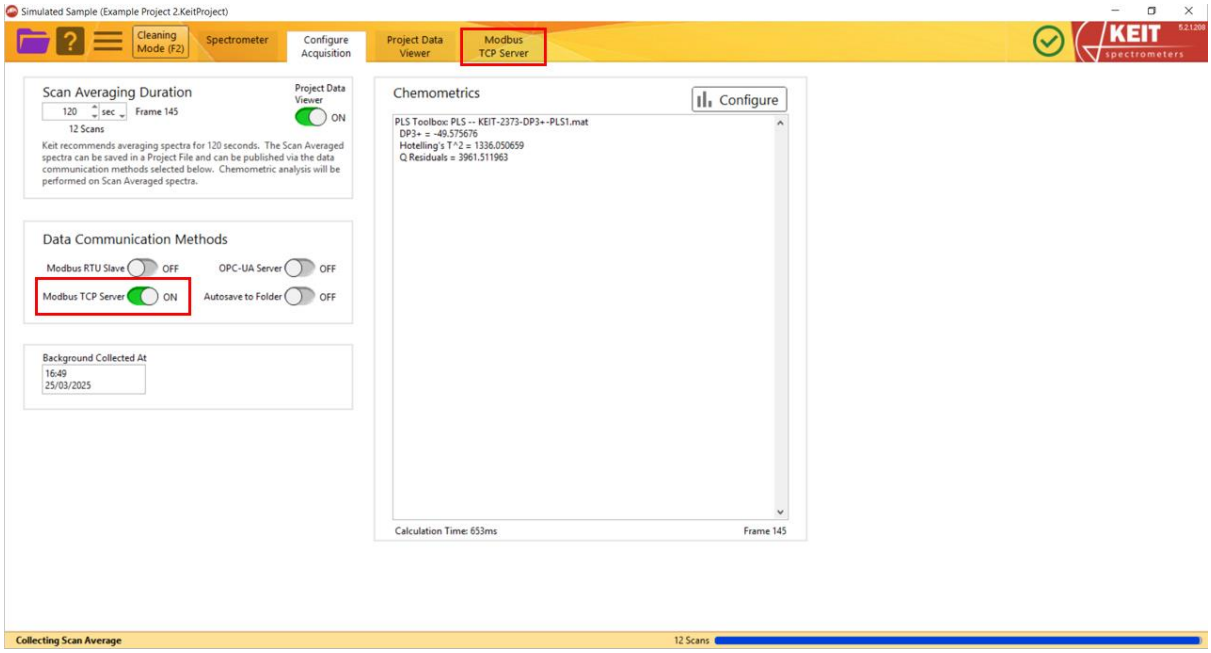


Figure 26: Enabling Modbus TCP Server

2. Open the **Modbus TCP Server** tab. A list of Input and Holding Registers is given on the panel on the right-hand side, showing the various outputs and their addresses. To enable the connection, toggle the **Enable Server** switch to the **ON** position. The text below will show **Connected** when the connection has been made.

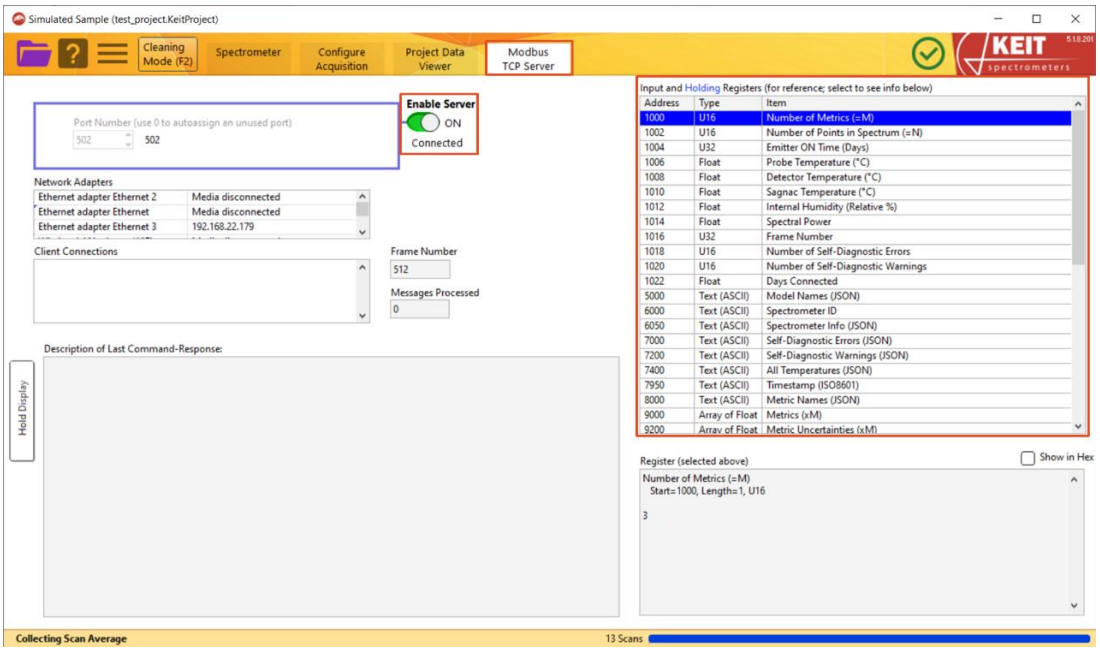


Figure 27: The Modbus TCP Server tab

3. For further details on connecting via Modbus TCP, refer to DOC0817 IRmadillo Commissioning Guide – data communication – Modbus TCP/IP.

1.8.3. OPC-UA Server

1. To enable OPC-UA Server, toggle the **OPC-UA Server** switch. This will create a new tab at the top of the window.

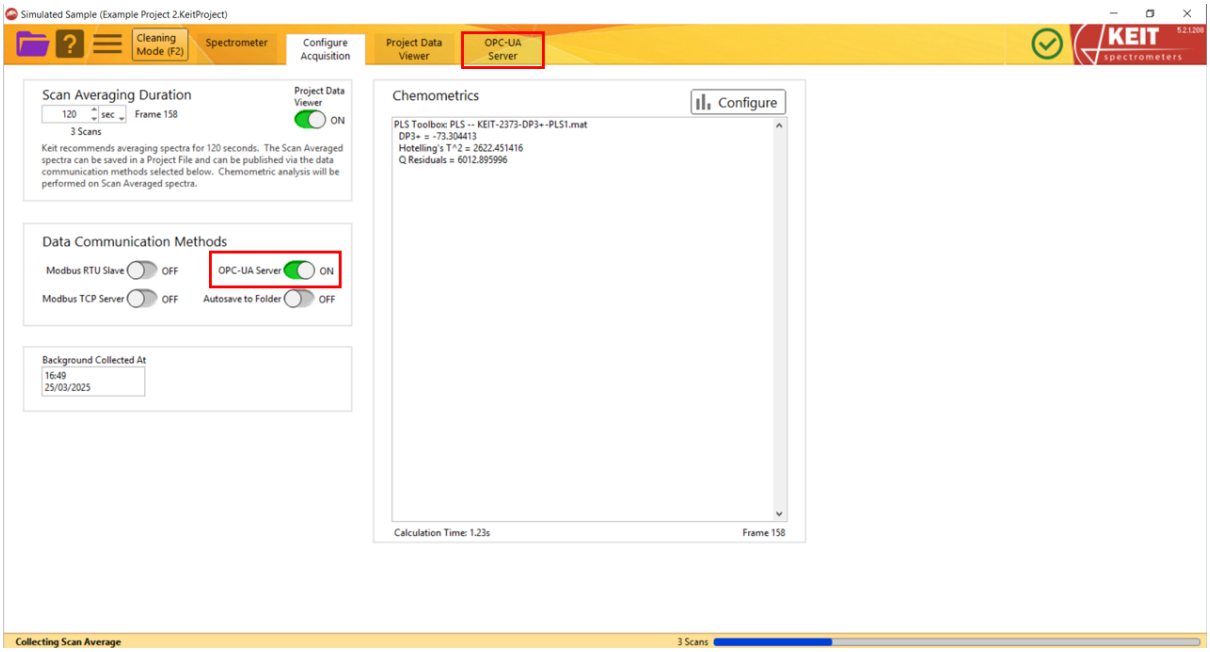


Figure 28: Enabling OPC-UA Server

2. Open the **OPC-UA Server** tab. To enable the connection, toggle the **Enable OPC-UA Server** switch to the **ON** position. The text below will show **Connected** when the connection has been made.

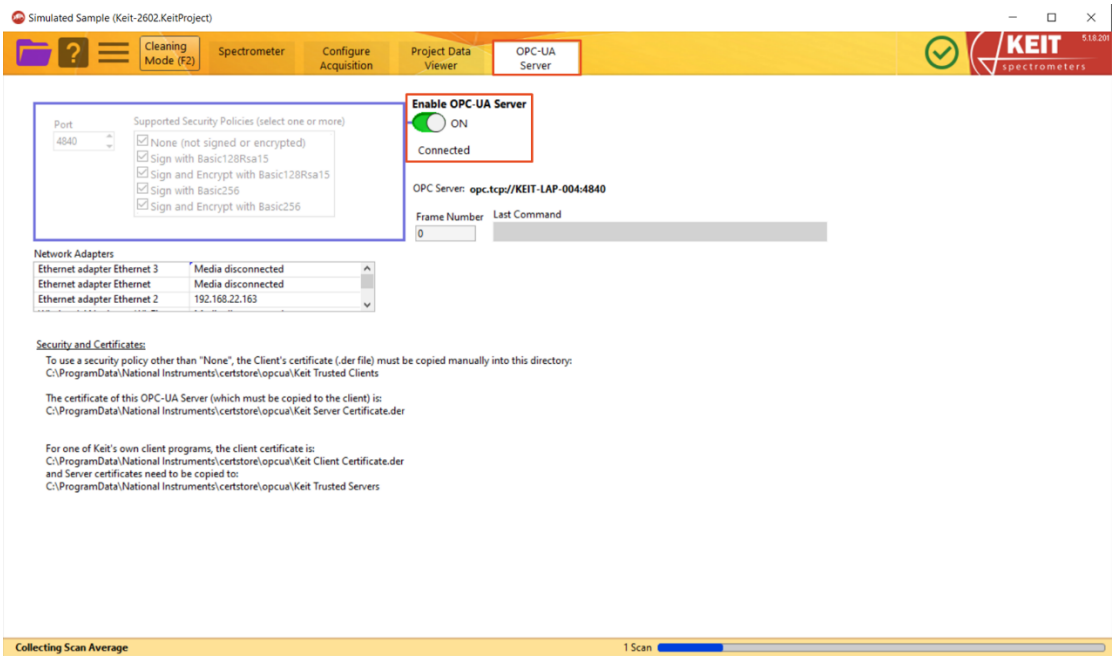


Figure 29: The OPC-UA Server tab

3. For further details on connecting via OPC-UA Server, refer to DOC0828 IRmadillo Commissioning Guide – data communication – OPC-UA.

1.8.4. Autosave to Folder

1. To enable autosaving to folder, toggle the **Autosave to Folder** switch. This will create a new tab at the top of the window.

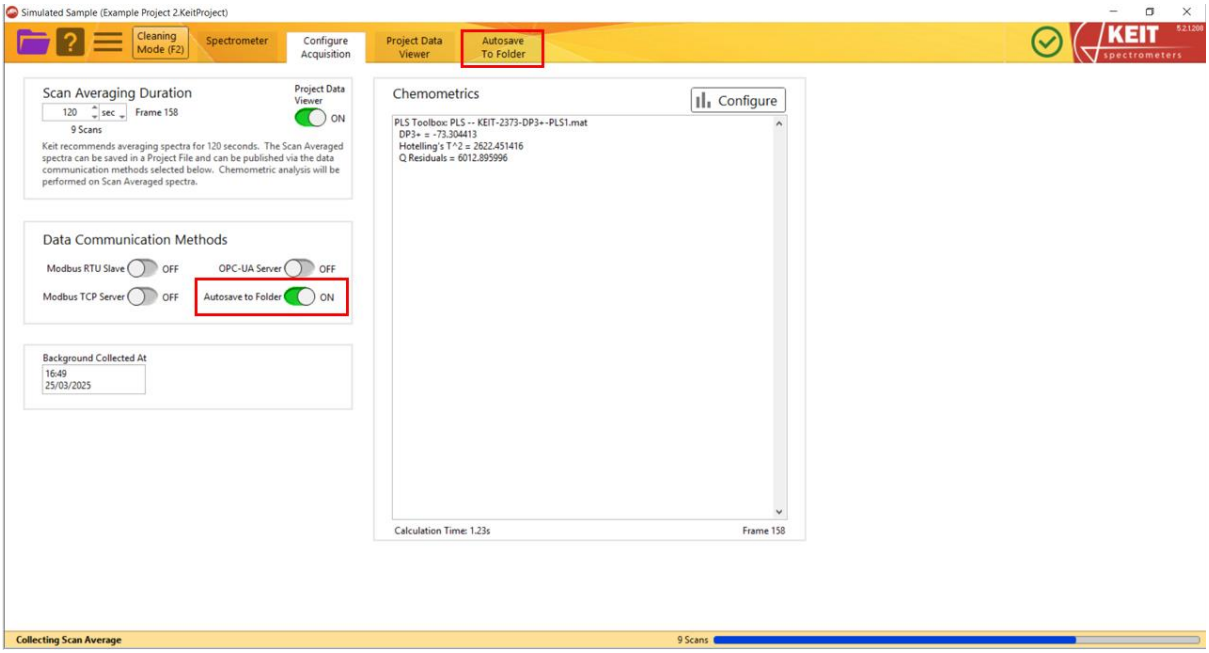


Figure 30: Enabling Autosave to Folder

2. Open the **Autosave to Folder** tab. The panel bounded by a blue rectangle allows you to navigate to a folder to save data into. The **Enable Saving** toggle enables automatic saving to the folder selected.

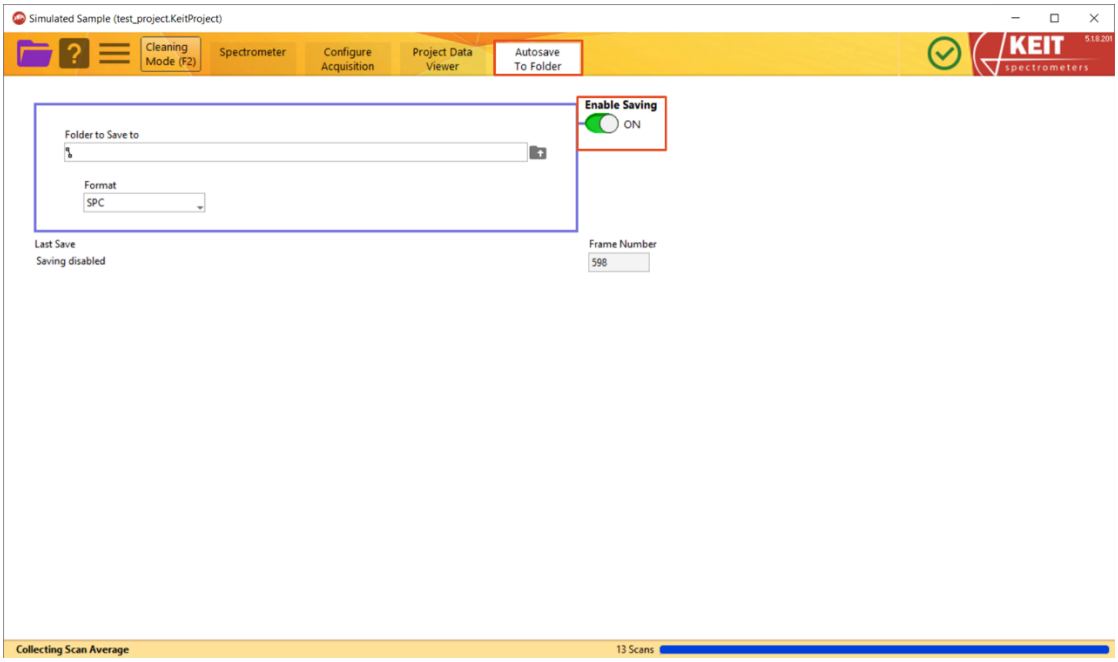


Figure 31: The Autosave to Folder tab

3. For further details on connecting via a watched folder, refer to DOC0876 IRmadillo Commissioning Guide – data communication – Watched Folder.

1.9. Manual sampling

These steps lead you through the process of creating a new manual sample acquisition project and how to collect spectra manually.

1. Create a new manual project by clicking the purple folder icon in the top left corner, then choose **New Project > Manual Sample Acquisition…**

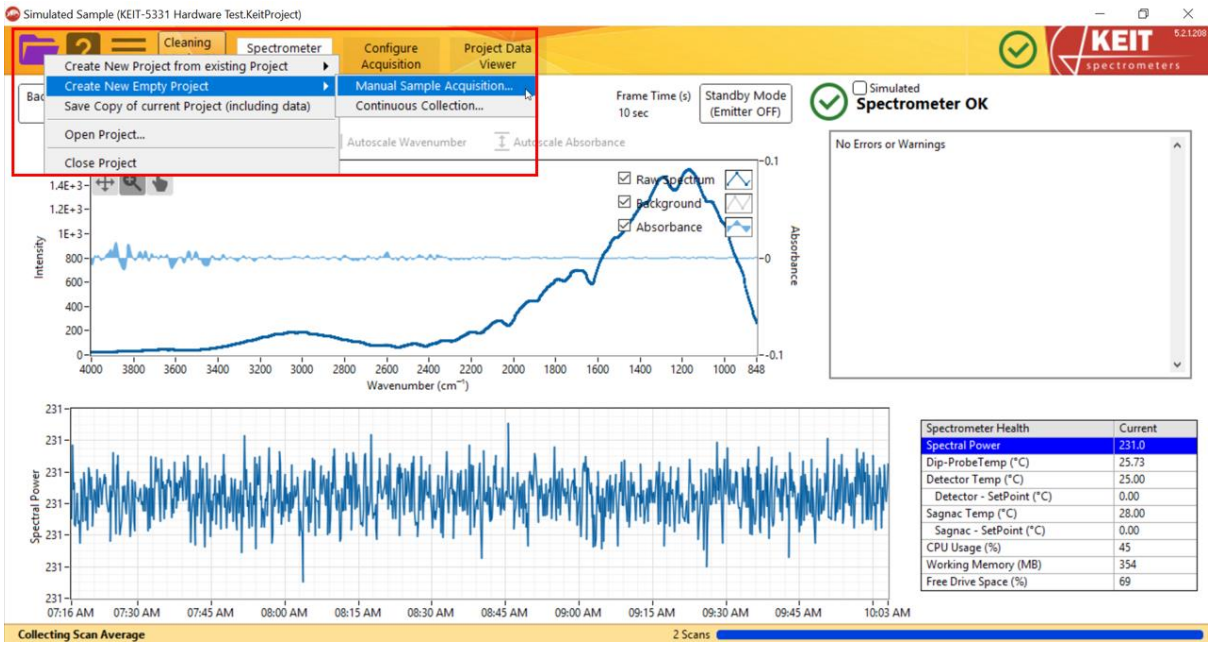


Figure 32: Creating a new Manual Sample Acquisition project

2. In the window that opens, navigate to the desired location and enter a name for your project. Click **OK** to create the project.

3. You should next record a background spectrum. Keit recommends a 30-minute background scan of air. Ensure that the probe ATR element is clean before doing so. The background scan duration can be adjusted using the **Time to Collect Background** inputs shown below.

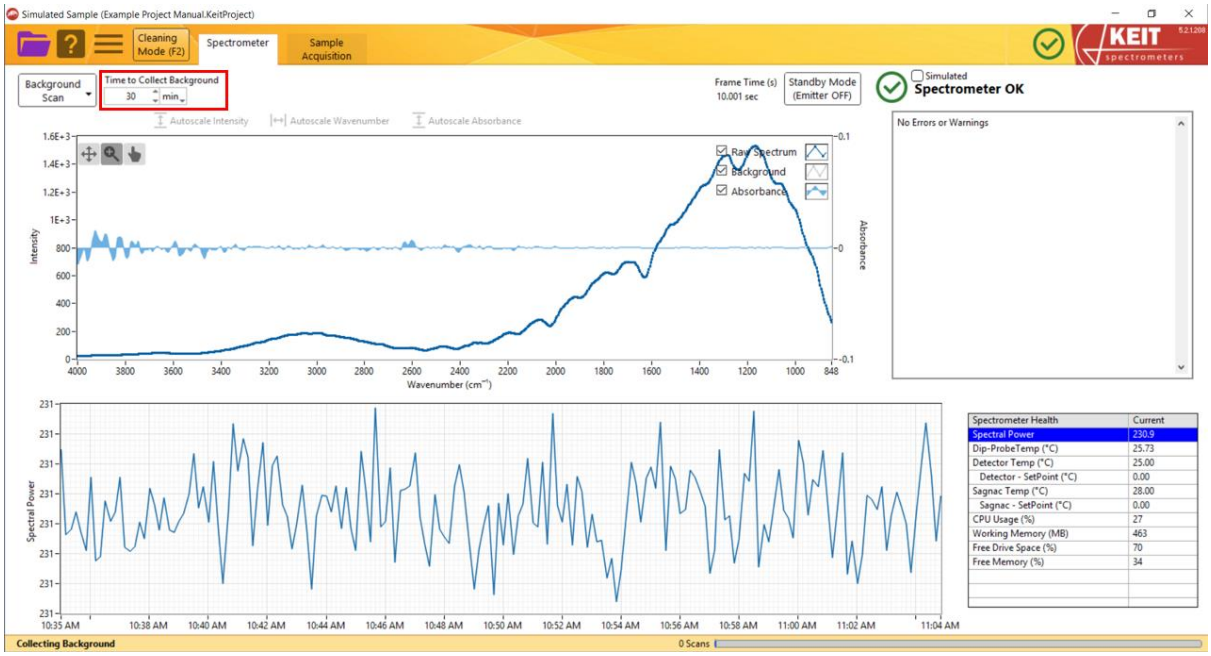


Figure 33: Changing background spectrum collection settings

Next, click **Background Scan > Collect New Background**.

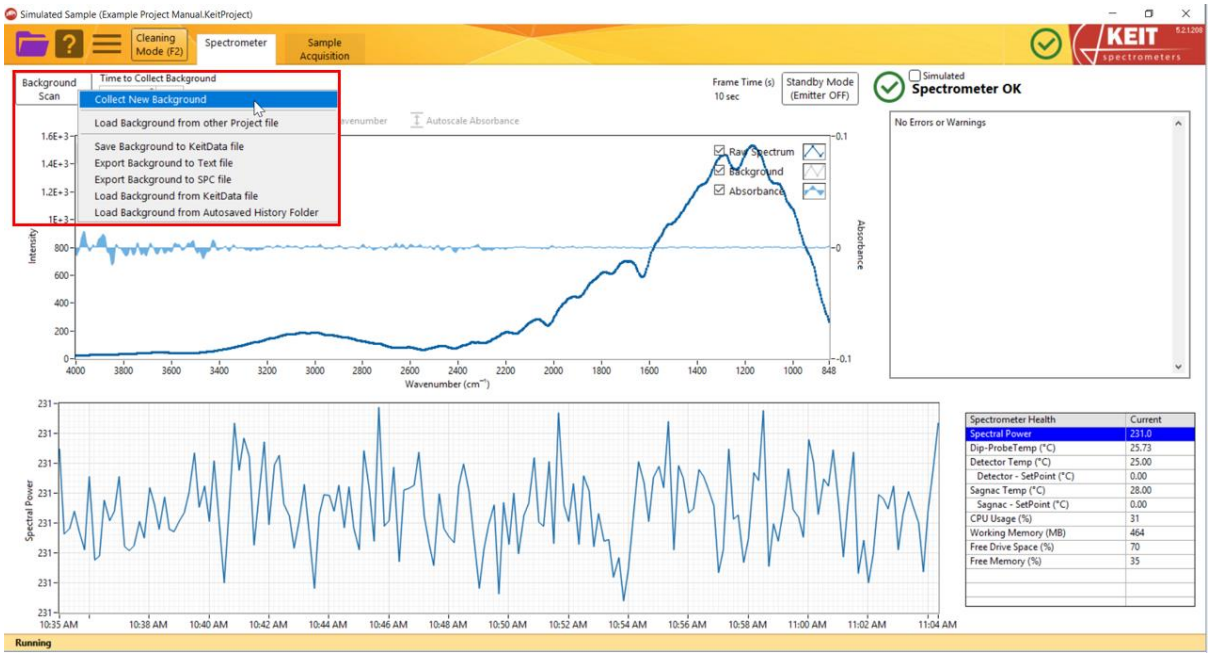


Figure 34: Recording a new background spectrum

The **Background Scan** button will turn green and a progress bar at the bottom right of the window will show the progress of the background scan. When the background scan has completed, the **Background Scan** button will return to its original white colour. Please note that background scan collection cannot be cancelled once it has been started.

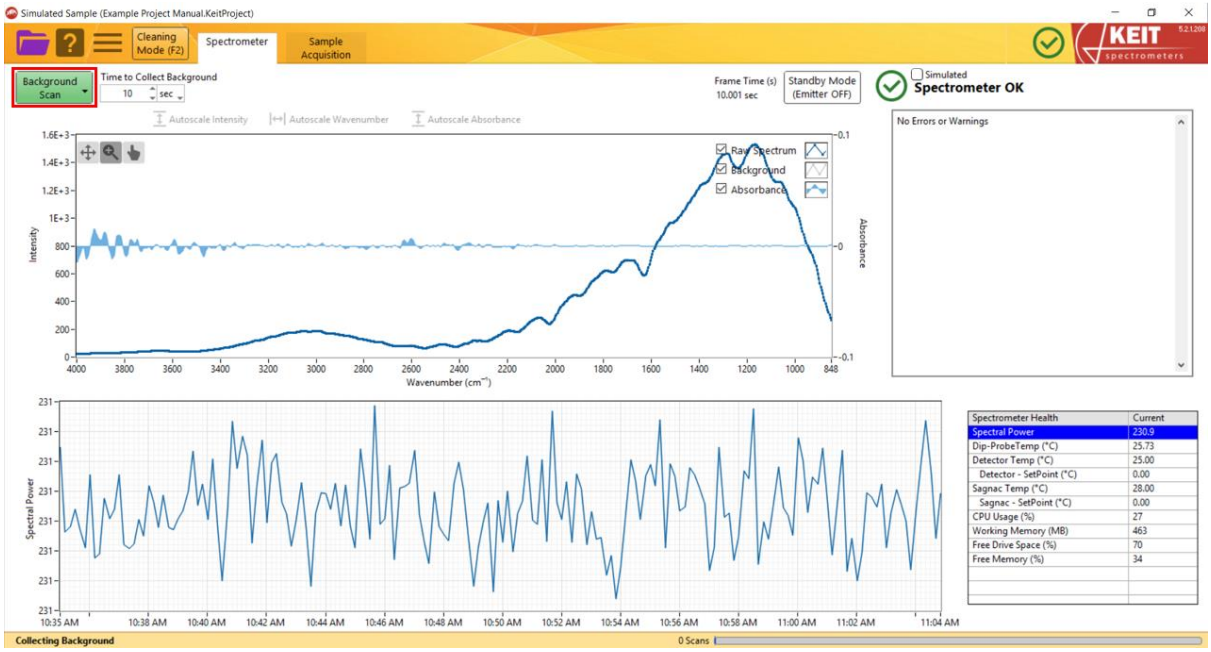


Figure 35: Recording of a new background spectrum in progress

4. You are now ready to collect spectra. On the **Sample Acquisition** tab, enter the name of the sample you are measuring and set the time to scan and number of samples. Keit recommends scanning for 120 seconds and taking three samples.

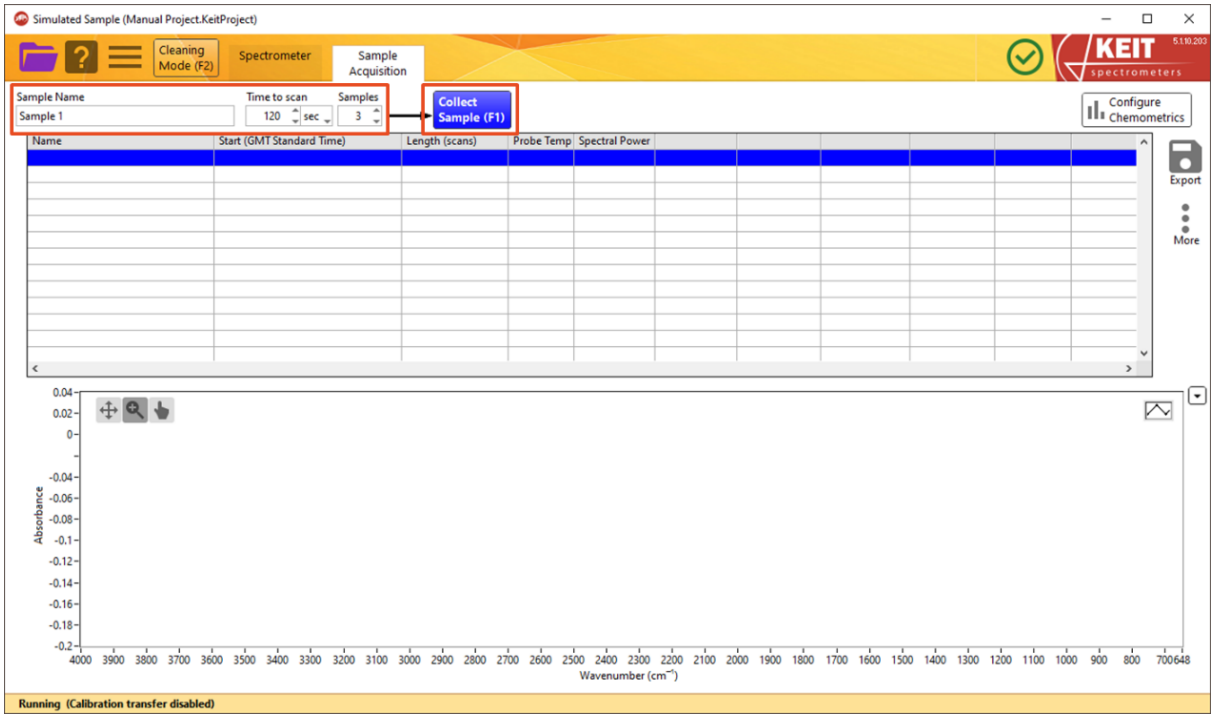


Figure 36: Collecting Manual Samples

5. Place your sample on the probe tip. Click the blue **Collect Sample** button or press F1 to collect samples. The **Collect Sample** button will go green during sample collection.

6. Spectra can be viewed once they have been saved in the Sample Acquisition tab. Click on a sample in the table to display its spectrum on the plot. You may select and display multiple spectra by ctrl+clicking or shift+clicking.

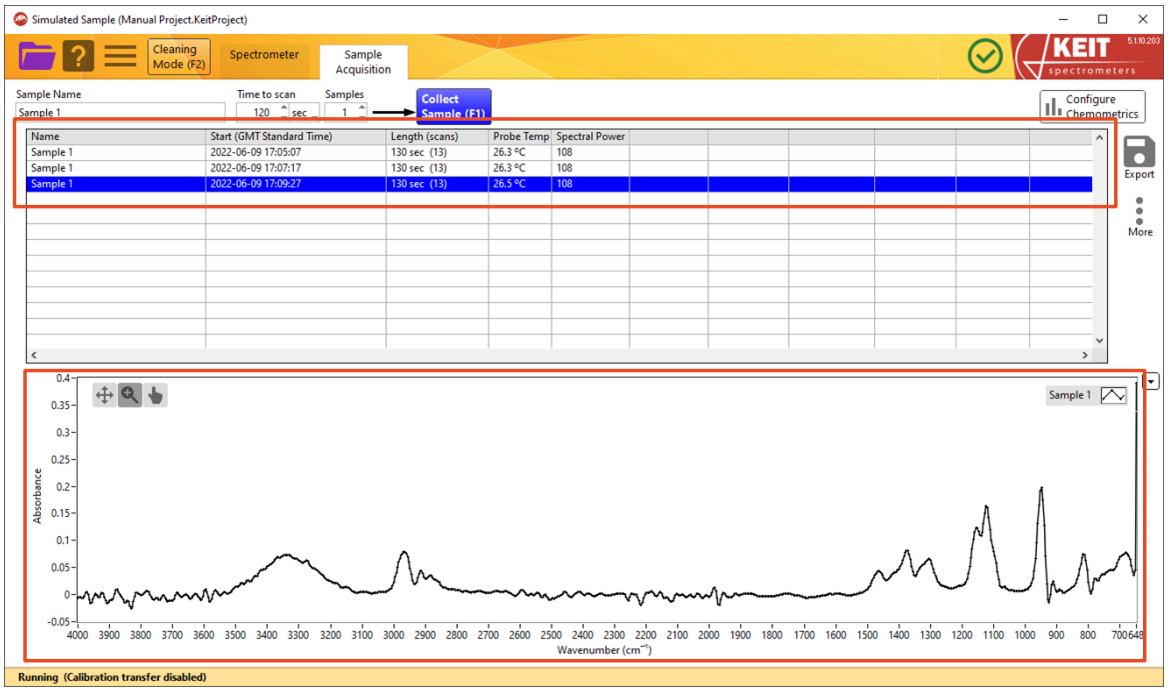


Figure 37: Viewing Manual Samples

7. To export the spectra of manual samples to a text file for import into a chemometrics modelling program, click the **Export** button, then select *Export Spectra to File > All Spectra*.

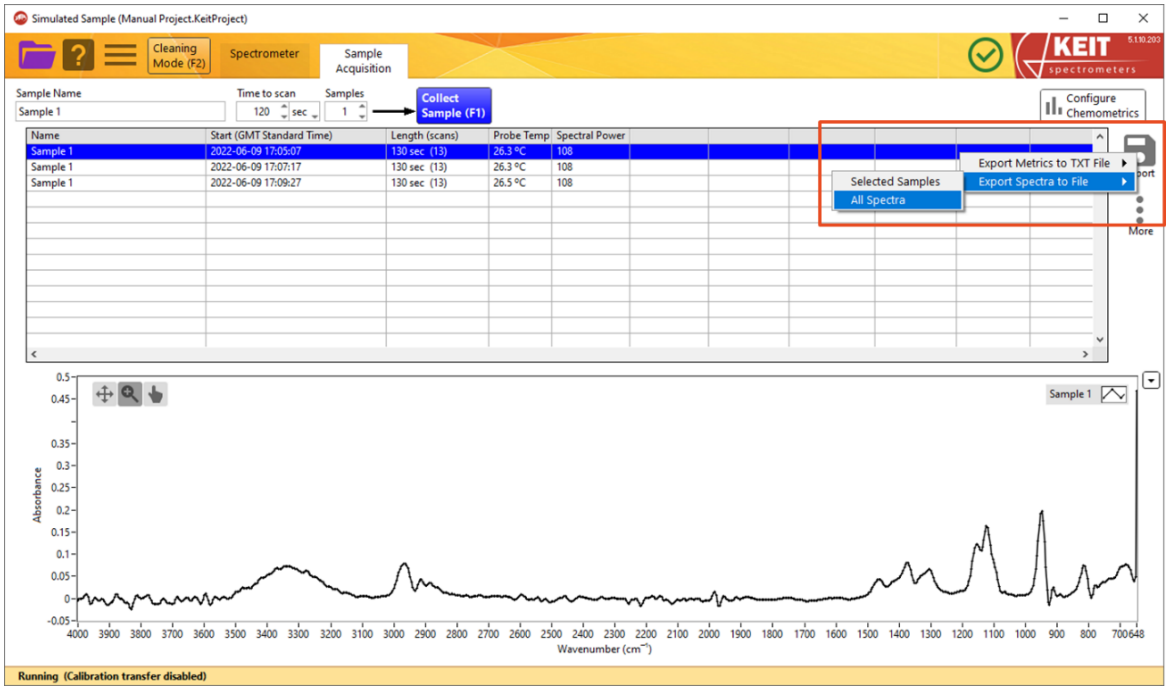


Figure 38**: Exporting spectra**

2. THE SPECTROMETER TAB

The Spectrometer tab provides setup information and ensures the instrument is working.

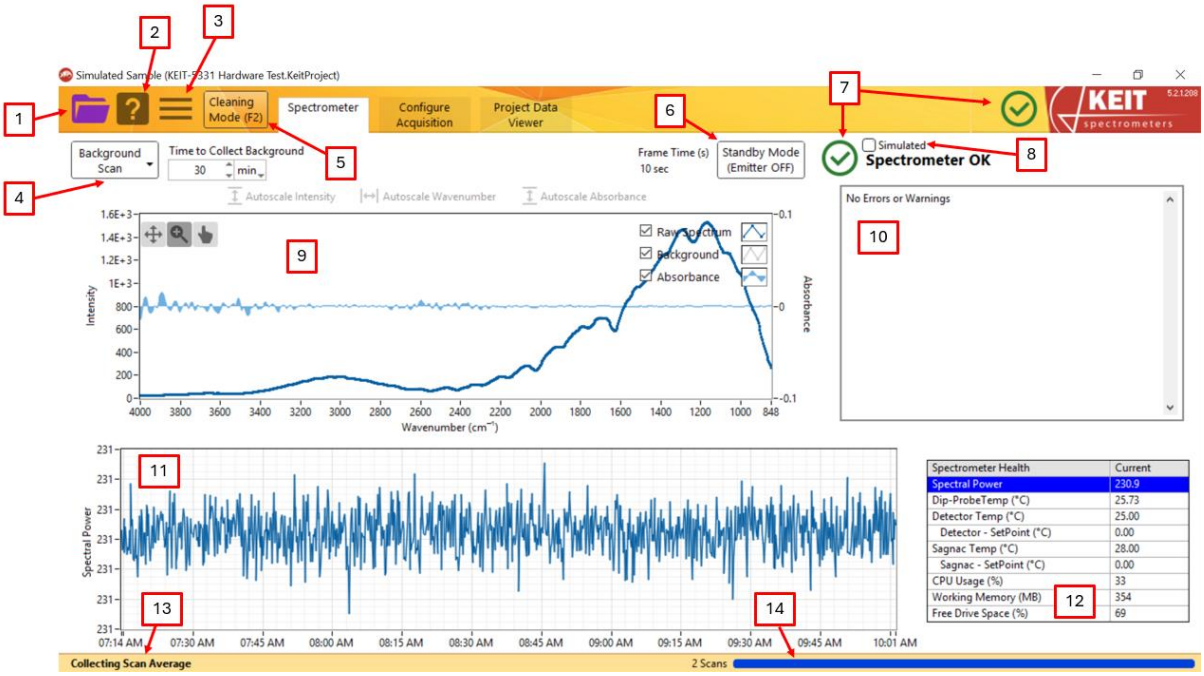


Figure 39: The Spectrometer tab

1. The File menu

a. **Create New Project from existing Project**: Creates a new project file of the same type (Continuous/Manual), copying all models, settings, and the background from the current open project file.

b. **Create new Empty Project**: Creates a new empty project file (either *Manual Sample Acquisition* or *Continuous Collection*).

c. **Save Copy of current Project (including data)**: Creates a copy of the current project, including all spectral data. This is the safest way to duplicate a project; copying in your file browser while the project is open in KeitSpec may corrupt the project file.

d. **Open Project:** Opens a project from disk. The project's background spectrum will replace the current background (if any). Use the Background Scan button options to load or collect a different background spectrum.

e. **Close Project**: This option can be used to safely close a project.

2. Context help

Context help appears in a floating window, providing information about the control or display the mouse pointer is hovering over. Use this feature to learn more about the software interface controls.

3. **More options**

   a. **Spectrometer Action**

      i. **Reset Spectrometer**: If the spectrometer stops responding, reset it using this dropdown.

      ii. **Reenable Sagnac TEC**: For some older models of IRmadillo (ASM0627-xx-x-**A**-x-x-x), exceeding the operating temperature range can damage electronics. Thermal stabilization will shut down automatically, and an error will appear in the Data Integrity pane (item 3110). Restart thermal stabilization when the IRmadillo returns to its specified temperature range.

   b. **Change Timezone**: Allows the user to change the timezone in which the project file is saved.

   c. **Create data package for Health Check**: Keit offers an annual health check as part of the IRmadillo's Maintenance and Support Programme (MSP). This control gathers the necessary files for Keit to perform the health check. To enrol in the MSP, contact your sales representative.

4. **Background scan**

FTIR requires a background spectrum (reference scan) before measuring absorption. Collect the background spectrum before inserting the probe into the reaction or process.

   a. **Collect New Background**: Collects a new background spectrum for the duration that is given in the Time to Collect Background boxes.

   b. **Load Background from other Project file**: Loads the background spectrum from another project file.

   c. **Save Background to KeitData file**: Saves the background spectrum in Keit's data format.

   d. **Export Background to Text file**: Saves the background spectrum as a human-readable text file.

   e. **Export Background to SPC file**: Saves the background spectrum as an SPC file.

   f. **Load Background from KeitData file**: Loads a background spectrum that has been saved in Keit's data format.

   g. **Load Background from Autosaved History Folder**: Background spectra are automatically stored on the IRmadillo's controller. This control allows these backgrounds to be reloaded into KeitSpec.

5. **Cleaning Mode**

Manual Cleaning Mode returns spectra every 2 seconds, useful for cleaning the probe tip. In this mode, spectra are not analyzed, stored, or reported via DCS. To return to Normal Running Mode, click 'Dismiss' or close the window.

6. **Standby Mode**

Standby mode disables the emitter (infrared light source) in the probe.

7. **Spectrometer Status**

Shows the status of the spectrometer. For more information, see Section 1.2 The Spectrometer tab: an overview.

8. Simulated Mode

Uses simulated data, allowing you to learn the software without a spectrometer.

9. Spectrum

Displays the current raw spectrum, absorption spectrum, and background reference spectrum. Use the top-left controls to zoom in on a specific spectral region.

10. Data Integrity pane

The spectrometer performs internal diagnostics to ensure reliable measurements. Any compromising conditions are shown in this panel, such as the instrument warming up. For more details, see Section 10 Troubleshooting.

11. Spectrometer health chart

Shows the metric that has been selected in the spectrometer health table.

12. Spectrometer health table

Relevant spectrometer performance metrics are shown in this table. Selecting a row plots the recent history of that metric in the spectrometer health chart.

13. Status bar

Instrument information appears in this bar, such as whether a background spectrum is loaded or if data is being collected. The status bar may show ‘(Calibration transfer disabled)’, referring to a spectral space transform technique. For most applications, calibration transfer between spectrometers is best done by augmenting the calibration with spectra from the second spectrometer. Some specialized applications benefit from using a spectral space transform on live data. Keit will advise on the best calibration transfer method during the calibration process if purchasing multiple instruments.

14. Progress bar

Shows the progress of the current scan.

3. CONTINUOUS COLLECTION: THE CONFIGURE ACQUISITION TAB

When you create a new project file in Continuous Collection mode, the Configure Acquisition tab will appear. This allows you to change the settings for data collection.

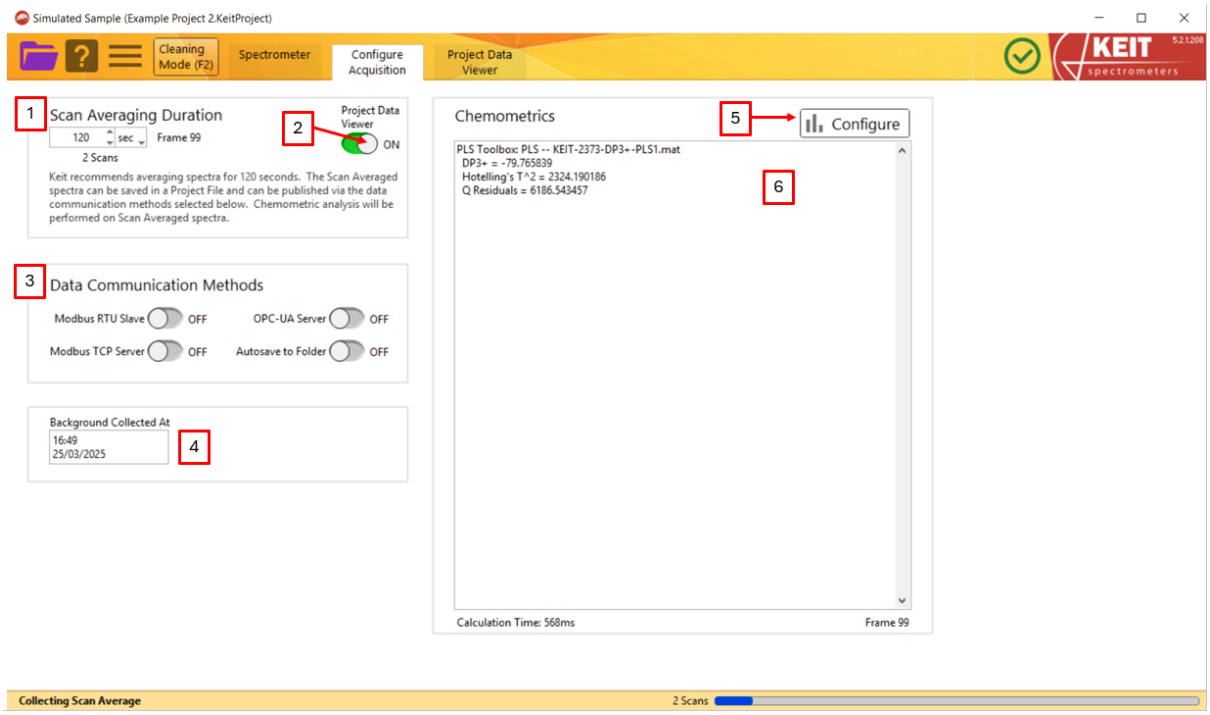


Figure 40: The Continuous Acquisition tab

1. Scan Averaging Duration

This sets the length of time for which spectra are averaged. Keit recommends averaging for 120 seconds for most applications.

2. Project Data Viewer toggle

When turned on, the Project Data Viewer tab will appear. This allows you to look at trends in the spectra over time. See Section 4 The Project Data Viewer tab for more information.

3. Data Communication Methods

KeitSpec can communicate data externally by four different methods: Modbus RTU (models ASM0627-xx-x-x-**O**-x-x only), Modbus TCP, OPC-UA (subject to the purchase of a separate OPC-UA licence), and by saving spectra to a folder over your local network. Use these toggles to enable the communication method(s) that are required.

4. Background collection time

This gives the date and time at which the background currently in use was collected.

5. Configure Chemometrics

KeitSpec includes analysis engines for chemometric models from various external software. The Configure Chemometrics button opens a window to adjust these models. When a model is loaded or changed, the software recalculates its outputs for all spectra in the Project file, which may take time for large files or complex models. See Section 3.1 Configure Chemometrics for details.

6. Chemometrics output pane

When chemometric models are loaded into KeitSpec, their outputs for the current spectrum will be shown in this pane. Any errors in the chemometric models will also be displayed here.

3.1. Configure Chemometrics

This allows chemometric models to be added or configured. The outputs of these chemometric models can be seen in the Project Data Viewer tab and are available over your DCS. No scaling is applied to the results as they are represented as floating point numbers.

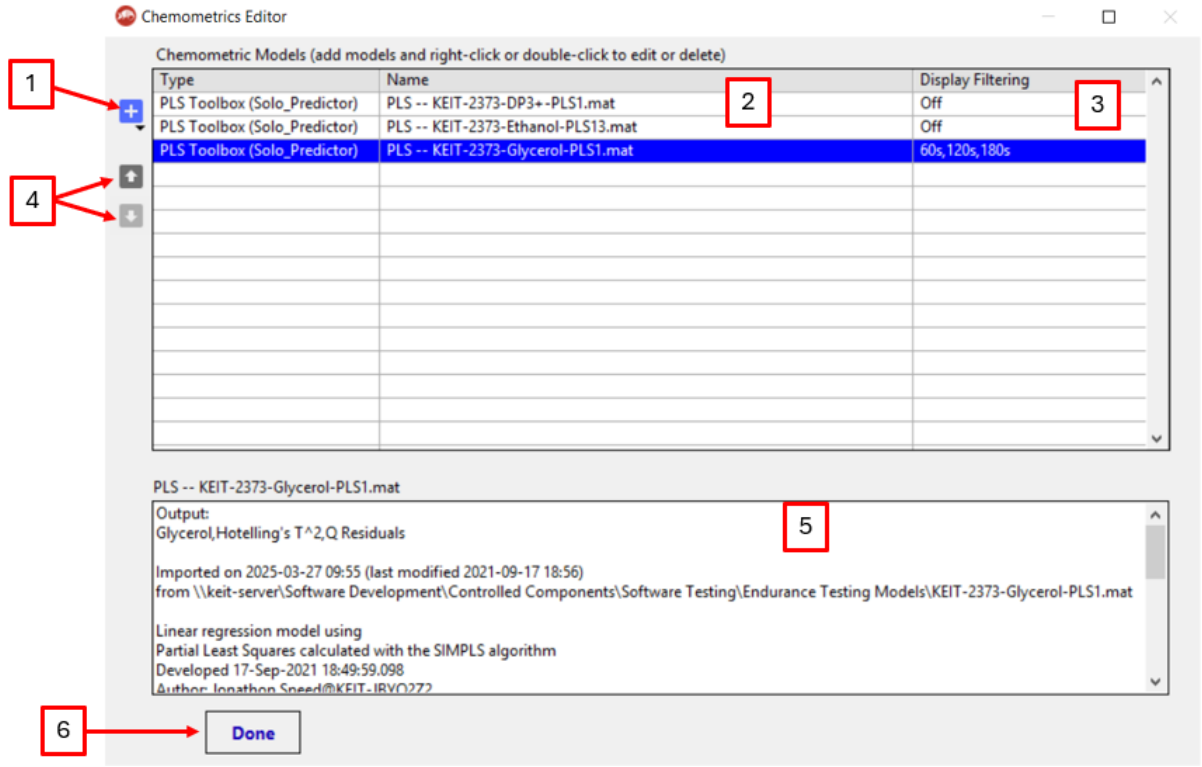


Figure 41: The Chemometrics Editor window

1. Add new model

This button is used to load chemometric models into KeitSpec. The following model types can be used:

a. **Unscrambler (Prediction)**: Quantitative models built using Unscrambler.
b. **Unscrambler (Classification)**: Qualitative models built using Unscrambler.

Unscrambler models are supported by the integration of the Unscrambler X engine version 11. A separate licence is required to use Unscrambler models.

c. **PLS Toolbox (Exported XML)**: Models built using EVRI's PLS Toolbox software and exported as XML files.
d. **PLS Toolbox (Solo_Predictor)**: Models built using EVRI's PLS Toolbox software and exported as Solo_Predictor (.mat) files.

Solo_Predictor models are run using Solo_Predictor version 4.1, shown below. This is installed on your controller as a standalone piece of software and runs automatically. A separate licence is required to use Solo_Predictor models.

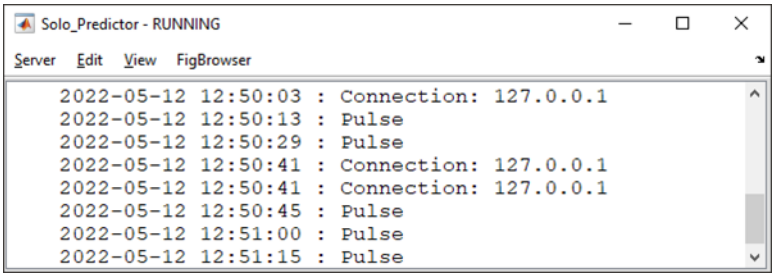


Figure 42: The Solo_Predictor window (standalone)

e. **Univariate**: Univariate models are based on peak height tracking and can be useful to monitor simple reactions.

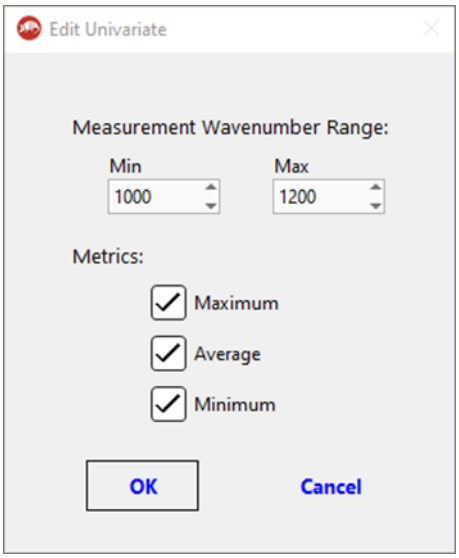


Figure 43: Editing Univariate models

f. **Calculation**: Calculation models perform calculations on the outputs of other chemometric models. Various mathematical operators are available, including Boolean logic and a time derivative (which is always performed as the final operation).

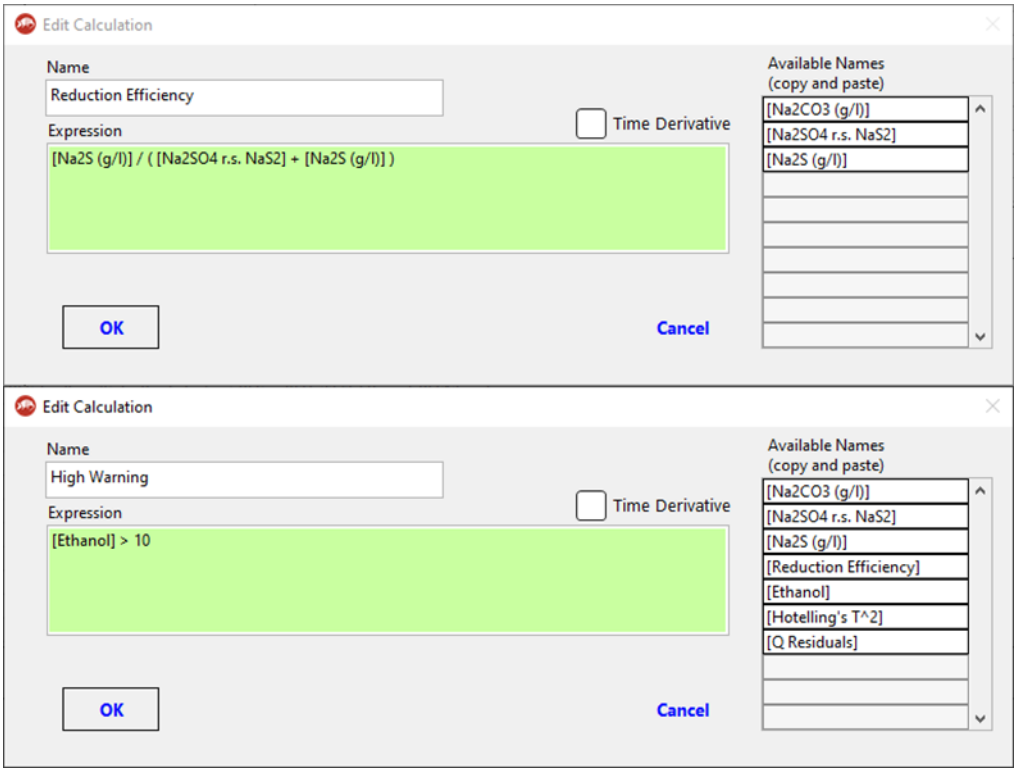


Figure 44: Examples of accepted syntax for Calculation models

2. List of currently loaded models

The models that are currently loaded into KeitSpec are listed here. Left-click to select a model, or right-click on a model to edit, duplicate or delete a model. Right-click anywhere inside this area to add an additional model.

For Solo_Predictor models only, it is possible to configure the outputs of the model. To do so, right-click on the model and select **Edit this Model**. The following dialogue will appear:

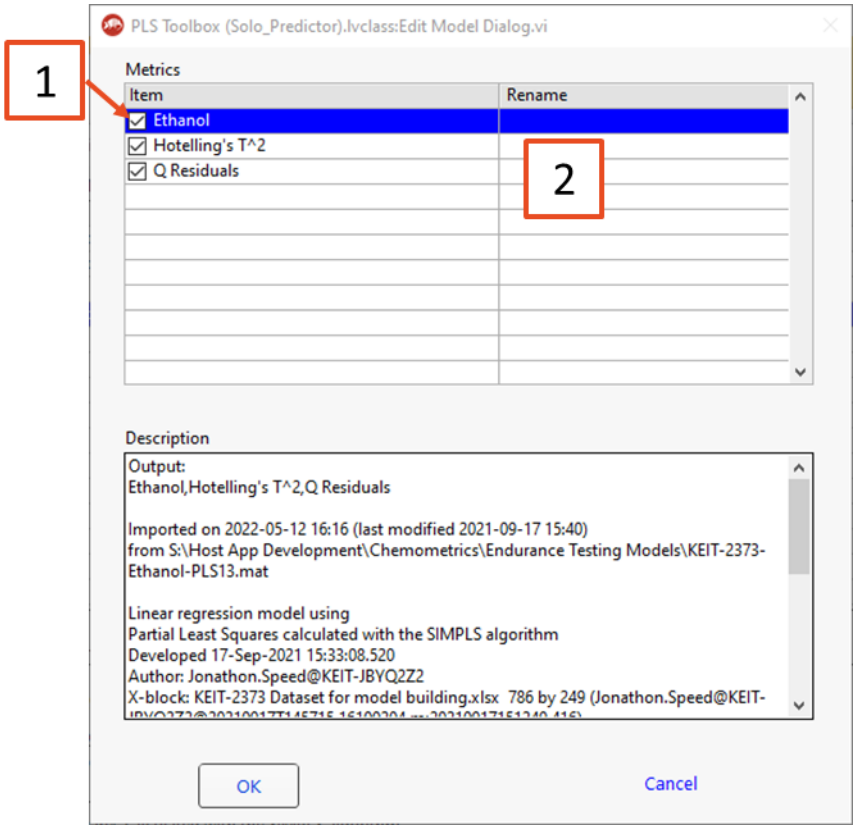


Figure 45: Editing Solo_Predictor model outputs

1. **Metric selector**. Metrics that are checked will be available for display in the Project Data Viewer tab and will be available over your DCS.
2. **Rename**. Click here to change the name of a metric.

3. Display Filtering Column

To apply an exponential filter, double-click the model in the display filtering column and enter the desired time constant.

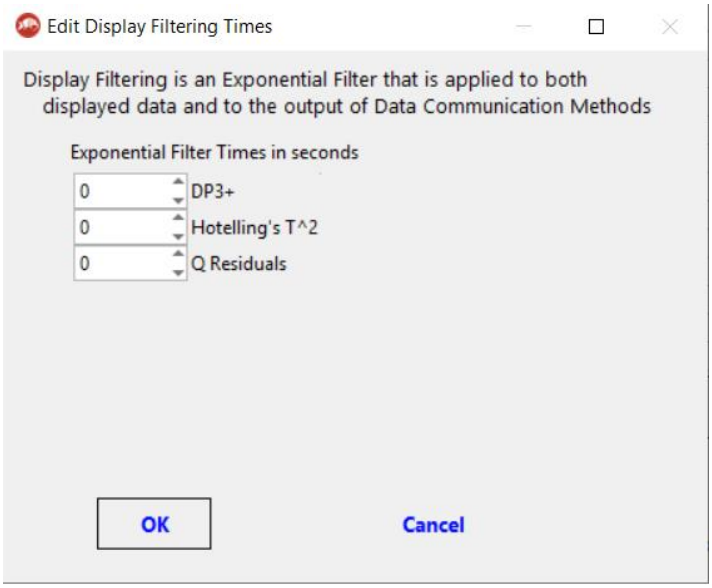


Figure 46 - Editing Display Filtering Times

4. Reorder buttons

To change the order of models, select a model and use the buttons to move it up or down the.

5. Model output pane

This shows a list of outputs and other information about the selected model.

6. Done

After configuring your models, press this to return to KeitSpec. This will apply the models to all spectra in the project file, which may take time for large files or complex models.

3.2. Chemometric Model Types

Supported Model Types			
Unscrambler Predictor	**Unscrambler Classifier**	**PLS Toolbox (Exported xml)**	**PLS Toolbox (Solo_Predictor)**
• PLS • PCR • SVR	• PLS-DA • SVC • SIMCA	• PLS • PCR • SVR • ANN	• PLS • PCR • MCR • LWR • SVR • ANN • PCA • PLS-DA • SIMCA • SVR-DA • ANN-DA

The following model types are not supported:

- Models which include non-wavenumber data (e.g., the dip probe temperature)
- PLS Toolbox (Exported xml) PCA models
- Solo_Predictor UMAP, ANNDL and ANNDLDA models

3.3. Notes on Building and Exporting Models

- KeitSpec can support Unscrambler models which have been exported in either Full or Short Prediction mode, but please note that Short Prediction mode does not support either Hotelling's T^2 or Q-residuals. These values will be shown as NaN in KeitSpec.
- When using OSC, MSC or EMSC pretreatments in Unscrambler, it is important to include these in the model when exporting for use in KeitSpec. For PLS models ensure that the option to include the pretreatment models is selected; for SVR models Keit recommends saving a separate Unscrambler file that includes the OSC/MSC/EMSC models of interest and the SVR calibration and loading that into KeitSpec for use. See Section 10.2 Common chemometrics errors for more details.
- Models built in PLS Toolbox must be exported correctly for them to work in KeitSpec. From the File menu, select Export Model > To File > MATLAB MAT file (*.mat).

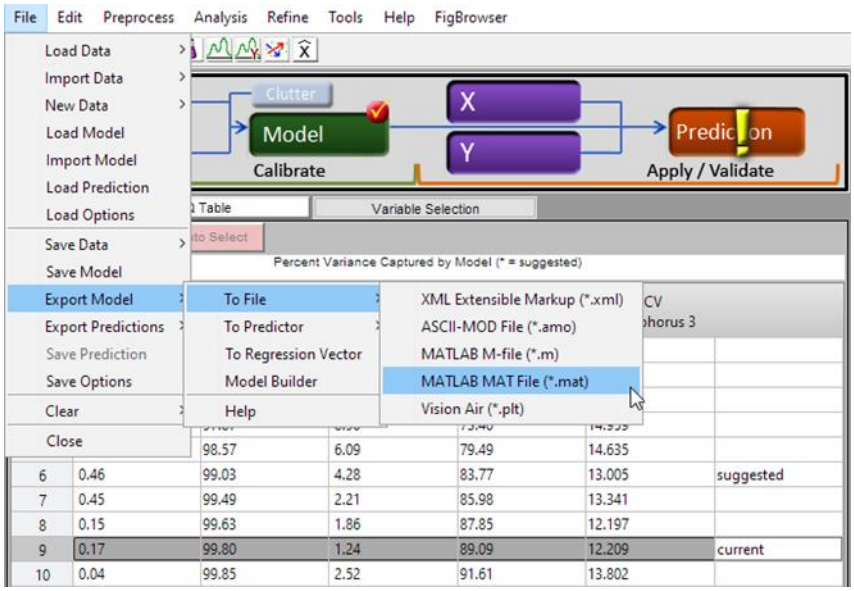


Figure 47: Exporting a model from PLS_Toolbox

3.4. Interpreting Confidence models

As part of calibration, Keit may build a model to indicate whether or not we are confident in the results from the IRmadillo. These models will return '0' if the results are within specification, and '1' if there is low confidence in the reported values.

There are a number of possible reasons why the IRmadillo's results may not be reported as low confidence, including:

- Your process has drifted outside its calibration space, e.g., your IRmadillo may have been calibrated for a range of ethanol concentrations between 0 and 15% but the current sample contains 18% ethanol.
- A change has been made to your process, e.g., a different enzyme has been used that the IRmadillo has never 'seen' before.
- The temperature or pressure of your process has moved outside the range over which your IRmadillo was calibrated.
- Water vapour or another contaminant is present in the air supply to your IRmadillo
- The spectrum from your IRmadillo has changed due to its components aging.

In most cases, your calibration models will need to be 'augmented' by rebuilding with additional sample points. Contact Keit on support@keit.co.uk to arrange this.

4. THE PROJECT DATA VIEWER TAB

The Project Data Viewer tab allows the display and export of the data that has been saved in the project file.

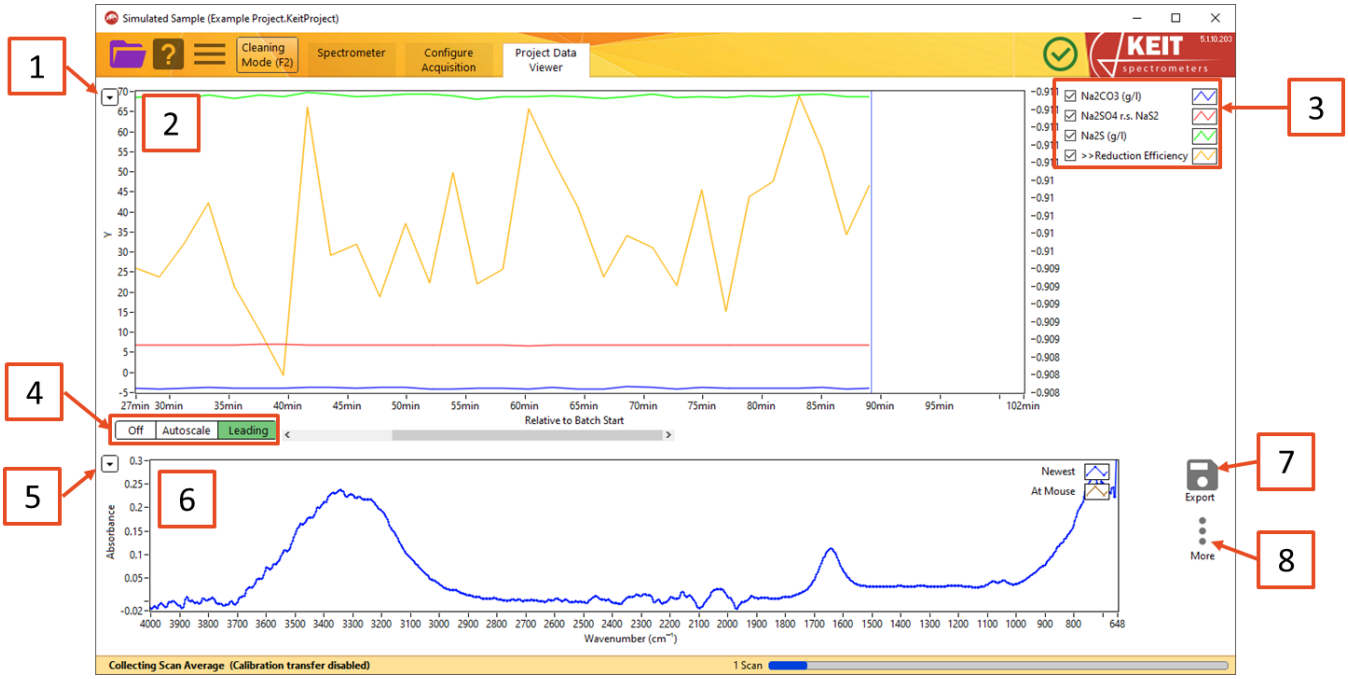


Figure 48: The Project Data Viewer tab

1. Trends plot options

Use this button to display a contextual menu to allow the trends plot display to be adjusted.

a. Time Axis: Choose whether the plot is displayed in hours since data collection started (*Relative to Batch Start*), in the timezone of the project file, or in UTC Standard Time.

b. Apply display Filtering: Choose whether filtered data will be displayed or not.

c. Export: Allows the data that are currently displayed in the trends plot to be exported to a range of different file types, including copying it directly to the Windows clipboard, to an Excel spreadsheet (requires a working copy of Microsoft Excel to be installed), or as an image.

d. Autoscale Y Axes: By default, the y-axis or axes are set to show the full range of data. If you wish to show a smaller range, uncheck this option so that the plot does not rescale whenever a new sample is displayed.

e. Export Metrics to TXT File: Allows the model outputs to be exported to a (human-readable) .txt file. You can choose to export either only the data that are currently being displayed on the plot, or all the data that has been collected.

f. Export Spectra to File: Allows the spectra themselves to be exported to a file. You can choose to export only the data that are currently being displayed on the plot (As Viewed); all the spectra that have been collected; or only the spectra which you have marked (by right-clicking on the Trends plot). You can then choose whether to export the spectra to a human-readable text file or to an SPC file.

g. **Import Spectra:** Allows the import of spectra from different project files to the current project file
h. **Time options**: The time period over which data are displayed may be adjusted as required.

2. Trends plot

Shows chemometric model outputs over time. If no models are present, the plot will be blank. Measurements can be displayed on the primary or secondary y-axis. Moving the cursor over the plot shows the spectrum measured at that time in the Spectra pane.
To mark individual spectra for correlation with external events (e.g., adding reactants or adjusting parameters), hover over the desired spectrum/time period, right-click, select 'Set Marker Here,' enter a name, and click OK.

3. Trends plot legend

This gives a key to the items that are plotted in the Trends plot. You can right-click on the text of an entry to change whether it is plotted against the left or right y-axis.

4. Trends plot range options

This control allows the time scale shown on the Trends plot to be changed.

Off holds the current view range unchanged as data are updated.

Autoscale (default) shows all the data that have been collected.

Leading shows the most recent data; the history is defined by the range chosen in the options for the trends plot.

5. Spectra plot options

Use this button to display a contextual menu to allow the spectra plot to be adjusted.

a. **Add Plot**: Add the spectrum of a marked sample to the plot.
b. **Display Type**: Allows you to choose whether to display absorbance spectra, transmission spectra or raw spectra.
c. **Autoscale X/Y**: The X and Y ranges of the plot are scaled to show the whole spectrum. If you wish to concentrate on a smaller range, unchecking these options will prevent the plot rescaling each time a new sample is displayed.
d. **Export**: Allows the data that are currently displayed in the spectra plot to be exported to a range of different file types, including copying it directly to the Windows clipboard, to an Excel spreadsheet (requires a working copy of Microsoft Excel to be installed), or as an image.

6. Spectra plot

This plot shows the most recent spectrum (‘Newest’), the spectrum under the cursor in the Trends plot (‘At Mouse’), and any marked spectra that have been selected.

7. Export

Allows spectra or trends to be exported.

a. **Export Metrics to TXT File**: Allows the model outputs to be exported to a (human-readable) .txt file. You can choose to export either only the data that are currently being displayed on the plot, or all the data that has been collected.

b. **Export Spectra to File**: Allows spectra export to a file. Choose to export data currently displayed (As Viewed), all collected spectra, or only marked spectra (right-click on Trends plot). Options include a human-readable text, or SPC files.

8. More

For each spectrum, diagnostic information is available to assess the instrument or calculation performance. The spectrum for which information is displayed is the one under the cursor if the cursor is over the Trends panel, or for the most recent spectrum if not.

a. **Show Frame Info**: Opens a floating window that displays diagnostic information about the spectrometer for that spectrum.

b. **Show Frame Info (Full)**: Opens a floating window that displays extensive diagnostic information about the spectrometer for that spectrum.

c. **Show Chemometrics Info**: Displays the model output from the current set of calculation parameters for that spectrum.

d. **Show Spectrometer Settings**: Displays a floating window with information about the spectrometer, including software version numbers and serial numbers.

e. **Backgrounds (Change or Export)**: Allows the saved spectra to be re-calculated using a new background (reference) scan and allows the export of the current background scan.

4.1. Changing and Exporting the Background Scan

This allows the background spectrum that was used to calculate the absorbance spectrum to be changed. This is useful if, for example, you discover that your probe was not clean when you calculated the original background spectrum, which would mean that all data collected subsequently would be incorrect.

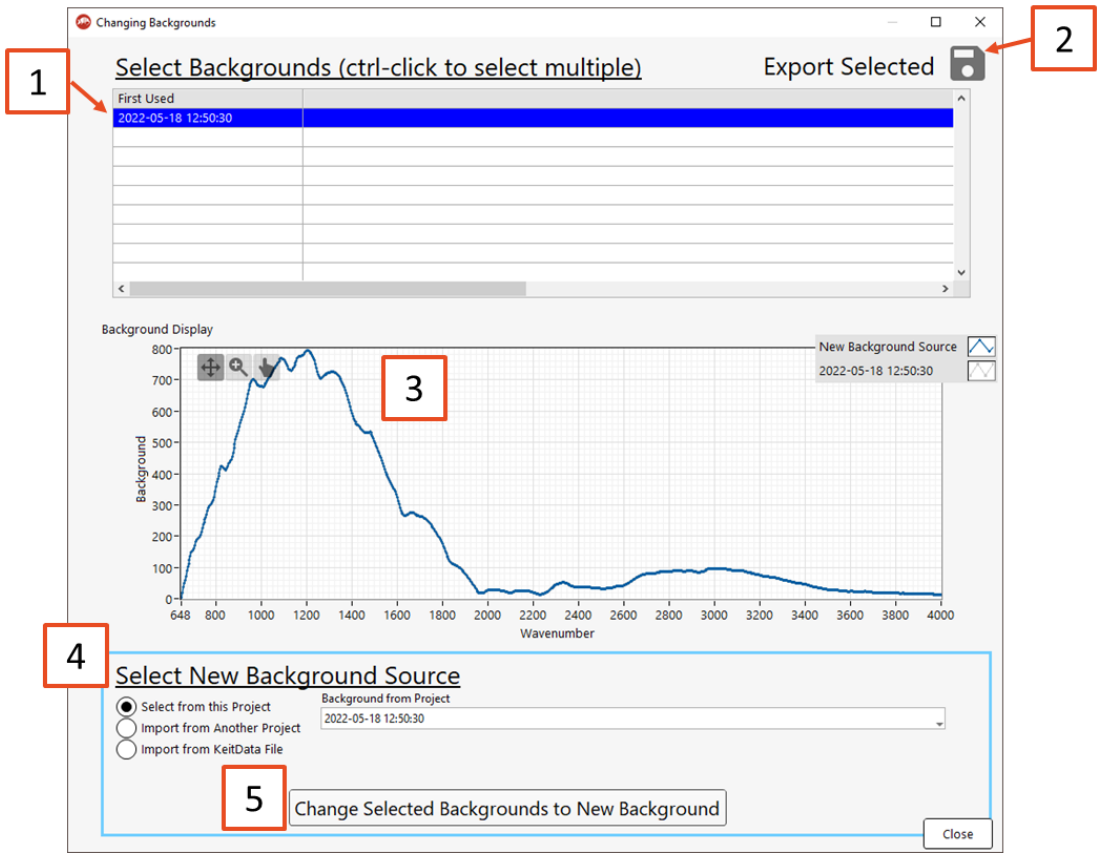


Figure 49: The Change Backgrounds window

1. Select Backgrounds

Choose the spectra for which you would like to change the background. The spectra are grouped by the background that is currently applied. Backgrounds that have been collected but with which no spectra have been taken will not appear in this list.

2. Export Selected

Allows the currently selected background spectra to be exported as a text file.

3. Background Display

This shows the currently selected and, if chosen, new background scans, in order to allow verification that the replacement background makes sense. Check to ensure that you are happy with the replacement background before proceeding with the substitution.

4. Select New Background Source

Select the source of the background that you wish to use to replace the current background. This can be a different background scan from the current project; a background scan saved in a different project file; or a spectrum that has been saved as a KeitData file.

5. Change Selected Backgrounds

Recalculates the absorbance spectra with the new background. This operation is irreversible, so please ensure that you have saved a copy of the project file before proceeding.

5. DATA COMMUNICATION – MODBUS RTU SLAVE

The IRmadillo (model numbers ASM0627-xx-x-x-**O**-x-x only) supports data communication using Modbus RTU.

5.1. Enabling the Modbus RTU Slave tab

To enable communication by Modbus RTU, one must first create or open a continuous project (see Section 1.3 Collecting spectra in a continuous process). Then, under Data Communication Methods, move the relevant Data Communication Methods switch to ON (**1**). This will reveal the Modbus RTU Slave tab (**2**).

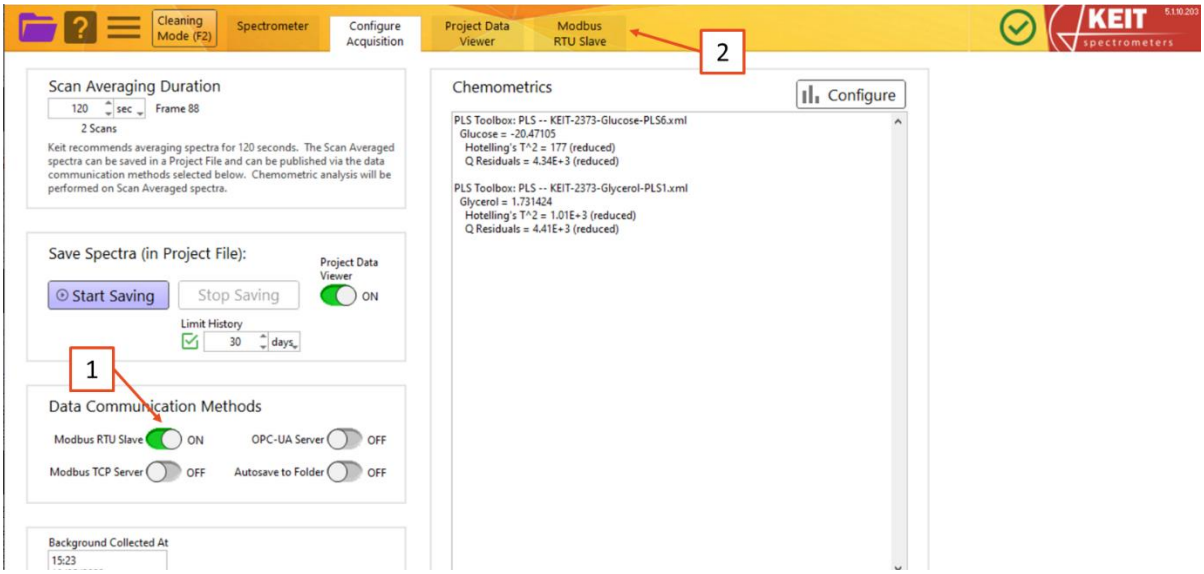


Figure 50: Enabling Modbus RTU Slave

For more information on implementing and configuring Modbus RTU, see DOC0871 Commissioning Guide: Data Communication – Modbus RTU.

5.2. Modbus RTU Slave tab

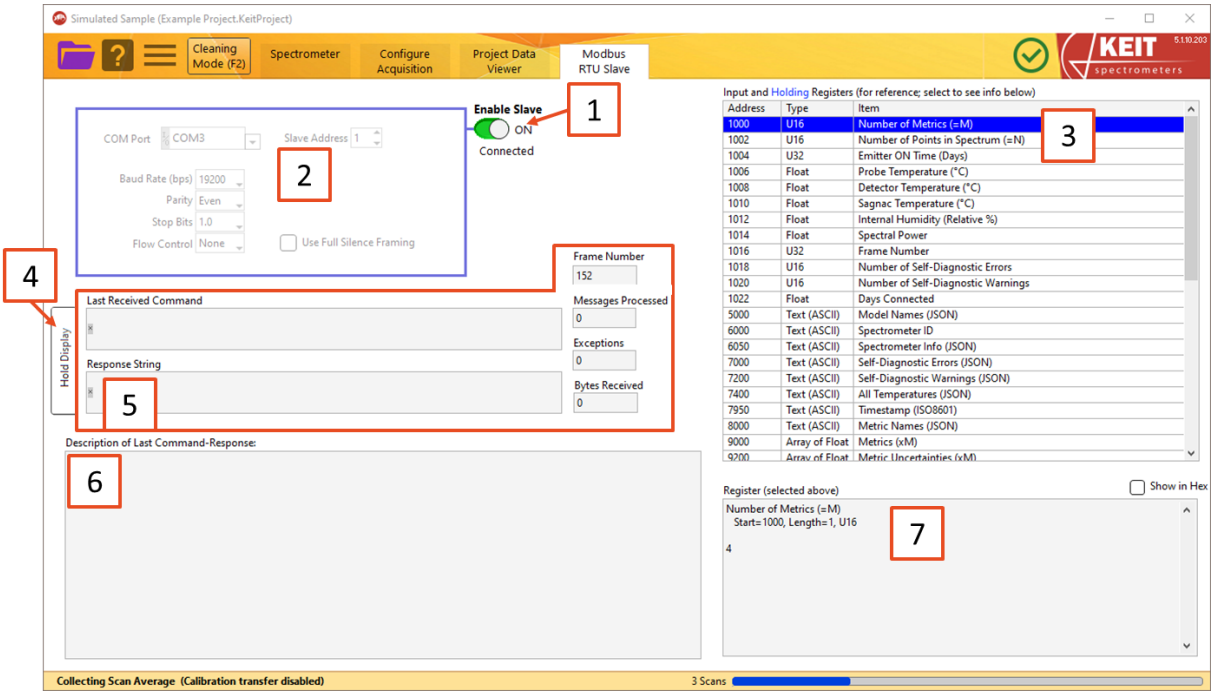


Figure 51: The Modbus RTU Slave tab

1. Enable Slave

Switch *Enable Slave* to ON to begin communicating with your DCS/Modbus server.

2. Modbus settings

Configure the slave settings as required to match your DCS settings. This can only be done while *Enable Slave* is switched to *OFF*.

3. Register List

The available data outputs, their data types, and register addresses are shown in the table. Select a register to view its contents in the *Register View* box below. The register numbers are given in decimal.

4. Hold Display

If the *Command Debug* view is changing too rapidly to read, use this button to freeze the display.

5. Command Debug

The last Modbus command that was received, along with the response that the instrument returned are shown in this box (as Modbus RTU strings). Various other metrics are shown to assist with debugging a connection to your DCS. Note that the frame number will update every averaging time.

6. Description of Last Command-Response

KeitSpec's response to the last command is shown here. The response will be interpreted in various ways to show you what you should expect from your Modbus RTU server.

7. Register View

Displays the contents of the register that is selected in the list above. Check the *Show in Hex* box to view the data in hexadecimal format.

6. DATA COMMUNICATION – MODBUS TCP SERVER

The IRmadillo supports data communication using Modbus TCP.

6.1. Enabling the Modbus TCP Server tab

To enable communication by Modbus TCP, one must first create or open a continuous project (see Section 1.3 Collecting spectra in a continuous process). Then, under Data Communication Methods, move the relevant Data Communication Methods switch to ON (**1**). This will reveal the Modbus TCP Server tab (**2**).

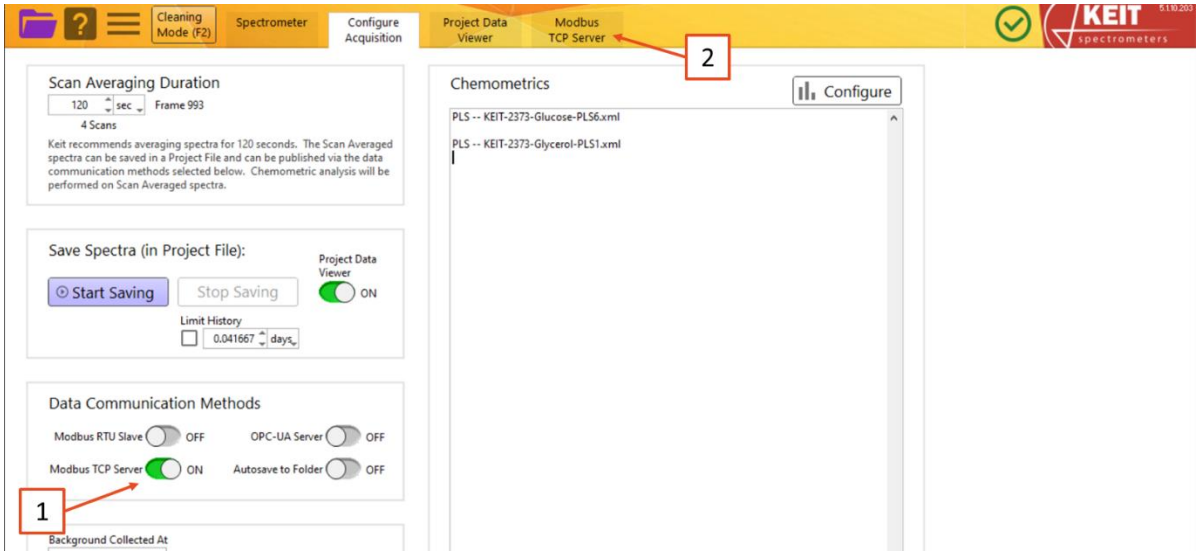


Figure 52: Enabling the Modbus TCP Server tab

For more information on implementing and configuring Modbus TCP, see DOC0817 Commissioning Guide – Data communications – Modbus TCP.

6.2. Modbus TCP Server tab

The Modbus TCP Server tab is shown below:

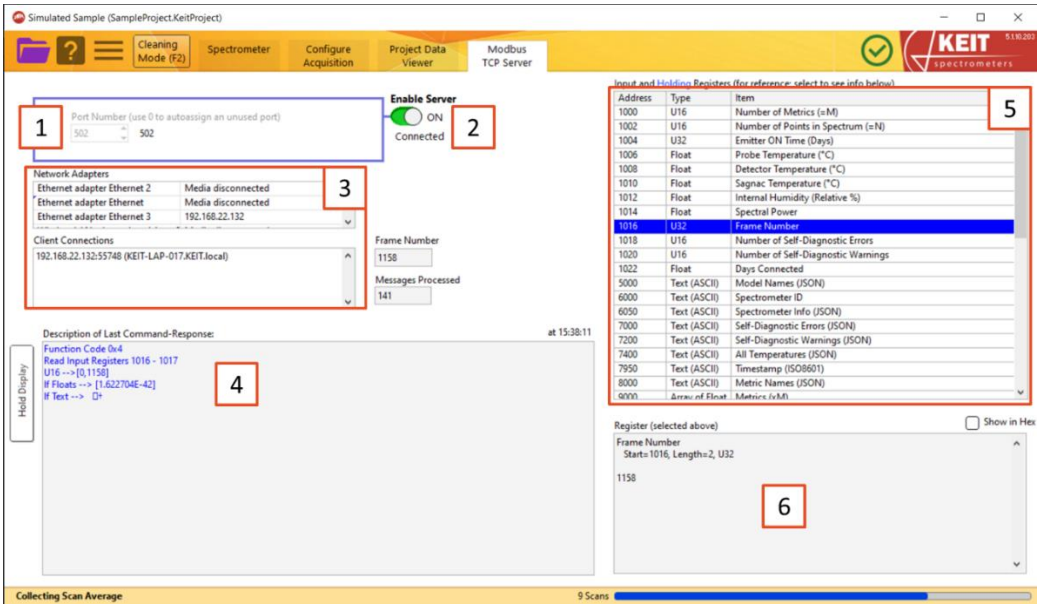


Figure 53: The Modbus TCP Server tab

1. **Port number selection**

Configure the server's port number as required to match your DCS settings. This can only be done while *Enable Server* is switched to *OFF*.

2. **Enable Server**

Once the port number is selected, switch *Enable Server* to *ON* to begin communicating with your DCS/Modbus client.

Windows Defender Firewall may prompt you to enter your administrator password on switching *Enable Server* on for the first time.

3. **Network Adapters and Client Connections**

Information on current network connections and their status (Network Adapters), and active Modbus TCP connections (Client Connections).

4. **Command Debug**

The last Modbus command that was received, along with the response that the instrument returned are shown in this box. Use the Hold Display button to freeze the display if the values change too rapidly to read. The number of messages processed and errors received are also shown to assist in debugging a connection to your DCS.

5. **Register List**

The available data outputs, their data types, and register addresses are shown in the table. Select a register to view its contents in the register box (6) below. In this example, 1016 "Frame Number" is selected. The contents of the chemometric results registers (registers 8000–20000) will depend on which chemometric analysis is being performed. The register numbers are given in decimal.

6. **Register View**

Displays the contents of the register that is selected in the list above. Check the *Show in Hex* box to view the data in hexadecimal format.

7. DATA COMMUNICATION – OPC-UA

The instrument can communicate over OPC-UA with a plant control system, subject to the purchase of an additional software license for the OPC server. This tab allows the communication to be set up and communications to be debugged.

OPC-UA requires an active connection to a local network that is shared with the computers or control hardware that will consume the data that the IRmadillo generates.

7.1. Enabling the OPC-UA tab

To enable communication by OPC-UA, one must first create or open a continuous project (see Section 1.3 Collecting spectra in a continuous process). Then, under Data Communication Methods, move the relevant Data Communication Methods switch to ON (**1**). This will reveal the OPC-UA tab (**2**).

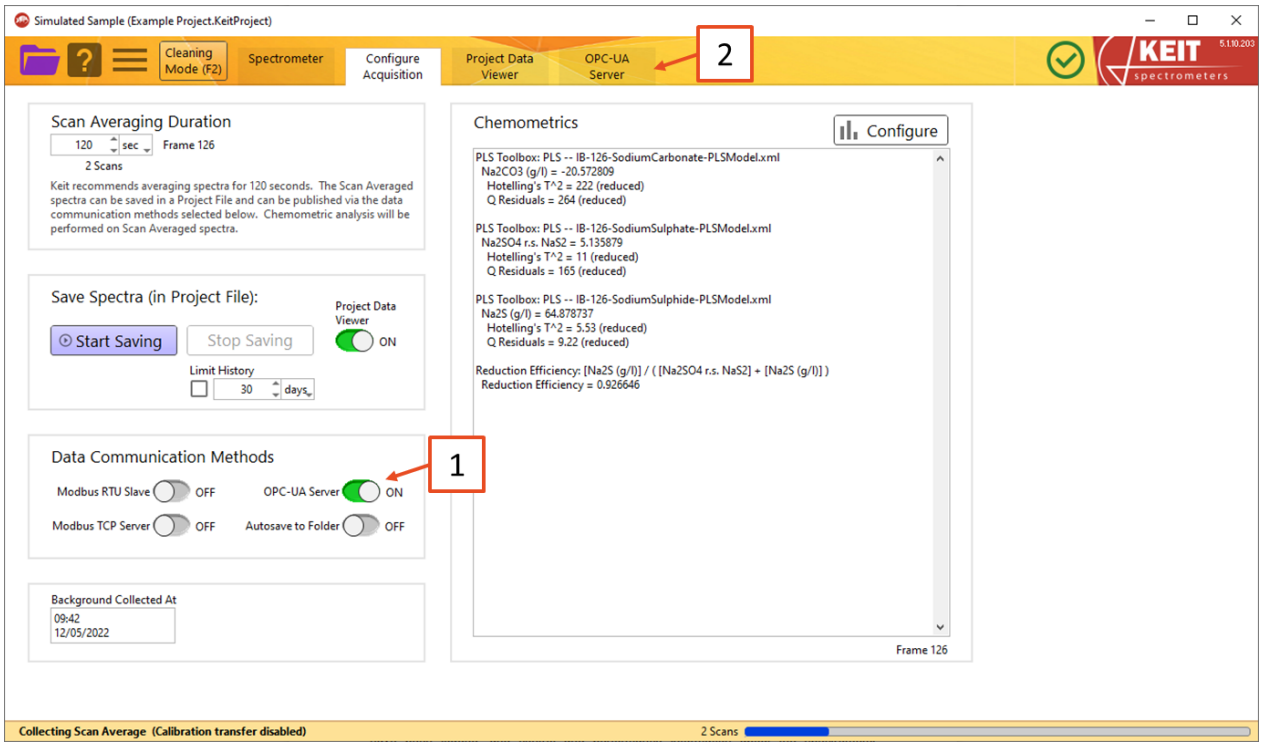


Figure 54: Enabling the OPC-UA tab

7.2. The OPC-UA tab

For more information on implementing and configuring OPC-UA, see DOC0828 Commissioning Guide – Data communications – OPC-UA.

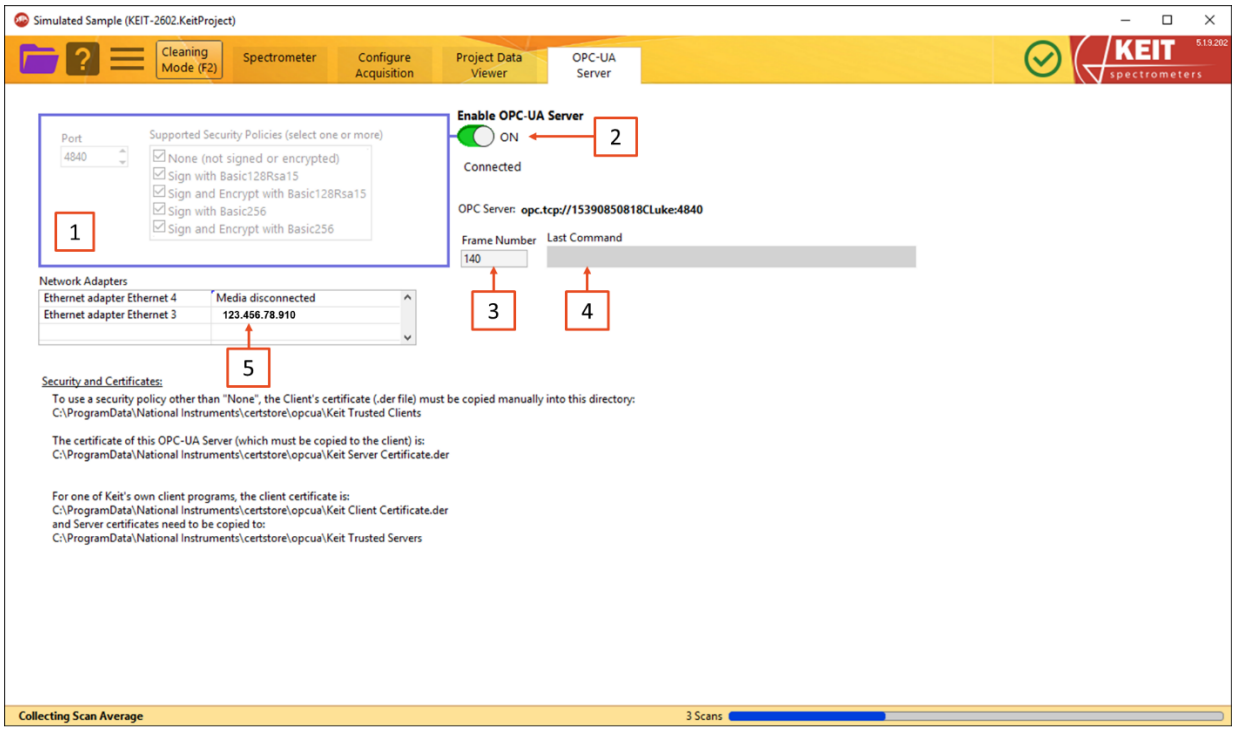


Figure 55: The OPC-UA tab

1. **Communications and security settings**

   Configure the OPC-UA server to match your plant control system's settings.

2. **Enable server**

   Once the settings are configured, use this switch to begin communicating with your OPC-UA client.

3. **Frame number**

   This displays the frame number in KeitSpec. This can be useful for debugging. It will update every scan averaging duration.

4. **Command Debug**

   The last OPC command that was received is displayed in this box to help with debugging the connection to the plant control system.

5. **Network Adapters**

   This gives a list of the available adapters and current connections to the controller.

8. DATA COMMUNICATION – AUTOSAVE TO FOLDER

The Autosave to Folder function allows you to save absorbance spectra to a folder automatically as they arrive, so that they can be read in real-time by another program (a 'watched folder').

8.1. Enabling the Autosave to Folder tab

To enable communication by autosaving to a watched folder, one must first create or open a continuous project (see Section 1.3 Collecting spectra in a continuous process. Then, under *Data Communication Methods*, move the relevant Data Communication Methods switch to *ON* (**1**). This will reveal the *Autosave to Folder* tab (**2**).

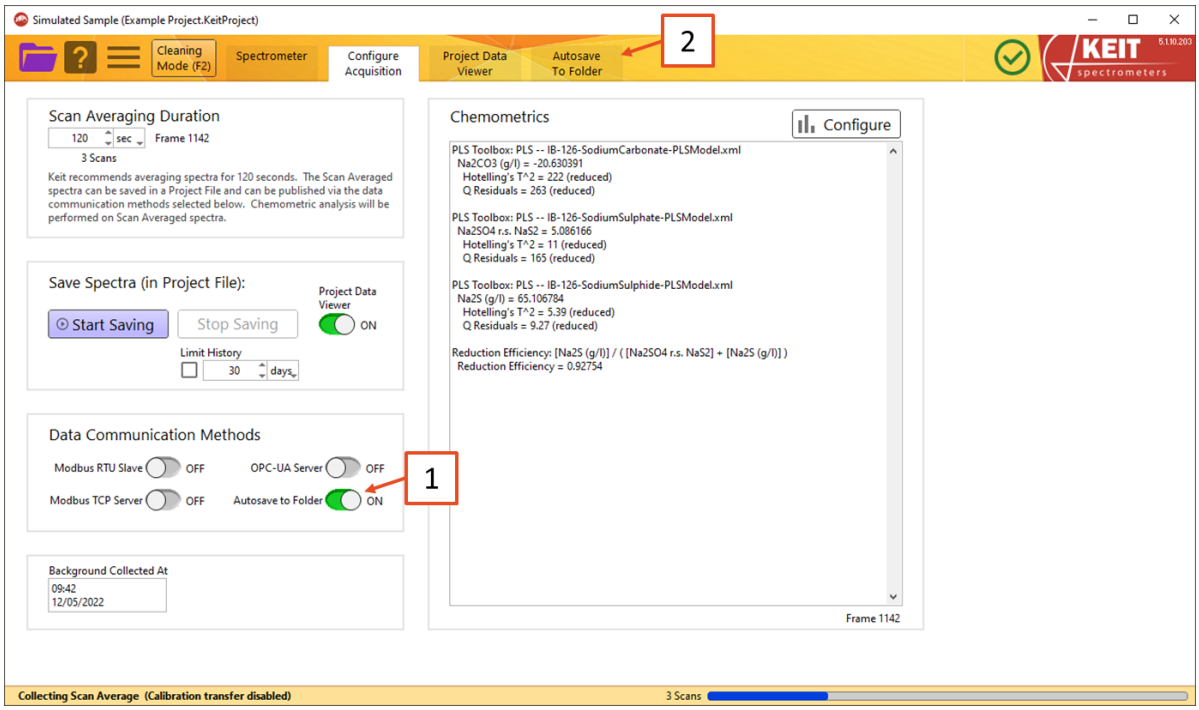


Figure 56: Enabling the Autosave to Folder tab

For more information on implementing and configuring autosaving to a watched folder, see DOC0876 Commissioning Guide – Data Communication – Watched Folder.

8.2. The Autosave to Folder tab

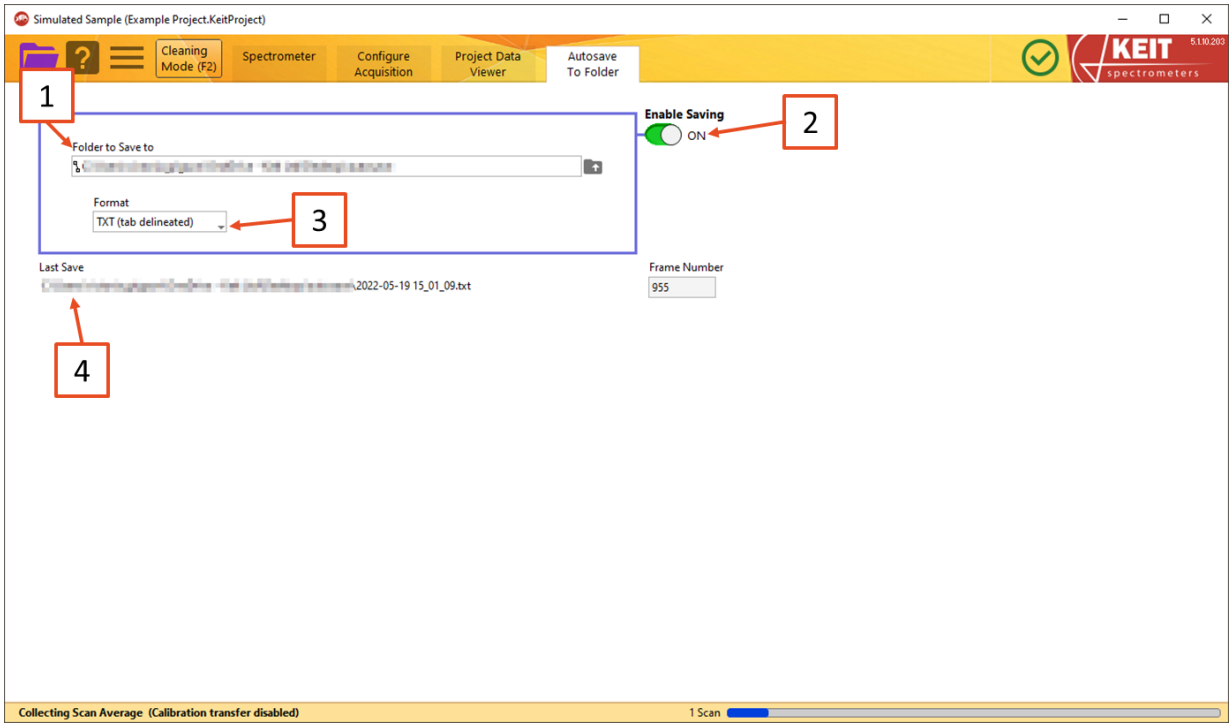


Figure 57: The Autosave to Folder tab

1. Folder to Save To

The folder in which spectra will be saved. This may be local or over a network.

2. Enable Saving

Turn data saving on and off using this toggle.

3. Format

Spectra can be saved either in text (.txt) or SPC format.

4. Last Save

The filename and full path of the most recent spectrum to be saved. Note that the filename is the time at which the spectrum was collected.

9. MANUAL SAMPLING: THE SAMPLE ACQUISITION TAB

Creating a new Manual Sample Acquisition project or opening a previously stored one will cause the Sample Acquisition tab to appear in the tab bar. This project type will allow you to collect individual spectra.

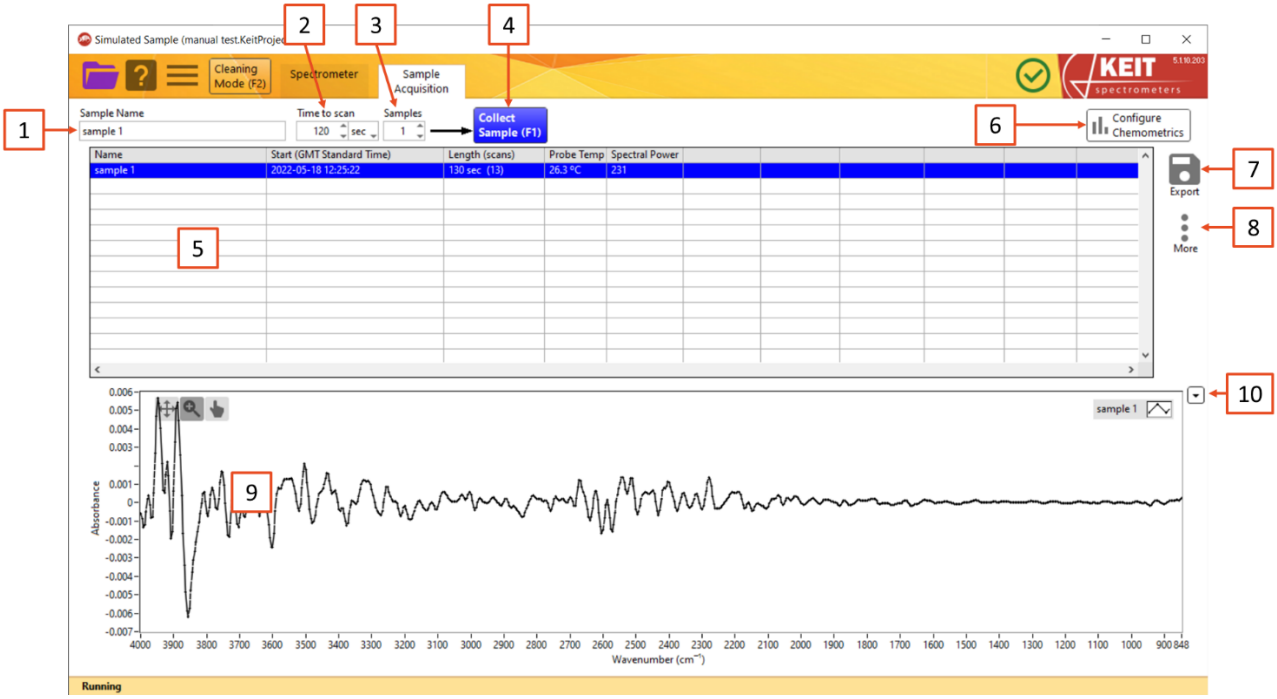


Figure 58: The Manual Sample Acquisition tab

1. Sample Name

Each sample that you collect can be named for later identification

2. Time to scan

Use this box to specify the sampling duration for each spectrum. Keit recommends sampling for 120 seconds.

3. Samples

If you wish to make several measurements of a single sample, specify the number in the Samples box. The instrument will make successive scans of the same sample. Keit recommends taking three measurements of each sample.

4. Collect Sample

Click this button, or press F1, to begin sampling.

As each measurement is collected, the number in the Samples box will automatically decrease to show the number that remain to be collected. Collection is also indicated by the button turning green and both the status bar and progress bar displaying the action. Samples are automatically saved to the current project – there is no separate 'Save' action.

5. Data panel

After each sample has been collected, information about it will appear in this panel. Each line refers to a different measurement. To display the absorption spectrum for that sample in the spectrum panel (9), click on it. Multiple spectra may be selected by Ctrl-clicking with the mouse. Right clicking a sample provides additional options.

a. **Edit this sample**: Allows you to rename a sample.
b. **Delete this sample**: Permanently erases a sample. A warning dialogue will appear.
c. **Show Sample Frame Info**: Opens a floating window that displays diagnostic information about the spectrometer for that sample.
d. **Show Sample Frame Info (Full)**: Opens a floating window that displays extensive diagnostic information about the spectrometer for that spectrum
e. **Backgrounds (Change or Export)**: Allows the saved spectra to be re-calculated using a new background (reference) scan, and allows the export of the current background scan. See Section 4.1 Changing and Exporting the Background Scan for more information on how to use this feature.

6. Configure chemometrics

The KeitSpec application contains analysis engines that can use chemometric models generated by a number of software vendors. When a model is configured, a summary of the results output is visible in the data panel (5).

This button opens a floating window to allow the chemometric model(s) to be configured and adjusted. When the model is loaded or changed, the software will reprocess all samples in this project against it. This may take a few minutes for a large batch or complex model. Refer to Section 3.1 on Chemometrics for further information about the chemometric models.

7. Export

Use this button to export data about the samples for use with analytical software (such as chemometric model-building software). You can export the sample metrics which contains all the data displayed in the data panel (5) or export the spectra which contains the raw data.

a. Export metrics to TXT file
   i. Selected samples
   ii. All data
b. Export spectra to file
   i. Selected samples
   ii. All data

8. More (see Section 4 The Project Data Viewer tab)

a. Show Sample Frame Info
b. Show Sample Frame Info (Full)
c. Backgrounds (Change or Export)

9. Spectrum panel

The spectrum of the currently selected sample(s) in the data panel (5) is displayed in this panel. Several spectra may be overlaid by selecting multiple samples in the data panel by Ctrl-clicking on multiple rows.

10. Graph panel options

Provides additional options for the Spectrum panel (9). These can also be accessed by right clicking the Spectrum panel.

a. Display Type

You can change what is displayed on the spectral panel depending on what provides the most value to you.

i. Absorbance
ii. Transmission
iii. Raw Spectrum

b. Visible items

i. Plot Legend

c. AutoScale X

The X range is scaled to show the whole spectrum. Uncheck this option to see sections of the range without rescaling

d. AutoScale Y

The Y range is scaled to show the whole spectrum. Uncheck this option to see sections of the range without rescaling

e. Export

Allows the data that is currently displayed in the spectrum panel (H) to be exported to a range of different file types, including copying it directly to the Windows clipboard, an Excel spreadsheet (requires a working copy of Microsoft Excel to be installed), or as an image.

i. Export Data to clipboard
ii. Export Data to Excel
iii. Export Data to DIAdem
iv. Export simplified image

10. TROUBLESHOOTING

If you encounter any issues during integration and use of the IRmadillo, please contact Keit (support@keit.co.uk).

10.1. Controller administrator guidance

When connecting the IRmadillo's controller to communicate to your distributed control system (DCS) using Ethernet, you will need to connect it to your local area network (LAN). Some changes may be required to ensure compliance with your internal Information Technology (IT) policies. Changes to the controller may cause the spectrometer to become unreliable. The information below should help to avoid problems.

Item	Guidance
User account to run spectrometer	A domain or local user account may be used. KeitSpec does not support simultaneous running by two different users. Keit recommends always using the same user account to run the spectrometer.
Automatic Login	The controller incorporates an auto-restart feature. To take advantage of this, the user account allocated to run the spectrometer **must** be set to automatically log in and run the KeitSpec software.
Domain Joining	You may join the IRmadillo to your domain network. When you do this be careful not to accidentally disable the auto-restart functionality. Examples of possible problems include: - Legal notices requiring user intervention on login - Automatic login being disabled If auto-restart is disabled then you will need to manually access the IRmadillo and login to the user account.
Administrator account	Do not use the administrator account for running the spectrometer. The administrator account should only be used to configure the controller. A domain or local user account may be used for normal operations.
Virus scanning software	You may install your own anti-virus software, but Keit does not guarantee reliability if you do so. When installing an anti-virus solution, please ensure it does not disrupt the spectrometer by consuming too much CPU when scanning or updating.
Windows updates	Windows updates may cause spectrometer outages, including automatic restarting of the controller. Windows updates are set to be run manually by default so that they can be installed during planned maintenance.
BIOS password	You may set a BIOS password if you wish.

Firewall	For Modbus TCP and OPC-UA communications, the KeitSpec application will need to be granted permission to communicate over your network. If you experience problems connecting, then check the controller's firewall policy.

10.2. Common chemometrics errors

Issue	Possible Cause	Potential Solution
Error 5115 occurred at Unscrambler: ERR_SUBMODEL_ERROR: Error in a sub-model file such as MSC/EMSC/OSC.	Multiple models have been applied in Unscrambler, but not all the models have been loaded into KeitSpec.	Import the whole Unscrambler file into KeitSpec, then select the correct model from within KeitSpec.
Error 5151 occurred at Unscrambler: ERR_INPUT_ERR: Some error in data used for prediction, e.g., column dimension mismatch.	Classifier models: The spectra on which the model was built has a different wavenumber range to that used by the spectrometer.	Rebuild the model using the full wavenumber range.
Error 5000 occurred at PLS Toolbox (Solo_Predictor). Error using parsemixed. No numerical data could be found in the file.	The model has not been correctly exported from PLS Toolbox.	Export the model correctly (see Section 3.3 Notes on Building and Exporting Models).
	The model is not communicating with Solo_Predictor.	Ensure that Solo_Predictor is running; delete the model from within KeitSpec; close and restart KeitSpec; then re-import the model.
Models return 0, NaN or no results	One or more unsupported models or pretreatments have been used.	Choose a different model or pretreatment. Refer to Section 3.2 Chemometric Model Types.
	An Unscrambler Classifier model has been imported as an Unscrambler Predictor model or vice versa.	Ensure that the correct model type has been imported.

Issue	Possible Cause	Potential Solution
Predictions that do not match those in Unscrambler, PLS_Toolbox or Solo	Wavenumber axis has been inverted.	Rebuild the models with the correct wavenumber axis.
	One or more unsupported models or pretreatments have been used.	Choose a different model or pretreatment. Refer to Section 3.2 Chemometric Model Types.

11. OFFLINE VIEWER

The KeitSpec Offline Viewer allows previously collected spectra to be explored and visualised. Opening KeitSpec Offline Viewer will automatically prompt you to select a file to load. Select a .KeitSpec file and click OK to load it, or else click Cancel to proceed without loading data to view.

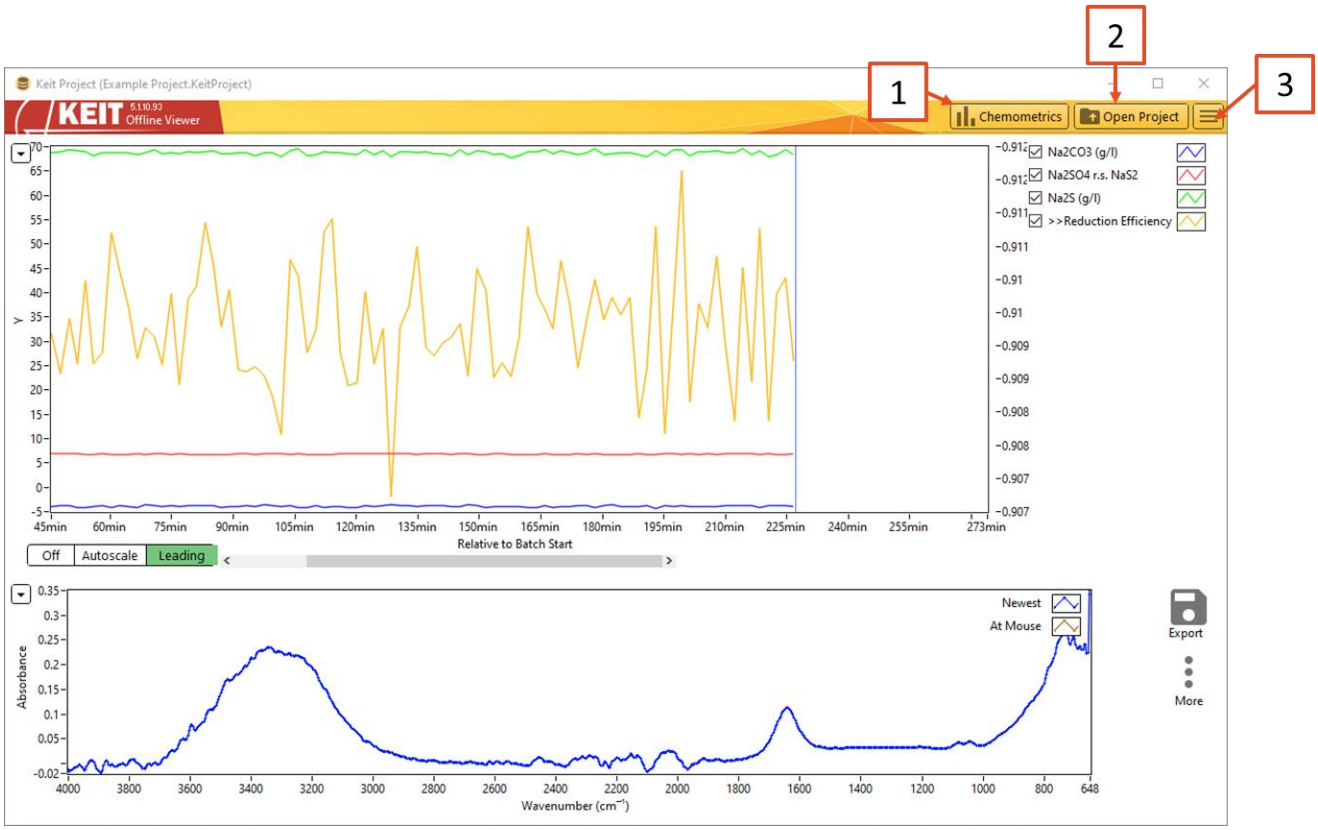


Figure 59: The Offline Viewer

1. Chemometrics

The Configure Chemometrics button opens a new floating window which allows the chemometric model(s) to be configured and adjusted. Please note that when a model is loaded or changed, the software will automatically recalculate the outputs of this model for all spectra stored in the Project file. For large Project files or complex models, this may take a long time.

Refer to Section 3.1 Configure Chemometrics for more information about chemometric models.

2. Open Project

Opens a file explorer dialogue to allow a project file to be opened.

3. More options

a. **Change Timezone**: Allows the user to change the timezone in which the project file is saved.

The appearance of the offline viewer will vary depending on whether the project that has been opened is a continuous or manual project.

11.1. Offline viewer: Continuous data collection

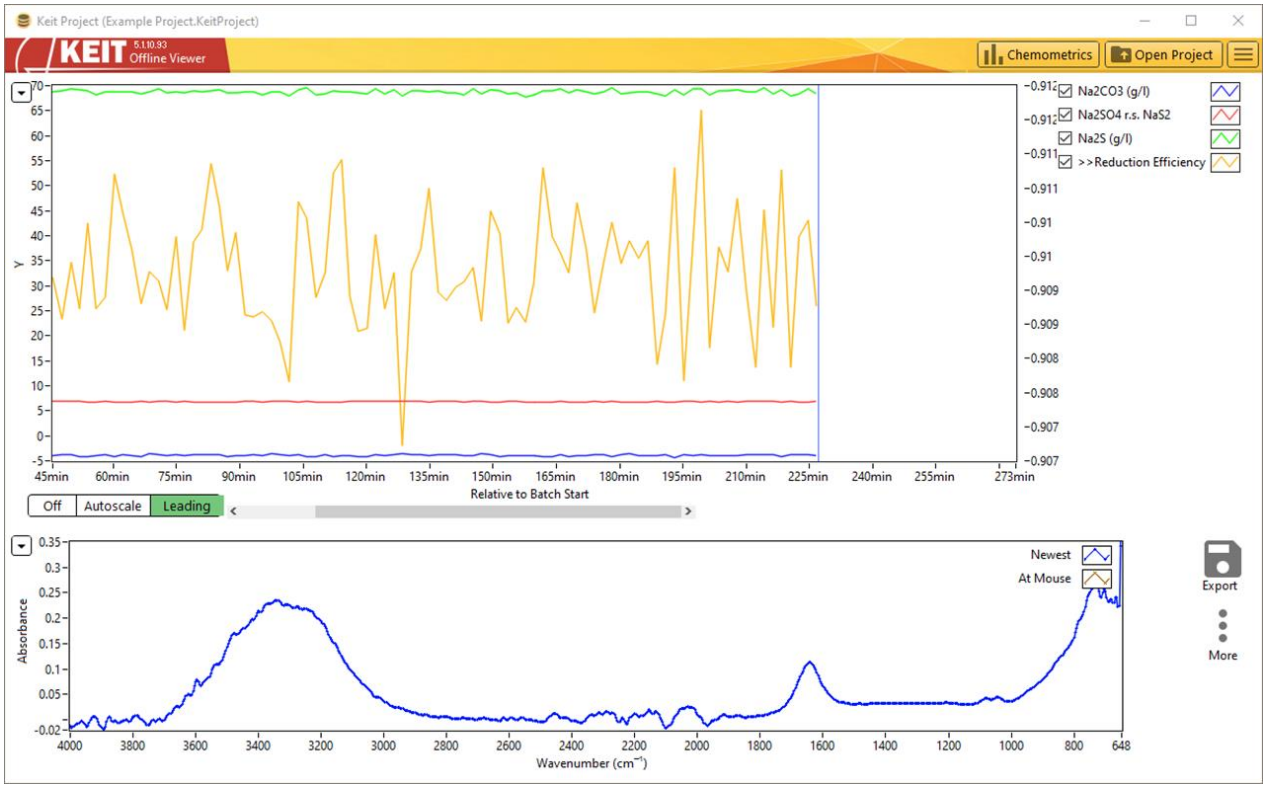


Figure 60: The Offline Viewer: Continuous Collection mode

When a Continuous Collection project is open, the settings and options in the offline viewer are identical to of the Project Data Viewer tab in KeitSpec. Please refer to Section 4 The Project Data Viewer tab for more information.

11.2. Offline viewer: Manually collected samples

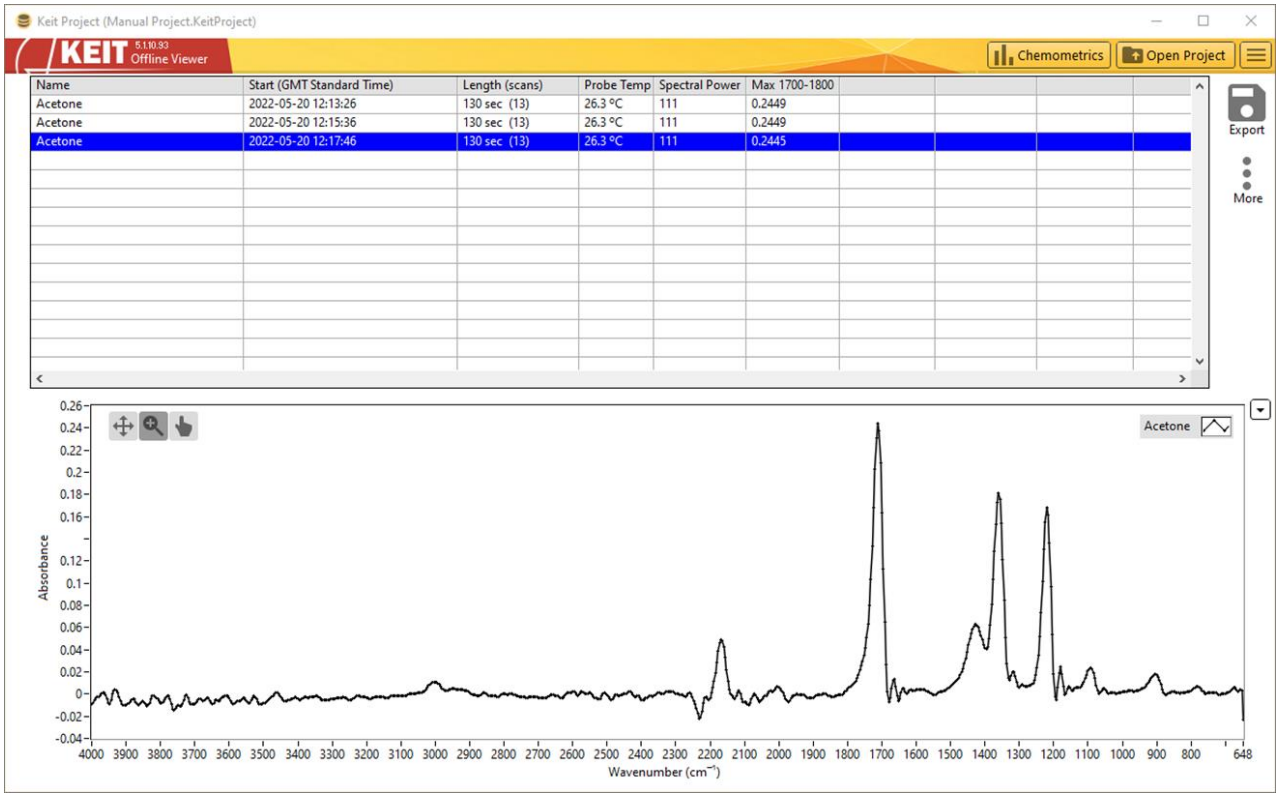


Figure 61: The Offline Viewer: Manual Sample Acquisition mode

When a Manual Sample Acquisition project is open, the settings and options in the offline viewer are identical to those of the Sample Acquisition tab in KeitSpec. Please refer to Section 9 Manual Sampling: The Sample Acquisition tab for more information.

12. LOG VIEWER

The KeitSpec application automatically logs various events, changes that are made to its configuration, and performance information about the spectrometer. Logs are also useful in case you need to contact Keit for service assistance. A log file is created for each month that the instrument is operating.

The log viewer software is installed on your computer when you install the main KeitSpec application. When you start the Log Viewer, it will prompt for you to choose the log file that you wish to view. These log files are stored by default in Users\Spectrometer User\Documents\LabVIEW Data\KeitSpec\Log.

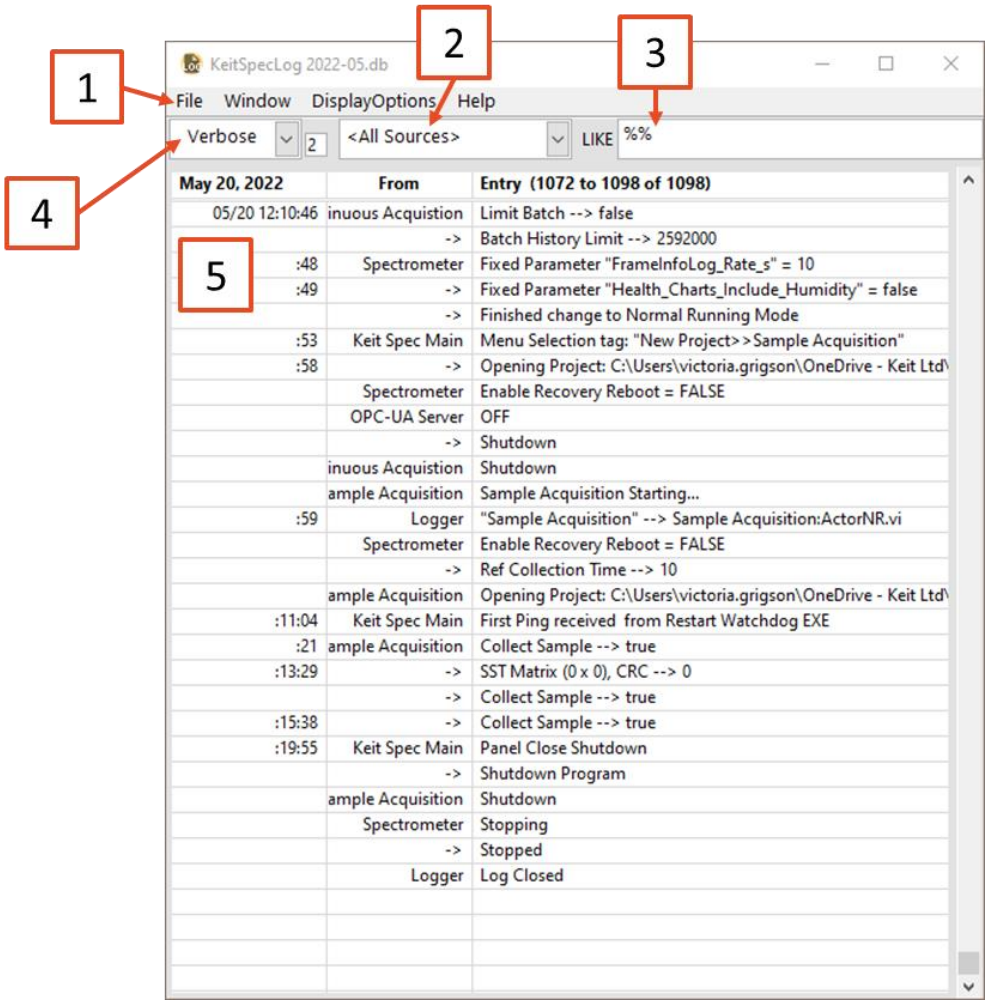


Figure 62: The KeitSpec Log Viewer

1. **Menu bar**
   a. **File**: Allows you to open a different log file, output the current log file to a variety of data formats, or close the KeitSpec log viewer.
   b. **Window**: Allows the display of a secondary window to show the full text of a log entry; to open a second log file for direct comparison with the first; or to expand the log viewer window to full screen.
   c. **DisplayOptions**: Allows you to display the full timestamp and source information rather than the sparse displays as shown in the above screengrab.
   d. **Help**: Allows the display of a contextual help window.

2. Sources dropdown

Filters the events displayed on the log file, so only events from, e.g., the spectrometer itself are displayed.

3. Search bar

Allows you to search through the events using a keyword. This search uses SQL syntax. Use % as a wildcard.

4. Log Levels

There are a series of different log levels that are recorded. Use this dropdown to choose the most appropriate level of detail.

Log Level	Serious	Standard	Verbose	Debug
Instrument errors	x	x	x	x
Application events (e.g., start/stop)		x	x	x
Settings changes			x	x
Settings configuration errors; non-fatal errors and warnings				x

5. Log entries

Each log entry is displayed in a new row in the table. Hover the mouse pointer over the field to display any information that overflows the space that is available.