In-situ Reaction Analysis

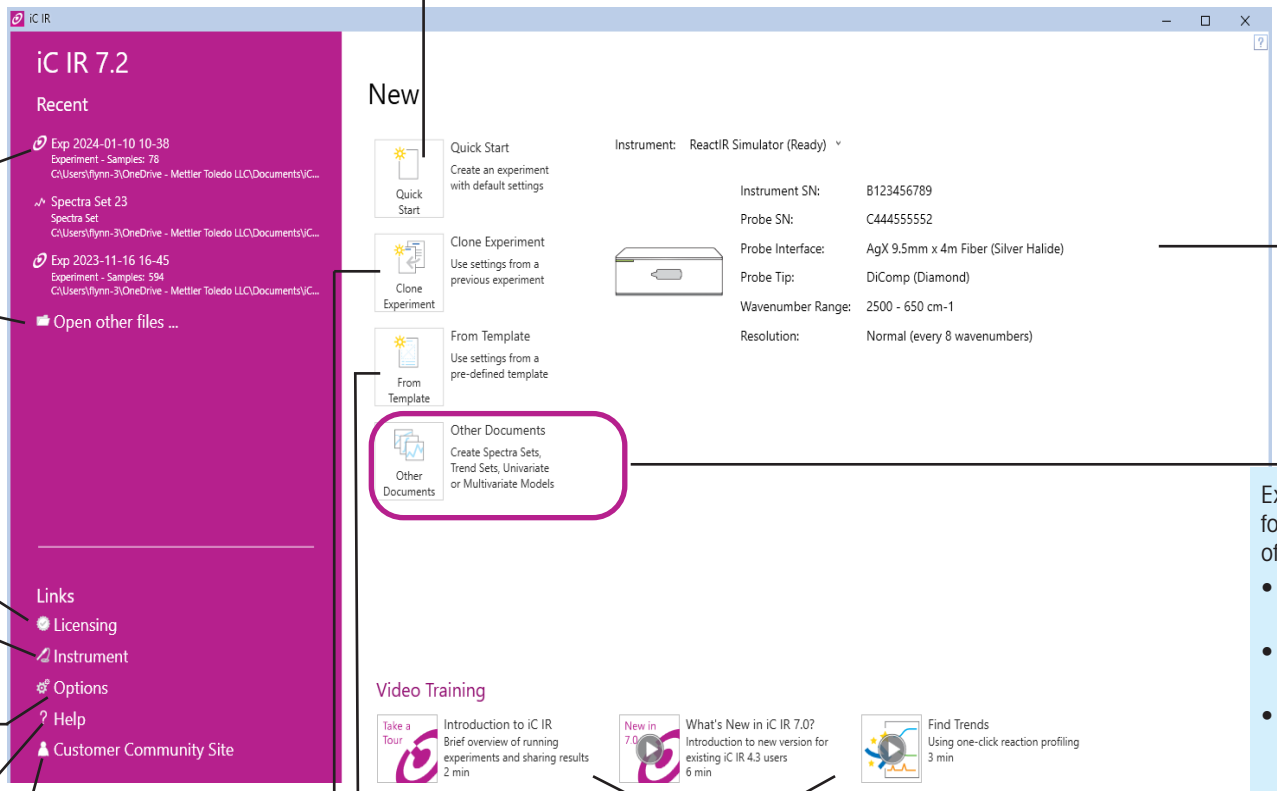
iC IR™ Quick Start Guide

iC IR software collects mid-infrared spectroscopic data and presents it graphically to help you **analyze** and **report** reaction information in real time. This guide introduces new users to the iC IR user interface (UI) and describes several choices for getting started. The Quick Start option is the fastest way to create an experiment and find the trends that provide insight into reaction dynamics. Each experiment automatically generates a report, and you can easily share spectra and trends of interest.

Start Page

A start page appears when you first open iC IR. At a glance you can see instrument configuration and begin an experiment, open a recent file, or view video tutorials. Always clean the probe after an experiment to ensure a clean, dry sensor before you take a background and begin monitoring your reaction.

Click **Quick Start** to quickly create a new iC IR experiment.



- Open recent experiments.
- Browse to other experiment, spectra set, or trend set files.

Open links to:

- Activate software licenses
- Edit instrument configuration
- Check options including templates and iC Data Center
- Access iC IR information and user assistance
- Go to AutoChem customer website

Alternatives for starting a new experiment include:

- Cloning an existing experiment allows you to tweak settings
- Or start an experiemnt from a template

Glance at instrument configuration details.

Expand to show menu for creating new types of files.

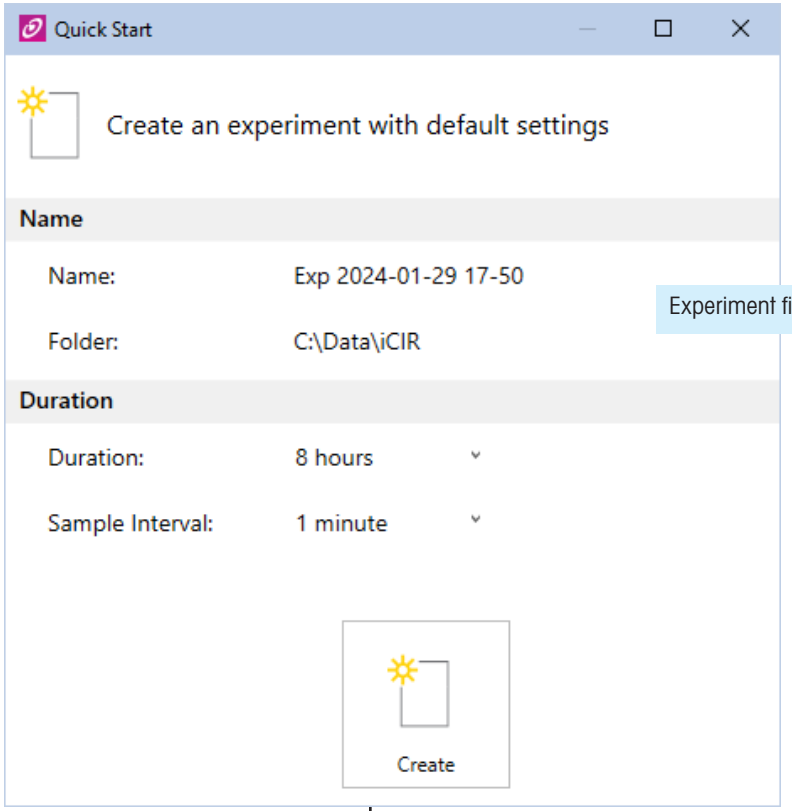
- Related spectra (Spectra Set)
- Trends (Trend Set)
- Quantitative Analysis models (univariate or multivariate)

Links to product video tutorials.

Next: Name experiment file and set timing options...

Name the Experiment File and Accept or Change Basic Options

After you click **Quick Start** on the Start Page, click **Create** to accept the default filename and location of the experiment file that will have either the default or specified sample interval and duration settings.



Edit or accept experiment file name and location.
If using iC Data Center, name the experiment according to your Standard Operating Procedure.

You can change these interval and duration settings now or during the experiment.

Experiment file holds up to 20,000 samples.

Click **Create** to make the experiment.

Next: Go to the paused experiment workspace...

Start Experiment

After you click **Create** to make the experiment, the main iC IR workspace appears in 'paused' mode with the LIVE ribbon. If you have a current background spectrum from a clean and dry probe sensor and if you have the necessary reference spectra, click the Play button ▶. When data collection starts, the LIVE experiment toolbar changes to green.

Adjust experiment schedule, as needed (interval and phases)

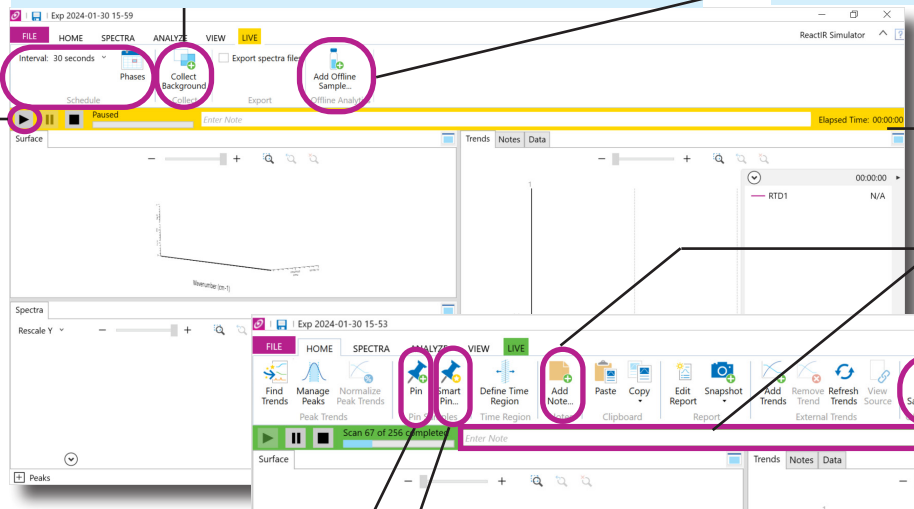
Collect a background, as needed. NOTE: This can only be done before the experiment starts (as well as after experiment completes).

Take an 'Offline Analytic Sample' from the reaction.

Multiple **ribbon tabs** show options and tools for the iC IR workspace. The LIVE ribbon is shown.

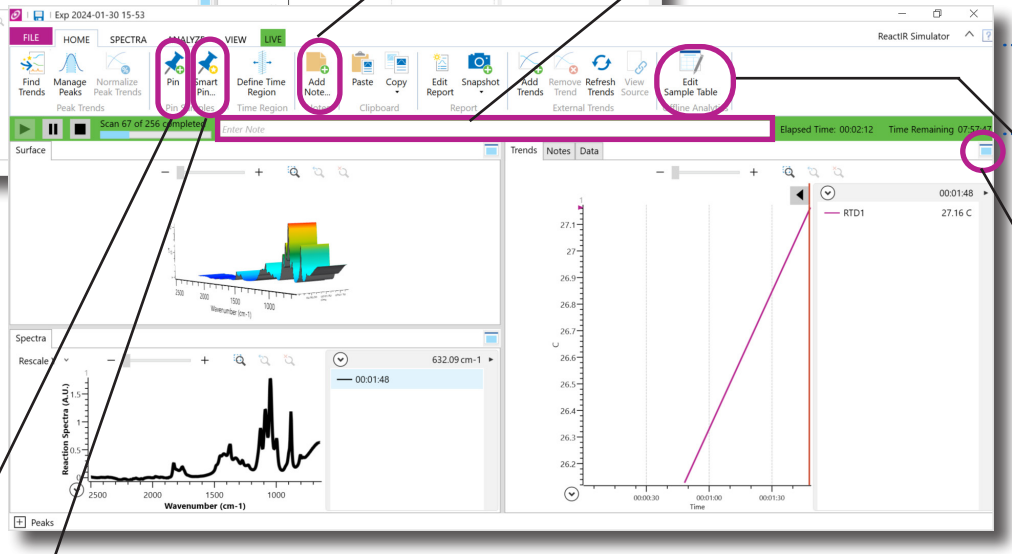
Click ▶ to start acquiring samples.

LIVE experiment toolbar (Paused)



Enter a process note

HOME ribbon



View and edit 'Offline Analytic data' for the reaction.

Use this corner button to expand a view to fill the entire window. (Click the button again to return to the multi-view layout)

Begin 'pinning' selected data points in the reaction by either:

- Clicking the **Pin** button after selecting data point in a reaction view—Spectra, Surface, Trend, Data, or Notes...

...OR

- Use the **SMART PIN** feature to automatically pin spectra around noted events or evenly across the experiment. Specify a time region in which to place a pin.

Next: The main workspace shows reaction data, with special features to Find Trends and Manage Peaks...

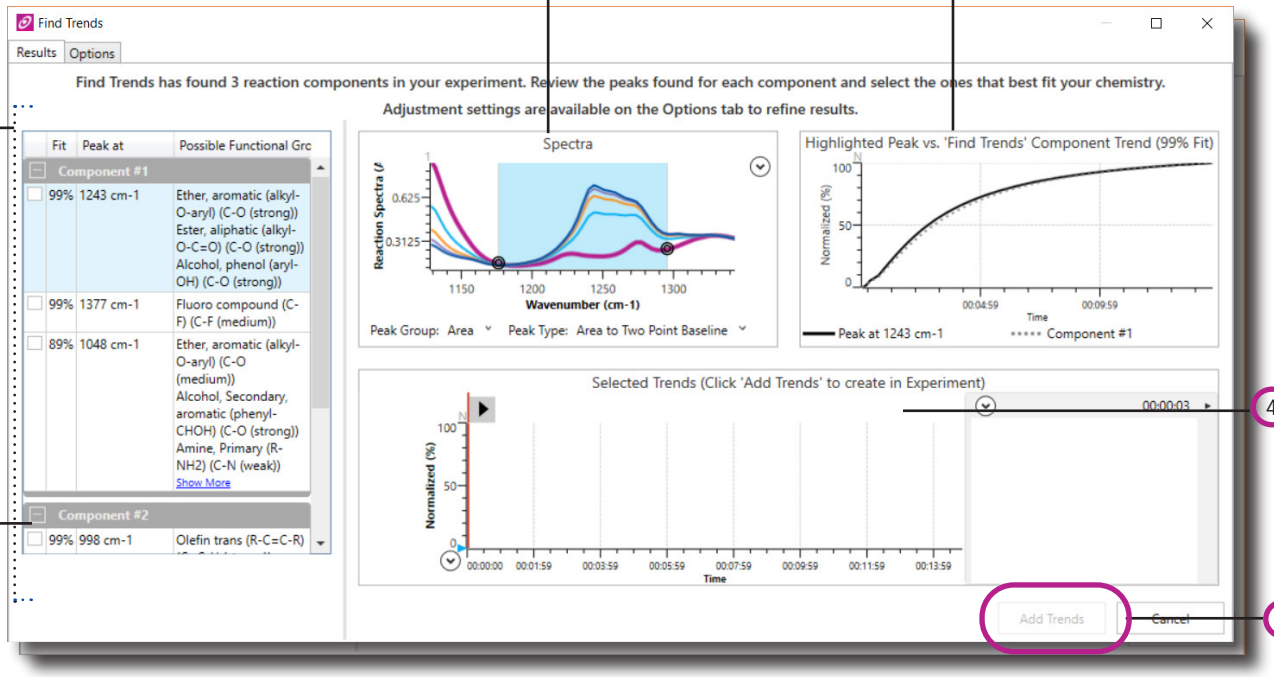
Find Trends

iC IR provides a powerful Find Trends feature on the HOME ribbon. Click the **Finds Trends** button to display a separate window.

After several scans, the software automatically processes the spectra and identifies probable reaction component concentrations in the chemistry. First, (1) select the components of interest from the table on the left, (2) review the peaks found for that component, and (3) observe the correlation graph. Then, (4) select one or more probable components with a high correlation between the calculated peak and the probable component. Finally, (5) click **Done** to add the displayed component trends to the current experiment.

Component spectra (zoomed in to selected peak) 2.

3. **Correlation graph** compares the shape of the selected component to "Find Trends' component to visualize a good match.



1. Results of 'Find Trend' calculation.

Shows the peaks that best match your reaction chemistry and the potential correlation to a class of compounds.

Select one or more peaks to observe:

- Component spectra (2) and
- Correlation (3)

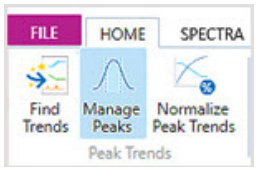
4. Component trends that are candidates to add to experiment...

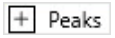
5. Click **Add Trends** to add the displayed component trends to the main experiment.

Next: Learn how to Manage Peaks...

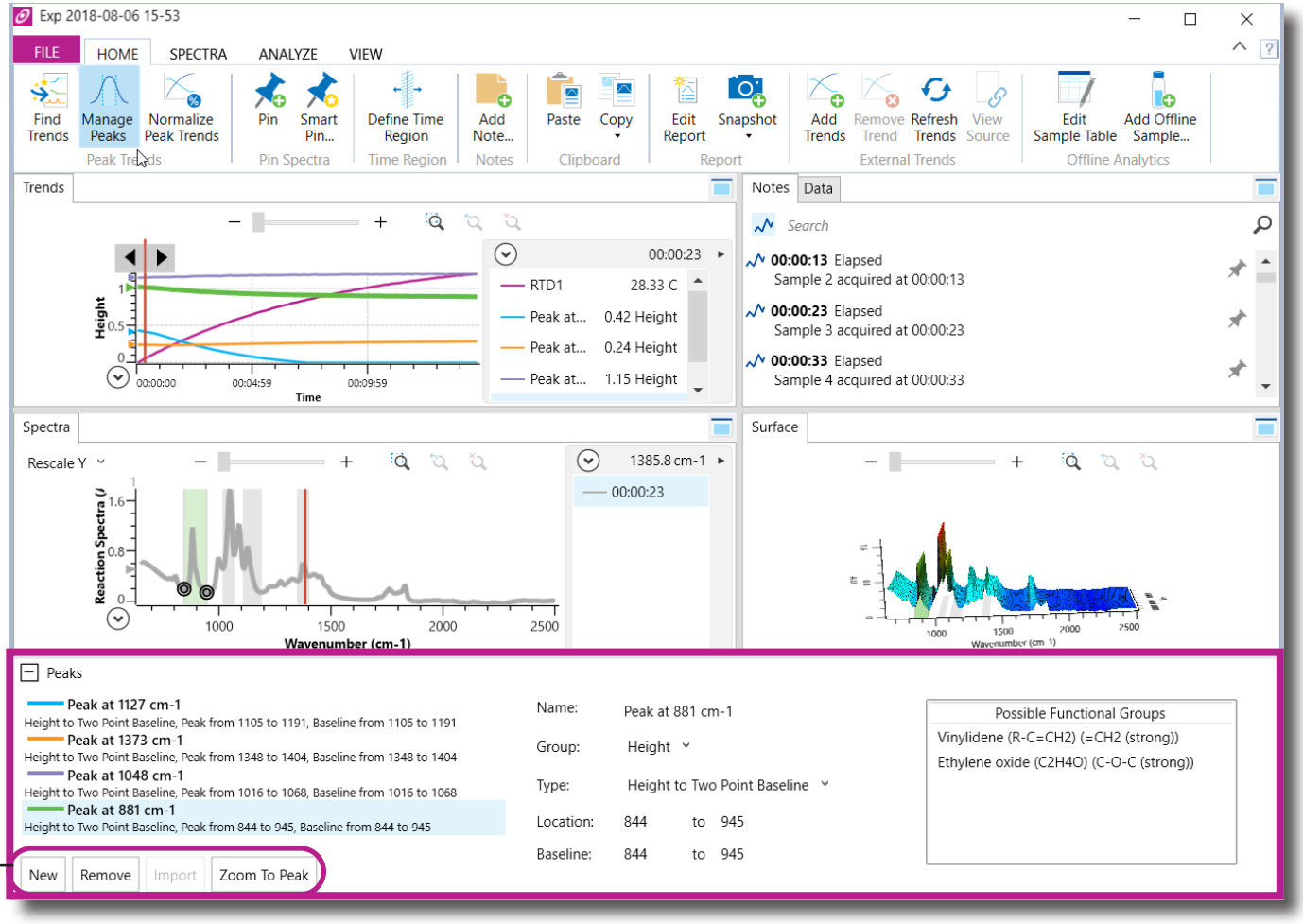
Manage Peaks

iC IR includes a special Manage Peaks feature on the HOME ribbon where you can add, edit, or remove peak trends. To expand the work section at the bottom of the main window, select the **Manage Peaks** button on the HOME ribbon.



Alternatively, click [+] Peaks at bottom left corner of the main window. 

Viewing the Spectra and Trends side-by-side allows easy graphical modifications to peak calculations and direct observation of resulting peak trend changes.

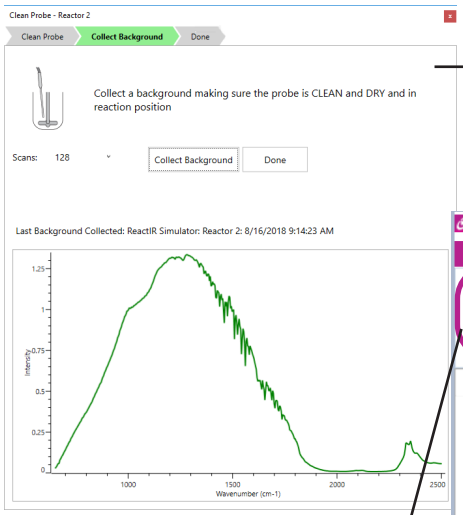


Use buttons to remove a trend, add a new one, or zoom to details about the highlighted peak, or observe the possible functional groups and adjust calculation settings.

Next: Review a completed experiment...

Review Completed Experiment

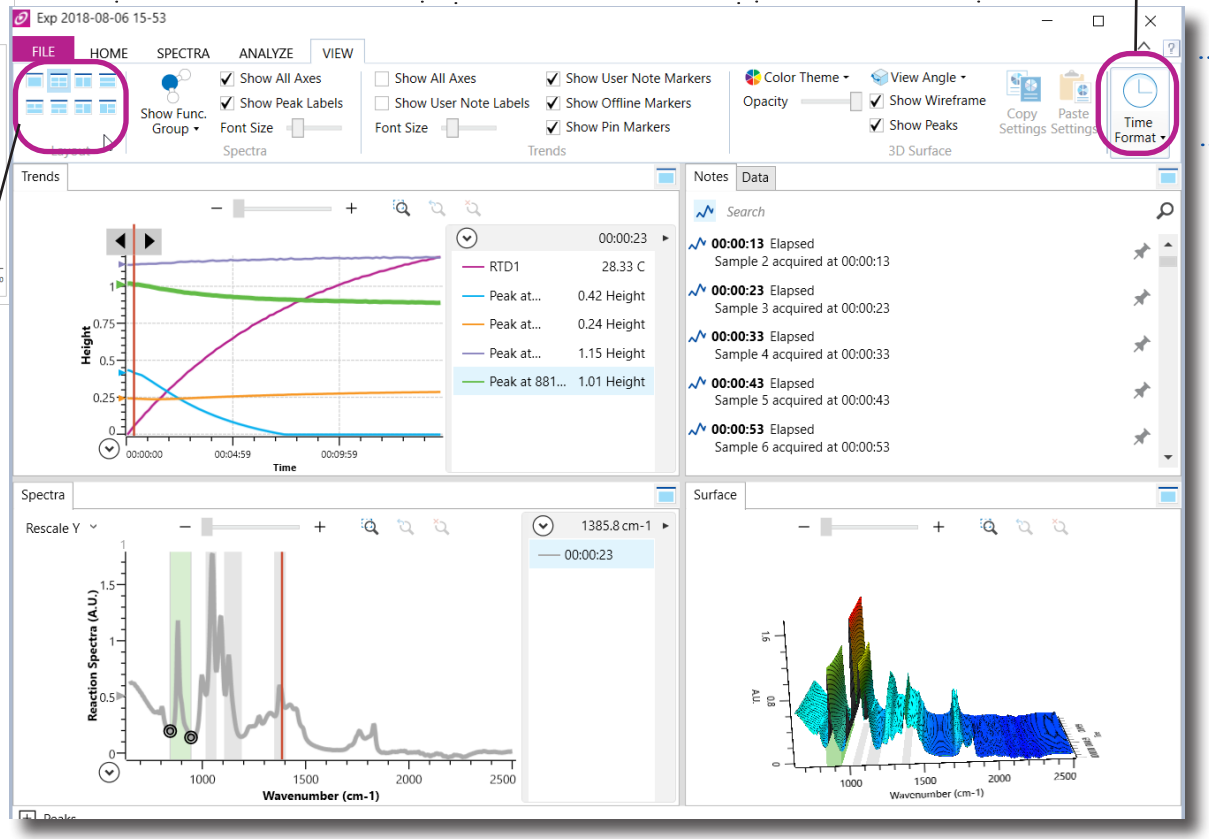
After you **Stop** ■ the experiment or when it completes the scheduled duration, the reaction information is ready for analysis, interpretation, and reporting. iC IR includes automatic reporting and a choice of export options, including single or multi-spectra files in SPC, SPA, or CSV format. Access both options from the HOME ribbon and FILE menu.



Best Practice: iC IR automatically prompts you to clean the probe and collect a background after the experiment completes.

Choose view options for Spectra, Trends, and the 3D Surface Viewer.

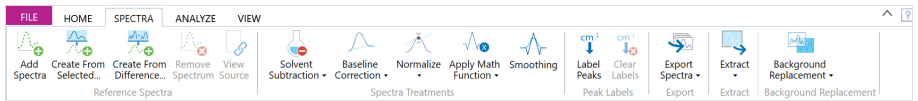
Choose X-axis time format: either the actual local time or time elapsed since experiment started.

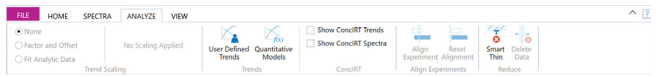


Select from many options, including eight layouts of the five possible tabbed viewers (three viewers shown ▥).

To rearrange tabs in the workspace layout, click-and-drag a tab to your preferred location.

Use the SPECTRA and ANALYZE ribbons to apply advanced data treatments and analysis.





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