iC IR™ 4.3 Quick Reference

Data Review and Analysis with iC IR™

iC IR displays dynamic linked views in live and review experiments. Four main 'views' provide a cross-section of experiment information, and a selection or change in one view dynamically appears in the other linked views. A 'toolbox' (I) enables you to control a variety of tasks.

I. Linked Views

- **Trends Viewer** (A)

  Displays real-time trends of each user-defined peak profile and ConcIRT™ LIVE! component in the experiment. Trends can also include Quant and Referee components plus user-defined math calculations.

- **Data/Events Viewer** (B)

  Select from two tabs. Data tab shows the time and value of each sample collected. Events tab shows a record of all user annotations and system/audit messages.

- **Spectra Viewer** (C)

  Shows a 2D view of pinned and selected spectra and allows definition of peak profiles.

- **Surface Viewer** (D)

  Presents a 3D view of the entire experiment and gives you the following options:

  - **Rotate or move**—Place cursor on the surface view, click the left mouse button and drag to ideal rotation. Use the right mouse button to move the 3D view.
  - **Enlarge or reduce size**—Place cursor in the view and rotate the mouse wheel.
  - **Additional options**—Right-click anywhere in the view to see more options.

II. Live Experiment Toolbar (E)

- Check current status of experiment by noting the background color of the toolbar: Green=Running, Yellow=Paused, Blue=Completed, Red=Error condition

(F)
- Control experiment status using the **Play/Pause** and **Stop** buttons.
  = Play = Pause = Stop

(G)
- Click the **Schedule** button to add/ edit/delete a phase of the experiment.

(K)
- Click the **Add Referee** button after taking a manual sample for HPLC or another chromatography method.

III. Annotations

Make any number of annotations on conditions or actions such as the beginning or end of additions, when a sample is extracted for offline analysis, modifications in reaction parameters, reaction color, bubbles, and so on. This provides useful details when you analyze results.

Adding an Annotation—Three Options

(H)
- **In Live Experiment**—Type the annotation in the Live Experiment Toolbar while the experiment is running. The Events Viewer logs the note.
  To see annotations in the Trend Viewer, click the **Show/Hide Annotation** button.
  To add annotations, click the **Add Annotation** button.

(A)
- **In Trends Viewer**
  Click to set the point where you want to add the annotation and use either the toolbar button or the right-click menu to open the annotation text box.

(B)
- **In Events Viewer**
  Select the Events tab, right-click a row in the events list, and select **Annotation/Add**.

To edit an annotation, double-click the annotation icon in the Trends or Events viewers or the row in the Events Viewer.

IV. Peak Profiles and Labels

(C) In the **Spectra Viewer**, you can define and edit profiles for peaks of interest and create or edit peak labels.

Defining a Peak Profile—Two Options

Both options create a peak profile definition that follows the maximum absorbance value over the specified region, based on the currently selected spectrum.

- Double-click above the spectrum to define a typically narrower region centered on the maximum absorbance value of the component of interest.
- Double-click below the spectrum to define a typically broader region determined by the inflection points of the component of interest.

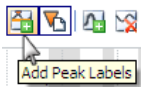
Changing a Peak Profile

- Ensure the Show Details option is checked in the context menu (Select **Show Details** button).
- Click the **Peaks** tab along the left side of the details table.
- Double-click a specific Peak Profile or graphically edit a peak by selecting it; then moving it or adjusting the width.
- Select the peak category from the drop-down menu in the Group field.
- Select the peak method from the drop-down menu in the Type field, and click **Apply**.

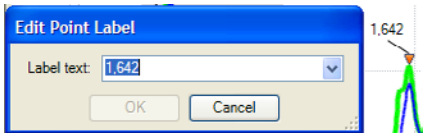
Creating/Editing a Peak Label

Create and edit peak labels in the Spectra View as well as in a Spectra Library.

1. Pin a spectrum by selecting it and clicking the **Pin Sample** button.
2. Click the **Add Peak Labels** toolbar button.



3. Click and drag across one or more peaks to select the ones to be labeled. The system creates a label with the peak center point value. Click and drag the label to move it.
4. Double-click on the label to edit it.



To edit an existing label, make sure the **Show Point Labels** button is selected , then double-click the label.

V. Process Spectral Data

From the Toolbox, select the **Data Treatments** task pane (I). In the default view, the most commonly used options appear under the following categories:

Reference Spectra

- **Correct for water vapor**—Apply a correction for water vapor based on a sample collection taken before the experiment (optional for sealed instruments: ReactIR 15, 247, 45P).
- **Subtract spectrum**—Subtract the selected reference spectrum from all sample spectra in the experiment.
- **Load or Remove**—Add reference spectra to or delete from the experiment.

Functions

The more common functions include:

- **Baseline offset**—Vertically shift each spectrum in the data set to zero at the selected reference wavenumber.
- **Normalize**—Correct each spectrum in the data set to a range of 0 at a single baseline point to 1.0 at the selected reference wavenumber. This normalization is useful to isolate effects such as temperature when you have a known standard in your reaction that should result in a constant peak height.
- **2nd derivative**—Apply a 2nd derivative function to each spectrum in a data set. This produces a spectrum that more easily processes weak remote or overlapping IR bands. The function multiplies results by –1 so traditionally negative peaks appear positive.

ConcIRT

- **Enable (ConcIRT LIVE!)**—Extract relative concentration profiles for products, intermediates, and starting materials, especially for chemical species that have overlapping peaks.
- **Show Components**—Show component spectra identified by ConcIRT LIVE!

Display Options

Use the 'Hide the DiComp "Diamond Region' check box to suppress display of the spectral region from 1950 to 2250cm^{-1} where the DiComp sensor absorbs the infrared energy. To specify a region other than the default, click the options button ...

Background Replacement

To replace the background with one loaded from an external source, mark "Show all options."

VI. Spectra Libraries

Create standard chemical references separately from an experiment and store them in spectra libraries.

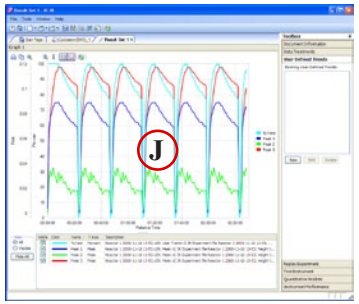
1. Click **New Spectra Library** from the Start Page.
2. Click either the **Sample Using Wizard**, or **Quick Collect** button to collect samples. Follow the steps under "Reference Spectra Needed?" in the 'Experiment Setup in iCIR' quick reference document.

Moving Spectra To or From a Library

Add selected spectra to the current experiment from a library, or add selected spectra from an open library to an experiment. Select spectra and use the drag-and-drop method.

VII. Result Sets

A result set is a separate file that contains trends. Data from a series of related experiments can be placed in one result set for comparison. To create the file, click **New Result Set** from the Start Page, select the trends, and save them using the 'File/Save as...' command.



Add trends to a result set by either of the following methods:

(J) • **In the graph area of the Results Set window**—Right-click on the graph and select **Add Trend** option.

(A) • **In the Trends Viewer for the experiment**—Click to highlight a trend., then drag-and-drop it to the target Result Set tab.

VIII. Templates

To enable running the same reaction multiple times with different conditions, create templates of frequently used trends and data treatments to reuse in subsequent experiments.

Watch the "Guided Tour" from the iC IR Start Page to see selected data review and analysis features in action.

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