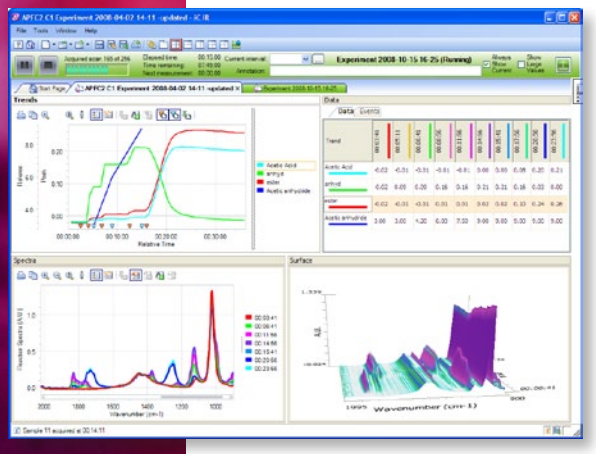
Software User Guide



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iC IR™ 4.3

Real-Time Results with *In Situ* Spectroscopy

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Contents

iC IR™

Introduction

iC IR is the next generation ReactIR software that combines essential reaction analysis functions with an easy to use user interface. iC IR is a wizard-based application that guides a user through the experience of collecting, analyzing and visualizing data. Key features include:

- Record in-situ reaction spectra
- Record pure component reference spectra
- Real-time peak profiling
- Real-time component analysis (ConcIRT LIVE)
- Real-time Solvent/Water Vapor Subtraction
- Linked Views (3D surface, 2D spectra, profile trends, event viewer)
- Export reaction data to ReactIR 3.0
- Replay reaction data (iC IR or ReactIR 3.0 formats)
- Export data to Excel
- Export graphs to Word
- Compare results from multiple experiments
- Manage libraries of reference spectra
- Univariate and Multivariate Modeling

iC IR allows full instrument control of the ReactIR iC10, the ReactIR 15, the ReactIR 45m and will also function with future ReactIR product releases.
iC IR allows chemists to focus on chemistry instead of instrumentation and analysis procedures.

Quick Reference Guides

The following Quick Start Guides will assist the user in setting up and using the iC IR software.
MK-PB-0013-AC QuickRef-Experiment Setup in iCIR.pdf
MK-PB-0012-AC QuickRef-Data Review and Analysis with iCIR.pdf

These documents are also available in the Documentation Portfolio (Help menu) for iC IR.

Guided Tour

This is a video presentation that is only available in the online help.

iC IR Data

iC IR organizes your data as various types of “documents” you view and edit from the application. Documents are stored as files on disk and displayed as windows within the application. The following document types are supported:

Experiments

Experiments (.iCIR files) are the heart of iC IR. They include reaction data plus all related pure component spectra, system messages, annotations, and analysis settings associated with your reaction. The Start Experiment Wizard guides you through the process of preparing your experiment. Once started, you can monitor and control your experiment from the Experiment Display which can also be used to analyze previously recorded experiments.

Result Sets

Result Sets (.iCResults files) are great for comparing results between experiments. Each result set consists of one or more trend graphs each containing one or more profiles.

The easiest way to add a trend profile from an experiment into a result set is to open both files, then simply drag and drop profiles into result sets.

Each profile in a result set has a link back to the original experiment it came from; right-click on the profile and select “Open Trend Source” to display and access the original experiment.

Spectra Libraries

Spectra Libraries (.iCSpectra files) provide a shared repository for reference spectra. The Creating a Spectra Library section guides you through the process of creating a new library. The Editing the Reference Spectra section explains how to view reference spectra and to add or remove spectra from a spectra library. New spectra can be collected from the instrument or copied from another spectra library.

Any experiment that contains reference spectra also functions as a spectra library. This is very convenient because it allows you to copy reference spectra from one experiment to another. To do so, select “Experiment Files” from the file type combo box of the Open Spectra Library dialog.

iC User Interface

The iC user interface combines power and simplicity to help you collect and analyze your data.

The **Menubar** provides standard Windows menus for accessing program functions. It also includes a toolbar or icons for common functions. The toolbar is positioned next to the menu items to eliminate wasted space and display useful functions for the current display. While recording data, it also provides a button to pause recording of the active experiment.

The Document area organizes multiple open document displays. By default, documents are shown as tabbed windows but can also be displayed as child windows if you prefer. You can group tabbed documents to compare documents side-by-side.

The figure above shows an Experiment Display which consists of four data viewers; Trend Viewer, Event Viewer, Spectra Viewer and Surface Viewer. The data viewers can be displayed, as shown here, in a tiled mode where all four viewers are displayed in a tiled arrangement in one window. The viewers can also be displayed as tabbed controls within the document display (tabbed mode). The default viewing mode is the tile mode. Several of these viewers have an associated information panel that can be opened to reveal additional details related to the particular viewer. The “active viewer” is highlighted to provide feedback on which data viewer will respond to keyboard commands.

The **Trend Viewer** displays profiles over time. The Trend List tab in its lower left corner opens an information panel with details on each available profile. You can show or hide profiles from the Trend List. You can also manipulate the trend view (zoom, change colors, show/hide legends, export data, etc) from the toolbar along the top edge of the Trend Viewer. Manipulation of trend profiles can also be performed by right-clicking the mouse to display context menus.

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The **Event Viewer** displays system messages and user annotations. A Sample message is appended each time the system acquires a reaction spectrum. The system also reports Info, Warning and Error messages, when appropriate. The Annotation panel can be displayed to create or edit user annotations. When a sample is annotated, you also have the option of having a marker displayed on the Trend Viewer.

The **Spectra Viewer** shows a 2D view of one or more spectra and also allows peak profiles to be defined. An associated information panel allows you to show/hide spectra and to create/edit peak definitions.

The **Surface Viewer** displays a 3D view of reaction spectra. Using the mouse you can view the surface from any perspective. The Surface Viewer automatically updates as you pan and zoom in the Trend Viewer or Spectra Viewer. The Viewing Options panel provides additional features such as overlaying a wire frame showing each reaction spectrum or selecting display colors for the surface.

The **Toolbox** provides access to a set of task panes which launch programs or manipulate the active document. For example, the Experiment task pane provides access to analysis functions such as water vapor and baseline corrections. The Toolbox can be popped open as needed or “pinned” to remain open and readily available.

The **Status bar** displays useful system information. The most recent system message is displayed on the left side.

The **Live Experiment Toolbar** contains experiment progress indicators and buttons to control experiment execution.

ConcIRT LIVE™ Overview

Relative concentration profiles are calculated by ConcIRT LIVE for products, intermediates and starting materials. ConcIRT LIVE is especially valuable for trending chemical species that have overlapping peaks. ConcIRT LIVE uses a type of mathematical algorithm known as curve-resolution. Curve-resolution algorithms have the capability to group wavenumber values that change absorbance intensity in the same manner. For each group, ConcIRT LIVE calculates the associated component spectrum and relative concentration profile. As each new reaction spectrum is acquired, ConcIRT LIVE re-analyzes all the reaction spectra and updates the individual component spectra and profiles. Thus, the calculation results evolve as the reaction proceeds and additional components such as intermediates are detected.

ConcIRT LIVE is a powerful tool that can analyze a broad range of reactions. It complements other iC IR features such as real-time peak profiling and the ability to collect and display reference spectra.

By default ConcIRT LIVE calculations analyze the “fingerprint” region of the mid-infrared spectrum from 1900 to 900 cm^{-1}. The region may be changed using the ConcIRT LIVE Region tool visible when the Show all options checkbox is activated. When enabled, ConcIRT LIVE begins reporting results as soon as six or more spectra have been acquired and two or more components have been detected.

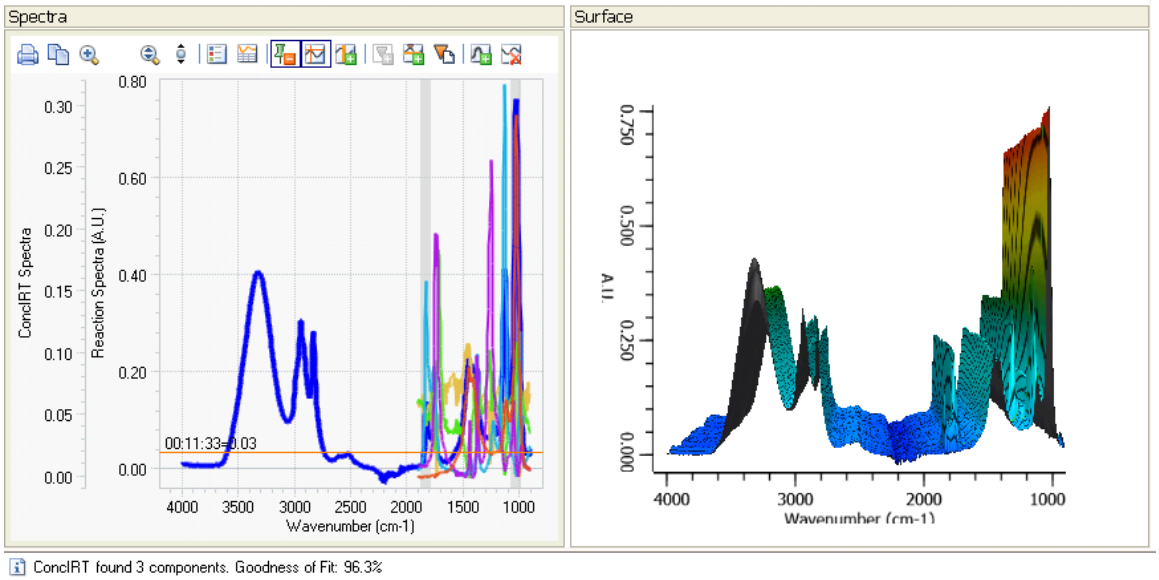
To aid the ConcIRT LIVE Analysis

- Be patient! If possible, wait for 3-4 spectral collections between additions or making changes to the reaction (i.e. changing a stir rate, changing temperature, adding more catalyst).
- If possible, add reagents in well defined ‘steps’. The discrete time increments of the additions help allow the algorithm to identify new chemical species.
- Choose a spectral region where changes are occurring. For example, try not to include regions containing strong bands from the solvent.
- If multiple additions or reaction steps are present in one data set, try analyzing each discrete step. For example, if an aqueous quench was used at the end of the reaction try ConcIRT LIVE processing including and excluding the quench step.
- If ConcIRT LIVE cannot find a component of interest during the reaction, try adding another aliquot of that material. For example, if one expects a low amount of reagent X to be present as it is slowly added to the reaction mixture, add a slight excess after the addition is complete. ConcIRT LIVE may have a better chance to now ‘see’ that reagent is in the mixture.
- The ConcIRT LIVE algorithm can work on a pre-processed experiment set. For example, a solvent subtraction, baseline offset or derivative can be applied before a ConcIRT LIVE calculation.
- If ConcIRT LIVE is not providing a satisfactory result (or no results at all) try changing the spectral region, time region, or pre-processing. One can also try to apply smoothing (5 or 7 points) in an effort to increase the signal-to-noise of the data set and the ability for ConcIRT LIVE to determine the different reaction components.

ALWAYS SANITY CHECK ConcIRT LIVE RESULTS! ConcIRT LIVE is an algorithm and has no inherent ‘chemical sense’, but we are interested in the chemical information. However, the algorithm is sensitive to changes in the reaction mixture. Infrared spectra can experience changes that are not due to the chemical reaction of interest. For example, temperature can influence the peak shape (intensity, position, width) of an infrared band, especially in strongly hydrogen bonded environments. The ConcIRT LIVE algorithm oftentimes calculates a component that tracks temperature quite well!

Use collected reference spectra to help confirm the identity of a ConcIRT LIVE generated component spectrum.

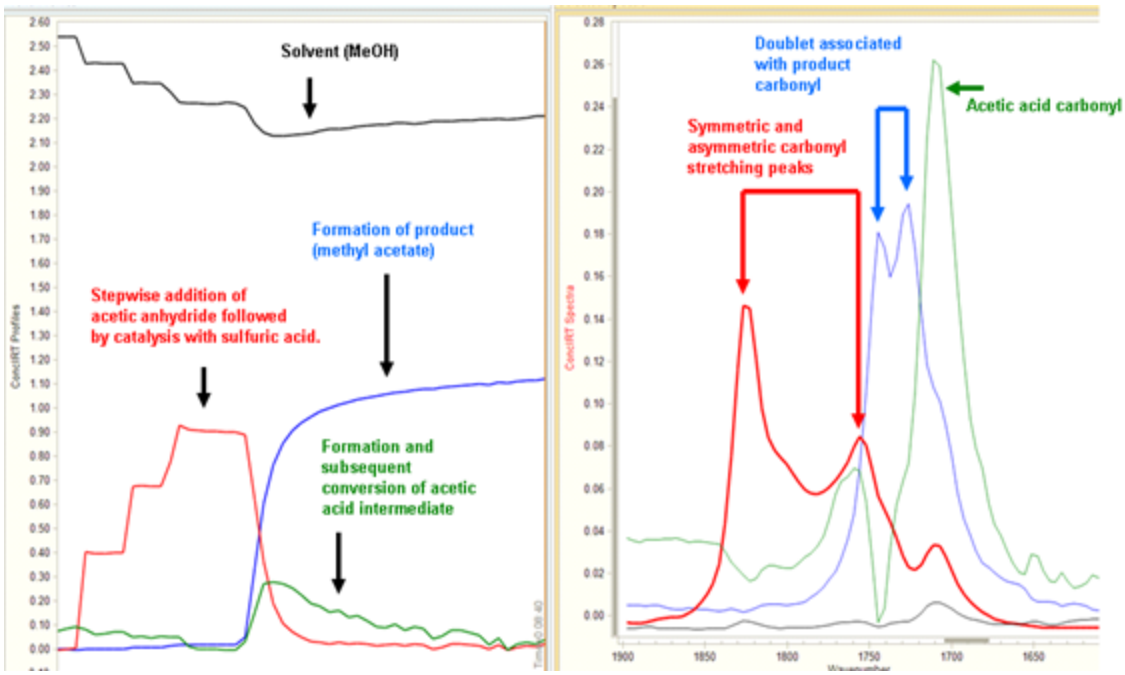
ConcIRT Live calculates a “goodness of fit” value and displays it in the Status area of the display. The value is updated as new calculations are completed.



The “goodness of fit” percentage is also displayed on the Data Treatments task pane, next to the Enable checkbox.

ConcIRT LIVE Example

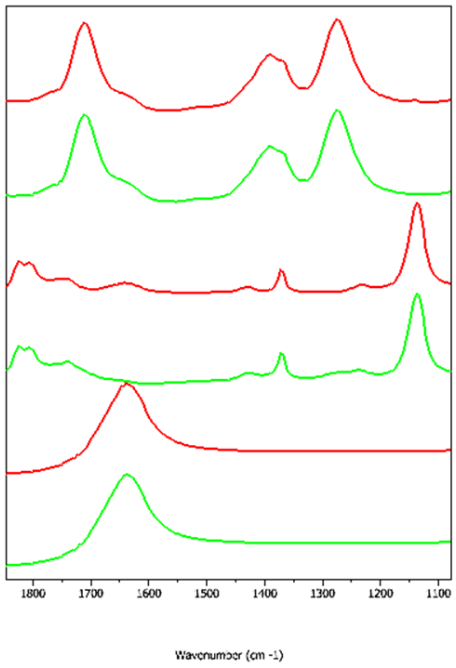
To illustrate the capabilities of ConcIRT LIVE, we will use the sulfuric acid catalyzed methanolysis of acetic anhydride. Through analysis of the 3D reaction surface the ConcIRT LIVE algorithm produces component profiles and component spectra for the solvent (methanol), starting material (acetic anhydride), intermediate (acetic acid), and product (methyl acetate). Comparison of the component spectra with authentic spectra was subsequently used to validate the results. It is important to note that while the results are closely related to the true chemical events in the reaction, there are noticeable deviations. The methanol profile for instance begins to rise late I the reaction progress. This is chemically impossible, because the methanol is both solvent and reactant and additional methanol is not introduced into the reactor. However, effect such as molecular interaction, temperature fluctuations and the degree to which component signatures resemble one another, can produce this type of outcome. This topic (deviation between spectroscopic and chemical results) will be explored in detail in the following example.



ConcIRT LIVE produces component profiles and spectra for the methanolysis of acetic anhydride.

ConcIRT LIVE Component Spectra

The correspondence between measured pure component spectra and the extracted spectra calculated by ConcIRT LIVE will vary from reaction to reaction because interactions, nonlinearities and severe overlap can affect the extracted spectra. Nevertheless, the correspondence is usually more than sufficient to identify reaction species. Especially useful, ConcIRT LIVE frequently makes it possible to determine when transient intermediates are present. The accompanying figure shows some examples of the correspondence between measured spectra (shown in green) and those extracted by ConcIRT LIVE (shown in red).



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You can use the Spectra Viewer in iC IR to visually compare ConcIRT LIVE component spectra with pure component reference spectra you collect as a means of identifying the chemicals associated with ConcIRT LIVE profiles. Simply use the checkboxes in the Spectra List panel to display the relevant components. As you identify each ConcIRT LIVE component spectrum, rename it with the chemical name. The labels on the corresponding ConcIRT LIVE profiles in the Trend Viewer will be auto-updated with the chemical name.

The benefit of ConcIRT LIVE is that it automatically produces relative concentration profiles and component spectra, in real-time, with no prior information or inputs needed. However, keep in mind that peak height profiling and ConcIRT LIVE are only two of the many methods used to help investigate chemistry. These tools are not a substitute for chemical intuition or results from off-line techniques (HPLC, GC, NMR, etc.). One could say that iC presents a qualitative ‘movie’ of the reaction providing process insight and understanding to complement quantitative ‘snapshots’ from off-line techniques.

ReactIR Instruments

The following instruments are supported by the iC IR application.

ReactIR iC 10— This base unit is similar to the ReactIR 15, but it supports mirror conduit as well as DS Series FiberConduit technologies.

ReactIR 15™ — This base unit has a built-in, single DS Optical Interface module SIM, so it can only be used with DS Series sampling technologies (mirrored conduits are not an option). It is factory-aligned and requires no rotational alignment. The base unit is sealed so an instrument purge is not required. The ReactIR 15 includes an integrated temperature monitor. The unit uses either a liquid nitrogen or Stirling engine MCT detector. If the Stirling MCT is used, an option in the Preferences dialog allows the engine to be shut down during idle periods to prolong its life.

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ReactIR 45m™ — This base unit is a full featured reaction analysis system for the most demanding applications. Designed to be flexible to use the full range of Comp™ probe and conduit technologies, the ReactIR 45m is the designed for the chemist or chemical engineer faced with the challenge of monitoring reactions across a wide range of temperature and pressure conditions and is ideal for kinetics and quantitative analysis. The 45m base unit supports MultiplexIR analysis using two sampling technologies. The unit uses either a liquid nitrogen or Stirling engine MCT detector. If the Stirling MCT is used, an option in the Preferences dialog allows the engine to be shut down during idle periods to prolong its life.

ReactIR 45P™ — This base unit is a Process Analytical Technology (PAT) tool designed for *in-situ*, FTIR monitoring of batch process chemistry. The system is available in two configurations for monitoring chemistry in the laboratory or in classified areas using a Stirling engine MCT detector. Designed to be flexible to use the full range of Comp™ probe and conduit sampling technologies, including a dual-probe option, the ReactIR 45P instrument can be controlled by iC IR or iC Process software. Use iC IR to develop a monitoring strategy in the lab that can be used as a method in iC Process for scale-up or full production.

ReactIR 247™ — This base unit is a Process Analytical Technology (PAT) tool designed for *in-situ*, FTIR monitoring of continuous process chemistry. The system is available in two configurations for monitoring chemistry in the laboratory or in classified areas using a DTGS detector. Designed for use with K4 conduit or direct Sentinel sampling technologies, a ReactIR 247 instrument can be controlled by iC IR or iC Process software. Use iC IR to develop a monitoring strategy in the lab that can be used as a method in iC Process for scale-up or full production.

FlowIR™— This dedicated FTIR instrument is designed for *in-situ*, real-time monitoring of continuous flow chemistry. The small footprint enables the unit to be placed virtually anywhere within the continuous reactor set-up. FlowIR™ sensors enable sensor types to meet application needs. Interchangeable Flow Cell Heads are available in heated or non-heated models with options for the internal volume.

Notes on the Stirling Engine MCT Operation

The ReactIR 15, ReactIR 45P and ReactIR 45m have the option of using a Stirling engine MCT as a detector. The following summarizes the automatic on/off operation of the Stirling engine.

Stirling Engine Turns On:

- When advancing past the initial page of the Configure Instrument Wizard
- When advancing past the Reference Spectra Needed page of the New Experiment Wizard.
- When starting a test in the Test Instrument task pane
- When collecting a sample directly into a spectra library
- When performing an IPA Calibration or Validation

When the Stirling engine is turned on automatically, a progress dialog is displayed until 5 consecutive scans with the MCT status of 'OK' is obtained, at which point, the dialog closes. The progress dialog does have a Cancel button so that the user can abort if the Mct OK diagnostic malfunctions for any reason.

Stirling Engine Turns Off:

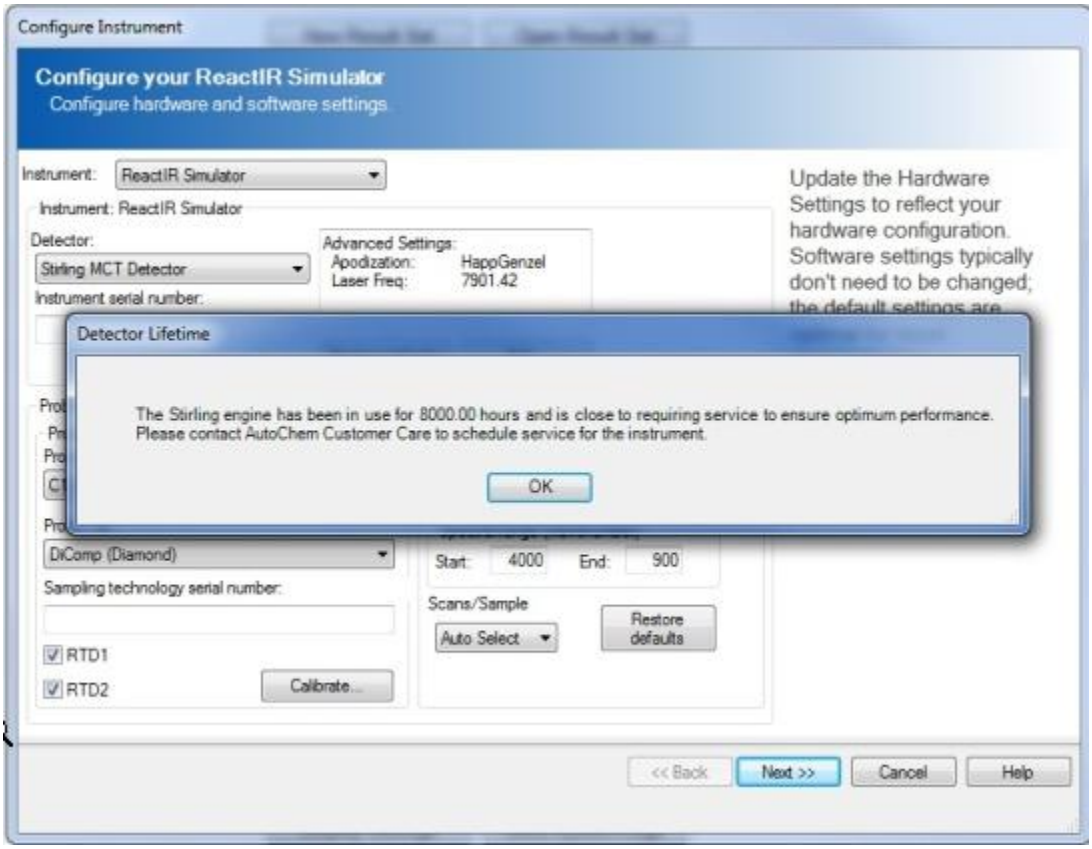
The Stirling engine will shut down immediately when shutting down iC IR. Also, if the "Auto-shutdown Stirling engine" user preference is enabled, the Stirling engine will be shut down after a delay after the most recent occurrence of any of the following:

- Completion of an experiment.
- Completion of a Contrast, Stability or Performance test executed from the Test Instrument task pane.
- Collection of a sample into a Spectra Library
- Completion/cancellation of the Configure Instrument wizard.
- Completion/cancellation of a IPA Calibration or Validation

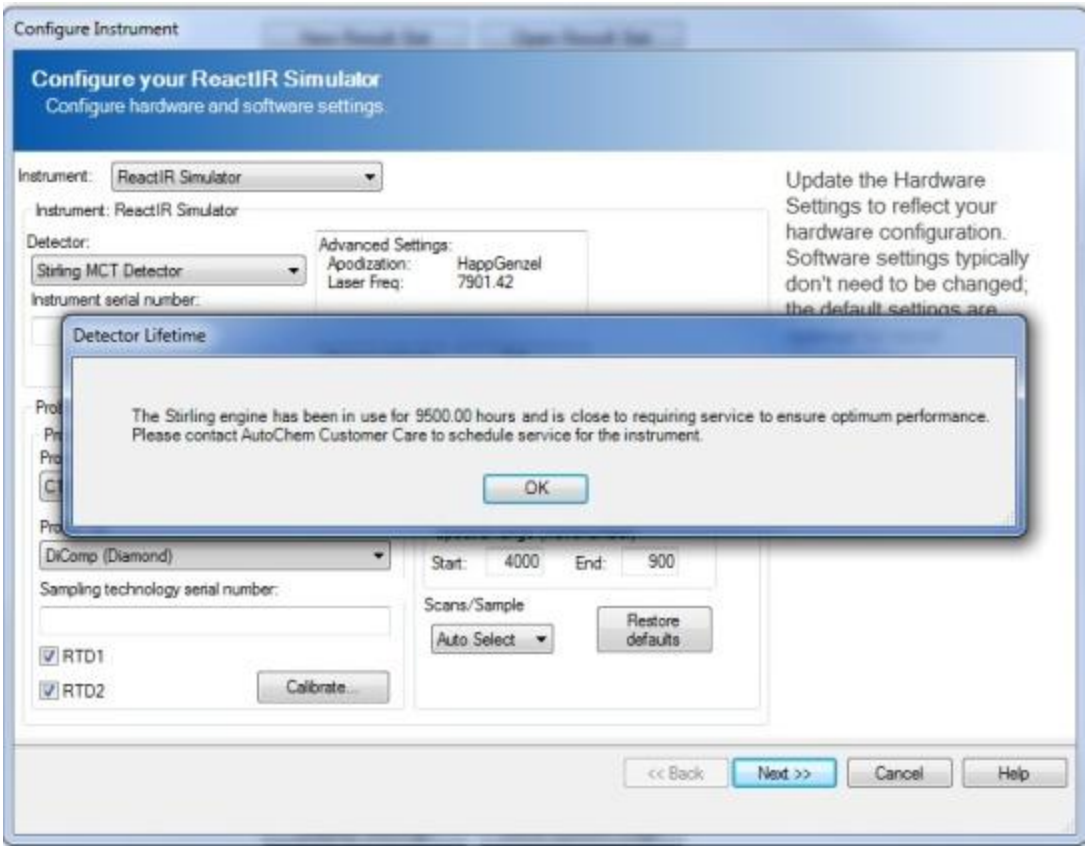
Stirling Engine Service

The Stirling engine has a lifetime of 10,000 hours. When engine usage approaches the 10,000 hour limit, AutoChem Customer Care should be contacted to schedule replacement of the engine. It is extremely important to replace the engine at this time in order to ensure optimum performance.

The instrument keeps track of Stirling engine usage and displays an initial reminder after the engine has been in use for 8000 hours. The message is displayed in the Configure Instrument wizard..



When Stirling engine usage reaches 9500 hours, a warning is displayed whenever an experiment is started. The warning is displayed when progressing through the Start Experiment wizard.



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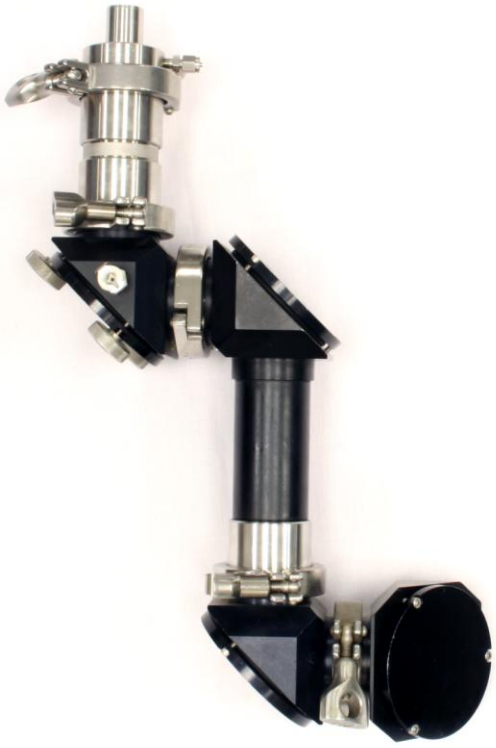
Conduits

AgX FiberConduit™

The FiberConduit™ is comprised of a flexible IR transmission fiber composed of silver chloride/ silver bromide. The flexible nature of the FiberConduit™ facilitates its use and easy integration with various reactors.

K4 Conduit

The K4 conduit is an articulated arm that provides a path for the infrared beam to travel to a sampling device (i.e. ATR-based probe) and back to the detector. The K4 conduit consists of four mirrors and a short tube between mirrors #2 and #3. Mirror #4 is used for alignment. The K4 conduit is used exclusively with Sentinel™ sampling technology.



K6 Conduit

The K6 conduit is an articulated arm that provides a purged path for the infrared beam to travel to a remote sampling device (i.e. ATR-based probe) and back to the detector. The K6 conduit consists of six mirrors and two tubes between mirrors #2 and #3 and #4 and #5. Mirror #6 is used for alignment. The K6 conduit is used exclusively with 16mm diameter Comp™ (composition) Probe sampling technology.

Sampling Technology

The Sentinel™ and Comp™ Probes are available in DiComp™ (Diamond) and SiComp™ (Silicon). These were developed specifically for spectroscopic monitoring of chemical, pharmaceutical and biological reactions. A diamond or silicon sensor is used as a multiple reflection ATR element; and the seal between the metal housing and the sensor is available in Teflon and Gold, to ensure chemical compatibility.

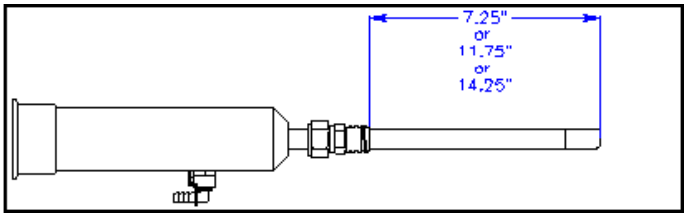
Sentinel™

Sentinels are available with a variety of options for interfacing to reaction vessels including: plant reactors, autoclaves, and other specialty vessels.

A Sentinel™ consists of a Hastelloy C-276 tube with a sensor at one end with a diameter of 1 inch (25.4 mm) attached to a base of 2 inches (51 mm) in diameter and approximately 1 inch (25.4 mm) in length.

Comp™ Probes

The Comp™ (composition) probes consist of a Hastelloy C-276 tube with the sensor at one end with a diameter of 0.625 inches (16 mm) attached to a base of 2 inches (51 mm) in diameter and approximately 9 inches (229 mm) in length. The base includes a flange that a clamp is used to fix the probe onto the conduit. The base also contains a hose barb for purge gas. The probe length is defined as the distance from the tip of the sensor to the threaded end of a fitting.



Note: It is the customer's responsibility to verify chemical compatibility of the probe with the chemistry intended to be monitored in advance. Test kits containing shavings of the probe body material, Diamond sensor and Gold sensor seal are available upon request.

The DiComp™ and SiComp™ composition probes are patented.

DS Micro Flow Cell

The DS Micro Flow Cell sampling technology is an inline analytical tool that enables processing of continuous flow chemistry without sampling. Attach the flow cell to a ReactIR instrument to enable real-time, in situ, measurement and monitoring of flow chemistry. The chemical stream flows to the sampling technology instead of the other way around. A heated model enables you to keep the stream at the desired temperature to ensure the highest quality measurements.

Heated Model

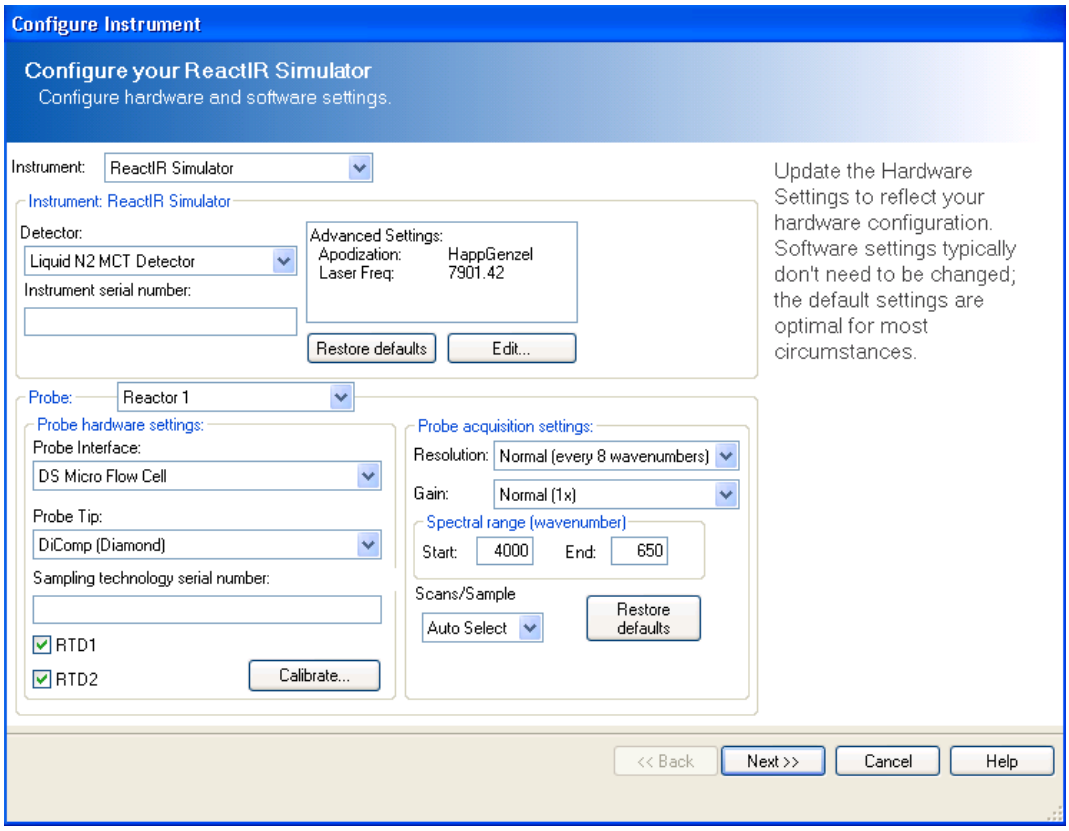
A DS Micro Flow Cell connects directly into a ReactIR 15 base unit. ReactIR iC10, and 45m require an adapter (a DS Optical Interface Module) into which the DS Micro Flow cell connects. ReactIR 45m MultiplexIR adapters enable you to maximize time and throughput by running two flow experiments with a single instrument and two flow cells, or you can monitor multi-stage flow processes.

Below is a ReactIR 45m with a MultiplexIR adapter and two DS Micro Flow Cells. One is the heated model and one is ambient.

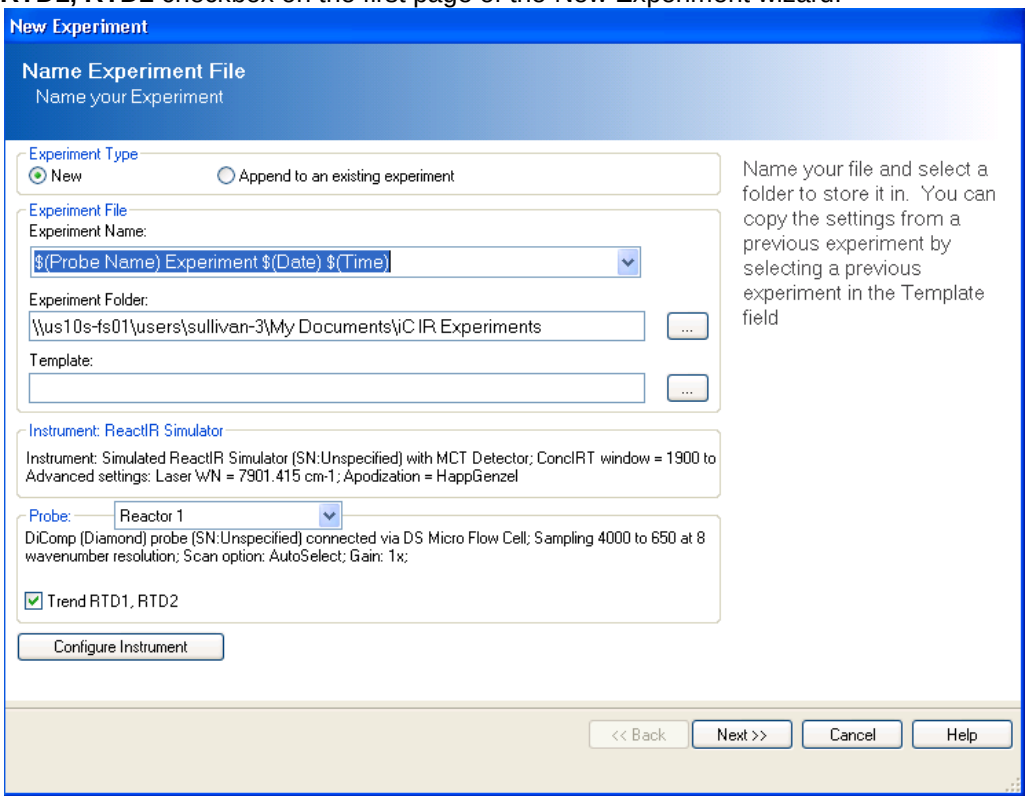
For more information, refer to the DS Micro Flow Cell data sheet or the *Sampling Technology Guide*.

RTDs

Some ReactIR instruments support RTD temperature sensing inputs. The RTDs can be used to monitor temperatures associated with the instrument or probe interface. When the instrument is configured, the user has the option of enabling or disabling the RTD inputs. RTD inputs are enabled/disabled using checkboxes on the first page of the Configure Instrument wizard.



The temperature values from enabled RTDs can be collected and displayed as a trend by checking the **Trend RTD1, RTD2** checkbox on the first page of the New Experiment wizard.



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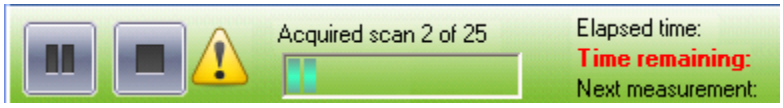
RTD Alarming

Alarming capabilities are available for RTDs used with the DS Micro Flow Cell .A low alarm limit of -45ºF and a high limit of 130ºF for each of the two RTDs are preset at the factory. RTD Alarming is also available for the AgXFiber6mm, AgXFiber95mmx15m, and AgXFiber6mmx15m (each with a high limit of 180 degrees C and no low limit. To enable the alarming function, the RTD values must be trended.

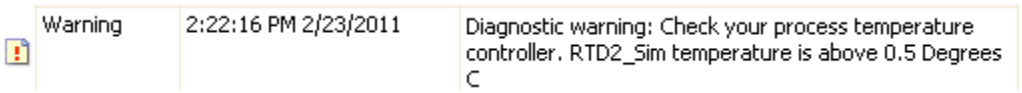
An RTD will alarm after a out of spec scans. The alarm will reset itself after a good scan. Three indications are provided for RTD alarms.

When an RTD goes into alarm, the large Value display will display the RTD temperature with a red background.

A yellow “caution icon” is also displayed on the Live Experiment toolbar.



Thirdly, an entry is made in the Event Log.



Configuring the ReactIR Instrument

You must configure iC IR with information about your ReactIR hardware before you can use it to conduct experiments. Configuration consists of the following steps:

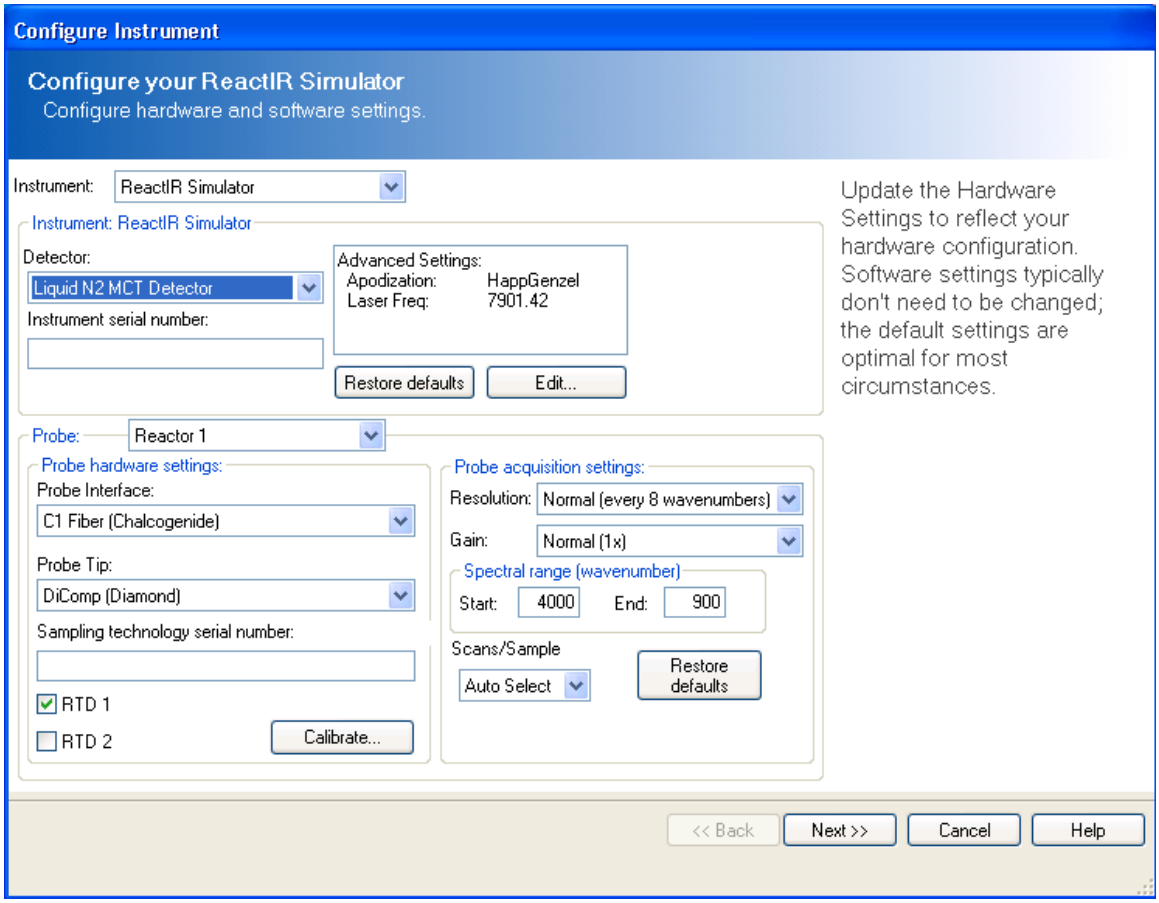
1. Specify hardware settings reflecting your ReactIR hardware configuration.
2. Optionally adjust software settings used when collecting and processing data from the ReactIR instrument.
3. Collect a reference background while the probe is clean and the system is well purged. This will be used subsequently as a baseline for accessing whether the probe tip is clean and the system purge is working properly.
4. Collect a reference background while the probe is clean and the system purge is off that will be used subsequently to support the water vapor correction feature.

These configuration steps are accomplished using the Configure Instrument Wizard. You can access this wizard by clicking the **Configure Instrument** button on the Start page.

Refer to: ReactIR Instruments.

Specify Hardware and Software Settings

The first page of the wizard is used to specify the particular ReactIR hardware options installed and to specify software settings that will influence how iC IR collects and processes the data it acquires from the ReactIR hardware.



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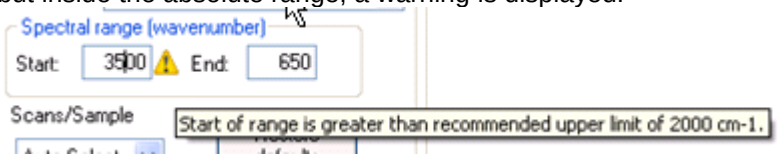
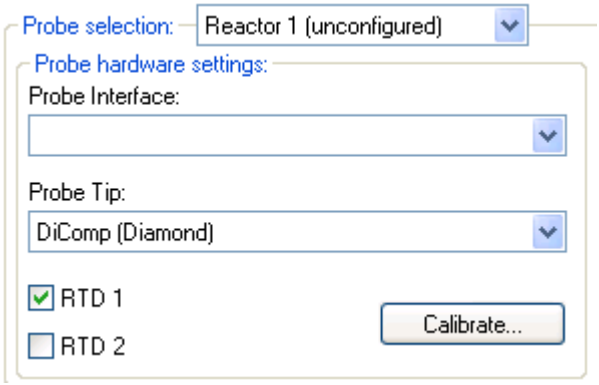
The configuration choices on the left side specify the particular hardware configuration you are using. The choices on the right affect software processing. The software settings are auto-initialized to default values based on the hardware settings you select. In most cases, you need not change the default software settings.

Instrument	The instrument type is selected from a droplist. Refer to Instrument Configuration Settings for a list of supported instruments.
Detector	The type of detector in the instrument. Supported types are as follows. **iC10** - DTGS (deuterated triglycine sulfate) or Liquid N2 MCT (mercuric cadmium telluride) **IR 15 and IR45m** - Liquid N2 MCT or Stirling MCT **IR45P** - DTGS or Stirling MCT **IR247** – DGTS only The DTGS detector is normally used for the acquisition of regular transmission spectra. The MCT detector has higher sensitivity than DTGS. If the Stirling MCT is used, an option in the Preferences dialog allows the engine to be shut down during idle periods to prolong its life.
Serial Number	The serial number of the instrument. This number is stored in the iC IR configuration and used in Stability and Performance test reports.
Advanced Settings	Refer to Instrument Configuration Settings for a list of the advanced settings used for each instrument type. Click the **Edit** button to change the advanced settings.
ConcIRT LIVE range	The range to use for ConcIRT LIVE processing.
Probe Interface	C1 Fiber (Chalcogenide) AgX Fiber (Silver Halide) K4 Conduit K6 Conduit DS Micro Flow Cell
Probe Tip	DiComp (Diamond) SiComp (Silicon)
Resolution	High - every 4 wavenumbers. This is unnecessary in most cases and will slow down scan rate, increase file size and slow application processing. It may be useful in certain reactions to help resolve overlapping peaks. Normal - every 8 wavenumbers. This is the best choice for most chemistry. Low - every 16 wavenumbers. This choice is only useful in reactions with broad, non-overlapped peaks that require a fast sampling rate. In such cases, the lower resolution allows for faster scanning which means a higher signal to noise ratio in samples taken more frequently than once a minute.
Spectral Range	There is an absolute minimum and maximum that the detector is capable of measuring. There is also a recommended minimum and maximum based on the probe interface. The spectral range displays the recommended range. This range is editable by the user. If the user selects a range outside of the recommended range, but inside the absolute range, a warning is displayed. 

	The recommended ranges (default) for the spectral range is: C1 Fiber 4000 900 AgX (6 mm x 2 m) 2000 650 AgX (9.5 mm x 2 m) 2000 650 AgX (6 mm x 1.5 m) 2800 650 AgX (9.5 mm x 1.5m) 2800 650 K4 Conduit 4000 650 K6 Conduit (6 mm probe) 4000 650 K6 Conduit (16 mm probe) 4000 650 K4 Sentinel 4000 650 AgX 1.5 m to Sentinel 2800 650 AgX 2 m to Sentinel 2000 650 DS Micro Flow Cell 4000 650 FlowIR 4000 650
Connect Button (on some instruments)	See ReactIR 247, FlowIR, ReactIR 45P and ReactIR 45P Dual Configuration.

If a ReactIR 15 or ReactIR 45 instrument is selected, additional checkboxes are added to the bottom of the configuration page of the wizard.



The RTD checkboxes allow the user to enable the instrument RTDs. There is one RTD checkbox for the ReactIR 15 and two for the ReactIR 45. When enabled, the RTD is displayed on the experiment wizard as a checkbox. When the checkbox on the experiment wizard is checked, the RTDs values are trended during the experiment. The 

button is used to calibrate the RTD.

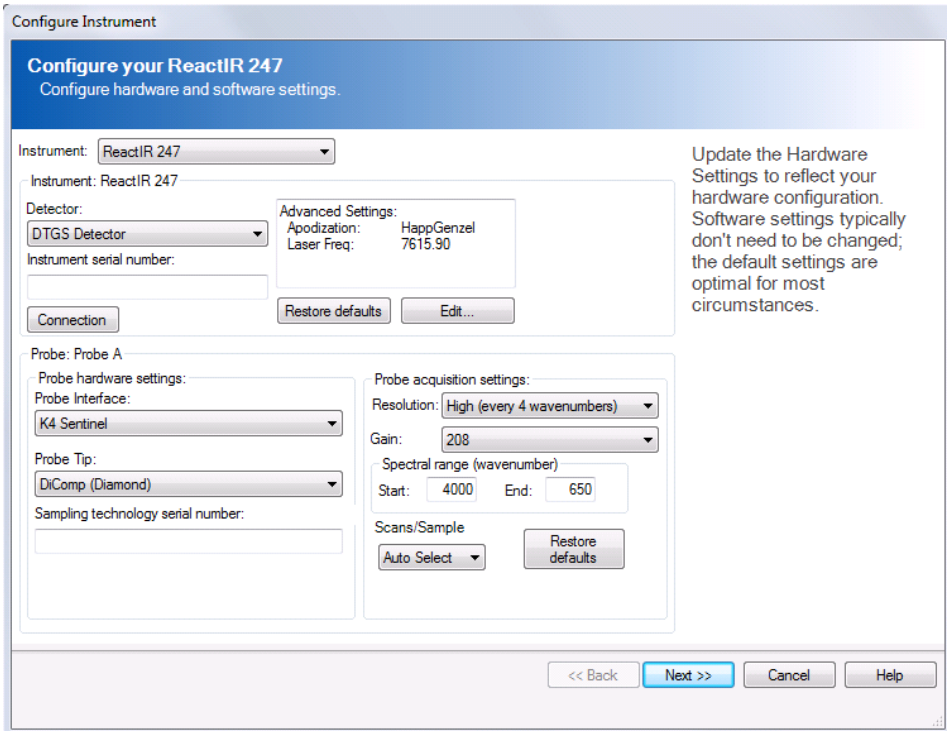
When the options are configured correctly, click the **Next** button to advance to the **Preparing to Clean the Probe** page of the wizard.

Note: If the user selects a MMIR instrument and the MMIR utility has not been run on that instrument, a warning dialog is displayed.

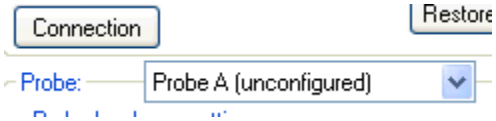
The user should exit the iC IR software, run the MMIR utility and restart the iC IR application.

ReactIR 247™, FlowIR™, ReactIR 45P™ and ReactIR 45P™ Dual Configuration

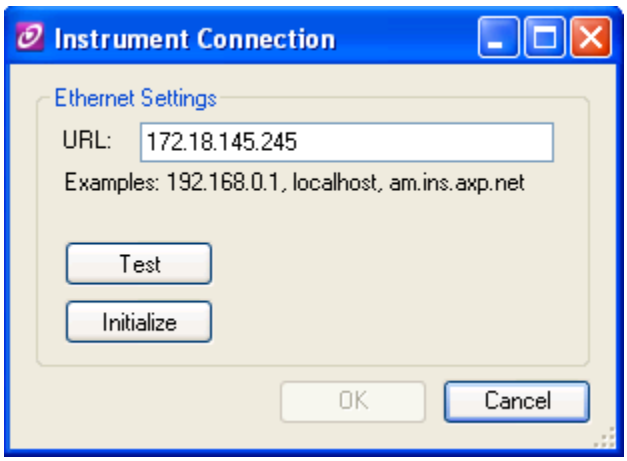
The Configuration page for the ReactIR 247, FlowIR, ReactIR 45P and ReactIR 45P Dual incorporate an additional **Connection** button.



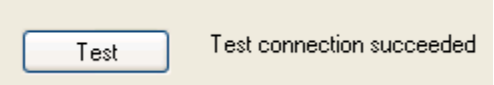
Note: The ReactIR 45P Dual configuration page has an additional field that allows the user to select the probe to be configured.



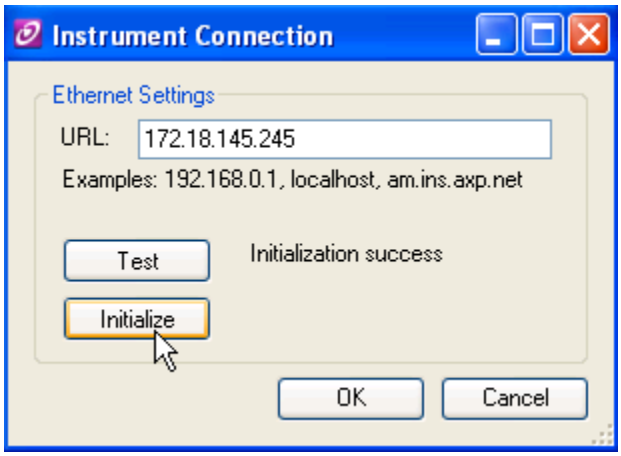
This **Connection** button is used to set up and test the address for the instrument. Click the button to open the Instrument Connection dialog.



Enter the instrument address using the formats listed on the dialog and click the **Test** button to verify that the iC IR software can communicate with the instrument. A success message will be displayed in the dialog.



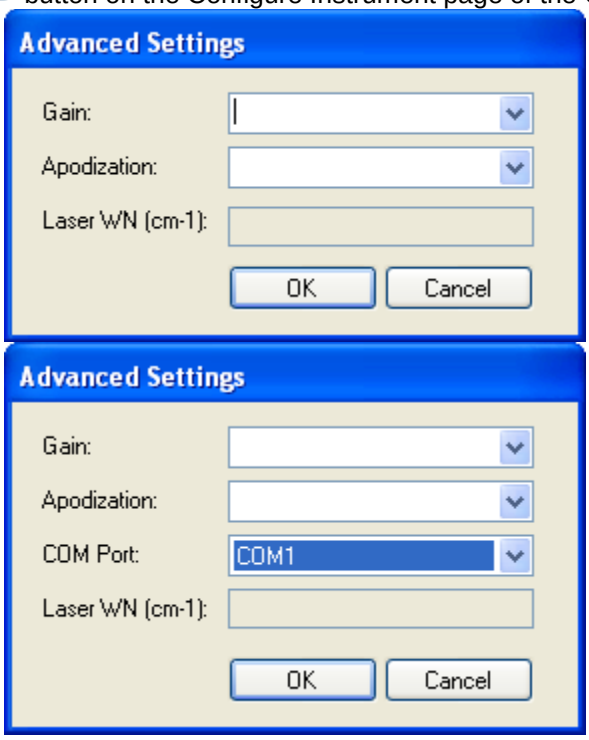
Click the **Initialize** button. When the instrument has been initialized, the **OK** button is enabled.



Click the **OK** button to close the dialog and continue with the instrument configurations outlined in the preceeding section.

Instrument Configuration Settings

The Advanced Setting dialog is used to edit the instrument setting for the instrument. The dialog is accedes by clicking the Edit... button on the Configure Instrument page of the Configuration wizard.



Note that the fields available will differ depending on whether the instrument employs a communications port.

Also note that the Configure Instrument page contains a Restore defaults button to restore a configuration to its factory default.

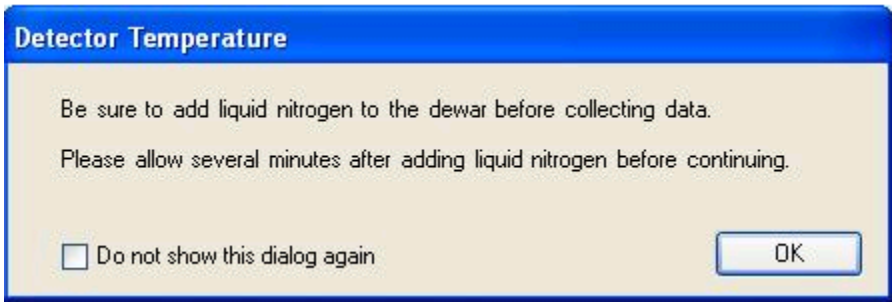
The following table describes the legal settings for the various instrument configurations.

Model	Probe Interface	Probe Tip	Resolution	Detector	Apodization	Gain	Scans per Sample
ReactIR™ iC10	C1, 1.0m AgX (Sentinel only), 1.5m AgX, >1.5m AgX, K4, K6, DS Flow Cell	DiComp, SiComp	4, 8, 16	LN2 MCT, DTGS	Happ-Genzel, Boxcar, Triangular	1-256	16, 32, 64, 128, 256, 512, 1024
ReactIR™ 45m	C1, 1.0m AgX (Sentinel only), 1.5m AgX, >1.5m AgX, K4, K6, DS Flow Cell	DiComp, SiComp	4, 8, 16	LN2 MCT, SE MCT	Happ-Genzel, Boxcar, Triangular	1-256	16, 32, 64, 128, 256, 512, 1024
Dual-Probe ReactIR™ 45 (Fiber MultiplexIR)	1.0m AgX (Sentinel only), 1.5m AgX, >1.5m AgX, DS Flow Cell	DiComp, SiComp	4, 8, 16	LN2 MCT, SE MCT	Happ-Genzel, Boxcar, Triangular	1-256	1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024
MMIR for ReactIR™ 45m	RB02-250, RB04-50	DiComp, SiComp	4, 8, 16	LN2 MCT, SE MCT	Happ-Genzel, Boxcar, Triangular	1-256	1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024
ReactIR™ 15	1.0m AgX (Sentinel only), 1.5m AgX, >1.5m AgX, DS Flow Cell	DiComp, SiComp	4, 8, 16	LN2 MCT, SE MCT	Happ-Genzel, Boxcar, Triangular	1-256	16, 32, 64, 128, 256, 512, 1024
ReactIR™ 247	K4, Sentinel	DiComp, SiComp	4, 8, 16	DTGS	Happ-Genzel, Boxcar, Triangular	192-255	16, 32, 64, 128, 256, 512, 1024
ReactIR™ 45P	C1, 1.0m AgX (Sentinel only), 1.5m AgX, >1.5m AgX, K4, K6, DS Flow Cell	DiComp, SiComp	4, 8, 16	SE MCT, DTGS	Happ-Genzel, Boxcar, Triangular	1-256	16, 32, 64, 128, 256, 512, 1024
ReactIR™ 45P Dual	1.0m AgX (Sentinel only), 1.5m AgX, >1.5m AgX, DS Flow Cell	DiComp, SiComp	4, 8, 16	SE MCT, DTGS	Happ-Genzel, Boxcar, Triangular	1-256	1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024
FlowIR™	FlowIR™ Sensor	DiComp, SiComp	4, 8, 16	DTGS	Happ-Genzel, Boxcar, Triangular	192-255	16, 32, 64, 128, 256, 512, 1024

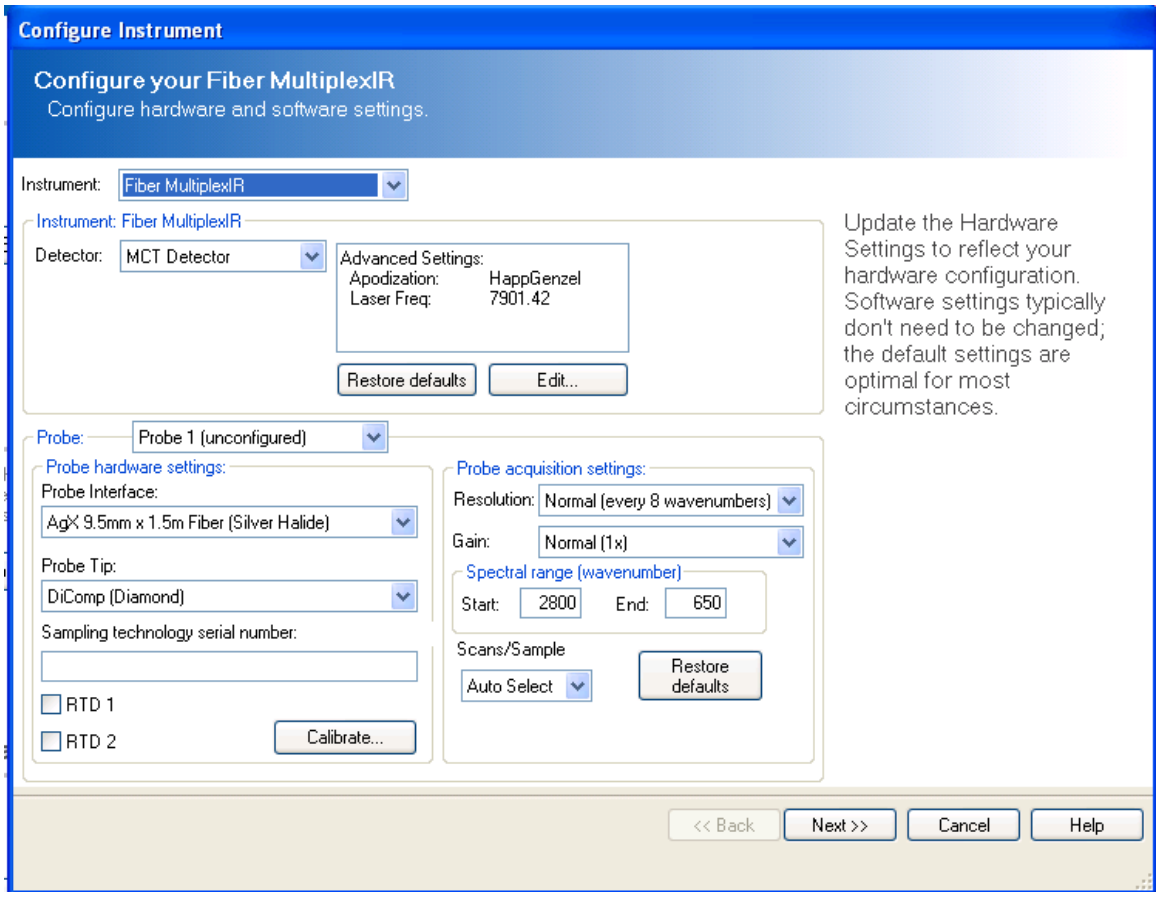
Multi-Probe Configuration

If a Multi-Probe configuration is selected in the instrument configuration, a droplist is provided on the Configure Instrument page of the configuration wizard to select the probe to use for an experiment. The probe is selected from the droplist and its properties are selected.

If the instrument is an R400 or an iC45M with a MCT diagnostic failure, the following reminder will be displayed.



The user has the option of turning off the reminder either with the checkbox in the dialog or through the Preferences options.



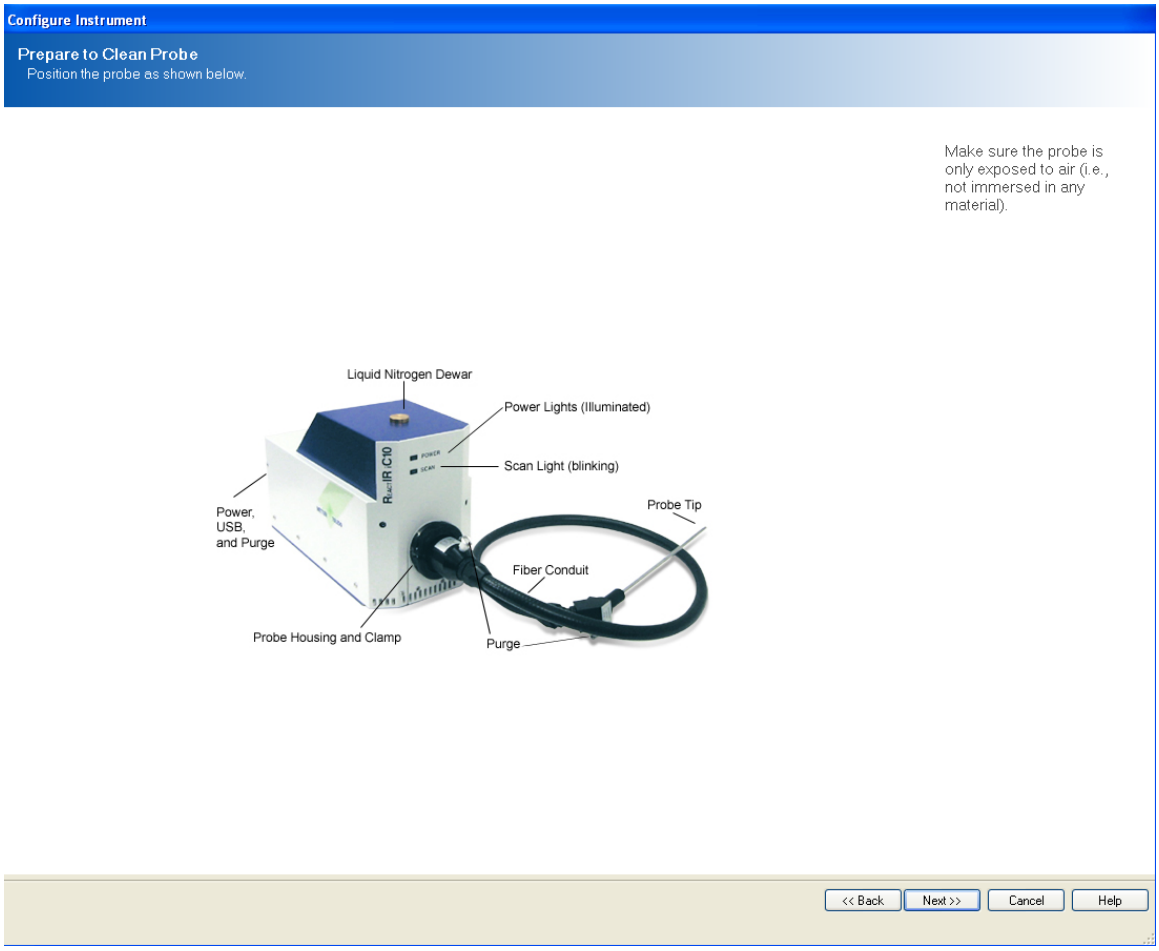
The following considerations apply to multi-probe configurations.

- Advanced Settings are shared among all probes of a multi-probe instrument.
- Settings for Probe Tip, Conduit, Resolution and Start/End WN can be set on a per-probe basis.
- Background and Water-vapor references are saved on a per-probe basis.

The alignment settings are saved independently for each probe.

Preparing to Clean the Probe

This page of the wizard is an informational page that shows the position of the probe for cleaning.

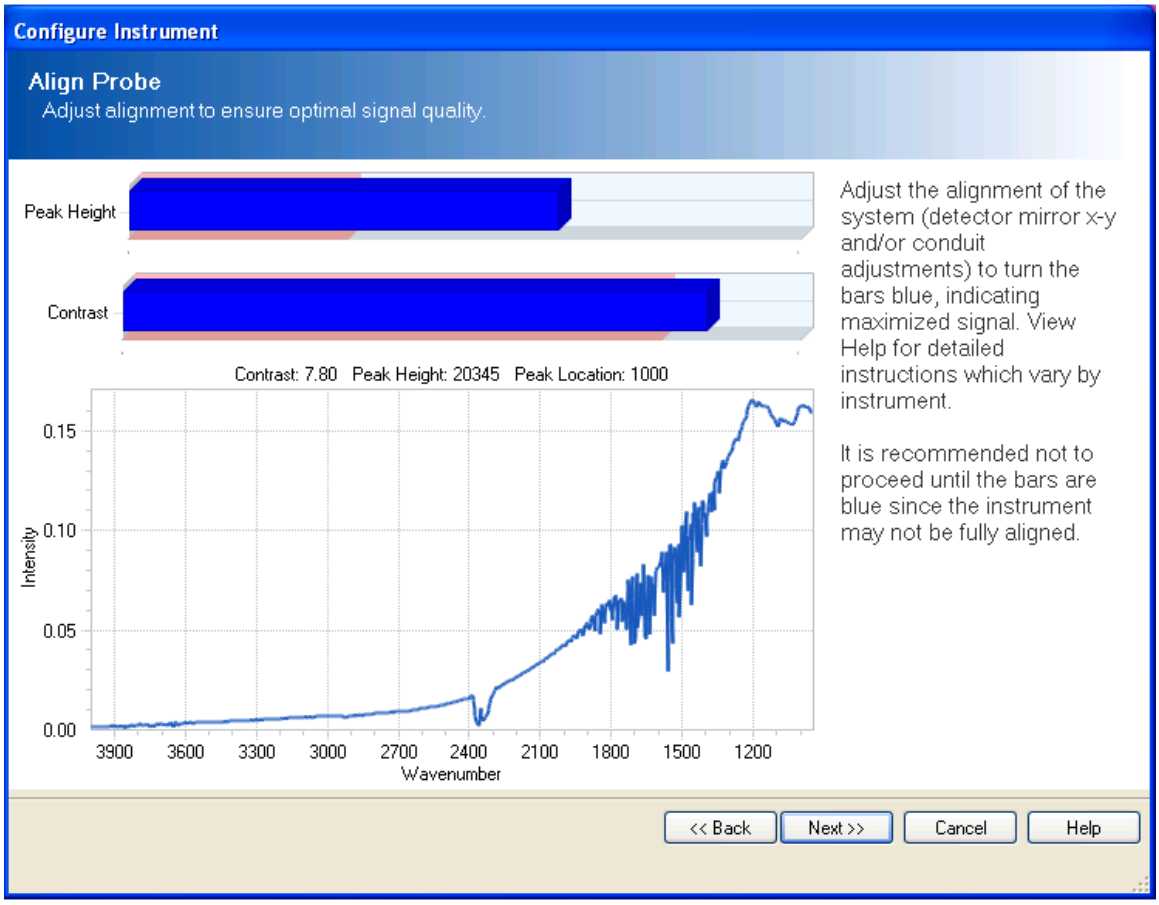


Note: The image shown in the wizard will differ depending on the instrument type specified in the configuration.

Position the probe as shown and click the **Next** button.

Aligning the Probe

This page of the wizard is used to physically align the probe. When the probe is aligned correctly, the indicator bars turn blue.



The alignment procedure varies depending on the instrument type and whether a flexible fiber or articulated conduit is used. Refer to:

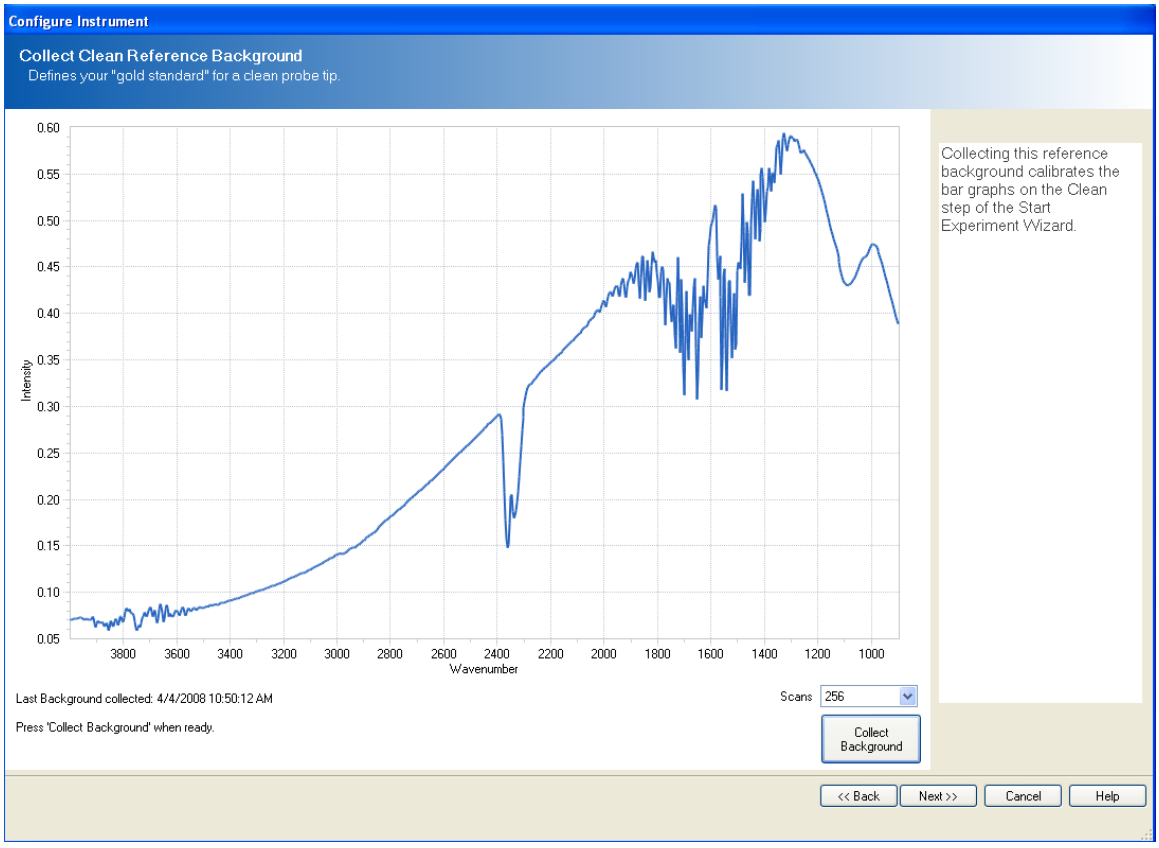
- ReactIR iC10 Setup Procedures
- ReactIR 45m Setup Procedures

Collecting a Clean Reference Background

This page of the wizard is used to collect a new spectral background of a clean, dry sensor in air. This reference background (or 'Gold Standard') will be used in the 'align' section to determine if the sensor is clean and the instrument sufficiently purged. It co-adds together 256 scans to ensure an accurate spectrometric background correction factor. The collection process is indicated by a time bar.

IMPORTANT: The system must be thermally stable, well purged with dry air or nitrogen, and have a clean sensor! To ensure a clean probe we recommend using the *BCS* (*Background…Clean…and Sample*) procedure. With this simple and effective approach a *Background* is obtained, the probe tip is *Cleaned* and then a *Sample* spectrum is obtained. If you have removed any contaminants from the sensor interface during the *Cleaning* step you will note a deviation in the *Sample* spectrum - which should essentially be a flat line, excluding the noise in the diamond region of the spectrum. If needed another round of *BCS* will continue to monitor the sensor interface for changes during the *Cleaning* step. *BCS* is **the** systematic approach to, arguably, the most critical aspect of setup for your system. It is hard to overstate the importance of a clean sensor as you move forward with monitoring your chemistry.

If you do not need to collect a fresh background, click the **Next** button to display the next page of the wizard.



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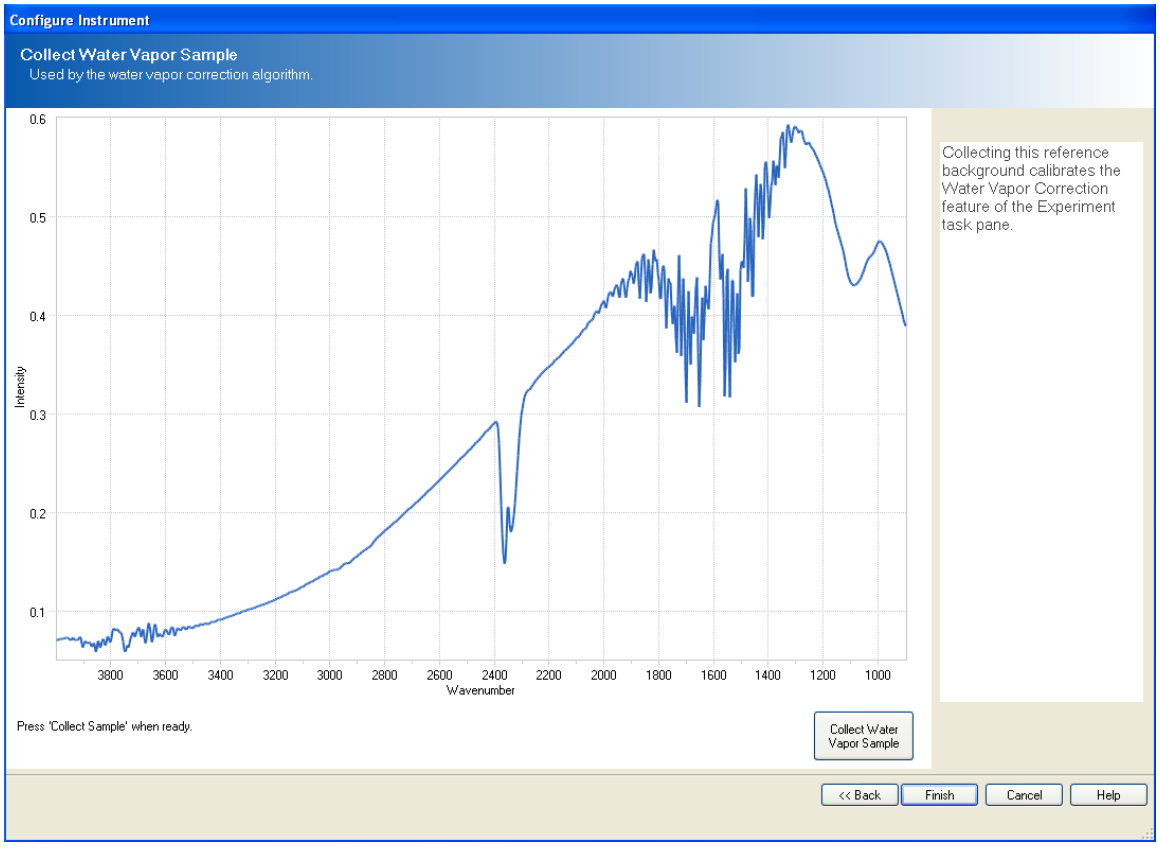
Collecting a Water Vapor Sample

This page of the wizard is used to collect a reference spectrum of water vapor. This reference spectrum is used for subtracting out water vapor from a data set. *It is not intended to be a replacement for an effective dry air or nitrogen purge.* The water vapor reference spectrum is simply a convenient way to remove small amounts of water vapor which may enter or leave the instrument over a long reaction period. The water vapor spectrum is displayed after the data is collected. Click the **Finish** button to complete the instrument configuration.

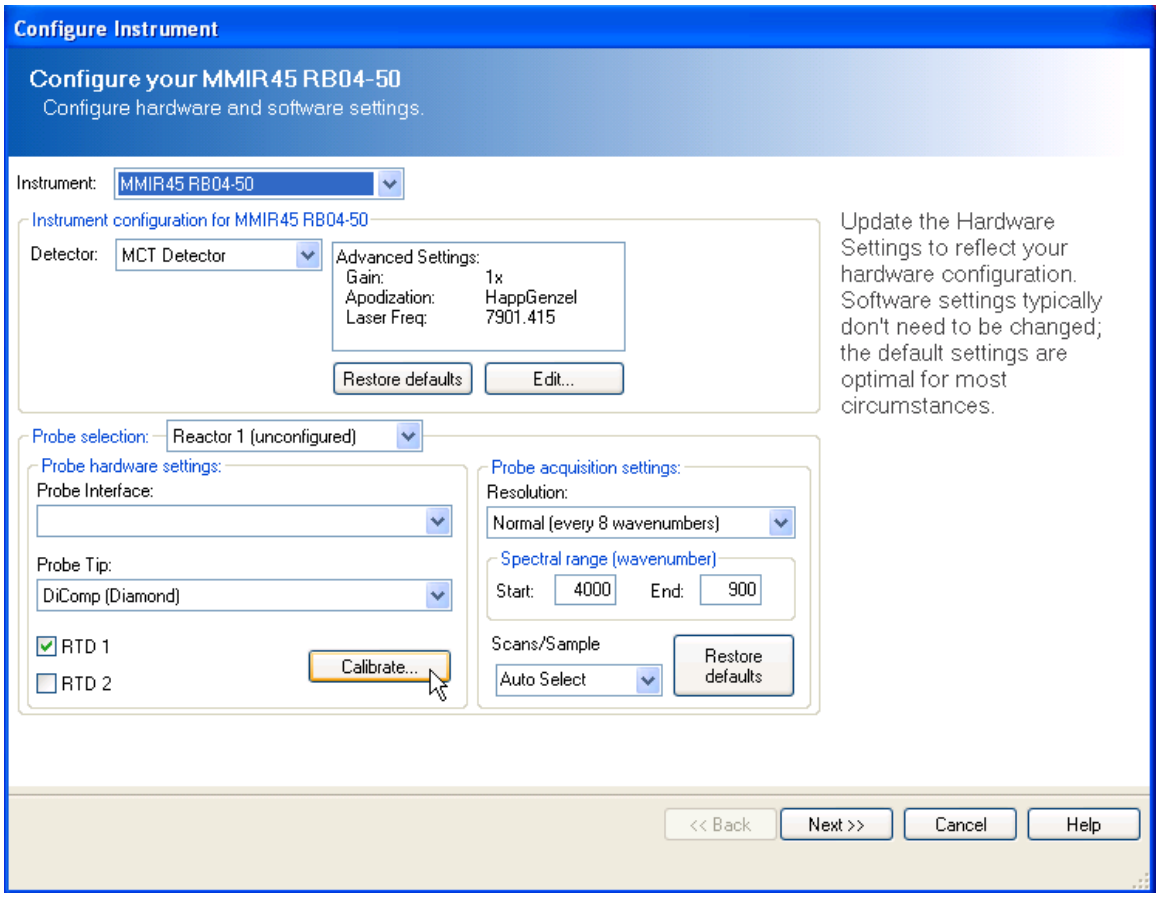
Note that the water vapor step is skipped for ReactIR 15 ReactIR 45P, ReactIR 45P Dual, FlowIR and ReactIR 247 instruments unless it is enabled in the User Preferences.

IMPORTANT: In order to collect a good reference spectrum of water vapor one must first obtain a good reference background with a well purged system and clean probe. Next, the system purge must be turned off for approximately 15 minutes to allow ambient moisture to collect within the system at levels which approximate the changes one might see over the period of a long experiment. This single beam reference (as shown below), ratioed to the “dry” background, will produce a sample spectrum of water vapor - recognizable by the many sharp absorbance bands in the 1800-1300 wavenumber region of the spectrum. This spectrum of water vapor is used to mathematically subtract interfering, ambient water vapor from your reaction spectra via an advanced algorithm specifically designed for this task.



RTD Calibration

RTDs are calibrated by clicking the Calibrate... button on the Configure Instrument page of the Configuration wizard.



The RTD Calibration wizard is launched.

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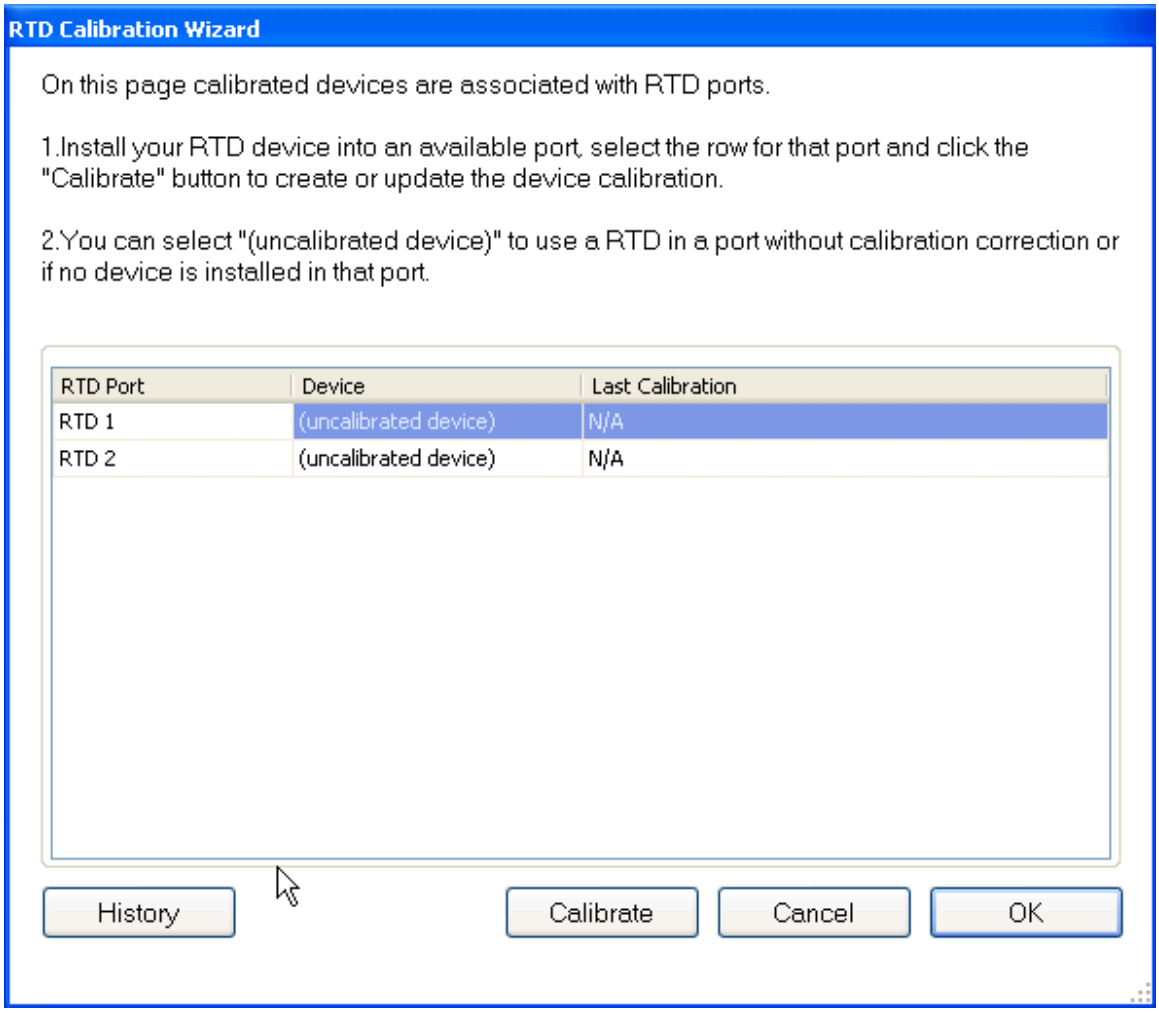


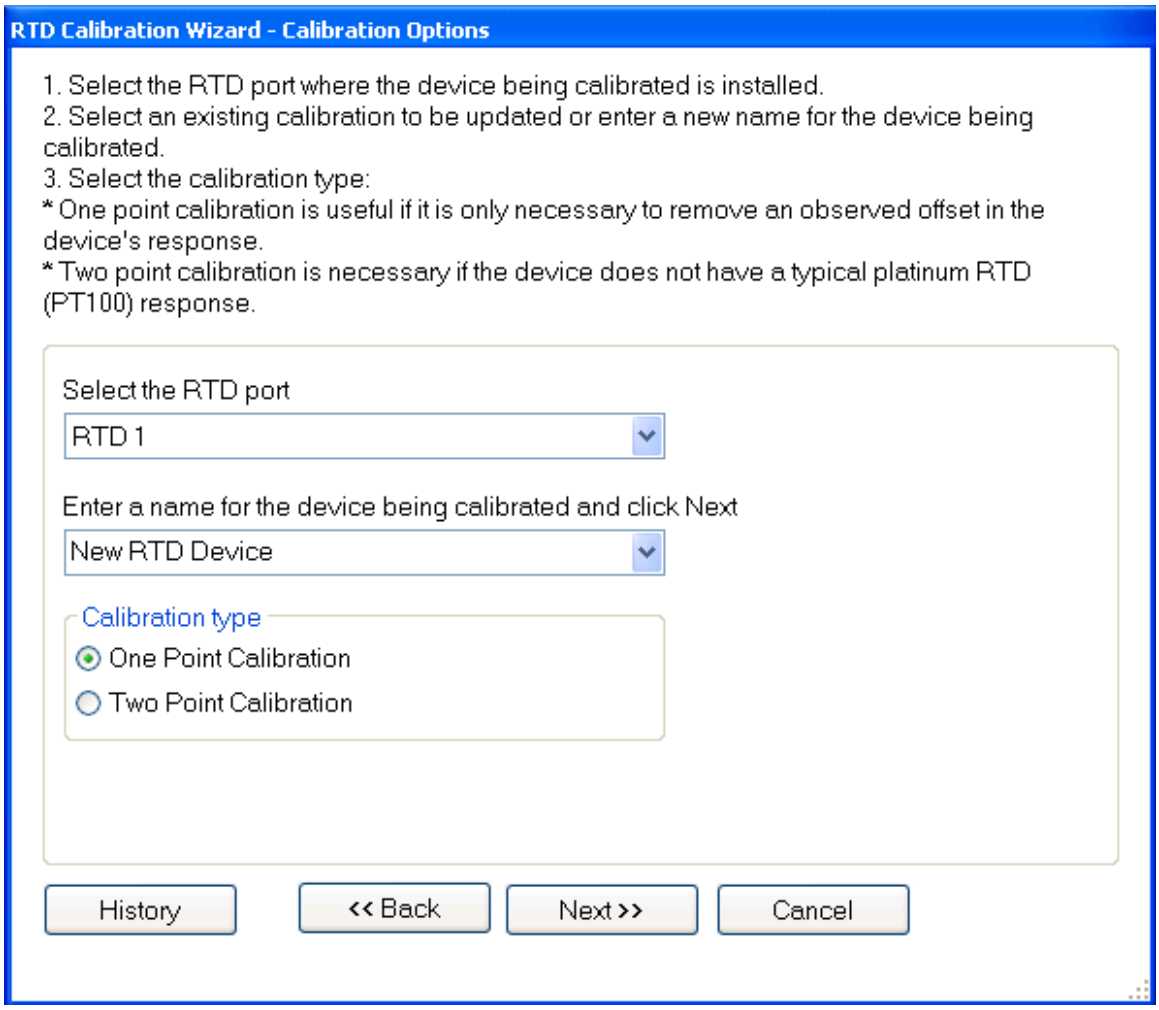
The first column lists all RTD ports on the instrument. The RTD Device column is a user-defined name for the RTD attached to the port. The last column lists the date when the RTD was last calibrated.

A RTD must be assigned a name before it can be calibrated. A droplist is provided in the RTD Device column that contains a list of all previously named RTDs. The user has the option of assigning a new name or using an existing name from the droplist. When an existing name is used, the calibration data from that RTD is used. Note that RTD Device names can be used for multiple RTD Ports. This does not imply that the physical RTD is connected to several ports, only that the calibration settings are the same for RTDs with the same device name.

A calibration history for an RTD can be viewed by selecting the RTD and clicking the **History** button. See RTD Calibration History Display.

Once a device name is assigned to the RTD, select the it and click the **Next** button to calibrate the RTD.

The next page of the wizard allows the user to select the type of calibration will be performed.



Select the calibration type and click Next.

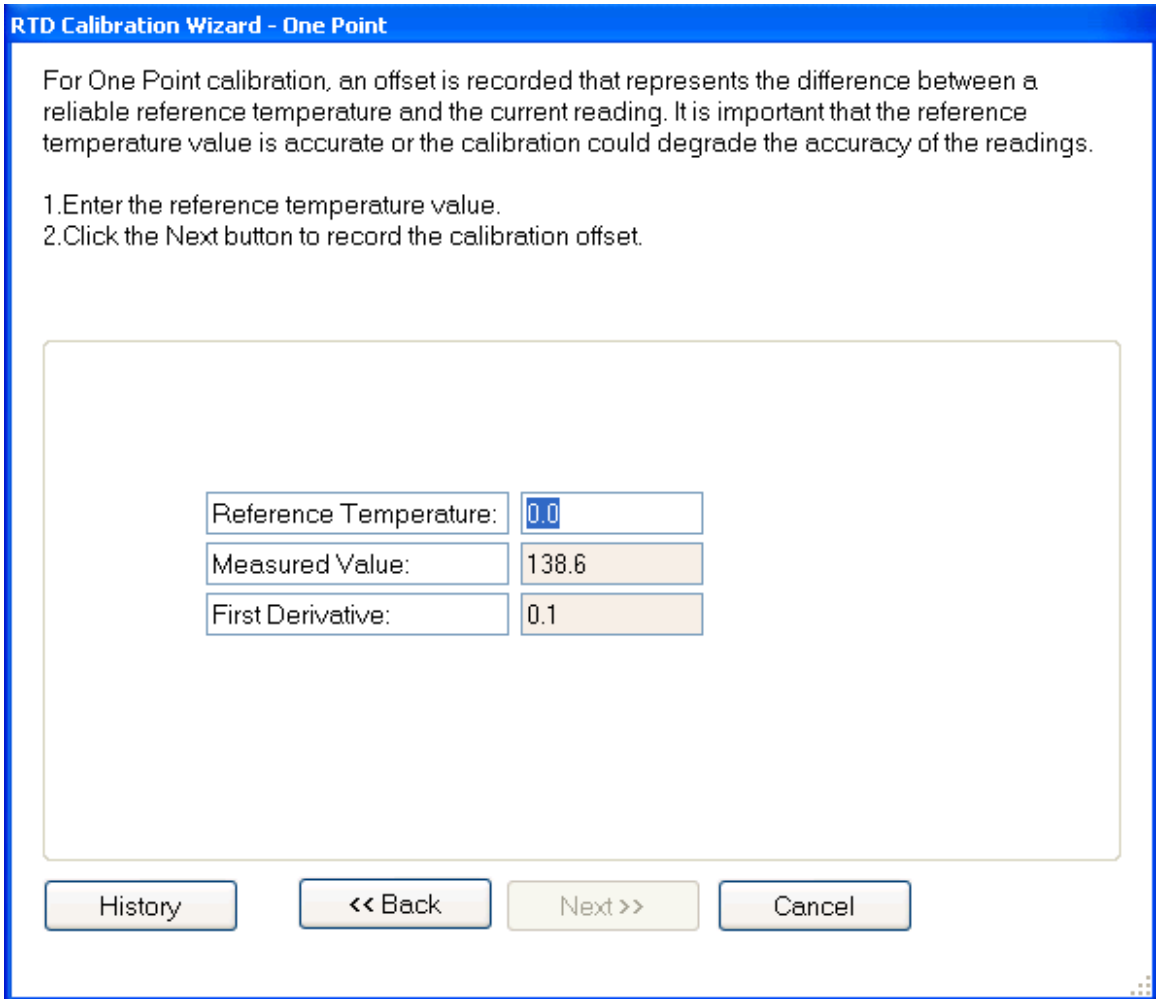
For One Point calibration, see Calibration Wizard: One Point (Offset Removal).

For Two Point calibration, see Calibration Wizard: Two Point Calibration (Response Correction).

Note that the FlowIR requires Two Point calibration. The One Point calibration button is disabled for the FlowIR.

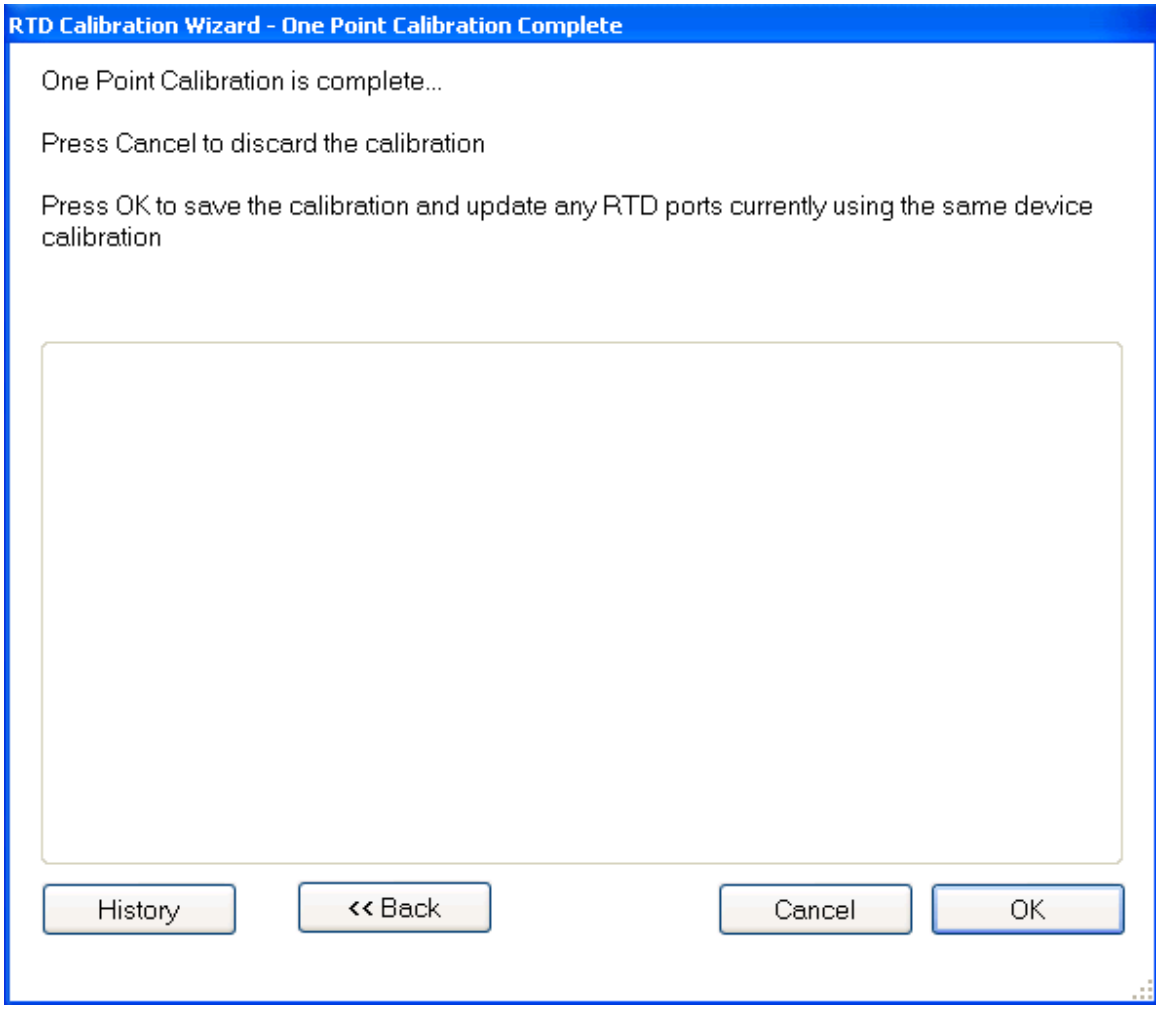
Calibration Wizard: One Point (Offset Removal)

This calibration mode assumes the current response curve is correct for the RTD in use and simply nulls out any offset from the actual and expected values – which are required inputs.



The user is urged to test the RTD's reported temperature at various set points using a calibrated temperature measuring device.

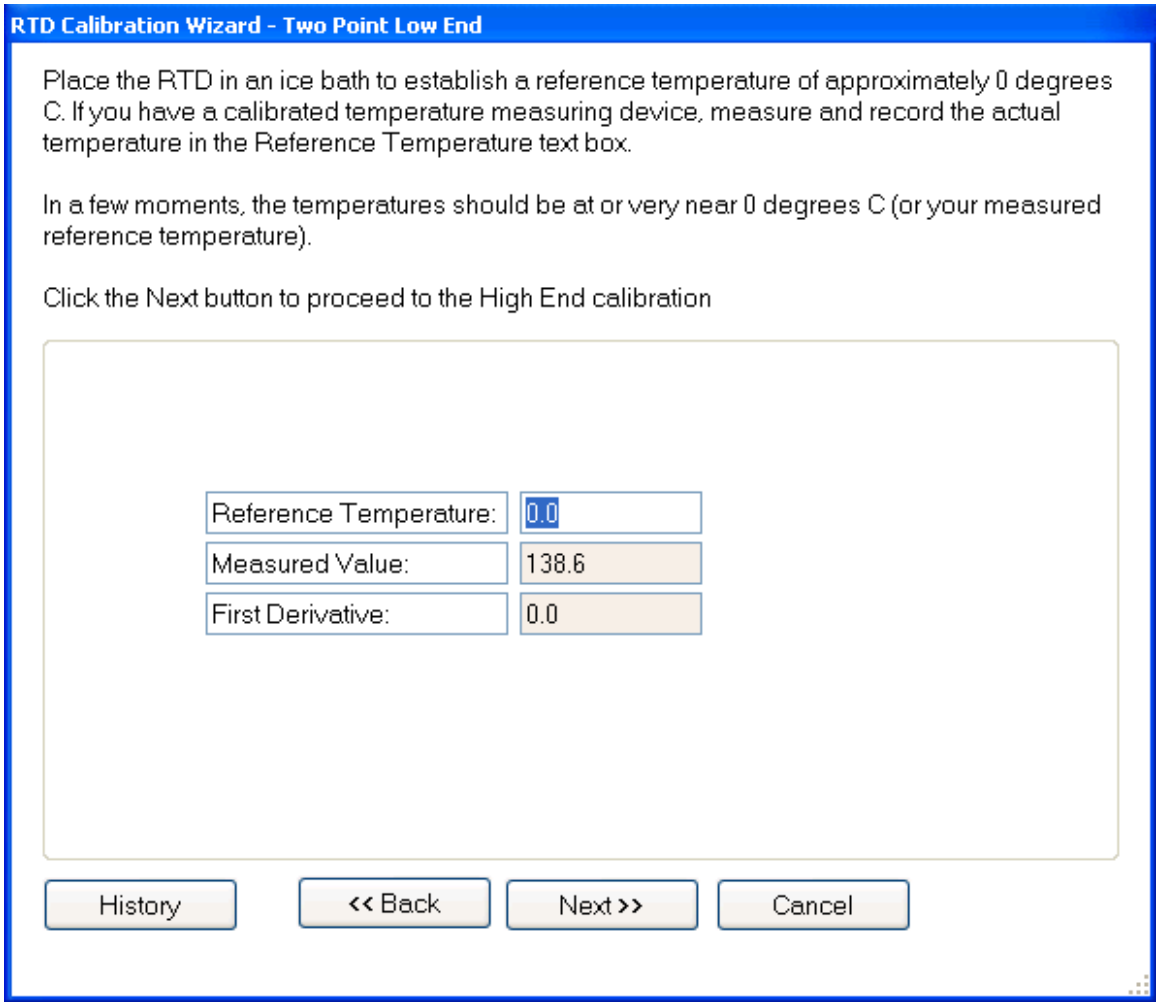
When the value settles out, the **Next** button is enabled and the offset is calculated. Click the **Next** button to advance to the calibration complete page.



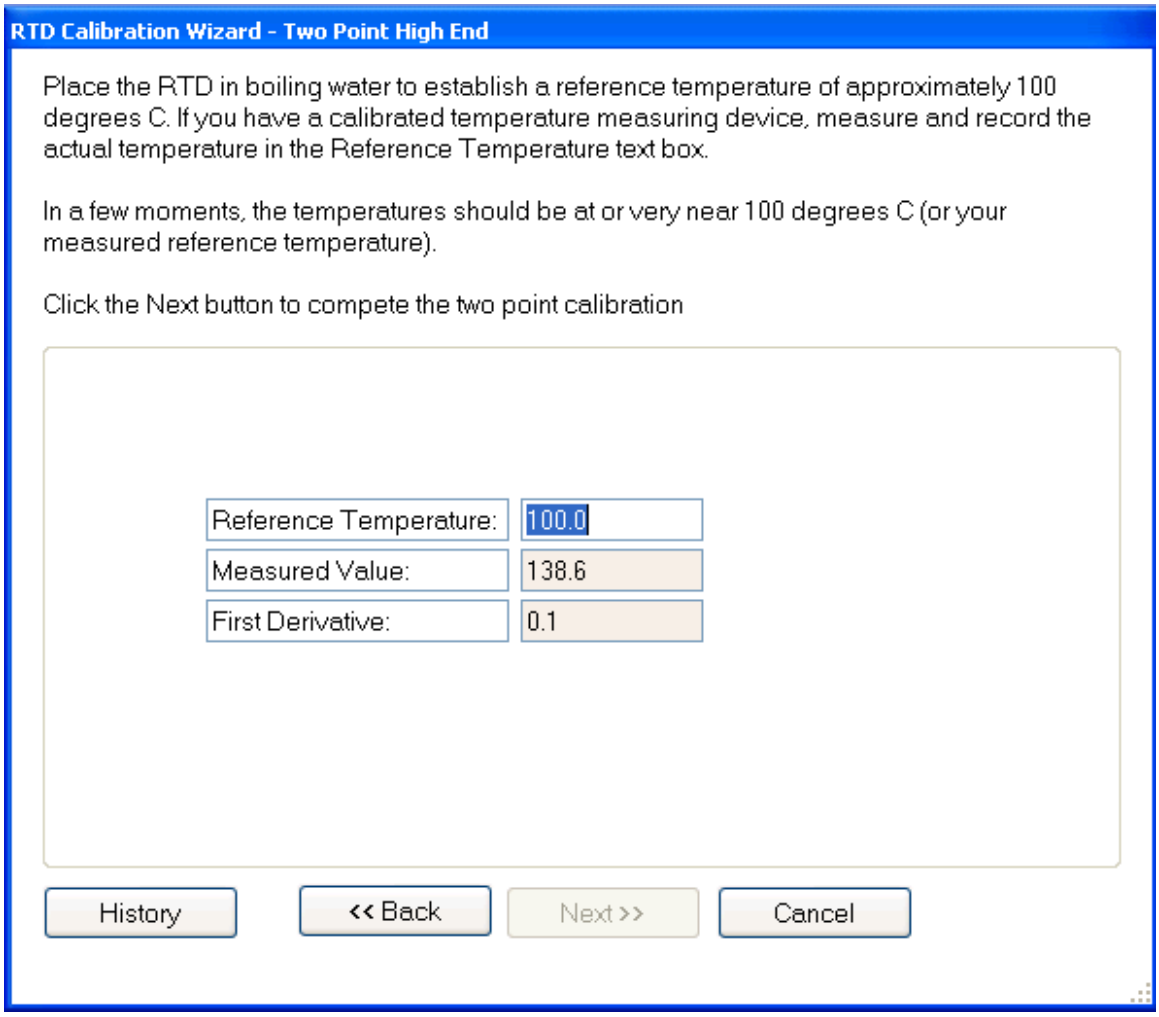
Clicking **Save** stores the offset correction value to disk for this instrument and RTD. At this point the probe is calibrated and ready to use.

Calibration Wizard: Two Point Calibration (Response Correction)

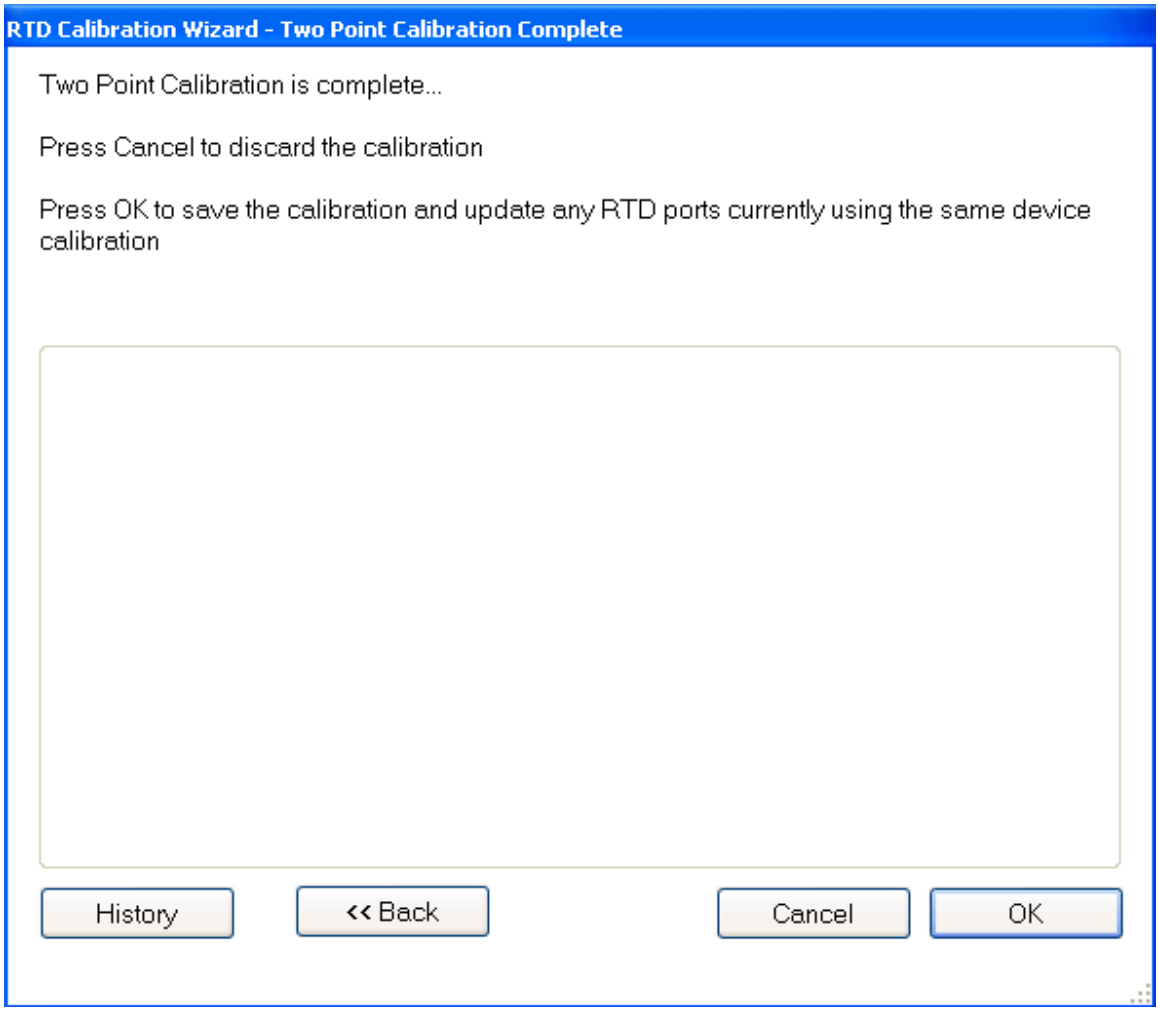
This calibration mode assumes that the response curve currently configured for the device is not correct and it is necessary to establish the correct response curve. This will require two points and is done at 0 degrees C and 100 degrees C. The Low Set Point is calibrated first. Note that the value fields are editable, allowing the user to fine tune the results.



When the value settles out, the **Next** button is enabled, click **Next** to proceed to the High Set Point calibration.



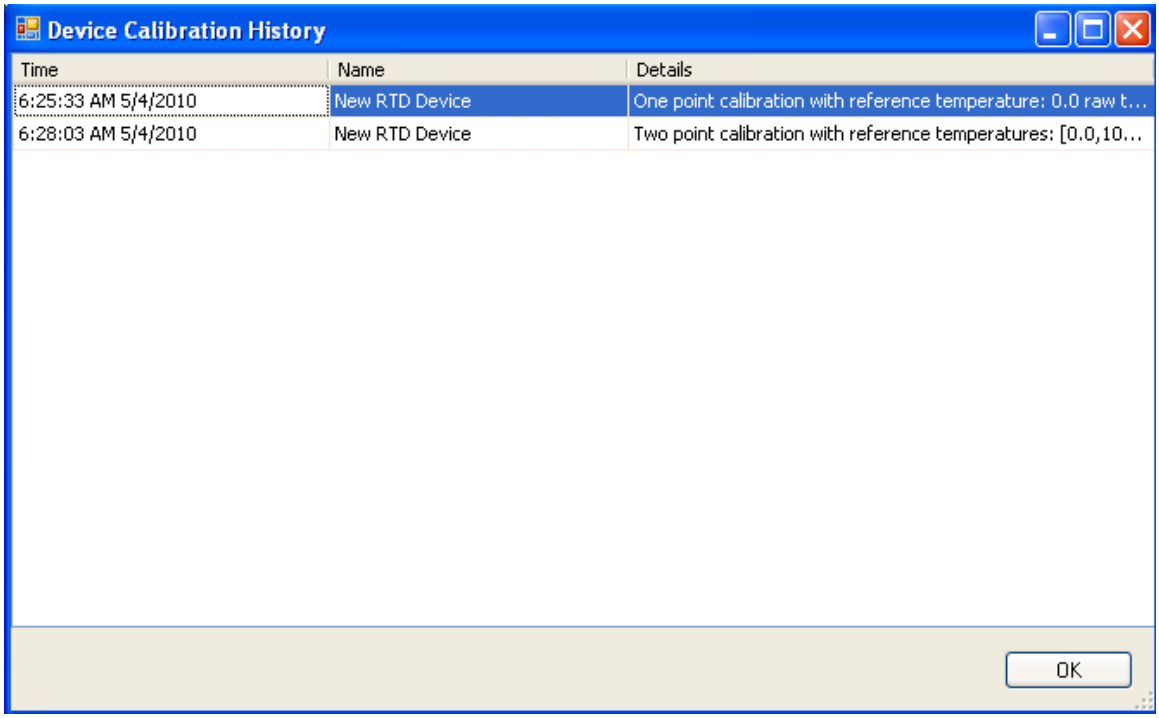
When the value settles out, the **Next** button is enabled and the offset is calculated. Note that the value fields are editable, allowing the user to fine tune the results. Click the **Next** button to advance to the calibration complete page.



Clicking **Cancel** cancels the calibration procedure and no changes are made to the curve. Clicking **Save** stores the response curve definition to disk for this instrument and RTD. At this point the probe is calibrated and ready to use.

RTD Calibration History Display

The RTD Calibration History display contains a table of all calibration procedure performed on a selected RTD. The display is accessed by clicking the History button on the bottom of the RTD Calibration wizard.



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Working with the iC User Interface

All iC data displays are interactive. Some of the behavior available with the interactive displays include:

- When a spectrum is selected in the Event Viewer, it is displayed in the Spectra Viewer.
- When a spectrum is chosen in the Spectra Viewer, its location in time is displayed in the Surface Viewer if associated with that plot.
- When a peak is double-clicked in the Spectra Viewer, the peak profile is added to the Trend display.

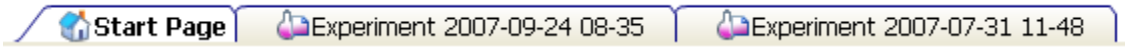
Tabbed Displays

iC makes use of tabbed displays at multiple levels within the user interface to provide flexibility and a maximum amount of available screen space for each analysis window.

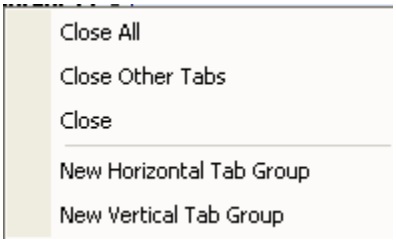
Multiple documents can be opened at once and shown as tabs across the top of the document area. Within a document, such as an experiment, multiple controls can be shown as tabs across the bottom of the document window.

Tab Groups allow you to view multiple documents at once

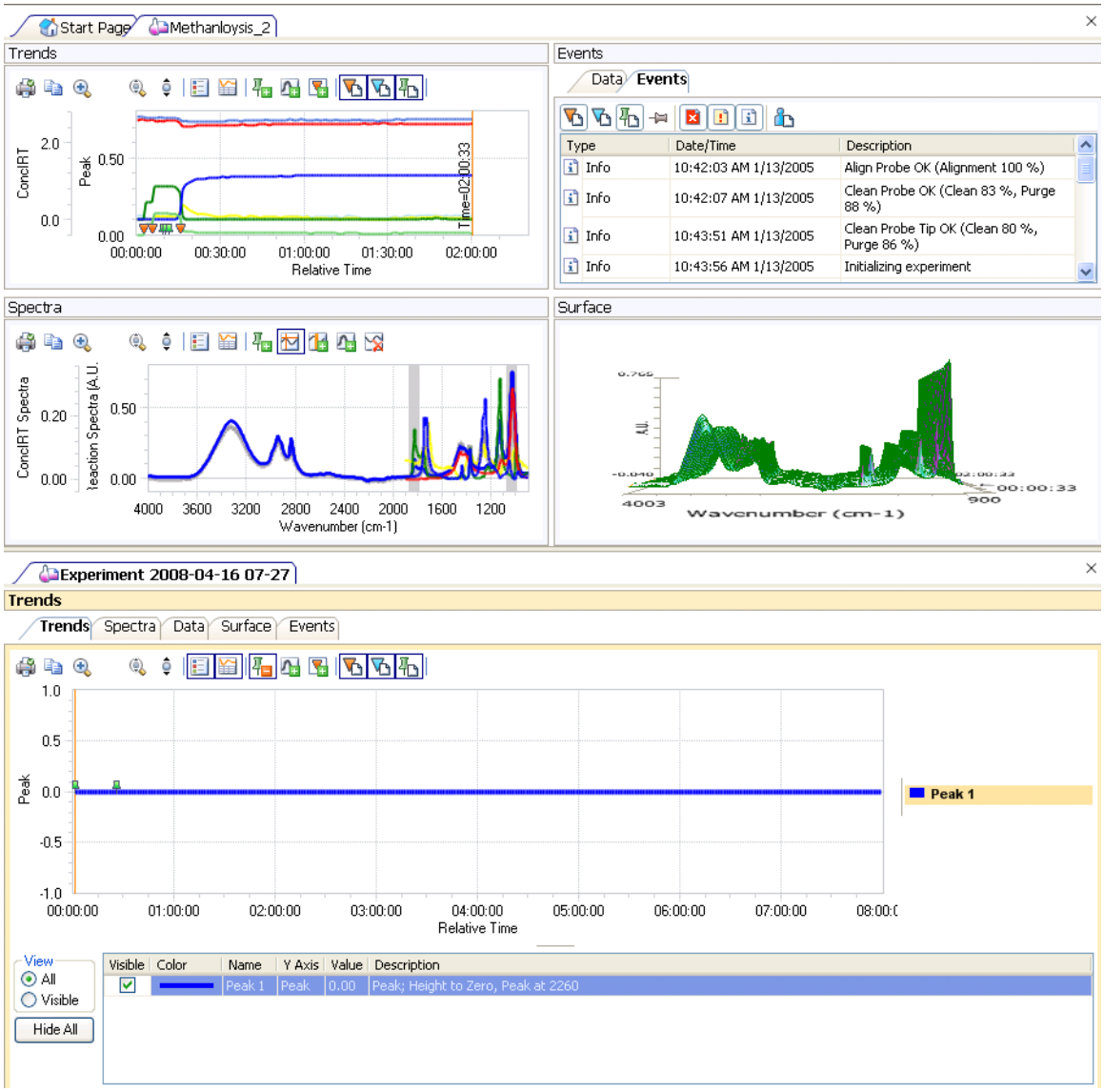
When multiple documents (e.g., experiments, results sets, etc) are opened, they are displayed as tabs located at the top of the display window. The user clicks on a tab to view that document.



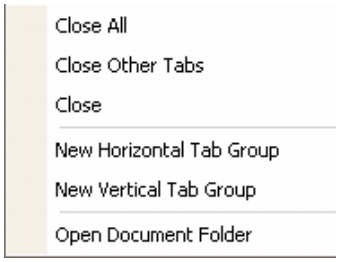
Two experiments can be viewed at once by right-clicking on a tab and selecting one of the tab group options from the context menu.



In the figure below, the New Horizontal Tab Group option was selected on an experiment. Note the screen is now divided into an lower tab group containing a single document and a upper tab group containing the remaining documents.



Once a new tab group has been created, the user can right-click on the tab again to rotate the tab grouping. The Move Next option rotates the selected tab group. Once all tabs have been rotated, the window returns to its original configuration.



The context menu also has several options for opening and closing document tabs.

Close All – closes all open tabs except the Start Page.

Close Other Tabs - closes all open tabs except the current tab and the Start Page.

Close – closes the current tab.

Open Document Folder – opens the folder (in a file browser) where the active document resides.

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Tabbed/Tiled Views Organize Data within a Document

The four viewer controls on the experiment display are normally tiled to show multiple perspectives on the experiment simultaneously. Alternately, the data displays can be organized as tabs with only one viewer control occupying the document area at a time. In the figure above, the lower experiment is viewed as tabbed which allows the profile to be seen in more detail.

When a document contains multiple tabbed controls, the tabs are displayed on the top portion of the display window.

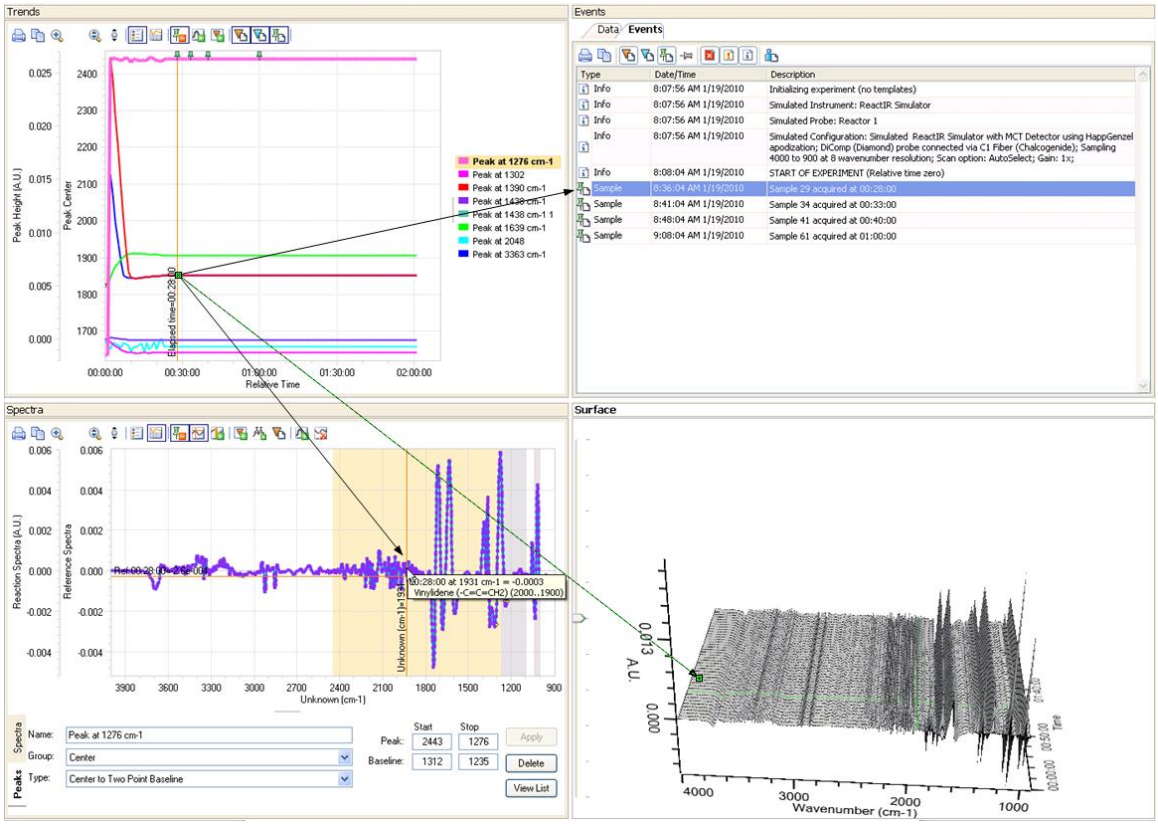
You can switch between Tabbed and Tiled views using the  buttons on the toolbar.

Linked Views

The four data viewers in the experiment display are linked interactively. For example, when a data element in one viewer is selected, the corresponding data elements in the other viewers are also highlighted.

Synchronized Highlighting

The spectral interval can be selected from the Trend Viewer, Event Viewer or Surface Viewer. The interval is highlighted on all displays automatically.



Select any reaction spectrum

If you select a reaction spectrum in the Spectra Viewer, click anywhere in the Trend Viewer, select a message in the Event Viewer or use the up/down arrow keys to highlight a spectrum in the Surface Viewer, all four viewer controls will update and highlight the chosen event:

- The thickness of the selected spectrum increases to visually highlight it.
- The associated y-axis title changes color to match the selected spectrum.
- The time line in the Trend Viewer moves to show the point in time when the spectrum was recorded.
- The Event Viewer highlights the selected event.
- The selected spectrum is highlighted on the Surface Viewer.

Selected Peak

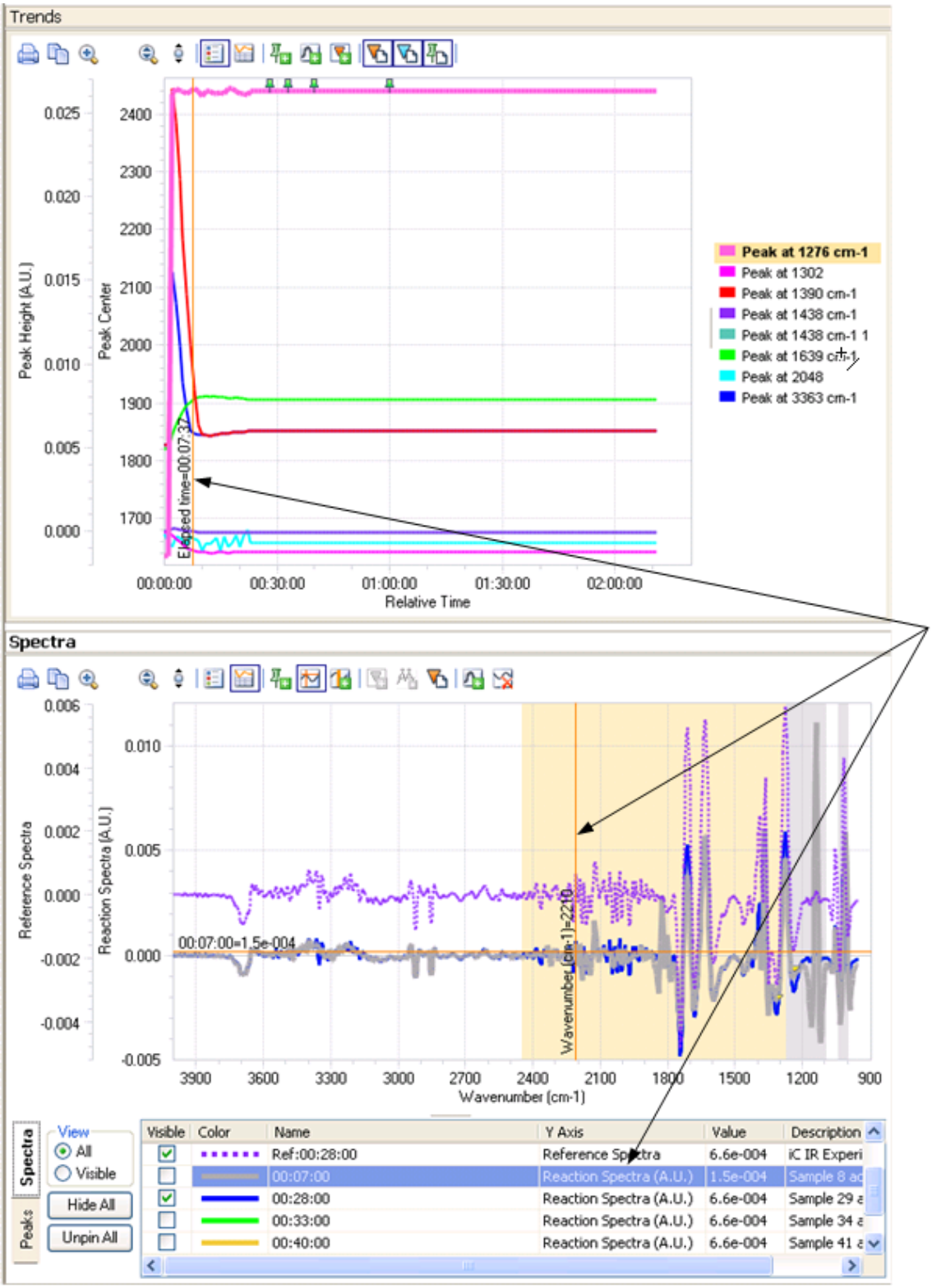
There are three ways to select an existing peak with a single mouse click:

Clicking a peak in the Spectra Viewer

Clicking a row in the Spectra Viewer grid

Clicking a peak profile trend in the Trend Viewer.

When any of these occur, the peak is highlighted in both the chart and grid in the Spectra Viewer and the trend line is widened in the Trend Viewer.



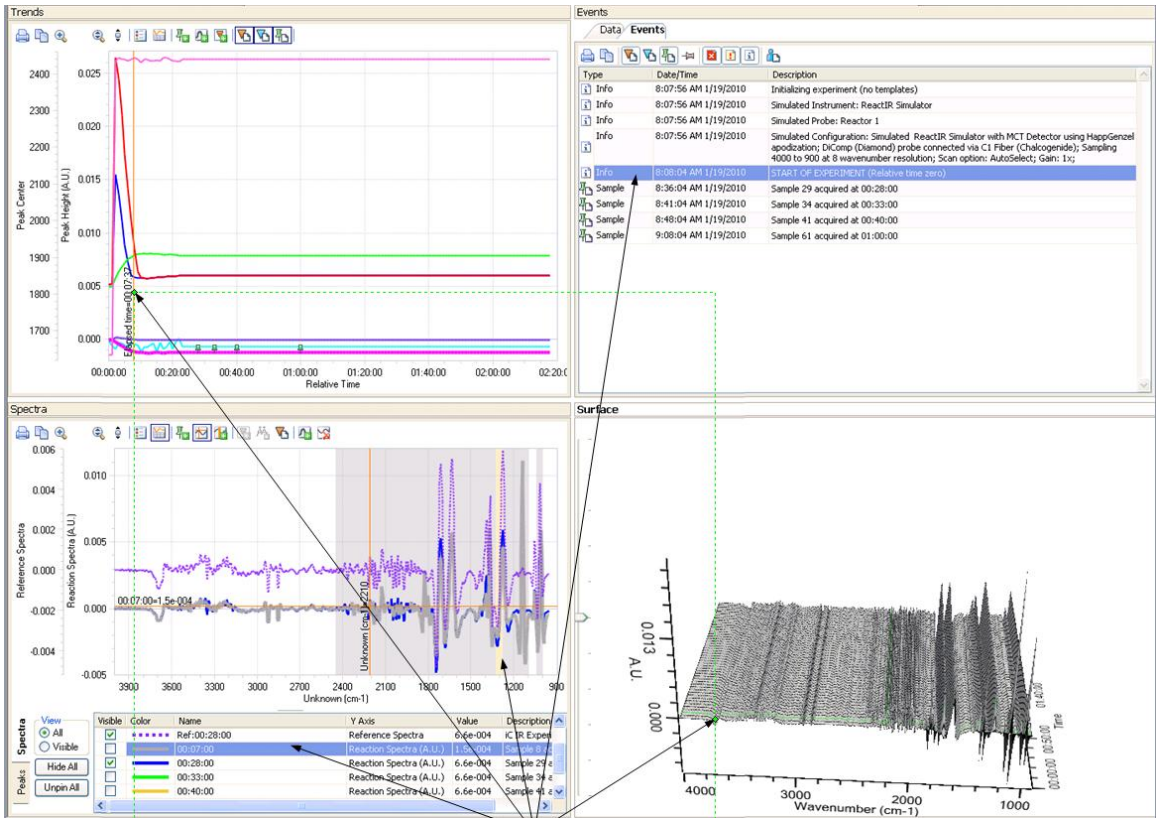
Selected Spectra

The spectra can be selected using one of these the following functions:

- Clicking on a sample in the Event Viewer.
- Dragging the time line in the Trend Viewer display
- Clicking on the spectrum in the Spectra Viewer
- Clicking on the selected spectrum in the Spectrum name list
- Clicking a point in the Surface Viewer.

When a specific spectrum is selected for analysis, all of the displays respond with the new data:

- Highlighting the row in the Event Viewer
- Positioning the Trend Viewer time line to the spectra's timestamp value
- Displaying the spectrum in the Spectra Viewer with a widened plot line
- Adding the spectrum to the Spectra Viewer's grid and highlighting it.
- Highlighting the spectrum in the Surface Viewer.



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Pinning

All measurements in the iC viewers can be pinned. When a measurement is pinned, it is displayed in the graph and in the corresponding Details Panel. Pinning is similar to the show/hide concept but pinning is application wide (one pin applies to all linked views), and show/hide is local to each individual viewer (or tile).

A Pin/Unpin button  is available on the viewers toolbar.

The following rules apply to pinning.

- Pin/Unpin is enabled/available whenever there is a selected measurement.
- When there is a selected measurement, the Pin button provides visual indication of whether the selected measurement is pinned or not.
- If unpinned, the selected measurement is gray in the Measurement/Distribution Viewer. It will change if another measurement is selected.
- Pinning from the Trend Viewer or Distribution Viewer assigns a color to the selected measurement and keeps it in the Measurement/Distribution Viewer even when another measurement is selected.
- Unpinning removes the permanent status of the selected sample and de-allocates its color, but the measurement is still selected and displayed in gray to reflect its temporary status. It will disappear entirely when another measurement is selected.
- The Remove button, removes the Reference Distribution

Show/Hide

The Distribution Viewer Details grid also has show/hide capabilities.

- Show displays the measurement or distribution in the Distribution Viewer.
- If the user clicks the checkbox to show an unpinned, selected measurement, the selected measurement becomes pinned.
- Hide removes the measurement or distribution in the Distribution Viewer and globally deselects the measurement (this will also cause the timebar in the Trend Viewer to disappear).
- Whether or not a selected, unpinned measurement is initially checked is a user preference (default value is pinned).

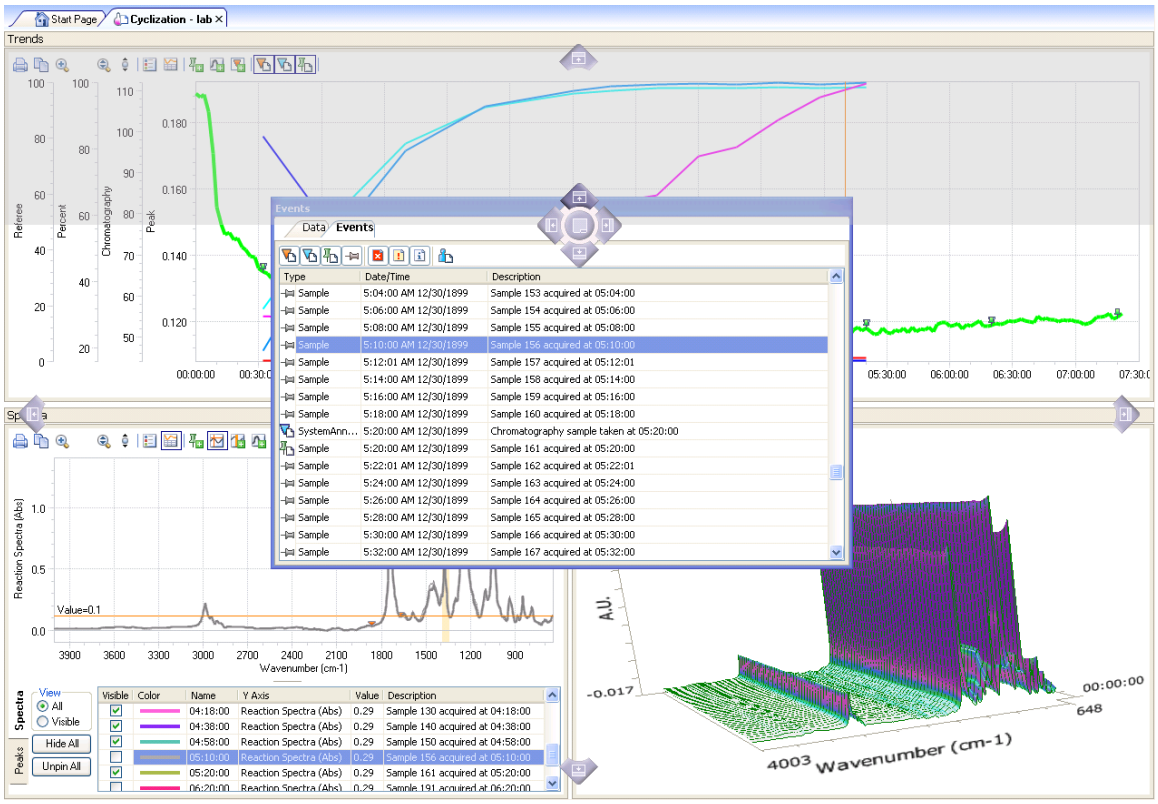
Dockable Viewers

The iC software allows the user to reposition the various viewers anywhere on the display window. In order to reposition viewers, the user clicks the  button on the toolbar. Note that the **Allow dockable controls to be undocked** option in the Tools menu must be checked in order for this button to be displayed.

The following example illustrates how to reposition the Event Viewer at the bottom of the Trend Viewer.

In the main toolbar, click the  button.

Click and drag the Event Viewer tab free from its normal position. A grey docking station control appears.



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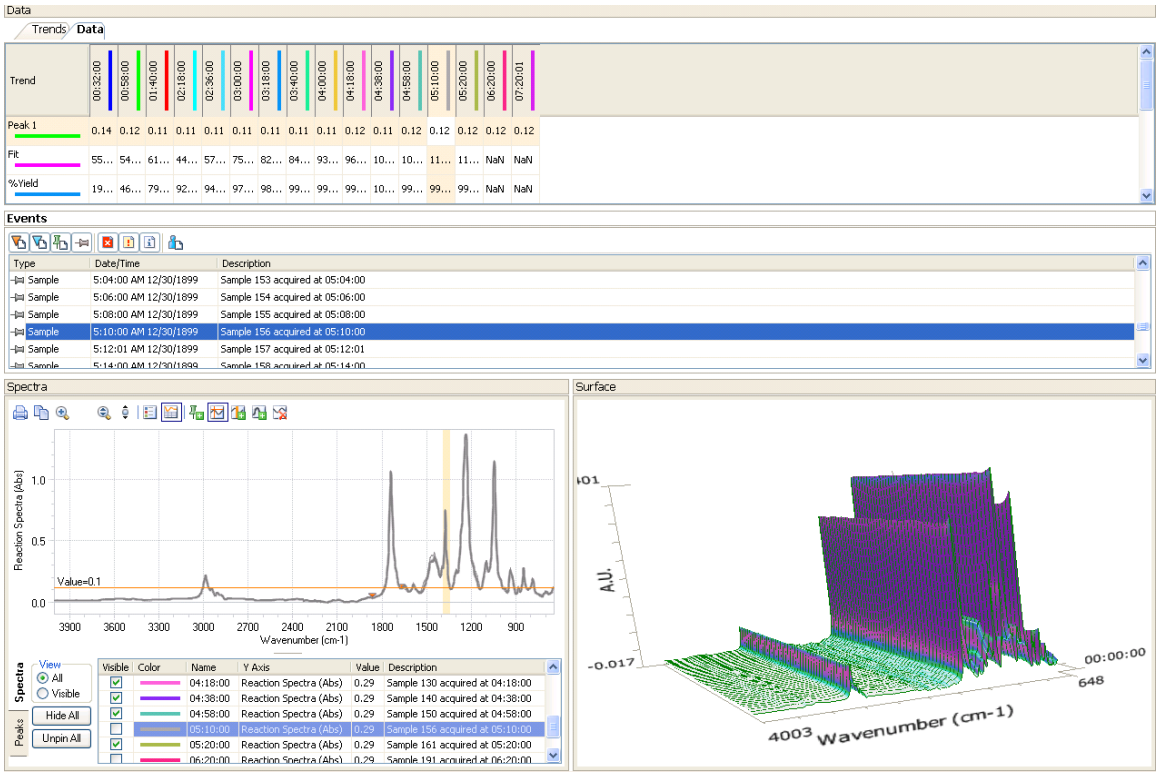
Release the mouse button while hovering over the bottom of the docking station bottom arrow.

The Event Viewer window will automatically be docked at the bottom of the Trend Viewer.



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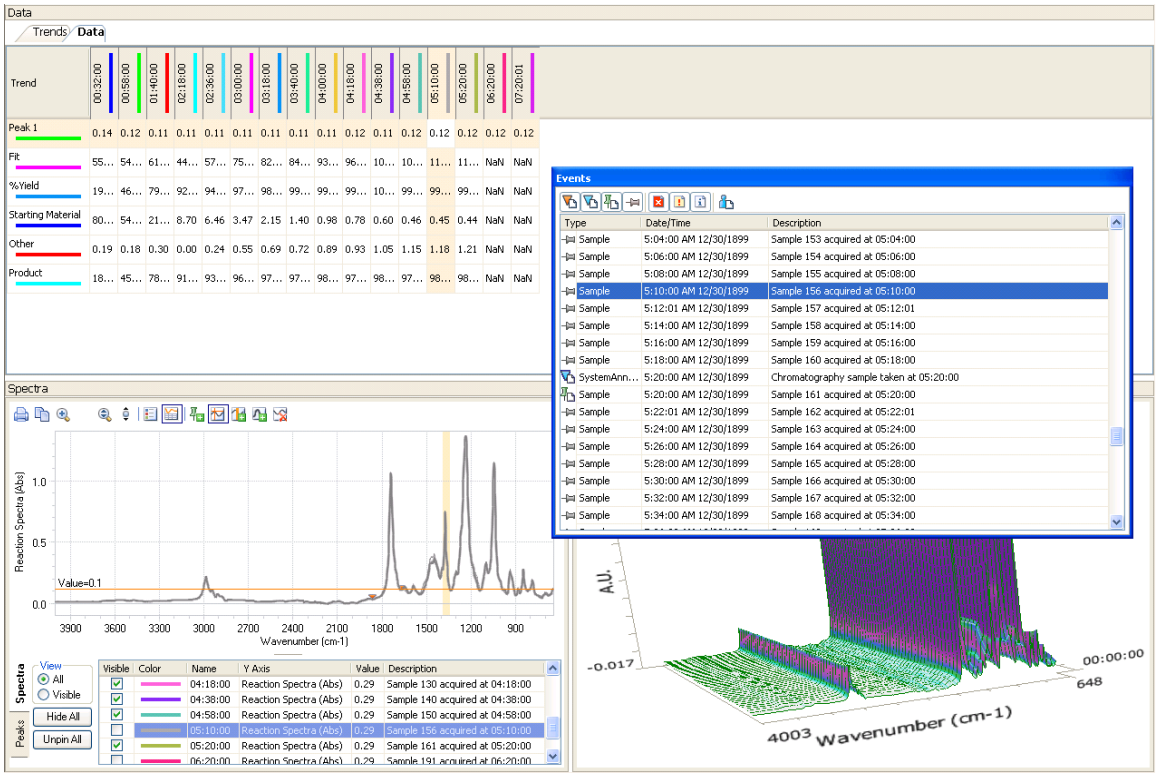
In addition to being docked, viewers can remain floating.



To return the window to one of the standard layouts, click on of the layout buttons on the toolbar.

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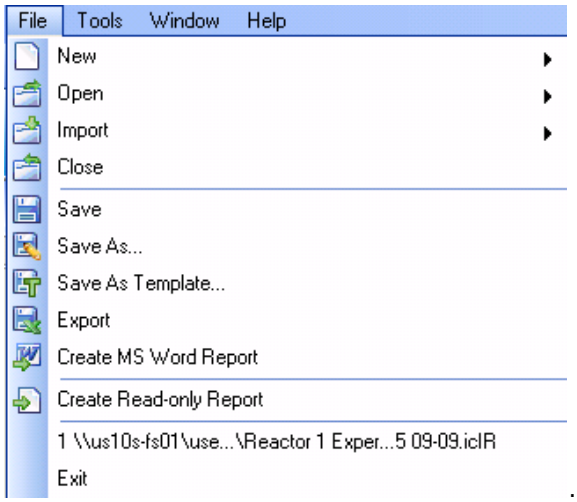
Using iC Menus

The iC application contains four pull-down menus located on the main menubar.

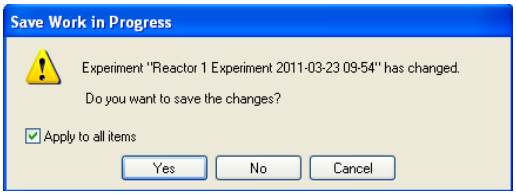
File Menu

The Files menu contains options relating to file functions such as opening and saving experiment documents.



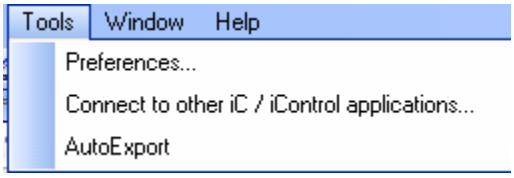
The menu contains the following options.

New	**Experiment** – Creates a new experiment document. **Spectra Library** – Creates a new spectra library for analysis or for copying into another file. **Result Set** – Creates a new Result set for analysis or for inserting additional spectra from other experiments. **Model** – Creates a new Model.
Open	**Experiment** - Opens an existing experiment document. Note that when an existing experiment is opened, a backup copy (.BAK file) of the experiment is automatically created. If necessary the extension of this file can be renamed to .EXP and opened. When the opened experiment is closed, the backup copy is automatically deleted. **Spectra Library** - Opens a current spectra library for analysis or for copying into another file. **Result Set** - Opens an existing Result set for analysis or for inserting additional spectra from other experiments. **Model** – Opens an existing Model.
Import	**Experiment** – Imports a iC IR, ReactIR or SPC Grams experiment file. **Result Set** – Imports trend files from other MT applications. **Spectra** - Imports a ReactIR spectra file. **Model** – Imports a QuantIR file. See Importing External Files.

Close	Closes the current document file.
Save	Saves the current opened document file.
Save As	Saves the current experiment as a new file with a name defined by the user.
Save as Template	Saves the current experiment as a template. See Saving an Experiment as a Template.
Export	Exports a iC IR, React IR or SPC Grams file.
Create Word Report	Generates a pre-formatted report of the current experiment in MS Word format.
Create Report	Generates a pre-formatted, read-only report of the current experiment in XPS format.
Exit	Closes all document files and closes the iC IR program. If there are any unsaved changes to open documents, a dialog is displayed giving the user the opportunity to save the changes before exiting.  The checkbox is used to save changes to all open documents.

Tools Menu

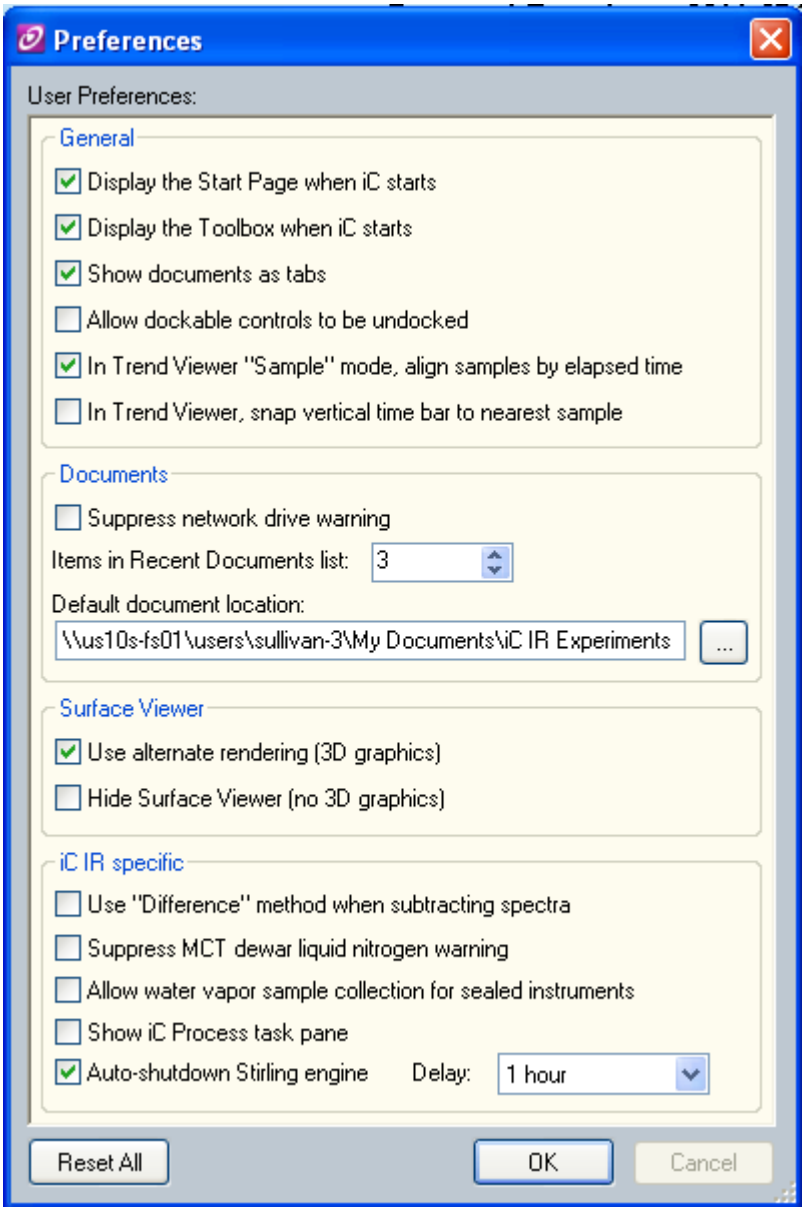
The Tools menu contains three items.



- Preferences – See Preferences Dialog
- Connect to other iC/iControl applications – See Sharing Trend Data with Other iC/iControl Applications
- AutoExport – See AutoExport Configuration Dialog

Preferences Dialog

Clicking the **Preferences** item in the Tools menu opens the Preferences dialog.



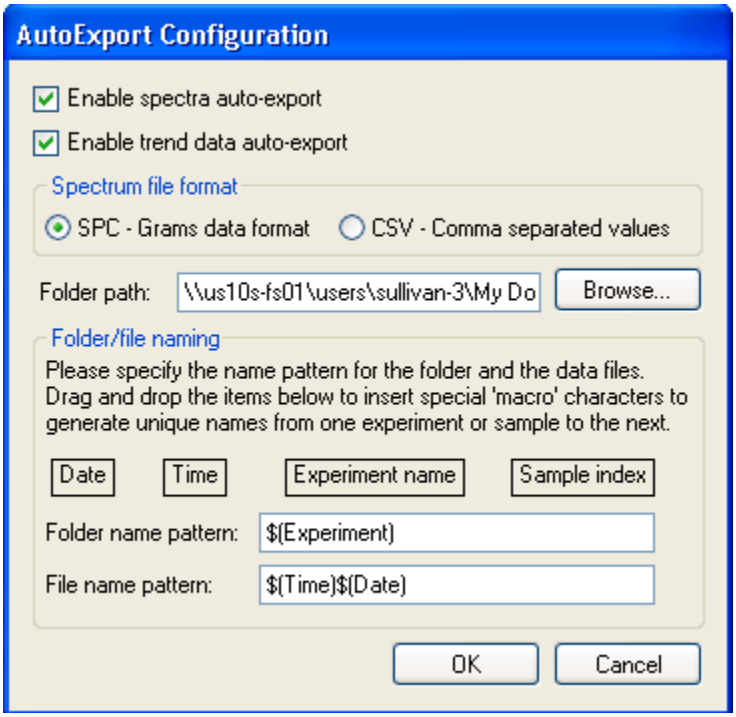
Preferences are enabled by clicking the checkbox. Clicking the **Reset All** button will reset the preferences to the state they were in when the dialog was opened. Clicking the **Cancel** will exit the dialog without saving changes. Clicking the **OK** button saves the changes and exits the dialog.

The dialog contains the following options.

Display the Start Page when iC Starts	If this option is checked, the Start Page with a list of top-level functions is displayed when the program starts. When it is unchecked, the program opens with a blank screen and the pull-down menus must be used to start a program.
Display the Toolbox when iC Starts	If this option is selected, the toolbox is initially displayed in a pinned open state when the application first starts. Otherwise, it is closed and can be opened when needed by clicking along the right edge of the application window.
Show documents as tabs	If this option is checked, multiple documents are displayed as tabs. Otherwise, multiple documents are shown as separate child windows similar to other Windows programs.
Allow docking controls to be undocked.	If this option is selected, you can drag controls such as the Surface Viewer off the form and arrange them as independent windows. This is particularly useful if you have a multi-monitor display. When this function is selected, it takes effect on new documents that are opened but has no effect on existing documents you already have open.
In Trend Sample Mode, Align Samples by Elapsed Time	If this option is selected, samples are aligned to the elapsed time from the start of the experiment.
In Trend Viewer, Snap Vertical Time Bar to Nearest Sample	When this option is on, when the mouse button is released, the vertical bar in the trend viewer snaps to the nearest sample position. If the option is off, when the mouse button is released, the vertical bar does not move
Suppress Network Drive Warning	If the option is checked, warning messages about saving data to a network drive are disabled.
Items in Recent Document List	A number to specify how many recent documents are displayed on the Start page and File menu.
Default Document Location	A user-selected default folder for all documents; Experiments, Result Sets, Distribution Libraries.
Use Alternate Rendering (3D Graphics)	Use this option if you are having problems with displaying 3D graphics in the Surface Viewer. Problems with 3D graphics are usually solved by switching the graphics card to 16-bit graphics. If that does not work, switch the graphics card back to 32-bit and then check this option.
Hide Surface Viewer	Hides the Surface Viewer in all viewing configurations.
Use “Difference” Method when Subtracting Spectra	When checked, the Differentiation method of solvent subtraction is used. If unchecked, the Savitzky Golay First Derivative method is used.
Allow Water Vapor Sample Collection for Sealed Instruments	When checked, the Water Vapor Correction step of the Configure Instrument wizard is enabled for ReactIR 15 ReactIR 45P, ReactIR 45P Dual, FlowIR and ReactIR 247 instruments.
Suppress MCT Dewar Liquid Nitrogen Warning	When checked, the liquid nitrogen reminder will be disabled. This only applies to iC 10 instruments, which do not have MCT temperature diagnostics."
Show iC Process Task Pane	When checked, the iC Process task pane is displayed to allow connection to the iC Process application.
Auto-shutdown Stirling Engine	Automatically shuts off the Stirling engine after the specified time delay.

AutoExport Configuration Dialog

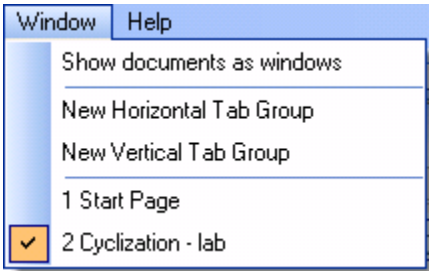
The AutoExport function is used to automatically export spectra and trend data at the end of an experiment. The AutoExport Configuration dialog is used to set up the export parameters.



The dialog contains the following fields.

AutoExport checkboxes	Specifies what type of data will be exported, Spectra and/or Trend.
Spectrum File Format	Specified whether the data is exported as an SPC or a CSV file.
Folder Path	Specifies the folder where the exported files will be stored.
Folder/File Naming	Used to format the naming pattern for the folder and file. To format a name, drag the items to the appropriate fields and location in the fields.

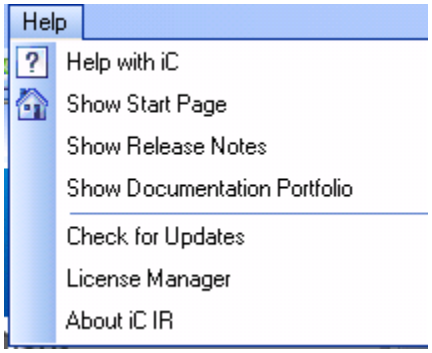
Window Menu



The menu contains the following options.

Show Documents as Windows/Tabs	Clicking on this menu when tabs are displayed will display the files as separate windows. Clicking on the menu when windows are displayed will change the files into a tabbed format.
New Tab Groups	Arranges the display as tabs. See Tabbed Displays.
File List	All of the open files are listed in the line. The file currently displayed is indicated by the check in the box next to the title. Clicking on another open file displays that file.

Help Menu

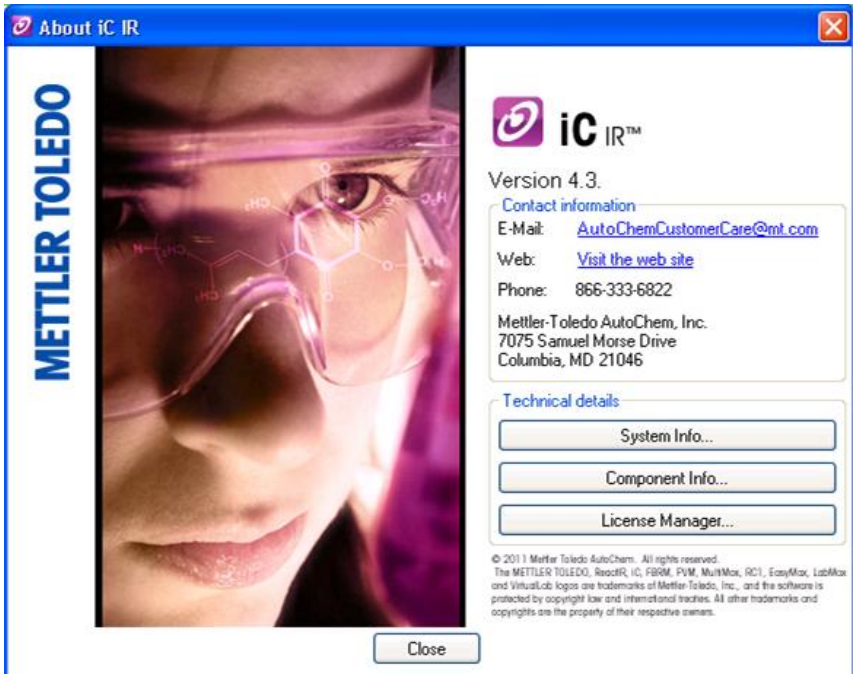


The menu contains the following options.

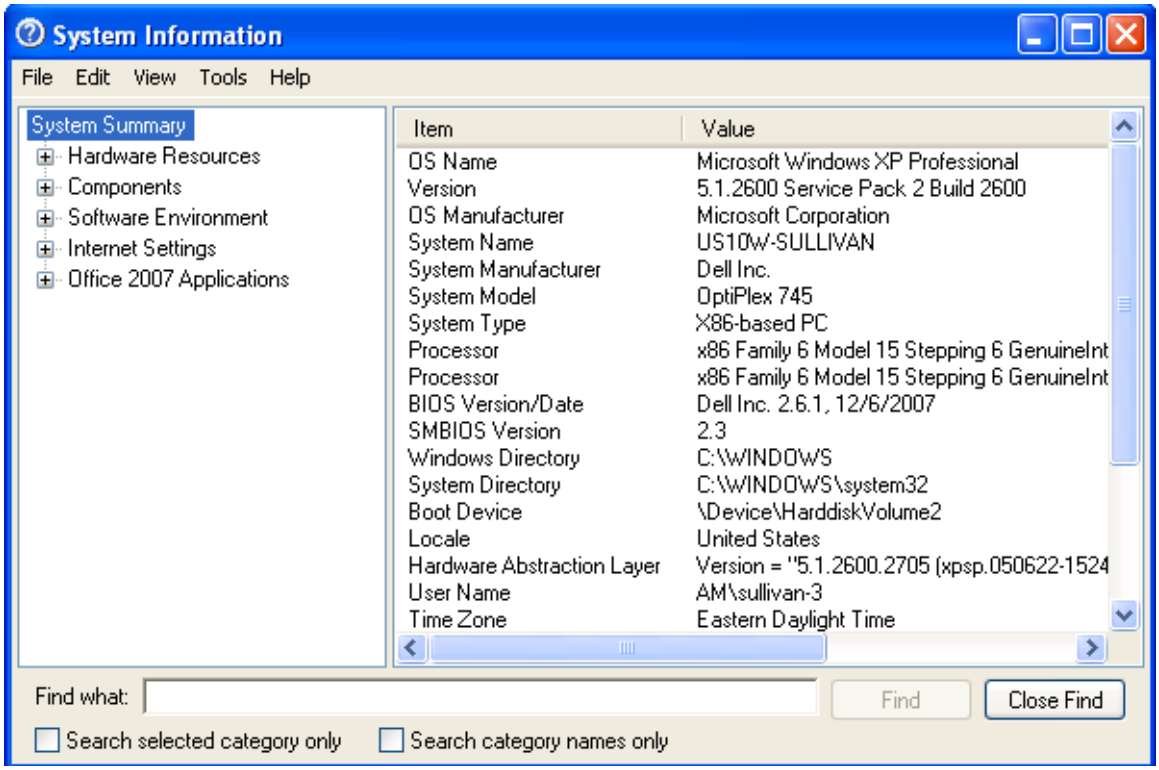
Help with iC	Opens the iC Help tool.
Show Start Page	Opens the Start Page. If the Start Page is already open, focus is given to the page.
Show Release Notes	Displays a list of changes for the installed release of the software.
Show Document Portfolio	Opens the PDF Portfolio document for iC IR.
Check for Updates	Connects to the MT website and checks for recent software updates. Note that an internet connection is necessary to use this option.
License Manager	Opens the License Manager dialog to enable the user to review and enter licenses.
About iC IR	Displays a list of the software associated with iC and their version number.

The About iC IR Dialog

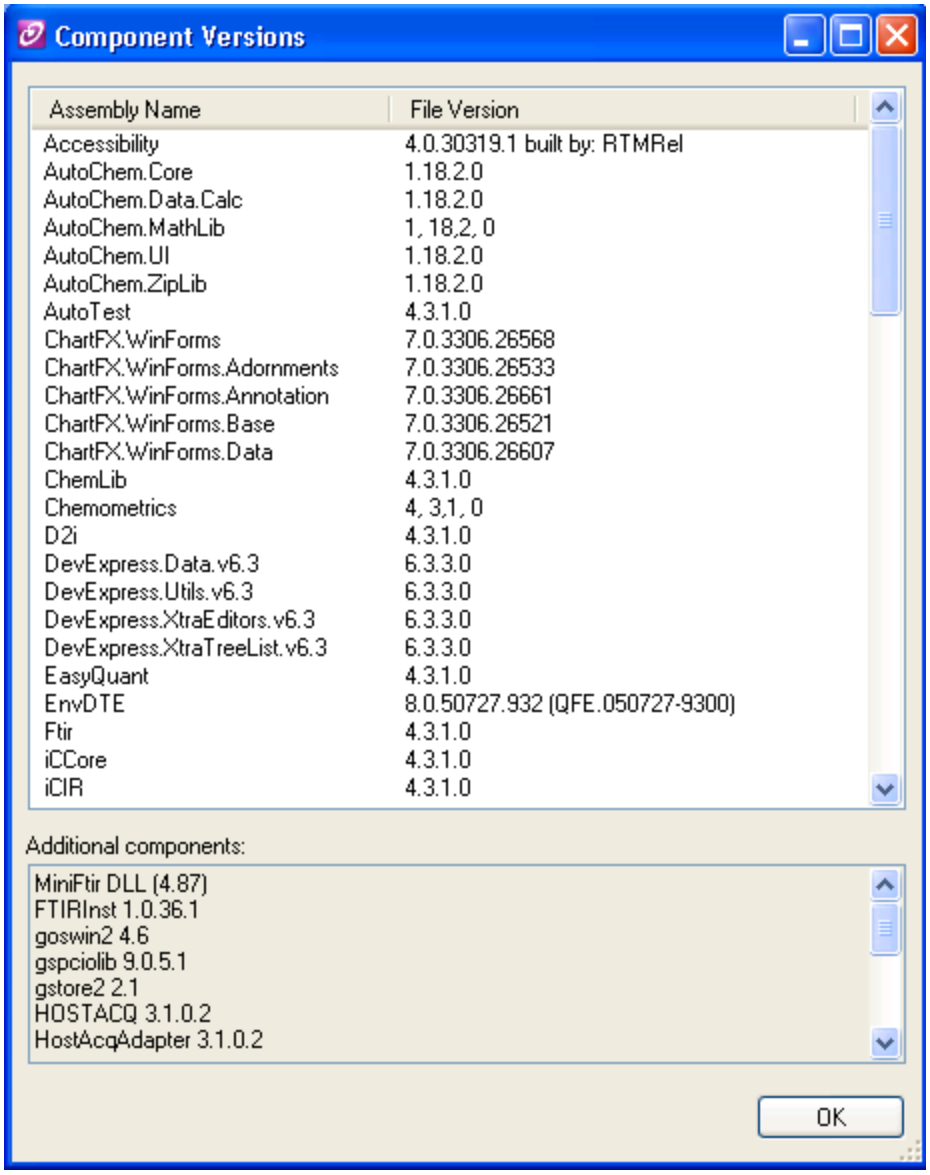
The About iC IR dialog displays information detailing the application version number and contains buttons to access various application/system tools.



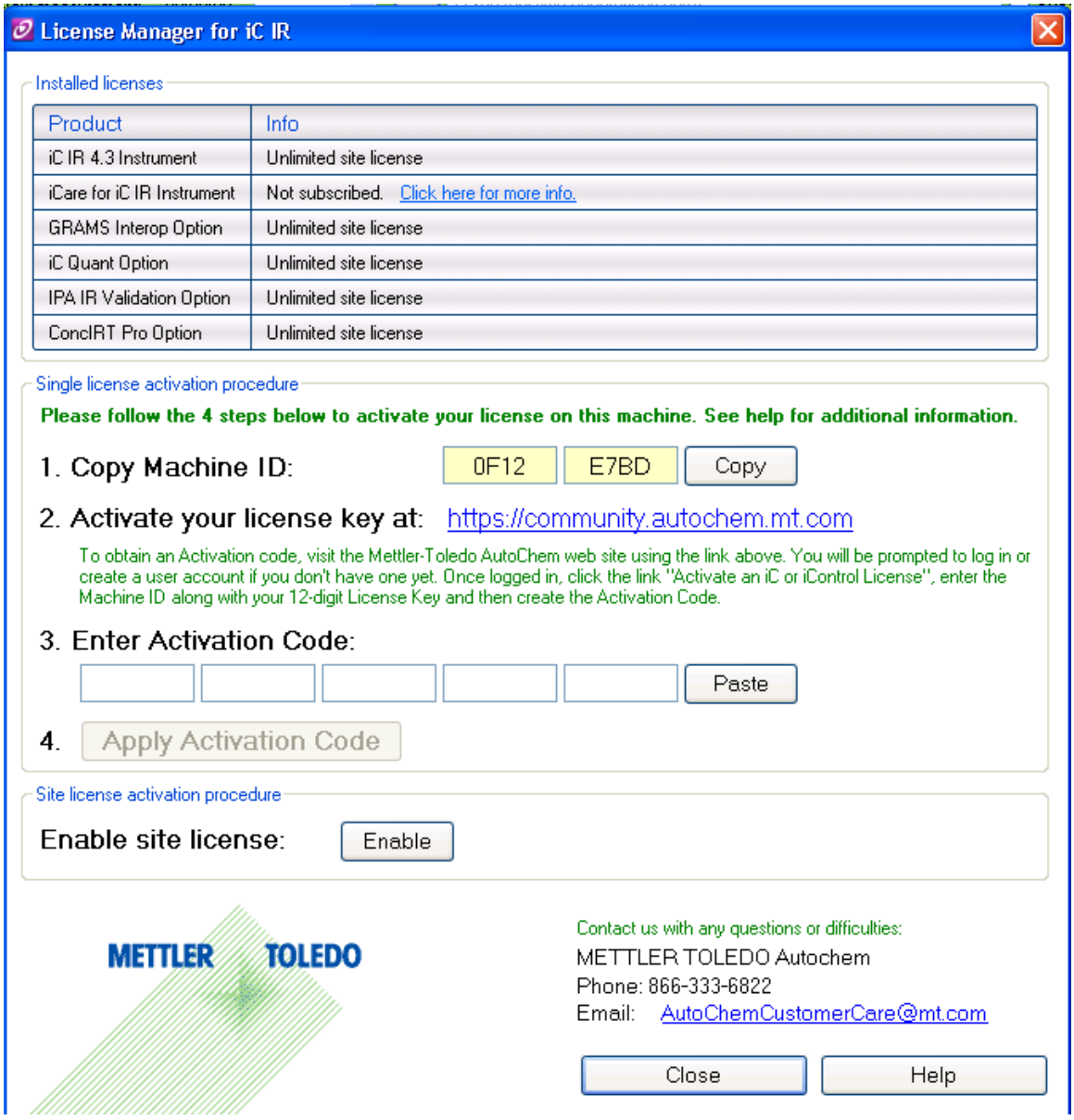
Clicking the **System Info** button opens the Windows System Information dialog. The dialog contains information about the Windows operating environment.



Clicking the **Components Info** button opens the Component Versions dialog. The dialog displays information detailing the version numbers of all iC IR software components.



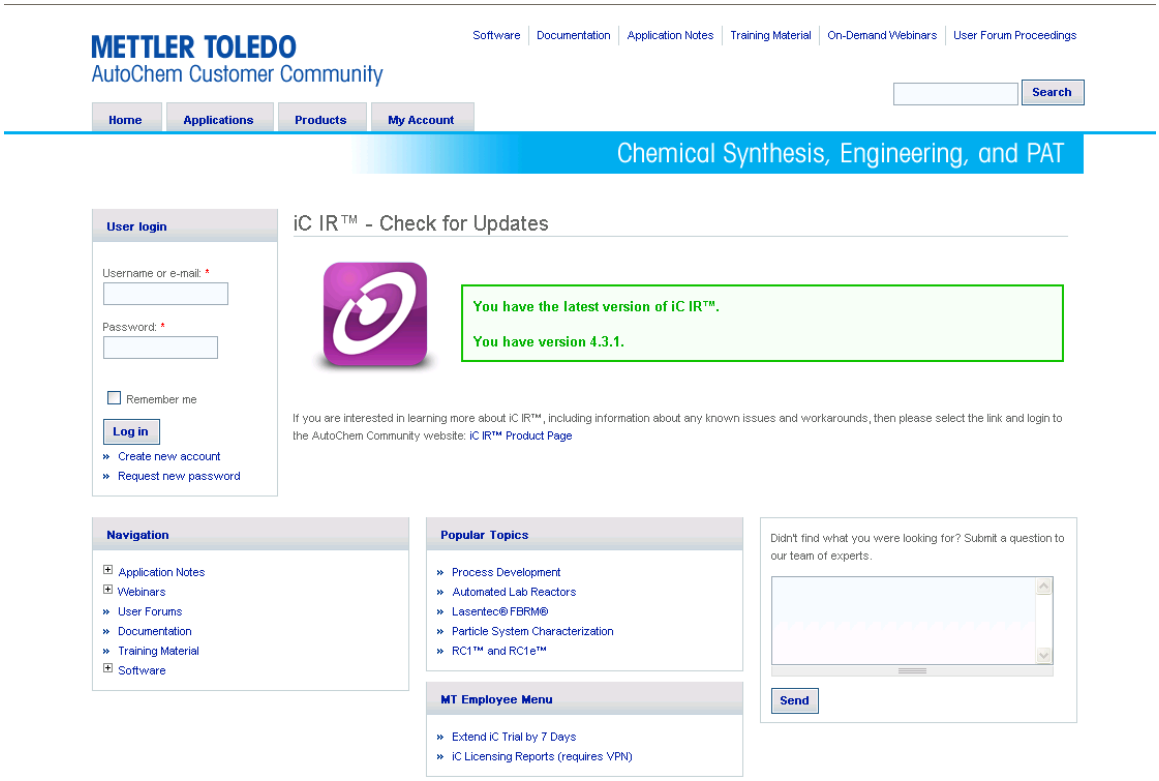
The **License Manager** button opens the License Manager,



Information about the License Manager is contained in the iC IR Installation Guide located on the Installation CD.

Check for Updates Menu Option

The Check for Updates option on the Help menu navigates the user to a website where an automatic check will be made to determine if the system is running the latest version of the iC software. Note that Internet access is required to use this feature.



The user has the option to download and install the latest version from the website.

Main Toolbar

The main toolbar contains a series of buttons that function as shortcuts to commonly used menu options.

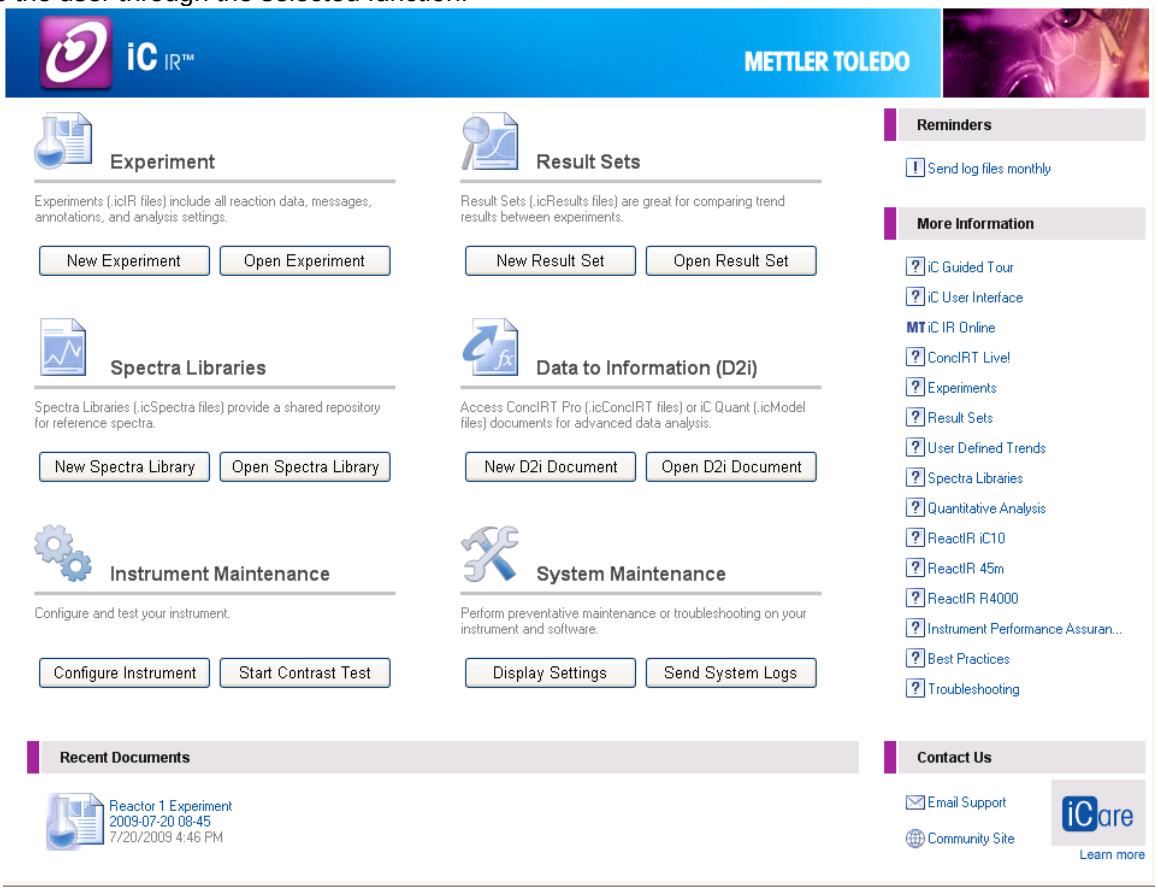
The buttons are only activated when the buttons function is available. Inactivated buttons appear as “grayed-out”.

The Toolbar contains the following buttons.

Button	Description
	Opens the iC Help system.
	Displays the Start Page.
	New Experiment Button - allows the user to create a new experiment.
	Open button - opens an existing experiment.
	Import button – used to import an external experiment or measurement file.
	Save button - saves changes to the active document.
	Save As button - saves changes to the active document with a new filename.
	Export button – Exports the selected experiment data to a CSV file.
	Dockable Viewer button – allows the user to reposition viewers within the viewing window. Refer to Dockable Viewers.
	Tab View button – displays the active documents as tabs. This button is mutually exclusive with the other layout buttons.
	Tiled View button – displays the active document in a four quadrant arrangement. This button is mutually exclusive with the other layout buttons.
	Horizontal Layout button – displays the active documents as horizontal panes. This button is mutually exclusive with the other layout buttons.
	Vertical Layout button – displays the active documents as vertical panes. This button is mutually exclusive with the other layout buttons.
	Trend Layout button – displays the Trend Viewer double sized with the Surface Viewer and Event Viewer tabbed. This button is mutually exclusive with the other layout buttons.
	Surface Layout button – displays the Surface Viewer double sized with the Surface Viewer and Event Viewer tabbed. This button is mutually exclusive with the other layout buttons.
	Referee Data button – opens the Referee Data dialog. Refer to The Referee Data Dialog.

Using the Start Page

The iC IR Start Page is used to perform the various functions available with the iC IR application. The functions are initiated by clicking on the appropriate button on the page. When a button is clicked, a wizard guides the user through the selected function.



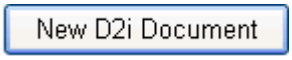
The following functions are available from the Start Page.

Button	Function
New Experiment	See Working with Experiments
Open Experiment	See Working with Experiments
New Result Set	See Working with Result Sets
Open Result Set	See Working with Result Sets
New Spectra Library	See Working with Spectra Libraries
Open Spectra Library	See Working with Spectra Libraries
New D2i Document	See D2i Documents
Open D2i Document	See D2i Documents
Configure Instrument	See Configuring the ReactIR
Start Contrast Test	See Aligning the Probe
Display Settings	See Viewing Display Settings
Send System Logs	See The Customer Care Log File Utility.

D2i Documents

The iC application supports several types of D2i (Data to Information) documents.

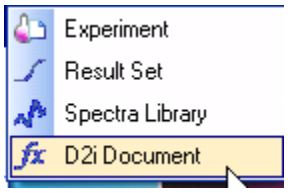
- Multivariate Models
- Univariate Models
- ConcIRT Pro Analysis

New D2i documents are created by clicking the 

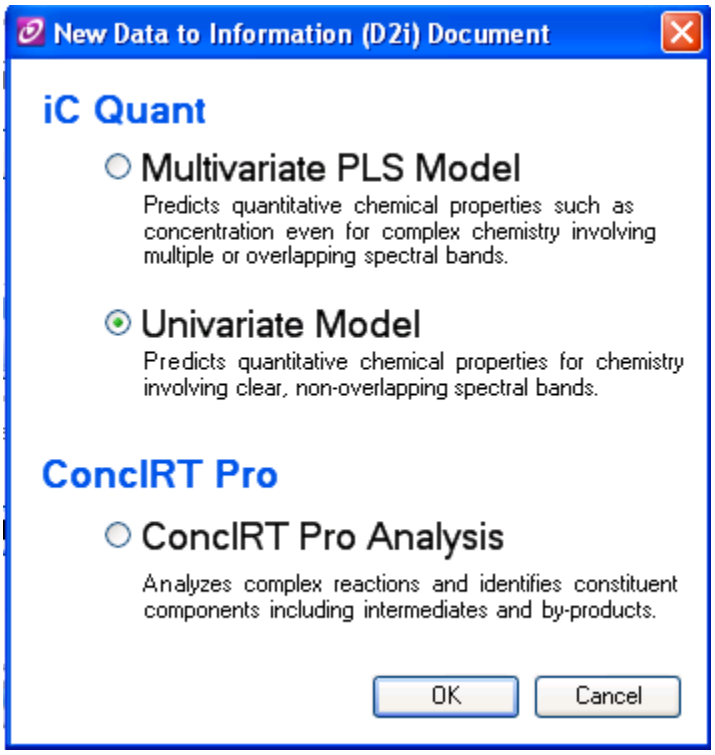
on the Start page

or

Selecting the **New/D2i Document** option from the **File** menu.



Either method opens the New Data to Information dialog.



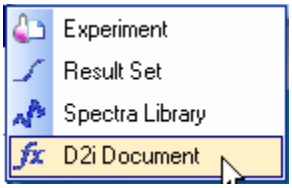
The dialog contains radio buttons to select the type of D2i document. The document type is selected and the **OK** button is clicked to create the new document.

Information about iC Quant models is contained in iC Quant help section and the ConcIRT Pro help section discusses ConcIRT Pro documents.

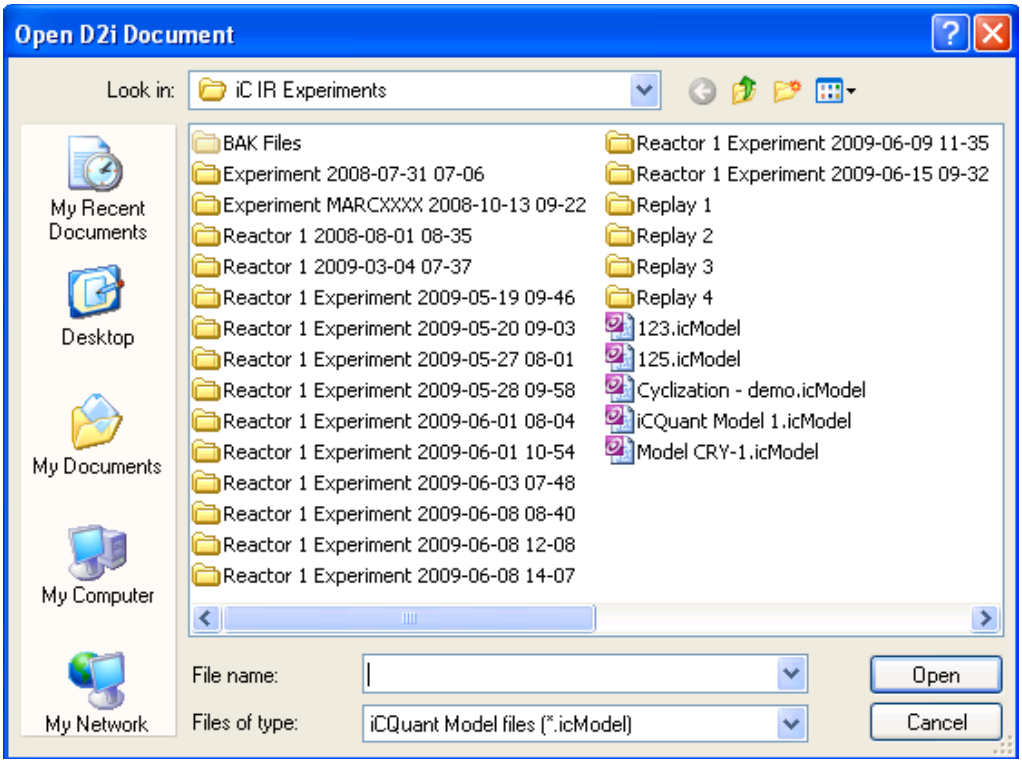
Existing D2i documents are opened by clicking the  on the Start page

or

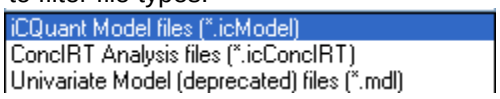
Selecting the **Open/D2i Document** option from the **File** menu.



Either method opens a file browser that is used to select the D2i document.



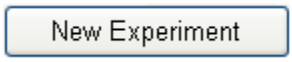
The **Files of Type** droplist is used to filter file types.



Working with Experiments

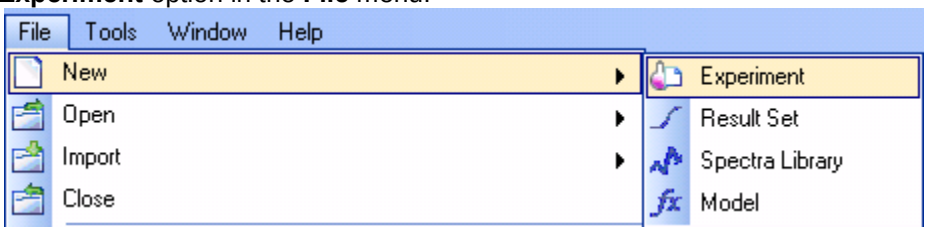
Experiments can be created using several methods:

The user can click the **New Experiment** button on the **Start Page**

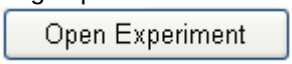


or

select the **New/Experiment** option in the **File** menu.



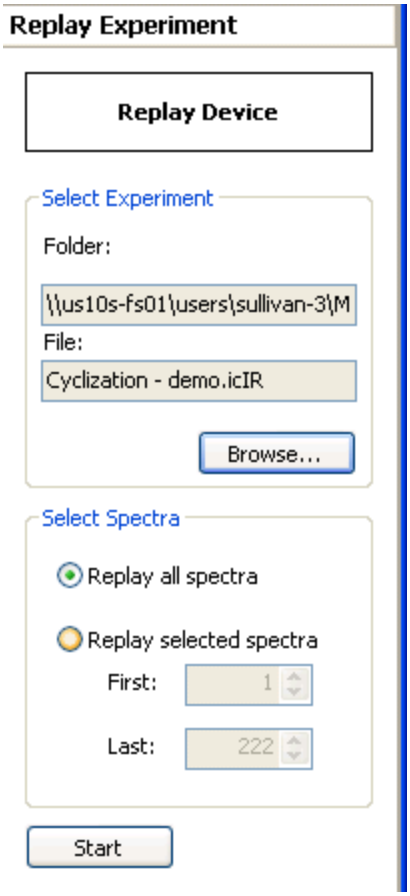
Both methods will open the **Start Experiment Wizard**.

Existing experiments can be opened by selecting the **Open/Experiment** option in the **File** menu or by clicking the 

button on the Start Page. The experiment is opened in the Experiment Display. Changes can be made to experiment (trends, annotations, peak types, etc.) and the experiment saved as another experiment file using the **Save As ...** option in the **File** menu.

Existing experiments can also be replayed using the **Replay Experiment Task Pane** of the **Toolbox**.

The Replay Experiment tool allows the user to replay all spectra or a selected group of spectra. In addition, the sampling interval for the replay can be specified and can be different from the original interval. The experiment replays with a default name of **Replay**. Once the experiment replay operation is completed, it can be saved as a new experiment using the **Save As ...** option in the **File** menu.



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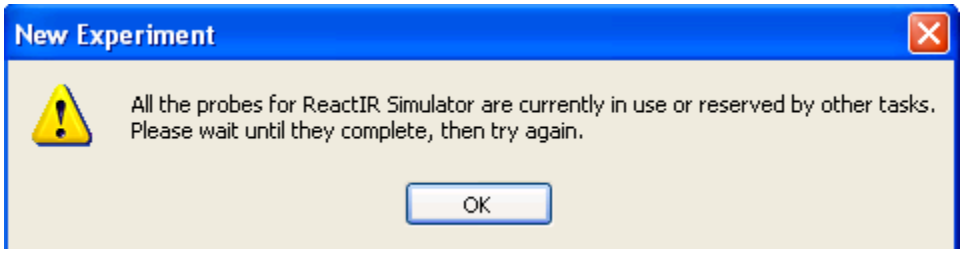
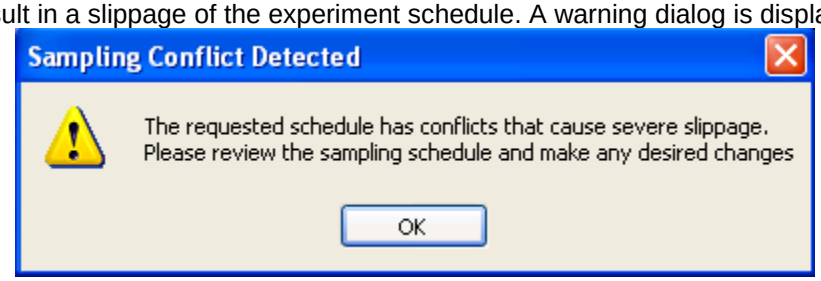
Multiple Experiments

On instruments that contain multiple probes, an experiment for each probe can be run simultaneously. Each experiment in run in a separate tab and contains its own Live Experiment Toolbar. Experiments are started in the normal manner. The experiment wizard will display the available probes for the experiment. If an experiment is running for all of the probes and a new experiment is started, an error dialog is displayed.



.
In this case, the user must wait until an experiment is complete, free up a probe or abort a running experiment.

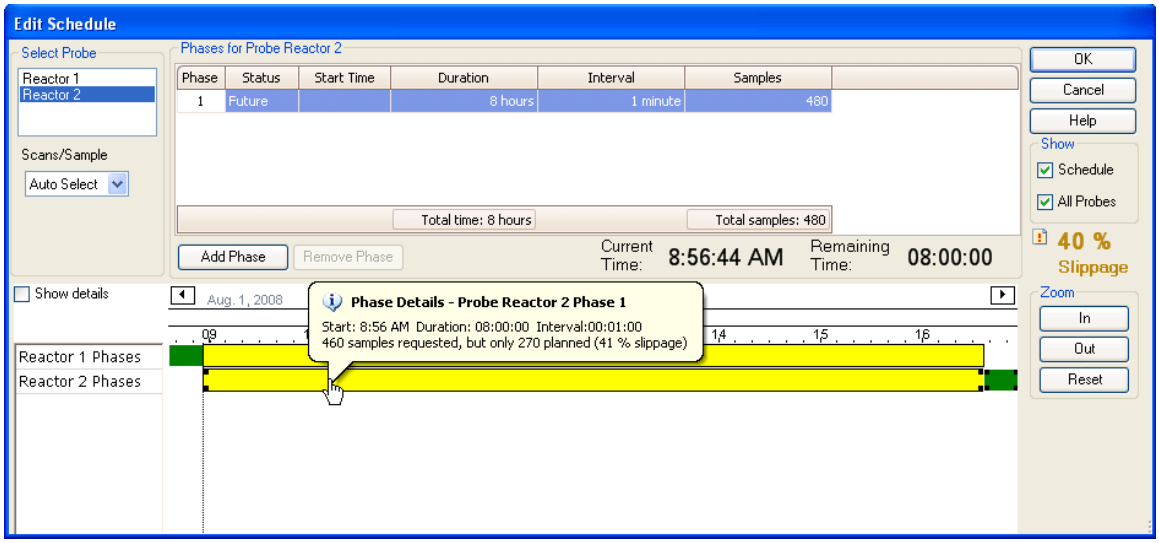
When multiple experiments are defined, the iC IR will check the sampling intervals and reports any scheduling conflicts that will result in a slippage of the experiment schedule. A warning dialog is displayed.



The user clicks the **OK** button to open the Edit Schedule dialog.

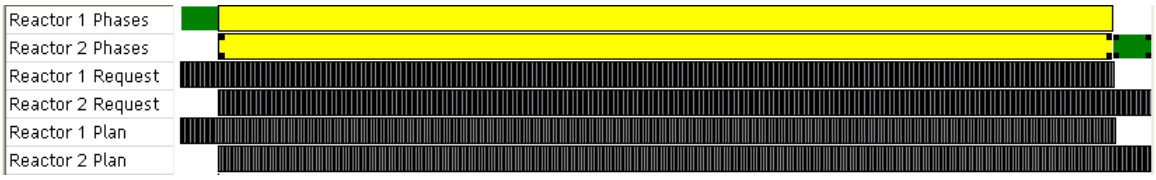
The Experiment Schedule

The Edit Schedule dialog allows the user to re-configure phases to eliminate any conflicts in the schedule.

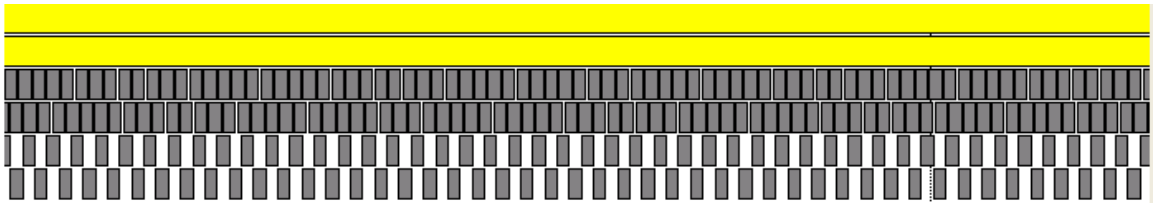


The **Slippage** field on the right-side of the dialog displays an estimate of the slippage. When the cursor hovers over a phase, a tooltip provides details of the estimated slippage for that phase and the number of samples that may be lost. The user can adjust sampling intervals to reduce the slippage. As sampling intervals are changed, the **Slippage** field updates to provide a current estimate. When the user is satisfied with the schedule, the **OK** button is clicked to create the experiment. It should be noted that the **OK** button is always enabled and an experiment can be created regardless of any severe scheduling conflicts.

The **Show Details** checkbox can be checked to display the individual scan for each probe.



The Zoom buttons allow the user to view the schedule in greater detail.



Click the **Reset** button to return the schedule display to it's original size.

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Start Experiment Wizard

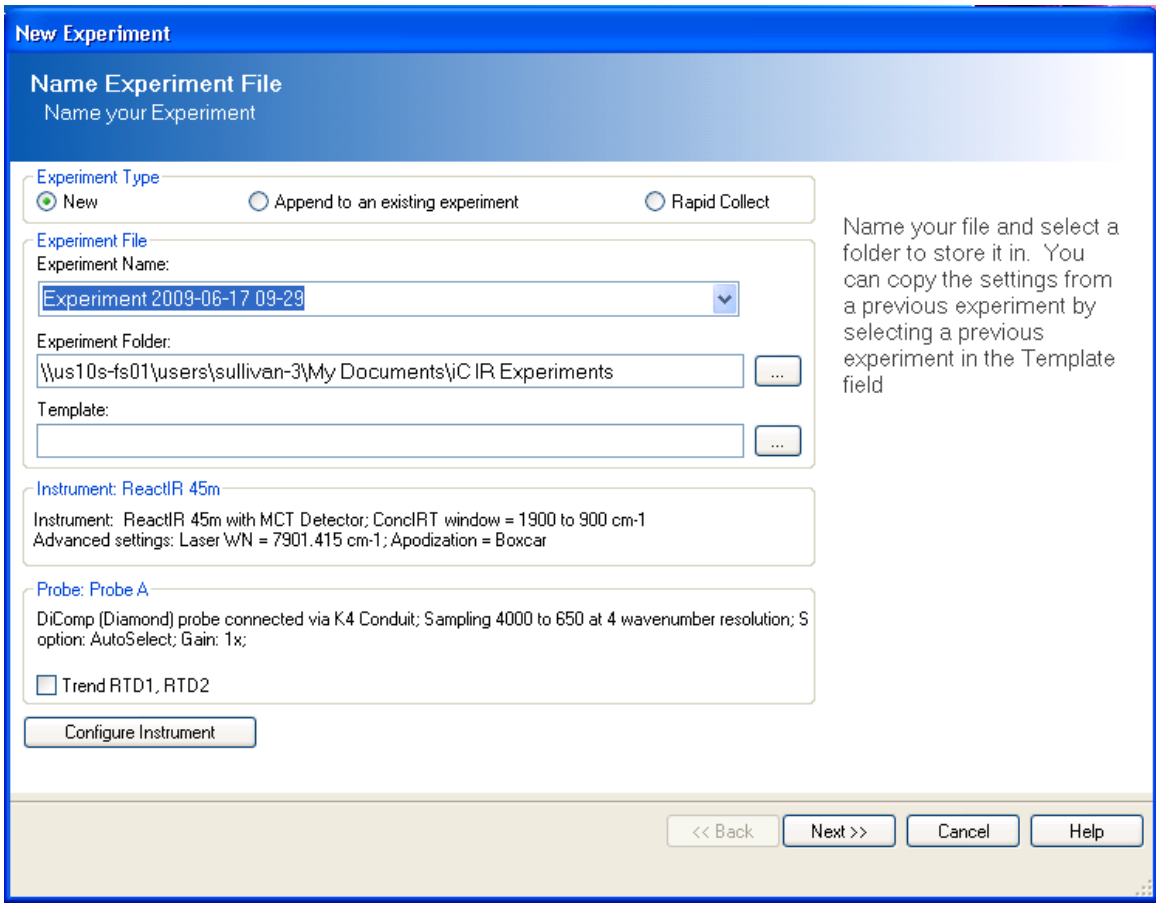
Check your instrument settings before recording an experiment by clicking on the 

button on the Start Page.

Once the configuration has been verified, click the 

button on the Start Page to start the Experiment Wizard.

The Start Experiment wizard is opened.



The first page of the Wizard is used to define the name and location of the experiment document. The page also displays the current instrument configuration. The **Configure Instrument** button can be used to correct any hardware configuration differences.

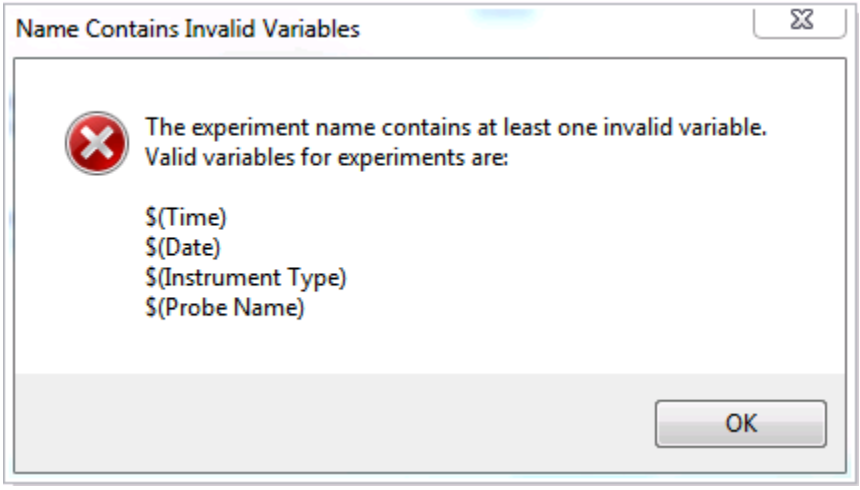
The user has the option of:

- Creating a new experiment data file.
- Appending this experiment to an existing experiment data file.
- Create a new experiment file with manual sampling. Refer to Manual Sampling.
- Rapid Collect (this option is only available for the ReactIR 45M and multiprobe variants). Refer to Rapid Collect Experiments.

The experiment name format can be configured by the user using tokens. The following tokens are supported.

- $(Date) - the current date
- $(Time) – the current time
- $(Instrument) – the instrument type by name
- $(Probe) – the probe type, available for multi-probe instruments only

iC checked the validity of the name before the wizard advances. If an invalid token is used, an error message is displayed. The error must be corrected before the experiment can be created.

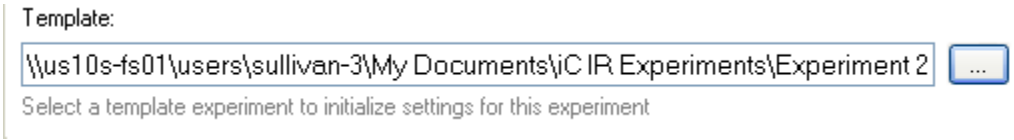


Note: It is recommended that experiments be saved to drives local to the PC running iC IR. You can move the experiment to a different drive after the experiment completes. If the experiment is being saved to a remote disk drive, a network interruption may cause an irrecoverable failure and the experiment will have to be re-run.

A droplist is provided that lists all previously defined name formats.

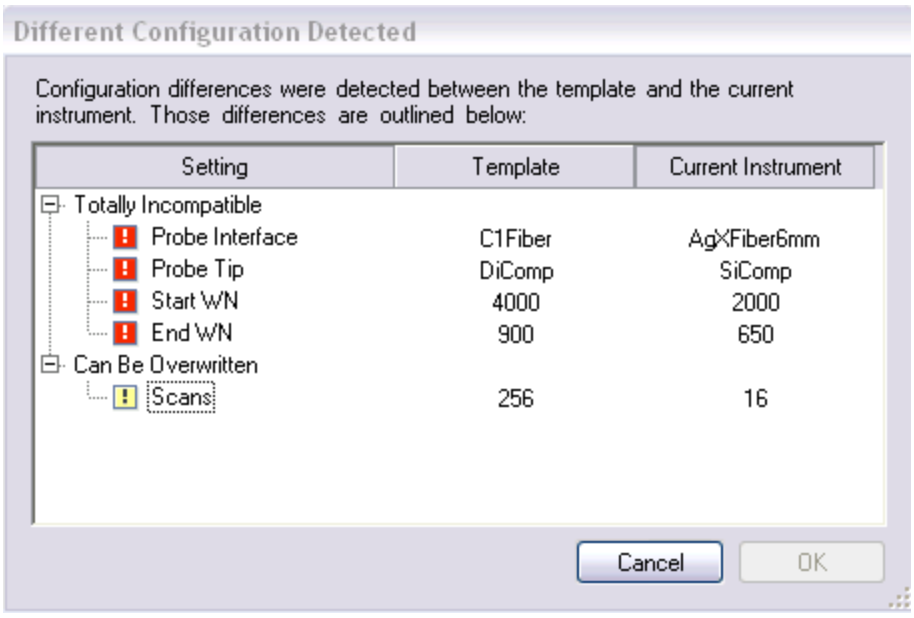
Templates

The user can select a template to use as a “method” for a new experiment. A template is actually an existing saved experiment. A template allows the user to automatically input all hardware settings, RTD configuration, measurement interval settings, phases, statistic settings, references and display settings from the previously saved experiment.



Click the **Next** button to advance to the next page of the wizard.

Note that when using templates, the instrument configuration defined in the template must match the configuration used for the current experiment. If a mismatch is detected, an error message is displayed that allows the user to correct the mismatch.

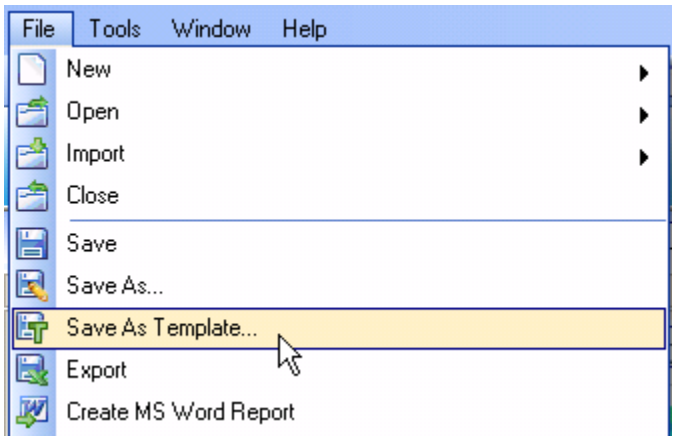


Saving an Experiment as a Template

The user can save a completed experiment as a template file. The template does not include any samples but include all experiment conditions (sampling interval, phases, averaging settings statistics definitions, scan speed, algorithm settings and serial IO configurations. When an experiment is saved as a template iC IR appends the term "- Template" (Reactor 1 Experiment 2010-01-25 09-09 - Template) to the filename.

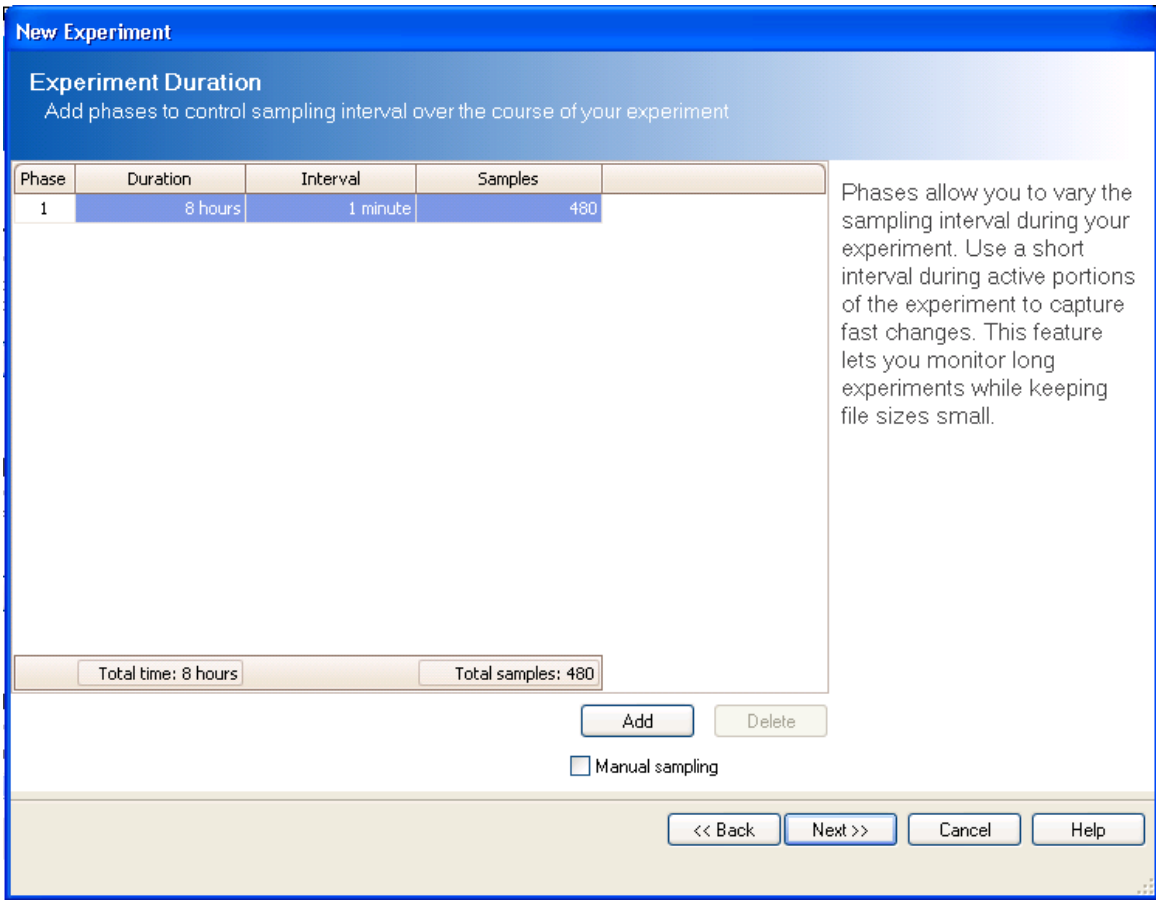
Experiments saved as templates are significantly smaller than the original experiment since all data, messages, and so on. are deleted.

An experiment is saved as a template by selecting the option on the **File** menu.

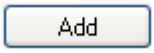


Creating the Experiment Schedule

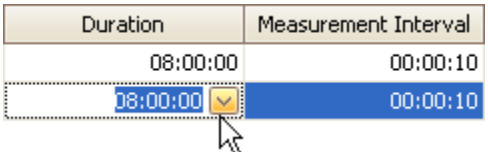
The next page of the wizard allows the user to configure the schedule for the experiment by partitioning it into multiple phases. Each phase can be defined with a specific duration and measurement interval. The phases are executed in sequence.



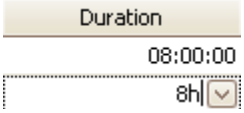
….

Click the  button to add a phase to the experiment. A new row is added to the Phases list. The **Duration** and **Measurement Interval** fields are edited as desired. The number of samples are calculated automatically. The maximum duration is 30 days with a measurement interval of 15 minutes.

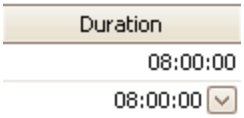
The **Duration** and **Measurement Interval** fields have a droplist from which the user can select the time values.



Alternatively, the user can enter a number into the fields followed by a “h” for hours, “m” for minutes or an “s” for seconds.



When the cursor leaves the field, the entered time is converted to the correct time format and displayed

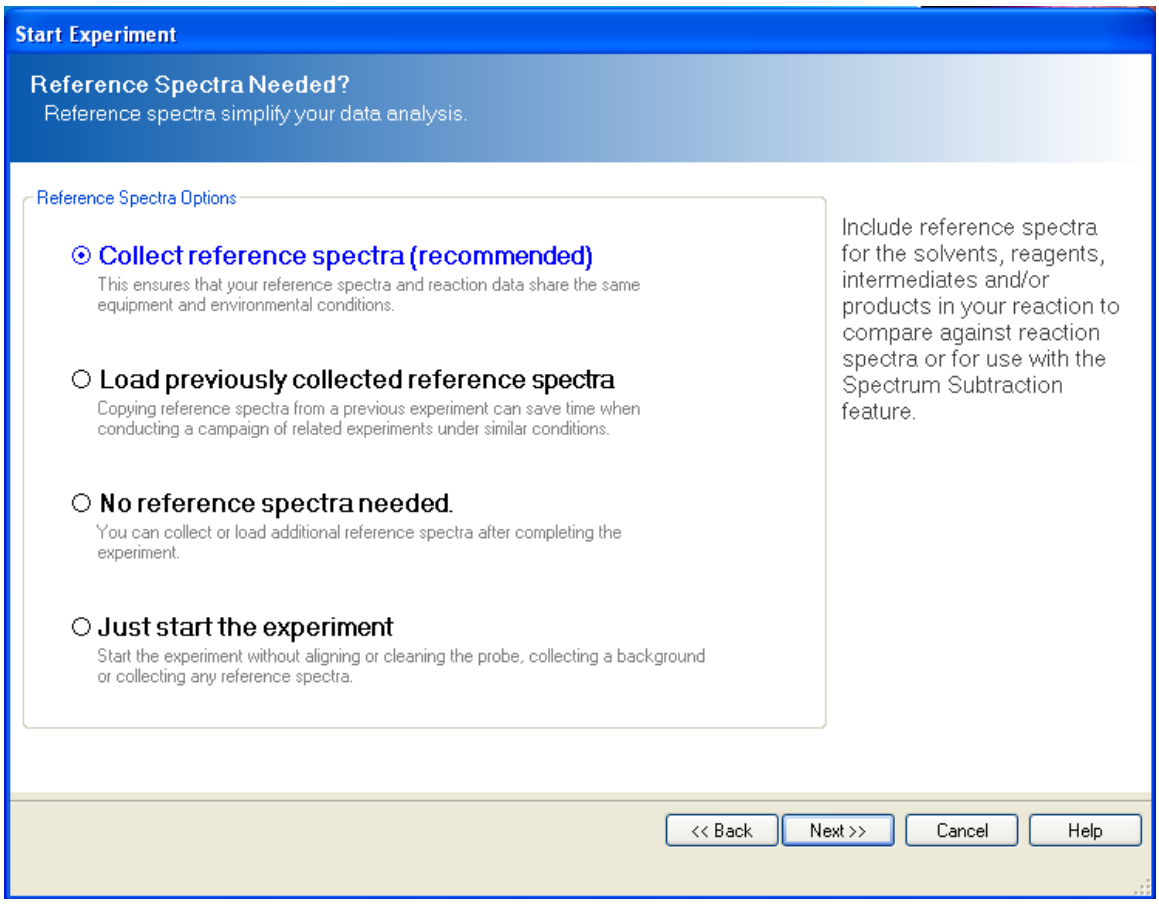


The Manual Sampling checkbox allows the user to manually take samples during the experiment. Refer to Manual Sampling.

Specifying Reference Spectra for the Experiment

The collection of reference spectra is highly recommended for each new experiment. Reference spectra, also referred to sometimes as pure component spectra, are useful for comparison to ConcIRT LIVE generated component spectra. This approach guides in data evaluation and acts as a check on the mathematically calculated results from ConcIRT LIVE. Additionally, a solvent spectrum must be associated with the experiment file in order to use the Solvent Subtraction feature on the Experiment task pane in the Toolbox. It is relatively simple to collect new pure component spectra before each experiment. Alternatively, they can be loaded into the current experiment file if taken previously. Having these reference spectra available during data analysis is invaluable. TIP: Solvents that exhibit strong hydrogen bonding (water, alcohols, etc.) will have a spectrum sensitive to temperature. Collect the reference solvent spectrum at the reaction temperature for the best auto-subtraction results.

Click one of the checkboxes to select the appropriate reference option.

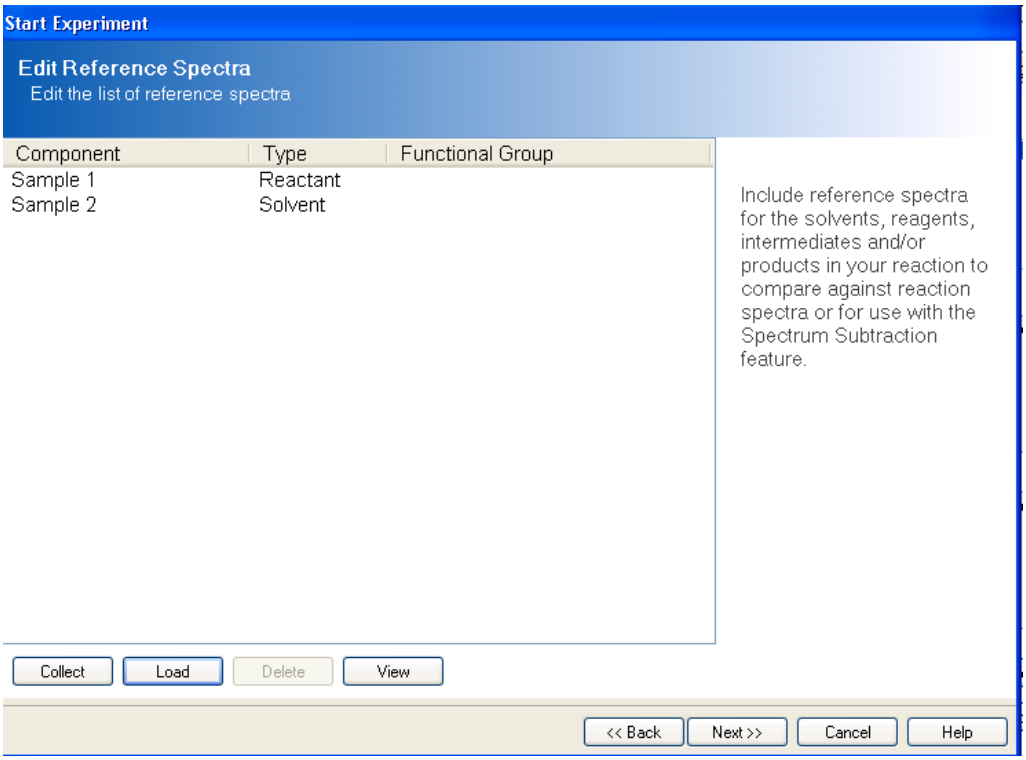


If you checked **Collect Reference Spectra**, the Wizard system cycles you through a spectrum collection procedure. Proceed to Positioning the Probe.

If you checked **No Reference Spectra Needed**, the wizard advances to the Aligning the Probe for the Experiment. Note that a reference can also be collected at the end of the experiment.

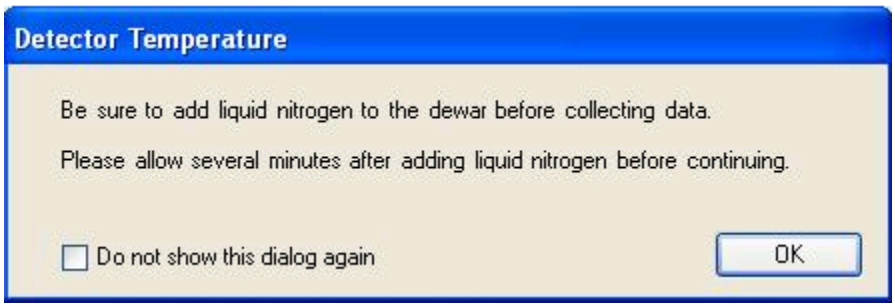
If you checked **Load Previous Collected Reference Spectra**, the **Edit Reference Spectra** page is opened to load a previously run spectra.

If you checked **Just Start the Experiment**, the wizard advances to The Live Experiment Toolbar.



Load a previously collected reference spectrum by clicking the **Load** button. A file browser is opened. Select the reference to use from the spectra library or experiment file and click OK. The **Edit Reference Spectra** page is populated with the selected spectrum file components. Select the component to use as a reference and click the **Next** button.

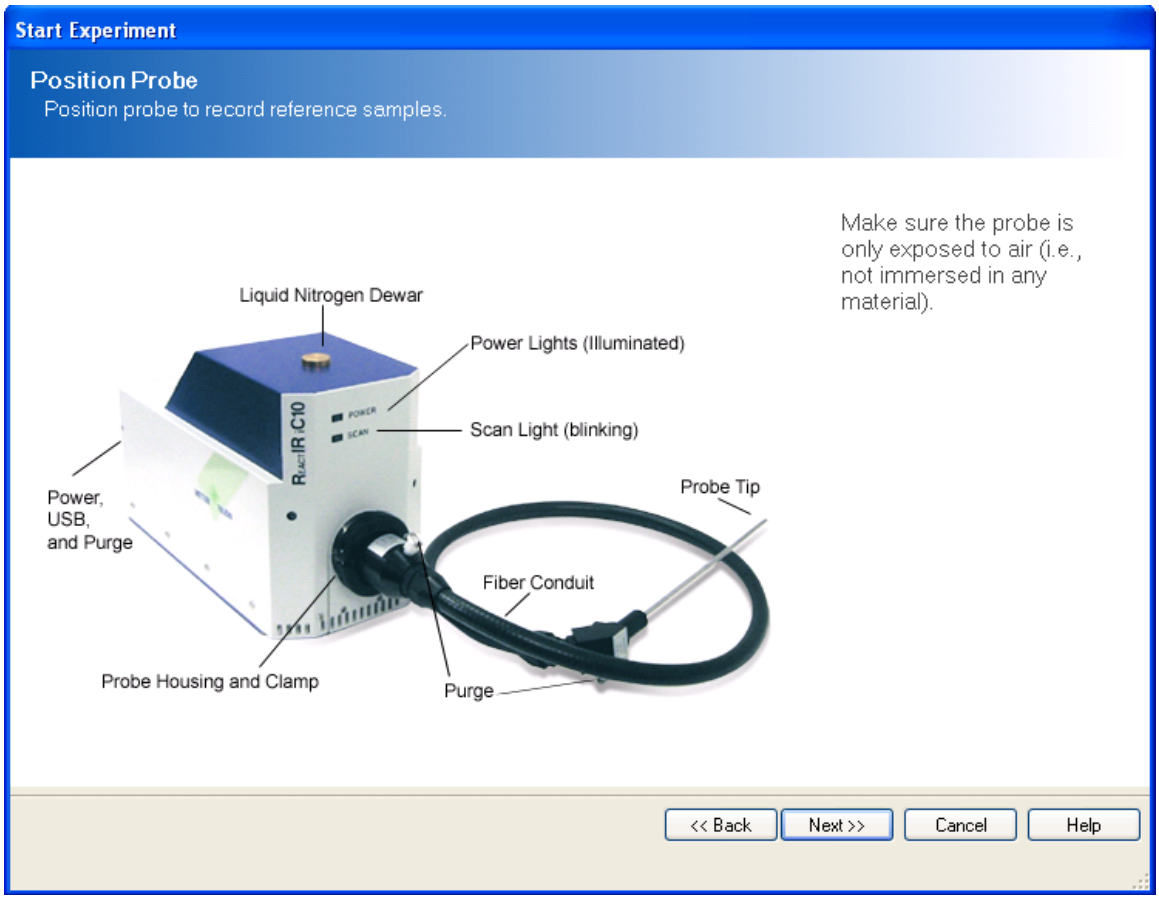
If the instrument is an ReactIR ReactIR15 or an ReactIR 45M that has a MCT diagnostic failure, the following reminder will be displayed.



The user has the option of turning off the reminder either with the checkbox in the dialog or through the Preferences options.

Positioning the Probe

This page of the wizard is an informational page that shows the position of the probe for cleaning. Note: the instrument image shown may be different depending upon your instrument configuration.

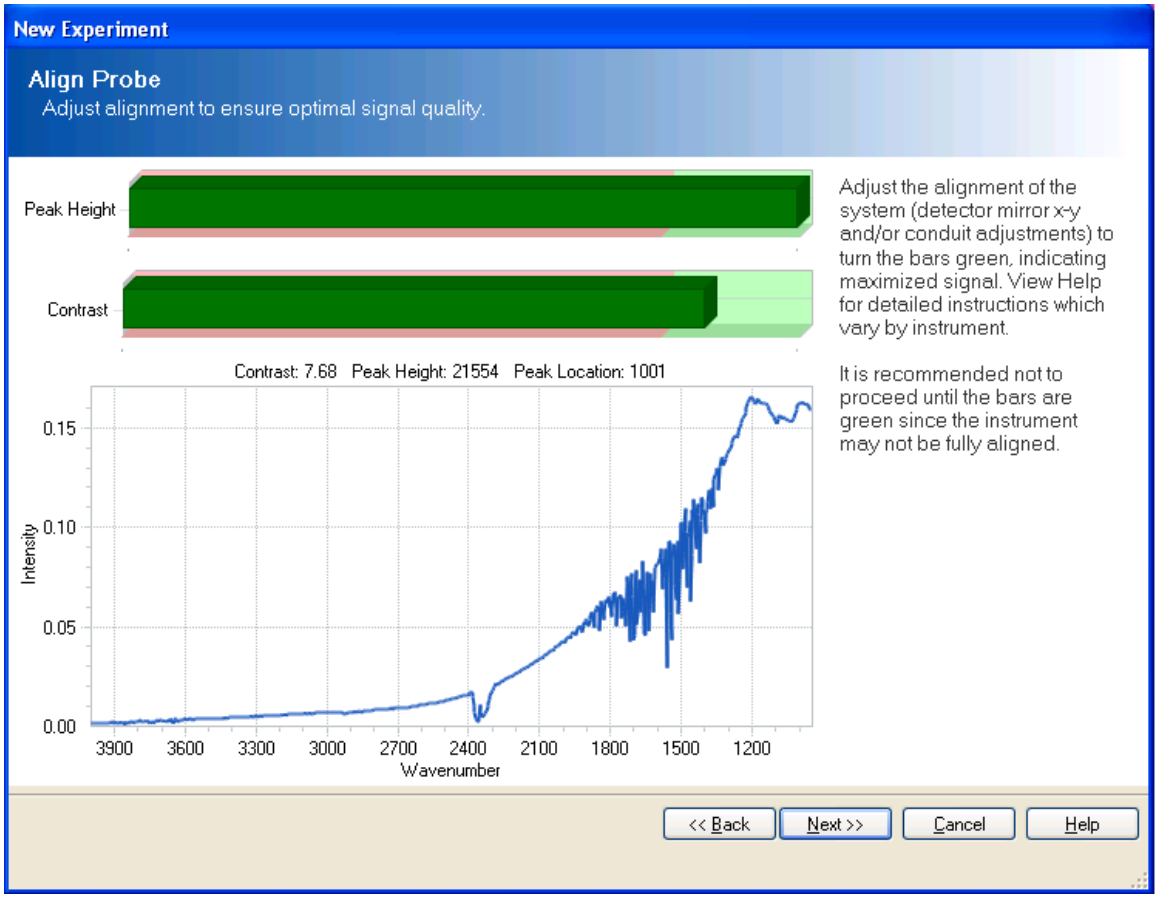


Position the probe for cleaning as shown and click the **Next** button.

Aligning the Probe for the Experiment

This page of the wizard is used to physically align the probe. When the probe is aligned correctly, the indicator bars turn green.

Refer to Alignment Indicators are Not for instructions about aligning the probe.



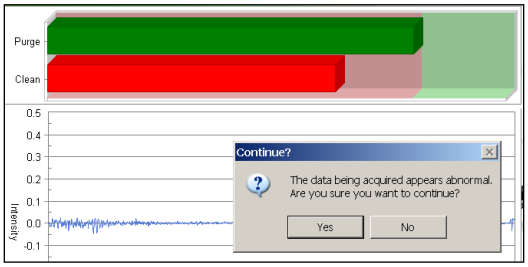
Cleaning the Probe

Clean the probe from the previous experiment using the most appropriate solvent(s) to dissolve the reaction species. A final cleaning with reagent grade acetone is recommended. A virgin cotton swab on a wooden stick makes an ideal cleaning tool for the slightly recessed sensor tip. NOTE: Q-tips and similar type swabs have lubricants and are not a great choice for a cleaning tool!

The two colored bars indicate if the probe is clean or dirty. If the bars are red and in the red area of the purge and clean zone, the probe surface is dirty.

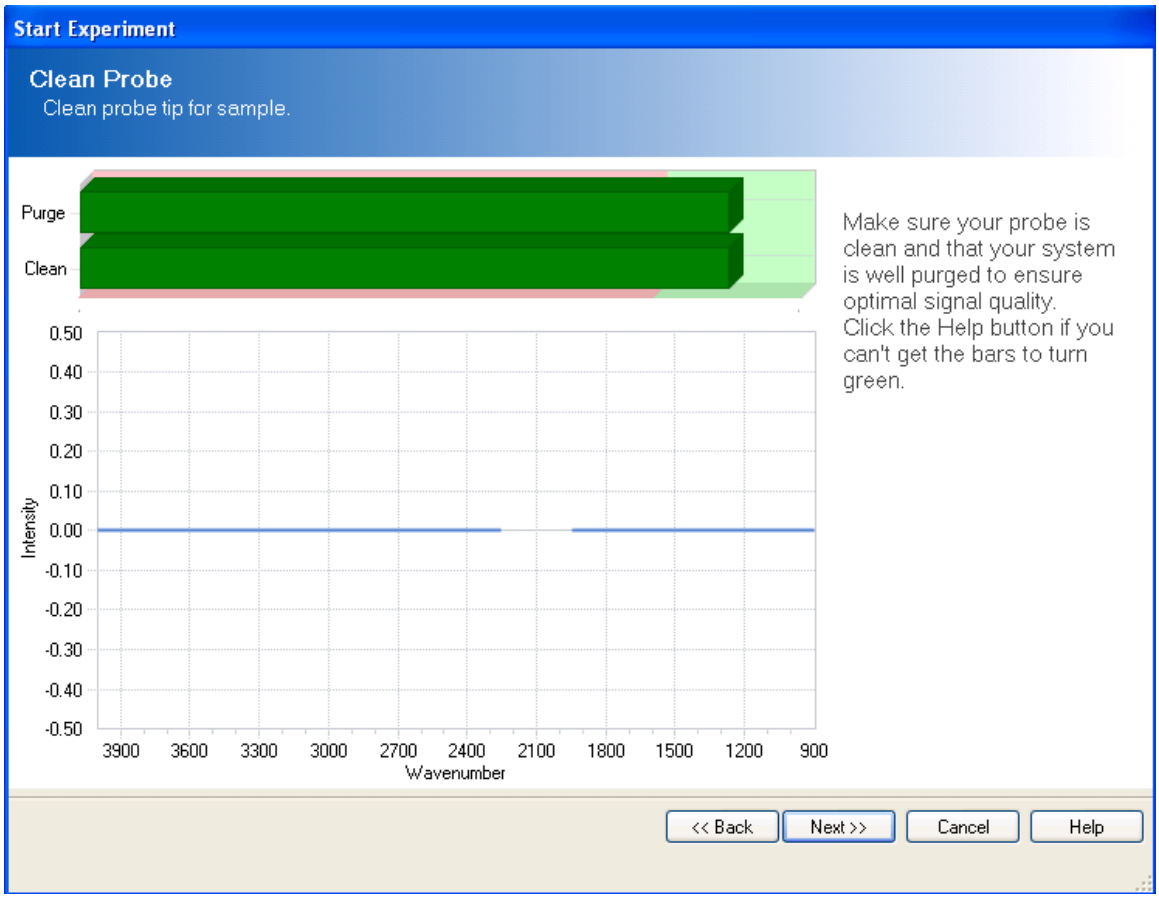
When both bars are green and extend into the green zone on the purge and clean zone, click Next to continue the setup.

If you click the **Next** button and the bar is red (indicating a dirty probe), the following display appears.



Note the spectrum is constantly refreshed indicating what is currently on the sensor. Therefore, one can see if the probe tip is still 'wet' with solvent by the presence of downward pointing peaks. The goal is a flat, straight line.

A clean probe with a well purged instrument is indicated below.



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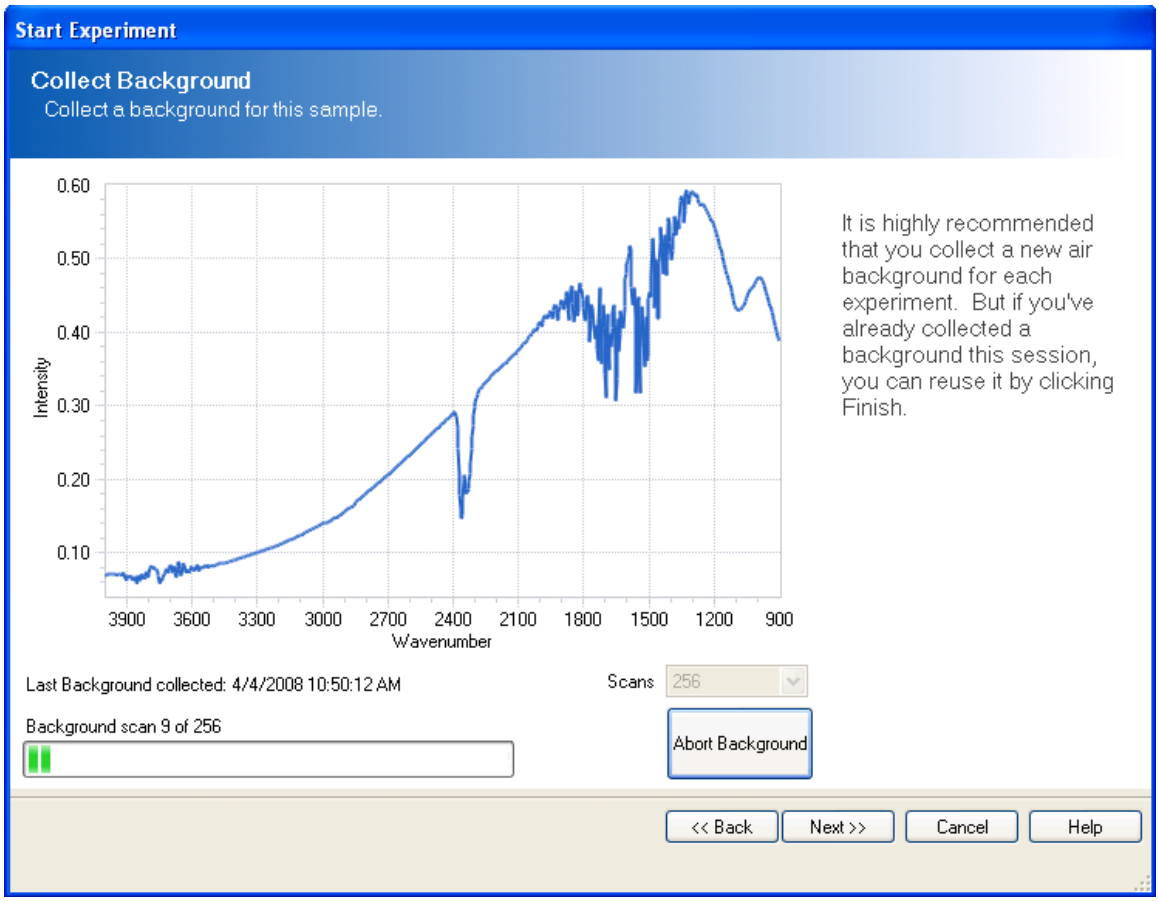
Collecting a Background

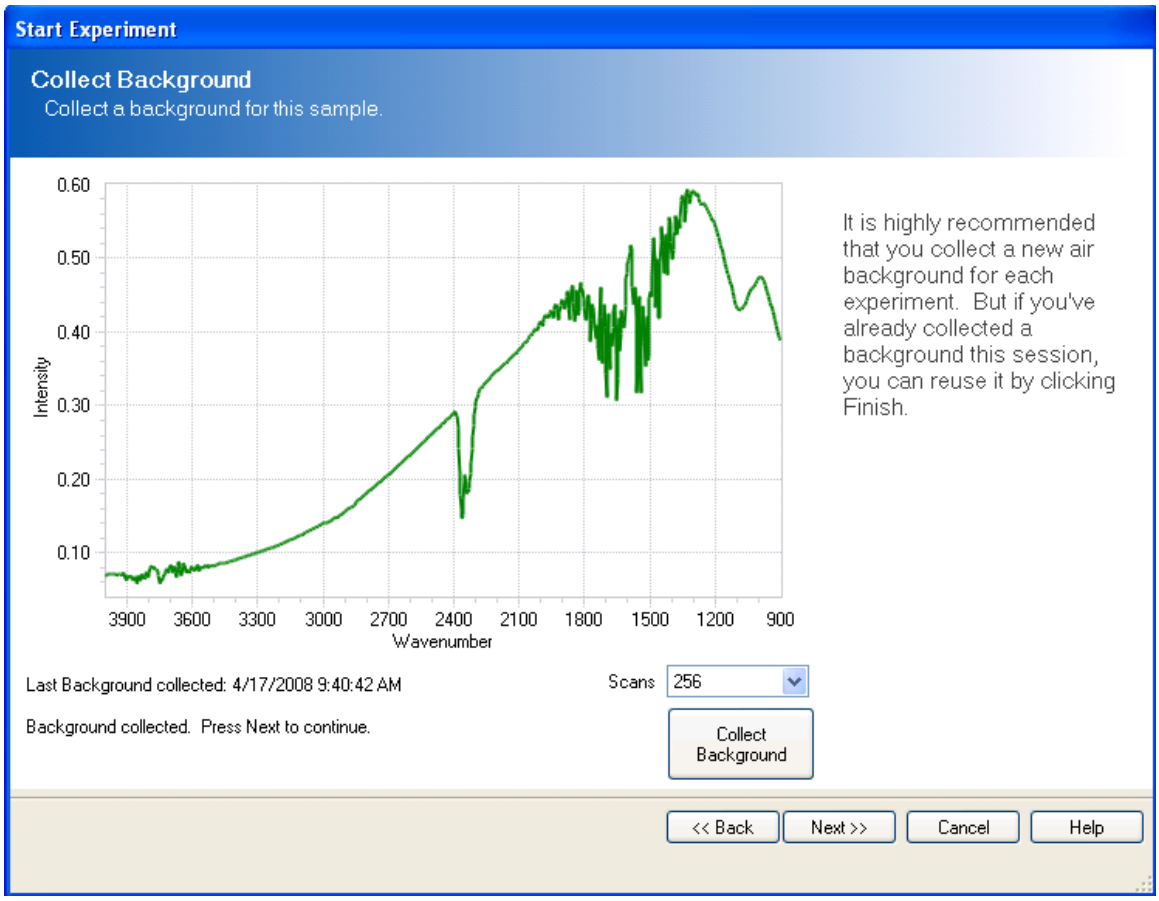
Note: A background spectrum should be collected for reference after the probe has been aligned properly and the sensor cleaned.

Modern FT-IR utilizes a background measurement to minimize the 'instrument response' from the desired spectrum. Historically, one is measuring I/Io where I is the intensity of the light after passing through a sample and Io is the intensity without any sample present. In order to collect good infrared data sets with the iC10 a background of a thermally stable, well purged system with a clean probe must be taken. This background will be collected before each new experiment is performed. The wizard leads one through this procedure.

Click on the **Collect Background** button to collect a background sample.



After the background is successfully collected, the displayed spectrum changes color from blue to green. Click the **Next** button.



Collecting a Reference Sample for the Experiment

The **Collect Sample** page of the wizard allows the user to collect reference spectra for an experiment. The wizard allows the user to collect any number of reference spectra for comparison and analysis purposes.

If you do not want to collect reference spectra, click the **Next** button.

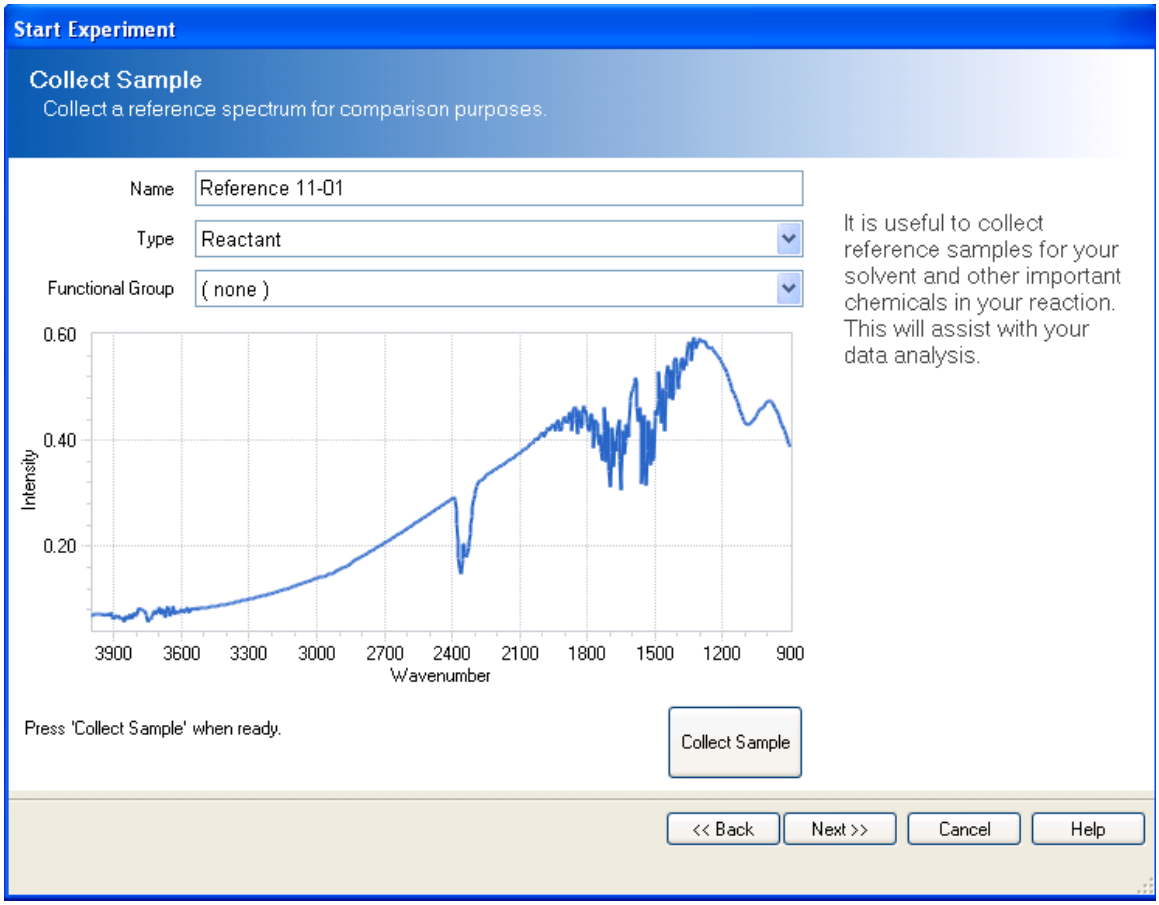
To collect reference spectra:

- Enter a name for the reference spectrum.
- Select a type for the sample from the drop-down list.
- Select the sample from a list by clicking on the **Select** button.
- Select a functional group, if desired, for the reference. Functional groups are useful to auto-define peaks.

Collect the sample by clicking on the Collect Sample button. When the button is clicked, the spectrum for the sample is displayed in the page. This process can be repeated to collect multiple reference samples.

NOTE: By selecting a functional group (i.e. secondary alcohol), iC-IR will automatically plot a peak profile (peak height to zero) once the experiment begins. Ideally, this peak is unique and does not overlap with peaks from the other materials in the experiment. The spectral regions for these suggestions come from a non-editable table of IR group frequencies. Within the Spectra Viewer, if the pointer is held over a single peak of interest, a tool tip window with suggestions for the possible identity of the peak will appear. Prior knowledge of the reaction species, potential intermediates and products will help to narrow the potential peak choices and minimize extraneous selections. Double-clicking the left mouse button will place a profile for the peak in the Trend Viewer. If desired, the new profile can be renamed for clarity by right-clicking the highlighted peak and selecting Trend - Rename. Note that the suggestions offered by the software are available as potential

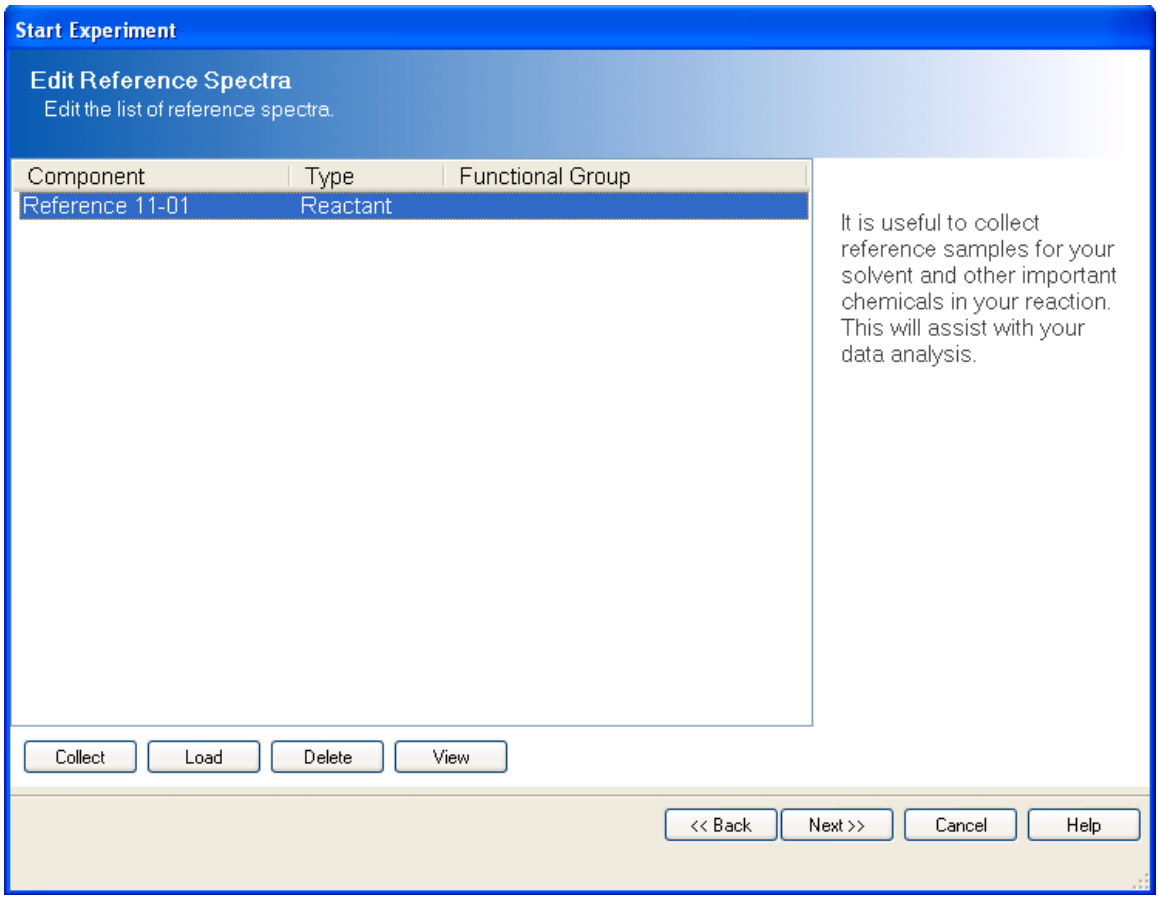
profile names. Additionally, the Type of profile may be changed from the default, peak height to zero, to a different choice under Trend -Types.



After the reference samples are collected, click **Next** button to advance to the next page of the wizard.

Edit Reference Spectra

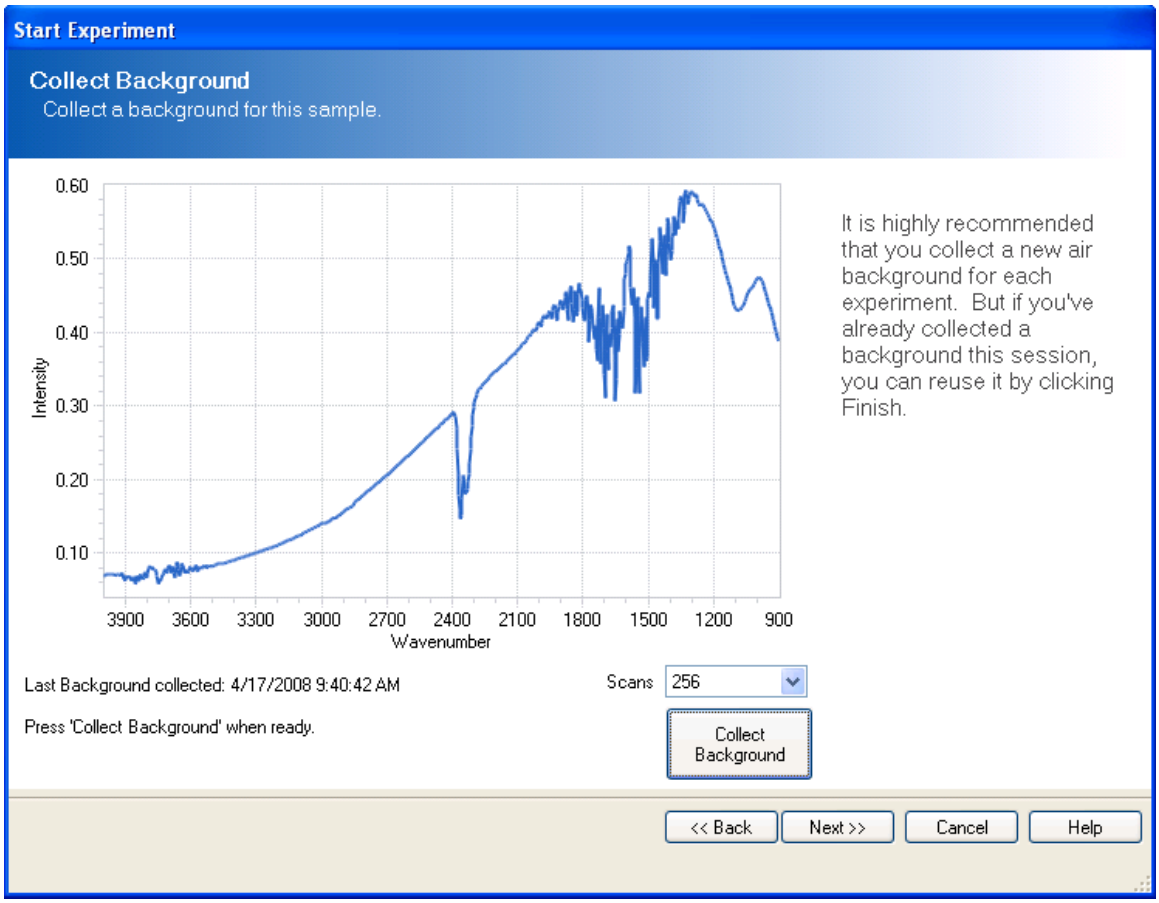
The **Edit Reference Spectra** page of the wizard displays a list of all collected reference spectra for the experiment.



Several options are available on the page.

- Clicking the **Load** button opens a file browser to allow the user to open an existing spectra library to use for the reference.
- Clicking the **View** button displays the spectra in a viewer. Refer to.
- Clicking the **Collect** button re-starts the spectra collection procedure to collect a new reference spectrum.

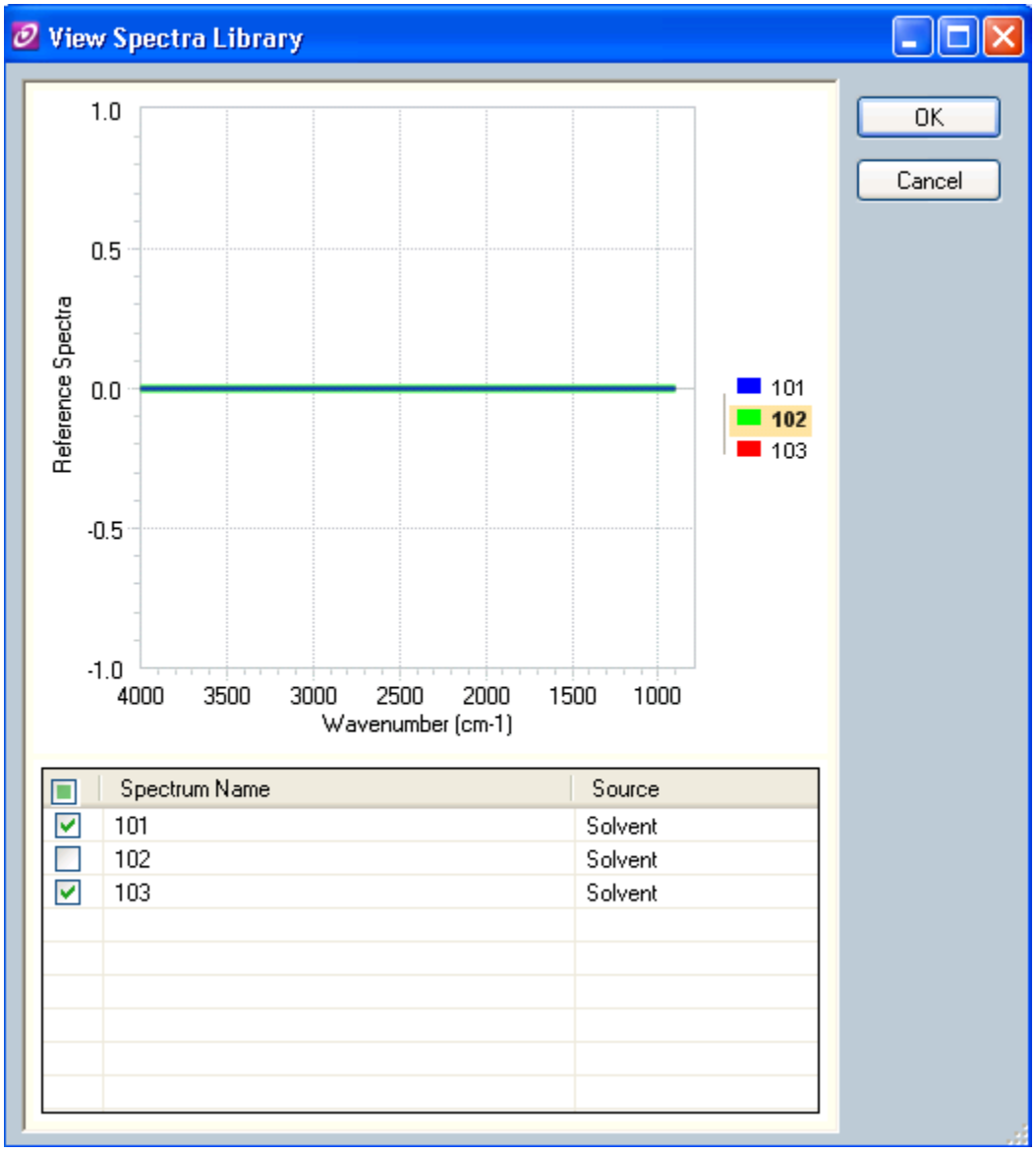
Click the **Next** button to advance to the next page of the wizard.
The next page of the wizard allows the user to collect another background for the experiment.



To collect another background, click the Collect Background button. Refer to Collecting a Clean Reference Background.

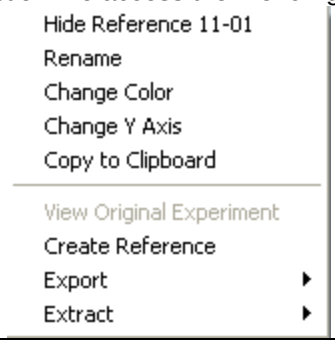
View Spectra Library Dialog

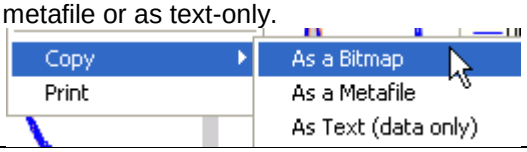
A library or collection of spectra can be created to serve as a reference for a group of experiments. The library is composed of the functional group of standard chemical references stored as a library document. Experiments run using standard functional references with your instrument can help determine the accuracy of data from your current experiment.



There is a checkbox next to each spectrum that is used to hide/show the spectrum on the graph. The checkbox at the top of the list functions as a “hide/show all”.

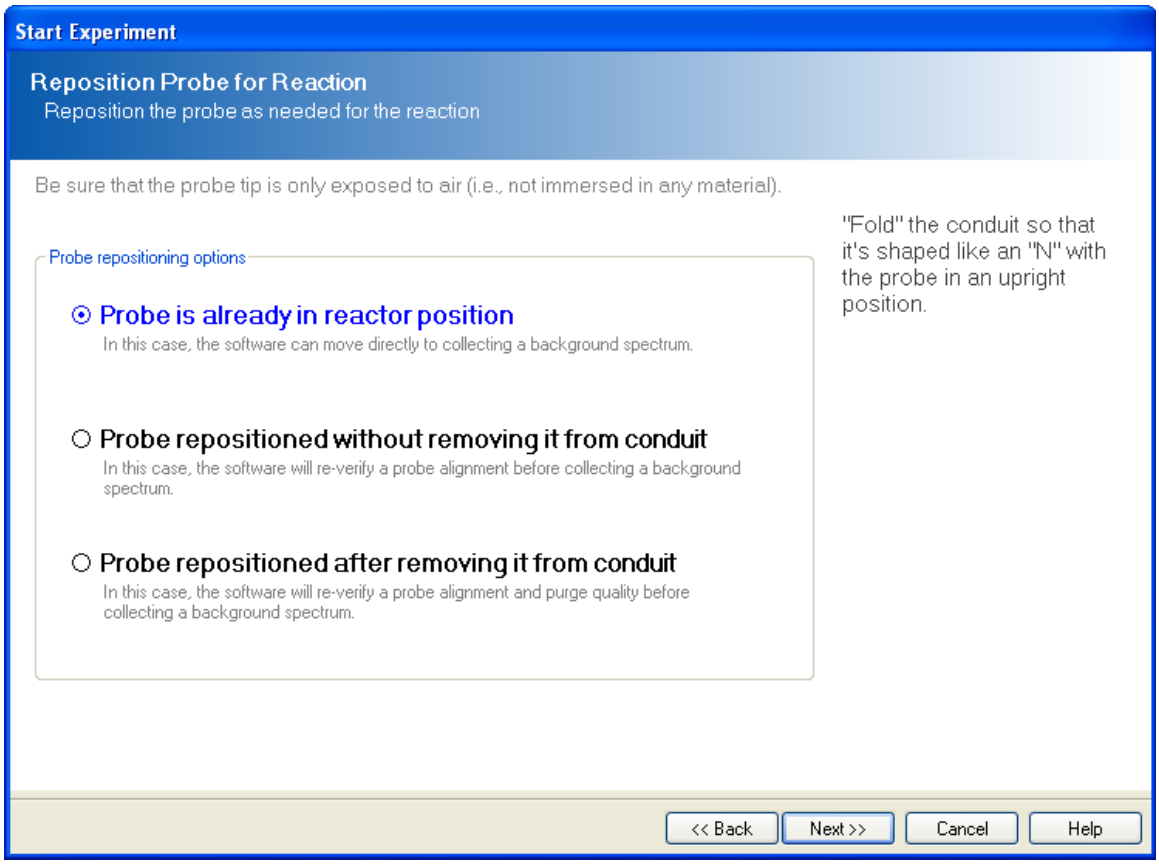
The dialog contains a context (right-mouse click) menu contains the following items.

Show Toolbar	Displays the toolbar at the top of the display.  The toolbar contains the following tools.  Prints the display.  Copies the display to the clipboard.  Zooms the display.  This button is only visible when the Zoom function is enabled. The button resets the zoom to its original scale.  Rescales only the X-axis on zoom.  Auto scales the Y-axis.  Displays the Legend Panel.  Displays crosshairs on the graph.
Show Legend	Displays a legend box which lists each trend and its name. The Legend also contains a context menu that allows the user to perform some of the functions discussed in this section. To access the menu right-click on the legend. 

Copy Chart to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
Print	Opens the Print dialog to print the display.
High Contrast	Displays the graph with a black background.
Zoom	Zooms the display. Refer to Trend Profiles Zoom Operation.
Reset Zoom	Resets the zoom to its original scale.
Rescale on zoom	Rescales only the X-axis on zoom.
Auto-scale	Auto scales the Y axis.
Line Thickness	Selects the line thickness for the plots.

Reposition the Probe for Reaction

If the specified probe is either a K4 or K6, this page of the wizard is displayed. If a fiber probe was specified, the user is directed to Cleaning the Probe.



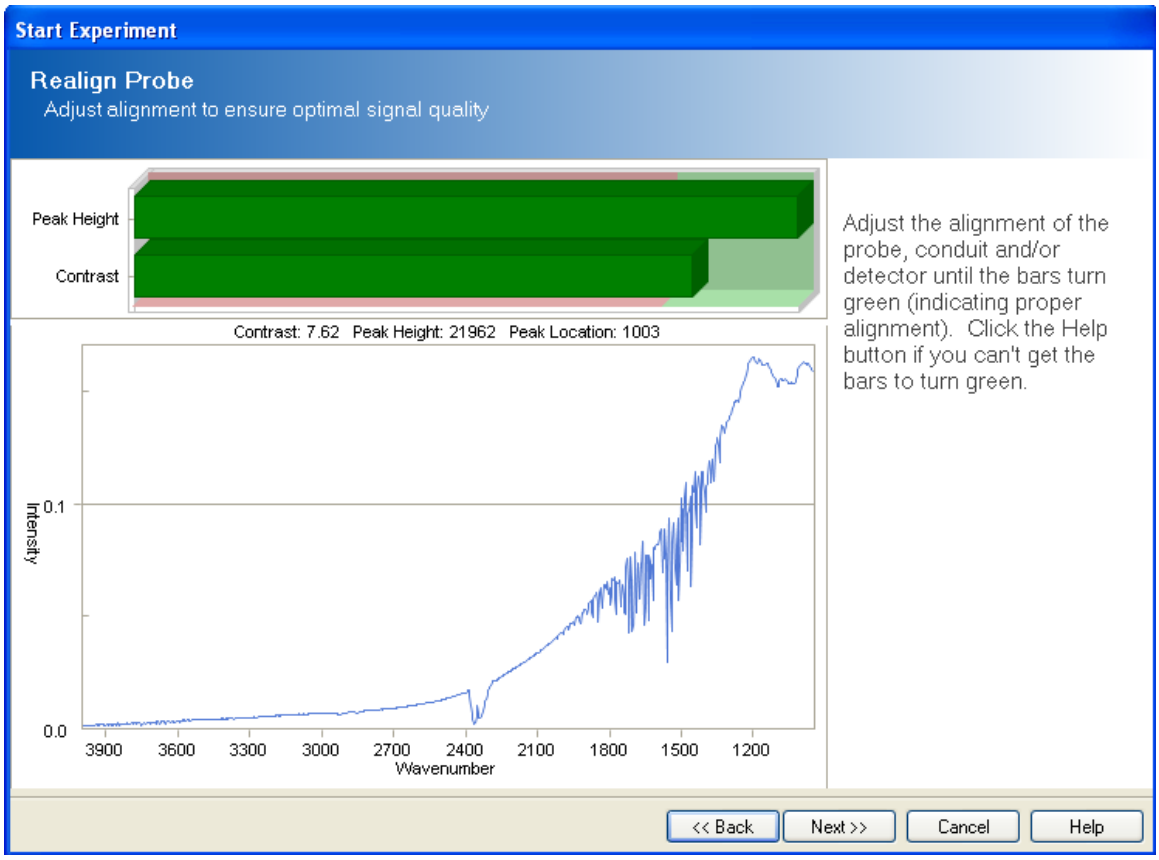
The user selects an option using the radio buttons.

If the **Probe is already in Reactor Position**, the wizard advances to Experiment. To start the experiment, click the **Finish** button.

If the **Probe repositioned without removing it from the conduit** or **Probe repositioned after removing it from the conduit** is selected, the wizard advances to the Realign Probe page to ensure maximum performance before data collection.

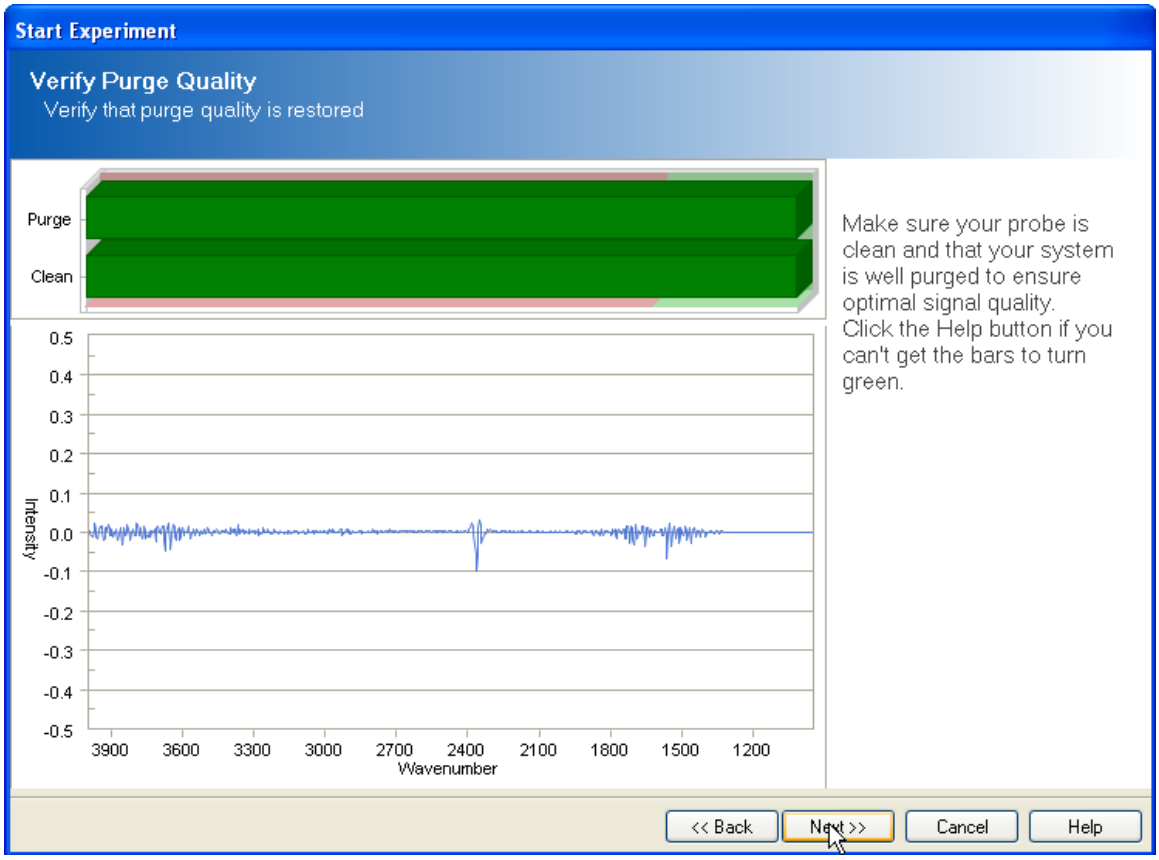
Realign Probe

If the probe is not in the reactor position, the alignment of the probe must be adjusted.



Adjust the probe until both bars are green and click the **Next** button. If the probe was removed from the conduit, the purge must be verified using the Verify Purge Quality page of the wizard. If the probe was not removed from the conduit, the wizard advances to Experiment. To start the experiment, click the **Finish** button.

Verify Purge Quality



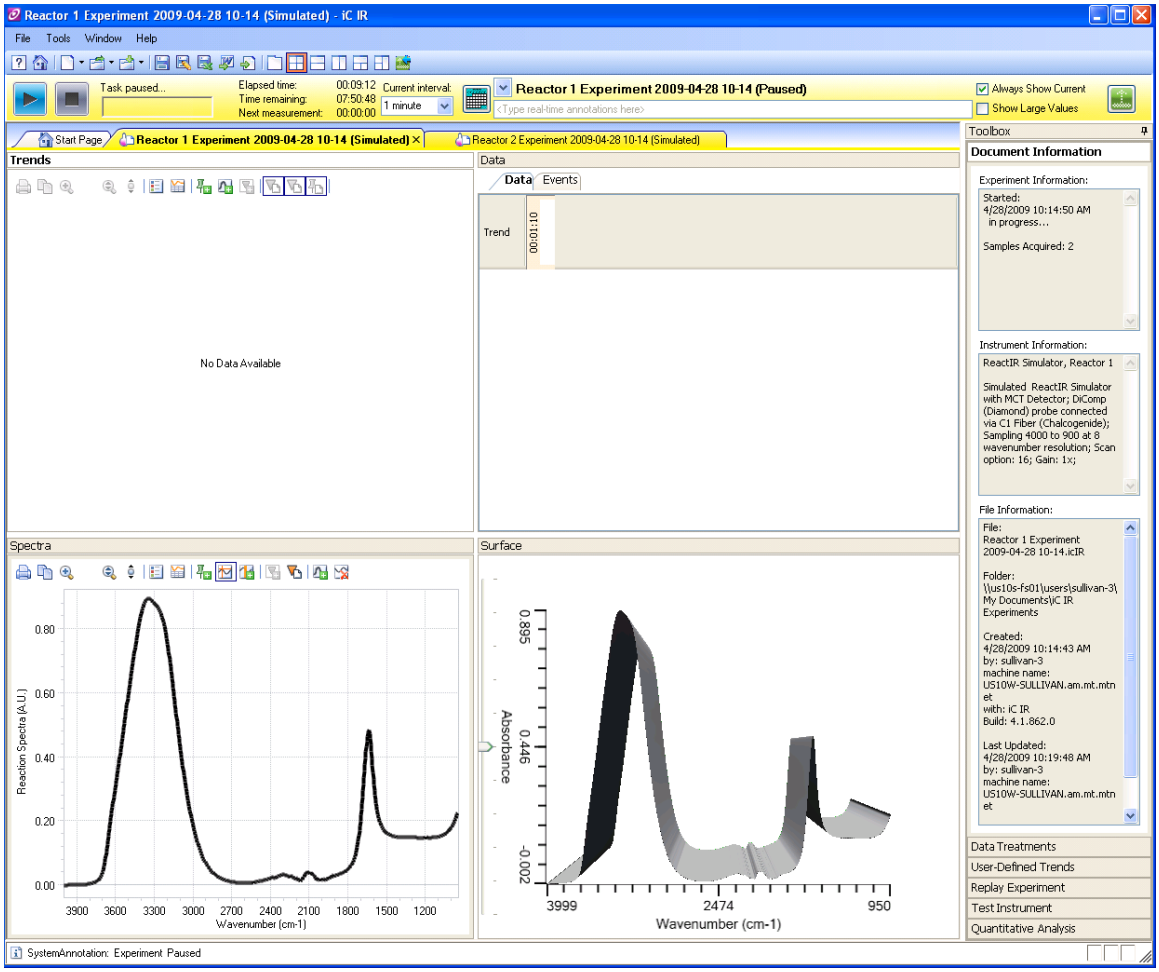
For best sampling results, after realigning the probe, you should wait while any water vapor is purged. Once the two indicators turn green, click Next to continue the setup.

Starting the Experiment

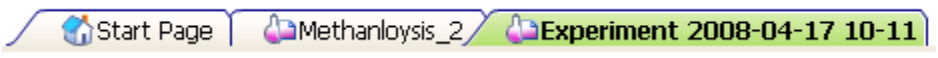
After all the preparation steps for the experiment are complete, the Live Experiment Toolbar is opened.

Note that the dialog contains a  button that allows the user to add additional phases to the experiment at this time.

When the experiment is opened, it is automatically in a paused state.



When the **Run** button is clicked to start the experiment, the experiment starts to collect data and the Live Experiment Toolbar and the experiment tab turn green.

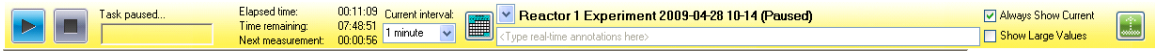


A running experiment can be paused by clicking the  button in the Live Experiment toolbar. When the button is clicked, the Live Experiment Toolbar and the experiment tab change to a yellow background.

If the  button is clicked the experiment is stopped and considered complete.

The Live Experiment Toolbar

The Live Experiment toolbar is displayed at the top of the main window and is only displayed when an experiment is in progress.



The toolbar initially is displayed in yellow indicating a paused experiment. When the **Start** button is clicked, the experiment is started and the toolbar changes to green.

When the experiment is complete, the toolbar changes to a completion verification message. A summary of samples taken and any error or warning messages is displayed on the toolbar.

The Live Experiment toolbar contains several tools:
The **Annotation** field allows the user to insert an annotation. The annotation is given a timestamp equal to the time indicated by the orange time line. By default the time line is positioned at the current time.

The Run -  - and Pause -  - buttons are used to control execution of the experiment. The buttons toggle depending on the current run state of the experiment.

The Stop button -  - permanently stops the experiment.

The **Current Interval** field allows the user to change the scan interval during the experiment.

The **Elapsed Time** field displays the total time of the experiment from when it was first started.

The **Time Remaining** field displays the calculated time remaining until the completion of the experiment.

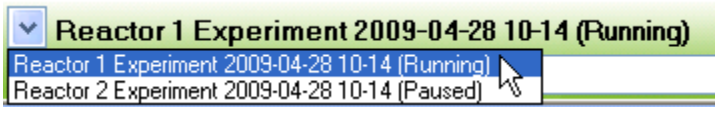
The **Next Measurement** field displays the time remaining until the next sampling.

The  button is used to add a manual sample from a HPLC or chromatography method. Refer to Adding Referee Data.

The 

checkbox open an additional display tab that displays the peaks in a matrix format. Refer to Large Values Viewer.

Clicking the  button displays a droplist of all active experiments. The user can select an experiment to view that experiment's Live Experiment Toolbar.



Click the  button to add a phase to the experiment.

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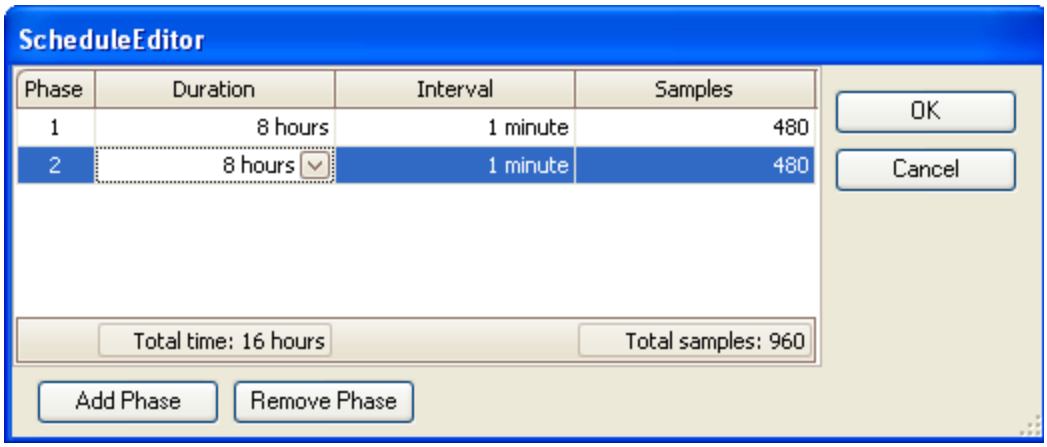
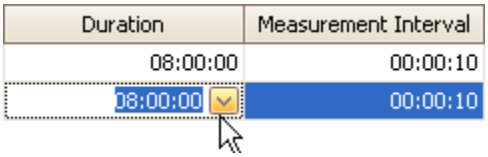
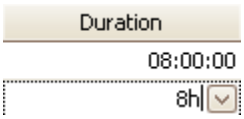


A new row is added to the Phases list. The **Duration** and **Measurement Interval** fields are edited as desired. The number of phases is calculated automatically.

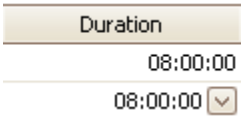
The **Duration** and **Measurement Interval** fields have a droplist from which the user can select the time values.



Alternatively, the user can enter a number into the fields followed by a “h” for hours, “m” for minutes or an “s” for seconds.

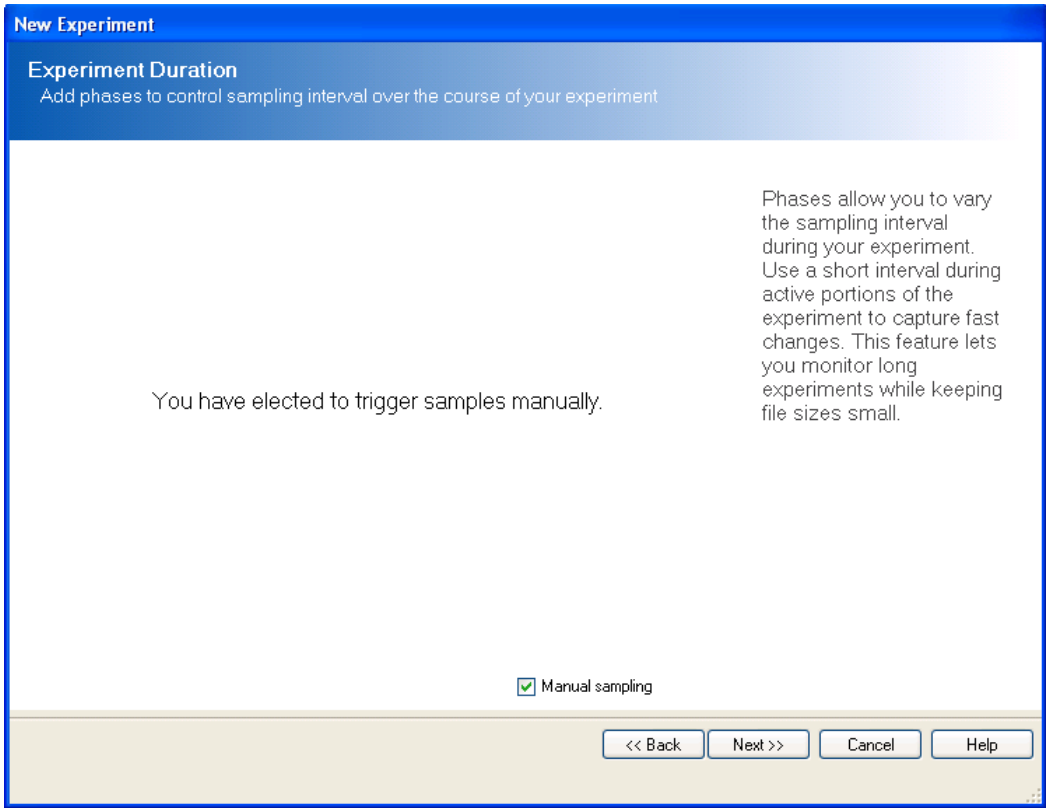


When the cursor leaves the field, the entered time is converted to the correct time format and displayed

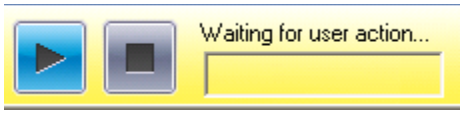


Manual Sampling

Experiments can be configured for manual sampling by clicking the manual Sampling checkbox on the Experiment Duration page of the experiment wizard.



If the experiment type is defined as Manual Sampling, iC IR will collect a sample each time the  button is clicked.



The button allows the user to manually take a sample during manually sampled experiments. When the user clicks the button, a manual sample is started. The Pause button is disabled during the sample scan and a progress bar displays the status of the scan.

When the sample scan is complete the data is added to the experiment and the experiment goes into a pause state until the  button is clicked again. The experiment continues to run, waiting for the next manual sample.

When the experiment is complete, the user clicks the  button to stop the experiment.

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Rapid Collect Experiments

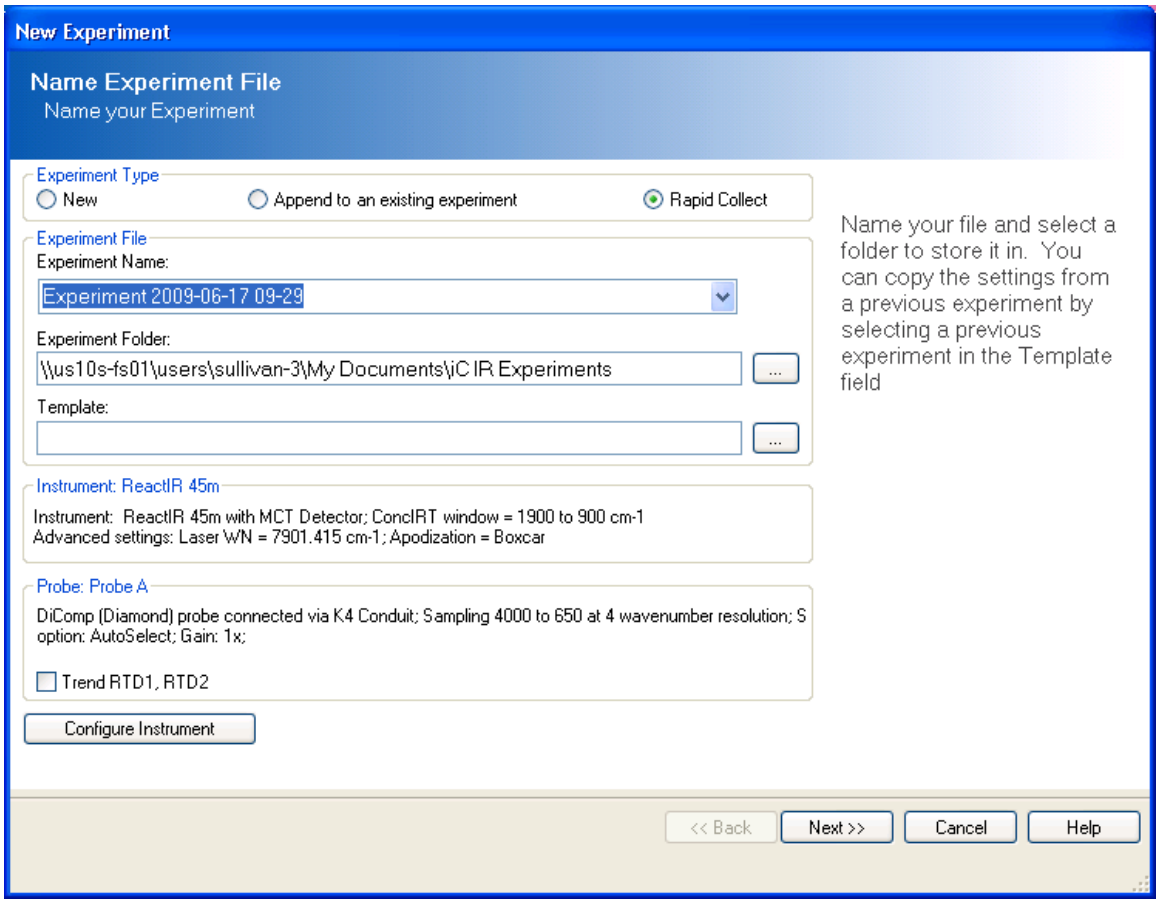
The Rapid Collect Experiment feature allows the user to effectively monitor short, fast moving reactions. The iC IR performs no processing on the acquired samples while the reaction is in progress, so real-time data analysis is not available during the execution of an experiment. The iC IR scans as rapidly as possible and the interferogram for each and every scan (no co-addition performed) is placed on a queue for the duration of the reaction. The Rapid Collect function also has the option to collect temperature data from the RTDs.

Note: The number of scans per second for a Rapid Collect experiment will decrease if RTD temperature values are trended.

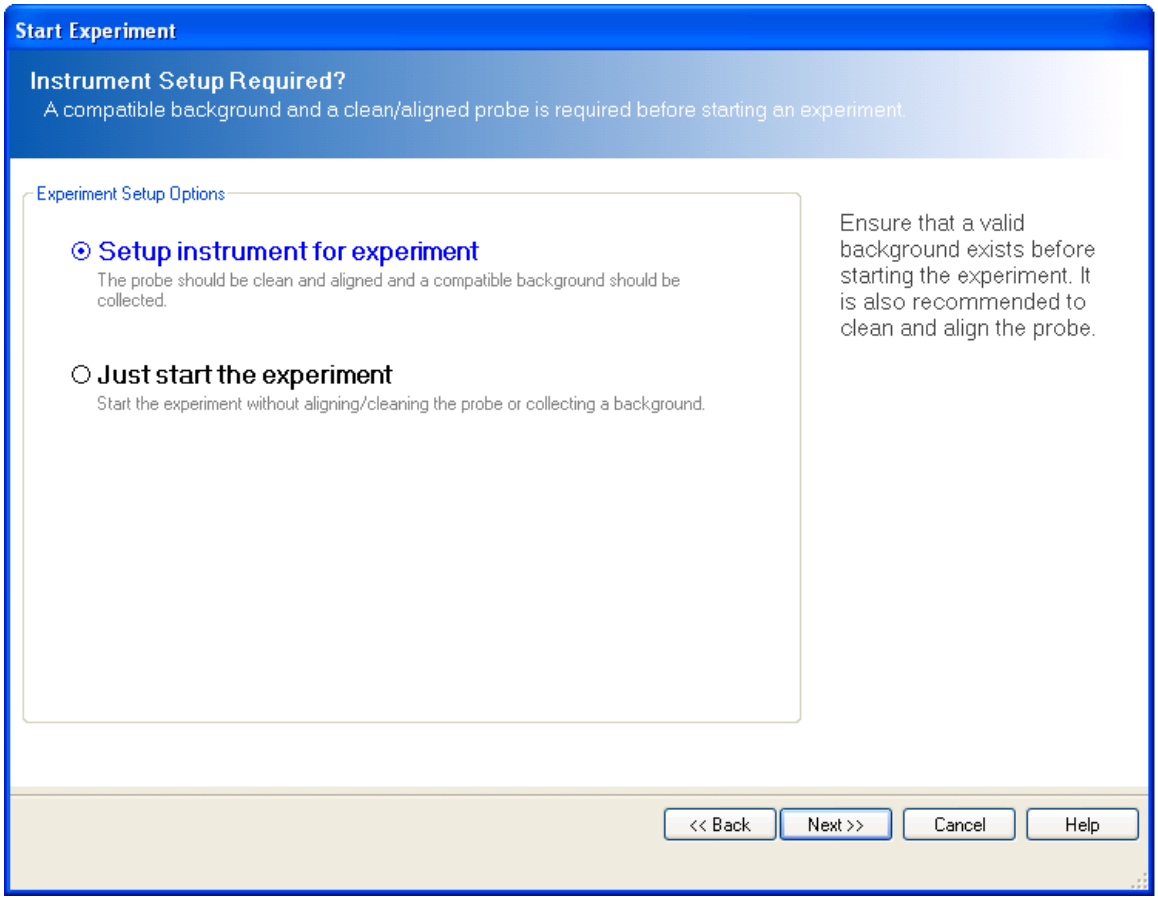
When the Rapid Collect Experiment is complete, the user can analyze the data like any other experiment. Using a data treatment option available to Rapid Collect Experiments only, the User is able to specify the number of interferograms to be co-added in the creation/recreation of the sample spectra collection.

A startup option is available on the Start Experiment wizard, Rapid Collect. This option is only available and displayed for the ReactIR 45m, ReactIR 15 and ReactIR 45P instruments.

The Rapid Collect Experiment option is also not available if any other probe is running for multi-probe instruments.

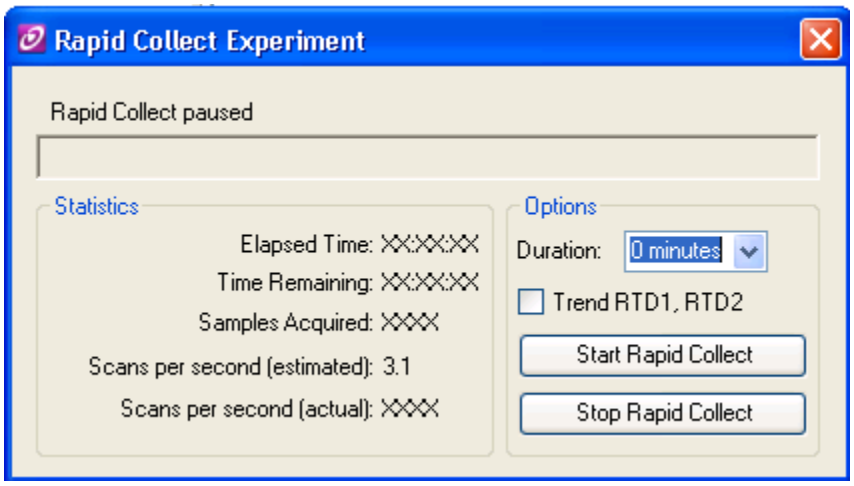


When the Rapid Collect option is selected, the wizard is modified to include clean, align, and background collection but no phase information is displayed. The system limits the experiment to a single phase with duration not to exceed 30 minutes. It is not possible for the user to specify any interval information.

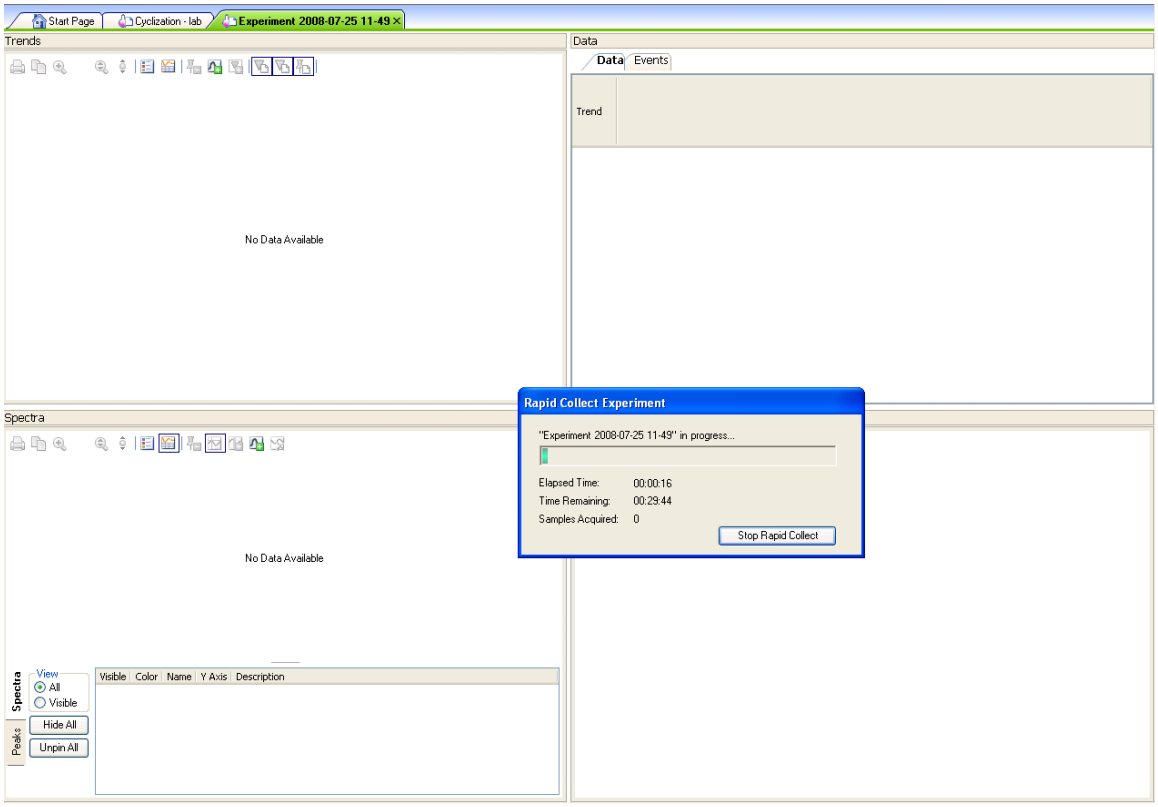


Refer to Positioning the Probe for a description of these wizard pages.

When the instrument has been set up for the experiment, a Rapid Collect Experiment dialog is displayed.

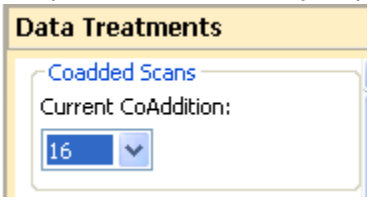


Click the **Start Rapid Collect** button to start the experiment. The iC IR displays a blank experiment document during a Rapid Collect Experiment.



The user can cancel the experiment by clicking the **Stop Rapid Collect** button. The iC IR prompts the user for confirmation before cancelling.

When the Rapid Collect Experiment is complete, the system uses the selected value for the number of interferograms to co-add and then processes the interferogram data into samples. The co-addition value is selected using the field on the Data Treatments task pane. This field is only displayed for Rapid Collect experiments.



The CoAddition option allows powers of two from 1 to 64. The chosen selection must be synchronized with the settings in the experiment used to co-add the interferogram data. If the CoAddition option is changed, the iC IR will delete the current collection and reprocess the raw interferograms using the new (co-addition) settings.

Experiment Display

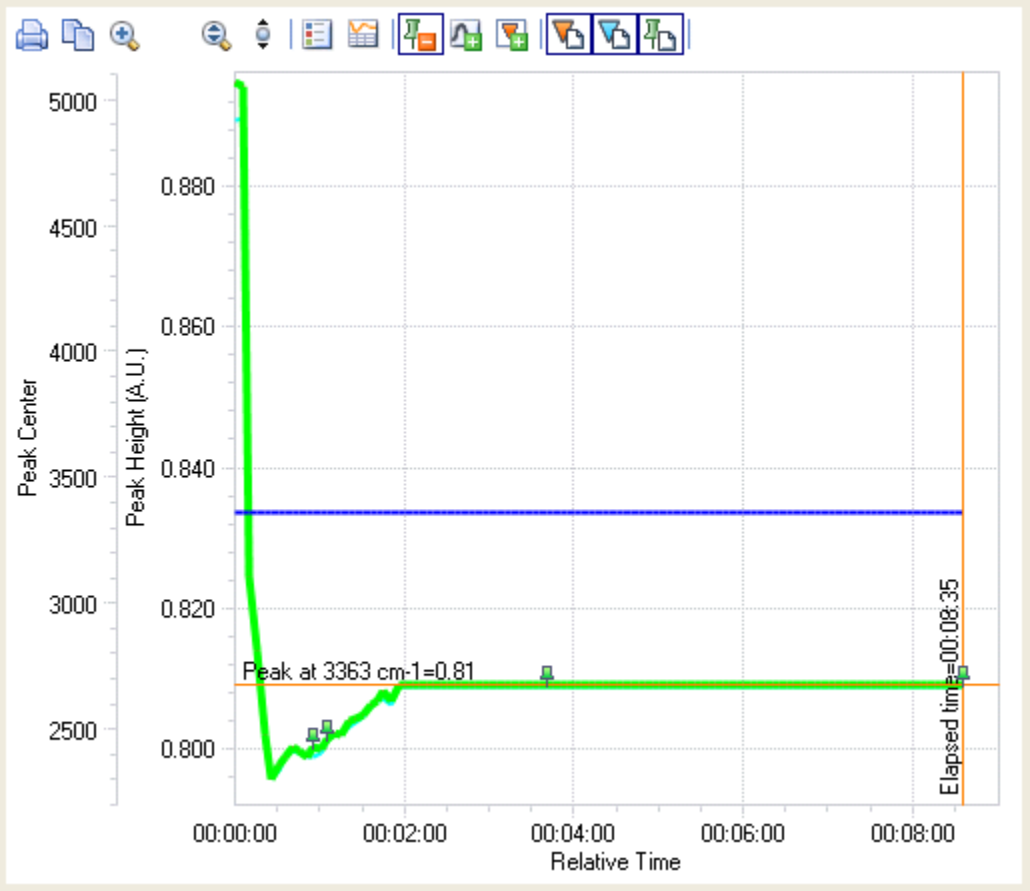
The experiment display is the primary tool for viewing experiment data. The display contains four viewers.

- Trend Viewer
- Spectra Viewer
- Surface Viewer
- Event Viewer.

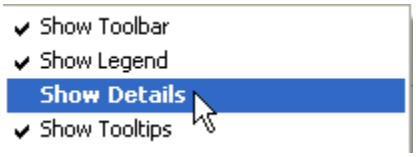
These viewers interact with each other to facilitate data interpretation and analysis. The viewers can also be displayed in a tiled configuration or singly as tabbed views.

Trend Viewer

Trend analysis of several selected components for the experiment are generated in real time and displayed in the Trend Profiles display. This enables the user to compare peak height profiles and ConcIRT LIVE generated profiles in one window. The display rescales automatically when different profiles are added.



The Trend List is displayed by either placing the cursor on a trend and double-clicking on it, which displays the corresponding trend along with the Trend List or by right-clicking on the trend plot area and then selecting the Show Details option.



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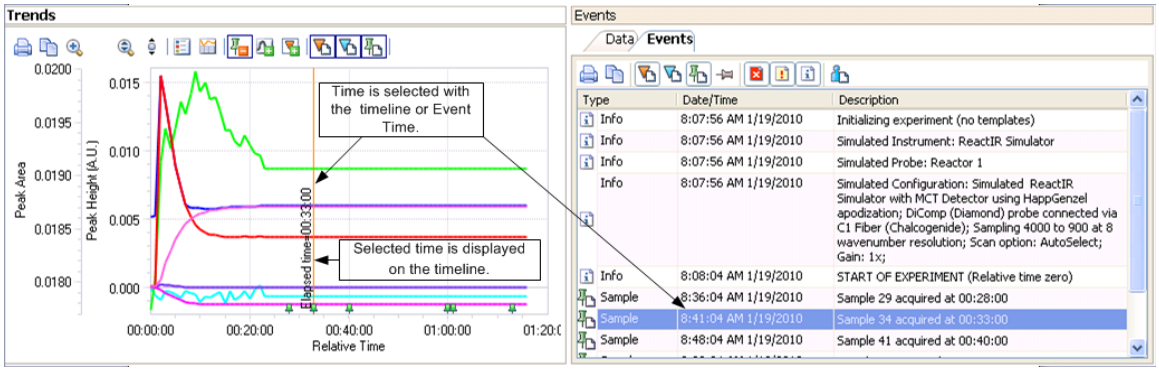
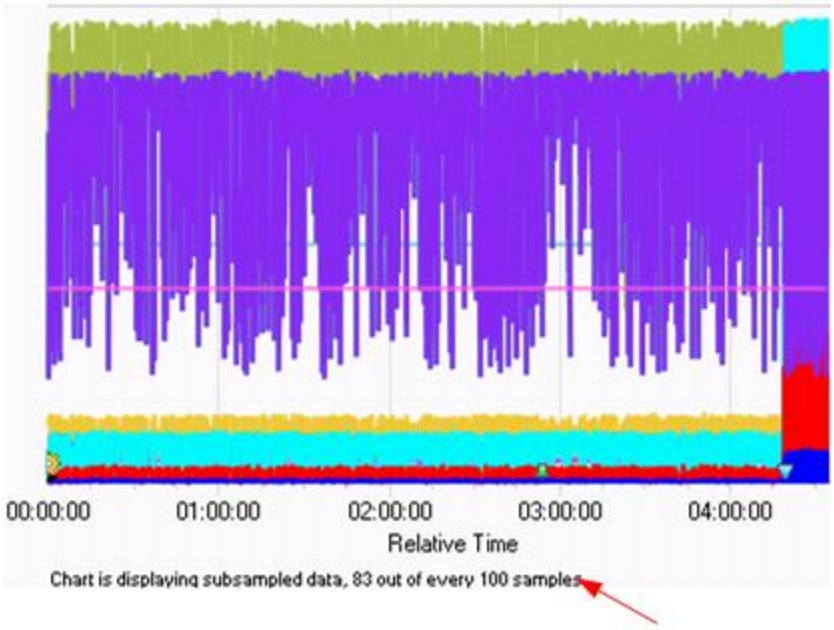
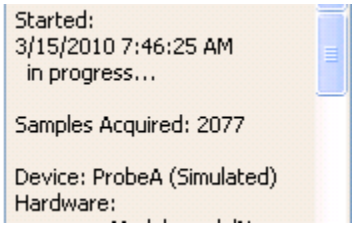
The value for each selected time is displayed for each component. Different times can be selected by selecting a different event in the event log.



Note that by default, the Trend Viewer chart displays a maximum of 20,000 data points. When the number of data points being trended exceeds this amount, trended values are subsampled. When subsampling occurs a message is displays at the bottom of the trend chart.



The message provides the ratio of subsamplng that is being performed. If it becomes necessary to view the full 100 percent of data, the user has the option of reducing the number of trends being displayed to bring the maximum number of data points below 20,000. The number of data points is calculated by multiplying the number of trends being displayed by the total number of samples acquired. The number of samples acquired is displayed in Document Information task pane.



It is important to note that subsampling only effects the data being displayed in the trend viewer, all data for every interval is always collected and stored.

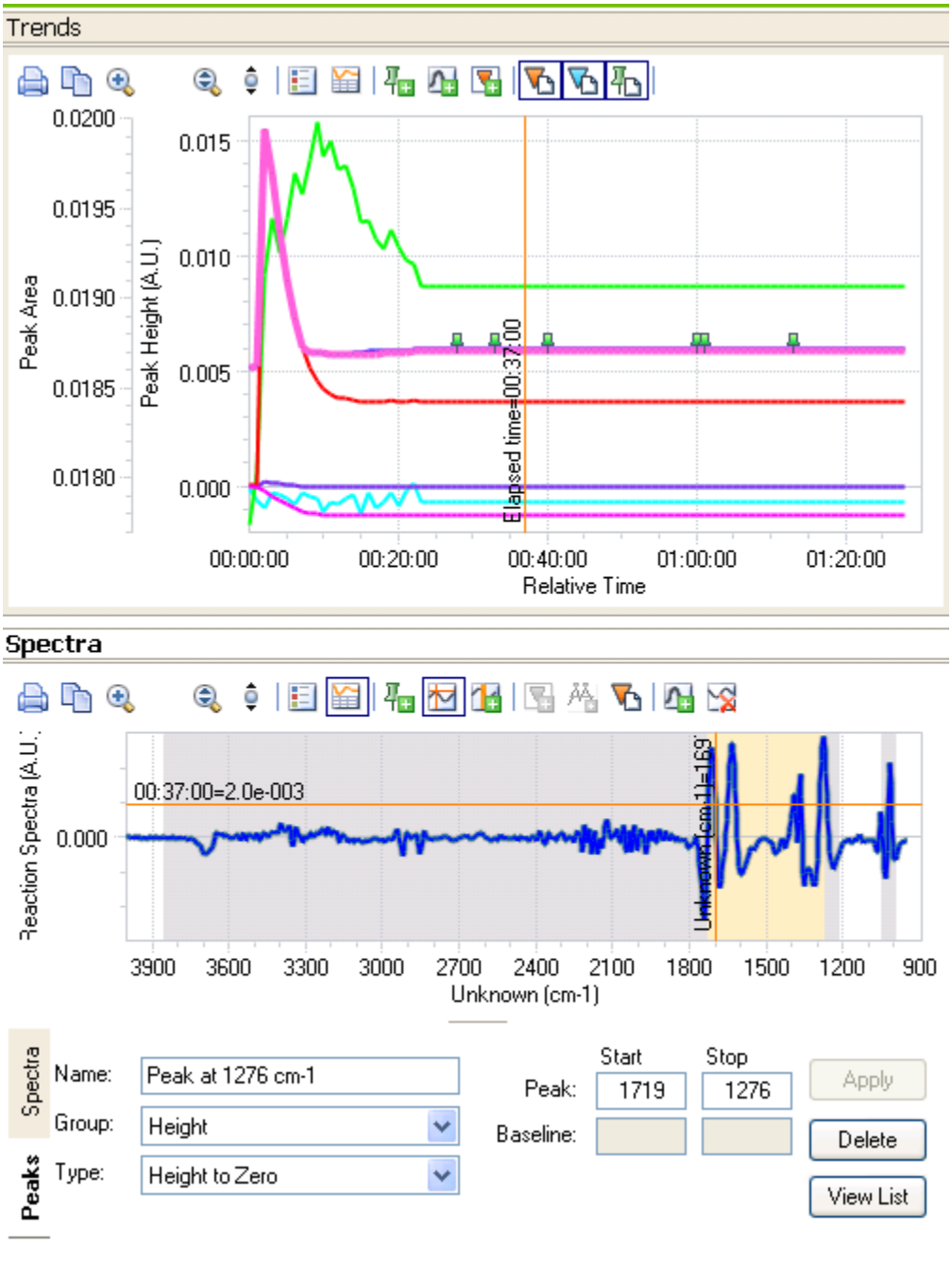
Trend Analysis from Selected Spectra

To create a trend of a specified spectra peak, click on the peak in selected spectra.

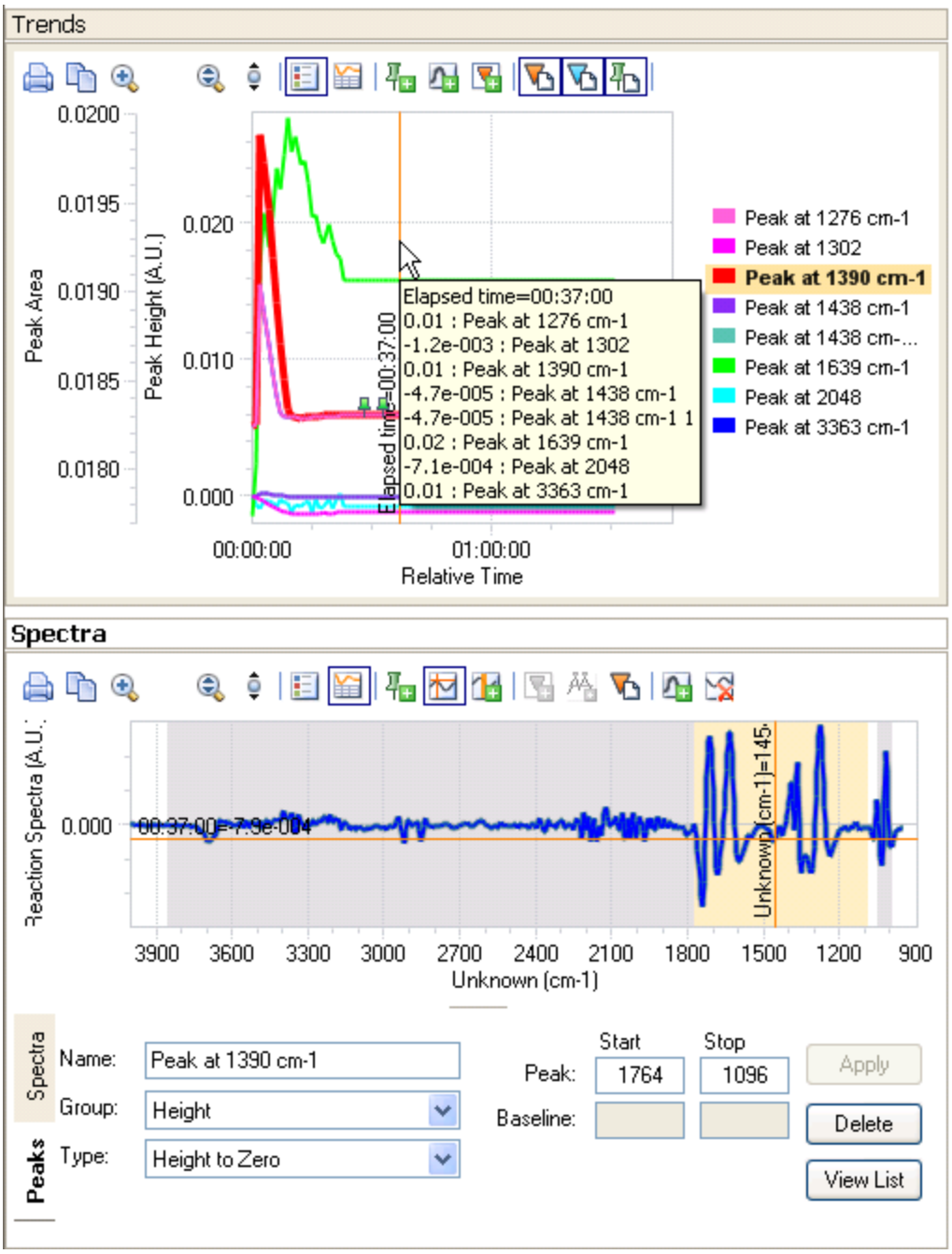
The selected spectrum is indicated in yellow and the profile is displayed in the Peak List.

Once it is displayed in the peak list, the type of peak can be edited. The trend is re-displayed when the type of peak profile is changed.

The Trend Profile, Peak Profile and profile description of one peak are shown below. The trend of the selected peak is displayed in the Trend Profile display.



Two peak profiles, their corresponding trend profiles and descriptions of two peaks are shown below. The trends of the selected peaks are displayed in the Trend Profile display.



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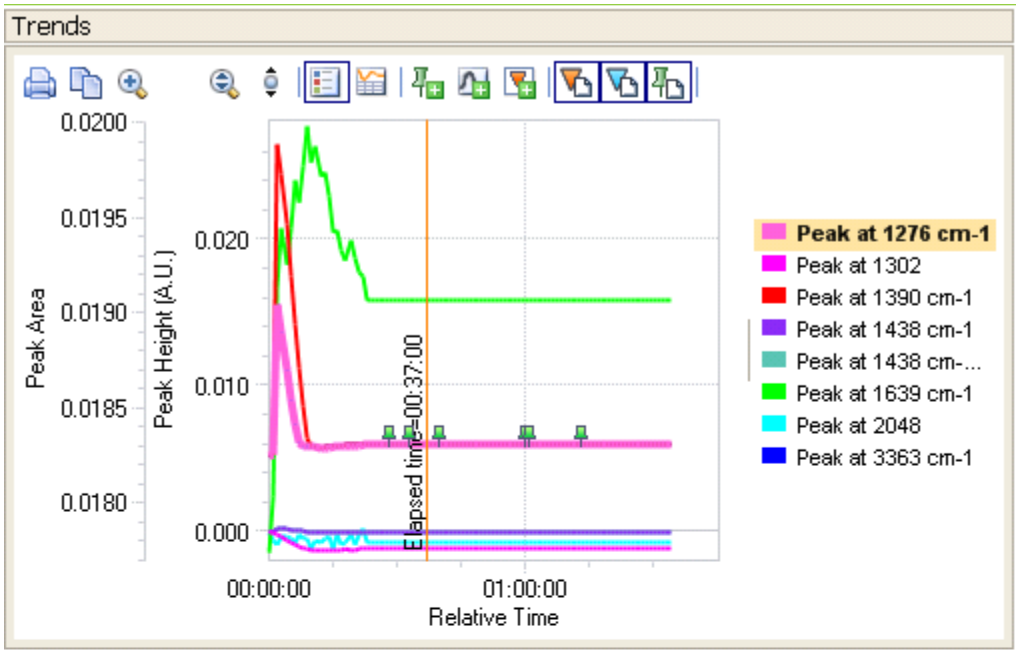
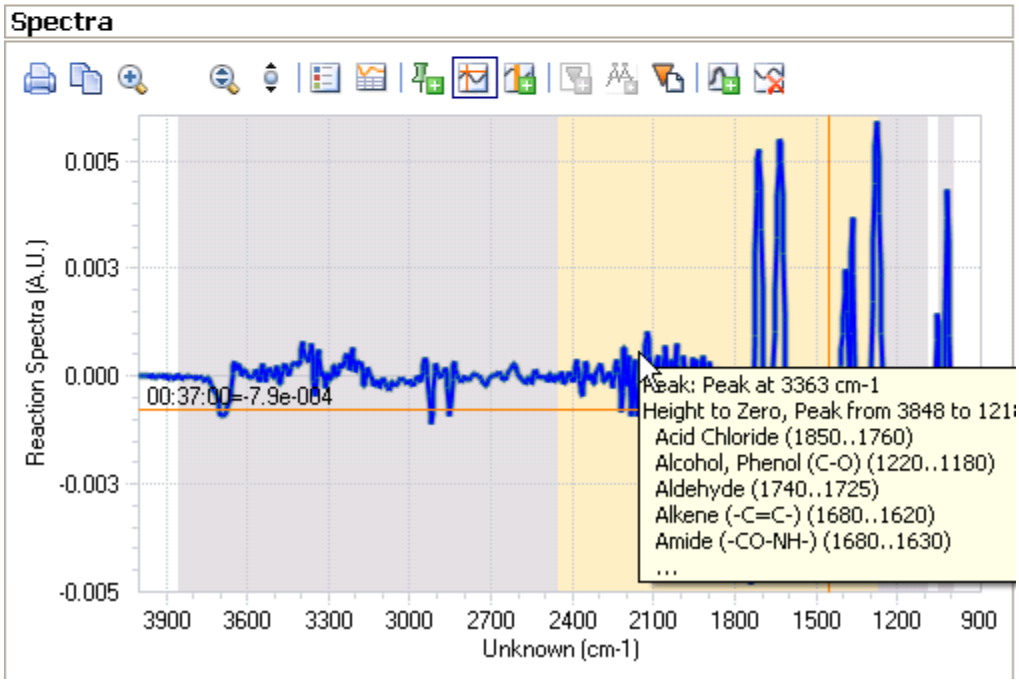
Highlighting a Trend Profile

Clicking on a trend with the cursor anywhere on the trend enlarges the trend line, changes the color of the corresponding title and highlights the selected peak as shown in the display below.





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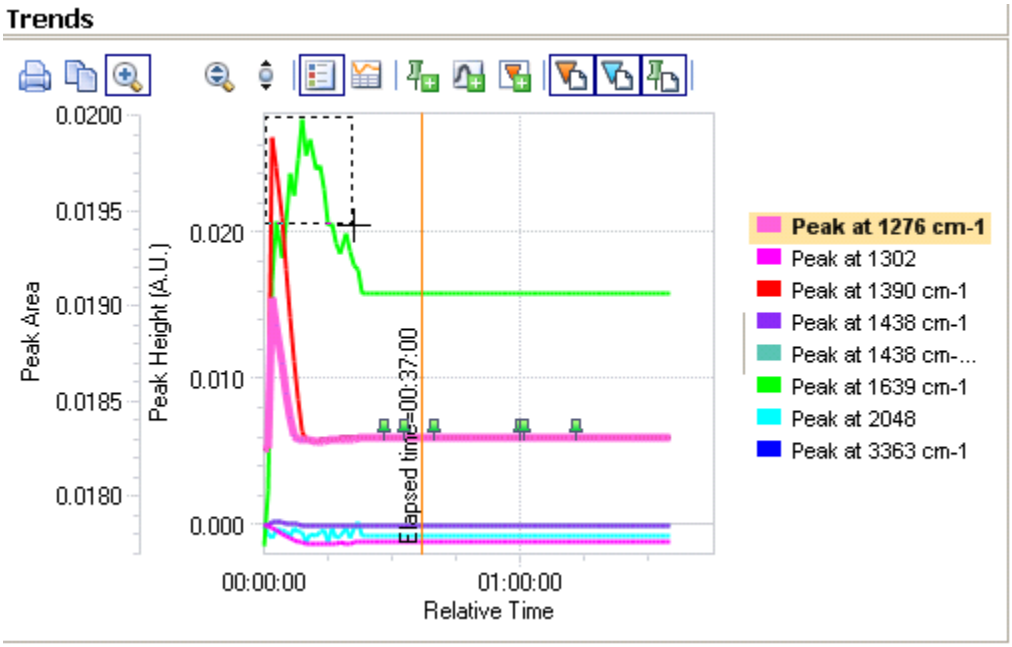
Trend Profiles Zoom Operation

There are two methods available for zooming the trend display.

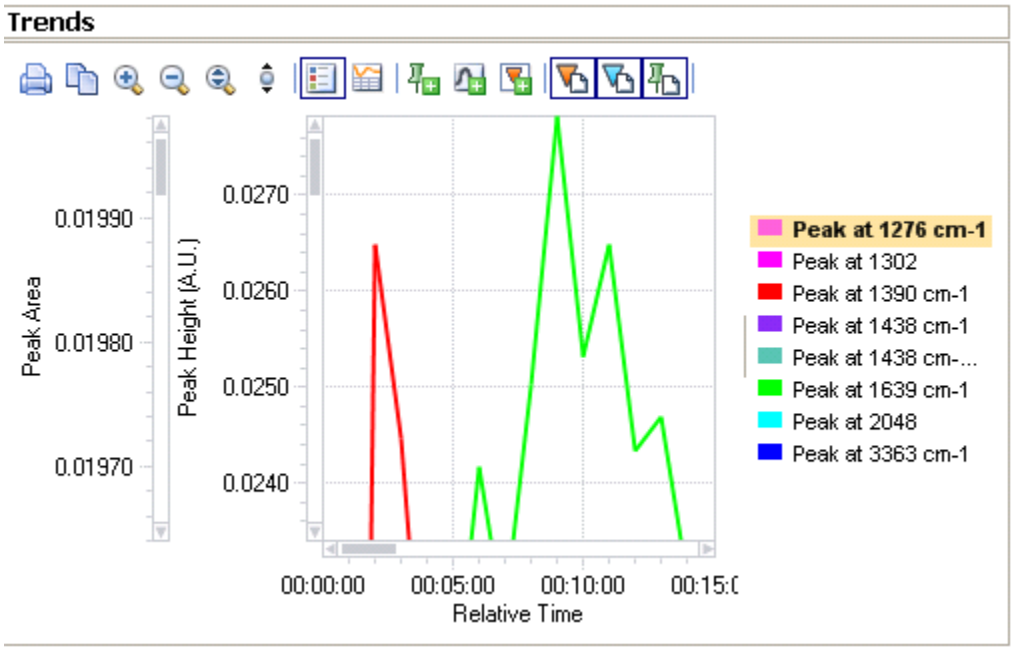
Right-clicking in the trend graph area and selecting the Zoom option from the right-click menu.

Dragging the mouse over the area you wish to enlarge, as shown below.



Both the selected Trend and Spectra enlarge.

The zoomed or enlarged image can be moved by moving the corresponding sliderbars with the mouse.



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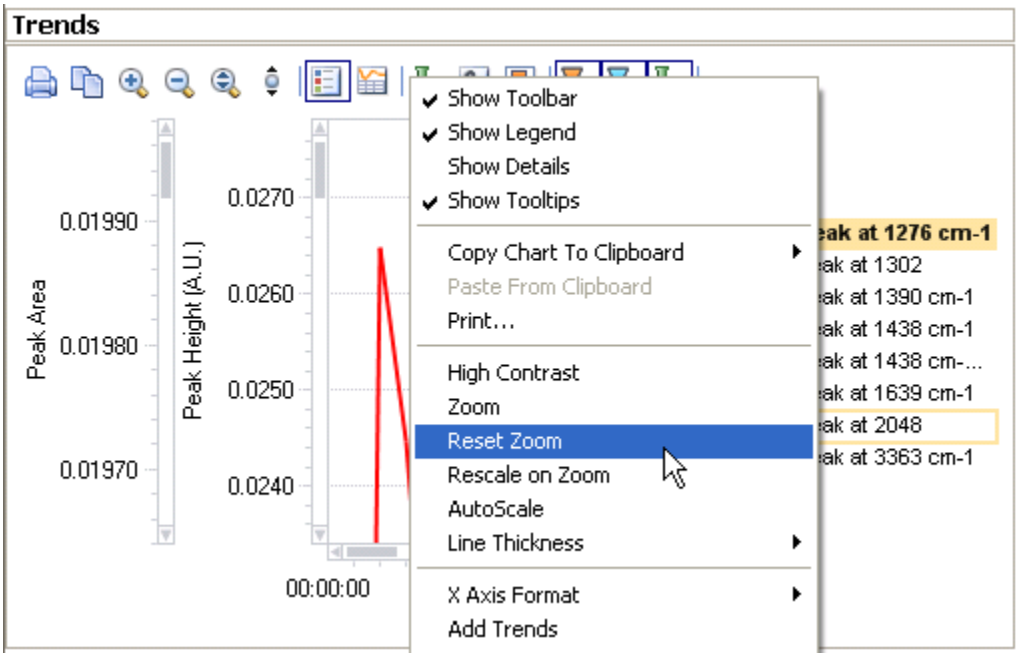
To return to the normal size display, right-click on the zoomed display and select the **Reset Zoom option from the menu or click the**  **button in the toolbar.**

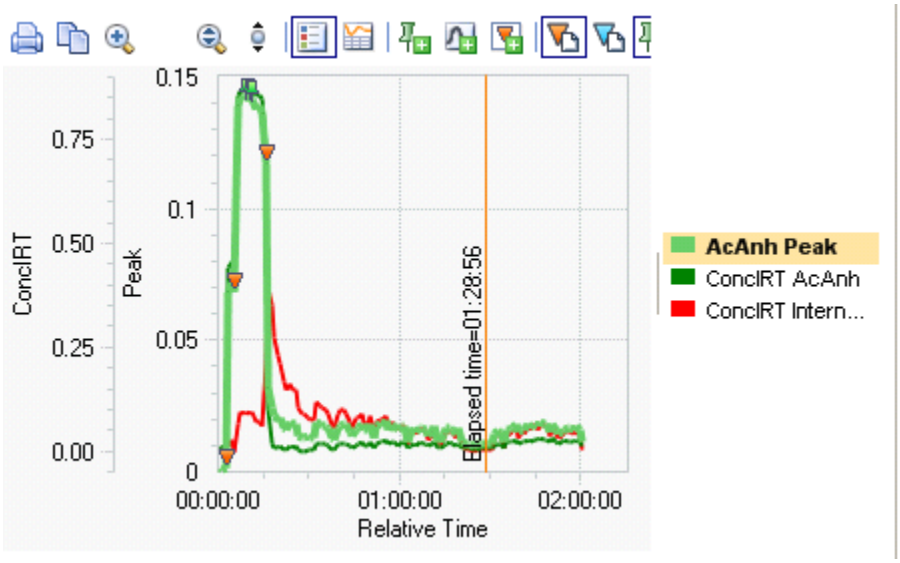


Trend Autoscale Operation

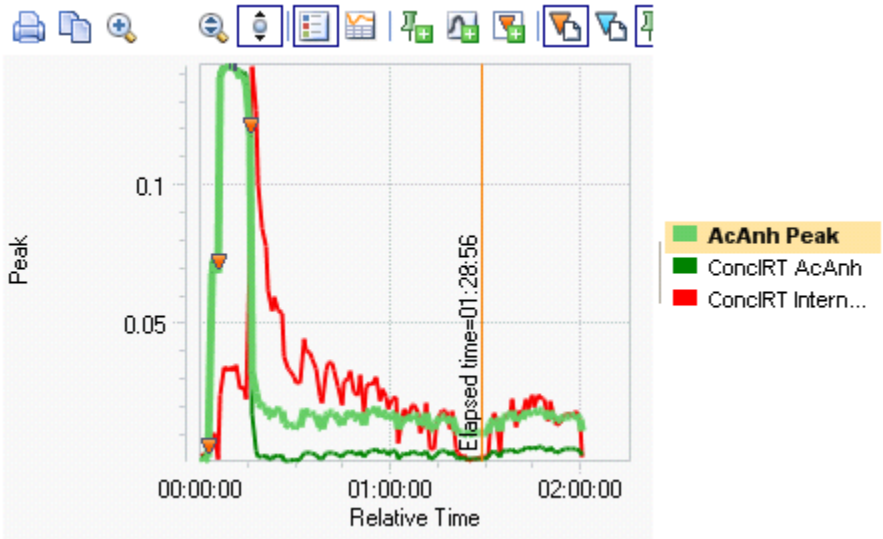
When autoscale is enabled, the y-axis is automatically autoscaled. The x-axis is the only portion of the graph that is selectable by the user.

AutoScale is intended to be used to visually compare the shape of a peak in two different spectra where the peak height in one spectrum is much smaller than in the other spectrum.

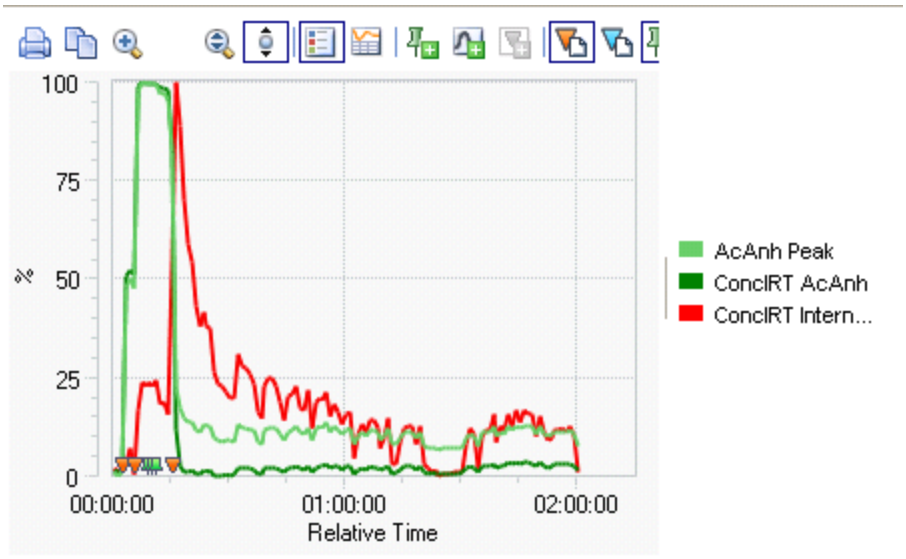
When the Autoscale button is clicked, the Y axis is scaled based on the selected plot in the graph. The remaining plots are scaled to their Y axis extents. The units used for the Y axis is the axis for the selected plot. For example, when autoscaled is enabled for the following graph,



The Y axis is autoscaled based on the selected plot.

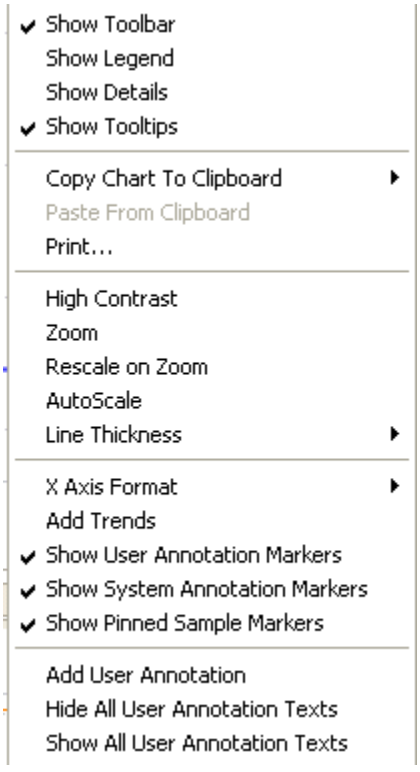


If no plots are selected, autoscaling uses the first plot in the graph as the basis and uses a Y axis scale of 0-100%.



The Trend Context Menus

The Trend Viewer display incorporates two right-click or context menus that contain tools for customizing the displayed data. The menu is displayed when the user right-clicks on the data area of the display.



The context (right-mouse click) menu contains the following items.

Show Toolbar	Displays the toolbar at the top of the display. 

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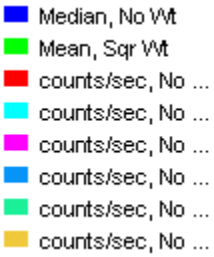
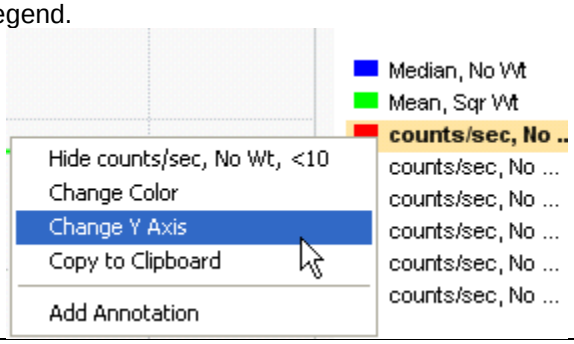
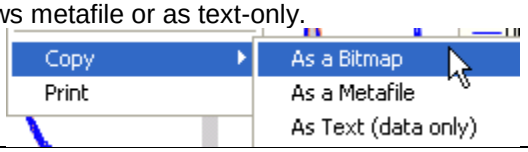
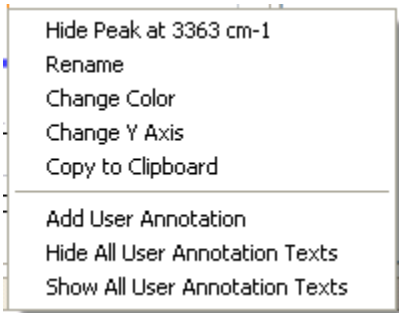
	The toolbar contains the following tools.  Prints the display.  Copies the display to the clipboard.  Zooms the display.  This button is only visible when the Zoom function is enabled. The button resets the zoom to its original scale.  Rescales only the X-axis on zoom.  Auto scales the Y-axis.  Displays the Legend Panel.  Displays the Details Panel.  Pins the spectra selected in the Event Viewer to the Spectra Viewer. Clicking the button when Spectra Viewer is already pinned, unpins those spectra. This tool can be used to add spectra from the Event Viewer to the spectra list.  Adds a Reference Trend to the graph. Clicking the button opens the Select Trend dialog.  Adds an annotation at the active point in the trend  Displays user-generated annotations on the graph.  Displays system generated annotations on the graph.  Displays all pinned sample markers.
Show Legend	Displays a legend box which lists each trend and its name.  The Legend also contains a context menu that allows the user to perform some of the functions discussed in this section. To access the menu right-click on the legend. 
Show Details	Displays information about the trends and allows access to hide and show options.

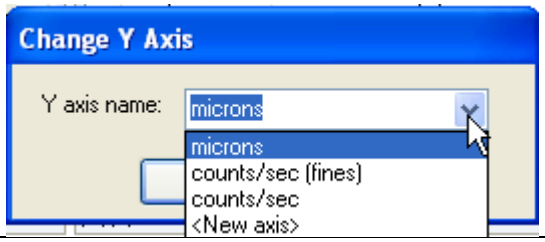
Copy to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
Paste from Clipboard	Pastes the contents of the clipboard into the trend graph.
Print	Opens the Print dialog to print the display.
High Contrast	Displays the graph with a black background.
Zoom	Zooms the display. Refer to Trend Profiles Zoom Operation.
Reset Zoom	Resets the zoom to its original scale.
Rescale on zoom	Rescales only the X-axis on zoom.
Auto-scale	Auto scales the Y axis.
Line Thickness	Selects the line thickness for the plots.
X Axis Format	Allows the user to change the format of the X axis as follows: • Record or Sample Number • Actual time of the measurement • Relative time (elapsed time during the experiment
Add Trends	Allows the user to add trends from open Experiments and Result Sets.
Show User Annotation Markers	Displays user-generated annotations on the graph.
Show System Annotation Markers	Displays system generated annotations on the graph.
Show Pinned Sample Markers	Displays all pinned sample markers.
Add Annotation	Adds a new annotation to the event log.
Hide All User Annotation Texts	Hides the text on user annotations. The marker is still displayed.
Show All User Annotation Texts	Displays the text in user annotations next to the marker. The text can be moved by dragging it to a new location.

If the user right-clicks on a trend line in the graph, another context menu is available.



The context (right-mouse click) menu contains the following items.

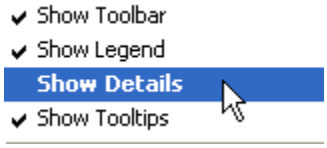
Hide . . .	Hides the selected trend.
Rename	Allows the user to rename the trend.
Change Color	Opens a color browser to change the color of the trend line.

Change Y Axis	Opens a dialog that allows the user to change the format of the Y axis. 
Copy to Clipboard	Copies the trend data to the clipboard as tab-delimited text.
Add Annotation	Adds an annotation to the to the trend point. Refer to Adding an Annotation.
Hide All User Annotation Texts	Hides the text on user annotations. The marker is still displayed.
Show All User Annotation Texts	Displays the text in user annotations next to the marker. The text can be moved by dragging it to a new location.

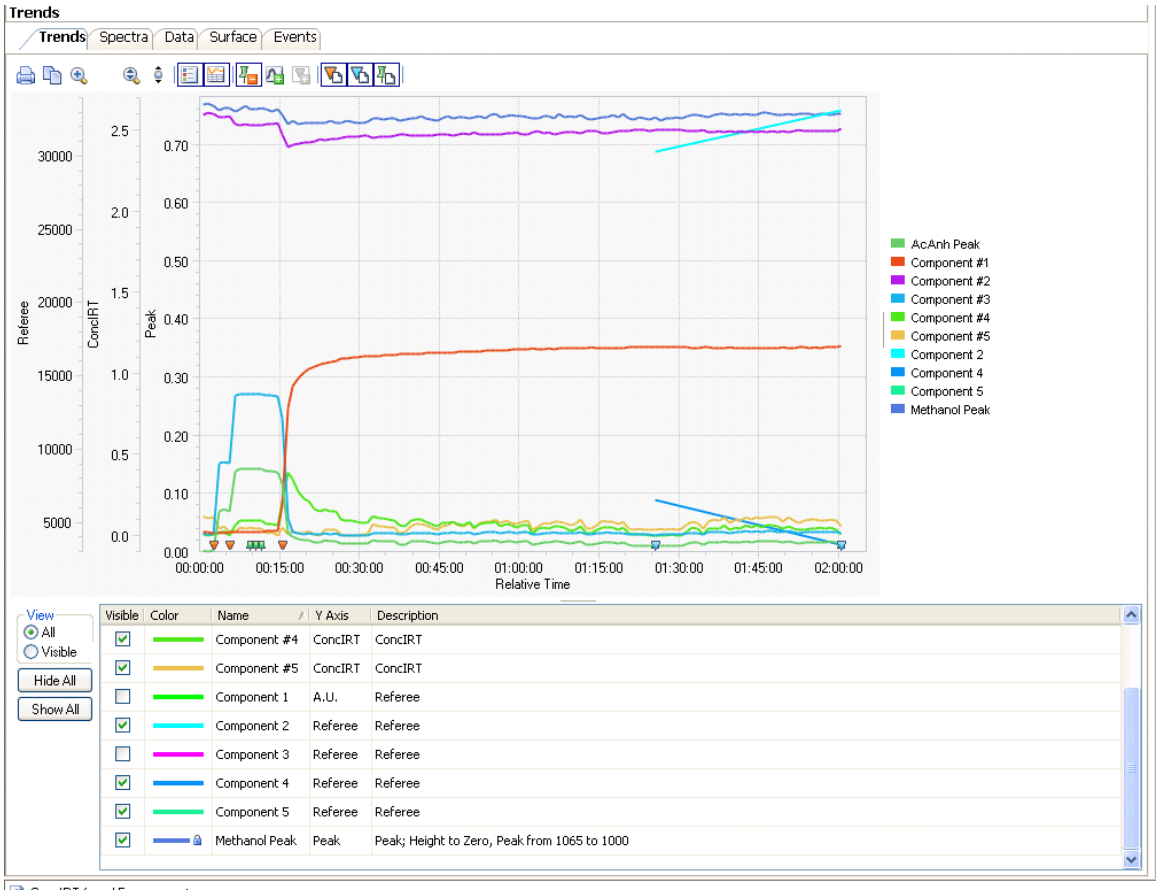
The Trend Details Panel

The **Details panel offers** a Detail list of current trends along with the value and source.

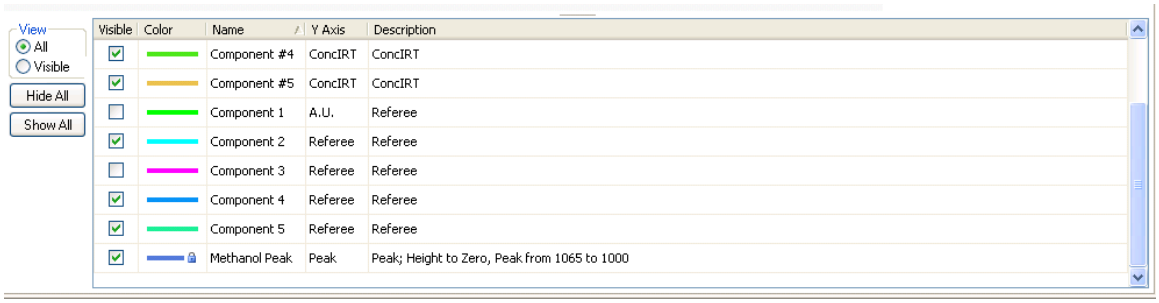
The Trend Details is displayed by either clicking on the detail button in the toolbar menu of the trend viewer, or placing the cursor on the trend viewer and double-clicking on it, which displays the corresponding trend along with the Trend Detail or by right-clicking on the trend plot area and then selecting the Show Details option.



Selecting the **Visible** checkbox displays the corresponding component as shown in the display below.



The Trend Details Panel allows the user to customize the trends in the viewer.



The **View** radio buttons are used to determine which trends are displayed on the graph. The All button displays all the trends in the trend list. When the **All** button is selected, the **Visible** checkboxes are used to select which trends are displayed. The **Hide All** button hides all visible data in the graph. The **Show All** button displays all visible data in the graph. The **Visible** checkboxes must be rechecked to view the spectra again.

Clicking on the **Y Axis** of a trend allows the user to select another Y axis to apply for the trend. The axis is selected from a droplist of available axes.

As a trend is selected, its Y axis legend moves to the left most position on the graph.

Changing the X Axis

The **X-axis** displays the trends either by:

Record or Sample Number

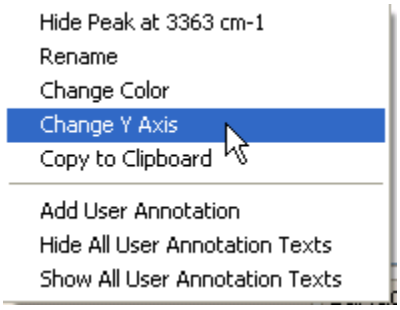
Actual time of the measurement

Relative time (elapsed time during the experiment

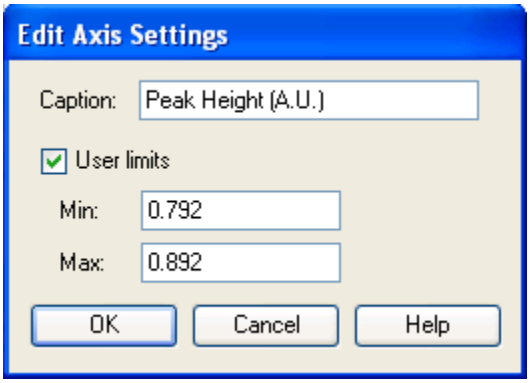
The **X-axis** is changed using a context menu activated when the cursor is right-clicked in the axis area.

Changing the Y Axis

The **Y-axis** can be changed to display different measurement units and scale through the use of a context menu. To access the menu, right-click on the graph area of the Trend Viewer.



The **Axis Settings** dialog is opened.

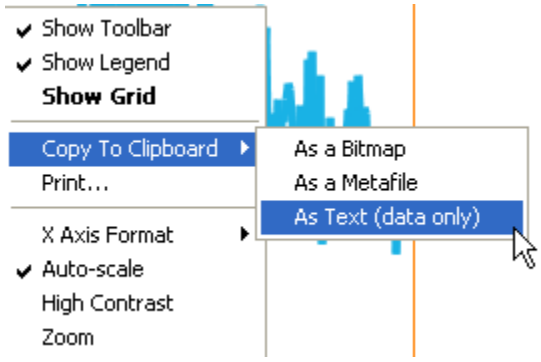


The dialog allows the user to enter a caption to use for the axis and to customize the min/max limits of the scale.

Copying Trend Data

Trend data can be copied to the Windows clipboard for use by other applications. The trend Viewer context (right-click) menu offers three copy functions for copying trend data.

- Bitmap – Copies the trend data as a bitmap (BMP) graphic file.
- Metafile – Copies the trend data as a Windows metafile (WMA) graphic file.
- Text – Copies the trend data as text. See the explanation below for a description of the textual format.



Copying Textual Trend Data to the Clipboard

When trend data is copied as textual data, the data is copied as tab delimited text. The format is illustrated below.

Time	Peak 6	Peak 13	Peak 14	Peak 15	Peak 16	Peak 17	Peak 18	Peak 19	Peak 20
00:02:05	0.867969	0.702798	0.24761	0.730396	0.178003	0.730396	0.0197286	0.0197286	0.298329
00:03:12	0.875022	0.700014	0.255044	0.745957	0.178498	0.745957	0.0280828	0.0280828	0.299953
00:04:19	0.809596	0.570456	0.560993	0.809596	0.162158	0.809596	0.276688	0.276688	0.29136
00:05:26	0.678432	0.470314	0.541923	0.678432	0.135537	0.678432	0.273884	0.273884	0.248191
00:06:33	0.637818	0.439062	0.517107	0.637818	0.125919	0.637818	0.261518	0.261518	0.231959
00:07:40	0.629253	0.433582	0.516048	0.629253	0.123884	0.629253	0.260199	0.260199	0.229347
00:08:47	0.627265	0.435176	0.518325	0.627265	0.124412	0.627265	0.260782	0.260782	0.230129
00:09:53	0.63284	0.440519	0.523852	0.63284	0.125392	0.63284	0.263767	0.263767	0.233211
00:11:00	0.645943	0.449623	0.535437	0.645943	0.128811	0.645943	0.269503	0.269503	0.238239
00:12:07	0.653781	0.457296	0.540745	0.653781	0.129734	0.653781	0.272924	0.272924	0.242323
00:13:13	0.658348	0.46302	0.547237	0.658348	0.130758	0.658348	0.275561	0.275561	0.245428
00:14:20	0.659227	0.461123	0.548293	0.659227	0.131023	0.659227	0.27593	0.27593	0.244629
00:15:27	0.655334	0.460125	0.545789	0.655334	0.129225	0.655334	0.273975	0.273975	0.243746
00:16:34	0.653815	0.458459	0.544491	0.653815	0.128305	0.653815	0.273049	0.273049	0.242936
00:17:40	0.651515	0.457564	0.543559	0.651515	0.128063	0.651515	0.271794	0.271794	0.242323
00:18:47	0.650269	0.456792	0.542892	0.650269	0.127905	0.650269	0.271136	0.271136	0.241926
00:19:54	0.62199	0.431866	0.519143	0.62199	0.119888	0.62199	0.256851	0.256851	0.227805
00:21:01	0.607383	0.420059	0.505784	0.607383	0.115383	0.607383	0.249794	0.249794	0.22096
00:22:07	0.604537	0.418337	0.503586	0.604537	0.114097	0.604537	0.24835	0.24835	0.220101
00:23:14	0.603749	0.41766	0.50202	0.603749	0.113787	0.603749	0.247669	0.247669	0.219756
00:24:21	0.599477	0.416067	0.499853	0.599477	0.112387	0.599477	0.246095	0.246095	0.218779
00:25:27	0.587144	0.405536	0.489012	0.587144	0.108986	0.587144	0.240034	0.240034	0.212861
00:26:34	0.581335	0.401462	0.485359	0.581335	0.107646	0.581335	0.237544	0.237544	0.21078
00:27:41	0.578652	0.400036	0.483484	0.578652	0.106979	0.578652	0.236497	0.236497	0.209917
00:28:48	0.576381	0.399327	0.481395	0.576381	0.10581	0.576381	0.235389	0.235389	0.209503
00:29:54	0.579418	0.399224	0.482206	0.579418	0.107649	0.579418	0.236244	0.236244	0.209669
00:31:01	0.571706	0.394537	0.476954	0.571706	0.10482	0.571706	0.232781	0.232781	0.206835
00:32:08	0.563354	0.388495	0.469971	0.563354	0.102829	0.563354	0.229203	0.229203	0.20355
00:33:14	0.563886	0.387179	0.469147	0.563886	0.10296	0.563886	0.228784	0.228784	0.202869
00:34:21	0.558435	0.384483	0.465884	0.558435	0.101107	0.558435	0.226431	0.226431	0.201303
00:35:28	0.558826	0.384137	0.465394	0.558826	0.101222	0.558826	0.226324	0.226324	0.201127
00:36:35	0.56047	0.384143	0.465325	0.56047	0.101346	0.56047	0.226667	0.226667	0.201082
00:37:41	0.559457	0.383615	0.465086	0.559457	0.100525	0.559457	0.226168	0.226168	0.200952
00:38:48	0.55812	0.383204	0.464709	0.55812	0.100087	0.55812	0.225618	0.225618	0.200668
00:39:55	0.557976	0.383459	0.465431	0.557976	0.100515	0.557976	0.225516	0.225516	0.200838
00:41:01	0.556714	0.38341	0.464674	0.556714	0.100007	0.556714	0.225193	0.225193	0.200725
00:42:08	0.558274	0.383404	0.464874	0.558274	0.100155	0.558274	0.225134	0.225134	0.200702
00:43:14	0.557738	0.383493	0.46449	0.557738	0.0999746	0.557738	0.225282	0.225282	0.200755

If the Trend Viewer contains data that were sampled at different time intervals, the format of the exported data varies depending upon which trend is selected, as explained below.

If a trend is selected in the Trend Viewer when the user selects the Copy function, iC IR exports the raw values for all the visible trends based on the set of timestamps associated with the selected trend. Note that in a typical experiment all the trends have the same timestamps, so data is copied without manipulation.

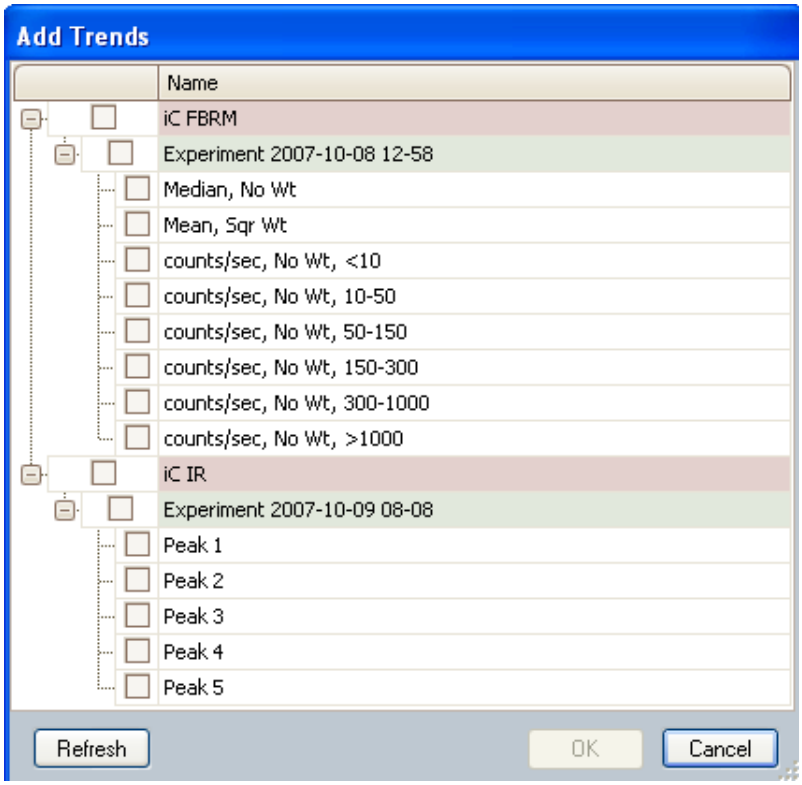
For the more complex case in which there are multiple sets of timestamps to deal with, interpolation is used on those trends with different timestamps to estimate the value at each timestamp in the selected trend. In this case the selected trends data is copied 'as is" since its timestamp is used as the master. Trends with different timestamps will have their data copied as interpolated data.

If there is no selected trend when the copy function is executed, the Trend Viewer creates a composite set of timestamps combining together ALL the timestamps for all the trends and then eliminates any duplicates. Timestamps that vary by less than second are also eliminated.

Interpolation based on the timestamps of the selected trend is useful for analyzing data collected across multiple experiments. On the other hand, to export the most complete data set when multiple sets of timestamps are involved, make sure that no trend is selected. That way, all the actual data points for each trend plus additional interpolated values are copied. To deselect all trends, click outside of the actual graph area in the Trend Viewer. This will de-select any selected trends.

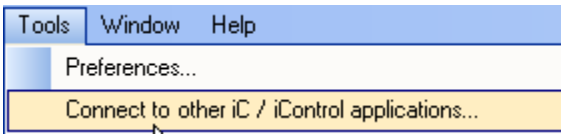
Sharing Trend Data with Other iC/iControl Applications

iC applications and iControl have the ability to share trend data with other applications in the iC software family. If the iC applications are running on the same PC, trend data from all open experiments in all running iC applications will automatically appear in the Result List Add Trends dialog for all the iC applications. This feature is useful for comparing trend data from various types of instrumentation. It should be understood that care must be taken when comparing trends from different types of instrumentation.

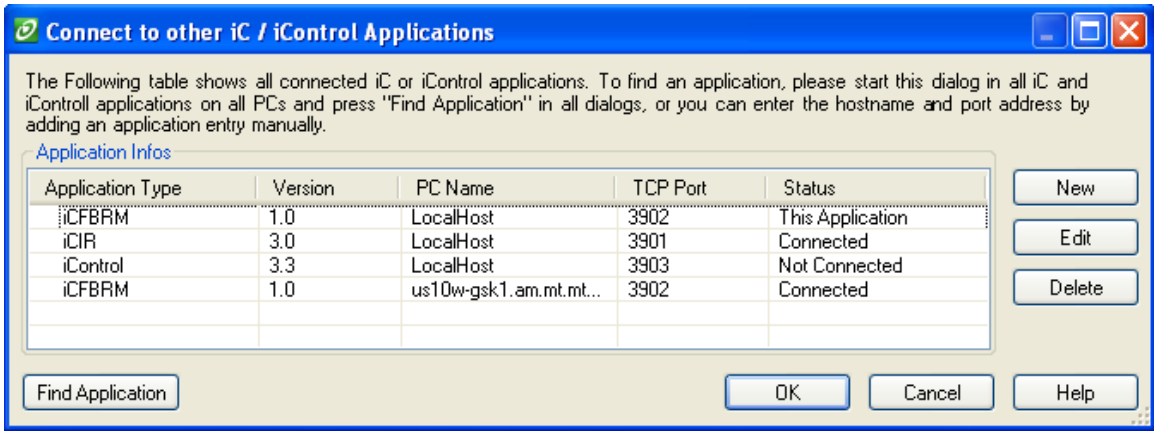


The Connect to Other iC/iControl Applications Dialog

For iC applications running on different PCs on the same network, the iC applications must first connect to one another. Connections to other iC application running on different PC is performed using the **Connect to other iC/iControl Applications** option on the Tools menu.



Clicking this option, opens the Connect to other iC/iControl Applications dialog.



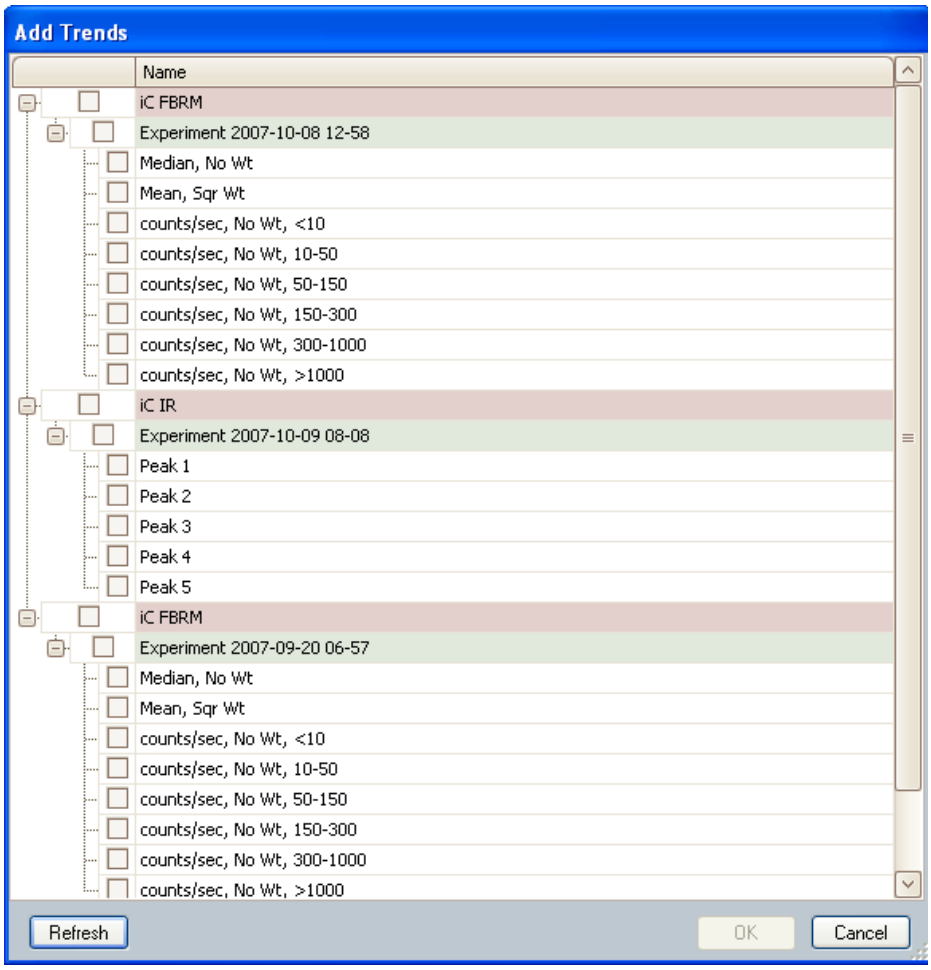
The user next clicks the **Find Applications** button to initiate a scan for other iC applications on the network. The user initiates this scan on all the PCs that will be sharing data. When the scan starts, these PCs will broadcast iC application identity information on the network and each PC will receive the broadcast and compile a “phone book” file containing the identity of other iC applications on the network. These PC and their respective iC applications will be populated in the Application Type list of the dialog.

Once this initial scan is performed the Application Type list automatically contains all iC applications running on the network.

There is no need to rescan all the network PCs in the future unless a new iC application or PC running iC applications is added to the network. In this case, a scan must be run on all PCs to update the “phone book” file.

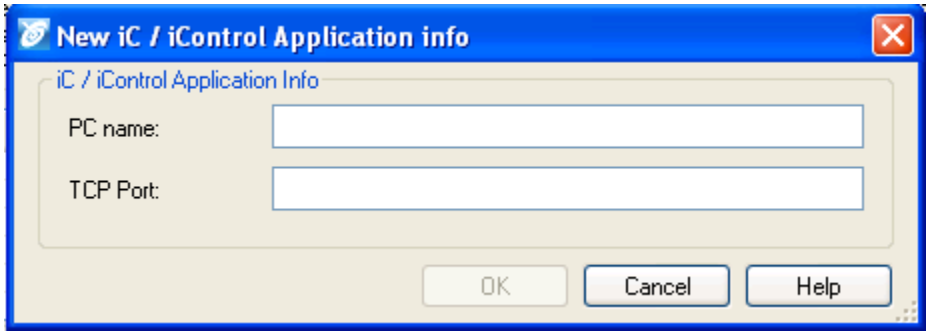
Once communications between the iC applications has be established, trend data for the applications is displayed in the Result List Add Trends list.

Note: Any PCs that will be coordinating live experiments should have the same regional settings and be in the same time zone.

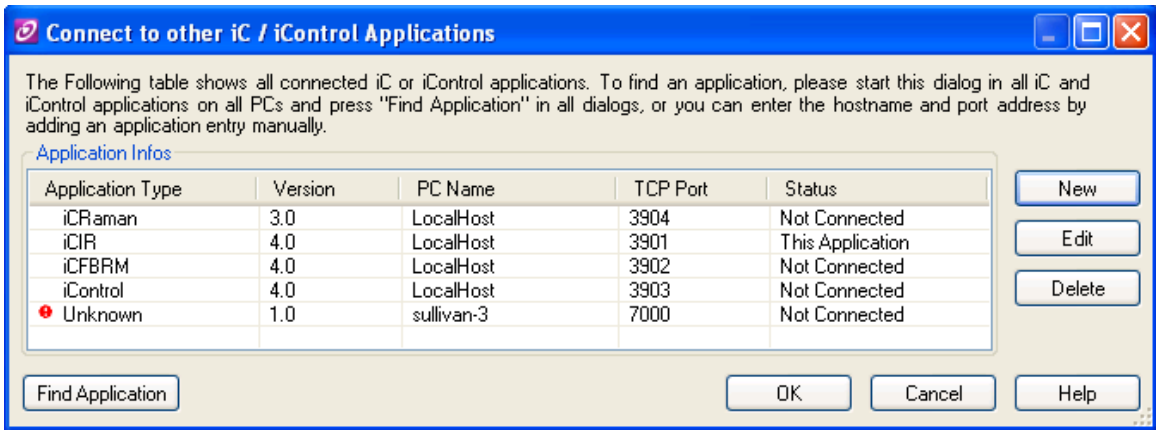


Defining a New Connection

A new application can be manually defined by clicking the **New** button on the Connect to other iC/iControl Applications dialog. The New iC/iControl Applications dialog is opened.

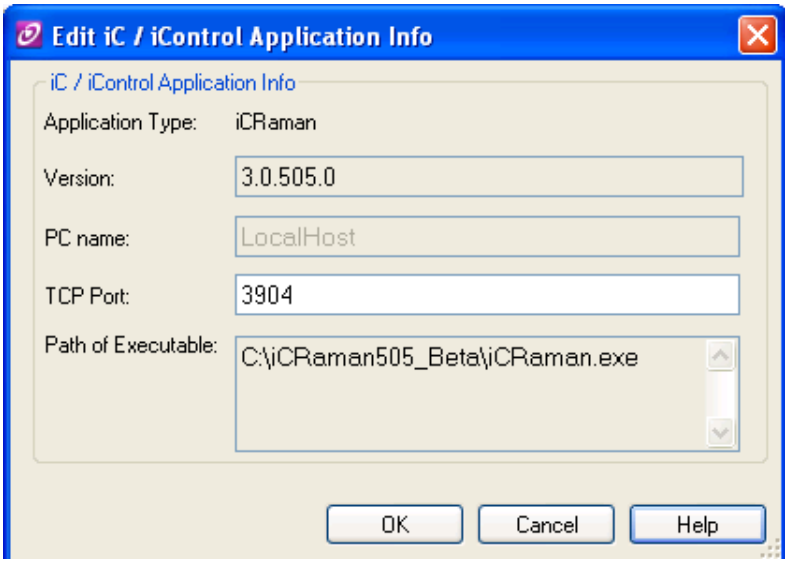


The user enters the network name for the PC and the port number that the application uses. When the **OK** button is clicked, the system verifies the connection to the application. If a connection cannot be made to the application, an error is displayed on the Connect to other iC/iControl Applications dialog.



Editing iC/iControl Application Info

The user can edit the port number for a application connection by clicking the Edit button on the Connect to other iC/iControl Applications dialog. The Edit iC/iControl Application Info dialog is opened. The dialog contains information about the application and has one editable field, TCP Port. Normally the TCP Port is auto-detected when the system scans for applications. If a port needs to be changed for some reason, the new port number can be edited here. When the **OK** button is clicked, the TCP Port is verified by the system.



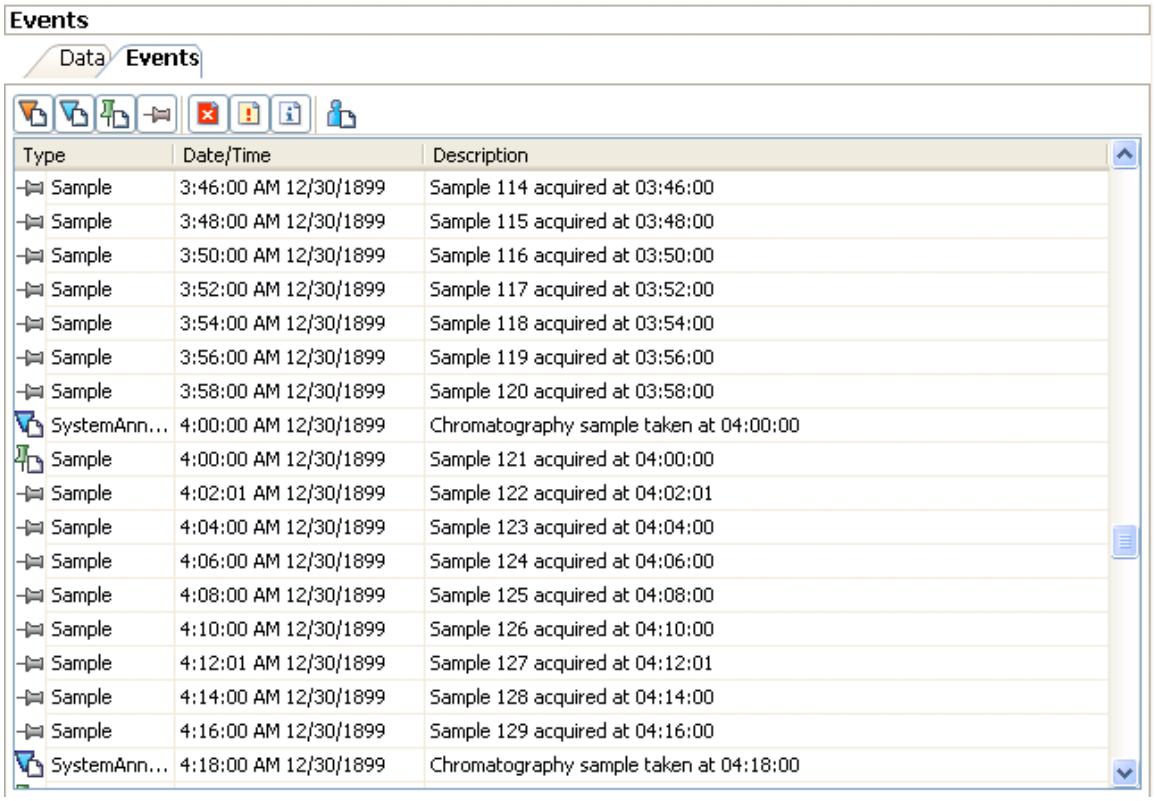
Event Viewer

The Event Viewer collects the time each sample spectrum was taken during an experiment. When the user clicks a sample in the list, the sample is displayed in the Spectra display.

The Event Viewer is a log of various events including:

- Annotations made by the user
- System messages including Pause and Resume actions
- Error and warning messages
- Audit events
- Sample events that record the date and time a sample was taken

IMPORTANT: Observations about an experiment can be added to the Event Viewer during an experiment by right-clicking on a row in the Event Viewer or by using The Live Experiment Toolbar. It is very important to note changes in the reaction conditions in the Event Viewer (i.e., changed stir rate, added 10 mg of material, solids being formed, instrument indicates 80% conversion).



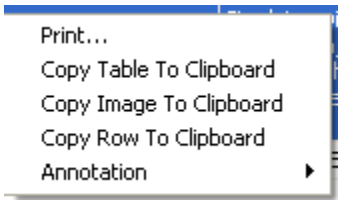
Multiple items can be selected in the Event Viewer using the Ctrl key (for individual), or Shift+Ctrl keys (for a range). When multiple items are selected, the user can pin or unpin the samples using the context menu.

Event Viewer Context Menu

The Event Viewer incorporates a right-click or context menu that contains an option for copying the contents of the viewer to the clipboard. The data can be copied as:

- A table of all events
- The table of events as an image
- Copy the selected row as text

A Print option can be used to print the contents of the display to a local or network printer.



Event Viewer Toolbar

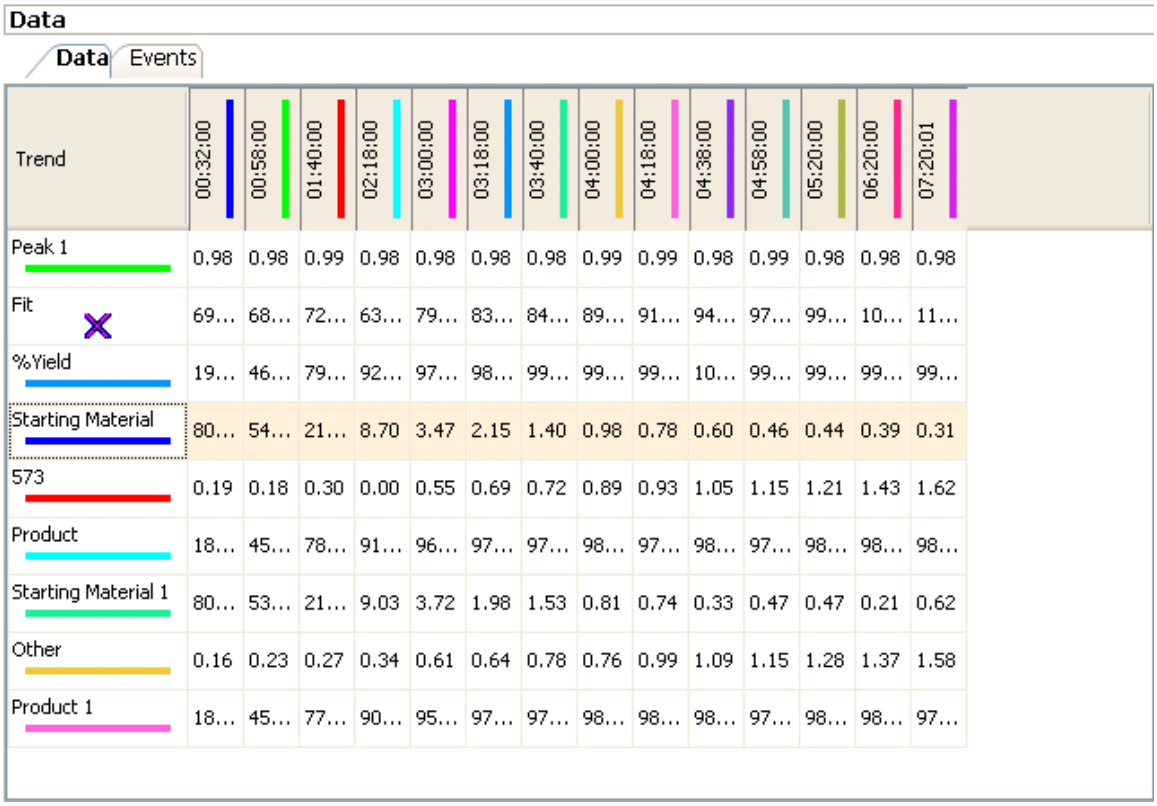
The Event Viewer contains a toolbar that provides filters for selecting which type of messages will be displayed. The toolbar contains the following filters.

	Prints the contents of the display.
	Copies the table to the clipboard.
	Displays all user messages
	Displays all system messages
	Displays all pinned system messages
	Displays all unpinned sample messages
	Displays all error messages
	Displays all warning messages
	Displays all informational messages
	Displays all audit messages

Note that the filters can be used in combination to provide a log suited to the users individual requirements.

Data Viewer

The Data Viewer collects the time each sample was taken and the value for each loaded sample.



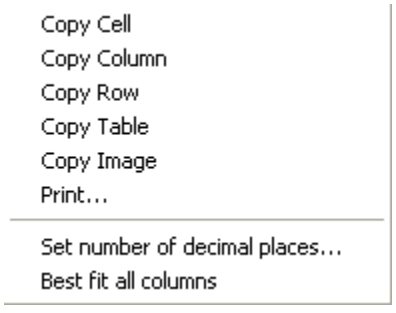
Trend	00:32:00	00:58:00	01:40:00	02:18:00	03:00:00	03:18:00	03:40:00	04:00:00	04:18:00	04:38:00	04:58:00	05:20:00	06:20:00	07:20:01
Peak 1	0.98	0.98	0.99	0.98	0.98	0.98	0.98	0.99	0.99	0.98	0.99	0.98	0.98	0.98
Fit	69...	68...	72...	63...	79...	83...	84...	89...	91...	94...	97...	99...	10...	11...
%Yield	19...	46...	79...	92...	97...	98...	99...	99...	99...	10...	99...	99...	99...	99...
Starting Material	80...	54...	21...	8.70	3.47	2.15	1.40	0.98	0.78	0.60	0.46	0.44	0.39	0.31
573	0.19	0.18	0.30	0.00	0.55	0.69	0.72	0.89	0.93	1.05	1.15	1.21	1.43	1.62
Product	18...	45...	78...	91...	96...	97...	97...	98...	97...	98...	97...	98...	98...	98...
Starting Material 1	80...	53...	21...	9.03	3.72	1.98	1.53	0.81	0.74	0.33	0.47	0.47	0.21	0.62
Other	0.16	0.23	0.27	0.34	0.61	0.64	0.78	0.76	0.99	1.09	1.15	1.28	1.37	1.58
Product 1	18...	45...	77...	90...	95...	97...	97...	98...	98...	98...	97...	98...	98...	97...

The Right and Left arrow keys can be used to step through the columns one column at a time. The Up and Down arrow keys can be used to step through the rows one row at a time.

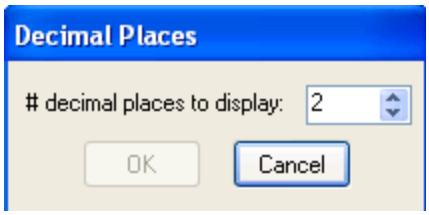
Data Viewer Context Menus

The Data Viewer incorporates several right-click or context menus.

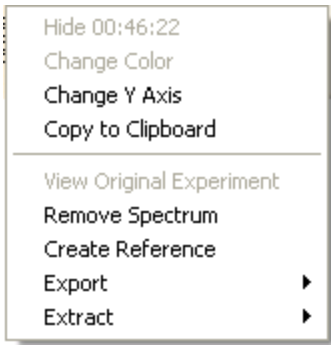
Right-clicking in a data cell opens a menu that contains an option for copying the contents of the viewer to the clipboard as text. Options are available to copy a single selected cell, row column or the entire table.
A Print option can be used to print the contents of the display to a local or network printer.



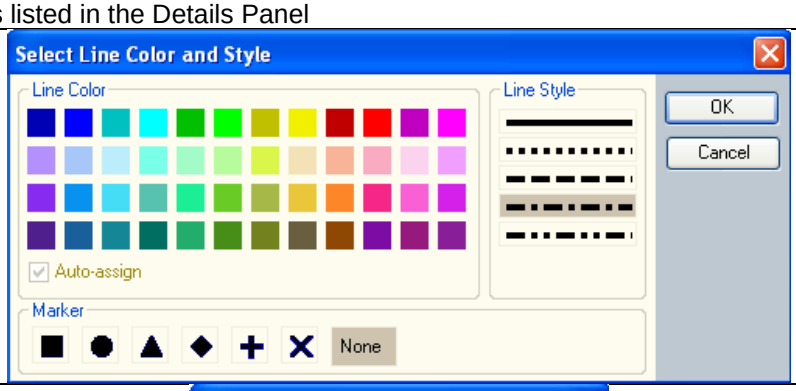
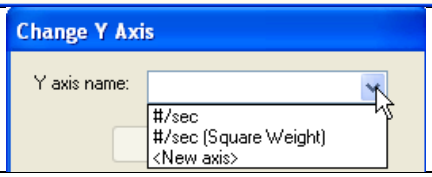
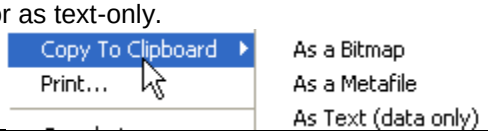
An additional option is available to set the number of decimal places that are displayed. The setting of this option affects every cell in the table.



Right-clicking on a trend heading opens another context menu allows the format of the data to be edited.

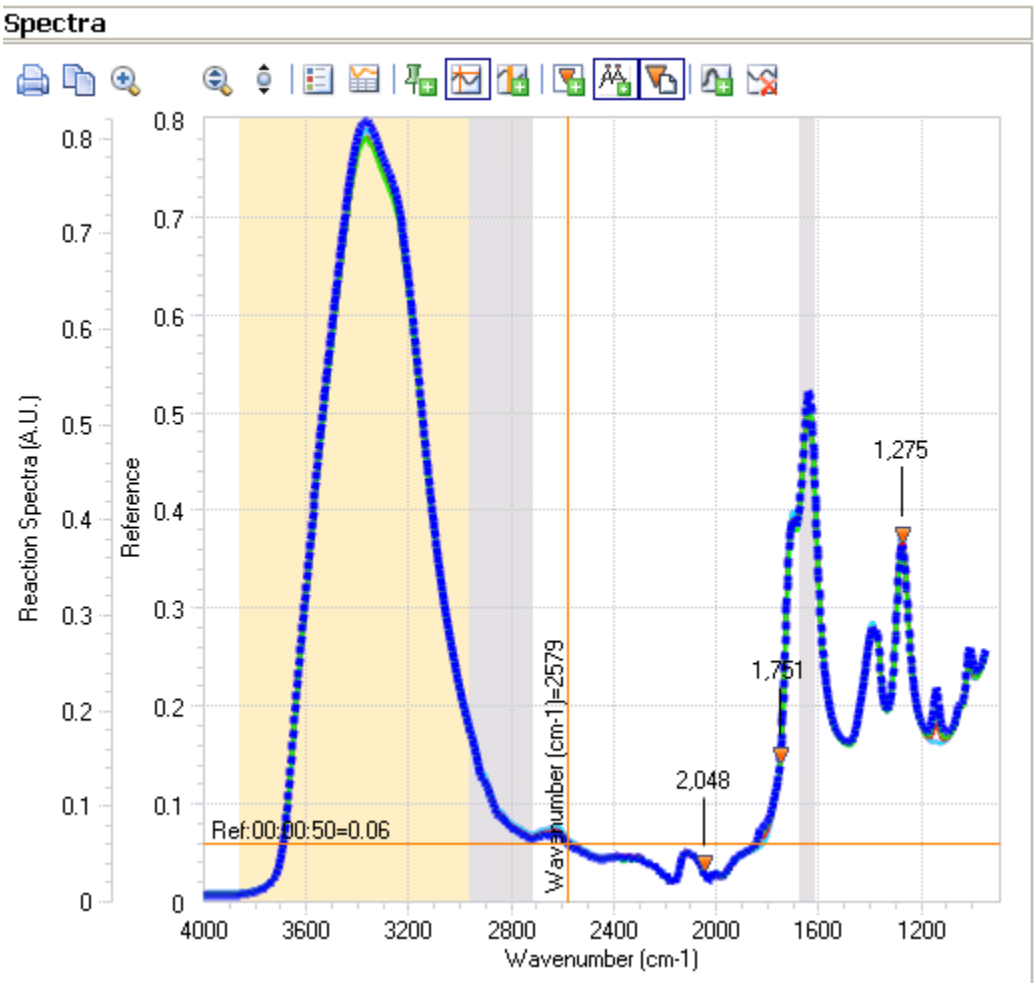


The menu contains the following options.

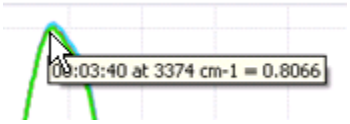
Show/Hide . . .	Shows or Hides the selected data. The data is hidden in the graphic area but remains listed in the Details Panel
Change Color	
Change Y Axis	
Copy to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
Remove Spectrum	Permanently removes the selected spectrum from the viewer. If the spectrum is a reference, a confirmation dialog is displayed before the spectrum is removed.
Create Reference	Designates the selected spectrum as a reference.
Export	Exports the selected spectra to a file. The user has the option of exporting only the selected spectra or all pinned spectra.
Extract	Allows the user to extract the background or single beam from the selected spectra.

Spectra Viewer

Reaction spectra from the experiment are shown in the Selected Spectra display. If the ConcIRT LIVE analysis feature is enabled, component spectra from the analysis are also shown in this display.



When the mouse hovers over any point in a spectrum, a tooltip shows the time, wavenumber (X axis) and absorbance (Y axis) for the point under the cursor.



The Spectra Display also allows you to create and edit peak definitions.

Working with Peak Definitions

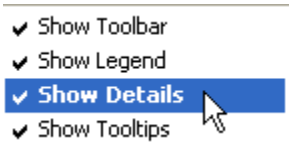
Peaks, by default, are automatically named with the center wave number of the peak. The user can rename peaks by clicking on the peak name in the Details panel and editing it.

Peaks can be selected in the Spectra Viewer using several techniques:

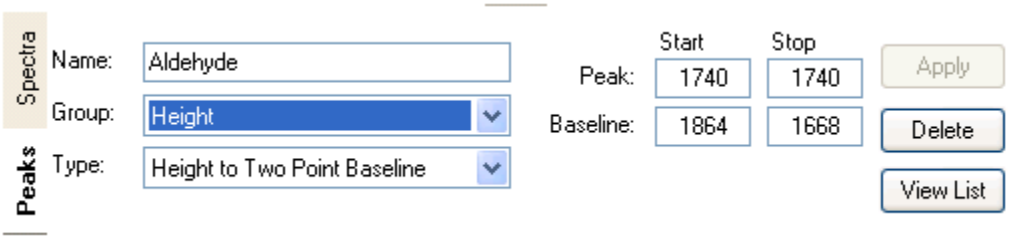
- Directly clicking on the peak in the Spectra Viewer.
- Click on a trend in the Trend Viewer. The corresponding peak is selected in the Spectra Viewer.
- Click on a peak in the Data Viewer. That peak is selected in the Spectra Viewer.
- Selecting the peak in the Surface Viewer.

It is often helpful to define the peak height as calculated relative to a baseline point.

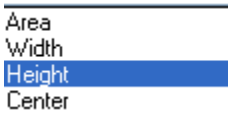
To change the peak type, first ensure the Show Details option is checked in the context right-click) menu.



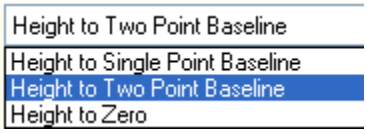
Next, click on the peak in the viewer. The grid displays the properties for the peak.



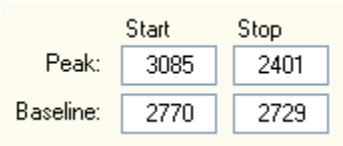
Select the desired functional group from the droplist in the Group field.



Select the desired peak type from the droplist in the Type field. Note that the options in the droplist will change depending on the group specified in the Group Field.



If a baseline type is selected, the baseline is specified in the Baseline fields.



Adding a new peak can be done in the following ways:

- Double-clicking under the peak adds the peak and calculates the start/end range
- Double-clicking above the peak creates a single wavenumber peak.
- Set the crosshairs to the desired peak position and do one of the following: a) click the New button in the Details panel (inside the Peak tab) b) click the New Peak toolbar button and c) Right-click in the chart and select the New Peak item in the context menu.
- To copy a peak definition from another experiment, click the **Add...** button in the Details panel. The other experiment must also be open in iC IR.

Graphically Editing a Peak Definition

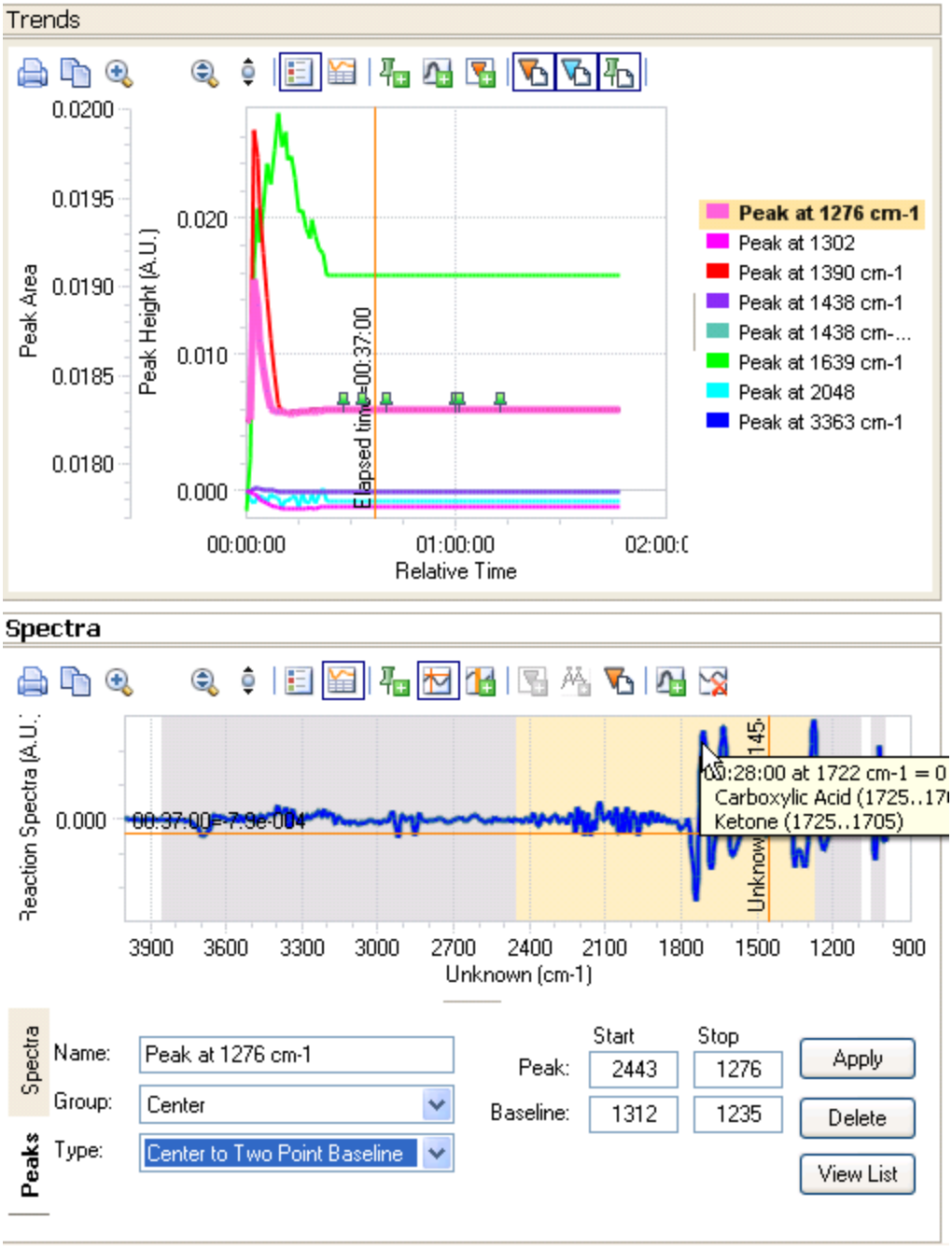
The peak region defined above can be moved, enlarged and reduced in width using the cursor. The default profiling technique is 'height to zero'. This will plot the maximum absorbance value within the defined box for each spectrum in the data set. Thus, a shifting peak will be able to be tracked appropriately.

If the peak name was auto-generated and the peak location is changed, the new peak location is reflected in the peak name.

Place the cursor over the peak you wish to change, when the cursor changes to a hand, move the highlighted region by dragging it, (clicking with the cursor on the peak and moving the mouse).

Enlarge or reduce the width of the peak by dragging the edge open or closed.

The peak dimensions change in the peak list, the highlighted yellow peak changes in size as well as position and the trend lines also change.



To rename a peak, double-click on the Peak Name field and type the new name in the field.

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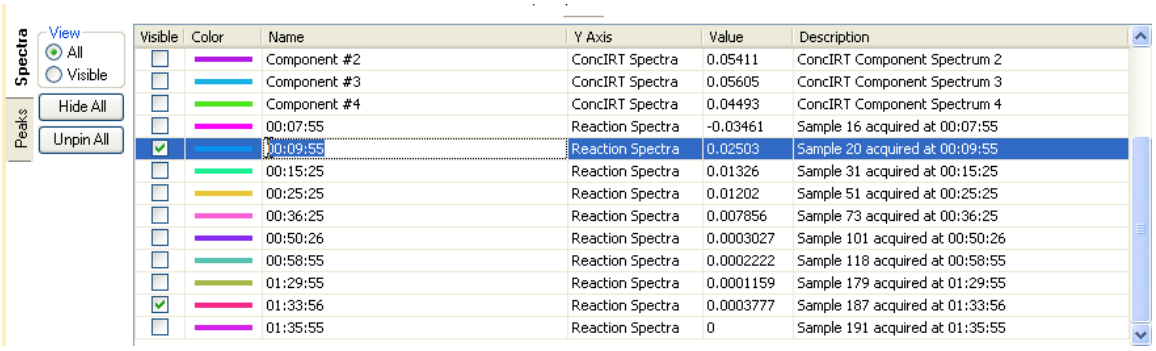
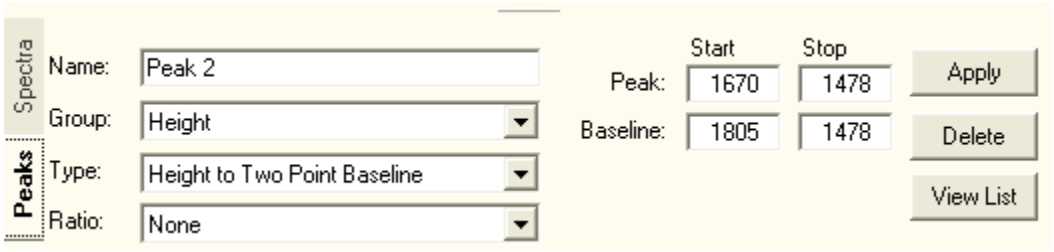
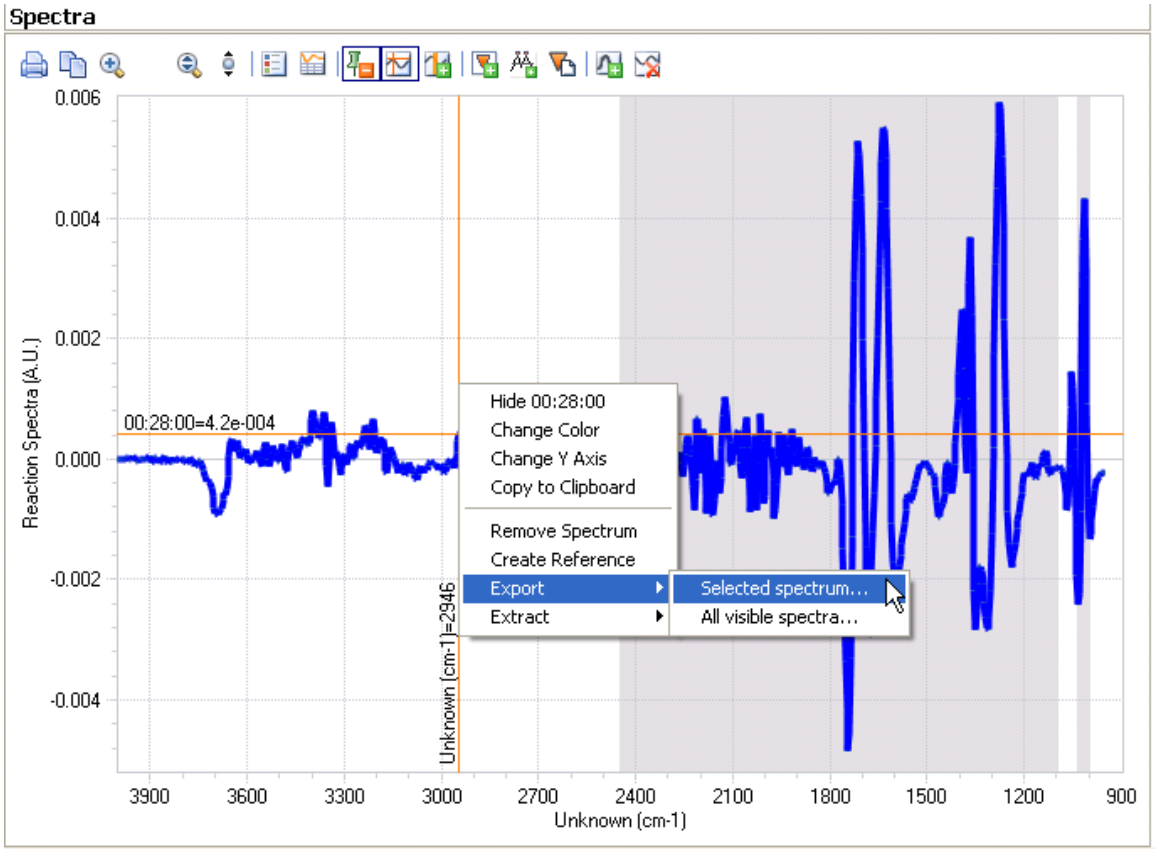


To change a peak type, double-click on the peak in the Peak Profile List and select the new peak type from the droplist in the peak properties panel.

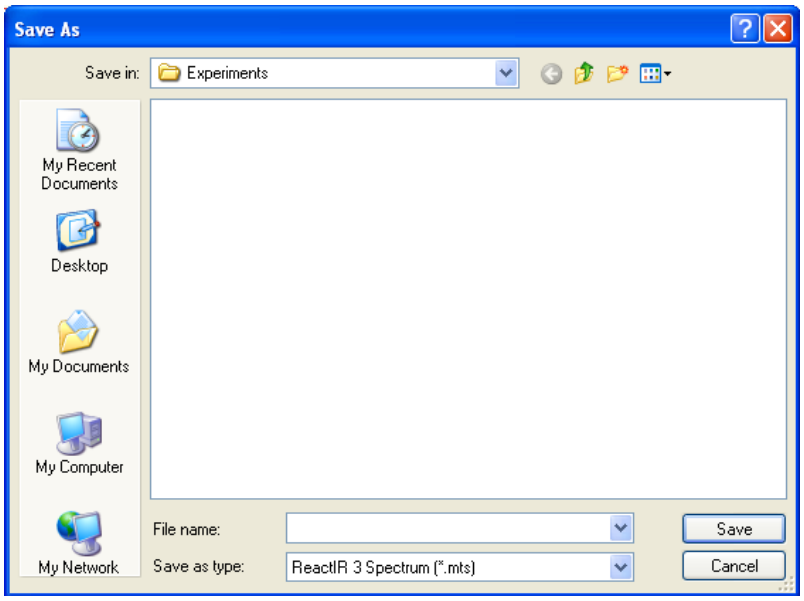


Exporting a Spectrum

By right-clicking on a spectrum in the Spectra Viewer, you have the option to export it as a .mts file for use with ReactIR 3.0.



There are two export options available, to export the selected spectra or to export all spectra that are pinned. A standard Windows “Save As . . .” browser is opened to allow the user to select a path/filename for the exported spectra.



The spectra can be saved in a ReactIR 2 or ReactIR 3 format.

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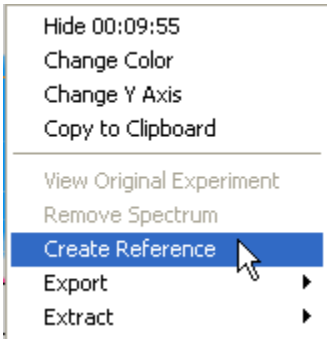
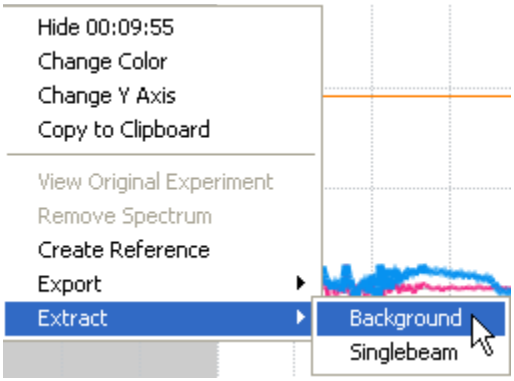
Creating a Reference Spectrum from the Spectra Viewer

You can create reference spectra from reaction spectra. Instead of collecting a solvent reference spectrum before you start your experiment, you can just right-click on the first reaction spectrum (which would contain pure solvent only) and select the option to Create Reference. The solvent is now immediately available for spectrum subtraction. The spectra is displayed on the graph.

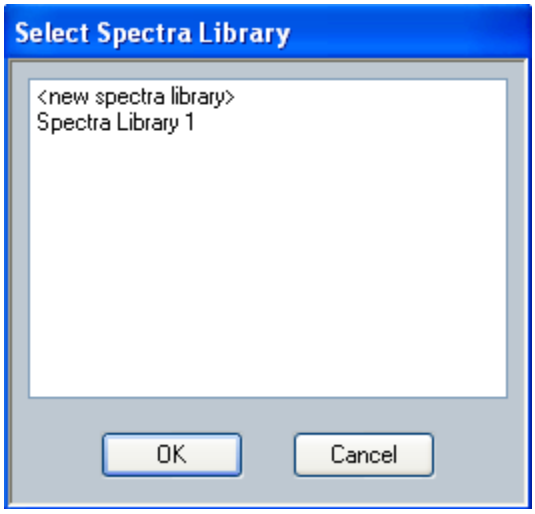


Extracting Spectra

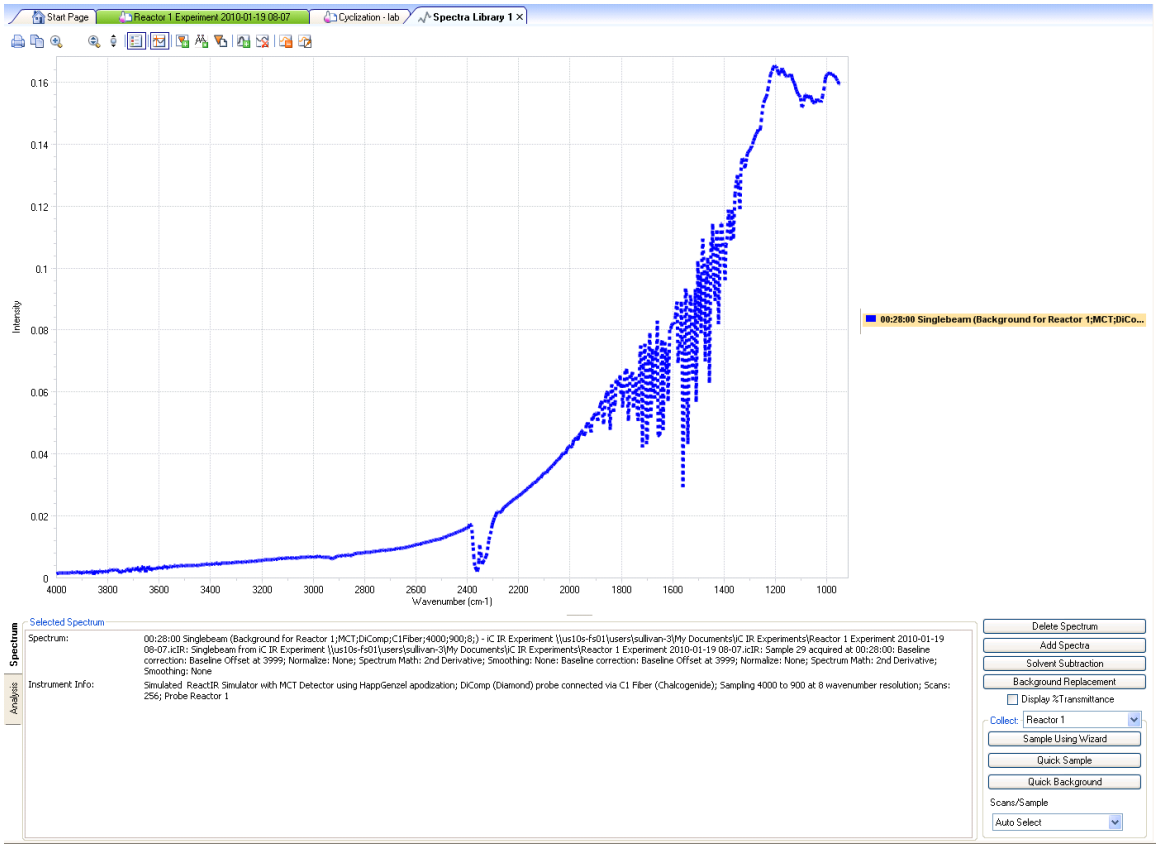
Spectra can be extracted and displayed in a Spectra Library by right-clinking on a spectra and selecting the Extract option.



The spectra can be extracted as a single beam or as a reference spectra. The spectra is extracted to a Spectra Library. If there are existing Spectra Libraries, the user is prompted to select which library should contain the spectra.



The spectra is extracted and the Spectra Library is displayed.



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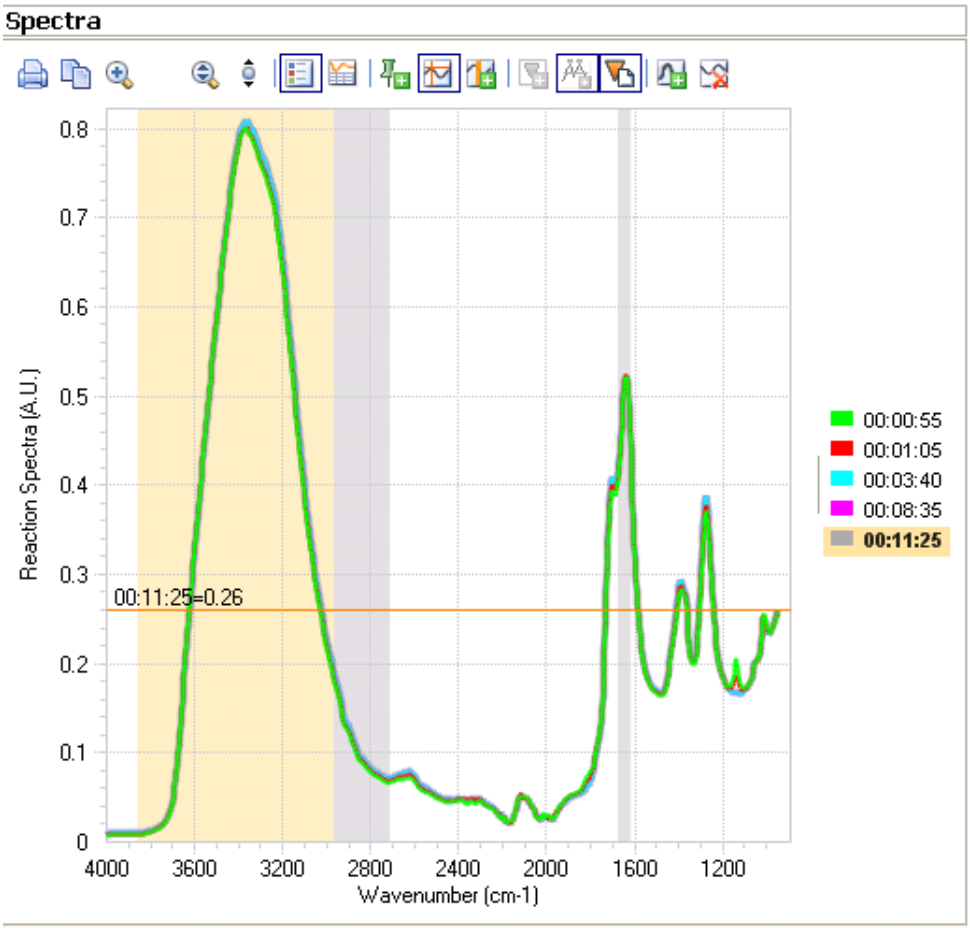
Displaying the Spectra Legend Box

A legend box containing a list of all Spectra Viewer with their color and corresponding time is displayed when the Show Legend button on the toolbar is clicked.



The legend can also be toggled from the right-click menu.

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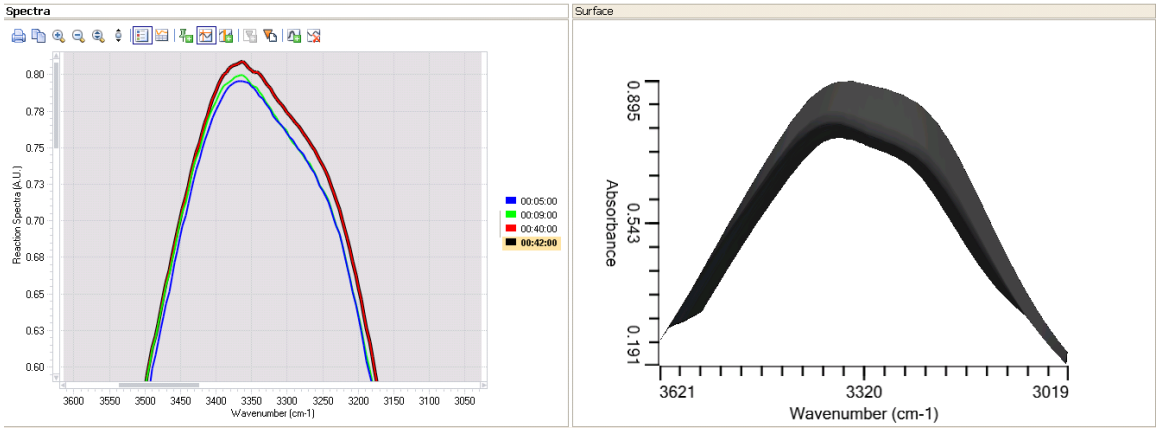
Spectra Zoom Operation

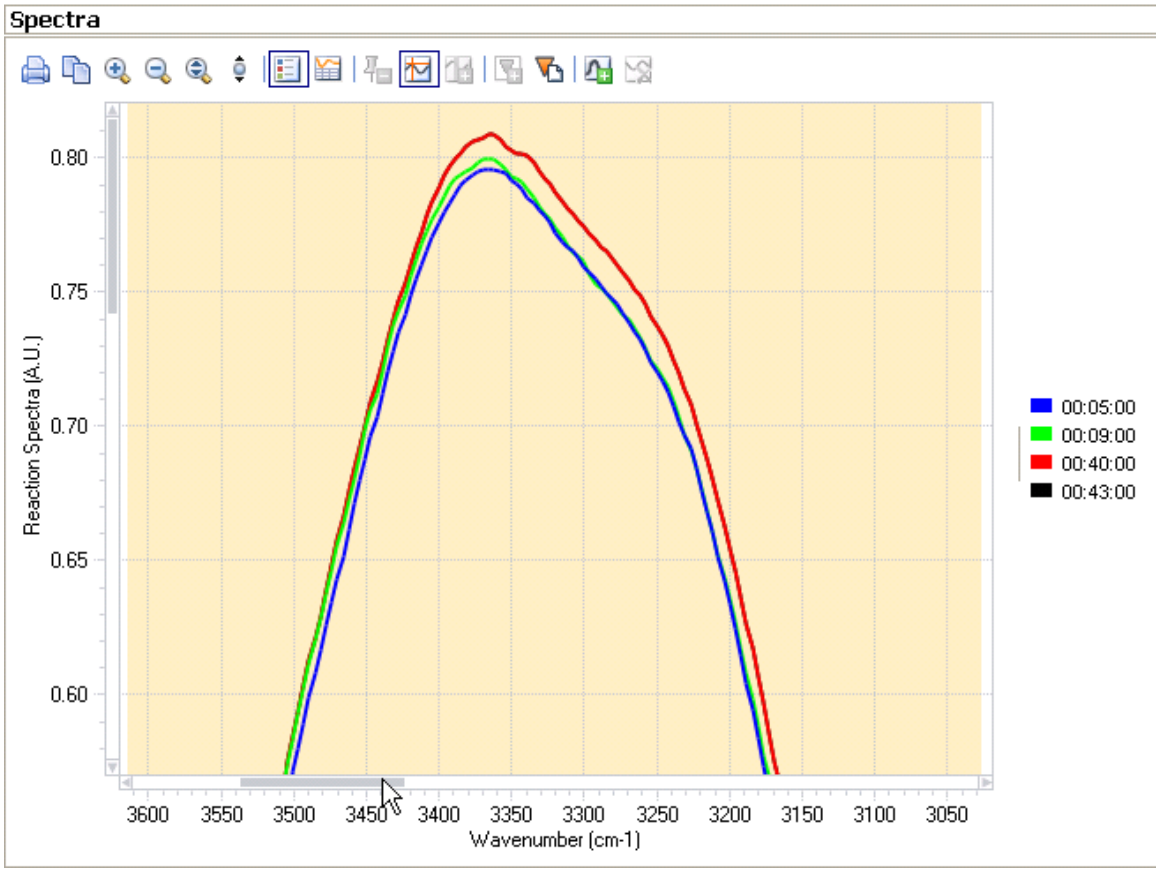
Zoom can be enabled by right-clicking on the chart and selecting the Zoom option or by clicking the button on the toolbar..

Using the mouse as a drawing tool, drag the mouse over the area you wish to enlarge, as shown below.

Both the Spectra Viewer and the Surface Viewer enlarge to the selected area as shown below.



The zoomed image can be moved by dragging the corresponding slider bars with the cursor.



An image can be enlarged several times by repeating the zoom function.

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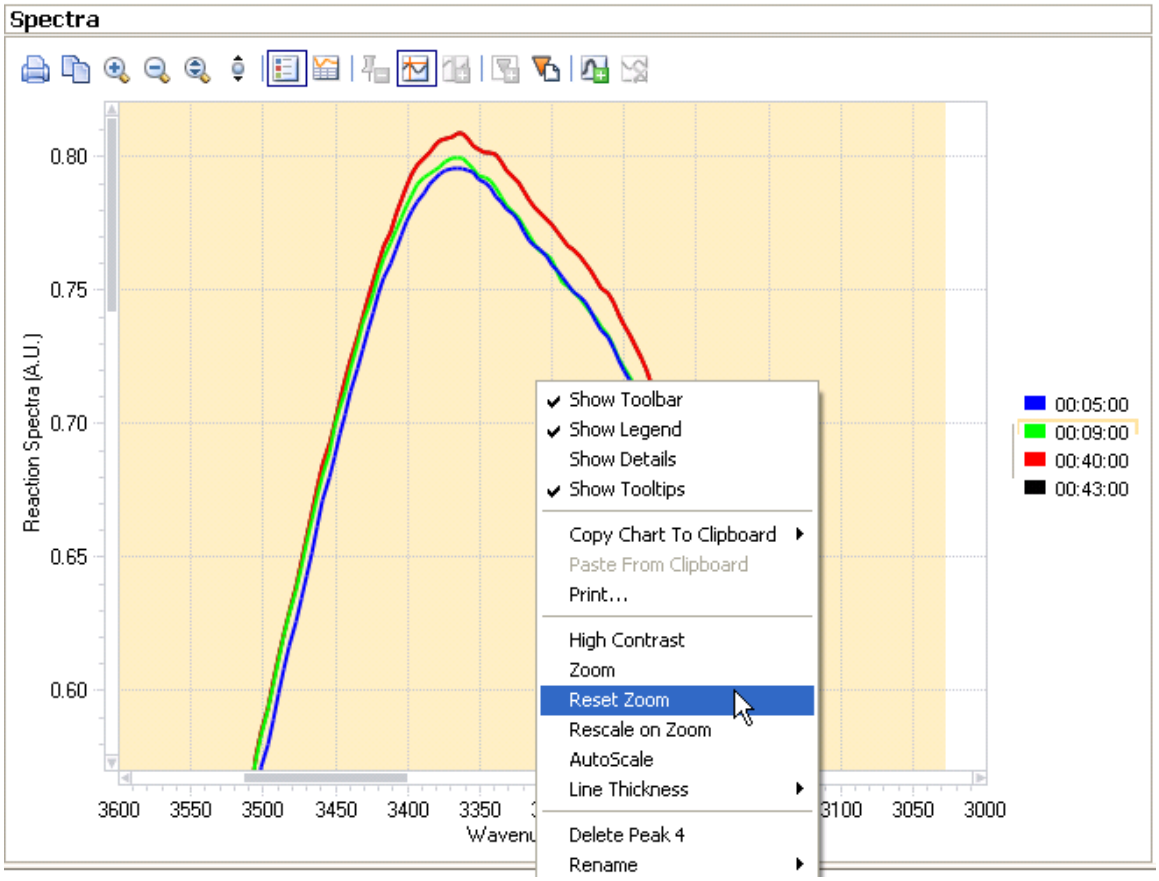
To return to the normal size display, right-click on the zoomed display and select **Reset Zoom**. The zoom can also be reset by clicking the button on the toolbar.

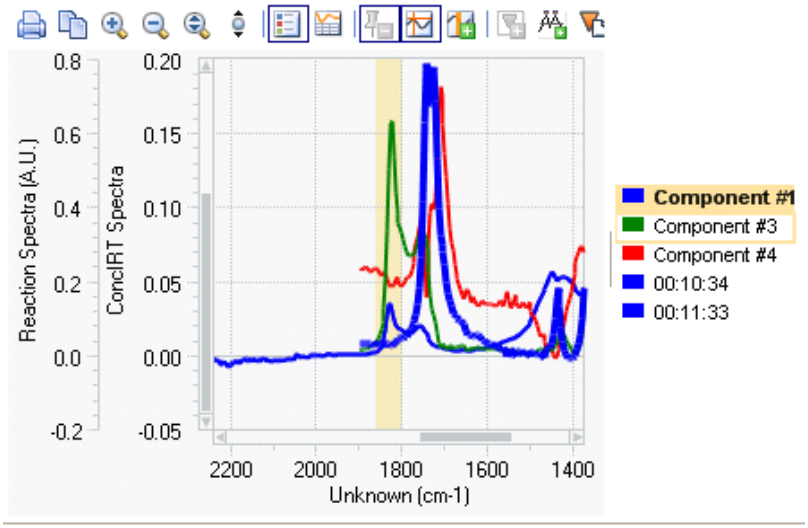


Spectra Autoscale Operation

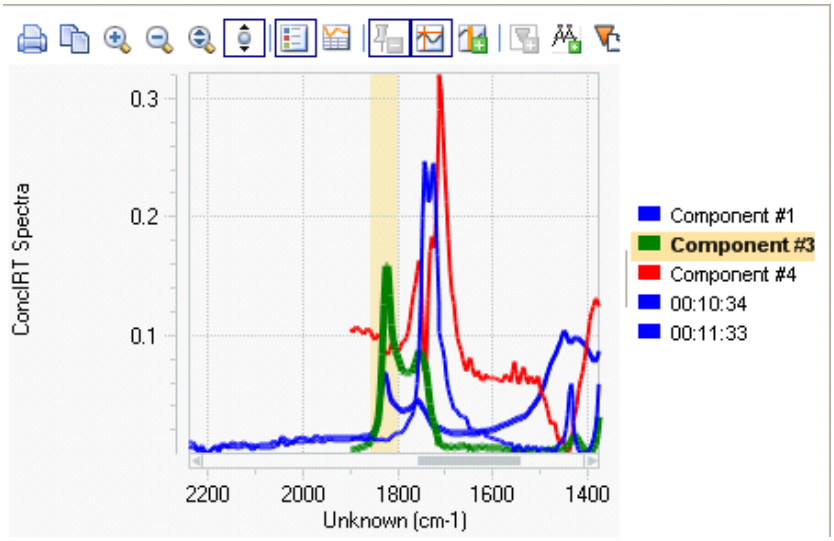
When autoscale is enabled, the y-axis is automatically autoscaled. The x-axis is the only portion of the graph that is selectable by the user.

AutoScale is intended to be used to visually compare the shape of a peak in two different spectra where the peak height in one spectrum is much smaller than in the other spectrum.

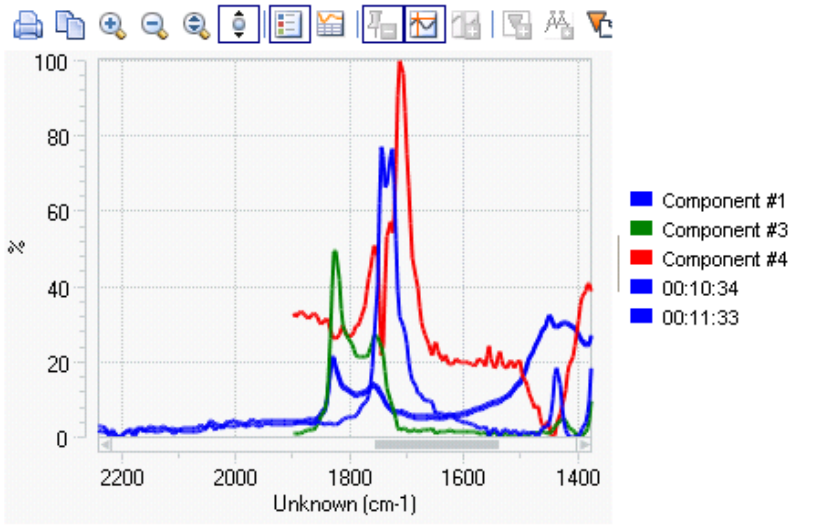
When the Autoscale button is clicked, the Y axis is scaled based on the selected plot in the graph. The remaining plots are scaled to their Y axis extents. The units used for the Y axis is the axis for the selected plot. For example, when autoscaled is enabled for the following graph,



The Y axis is autoscaled based on the selected plot.



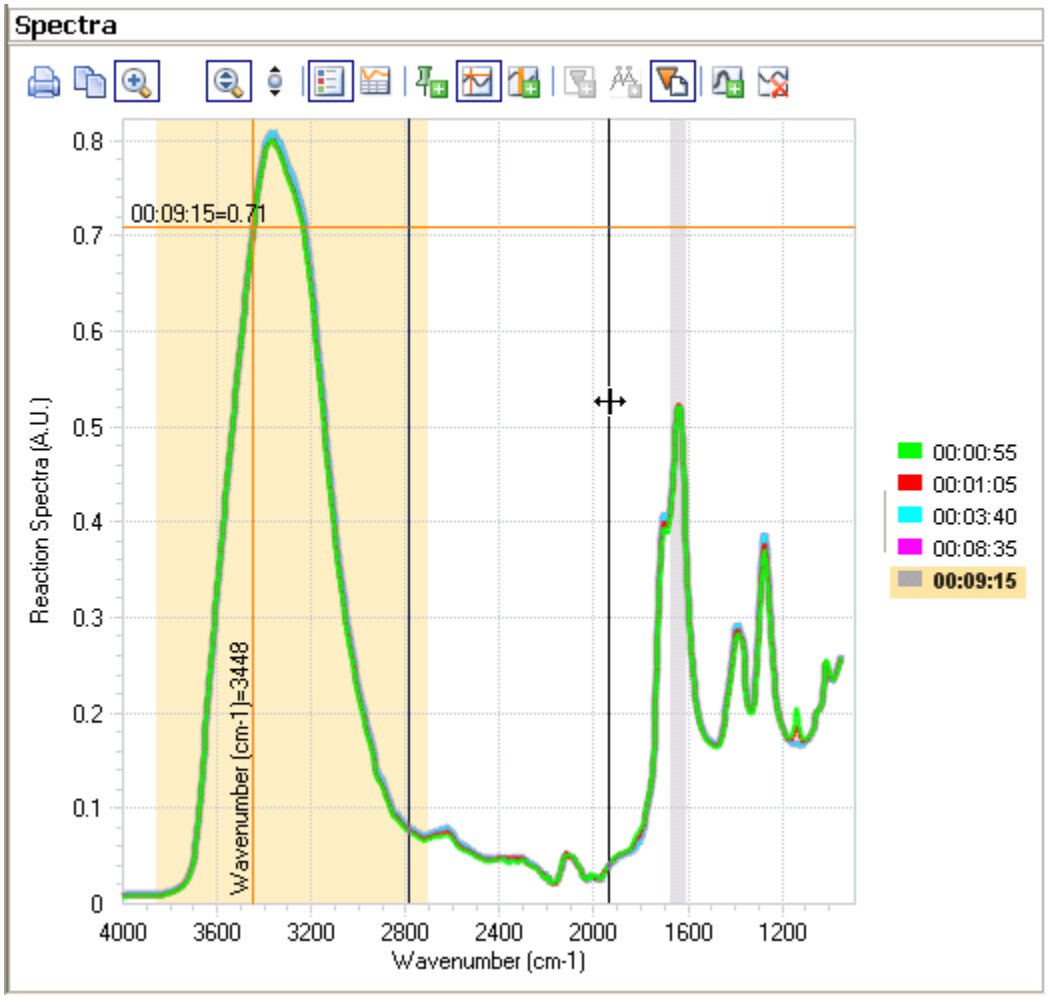
If no plots are selected, autoscaling uses the first plot in the graph as the basis and uses a Y axis scale of 0-100%.



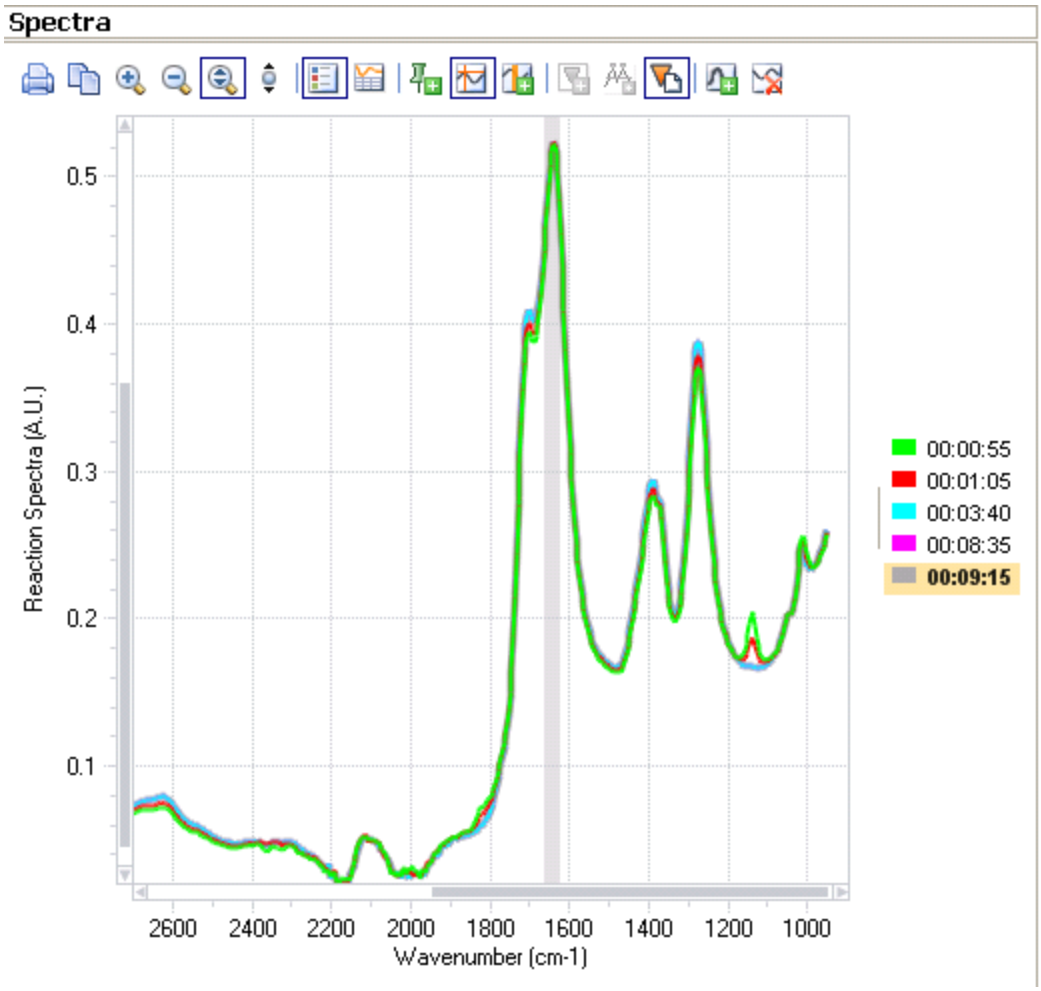
Spectra Zoom Operation with Rescale on Zoom Enabled

When Rescale on Zoom is enabled, zooming has a slightly different effect. The x-axis is the only portion of the graph that is selectable by the user. The y-axis is automatically autoscaled.

When the Zoom button is clicked the cursor changes to an icon. The user moves the cursor to the beginning point of the area to be zoomed. A vertical bar is displayed. Holding the mouse button, the user drags the cursor to the end point of the zoon area.



When the mouse button is released, the zoomed graph is displayed with the y-axis autoscaled



Pinning Spectra

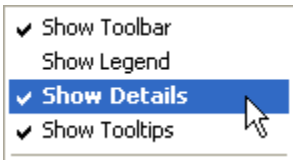
Spectra can be pinned to the spectra display by selecting the appropriate spectra in the Spectra Viewer or Event Viewer and clicking the  button in the toolbar. As spectra are pinned, they are automatically assigned a color by the iC IR software.

These colors can be changed using the context menu.

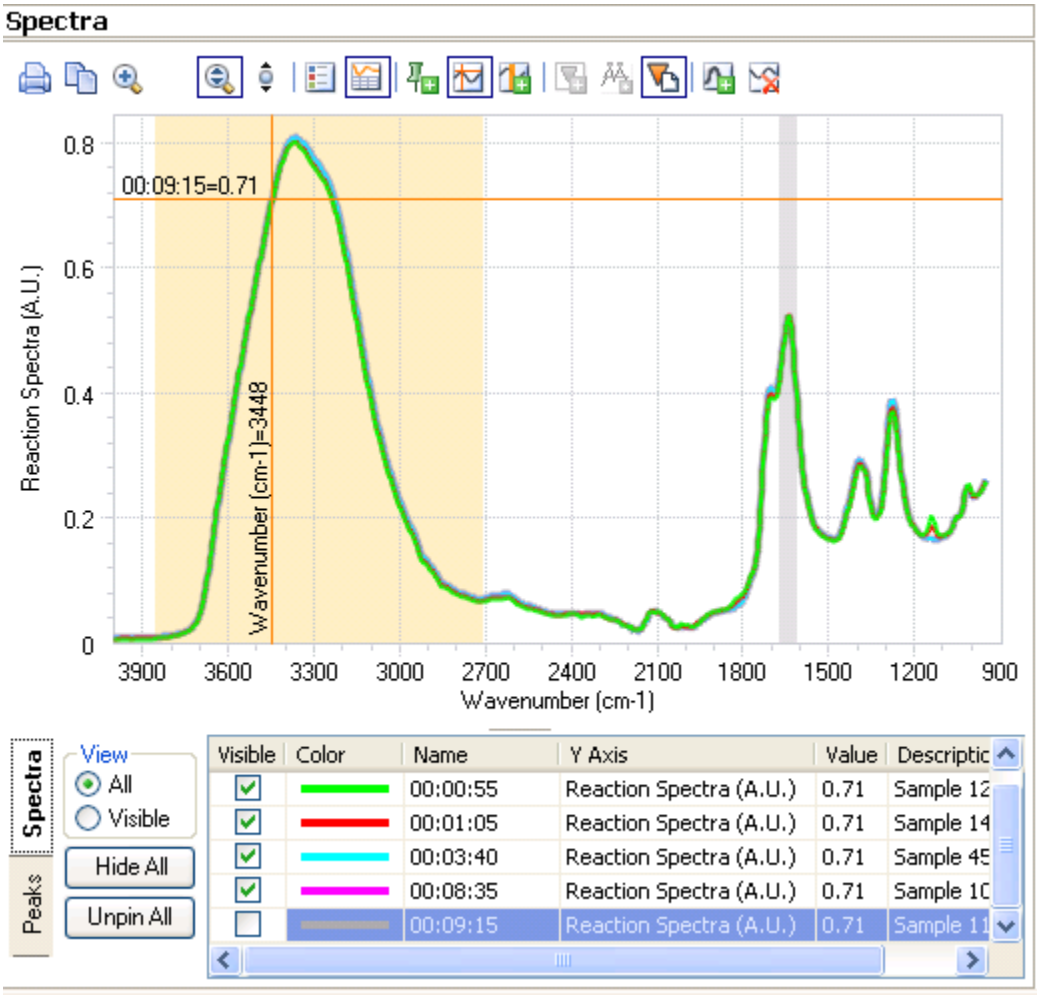
Pinned spectra can be unpinned by clicking the  button in the toolbar.

Spectra List Details Panel

The Spectra List details panel is used to select which spectra are displayed. The pane is opened by clicking the  toggle button in the toolbar or by selecting the **Show Details** option in the right-click menu.



The pane contains a list of all collected spectra. The **Visible** checkbox indicates which spectra are displayed. Multiple spectra can be compared by displaying those spectra and hiding all others.



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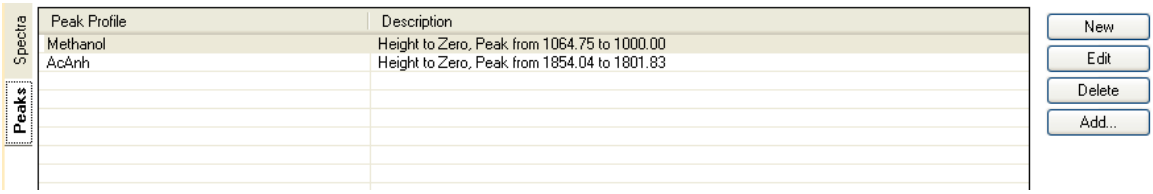
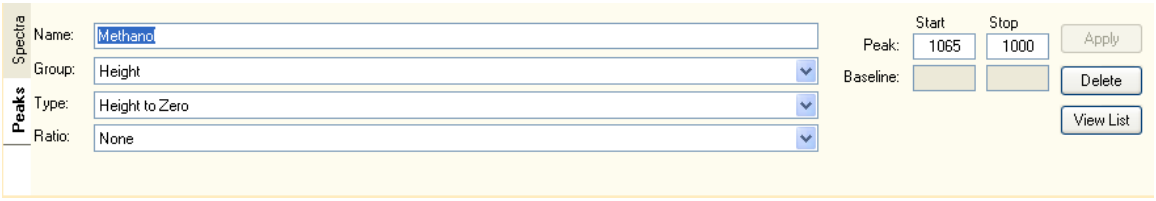
Adding and Editing Peaks

Peaks are edited by clicking the **Edit** button and selecting the peak in the grid.

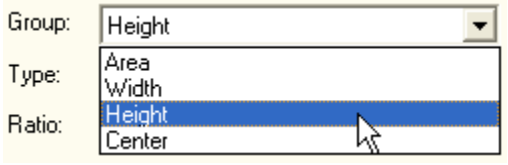


To define a new peak, click the **New** button. A new peak is added to the list. When the **Add** button is clicked, the Select Peaks Dialog is opened."

To edit a peak, select the peak in the list and click the **Edit** button. The list pane changes to an editing pane where the user can change the Peak Name, Start and Stop times, Base Lines and the Analysis Type. The Up and Down arrow keys can be used to increment/decrement the Start and Stop values. If decimal places are used when editing the peak, the value is rounded off when the **Apply** button is clicked.

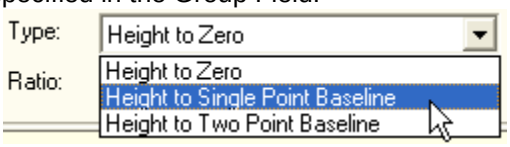


Select the desired peak group from the droplist in the Group field.



- Peak area is the total area (calculated by integration) which is under the peak profile, and above the baseline.
- Peak width at zero is the width of the peak at half of the peak height. If single point baseline is selected, then the peak is subtracted by the single point baseline first then get half of the height.
- Peak height is the actual absorbance reading at the wavenumber which is considered peak center. If single point baseline is selected, then the peak is subtracted by the single point baseline. Similarly for the 2 point baseline.
- Peak center is the wavenumber which gives largest absorbance, and also 1st derivative closest to zero. In other words, the peak center is the flat and tallest point of the peak. It is calculated via cubic spline interpolation.

Select the desired peak type from the droplist in the Type field. Note that the options in the droplist will change depending on the group specified in the Group Field.



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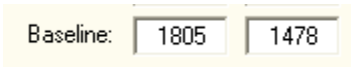
If a baseline type is selected, the baseline is specified in the Baseline fields. The Up and Down arrow keys can be used to increment/decrement the values.

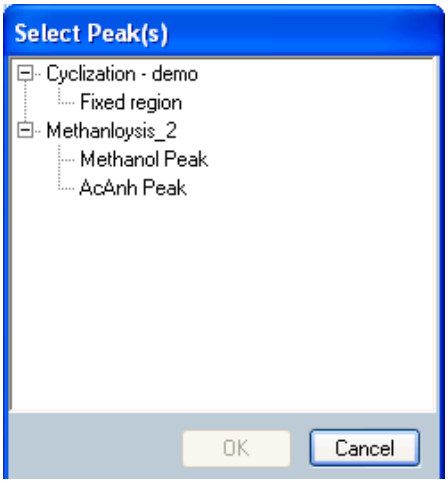


Click the **Apply** button to save the edits.

Click on the **View List** button to return to the Peak List.
Note that if decimal places are used when editing the peak or baseline, the value is rounded off when the **Apply** button is clicked.

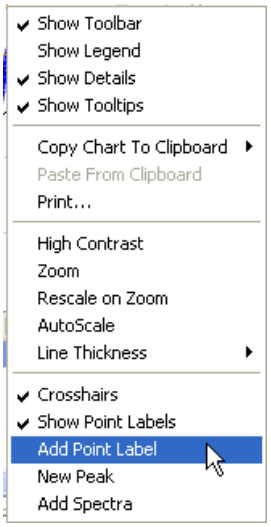
Select Peaks Dialog

The Select Peaks dialog is used to insert a peak into a Spectra Viewer display. The dialog provides a tree-view of available peaks from all open experiments.



Adding Point Labels to a Spectra

A Point Label can be added to a point by selecting the point and selecting the Add Point label option from the context menu.

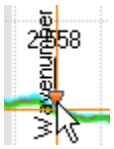


or

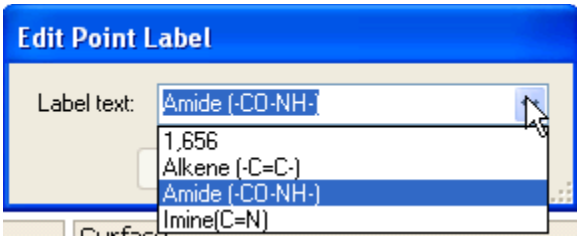
Selecting the point and clicking the  button on the toolbar.

A label containing the wavenumber (default) of the point is displayed on the graph.

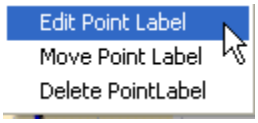
A point label can be edited by double-clicking on the point marker.



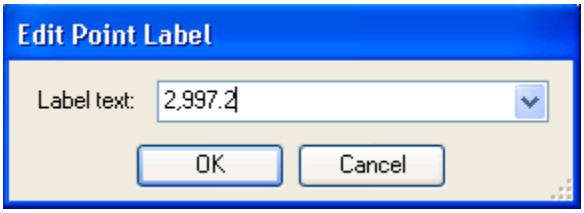
Select the new label from the droplist or enter a name in the field.



The point label can be edited, moved or detected by right-clicking on the label and selecting the appropriate option.

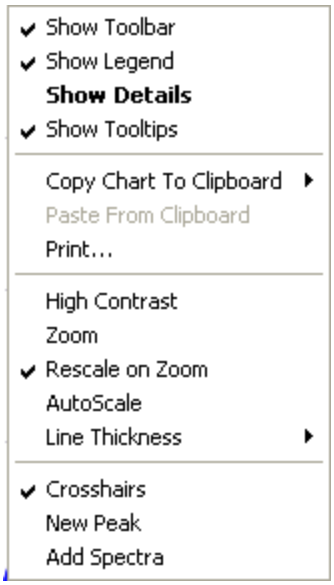


When the edit option is selected, the Edit Point label dialog is opened. Enter the desired text or select a label from the droplist and click the **OK** button.



Spectra Viewer Context Menu

The Spectra Viewer incorporates a several right-click or context menus that contain tools for customizing the displayed data. The first menu is displayed when the user right-clicks on the data area of the display.

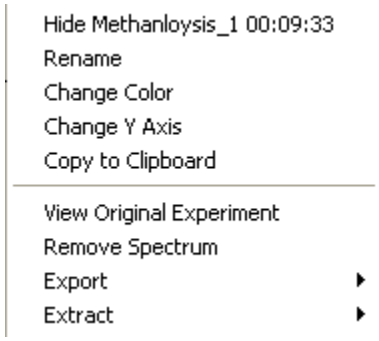


The menu contains the following items.

Show Toolbar	Displays the toolbar at the top of the display.  The toolbar contains the following tools.  Prints the display.  Copies the display to the clipboard.  Zooms the display.  This button is only visible when the Zoom function is enabled. The button resets the zoom to its original scale.  Rescales only the X-axis on zoom.  Auto scales the Y-axis.  Displays the Legend Panel.  Displays the Details Panel.  Pins the selected spectra in the Event Viewer to the Spectra Viewer. Clicking the button when spectra are already pinned, unpins those spectra. This tool can be used to add spectra from the Event Viewer to the spectra list.  Displays crosshairs on the graph.  Adds a new peak.  Adds a point label.  Adds peak labels.  Displays point labels.

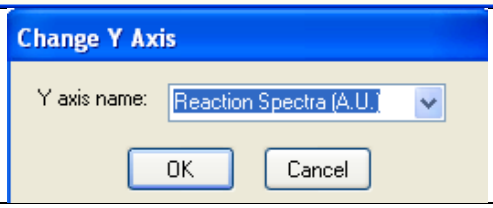
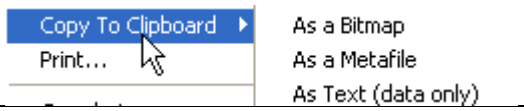
	 Adds a new spectra.  Removes a selected spectra.
Show Legend	Displays the Legend Box.
Show Details	Displays the Details panel.
Show Tooltips	Displays tooltips on the graph as data points are selected.
Copy to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
Paste from Clipboard	Pastes tab delimited numeric data into the graph.
Print	Opens the Print dialog to print the contents of the display.
High Contrast	Displays the graph with a black background.
Zoom	Zooms the display. Refer to Spectra Zoom Operation
Reset Zoom	Resets the zoom to its original scale. This button is only displayed when the display is in a zoomed condition.
Rescale on zoom	Rescales only the X-axis on zoom.
Auto-scale	Auto scales the Y axis.
Line Thickness	Selects the line thickness for the plots.
Crosshairs	Displays crosshairs on the Spectra Viewer. Crosshairs immediately jump to the selected point and a tool tip displays information about that point. The Trend Viewer and Log Viewer highlight the corresponding time. When you turn on the crosshairs option in the Spectra Viewer, they will jump to the highlighted point. Conversely, moving the crosshairs in the Spectra Viewer changes the crosshair position in the Surface Viewer. You can also use the arrow keys in the Surface Viewer to “nudge” the crosshairs exactly where you want them.
New Peak	Adds a height to zero peak exactly at the crosshairs.
Add Spectra	Adds a new spectra from a Spectra Library.

The second menu is displayed when the user right-clicks on a data point in the display and contains tools for customizing the data. The menu is accessed by right-clicking on a data point in the distribution or by right-clicking on a measurement in the legend. This method may be preferable because it might be difficult to select a precise data point.



The menu contains the following items.

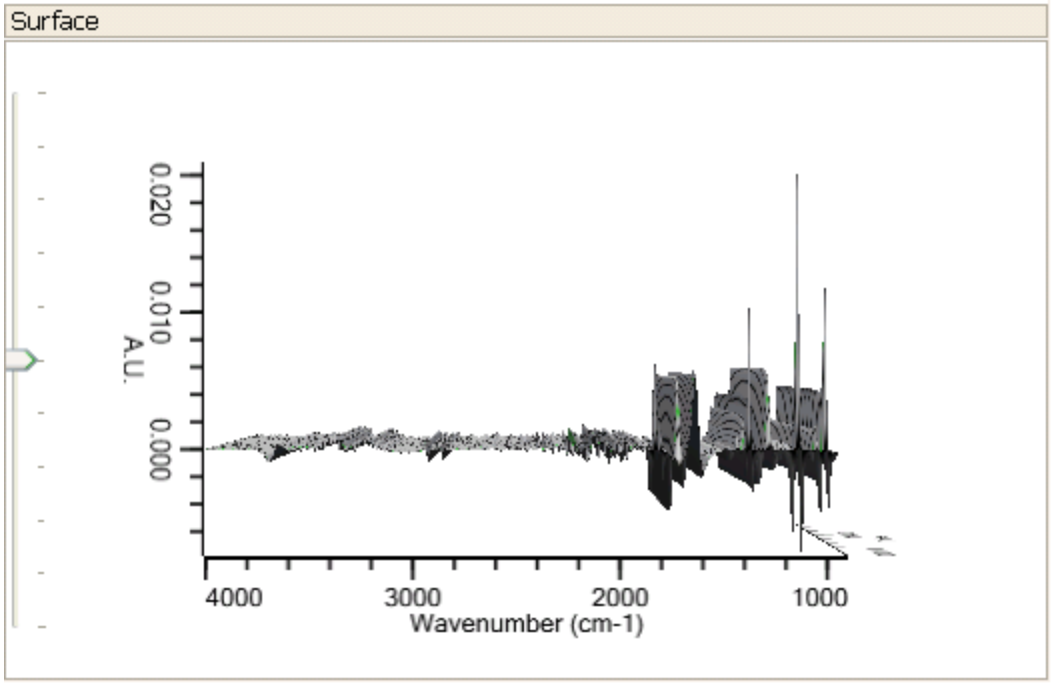
Hide . . .	Hides the selected distribution. The distribution is hidden in the graphic area but remains listed in the Details grid.
Rename	Opens a dialog allowing the user to rename the spectra
Change	

Color	
Change Y Axis	
Copy to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
View Original Experiment	Opens the experiment containing the original spectra in a new tab.
Remove Spectrum	Permanently removes the selected spectra from the viewer.
Export	Exports the selected spectra to a file. The user has the option of exporting only the selected spectra or all pinned spectra.
Extract	Allows the user to extract the background or single beam from the selected spectra.

Surface Viewer

The Surface Viewer shows a three dimensional view of the entire experiment with a time line and two planes, one in the x axis and one in the z axis for an in-depth analysis. The display can be enlarged or reduced in size, completely rotated about all three axes, and moved within the Surface Viewer.

Colors can be changed to emphasize different parts of the reaction and a wire frame can be added for detailed analysis.



Rotating the Surface Viewer about its three axes:

To rotate the display, place the cursor on the display, hold down the mouse button and move the cursor. The display will rotate about its axis in response to vertical and horizontal movements of the mouse.

Moving the display up, down, or sideways in the display area:

Put the cursor anywhere on the display, click the right mouse button and move the mouse in the desired direction. The display moves in the same direction as the mouse.

Enlarging or Reducing the Size of the Surface Viewer:

To enlarge or reduce the size of the display, place the cursor anywhere on the Surface Viewer and then press and release the left mouse button. Rotating the mouse wheel counterclockwise reduces the size of the display, rotating the mouse wheel clockwise enlarges the display.

Keyboard Control Keys

Pressing the **C** key changes the color to one of the selections in the pull down display. Each time the **C** key is pressed, the color display changes.

Pressing the **W** key displays the wire frame display. Pressing it again turns off the wire frame display.

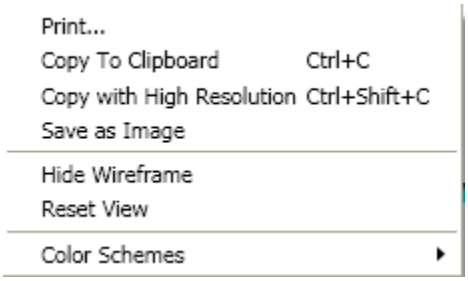
Pressing the **R** key resets the Surface Viewer display.

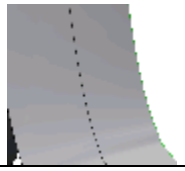
Pressing the cursor up or down key ↑↓ moves the time sequence on the topographic surface.

Pressing the x key displays the wave length on the topographic display. Pressing the left or right cursor keys ←→ move the wave length line to the right or left.

Surface Viewer Context Menu

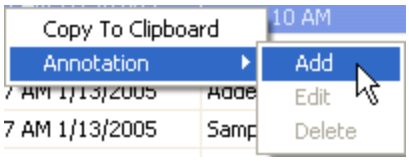
There are several options available in the Surface Viewer context (right-click) menu.



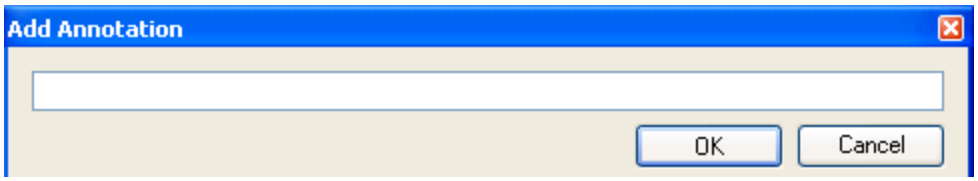
Print	Prints the graph to a local or network printer.
Copy to Clipboard	The Copy function copies a bitmap image of the reaction surface to the clipboard. The image can be pasted into any application supporting bitmaps.
Save as Image	Saves the view as a PNG image file.
Show/Hide Wire Frame	Show wire frame – When checked, displays a wire frame on the surface. 
Reset View	To reset the display to its default setting, select Reset View.
Color Scheme	To select a color scheme for the Surface Viewer, select the desired color scheme from the drop-down list. 

Adding an Annotation

Annotations can be added to the Event Viewer by right-clicking on a row in the Event Viewer or by using The Live Experiment Toolbar (only while an experiment is running).



A blank annotation popup is opened. Enter the text for the annotation and click the **OK** button to save it and close the popup.



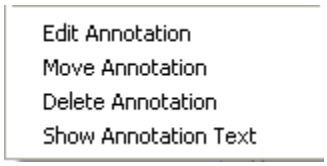
- A icon is displayed on the Trend Viewer at the time reference when the user annotation was made.
- A icon is used to designate a pinned sample marker
- A icon is used to designate a system message.

When the mouse hovers over the marker on the Measurement display, a tool tip is displayed that contains the annotation text. Double-clicking the marker will open a popup displaying the annotation.

Existing annotations can be edited by double-clicking the annotation in the Event Viewer or by using the Edit option in the right-click menu.

The menu also contains options for deleting an annotation.

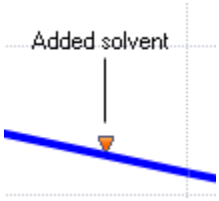
Right-clicking on an Annotation in the Trend Viewer displays a context menu with two additional options.



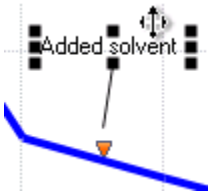
When choosing the Move Annotation option, the marker can be dragged to the new location with the cursor. When the marker is at the desired location, click the mouse button to set the marker at that location. The annotation can be moved by right-clicking either directly on the marker or the marker text.

The annotation text can be moved by clicking on the text. The cursor changes to an arrow that can be moved to the decided location on the graph.

The Show/Hide Annotation Text will display or hide the text of the annotation next to the annotation marker.



The text can be moved by dragging the text box to a new location on the graph.

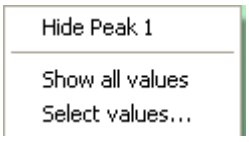


Large Values Viewer

The Large Values viewer displays the current values of the peaks and components in a large table format.

The window is available during the execution of a live experiment and is opened by clicking the checkbox in the Live Experiment toolbar. The values are updated as samples are taken.

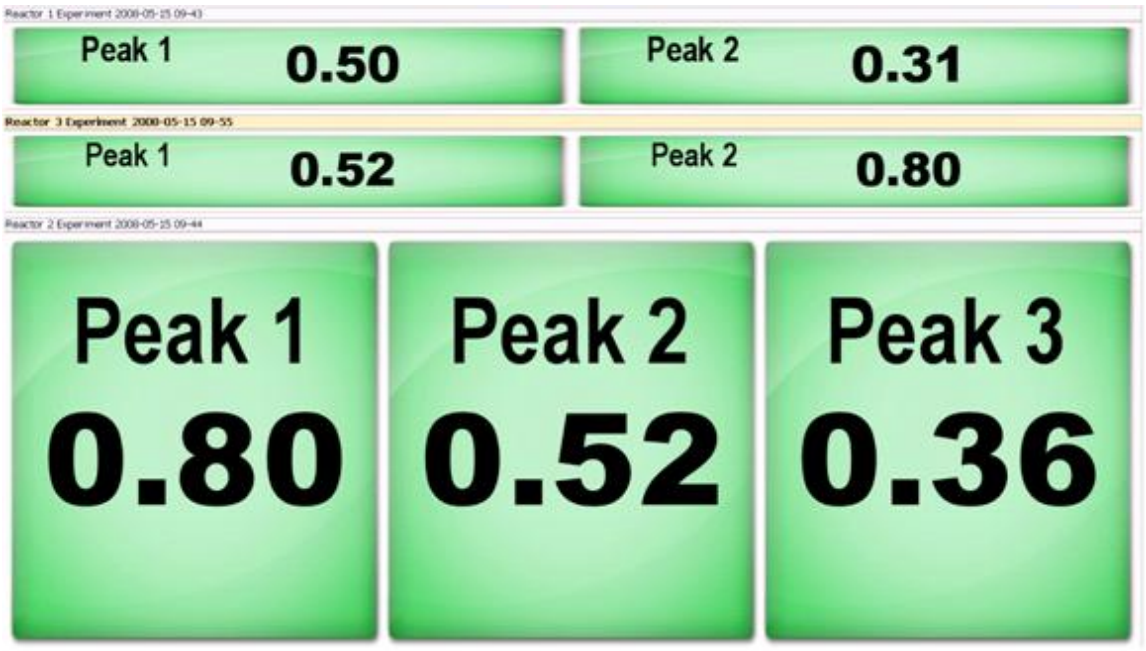
By default the values for all defined peaks and components are displayed. A right-click (context) menu is available to customize the display window.



The following options are available.

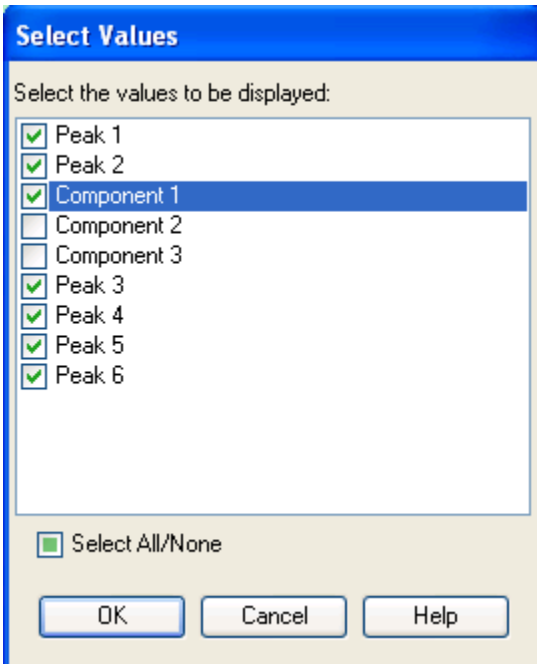
Hide . . .	Hides the currently selected peak or component.
Show All Values	Displays all defined statistics.
Select Values	Opens the Select Values dialog that allows the user to select which statistics are displayed.

In multi-probe systems large values can be displayed for each running experiment on the same display. The **Show Large Values** checkbox must be checked in each experiments Live Experiment Toolbar in order for the large values to be displayed for that experiment.



Select Values Dialog

The Select Values dialog is used to select which peaks and components are displayed on the Large Values display. The dialog displays a list of all defined peaks and components. The user checks the peaks and components to be displayed.



When multiple experiments are displayed, the user must click on a specific experiment to select the values for that experiment.

Zooming Interactions between Viewers

A Zoom function is available for the Spectra Viewer and Trend Viewer. When the zoom function is operated with either display, the Surface Viewer also changes accordingly.

Only two displays zoom in tandem; the Spectra Viewer and Surface Viewer or Trend Viewer and Surface Viewer.

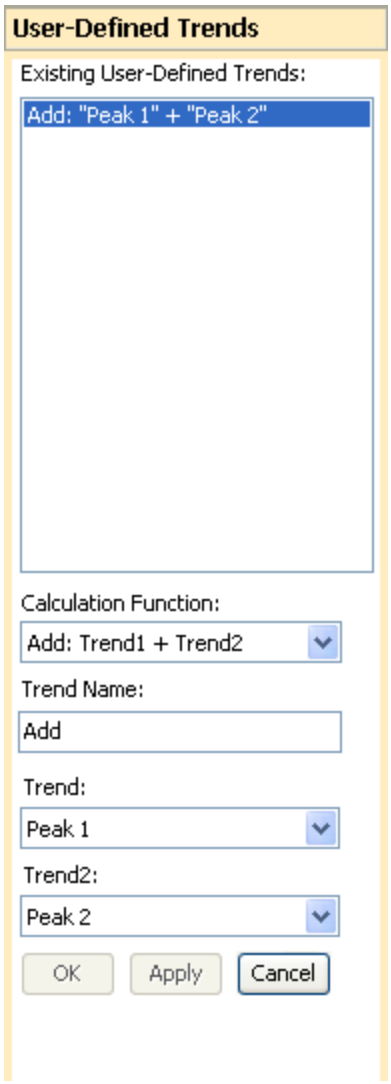
User-Defined Trends

The user can define custom trends that perform math functions on one or more trends to show information or relationships that might not otherwise be apparent. Once a trend is created, it is displayed in the Trend Viewer where it can be analyzed. User-defined trends are treated the same as other trends in the Trend Viewer.

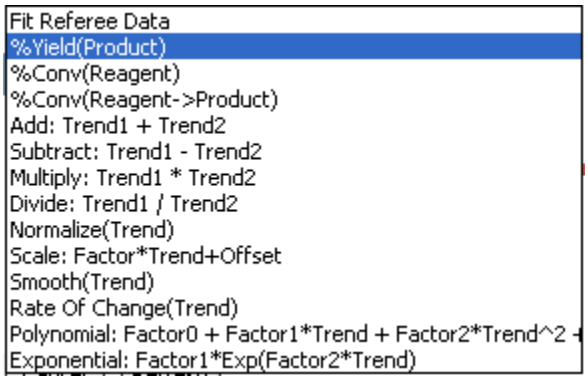
Any number of user-defined trends can be created. User-defined trends can be chained so that the result of one user-defined trend can be used in another user-defined trend. The iC software has internal checks to ensure that circular dependencies are not introduced when referencing other user-defined trends in a trend equation.

The User-defined Trends task pane in the toolbox is used to create a user-defined trend.

The user clicks the Add button to create a new user-defined trend. The task pane expands to display the definition fields.



The Calculation Function droplist is used to select the calculation that will be used to define the trend. The following options are available:



Fit Referee Data - scales a relative trend (ex ConcIRT LIVE, peak profile, etc) to quantitative data from HPLC or other offline analytical data source. The quantitative data is entered in The Referee Data Dialog. The function calculates the linear equation correlating the relative trend to the chromatography data (based on a least squares fit). This linear equation is then applied to each point in the relative trend to scale to the quantitative data.

A checkbox is available to show the result as %Conversion rather than the units of the quantitative data. For this option the max value (i.e. starting amount for a reagent or theoretical limit for a product) can be entered in the Chromatography Data dialog for the selected component. If no value is entered, the largest entered value is used. Refer to The Referee Data Dialog for more information.

%Yield - is calculated as trend/max, where max is a constant entered by the user representing the theoretical yield for the selected trend (presumably the product). If no max value is entered, the maximum value in the selected trend is mapped to 100%.

%Conversion - estimates the %conversion based on parameters. The formula is 1 – trend/max where max is a constant representing the starting amount for the selected trend (presumably the limiting reagent).. If no max value is entered, the maximum value in the selected trend is mapped to 100%.

Add – create a third trend based on the sum of the two specified trends.

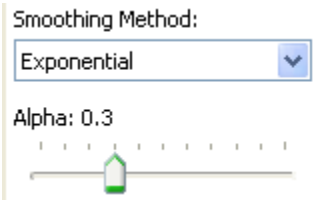
Subtract – create a third trend based on the difference between the two specified trends.

Multiply – create a third trend based on the product of the two specified trends.

Divide – create a third trend based on the ratio of the two specified trends.

Scale – scales a trend based on a used-specified factor and/or an offset.

Smooth – smoothes a trend over a user-specified range using Savitsky-Golay smoothing or Exponentially Weighted Moving Average with a user-specified smoothing window. The smoothing type is selected from a droplist and the smoothing value is set by a slidebar.



Rate of Change - creates a new trend that is the 1st derivative of the selected tracking trend based on a user-specified sample window. In other words, for each point T[i], rate is calculated based on the different with point T[i – w], where w represents the window size. The Time Basis parameter allows the rate of change to be calculated on a per second, per minute or per hour basis.

Polynomial – is commonly used to support solubility in a crystallization workflow. Solubility C* is often a polynomial function of the temperature of the solution. C* = a + bT + cT2+……
Example:

Exponential - is commonly used to support solubility in a crystallization workflow. Solubility C* can also be expressed as exponential function of the temperature of the solution. C* = a*ebT.
Example:

The remaining fields in the task box will vary depending on the calculation selected. If the **Apply** button is clicked, the trend is added/updated in the Existing User-defined Trends list, the trend is displayed in the Trend Viewer, and the task pane remains expanded allowing the user to create additional user-defined trends or adjust trend parameters. If the **OK** button is clicked, the trend is added/updated in the Existing User-defined Trends list, the trend is displayed in the Trend Viewer, and the task pane collapses to its original view.

To edit an existing user-defined trend, the user selects the trend in the Existing User-defined Trends list and clicks the **Edit** button. Alternately, the user can double-click on the trend in the list.

To delete an existing user-defined trend, the user selects the trend in the Existing User-defined Trends list and clicks the **Delete** button. Alternately, the user can select the trend in the list and press the Delete key on the keyboard.

Adding Referee Data

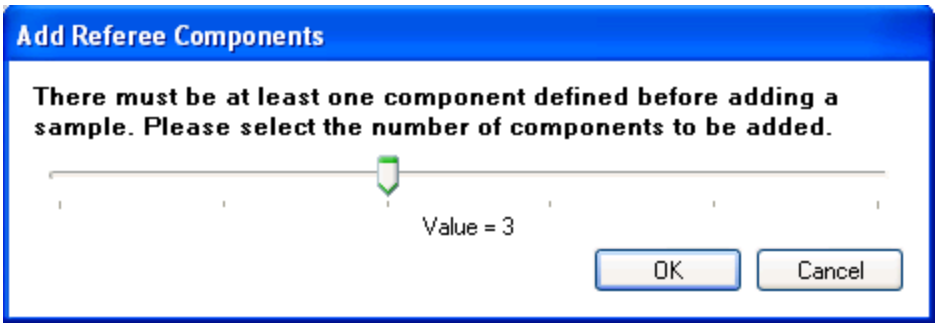
Data from a manual sample from a HPLC or chromatography method can be added to an experiment by clicking the  button on the Live Experiment toolbar. Click the button immediately after taking a manual sample for HPLC or other chromatography method.

Clicking the button performs the following functions.

- Identifies the most recent sample
- Pins that sample
- Adds an annotation at that point in time: Took Referee Sample <1>
- Adds a row to the Chromatography data table in the database

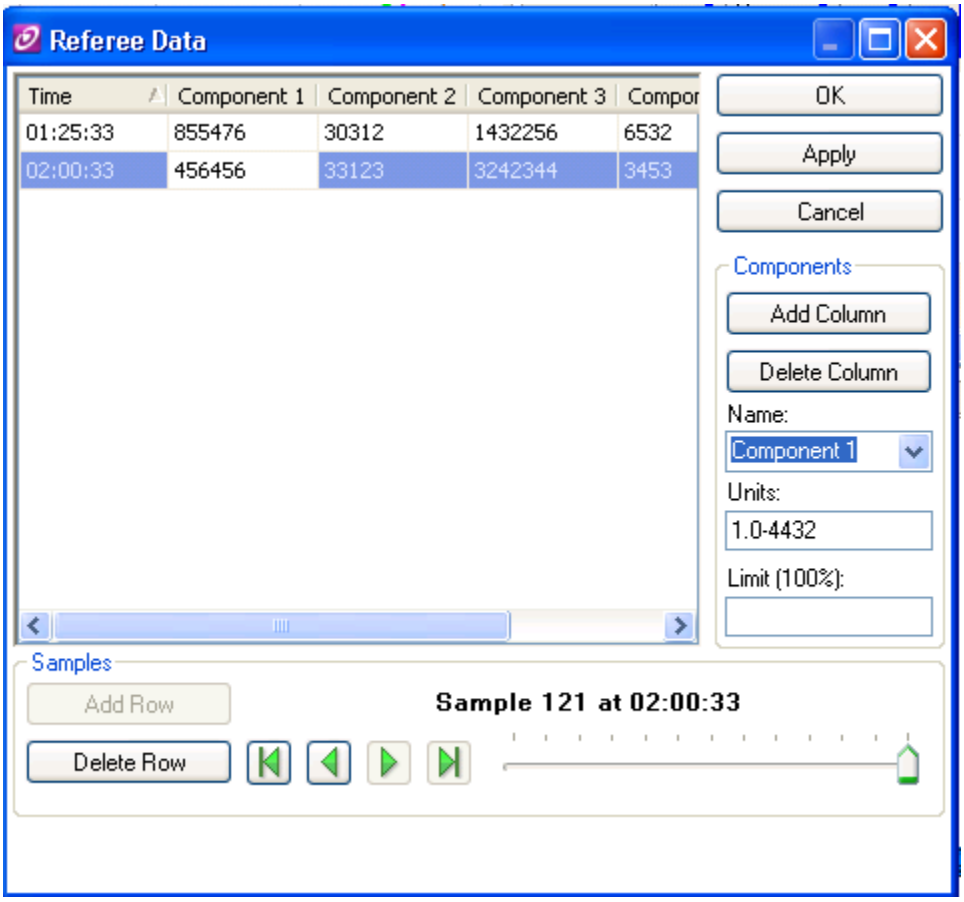
For best results, extract the sample right as the iC sample is being collected.

The first time a sample is taken, a dialog is opened that requires the user to specify the number of components to use for the sample.



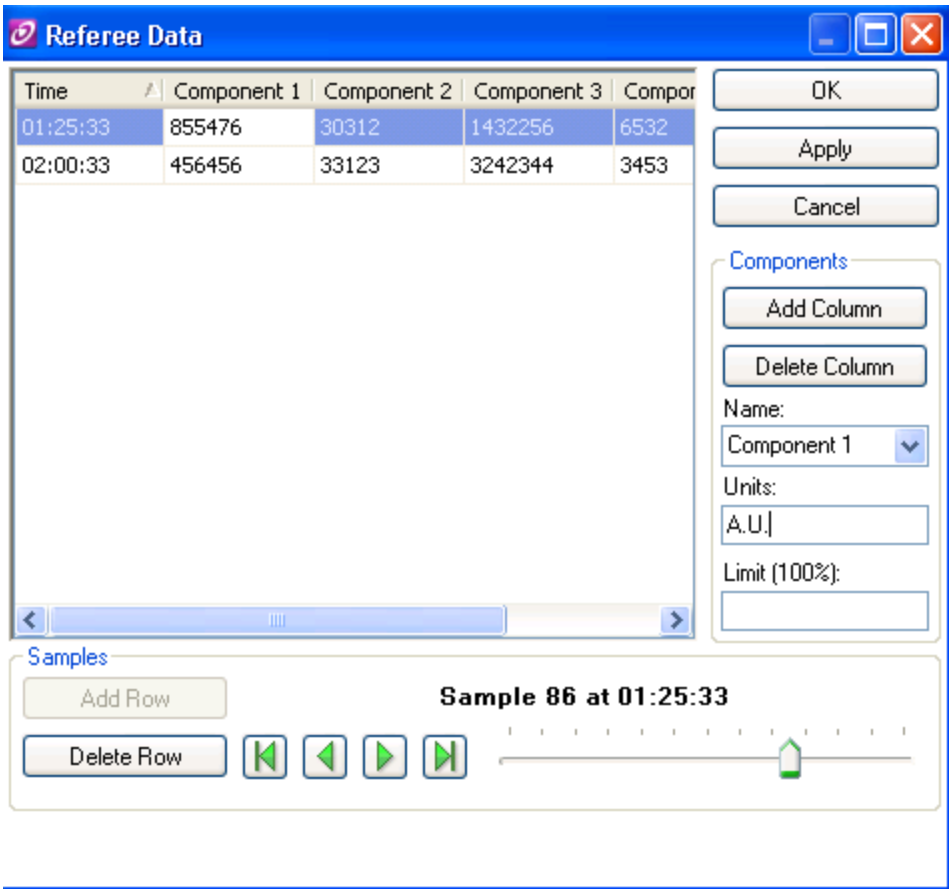
The Referee Data Dialog

The Referee Data dialog is used to enter/edit quantitative data from a HPLC or other chromatography method. This data can then be used to create User-Defined Trends or be imported into an iC Quant model.



The user uses the slider bar or arrow keys at the bottom of the dialog to select a sample. As the slider bar or arrow keys are moved, the sample is selected in the Spectra, Trend and Event Viewers. Once the desired sample is selected, the **Samples/New** button is clicked to add the sample to the list. Alternately, the user can click in the Trend Viewer, Event Viewer or Spectra Viewer to select the desired sample time.

The units field is used to group the trends on a shared axis.



Component information is added for the samples by clicking the **Components/Add Column** button. A Name, Units and Limit are specified for each component. Finally, the values for each component are entered for each sample.

Clicking the **Apply** button is saves the information. Clicking the **OK** button is saves the information and closes the dialog.

Helpful Hints for Real-Time Peak Profiling

This is the simplest and most direct approach to produce a relative concentration vs. time profile. The absorbance value in an infrared spectrum holds quantitative information as described in the Beer-Lambert Law: A=abc. This states that the absorbance is linearly proportional to the molar absorptivity a, the pathlength b, and the concentration c. For peak measurements performed with the iC10 and DiComp probe we approximate a and b as constants. Therefore, the peak height is directly related to the concentration of the species in solution. Some simple guidelines will carry you through the peak height profiling process.

1. It is usually best to profile a peak height to a single point baseline. This will ensure that any changes in the baseline due to temperature or other effects will be negated in the resulting concentration profile.

2. Use the following guidelines to select a component peak to profile. A simple mnemonic using the iC letters will help you to remember!

i → **isolated:** ***Peaks that are isolated and*** not overlapped.

intense: Peaks that are intense are the easiest to profile and provide the best profiles. The larger the peak the better!

involved: Peaks associated with a functional group that is either being formed or consumed are good candidates for profiling. Do not forget to look at functional groups that are structurally close to the reactive groups.

3. Similarly, we can use the following guidelines for the baseline point selection.

C → **Close:** Because the baseline and other sub structural features vary in different regions of the spectrum, it is a good idea to choose a baseline point as near as possible to the peak.

Calm: Of course we are going to look for a flat section of the spectrum to choose a baseline point, but what if a peak associated with an intermediate begins to form at that wavenumber value? In these cases we will need to change baseline points**.**

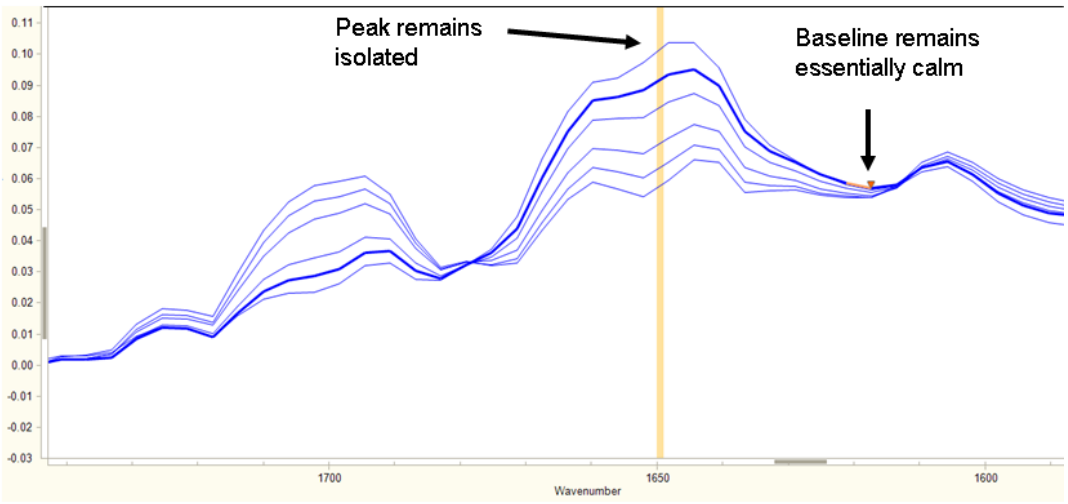
Concentration: Be aware that dilution and/or concentration effects will be observed as relative concentration changes in a reaction. Thus, what appears to be a drop in concentration of an analyte from a direct chemical reaction may only be a dilution effect caused by adding solvent. This is an example of why it is important to annotate your reaction!

NOTE: By default, peaks defined in iC are defined as 'Peak height to zero'. It is often useful to define a single point baseline point. To compensate for overlapping peaks (i.e. a shoulder), it is often useful to choose a two point baseline such that one point moves with the overall spectral baseline and the other moves with the overlapping peak.

Example of Real-Time Peak Height Profiling

For this exercise, we will use the decomposition of an enolate to an ester as it is allowed to warm up. The following figure shows the first spectrum of the reaction. At this point a peak value and baseline point are chosen according to the criteria above.

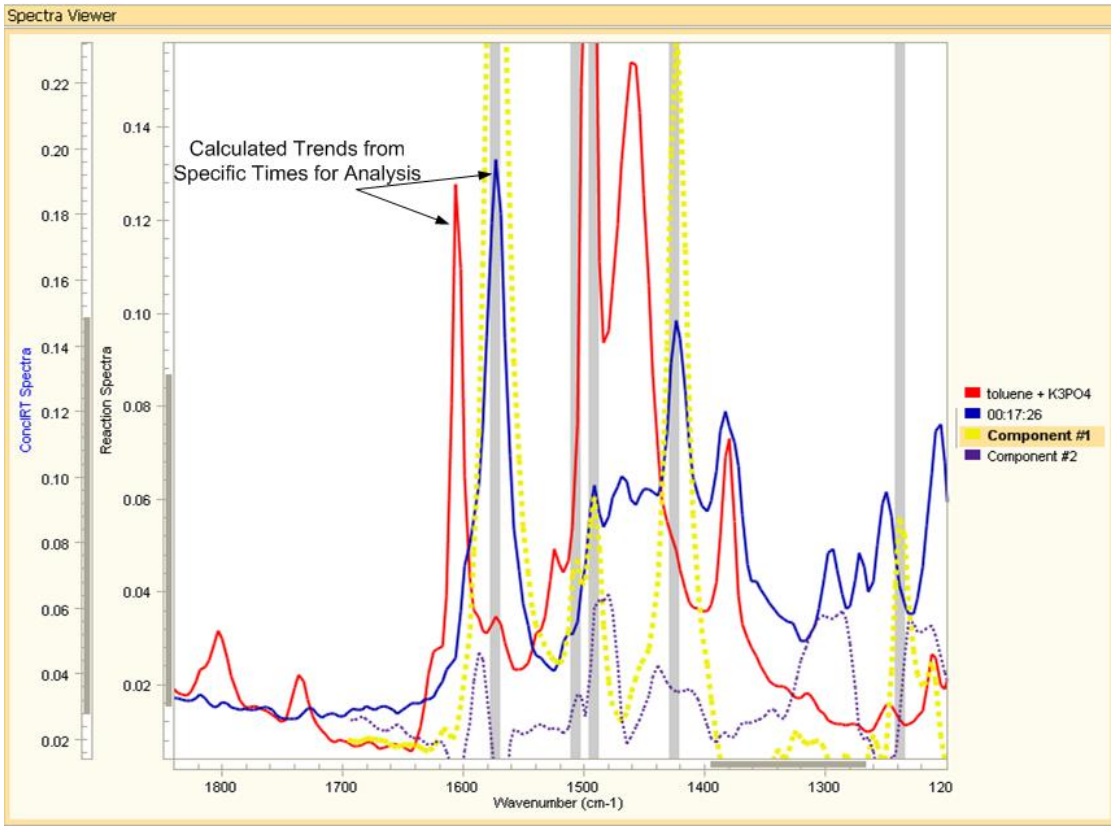
Spectrum with enolate peak, prior to the onset of decomposition.



Spectra extracted from enolate decomposition, new peak forms, but is not overlapped with either peak or baseline point.

Real-time Peak Profiles vs. ConcIRT LIVE Profiles

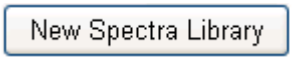
Reaction trends for spectra selected by the user can be compared with the three generated component trends for further analysis. Each plotted trend can be labeled by the user. Trend analysis is generated in real time. The timestamp associated with each spectrum can be observed with the time slider bar.



Working with Spectra Libraries

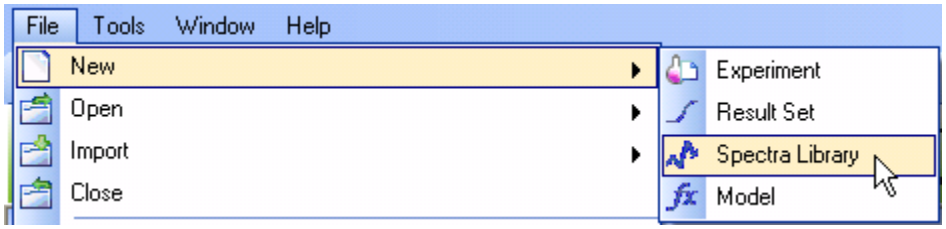
Standard chemical references in the library are created separately from an experiment. The instrument is cleaned and aligned separately from that used in an experiment as well.

The Spectra Library is created using a Wizard that guides the user through the process.

To create a spectra library click the 

button on the Start Page

or select the **New/Spectra Library** option in the **File** menu.



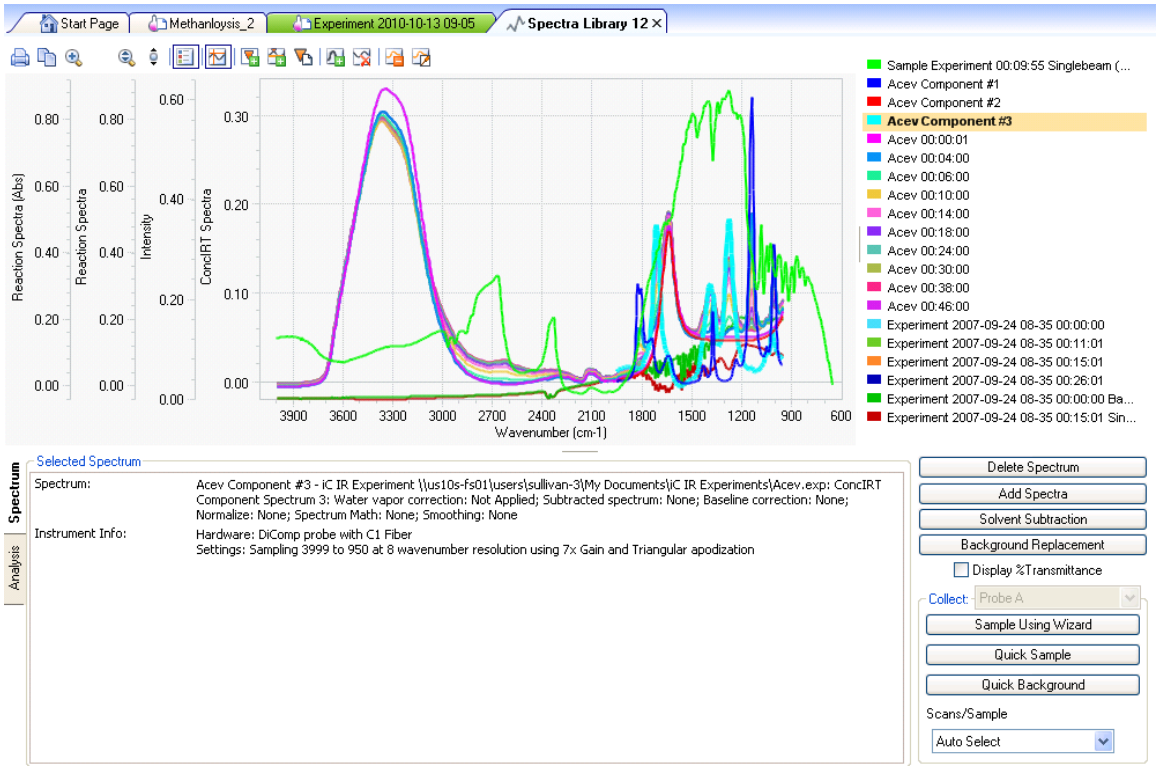
The dialog for adding spectra is opened. See Adding Spectra to a Spectra Library

An existing spectra library can be opened and edited by selecting the **Open/Spectra Library** option in the **File** menu. The library can be edited and resaved or a new spectra library can be created from the edited library file using the **Save As . . .** option in the **File** menu.

Note: To prevent data loss during a system malfunction, a backup copy of the spectra library document is saved to the application data directory (e.g. C:\ProgramData\METTLER TOLEDO\iC IR\<version>\...) whenever a sample is collected. This backup file is automatically deleted when the document is saved or closed.

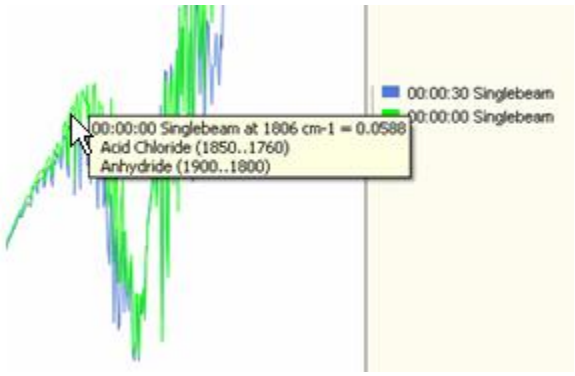
Creating a Spectra Library

A library or collection of spectra can be created to serve as a reference for a group of experiments. The library is composed of the functional group of standard chemical references stored as a library document. Experiments run using standard functional references with your instrument can help determine the accuracy of data from your current experiment.

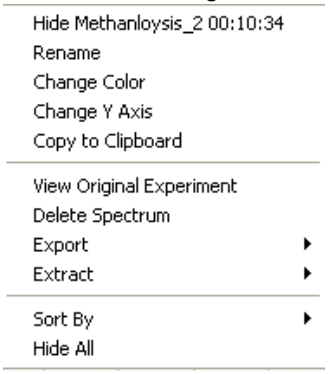


The spectra can be view as a percent of transmittance instead of absorbance by checking the **Display % Transmittance** checkbox.

When the mouse hovers over a data point, a tooltip is displayed that provides details about the data.

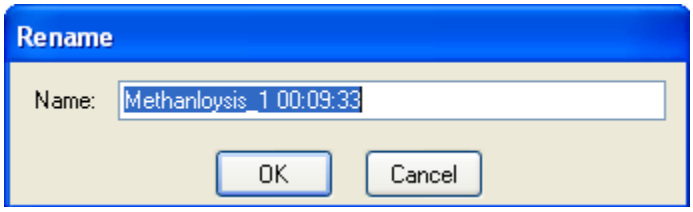


The Spectra Library display contains all plots for all spectra currently in the library. Individual spectra can be hidden from view by right-clicking on the trace and selecting the **Hide . . .** option from the menu.

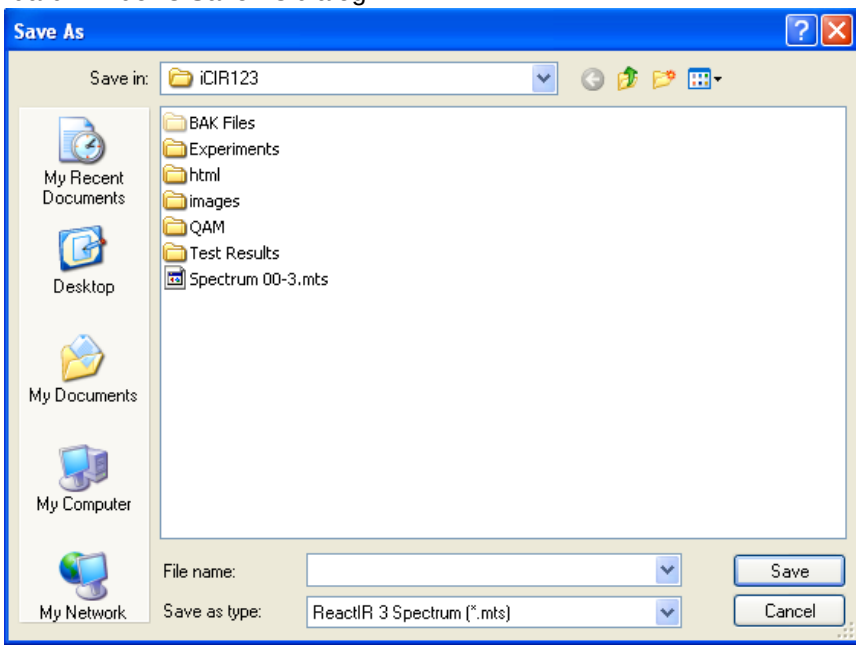


The same menu and method can be used to remove spectra from the library.

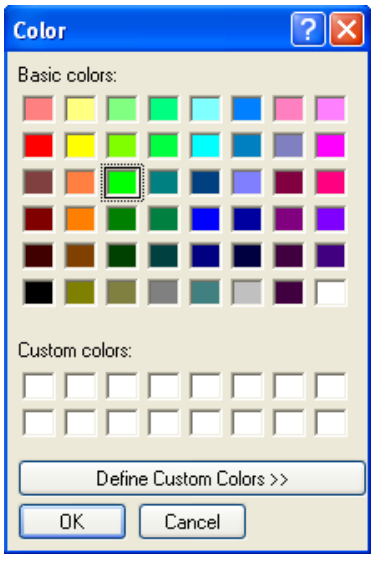
To rename spectra right-click on the trace and select the **Rename** option. The rename reference Spectrum dialog is opened, allowing the user to enter a new name.



The **Export** option on the right-click (context) menu allows the user to export spectra to an external file. The option opens a standard Windows Save As dialog.

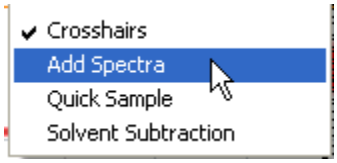


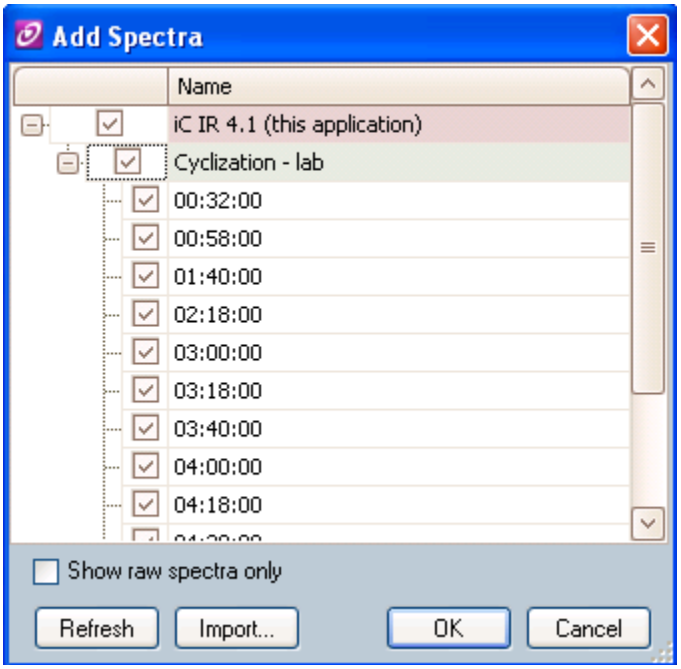
The color of a trace can be changed using the **Change Color** option on the context menu. The option opens a color browser from which the user selects a color.



Adding Spectra to a Spectra Library

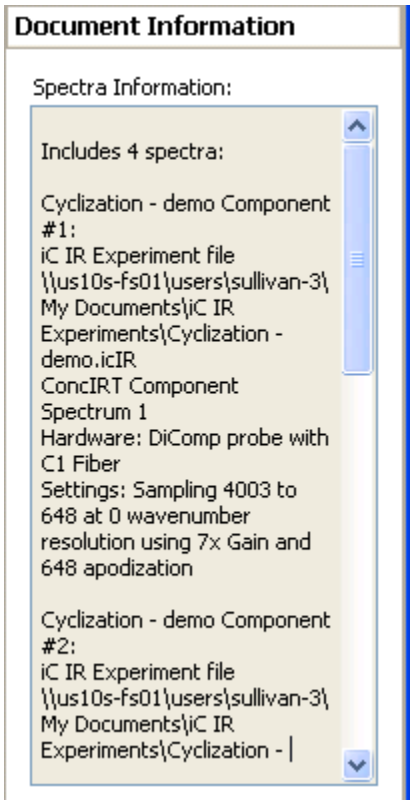
Spectra is added to a library using the Select Spectra dialog. The dialog contains a list of existing spectra in a collapsible tree-view. The dialog is accessed by clicking the Add Spectra button or by selecting the **Add Spectra** option in the context menu.





The user can either select existing spectra to open or click the **Cancel** button to open a blank Spectra Library display. Refer to Creating a Spectra Library for a description of the Spectra Library display.

The Document Information task pane contains information about each spectra in the Spectra Library. As spectra are added to the library, the Document Information task pane is updated with information about that spectra.

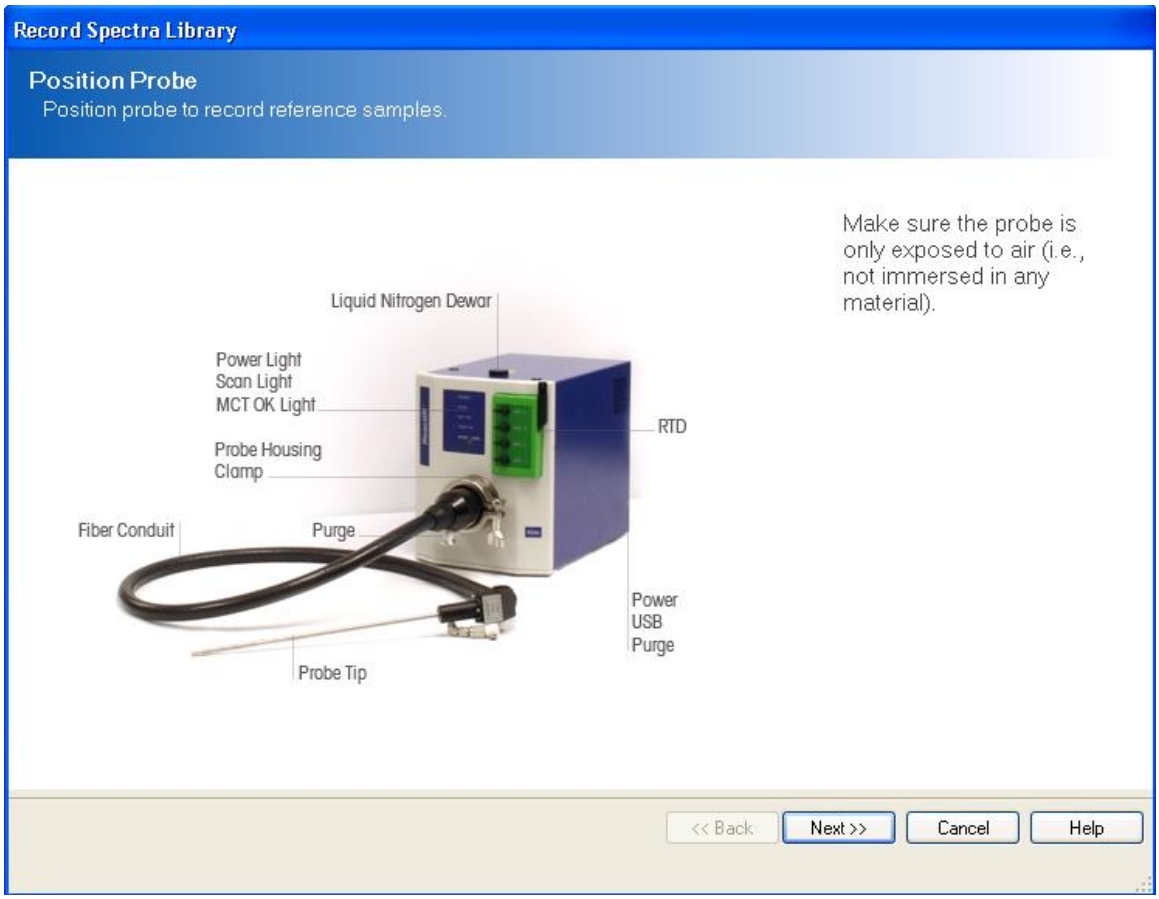


Collecting a Spectrum for a Spectra Library

A Wizard is used to collect a reference spectra. The wizard guides the user through the process with the following steps. The wizard is accessed by clicking the Sample Using Wizard button.

Positioning the Probe for Recording Spectra

This page of the wizard is an informational page that shows the position of the probe for cleaning. Note: the instrument image shown may be different depending on your instrument configuration.

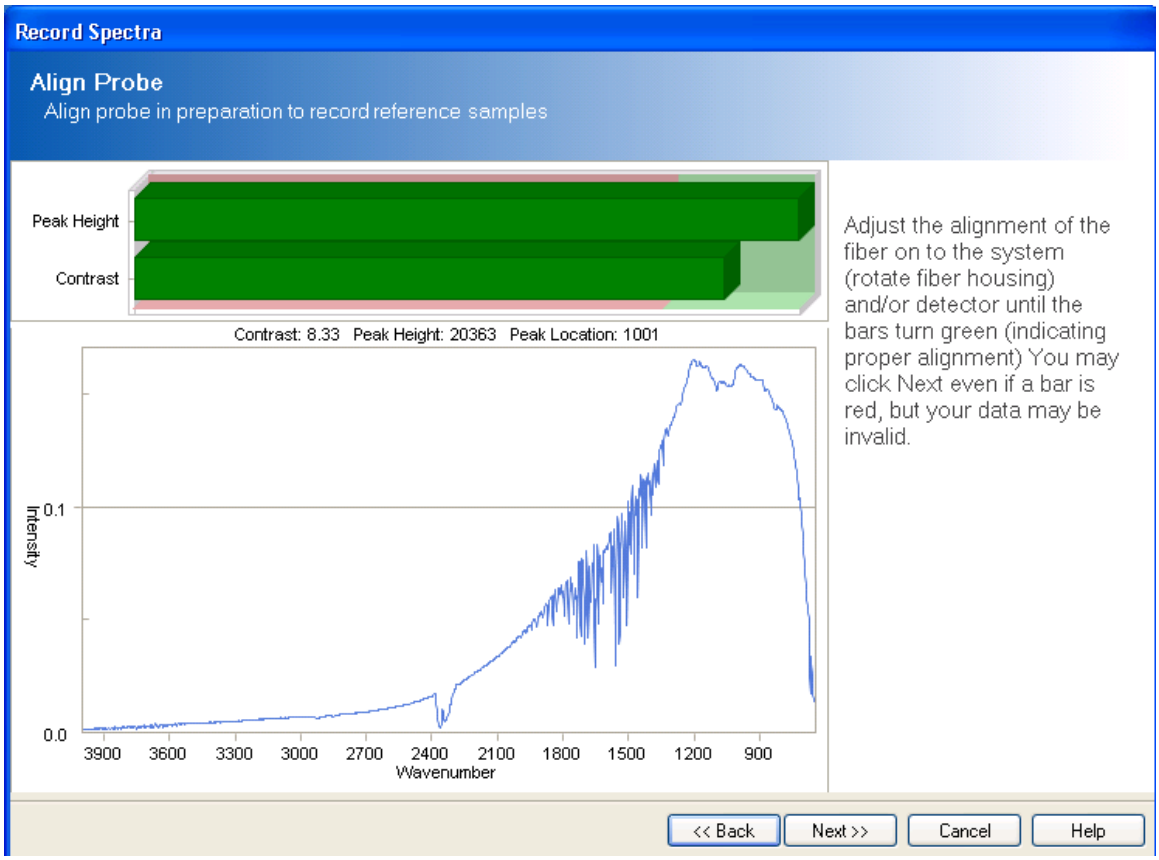


Click the **Next** button.

Aligning the Probe for Recording Spectra

This page of the wizard is used to physically align the probe. When the probe is aligned correctly, the indicator bars turn green.

Refer to Aligning the Probe for instructions about aligning the probe.



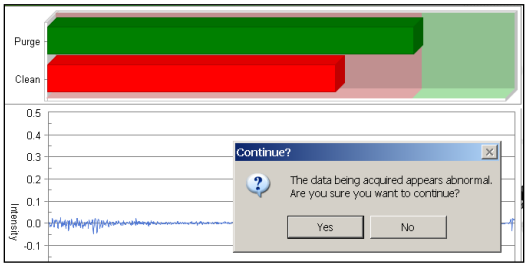
Cleaning the Probe for Recording Spectra

Acetone is recommended as a solvent.

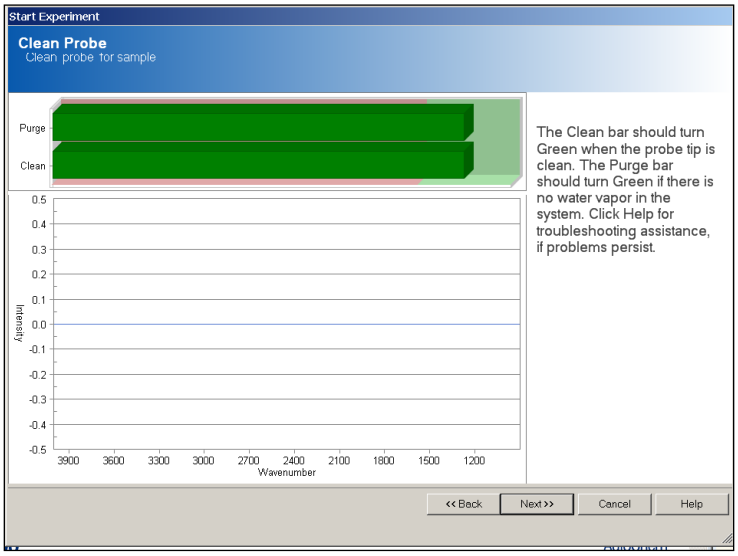
The two colored bars indicate if the probe is clean or dirty. If the bars are red and in the red area of the purge and clean zone, the probe surface is dirty.

When both bars are green and extend into the green zone on the purge and clean zone, click Next to continue the setup.

If you click on the Next button and the probe indication is a dirty probe, the following display appears.



A clean probe is indicated below.



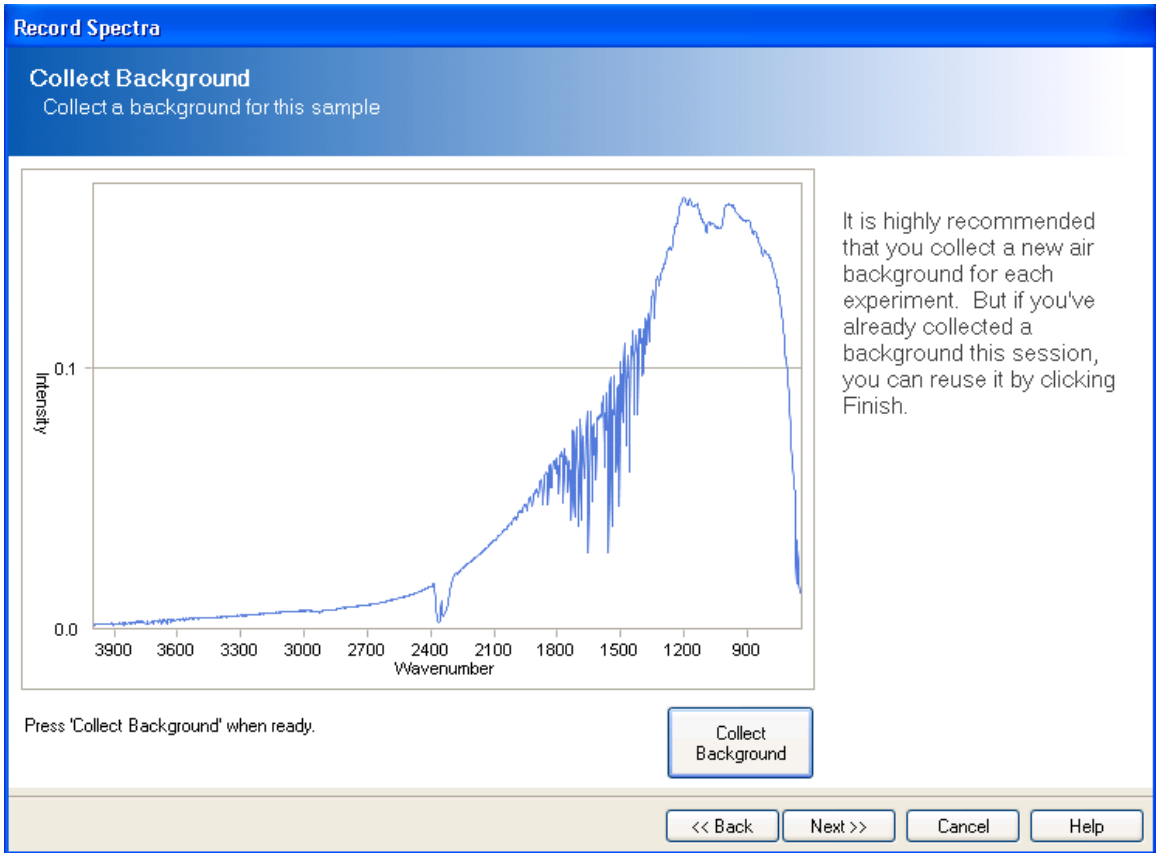
Collecting a Background for the Spectra

Note: A background spectrum should be collected for reference after the probe has been aligned properly and the sensor cleaned.

Modern FT-IR utilizes a background measurement to eliminate any instrument response in the desired spectrum. Historically, one is measuring I/Io where I is the intensity of the light after passing through a sample and Io is the intensity without any sample present. In order to collect good infrared data sets with the iC10 a background of a thermally stable, well purged system with a clean probe must be taken. This background will be collected before each new experiment is performed. The wizard leads one through this procedure.

Click on the **Collect Background** button to collect a background sample.

When the background spectrum is successfully collected, the displayed spectrum changes color from blue to green. Click the **Next** button.



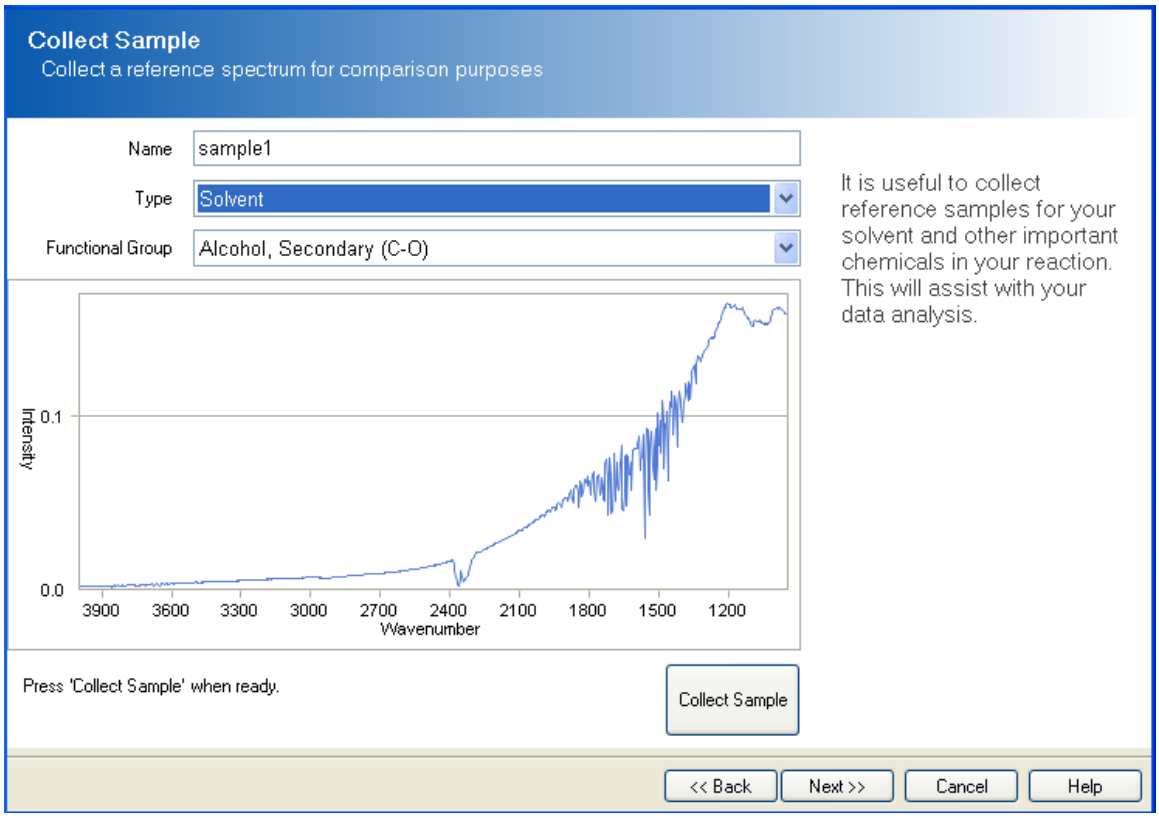
Collecting a Reference Sample for the Spectra

The **Collect Sample** page of the wizard allows the user to collect reference spectra for an experiment. The wizard allows the user to collect any number of reference spectra for comparison and analysis purposes.

If you do not want to collect reference spectra, click the **Next** button.

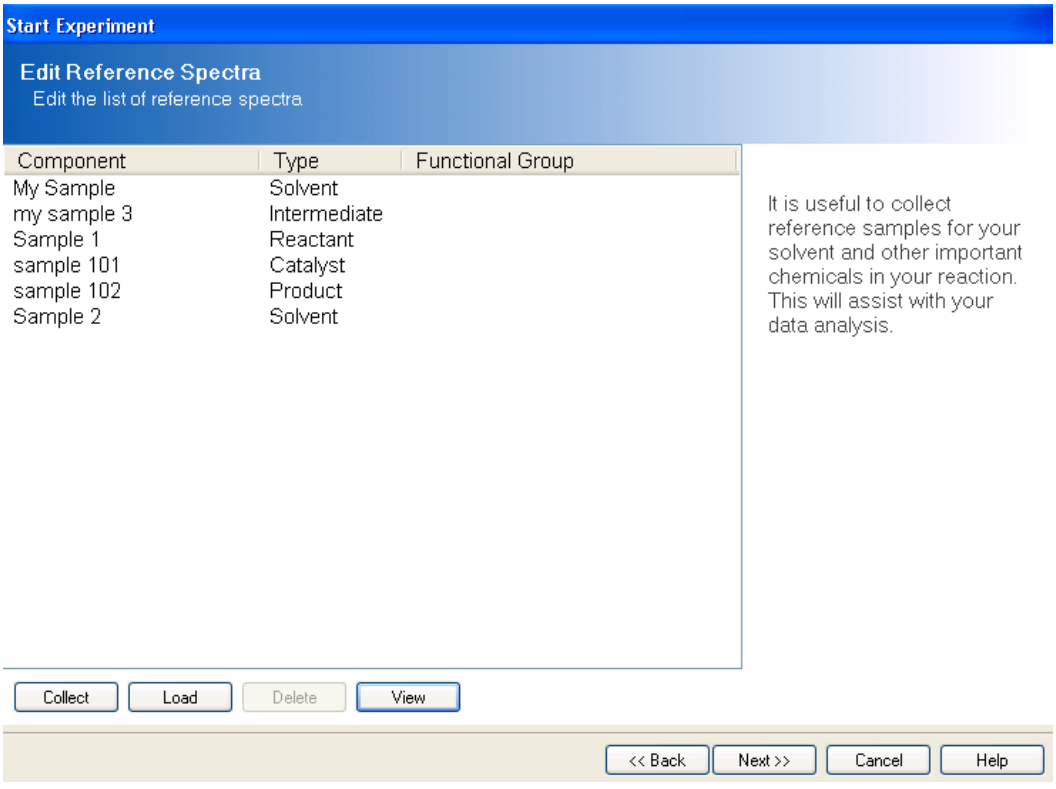
To collect reference spectra:

- Enter a name for the reference spectrum.
- Select a type for the sample from the drop-down list.
- Select the sample from a list by clicking on the **Select** button.
- Select a functional group, if desired, for the reference. Functional groups are useful to auto-define peaks.
- Collect the sample by clicking on the **Collect Sample** button. When the button is clicked, the spectrum for the sample is displayed in the page.

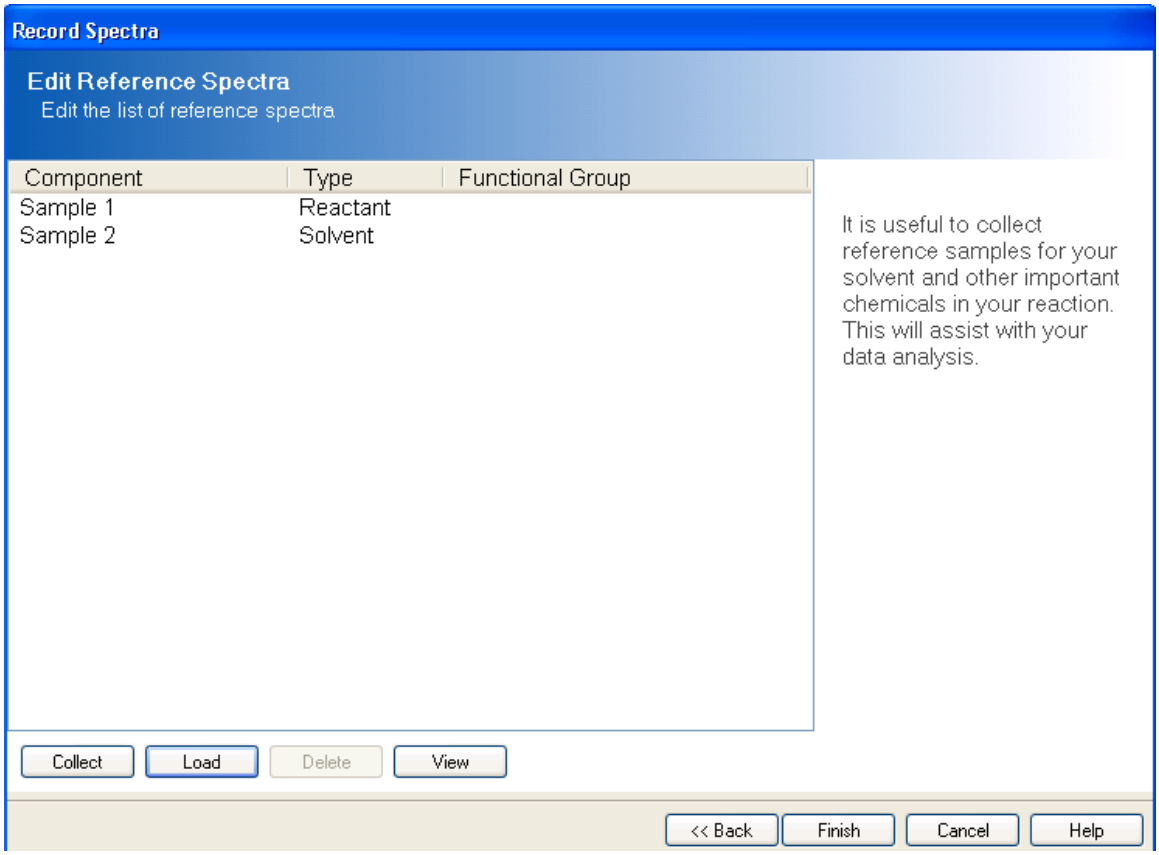


After the reference samples are collected, click **Next** button to advance to the next page of the wizard.

The **Edit Reference Spectra** page of the wizard displays a list of all collected reference spectra for the experiment.



Editing the Reference Spectra



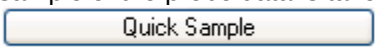
Several options are available on the page.

- Clicking the **Load** button opens a file browser to allow the user to open an existing spectra library to use for the reference.
- Clicking the **View** button displays the spectra in a viewer. Refer to View Spectra Library Dialog.
- Clicking the **Collect** button re-starts the spectra collection procedure to collect a new reference spectrum.

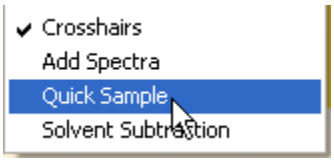
Click the **Finish** button to complete the spectra library and close the wizard.

Collecting a Quick Sample

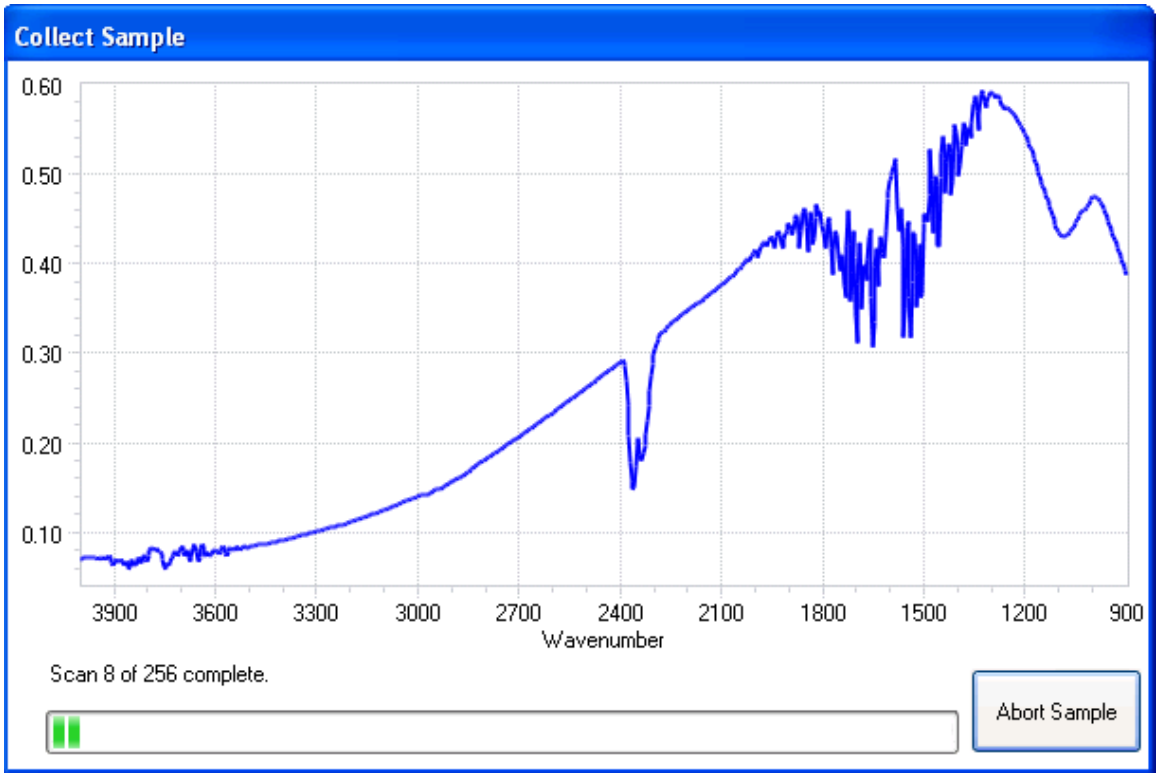
A quick sample of live data can be taken for the Spectra Library. When a quick sample is initiated a single sample of the probe data is taken. A quick sample is operation is started by clicking the



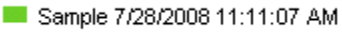
button or by selecting the Quick Sample option on the context menu.



The sample is immediately taken and the result is displayed on the Collect Sample dialog.



When the sample is complete, it is added to the spectra library. The name of the sample is reference by the date and time.

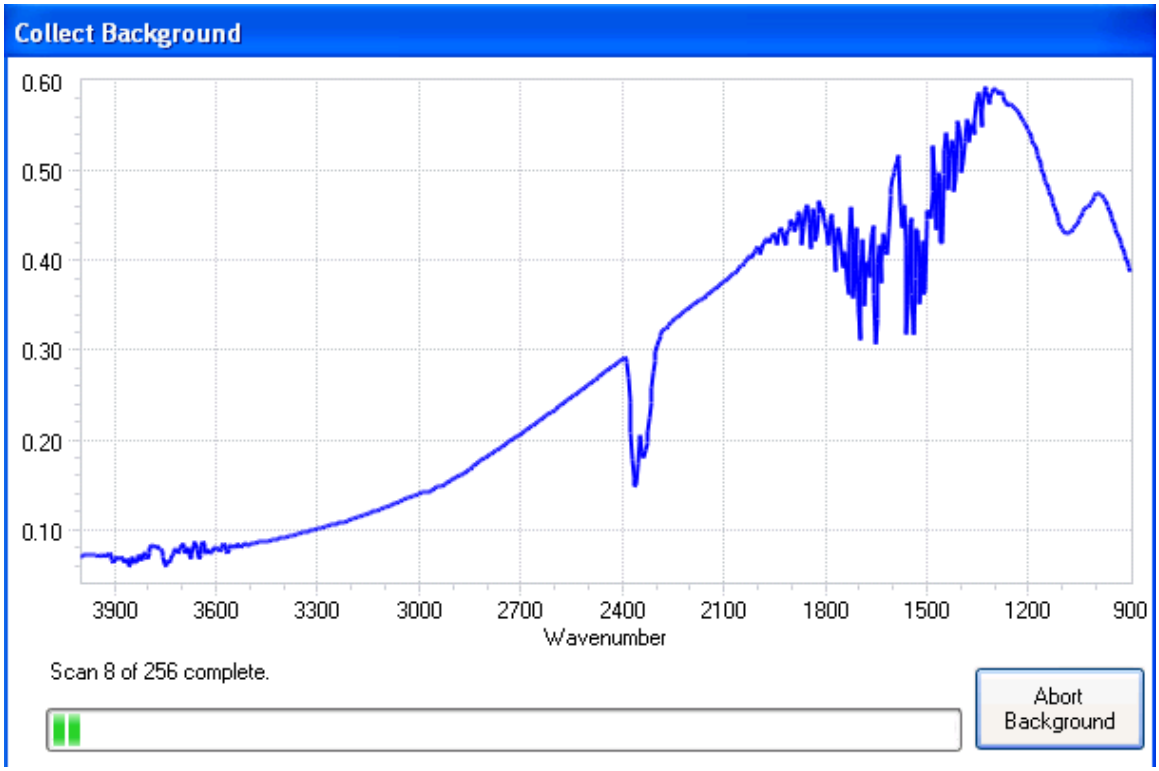


Collecting a Quick Background Sample

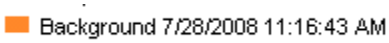
A quick sample of background data can be taken for the Spectra Library. When a quick background scan is initiated a single sample of the background data is taken. A quick background is operation is started by clicking the 

button.

The sample is immediately taken and the result is displayed on the Collect Background dialog.



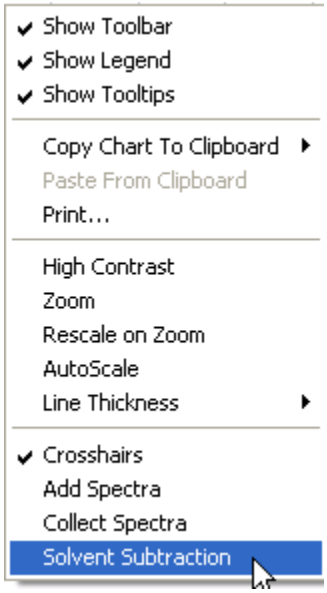
When the background sample is complete, it is added to the spectra library. The name of the background sample is reference by the date and time.



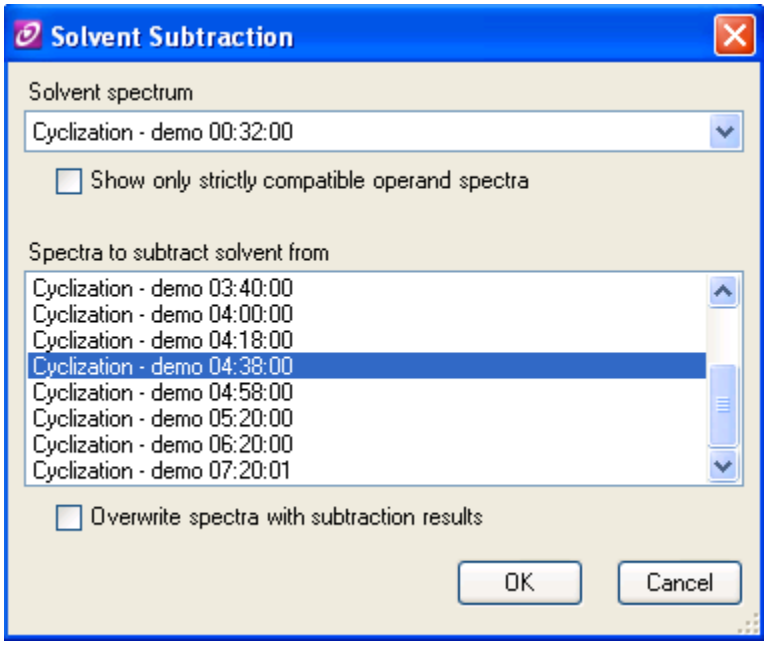
Solvent Subtraction

The Solvent Subtraction dialog is used to remove the effects of a solvent from spectra. The dialog is accessed clicking the 

button or by right-clicking in the graph area of the Spectra Library window and selecting the **Solvent Subtraction** option from the menu.

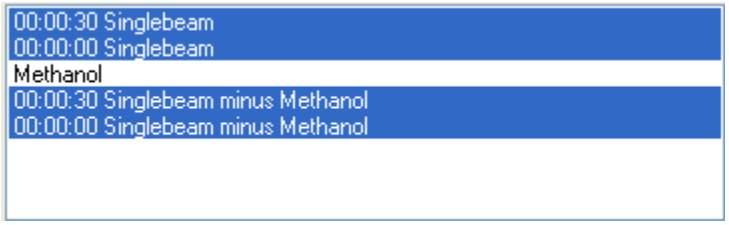


The Solvent Subtraction dialog contains a droplist of all defined solvents.



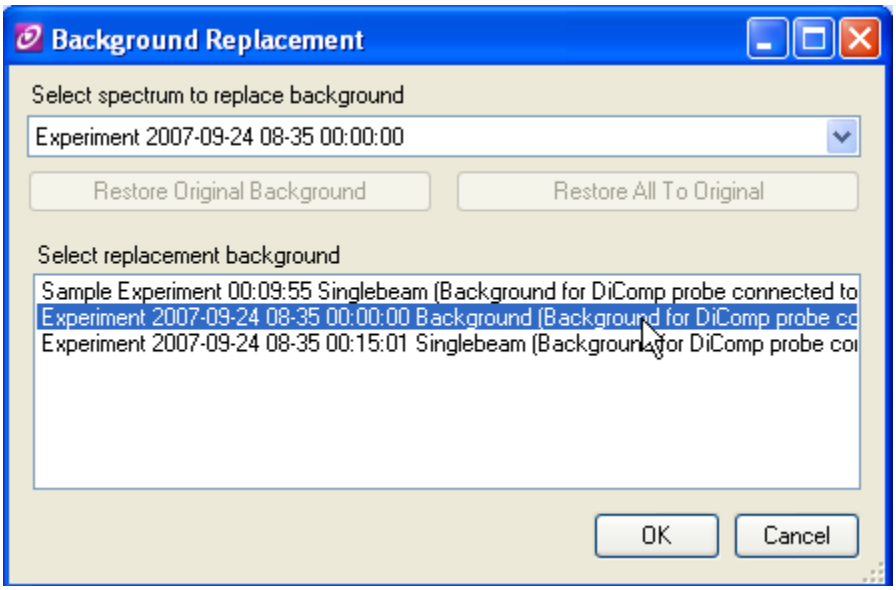
The user selects the solvent to subtract from the droplist and then selects the spectra from which the solvent will be subtracted. If the Overwrite Spectra with Subtraction Results checkbox is checked, the original spectra

will be replaced with the subtracted spectra. Otherwise, the subtracted spectra is added to the library as shown below.



Replacing a Background

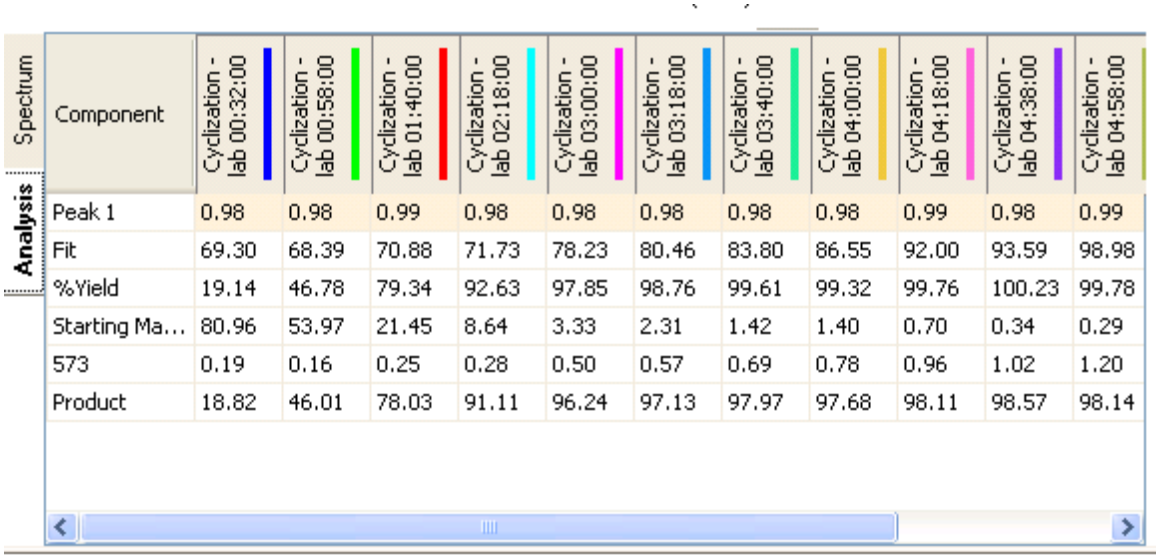
The current background spectra can be replaced by clicking the Background Replacement button. Clicking the button opens the Background Replacement dialog.



The dialog contains a list of currently loaded backgrounds. The section Background Replacement describes how to load backgrounds.

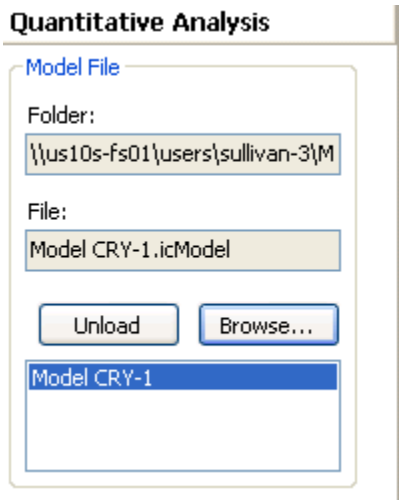
Spectra Library Analysis Tab

The Analysis tab of the Spectra Library viewer displays a table of results from a Quantitative Analysis.



Component	Cyclization - lab 00:32:00	Cyclization - lab 00:58:00	Cyclization - lab 01:40:00	Cyclization - lab 02:18:00	Cyclization - lab 03:00:00	Cyclization - lab 03:18:00	Cyclization - lab 03:40:00	Cyclization - lab 04:00:00	Cyclization - lab 04:18:00	Cyclization - lab 04:38:00	Cyclization - lab 04:58:00
Peak 1	0.98	0.98	0.99	0.98	0.98	0.98	0.98	0.98	0.99	0.98	0.99
Fit	69.30	68.39	70.88	71.73	78.23	80.46	83.80	86.55	92.00	93.59	98.98
%Yield	19.14	46.78	79.34	92.63	97.85	98.76	99.61	99.32	99.76	100.23	99.78
Starting Ma...	80.96	53.97	21.45	8.64	3.33	2.31	1.42	1.40	0.70	0.34	0.29
573	0.19	0.16	0.25	0.28	0.50	0.57	0.69	0.78	0.96	1.02	1.20
Product	18.82	46.01	78.03	91.11	96.24	97.13	97.97	97.68	98.11	98.57	98.14

An existing Quantitative Analysis Model can be opened from the Quantitative Analysis task pane and viewed.



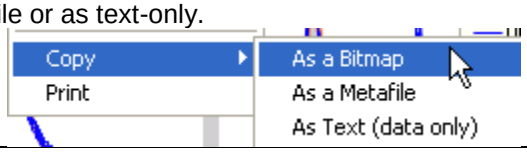
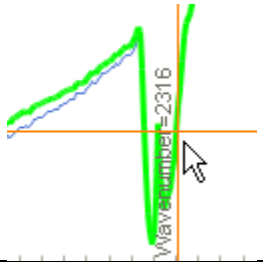
Only existing models can be viewed. In order to create Quantitative Analysis Models, the optional QAM add-on must be installed.

Spectra Library Context Menu

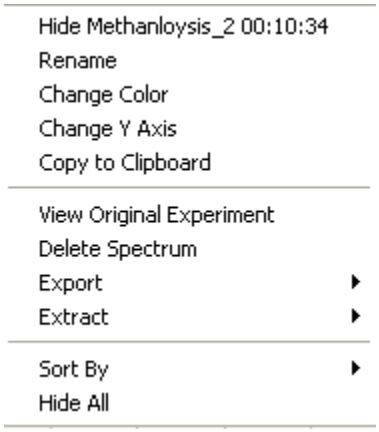
The Spectra Library display incorporates several right-click or context menus that contain tools for customizing the displayed data. The first menu is displayed when the user right-clicks on the data area of the display.

The menu contains the following items.

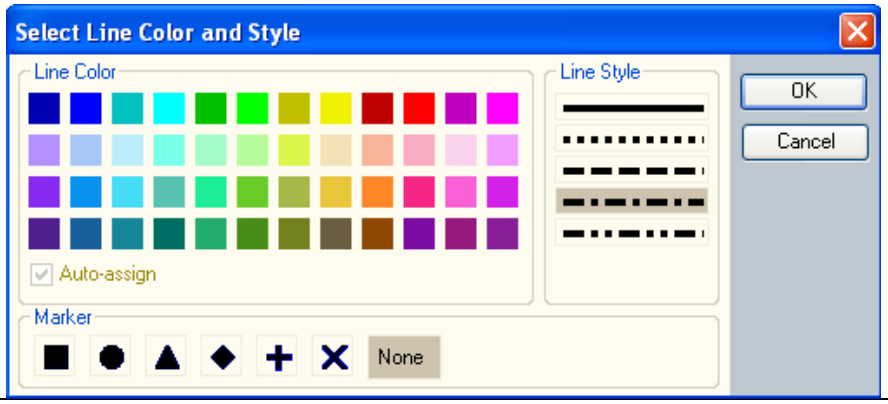
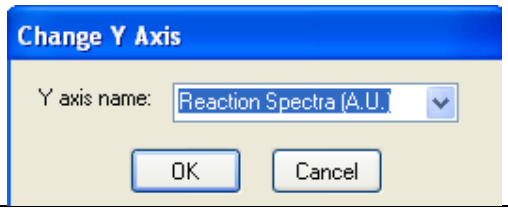
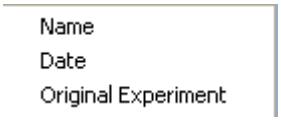
Show Toolbar	Displays the toolbar at the top of the display.  The toolbar contains the following tools.  Prints the display.  Copies the display to the clipboard.  Zooms the display.  This button is only visible when the Zoom function is enabled. The button resets the zoom to its original scale.  Rescales only the X-axis on zoom.  Auto scales the Y-axis.  Displays the Legend Panel.  Adds a new spectra from a Spectra Library.  Opens the Solvent Subtraction dialog.  Collects opens the Collect Spectra wizard.

Show Legend	Displays the Legend Box.
Show Tooltips	Displays tooltips on the graph as data points are selected.
Copy to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
Paste from Clipboard	Pastes tab delimited numeric data into the graph.
Print	Opens the Print dialog to print the display.
High Contrast	Displays the graph with a black background.
Zoom	Zooms the display. Refer to Spectra Zoom Operation
Reset Zoom	Resets the zoom to its original scale. This button is only displayed when the display is in a zoomed condition.
Rescale on zoom	Rescales only the X-axis on zoom.
Auto-scale	Auto scales the Y axis.
Line Thickness	Selects the line thickness for the plots.
Crosshairs	Displays crosshairs at the location of the cursor. 
Add Spectra	Opens the Select Spectra dialog. See Adding Spectra to a Spectra Library.
Quick Sample	Opens the Collect Sample dialog. See Collecting a Spectrum for a Spectra Library.
Solvent Subtraction	Opens the Solvent Subtraction dialog.

The second menu is displayed when the user right-clicks on a data point in the display and contains tools for customizing the data. The menu is accessed by right-clicking on a data point in the distribution or by right-clicking on a measurement in the legend. This method may be preferable because it might be difficult to select a precise data point.



The menu contains the following items.

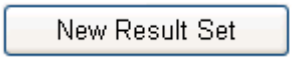
Hide . . .	Hides the selected distribution. The distribution is hidden in the graphic area but remains listed in the Details grid.
Rename	Opens a dialog allowing the user to rename the spectra
Change Color	
Change Y Axis	
Copy to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
View Original Experiment	Opens the experiment containing the original spectra in a new tab.
Remove Spectrum	Permanently removes the selected spectra from the viewer.
Export	Exports the selected spectra to a file. The user has the option of exporting only the selected spectra or all pinned spectra.
Extract	Allows the user to extract the background or single beam from the selected spectra.
Sort By	Sorts the spectra in the legend and detail area. The spectra can be sorted by:  Selecting a sort option a multiple times will reverse the sort order; ascending, descending and remove sort.
Sort/Hide All	Hides or displays all spectra on the graph. This option is useful when displaying many spectra on a graph.

Working with Result Sets

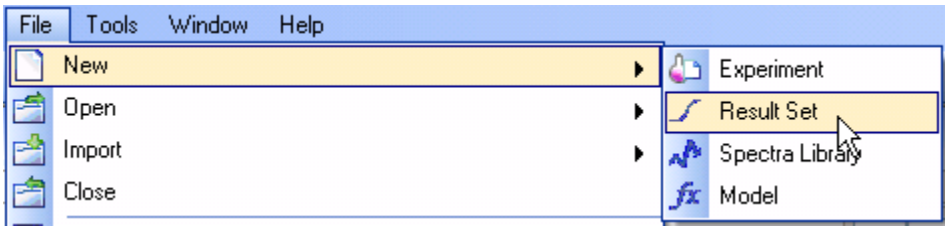
A Result Set is a separate file containing spectra and trend analysis selected by the user. Data from several experiments can be put into one result set for comparison.

Creating a Result Set

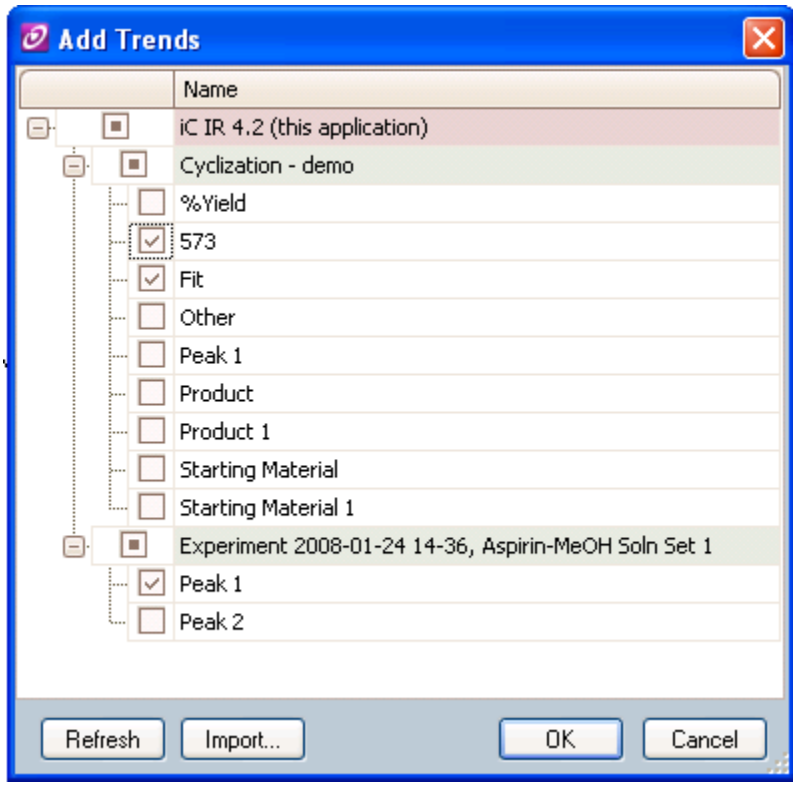
Spectra and trends from a file can be easily transferred to another file called a **Result Set**.

To create a new Result Set, click the 

button on the Start Page or select the **New/Result Set** option from the **File** menu.



The **Add Trends** dialog is opened.



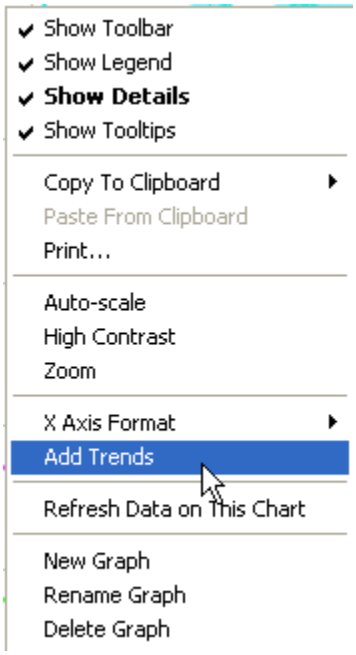
The dialog contains a tree-view of all trends in open documents from all iC applications. Select the trends to include in the new Result Set and click the **OK** button. When the **OK** button is clicked, the dialog closes and the new **Result Set** is displayed.

It is good practice to save the new Result Set for future reference. To save the set, select the **File/Save As..** menu option.

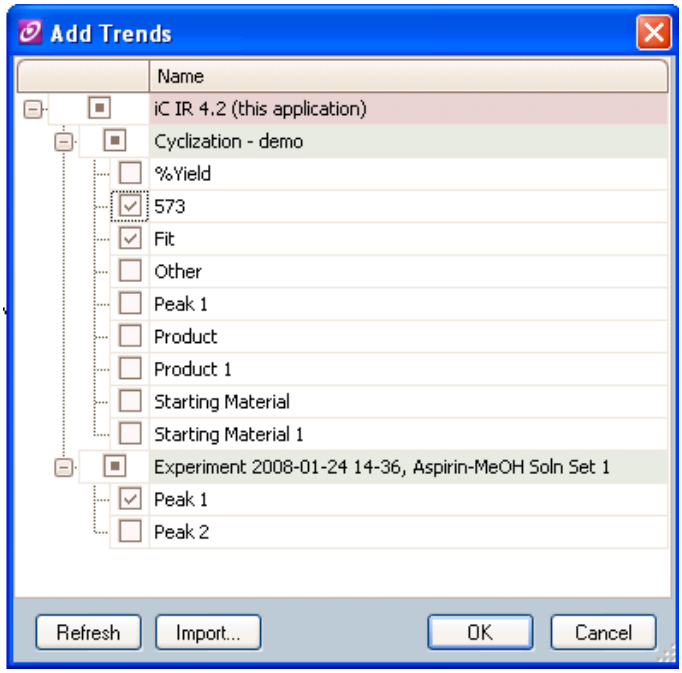
Adding Trends to a Result Set

Additional trends can be added to an existing Result Set using two methods.

The user can right-click in the graph area of the display and select the **Add Trend** menu option.



The Add Trends dialog is open. The dialog allows the user to select trends from multiple experiments.

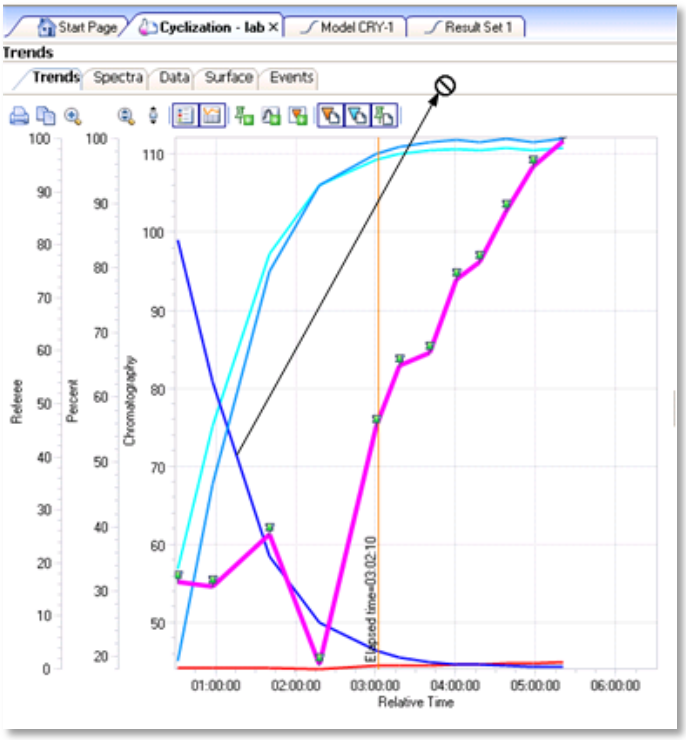


The user can also drag trends from an experiments from a Trend display to the Result List display.

To add trends by this method:

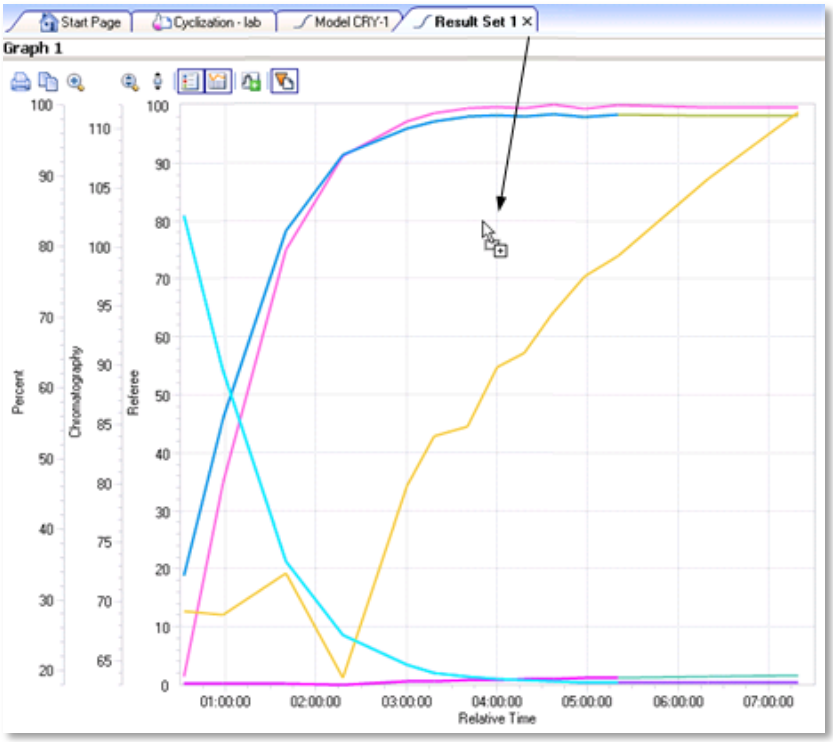
On a Trend display, click on trend to be included in new Result Set. The cursor changes to a ⃠ if the plot was correctly selected.

Drag the cursor to the Result Set tab.



When the cursor hovers on the Result Set tab, focus is given to the tab and the Result Set is displayed.

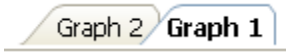
The cursor changes to a shortcut icon,



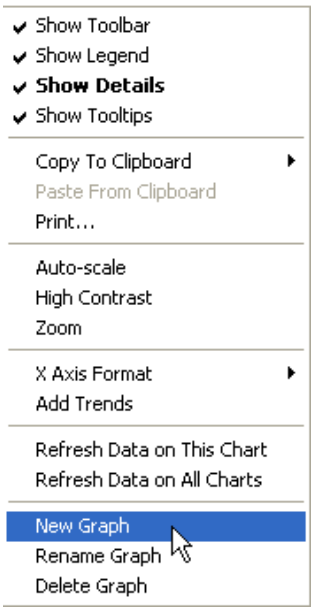
The dragged trend is copied to the Result Set.

Adding a New Graph to a Result Set

New graphs can be added to result sets. New graphs appear as tabs along the top of the Result Set display.



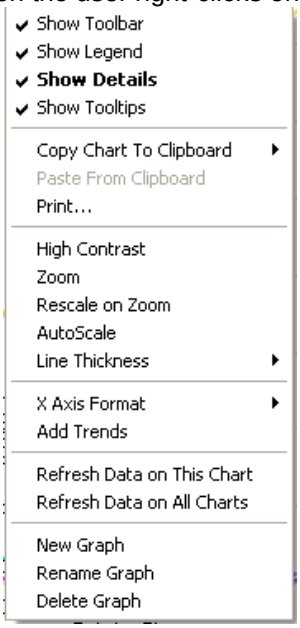
New graphs are created by selecting the New Graph option from the right-click menu.



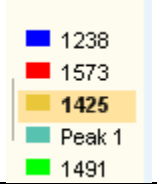
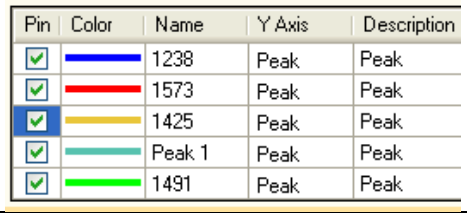
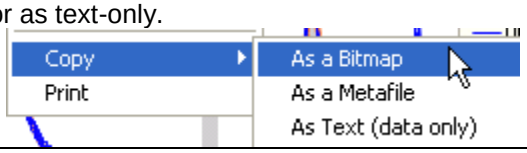
A new blank graph is opened. Trends are added to the graph as described previously. Refer to Adding Trends to a Result Set.

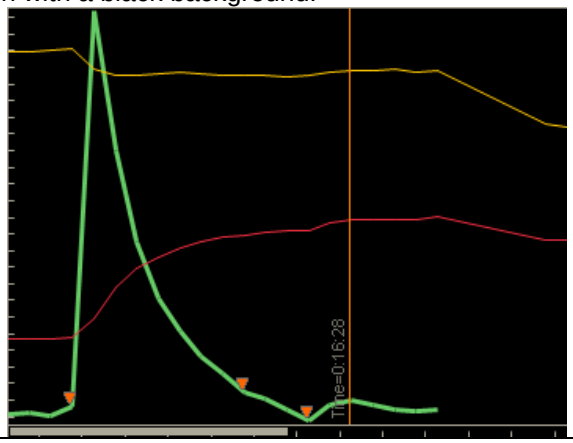
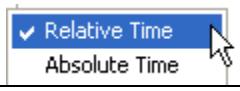
The Result Set Context Menu

The Result Set display incorporates a right-click or context menu that contains tools for customizing the displayed data. The menu is displayed when the user right-clicks on the data area of the display.

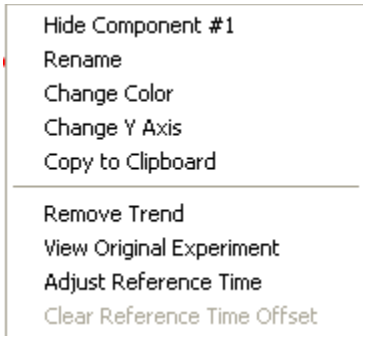


The menu contains the following items.

Show Toolbar	Displays the toolbar at the top of the display.  The toolbar contains the following tools.  Prints the display.  Copies the display to the clipboard.  Zooms the display.  This button is only visible when the Zoom function is enabled. The button resets the zoom to its original scale.  Rescales only the X-axis on zoom.  Auto scales the Y-axis.  Displays the Legend Panel.  Displays the Details Panel.  Adds a Reference Trend to the graph. Clicking the button opens the Select Trend dialog.  Displays user-generated annotations on the graph.
Show Legend Box	Displays a legend box which lists each trend and its name. 
Show Grid	Displays the grid. 
Copy to Clipboard	Copies the display to the clipboard. The display can be copied as a bitmap, Windows metafile or as text-only. 
Paste from Clipboard	Pastes numerical data into the graph as a plot.
Print	Opens the Print dialog to print the display.

High Contrast	Displays the graph with a black background. 
Zoom	Zooms the display. Refer to Zooming.
Reset Zoom	Resets the zoom to its original scale.
Rescale on zoom	Rescales only the X-axis on zoom.
Autoscale	Autoscales the Y-axis
X Axis Format	Selects the time format for the X axis. 
Add Trends	Adds a new trend to the graph.
Refresh data on this Chart	Refreshes trend data on this graph only.
Refresh data on all Charts	Refreshes trend data on all graphs (in all tabs) in the Result Set.
New Graph	Creates a new blank graph in the Result Set.
Rename graph	Renames the selected graph.
Delete graph	Deletes the selected graph.

When the user right-clicks on a trend plot, another context menu Is displayed.



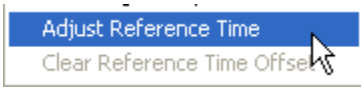
The menu contains the following items.

Hide . .	Hides the selected plot.
Rename	Opens a dialog allowing the user to rename the plot.
Change Color	Opens a color browser to select a color for the plot. Note that the color is only changed for the selected trend.
Change Y Axis	Allows the user to change the Y axis reference from a droplist. 

Copy to Clipboard	Copies the trend data to the clipboard as tab-delimited data.
Remove Trend	Permanently removes the trend from the Result List.
View Original	Views the experiment where the trend resides.
Adjust Reference Time	Refer to Adjusting the Reference Time for a Trend.
Clear Reference Time Offset	Refer to Adjusting the Reference Time for a Trend.

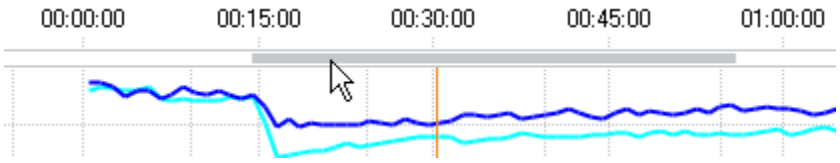
Adjusting the Reference Time for a Trend

The reference time offset for a trend in a result Set can be adjusted by clicking the **Adjust Reference Time** option from the context menu.



A slider bar is displayed at the top of the graph and two buttons are added to the toolbar.

Slide the bar to the desired offset.



Click the  button to save the change. Clicking the  button resets the offset and cancels the adjustment.

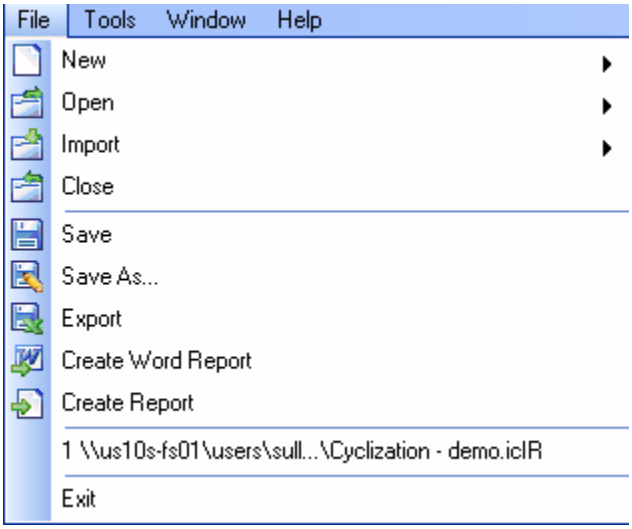
To return to the original reference time, select the **Clear Reference Time Offset** from the context menu.

Generating Reports of iC Data

Data from the various viewers in the iC software can be used to create experiment reports. The Microsoft Office® Clipboard is used to copy and paste data into a suitable application such as MS Excel® . In addition, a One-click reporting function is available to generate a preformatted experiment reports in either MS Word or XPS format.

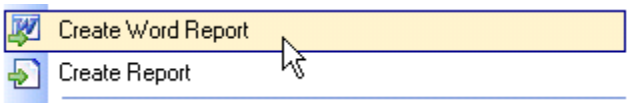
One-click Reporting Function

The One-click Reporting Function creates a pre-formatted report in MS Word or Microsoft XPS format. Reports can be made for any current document; Experiments, Spectra Libraries, and Result Sets. The Report contains all data in the document.

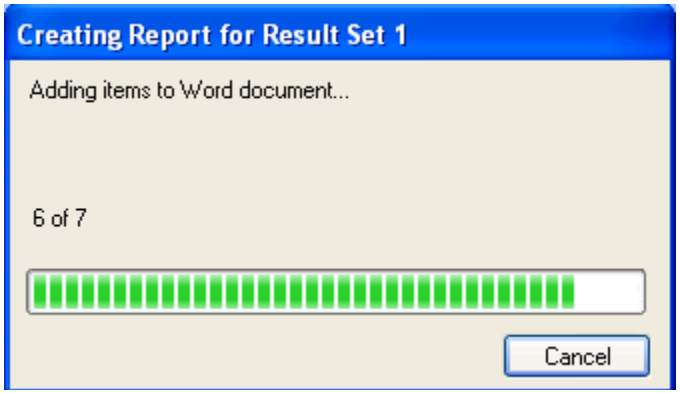


Creating a MS Word Report

The Word Report function is accessed from the **File/Create Word Report** menu.



When the Create Word Report menu option is selected, iC creates a report of the selected experiment. A progress indicator is displayed during the creation process.



When the report is created it is opened in MS Word as a new document.

Note that the format of the report is based on a MS Word template, iC Report Template.dot located in the Program folder for the iC application. This template can be edited by the user to create custom report formats. It is advisable to make a backup copy of the template file before any edits are made. The name of the template file should not be changed.

iC IR Experiment: Methanloysis_2 Author: AM\sullivan-3

1. Document Information

File Information:
File:
Methanloysis_2.icIR

Folder:
\\us10s-fs01\users\sullivan-3\My Documents\iC IR Experiments

Created:
4/11/2008 9:52:13 AM
Eastern Standard Time (-04:00:00)
by: joyce-2
machine name:
with: iC IR Software
Build 1.5.110.0

Last Updated:
4/11/2008 9:52:13 AM
by: flynn-3
machine name:
with: iC IR
Build 3.0.404.3

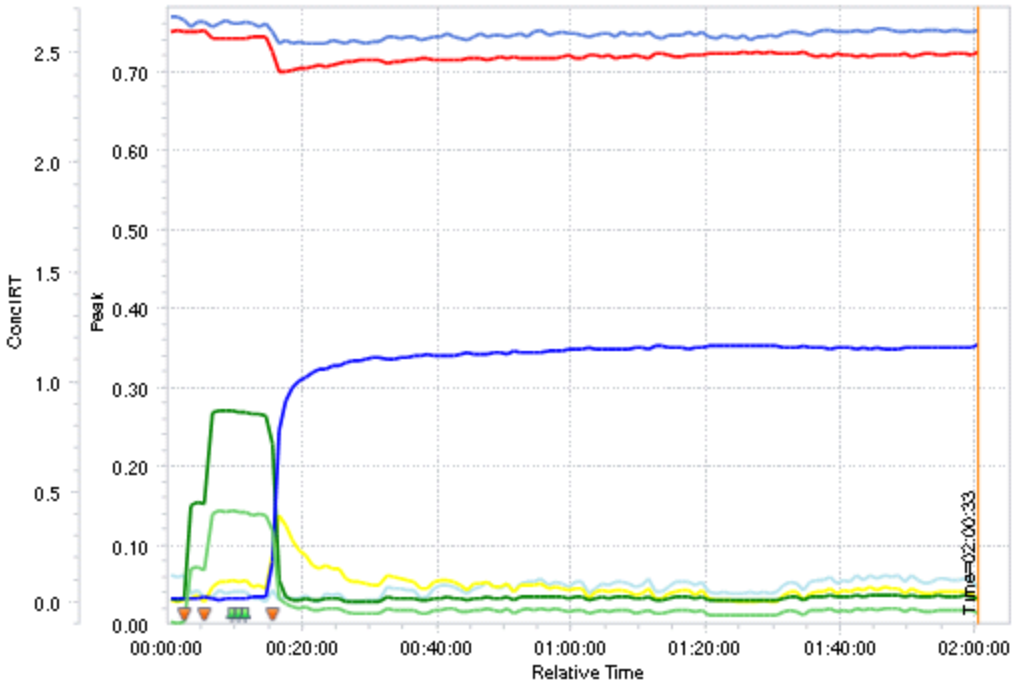
Experiment Information:
Started:
1/13/2005 10:45:34 AM
Completed:
1/13/2005 12:46:10 PM

Samples Acquired: 121
Instrument Information:
FTIR

Hardware: DiComp probe connected to an MCT detector with C1 Fiber
Settings: Sampling 4000 to 900 at 8 wavenumber resolution

iC IR Experiment: Methanloysis_2 Author: AM\sullivan-3

2. Trends

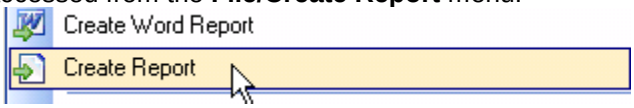


3. Legend

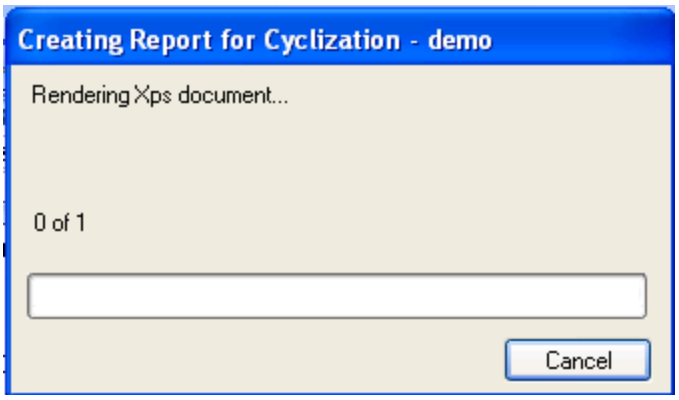
Visible	Color	Name	Y Axis	Value	Description
X		Methanol Peak	Peak	0.77	Peak; Height to Zero, Peak from 1065 to 1000
X		AcAnh Peak	Peak	0.00	Peak; Height to Zero, Peak from 1854 to 1802
X		ConcIRT Product	ConcIRT	0.02	ConcIRT
X		ConcIRT Methanol	ConcIRT	2.59	ConcIRT
X		ConcIRT AcAnh	ConcIRT	0.01	ConcIRT
X		ConcIRT Intermediate	ConcIRT	0.01	ConcIRT
X		Component#5	ConcIRT	0.12	ConcIRT

Creating an XPS Report

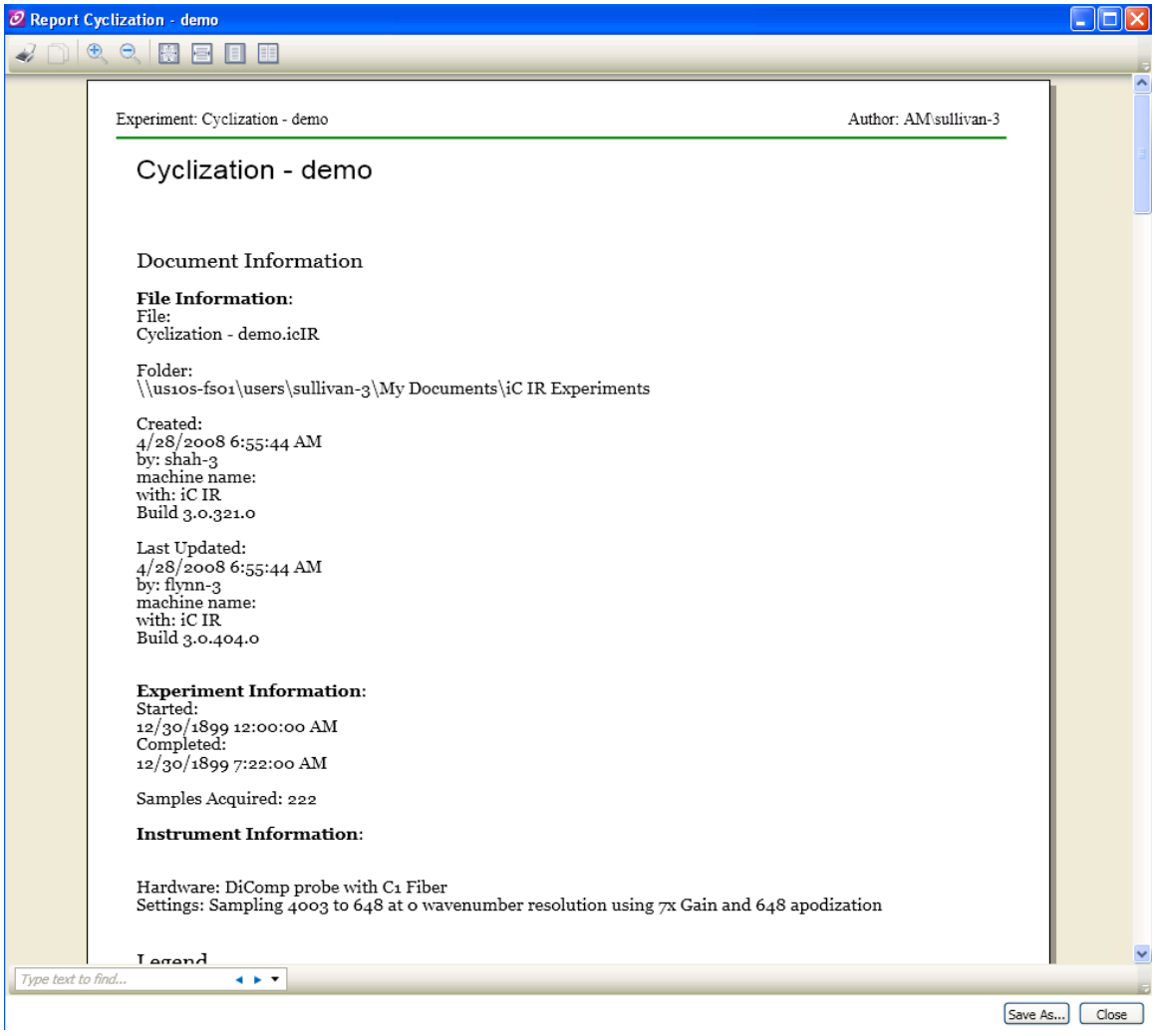
The XPS report function is accessed from the **File/Create Report** menu.



When the Create Report menu option is selected, iC creates a report of the selected experiment. A progress indicator is displayed during the creation process.



When the report is completed, it is opened in a viewer.

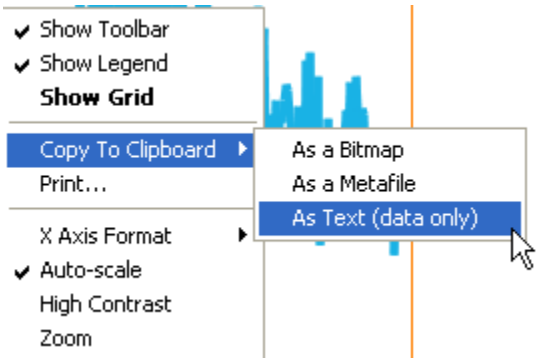


The report resides in a temporary directory and must be saved to permanently store the report. Note that the report is read-only and can be opened by any application supporting the XPS format (Internet Explorer, Microsoft XPS Viewer, etc.)

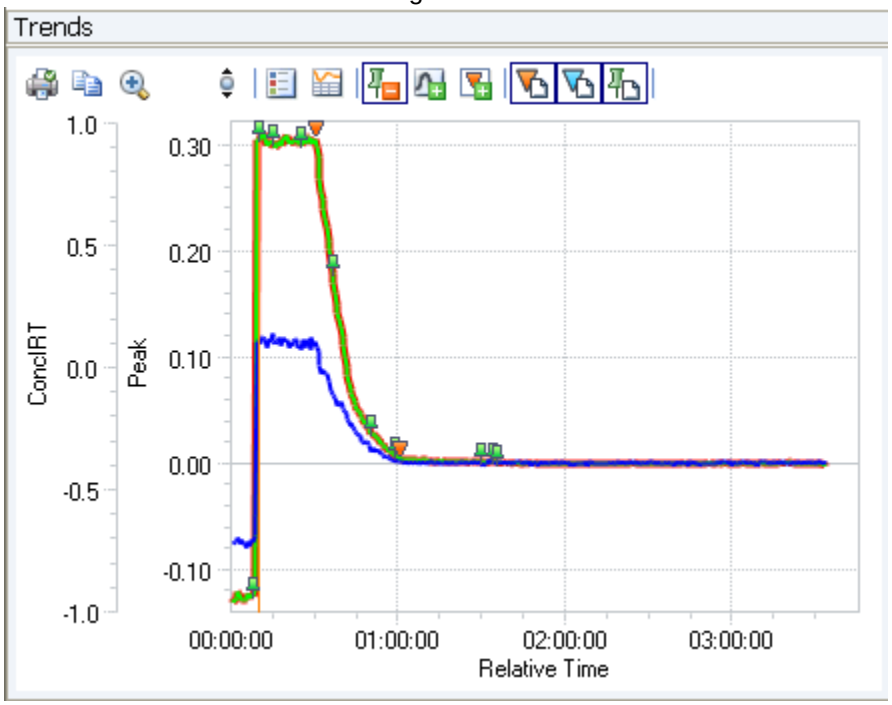
Copying Experiment Data

Data can be copied to the Clipboard using the viewers context (right-click) menu. The menu offers three copy functions for copying data.

- Bitmap – Copies the trend data as a bitmap (BMP) graphic file.
- Metafile – Copies the trend data as a Windows metafile (WMA) graphic file.
- Text – Copies the trend data as text. See the explanation below for a description of the textual format.



Both the Bitmap (BMG) and Metafile (WMA) options copy the data as a graphic image. The Windows Metafile format provides a clearer image but is not supported by some non-Microsoft applications. A bitmap image is universally supported but the file size tends to be large.



When trend data is copied as textual data, the data is copied as tab-delimited text. This format can readily be pasted into an Excel spreadsheet as a table. The first row of the data always contains the column headings for the table. This format is illustrated below.

Relative Time	Peak 1	Peak 2	Peak 3	Annotations
00:00:25	-0.075283	-0.129418	-0.129418	
00:00:55	-0.0757392	-0.129898	-0.129898	
00:01:25	-0.0733607	-0.127831	-0.127831	
00:01:55	-0.0730829	-0.126375	-0.126375	

00:02:25	-0.0695092	-0.120724	-0.120724	
00:02:55	-0.0719094	-0.12377	-0.12377	
00:03:25	-0.0749703	-0.129621	-0.129621	
00:03:55	-0.0713097	-0.128329	-0.128329	
00:04:25	-0.0757192	-0.12963	-0.12963	
00:04:55	-0.0768396	-0.128137	-0.128137	
00:05:25	-0.0803207	-0.129544	-0.129544	
00:05:55	-0.0739381	-0.123816	-0.123816	
00:06:25	-0.0785219	-0.126326	-0.126326	
00:06:55	-0.0740753	-0.123604	-0.123604	
00:07:25	-0.0728557	-0.122295	-0.122295	
00:07:55	-0.0748924	-0.124245	-0.124245	
00:08:25	-0.0677285	-0.119897	-0.119897	Sample 16 acquired at 00:07:55
00:08:55	-0.0500758	-0.0786976	-0.0786976	
00:09:25	0.115091	0.304483	0.304483	
00:09:55	0.114271	0.30542	0.30542	
00:10:25	0.112993	0.305691	0.305691	Sample 20 acquired at 00:09:55
00:10:55	0.118845	0.308429	0.308429	
00:11:25	0.118478	0.30985	0.30985	
00:11:55	0.115791	0.304085	0.304085	
00:12:25	0.116571	0.305012	0.305012	
00:12:55	0.108204	0.299243	0.299243	
00:13:25	0.115918	0.301942	0.301942	
00:13:55	0.115443	0.30222	0.30222	
00:14:25	0.115471	0.301603	0.301603	
00:14:55	0.121372	0.303738	0.303738	
00:15:25	0.114449	0.30034	0.30034	
00:15:55	0.11312	0.298218	0.298218	Sample 31 acquired at 00:15:25
00:16:25	0.115283	0.299927	0.299927	
00:16:55	0.116913	0.301626	0.301626	
00:17:25	0.11786	0.303789	0.303789	

If the viewer contains data that were sampled at different time intervals, the format of the exported data varies depending upon which data is selected, as explained below.

If data is selected in the viewer when the user selects the Copy function, iC exports the raw values for all the visible data based on the set of timestamps associated with the selected data. Note that in a typical experiment all the data have the same timestamps, so data is copied without manipulation.

For the more complex case in which there are multiple sets of timestamps to deal with, interpolation is used on those data with different timestamps to estimate the value at each timestamp in the selected data. In this case the selected data is copied ‘as is” since its timestamp is used as the master. Data with different timestamps will have their data copied as interpolated data.

If there is no selected data when the copy function is executed, the viewer creates a composite set of timestamps combining together ALL the timestamps for all the data and then eliminates any duplicates. Timestamps that vary by less than second are also eliminated.

Interpolation based on the timestamps of the selected data is useful for analyzing data collected across multiple experiments. On the other hand, to export the most complete data set when multiple sets of timestamps are involved, make sure that no data is selected. That way, all the actual data points plus additional interpolated values are copied. To deselect all data, click outside of the actual graph area in the viewer. This will de-select any selected data.

Copying Experiment Events

Annotations and messages from the Event Viewer can also be copied to the clipboard for inclusion in experiment reports. The events are copied as tab-delimited text that can be pasted as a table into MS Excel or Word.

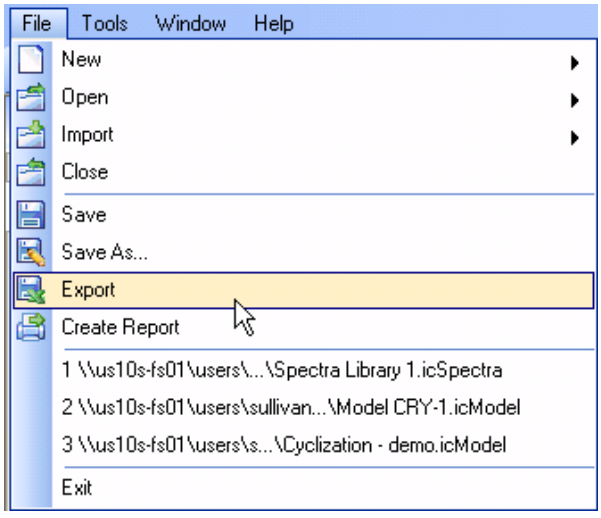
Before copying event data, the user should first format the data displayed in the Event Viewer window. This is done by using the filter buttons on the Event Viewer toolbar to select which types of events are displayed. The Copy function copies all the event data currently displayed in the window.

Type	Date/Time	Description
Audit	10:00:21 AM on 7/30/2007	Created Experiment Experiment 2007-07-30 10-00 in C:\iCIR306\Experiments
Audit	10:00:29 AM on 7/30/2007	Opened by John Doe
Audit	10:00:29 AM on 7/30/2007	Experiment started.
Audit	10:00:29 AM on 7/30/2007	Phase 1 started: Interval=10 sec. Duration=24:00:00
Audit	10:00:29 AM on 7/30/2007	Experiment initially paused. Awaiting start.
Audit	10:01:15 AM on 7/30/2007	Experiment resuming.
Audit	10:01:16 AM on 7/30/2007	Experiment AutoSaved
Annotation	10:02:02 AM on 7/30/2007	Increased heat by 50 deg C - JG
Audit	10:02:57 AM on 7/30/2007	Experiment paused by user.
Audit	10:03:36 AM on 7/30/2007	Experiment resuming.
Annotation	10:04:33 AM on 7/30/2007	Experiment paused to remove dirt from lens
Annotation	10:04:51 AM on 7/30/2007	Heat stabilized
Audit	10:05:31 AM on 7/30/2007	Experiment paused by user.
Audit	10:06:01 AM on 7/30/2007	Experiment resuming.
Audit	10:06:16 AM on 7/30/2007	Experiment AutoSaved
Audit	10:10:53 AM on 7/30/2007	Experiment paused by user.
Audit	10:11:01 AM on 7/30/2007	Experiment resuming.
Audit	10:11:17 AM on 7/30/2007	Experiment AutoSaved
Audit	10:11:46 AM on 7/30/2007	Experiment paused by user.
Audit	10:12:04 AM on 7/30/2007	Experiment resuming.

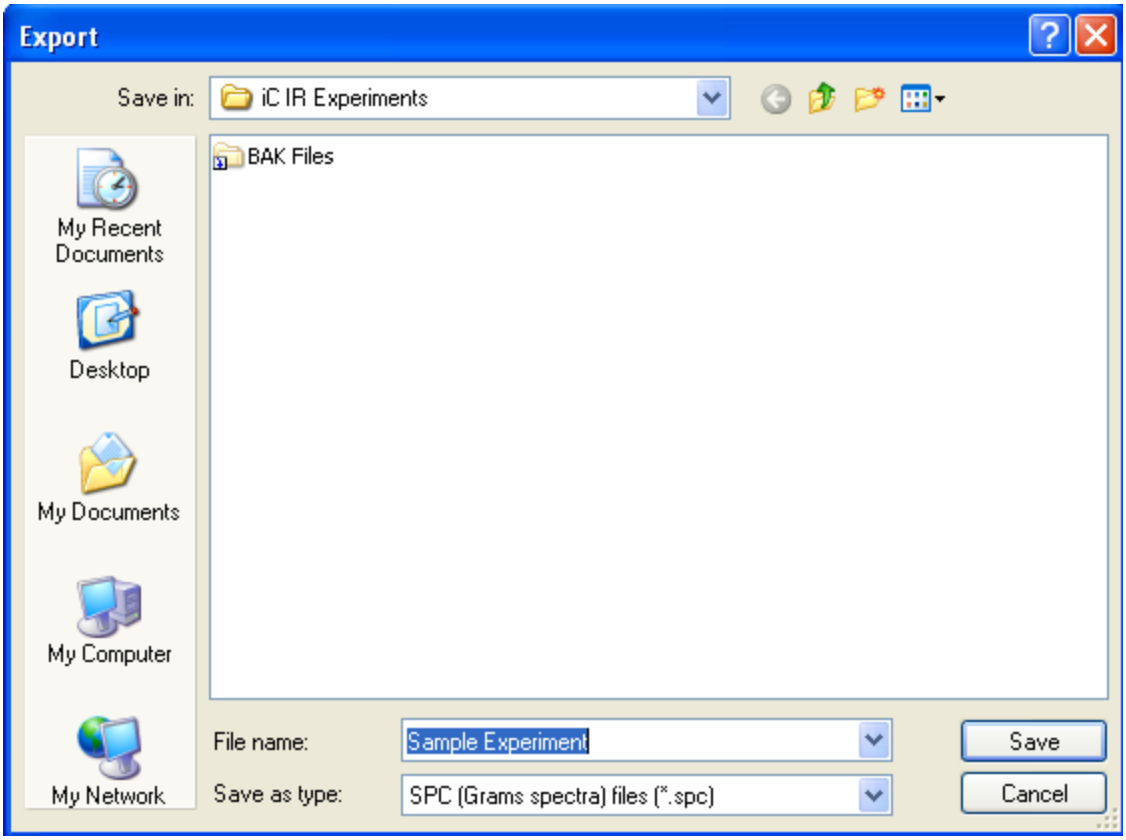
Exporting Experiment Data

Data from an entire experiment can be exported to an external CSV file. A CSV file can be directly opened by MS Excel. Depending on the actual experiment, the resulting file can be very large.

To export experiment data, select the **Export** button in the **File** menu.

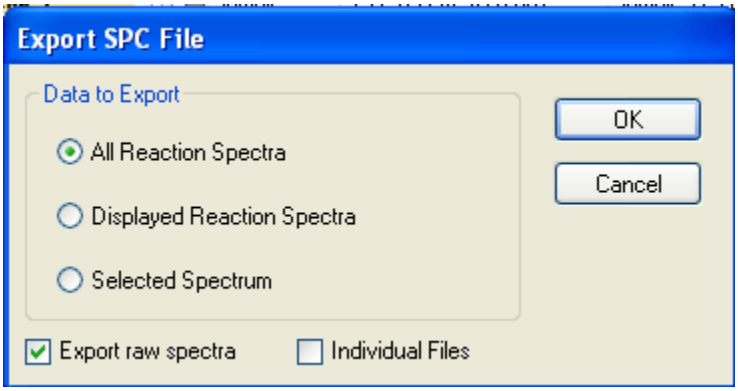


A standard **Save As** dialog is opened.



Enter a filename for the file and click the **Save** button.

The following dialog is displayed.



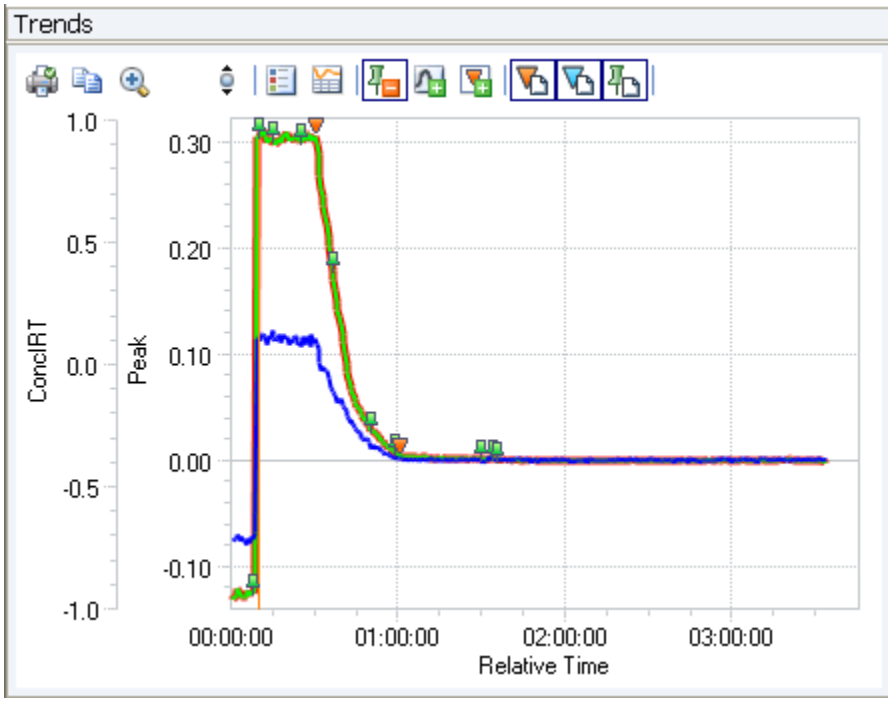
Select the data to be exported. To proceed with the export, click **OK**.

The saved CSV file can be opened directly with GRAMS or other applications that are SPC compatible.

Example Report

The following report is provided as an example of iC data that can readily be incorporated into experiment reports.

Control Number: 10A-879870-2	Prepared by: J. Doe
Title:	
Abstract:	



Relative Time	Peak 1	Peak 2	Peak 3	Annotations
00:00:25	-0.075283	-0.129418	-0.129418	
00:00:55	-0.0757392	-0.129898	-0.129898	
00:01:25	-0.0733607	-0.127831	-0.127831	
00:01:55	-0.0730829	-0.126375	-0.126375	
00:02:25	-0.0695092	-0.120724	-0.120724	
00:02:55	-0.0719094	-0.12377	-0.12377	
00:03:25	-0.0749703	-0.129621	-0.129621	
00:03:55	-0.0713097	-0.128329	-0.128329	
00:04:25	-0.0757192	-0.12963	-0.12963	
00:04:55	-0.0768396	-0.128137	-0.128137	
00:05:25	-0.0803207	-0.129544	-0.129544	
00:05:55	-0.0739381	-0.123816	-0.123816	
00:06:25	-0.0785219	-0.126326	-0.126326	
00:06:55	-0.0740753	-0.123604	-0.123604	
00:07:25	-0.0728557	-0.122295	-0.122295	
00:07:55	-0.0748924	-0.124245	-0.124245	
00:08:25	-0.0677285	-0.119897	-0.119897	Sample 16 acquired at 00:07:55
00:08:55	-0.0500758	-0.0786976	-0.0786976	
00:09:25	0.115091	0.304483	0.304483	
00:09:55	0.114271	0.30542	0.30542	
00:10:25	0.112993	0.305691	0.305691	Sample 20 acquired at 00:09:55
00:10:55	0.118845	0.308429	0.308429	

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00:11:25	0.118478	0.30985	0.30985	
00:11:55	0.115791	0.304085	0.304085	
00:12:25	0.116571	0.305012	0.305012	
00:12:55	0.108204	0.299243	0.299243	
00:13:25	0.115918	0.301942	0.301942	
00:13:55	0.115443	0.30222	0.30222	
00:14:25	0.115471	0.301603	0.301603	
00:14:55	0.121372	0.303738	0.303738	
00:15:25	0.114449	0.30034	0.30034	
00:15:55	0.11312	0.298218	0.298218	Sample 31 acquired at 00:15:25
00:16:25	0.115283	0.299927	0.299927	
00:16:55	0.116913	0.301626	0.301626	
00:17:25	0.11786	0.303789	0.303789	

Events:

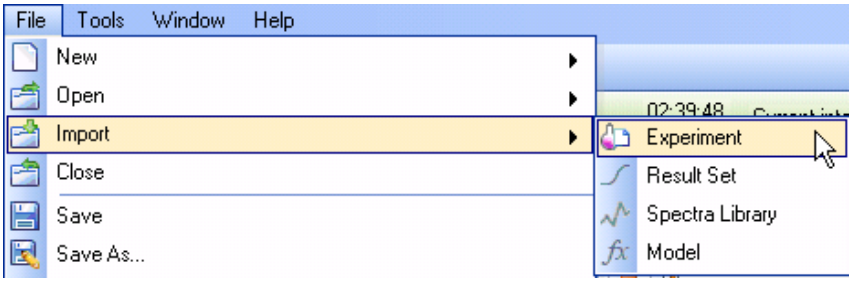
Type	Date/Time	Description
Audit	10:00:21 AM on 7/30/2007	Created Experiment Experiment 2007-07-30 10-00 in C:\iCIR306\Experiments
Audit	10:00:29 AM on 7/30/2007	Opened by John Doe
Audit	10:00:29 AM on 7/30/2007	Experiment started.
Audit	10:00:29 AM on 7/30/2007	Phase 1 started: Interval=10 sec. Duration=24:00:00
Audit	10:00:29 AM on 7/30/2007	Experiment initially paused. Awaiting start.
Audit	10:01:15 AM on 7/30/2007	Experiment resuming.
Audit	10:01:16 AM on 7/30/2007	Experiment AutoSaved
Annotation	10:02:02 AM on 7/30/2007	Increased heat by 50 deg C - JG
Audit	10:02:57 AM on 7/30/2007	Experiment paused by user.
Audit	10:03:36 AM on 7/30/2007	Experiment resuming.
Annotation	10:04:33 AM on 7/30/2007	Experiment paused to remove dirt from lens
Annotation	10:04:51 AM on 7/30/2007	Heat stabilized
Audit	10:05:31 AM on 7/30/2007	Experiment paused by user.

Importing External Files

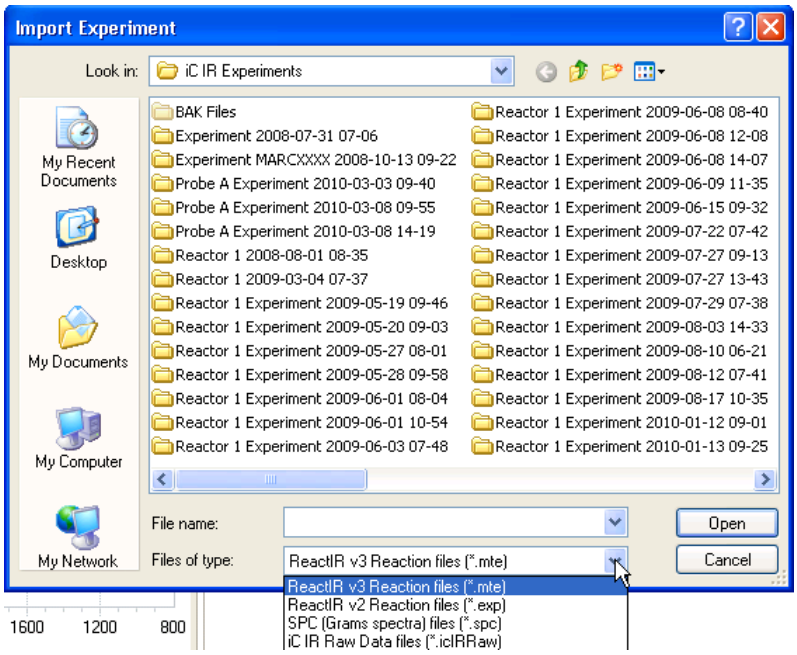
The iC IR application has the ability to import a variety of files from other application. The following table listed the type of files and their supported formats

Experiment Files	ReactIR version 2 reaction files (.exp)
	ReactIR version 3 reaction files (.mte)
	Grams spectral files (.spc)
	iC IR raw data files .icIRRaw)
Result Sets	WinRC trend files (.mtd)
	iControl RC1e experiment files (.iControlRC1e)
	iControl LabMax experiment files (.iControlLM)
	iControl EasyMax experiment files (.iControlEM)
	ConcIRT analysis files (.icConcIRT)
	iC IR experiment files (.icIR)
	iC FBRM experiment files (.icFbrm)
	iC Raman experiment files (.icRaman)
	iC UV-VIS experiment files (.icUV)
Spectra Libraries	ReactIR version 2 spectrum files (.spa)
	ReactIR version 3 spectrum files (.mts)
	Grams spectra files (.spc)
Model files	ReactIR version2 QuantIR files (.qnt)

Files are imported by selecting the **Import** option in the **File** menu.



When a document type is selected, a standard File Open dialog is opened.



A droplist is available to filter the files based on the supported file types. When the **Open** button is clicked, the selected file is imported into iC IR and opened in a new document.

Using the Toolbox

The IR Toolbox is a windowed pane that provides a collection of “task panes”. Each task pane provides a set of controls relevant to performing a task. For example, the Experiment Task pane provides ready access to various data analysis functions that may be applied to the current experiment being viewed in the document area.

To open the Toolbox, click on the 

icon in the upper-right corner of the main window.

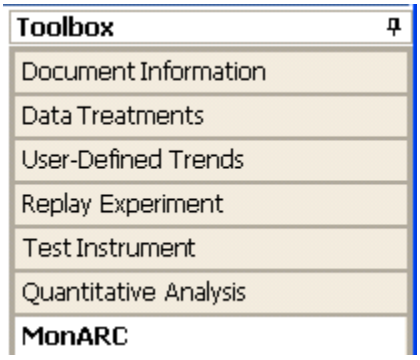
The Toolbox features an auto-hide function. When the toolbox is expanded, it remains open until you move the cursor out of the Toolbox window; it then closes (i.e. auto-hides).

Alternatively, the Toolbox can be pinned so that it is always displayed by clicking the  icon in the upper-right corner of the Toolbox window. Auto-hide is useful when you want to maximize the viewing area of document area. Pinning is useful if you want to monitor or interact with the Toolbox (or one of its task panes) frequently.

The Toolbox is organized as a button bar representing the set of task panes available to you based on an XML configuration file stored under your account in the Documents and Settings folder. This configuration file is typically stored under the hidden folder:

C:\Documents and Settings\<your username>\Local Settings\Application Data\Mettler Toledo\

The standard task panes configured with iC are described in the following sections. Note that there may be additional task panes for optional components installed with the iC IR software. The task panes for optional components are discussed under the topic for the optional component.

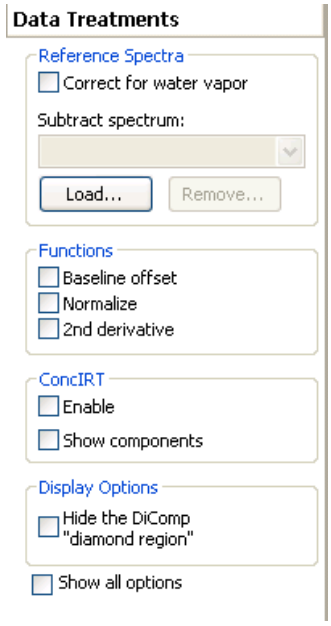


Data Treatments Task Pane

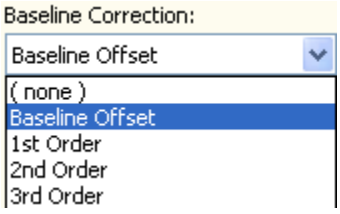
The Data Treatments task pane provides data analysis tools for the currently displayed experiment.

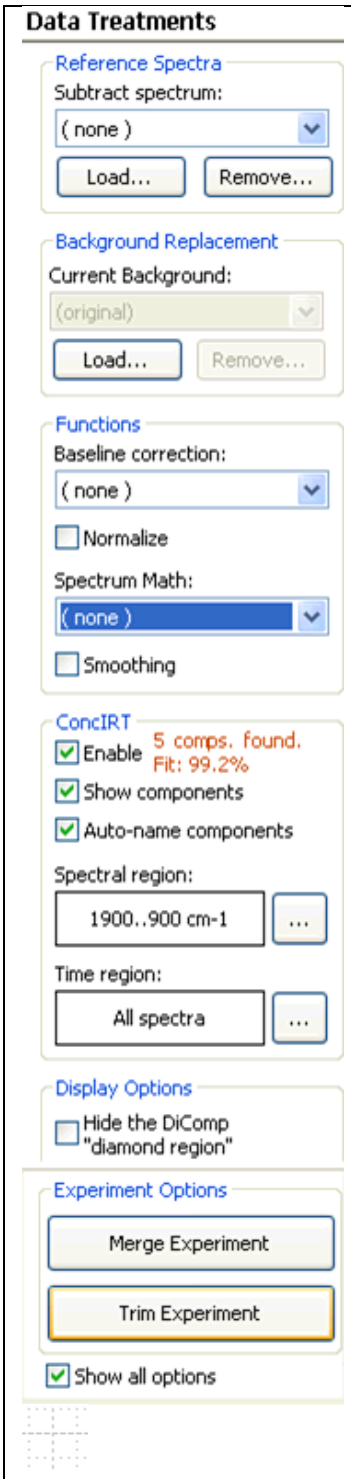
There are two display options available for the toolbox. In the Normal view, the most commonly used tools are displayed as checkboxes. When the Show All Options checkbox is checked, the tools are displayed as drop-down lists that allow the user to select another option instead of the most commonly used one.

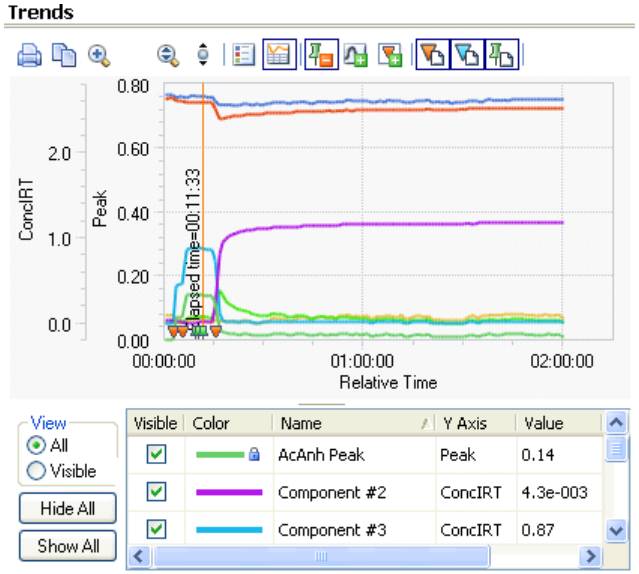
The following options can be selected from the task pane.

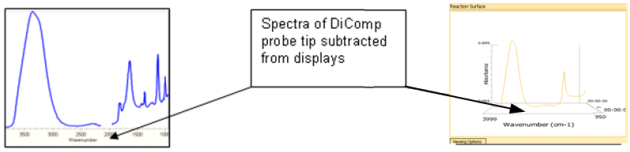
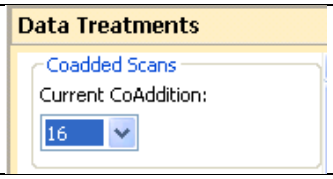


With Show all Options checked:

Correct for Water Vapor	Apply a correction for water vapor (spectrum which was taken before the experiment) by selecting the check box.
Reference Spectrum Subtraction	Subtracts a reference spectrum from the current data set that was previously saved in the spectra library during the experiment set up. This is useful, for example, to remove the solvent peaks from the data set. The Load button is used to load a new reference Spectra. The Remove button opens a dialog that allows the user to remove Reference Spectra from the experiment.
Background Replacement	Allows the user to change the background for a sample spectrum or a complete experiment. The original data is not corrupted. A copy of the spectrum/experiment is created with the new ratioed data and the replaced background installed. This option is only available for an spectrum/experiment containing an original embedded background.
Baseline Offset	In the Normal view, this checkbox is used to vertically shift each spectrum in the dataset such that the value is zero at the selected reference wavenumber which is chosen from the Baseline Offset dialog. Refer to Baseline Offset Dialog In the Show All Options view, the checkbox changes to a Baseline Correction drop-down list that allows the user to select additional options.  1st order correction adjusts the spectra to a straight baseline. Similarly, 2nd and 3rd order corrections adjust the baseline to a 2nd or 3rd order curve. Be very cautious about higher order corrections as they can distort your data.
Normalize	This checkbox is used to normalize each spectrum in the dataset such that the value is 1.0 at the selected reference wavenumber. This correction 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. Refer to Normalization Dialog.
2nd Derivative	In the Normal view, checking this box applies a 2nd derivative function to each spectrum in your dataset. As a convenience, it also multiplies the results by -1 so that the peaks point upwards. In the Show All Options view, the checkbox changes to a Spectrum Math drop-down list that allows the user to select additional options.

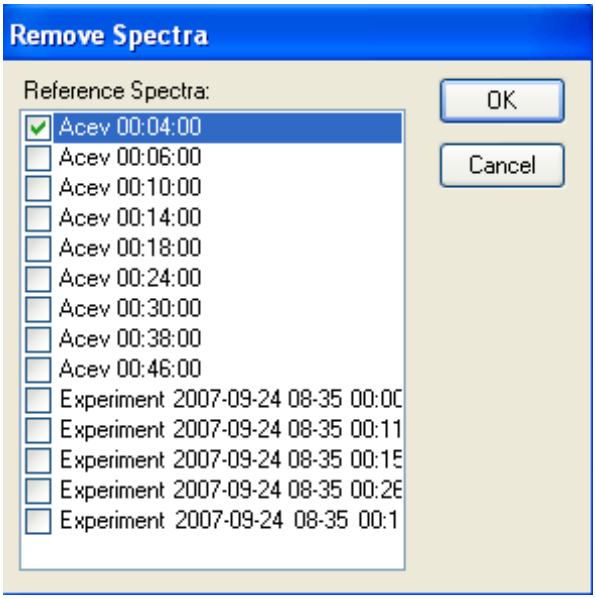


	(none) 1st Derivative 2nd Derivative 3rd Derivative Square Root
Smoothing	When this box is checked, the Smoothing Window is opened to allow the user to apply smoothing to the trend. Note that this option is only displayed when the Show All Options checkbox is checked. Be careful about over-smoothing your data. In particular, smoothing may prevent ConcIRT LIVE form being able to correctly isolate component spectra.
Enable/Hide ConcIRT LIVE analysis module	Click the checkbox to run the ConcIRT LIVE analysis module.  The “goodness of fit” value is displayed next to the checkbox. The value is updated as new values are calculated.
Show Components	When checked, the component spectra identified by ConcIRT LIVE will be shown in the Spectra Viewer. Conversely, clearing this checkbox will hide ConcIRT LIVE component spectra.
Auto-name Components	If the experiment contains any reference spectra and/or referee trends (more than 8 data points), ConcIRT LIVE components are auto-named after these references. When the user renames a spectra, this name is retained during the same ConcIRT LIVE session.
Spectra Region	Displays the region over which the Relative concentration profiles are calculated. The region can be changed by clicking the ... button to open the ConcIRT LIVE Region Dialog.
Time Region	Displays the time region which the Relative concentration profiles are calculated. The time can be changed by clicking the ... button to open the ConcIRT LIVE Time Region Dialog.

	Hide the DiComp diamond region of the spectra	This option suppresses display of the spectral display of the region from 1950 to 2250 cm-1 (default). This is done because the DiComp probe tip absorbs so much light in this region that the no useful information is available in this region.  When the option is checked, the range of the region and a  button is displayed. Clicking the button opens a dialog that allows the user to edit the region.
	Merge Experiment	Allows the user to merge two completed experiments into a composite experiment file. Clicking the button opens a file browser to select the experiment that will be merged into the currently selected one.
	Trim Experiment	Allows the user to trim (delete) unnecessary samples from an experiment. Clicking the button opens The Trim Experiment Dialog.
	**Coadded Scans**	This option is only displayed for Rapid Collect experiments. Refer to Rapid Collect Experiments.

Remove Spectra Dialog

The Remove Spectra dialog is opened when the Remove button on the Data Treatments Task Pane is clicked. The dialog is used to remove Reference Spectra from the experiment.



The user checks the spectra to remove, and clicks the **OK** button.

Background Replacement

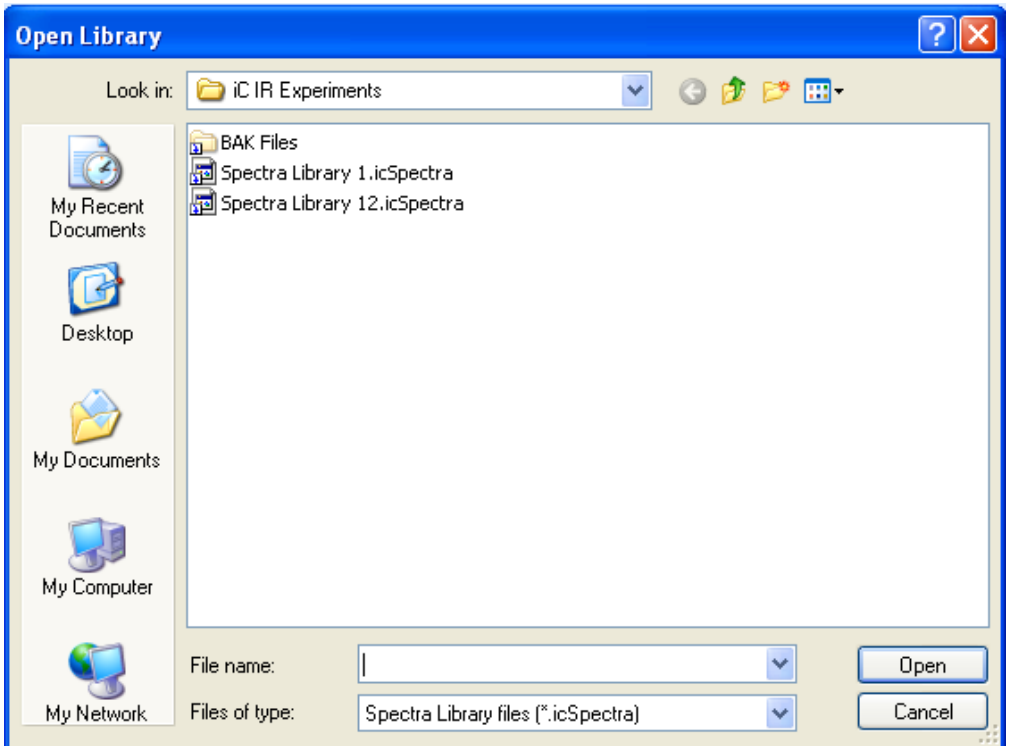
The Background Replacement portion of the Data Treatments task pane allows the user to change the background for a sample spectrum or a complete experiment.

The original data is not corrupted. A copy of the spectrum/experiment is created with the new ratioed data and the replaced background installed.

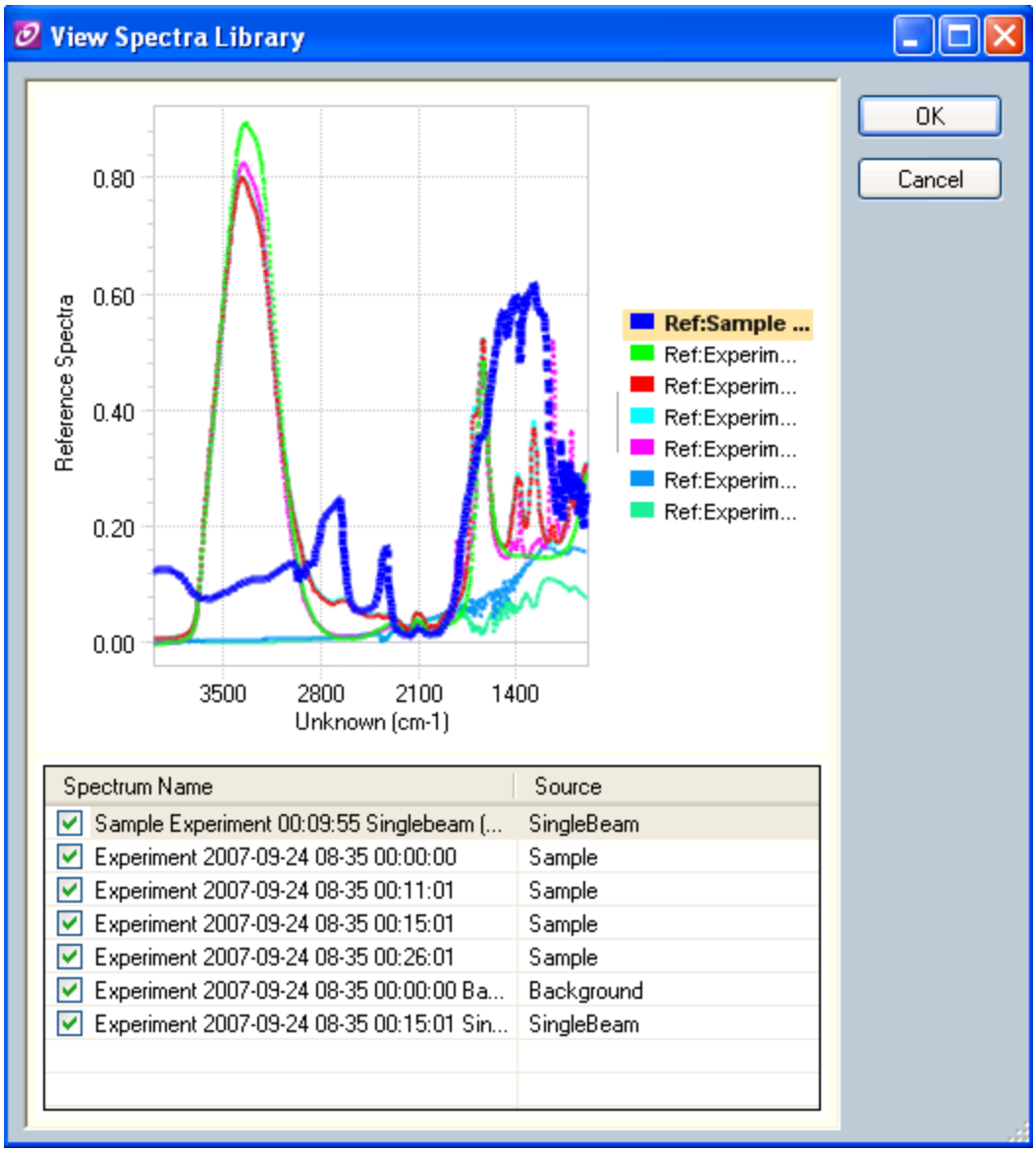
This option is only available for an spectrum/experiment containing an original embedded background.

To replace a background, the user clicks the **Load** button.

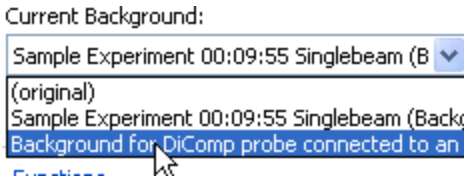
A file browser is opened to select the Spectra Library or Experiment file where the desired replacement background is located.



The user selects the file and clicks the **Open** button. The View Spectra Library dialog is opened.



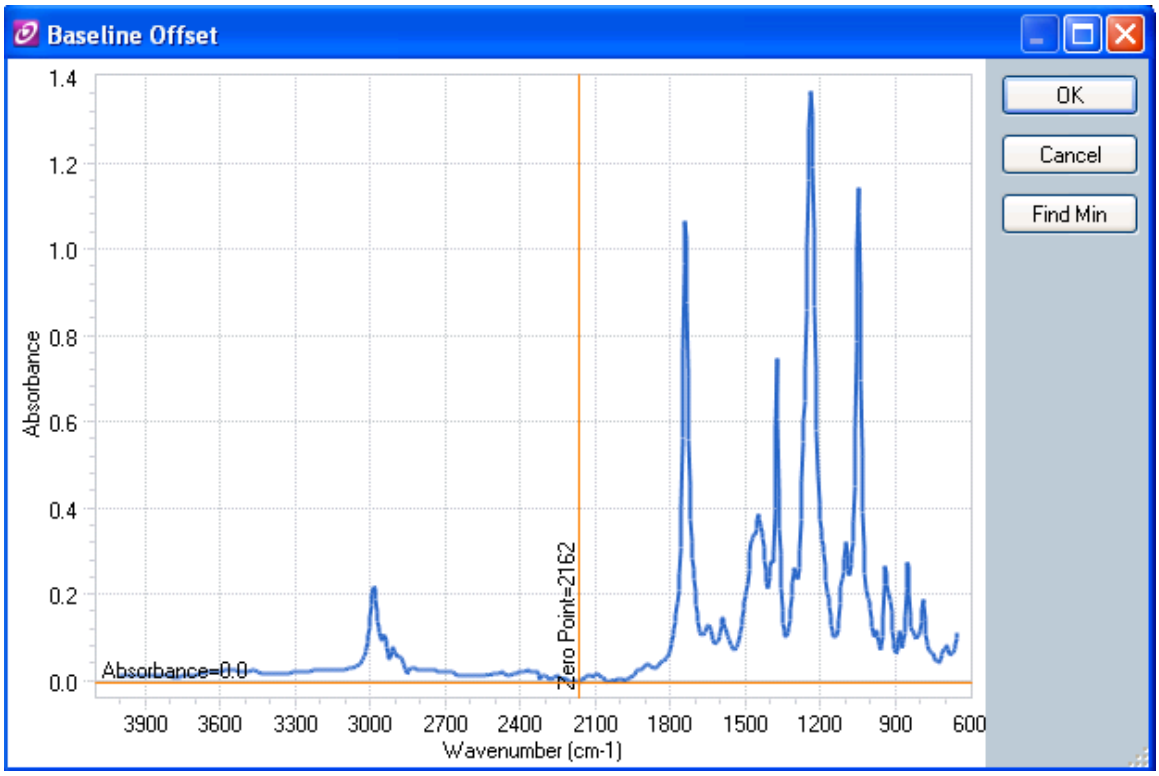
Select the background and click the **OK** button. The selected background is added to the droplist in the Data Treatments task pane and can be selected as a replacement background.



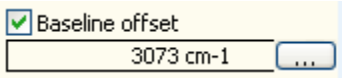
Also refer to Replacing a Background.

Baseline Offset Dialog

The Baseline Offset dialog is used to select a position along the X axis for the Baseline Offset function. The most recently selected reaction spectrum is displayed for your reference. When baseline offset is applied, each reaction spectra is shifted such that the value at this position is zero. Typically, you would want to use the minimum value, so this position is chosen by default. You have the option of clicking in the graph to choose any position or clicking the **Find Min** button to reselect lowest value on the graph.

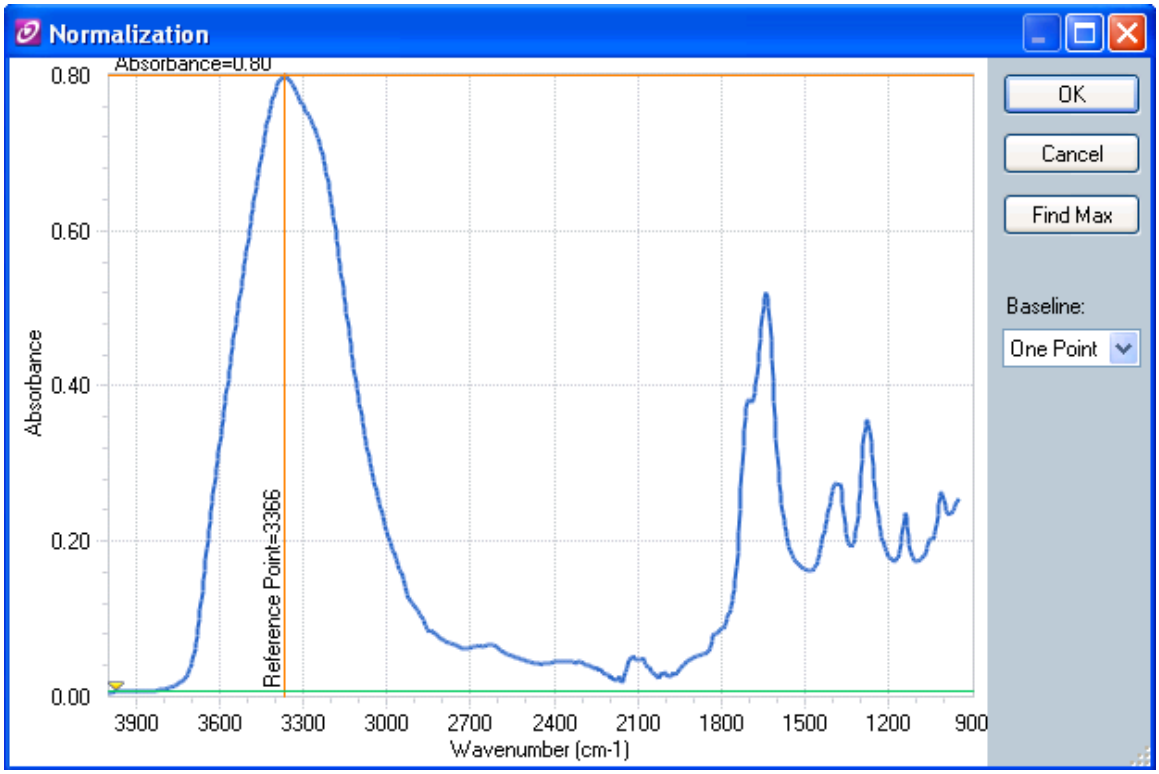


When the baseline is set, its value is displayed in the Data Treatments toolbox. The offset can be adjusted at any time by clicking the ... button next to the value field.



Normalization Dialog

The Normalization dialog is used to select a position along the X axis for the Normalize Offset function. The most recently selected reaction spectrum is displayed for your reference. A green line is displayed at the baseline point. When normalize is applied, each reaction spectra is scaled such that the value at this position is 1.0. Typically, you would want to use the maximum value, so this position is chosen by default. You have the option of clicking in the graph to choose any position or clicking the **Find Max** button to reselect the largest value on the graph.

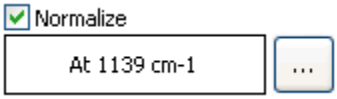


Note: The iC software allows normalization against the height to a single-point baseline as follows:

$$YNorm[i] = (YRaw[i] - YBase) / (YMax - YBase)$$

To do this, the user selects the 'One Point' for the Baseline dropdown. The user then specifies a reference point for Normalization typically by normalizes using the Find max button in the Normalization dialog. Then user specifies the Baseline Offset by moving the cursor in the dialog window.

When the normalization is set, its value is displayed in the Data Treatments toolbox. The value can be adjusted at any time by clicking the ... button next to the value field.



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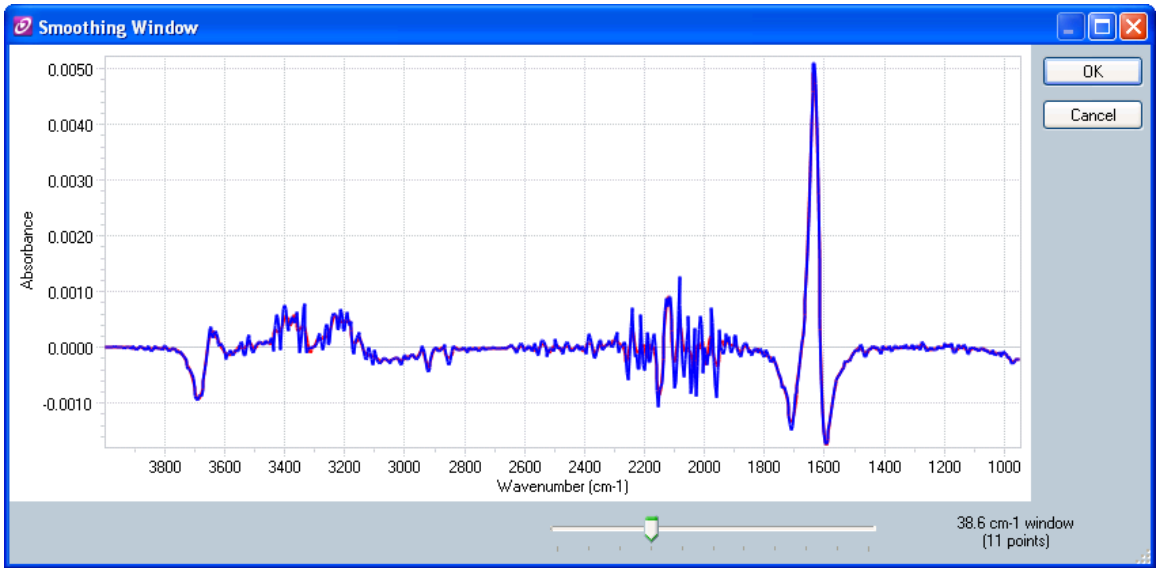
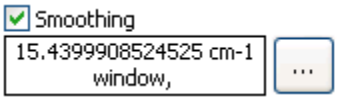
Smoothing Window Dialog

The Smoothing function is used to remove noise from the spectra by applying Savitsky-Golay smoothing. The most recently selected reaction spectrum is displayed for your reference at the current zoom settings. The dialog is opened when the Smoothing checkbox is checked. The Smoothing Window allows you to specify the number of points to consider in calculating the smoothed value for each point along the spectrum.



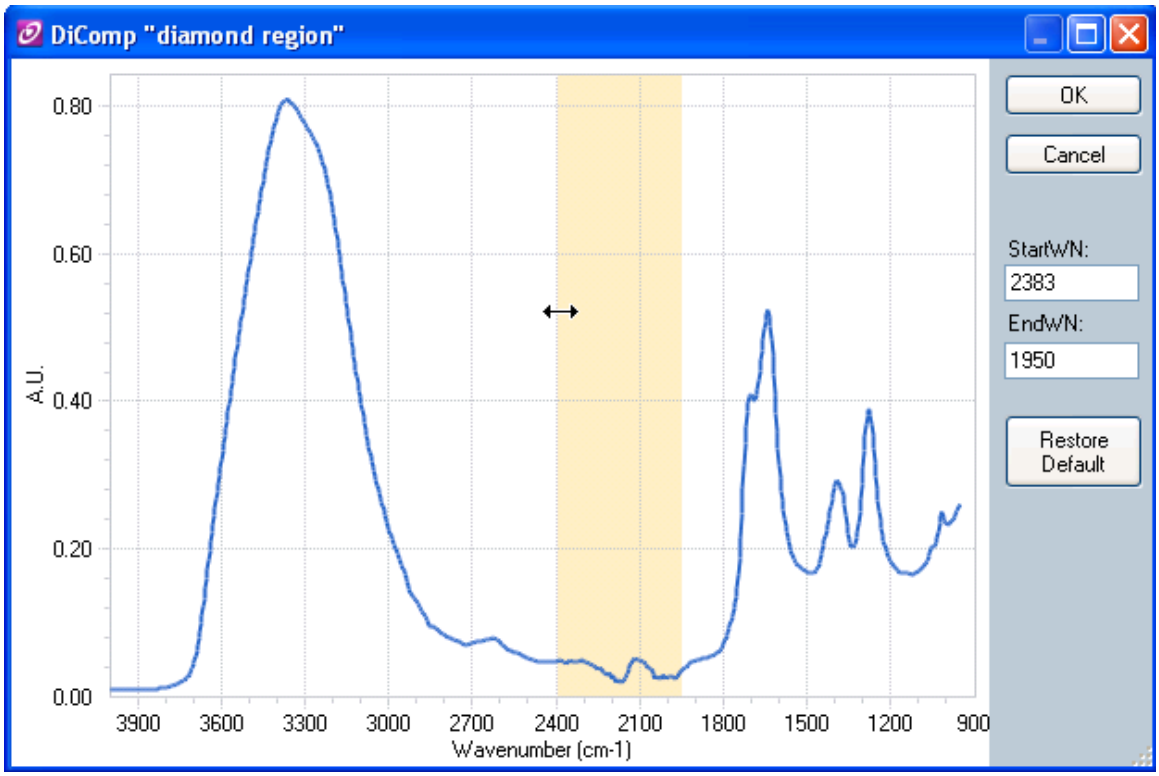
Smoothing is adjusted by moving the slider bar at the bottom of the dialog. The amount of smoothing can be set from 5 to 25 points.

When smoothing is applied, its value is displayed in the Data Treatments toolbox. The size of the smoothing window can be adjusted at any time by clicking the ... button next to the value field.



DiComp Diamond Region Dialog

The DiComp Diamond Region dialog allows the user to make adjustments to the range that is hidden in the spectral display to compensate for the characteristic of diamond probe tips to absorb so much light in the region that no useful information is available. The default range is from 1950 to 2250 cm-1.



To adjust the range, the user moves the cursor to the edge of the existing region. The cursor will change to an arrow, ↔. The user then drags the arrow to increase or decrease the range.

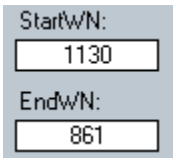
ConcIRT LIVE Region Dialog

The ConcIRT LIVE Region dialog is used to adjust the region over which the relative concentration profiles are calculated.

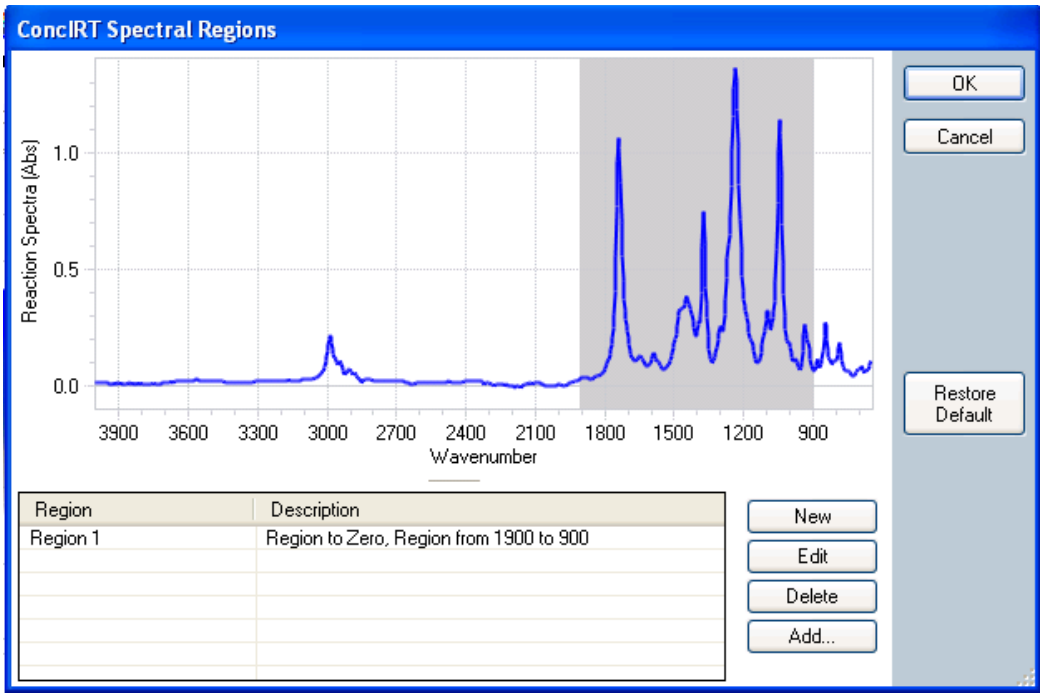
The region is highlighted in yellow. The size of the region is adjusted by placing the cursor on the edge of the yellow shading. The cursor will change to a ↔. The arrow can then be moved to resize the region.

The region can be moved by clicking the mouse button while the cursor is in the highlighted region. The cursor changes to a ✋. The region can then be moved to the desired area of the window.

The actual wave numbers of the region are displayed on the dialog.



The default region can be restored at any time be clicking the **Restore Default** button. The default region is dependent on the type of hardware probe in use.

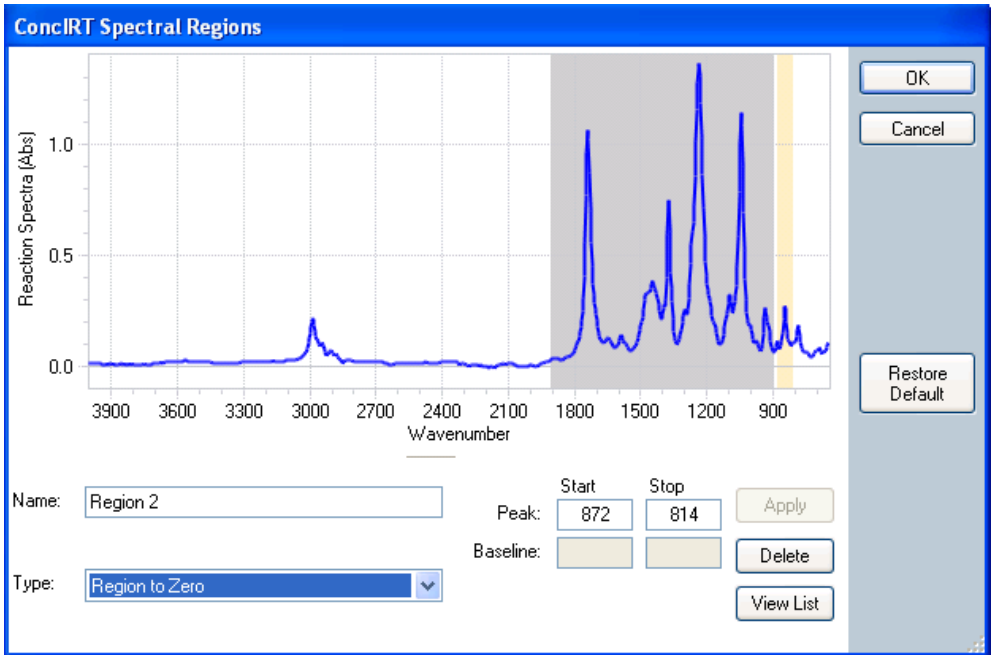


NOTE: The larger the spectral window the longer ConcIRT LIVE may need to process the information. Therefore, ConcIRT LIVE may not be able to 'keep up' when certain interval times are selected.

Multiple ConcIRT LIVE Spectral Regions can be defined by clicking the **New** button. The dialog changes to the Edit ConcIRT LIVE Spectral Regions dialog.

Edit ConcIRT LIVE Spectral Regions Dialog

The Edit ConcIRT LIVE Spectral Regions dialog is used to define new spectral regions and edit existing ones. The user can define and edit the name of the spectral region, as well as its type. When changes are made, the **Apply** button is clicked to save the edits. The user can return to the spectral region list by clicking the **View List** button. Clicking the **OK** button closes the dialog.



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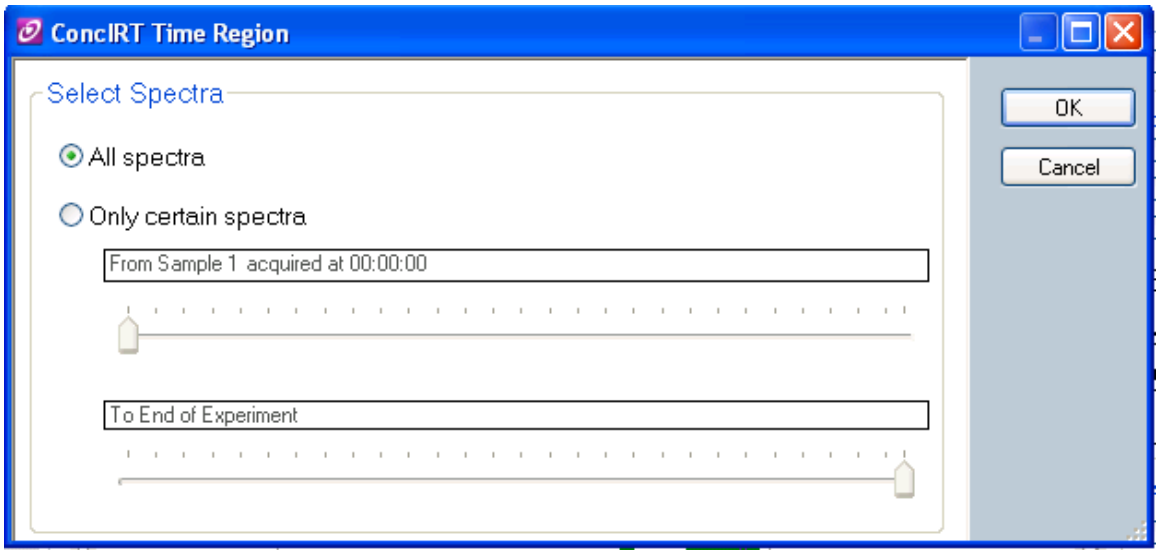
ConcIRT LIVE Time Region Dialog

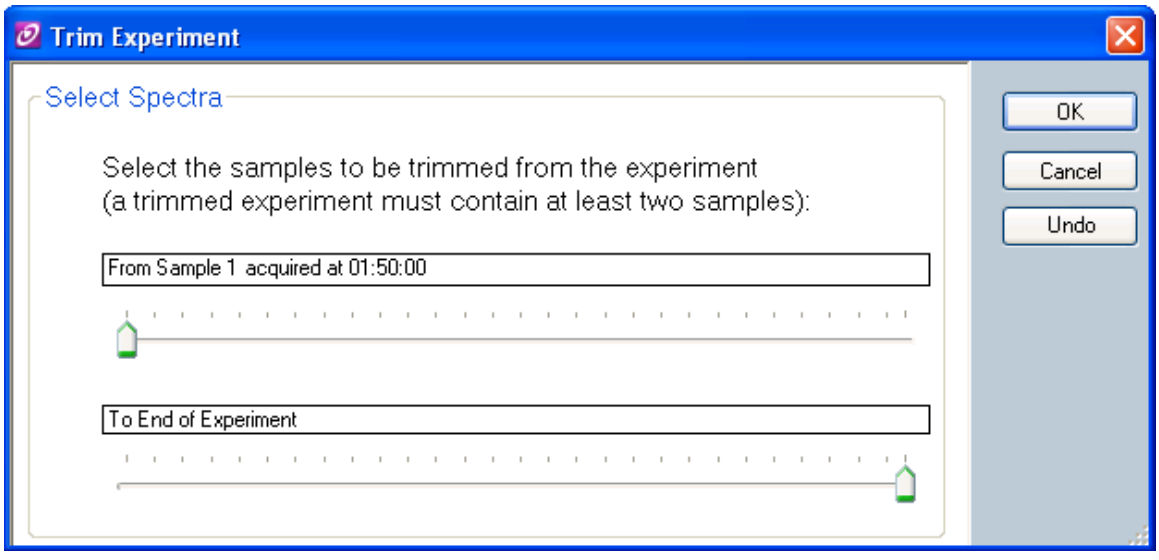
The ConcIRT LIVE Time Region dialog is used to select the time period over which the relative concentration profiles are calculated.

The user has the option to include all spectra or to select spectra samples for a specific time period. Slider bars are used to specify the “From and To” time window.



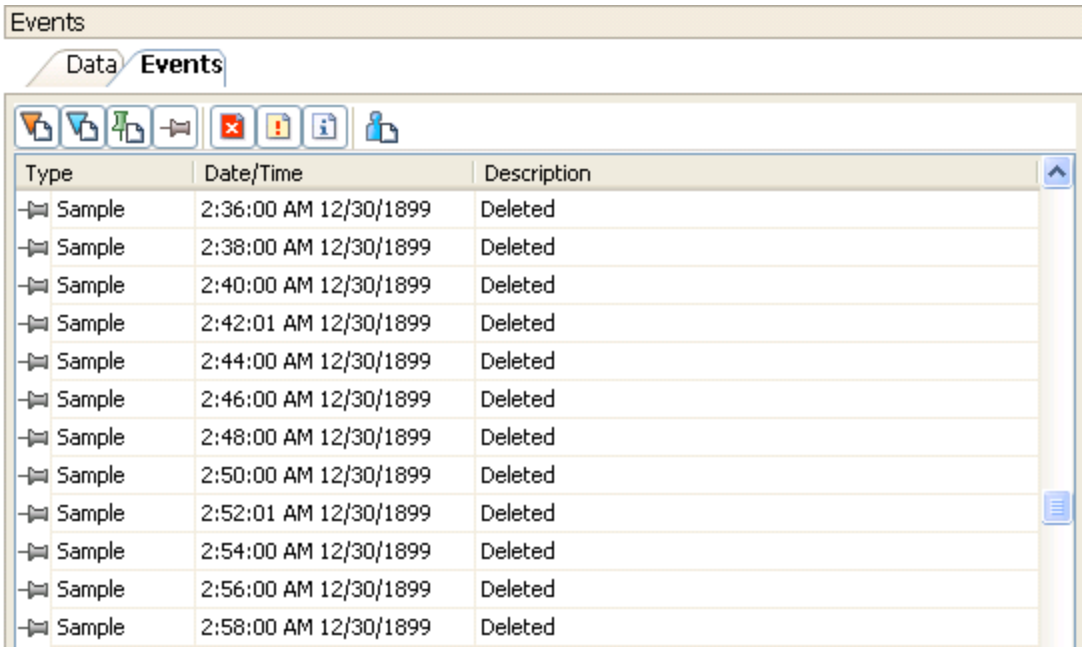
The Trim Experiment Dialog

The Trim Experiment Dialog is used to trim samples from a completed experiment. This feature is useful to remove insignificant samples from an experiment. It is important to note that when an experiment is trimmed the samples are deleted from the experiment and cannot be recovered. It is advisable to save a trimmed experiment to a different filename leaving the original experiment intact.



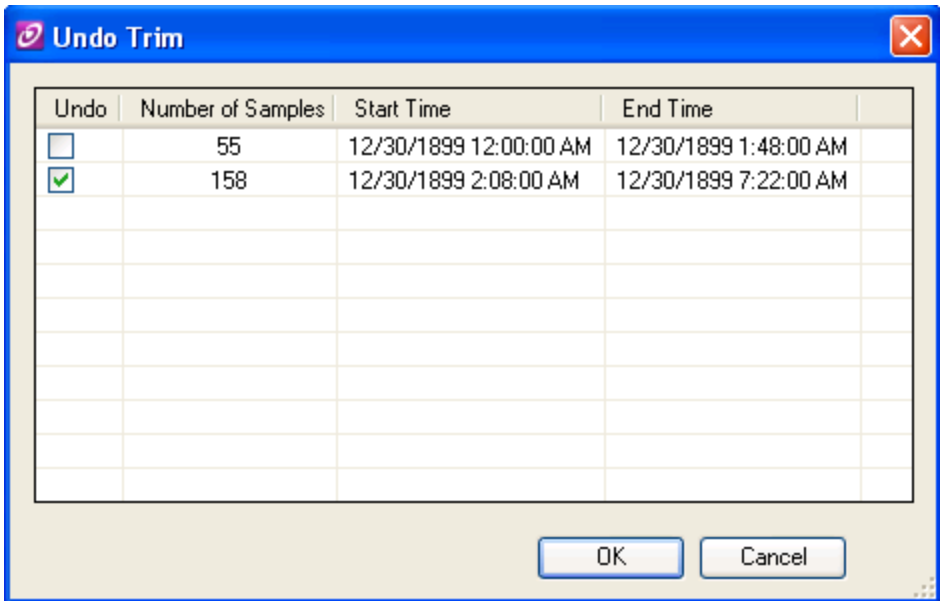
The slider bars in the dialog are used to select which samples will be deleted from the experiment. The arrow keys can be used to advance the slider bar in one sample increments.

In the above example, samples 123 through 145 are selected to be deleted from the experiment.



The trimmed samples remain listed in the Event Viewer and are marked as Deleted.

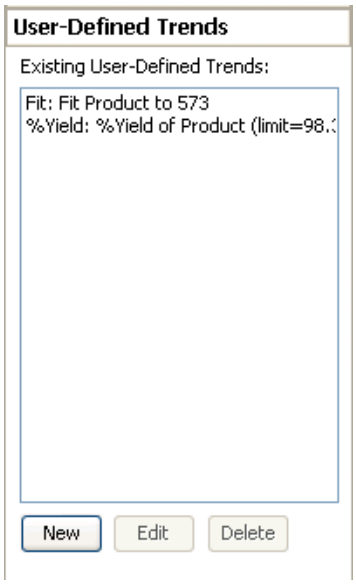
The **Undo** button is used to reverse a trim operation. When the button is clicked, a Undo Trim dialog is displayed.



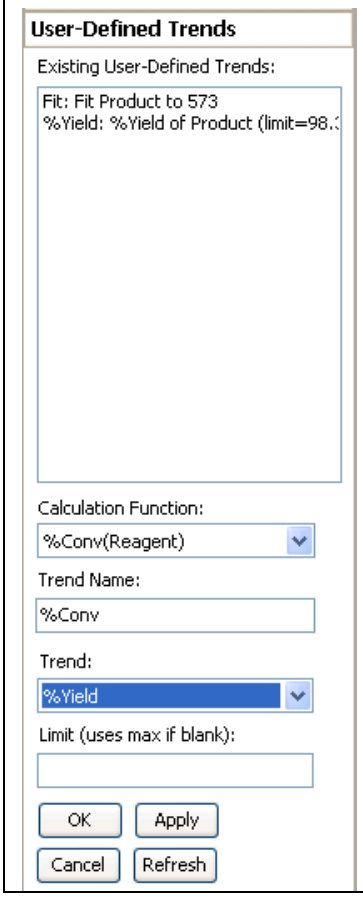
The dialog contains a list of all Trim operations that have been performed on the experiment. The user checks the appropriate operation and clicks the **OK** button. The trimmed samples are reinserted into the experiment.

User-Defined Trends Task Pane

The User-defined Trends task pane is used to create and perform math functions on trends. The User-defined Trends task pane for an Experiment includes the following information.



Existing User-defined Trends	A list of trends created by the user.



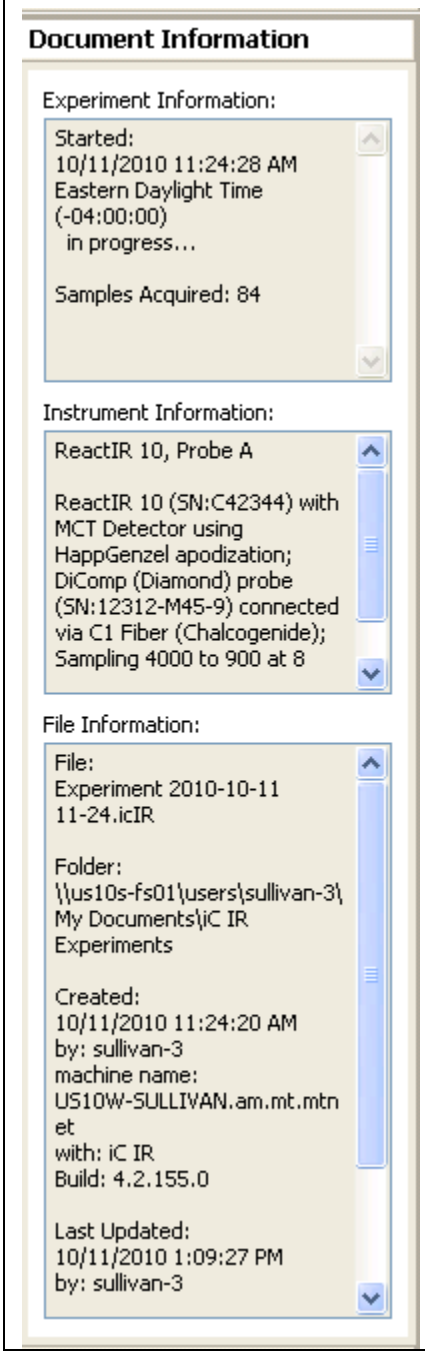
When the **New** or **Edit** button is clicked, the task pane is expanded to include additional fields that define the trend. Refer to User-Defined Trends for more information.

Document Information Task Pane

The Document Information task pane is an informational display that provides chronological and summary about the currently displayed data document.

The document information pane displays different information depending on the type of document (Experiment, Result List, Spectra Library).

The document information pane for an Experiment includes the following information.

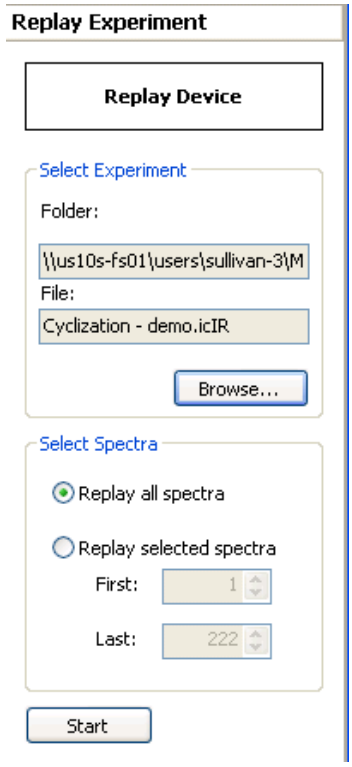


Experiment Information	Provides statistical information about the experiment. Date and time of start of the experiment Date and time of finish of the experiment Samples Acquired
Instrument Information	Describes the hardware configuration of the instrument. If the instrument uses a multi-probe, the channel number is listed. Gain and Apodization are also displayed.
File Information	The Filename for the experiment document. (test1.iCIR) (example)
Folder:	The folder where the file resides. Example: C:\\iC IR\Experiments
Created:	Date, time, author, file name and build number.
Last Updated:	Date, time, author, file name and build number for last update.

Replay Experiment Task Pane

The Replay Experiment task pane is used to replay a saved experiment. For in-depth spectra analysis and for greater analysis comparison, you can replay a saved experiment. By replaying an experiment you can select different peaks for analysis, subtract different spectra saved in the spectra library, apply a correction for water vapor, and use the ConcIRT LIVE software for analysis if it was not done initially.

Note: Both .MTE files (ReactIR 3.0) and .EXP iC experiment files can be replayed with the current software version.



Select Experiment	To replay an experiment, the path/experiment document is first selected by clicking the Browse... button on the Replay Experiment tool. The standard file browser is opened. Note that the browser allows the user to filter on .MTE files (ReactIR 3.0) or .EXP (iC) experiment files
Select Spectra	The user clicks the appropriate radio button to replay all of the spectra for an experiment or a selected part of the spectra.
Sampling Interval	The user can change the sampling interval to speed up the review process. Replaying the sampling speed has no relation to the speed at which the samples were recorded. The Start button is clicked to initiate the replay function. The status indicator at the top of the Replay Experiment task pane display indicates that the experiment replay is in progress. **Replay is Running** When the experiment starts replaying, an additional button is displayed; Pause Stop Pause When the Pause button is clicked, the experiment is paused and the button label changes to Resume. Resume Clicking the button resumes the experiment replay.

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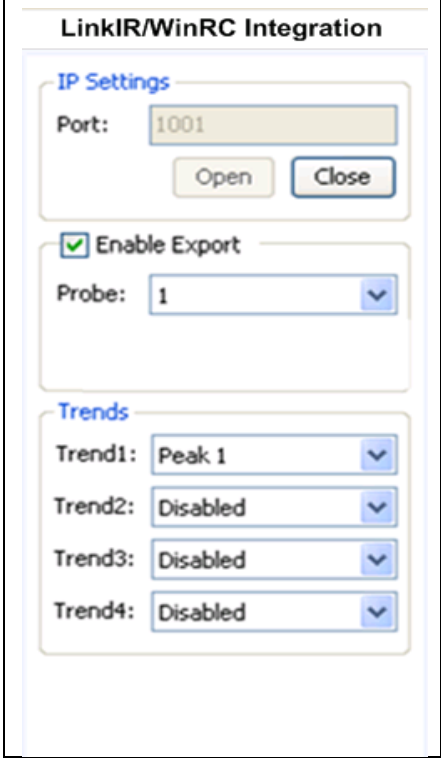
LinkIR/WinRC Integration Task Pane

The LinkIR/WinRC Integration task pane is used to export trends to WinRC or LabMax software applications. The task pane is only functional during a live experiment. The trend data is automatically updated on a running WinRC application as data is collected. Up to four trends can be exported.

First, the iC application is set up to export trends and then the WinRC. The LinkIR/WinRC Integration task pane is used to establish and control communications with WinRC.

The task pane includes the following information.

<table>
<tr>
<td rowspan="3"> 
</td>
<td>IP Settings</td>
<td>The IP port that the WinRC software is using is specified and the Open button is clicked to establish communications with WinRC.

The Close button is used to disconnect the connection with WinRC.

Note: An experiment should be running on the iC and the WinRC application should be running at this time.</td>
</tr>
<tr>
<td>Probe Settings</td>
<td>The Enable Export checkbox allows the iC software to export trend data to the WinRC. the

The Probe droplist is used to select which probe input port will be used to input the data in WinRC.</td>
</tr>
<tr>
<td>Trends</td>
<td>The iC software can export up to four trends to the WinRC. The droplists displayed in the Trends section of the task pane are populated with all trends from the Trend Viewer.</td>
</tr>
</table>

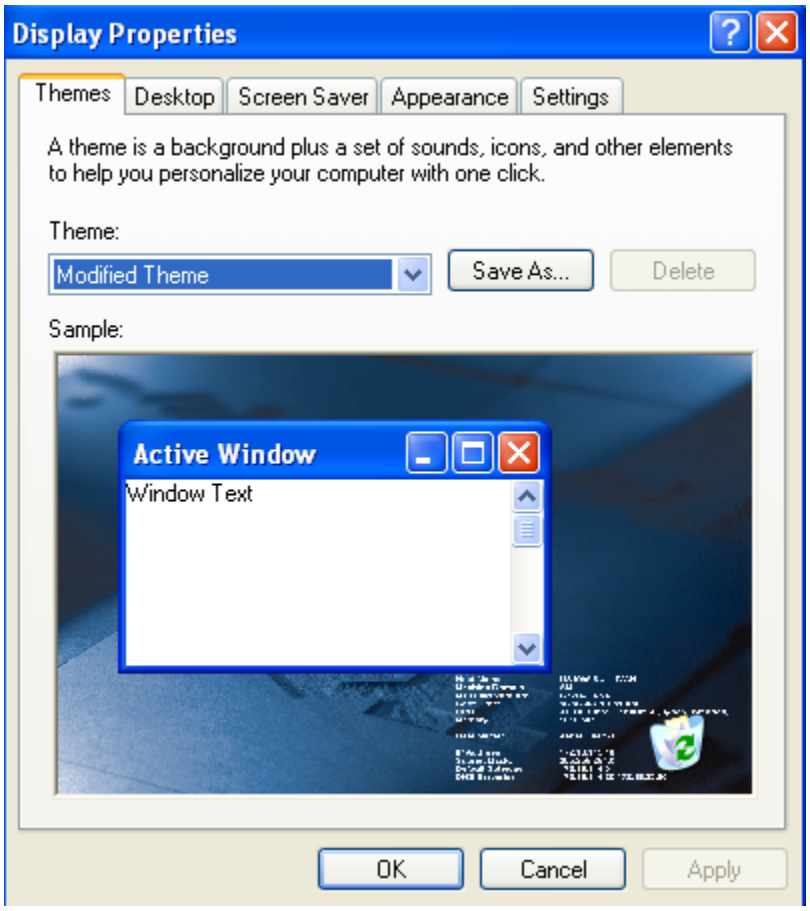
Setting up the WinRC to Import iC Trends

The following steps should be performed in WinRC to import iC trends. The WinRC documentation should be consulted for additional detailed information.

- Start the WinRC application then click on the **Tools** menu item and choose **Options**.
- Check "Reactor Box 1" checkbox and select reactor block "RB04-50 No. 1",
- Select the COM port that is connected to the reactor block.
- Click on the **"Instruments"** tab and check the "ReactIR 1" checkbox.
- Type in the iC IR computer's IP address in the **PC name or TCP/IP address** field, then type in port number 1001 (or the one you entered in the iC application.
- Click on the Test Connection button.
- After the connection is established click on the **OK** button to close Options dialog.
- Start a new experiment in WinRC, deselect all reactor block values and activate the four trends in the eval graph control.

Viewing Display Settings

The View Display Settings button on the Start Page opens the MS Windows Display Properties dialog to enable the user to change display setting for optimal performance of the iC application. This option is provided as a convenience to the user.



iC Licensing

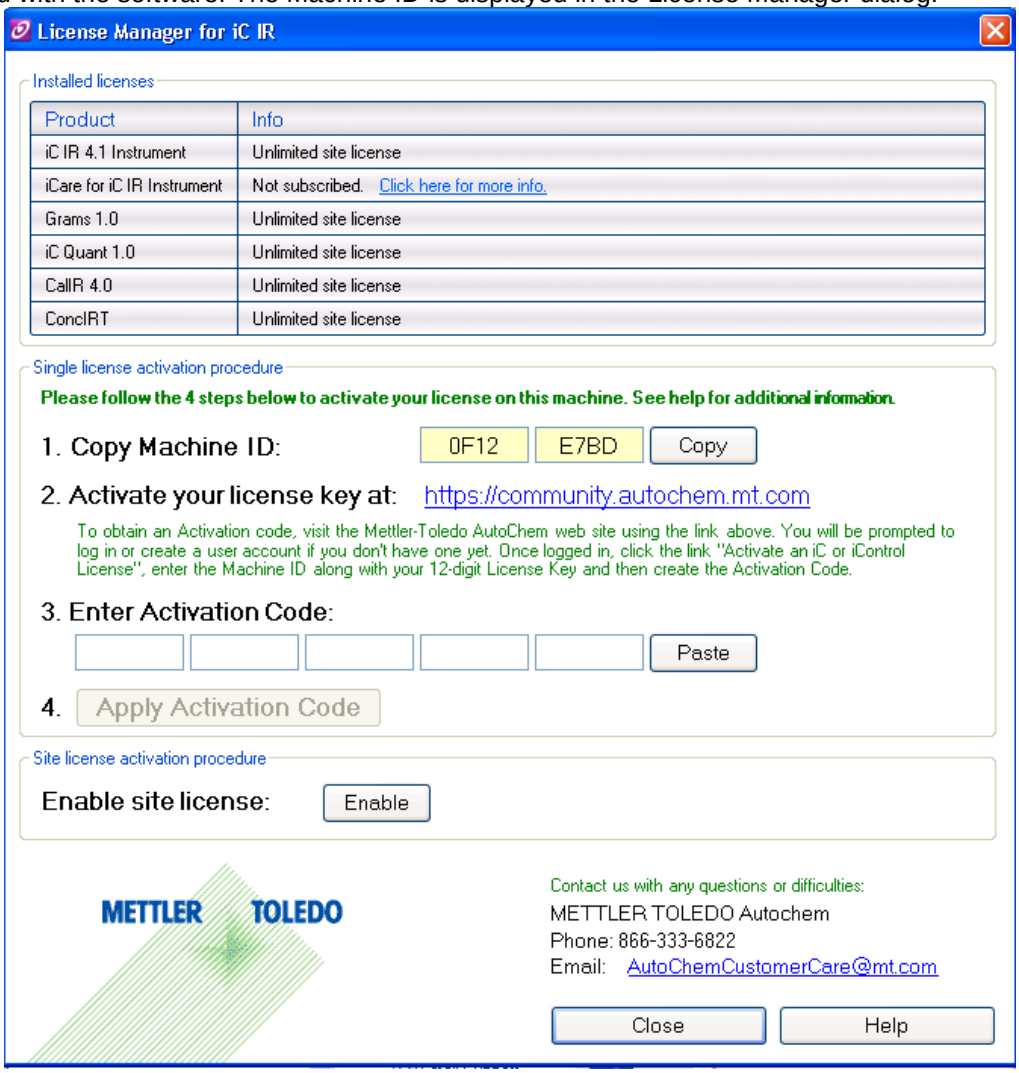
iC applications incorporate a licensing scheme to control distribution and use of the software.

There are three types of licenses.

- Instrument version– Allows the application to connect to a live instrument and run experiments.
- Office version – Allows the user to run the application without a connection to an instrument. Experiment data obtained from a computer with an Instrument license can be viewed and analyzed.
- Demo version – A demo version is equivalent to an Instrument license with a 30 day time limit.

In addition a Site License is available for multiple installations of the software.

The iC License manager is used to view and manage iC licenses. Activating a software license is performed through a website. The user must have the Machine ID from the License Manager dialog and the software key provided with the software. The Machine ID is displayed in the License Manager dialog.



Detailed instructions on activating a license are contained in the Installation Guide.

Best Practices

This section provides guidance on best practices for getting the most out of iC IR and your ReactIR instruments.

Tips for obtaining good results

- Collect background with a clean sensor in air
- Collect pure component spectra of solvent and major reagents.
- Start your reaction collection with just solvent in the reactor.
- Make sure no bubbles are trapped on the sensor (especially in aqueous systems).
- Check that the probe remains immersed in the solvent when stirring is on.
- Add components one at a time and collect at least four spectra between each addition.
- Make copious annotations (Adding an Annotation.) Label the beginning and end of additions, results from grab samples, modifications in reaction parameters (e.g., temperature, stirring speed), and events that you see (e.g., precipitation, color change, gas release).
- Make sure concentration of the species of interest is within the detection limits of your ReactIR system and chosen sampling technology.
- Make changes to see the effect upon the reaction profiles (add another aliquot (spiking), increase stirring, change temperature). This can increase your knowledge about the chemistry.
- Since absorbance is proportional to concentration, the ReactIR iC10 provides a qualitative 'movie' of concentration trends over the course of the reaction. Grab samples for off-line analysis can provide the quantitative 'snapshots' for putting the ReactIR iC10 profiles in the correct context.
-

Good/Poor application choices

- A major advantage of ReactIR instruments is the ability to measure in real-time what is going on inside the reactor under actual reaction conditions. Thus, reactions involving air sensitive reagents, extremes in temperature or pressure, toxic or corrosive reagents, or unstable intermediates are good candidates for monitoring.
- ATR (Attenuated Total Reflection) sensors such as the DiComp are essentially measuring the LIQUID phase of the reaction mixture. The probe is NOT sensitive to bubbles and solids in a well mixed solution. Be observant for dissolution and precipitation of solids!
- Often times impurities are very structurally similar to the desired product and are at low concentration. These facts make it difficult to track low level impurity profiles using the ReactIR. However, there are exceptions, especially when impurities form at higher concentrations. Under these conditions impurities may be tracked with the ReactIR.
- Although infrared spectra are very specific for functional groups, these groups vary in their ability to absorb mid-infrared energy. Functional groups with strong dipoles (such as carbonyls) will yield large peaks versus groups with smaller dipoles (such as alkenes). The stronger the peak, the easier it is to profile. Check the references for functional groups that absorb strongly.
-

Functional groups in the diamond 'blind spot'

Diamond absorbs infrared energy in the region 1950 to 2250 cm-1. This 'blind spot' masks the following functional group frequencies:

- isocyanate (~2275 cm^{-1})
- acetylene (~2200 cm^{-1})
- isothiocyanate
- cyanide, thiocyanate, cyanate (2200-2000 cm^{-1})
- C=N (~2150 cm^{-1})

- azide (~2100 cm^{-1})
- silane (~2050 cm^{-1})
- BH_3 (~2100 cm^{-1})
- ketene (~2200 cm^{-1})
- allene (~1975 cm^{-1})

Refer to: Data Treatments Task Pane

If you wish to monitor any of these functional groups directly, then both the SiComp (Silicon sensor) and ZrComp (Zirconium sensor) are excellent alternatives to have accessible in your laboratory. In fact, the SiComp ATR element transmits IR energy throughout the entire mid-IR region, so it is recommended that both the DiComp and SiComp are available to the user as this extends the utility of the instrumentation for monitoring all types of chemistry.

How do I perform the test(s)?

1. Weigh the test material and record the mass to the nearest milligram.
2. Examine the test material (preferably under low magnification) and record your observations.
3. Suspend the test material in the process matrix for the duration of the process. Ensure that the material is not mechanically damaged by the agitator.
4. Remove the material from the process matrix at the end of the process and rinse gently with an appropriate solvent. Dry with air or nitrogen.
5. Repeat steps 1 and 2.
6. Evaluate the differences (if there are any) between the mass and appearance of the test material before and after the reaction.

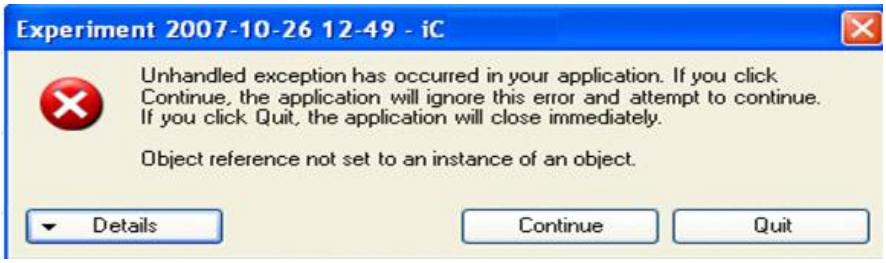
If there are differences, then it could be that your process conditions are incompatible with the test material. Contact your local Mettler Toledo AutoChem representative, or call (US) 410-910-8100 ext. 2 and ask to speak with a ReactIR specialist.

Error Messages

The iC software has extensive error handling capabilities. These capabilities range from verifying correct program execution and hardware functionality to the validity of variables entered by the user for data manipulation. The content of error and warning messages provides valuable information for AutoChem personnel when diagnosing problems.

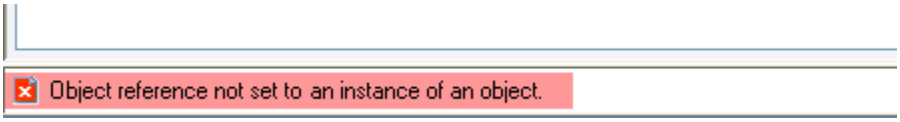
Instrument-type errors turn the Live Experiment toolbar red and displays the error as a tooltip on the toolbar. In addition, the errors are logged in the Event Viewer and in the iC Log Manager logs. Instrument type errors consist of actual failures with the hardware and communication errors between the iC software and the instrument. Communication errors include failures with the PC communications port and cabling issues. Many times the tooltip will provide hints for resolving the problem.

System type errors generate an error dialog as shown below.



Normally the user should try and continue. In the event the error dialog continues to pop up, the user should quit. Clicking the **Quit** button closes the iC application. The user can then restart the iC application and try and continue operation.

General error and warning messages are displayed in the status area at the bottom of the main window.



These errors are also logged in the Event Viewer and in the iC Log Manager logs.

Info	12:50:13 PM 10/26/2007	Experiment Started
SystemAnnotation	12:50:13 PM 10/26/2007	Experiment Paused
Error	12:50:20 PM 10/26/2007	Object reference not set to an instance of an object.
Error	12:50:20 PM 10/26/2007	Object reference not set to an instance of an object.

The section, The Customer Care Log File Utility describes how to send Log Manager reports to AutoChem.

ReactIR Troubleshooting

This section provides guidance for resolving various situations you may encounter working with iC IR and/or the ReactIR iC10. Each troubleshooting procedure includes a summary of the situation it addresses and step-by-step instructions for diagnosing and resolving the problem.

Alignment Indicators are Not in Spec

(For the ReactIR 15 instrument, refer to ReactIR15 Alignment Indicators are Not in Spec)

This troubleshooting procedure addresses common problems you may be having related to getting the Peak Height and Contrast indicator bars to turn green on the Align pages of the Start Experiment and Create Spectra Library wizards and blue on the Configure Instrument wizard.

1. If you have any doubts that the instrument set up properly, please refer to the ReactIR iC 10 Setup Procedure or the ReactIR 45m Setup Procedures.
2. Verify that the ReactIR instrument has been turned on for at least three hours to allow sufficient time for system stabilization.
3. Verify that the ReactIR instrument is properly purged. Allow at least one hour for purging. See the Purge Quality Indicator is Not Green troubleshooting procedure for additional details.
4. Verify that the ReactIR Dewar been filled with liquid nitrogen for at least 20 minutes to allow the detector sufficient time to cool.
5. Maximize the peak height and contrast according to the correct procedure below: section a. for fiber conduits or section b. for optical conduits.

    a. When using a fiber conduit; verify that the purge fitting on the probe housing connected to the instrument is in a vertical orientation either pointing straight up or straight down and verify that the probe housing is snuggly fitted to the instrument and that the clamp is tight.

    If you have confirmed that the orientation and the connection are correct and the contrast and / or peak height bars are still red, loosen the clamp on the probe housing and rotate the probe housing slightly to the left or right (5 to 10 degrees should be sufficient). Rarely, you may need to readjust the detector mirror. Alternating back and forth between the two adjustment screws on the front of the instrument, slowly adjust the screws about a ¼ turn or less at a time. You should not have to change either screw by more than a full turn total in either direction. If you still cannot get the peak height and Contrast bars to turn green, contact customer service.

    b. When using a K6 or K4 optical conduit, use the three step alignment procedure:
        i. rotate the probe to maximize contrast
        ii. adjust the knurled knobs on the knuckle adjacent to the probe to maximize peak height
        iii. adjust the MCT detector mirror to further maximize peak height. Two to four iterations of this process are usually needed optimize alignment. If you still cannot get the peak height and Contrast bars to turn green, contact customer service.

ReactIR 15 Alignment Indicators are Not in Spec

The ReactIR 15 is factory aligned and requires no system purge. Therefore, if the bars indicate the alignment is not within specifications, follow the steps below:

1. Verify that the hardware settings reflect your hardware configuration (Start Page > Configure Instrument).
2. Verify that the ReactIR Dewar has been filled with liquid nitrogen for at least 20 minutes to allow the detector sufficient time to cool and ensure the ReactIR 15 base unit has been powered on for at least four hours.
3. Collect a reference background while the probe is clean and exposed to the air (Start Page > Configure Instrument > Clean Probe > Align Probe). This background will become the baseline for determining that the probe alignment is within specifications.

Clean Probe Indicator is Not Green

This troubleshooting procedure addresses common problems you may be having related to getting the Clean indicator bar to turn green on the Clean pages of the Configure Instrument, Start Experiment and Create Spectra Library wizards.

1. Verify that the system is properly aligned, see Alignment Indicators are Not in Spec.
2. Visually inspect the sensor which at the tip of the probe. It should have a mirror-like appearance.
3. Rinse the probe with an appropriate solvent to dissolve or rinse away any visible residue.
4. Dry the sensor with a lint-free towel or pure cotton swab (not a Q-tip, which have oils!). Perform a final swabbing using a pure cotton swab wetted with reagent grade acetone and a circular motion around the sensor. Repeat as necessary. Refer to: Configuring the ReactIR section.
5. To remove material stuck to DiComp or ZrComp sensor, you may scrape the sensor with the wooden end of a cotton swab. For a SiComp sensor, continue rinsing with room temperature or hot solvent until clean. Do not scrape a SiComp sensor – strong physical action will damage the sensor.
6. If the probe is still not clean, try cleaning the probe tip in an ultrasonic cleaner.
7. If none of above works, contact customer service.

Purge Quality Indicator is Not Green

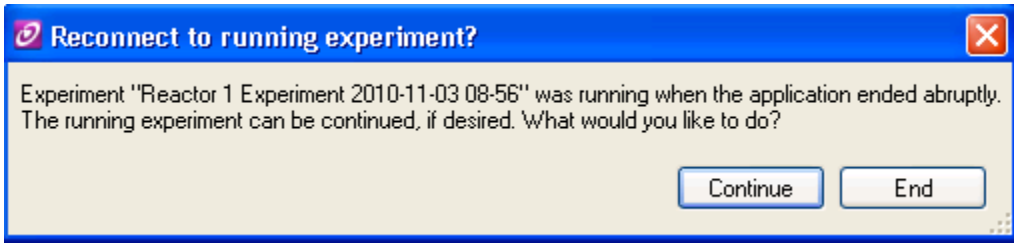
This troubleshooting procedure addresses common problems you may be having related to getting the Purge Quality indicator bar to turn green on the Clean Probe pages of the Configure Instrument, Start Experiment and Create Spectra Library wizards.

1. Verify that the system is properly aligned (see Alignment Indicators are Not in Spec) and that the probe is clean (see Clean Probe Indicator is Not Green).
2. Verify that all purge lines are properly connected.
    a. For a C1 probe, there are three purge fittings: on the rear of the instrument, near the fiber optic housing connected to the instrument and at the probe.
    b. For an AgX (Silver Halide) probe, there are two purge fittings: on the rear or the instrument and the fiber optic housing connected to the instrument.
    c. For a K4 or K6 connect the purge tubing at all of the available fittings: on the rear of the instrument, one on the probe and 1 or 2 on the conduit.

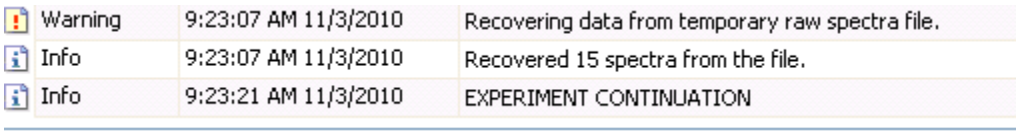
3. Verify that nominal purge pressure is 10psig (0.69barg) with a flow rate of 10 SCFH (4.7lpm).
4. Verify that the purge system is using instrument grade air, Nitrogen or other suitable inert gas.
5. If none of above works, contact customer service.

Possible Data Loss during an Application Failure

If the iC IR application fails or becomes inoperable, possible loss in the data can occur. During the period of time when the application is not operational, the instrument will likely continue to run the experiment. If the user restarts the iC IR application, it will attempt to reload any running experiments and resume collecting data. It this event, the user is given the option of continuing the experiments or ending them.

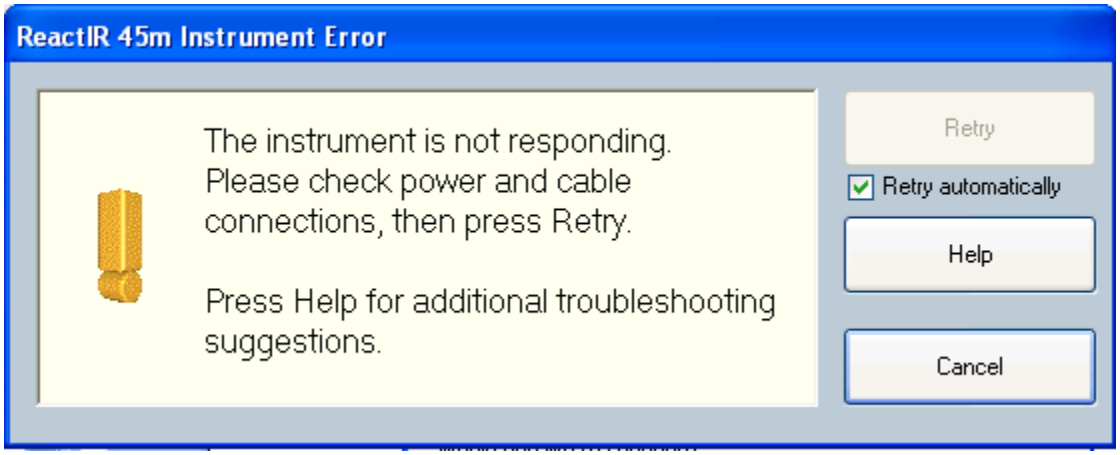


If the user elects to continue the experiments, data collection is resumed and any data in the temporary raw data file is recovered. A message is also entered into the event log.

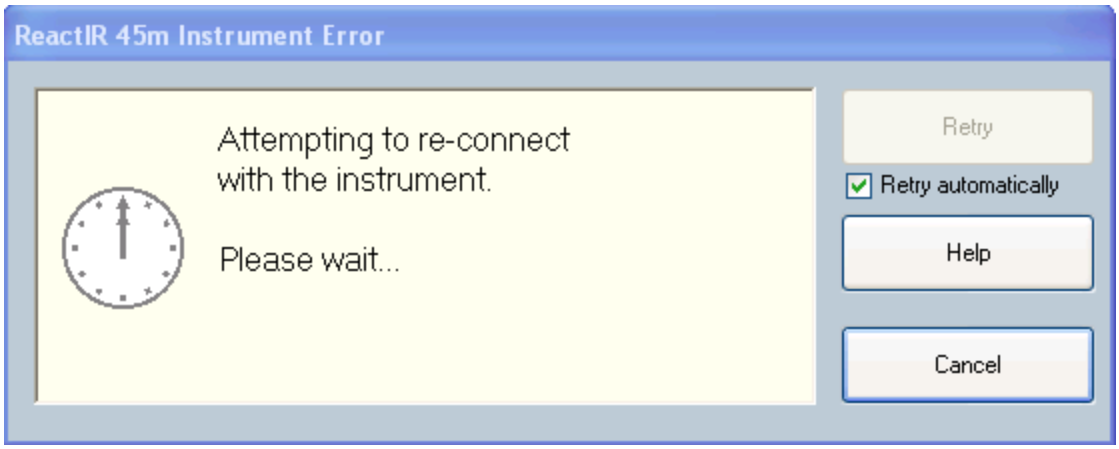


Instrument Error

If communication with the instrument is lost, an error dialog is displayed.



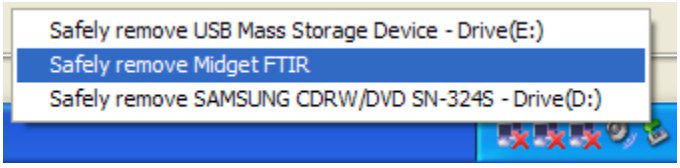
The iC IR software will attempt to re-establish communications with the instrument either automatically or manually as specified in the dialog.



If iC IR cannot communicate with the ReactIR instrument, verify the following:

1. Verify that the iC10 is plugged in and turned on. The green Power LED on the front of the instrument should be on.
2. Verify that the USB cable is fully plugged in to the back of the iC instrument.
3. Verify that the other end of the USB cable is fully plugged in to a USB port on the computer running the iC IR software.
4. Verify that the Midget FTIR device driver is loaded. Look for the USB Device icon in the system tray in the lower right edge of your screen.

5. Click on the USB Device icon and verify that the pop-up menu includes an option to “Safely remove Midget FTIR”. DO NOT select that option.



6. Turn off power to the hardware. Wait 15 seconds. Turn power back on.
7. Wait another minute allowing iC IR to retry establishing communications.

If communications are still not re-established, do the following:

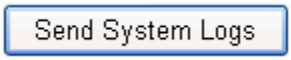
8. Exit iC IR.
9. Turn off power to the hardware. Wait 15 seconds. Turn power back on.
10. Verify that the Midget FTIR device driver is loaded. Look for the USB Device icon in the system tray in the lower left edge of your screen.
11. Click on the USB Device icon and verify that the pop-up menu includes an option to “Safely remove Midget FTIR”. DO NOT select that option.
12. Restart iC IR.

If the problem persists, contact customer service.

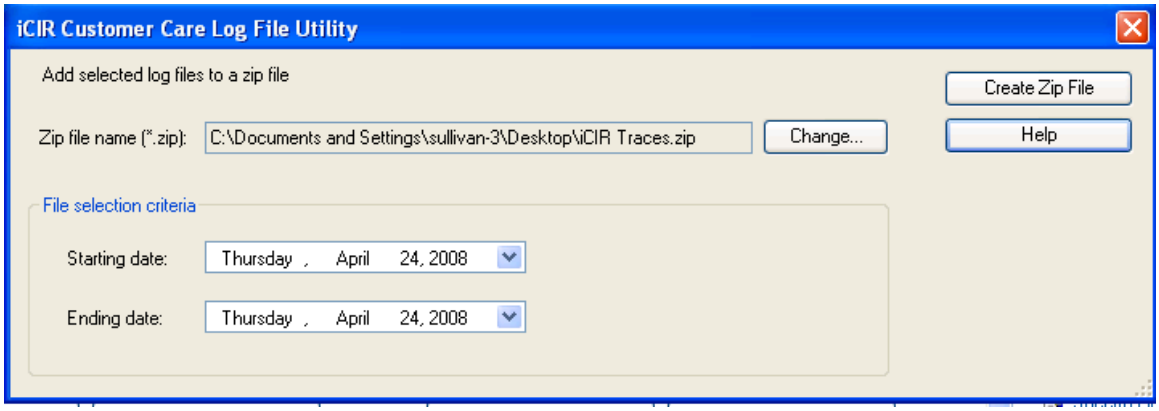
The Customer Care Log File Utility

The Customer Care Log File Utility creates a compressed (ZIP) folder of all system log files, licensing information and remote instrument diagnostic data (on supported instruments only). These log files are used by Mettler Toledo Customer Care as an aid in diagnosing problems with the iC software.

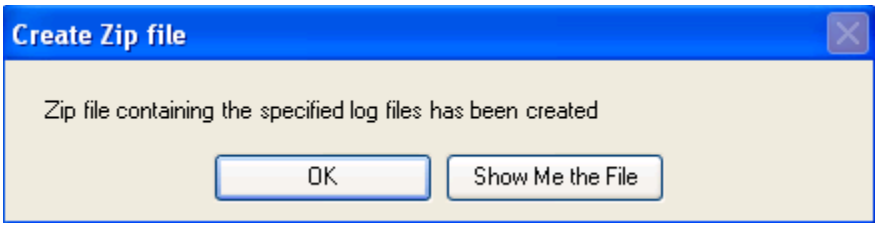
It is advisable to create a log file folder and include it with any problem reports. To create a log file, click the



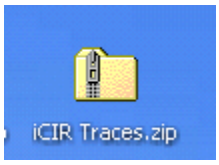
button on the Start Page.



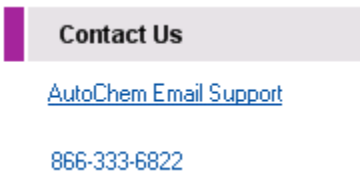
Select the date period in which you encountered the issue and click on the **Create Zip File** button. A log folder is created on the Desktop and a completion message is displayed.



The log folder is saved to the Desktop or the location specified in the Zip File Name field. The filename for the folder is ICIR Traces.Zip



The hyperlink on the Start Page can be used to email the report to Mettler Toledo Customer Care.



ReactIR Technical References

Over the past 15 years, ReactIR technology has been applied extensively in the fields of catalysis[1-3], crystallization[4-6], safety / scale-up[7-9], mechanistic studies[10-12], and polymerization[13-16]. The iC IR Software uses two complementary techniques to produce time vs. relative concentration profiles. The first of these is referred to as peak profiling (see Real-time Peak Profiles vs. ConcIRT LIVE Profiles) and the second utilizes Mettler Toledo's proprietary self-modeling curve resolution algorithm; ConcIRT LIVE The ReactIR iC utilizes the highly selective mid-infrared region of the spectrum. Although a thorough discussion of infrared spectroscopy is outside the scope of this introduction, there are many excellent references to guide the reader through the theory underlying the application of mid-infrared spectroscopy to the industrial and academic investigations[17,18].

Catalysis

1. "Dynamic Ligand Exchange of the Lanthanide Complex Leading to Structural and Functional Transformation: One-Pot Sequential Catalytic Asymmetric Epoxidation-Regioselective Epoxide-Opening Process", Tosaki, S., Tsuji, R. Ohshima, T., Shibasaki, M. JACS, 127, 2147-2155.

2. "Enantioselective and Diastereoselective Maukaiyama-Michael Reactions Catalyzed by Bis(Oxazoline) Copper (II) Complexes", Evans, D. A., Willis, M. C., Johnston, J. N., JACS, 123, 2001, 4480.

3. "Cooperative Asymmetric Catalysis Using Dimeric Salen Complexes", Konsler, R., Karl, J., Jacobsen, E. JACS, 120, 1998, 10780-10781,

Crystallization

4. "Monitoring and Feedback Control of Supersaturation Using ATR-FTIR to produce an Active Pharmaceutical Ingredient of a Desired Crystal Size", Vincenzo Liotta, Vijay Sabesan, *Organic Process Research and Development*, 2004, 8, 488-494.

5. "Influence of Solvent and Operating Conditions on the Crystallization of Racemic Mandelic Acid", Crystal Growth and Design, 2004, Vol. 4, No. 2, 315-323. Veronica M. Profir, Ake C. Rasmuson

6. "Solution Concentration Prediction for Pharmaceutical Crystallization Processes Using Robust Chemometrics and ATR FTIR Spectroscopy"; Togkalidou T., Tung H.-H., Sun, Y., Andrews A., Braatz R. D., Organic Process Research & Development, 6, 2002, 317-322

Safety/Scale-Up

7. "A Calorimetric Investigation to Safely Scale-Up a Curtius Rearrangement of Acryloyl Azide", am Ende, D., DeVries, K., Clifford, P., Brenek, S., *Org. Proc. R&D*., 2, 1998, pp 382-392

8. "Preparation of Grignard Reagents: FTIR and Calorimetric Investigation for Safe Scale-up", am Ende, D. J., Clifford, P. J., DeAntonis, D. M., SantaMaria, C., Brenek, S. J., *Org. Proc. Res. Dev.*, 3(5), 1999, pp 319-329

9. "Streamlining Process R&D Using Multidimensional Analytical Technology", McConnell, J. R.; Barton, K. P.; LaPack, M. A.; DesJardin, M. A.; *Org. Process Res. Dev.;* (Technical Note); 2002; ASAP Article. DOI: 10.1021/op0255332 (Published on the ACS website)

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11. **Computational, ReactIR-, and NMR-Spectroscopic Investigations on the Chiral Formyl Anion Equivalent *N*-(α-Lithiomethylthiomethyl)-4-isopropyl-5,5-diphenyloxazolidin-2-one and Related Compounds** Christoph Gaul, Per I. Arvidsson, Walter Bauer, Robert E. Gawley, Dieter Seebach Chemistry-AEuropeanJournal Volume 7, Issue 19, 2001. Pages 4117-4125

12. On the Mechanism of Catalytic, Enantioselective Allylation of Aldehydes with Chlorosilanes and Chiral Lewis Bases", Denmark S. E., Fu J., *J. Am. Chem. Soc.* 122, 2000, 12021-12022

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13. “In-Line Monitoring of Butyl Acrylate and Vinyl Acetate Emulsion Copolymerizations Using ATR-FTIR Spectroscopy. Jovanovic, R., and M.A. Dubé, Polym. React. Eng. J., 11, 233-257 (2003).

14. **Photocuring of a thiol-ene system based on an unsaturated polyester**
Y. B. Kim, H. K. Kim, H. C. Choi, J. W. Hong
Journal of Applied Polymer Science
Volume 95, Issue 2, 2005. Pages 342-350

15. Real-Time Monitoring of Carbocationic Polymerization of Isobutylene Using in Situ FTIR-ATR Spectroscopy with Conduit and Diamond-Composite Sensor Technology”, Storey, R., Donnalley, A., Maggio, T., *Macromolecules*, 31, 1998, pp 1523-1526

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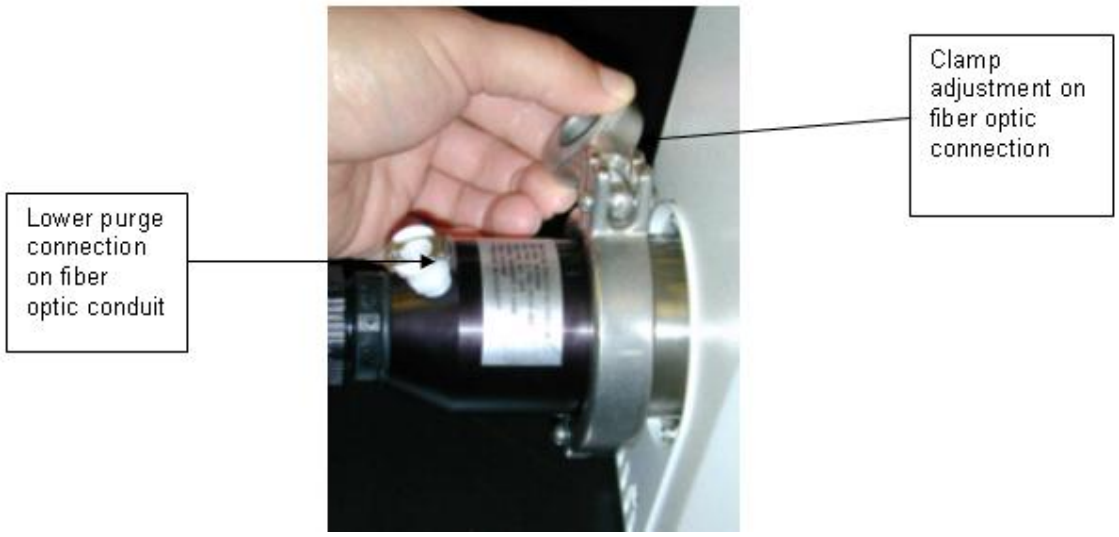
17. Infrared Raman Characteristic Group Frequencies Tables and Charts by George Socrates published by Wiley, 3rd Edition, ISBN: 0-470-09307-2

18. Introduction to Infrared and Raman Spectroscopy”, Norman B. Colthup, Lawrence H. Daly, Stephen E. Wiberley, Stephen E. Wiberly Academic Pr ISBN: 012182554X 3rd Ed. 1997

ReactIR Setup Procedure

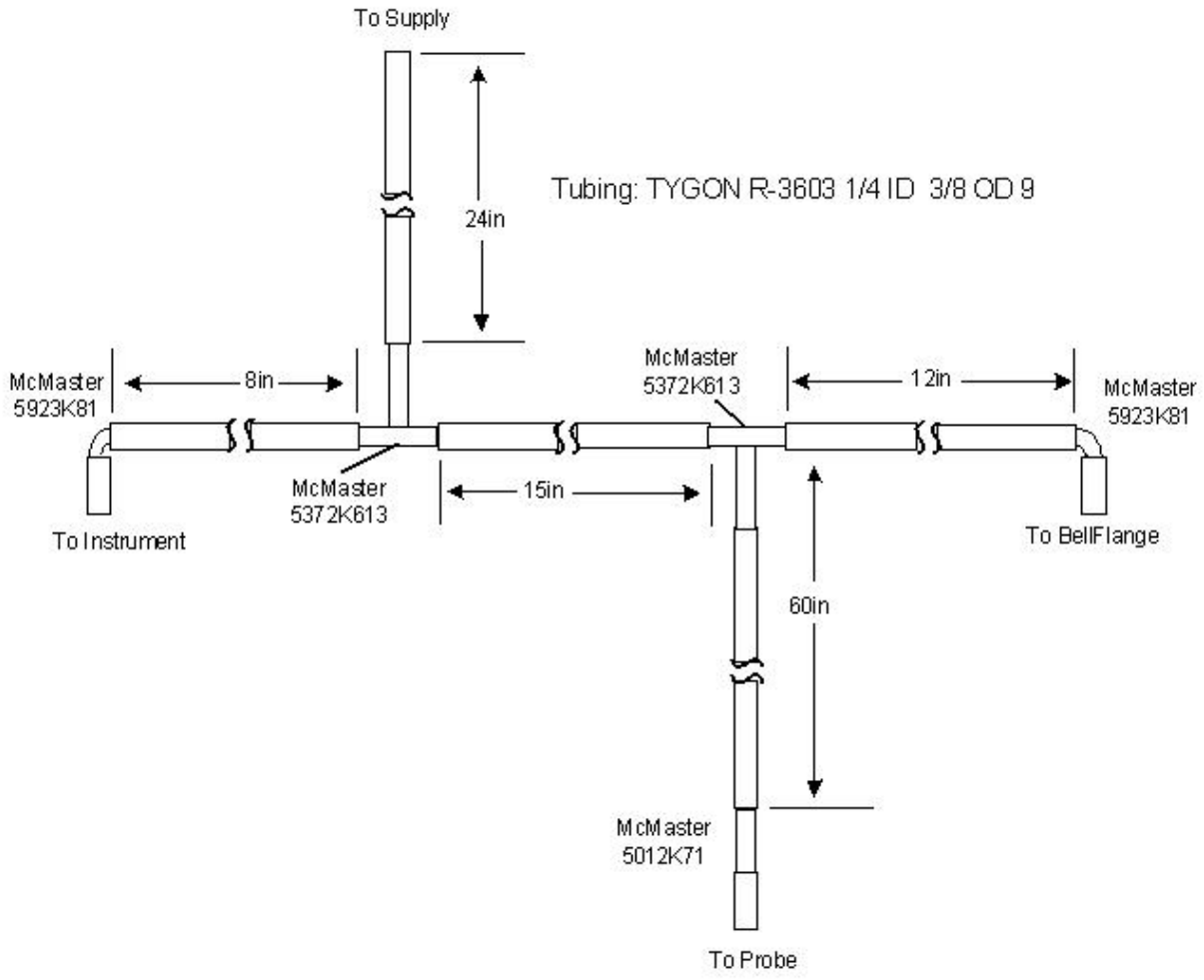
This procedure describes the setup procedure for setting up the ReactIR. Note that initial setup, testing and calibration should be done by a qualified METTLER TOLEDO AutoChem Service Engineer **and are not described here.**

1. **Position the ReactIR on a laboratory bench or in a laboratory hood configuration following the recommended Instrument Handling Instructions.**
2. **Connect the fiber optic conduit as indicated below.**



Connecting the Fiber Optic Conduit

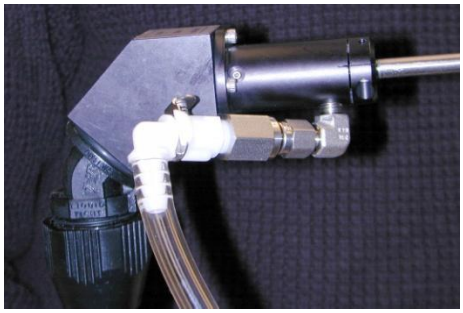
3. **Connect the purge lines to the probe.**
    a. **For a C1 probe, there are three purge fittings: the rear of the instrument, the fiber optic housing connected to the instrument and the probe.**
    b. **For a AgX (Silver Halide) probe, there are two purge fittings: the rear or the instrument and the fiber optic housing connected to the instrument.**



Purge Line tubing for ReactIR iC10

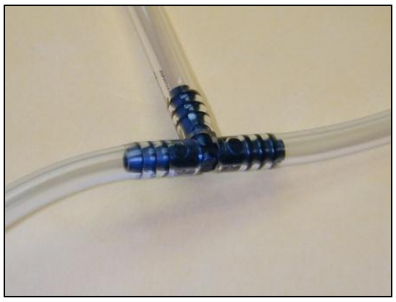
Main connection of fiber optic unit with purge line connected.

For alignment purposes, the purge connector on the instrument end of the 6.3mm Fiber Conduit probe should either be facing upwards (12 o'clock) or downwards (6 o'clock). On a 9.5mm Fiber Conduit probe the purge fitting should be oriented to the left (9 o'clock) or to the right (3 o'clock) positions.

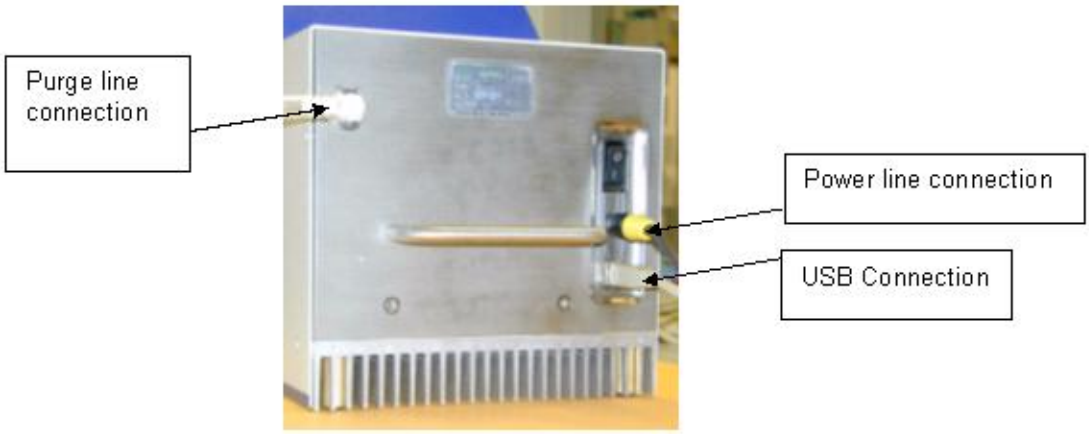


Probe with purge line attached.

Use a "y" adapter to connect the purge lines.



"Y" adapter for purge lines



Connections at rear of ReactIR iC10

4. **Adjust purge pressure to nominal 10psig (0.69barg) and 10SCFH (4.7lpm) flow rate.**
    a. **NOTE a flow regulator is not supplied by Mettler Toledo.**
5. **Connect the power cable to rear to the instrument.**
6. **Connect the AC plug of the power supply to the power outlet.**
7. **Turn on power to the ReactIR iC10.**

8. **Connect the USB communications cable to the rear panel as shown below.**
9. **Connect the other end of the communications cable to the USB port on the workstation.**
10. **Fill the MCT cooling chamber with liquid nitrogen (N_2) until the chamber is full. The port is located on the top of the unit as shown in the photo below.**

Filling the liquid nitrogen chamber

Always wear a face shield, goggles and insulating gloves when filling the iC10 with liquid nitrogen.

Liquid nitrogen boiling in funnel.

Use care in pouring liquid nitrogen into the ReactIR iC10. The sudden drop in temperature my fracture the funnel. Let the liquid nitrogen stabilize in the funnel and vent off. Do not overfill. Liquid nitrogen is explosive when not allowed to vent properly.

11. **Allow sufficient time for the system to stabilize considering each of the factors below:**
    a. **The system should be powered on for at least three hours from a cold start to allow sufficient time for the optics to stabilize to the ambient temperature.**
    b. **The purge needs to be connected and active for at least one hour to allow sufficient time for water vapor to be purged from the system.**
    c. **The system requires at least 20 minutes after adding liquid nitrogen for the interferometer in the instrument to fully cool.**

Note: The iC10 will function for 24 hours with one load of liquid nitrogen. This includes a stabilization time as described above.

CAUTION: The system can be awkward when handling.

When moving the ReactIR iC10 system, it is highly recommended to use a cart or similar type device. The system can be hand-carried by using the integrated handle on the rear of the system along with using the front sampling attachment port.

DO NOT hand carry the system with the fiber optic or the mirror conduit attached to the system. Remove the conduit first before moving the unit.

ONLY move the system with the conduit attached by using a cart or similar device. This will prevent any possible damage to the unit or personnel.

ONLY lift the system using BOTH the handle in the rear and the sampling port on the front of the unit. Lifting the unit in other manners may cause damage to the system or personal injury should the cover unexpectedly become detached.

Maintenance and Cleaning

- Ensure the unit is powered off before doing any cleaning.
- Clean all exterior surfaces only with water and mild detergent.
- Do not use any alcohols, acids, bases or any flammable material to clean any part of the system.
- Be careful not to submerse any parts of the system with washing liquid.
- Be certain to dry all surfaces of the system after washing to avoid pooling of any liquid.

Leave system powered off for at least 30 minutes after washing to avoid accidental short circuit of the electronics.

ReactIR Safety

Be sure read and follow all guidelines and recommendations in your Chemical Hygiene Plan to ensure safe operation of ReactIR. Use of ReactIR in a manner other than that described in this manual and all associated safety procedures may result in serious injury, damage to equipment and/or void the warranty of the system.

The ReactIR is designed to be used in a ventilated fume hood. Alternatively, this system can be used on a bench top with the flexible fiber optic conduit positioned inside the fume hood where the reactor is located.

LASER Safety

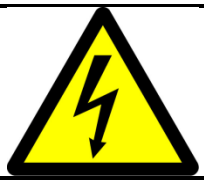
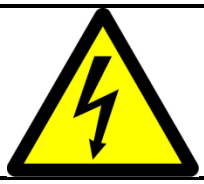
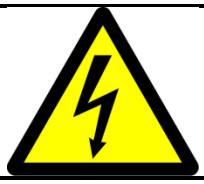
The ReactIR System contains a LASER. Protective warning labels are located on the system at points where laser radiation may be accessible. Located on and next to removable cover of interferometer:

CAUTION
Laser light when open
DO NOT STARE INTO BEAM

To ensure that no exposure to laser radiation in excess of that allowed for Class 1 laser products, do not attempt adjustment or repair of this unit beyond that described in this manual. Access to a HeNe laser power up to 5 mW could be accessible if the interior of the inner cover is removed.

CAUTION: Use of controls or adjustments or performance of procedures other than those specified herein may result in hazardous laser light exposure.
CAUTION: The use of optical instruments with this product will increase eye hazard. Note that this statement applies to binoculars, telescopes, SLR cameras, and other instruments with collecting optics, and it does not apply to eyeglasses or contact lenses.

Measures for your protection

System Unit - Interferometer	
	Opening access door on side of system unit will expose interior components. Do not remove the cover from the top of the interferometer while power is supplied to system unit.
Interface Board	
	Opening access door on side of system unit will expose interior components. Do not touch contact points on board.
Node Computer	
	Opening access door on side of system unit will expose interior components. Do not touch contact points on board.
Heat Exchanger	
	Do not touch heat exchanger on top of system unit. Do not touch heat exchanger on outside rear of system unit. Opening access door on right side of system unit will expose interior components.
Power Supply Connections	
	Do not supply power with any power cord except the one supplied with the system unit.

Power Supply Conduit Orientation	
	Extending the conduit with sampling technology attached may cause system to become unstable if not secured on mounting base.
 Risk of an electric shock	**Grounding the power supply outlet** Make sure that you plug the power cable supplied with the ReactIR system into power supply outlets that are grounded. A technical fault could otherwise result in death or serious injury.
Measures for operational safety	
 Caution	**Connection of cables** Connect all cables (power and communications) of ReactIR system to their respective inputs and outputs before you switch on the system. Do not disconnect any cables while the system is in operation as this may cause damage to internal electrical components.
 Caution	**Handling Liquid Nitrogen** Liquid Nitrogen is used with the ReactIR system to cool the MCT detector for optimum detector performance. Liquid Nitrogen will cause severe burns to exposed skin. Ensure use of proper clothing (gloves) and eye protection before handling liquid Nitrogen. **NOTE: A caution label is located on the top of the ReactIR next to the Liquid Nitrogen fill port.**
 Caution	**Liquid Nitrogen "Blow Off"** When filling the MCT detector with Liquid Nitrogen there is a chance that the Liquid Nitrogen may "Blow Off" once sufficient pressure is reached inside the detector cooling chamber. It is recommended to add liquid Nitrogen slowly to allow sufficient time for entrained pressure to release from the cooling chamber and prevent "Blow Off".
 Caution	**Cold Surfaces (Liquid Nitrogen Spills)** Spills will most likely occur when filling the MCT cooling chamber with Liquid Nitrogen. Normal Liquid Nitrogen spillage (i.e. Blow Off) will not damage components of the ReactIR system BUT will create COLD surfaces. Avoid touching these cold surfaces without proper protective clothing. These cold surfaces typically warm to room temperature within a few minutes (~15min).

 Caution	**Instrument Purge** The ReactIR system should be purged at all times (whether system is powered on or not) using instrument grade air, Nitrogen or other suitable inert gas. The purge prevents water vapor from collecting inside the optics that otherwise can obscure the spectral data. The purge fittings are located (1) on the rear panel of the unit and (1) located at the fiber housing that connects to the instrument. In the case of the C1 probe, there is also a second purge fitting on the probe. Nominal purge settings: 10psig (0.69barg), 10SCFH (4.7lpm) flow rate, -50C Dew Point
 Caution	**General** Exclude the following environmental influences: • powerful vibrations • direct sunlight • atmospheric humidity greater than 60% • temperatures below 15C and above 40C • powerful electric or magnetic fields
 Caution	**Service** Never open the enclosure of the ReactIR system or any of its components. These items are serviced only by a qualified METTLER TOLEDO AutoChem Service Engineer.

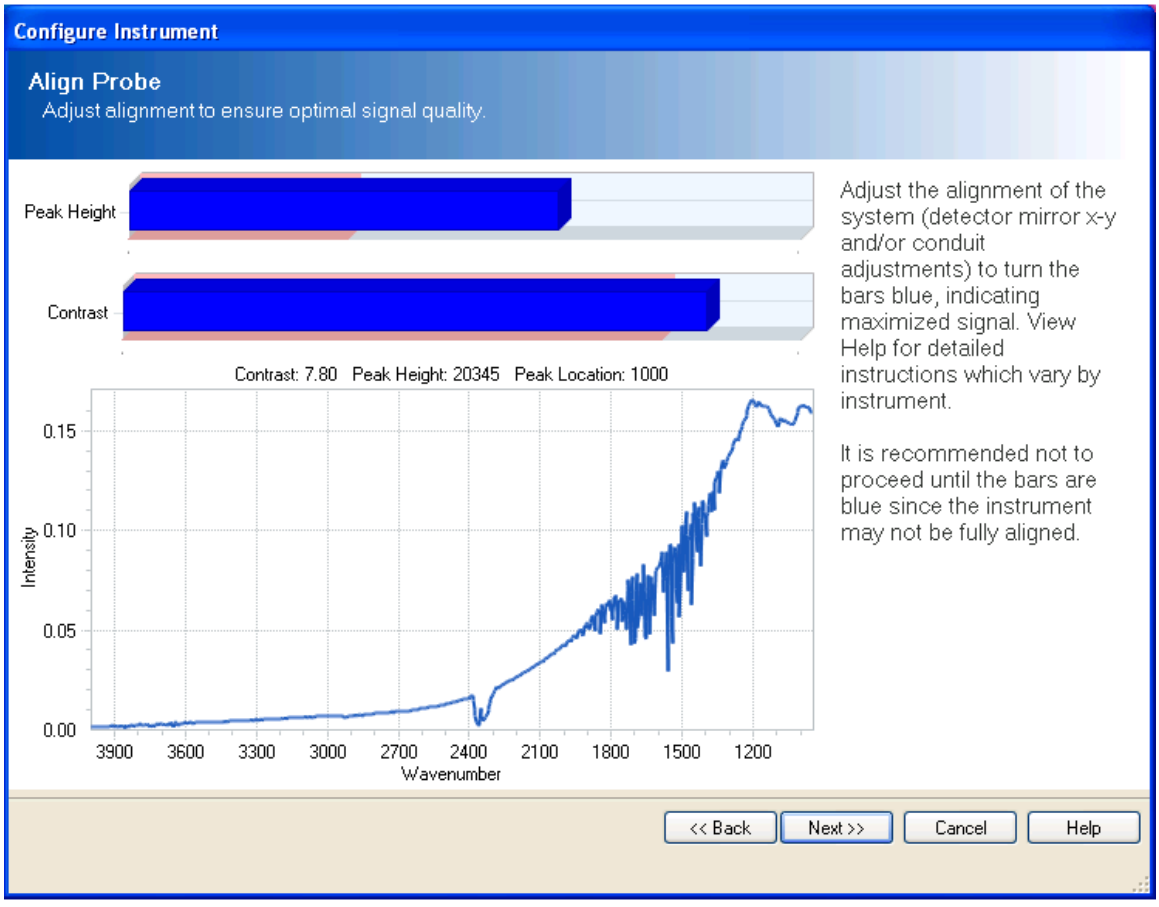
ReactIR iC10 Setup Procedures

You must configure the iC IR software with information about your ReactIR iC10c hardware before you can use it to conduct experiments. Configuration consists of the following steps:

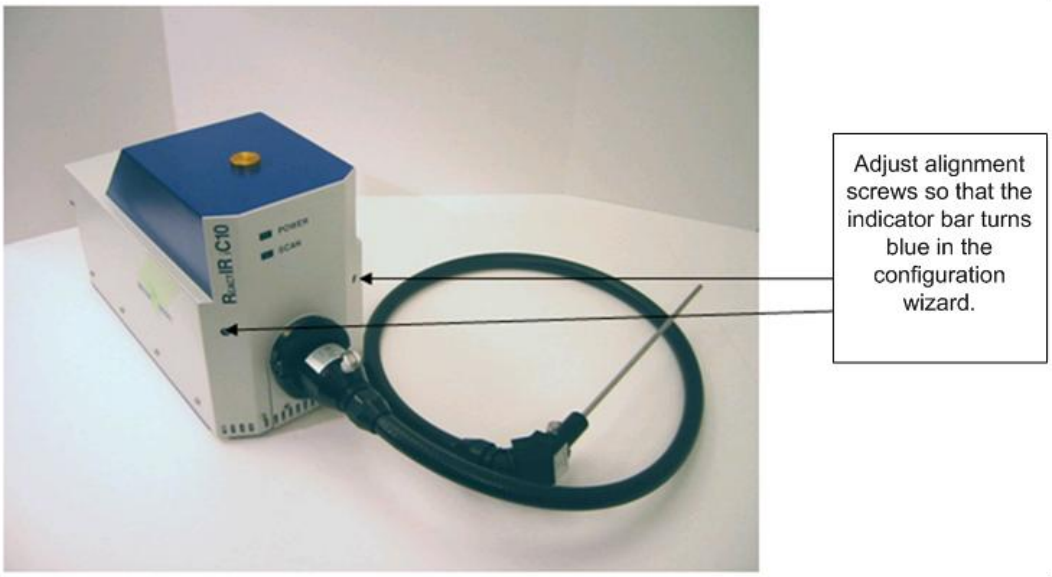
1. Specify hardware settings reflecting your hardware configuration.
2. Optionally adjust software settings used when collecting and processing data from the instrument.
3. Collect a reference background while the probe is clean and the system is well purged. This will be used subsequently as a baseline for accessing whether the probe tip is clean and the system purge is working properly.
4. Collect a reference background while the probe is clean and the system purge is off that will be used subsequently to support the water vapor correction feature.

These configuration steps are accomplished using the Configure Instrument Wizard in the iC IR software. You can access this wizard by clicking the Configure Instrument button on the Start page of the iC IR software. Refer to the iC IR Help for additional information.

The Align Probe page of the wizard is used to physically align the probe. When the probe is aligned correctly, the indicator bars turn blue.



METTLER TOLEDO



System Alignment for C1 **FIBER INTERFACE with 6.3 mm (1/4") diameter Probe**

- At the Start Page, Click on the button **Configure/Test Instrument**.
- Select **Contrast** in the dialog box on the right.
- Click **Start**
- Rotate fiber optic conduit at the front of the instrument by ¼ turn CW (Clock Wise) and CCW (Counter Clock Wise) to maximize Contrast and Peak Height values.
- Adjust the detector mirror by turning adjustment screws located on the front left and right sides of the unit until Contrast and Peak Height are maximized.
- Acceptable Contrast is **> 10**.
- Acceptable Peak Height is **> 18,000**.

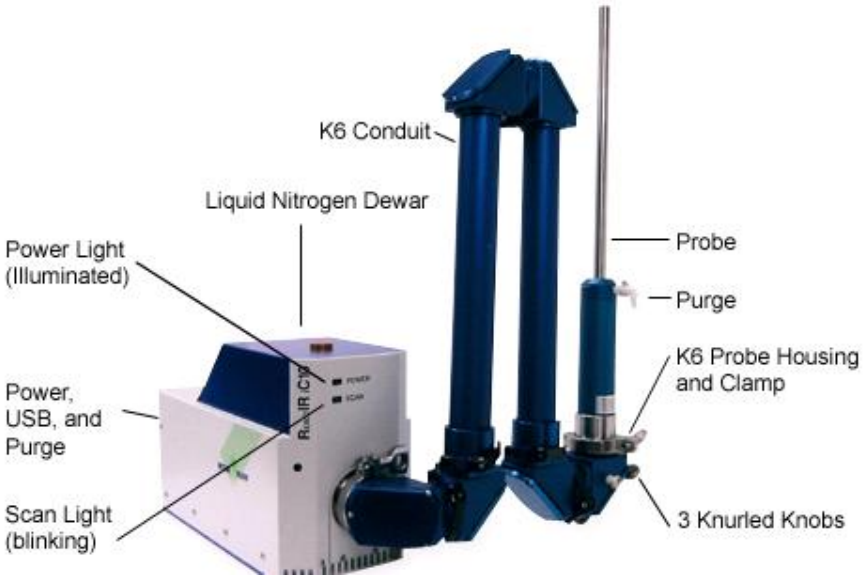
System Alignment for AgX **FIBER INTERFACE with 6.3 mm (1/4") diameter Probe**

- At the Start Page, Click on the button **Configure/Test Instrument**.
- Select **Contrast** in the dialog box on the right.
- Click **Start**
- Connect the fiber to the instrument with the purge fitting in the 12:00 or 6:00 position. Rotate fiber optic conduit at the front of the instrument by ¼ turn CW and CCW to maximize Contrast and Peak Height values.
- Adjust the detector mirror by turning adjustment screws located on the front left and right sides of the unit until Contrast and Peak Height are maximized.
- Acceptable Contrast is **> 10**.
- Acceptable Peak Height is **> 18,000**.

System Alignment for AgX **FIBER INTERFACE with 9.5 mm (3/8") diameter Probe**

- At the Start Page, Click on the button **Configure/Test Instrument**.
- Select **Contrast** in the dialog box on the right.
- Click **Start**
- Connect the fiber to the instrument with the purge fitting in the 3:00 or 9:00 position. Rotate fiber optic conduit at the front of the instrument by ¼ turn CW and CCW to maximize Contrast and Peak Height values.

- Adjust the detector mirror by turning adjustment screws located on the front left and right sides of the unit until Contrast and Peak Height are maximized.
- Acceptable Contrast is **> 10**.
- Acceptable Peak Height is **> 18,000**.



System Alignment for **K6 CONDUIT INTERFACE with 16 mm (5/8") diameter Probe**

- At the Start Page, Click on the button **Configure/Test Instrument**.
- Select **Contrast** in the dialog box on the right.
- Click **Start**
- Rotate probe on the end of the conduit 180 degrees CW and CCW to maximize Contrast and Peak Height values.
- Adjust detector mirror by turning adjustment screws located on the front left and right sides of the unit until Contrast and Peak Height are maximized.
- Acceptable Contrast for DiComp is **> 45**, acceptable Contrast for SiComp is > 30.
- Acceptable Peak Height is **> 20,000**.

System Alignment for **K4 CONDUIT INTERFACE with 25 mm diameter Sentinel Probe**

- At the Start Page, Click on the button **Configure/Test Instrument**.
- Select **Contrast** in the dialog box on the right.
- Click **Start**
- Rotate probe on the end of the conduit 180 degrees CW and CCW to maximize Contrast and Peak Height values.
- Adjust detector mirror by turning adjustment screws located on the front left and right sides of the unit until Contrast and Peak Height are maximized.
- Acceptable Contrast for DiComp is **> 50**, acceptable Contrast for SiComp is > 30.
- Acceptable Peak Height is **> 20,000**.

When the probe is aligned correctly the indicator bars turn blue as shown below.

ReactIR 15 Setup Procedures

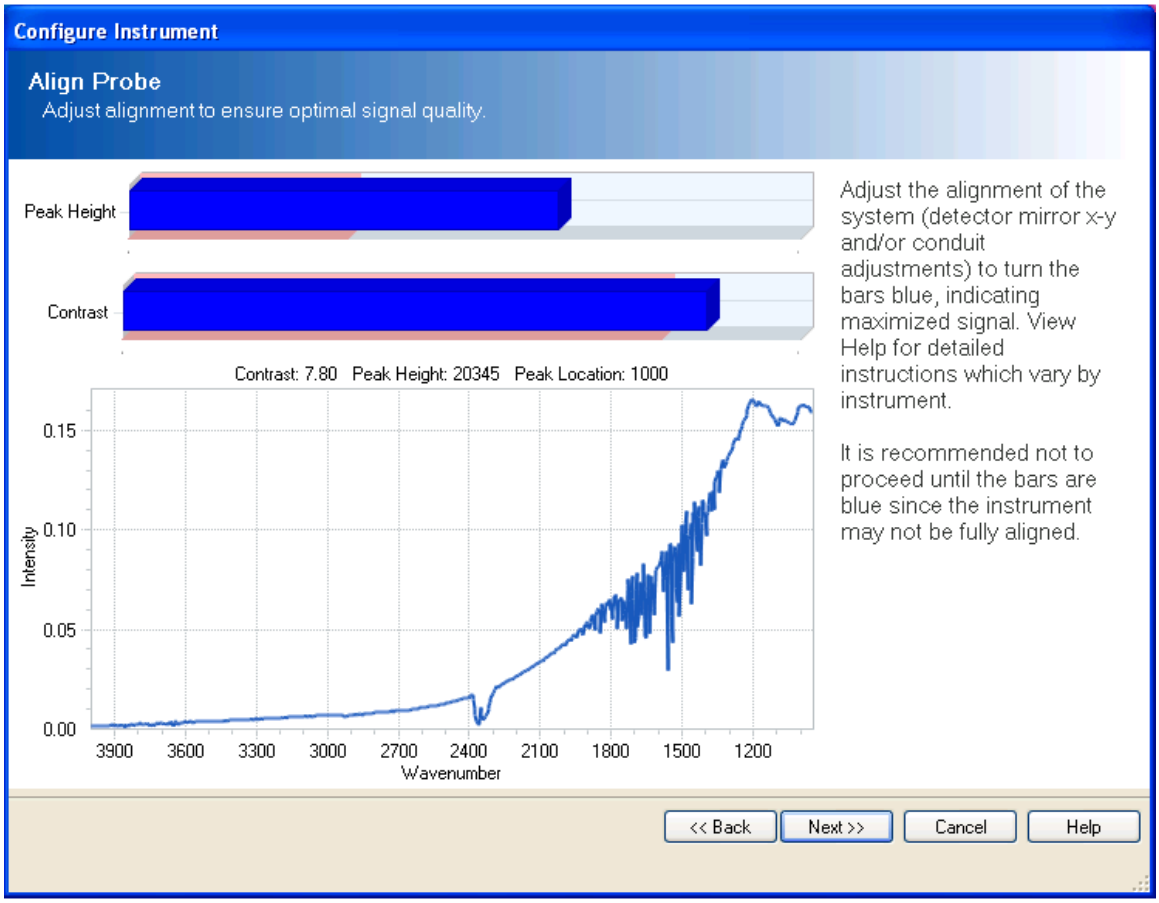
.You must configure the iC IR software with information about your ReactIR 15 hardware before you can use it to conduct experiments. Configuration consists of the following steps:

1. Specify hardware settings reflecting your hardware configuration.
2. Optionally adjust software settings used when collecting and processing data from the instrument.
3. Collect a reference background while the probe is clean. This will be used subsequently as a baseline for accessing whether the probe tip is clean.

These configuration steps are accomplished using the Configure Instrument Wizard in the iC IR software. You can access this wizard by clicking the Configure Instrument button on the Start page of the iC IR software.

Note: The final page in the wizard, which is entitled “Collect Water Vapor Sample”, is skipped for the ReactIR 15 instrument unless it is enabled in the User Preferences

The Align Probe page of the wizard is used to physically align the probe. When the probe is aligned correctly, the indicator bars turn blue.



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System Alignment for AgX **FIBER INTERFACE with 6.3 mm (1/4”) diameter Probe**

- At the Start Page, Click on the button **Start Contrast Test**.
- Connect the fiber to the instrument. Rotate fiber optic conduit at the front of the instrument by ¼ turn CW and CCW to maximize Contrast and Peak Height values.
- Acceptable Contrast is **> 10**.
- Acceptable Peak Height is **> 18,000**.

System Alignment for AgX **FIBER INTERFACE with 9.5 mm (3/8”) diameter Probe**

- At the Start Page, Click on the button **Start Contrast Test**.
- Connect the fiber to the instrument. Rotate fiber optic conduit at the front of the instrument by ¼ turn CW and CCW to maximize Contrast and Peak Height values.
- Acceptable Contrast is **> 10**.
- Acceptable Peak Height is **> 18,000**.

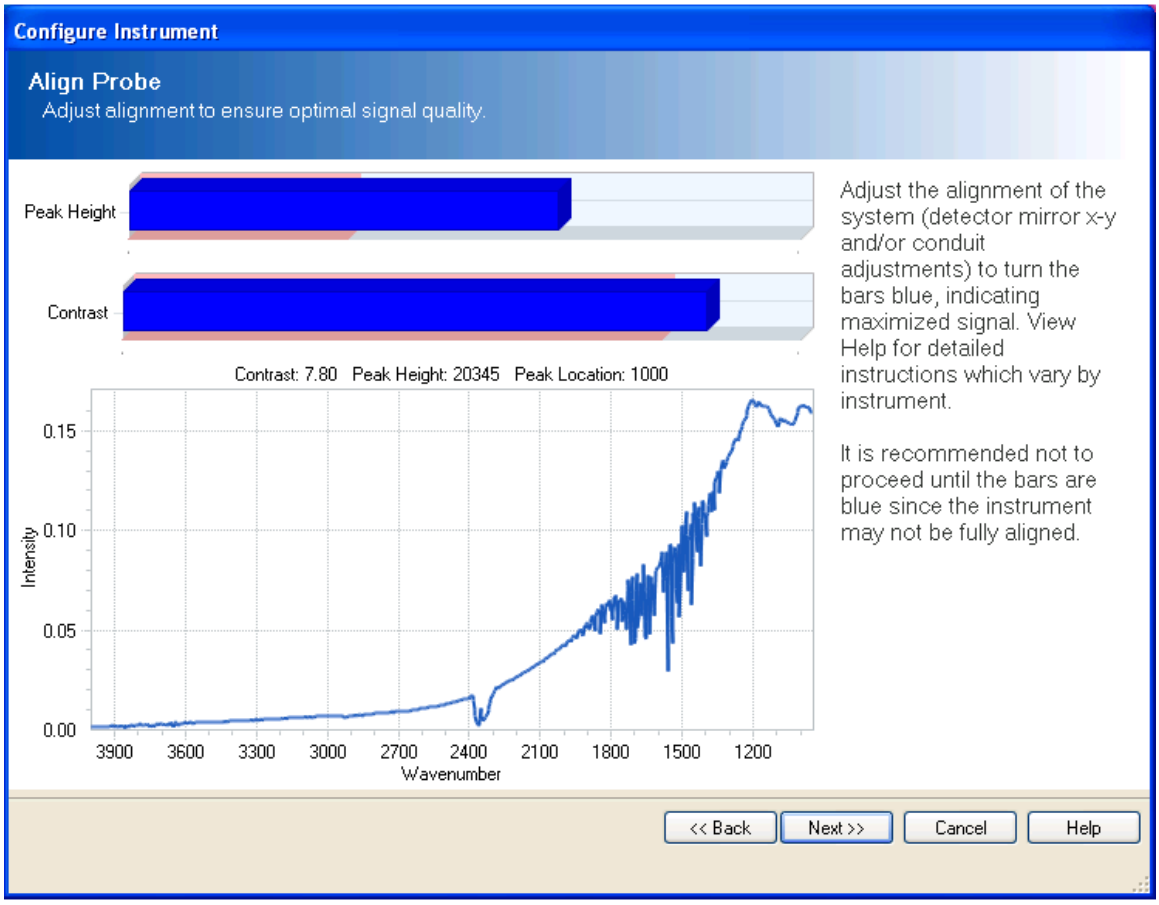
ReactIR 247 Setup Procedures

You must configure the iC IR software with information about your ReactIR 247 hardware before you can use it to conduct experiments. Configuration consists of the following steps:

1. Specify hardware settings reflecting your hardware configuration.
2. Optionally adjust software settings used when collecting and processing data from the instrument.
3. Collect a reference background while the probe is clean and the system is well purged. This will be used subsequently as a baseline for accessing whether the probe tip is clean and the system purge is working properly.
4. Collect a reference background while the probe is clean and the system purge is off that will be used subsequently to support the water vapor correction feature.

These configuration steps are accomplished using the Configure Instrument Wizard in the iC IR software. You can access this wizard by clicking the Configure Instrument button on the Start page of the iC IR software. Refer to the iC IR Help for additional information.

The Align Probe page of the wizard is used to physically align the probe. When the probe is aligned correctly, the indicator bars turn blue.



System Alignment for **K4 CONDUIT INTERFACE with 25 mm diameter Sentinel Probe**

- At the Start Page, Click on the button **Configure/Test Instrument**.
- Select **Contrast** in the dialog box on the right.
- Click **Start**

- Rotate probe on the end of the conduit 180 degrees CW and CCW to maximize Contrast and Peak Height values.
- Acceptable Contrast for DiComp is **> 50**, acceptable Contrast for SiComp is > 30.
- Acceptable Peak Height is **> 20,000**.

When the probe is aligned correctly the indicator bars turn blue as shown below.

System Alignment for **Direct ReactIR 247 INTERFACE with 25 mm diameter Sentinel Probe**

- At the Start Page, Click on the button **Configure/Test Instrument**.
- Select **Contrast** in the dialog box on the right.
- Click **Start**
- Rotate probe on the end of the conduit 180 degrees CW and CCW to maximize Contrast and Peak Height values.
- Acceptable Contrast for DiComp is **> 50**, acceptable Contrast for SiComp is > 30.
- Acceptable Peak Height is **> 20,000**.

When the probe is aligned correctly the indicator bars turn blue as shown below.

ReactIR 45m Setup Procedures

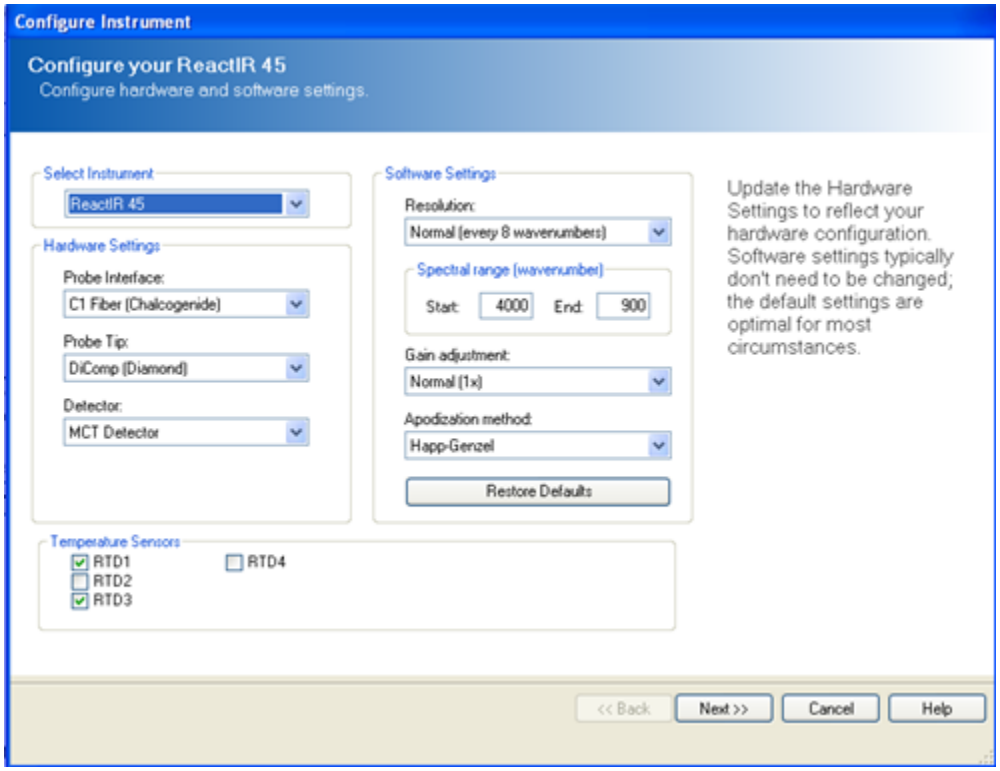
You must configure the iC IR software with information about your ReactIR 45m hardware before you can use it to conduct experiments. Configuration consists of the following steps:

1. Specify hardware settings reflecting your ReactIR 45mhardware configuration.
2. Optionally adjust software settings used when collecting and processing data from the ReactIR 45m instrument.
3. Collect a reference background while the probe is clean and the system is well purged. This will be used subsequently as a baseline for accessing whether the probe tip is clean and the system purge is working properly.
4. Collect a reference background while the probe is clean and the system purge is off that will be used subsequently to support the water vapor correction feature.

These configuration steps are accomplished using the Configure Instrument Wizard in the iC IR software. You can access this wizard by clicking the Configure Instrument button on the Start page of the iC IR software. Refer to the iC IR Help for additional information.

Specify Hardware and Software Settings

The first page of the wizard is used to specify the particular ReactIR hardware options installed and to specify software settings that will influence how iC IR collects and processes the data it acquires from the ReactIR hardware.

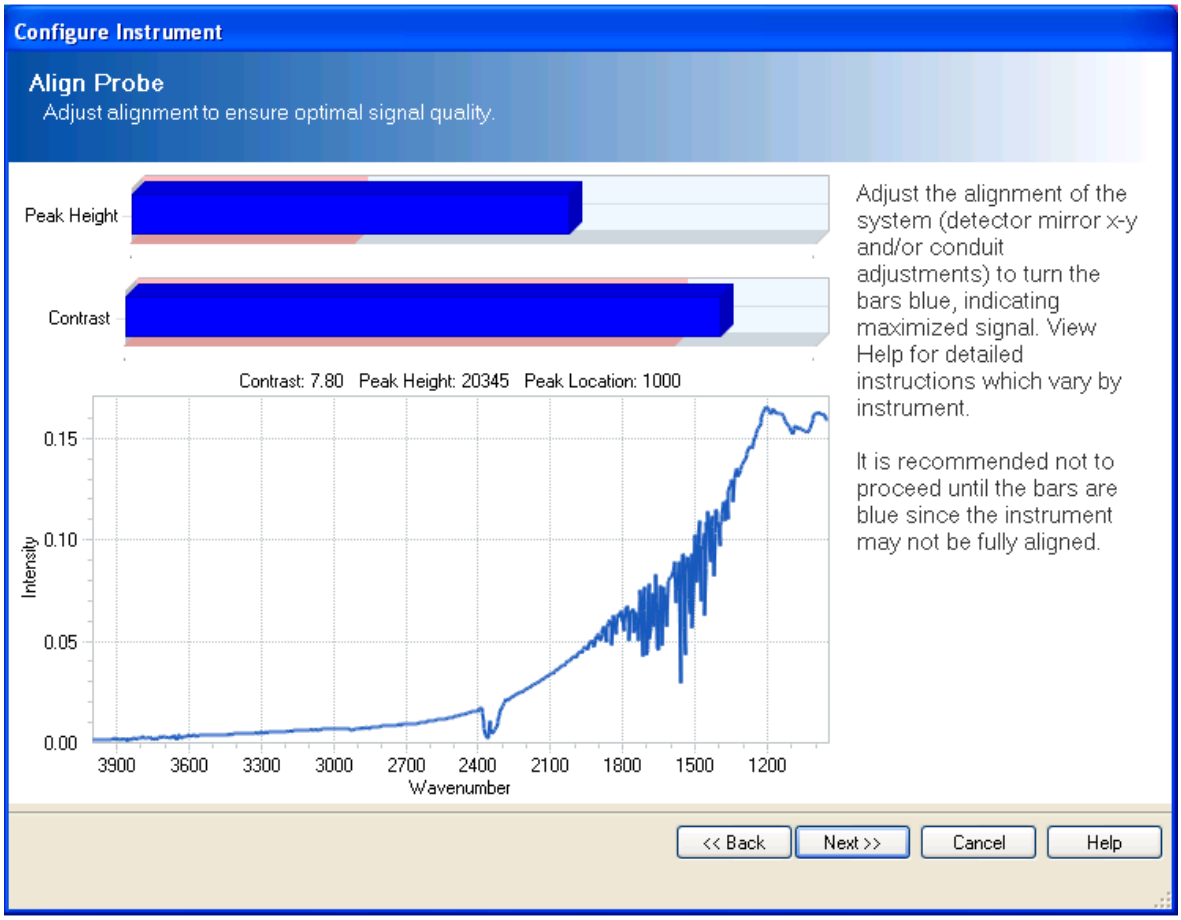


The configuration choices on the left side specify the particular hardware configuration you are using. The choices on the right affect software processing. The software settings are auto-initialized to default values based on the hardware settings you select. In most cases, you need not change the default software settings.

Probe Interface	C1 Fiber (Chalcogenide) AgX Fiber (Silver Halide) K4 Conduit K6 Conduit
Probe Tip	DiComp (Diamond) SiComp (Silicon)
Detector	MCT Detector (Mercury Cadmium Telluride, HgCdTe) DTGS Detector (Deuterated Triglycine Sulfate)
Resolution	High - every 4 wavenumbers. This is unnecessary in most cases and will slow down scan rate, increase file size and slow application processing. It may be useful in certain reactions to help resolve overlapping peaks. Normal - every 8 wavenumbers. This is the best choice for most chemistry. Low - every 16 wavenumbers. This choice is only useful in reactions with broad, non-overlapped peaks that require a fast sampling rate. In such cases, the lower resolution allows for faster scanning which means a higher signal to noise ratio in samples taken more frequently than once a minute.
Gain Adjustment	Gain Adjustment should always be set the default Normal 1x setting. The other choices are provided only to support hardware troubleshooting.
Apodization Method	Apodization is a part of the process of converting the raw interferogram from the ReactIR 45m into a spectrum. There are several standard mathematical methods for this process. Happ-Genzel is, by far, the most common. The other methods are provided for expert implementations with very specific requirements.
RTD1 -4	The RTD1-4 checkboxes allow the user to enable the instrument RTDs. When enabled, the RTD is displayed on the experiment wizard as a checkbox. When the checkbox on the experiment wizard is checked, the RTDs values are trended during the experiment.

When the options are configured correctly, click the **Next** button to advance to the next page of the wizard.

The Align Probe page of the Configuration wizard is used to physically align the probe. When the probe is aligned correctly, the indicator bars turn blue.



The detector mirror and conduit are adjusted to properly align the probe. These adjustments are detailed in the sections that follow.

Detector Mirror Alignment

The Detector mirror on the ReactIR 45 is adjusted using the N, E, S, W buttons on the details panel. The Detector can also be adjusted using the Auto-align feature.

The Auto-align feature is only enabled if the **Detector XY** checkbox is checked.

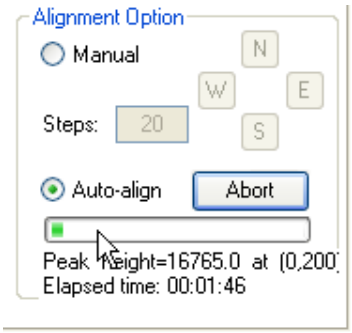
During the auto-align process, the progress bar displays a visual indication of the auto-align process.

The system shall be able to find the best-aligned mirror position automatically within 5 minutes.

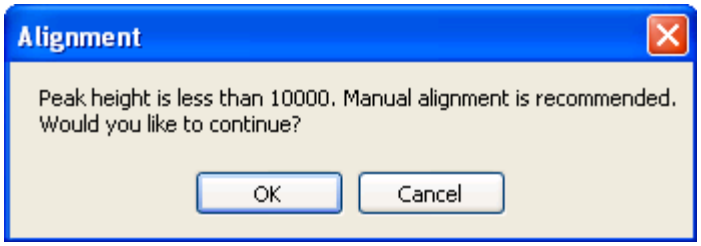
The user may abort the auto-align process at any time. If the process is aborted before completion, the iC IR uses the best mirror position found so far.

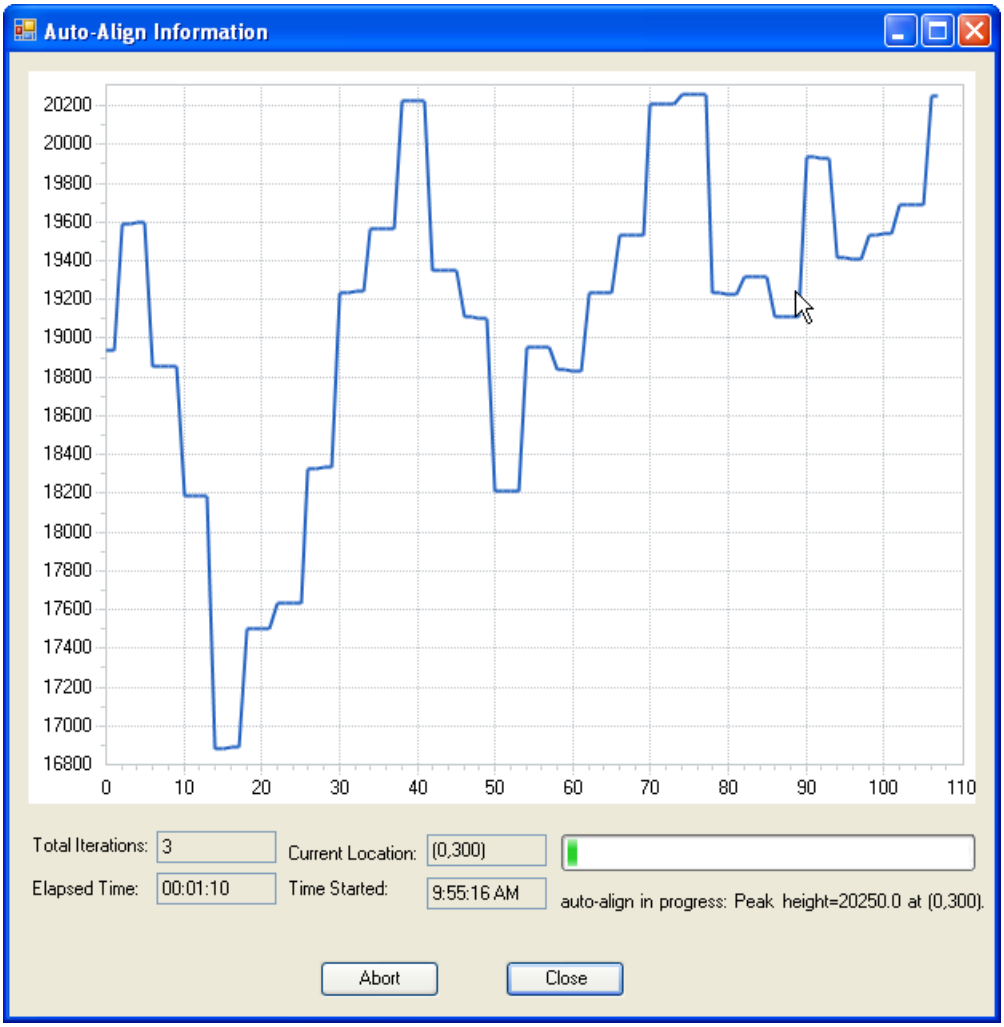
During the auto-align process, the iC IR does not allow user to select a different mirror or manually adjust the mirror positions.

Click on the progress bar under the **Auto-align** checkbox to open the Auto-Align Information dialog.



The dialog displays information about the Auto-align process.
When the peak height is less than 10k, a message is displayed when user clicks on 'Start' button for auto-align.

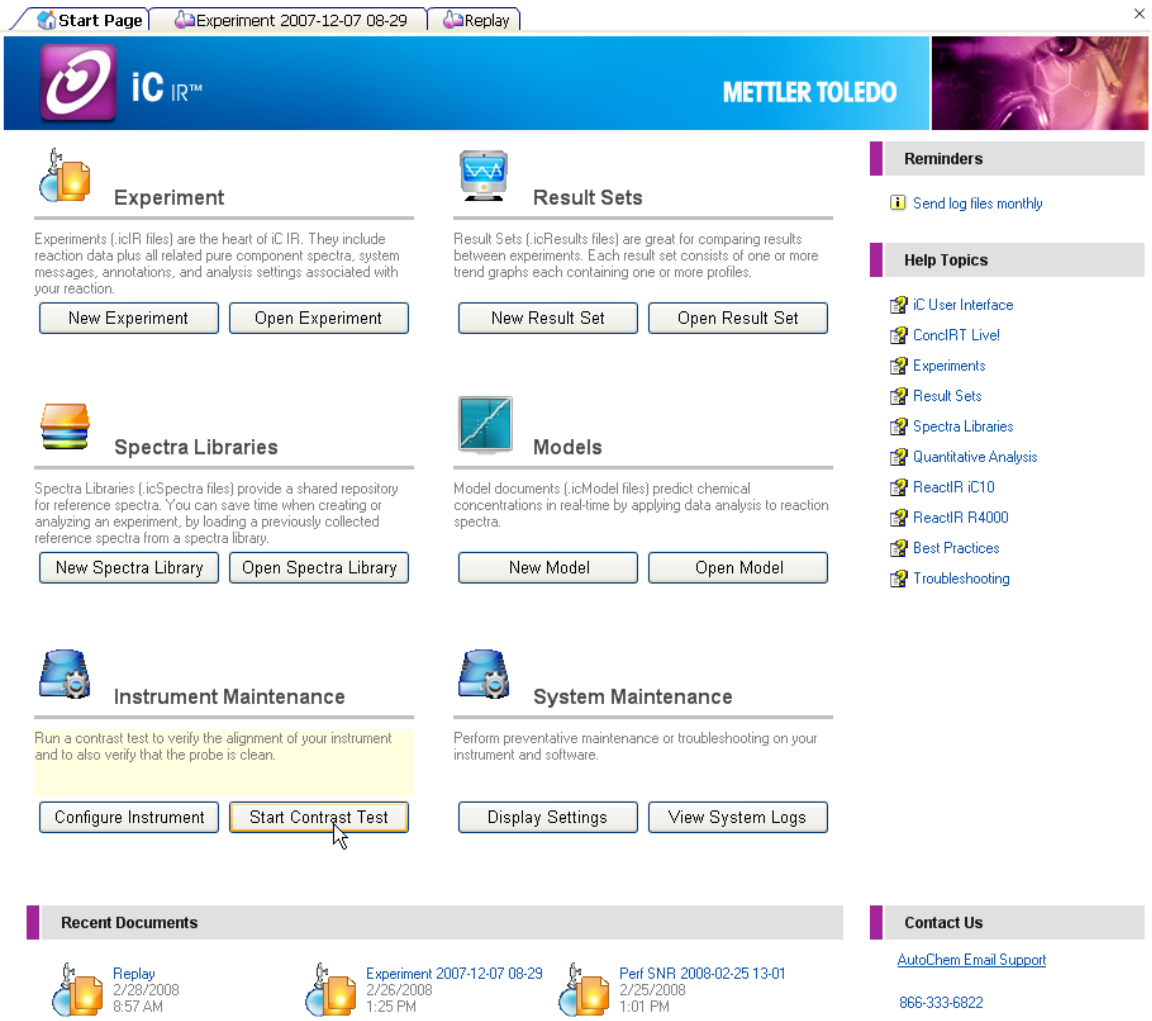




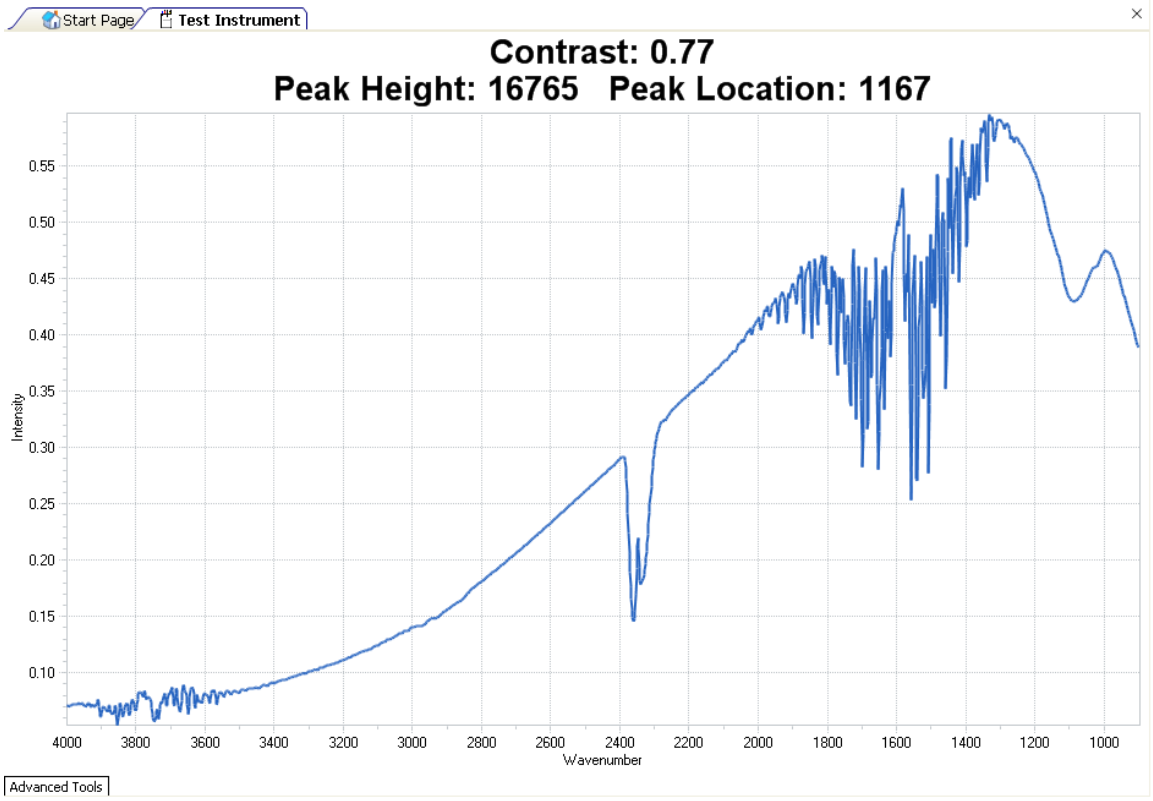
C1 Fiber Interface Alignment

The ReactIR™ 45m is factory aligned for the sampling technology ordered with the base unit (if applicable). Therefore, it is expected that if a Fiber technology is ordered, the only alignment procedure that must be performed is rotation of the FiberConduit. The best alignment will always correspond to a position where the purge fitting of on the FiberConduit is positioned at the 12 o'clock or 6 o'clock position for a 6.3mm diameter probe or the 3 o'clock or 9 o'clock position for a 9.5mm diameter probe.

Before beginning the rotation adjustment, click on the **Start Contrast Test** on iC IR **Start** page.



- Once the contrast screen appears, loosen the conduit clamp and rotate the Fiber Conduit. Note that the purge fitting will be positioned near the 12 o'clock or 6 o'clock position for the 6.3mm diameter probe or the 3 o'clock/ 9 o'clock for the 9.5mm probe, so the amount of rotation needed is minimal.



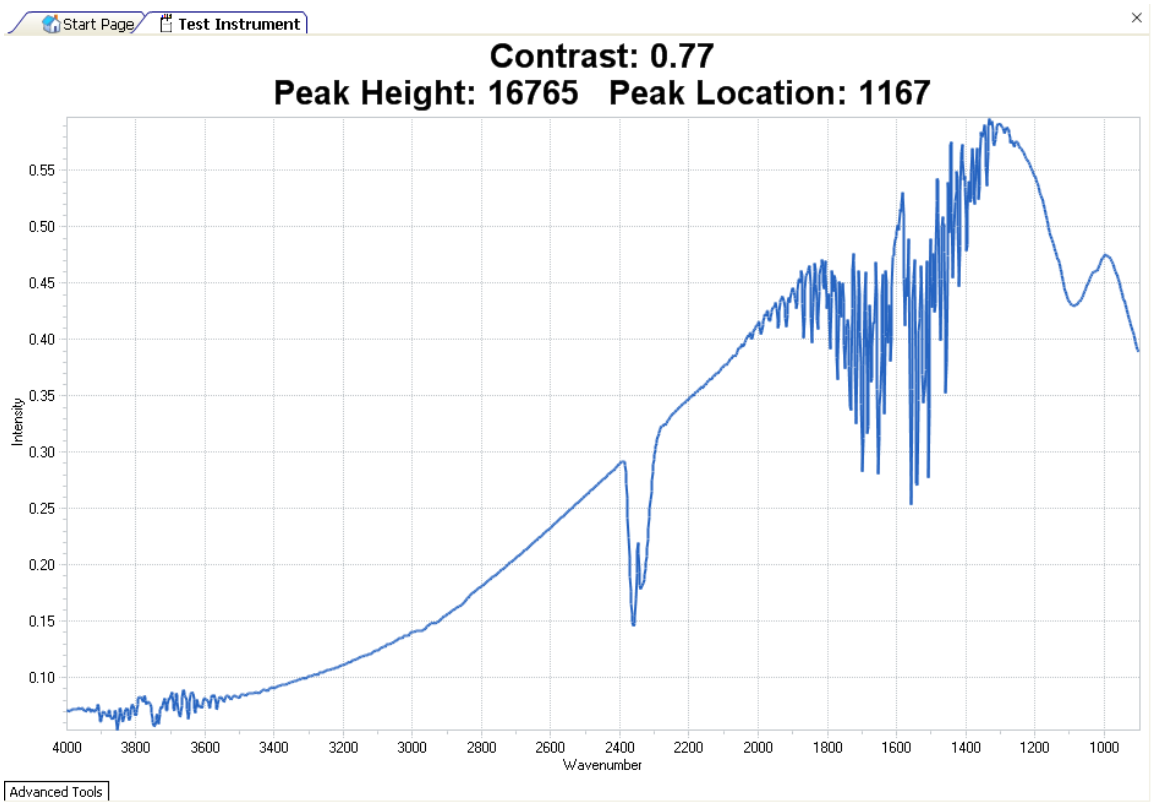
- While rotating the Fiber Conduit, maximize the contrast and peak height. The minimum specification for contrast is 5.0 and the minimum specification for peak height is 18,000.
- Once the contrast and peak height have been maximized, retighten the clamp.
- Ensure that the unit has passed all tests listed in the Toolbox.

Name	Value
SourceOK	OK
LaserOK	OK
Minus15OK	OK
Plus15OK	OK
LaserDcOK	OK
TempOK	OK
PeakLocationOK	OK
PeakHeightOK	OK

- Record the values for contrast and peak height in a log book.

- Before beginning the rotation adjustment, click on the **Start Contrast Test** on iC IR **Start** page.

- Connect the fiber to the instrument with the purge fitting in the 12:00 or 6:00 position for a 6.3 mm diameter probe or 3:00 or 9:00 position for a 9.5 mm diameter probe. Rotate fiber optic conduit at the front of the instrument by ¼ turn CW and CCW to maximize Contrast and Peak Height values.



- Once the contrast and peak height have been maximized, retighten the clamp.
- Acceptable Contrast is > 10.
- Acceptable Peak Height is > 18,000.
- Ensure that the unit has passed all tests listed in the Toolbox.

Name	Value
SourceOK	OK
LaserOK	OK
Minus15OK	OK
Plus15OK	OK
LaserDcOK	OK
TempOK	OK
PeakLocationOK	OK
PeakHeightOK	OK

- Record the values for contrast and peak height in a log book.

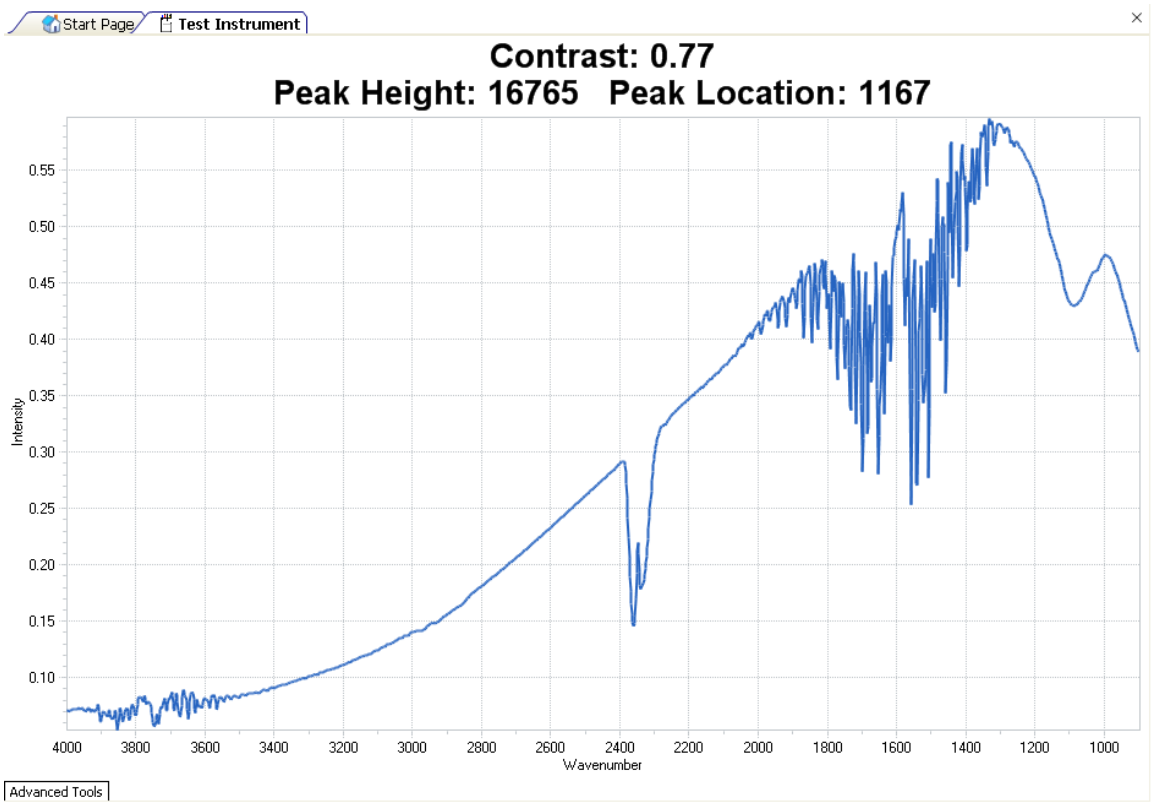
K6 Conduit Interface Alignment

Before beginning the rotation adjustment, click on the **Start Contrast Test** on iC IR **Start** page.

Select the appropriate fiber, probe and MCT detector options.

Click on **Contrast** to highlight and click **Start**.

- Once the contrast screen appears, loosen the probe clamp and rotate the probe to maximize peak height and contrast.



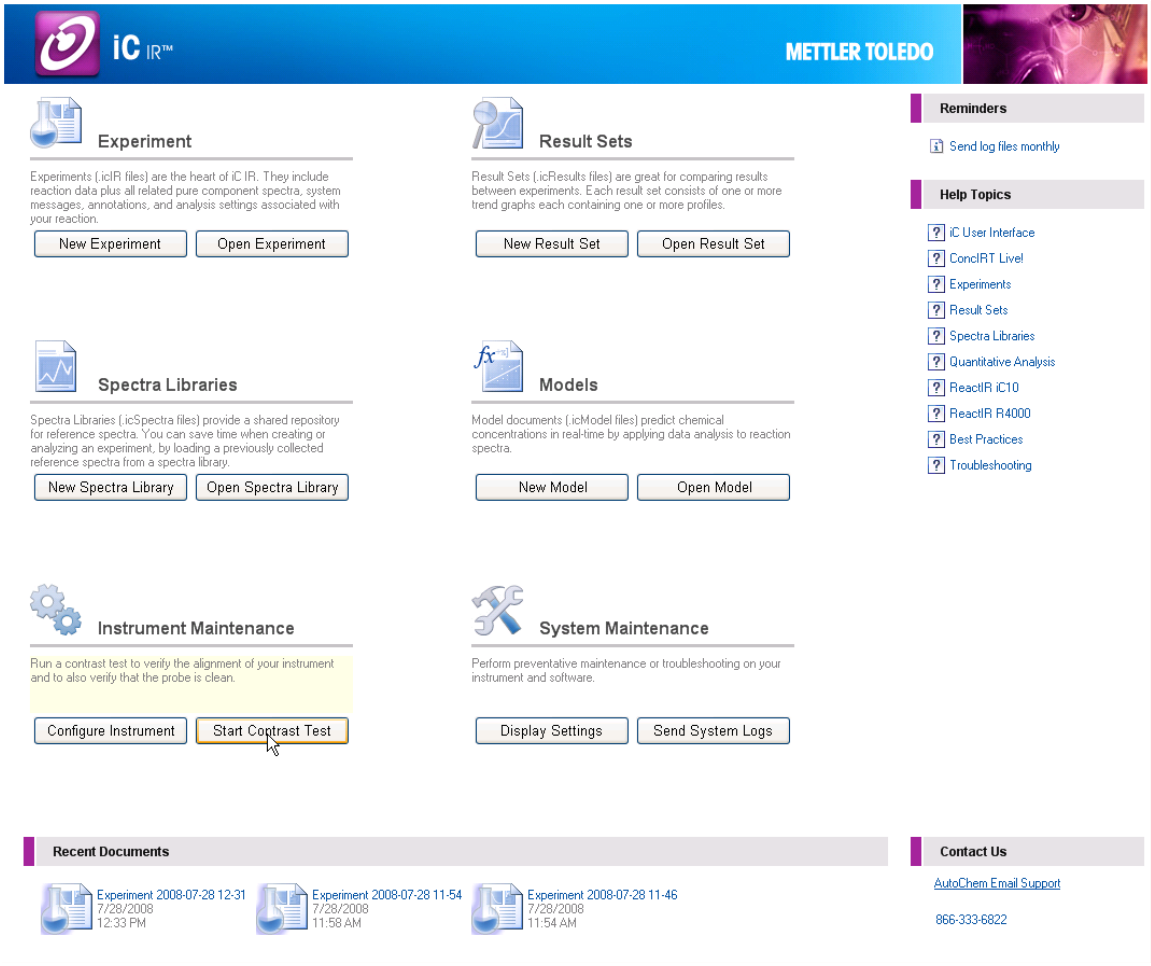
- Following rotation of the probe, adjust the 3 knobs on knuckle 4 or 6 (i.e. last knuckle of the conduit) to maximize peak height and contrast.
- Repeat probe rotation, last knuckle adjustment knobs and detector mirror adjustments as necessary to maximize peak and contrast.
- Ensure that the unit has passed all tests listed in the Toolbox.

Name	Value
SourceOK	OK
LaserOK	OK
Minus15OK	OK
Plus15OK	OK
LaserDcOK	OK
TempOK	OK
PeakLocationOK	OK
PeakHeightOK	OK

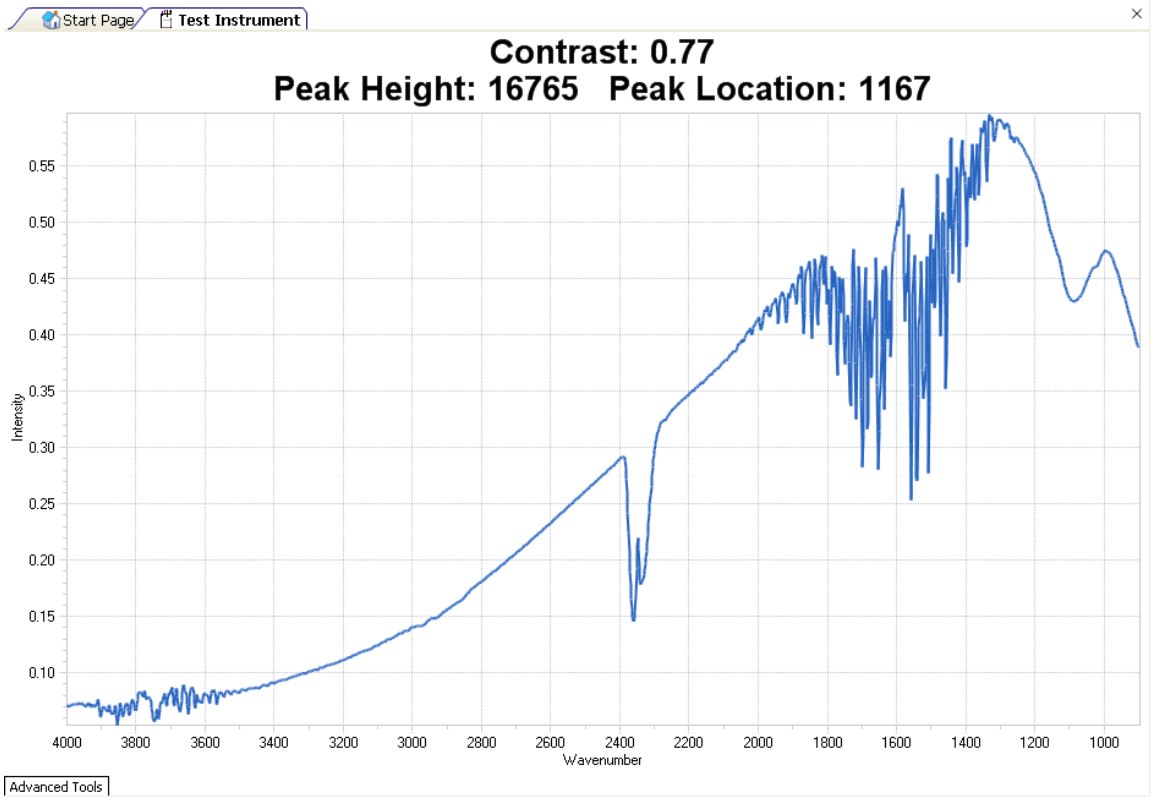
- Record the values for contrast and peak height in a log book.

K4 Conduit Interface Alignment

Before beginning the rotation adjustment, click on the **Start Contrast Test** on iC IR **Start** page.



- Once the contrast screen appears, loosen the probe clamp and rotate the probe to maximize peak height and contrast.



- Following rotation of the probe, adjust the 3 knobs on knuckle 4 or 6 (i.e. last knuckle of the conduit) to maximize peak height and contrast.

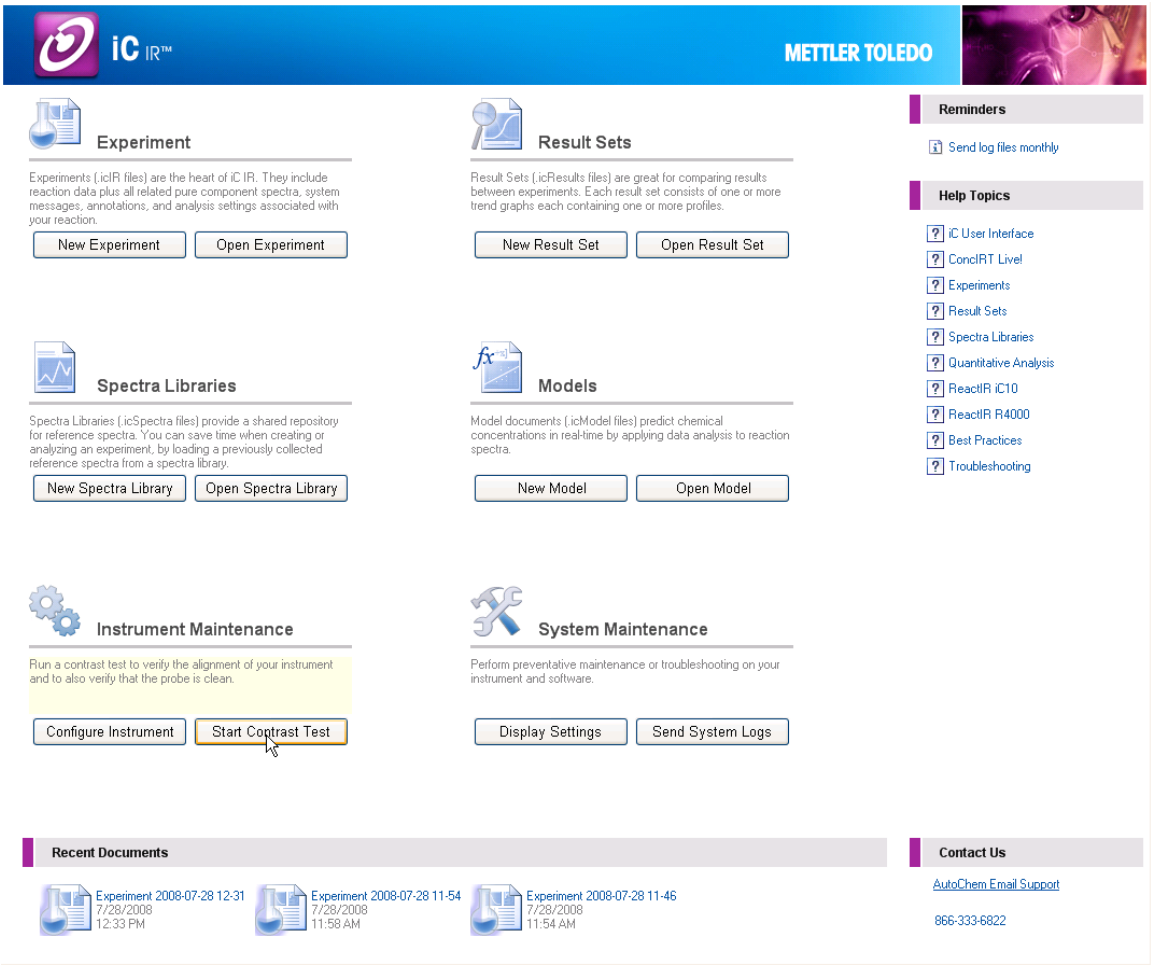
- Repeat probe rotation, last knuckle adjustment knobs and detector mirror adjustments as necessary to maximize peak and contrast.

- Ensure that the unit has passed all tests listed in the Toolbox.

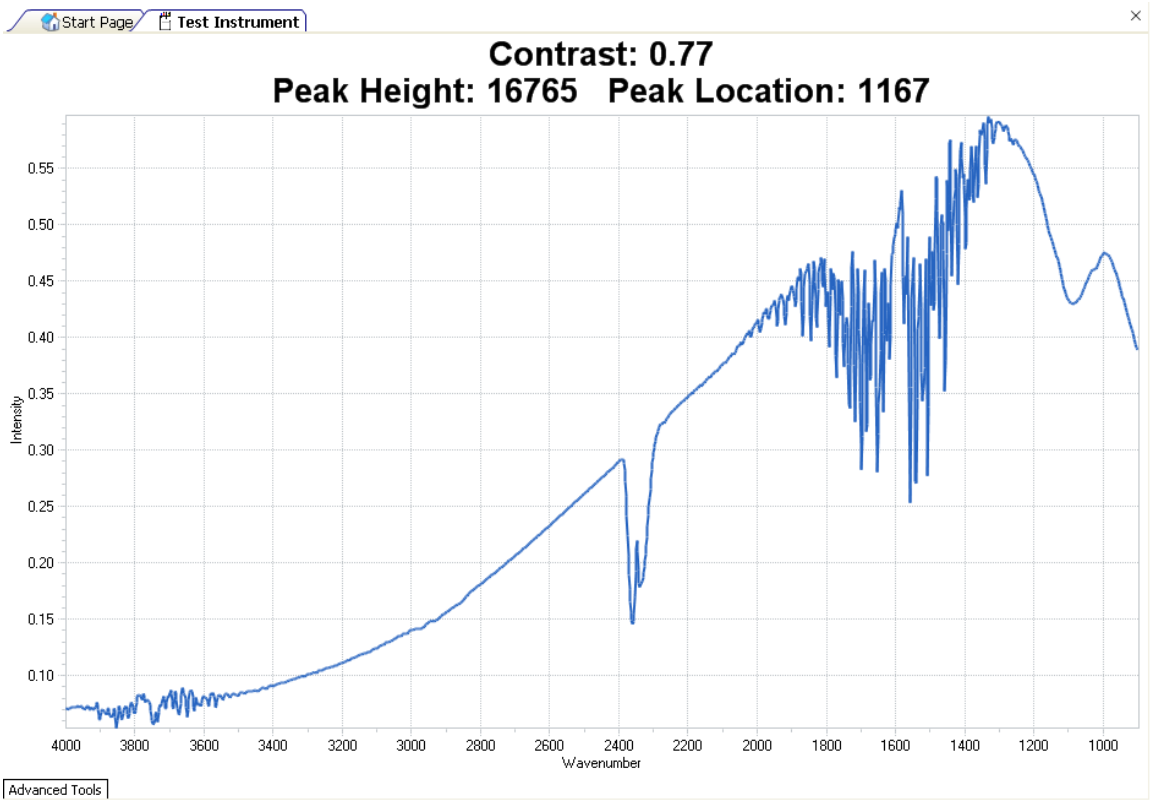
Name	Value
SourceOK	OK
LaserOK	OK
Minus15OK	OK
Plus15OK	OK
LaserDcOK	OK
TempOK	OK
PeakLocationOK	OK
PeakHeightOK	OK

- Record the values for contrast and peak height in a log book.

Before beginning the rotation adjustment, click on the **Start Contrast Test** on iC IR **Start** page.



- Once the Contrast window is opened, rotate probe on the end of the conduit 180 degrees CW and CCW to maximize Contrast and Peak Height values.



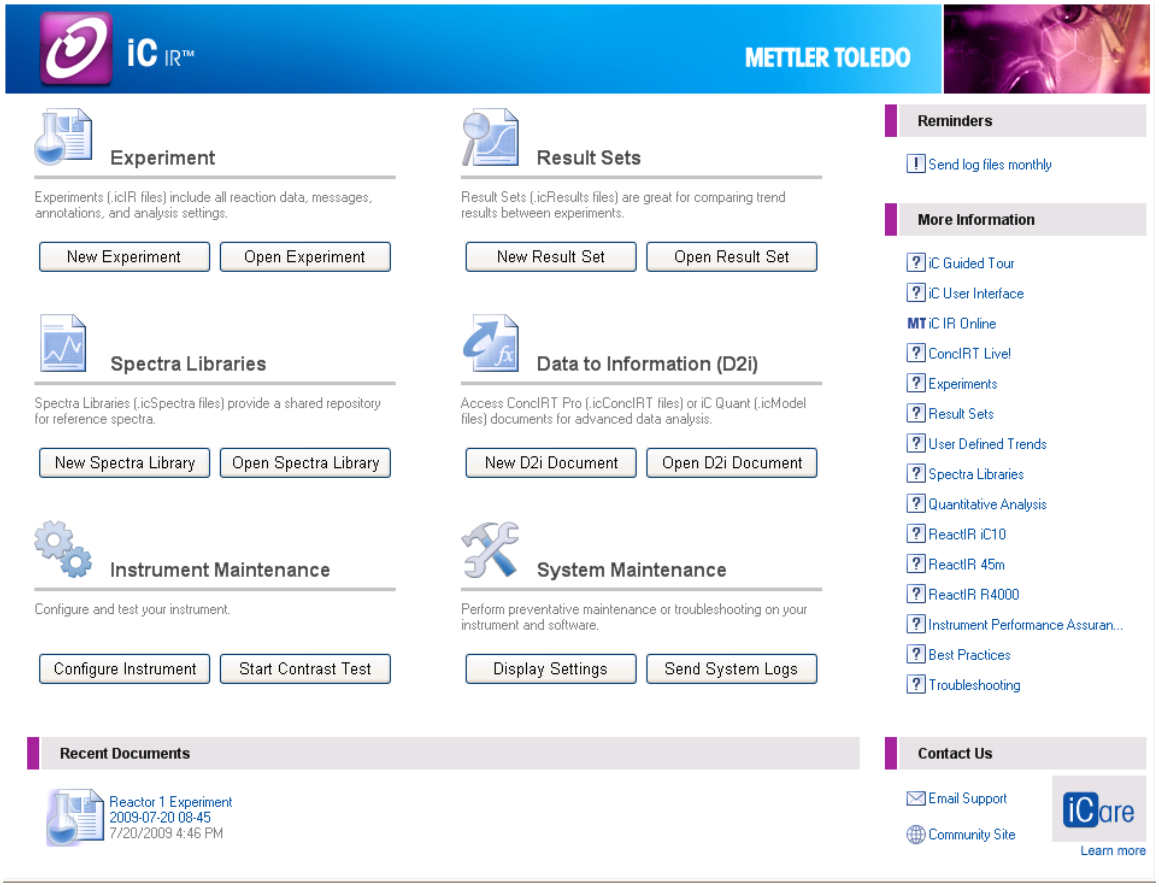
- Acceptable Contrast for DiComp is **> 50**, acceptable Contrast for SiComp is > 30.
- Acceptable Peak Height is **> 20,000**.
- Ensure that the unit has passed all tests listed in the Toolbox.

Name	Value
SourceOK	OK
LaserOK	OK
Minus15OK	OK
Plus15OK	OK
LaserDcOK	OK
TempOK	OK
PeakLocationOK	OK
PeakHeightOK	OK

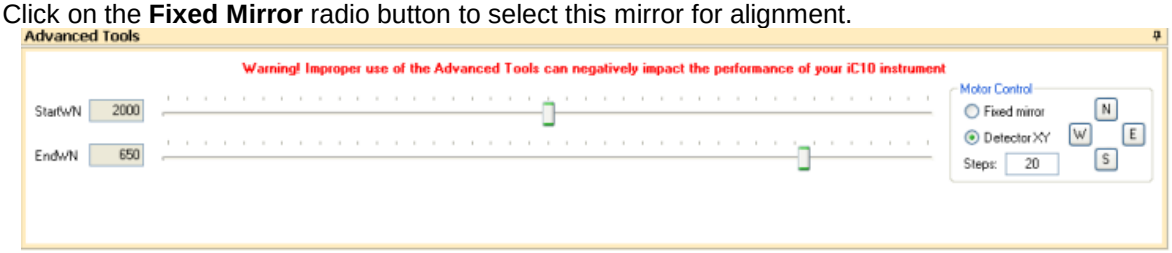
- Record the values for contrast and peak height in a log book.

Note: It is possible that the fixed mirror alignment position has moved slightly out of optimum position after shipment of the system. To check the alignment of this mirror, you need to launch the fixed mirror test program.

Before beginning the mirror adjustment, click on the **Start Contrast Test** on iC IR **Start** page.



- The mirror adjustment controls are displayed on the details panel of the Contrast Test window. The user can double-click in the chart area of the window to show or hide the details panel.
- Click on the **Fixed Mirror** radio button to select this mirror for alignment.



- Using the toggle buttons (N, E, S, and W) verify/ optimize proper alignment of the fixed mirror for maximum peak height and contrast levels.
- Verify the shape of the single beam is consistent with the sampling technology (i.e. region from 1950 – 2200 cm-1 show the characteristic diamond absorption when using a DiComp™ probe)
- Record the Peak Height and Contrast values.

Safety Hazards Associated with Handling Liquid Nitrogen

1. The extremely low temperature of the liquid can cause severe frostbite or eye damage upon contact. Items in contact with liquid nitrogen become extremely cold. Touching these items may result in torn flesh. Many substances become brittle upon contact with liquid nitrogen and may shatter when cold (such as common glass and large solid plastics), sending pieces of the material flying.

2. On vaporization it expands by a factor of 700; one liter of liquid nitrogen becomes 24.6 cubic feet of nitrogen gas. This can cause explosion of a sealed container. This release of nitrogen can also displace oxygen in the room and cause asphyxiation without warning.

3. Because the boiling point of oxygen is above that of nitrogen, oxygen can condense from the air into the liquid nitrogen. If dewars and insulated flasks containing liquid nitrogen are left uncovered for an extended period of time, liquid oxygen can build up to levels which may cause violent reactions with organic materials (i.e. a severe clothing fire could result).

Personal Protective Equipment (PPE) Required When ***Handling Liquid Nitrogen***

- Safety goggles (unvented)
- Face shield
- Insulating gloves (gloves should be loose fitting, so they can be thrown off if liquid pours inside them, or they should be elastic cuff insulated gloves).
- A lab coat or long sleeves is required to minimize skin contact. Also, trousers should be worn on the outside of boots or work shoes to prevent shoes filling in the event of a spillage.

Important Precautions for Handling Liquid Nitrogen

- Always wear a face shield when handling liquid nitrogen.
- Use liquid nitrogen only in well ventilated places. Never dispose of liquid nitrogen by pouring it on the floor. It could displace enough oxygen to cause suffocation. Nitrogen is colorless and odorless – the cloud that forms when you pour liquid nitrogen is condensed water vapor from the air, not nitrogen gas.
- Do not allow any liquid nitrogen to touch any part of your body or become trapped in clothing near the skin.
- Do not touch any item that has been immersed in liquid nitrogen until it has warmed to room temperature.
- Do not store liquid nitrogen in any container with a tight fitting lid. A tightly sealed container will build up pressure as the liquid boils and may explode after a short time. Use only approved unsealed containers.
- Do not store liquid nitrogen for long periods in an uncovered container. Use only fittings that have been designed specifically for use with cryogenic liquids as non-specialized equipment may crack or fail.

- Never dip a hollow tube into liquid nitrogen; it may spurt liquid.
- Never ride in an elevator with liquid nitrogen! When using passenger elevators, use an elevator key to prevent the door from being opened by unauthorized persons. If a key is not available, then station a person at each floor to ensure no one enters.
- Always fill warm Dewars slowly to reduce temperature shock effects and to minimize splashing.
- Always make sure that containers of liquid nitrogen are suitably vented and unlikely to block due to ice formation.
- Do not fill cylinders and Dewars to more than 80% of capacity, since expansion of gases during warming may cause excessive pressure buildup.

Appendix A: Guidance Document for the use of iC FBRM®, iC IR™, iC Raman and iC Quant in 21CFR11-regulated environments

This document outlines the means by which users of METTLER TOLEDO iC FBRM, iC IR, iC Raman and iC Quant software can achieve compliance with specific aspects of Title 21, Part 11 of the Code of Federal Regulations (commonly known as 21CFR11).

All references in *italics* are taken from the regulation.

Definitions (*from Sec. 11.3*):

(4) Closed System means an environment in which system access is controlled by persons who are responsible for the content of electronic records that are on the system.

(6) Electronic record means any combination of text, graphics, data, audio, pictorial, or other information representation in digital form that is created, modified, maintained, archived, retrieved, or distributed by a computer system.

Subpart B--Electronic Records

Sec. 11.10 -- Controls for closed systems

iC FBRM, iC IR, iC Raman and iC Quant software are closed systems; therefore, these provisions apply.

a) Validation of systems to ensure accuracy, reliability, consistent intended performance, and the ability to discern invalid or altered records.

The software was developed and tested following approved and controlled SDLC practices within AutoChem's ISO9001:2000 certified Quality Management System. Invalid or altered records are detected by the software using CRC algorithm technology. When the software detects invalid or altered records, the user is presented with a warning dialog as well as a notation in the Document Information pane. The user can choose to open the experiment even with invalid or altered data; however, the notation in the Document Information pane remains.

b) The ability to generate accurate and complete copies of records in both human readable and electronic form suitable for inspection, review, and copying by the agency. Persons should contact the agency if there are any questions regarding the ability of the agency to perform such review and copying of the electronic records.

Records can be viewed in electronic form within the software. Analyzed data records can be printed by using the reporting function in our software.

c) Protection of records to enable their accurate and ready retrieval throughout the records retention period.

Records created by the software are saved as files. It is up to the customer to create SOPs surrounding the proper storage and archiving of such files.

d) Limiting system access to authorized individuals.

Access to the software is provided to licensed users through the use of the Windows NT logon and authentication. Management of user IDs, passwords and control of physical access must be addressed through customer SOPs.

e) Use of secure, computer-generated, time-stamped audit trails to independently record the date and time of operator entries and actions that create, modify, or delete electronic records. Record changes shall not obscure previously recorded information. Such audit trail documentation shall be retained for a period at least as long as that required for the subject electronic records and shall be available for agency review and copying.

All raw data is secure and cannot be altered once the experiment has been saved as per customer SOPs. Any change in the presentation of data, i.e. statistics, averaging, etc., is written to the audit log. The user can re-create the presentation of data at a later time. The audit trail cannot be edited, only appended to and is retained as long as the experiment document. Retention of document files is addressed in 11.10c above. The audit log can be reviewed within the software and can be copied using the 'Copy to Clipboard' feature.

f) Use of operational system checks to enforce permitted sequencing of steps and events, as appropriate.

Customer SOPs ensure proper instrument calibration and usage. iC software assists by providing wizards that guide the user through instrument configuration and experiment set-up.

g) Use of authority checks to ensure that only authorized individuals can use the system, electronically sign a record, access the operation or computer system input or output device, alter a record, or perform the operation at hand.

The software relies on Windows NT logon security for authorization. Management of user IDs, passwords and control of physical access is addressed through customer SOPs.

h) Use of device (e.g., terminal) checks to determine, as appropriate, the validity of the source of data input or operational instruction.

The software warns the user if the instrument has not been calibrated within the last 3 months. Instrument readiness is also displayed to the user during the Start Experiment Wizard workflow. Customer SOPs must be in place to ensure proper instrument calibration and usage.

i) Determination that persons who develop, maintain, or use electronic record / electronic signature systems have the education, training, and experience to perform their assigned tasks.

Education and training of customer personnel is provided at installation by qualified MT employees.

j) The establishment of, and adherence to, written policies that hold individuals accountable and responsible for actions initiated under their electronic signatures, in order to deter record and signature falsification.

Establishment of policies related to personnel accountability is the responsibility of the customer.

k) Use of appropriate controls over systems documentation including:

(1) Adequate controls over the distribution of, access to, and use of documentation for system operation and maintenance.

(2) Revision and change control procedures to maintain an audit trail that documents time-sequenced development and modification of systems documentation.

Document management is addressed through customer SOPs. This includes document version control. Version control of iC software and documentation is addressed by the AutoChem QMS.

Subpart C--Electronic Signatures

iC FBRM, iC IR, iC Raman and iC Quant software do not have electronic signature capability.

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