

Software User Guide



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DCN 1428



iC IR™ 4.3 IPA

Instrument Performance Assurance

METTLER TOLEDO

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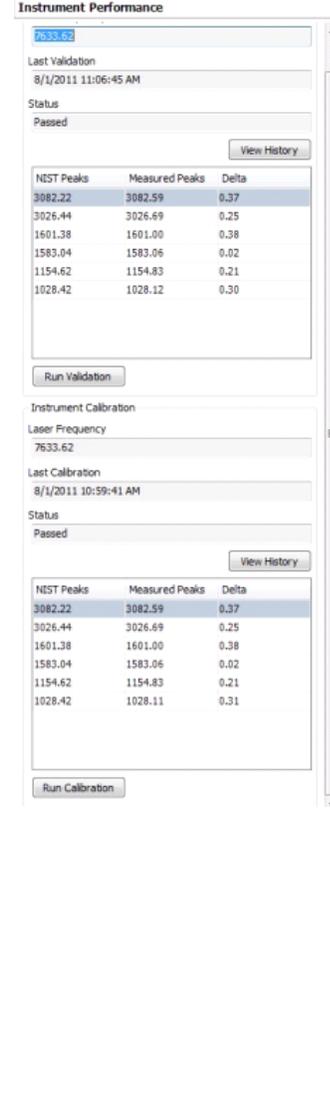
Instrument Performance Assurance Package

The Instrument Performance Assurance Package (IPA) is an optional add-on that is used to perform validation and calibration of an instrument using a polystyrene film standard supplied with the option. The validation and calibration procedures are wizard-based and controlled through the Instrument Performance Assurance task pane. The Instrument Performance Assurance package supports the ReactIR iC10, ReactIR 15, ReactIR 45P, ReactIR 247 and the ReactIR 45m.

It should be noted that a valid license is required to use the Instrument Performance Assurance Package.

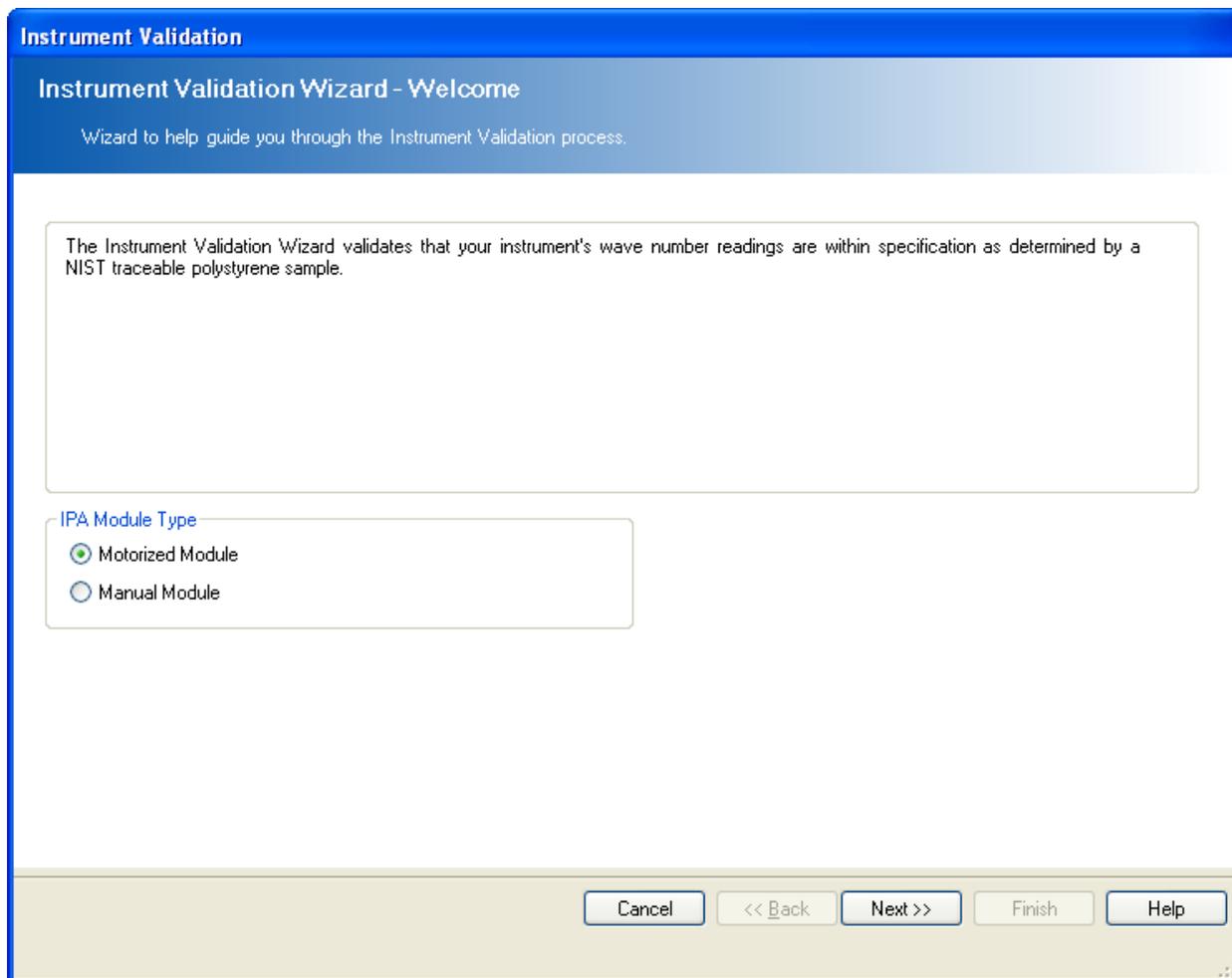
Instrument Performance Assurance Task Pane

The Instrument Performance Assurance task pane is displayed in the toolbox and is used to perform validation and calibration tasks for the instrument. The task pane contains the following items.

 <p>The screenshot shows the Instrument Performance Assurance Task Pane. It is divided into two main sections: Instrument Validation and Instrument Calibration. Each section includes a 'Last Validation' or 'Last Calibration' status, a 'Run' button, and a table of NIST Peaks with columns for NIST Peaks, Measured Peaks, and Delta. The validation section shows a 'Last Validation' of 8/1/2011 11:06:45 AM with a 'Passed' status. The calibration section shows a 'Last Calibration' of 8/1/2011 10:59:41 AM with a 'Passed' status. A smaller inset screenshot shows the 'Instrument Performance' window with 'Temperature Dependent' selected for the Laser Frequency.</p>	Instrument Validation	
	Laser Frequency	Displays the laser wavenumber that was used for the last validation test.
	Last Validation	Displays the date and time the system was last validated.
	Status	Displays the results of last validation.
	View History	Displays a history of all validations on record.
	NIST Peaks Table	Displays NIST peaks (in scope peaks based on the sampling technology) and their value from the last validation test.
	Run Validation	Starts the Validation wizard. Refer to The Validation Wizard
	Instrument Calibration	
	Laser Frequency	Displays the current laser wave number the system is using which could be updated by the calibration activity. The ReactIR 247, ReactIR 45P and the ReactIR 15 support a temperature corrected laser frequency. For these instruments the laser frequency is corrected based on the base temperature. The Validation and Calibration sections for these instruments displays the term "Temperature Dependent" instead of a laser frequency value.
	Last Calibration	Displays the date and time the system was last calibrated.
Status	Results of last calibration	
View History	Displays a history of calibration data.	
NIST Peaks Table	NIST peaks in scope based on sampling technology and their value before calibration and their value after calibration.	
Run Calibration	Launches the Calibration Wizard.	

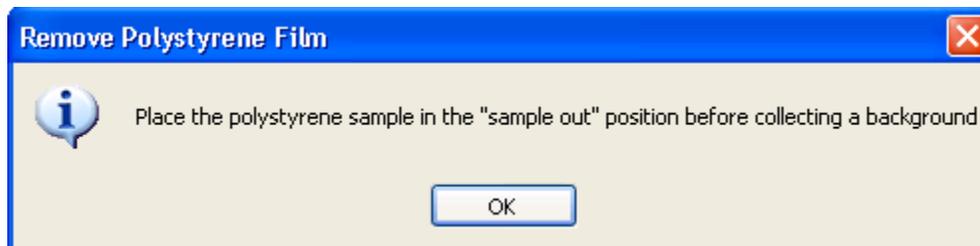
The Validation Wizard

The Instrument Validation wizard is used to verify that the instrument's wavenumber is within specifications. The validation used a NIST traceable polystyrene film sample. The wizard is launched by clicking the **Run Validation** button in the Instrument Performance Assurance task pane.



The first page of the wizard is a welcome page. If the instrument is a ReactIR 45m, radio buttons are displayed that allow the selection of the Motorized or Manual Module. The ReactIR 247, ReactIR 15 and IC10 only use manual operation and the ReactIR 45P only uses motorized operation. Click the **Next** button to continue.

A message dialog is displayed that instructs the user to insert the polystyrene sample into the optical path.



Note that this dialog is not displayed for the motorized module.

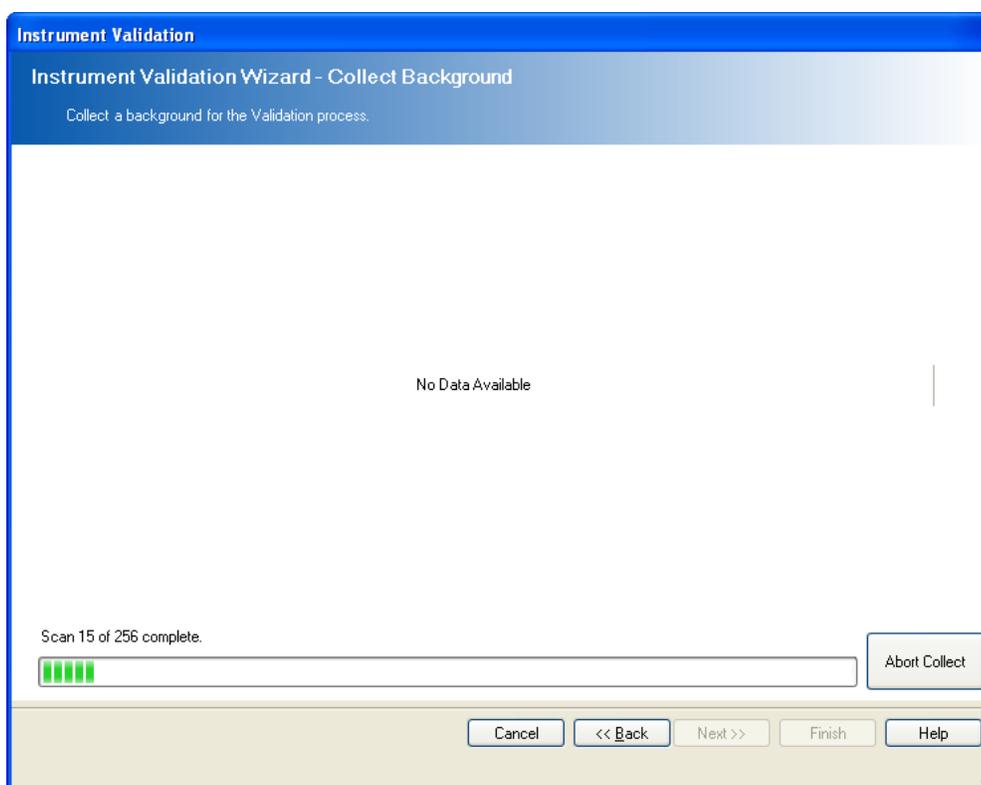
Validation Wizard – Collect Background Page

The next page of the wizard is used to collect a background.

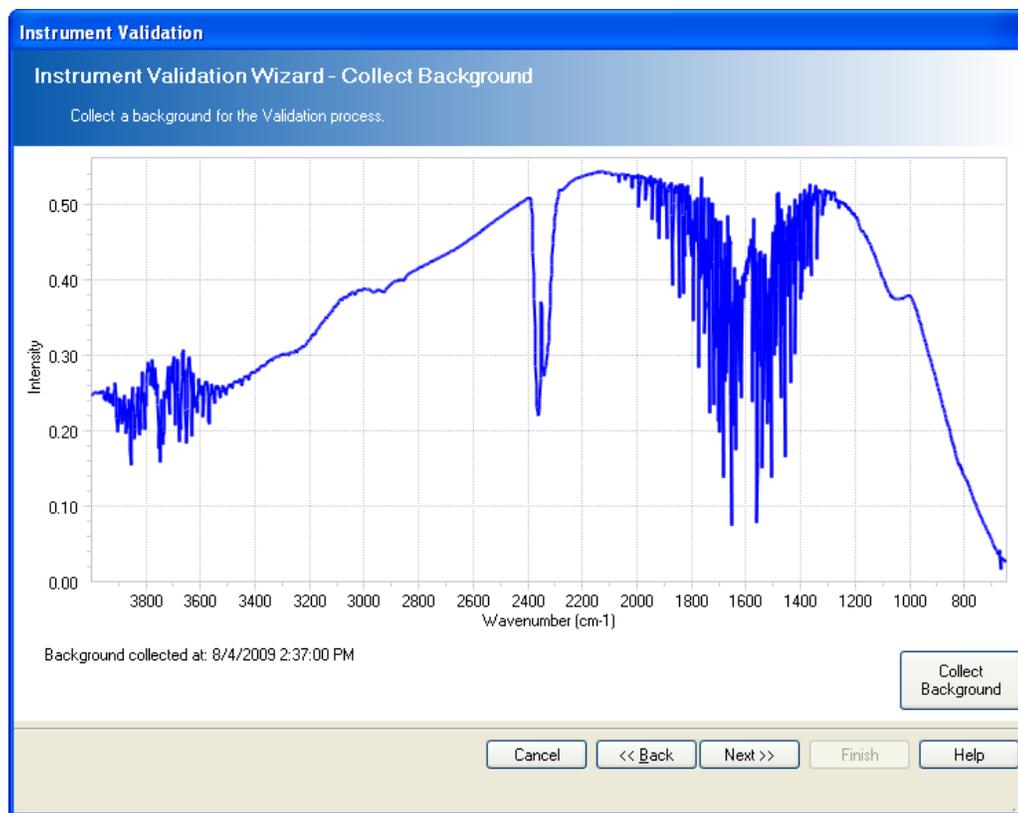
Note: A background spectrum should be collected for reference after the probe has been aligned properly and the sensor cleaned.

ReactIR instruments utilize a background measurement to minimize the 'instrument response' from the desired spectrum. Historically, one is measuring I/I_0 where I is the intensity of the light after passing through a sample and I_0 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. You can run multiple tests without collecting a new background. However if you close and reopen the wizard, a new background must be collected. The wizard leads you through this procedure.

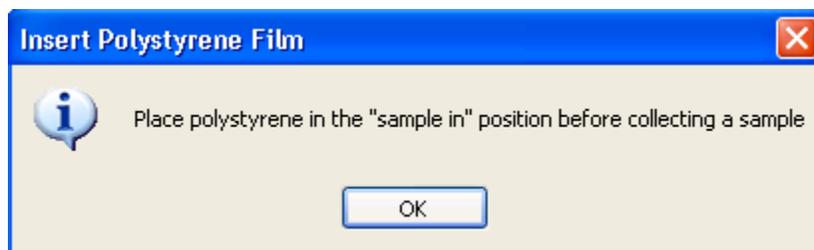
Click on the **Collect Background** button to collect a background sample.



After the background has been collected, click the **Next** button.



A message dialog is displayed that instructs the user to insert the polystyrene sample into the optical path. Note that this dialog is not displayed for the motorized module.

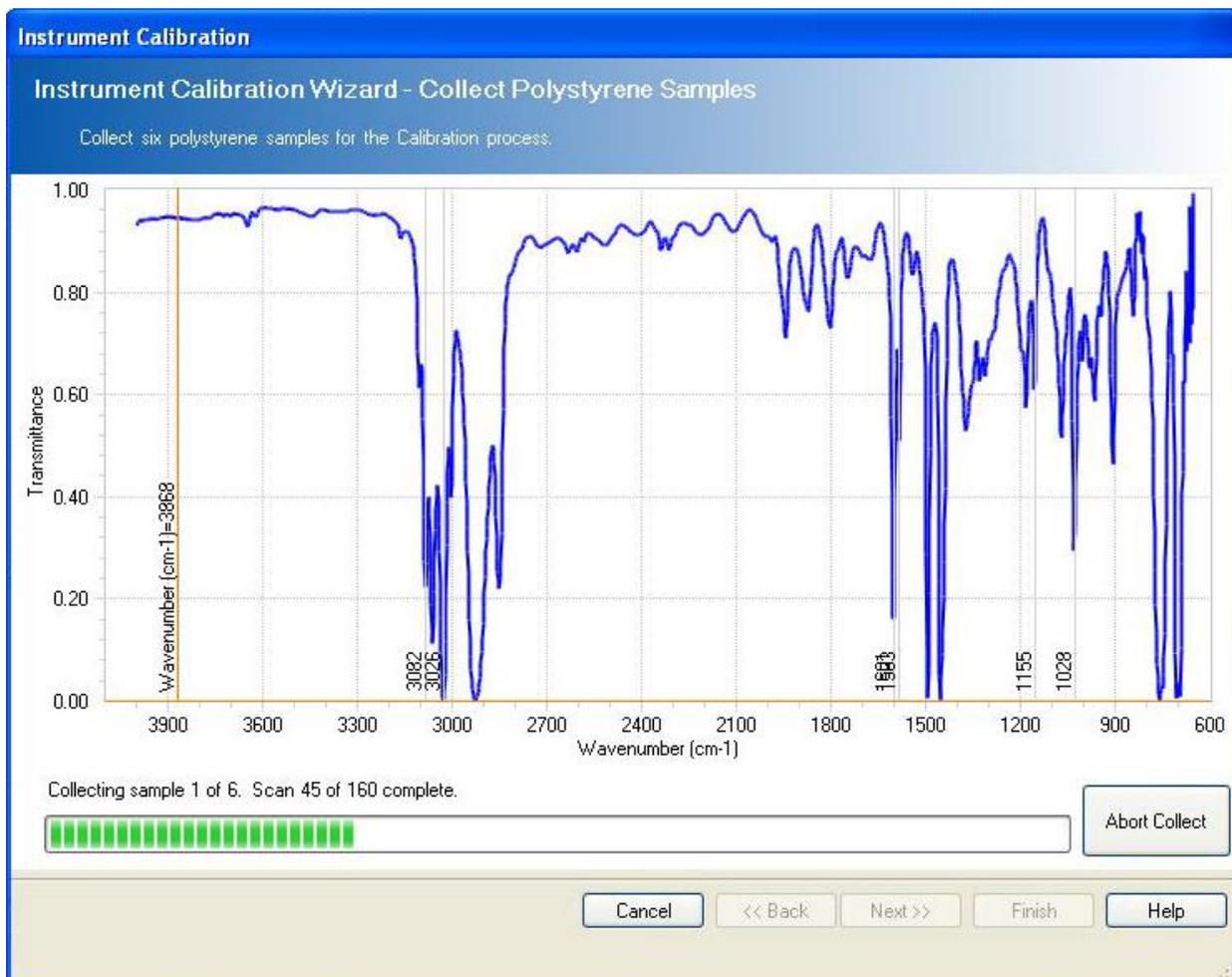


Insert the sample and click **OK**.

The last page of the wizard is used to take a sample of the polystyrene film.

Validation Wizard – Collect Polystyrene Sample Page

Click the **Collect Sample** button to take a sample.



When the sampling is complete, click the **Next** button.

The results of the validation are displayed on the next page of the wizard.

Validation Wizard – Validation Results Page

The last page of the wizard displays the results of the validation.

The screenshot shows the 'Instrument Validation Wizard - Validation Results' window. The title bar reads 'Instrument Validation'. The main header is 'Instrument Validation Wizard - Validation Results'. Below the header, it says 'Results of the Validation test.' A 'Test Details' box contains the following information:

Time of Run:	8/1/2011 11:06:45 AM	Test Type:	Validation
Instrument Name:	ReactIR 45m	Test Status:	Passed
Serial Number:	4392	Laser Frequency:	7633.62

Below the test details is a table with the following data:

NIST Peaks	Measured Peaks	Delta	Allowed Delta	Passed/Failed
3082.22	3082.59	0.37	1.00	Passed
3026.44	3026.69	0.25	1.00	Passed
1601.38	1601.00	0.38	1.00	Passed
1583.04	1583.06	0.02	1.00	Passed
1154.62	1154.83	0.21	1.00	Passed
1028.42	1028.12	0.30	1.00	Passed

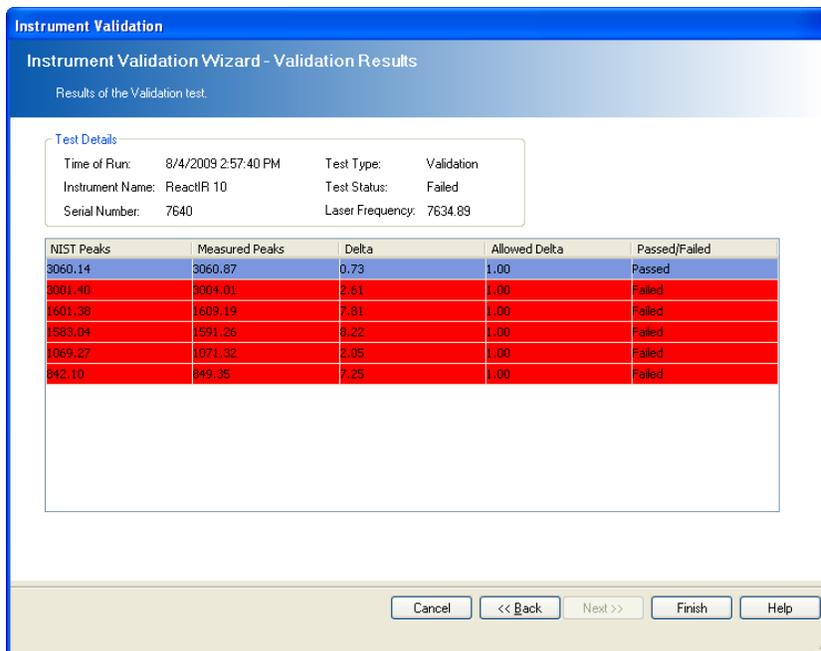
At the bottom of the window are five buttons: 'Cancel', '<< Back', 'Next >>', 'Finish', and 'Help'.

The ReactIR 247, ReactIR 45P and the ReactIR 15 support a temperature corrected laser frequency. For these instruments the laser frequency is corrected based on the base temperature. The Validation Results page for these instruments displays the term "Temperature Dependent" instead of a laser frequency value.

The screenshot shows the 'Instrument Validation Wizard - Validation Results' window for a ReactIR 45P instrument. The title bar reads 'Instrument Validation'. The main header is 'Instrument Validation Wizard - Validation Results'. Below the header, it says 'Results of the Validation test.' A 'Test Details' box contains the following information:

Time of Run:	8/1/2011 3:47:56 PM	Test Type:	Validation
Instrument Name:	ReactIR 45P	Test Status:	Passed
Serial Number:	9162	Laser Frequency:	Temperature Dependent

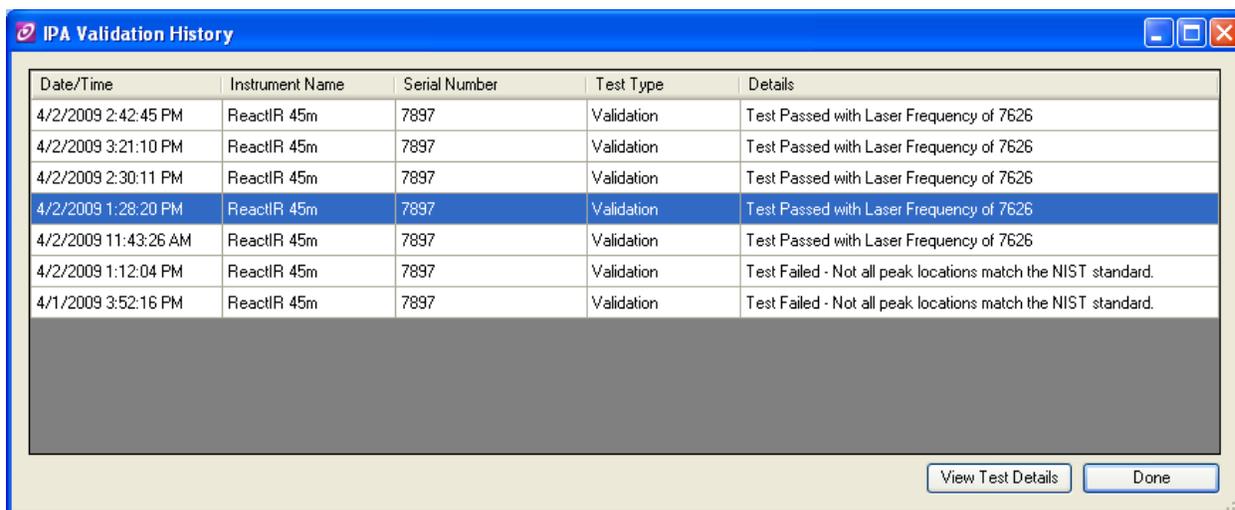
Any failed results are displayed in red on the display.



Click the **Finish** button to close the wizard and save the results. The NIST Peaks table is also updated with the results of the validation.

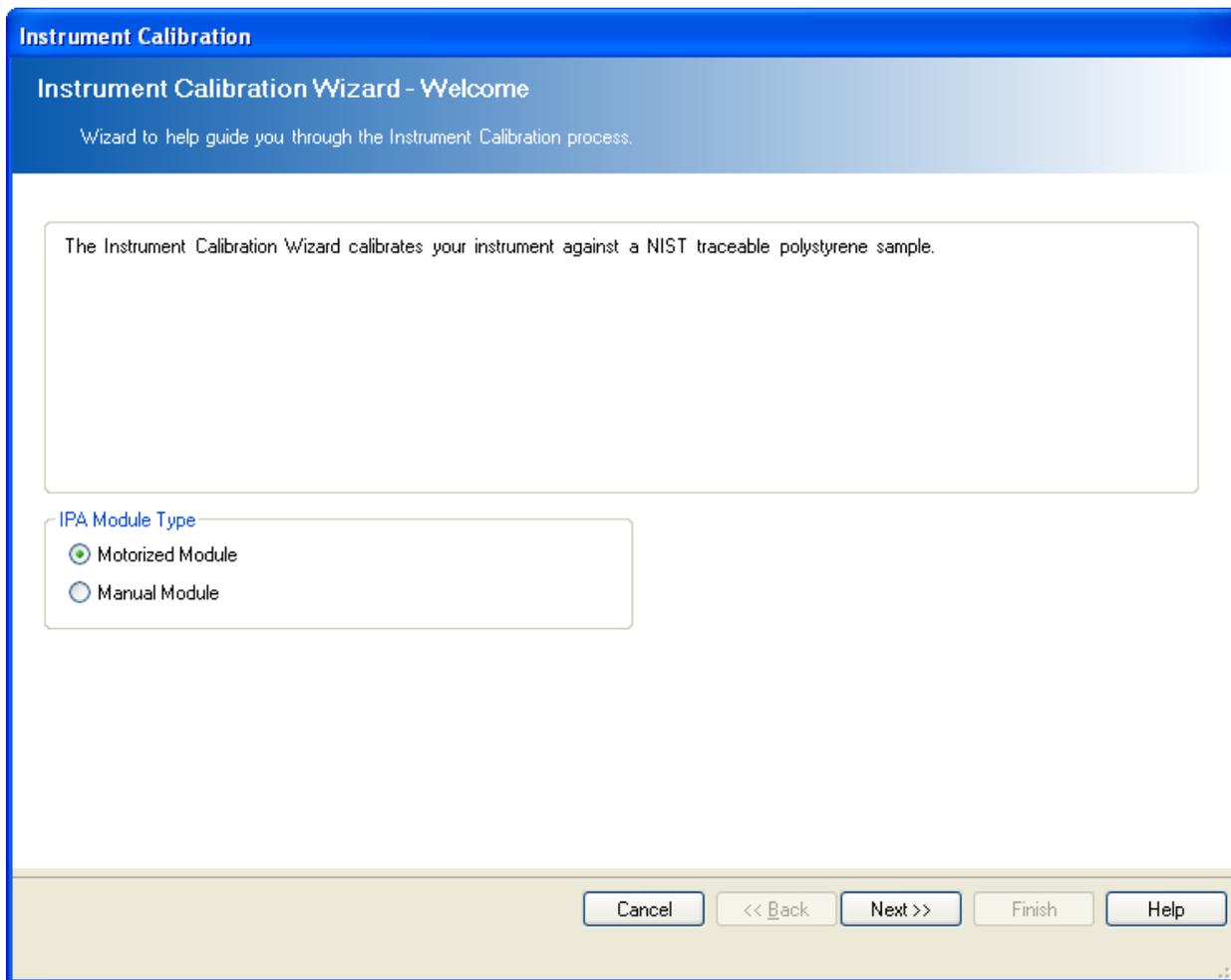
NIST Peaks	Measured Peaks	Delta
3082.22	3082.59	0.37
3026.44	3026.69	0.25
1601.38	1601.00	0.38
1583.04	1583.06	0.02
1154.62	1154.83	0.21
1028.42	1028.12	0.30

The Validation History is updated with the details of the validation.



The Calibration Wizard

The Instrument Calibration wizard is used to calibrate an instrument against a NIST traceable polystyrene film sample. The wizard is launched by clicking the **Run Calibration** button in the **Instrument Performance Assurance** task pane.



The first page of the wizard is a welcome page. If the instrument is a ReactIR 45m, radio buttons are displayed that allow the selection of the Motorized or Manual Module. The ReactIR 247, ReactIR 15 and IC10 only use manual operation and the ReactIR 45P only uses motorized operation. Click the **Next** button to continue.

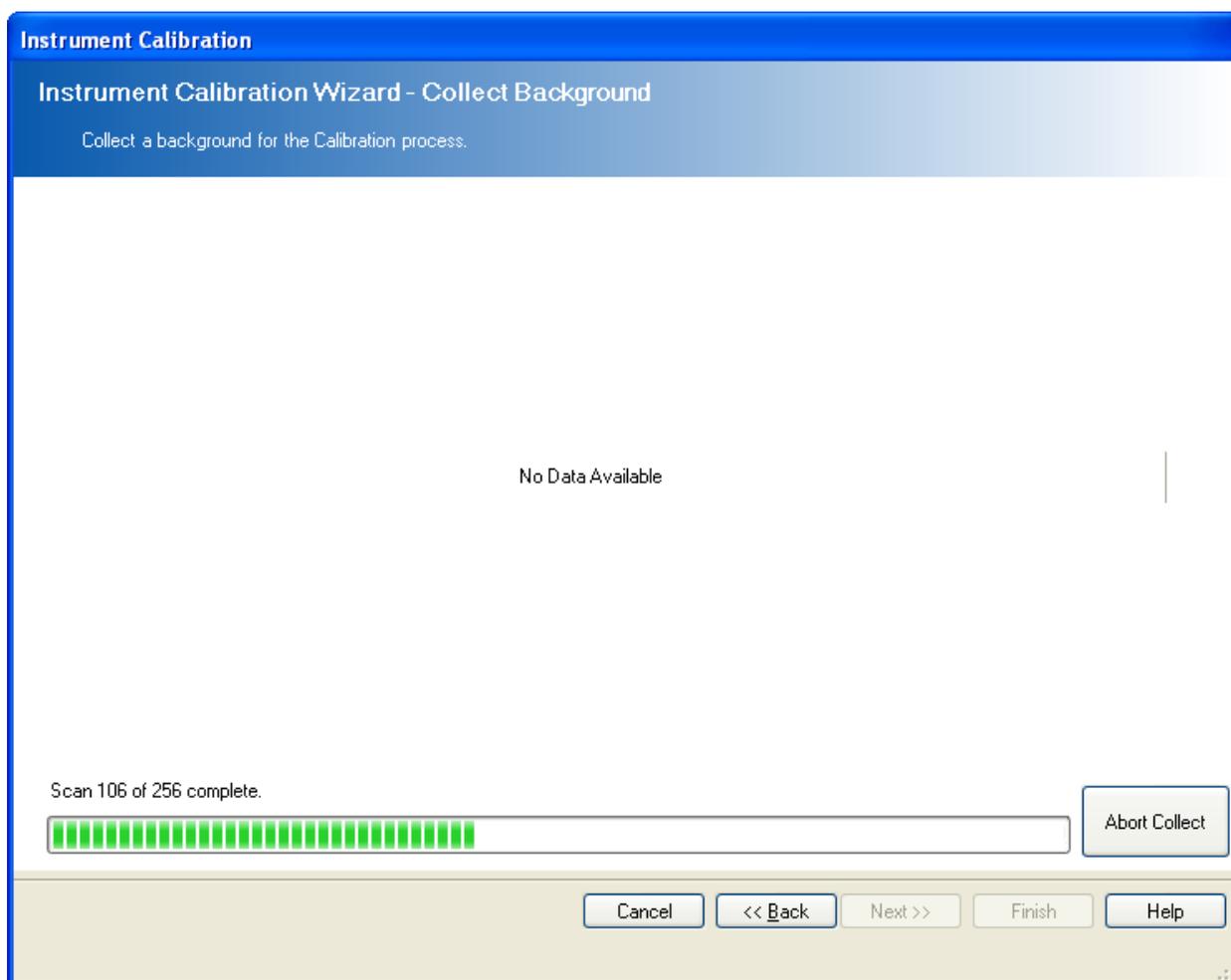
Calibration Wizard – Collect Background Page

The next page of the wizard is used to collect a background.

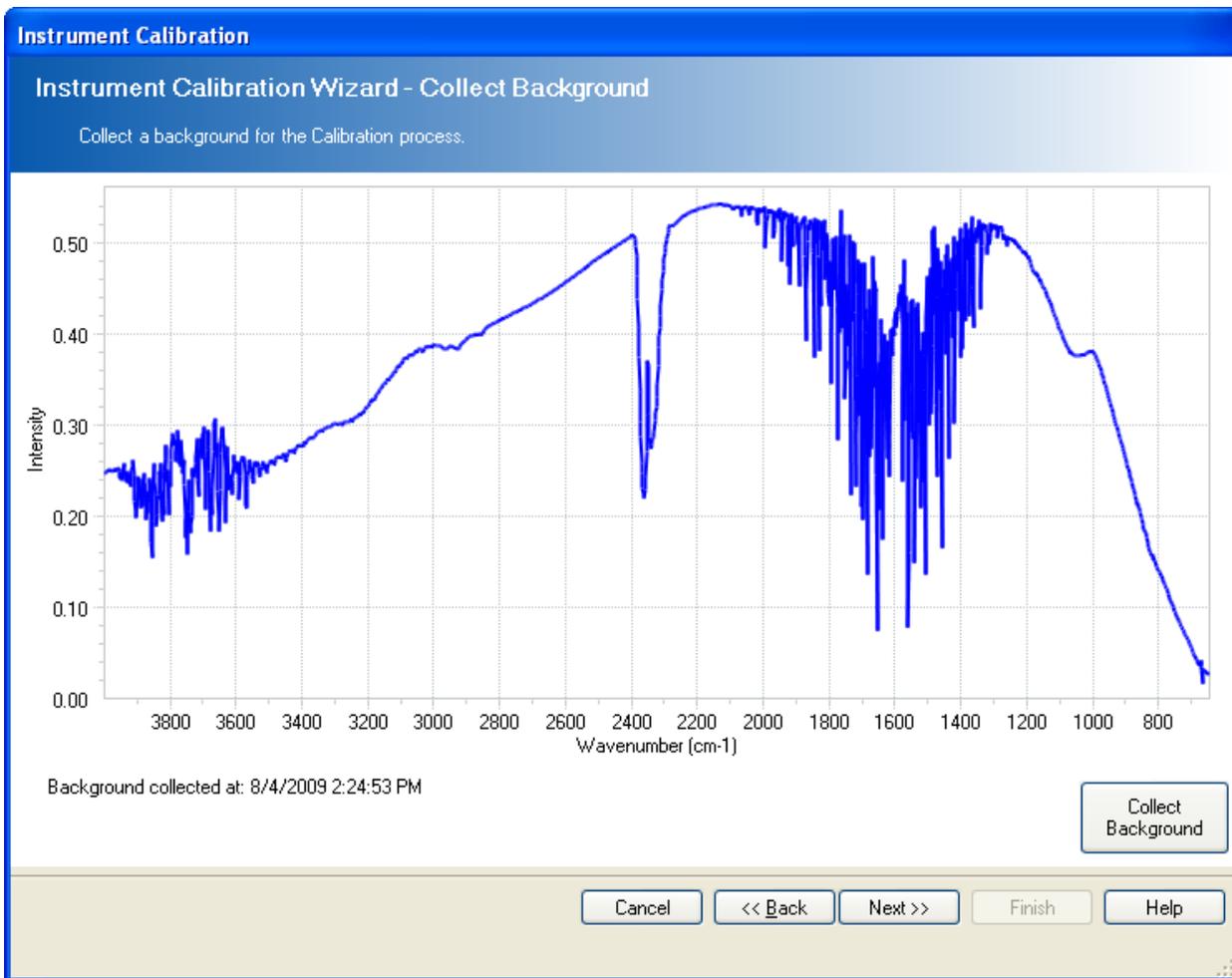
Note: A background spectrum should be collected for reference after the probe has been aligned properly and the sensor cleaned.

The React IR utilizes a background measurement to minimize the 'instrument response' from the desired spectrum. Historically, one is measuring I/I_0 where I is the intensity of the light after passing through a sample and I_0 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. You can run multiple tests without collecting a new background. However if you close and reopen the wizard, The wizard leads you through this procedure.

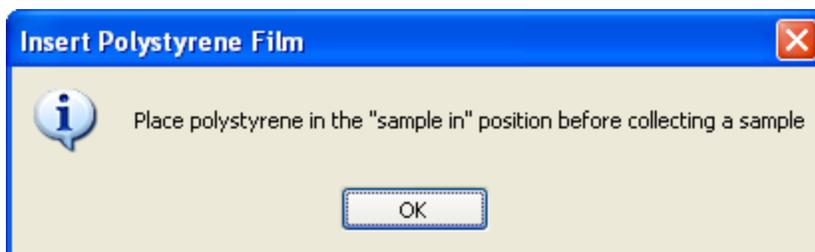
Click on the **Collect Background** button to collect a background sample.



When the background has been collected, click the **Next** button.



A message dialog is displayed that instructs the user to insert the polystyrene sample into the optical path. Note that this dialog is not displayed for the motorized module.

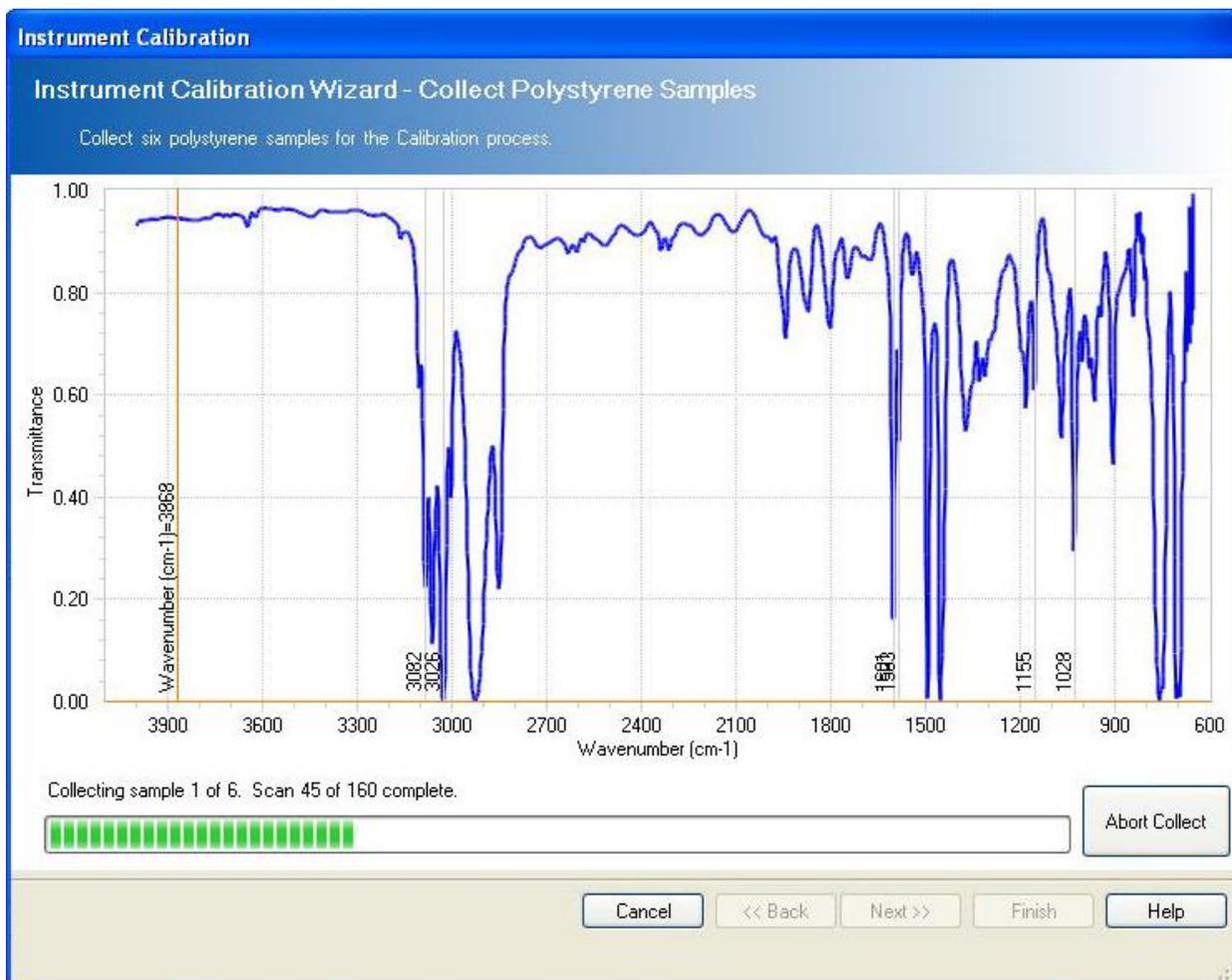


Insert the sample and click **OK**.

Calibration Wizard – Collect Polystyrene Sample Page

The next page of the wizard is used to take a sample of the polystyrene film.

Click the **Collect Sample** button to take a sample.



When the sampling is complete, click the **Next** button.

The results of the validation are displayed on the next page of the wizard.

Calibration Wizard – Calibration Results Page

The last page of the wizard displays the results of the calibration.

The screenshot shows the 'Instrument Calibration Wizard - Calibration Results' window. The title bar reads 'Instrument Calibration'. Below the title bar, the main heading is 'Instrument Calibration Wizard - Calibration Results'. Underneath, it says 'Results of the Calibration test.'.

The 'Test Details' section contains the following information:

Time of Run:	8/1/2011 10:59:41 AM	Test Type:	Calibration
Instrument Name:	ReactIR 45m	Test Status:	Passed
Serial Number:	4392	Laser Frequency:	7633.62

Below the test details is a table with the following data:

NIST Peaks	Measured Peaks	Delta	Allowed Delta	Passed/Failed
3082.22	3082.59	0.37	1.00	Passed
3026.44	3026.69	0.25	1.00	Passed
1601.38	1601.00	0.38	1.00	Passed
1583.04	1583.06	0.02	1.00	Passed
1154.62	1154.83	0.21	1.00	Passed
1028.42	1028.11	0.31	1.00	Passed

At the bottom right of the main content area, there is a button labeled 'Commit New Laser Frequency'. At the very bottom of the window, there are navigation buttons: 'Cancel', '<< Back', 'Next >>', 'Finish', and 'Help'.

The ReactIR 247, ReactIR 45P and the ReactIR 15 support a temperature corrected laser frequency. For these instruments the laser frequency is corrected based on the base temperature. The Calibration Results page for these instruments displays the term "Temperature Dependent" instead of a laser frequency value.

The screenshot shows the 'Instrument Calibration Wizard - Calibration Results' window for a ReactIR 45P instrument. The title bar reads 'Instrument Calibration'. Below the title bar, the main heading is 'Instrument Calibration Wizard - Calibration Results'. Underneath, it says 'Results of the Calibration test.'.

The 'Test Details' section contains the following information:

Time of Run:	8/1/2011 2:26:39 PM	Test Type:	Calibration
Instrument Name:	ReactIR 45P	Test Status:	Passed
Serial Number:	9162	Laser Frequency:	Temperature Dependent

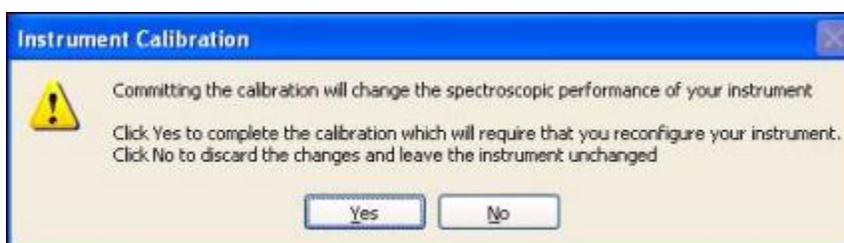
The **Commit New Laser Frequency** button is enabled if the calibration succeeds allowing the user the option to save the new laser frequency found by the calibration to the instrument

There is only one calibration attempt which is performed on all six samples (i.e. all six samples are collected first and then an attempt is made to calibrate the instrument).

During the calibration attempt, IPA adjusts the laser frequency looking for a laser frequency value that will give the closest peak values (averaged over the six peaks) to the NIST peaks. ALL peaks must lie within the allowable delta for the calibration to pass. The laser frequency that is found to have the closest peak values to the NIST peaks is the value found for the test.

If no peaks can be found at any laser frequency value that are ALL within the allowable delta then the test fails.

The Calibration History is not updated until/unless the **Commit New Laser Frequency** button is enabled and clicked. This requires that the calibration succeeded and the laser wavenumber changed as a result of performing the calibration. When the **Commit New Laser Frequency** button is clicked a confirmation dialog is displayed.



Click **Yes** to submit the calibration changes.



Click **OK** to verify that changes are to be made to the instrument calibration. Note that the instrument must be reconfigured after the changes are submitted.

Click the **Finish** button to close the wizard and save the results. The NIST Peaks table is also updated with the results of the validation.

The NIST Peaks table is updated with the results of the calibration.

NIST Peaks	Measured Peaks	Delta
3082.22	3082.59	0.37
3026.44	3026.69	0.25
1601.38	1601.00	0.38
1583.04	1583.06	0.02
1154.62	1154.83	0.21
1028.42	1028.12	0.30

The Calibration History is updated with the results of the calibration.

Date/Time	Instrument Name	Serial Number	Test Type	Details
8/3/2009 2:33:50 PM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.3
8/3/2009 12:10:58 PM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.29
8/3/2009 11:54:27 AM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.29
8/3/2009 11:37:16 AM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.29
8/3/2009 11:22:55 AM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.29
8/3/2009 9:02:20 AM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.26
8/3/2009 8:17:33 AM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.28
7/31/2009 3:31:12 PM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.27
7/31/2009 3:22:28 PM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.27
7/31/2009 3:12:32 PM	ReactIR 10	7640	Calibration	Test Passed with Laser Frequency of 7635.28

The Calibration/Validation History Dialog

The Calibration/Validation History dialog displays a history listing each calibration and validation performed on the instrument. The list also contains a details field that contains the result of the calibration/validation. If a calibration or validation attempt fails, the reason for the failure is noted in the Details field.

Date/Time	Instrument Name	Serial Number	Test Type	Details
3/24/2009 9:34:57 AM	ReactIR 45m	7897	Calibration	Test Passed with Laser Frequency of 7624.96
3/24/2009 9:38:17 AM	ReactIR 45m	7897	Calibration	Test Passed with Laser Frequency of 7624.81
3/24/2009 9:55:03 AM	ReactIR 45m	7897	Calibration	Test Failed - Not all peak locations match the NIST standard.
3/26/2009 9:35:48 AM	ReactIR 45m	7897	Calibration	Test Passed with Laser Frequency of 7624.75
3/26/2009 9:43:39 AM	ReactIR 45m	7897	Calibration	Test Passed with Laser Frequency of 7624.73
3/26/2009 10:17:48 ...	ReactIR 45m	7897	Calibration	Test Passed with Laser Frequency of 7626
3/26/2009 11:10:03 ...	ReactIR 45m	7897	Calibration	Test Passed with Laser Frequency of 7626

When the user clicks on the View Test Details button, the results for the selected test are displayed.



The **Print Test Results** button is used to generate an XPS report of the test results. This report can be saved and viewed by any XPS compliant application (Internet Explorer, etc.)

IPA Validation Test Results

IPA Test Information

Date/Time: 8/3/2009 11:07:35 AM

Instrument Name: ReactIR 10

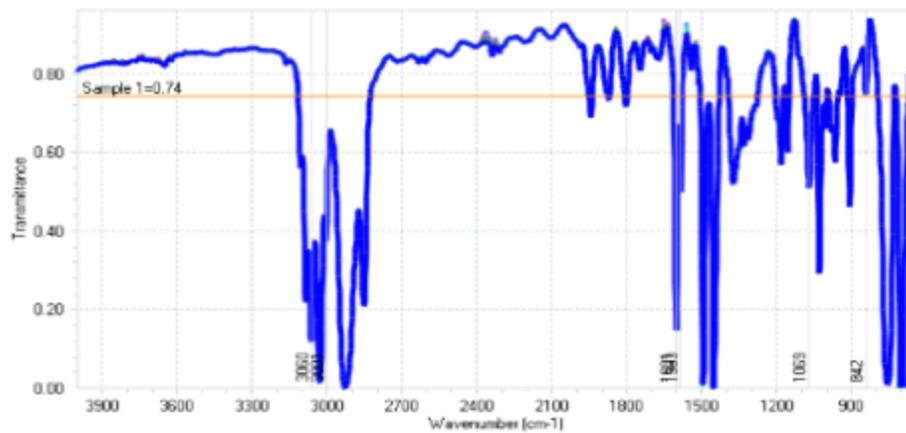
Serial Number: 7640

Test Type: Validation

Laser Frequency: 7635.26

Test Status: Passed

IPA Spectra



IPA Test Results

NIST Peaks	Measured Peaks	Delta	Allowed Delta	Passed/Failed
3060.14	3060.06	0.08	1	Passed
3001.4	3001.12	0.28	1	Passed
1601.38	1600.98	0.4	1	Passed
1582.04	1582.72	0.68	1	Passed
1069.17	1069.44	0.27	1	Passed
842.1	841.91	0.19	1	Passed

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A Note for Users of Fiber Multiplex Sampling Technology

The motorized IPA module should not be used with the iC IR configured as a Fiber Multiplexer. The user should configure a fiber multiplexer as a ReactIR 45 instrument, run the Validation/Calibration and then reconfigure it as a Fiber Multiplexer.

Replacing the Polystyrene Film

The polystyrene film in the IPA should be replaced on a yearly basis. The following document provides a procedure for replacing the film.

This document is available in the iC IR Documentation Portfolio.

[MK-PB-0003-AC Replacing Polystyrene Film in IPA Module.pdf](#)

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