Chapter 9:

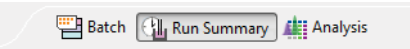
Run Status

Chapter Overview

- Run Summary Screen Overview
- Opening Run Files
- Batch Injection Information
- Run Status Information
- Viewing the Focus Series (cIEF Only)
- Viewing the Separation (CE-SDS Only)
- Current and Voltage Plots
- Run History
- Viewing Run Errors
- Injection Reports
- Switching Between Open Run Files
- Closing Run Files

Run Summary Screen Overview

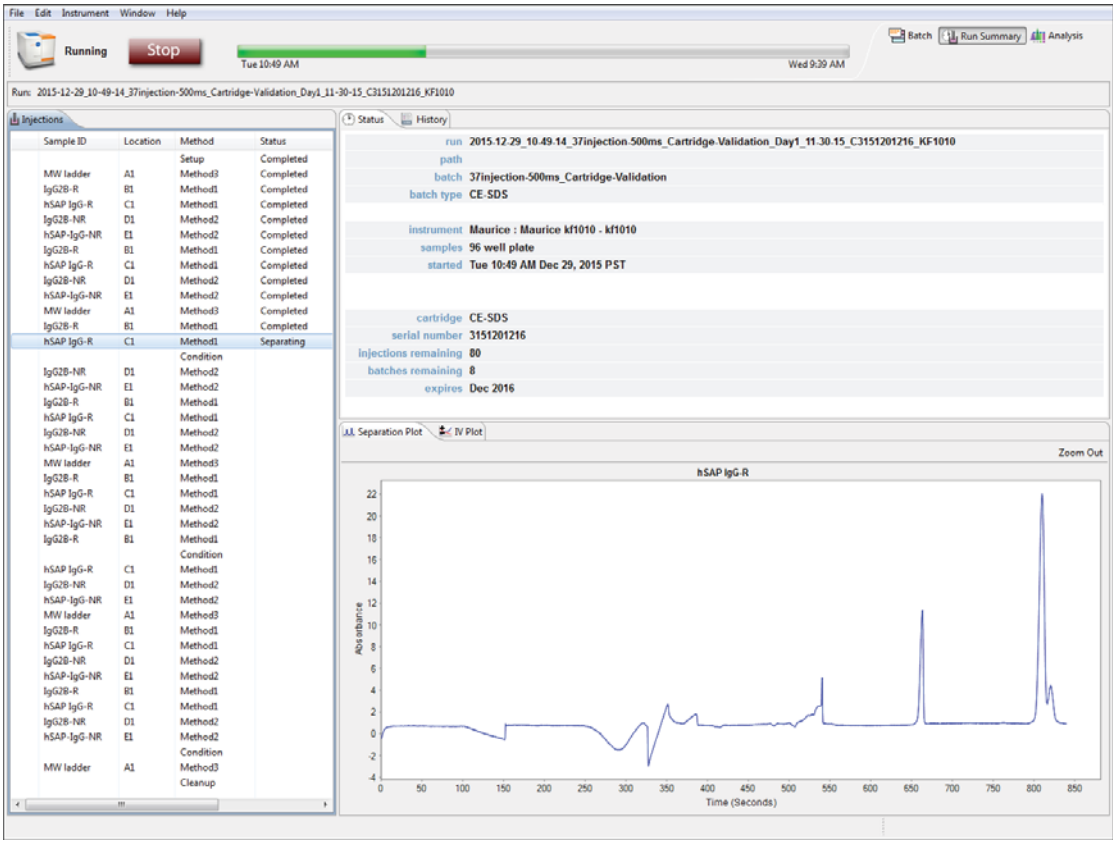
You can use the Run Summary screen to monitor the stats of a batch in progress, see the CE-SDS separation or cIEF Focus series for your injections or the current and voltage plots for each injection. To get to this screen, click the **Run Summary** screen tab:

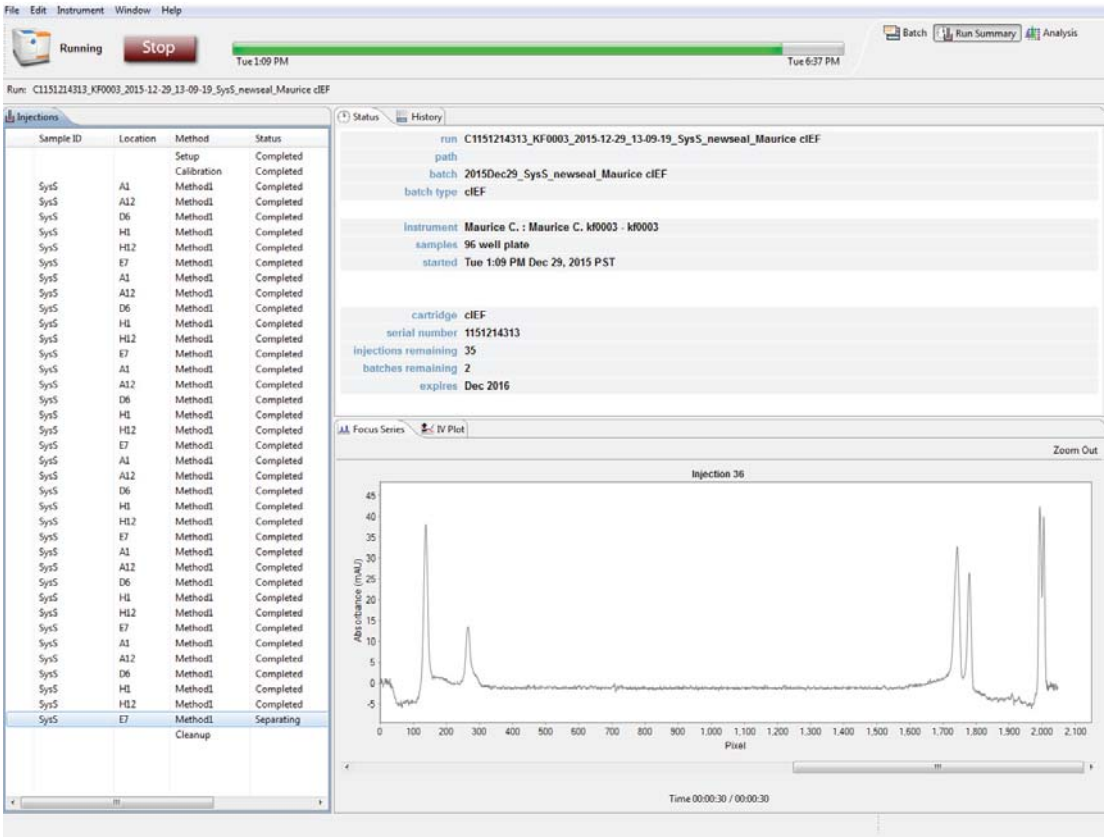


Run Summary Screen Panes

The Run Summary screen has five panes:

- **Injections** - Lists the sample IDs, sample locations and methods used for each injection in the run. It also shows the status of the current injection if a run is in progress.
- **Status** - Displays run file information and the current status of a run if one's in progress.
- **History** - Running history of all run file events from when the run was first started to the most current analysis update.
- **Separation Plot (CE-SDS only)**- Lets you view the raw protein separation in the capillary for each injection.
- **Focus Series (cIEF only)** - Lets you view the recorded focusing of proteins along the pH gradient in the capillary for each injection.
- **IV Plot** - Lets you view plots of the total current and voltage measured during the separation for each injection.


File Edit Instrument Window Help
Running
Stop
Tue 10:49 AM
Wed 9:39 AM
Batch
Run Summary
Analysis
Run: 2015-12-29_10-49-14_37injection-500ms_Cartridge-Validation_Day1_11-30-15_C3151201216_KF1010
Injections
Sample ID Location Method Status
Status
History
run 2015.12.29_10.49.14_37injection.500ms_Cartridge.Validation_Day1_11.30.15_C3151201216_KF1010
path
batch 37injection-500ms_Cartridge-Validation
batch type CE-SDS
instrument Maurice : Maurice kf1010 - kf1010
samples 96 well plate
started Tue 10:49 AM Dec 29, 2015 PST
cartridge CE-SDS
serial number 3151201216
injections remaining 80
batches remaining 8
expires Dec 2016
Separation Plot
IV Plot
Zoom Out
hSAP IgG-R
Absorbance
Time (Seconds)



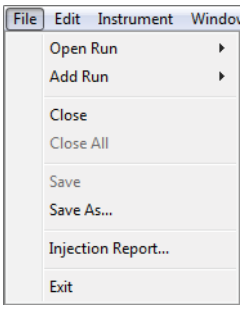
Software Menus Active in the Run Summary Screen

These main menu items are active in the Run Summary screen:

- File
- Edit
- Instrument (when the software is connected to an instrument)
- Window
- Help

File Menu

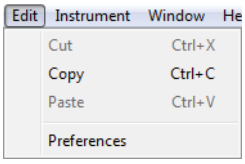
These File menu options are active:



- **Open Run** - Opens a run file.
- **Add Run** - Lets you open and view other run files besides the one that's already open.
- **Close** - Closes the run file currently being viewed.
- **Close All** - Closes all open run files.
- **Save/Save As** - If you made changes in the Analysis screen before you went to the Run Summary screen, this saves your changes to the run file.
- **Injection Report** - Exports the raw and analyzed data, IV plot, peaks table, sample and system info for individual injections as PDF files. You can also export the run history with all analysis events.
- **Exit** - Closes Compass for iCE.

Edit Menu

These Edit menu options are active:



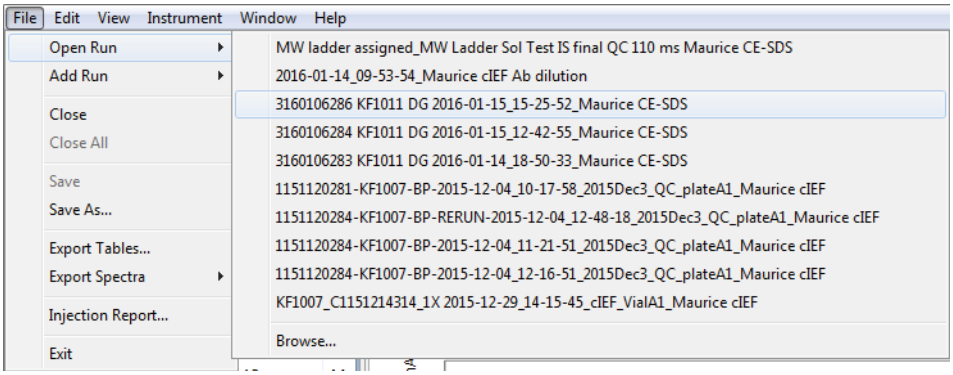
- **Copy** - Copies the information in the History pane so you can paste it into other documents.
- **Preferences** - Lets you set and save your preferences for data export, graph colors, grouped data and Twitter settings. See Chapter 13, *"Setting Your Preferences"* for more information.

Opening Run Files

You can open one run file or multiple files at the same time to compare information between runs.

Opening One Run File

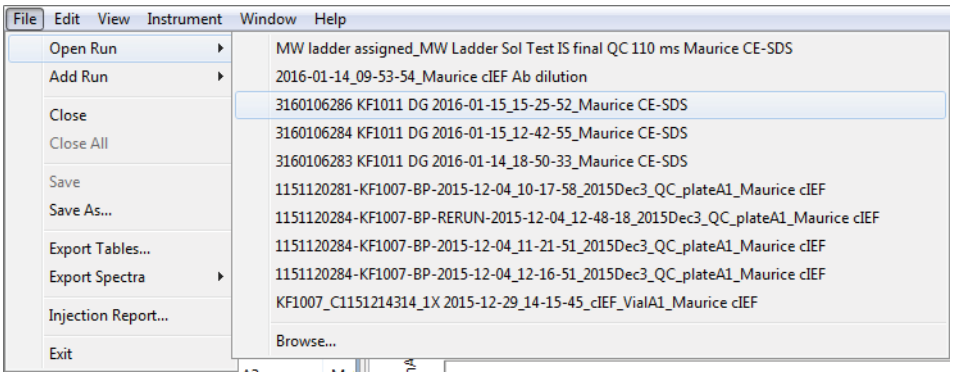
1. Select **File** in the main menu and click **Open Run**.



2. A list of the last 10 runs opened will display. Select one of these runs or click **Browse** to open the Runs folder and select a different file.

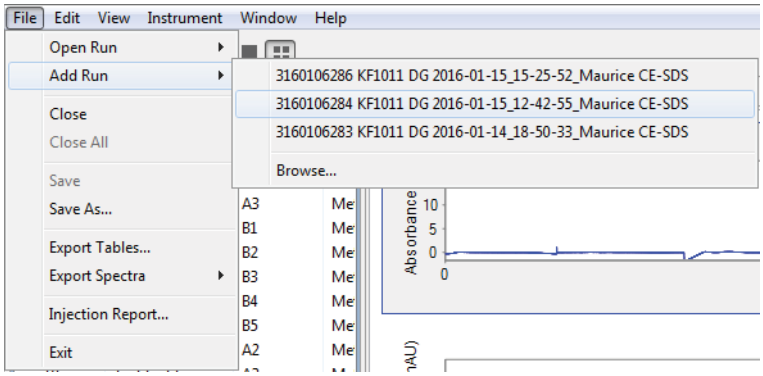
Opening Multiple Run Files

1. To open the first run file, select **File** in the main menu and click **Open Run**.



2. A list of the last 10 runs opened will display. Select one of these runs or click **Browse** to open the Runs folder and select a different file.

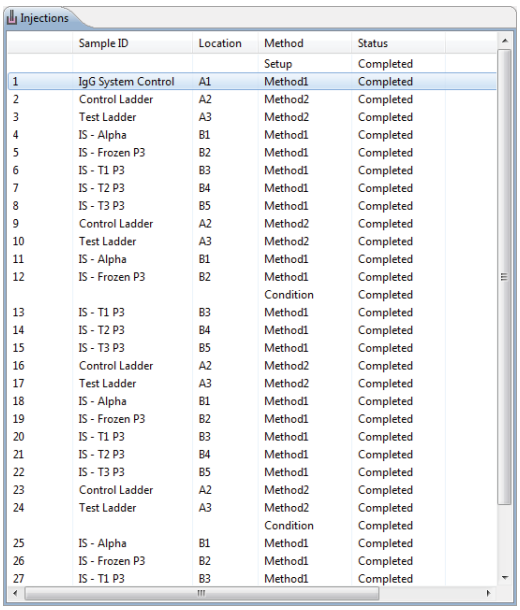
3. To open another run file, select **File** in the main menu and click **Add Run**.

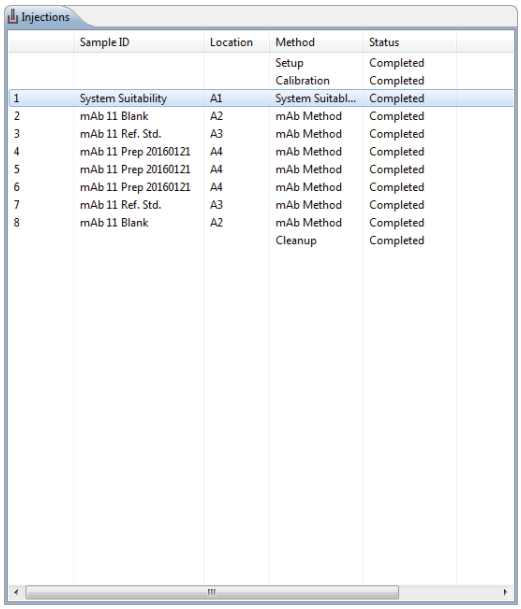


4. A list of runs will display. You can only open a run that uses the same application as the run that's already open (cIEF or CE-SDS), so the run files displayed are only for that application. Select one of these runs or click **Browse** to open the Runs folder and select a different file.
5. Repeat the last two steps to open additional runs.

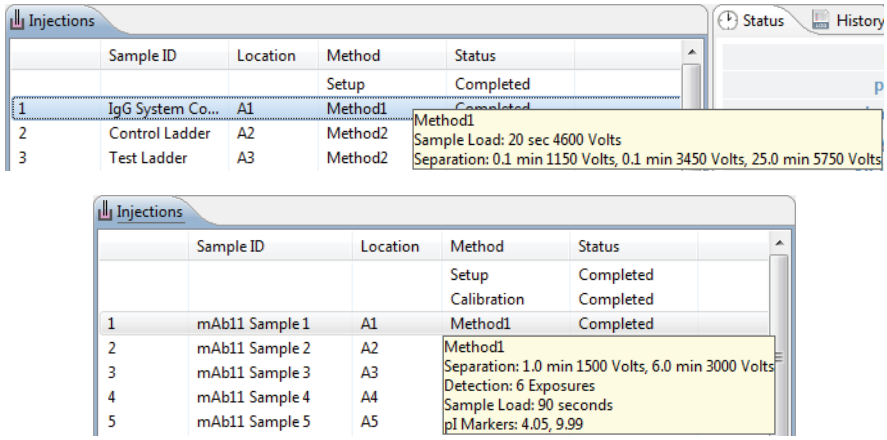
Batch Injection Information

The Injections pane lists the system protocols (Setup and Cleanup) and injections performed during the run.



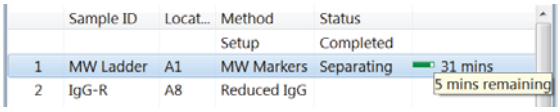


- Clicking on an injection displays its data in the Focus Series (cIEF) or Separation (CE-SDS) and IV Plot panes.
- Hovering over a method name displays the method parameters:



For runs in progress, the Status column displays:

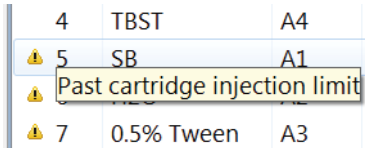
- **Running** for Setup, Conditioning (CE-SDS only) and Cleanup protocols that are in progress
- **Loading** or **Separating** for injections in progress. Once the separation starts, a status bar displays next to the injection so you know when the separation will be done. Hovering your mouse over the progress bar tells you the time left for the injection.
- **Completed** for Setup, Conditioning and Cleanup protocols and injections that are done.



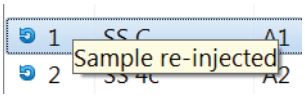
Injection Flags

If Compass for iCE detects a potential injection issue, a flag icon will display next to the injection row in the Injections pane.

⚠ **Past cartridge injection limit notification** - This means the injection is over the guaranteed number of injections for the cartridge. Roll your mouse over the icon to display details.



Reinjection notification (CE-SDS only) - This means the current during the separation dropped below the minimum value, so the separation was stopped and the sample was reinjected. The second injection always runs to completion even if the current drops again. Roll your mouse over the icon to display details.

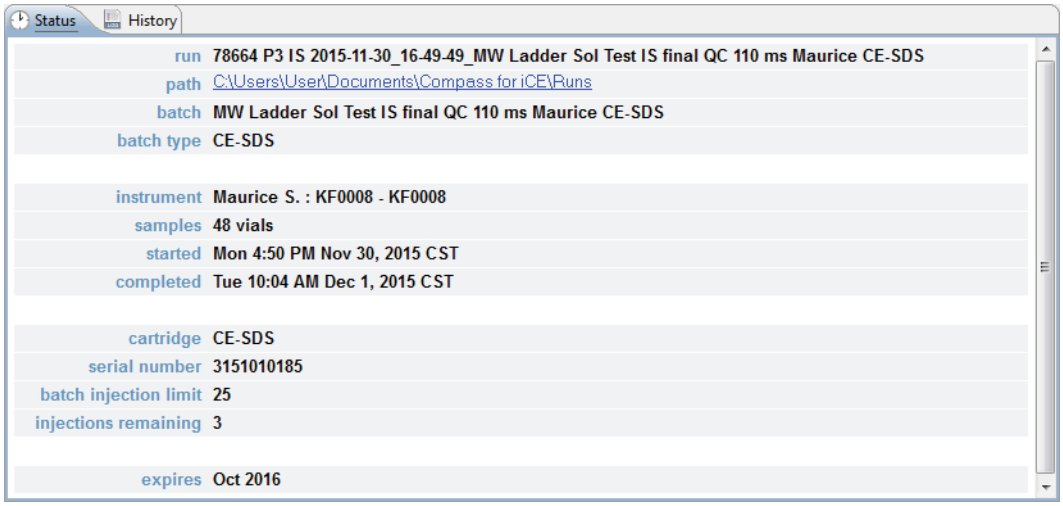


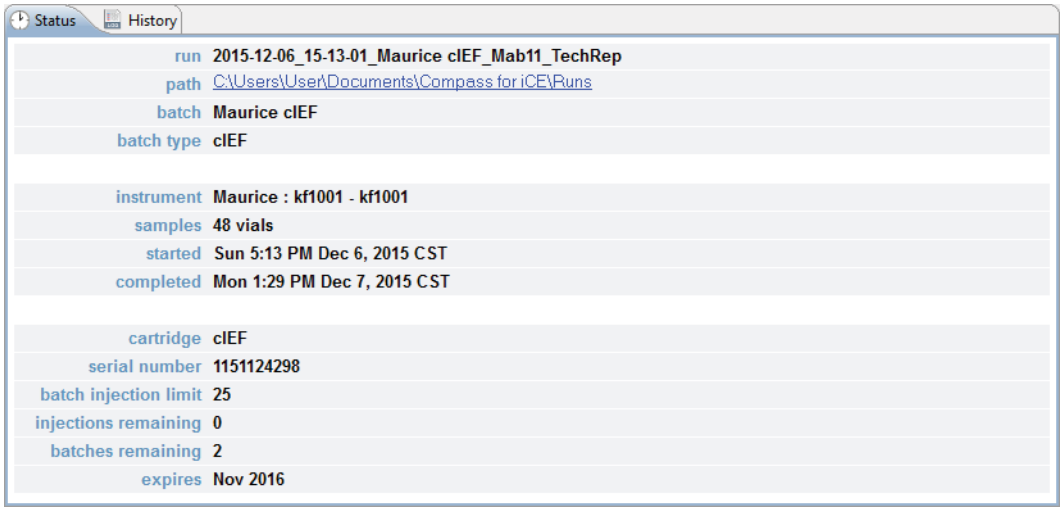
Run Status Information

The Status pane shows info specific to each run file:

- Run file name and path (directory location)
- Batch name and type
- Instrument and serial number
- Type of sample tray used
- Run start/complete date and time
- Type of cartridge
- Cartridge serial number

- Cartridge batch injection limit, injections/batches remaining and expiration date





- **To go to the run file directory location** - Double click the path hyperlink, or right-click and select **Open Directory**.
- **To copy the path** - Right-click on the path hyperlink and click **Copy**. The path can then be copied into documents. The path can also be copied into the Windows Explorer address bar to launch Compass for iCE and open the run file automatically.

Viewing the Focus Series (cIEF Only)

You can view your proteins focusing along the pH gradient in the capillary for each injection in the Focus Series pane.

NOTE: The Focus Series plot displays in absorbance only, even if the fluorescence detection mode is selected in the Analysis settings.

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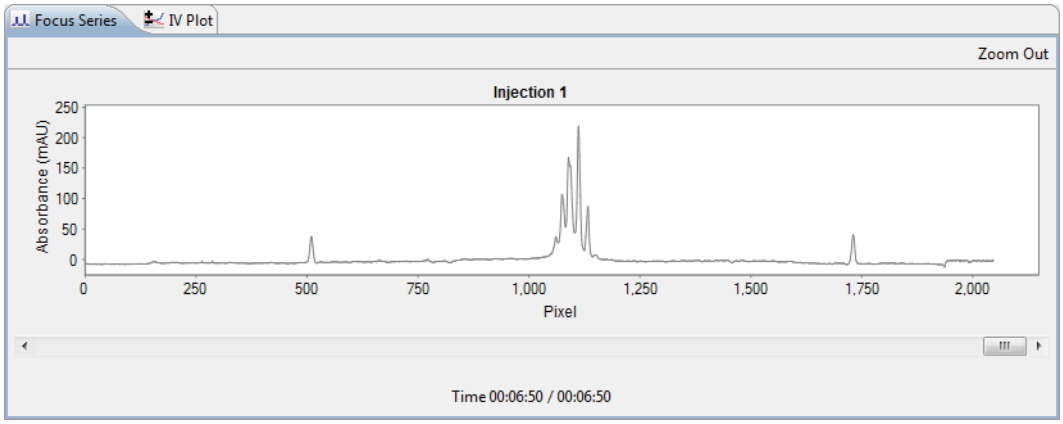
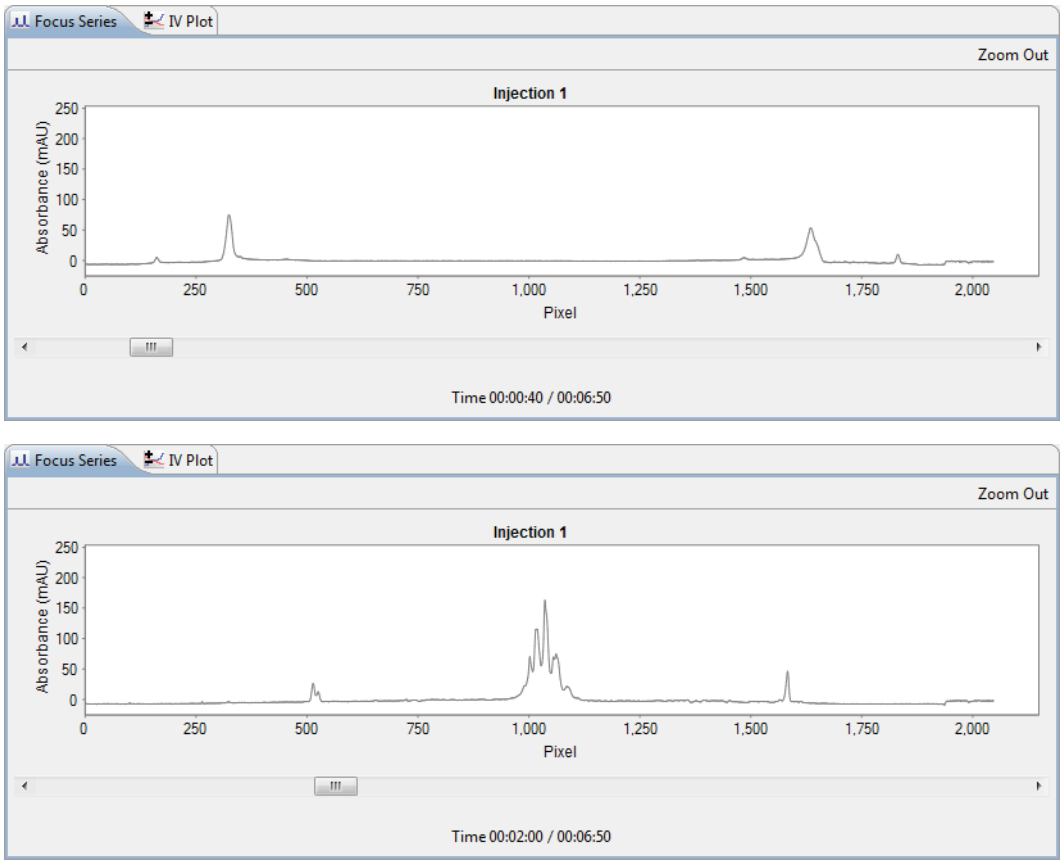
1. Select an injection in the Injections pane.
2. Click the **Focus Series** pane. It'll display the final focusing plot:



3. To view the focusing as it happened, drag the slider bar under the plot to the left or right. To view it frame by frame, click the left/right arrows.



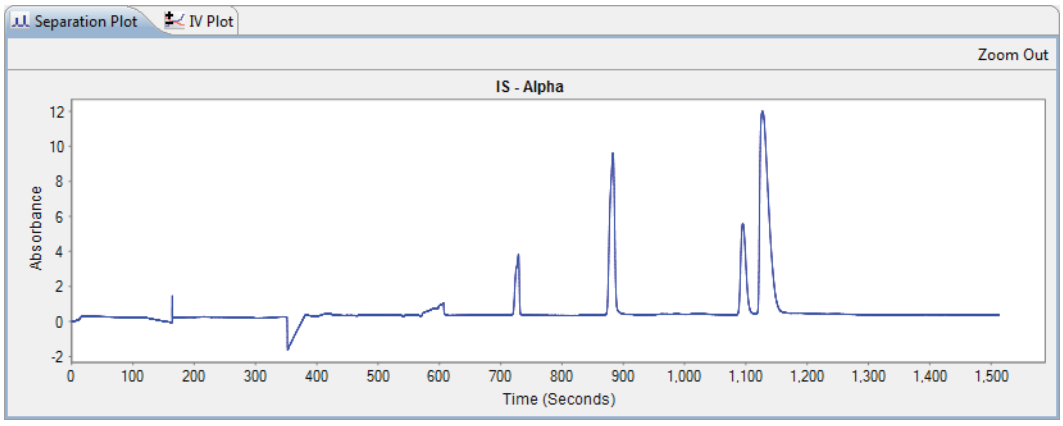
- **To zoom in on an area of the plot** - Hold the mouse button down and draw a box around the area with the mouse.
- **To zoom out** - Click **Zoom Out** in the upper right corner of the pane.

NOTE: Focus Series data for a run in progress won't be available until the injection is executing. Once it starts, the plot displays data up to the current point in time.

Viewing the Separation (CE-SDS Only)

You can view your protein separation in the capillary for each injection in the Separation pane.

1. Select an injection in the Injections pane.
2. Click the **Separation** pane. It'll display a plot of the raw separation data.



- **To zoom in on an area of the plot** - Hold the mouse button down and draw a box around the area with the mouse.
- **To zoom out** - Click **Zoom Out** in the upper right corner of the pane.

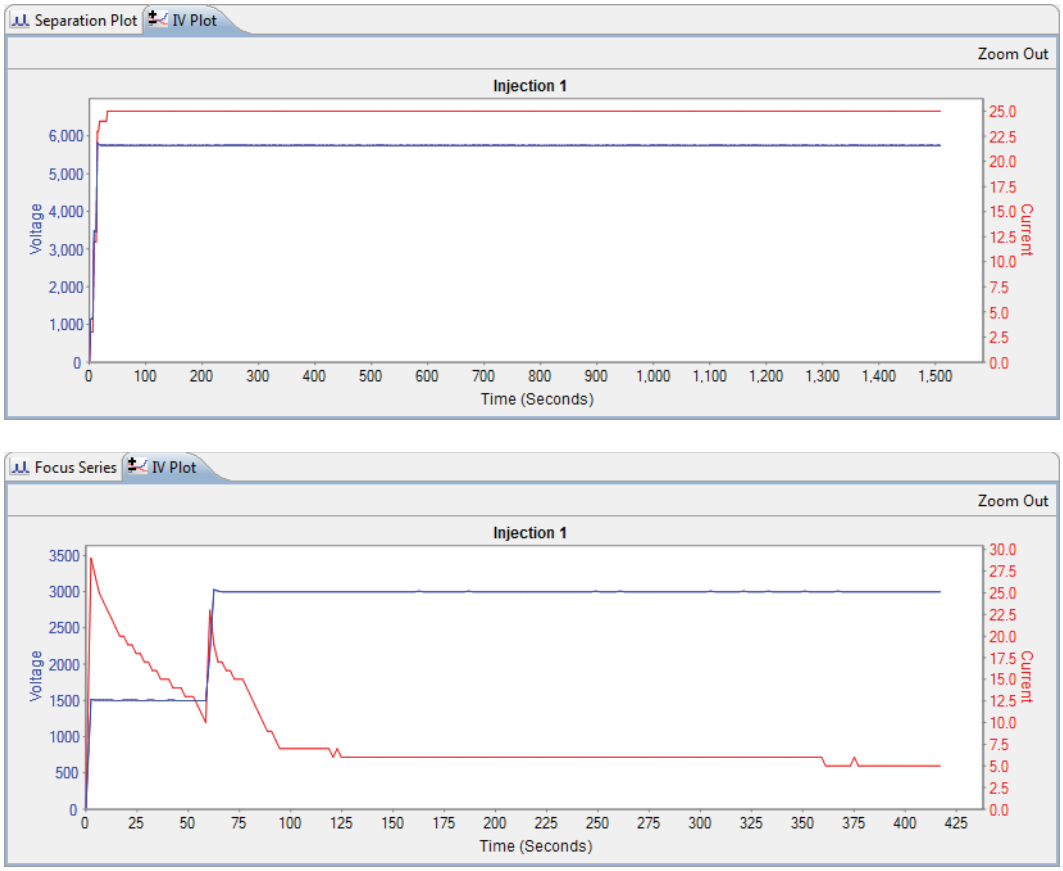
NOTE: Separation data for a run in progress won't be available until the injection is executing. Once it starts, the plot displays data up to the current point in time.

Current and Voltage Plots

To view plots of the total current and voltage measured during an injection:

1. Select an injection in the Injections pane.

2. Click the **IV Plot** pane.



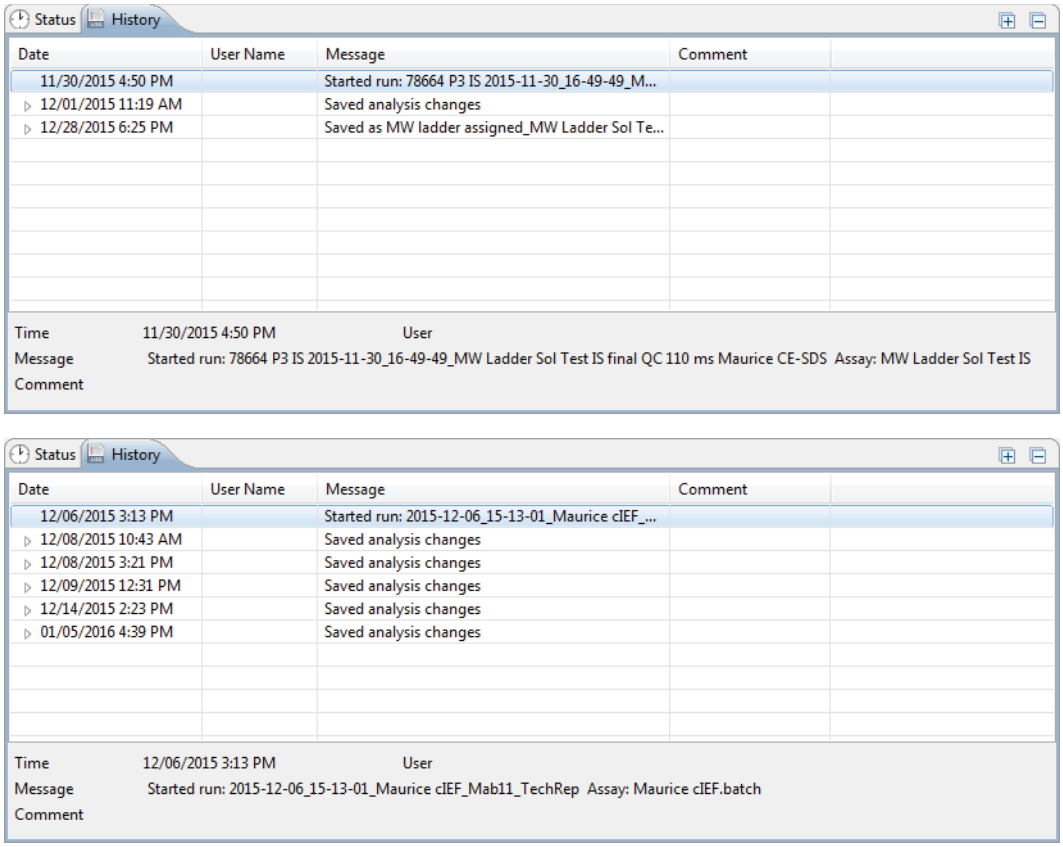
The blue Y-axis and plot shows the run voltage in volts (V), and the red Y-axis and plot shows the run current in microamps (µA). The X-axis displays time in seconds.

- **To zoom in on an area of the plot** - Hold the mouse button down and draw a box around the area with the mouse.
- **To zoom out** - Click **Zoom Out** in the upper right corner of the pane.

NOTE: IV Plots for a run in progress won't be available until the injection is executing. Once it starts, the plot displays in real time.

Run History

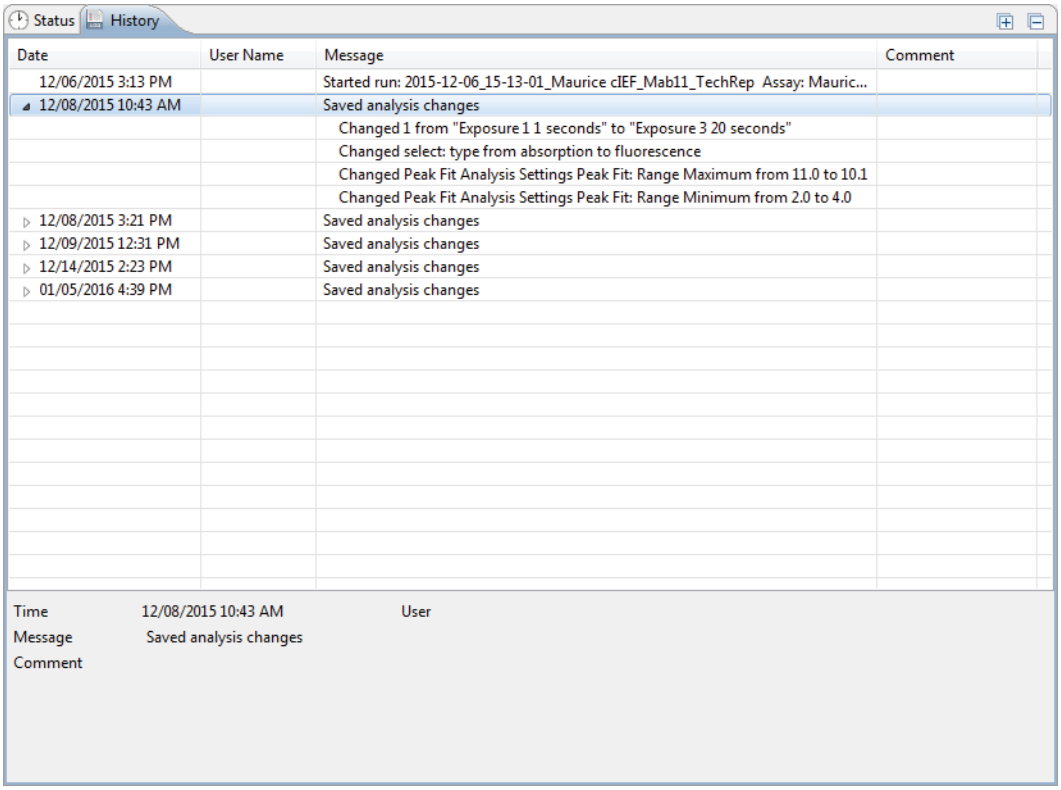
The History pane shows the run file event history, starting with the date and time the run was started through the most current analysis event. Clicking on a row in the table displays the full event details in the box under the table.



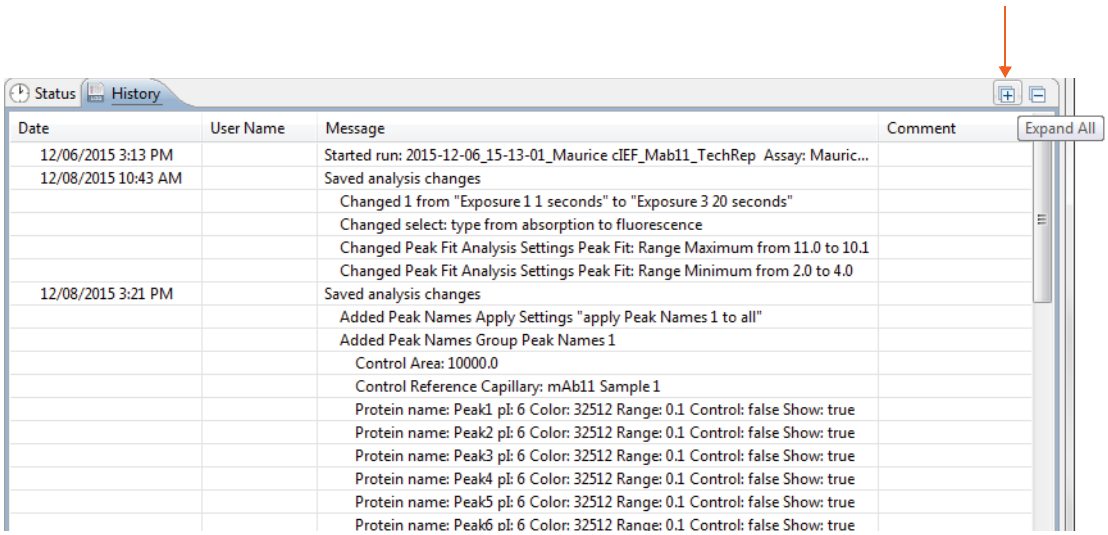
- **Date:** Date and time of the run event.
- **User Name:** User that initiated the event. User names only display if you're using the Access Control feature to help satisfy the 21CFR Part 11 data security requirements.
- **Message:** Description of the event that took place.
- **Comment:** Comments entered by the user when the batch was saved.

Viewing Multiple Events

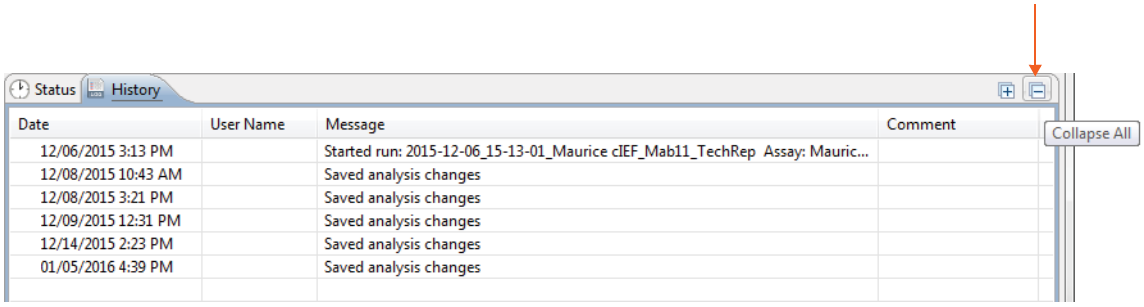
Items in the table with multiple analysis events have an arrow next to the date and time. You can view or hide these details by toggling the arrow:



- To view details for all items with multiple analysis events in the run, click the **Expand All** button.



- To hide all items with multiple analysis events, click the **Collapse All** button.



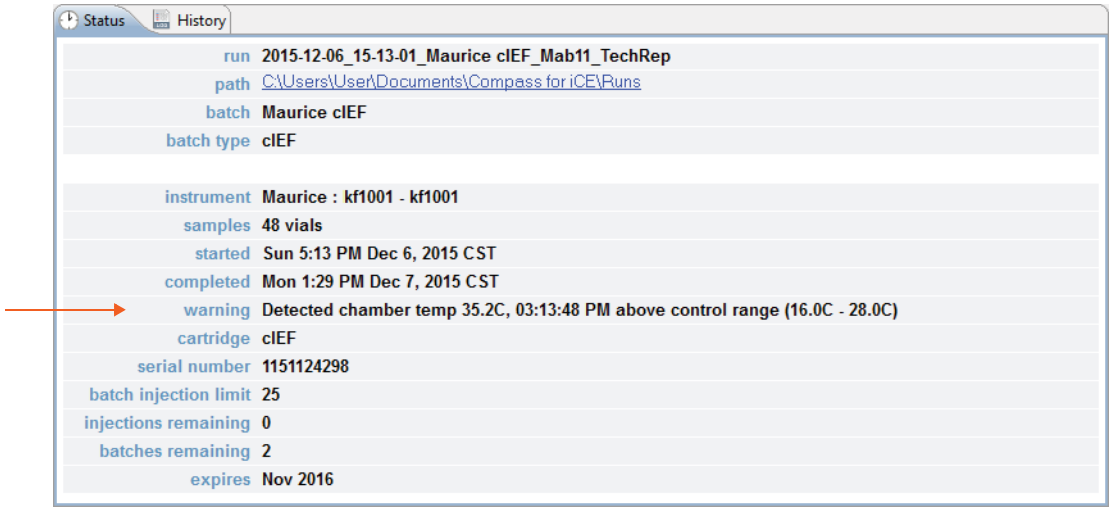
Copying History Info

You can copy the information in the History pane to use in other documents:

1. Click the **History** pane to make sure it's active.
2. Click **Edit** in the main menu and select **Copy**.
3. Open a document and click **Paste**.

Viewing Run Errors

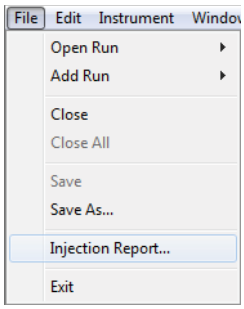
If an error is detected during the run it will display in the Status pane:



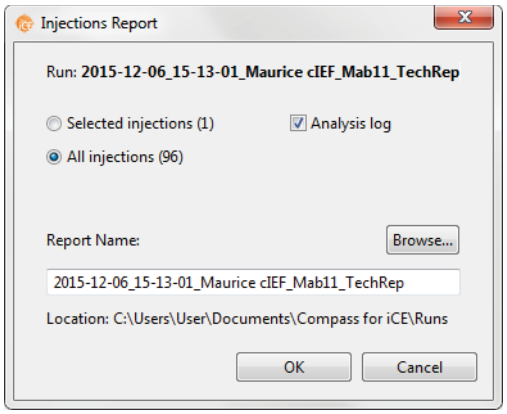
Injection Reports

You can export PDF files of the raw and analyzed data, IV plot, peaks table, sample and system info for individual or all injections in a run file. You can also export the run history with all analysis events.

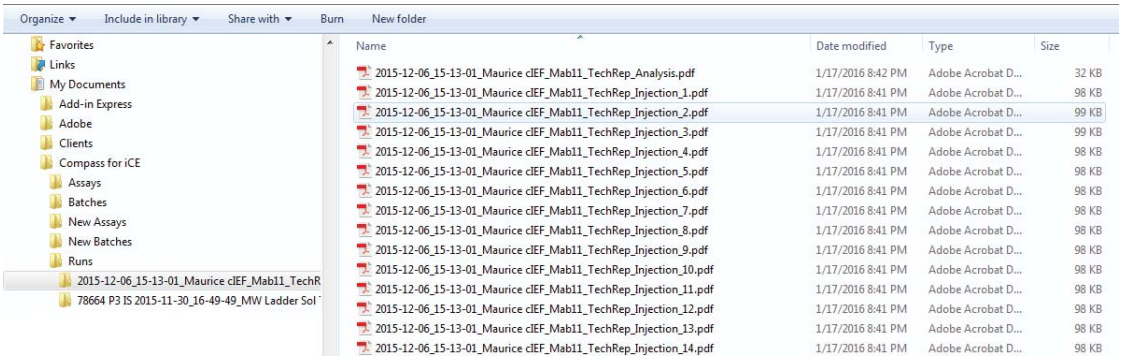
1. Click **File** > **Open Run** and select a run file.
2. If you want reports for all injections, skip to the next step. Otherwise, select the injection in the Injection pane that you want a report for.
3. Select **File** from the main menu in either screen and click **Injection Report**.



4. In the Injection Reports window:
   a. Choose either **Selected injections** or **All injections**.
   b. Select the **Analysis log** checkbox if you want a run history report with all analysis events.
   c. The report name defaults to the run file name. If you want to change it, type in the **Report Name** box to make updates.
   d. Click **OK**.



5. The Injection Report PDF(s) are exported to the Runs folder in the Compass for iCE directory. They'll be in a folder with the report name used in the prior step. When the reports are done, the folder opens for you automatically.



Example Analysis and Injection Report: CE-SDS

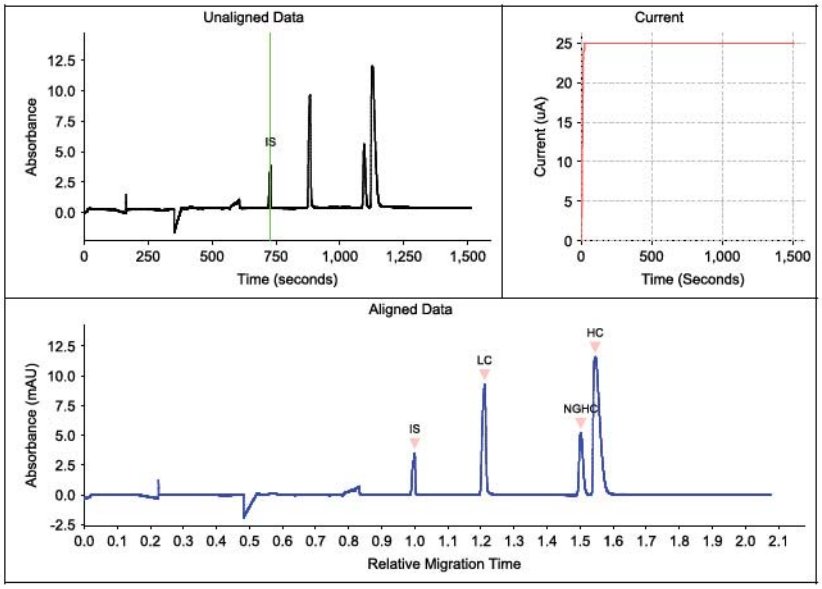
Run 78664 P3 IS 2015-11-30_16-49-49_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS

Analysis Log

Date	User Name	Message	Comment
11/30/2015 4:50 PM		Started run: 78664 P3 IS 2015-11-30_16-49-49_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS_Assay: MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.batch	
12/01/2015 11:19 AM		Saved analysis changes	
		Added Peak Names Apply Settings "apply Internal Standard to all"	
		Added Peak Names Apply Settings "apply IgG-Red to Method1"	
		Added Peak Names Apply Settings "apply MW ladder to Method2"	
		Added Peak Names Group Internal Standard	
		Protein name: IS RMT: 1.0 Color: 32512 Range: 10.0	
		Added Peak Names Group IgG-NR	
		Protein name: IgG RMT: 2.25 Color: 32512 Range: 10.0	
		Protein name: NG-IgG RMT: 2.18 Color: 32512 Range: 10.0	
		Protein name: frag1 RMT: 2.13 Color: 32512 Range: 10.0	
		Protein name: frag2 RMT: 2.07 Color: 32512 Range: 10.0	
		Protein name: frag3 RMT: 2.0 Color: 32512 Range: 10.0	
		Protein name: frag4 RMT: 1.95 Color: 32512 Range: 10.0	
		Protein name: frag5 RMT: 1.92 Color: 32512 Range: 10.0	
		Protein name: frag6 RMT: 1.77 Color: 32512 Range: 10.0	
		Protein name: frag7 RMT: 1.72 Color: 32512 Range: 10.0	
		Protein name: frag8 RMT: 1.57 Color: 32512 Range: 10.0	
		Protein name: frag9 RMT: 1.5 Color: 32512 Range: 10.0	
		Protein name: frag10 RMT: 1.22 Color: 32512 Range: 10.0	
		Added Peak Names Group IgG-Red	
		Protein name: HC RMT: 1.55 Color: 32512 Range: 10.0	
		Protein name: NGHC RMT: 1.5 Color: 32512 Range: 10.0	
		Protein name: LC RMT: 1.2 Color: 32512 Range: 10.0	
		Added Peak Names Group MW ladder	

Created: Thu 3:16 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\MW ladder assigned_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.mbz
Computer: JRichards

Injection 4: IS - Alpha



Peaks

Peak	Name	Time	RMT	MW (kDa)	Height	Raw Area	Area	%Total	%Area	Width	Baseline	Resolution
1	IS	727.0	0.997	10.00	3.5	217	298.4		100.0	7.2	0.4	
2	LC	881.8	1.209	24.61	9.2	762	863.7	30.7	30.7	9.1	0.4	11.21
3	NGHC	1096.3	1.503	55.39	5.2	458	417.7	14.9	14.9	9.3	0.4	13.72
4	HC	1130.4	1.550	63.27	11.6	1731	1530.	54.4	54.4	15.5	0.4	1.61

Created: Thu 1:58 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\MW ladder assigned_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.mbz
Computer: JRichards

Injection 4: IS - Alpha

Sample Information

Sample ID	IS - Alpha
Location	Plate Well B1
Batch Name	78664 P3 IS 2015-11-30_16-49-49_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS
Run Started	Mon 4:50 PM Nov 30, 2015 CST
Run Completed	Tue 10:04 AM Dec 1, 2015 CST
Reinjection	No

Injection Conditions

Focus Period 1	1150V for 0.1 min
Focus Period 2	3450V for 0.1 min
Focus Period 3	5750V for 25.0 min
Sample Load	20 sec 4600 Volts
Tray Temperature	

Maurice Settings

Model	Maurice S.
Instrument S/N	KF0008
Software Version	1.0.15, Build ID: 0222
Firmware Version	2.0.2015.11.13.18.34.39.f6fbaa9
Tray Type	48 vials
Cartridge Type	CE-SDS
Cartridge S/N	3151010185
Cartridge Expiration	Oct 2016
Injections Remaining	3

Created: Thu 1:58 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\MW ladder assigned_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.mbz
Computer: JRichards

Example Analysis and Injection Report: cIEF

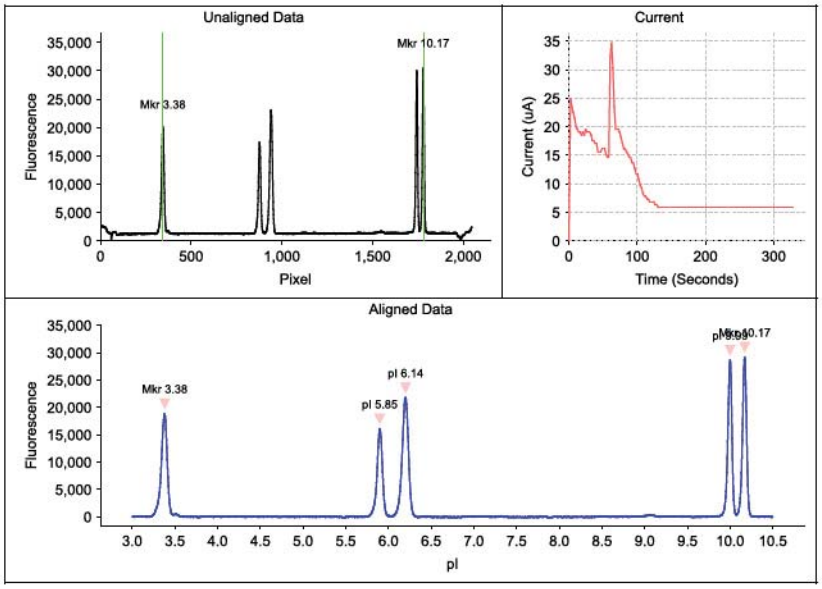
Run 2016-01-21_09-46-39_mAb11_Prep20160121_QC

Analysis Log

Date	User Name	Message	Comment
01/21/2016 9:47 AM		Started run: 2016-01-21_09-46-39_mAb11_Prep20160121_QC Assay: Maurice cIEF.batch	
01/21/2016 12:53 PM		Saved as 2016-01-21_09-46-39_mAb11_Prep20160121_QC(0)	
		Changed Detection: Method from Absorbance to Fluorescence	
01/21/2016 1:11 PM		Saved analysis changes	
		Added Peak Fit Apply Override "apply System Suitability to System Suitability"	
		Added Peak Fit Apply Override "apply mAb 11 to mAb Method"	
		Added Peak Names Apply Settings "apply System Suitability to System Suitablity"	
		Added Peak Names Apply Settings "apply mAb 11 to mAb Method"	
		Added Peak Fit Analysis Settings mAb 11	
		Range Minimum: 6.0	
		Range Maximum: 8.0	
		Range View: Analysis	
		Baseline Threshold: 0.2	
		Baseline Window: 25.0	
		Baseline Stiffness: 1.0	
		Peak Find Threshold: 20.0	
		Peak Find Width: 10.0	
		Peak Find Area Calculation: Dropped Lines	
		Added Peak Names Group System Suitability	
		Protein name: pI 3.38 pI: 3.4 Color: 255 Range: 0.1	
		Protein name: pI 5.85 pI: 6.0 Color: 255 Range: 0.1	
		Protein name: pI 6.14 pI: 6.2 Color: 255 Range: 0.1	
		Protein name: pI 9.99 pI: 10.0 Color: 255 Range: 0.1	
		Protein name: pI 10.17 pI: 10.2 Color: 255 Range: 0.1	
		Added Peak Names Group mAb 11	
		Protein name: Peak1 pI: 6.55 Color: 255 Range: 0.1	

Created: Thu 2:02 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\2016-01-21_09-46-39_mAb11_Prep20160121_QC(0).mbz
Computer: JRichards

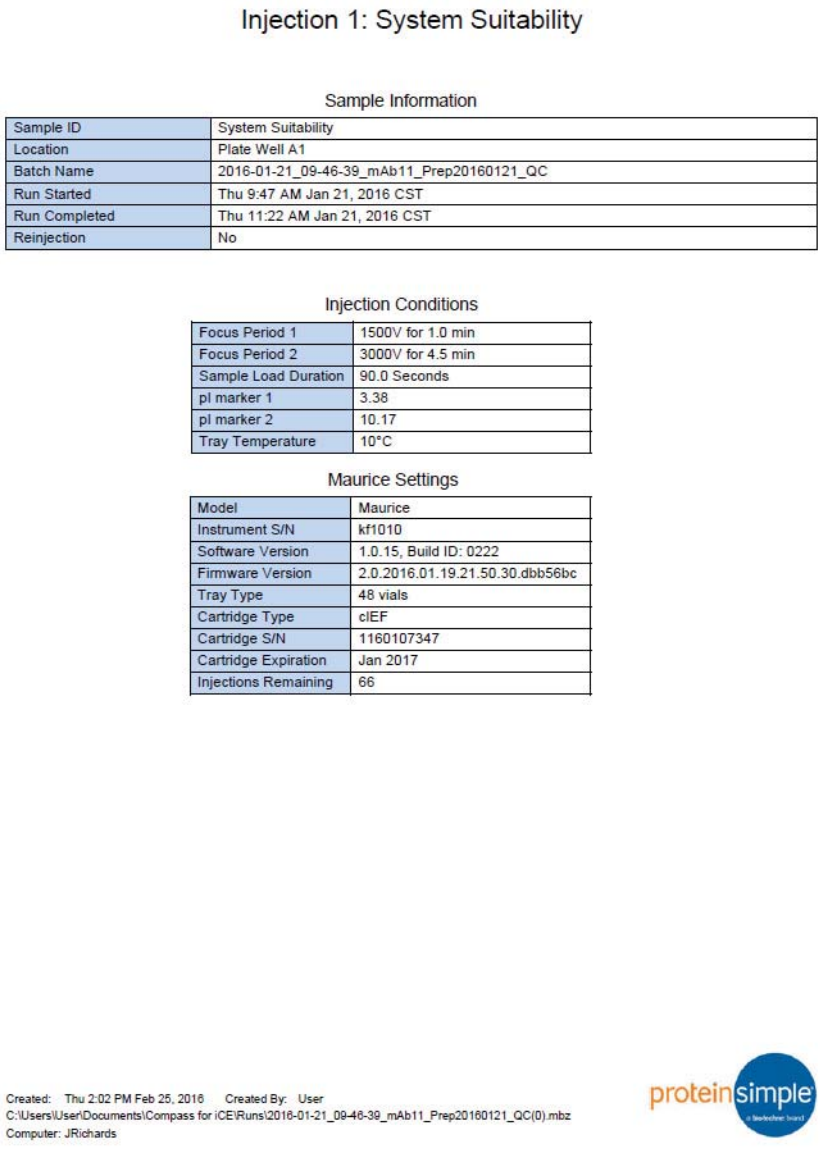
Injection 1: System Suitability



Peaks

Peak	Name	Position	pI	Height	Area	%Total	%Area	Width	Baseline	Resolution
1	Mkr 3.38	344	3.380	18510.8	315487		19.3	0.0757	-1331.2	
2	pI 5.85	877	5.899	15831.0	243987	25.1	14.9	0.0685	-1283.2	20.59
3	pI 6.14	941	6.198	21741.0	394316	40.5	24.1	0.0806	-1277.4	2.36
4	pI 9.99	1744	9.998	28505.6	334653	34.4	20.5	0.0522	-1205.0	33.69
5	Mkr 10.17	1780	10.170	28991.0	344549		21.1	0.0528	-1201.7	1.92

Created: Thu 2:02 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\2016-01-21_09-46-39_mAb11_Prep20160121_QC(0).mbz
Computer: JRichards



Injection 1: System Suitability

Sample Information

Sample ID	System Suitability
Location	Plate Well A1
Batch Name	2016-01-21_09-46-39_mAb11_Prep20160121_QC
Run Started	Thu 9:47 AM Jan 21, 2016 CST
Run Completed	Thu 11:22 AM Jan 21, 2016 CST
Reinjection	No

Injection Conditions

Focus Period 1	1500V for 1.0 min
Focus Period 2	3000V for 4.5 min
Sample Load Duration	90.0 Seconds
pI marker 1	3.38
pI marker 2	10.17
Tray Temperature	10°C

Maurice Settings

Model	Maurice
Instrument S/N	kf1010
Software Version	1.0.15, Build ID: 0222
Firmware Version	2.0.2016.01.19.21.50.30.dbb56bc
Tray Type	48 vials
Cartridge Type	cIEF
Cartridge S/N	1160107347
Cartridge Expiration	Jan 2017
Injections Remaining	66

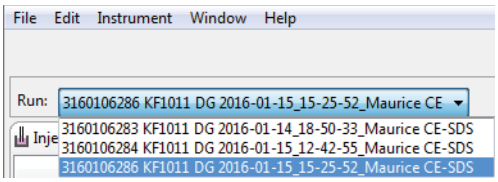
Created: Thu 2:02 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\2016-01-21_09-46-39_mAb11_Prep20160121_QC(0).mbz
Computer: JRichards

proteinsimple

Switching Between Open Run Files

If you've got more than one run file open, you can switch between viewing the run information in each.

1. Click the down arrow in the Run box.



2. Select the run you want to view from the drop down list.

Closing Run Files

If you've got more than one run file open, you can close just one file or all the open files at the same time.

- **To close the run file being viewed** - Select **File** from the main menu and click **Close**.
- **To close all open run files** - Select **File** from the main menu and click **Close All**.

Chapter 10:

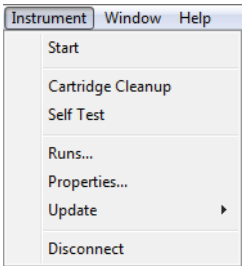
Controlling Maurice, Maurice C. and Maurice S.

Chapter Overview

- Instrument Control
- Stopping a Run
- Status Modes
- Instrument Software (Embedded) Updates
- Self Test
- Viewing and Changing System Properties
- Checking Cartridge Status
- Viewing Log Files

Instrument Control

The Instrument menu lets you to control Maurice, Maurice C. and Maurice S.



NOTE: Instrument menu options are only active when you've got a computer with Compass for iCE software connected directly to your Maurice system.

Starting a Run

To start your run, click the **Start** button in the Batch screen. You can also start a run by selecting **Instrument** in the main menu and clicking **Start**. For more info on creating and starting batches check out Chapter 7, *"Running cIEF Applications on Maurice and Maurice C."* or Chapter 8, *"Running CE-SDS Applications on Maurice and Maurice S."*

Cleaning

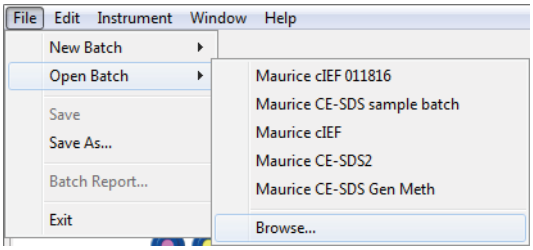
Cartridge Cleanup (CE-SDS Cartridges Only)

If you've still got injections left after your last run and you won't use the cartridge again within 2 hours, you'll need to run a clean up and store it. Check out page 137 for the details on how to do that.

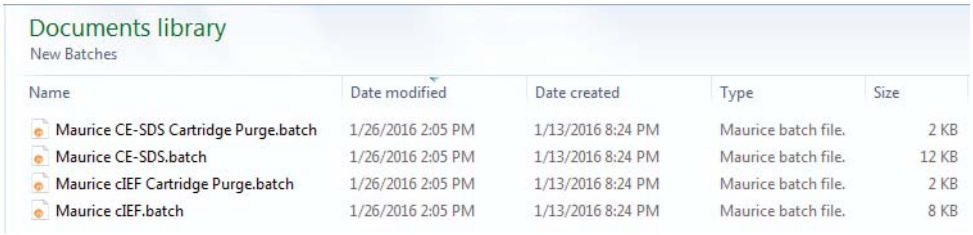
Cartridge Purge

You'll want to run the Cartridge Purge any time you have to stop a run manually or if the run stops because of an error. This runs the Cleanup step that normally happens at the end of a batch. It flushes the cartridge of any reagents and samples so it's ready to go for the next run.

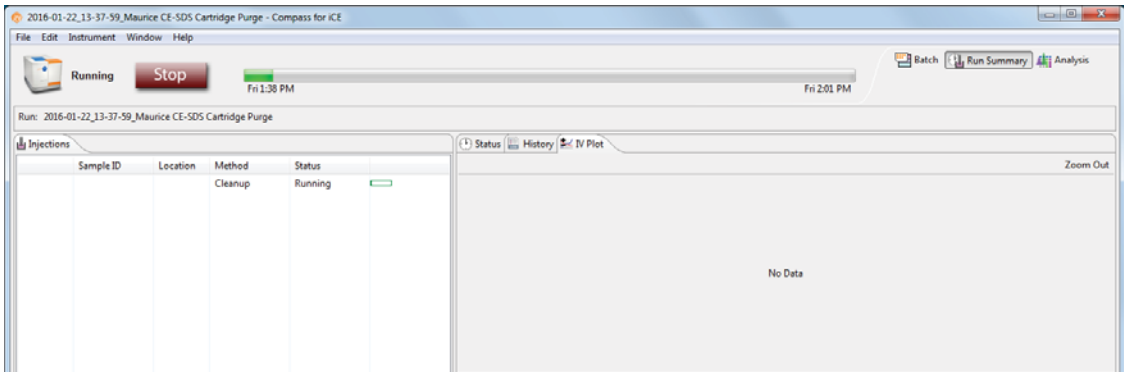
1. In the Batch screen, select **File** > **Open Batch** and click **Browse**.

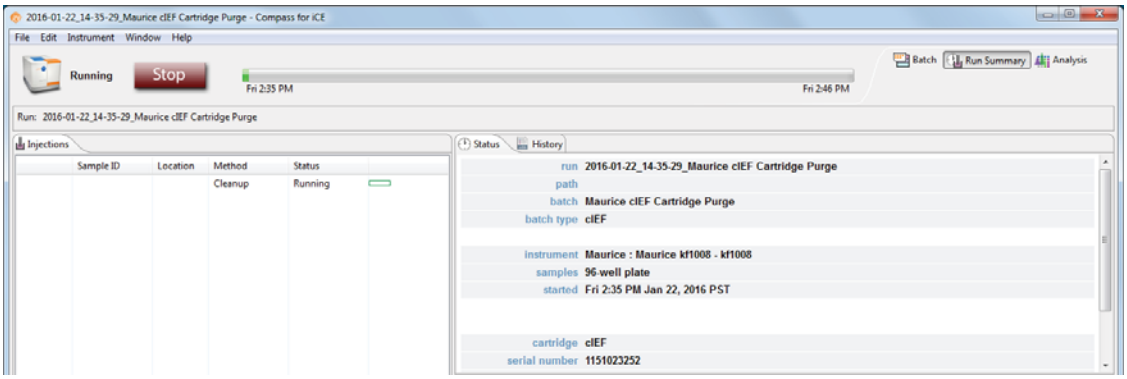


2. Go to the New Batches folder and select either **Maurice cIEF Cartridge Purge** or **Maurice CE-SDS Cartridge Purge**, depending on what cartridge you're using.



3. After the purge batch loads, just click **Start**. The CE-SDS Cartridge purge takes about 25 minutes, and the cIEF one takes a little over 10 minutes.





4. Once the purge is done, if you'll be starting a new run:

   - **cIEF Cartridges:** If you've still got injections left and the cartridge will be used again within 24 hours, you don't need to do anything. Just leave the cartridge in Maurice.
   - **CE-SDS Cartridges:** If you've still got injections left and the cartridge will be used again within 2 hours, you'll just need to put in a new Top Running Buffer vial in the cartridge insert.

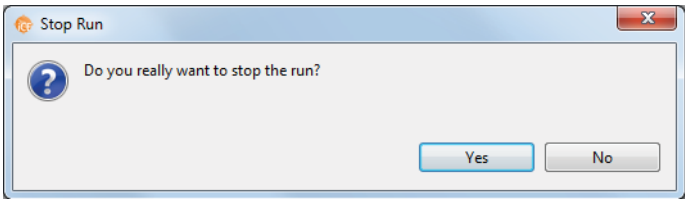
   If you won't be starting a new run:

   - **cIEF Cartridges:** Follow the steps in "Post-batch Procedures" on page 102.
   - **CE-SDS Cartridges:** Follow the steps in "Post-batch Procedures" on page 135.

Stopping a Run

1. Click **Stop**.

2. Click **Yes** in the pop-up window.



3. When the run stops, run the "Cartridge Purge" on page 178.
4. Once the purge is done:

   If you'll be starting a new run:

   - **cIEF Cartridges:** If you've still got injections left and the cartridge will be used again within 24 hours, you don't need to do anything. Just leave the cartridge in Maurice.
   - **CE-SDS Cartridges:** If you've still got injections left and the cartridge will be used again within 2 hours, you don't need to do anything other than prepare the cartridge for the next batch as described "Step 2: Prep the Cartridge" on page 120.

   If you won't be starting a new run:

   - **cIEF Cartridges:** Follow the steps in "Post-batch Procedures" on page 102.
   - **CE-SDS Cartridges:** Follow the steps in "Post-batch Procedures" on page 135.

Status Modes

The instrument status bar displays status, buttons and progress bars depending on what Maurice, Maurice C. or Maurice S. are doing.

- **Ready/Start button** - The instrument is ready and a batch is loaded. Click **Start** to begin a run.
- **Not Ready/Reset button** - The instrument isn't ready and needs to reinitialize. Click **Reset** to start the initialization protocol.
- **Running/Stop button** - The instrument is running. The run name, time it started and when it will be done show in the run progress bar. Click **Stop** to stop the run.
- **Cleaning/Stop button** - The instrument is running a cleaning protocol. The time the cleaning protocol started and when it will be done show in the run progress bar.
- **Error/Reset button** - There's an error. Go to the **Status** pane in the **Run Summary** screen to view details. When you've fixed the source of the error, click **Reset**.

Shutdown

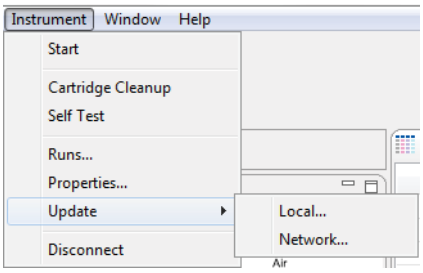
Close Compass for iCE software. Maurice can stay on unless he won't be used for an extended period.

Instrument Software (Embedded) Updates

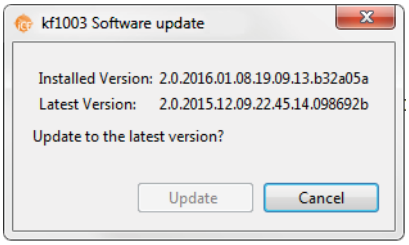
To check for embedded software updates:

If you're on the network:

1. Select **Instrument > Update**, then select **Network**.

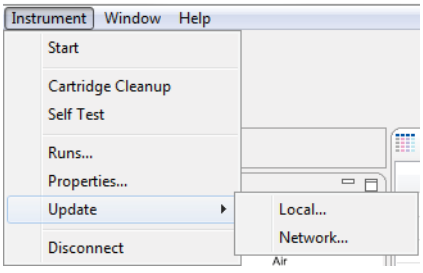


2. The following screen displays. Click **Update**.

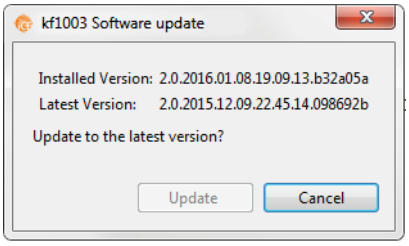


If you're not on the network:

1. Call ProteinSimple Technical Support or your FAS for assistance on getting the latest update.
2. Copy the new embedded software file onto Maurice's computer.
3. Select **Instrument > Update**, then select **Local**.



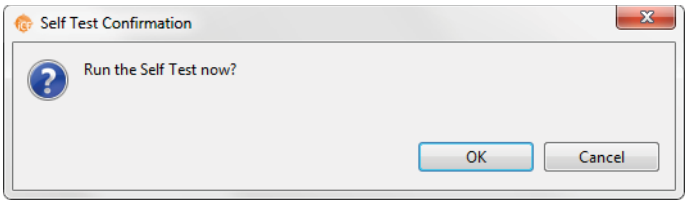
4. Browse to the location of the embedded software file, select it and click **OK**.
5. The following screen displays. Click **Update**.



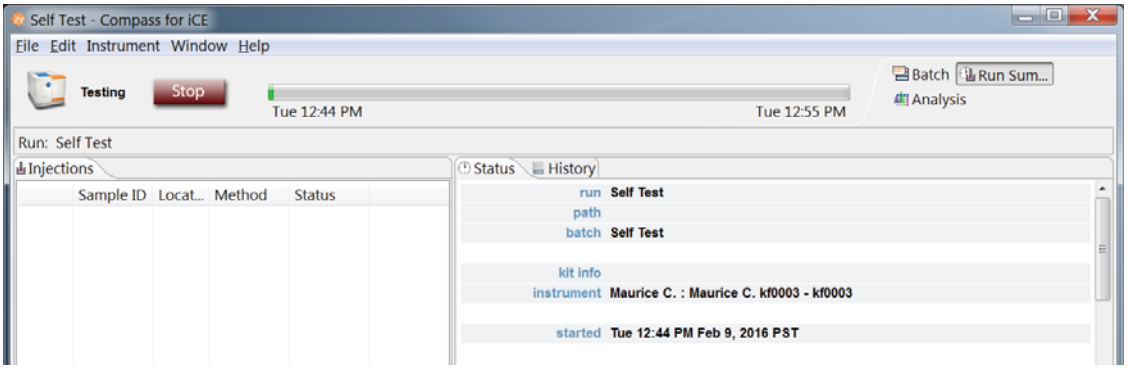
Self Test

Maurice, Maurice C. and Maurice S. can run a series of self tests for you to make sure they're operating properly.

1. To start the test, select **Instrument > Self Test**.
2. The following screen displays. Click **OK**.



The test takes approximately 11 minutes.



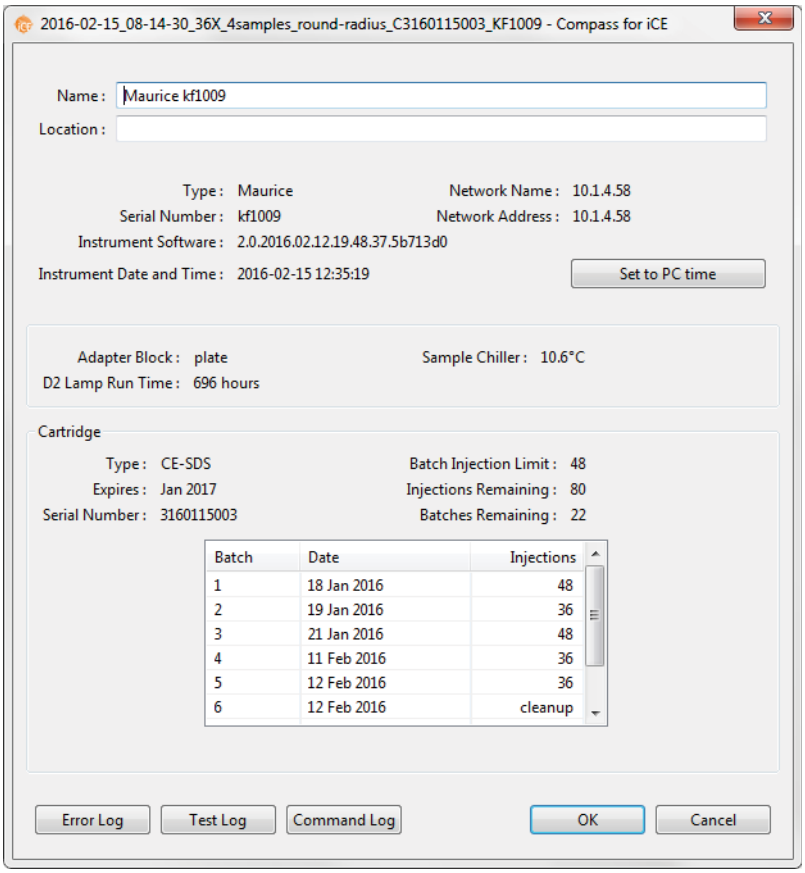
NOTE: We recommend running the self test before you start a run.

To view the results when the test's done, select **Instrument** > **Properties** and click **Test Log**. See "Self Test Logs" on page 192 for more info.

Viewing and Changing System Properties

Selecting **Instrument** > **Properties** displays your system properties. They include:

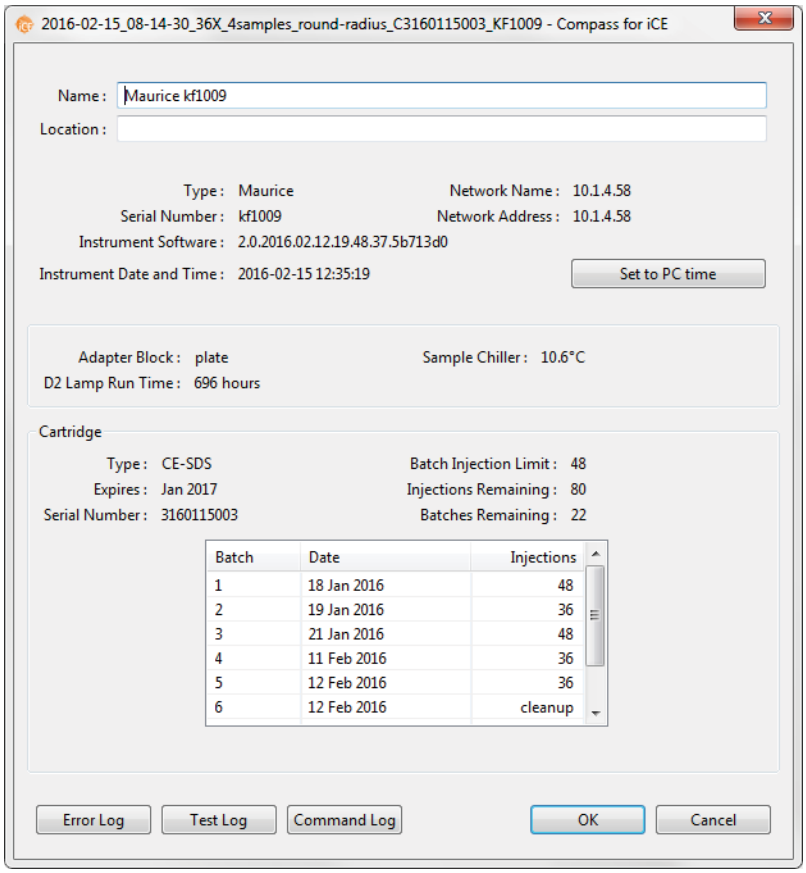
- System Name
- System Location
- Instrument Type
- Serial number
- Instrument software version (firmware)
- Network name and address
- Date and time of the instrument clock
- Adapter block currently in use
- Number of hours on the Deuterium (UV) lamp
- Current sample chiller temperature



- **To change the system name or location:** Click in the name or location boxes and enter your new info, then click **OK**.
- **To sync the instrument clock with the computer:** Click **Set to PC time**.

Checking Cartridge Status

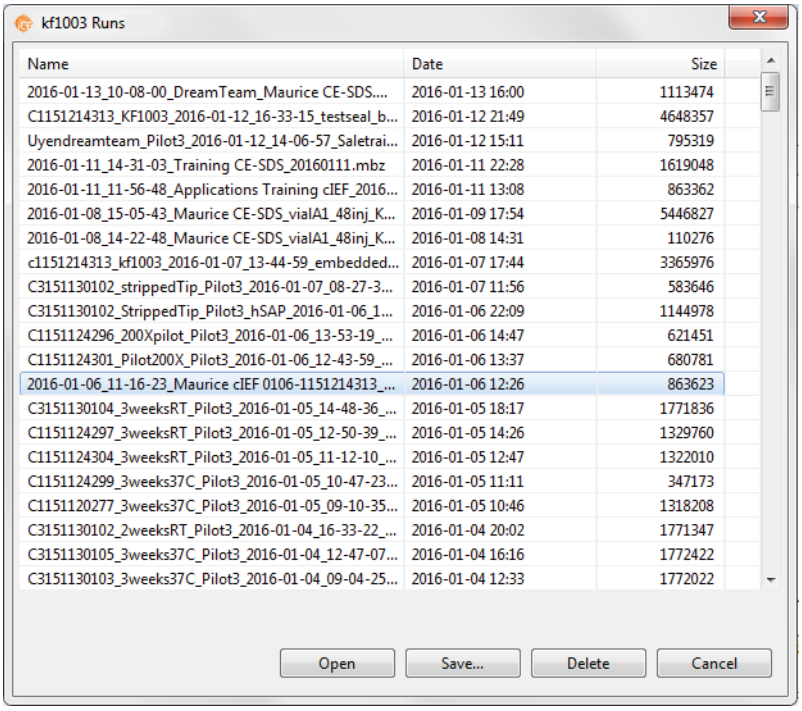
If you've got a cartridge installed in the system, you can see its serial number, the injections and batches it still has available, and a history of batches and injections its run to date. To view this info, select **Instrument** > **Properties**.



Viewing Log Files

Runs Log

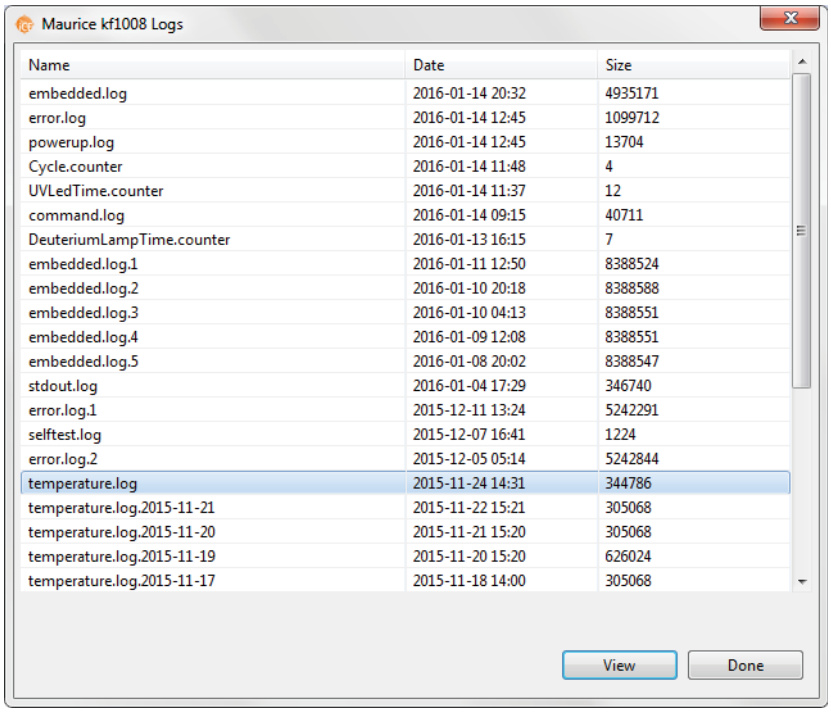
To see a history of all runs your system has performed, select **Instrument** > **Runs**:



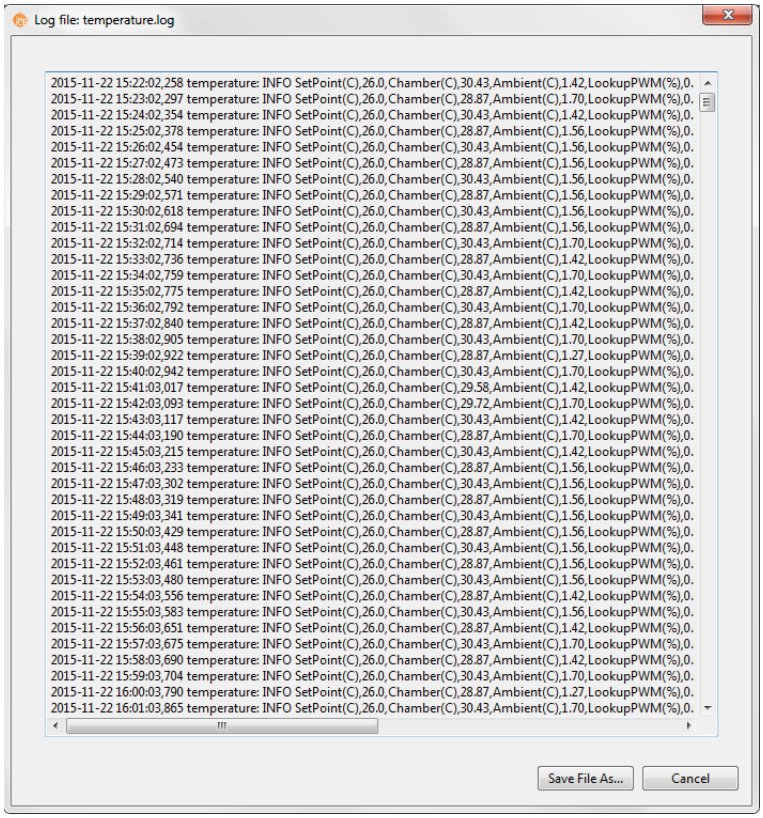
- **To open a run file:** Select a run file from the list and click **Open**.
- **To save a run file:** Select a run file from the list and click **Save**. This lets you save a copy of a completed run or one in progress to either a USB drive or the local computer.
- **To delete a run file:** Select a run file from the list and click **Delete**. The run file will be deleted from the history and from the Run file in the Compass for iCE directory.

System Logs

1. Select **Instrument** > **Properties** to display your system's properties.
2. Click **Error Log**. A list of system logs displays:



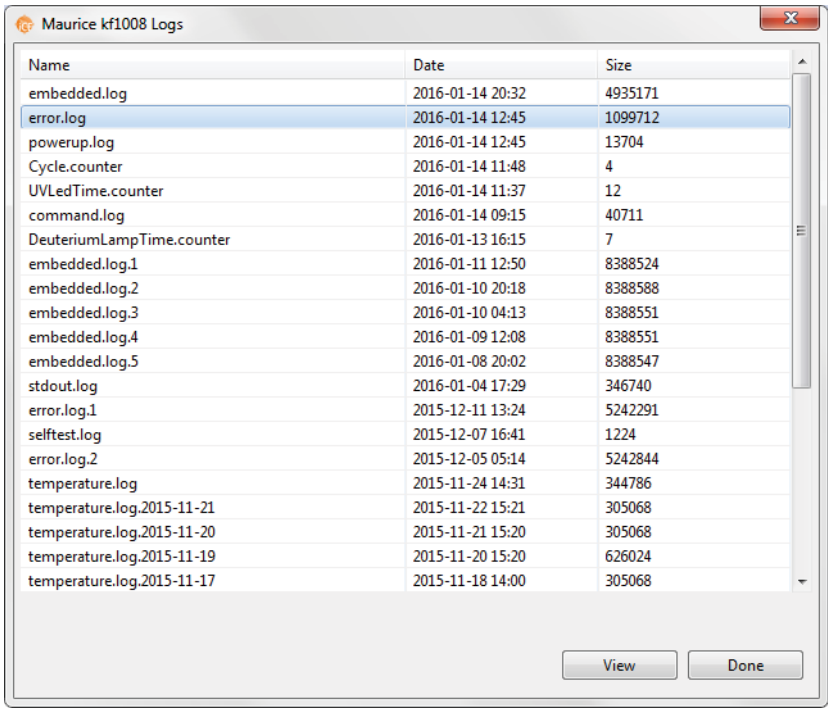
3. To view a log, select it in the list and click **View**.



4. Click **Save File As** to save a copy of the log file.

Error Log

1. Select **Instrument** > **Properties** to display your system's properties.
2. Click **Error Log**. A list of system logs displays:

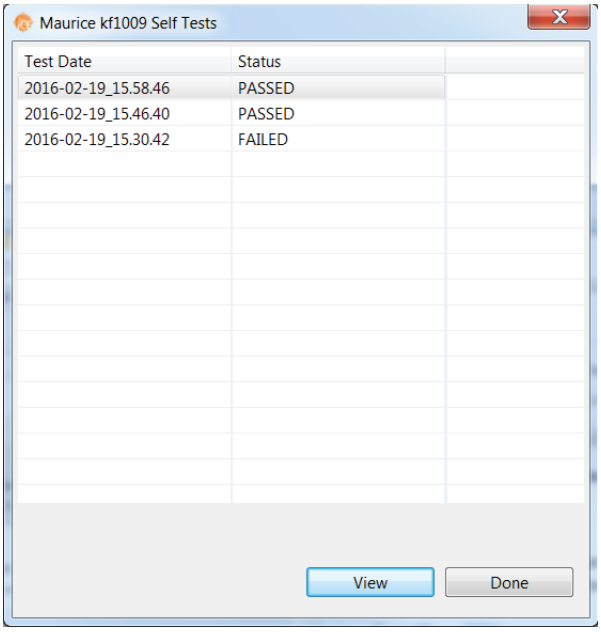


3. Select the **error.log** you're interested in from the list and click **View**.

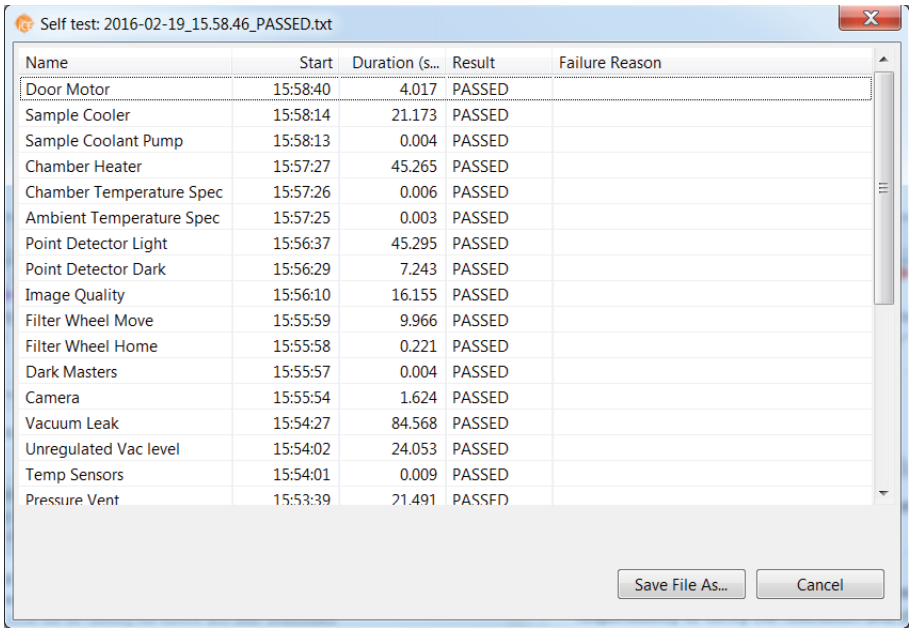
4. Click **Save File As** to save a copy of the log file.

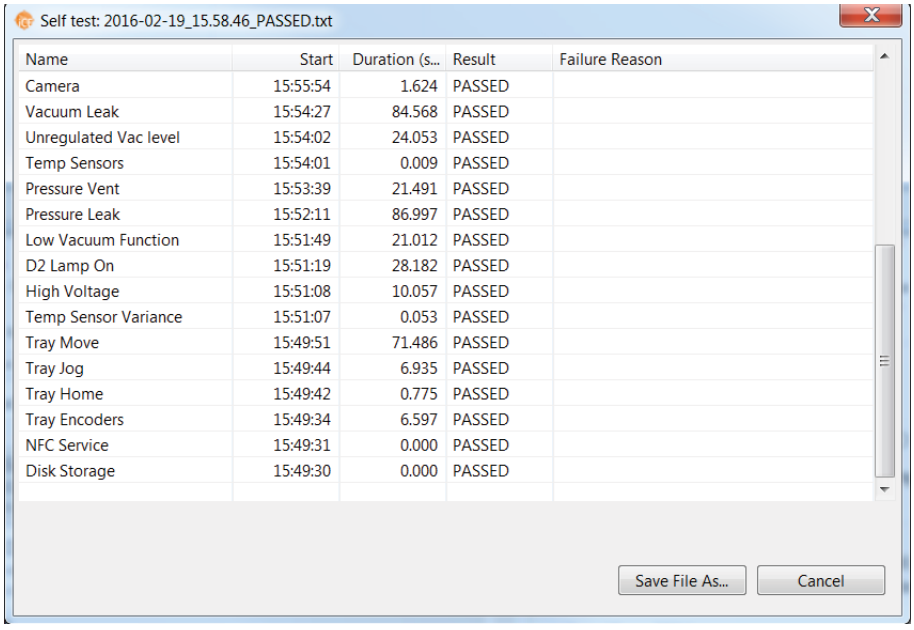
Self Test Logs

1. Select **Instrument** > **Properties**.
2. Click **Test Log**. A list of dates each self test was run displays:



3. Select a test date in the list and click **View** to see the individual test results:

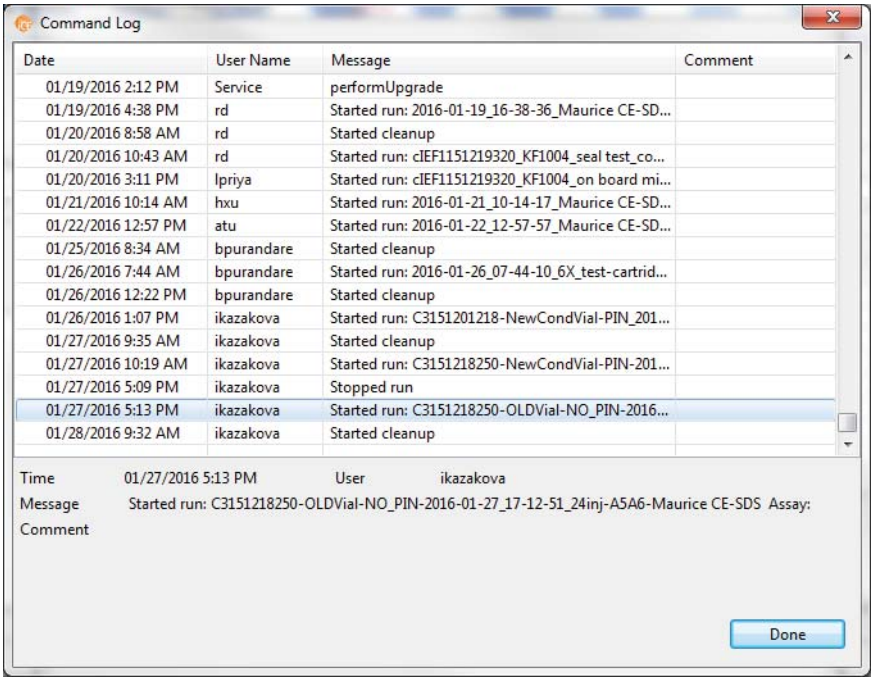




4. Click **Save File As** to save a copy of the test log file.

Command Log

1. Select **Instrument** > **Properties** to display your system's properties.
2. Click **Command Log**. A list of system commands displays:



Chapter 11:

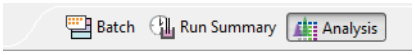
CE-SDS Data Analysis

Chapter Overview

- Analysis Screen Overview
- Opening Run Files
- How Run Data is Displayed
- Viewing Run Data
- Data Notifications and Warnings
- Checking Your Results
- Group Statistics
- Copying Results Tables and Graphs
- Exporting Run Files
- Changing Sample Protein Identification
- Changing the Electropherogram View
- Closing Run Files
- Analysis Settings Overview
- Advanced Analysis Settings
- Markers Analysis Settings
- Peak Fit Analysis Settings
- Peak Names Settings
- Injection Reports
- Importing and Exporting Analysis Settings

Analysis Screen Overview

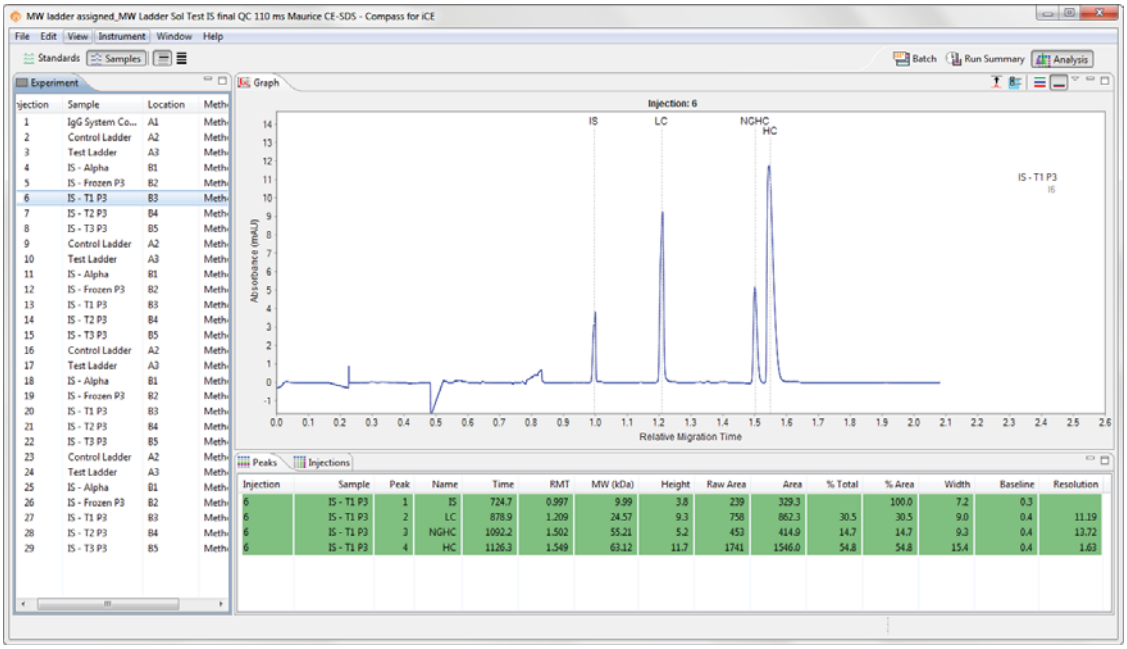
You can use the Analysis screen to view electropherograms and tabulated results for your injections. If any post-run analysis is needed, you can do it here too. To get to this screen, click the **Analysis** screen tab:



Analysis Screen Panes

The Analysis screen has four panes:

- **Experiment** - Lists the injection number, sample IDs, sample locations and methods for each injection in the run and lets you get a quick view of method parameters.
- **Graph** - Displays the electropherograms for sample proteins or standards.
- **Peaks** - Shows the tabulated results for sample proteins, internal standards and CE-SDS MW Markers.
- **Injections** - Displays a list of the sample proteins Compass for iCE names automatically using the user-defined peak name analysis parameters.



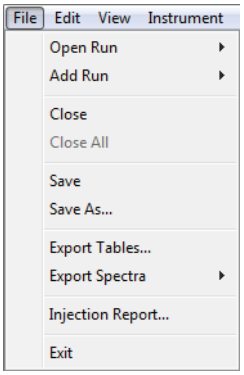
Software Menus Active in the Analysis Screen

These main menu items are active in the Analysis Screen:

- File
- Edit
- View
- Instrument (when Compass for iCE is connected to Maurice, Maurice C. or Maurice S.)
- Window
- Help

File Menu

These File menu options are active:

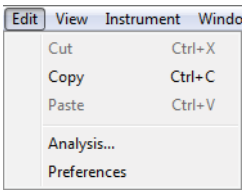


- **Open Run** - Opens a run file.
- **Add Run** - Lets you open and view other run files besides the one that's already open.
- **Close** - Closes the run file currently being viewed.
- **Close All** - Closes all open run files.
- **Save/Save As** - If you made changes in the Analysis screen before you went to the Run Summary screen, this saves your changes to the run file.
- **Export Tables** - Exports the results for all injections in the run in .txt format.
- **Export Spectra** - Exports the raw and analyzed data traces and background for each injection in the run in .txt or .cdf format.
- **Injection Report** - Exports the raw and analyzed data, IV plot, peaks table, sample and system info for individual injections as PDF files. You can also export the run history with all analysis events.

- **Exit** - Closes Compass for iCE.

Edit Menu

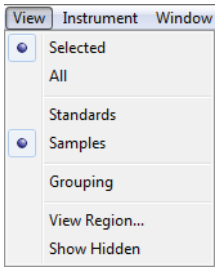
These Edit menu options are active:



- **Copy** - Copies the information in the History pane so you can paste it into other documents.
- **Analysis** - Displays the analysis settings used to analyze the run data and lets you change them as needed. See "Analysis Settings Overview" on page 244 for more information.
- **Preferences** - Lets you set and save your preferences for data export, graph colors, grouped data and Twitter settings. See Chapter 13, *"Setting Your Preferences"* for more information.

View Menu

These View menu options are active:



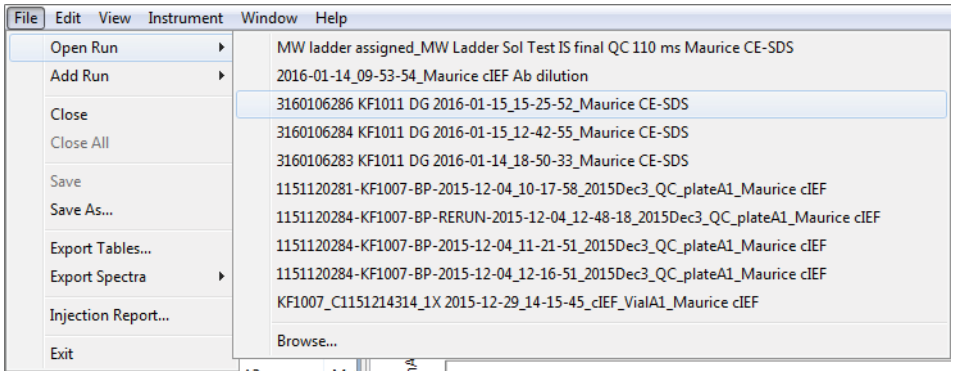
- **Single View** - Displays the data for only the injections selected.
- **Multiple View** - Displays data for all injections so you can scroll through them.
- **Standards** - Lets you view data just for the internal standards in your injections.
- **Samples** - Lets you view data just for sample proteins in your injections.
- **Grouping** - Displays data for injection groups.
- **View Region** - Lets you change the x-axis range of the data displayed.
- **Show Hidden**- Shows injections that are hidden from the data view.

Opening Run Files

You can open one run file or multiple files at the same time to compare information between runs.

Opening One Run File

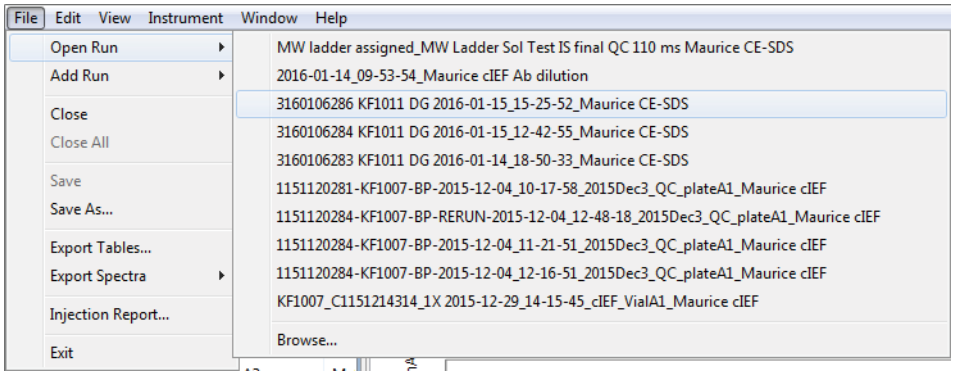
1. Select **File** in the main menu and click **Open Run**.



2. A list of the last 10 runs opened will display. Select one of these runs or click **Browse** to open the Runs folder and select a different file.

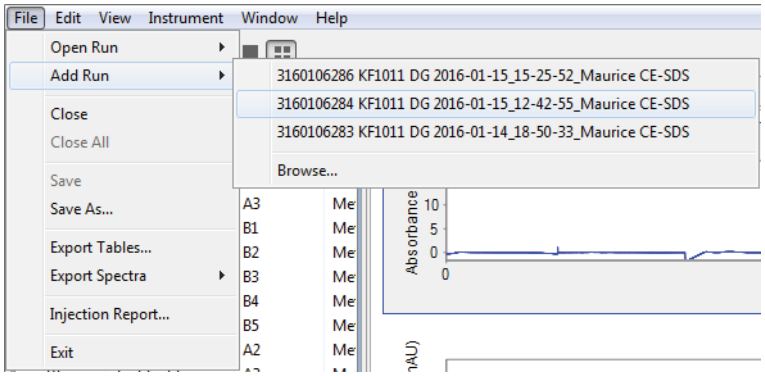
Opening Multiple Run Files

1. To open the first run file, select **File** in the main menu and click **Open Run**.



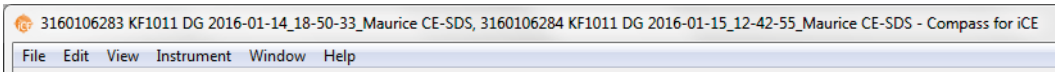
2. A list of the last 10 runs opened will display. Select one of these runs or click **Browse** to open the Runs folder and select a different file.

3. To open another run file, select **File** in the main menu and click **Add Run**.



4. A list of CE-SDS runs will display. Select one of these runs or click **Browse** to open the Runs folder and select a different file.

   When a run is added, its data appends to the open run file and displays as a second set of injections in all screen panes. The second run file name also appears in the title bar:



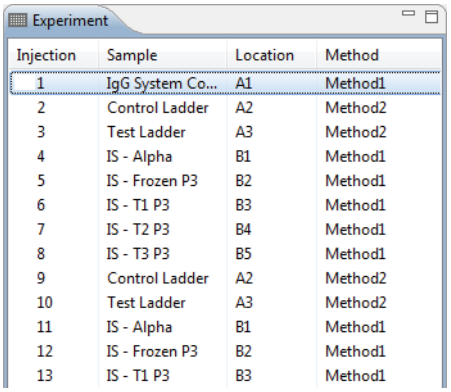
5. Repeat the last two steps to add additional runs.

How Run Data is Displayed

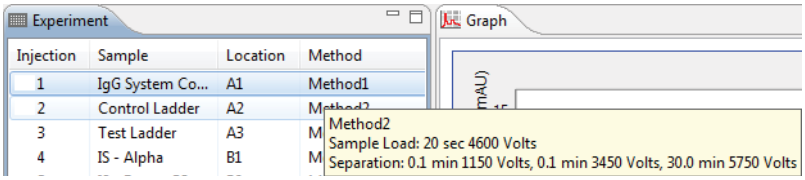
Data in the run file is organized for easy review.

Experiment Pane: Batch Injection Information

The Experiment pane lists all the injections performed in the run, which samples were used for each, the sample location in the 96-well plate or 48-vial tray and the method used.



- **To view all columns** - Use the scroll bar or click **Maximize** in the upper right corner.
- **To resize columns** - Roll the mouse over a column border until the sizing arrow appears, then click and drag to resize.
- **To view method parameters** - Hover the mouse over a method name.

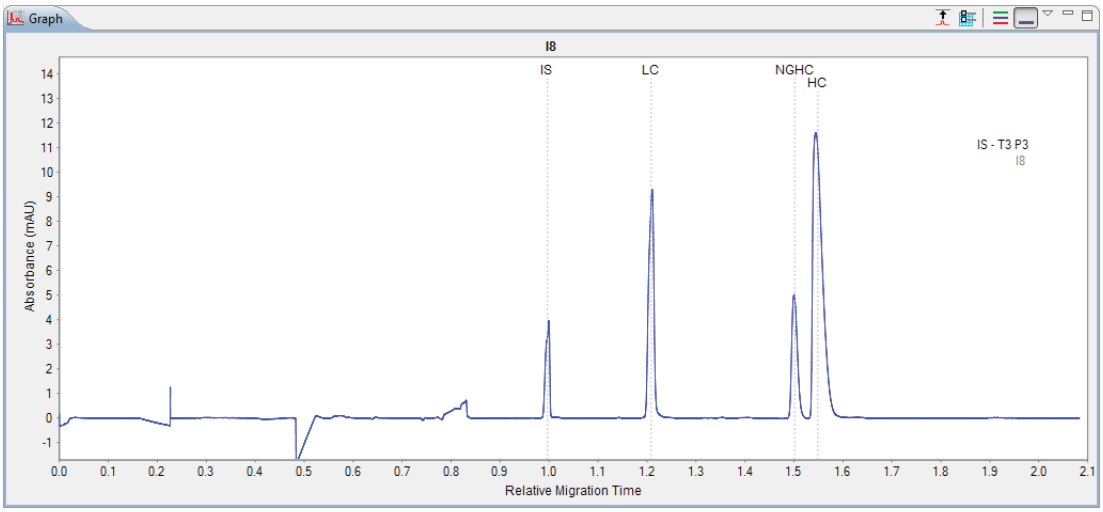


NOTE: Data notification icons will display in the Injection column if Compass for iCE detects a potential analysis issue or data was manually modified by the user. For more information see "Data Notifications and Warnings" on page 214.

Graph Pane: Electropherogram Data

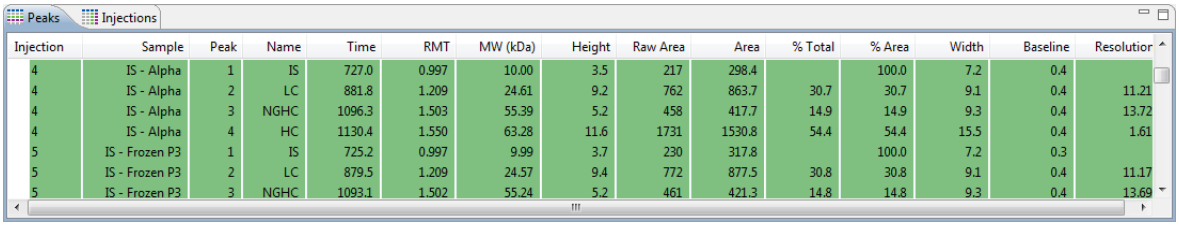
The Graph pane displays the electropherogram(s) for sample proteins or internal standards depending on the view options you've selected.

You can get more info on graph view options in "Changing the Electropherogram View" on page 226.



Peaks Pane: Calculated Results

The Peaks pane shows the tabulated results for your sample proteins or internal standards. Each row in the table has the individual results for each peak detected in an injection. Results shown will either be for one injection or multiple injections, samples or standards depending on the view options you're using. Check out "Viewing Run Data" on page 205 for more info.



Injection	Sample	Peak	Name	Time	RMT	MW (kDa)	Height	Raw Area	Area	% Total	% Area	Width	Baseline	Resolution
4	IS - Alpha	1	IS	727.0	0.997	10.00	3.5	217	298.4		100.0	7.2	0.4	
4	IS - Alpha	2	LC	881.8	1.209	24.61	9.2	762	863.7	30.7	30.7	9.1	0.4	11.21
4	IS - Alpha	3	NGHC	1096.3	1.503	55.39	5.2	458	417.7	14.9	14.9	9.3	0.4	13.72
4	IS - Alpha	4	HC	1130.4	1.550	63.28	11.6	1731	1530.8	54.4	54.4	15.5	0.4	1.61
5	IS - Frozen P3	1	IS	725.2	0.997	9.99	3.7	230	317.8		100.0	7.2	0.3	
5	IS - Frozen P3	2	LC	879.5	1.209	24.57	9.4	772	877.5	30.8	30.8	9.1	0.4	11.17
5	IS - Frozen P3	3	NGHC	1093.1	1.502	55.24	5.2	461	421.3	14.8	14.8	9.3	0.4	13.69

NOTES:

Peaks that Compass for iCE names automatically with user-defined peak name settings are color-coded.

When the Standards view is selected, the information in the Peaks table includes only injection, sample, peak, time and height. Internal standards the software has identified are marked with an ***S****.*

- **To view all rows** - Use the scroll bar or click **Maximize** in the upper right corner.

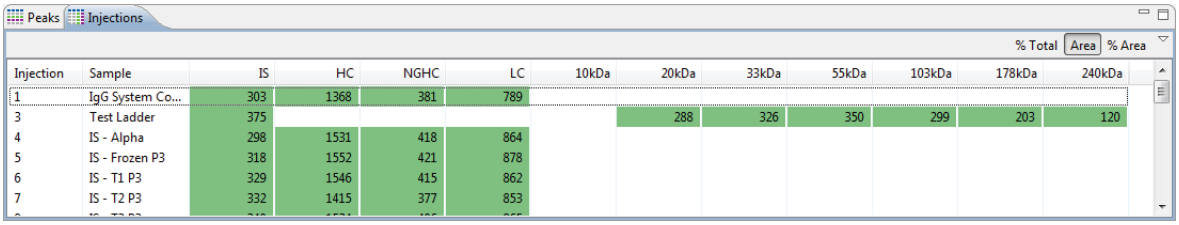
- **To resize columns** - Roll the mouse over a column border until the sizing arrow appears, then click and drag to resize.

The following results and info are listed in the Peaks table:

- **Injection** - Injection number.
- **Sample** - If sample names were entered in the batch, those names will display here. Otherwise, Sample (default name) will display.
- **Peak** - Peaks are numbered in order of detection.
- **Name** - Displays peaks Compass for iCE named automatically using the user-defined peak name analysis parameters. These cells are blank if the software wasn't able to name the peak or if you didn't enter naming parameters.
- **Time** - Peak detection time (seconds). This is the elapsed time between the start of the separation and when the peak is detected.
- **RMT** - Relative migration time of the peak to the Internal Standard which has an RMT of 1.0.
- **MW (kDa)** - Displays the relative molecular weight in kDa for sample peaks. MW only displays if you've run the CE-SDS MW Markers as one of the injections in the run and identified that injection in your analysis parameters.
- **Height** - The calculated peak height.
- **Raw Area** - Displays the uncorrected peak area.
- **Area** - Displays the time-corrected peak area. This includes corrections for big and/or slow moving peaks which can be artificially large when uncorrected.
- **% Total** - Displays the peak area ratio compared to the sum of all peak areas (excluding the Internal Standard peak). This value results from dividing the individual peak area by the sum of all peak areas for the injection and multiplying by 100.
- **% Area** - Displays the calculated percent area for the named peak compared to all named peaks. This value results from dividing the individual peak area by the sum of all named peak areas for the injection and multiplying by 100 (shown for named peak sample data only).
- **Width** - Displays the calculated peak width (sample data only).
- **Baseline** - Displays the raw baseline signal of each peak.
- **Resolution** - Displays resolution of the peak compared to neighboring peaks. Two peaks that are baseline resolved will have a resolution value of 1.5. Smaller values means the peaks are not completely resolved, larger values mean the peaks are fully resolved.

Injections Pane: User-Specified Peak Names

The Injections pane shows tabulated results for sample proteins Compass for iCE labels automatically using user-defined peak name settings. Each row in the table shows the individual results for the named peaks detected in each injection.



Injection	Sample	IS	HC	NGHC	LC	10kDa	20kDa	33kDa	55kDa	103kDa	178kDa	240kDa
1	IgG System Co...	303	1368	381	789							
3	Test Ladder	375					288	326	350	299	203	120
4	IS - Alpha	298	1531	418	864							
5	IS - Frozen P3	318	1552	421	878							
6	IS - T1 P3	329	1546	415	862							
7	IS - T2 P3	332	1415	377	853							

NOTES:
Peaks that Compass for iCE names automatically with user-defined peak name settings are color-coded.

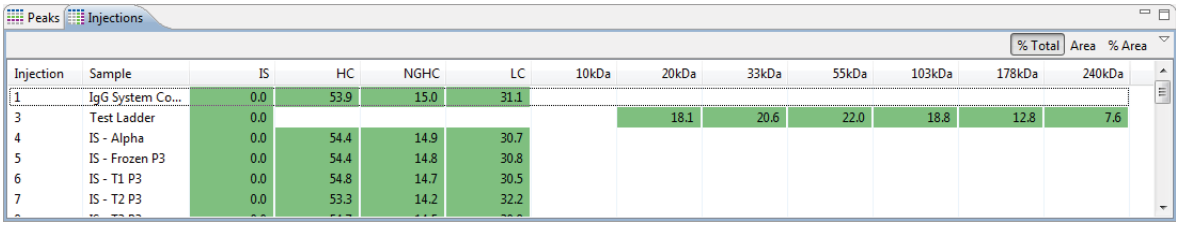
When the Standards view is selected, the information in the Injections table includes only injection, sample and std 1 (the migration time of the standard peak).

- **To view all rows** - Use the scroll bar or click **Maximize** in the upper right corner.
- **To resize columns** - Roll the mouse over a column border until the sizing arrow appears, then click and drag to resize.

The following results and info are listed in the Injections table:

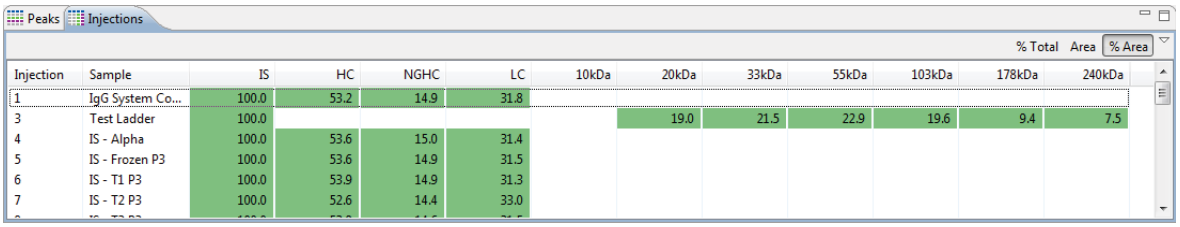
- **Injection** - Injection number.
- **Sample** - If sample names were entered in the batch, those names will display here. Otherwise, Sample (default name) will display.
- **Peak Name Columns** - An individual column per peak name will display for every peak identified by name or as a MW Marker peak in the run data. Cells for injections in these columns will be blank if Compass for iCE didn't find peaks automatically using the user-defined peak name analysis and maker parameters (or none were entered).
  - **To view peak area in the peak name columns (default)** - Select **Area** in the upper right corner of the pane. This displays calculated peak area for the individual peak only.
  - **To view % total in the peak name columns** - This displays the calculated percent area for the named peak compared to all named peaks. This value results from dividing the individual peak area by the sum of all named peak areas for the injection and multiplying by 100.

NOTE: The sum of the named peak percentages can be less than 100% if some peaks aren't named.



Injection	Sample	IS	HC	NGHC	LC	10kDa	20kDa	33kDa	55kDa	103kDa	178kDa	240kDa
1	IgG System Co...	0.0	53.9	15.0	31.1							
3	Test Ladder	0.0					18.1	20.6	22.0	18.8	12.8	7.6
4	IS - Alpha	0.0	54.4	14.9	30.7							
5	IS - Frozen P3	0.0	54.4	14.8	30.8							
6	IS - T1 P3	0.0	54.8	14.7	30.5							
7	IS - T2 P3	0.0	53.3	14.2	32.2							

- **To view % area in the peak name columns** - This displays the peak area ratio compared to the sum of all named peak areas. This value results from dividing the individual peak area by the sum of all peak areas for the injection and multiplying by 100.



Injection	Sample	IS	HC	NGHC	LC	10kDa	20kDa	33kDa	55kDa	103kDa	178kDa	240kDa
1	IgG System Co...	100.0	53.2	14.9	31.8							
3	Test Ladder	100.0					19.0	21.5	22.9	19.6	9.4	7.5
4	IS - Alpha	100.0	53.6	15.0	31.4							
5	IS - Frozen P3	100.0	53.6	14.9	31.5							
6	IS - T1 P3	100.0	53.9	14.9	31.3							
7	IS - T2 P3	100.0	52.6	14.4	33.0							

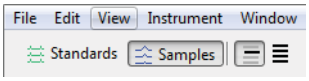
Viewing Run Data

The Analysis screen lets you view data for just one injection, specific injections or all injections in the run. Each run file has data for the sample proteins and the Internal Standard detected in each injection.

Switching Between Samples and Standards Data Views

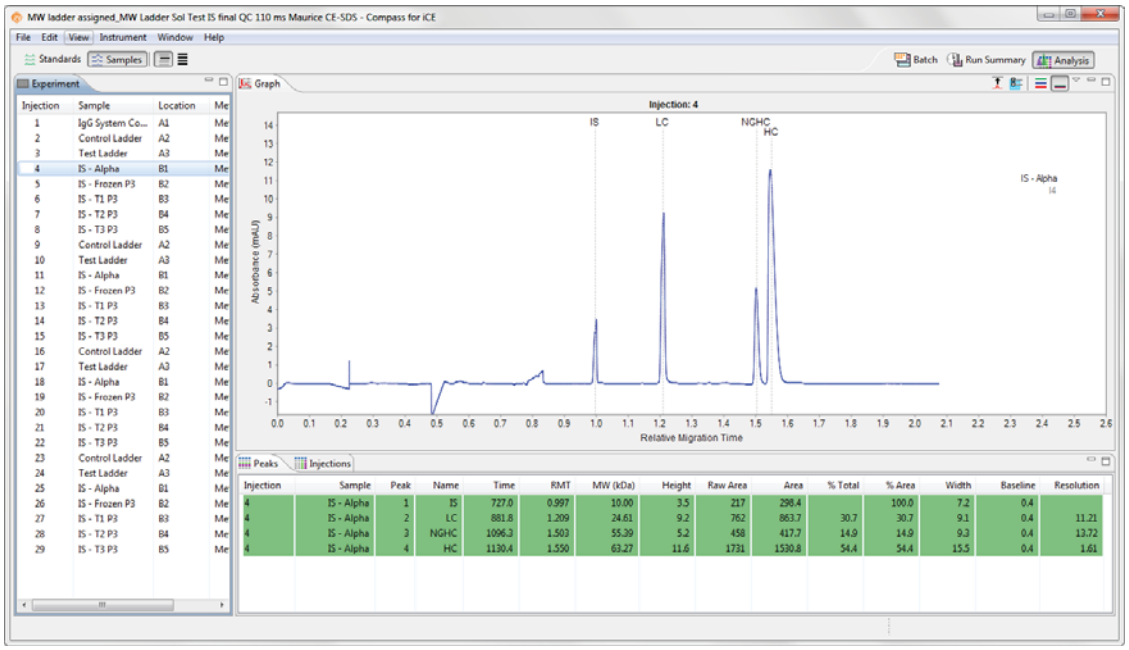
Here's how you switch between viewing data for your samples and standards:

- **To view sample data** - Click **Samples** in the View bar or select **View** in the main menu and click **Samples**.



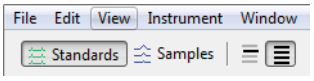
  - Data in this view is for sample proteins only.

- The graph displays electropherograms with a y-axis of Absorbance units (mAU) and an x-axis of RMT (relative migration time).
- Results for each protein are shown in the Peaks and Injections panes.



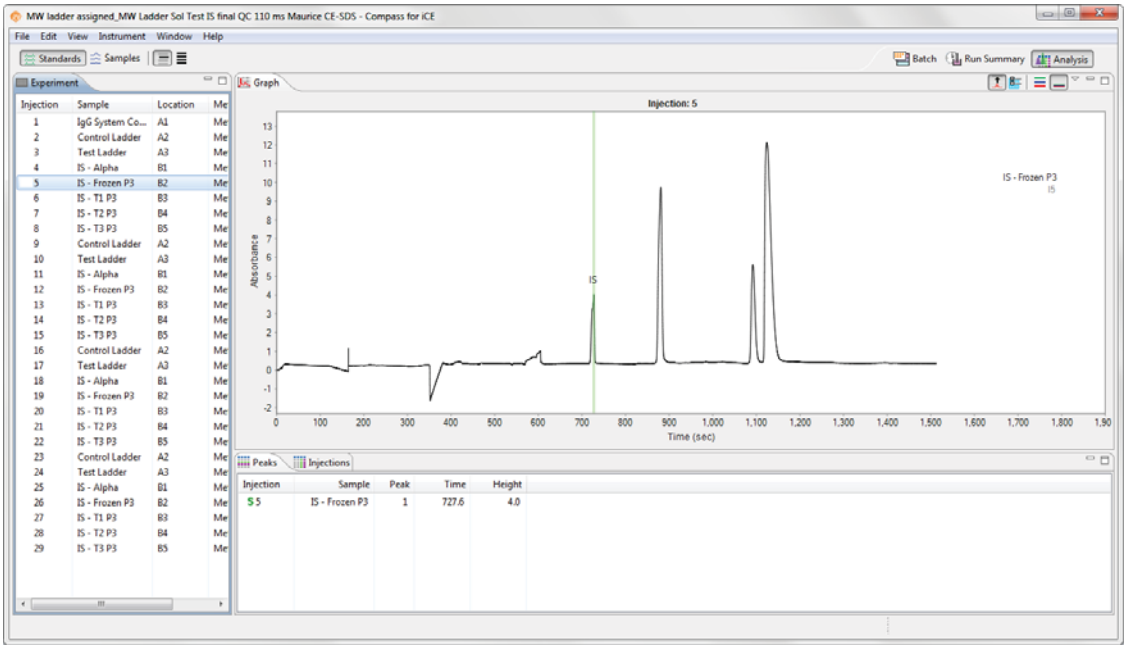
For information on checking and identifying sample peaks, see "Checking Your Data" on page 139.

- **To view Internal Standard data** - Click **Standards** in the View bar or select **View** in the main menu and click **Standards**.



- Data in this view is for analyzing standards only. This is the Internal Standard you add to your samples during prep.
- The graph displays electropherograms with a y-axis of Absorbance units (mAU) and an x-axis of time in seconds.

- The Internal Standard is identified in the Peaks pane with an **S** and as Std1 in the Injections pane.

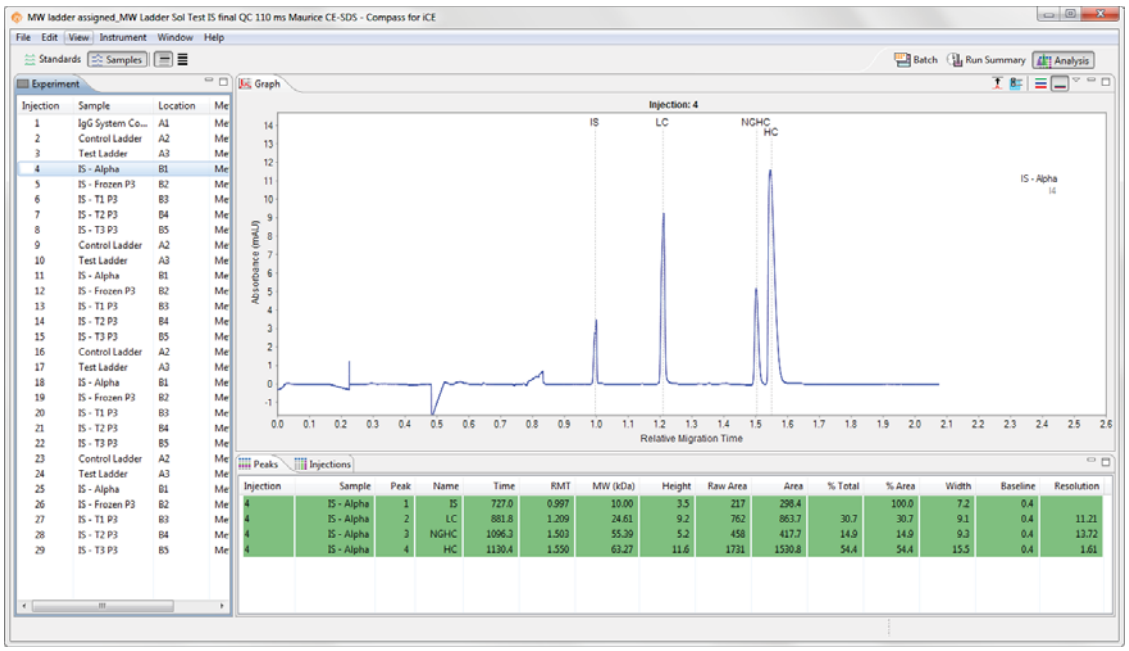


For information on checking and identifying the Internal Standard peak, see “Checking Your Data” on page 139.

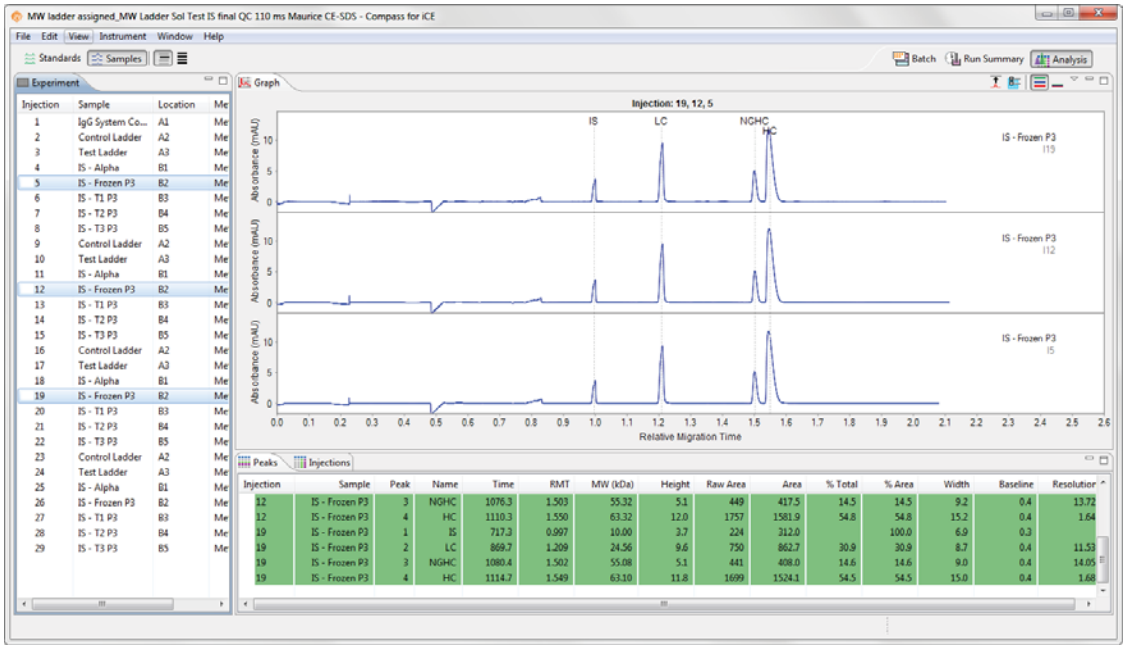
Selecting and Displaying Injection Data

You can view data from one, multiple, or all injections at once.

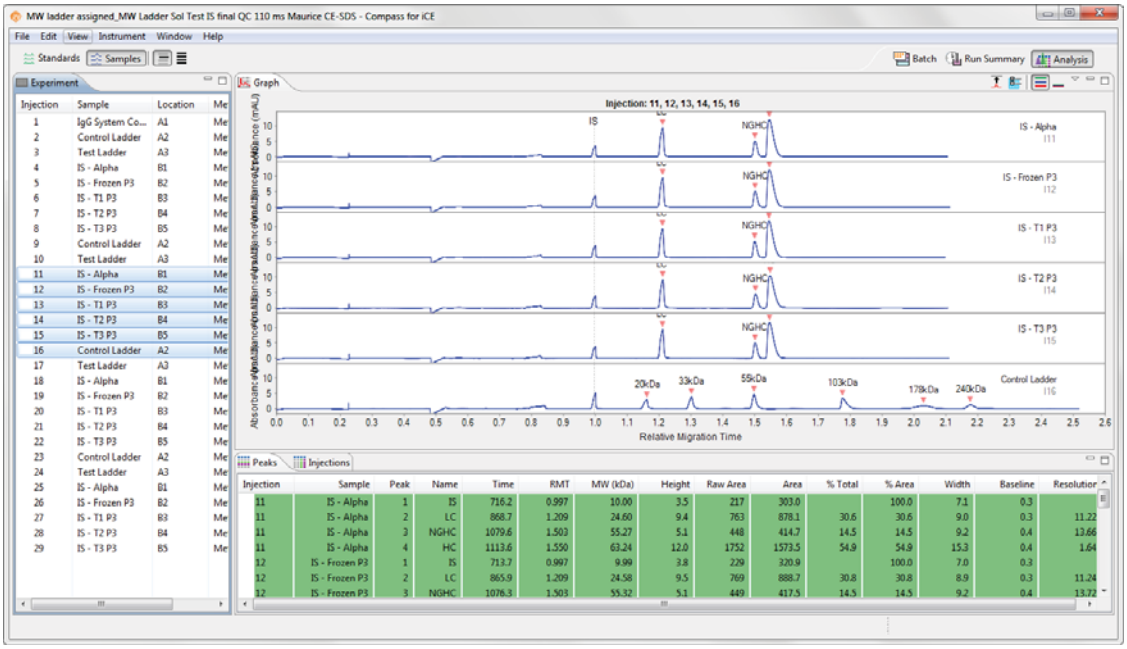
- **To look at data for one injection** - Click an injection row in the Experiment pane. Data for just that injection displays in the graph and tables.



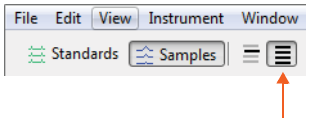
- **To look at data for specific injections** - Hold the **Ctrl** key and select just the injection rows you want to view in the Experiment pane. Data for only the injections selected display in the graph and tables.



- **To look at data for sequential injections** - Select the first injection row in the Experiment pane that you want to view, then hold the **Shift** key and select the last. This selects all rows between the two injections. Data for only the injections selected display in the graph and tables.



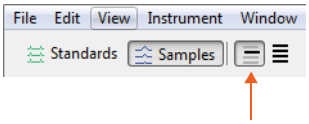
- **To look at data for all injections** - Just click **View All** in the View bar. Data for all injections displays in the graph and tables.



Switching Between Single and Multiple Views of Injections

You can switch between displaying run data in a single, per-injection format or a multi-injection format.

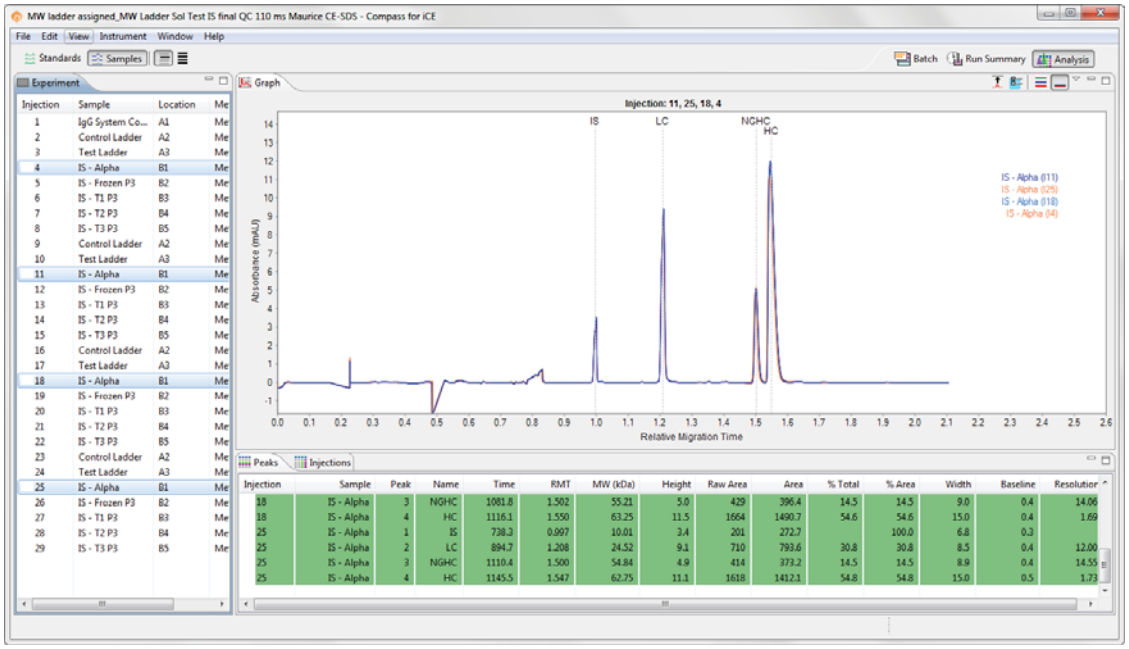
- **To view data per in a per-injection format** - Click **Single View** in the View bar or select **View** in the main menu and click **Single View**.



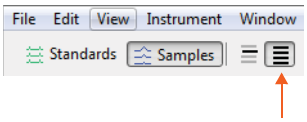
Data for the injection row(s) selected in the Experiment pane:

- Displays with electropherograms either overlaid or stacked in the Graph pane depending on the option you've got chosen.

- Shows only results for the selected row(s) in the Peaks and Injections panes.

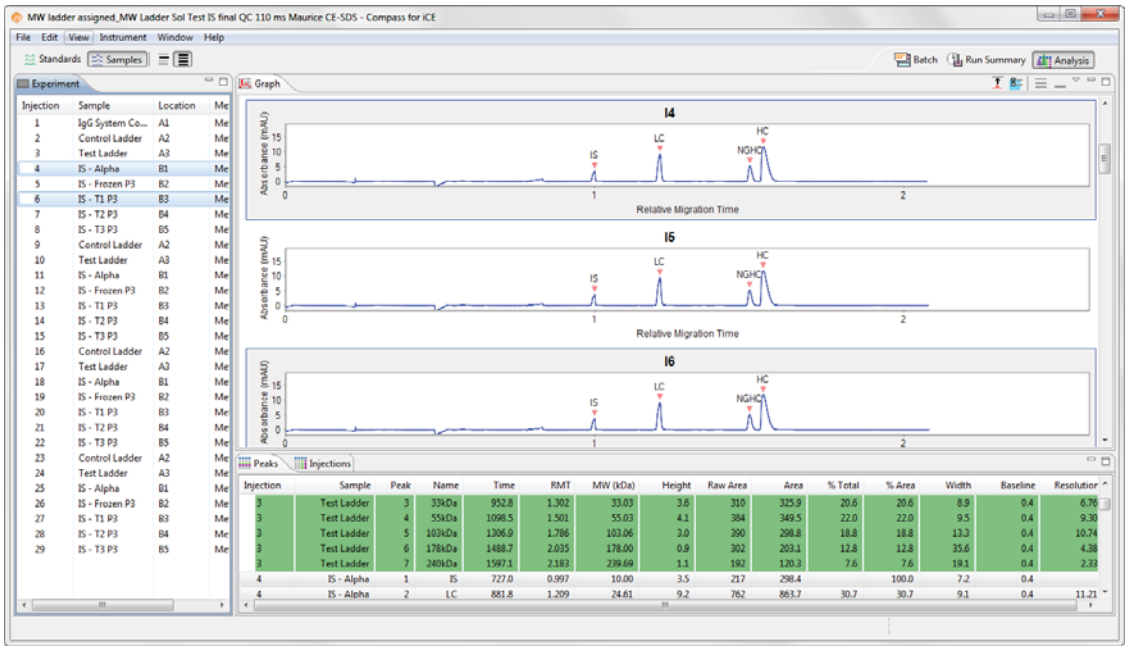


- **To view data in a multi-injection format** - Click **View All** in the View bar or select **View** in the main menu and click **Multiple View**:



Data for the injection row(s) selected in the Experiment pane:

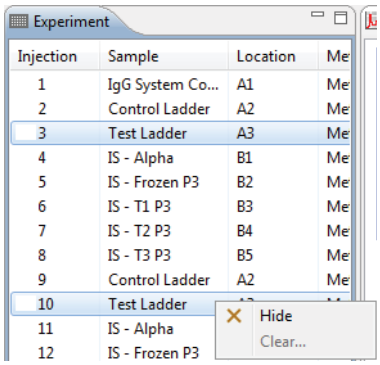
- Displays with the electropherograms of the selected injections highlighted in the Graph pane.
- Shows the results for the selected injections highlighted in the Peaks and Injections panes.



Hiding Injection Data

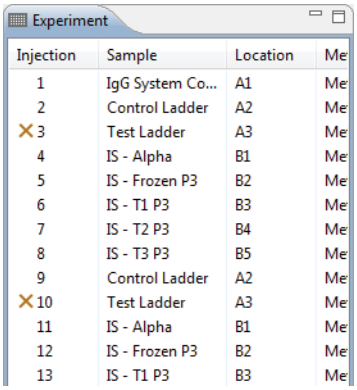
You can hide injection data from the view if needed.

- **To hide injections** - Select the injection rows you want to hide in the Experiment pane, then right click one and select **Hide**.



Data for the injections will be hidden in all data views and results tables.

- **To view hidden injections** - Select **View** in the main menu and click **Show Hidden**. Hidden rows will become visible again in all panes, and are marked with an X in the Experiment pane.

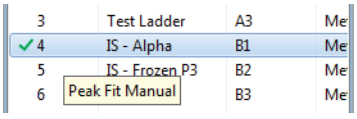


- **To unhide injections** - Select the hidden row(s). Right click on one and click **Unhide.**

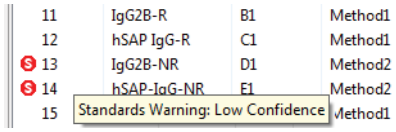
Data Notifications and Warnings

If Compass for iCE detects a potential data issue, a notification or warning icon will display next to the injection row in the Experiment pane.

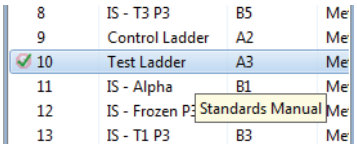
Manual correction of sample data notification - This means the sample data was manually changed by a user, for example to add or remove a sample peak. Roll your mouse over the icon to display the type of modification that was made.



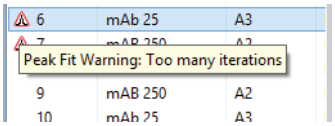
Standards warning - This means the Internal Standard may not be identified properly. You can fix this by manually identifying the standard using the steps in "Step 1: Check Your Internal Standard" on page 139. Roll your mouse over the icon to display warning details.



Manual correction of standards data notification - This means a user changed the standards data manually. Roll your mouse over the icon to display the type of modification that was made.



Peak fit warning - Means that a peak can't be fit properly. This can sometimes be caused when a broad peak is fitted as multiple narrow peaks. Changing the peak width can help in this case. The warning is also caused by very small peaks around main peaks, or small peaks that are close to the end of the separation range. You can often fix this by removing the peak(s) using the steps in "Step 3: Checking Sample Peaks" on page 147. Roll your mouse over the icon to display warning details.



Checking Your Results

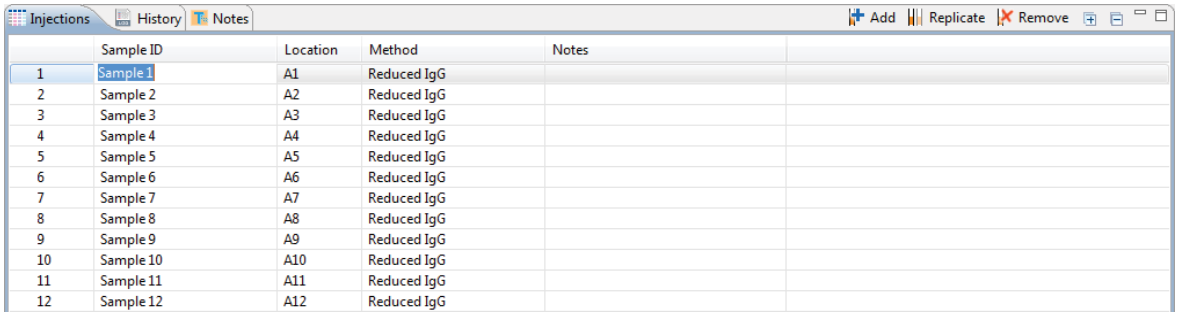
Compass for iCE detects your sample protein, CE-SDS MW Markers and Internal Standard peaks and reports results automatically. But, we always recommend you review and check your data as a good general practice to make sure your results are accurate. Please see the step by step procedure in "Checking Your Data" on page 139 to do this. If you see a data warning in the Experiment pane, these steps will also help you identify and correct any issues.

Group Statistics

You can use the Grouping view to have Compass for iCE do a statistical analysis of named proteins in your injections (see "Peak Names Settings" on page 271 for more info on setting named peaks up). Statistics for each protein are also plotted for easy comparison.

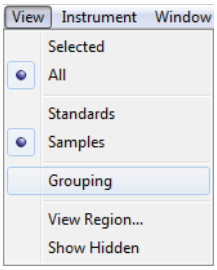
Using Groups

1. Groups are automatically created for injections that use the same sample name and method, so to use this feature, you need to make sure you've got sample names entered.
   a. Go to the **Batch** screen.
   b. Click the **Sample ID** cells in the Injection pane and type a name for any samples you want to calculate statistics for.



	Sample ID	Location	Method	Notes
1	Sample 1	A1	Reduced IgG	
2	Sample 2	A2	Reduced IgG	
3	Sample 3	A3	Reduced IgG	
4	Sample 4	A4	Reduced IgG	
5	Sample 5	A5	Reduced IgG	
6	Sample 6	A6	Reduced IgG	
7	Sample 7	A7	Reduced IgG	
8	Sample 8	A8	Reduced IgG	
9	Sample 9	A9	Reduced IgG	
10	Sample 10	A10	Reduced IgG	
11	Sample 11	A11	Reduced IgG	
12	Sample 12	A12	Reduced IgG	

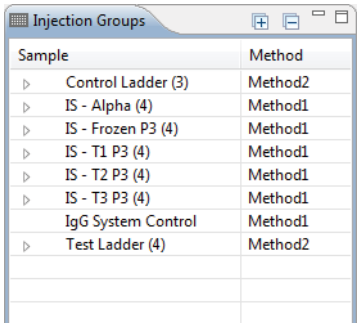
2. Go back to the **Analysis** screen. Click **View** in the main menu and select **Grouping**.



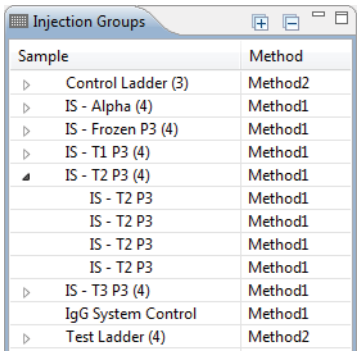
*NOTE: To turn Grouping off, select **View** in the main menu and deselect **Grouping**.*

Viewing Sample Injection Groups

Compass for iCE automatically groups all injections using the same sample name together in the Injection Groups pane.



- **To expand a group** - Click the arrow next to a group to see the individual injections in the group and reported data for each

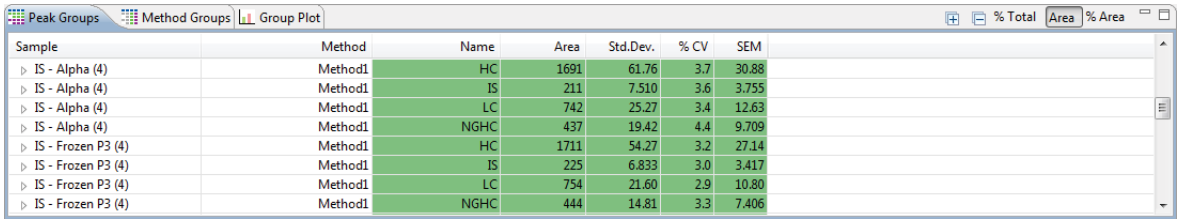


- **To expand all groups** - Click **Expand All (+)** in the upper right corner of the pane.
- **To collapse all groups** - Click **Collapse All (-)** in the upper right corner of the pane.

Viewing Statistics

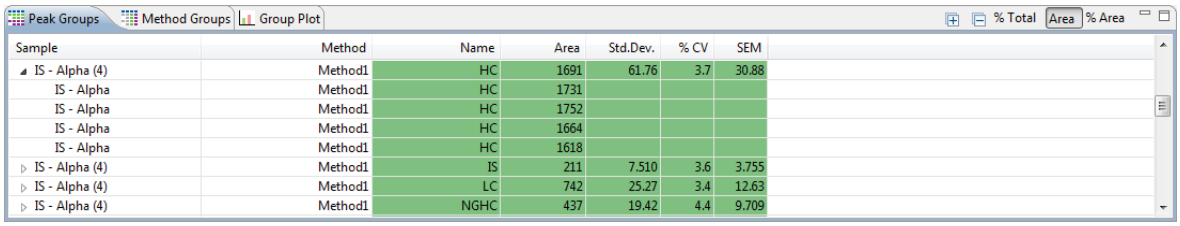
Peak and Method Groups

The Peak Groups pane reports statistics for each named protein in every group. Each group shows the statistics for named proteins which includes average area, standard deviation, %CV and SEM (standard error measurement). The number in parenthesis after the sample name is the number of injections in the group.



Sample	Method	Name	Area	Std.Dev.	% CV	SEM
IS - Alpha (4)	Method1	HC	1691	61.76	3.7	30.88
IS - Alpha (4)	Method1	IS	211	7.510	3.6	3.755
IS - Alpha (4)	Method1	LC	742	25.27	3.4	12.63
IS - Alpha (4)	Method1	NGHC	437	19.42	4.4	9.709
IS - Frozen P3 (4)	Method1	HC	1711	54.27	3.2	27.14
IS - Frozen P3 (4)	Method1	IS	225	6.833	3.0	3.417
IS - Frozen P3 (4)	Method1	LC	754	21.60	2.9	10.80
IS - Frozen P3 (4)	Method1	NGHC	444	14.81	3.3	7.406

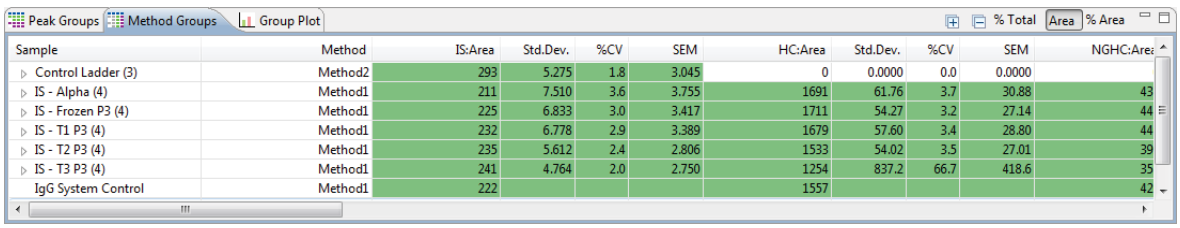
- **To display results using area** - Click **Area** in the upper right corner of the pane.
- **To display results using % total** - Click **% Total** in the upper right corner of the pane to display the calculated percent area for the named peak compared to the total area measured in the injection. This value results from dividing the individual peak area by the sum of all peak areas for the injection and multiplying by 100.
- **To display results using % area** - Click **% Area** in the upper right corner of the pane to display the calculated percent area for the named peak compared to all named peaks. This value results from dividing the individual peak area by the sum of all named peak areas for the injection and multiplying by 100 (shown for named peak sample data only).
- **To expand a group** - Click the arrow next to a group to see the individual injections in the group and reported data for each



Sample	Method	Name	Area	Std.Dev.	% CV	SEM
IS - Alpha (4)	Method1	HC	1691	61.76	3.7	30.88
IS - Alpha	Method1	HC	1731			
IS - Alpha	Method1	HC	1752			
IS - Alpha	Method1	HC	1664			
IS - Alpha	Method1	HC	1618			
IS - Alpha (4)	Method1	IS	211	7.510	3.6	3.755
IS - Alpha (4)	Method1	LC	742	25.27	3.4	12.63
IS - Alpha (4)	Method1	NGHC	437	19.42	4.4	9.709

- **To expand all groups** - Click **Expand All (+)** in the upper right corner of the pane.
- **To collapse all groups** - Click **Collapse All (-)** in the upper right corner of the pane.

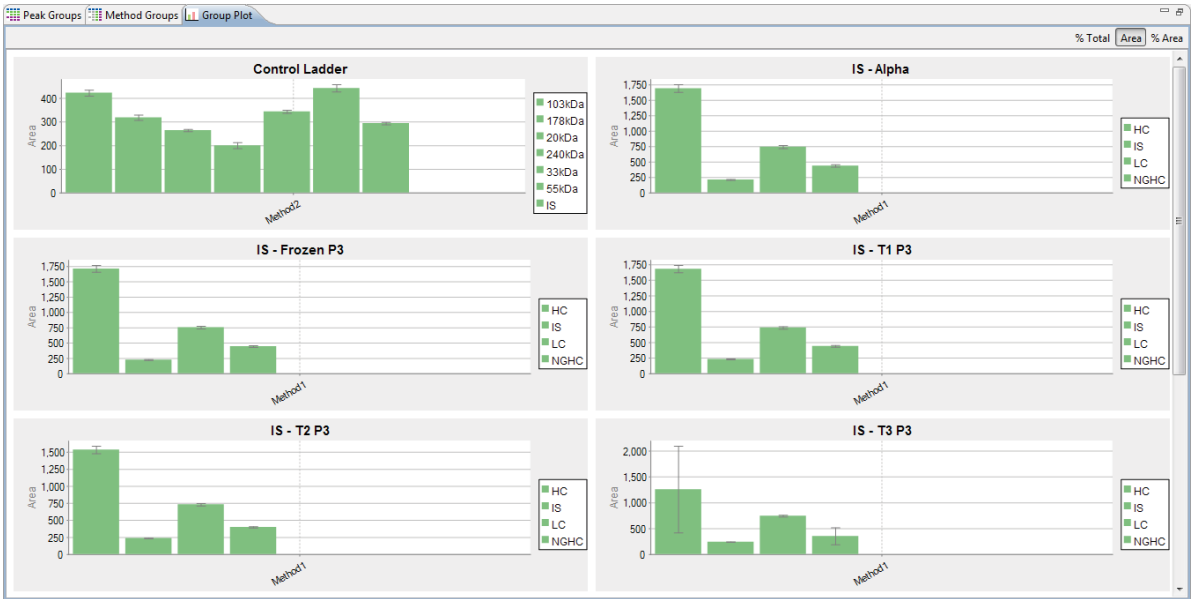
The Method Groups pane pivots the Peak Groups pane results to show statistics for named protein peaks in individual columns.



Sample	Method	IS:Area	Std.Dev.	%CV	SEM	HC:Area	Std.Dev.	%CV	SEM	NGHC:Area
Control Ladder (3)	Method2	293	5.275	1.8	3.045	0	0.0000	0.0	0.0000	
IS - Alpha (4)	Method1	211	7.510	3.6	3.755	1691	61.76	3.7	30.88	43
IS - Frozen P3 (4)	Method1	225	6.833	3.0	3.417	1711	54.27	3.2	27.14	44
IS - T1 P3 (4)	Method1	232	6.778	2.9	3.389	1679	57.60	3.4	28.80	44
IS - T2 P3 (4)	Method1	235	5.612	2.4	2.806	1533	54.02	3.5	27.01	39
IS - T3 P3 (4)	Method1	241	4.764	2.0	2.750	1254	837.2	66.7	418.6	35
IgG System Control	Method1	222				1557				42

Group Plots

The mean values for named peaks using the same method in each injection group are plotted in bar graphs with error bars showing the standard deviation in the Group Plots pane. You'll also get plots that compare samples using the same method in the run.



Hiding or Removing Injections in Group Analysis

Hidden injections are not included in injection groups. But, hiding injections gives you an easy way to reject individual injections from the statistical analysis. See "Hiding Injection Data" on page 213 for details on how to do this.

Copying Results Tables and Graphs

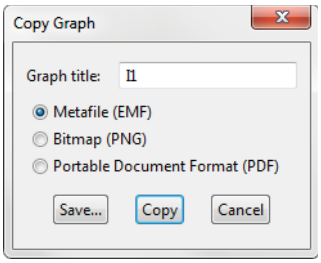
You can copy and paste data and results tables into other documents, or save the electropherogram as a graphic file.

Copying Results Tables

1. Click in the Peaks or Injections pane.
2. Select one or multiple rows.
3. Select **Edit** in the main menu and click **Copy**, or right click on row(s) you selected and click **Copy**.
4. Open a document (Microsoft® Word®, Excel®, PowerPoint®, etc.). Right click in the document and select **Paste**. Data for the rows selected will be pasted into the document.

Copying the Graph

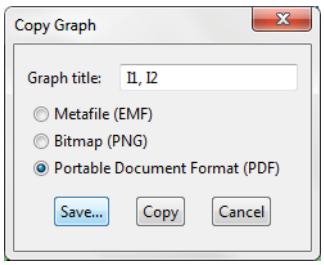
1. Select the Graph pane.
2. Select **Edit** in the main menu and click **Copy**, or right click in the Graph pane and select **Copy**.
3. Select an image option (EMF, PNG or PDF) in the pop-up window, then click **Copy**.



4. Open a document (Microsoft® Word®, Excel®, PowerPoint®, etc.). Right click in the document and select **Paste**. A graphic of the copied electropherogram will be pasted into the document.

Saving the Graph as an Image File

1. Select the Graph pane.
2. Select **Edit** in the main menu and click **Copy**, or right click in the Graph pane and select **Copy**.
3. Select an image option (EMF, PNG or PDF) in the pop-up window, then click **Save**.



4. Select a directory to save the file to, enter a file name, then click **OK**.

Exporting Run Files

Results tables and raw plot data can be exported for use in other applications.

Exporting Results Tables

To export the information in the Peaks and Injections tables:

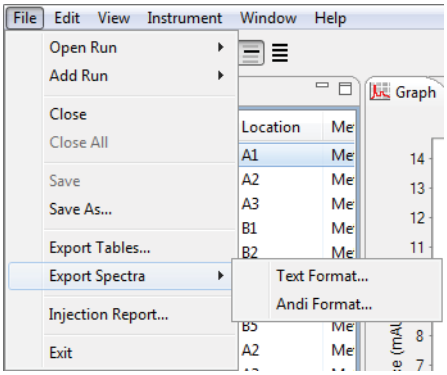
1. Click **File** in the main menu and click **Export Tables**.
2. Select a directory to save the files to and click **OK**. Data will be exported in .txt format.

NOTE: To exclude export of standards data or export results table data in .csv format, see "Setting Data Export Options" on page 379.

Exporting Raw Sample Electropherogram Data

To export raw sample plot and background data:

1. Click **File** in the main menu and click **Export Spectra**.



- **To export data in .txt format** - Select **Text Format**. Data will be exported in one file for all injections.
- **To export data in .cdf format** - Select **Andi Format**. Data will be exported in one file per injection.

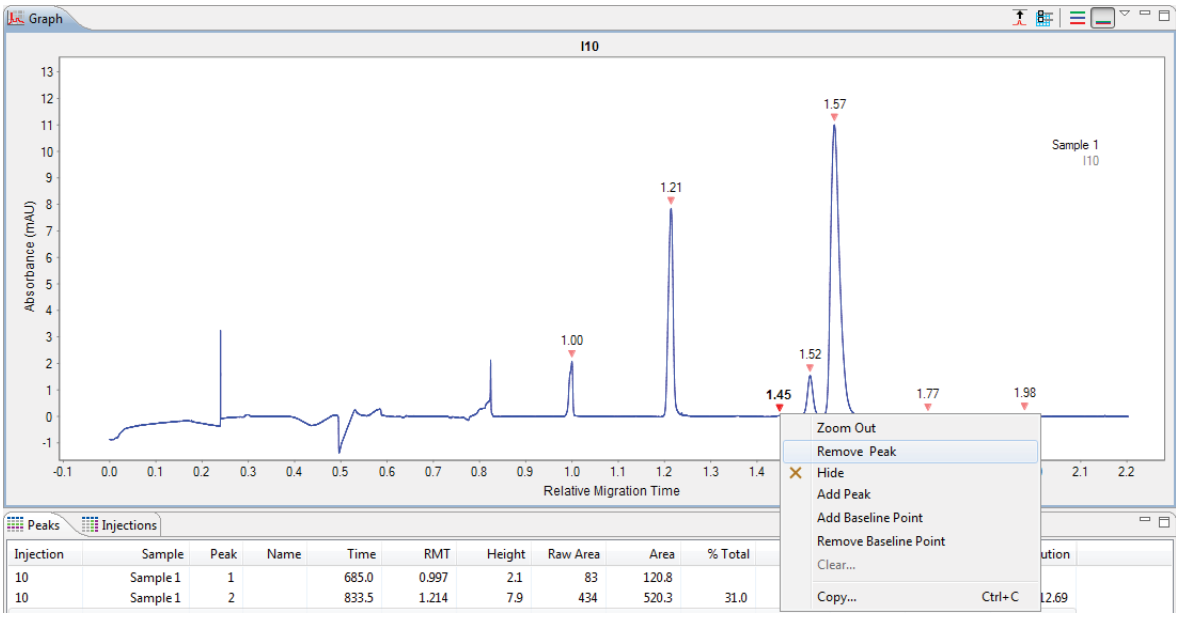
2. Select a directory to save the files to and click **OK**. Data will be exported in the selected format.

Changing Sample Protein Identification

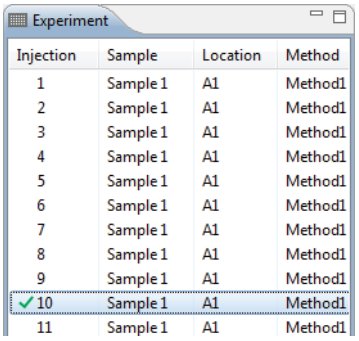
Compass for iCE lets you customize what sample proteins are reported in the results tables by making manual adjustments in the electropherogram or Peaks table.

Adding or Removing Sample Data

1. Click **Show Samples** in the View bar.
2. Click **Single View** in the View bar.
3. Click on the row in the experiment pane that has the injection you want to correct, then click the **Graph** tab.
    - **To remove a peak from the data -** Right click the peak in the electropherogram or Peaks table and select **Remove peak**. The software will no longer identify it as a sample peak in the electropherogram, and the peak data will be removed in the results tables.



A check mark will appear next to the injection in the Experiment pane to indicate a manual correction was made.



- **To add an unidentified peak to the data -** Right click the peak in the electropherogram or peaks table and select **Add Peak**. The software will calculate and display the results for the peak in the results tables and identify the peak in the electropherogram.

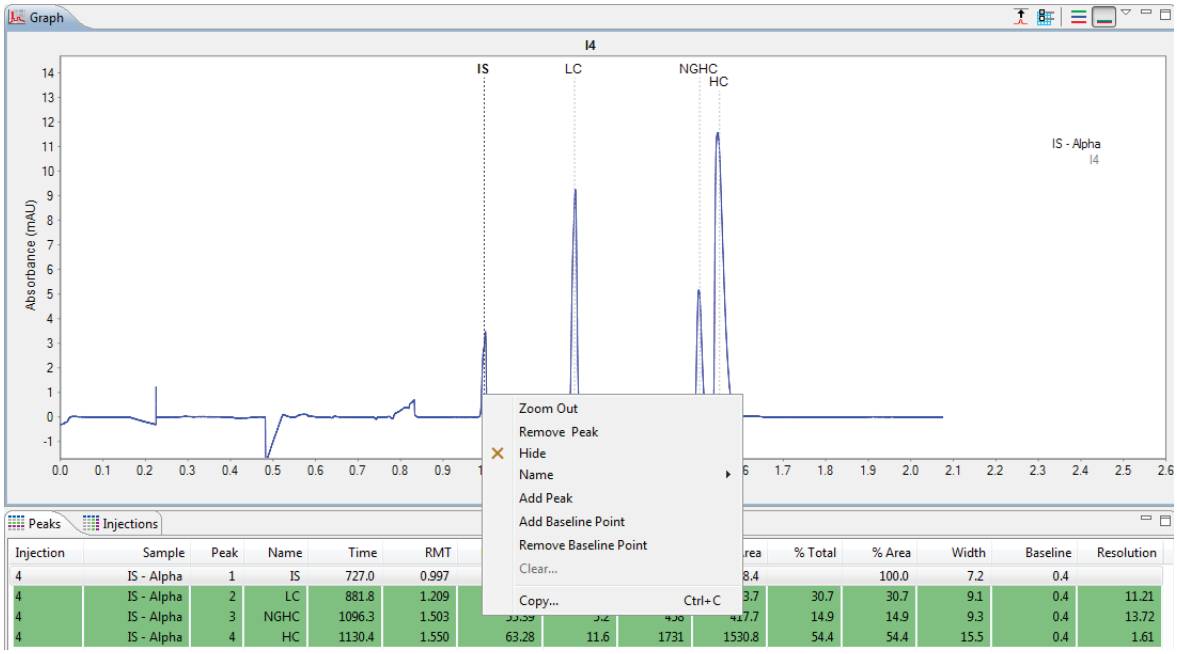
  A check mark will appear next to the injection in the Experiment pane to indicate a manual correction was made.

*NOTE: To remove sample peak assignments that were made manually and go back to the original peak data, right-click the peak in the electropherogram and select **Clear** for the current injection or **Clear All** for all injections in the batch.*

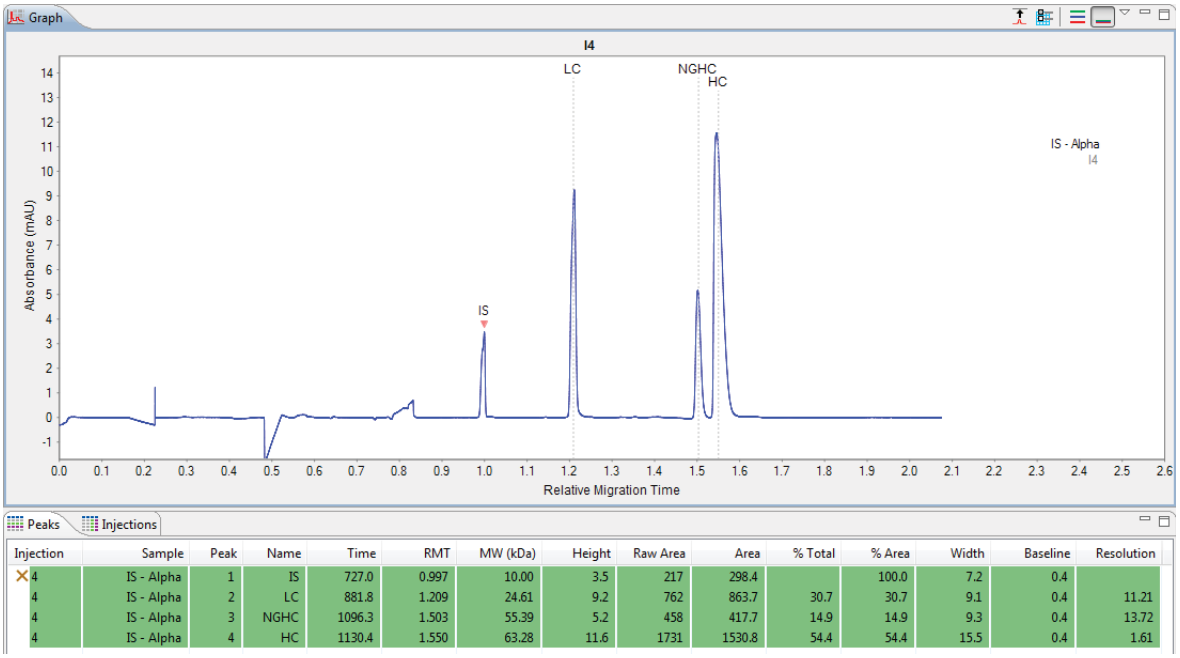
Hiding Sample Data

You can hide the results for a sample protein in the results tables without completely removing it from the reported results.

1. Click **Show Samples** in the View bar.
2. Click **Single View** in the View bar.
3. Click on the row in the experiment pane that contains the injection you want to correct, then click the **Graph** tab.
4. Right click the peak in the electropherogram or Peaks table and select **Hide**. Compass for iCE will hide the peak data in the results tables.



5. To view hidden peak data, click **View** in the main menu and click **Show Hidden**. Hidden peak data will display in the results table and be marked with an X.



Injection	Sample	Peak	Name	Time	RMT	MW (kDa)	Height	Raw Area	Area	% Total	% Area	Width	Baseline	Resolution
4	IS - Alpha	1	IS	727.0	0.997	10.00	3.5	217	298.4		100.0	7.2	0.4	
4	IS - Alpha	2	LC	881.8	1.209	24.61	9.2	762	863.7	30.7	30.7	9.1	0.4	11.21
4	IS - Alpha	3	NGHC	1096.3	1.503	55.39	5.2	458	417.7	14.9	14.9	9.3	0.4	13.72
4	IS - Alpha	4	HC	1130.4	1.550	63.28	11.6	1731	1530.8	54.4	54.4	15.5	0.4	1.61

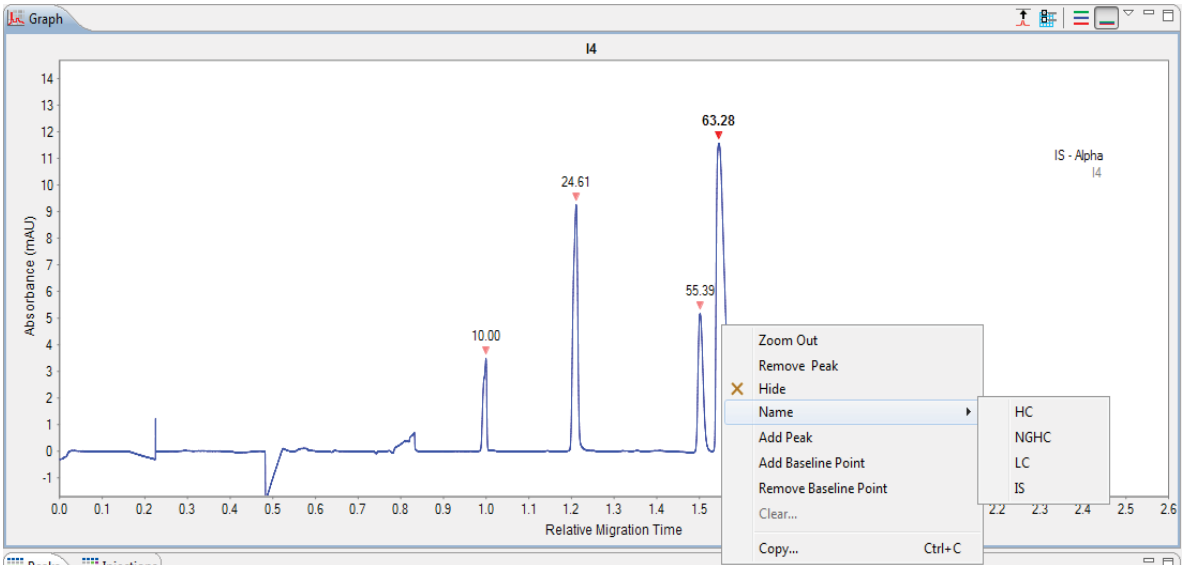
6. To unhide a peak, right click on the peak in the electropherogram or peaks table and select **Unhide**.

Changing Peak Names for Sample Data

If Compass for iCE did not automatically name a sample protein peak, you can do it manually.

1. Click **Show Samples** in the View bar.
2. Click **Single View** in the View bar.
3. Click on the row in the experiment pane that has the sample you want to correct, then click the **Graph** pane.

4. Right click the peak in the electropherogram or Peaks table and click **Name**, then select a name from the list. Compass for iCE will change the peak name in the electropherogram and results tables, and adjust peak names for other sample proteins accordingly.



NOTE: For details on how to specify peak name settings, see "Peak Names Settings" on page 271.

Changing the Electropherogram View

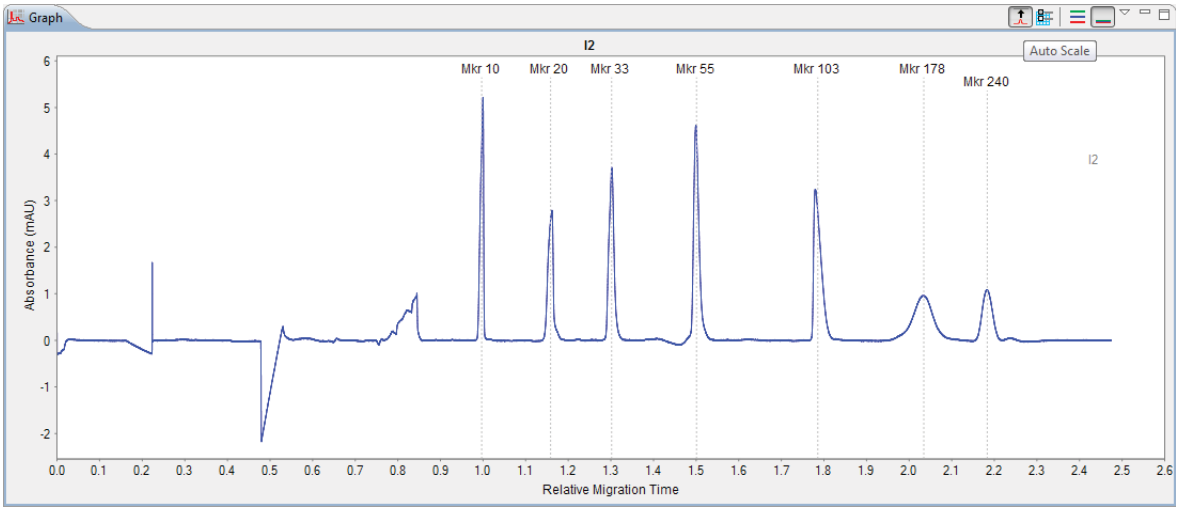
Options in the Graph pane let you zoom and rescale electropherograms, overlay or stack plots and change the peak and plot info displayed.

The Graph pane toolbar has these options:

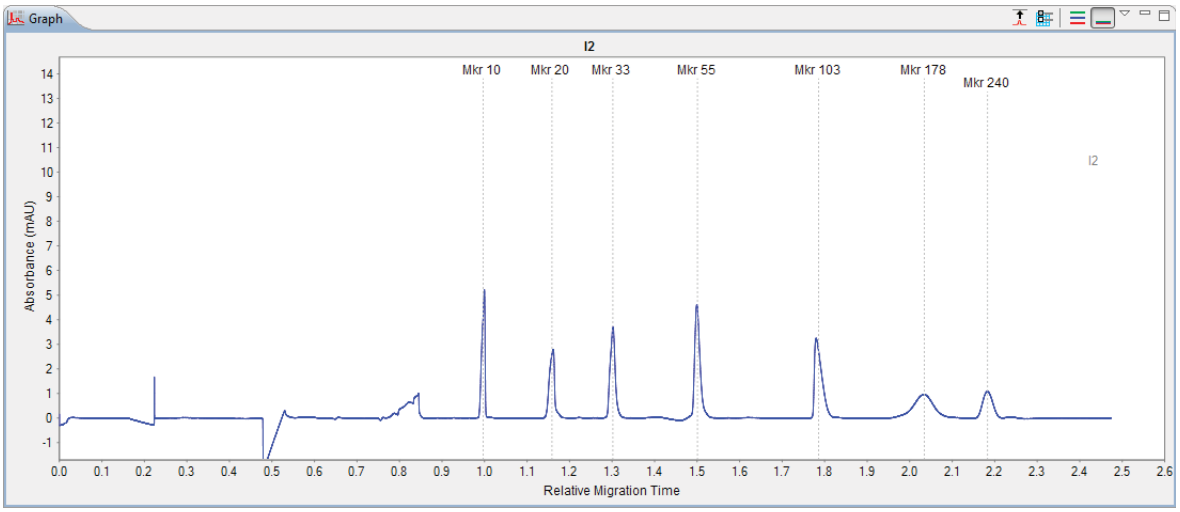
- Auto Scale
- Graph Options
- Stack the Plots
- Overlay the Plots

Autoscaling the Electropherogram

Click the **Auto Scale** button to scale the y-axis to the largest peak in the electropherogram.

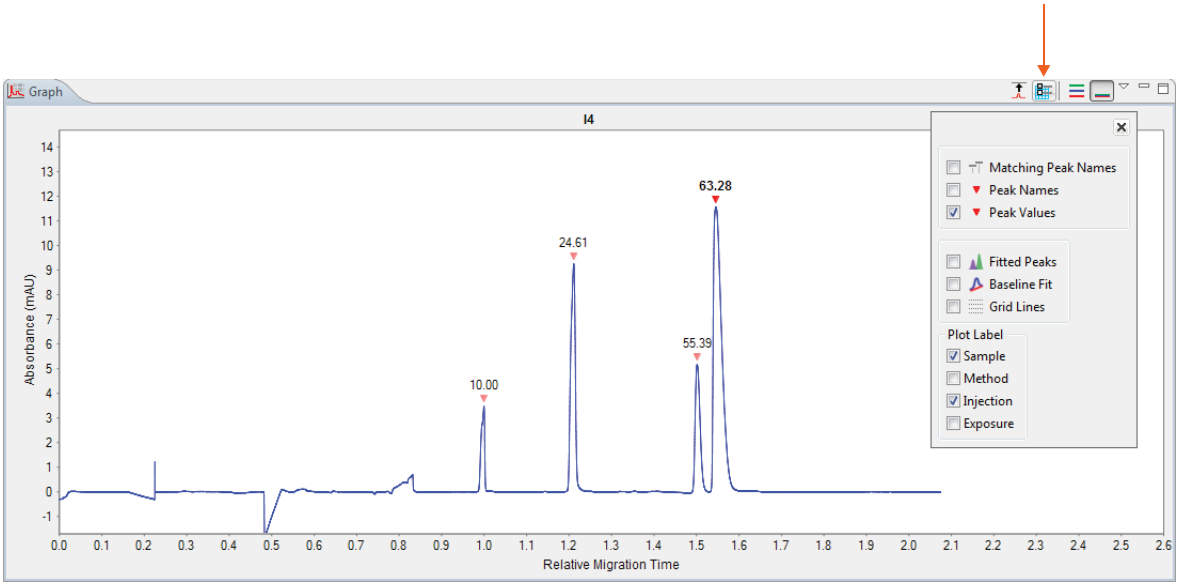


Click the **Auto Scale** button again to return to default scaling.



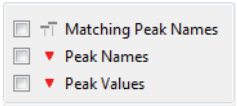
Customizing the Data Display

You can customize electropherogram peak labels, plot labels and display options. To do this, just select the **Graph Options** button.

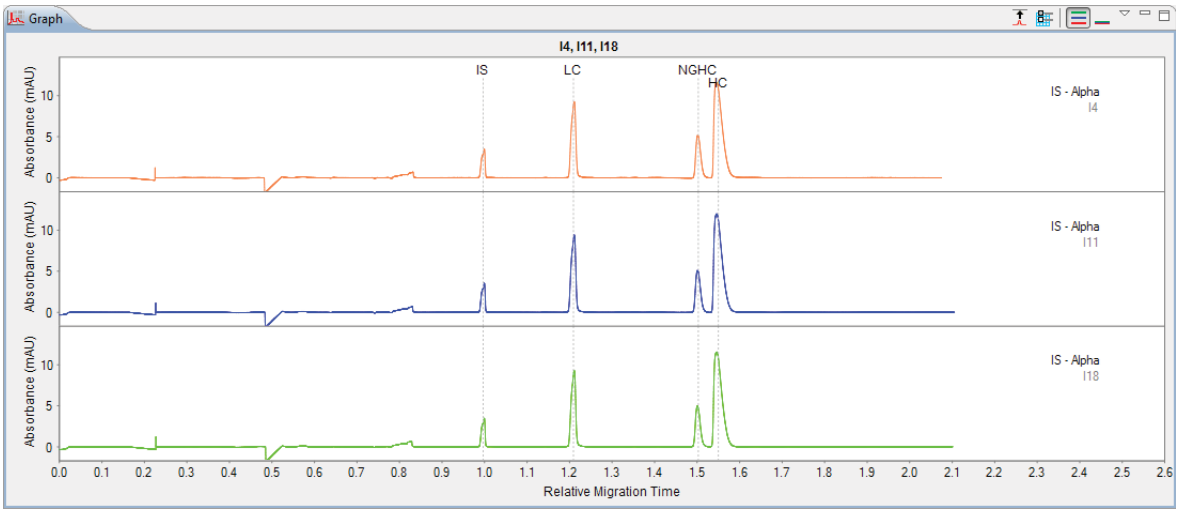


Peak Labels

You can customize the labels used to identify peaks in the electropherogram with these options:

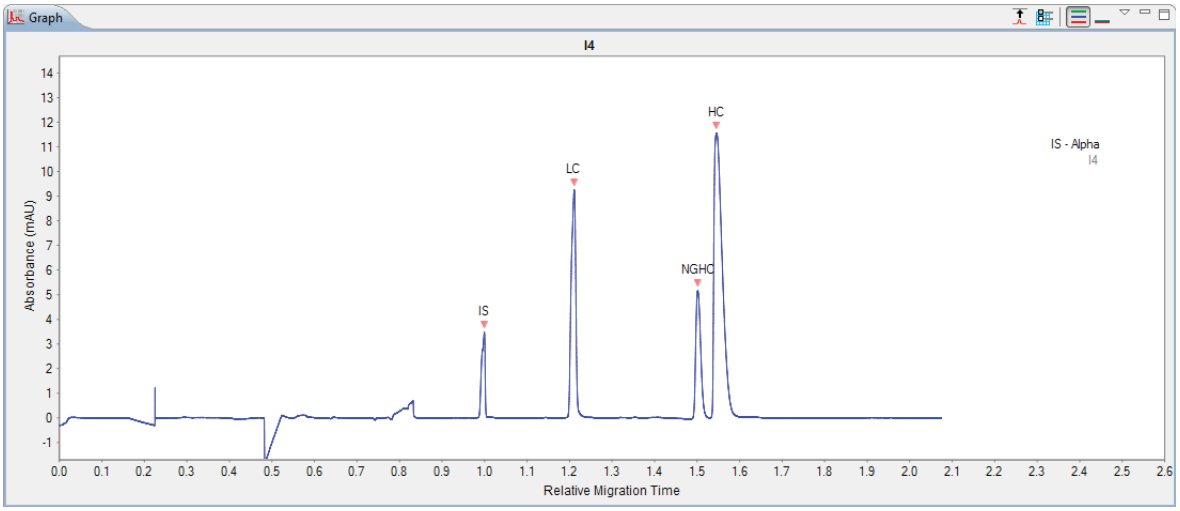


- **Matching Peak Names** - Checking this box will draw vertical lines through each named peak. Using this option with Stack the Plots or Overlay the Plots features is helpful for visually comparing your named peaks across multiple injections.



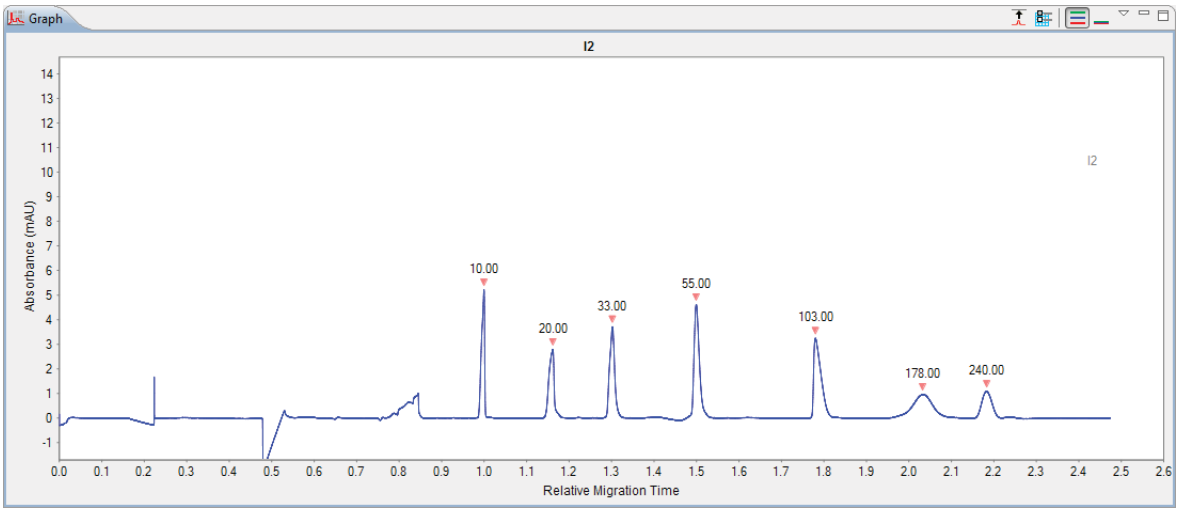
- **Peak Names** - Checking this box displays peak name labels on all named peaks in the electropherogram.

NOTE: If more than one peak label option is selected, peak name labels will always be used for named peaks.



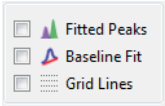
- **Peak Values** - Checking this box will display the molecular weight labels on all peaks in the electropherogram.

NOTE: If more than one peak label option is selected, peak name labels will always be used for named peaks.



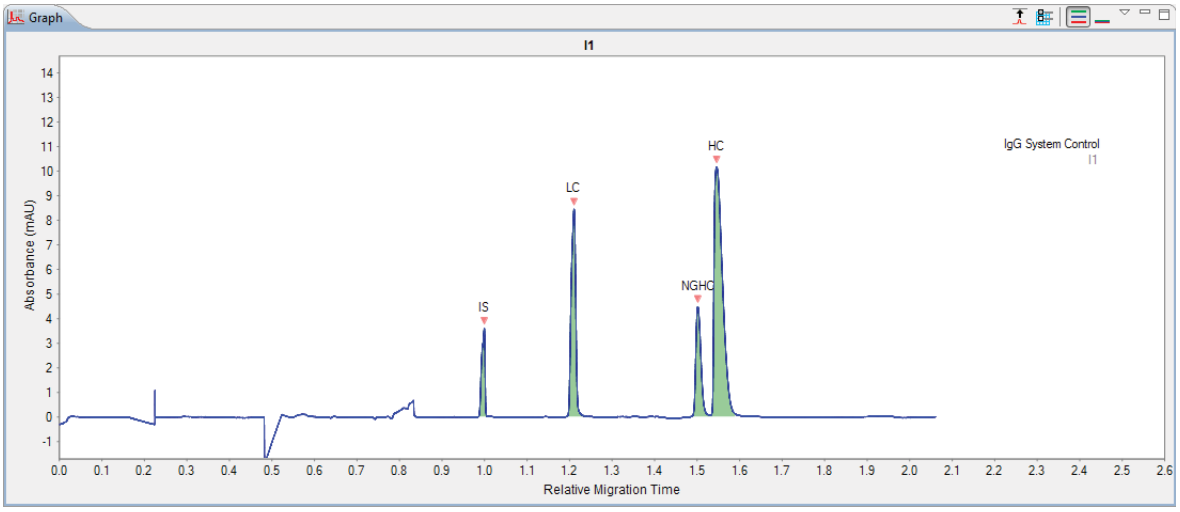
Baseline and Grid Options

You can view the calculated baseline fit, peak integration and show grid lines with these options.



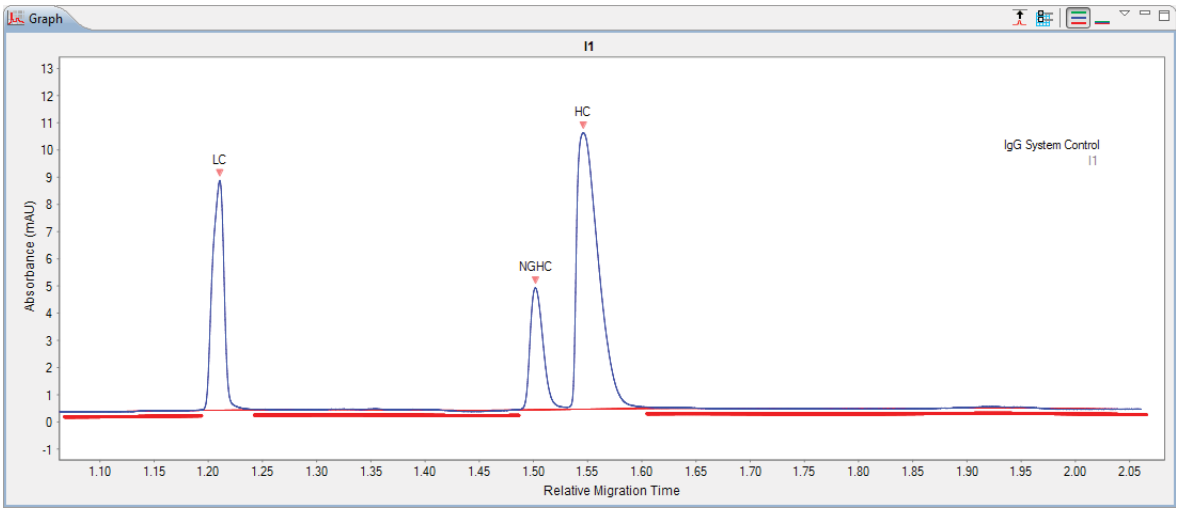
- **Fitted peaks** - Checking this box displays how the peaks were fit by the software. For CE-SDS runs, the software uses Gaussian fit by default.

NOTE: This option is only available for sample data.

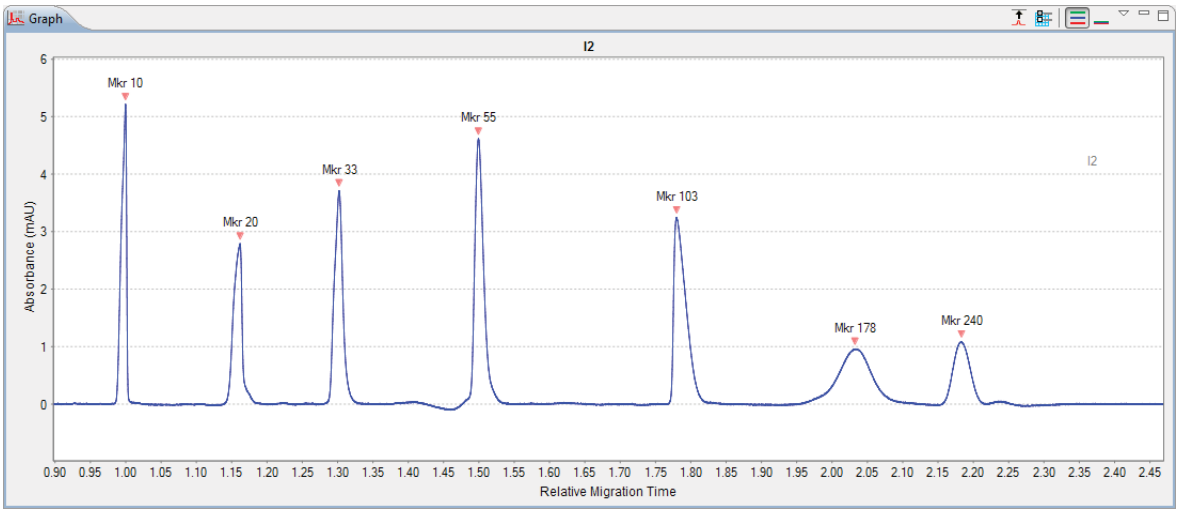


- **Baseline Fit** - Checking this box displays the calculated baseline for the peaks. Baseline points will also display for regions of the electropherogram considered to be at baseline.

NOTE: This option is only available for sample data.

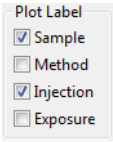


- **Grid Lines** - Checking this box adds grid lines in the graph.



Plot Labels

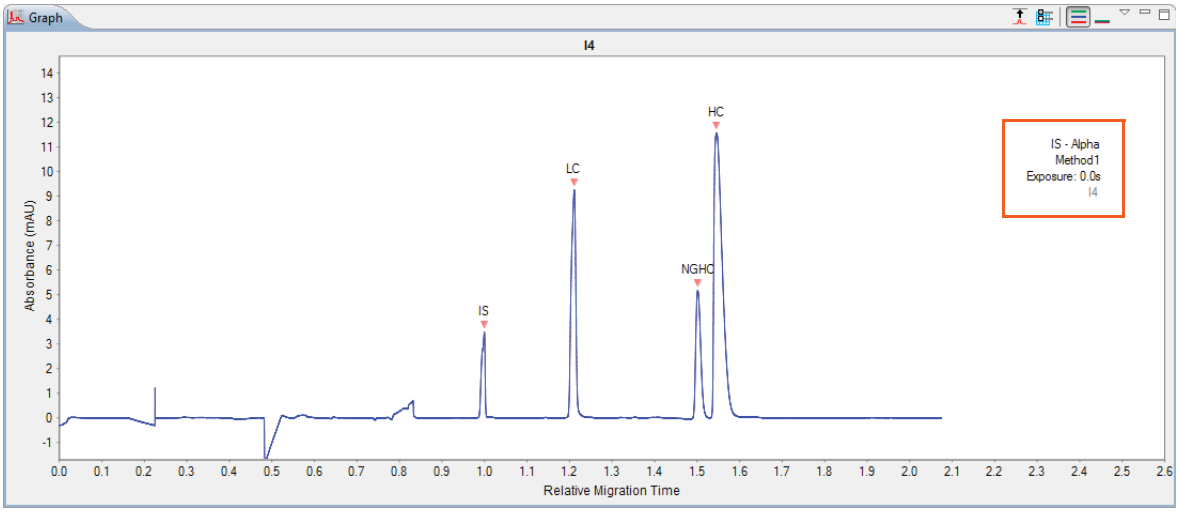
You can customize the plot labels displayed on the electropherogram with these options.



Plot labels are shown in the upper right side of the graph.

- **Sample** - Checking this box displays the sample name used for the injection. If sample names were entered with the batch, those names will display here. If not, Sample (default name) displays.
- **Method** - Checking this box displays the method used for the injection.
- **Exposure** - Checking this box display the exposure time(s) used for the data. For CE-SDS data this value will be 0.0 seconds.
- **Injection** - Checking this box displays the injection number. For example, I4 for injection 4 in the run.

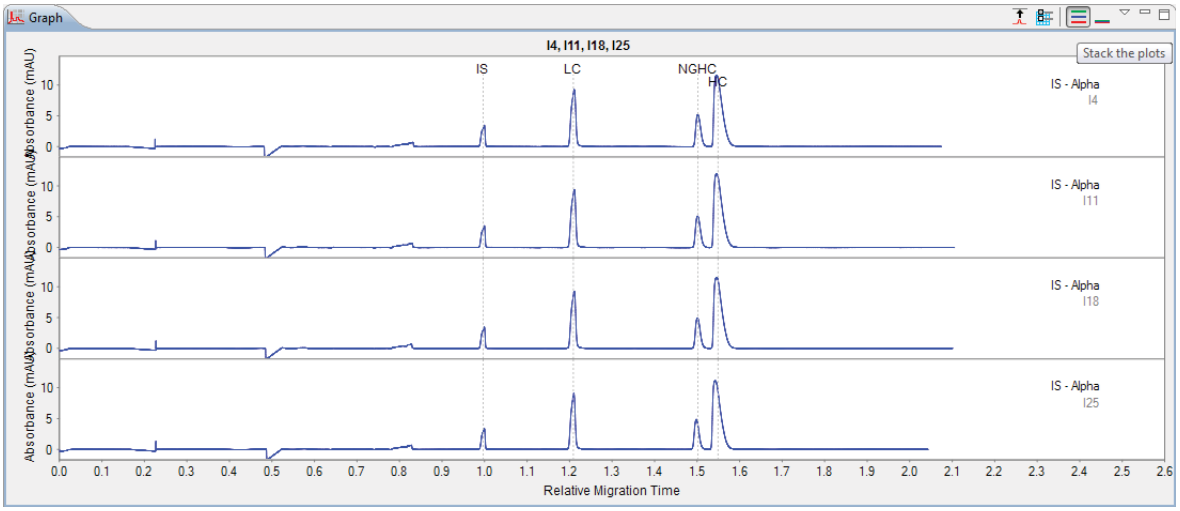
Here's an example of an electropherogram with all plot labels selected:



Stacking Multiple Electropherograms

You can stack electropherograms for multiple injections vertically in the Graph pane for comparison.

1. Click **Single View**.
2. Select multiple injection rows in the Experiment pane.
3. Click the **Stack the Plots** button. The individual electropherograms for each injection you selected will stack in the Graph pane.

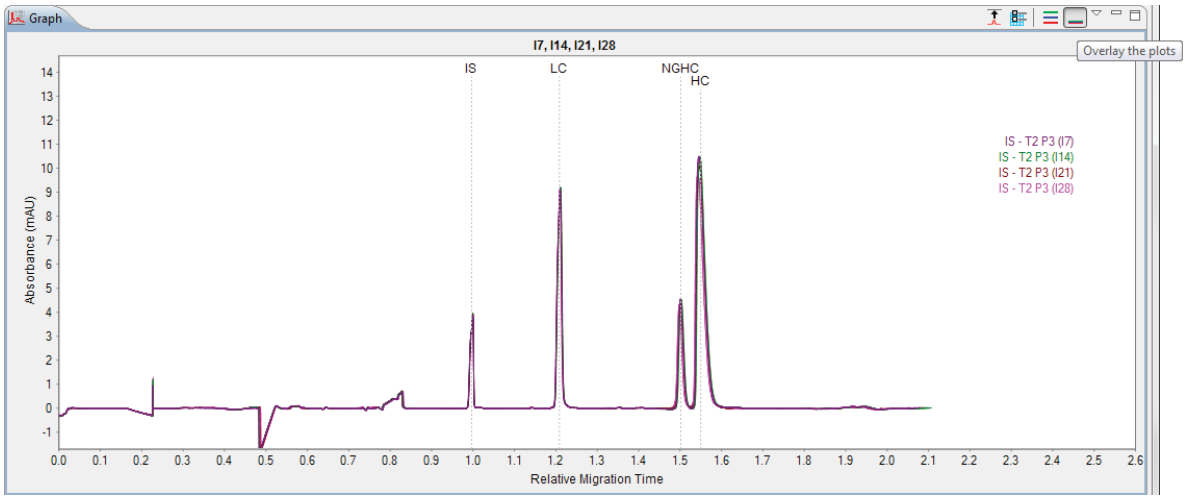


You can also customize the colors used for the stacked plot display. To do that go to "Selecting Custom Plot Colors for Graph Overlay" on page 380.

Overlaying Multiple Electropherograms

You can overlay electropherograms for multiple injections on top of each other for comparison in the Graph pane.

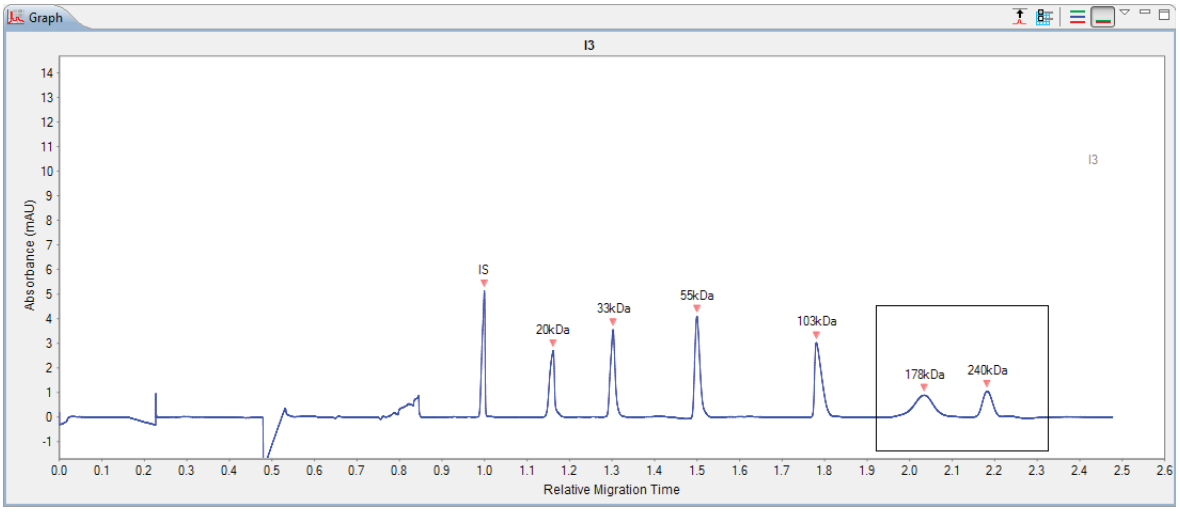
1. Click **Single View**.
2. Select multiple injection rows in the Experiment pane.
3. Click the **Overlay the Plots** button. The individual electropherograms for each injection you selected will overlay in the Graph pane.



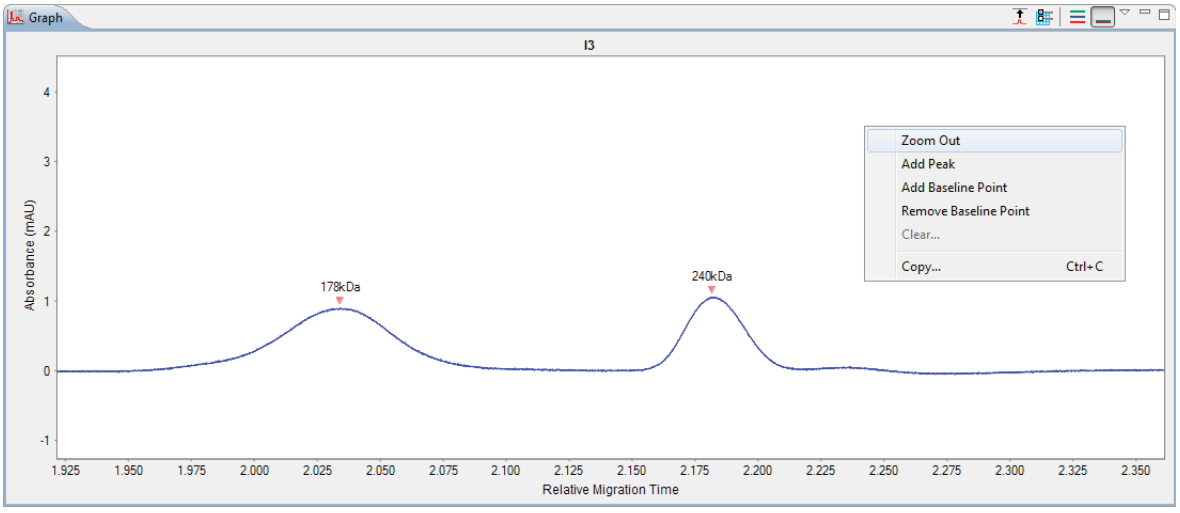
You can also customize the colors used for the overlay plot display. To do that go to "Selecting Custom Plot Colors for Graph Overlay" on page 380.

Zooming

To zoom in on a specific area of the electropherogram, hold the mouse button down and draw a box around the area with your mouse:

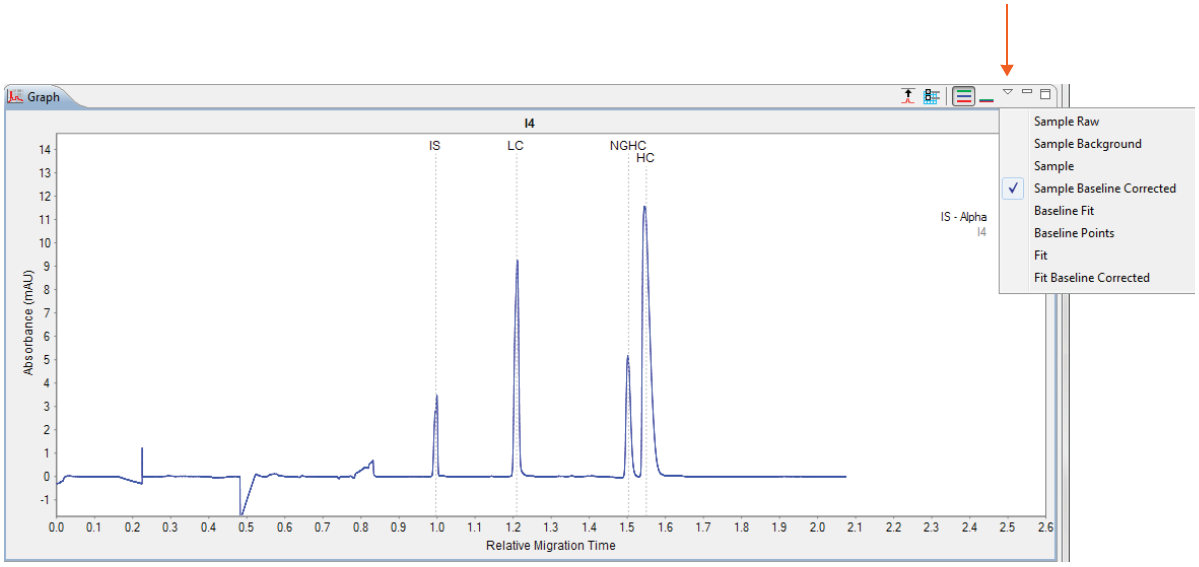


To return to default scaling, right click in the electropherogram and click **Zoom Out**.



Selecting Data Viewing Options

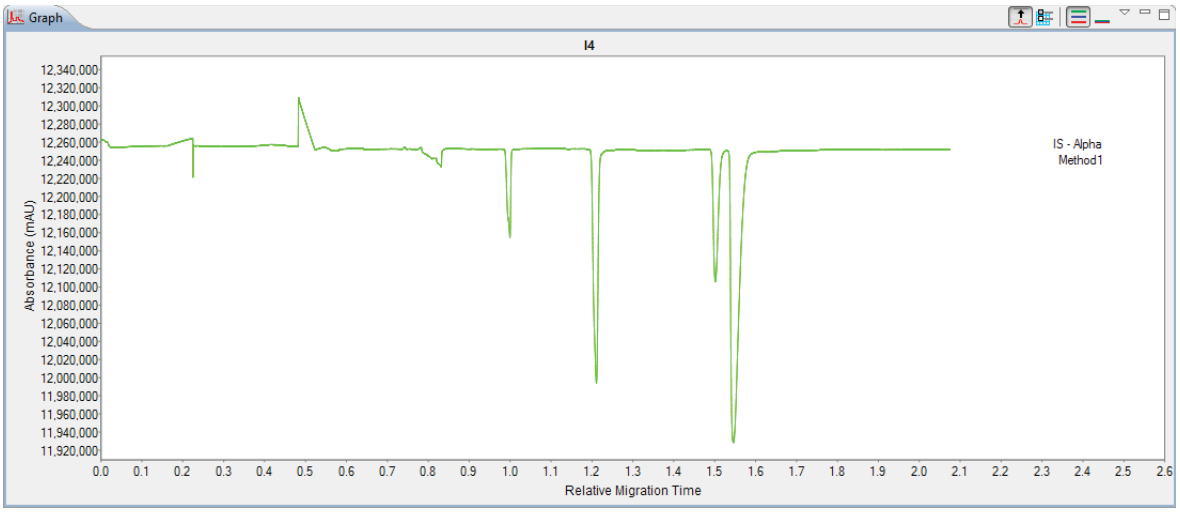
The graph view menu gives you multiple options for changing what type of electropherogram data is displayed. Just click the down arrow next to the graph pane toolbar to view the menu:



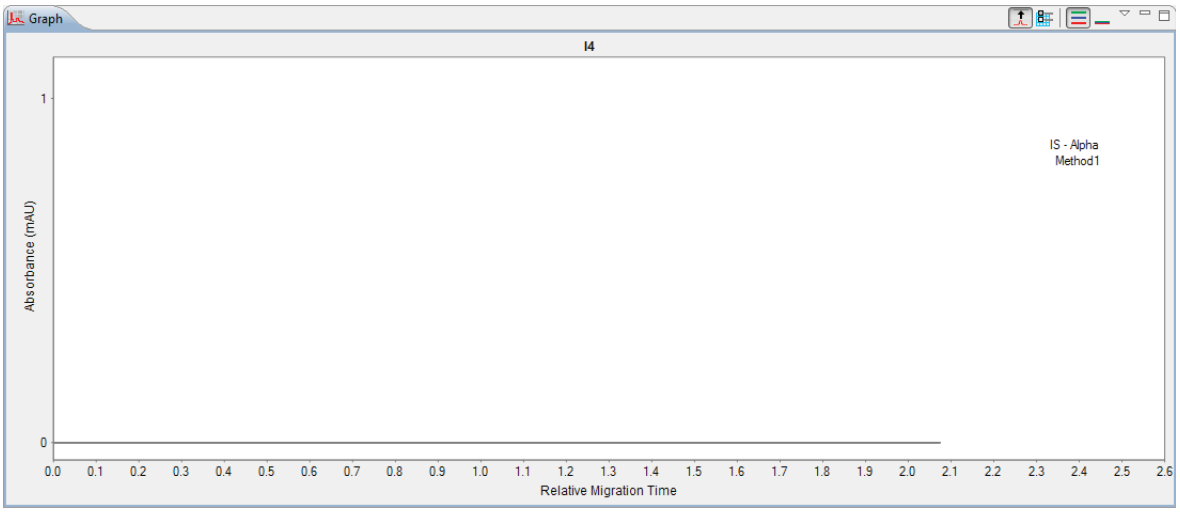
A check mark next to the menu option indicates it's currently selected, and you can select multiple options at once.

NOTE: Unless noted otherwise, graph view menu options are available for sample data only.

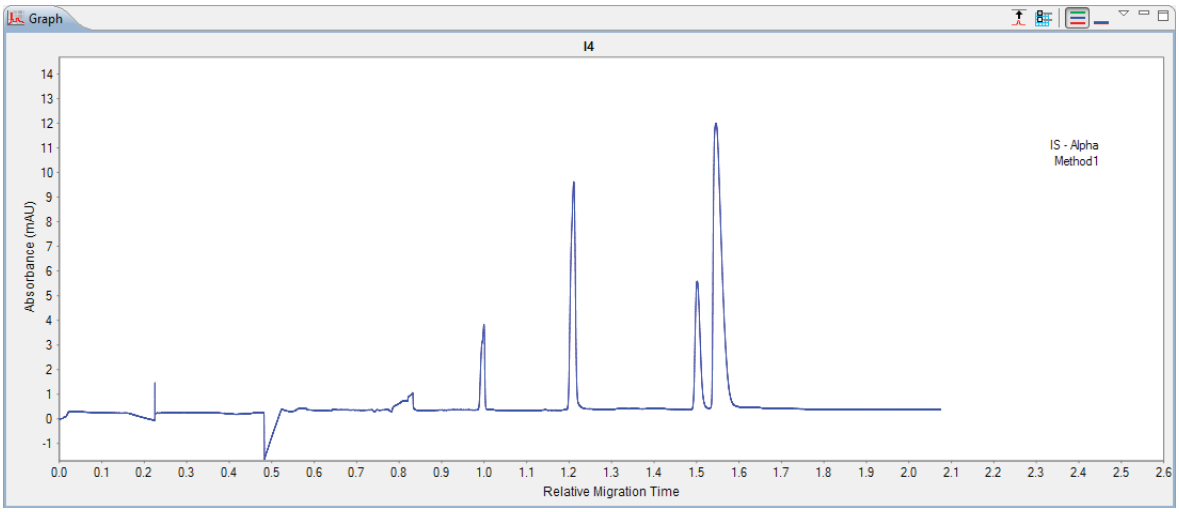
- **Sample Raw** - Clicking this option displays the basic detector values used to calculate peak absorbance. To view this you'll need to select **Auto Scale** in the Graph pane tool bar.



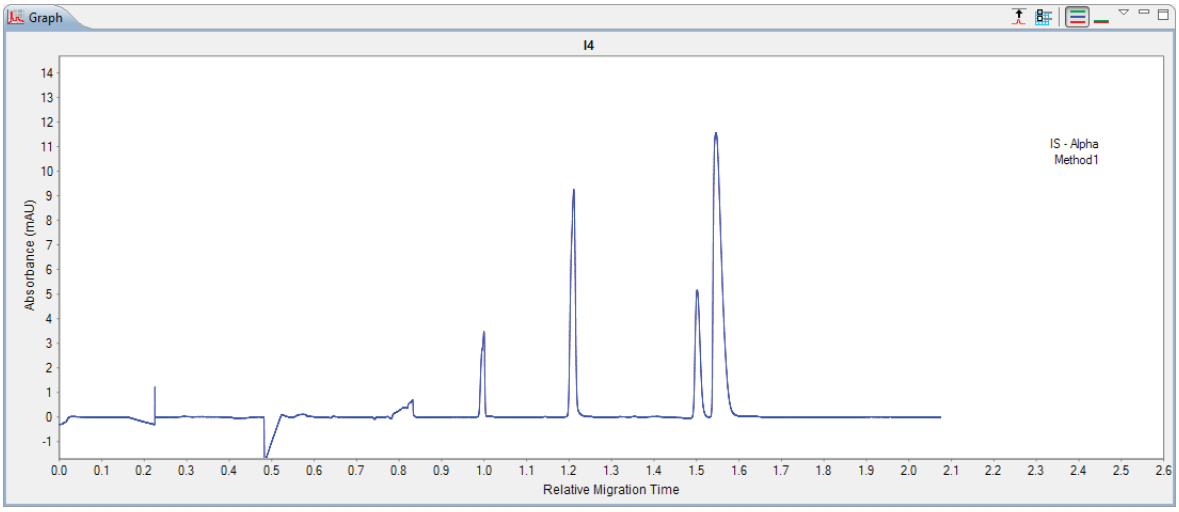
- **Sample Background** - Clicking this option displays the basic detector values used to calculate baseline absorbance. To view this you'll need to select **Auto Scale** in the Graph pane tool bar.



- **Sample** - Clicking this option displays raw, uncorrected sample data.

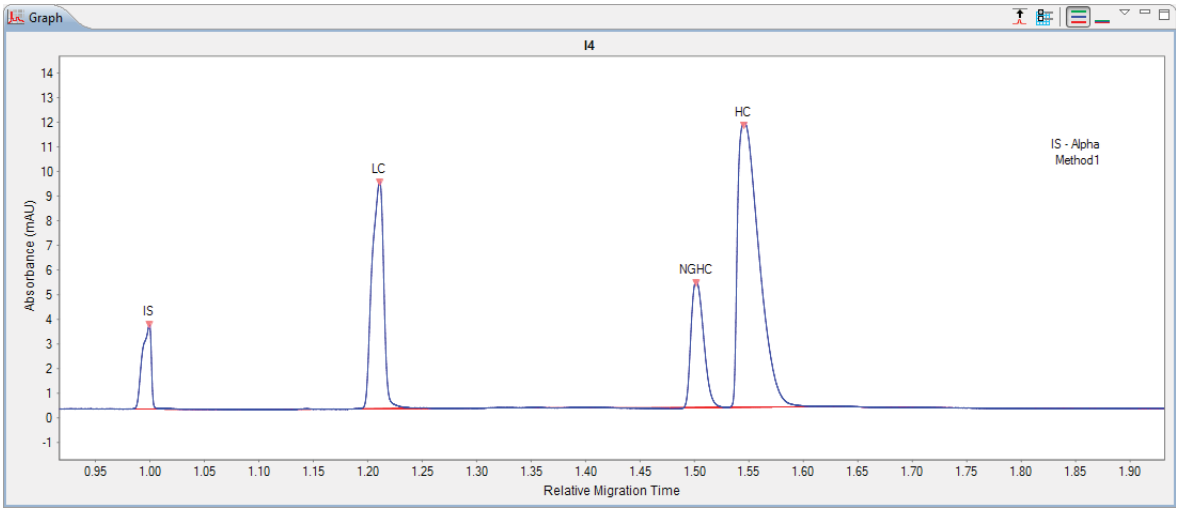


- **Sample Baseline Corrected** - Clicking this option displays sample data with the baseline subtracted (zeroed). This is the default view.



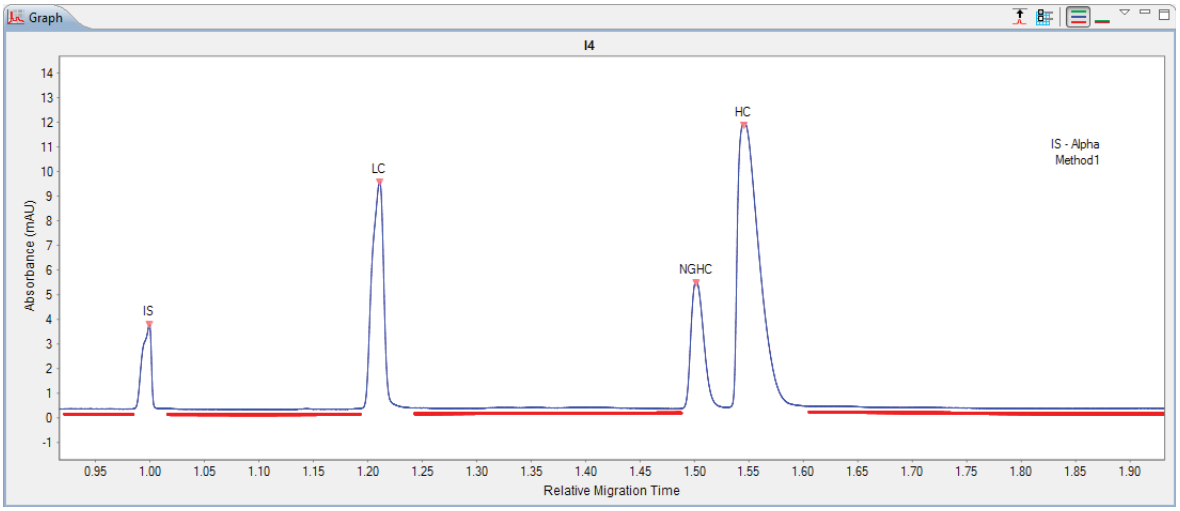
- **Baseline Fit** - Clicking this option displays the calculated baseline for the raw sample data. In this next example, both Baseline Fit and Sample are selected.

NOTE: This option is selected automatically when Baseline Fit is selected in graph options.

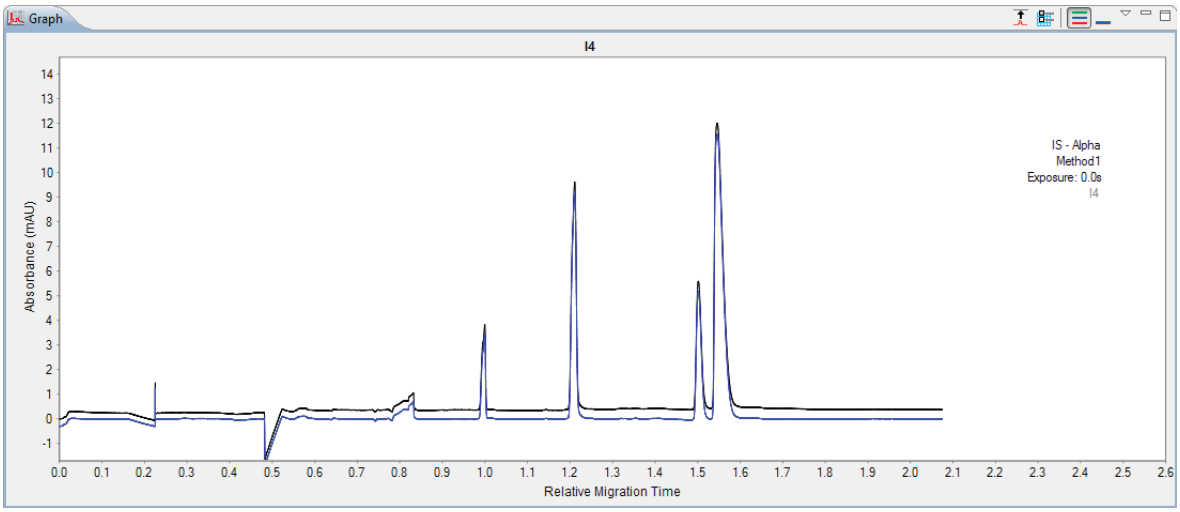


- **Baseline Points** - Clicking this option displays regions of the electropherogram considered to be at baseline. In this example, both Baseline Points and Sample are selected.

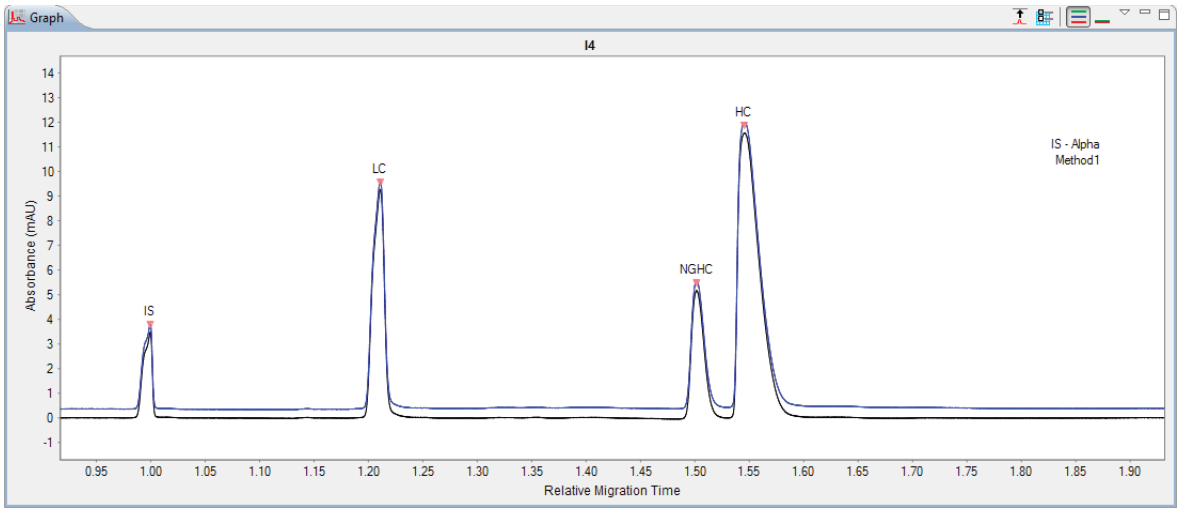
NOTE: This option is selected automatically when Baseline Fit is selected in graph options.



- **Fit** - Clicking this option displays the bounding envelope of the fitted peaks as calculated by the software for the raw sample data. In this example, both Fit and Sample Baseline Corrected are selected.



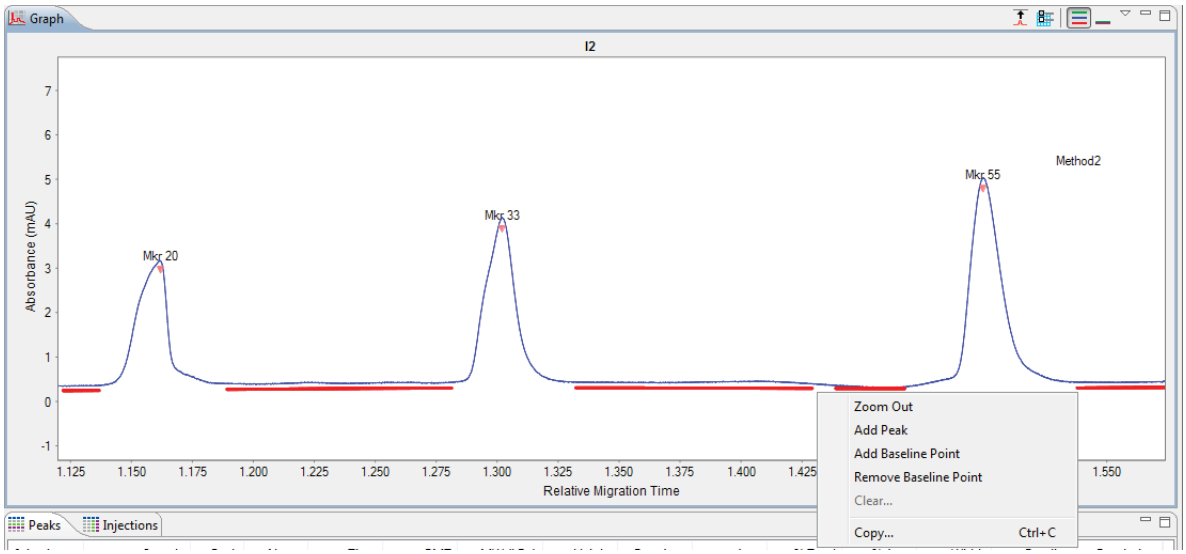
- **Fit Baseline Corrected** - Clicking this option displays the fitted peaks as calculated by the software for the sample baseline corrected data. In this example, both Fit Baseline Corrected and Sample are selected, the fit plot is on the bottom.



Adding and Removing Baseline Points

Points in the baseline can be added or removed as needed.

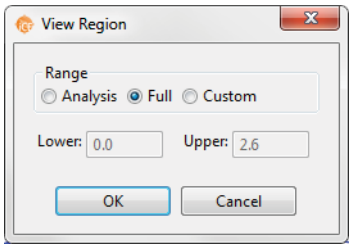
1. Click the **Graph Options** button in the graph pane toolbar and check **Baseline Points**. This will display baseline points for the raw sample data.
2. Use the mouse to draw a box around the area you want to correct. This will zoom in on the area.
3. Right click a baseline point and select **Add Baseline Point** or **Remove Baseline Point**.



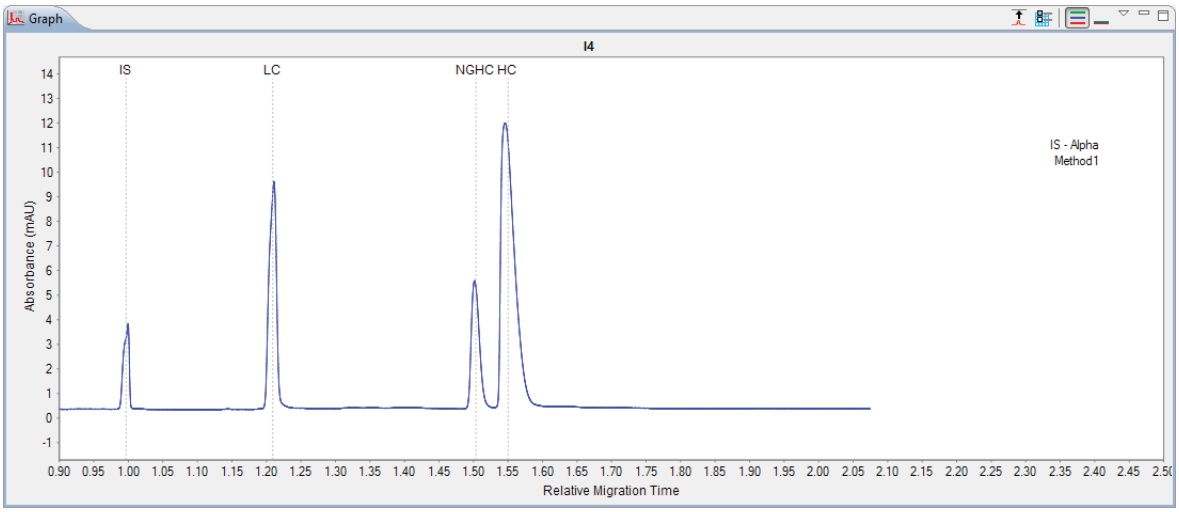
*NOTE: To clear the manual addition or removal of baseline points and go back to the original view of the data, right click in the electropherogram and click **Clear All**.*

Selecting the Graph X-axis Range

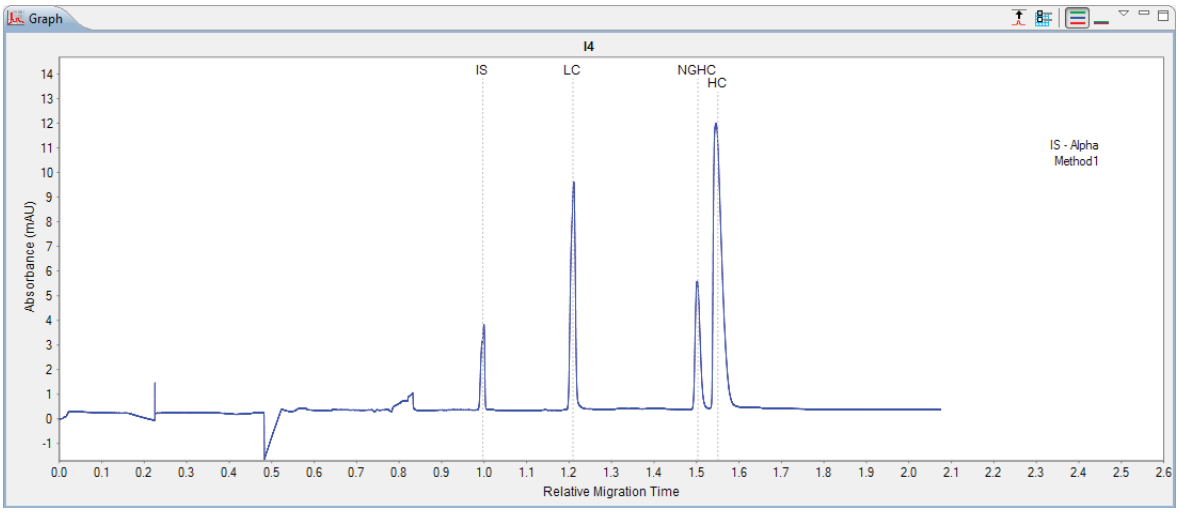
The RMT (relative migration time) range used for the x-axis can be changed. Just select **View** in the main menu and click **View Region**.



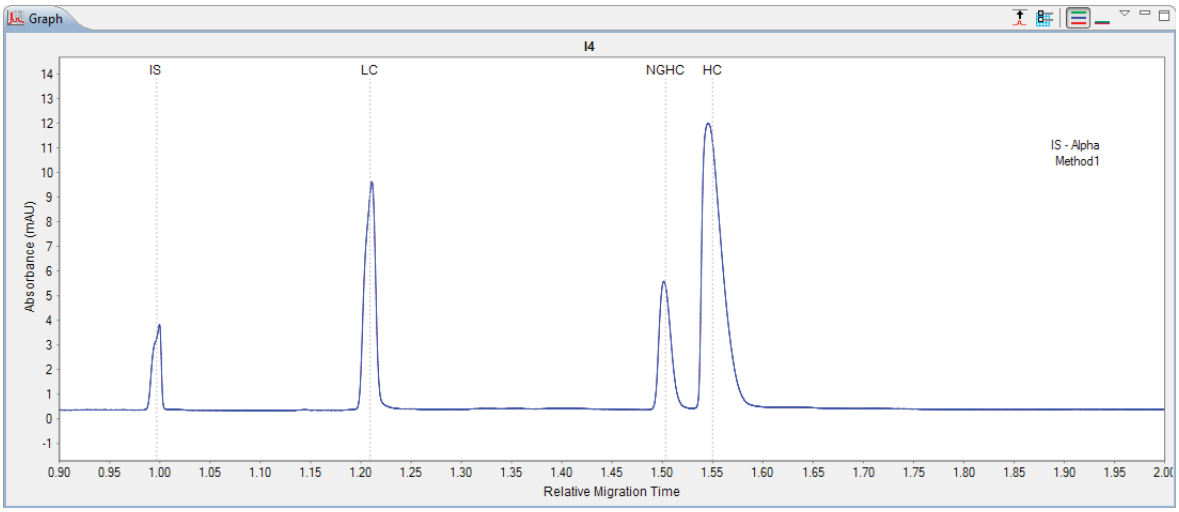
- **Analysis** sets the x-axis range of the electropherogram to what is selected in the Peak Fit range settings. To view or change these analysis settings, go to **Edit** > **Analysis** and click **Peak Fit** in the left sidebar. In this example, the lower and upper range settings are 0.9 and 2.5.



- **Full** displays the entire separation in the electropherogram. This is the default setting. In this example the lower and upper range settings are 0 and 2.6.



- **Custom** lets you manually enter the lower and upper range settings to display in the electropherogram. In this example the lower and upper range settings are 0.9 and 2.0.



NOTE: You can change the default x-axis range that Compass for iCE uses. Go to "Advanced Analysis Settings" on page 246 for more info.

Closing Run Files

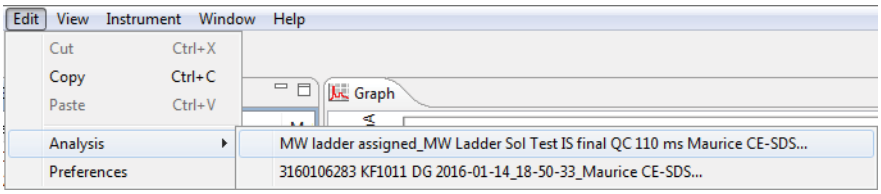
If more than one run file is open, you can close just one file or all the open files at the same time.

- **To close one run file** - In the Experiment pane, click on one of the sample rows in the file. Then click **File** from the main menu and click **Close**.
- **To close all open run files** - Select **File** from the main menu and click **Close All**.

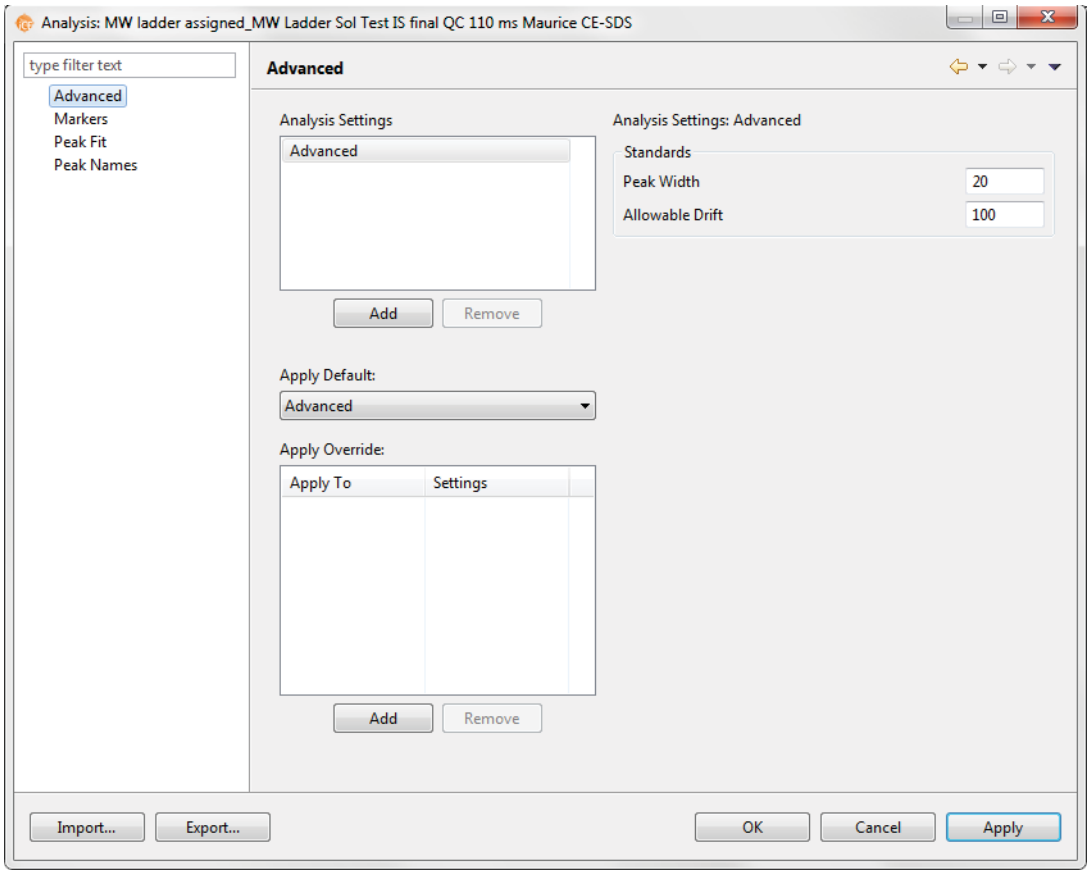
Analysis Settings Overview

Compass for iCE has many analysis features and settings that you can change to enhance your run data.

Select **Edit** in the main menu and click **Analysis**. If more than one run file is open, select the run file you want to view settings for from the list:



This opens the Analysis window:



To move between pages in the window, click on an option in the left sidebar.

- **Advanced** - Lets you customize analysis settings for the Internal Standard.
- **Markers** - Lets you customize the Internal Standard migration time, and the molecular weight and RMT Compass for iCE uses to identify your CE-SDS MW Markers.
- **Peak Fit** - Lets you customize peak fit settings for sample data.
- **Peak Names** - Lets you enter custom naming settings for sample proteins and have Compass for iCE automatically label the peaks in the run data.

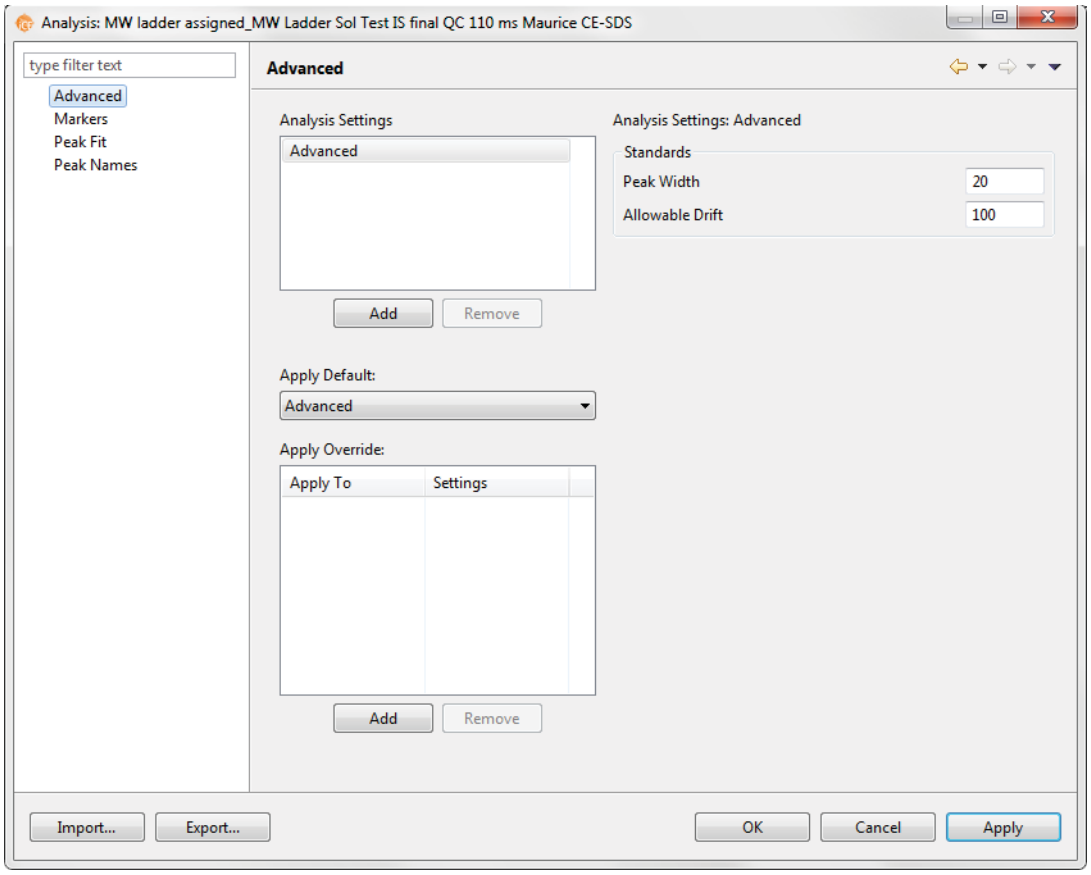
On all pages in the Analysis window:

- Click **Import** to import an analysis settings file. Go to "Importing Analysis Settings" on page 283 to learn how to do this.
- Click **Export** to export the current analysis settings file. Go to "Exporting Analysis Settings" on page 283 to learn how to do this.
- Click **Apply** to apply changes to the run file and update results in real time.
- Click **OK** to save changes to the run file and exit.
- Click **Cancel** to exit without saving changes.

Advanced Analysis Settings

This page lets you view and change analysis settings for the Internal Standard data. Select **Edit** in the main menu and click **Analysis**, then click **Advanced** in the left sidebar:

NOTE: Settings can be changed in batches before you start the run, or in run files once they're completed. If you make analysis settings changes to an executing run, they won't be saved to the final run file.



Internal Standard Settings

- **Peak Width** - The approximate width (at full width half max) used to filter out absorbance artifacts which improves recognition of standards.
- **Allowable Drift** - The distance the Internal Standard is expected to move compared to the entered number of seconds on the Markers page. This setting helps with recognition of the Internal Standard.

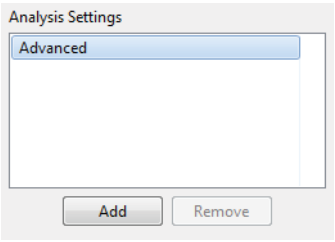
Advanced Analysis Settings Groups

Advanced analysis settings are saved as a group, and you can create multiple settings groups. Specific group settings can be applied to methods, injections, sample names or other attributes in the run data.

NOTES:
We recommend using the Compass for iCE default values for advanced analysis settings. These settings are included in the default Advanced group.

Analysis settings are run-file specific. But, settings can be imported or exported for use with other run files. See "Importing and Exporting Analysis Settings" on page 283 for more info.

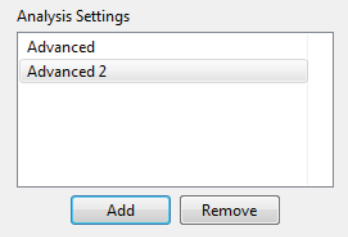
Analysis groups are displayed in the analysis settings box:



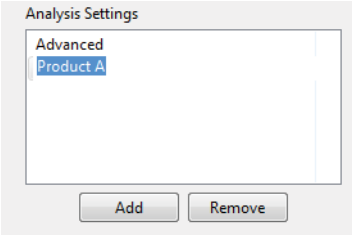
The Advanced group shown contains the Compass for iCE default analysis settings. You can make changes to this group and create new groups. To view settings for a group, click on the group name.

Creating a New Analysis Group

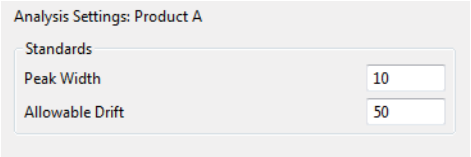
1. Select **Edit** > **Analysis**, and select **Advanced** in the left sidebar.
2. Click **Add** under the analysis settings box. A new group will be created:



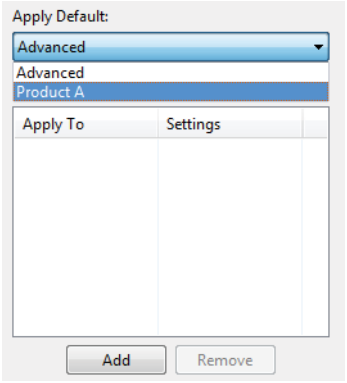
3. Click on the new group and enter a new name.



4. Change the settings in the Standards box as needed.



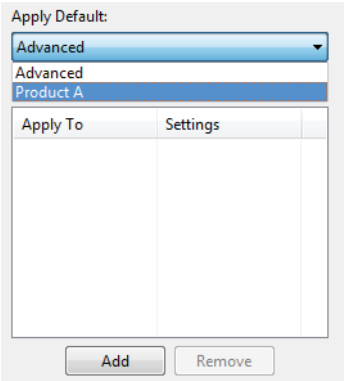
5. To use the new group as the default analysis settings for the run data, click the arrow in the drop down list next to Apply Default, then click the new group from the list. Analysis settings in the new group will then be applied to the run data.



6. Click **OK** to save changes.

Changing the Default Analysis Group

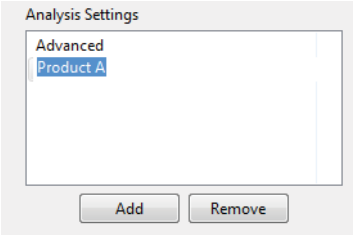
1. Select **Edit** > **Analysis**, and select **Advanced** in the left sidebar.
2. Click the arrow in the drop down list next to Apply Default, then click a new default group from the list.



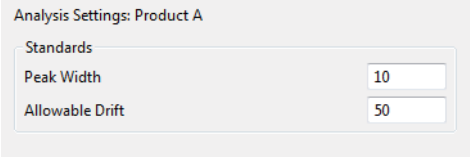
3. Click **OK** to save changes. Analysis settings in the group selected will be applied to the run data.

Modifying an Analysis Group

1. Select **Edit** > **Analysis**, and select **Advanced** in the left sidebar.
2. Click on the group in the analysis settings box you want to modify.



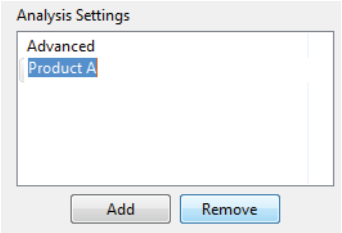
3. Change the settings in the Standards box as needed.



4. Click **OK** to save changes. The new analysis settings will be applied to the run data.

Deleting an Analysis Group

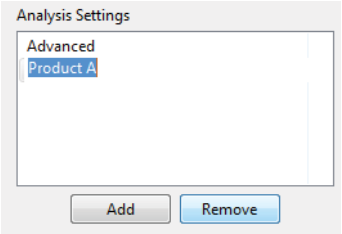
1. Select **Edit** > **Analysis**, and select **Advanced** in the left sidebar.
2. Click on the group in the analysis settings box you want to delete and click **Remove**.



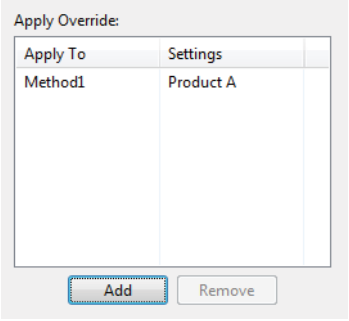
3. Click **OK** to save changes.

Applying Analysis Groups to Specific Run Data

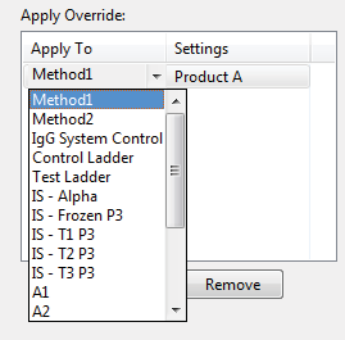
1. Select **Edit** > **Analysis**, and select **Advanced** in the left sidebar.
2. Click on the group in the analysis settings box you want to apply to specific run data.



3. Application of analysis groups to specific run data is done in the override box. Click **Add** under the override box. A default override data set will be created from sample information found in the run file.

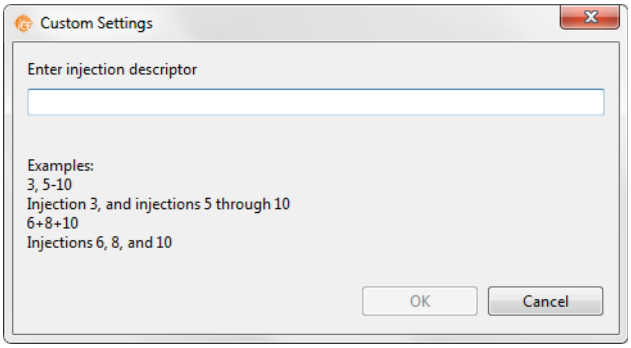


4. Click the cell in the **Apply To** column, then click the down arrow.

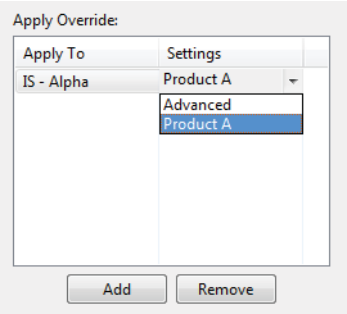


5. Select an option from the drop down list. This applies the settings group selected to specific run data as follows:

   - **Methods** - All methods in the run file display in the list. Selecting a method applies the group settings to all injections that used that method.
   - **Sample names** - All sample names in the run file display in the list, otherwise the default name of Sample shows. Selecting a sample name applies the group settings to all injections that used that sample name.
   - **Wells or vials** - All well or vial numbers used in the run display in the list. Selecting a well/vial number applies the group settings to all injections that used that well/vial.
   - **Custom settings** - Lets you choose specific injections to apply the group settings to. When you select this in the list, a pop-up box displays to let you enter a specific injection number or range of injections:



6. If you need to change the analysis group used for a data set, click the cell in the **Settings** column and click the down arrow. Select a group from the drop down list.

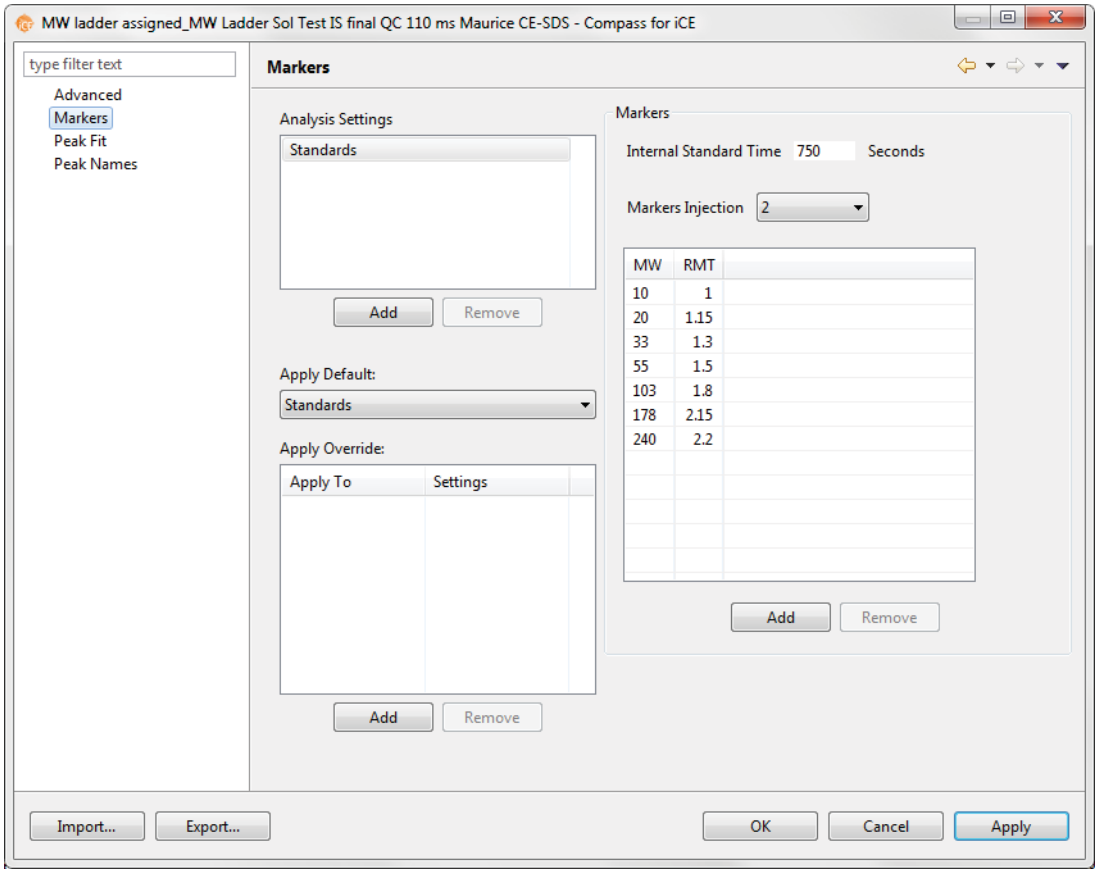


7. Repeat the previous steps to apply other groups to specific run data.
8. To remove a data set, click on its cell in the **Apply To** column, then click **Remove**.
9. Click **OK** to save changes.

Markers Analysis Settings

This page lets you select the injection for your CE-SDS MW Markers, enter a list of molecular weights and RMTs for each marker peak, and set the expected migration time of the Internal Standard for all injections. Select **Edit** in the main menu and click **Analysis**, then click **Markers** in the left sidebar.

NOTE: Settings can be changed in the batch default analysis before you start the run, or in run files once they're completed. If you make analysis settings changes to an executing run, they won't be saved to the final run file.



Markers Settings

- **Internal Standard Time** - The approximate migration time (in seconds) of the Internal Standard. This is applied to all injections.

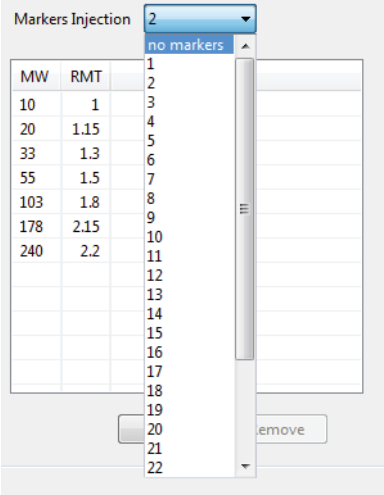
Changing the Injection Used for the CE-SDS MW Markers

You can use known markers to calculate molecular weights of your unknown sample proteins. You can select the injection you ran your CE-SDS MW Markers in, or opt to not use one.

NOTE: When the markers injection is set to no markers, the molecular weight for sample proteins in the run isn't displayed.

To change the markers injection:

1. Select **Edit** > **Analysis**, and select **Markers** in the left sidebar.
2. Click the arrow in the drop down list next to Markers Injection, then select an **injection number** or **no markers** from the list.



Compass for iCE will use the data in the selected injection to calculate molecular weights for sample proteins in the run data using the information in the table. If no markers is selected, Compass for iCE doesn't display molecular weight for sample proteins.

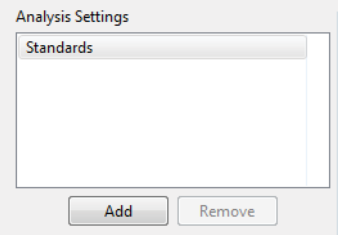
Standards Analysis Settings Groups

Standards settings are saved as a group, and you can create multiple settings groups. Specific group settings can be applied to methods, injections, sample names or other attributes in the run data.

NOTES:
We recommend using the Compass for iCE default values. These settings are included in the default Standards group.

Analysis settings are run-file specific. But, settings can be imported or exported for use with other run files. For more information see "Importing and Exporting Analysis Settings" on page 283.

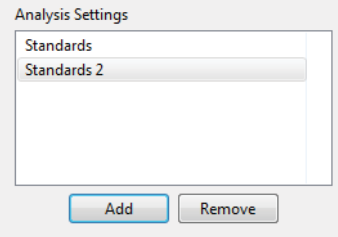
Standards groups are displayed in the analysis settings box:



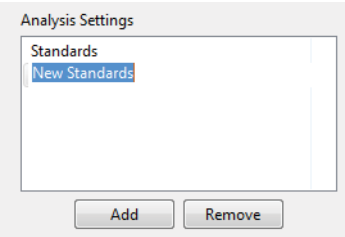
The Standards group shown uses the Compass for iCE default settings. You can make changes to this group and create new groups. To view settings for a group, click on the group name.

Creating a New Standards Group

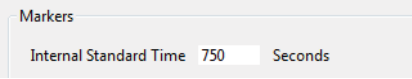
1. Select **Edit** > **Analysis**, and select **Markers** in the left sidebar.
2. Click **Add** under the analysis settings box. A new group will be created:



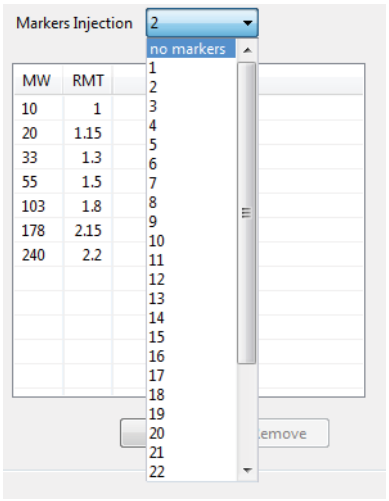
3. Click on the new group and enter a new name.



4. Change the Internal Standard time as needed.



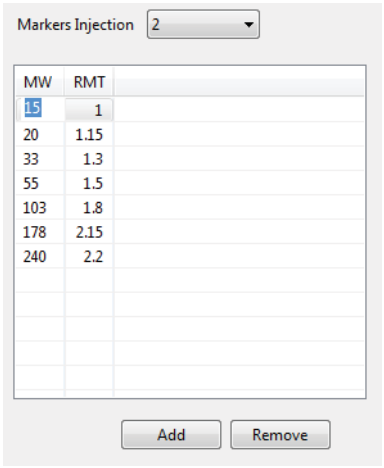
5. Click the arrow in the drop down list next to Markers Injection, then click an injection number or no markers from the list.



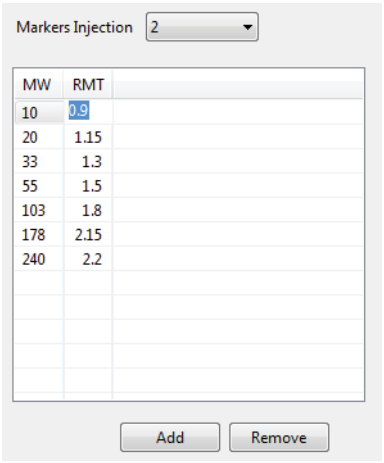
Compass for iCE will use the data in the selected injection to recalculate molecular weights for sample proteins in the run data using the information in the table. If no markers is selected, Compass for iCE doesn't display molecular weight for sample proteins.

6. If a markers injection was selected, the default Maurice CE-SDS MW Markers molecular weights and relative migration time (RMT) values are already populated in the table. If you'd like to use these values, skip to the next step. If you're using different markers, here's how to change the values:

   a. Click in the first cell in the MW column in the table and enter the molecular weight (in kDa) for the marker.



   b. Click in the first cell in the RMT column and enter a value for the marker.



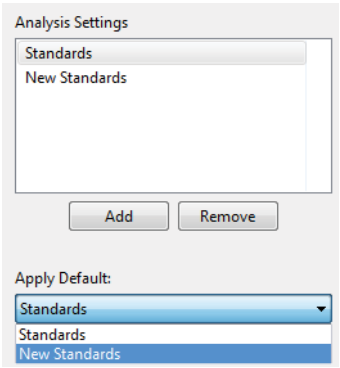
NOTE: Marker peak positions are relative to each other. Only the difference in RMT is used to help identify them. When entering marker peak information for the first time, review the marker data in the Analysis screen to find the correct peak RMT.

---

c. Repeat the steps above for the remaining markers in the table.

- **To add another marker** - Click **Add** under the table, then change the information in the new row.
- **To remove a marker** - Select its row and click **Remove**.

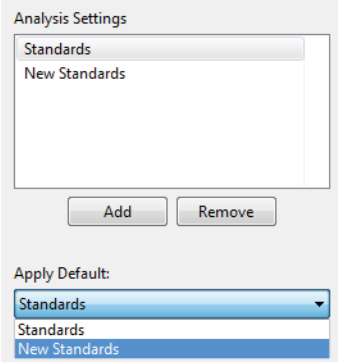
7. To use the new group as the default settings for the run, click the arrow in the drop down list next to Apply Default, then click the new group in the list. The settings in the new group will then be applied to the run data.



8. Click **OK** to save changes.

Changing the Default Standards Group

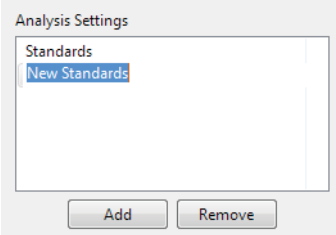
1. Select **Edit** > **Analysis**, and click **Markers** in the left sidebar.
2. Click the arrow in the drop down list next to Apply Default, then select a new default group from the list.



3. Click **OK** to save changes. Analysis settings in the group selected will be applied to the run data.

Modifying a Standards Group

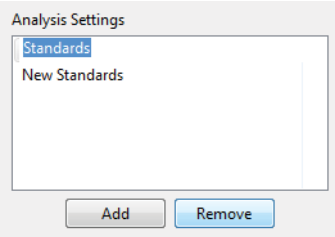
1. Select **Edit** > **Analysis**, and click **Markers** in the left sidebar.
2. Click on the group in the analysis settings box you want to modify.



3. Change the marker info as needed as in "Creating a New Standards Group" on page 255.
4. Click **OK** to save changes. The new analysis settings will be applied to the run data.

Deleting a Standards Group

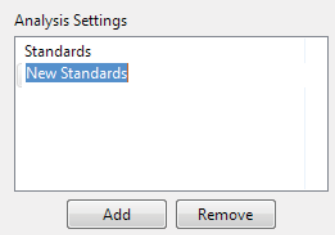
1. Select **Edit** > **Analysis**, and click **Markers** in the left sidebar.
2. Click on the group in the analysis settings box you want to delete and click **Remove**.



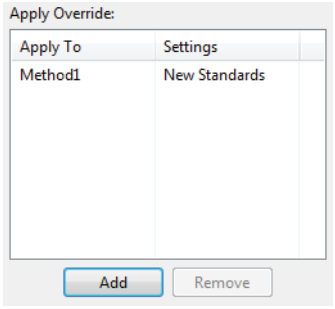
3. Click **OK** to save changes.

Applying Standards Groups to Specific Run Data

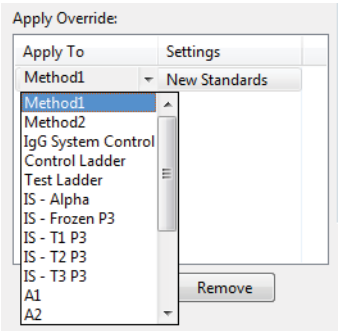
1. Select **Edit** > **Analysis**, and select **Markers** in the left sidebar.
2. Click on the group in the analysis settings box you want to apply to specific run data.



3. Application of standards groups to specific run data is done in the override box. Click **Add** under the override box. A default override data set will be created from sample information found in the run file.

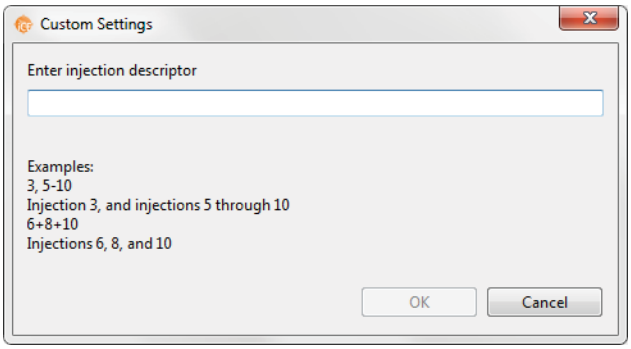


4. Click the cell in the **Apply To** column, then click the down arrow.

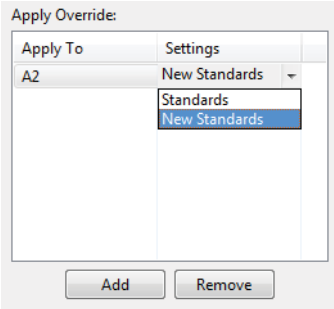


5. Select an option from the drop down list. This applies the settings group selected to specific run data as follows:

   - **Methods** - All methods in the run file display in the list. Selecting a method applies the group settings to all injections that used that method.
   - **Sample names** - All sample names in the run file display in the list, otherwise the default name of Sample shows. Selecting a sample name applies the group settings to all injections that used that sample name.
   - **Wells or vials** - All well or vial numbers used in the run display in the list. Selecting a well/vial number applies the group settings to all injections that used that well/vial.
   - **Custom settings** - Lets you choose specific injections to apply the group settings to. When you select this in the list, a pop-up box displays to let you enter a specific injection number or range of injections:



6. If you need to change the analysis group used for a data set, click the cell in the **Settings** column and click the down arrow. Select a group from the drop down list.

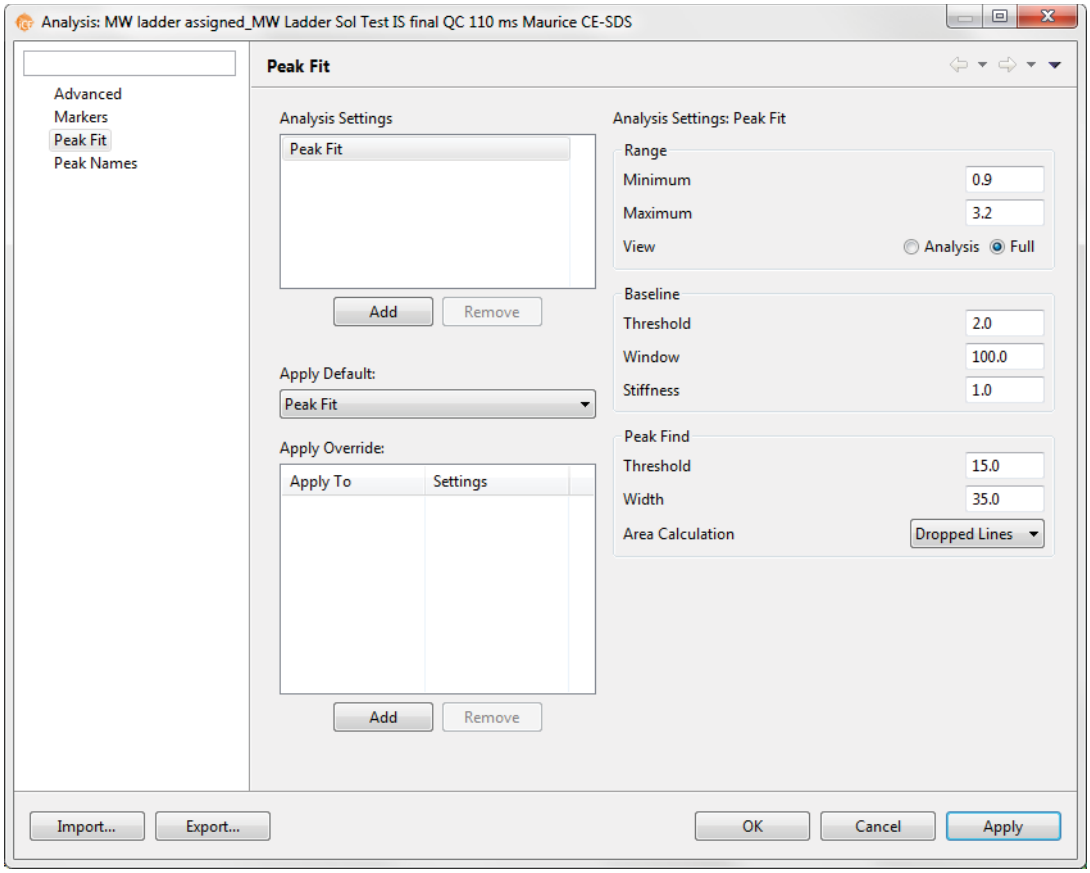


7. Repeat the previous steps to apply other groups to specific run data.
8. To remove a data set, click on its cell in the **Apply To** column, then click **Remove**.
9. Click **OK** to save changes.

Peak Fit Analysis Settings

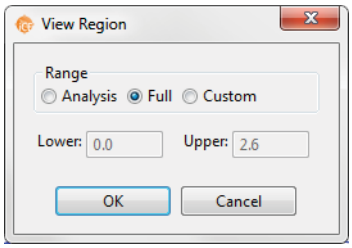
This page lets you view and change peak fit settings for sample data. Select **Edit** in the main menu and click **Analysis**, then click **Peak Fit** in the left sidebar:

NOTE: Settings can be changed in the batch default analysis before you start the run, or in run files once they're completed. If you make analysis settings changes to an executing run, they won't be saved to the final run file.



Range Settings

- **Minimum** - The RMT value below which peaks won't be identified. This value is also used as the default lower RMT range for data displayed in the electropherogram.
- **Maximum** - The RMT value above which peaks won't be identified. This value is also used as the default upper RMT range for data displayed in the electropherogram.
- **View** - Sets the default range to either Full or Analysis for the electropherogram x-axis range in the View Region window (select **View** in the main menu and click **View Region**).



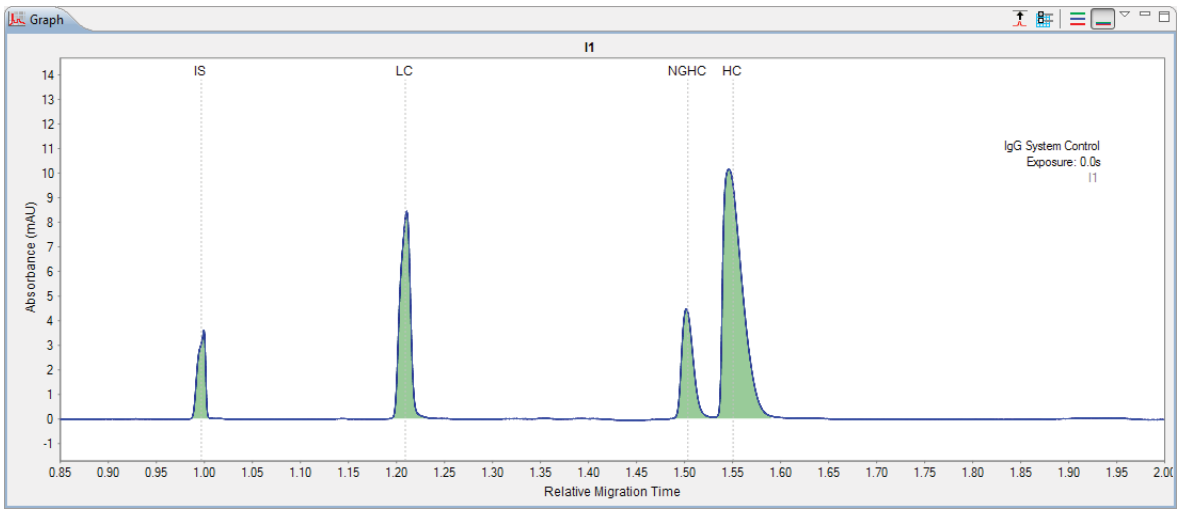
- **Analysis** sets the x-axis range of the electropherogram to the Peak Fit range minimum and maximum settings in the electropherogram.
- **Full** displays the entire separation range of the run data in the electropherogram. This is the default setting.

Baseline Settings

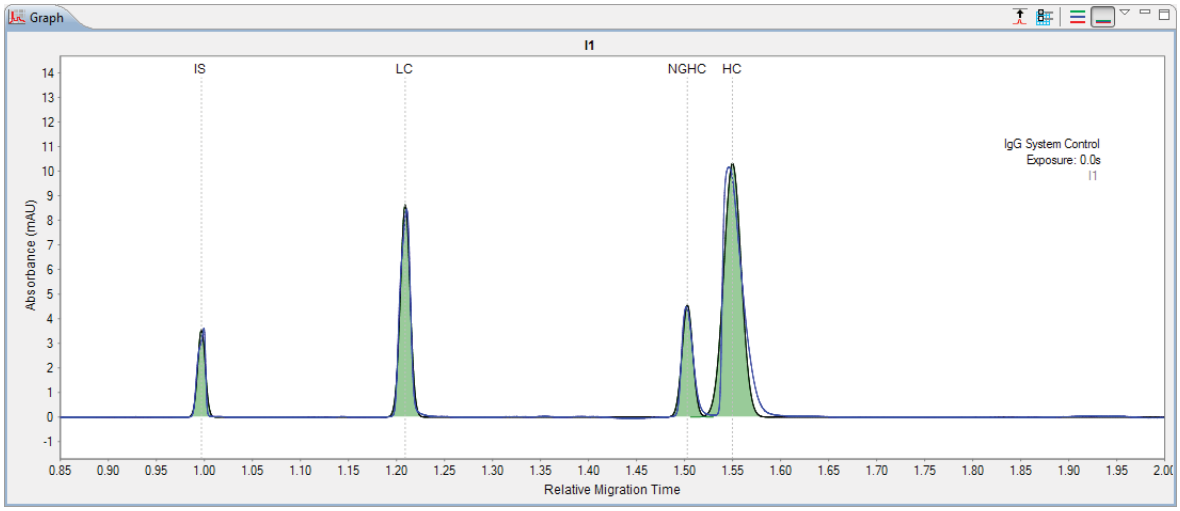
- **Threshold** - The variance, or roughness, in a baseline data segment below which a point is called part of the baseline.
- **Window** - How long baseline data segments are expected to be in pixels. Shorter segments let the baseline follow plateau sections of the signal.
- **Stiffness** - The amount the baseline is allowed to vary from a straight line. Settings between 0.1 and 1.0 make the baseline fit closer to a straight line. Settings from 1.0 to 10.0 will make the baseline fit follow the data more closely.

Peak Find Settings

- **Threshold** - The minimum signal to noise ratio required for a peak to be identified. A setting of 1.0 will detect many peaks, a setting of 10.0 will detect fewer peaks.
- **Width** - The approximate peak width (at full width half max) in pixels used to detect peaks. The minimum value for this setting is 3.0. Larger widths help eliminate the detection of shoulder and noise peaks.
- **Area Calculation** - Two fits are used, either Gaussian Fit or Dropped Lines. These settings can be changed before or after the run is finished.
  - For CE-SDS applications, peak area is calculated using Dropped Lines by default. This type of area calculation is also often called the perpendicular drop method. This is the preferred method when peaks overlap or are close to each other. It draws two vertical lines from the left and right bounds of the peak down to the x-axis and then measures the total area bounded by the signal curve, the x-axis (y=0 line), and the two vertical lines.



- This next view is of the same data using Gaussian fit instead:



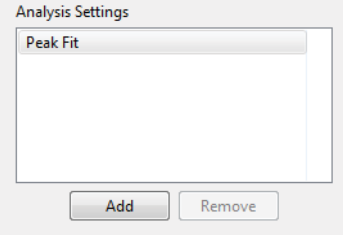
Peak Fit Analysis Settings Groups

Peak fit settings are saved as a group, and you can create multiple settings groups. Specific group settings can then be applied to methods, injections, sample names or other attributes in the run data.

NOTES:
We recommend using the Compass for iCE default values for peak fit analysis settings. These settings are included in the default Peak Fit group.

Analysis settings are run-file specific. But, settings can be imported or exported for use with other run files. For more information see "Importing and Exporting Analysis Settings" on page 283.

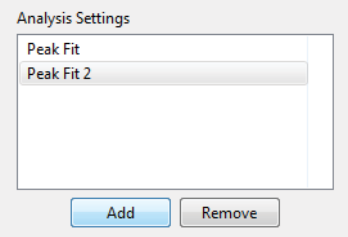
Peak fit groups are displayed in the analysis settings box:



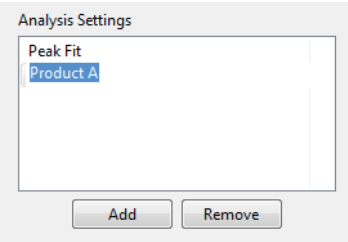
The Peak Fit group shown contains the Compass for iCE default analysis settings. You can make changes to this group and create new groups. To view settings for a group, click on the group name.

Creating a New Peak Fit Group

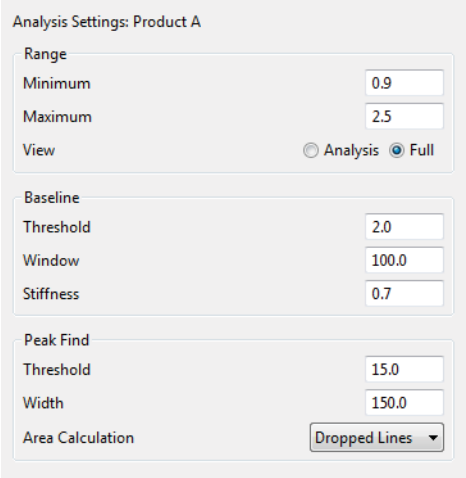
1. Select **Edit** > **Analysis**, and select **Peak Fit** in the left sidebar.
2. Click **Add** under the analysis settings box. A new group will be created:



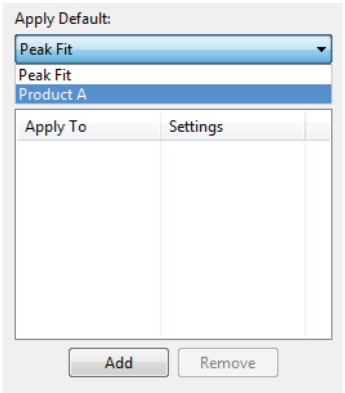
3. Click on the new group and enter a new name.



4. Change the settings in the range, baseline or peak find boxes as needed.



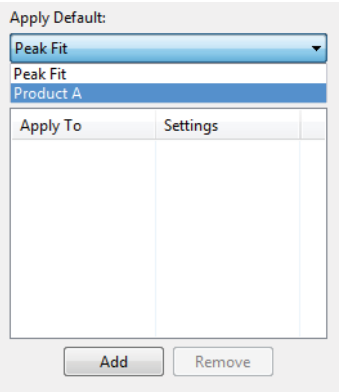
5. To use the new group as the default peak fit settings for the run file data, click the arrow in the drop down list next to Apply Default, then click the new group from the list. Peak fit settings in the new group will then be applied to the run data.



6. Click **OK** to save changes.

Changing the Default Peak Fit Group

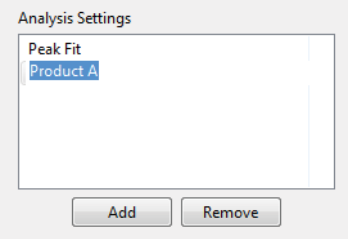
1. Select **Edit** > **Analysis**, and select **Peak Fit** in the left sidebar.
2. Click the arrow in the drop down list next to Apply Default, then click a new default group from the list.



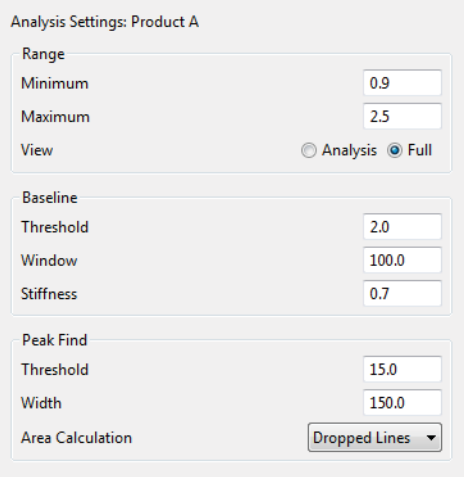
3. Click **OK** to save changes. Peak fit settings in the group selected will be applied to the run data.

Modifying a Peak Fit Group

1. Select **Edit** > **Analysis**, and click **Peak Fit** in the left sidebar.
2. Click on the group in the analysis settings box you want to modify.



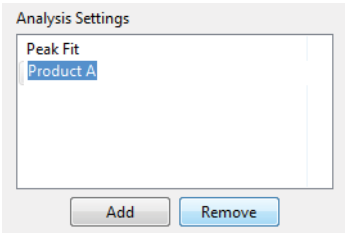
3. Change the settings in the range, baseline or peak find boxes as needed.



4. Click **OK** to save changes. The new peak fit settings will be applied to the run data.

Deleting a Peak Fit Group

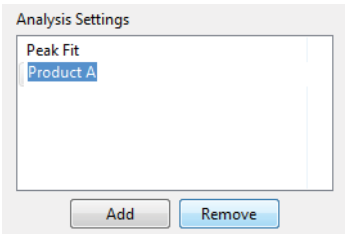
1. Select **Edit** > **Analysis**, and select **Peak Fit** in the left sidebar.
2. Click on the group in the analysis settings box you want to delete and click **Remove**.



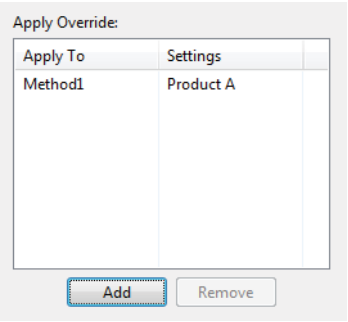
3. Click **OK** to save changes.

Applying Peak Fit Groups to Specific Run Data

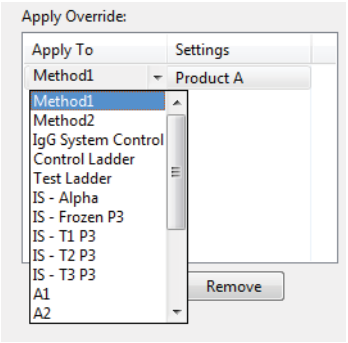
1. Select **Edit** > **Analysis**, and select **Peak Fit** in the left sidebar.
2. Click on the group in the analysis settings box you want to apply to specific run data.



3. Application of analysis groups to specific run data is done in the override box. Click **Add** under the override box. A default override data set will be created from sample information found in the run file.



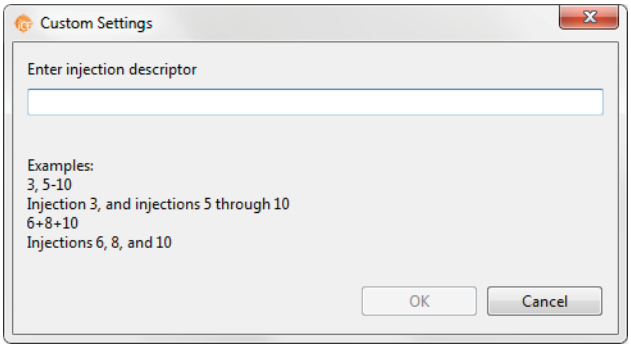
4. Click the cell in the **Apply To** column, then click the down arrow.



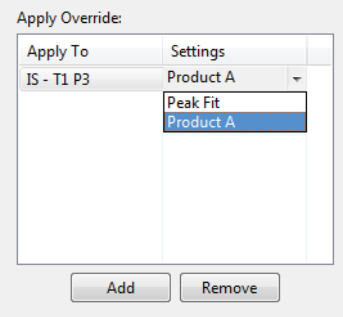
5. Select an option from the drop down list. This applies the settings group selected to specific run data as follows:

   - **Methods** - All methods in the run file display in the list. Selecting a method applies the group settings to all injections that used that method.
   - **Sample names** - All sample names in the run file display in the list, otherwise the default name of Sample shows. Selecting a sample name applies the group settings to all injections that used that sample name.

- **Wells or vials** - All well or vial numbers used in the run display in the list. Selecting a well/vial number applies the group settings to all injections that used that well/vial.
- **Custom settings** - Lets you choose specific injections to apply the group settings to. When you select this in the list, a pop-up box displays to let you enter a specific injection number or range of injections:



6. If you need to change the analysis group used for a data set, click the cell in the **Settings** column and click the down arrow. Select a group from the drop down list.

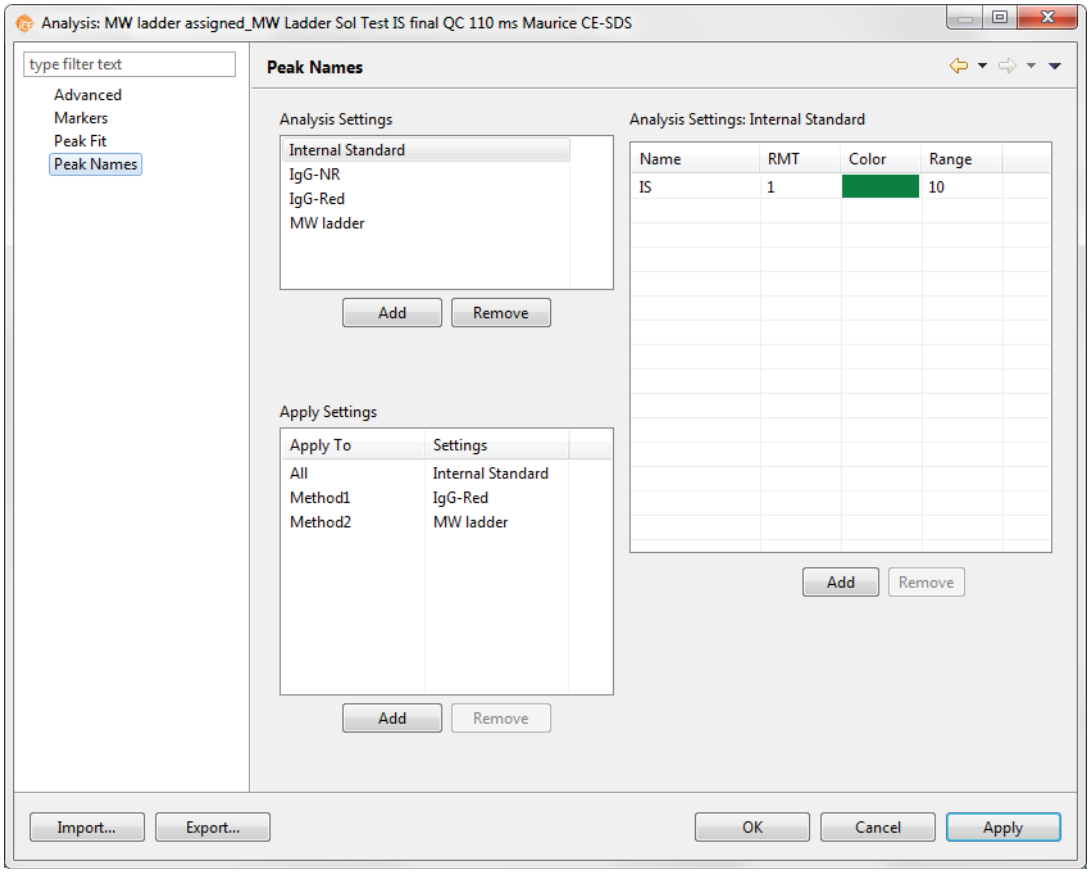


7. Repeat the previous steps to apply other groups to specific run data.
8. To remove a data set, click on its cell in the **Apply To** column, then click **Remove**.
9. Click **OK** to save changes.

Peak Names Settings

This page lets you view and change custom naming settings for sample proteins. Select **Edit** in the main menu and click **Analysis**, then click **Peak Names** in the left sidebar.

NOTE: Settings can be changed in the batch default analysis before you start the run, or in run files once they're completed. If you make analysis settings changes to an executing run, they won't be saved to the final run file.

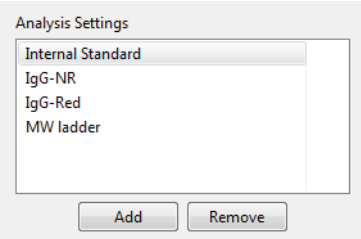


Peak Names Analysis Settings Groups

Peak name settings are saved as a group, and you can create multiple settings groups. Specific group settings can be applied to methods, injections, sample names or other attributes in the run data.

NOTE: Analysis settings are run-file specific. But, settings can be imported or exported for use with other run files. For more information see "Importing and Exporting Analysis Settings" on page 283.

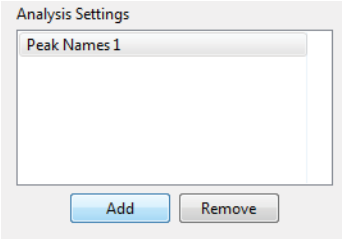
Peak name groups are displayed in the analysis settings box:



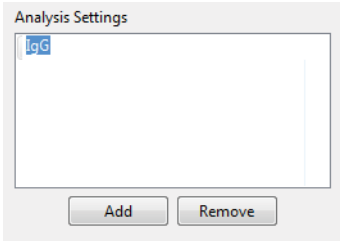
There aren't any Compass for iCE default settings groups, but you can make changes to groups you've created and create new groups. To view settings for a group, click on the group name in the analysis settings box.

Creating a Peak Names Group

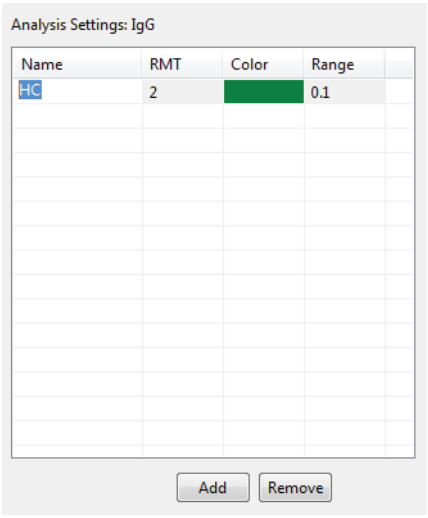
1. Select **Edit** > **Analysis**, and select **Peak Names** in the left sidebar.
2. Click **Add** under the analysis settings box.



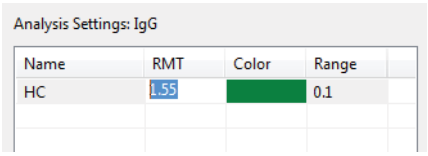
3. Enter a new name for the group.



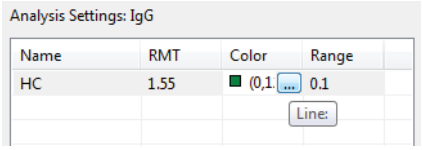
4. Click in the first cell in the **Name** column in the analysis settings peak table and enter a sample protein name.



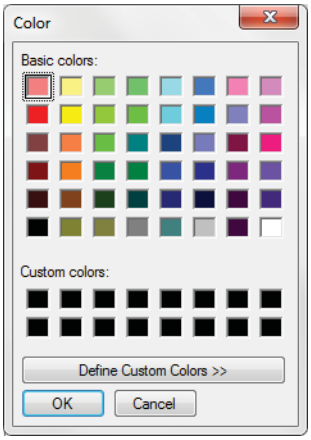
5. Click in the first cell in the **RMT** column and enter the relative migration time for the sample protein.



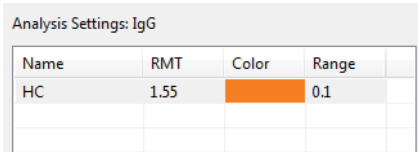
6. Click in the first cell in the **Color** column, then click the button.



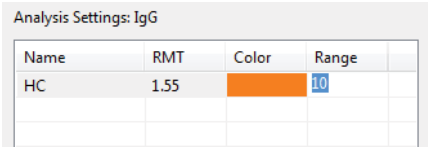
The color selection box displays:



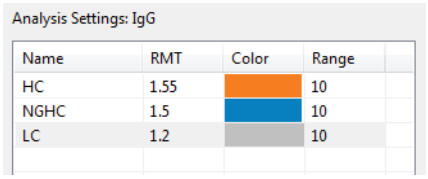
7. The color you pick is used to identify the sample protein peak in the Peaks and Injections panes in the Analysis screen. Click a color or define a custom color and click **OK**. The color selection will update in the table:



8. Click in the first cell in the **Range** column.



9. Enter a % range for the RMT entered. Compass for iCE will automatically name peaks found within this percent of the RMT. For example, if the RMT entered is 2 and a 10% range is used, all peaks with RMTs between 1.8 and 2.2 will be identified with this peak name and color.
10. To add another sample protein, click **Add** under the peak table. Repeat the previous steps for other sample proteins. In this example, three proteins were entered:

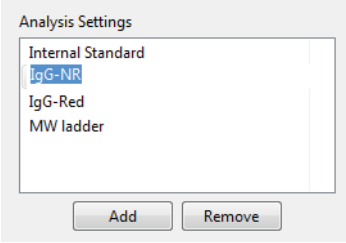


To remove a sample protein, select its row and click **Remove**.

11. Click **OK** to save changes.

Modifying a Peak Names Group

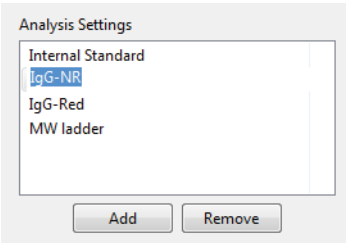
1. Select **Edit** > **Analysis**, then click **Peak Names** in the left sidebar.
2. Click on the group in the analysis settings box you want to modify.



3. Change the information in the analysis settings peak table as described in "Creating a Peak Names Group" on page 272.
4. Click **OK** to save changes.

Deleting a Peak Names Group

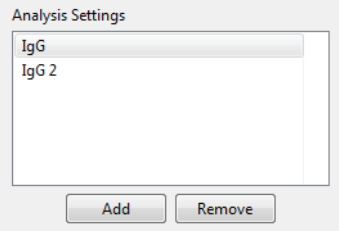
1. Select **Edit** > **Analysis**, then click **Peak Names** in the left sidebar.
2. Click on the group in the analysis settings box you want to delete and click **Remove**.



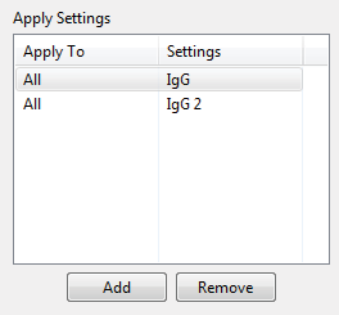
3. Click **OK** to save changes.

Applying Peak Names Groups to Run Data

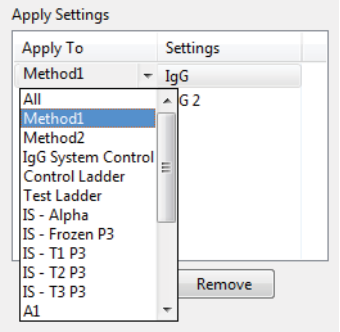
1. Select **Edit** > **Analysis**, then click **Peak Names** in the options list.
2. Click on the group in the analysis settings box you want to apply to specific run data.



3. Application of peak names groups to specific run data is done in the apply settings box. A default data set automatically gets created whenever you create a new group and it's applied to all injections in the run. You can either modify the default group or click **Add** under the box to create a new one.

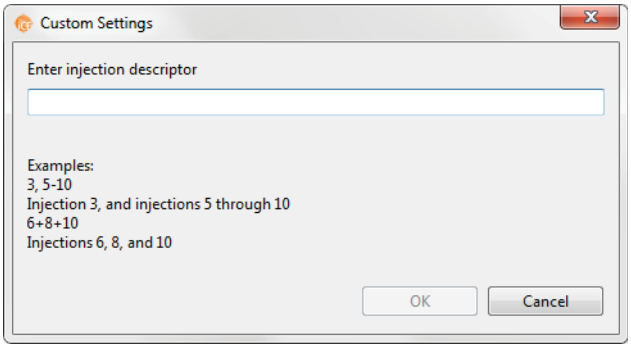


4. Click the cell in the **Apply To** column, then click the down arrow.

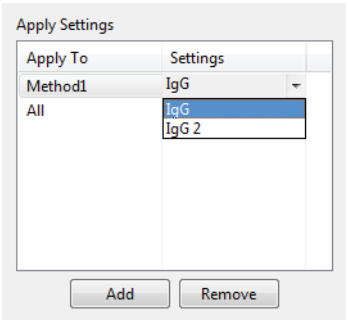


5. Select an option from the drop down list. This applies the peak names group selected to specific run data as follows:

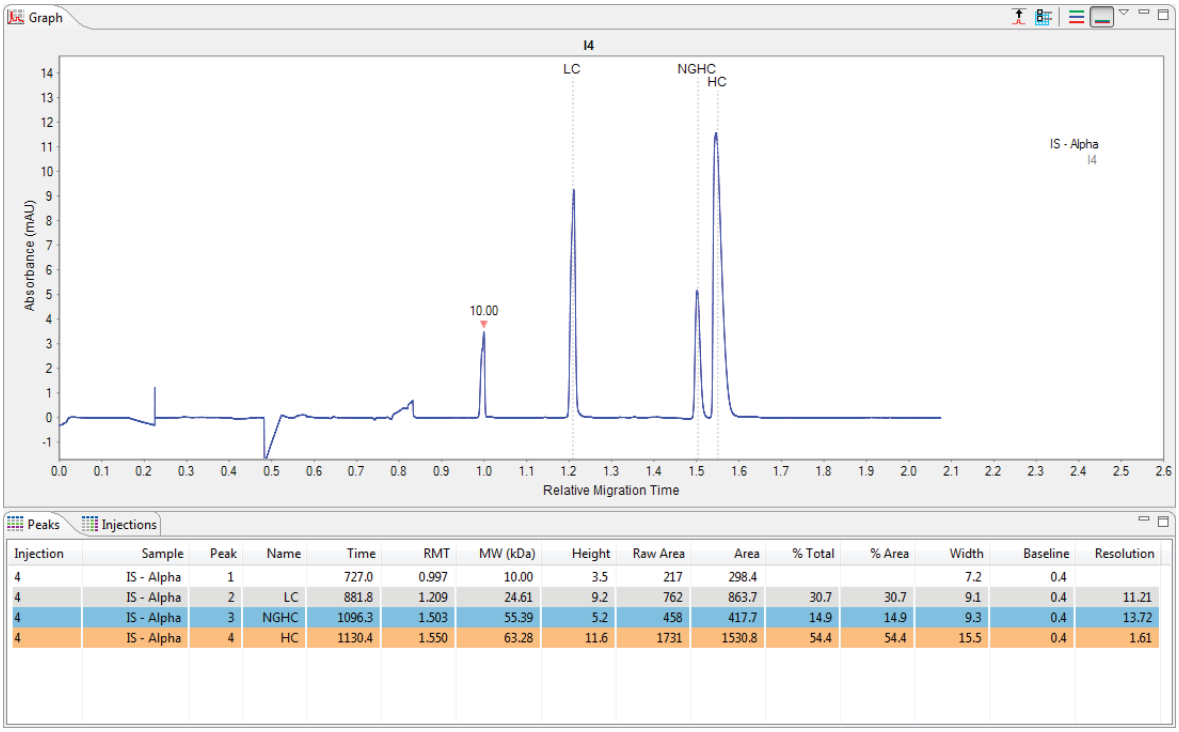
- **All** - Selecting this applies peak names group settings to all injections.
- **Methods** - All methods in the run file display in the list. Selecting a method applies the group settings to all injections that used that method.
- **Sample names** - All sample names in the run file display in the list, otherwise the default name of Sample shows. Selecting a sample name applies the group settings to all injections that used that sample name.
- **Wells or vials** - All well or vial numbers used in the run display in the list. Selecting a well/vial number applies the group settings to all injections that used that well/vial.
- **Custom settings** - Lets you choose specific injections to apply the group settings to. When you select this in the list, a pop-up box displays to let you enter a specific injection number or range of injections:



6. If you need to change the peak names group used for a data set, click the cell in the **Settings** column and click the down arrow. Select a group from the drop down list.



7. Repeat the previous steps to apply other groups to specific run data.
8. To remove a data set, click on its cell in the **Apply To** column, then click **Remove**.
9. Click **OK** to save changes. Named peaks will be identified with a peak name label in the electropherogram and color-coded in the Peaks and Injections panes:

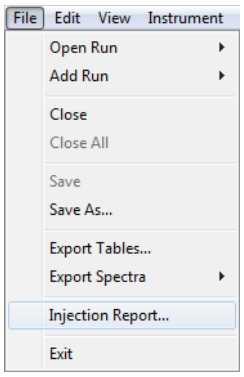


Injection	Sample	Peak	Name	Time	RMT	MW (kDa)	Height	Raw Area	Area	% Total	% Area	Width	Baseline	Resolution
4	IS - Alpha	1		727.0	0.997	10.00	3.5	217	298.4			7.2	0.4	
4	IS - Alpha	2	LC	881.8	1.209	24.61	9.2	762	863.7	30.7	30.7	9.1	0.4	11.21
4	IS - Alpha	3	NGHC	1096.3	1.503	55.39	5.2	458	417.7	14.9	14.9	9.3	0.4	13.72
4	IS - Alpha	4	HC	1130.4	1.550	63.28	11.6	1731	1530.8	54.4	54.4	15.5	0.4	1.61

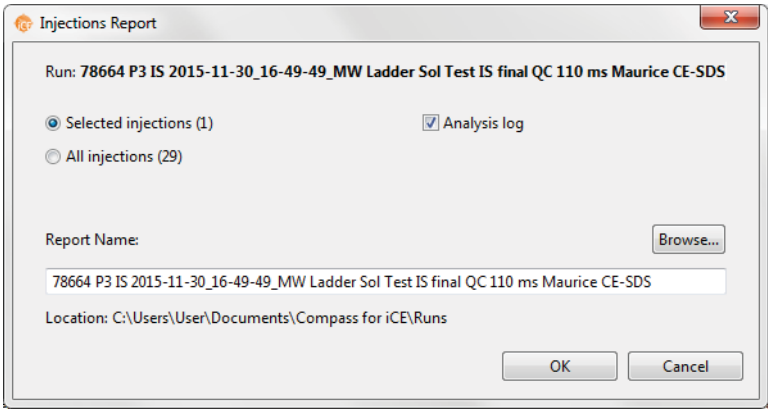
Injection Reports

You can export PDF files of the raw and analyzed data, IV plot, peaks table, sample and system info for individual or all injections in a run file. You can also export the run history with all analysis events.

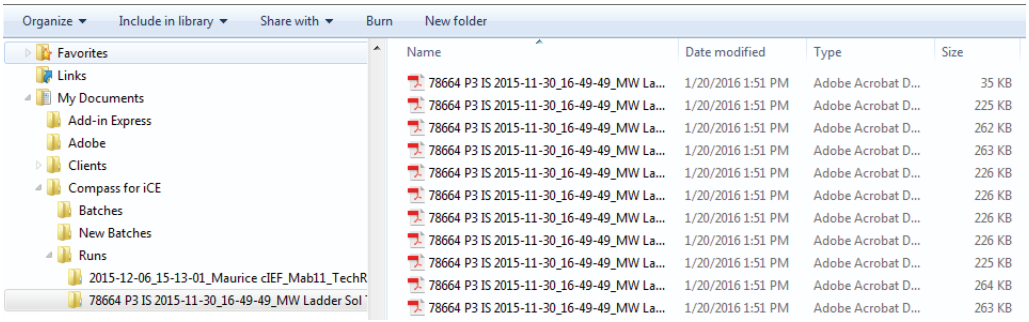
1. Click **File > Open Run** and select a run file.
2. If you want reports for all injections, skip to the next step. If you only want reports for certain injections, in the Experiment pane:
   - **To select sequential injections:** Select the first injection, then hold the **Shift** key and select the last injection you want a report for. This selects all rows between the two injections.
   - **To select specific injections:** Hold the **Ctrl** key and select just the injections you want reports for.
3. Select **File** from the main menu in either screen and click **Injection Report**.



4. In the Injection Reports window:
   d. Choose either **Selected injections** or **All injections**.
   e. Select the **Analysis log** checkbox if you want a run history report with all analysis events.
   f. The report name defaults to the run file name. If you want to change it, type in the **Report Name** box to make updates.
   g. Click **OK**.



5. The Injection Report PDF(s) are exported to the Runs folder in the Compass for iCE directory. They'll be in a folder with the report name used in the prior step. When the reports are done, the folder opens for you automatically.



Example Analysis and Injection Report

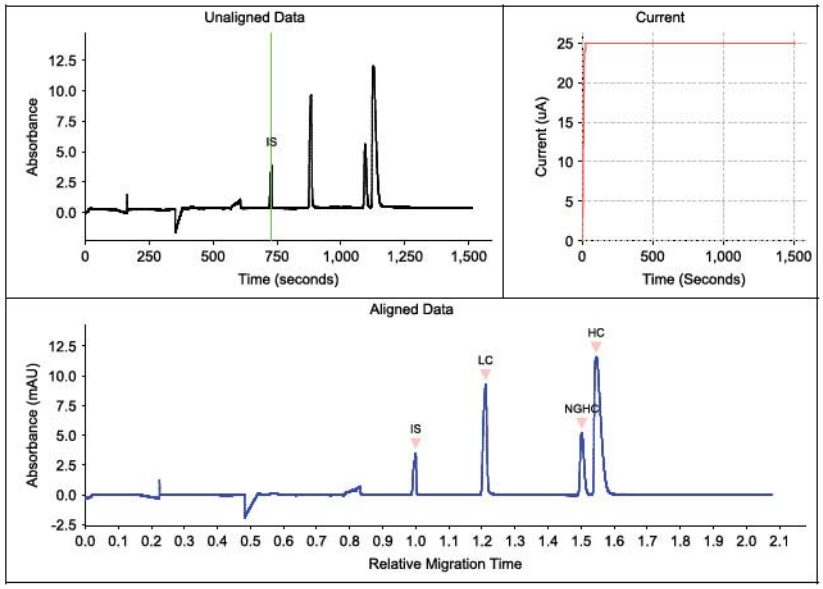
Run 78664 P3 IS 2015-11-30_16-49-49_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS

Analysis Log

Date	User Name	Message	Comment
11/30/2015 4:50 PM		Started run: 78664 P3 IS 2015-11-30_16-49-49_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS_Assay: MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.batch	
12/01/2015 11:19 AM		Saved analysis changes	
		Added Peak Names Apply Settings "apply Internal Standard to all"	
		Added Peak Names Apply Settings "apply IgG-Red to Method1"	
		Added Peak Names Apply Settings "apply MW ladder to Method2"	
		Added Peak Names Group Internal Standard	
		Protein name: IS RMT: 1.0 Color: 32512 Range: 10.0	
		Added Peak Names Group IgG-NR	
		Protein name: IgG RMT: 2.25 Color: 32512 Range: 10.0	
		Protein name: NG-IgG RMT: 2.18 Color: 32512 Range: 10.0	
		Protein name: frag1 RMT: 2.13 Color: 32512 Range: 10.0	
		Protein name: frag2 RMT: 2.07 Color: 32512 Range: 10.0	
		Protein name: frag3 RMT: 2.0 Color: 32512 Range: 10.0	
		Protein name: frag4 RMT: 1.95 Color: 32512 Range: 10.0	
		Protein name: frag5 RMT: 1.92 Color: 32512 Range: 10.0	
		Protein name: frag6 RMT: 1.77 Color: 32512 Range: 10.0	
		Protein name: frag7 RMT: 1.72 Color: 32512 Range: 10.0	
		Protein name: frag8 RMT: 1.57 Color: 32512 Range: 10.0	
		Protein name: frag9 RMT: 1.5 Color: 32512 Range: 10.0	
		Protein name: frag10 RMT: 1.22 Color: 32512 Range: 10.0	
		Added Peak Names Group IgG-Red	
		Protein name: HC RMT: 1.55 Color: 32512 Range: 10.0	
		Protein name: NGHC RMT: 1.5 Color: 32512 Range: 10.0	
		Protein name: LC RMT: 1.2 Color: 32512 Range: 10.0	
		Added Peak Names Group MW ladder	

Created: Thu 3:16 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\MW ladder assigned_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.mbz
Computer: JRichards

Injection 4: IS - Alpha



Peaks

Peak	Name	Time	RMT	MW (kDa)	Height	Raw Area	Area	%Total	%Area	Width	Baseline	Resolution
1	IS	727.0	0.997	10.00	3.5	217	298.4		100.0	7.2	0.4	
2	LC	881.8	1.209	24.61	9.2	762	863.7	30.7	30.7	9.1	0.4	11.21
3	NGHC	1096.3	1.503	55.39	5.2	458	417.7	14.9	14.9	9.3	0.4	13.72
4	HC	1130.4	1.550	63.27	11.6	1731	1530.	54.4	54.4	15.5	0.4	1.61

Created: Thu 1:58 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\MW ladder assigned_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.mbz
Computer: JRichards

Injection 4: IS - Alpha

Sample Information

Sample ID	IS - Alpha
Location	Plate Well B1
Batch Name	78664 P3 IS 2015-11-30_16-49-49_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS
Run Started	Mon 4:50 PM Nov 30, 2015 CST
Run Completed	Tue 10:04 AM Dec 1, 2015 CST
Reinjection	No

Injection Conditions

Focus Period 1	1150V for 0.1 min
Focus Period 2	3450V for 0.1 min
Focus Period 3	5750V for 25.0 min
Sample Load	20 sec 4600 Volts
Tray Temperature	

Maurice Settings

Model	Maurice S.
Instrument S/N	KF0008
Software Version	1.0.15, Build ID: 0222
Firmware Version	2.0.2015.11.13.18.34.39.f6fbaa9
Tray Type	48 vials
Cartridge Type	CE-SDS
Cartridge S/N	3151010185
Cartridge Expiration	Oct 2016
Injections Remaining	3

Created: Thu 1:58 PM Feb 25, 2016 Created By: User
C:\Users\User\Documents\Compass for iCE\Runs\MW ladder assigned_MW Ladder Sol Test IS final QC 110 ms Maurice CE-SDS.mbz
Computer: JRichards

Importing and Exporting Analysis Settings

The analysis settings in a run file can be exported as a separate file. This allows the same analysis settings to be imported into other batches or run files at a later time, rather than you having to re-enter them manually.

Importing Analysis Settings

NOTE: Importing an analysis settings file populates the settings in all analysis pages.

---

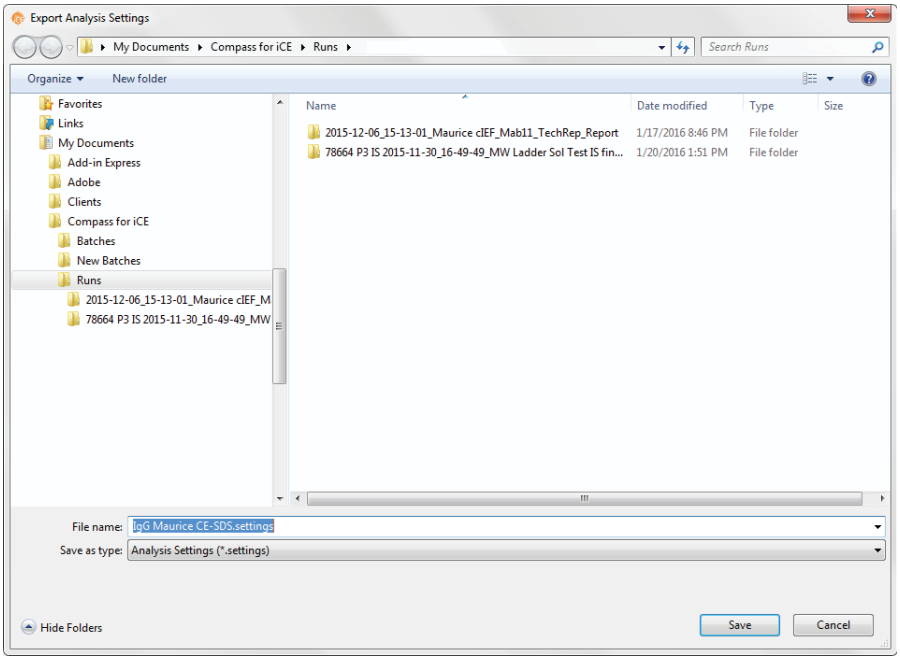
1. Open the run file or batch you want to import analysis settings to.
2. Select **Edit** in the main menu and click **Default Analysis** (Batch screen) or **Analysis** (Analysis screen).
3. Click **Import** on any page.
4. Select a settings file (*.settings) and click **OK**. The imported settings will display in all analysis pages.

Exporting Analysis Settings

NOTE: Exporting an analysis settings file exports the settings in all analysis pages.

---

1. Open the run file or batch you want to export analysis settings from.
2. Select **Edit** in the main menu and click **Default Analysis** (Batch screen) or **Analysis** (Analysis screen).
3. Click **Export** on any page. The following window displays:



4. The default directory is Compass for iCE/Runs. Change the directory if needed.
5. Enter a file name and click **Save**. The settings will be saved as a *.settings file.