White Paper

Agilent
Trusted Answers

GC Intelligence: Peak Evaluation

Contents

Introduction

The recent GC hardware revisions of the Agilent Intuvo 9000 GC and Agilent 8890 GC have provided an opportunity to significantly improve the user's day-to-day experience in many ways. Many of these enhancements are due to the addition of Smart GC features contained within the instrument's firmware. Additionally, new user interfaces such as the touch screen and browser interface provide new ways to interact with the instruments. Some of these new features include integrated diagnostic and maintenance procedures, onboard instrument help content, and GC intelligence[1] (such as Peak Evaluation, User-Guided Troubleshooting, and Trend Plots). This white paper focuses on the features and usage of the GC Intelligence feature, Peak Evaluation.

What is Peak Evaluation?

Peak Evaluation is an automated and customizable tool for the comparison of chromatographic data to a previously collected reference chromatogram. Unlike other forms of GC Intelligence (such as Detector Evaluation), Peak Evaluation allows the user to specify analytes of interest from their separation and define acceptable criteria for their method and analysis they are running. Throughout a sequence, Peak Evaluation can monitor the user-specified analytes of interest for changes in peak retention time, area, height, width, symmetry, resolution, and relative related attributes. When Peak Evaluation is enabled, the GC examines the data internally and compares it to the user-defined reference chromatogram after each run.

If any user-specified criteria fail, the system will alert the user and can suggest maintenance procedures or guide the user to the onboard troubleshooting feature to help determine the cause of the failure. The user can also elect to stop a sequence from continuing onto the next sample upon failure if desired, thus allowing the opportunity to perform any maintenance or troubleshooting steps and prevent the loss of samples.

Users can also monitor the Peak Evaluation results through Trend Plotting by plotting desired user-defined Peak Evaluation parameters. See the Troubleshooting[2] and Trend Plotting[3] white papers (or the instrument help) for more details about other GC Intelligence Features of Troubleshooting and Trend Plotting.

General Peak Evaluation workflow

Figure 1 shows the general workflow for how to set up Peak Evaluation.

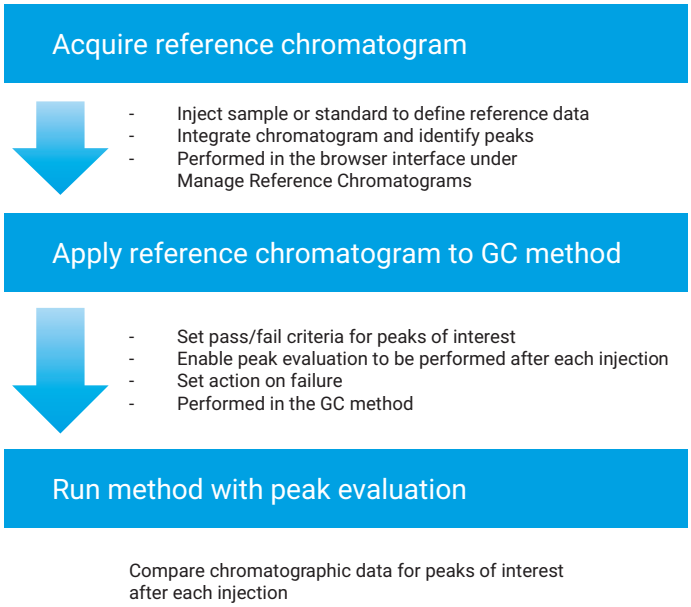


Figure 1. General Peak Evaluation workflow.

The following section will go into the specifics of the workflow in Figure 1.

How to generate a Reference Chromatogram

The first step in the Peak Evaluation workflow is for the user to generate a Reference Chromatogram. To generate a reference chromatogram, first click the Diagnostics tab at the top of the browser interface screen. For more information about the Browser Interface[4], see the associated white paper found within the GC help documentation or search on Agilent.com.

Within the Diagnostics tab, click **Manage Reference Chromatograms** on the left side of the screen to open the Manage Reference Chromatograms window. On the left side of the Manage Reference Chromatograms screen in the Select Reference Chromatogram section are the previously collected reference chromatograms (if present). If one of the previously collected reference chromatograms is selected, the chromatogram will appear to the right of the Select Reference Chromatogram section. If multiple versions of the same reference chromatogram are available, the version number will appear below the Select Reference Chromatogram section in the Details pane (see Figure 2). An updated version of the reference chromatogram might be needed if a method was updated or modified on the instrument (or instrument maintenance was performed).

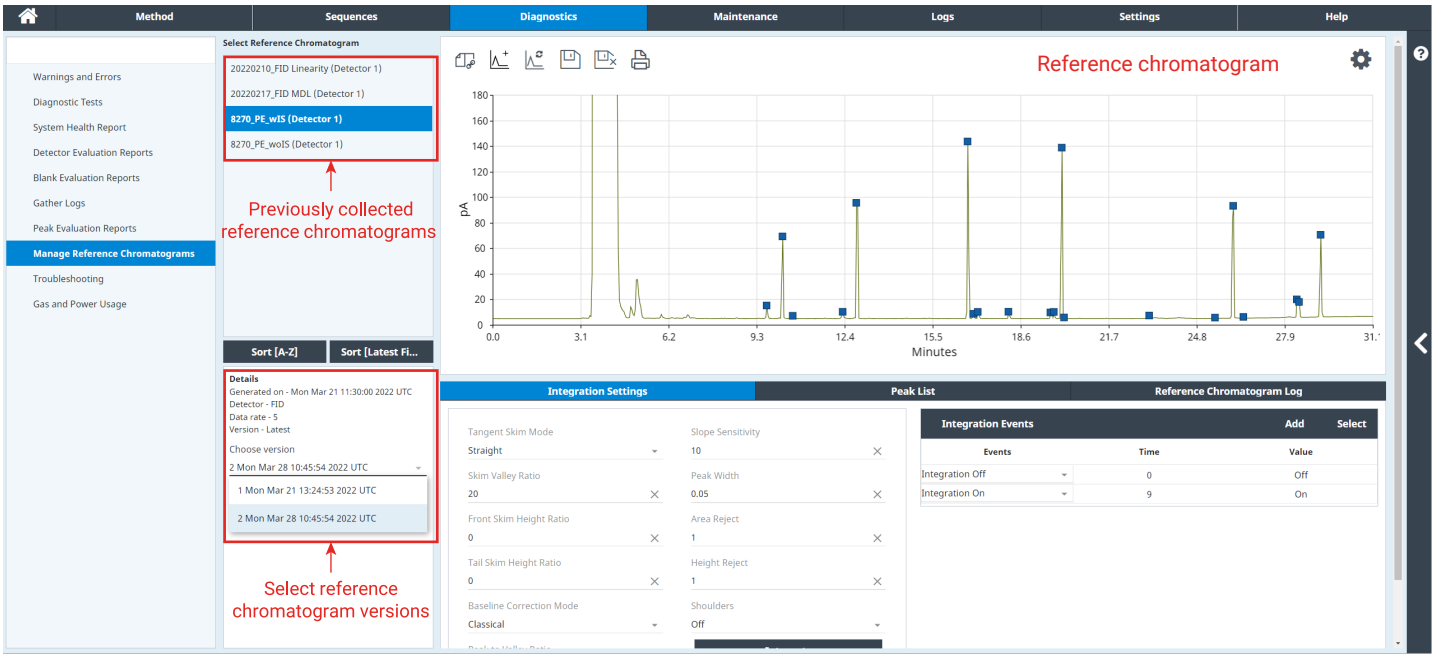


Figure 2. Different parameters in the Manage Reference Chromatograms screen.

Below the chromatogram are three tabs–Integration Settings, Peak List, and Reference Chromatogram Logs–for the selected reference chromatogram. More details about each of these tabs can be found later. A settings icon can be found in the upper-right hand corner of the Manage Reference Chromatograms screen; when clicked, it opens the Settings window (see Figure 3). In this window, the X- and Y-axis limits of the of the reference chromatogram can be adjusted.

The reference chromatogram can also be zoomed in on by clicking and dragging to draw a box around the area of interest. Double-clicking will zoom back out to the previous level. At the top of the chromatogram, there are six icon buttons that are used to: apply a reference chromatogram to a method, generate new reference chromatogram, update reference chromatogram, save, or delete a reference chromatogram, as well as a method print button (see Figure 4).

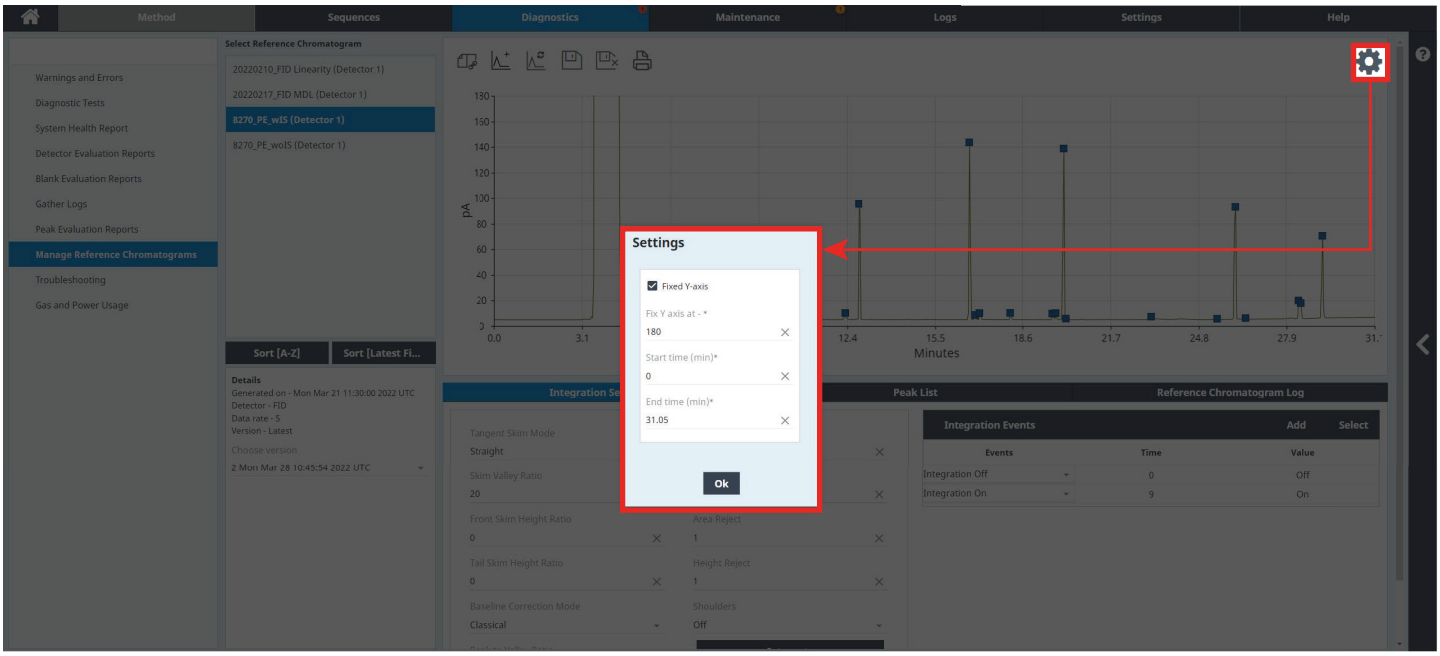


Figure 3. Settings pop-up window opened from the Manage Reference Chromatograms screen via the settings icon.

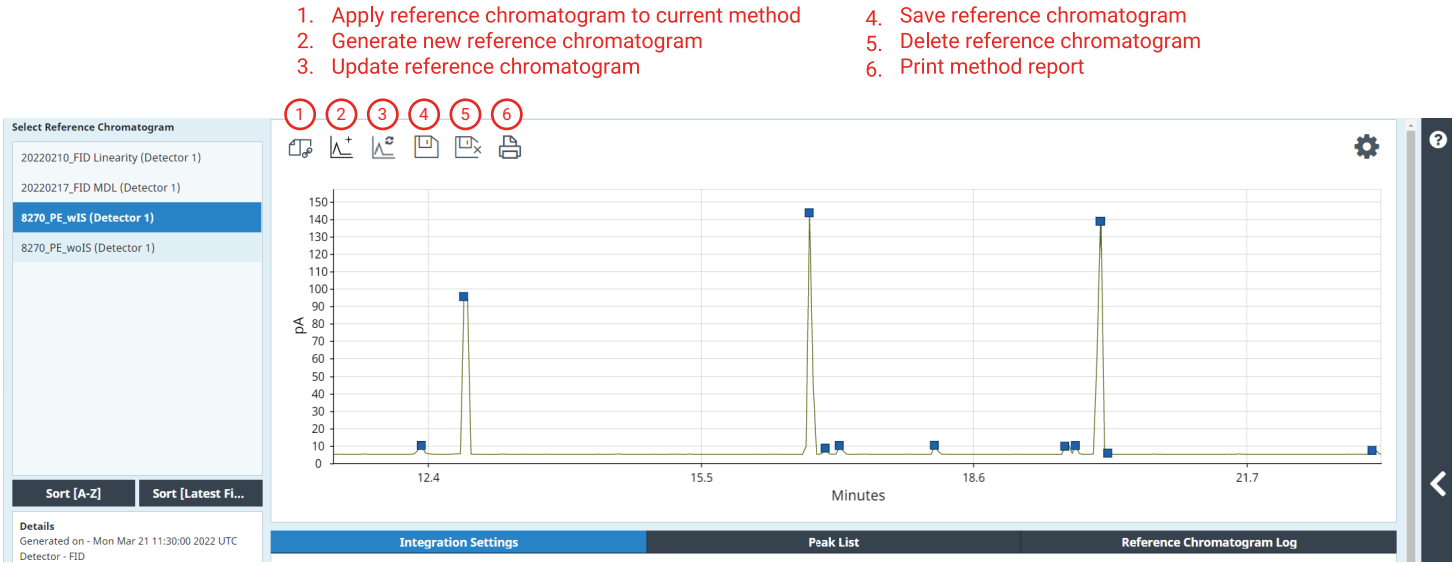


Figure 4. Icons at the top of the Manage Reference Chromatograms screen.

To first generate a new reference chromatogram, select the Generate New Reference Chromatogram icon located at the top left side of the chromatogram (see Figure 5).

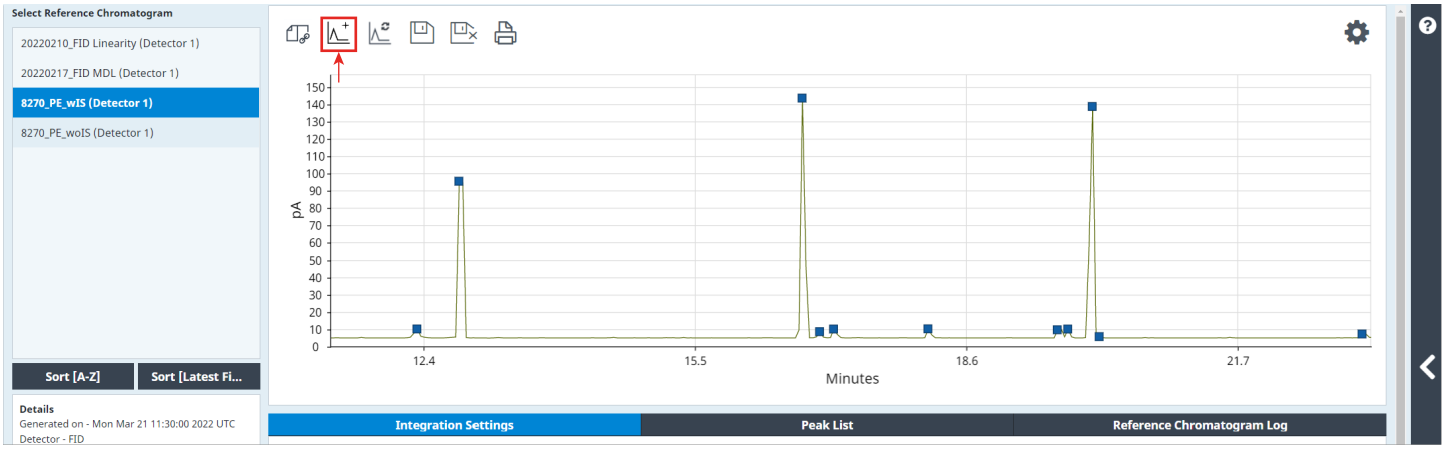


Figure 5. Generate a new reference chromatogram from the Manage Reference Chromatograms screen.

Clicking the Generate new Reference Chromatogram icon will start the process of generating a new reference chromatogram on the instrument. Note that, to collect a new reference chromatogram, the instrument must not be actively connected to a Data System. This is because the instrument is making a browser interface-based injection, which would be prevented by the Data System. After selecting the Generate new Reference Chromatogram icon, a new window will appear allowing the user to input the reference chromatogram run parameters (see Figure 6).

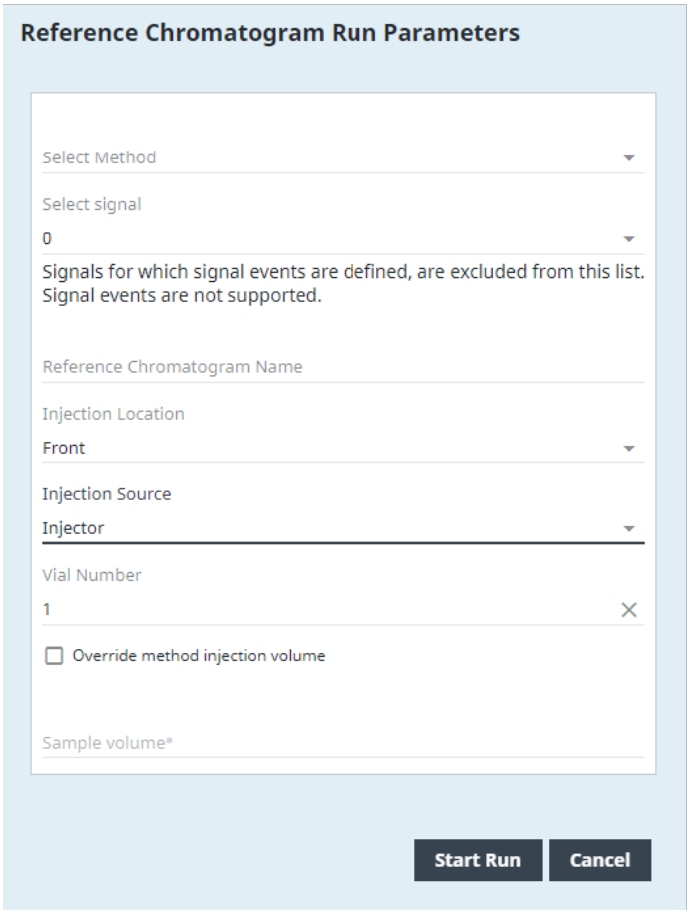


Figure 6. The Reference Chromatogram Run Parameters pop-up window opened from the Manage Reference Chromatograms screen.

After the pop-up window appears, the following parameters need to be completed to start the reference chromatogram run:

- Select the GC method to be used for generating the reference chromatogram.
- Select the detector signal (should be the same ones listed as those in the GC method).
- Type the reference chromatogram name.
- Select the injection location.
  - This will be *Front* or *Back* for automatic liquid sampler (ALS) injections on the 8890 GC.
  - A value of 1 will be present on the Intuvo 9000 GC for the injection location because the Intuvo 9000 GC only has a single injection location.
- Select the sample source under Injection Source.
  - Select **Injector** for ALS injections.
  - Select **Valve** if making a valve-based injection.
  - You can also select **Headspace** if an Agilent 8697 headspace sampler is installed on the system.
- Type the vial number to make the injection from.
- If desired, modify the injected sample volume by selecting the **Override method injection volume** check box.

Once all the above parameters are completed, click **Start Run** at the bottom of the pop-up window (see Figure 7).

The instrument will then make an injection and start collecting a new reference chromatogram. Users can monitor the progress of the reference chromatogram collection by going to the real-time plot on the main browser interface screen. This will display the chromatogram as it is collected from the instrument. After the run ends, a new alert will appear under Warning and Errors within the Diagnostics tab on the browser. When the alert is selected, a pop-up window will appear alerting the user that a new reference chromatogram was collected and will direct the user to Manage Reference Chromatograms to modify the integration settings and peak list table (see Figure 8).

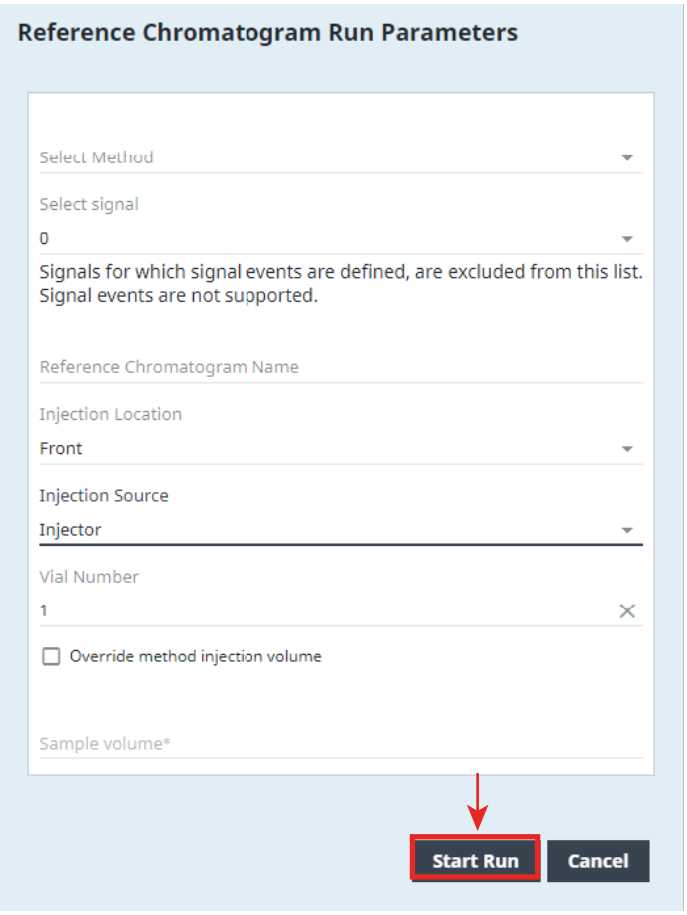


Figure 7. Clicking Start Run to collect a new reference chromatogram.

After the reference chromatogram is collected, navigate back to the Manage Reference Chromatograms screen under the Diagnostics tab on the browser. Once in Manage Reference Chromatograms, select the reference chromatogram that was just collected on the instrument from the Selected Reference Chromatogram list on the left side of the screen. After selecting the reference chromatogram, an image of the collected reference chromatogram will appear to the right. The X- and Y-axis ranges can be modified by clicking the settings icon in the upper right side of the chromatogram window (see Figure 9). A pop-up window will appear allowing the user to adjust the start and end time (X-axis). The Y-axis can also be adjusted by selecting the **Fixed Y-axis** check box and typing a value in the user-entry field.

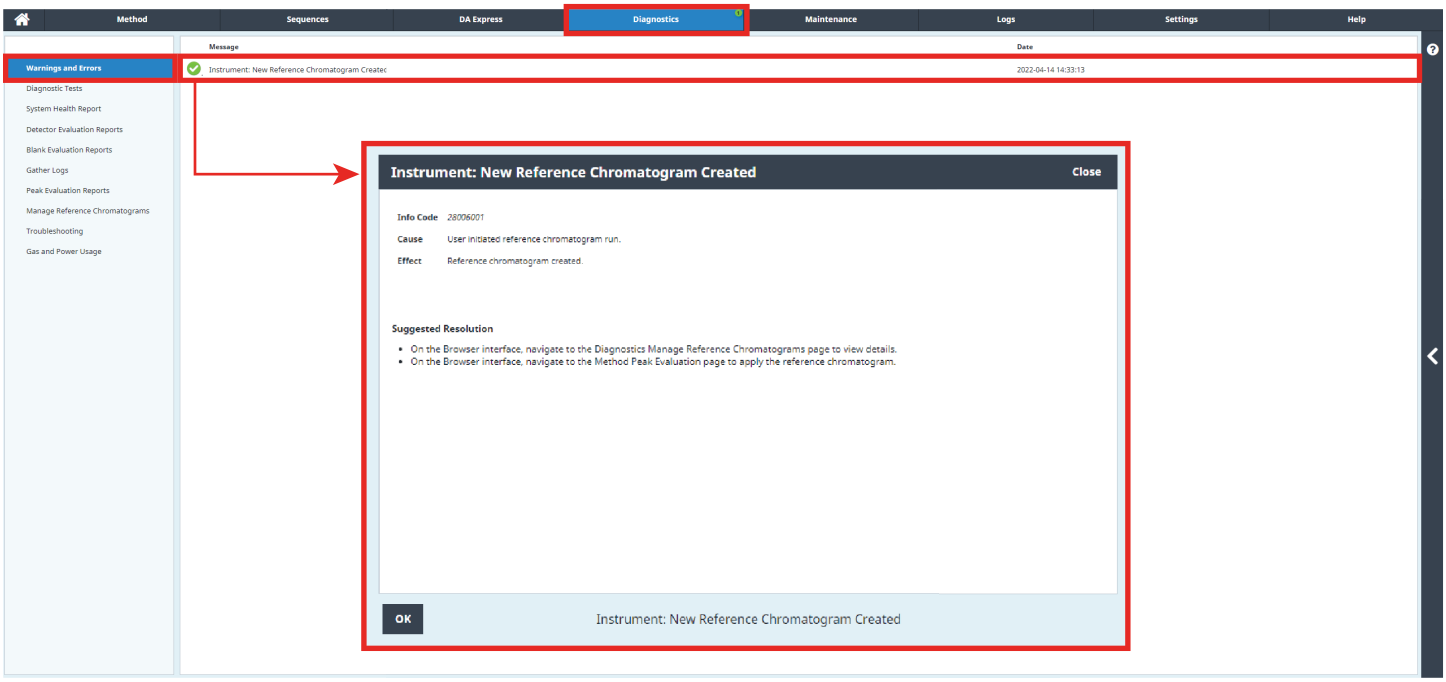


Figure 8. Pop-up window from the Warning and Errors screen on the Diagnostics tab, which appears after collecting a new reference chromatogram.

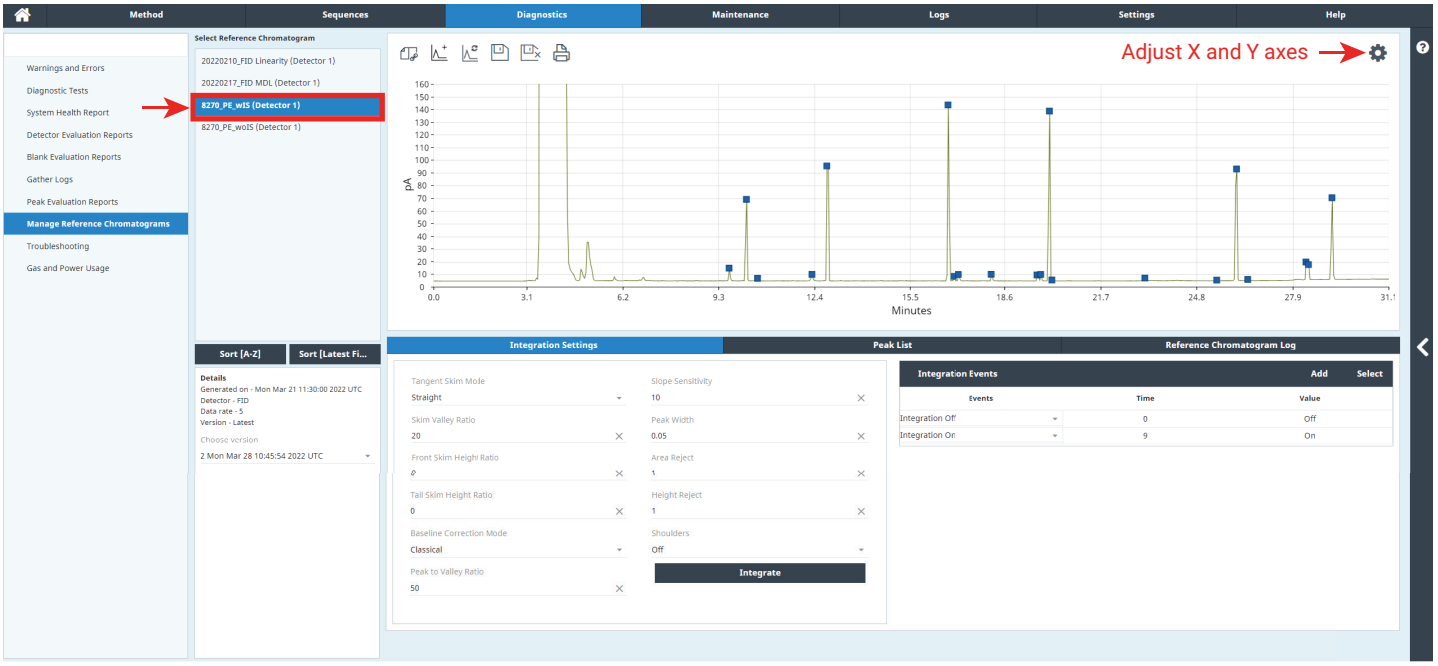


Figure 9. Select the reference chromatogram that was generated on the left.

After adjusting the X and Y axes of the chromatogram, the next step is to adjust the integration parameters to integrate the chromatogram. When the reference chromatogram is first collected, it is integrated using default settings. In the Integration Settings tab below the chromatogram, the user can adjust the integration parameters to ensure all the peaks or analytes of interest are found and properly integrated. These integration settings are similar to those found in data systems such as Agilent OpenLab software. The Integration Events section is also available to the right of the integration settings if users wish to set particular timed integration events (such as removing the solvent peak integration). After setting the integration parameters, click **Integrate** to apply the parameters to the reference chromatogram (see Figure 10). Repeat the process of adjusting parameters and clicking **Integrate** until peaks of interest are integrated as desired.

Once the chromatogram has been integrated, label the peaks of interest with the corresponding analyte names. Under the Peak List tab (to the right of the Integration Settings tab), the user will see the retention times and analyte areas of the integrated peaks that were integrated in the reference chromatogram. When the default integration settings are initially applied to the chromatogram, the peak names are filled out by default with the title "Default Retention Time", where "Retention Time" is the retention time of the peak. If the user adjusts the integration settings and reintegrates the chromatogram, the peak list is cleared. Users may enter the analyte name next to the retention time/area column of the analytes of interest. The chemical CAS ID number may also be listed if desired, but it is not required. After naming the analytes of interest, the reference chromatogram should be saved by clicking **Save** in the upper left corner of the chromatogram window (see Figure 11). A confirmation dialog will appear afterwards.

After completing these steps from within the Manage Reference Chromatograms screen, the user can transfer the reference chromatogram with all the saved parameters to the GC method for use in the analytical injections. The following section will demonstrate how to apply a reference chromatogram to a GC method.

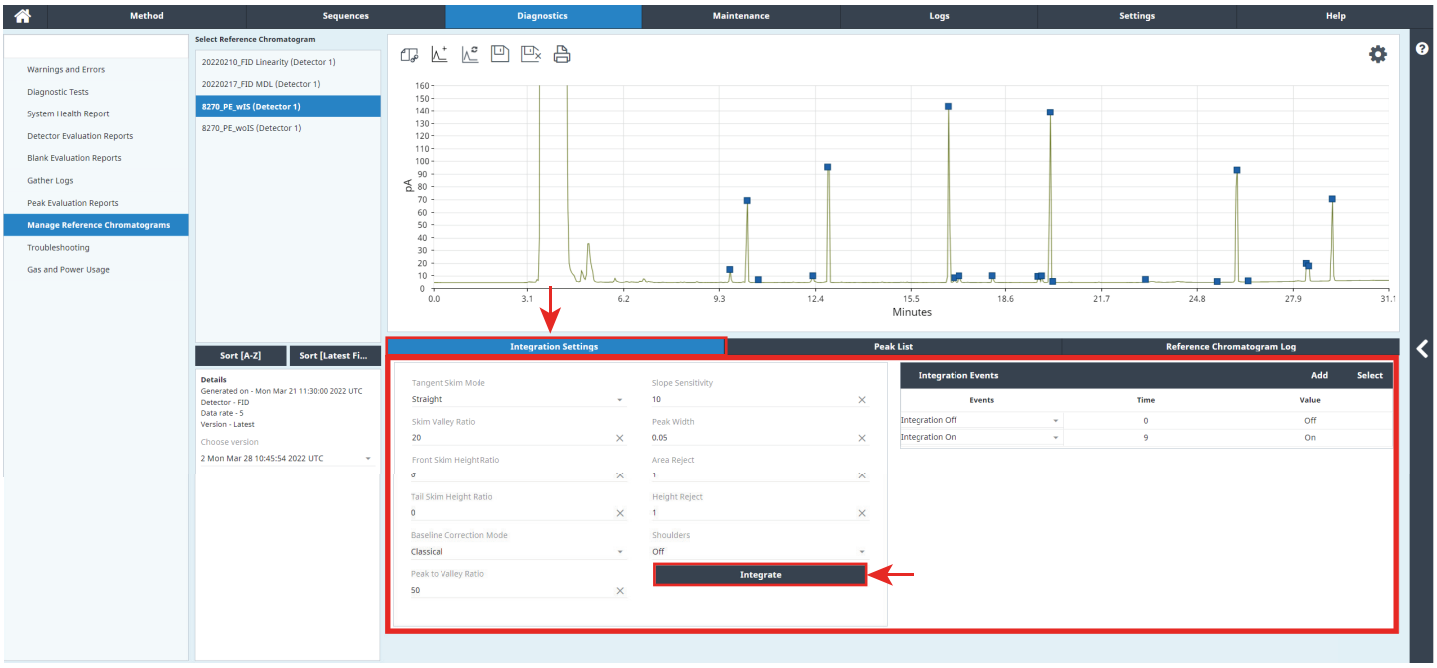


Figure 10. The Integration Settings tab within the Manage Reference Chromatograms screen.

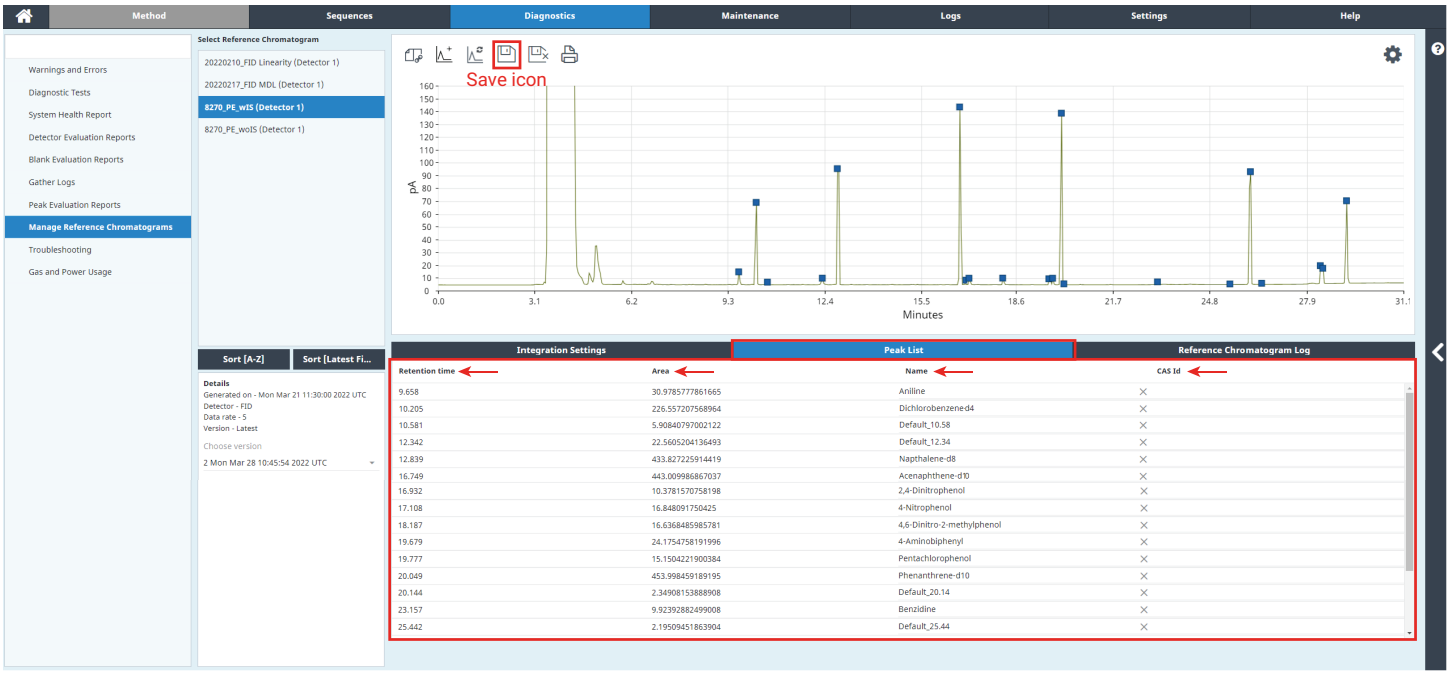


Figure 11. The Peak List tab within the Manage Reference Chromatograms screen.

How to set up a GC method to use Peak Evaluation

Before applying the reference chromatogram to the GC method, verify the correct GC method is loaded on the browser interface. To apply the reference chromatogram from Manage Reference Chromatograms to the GC method, select the Apply reference chromatogram to current method icon, located in the upper left corner of the reference chromatogram (see Figure 12).

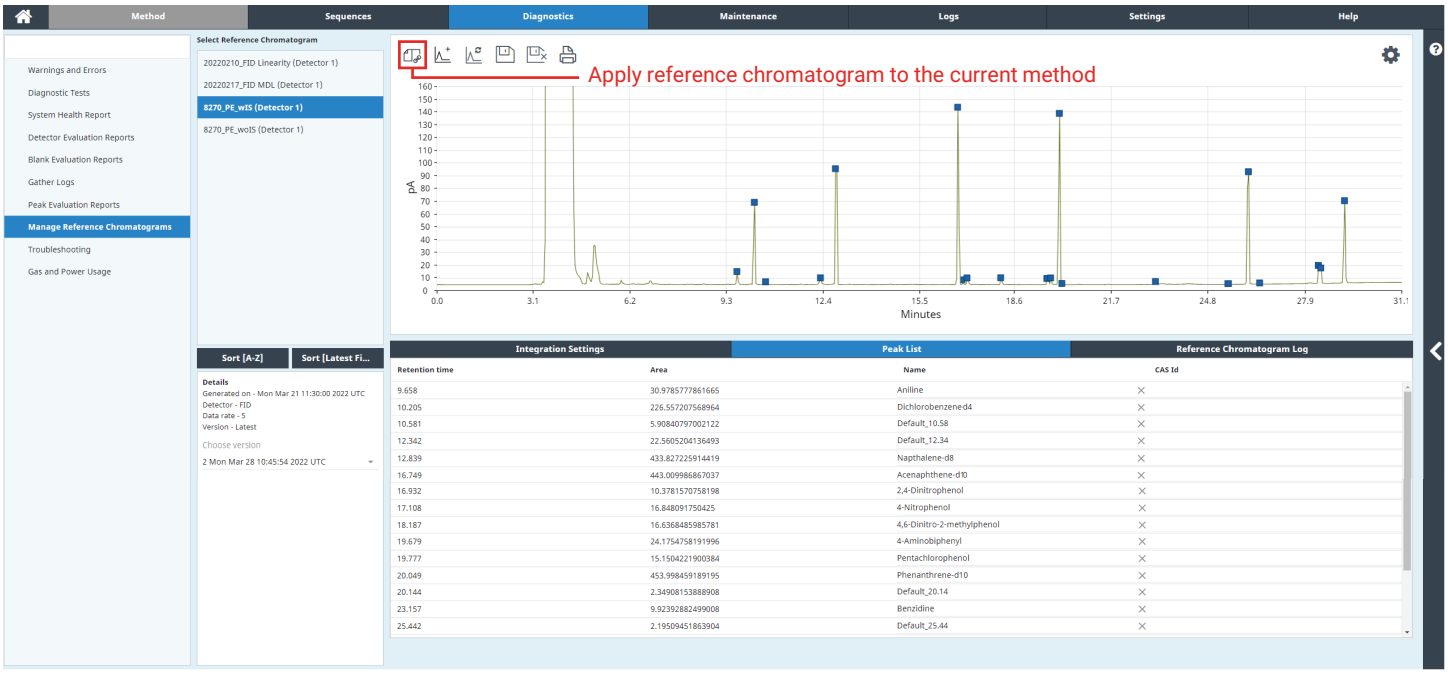


Figure 12. Apply the reference chromatogram to the current GC method.

After selecting the icon to apply the reference chromatogram to the current method, a pop-up window will appear asking the user to verify if they wish to apply the reference chromatogram to the currently loaded method (the currently loaded method name will be displayed). Clicking **Yes** will transfer the reference chromatogram to the active GC method on the browser, and the screen will move to the Methods tab of the browser interface. Clicking **No** will close the pop-up window and return to the Manage Reference Chromatograms screen (see Figure 13).

If the user clicks **Yes**, the GC method used to collect the reference chromatogram is compared against the GC method that is currently loaded, to ensure that the correct method is loaded. If any method setpoints differ, a pop-up window will appear showing any method or configuration differences (see Figure 14). Significant method setpoint differences between the two methods (such as injection volume, column flow rate, or oven program) can cause the peak evaluation to fail, so the user can review this comparison to decide whether to cancel or proceed.

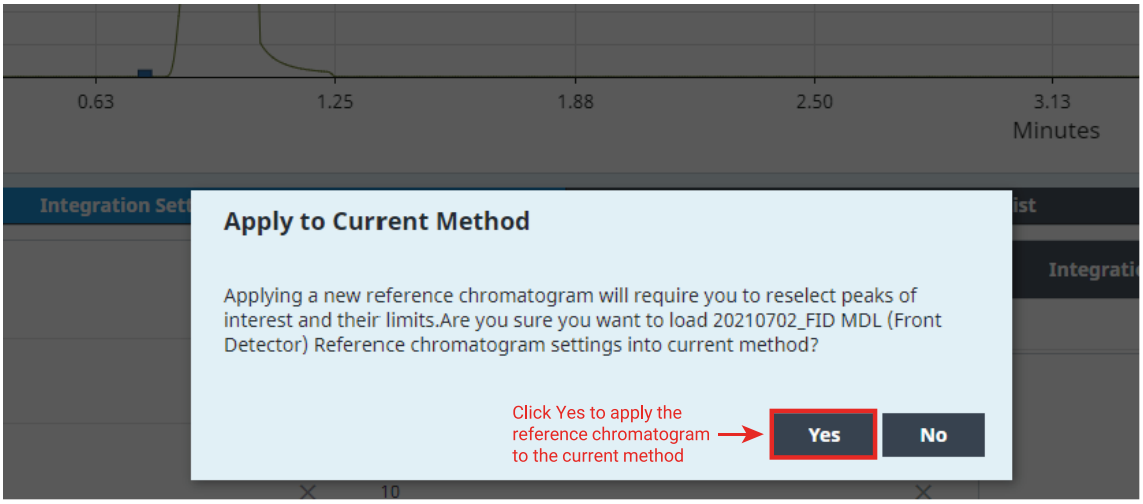


Figure 13. Click **Yes** to apply the reference chromatogram to the current GC method.

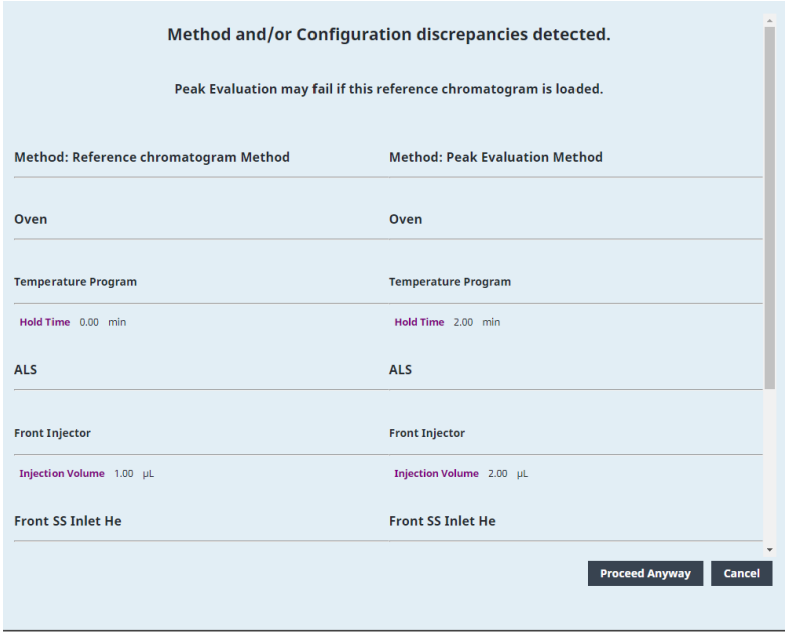


Figure 14. Pop-up window displaying method or configuration differences.

After transferring the reference chromatogram to the GC method, the user will be within the Method > GC Performance > Peak Evaluation screen of the browser interface. First verify that the **Enable Peak Evaluation** check box has been selected. It should be selected by default after applying the reference chromatogram. It should be noted that only one type of GC performance evaluation (Peak, Detector, or Blank Evaluation) can be enabled per method. If multiple evaluations are needed, separate injections using separate methods will need to be used in a sequence. Also verify that the Compare Reference chromatogram with field is showing the correct detector signal. (The signal should match the same detector signal as was used to collect the reference chromatogram.) Next, select a warning level to be used for peak evaluation in the GC method under Choose warning level (see Figure 15).

The warning level can be set as *None*, *Lenient*, or *Strict*. Selecting **None** will turn off use of the warning levels for the different analyte parameters found within Peak Evaluation; selecting **Lenient** will set the warning level at 80% of the tolerance band; and selecting **Strict** will set a warning level at 60% of the tolerance band. When warning levels are used, a Peak Evaluation result falling between the warning level and the failure limit will trigger a warning diagnostic. This allows the user to be alerted that the Peak Evaluation is approaching the failing limit of the tolerance band but does not trigger a sequence action. See Figure 16 for a visual representation of the warning level tolerance limits.

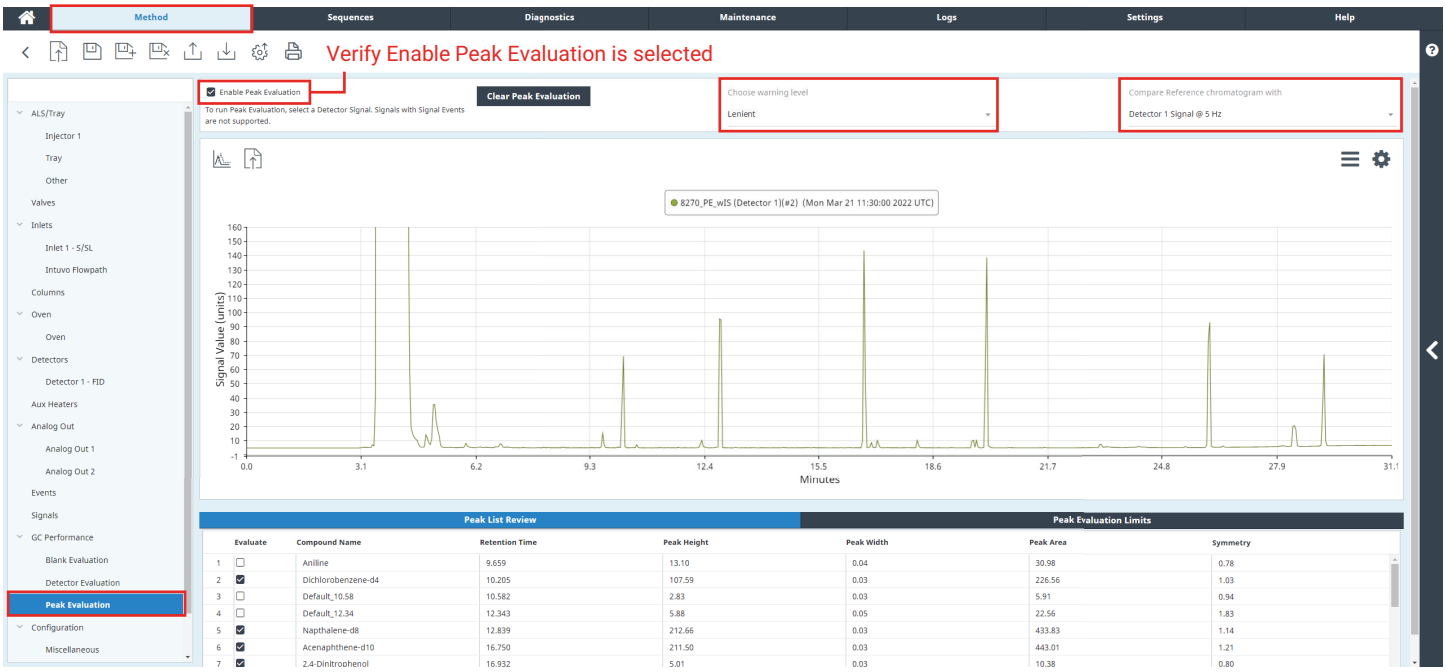


Figure 15. Peak Evaluation screen once transferred to the Method tab.

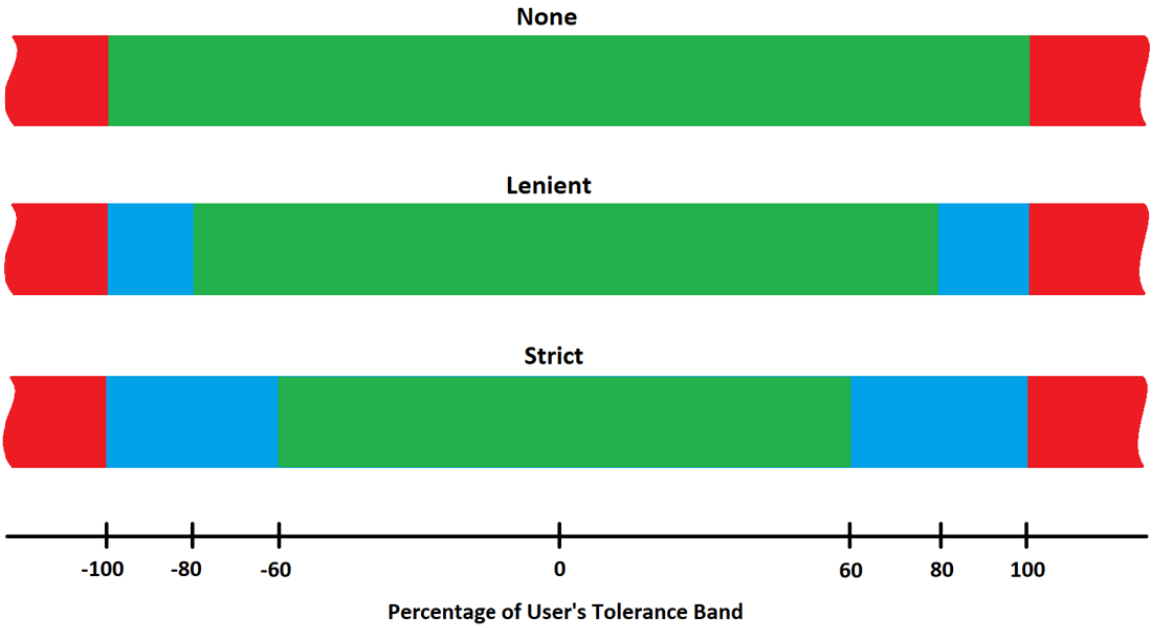


Figure 16. Visual representation of the tolerance limits (warning levels) used within the Peak Evaluation.

Directly below the Choose warning level field will be the reference chromatogram that was transferred from the Manage Reference Chromatograms screen. Above the reference chromatogram is a label displaying the reference chromatogram name, detector used, version number, and the date and time stamp when the reference chromatogram was collected (see Figure 17).

Next to the settings icon is a hamburger icon (see Figure 18). When clicked, it displays the integration settings that were used in the Manage Reference Chromatograms screen. An Integration Settings pop-up window will appear showing the integration settings and events used prior to transferring the reference chromatogram to the GC method. The integration settings can only be viewed and not edited from within this

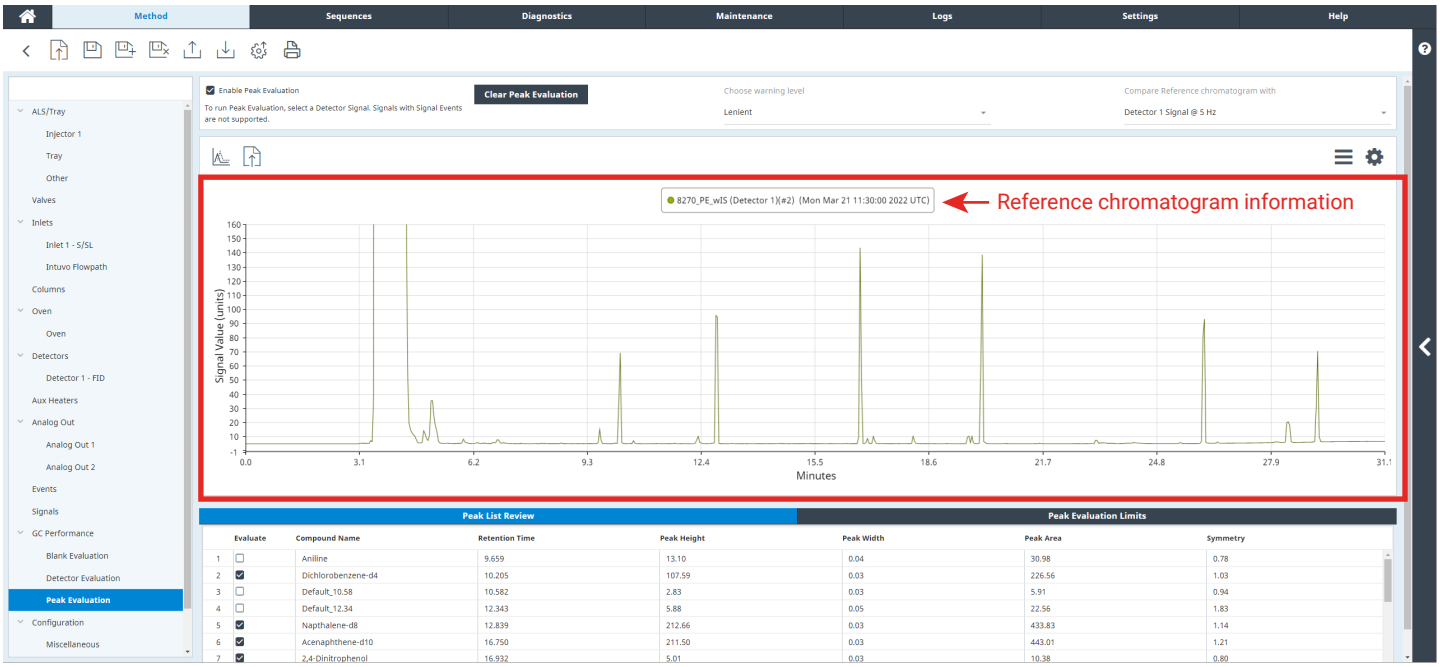


Figure 17. Image of reference chromatogram within the Peak Evaluation screen in the Method tab.

pop-up window (values can only be edited from the Manage Reference Chromatograms screen).

Two icons on the upper left side of the chromatogram window will allow the user to load another reference chromatogram (replace the one which is currently being viewed) and go back to the Manage Reference Chromatograms screen of the browser interface (see Figure 19).

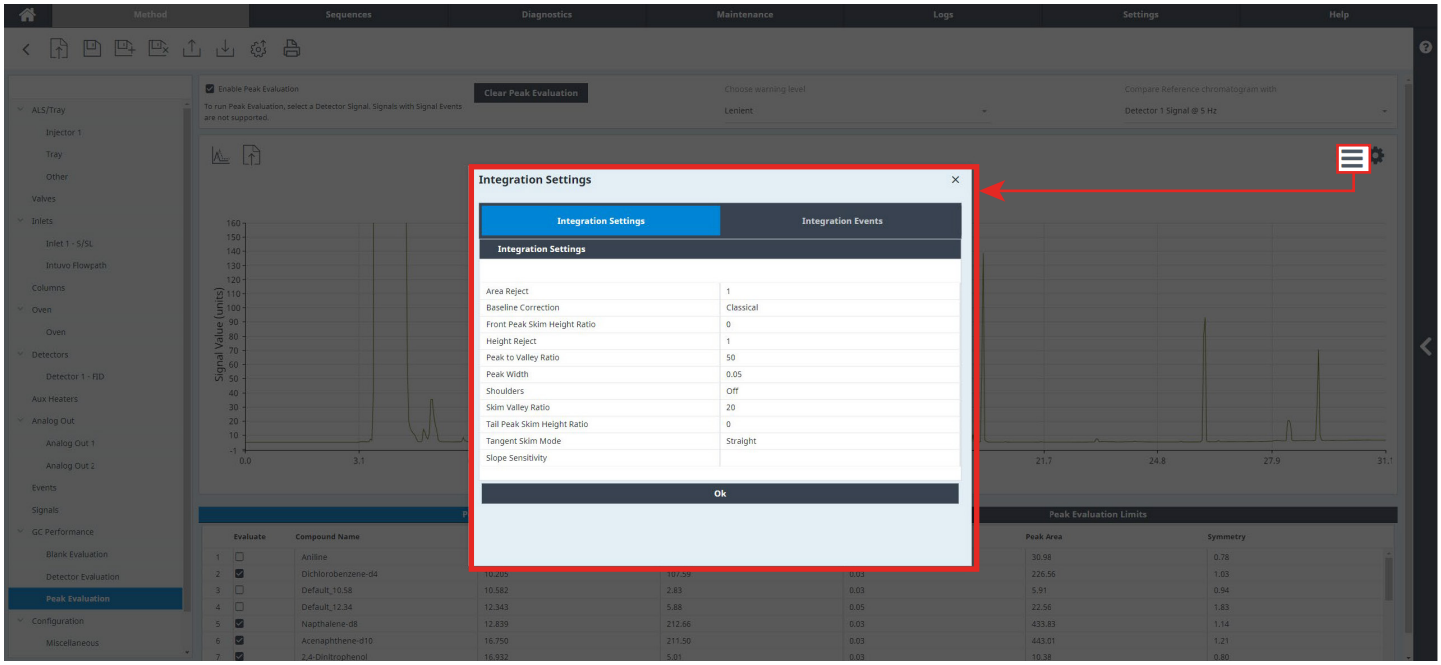


Figure 18. Integration Settings window within the Peak Evaluation screen in the Method tab.

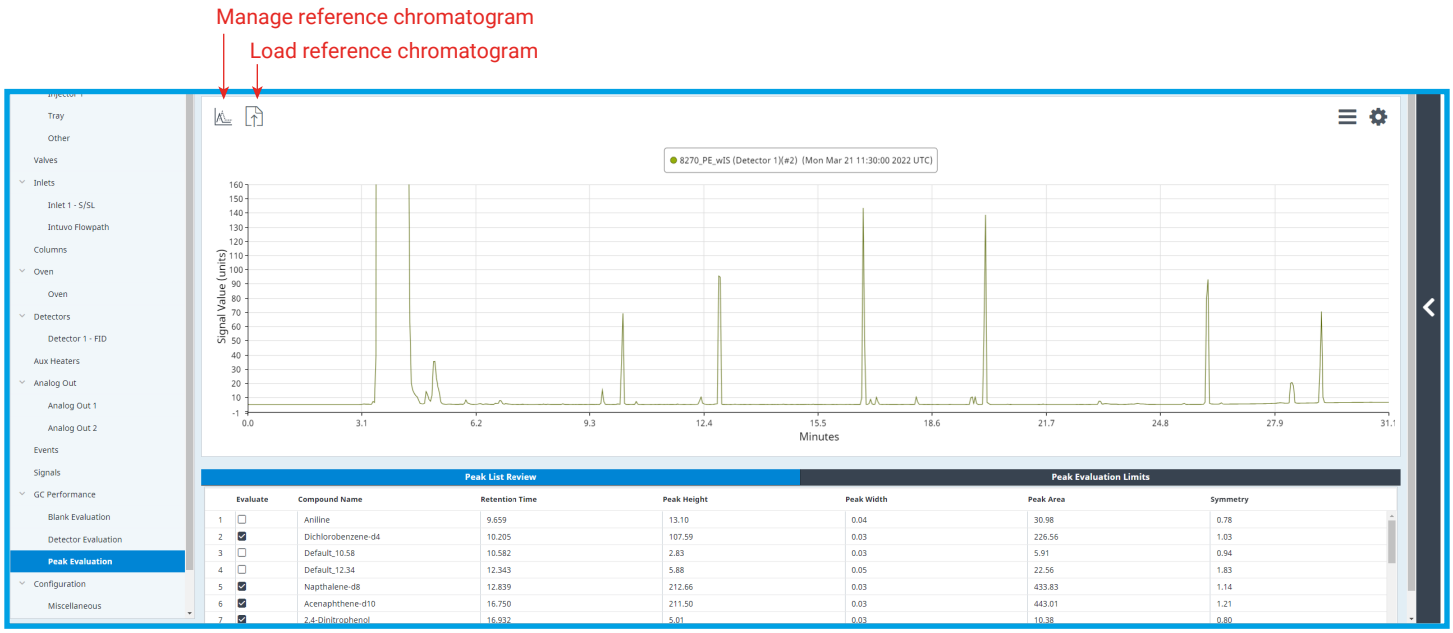


Figure 19. Icons to load and manage the reference chromatogram from within the Peak Evaluation screen in the GC method.

Below the reference chromatogram are two tabs, Peak List Review and Peak Evaluation Limits, which will be used to select the analytes of interest for monitoring during Peak Evaluation and to set their corresponding tolerance limits (see Figure 20).

Under the Peak List Review tab, the peaks that were integrated in the Manage Reference Chromatograms screen will be shown. The different peak parameters (retention time, peak height, peak width, peak area, and symmetry) for each peak will also be listed. In the Evaluate column, users may select up to 10 peaks of interest to be used for evaluation (see Figure 21).

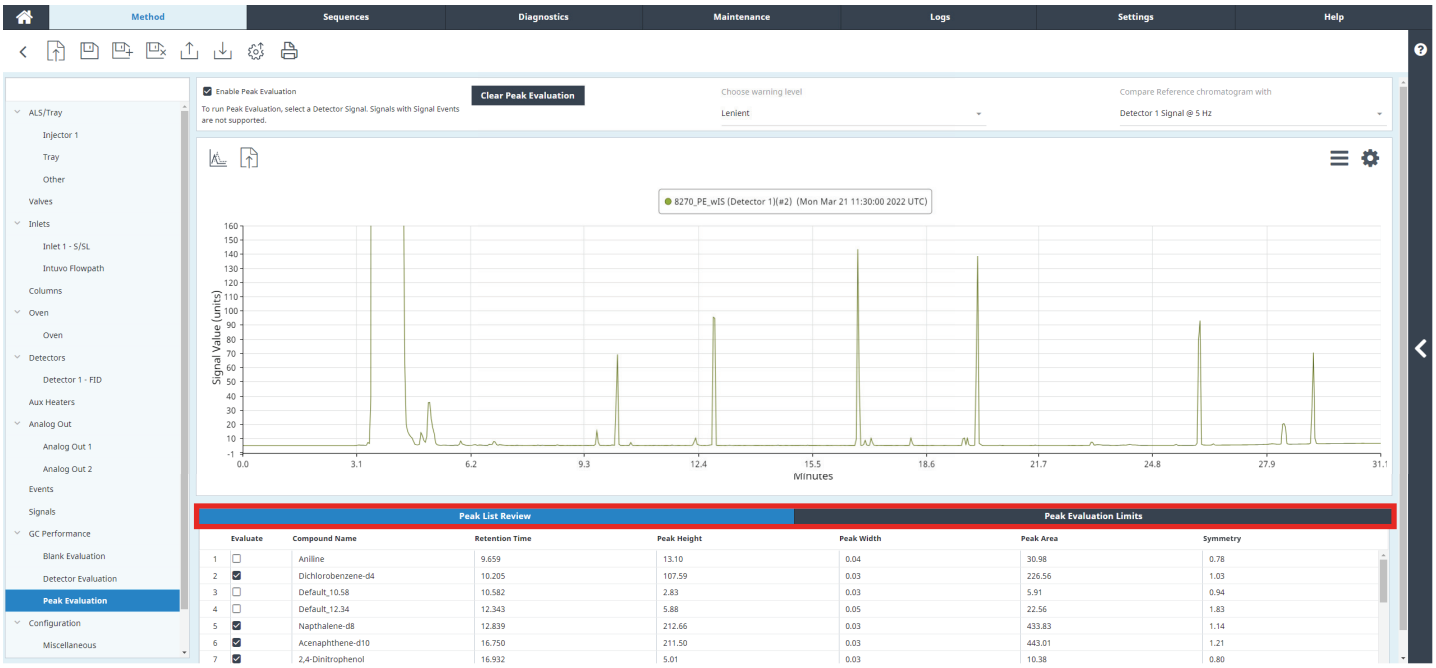


Figure 20. Peak List Review and Peak Evaluation Limits tabs on the Peak Evaluation screen in the Method tab.

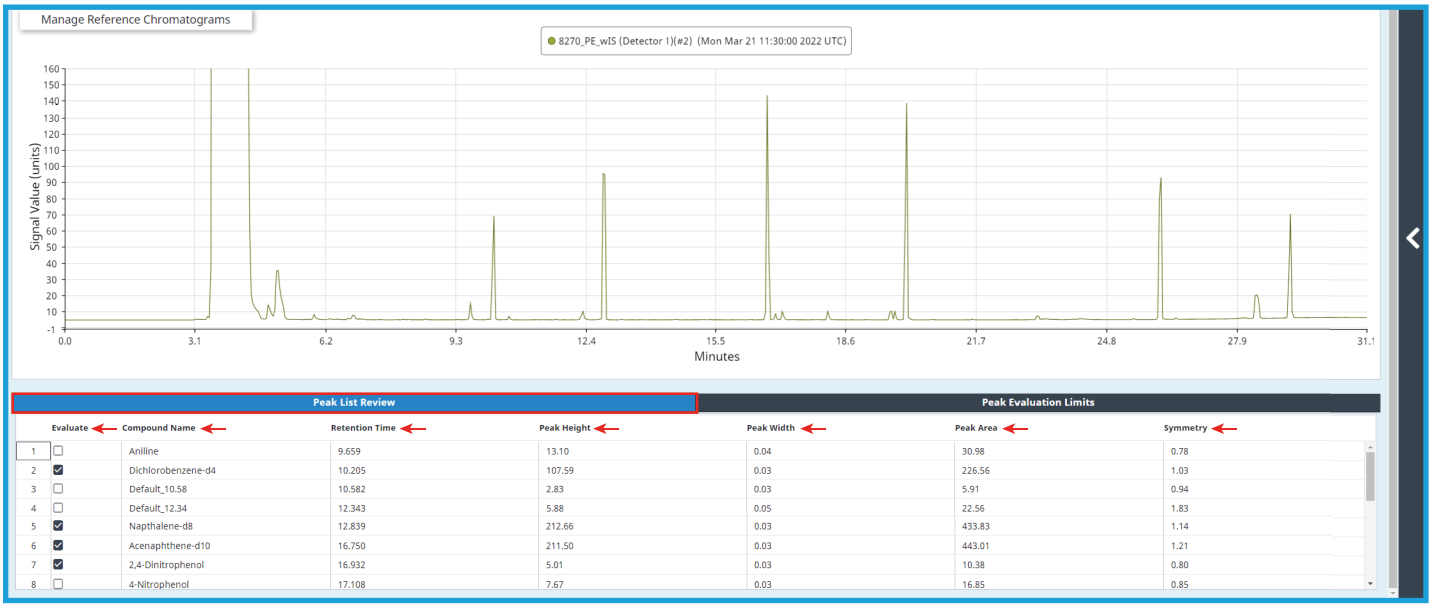


Figure 21. Peak List Review tab showing the parameters that can be evaluated from within Peak Evaluation.

The Peak Evaluation Limits tab will display the different tolerance limits that can be used during Peak Evaluation. The section labeled Peak Attributes has the tolerance limits the user may set for the pass/fail criteria for the different analyte attributes. Different analyte parameters (such as peak height, peak width, peak area, and symmetry) can be enabled or disabled as needed for the type of analysis being run. The Retention Time parameter will always be enabled by default. The tolerance limits are a ± pass/fail percentage value using the reference values taken from the reference chromatogram. For example, if the retention time of one of the analytes was 10 minutes in the reference chromatogram with a tolerance limit set to 10%, then the pass/fail tolerance band would be 9 to 11 minutes for that analyte. Default values are initially present for all the tolerance bands but can be modified as needed (see Figure 22).

Above the Peak Attributes table are two check boxes that will allow the user to enable/disable setting Peak Evaluation metrics individually for each of the selected analytes and enable/disable the baseline attributes aspects of Peak Evaluation (see Figure 23).

If the **Set limits for each peak individually (Advanced)** check box is selected, the Peak Attributes table will be cleared and a drop-down list for Compound Name will appear (see Figure 24).

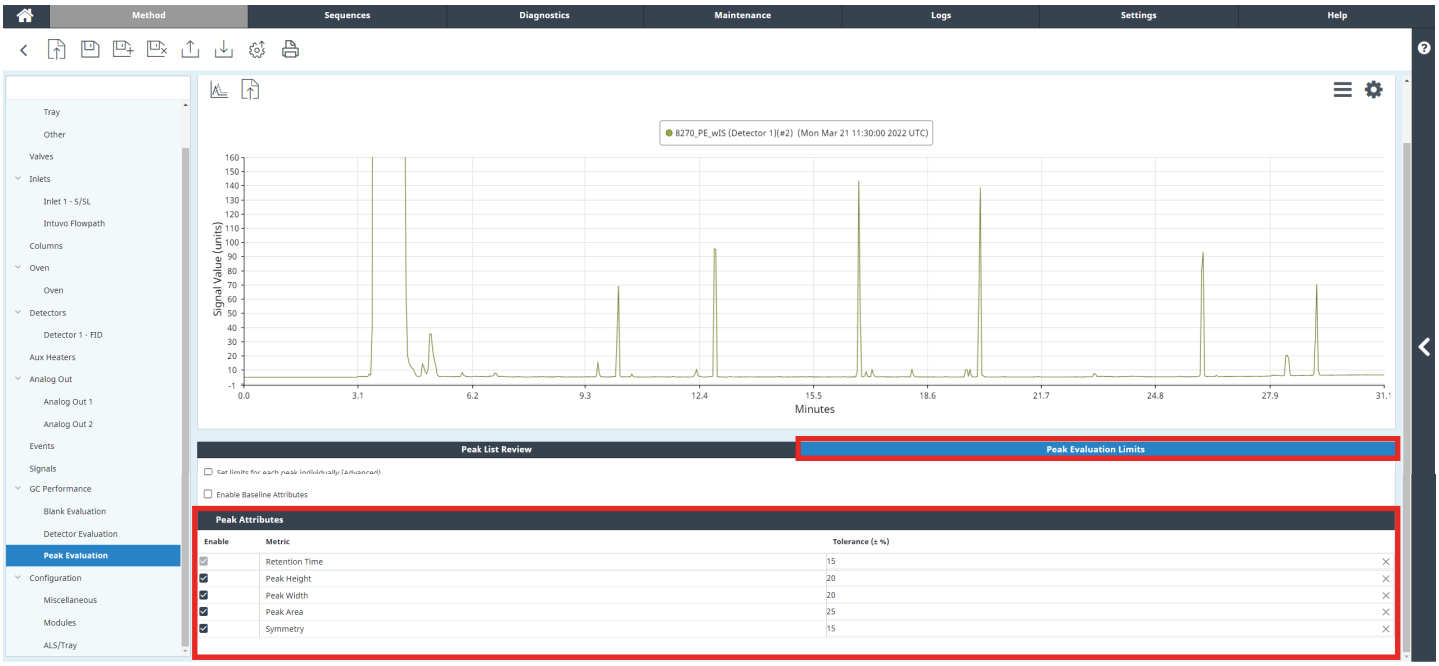


Figure 22. Peak Evaluation Limits tab showing the tolerance limits for the difference peak attributes.

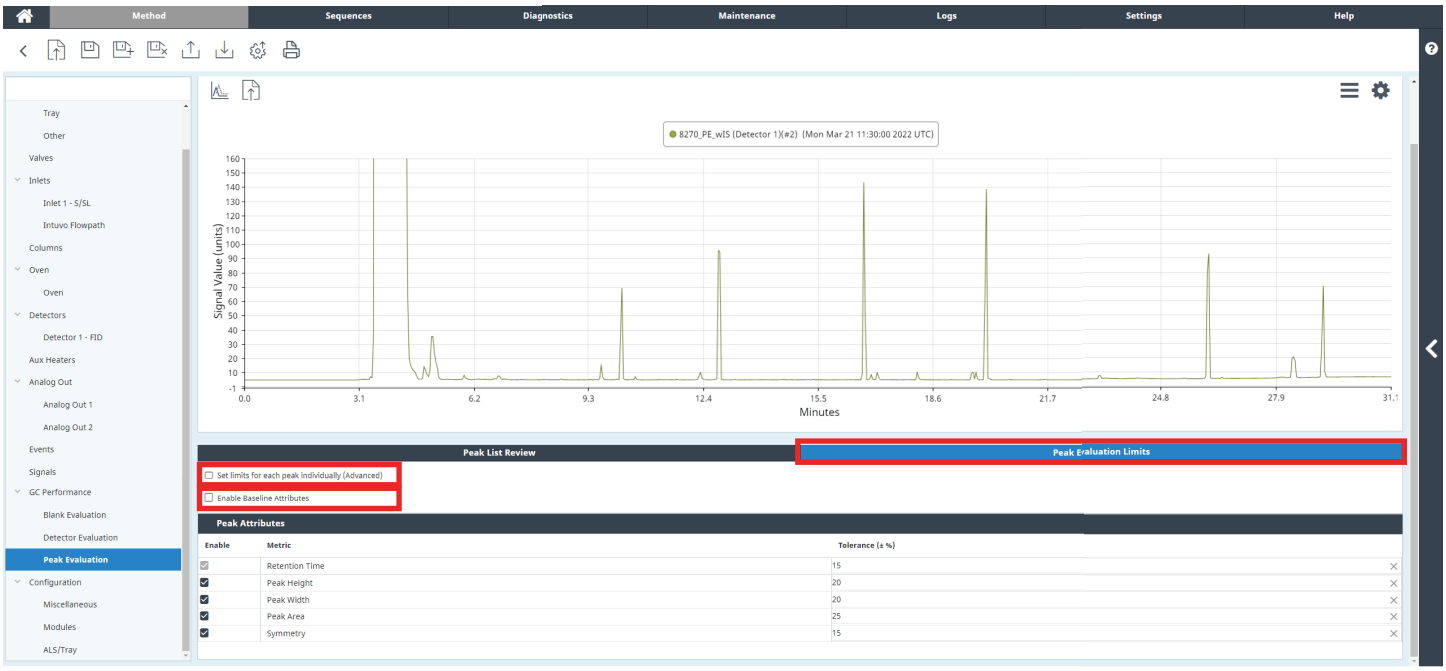


Figure 23. Within the Peak Evaluation Limits tab, showing the two check boxes to enable setting limits for each individual analyte and enabling the baseline attributes.

Figure 24. Within the Peak Evaluation Limits tab, selecting the Set limits for each peak individually (Advanced) check box.

On the right side of the compound name is a drop-down arrow that will display the selected analytes that were chosen in the Peak List Review tab (see above). After a compound is selected, the Peak Attributes table will be populated, allowing the user to individually set the upper and lower limits (percentages) for each analyte separately. This allows for more advanced and customizable peak by peak limits. Also appearing at the bottom of the Peak Attributes table is another field for the Resolution metric that may only be monitored if the user selects **Set limits for each peak individually (Advanced)**. The user will also need to specify a comparison peak if the resolution parameter is selected (see Figure 25).

Another feature of selecting the setting limits for each peak individually is the ability to monitor not only the absolute vales of the selected analytes but also the relative values, by applying a comparison peak. As with the peak resolution parameter, a comparison peak will also need to be selected if the user wants to monitor the relative parameters. Relative Peak Evaluation parameters also have default upper and lower limits present, which can be modified as needed (see Figure 26).

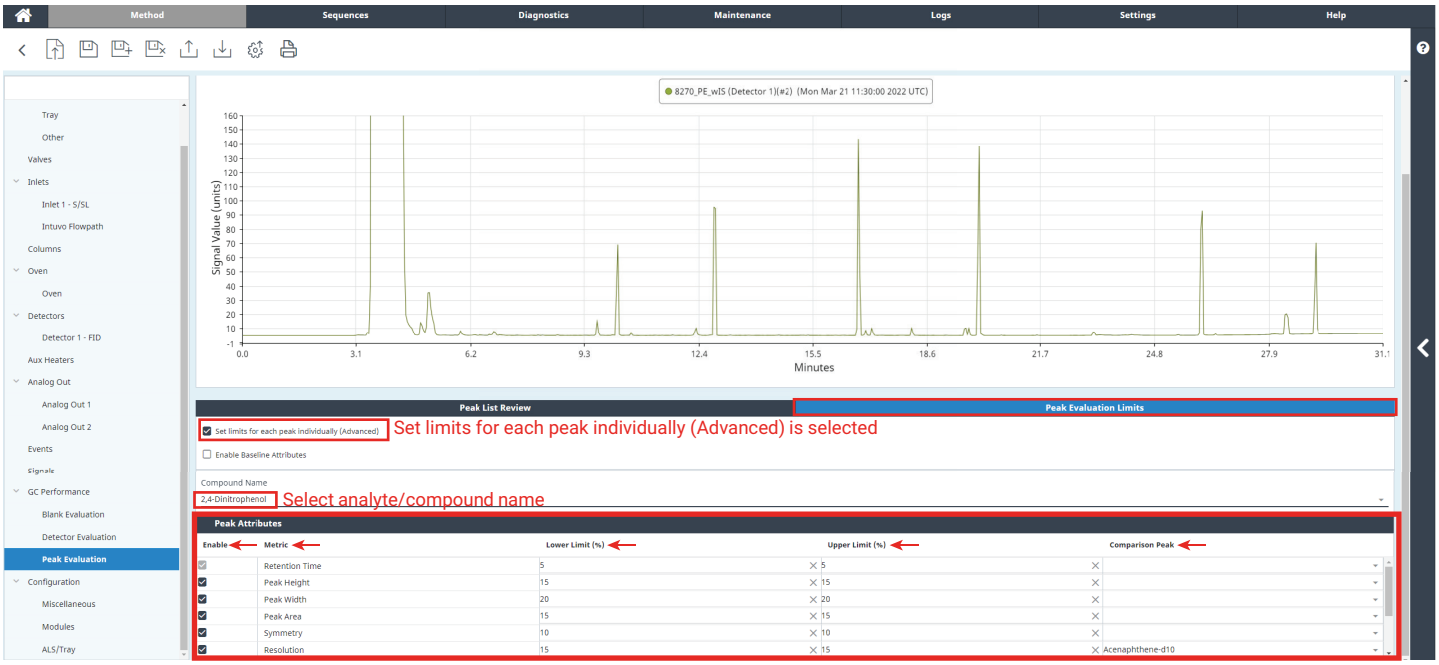


Figure 25. Within the Peak Evaluation Limits tab, selecting the Set limits for each peak individually (Advanced) check box and selecting an analyte.

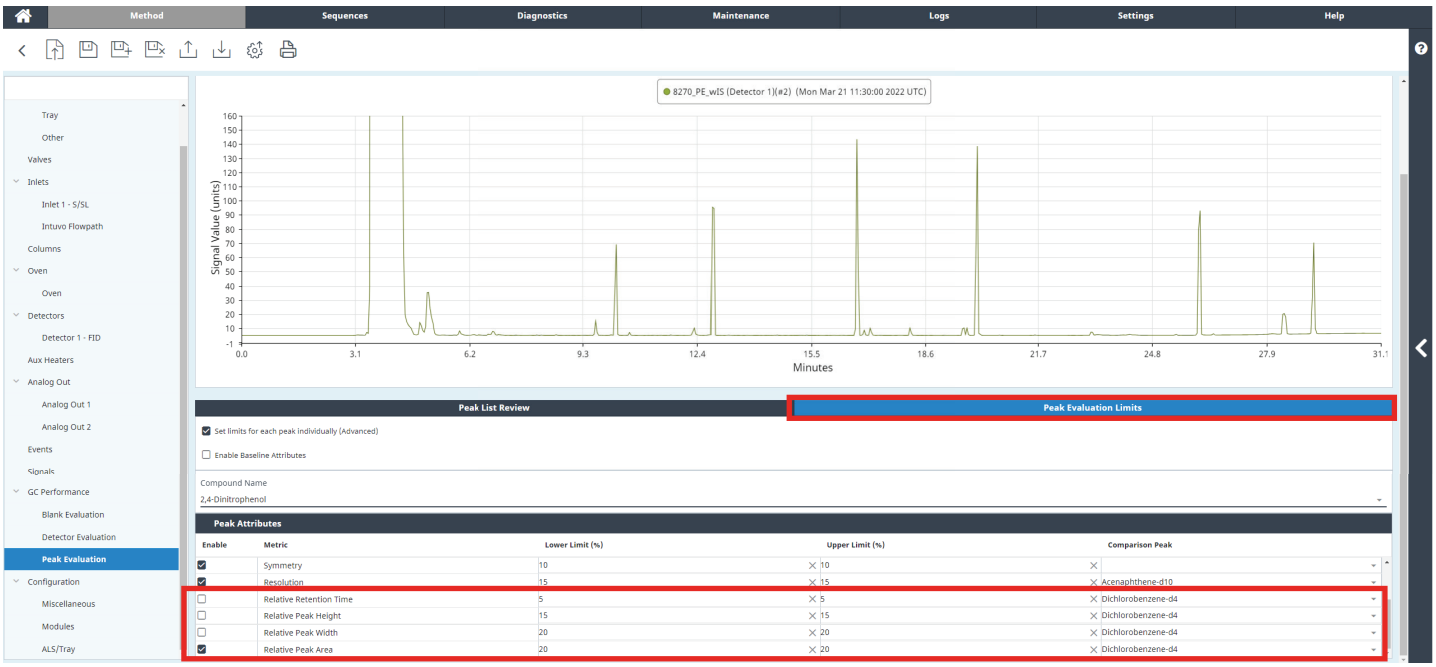


Figure 26. Within the Peak Evaluation Limits tab, selecting the Set limits for each peak individually (Advanced) check box and selecting relative parameters to be monitored.

Also within the Peak Evaluation Limits tab is the ability to select/deselect the **Baseline Attributes** check box at the top of the Peak Evaluation Limits screen. Once selected, a Baseline Attributes window will appear that allows the user to input parameters associated with baseline monitoring from within the Peak Evaluation screen. Default values are present in all the fields, which the user can modify as needed. The first two metrics are the initial and final baseline values. Both minimum and maximum values are monitored at the start and end of the run from the detector signal that was saved when the reference chromatogram was collected. Baseline noise (six-sigma noise is calculated) is another parameter that may be monitored, in a specified time window. Users should select a time window which no known eluting peaks are expected to be present for best results. The final baseline attribute metric is total peak area. As with baseline noise, minimum and maximum values are used to monitor the total peak area during a particular time window. Again, the user should choose a time window when no known peaks are expected to elute from the system (see Figure 27).

Once the Peak List Review and Peak Evaluation Limits are set, the user can save the GC method and parameters by clicking the save icon. Users should then download the method to the GC by clicking the download icon, so that this method is the active method on the instrument (see Figure 28).

If a data system is being used to run the instrument, the GC method will need to be uploaded from the instrument from within the data system. This will put the active method (with Peak Evaluation enabled) from the instrument into the data system method. Users will then need to resave the data system method to allow use of Peak Evaluation from within the data system. Another section below will describe the use of Peak Evaluation from within the Data System.

After a method with Peak Evaluation enabled has been run, an alert will appear in the Warnings and Errors section under the Diagnostics tab of the browser interface. After the user clicks the message, a pop-up window appears notifying the user if the Peak Evaluation passed or failed (see Figure 29).

If the Peak Evaluation has failed, the option to initiate the onboard troubleshooting will be present, and the user can choose to start troubleshooting to resolve the Peak Evaluation issue if needed (see Figure 30).

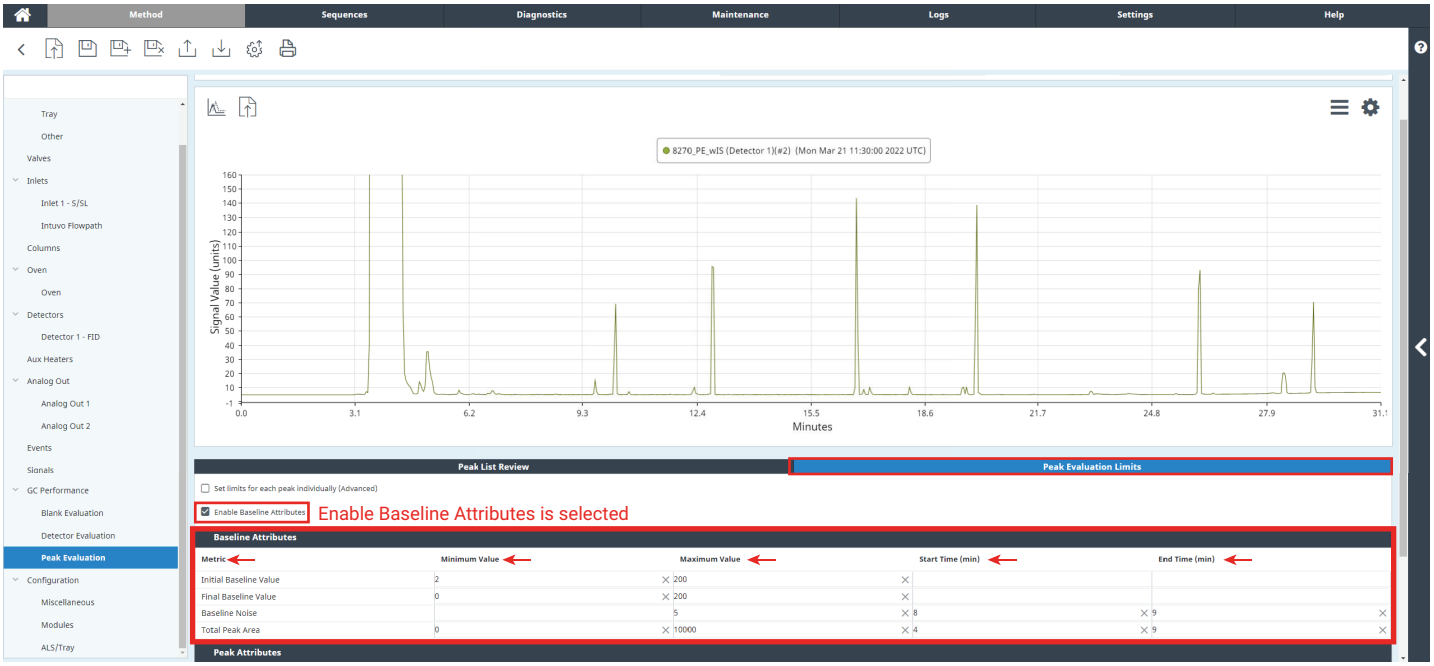


Figure 27. Selecting Enable Baseline Attributes from within the Peak Evaluation screen.

Figure 28. Save and download the method to the GC.

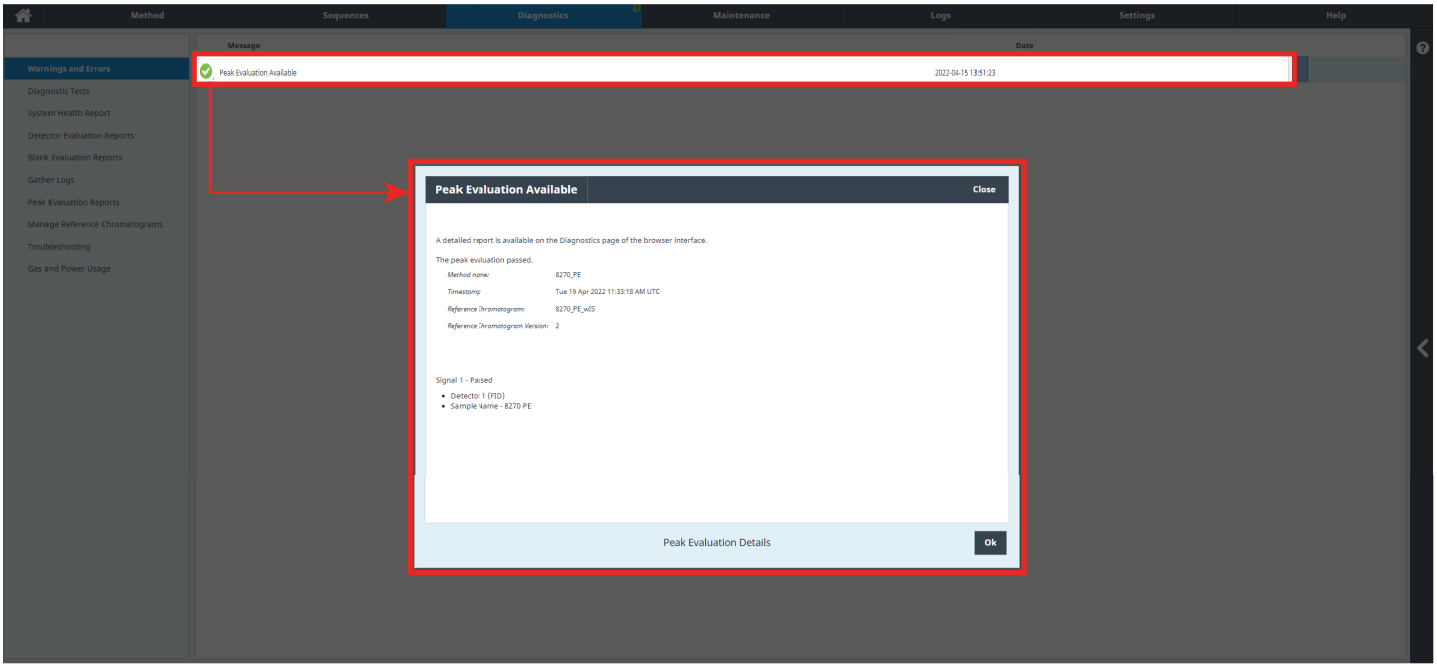


Figure 29. Pop-up window within the Warnings and Errors screen showing a passed peak evaluation after running a method with Peak Evaluation enabled.

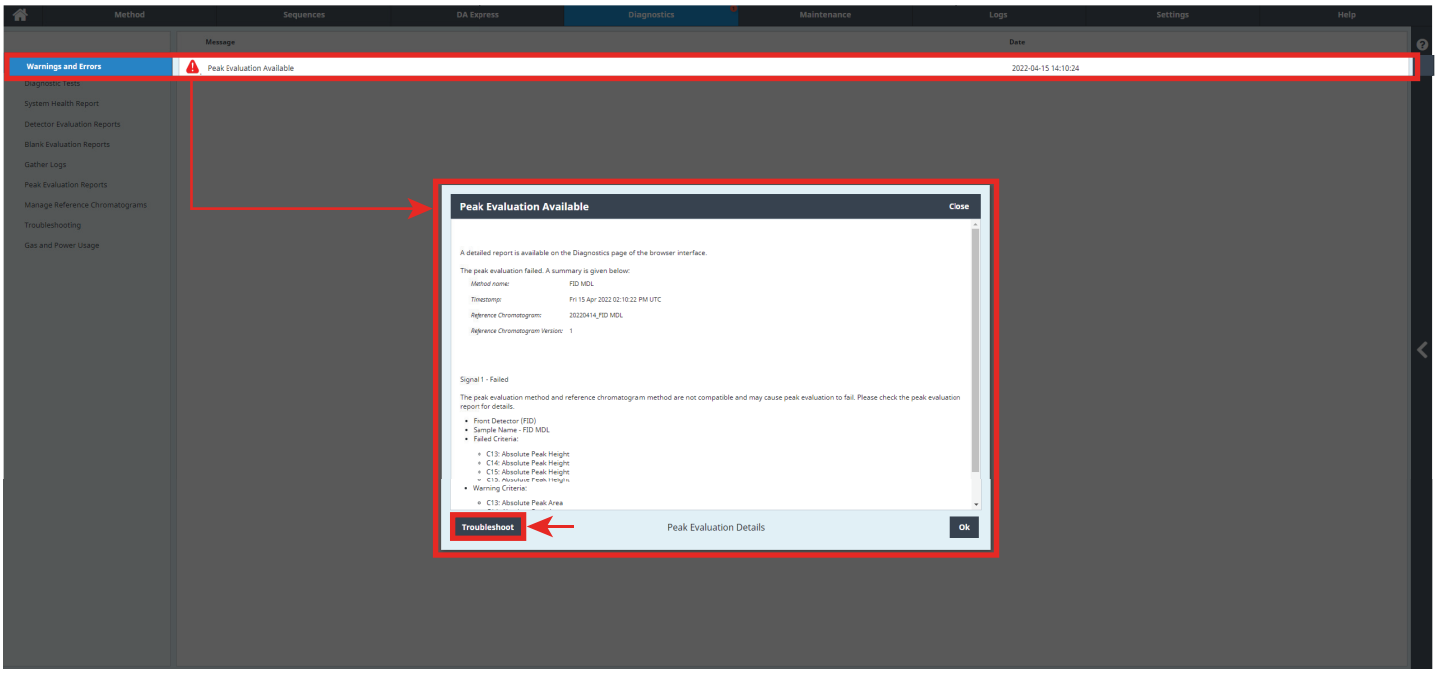


Figure 30. Pop-up window within the Warnings and Errors screen showing a failed peak evaluation after running a method with peak evaluation enabled. Clicking **Troubleshoot** can resolve the peak evaluation issue.

Previous Peak Evaluation results can also be obtained by selecting **Peak Evaluation Reports** in the Diagnostics tab. A report of the individual Peak Evaluations will be displayed when the result is selected (see Figure 31). Reports can then be printed if the user desires.

A chromatographic trend plot may also be generated if the user clicks **Chromatographic Trend Plot** in the upper right corner of the screen (see Figure 32).

See the Trend Plot white paper[3] for additional information on how to generate a trend plot.

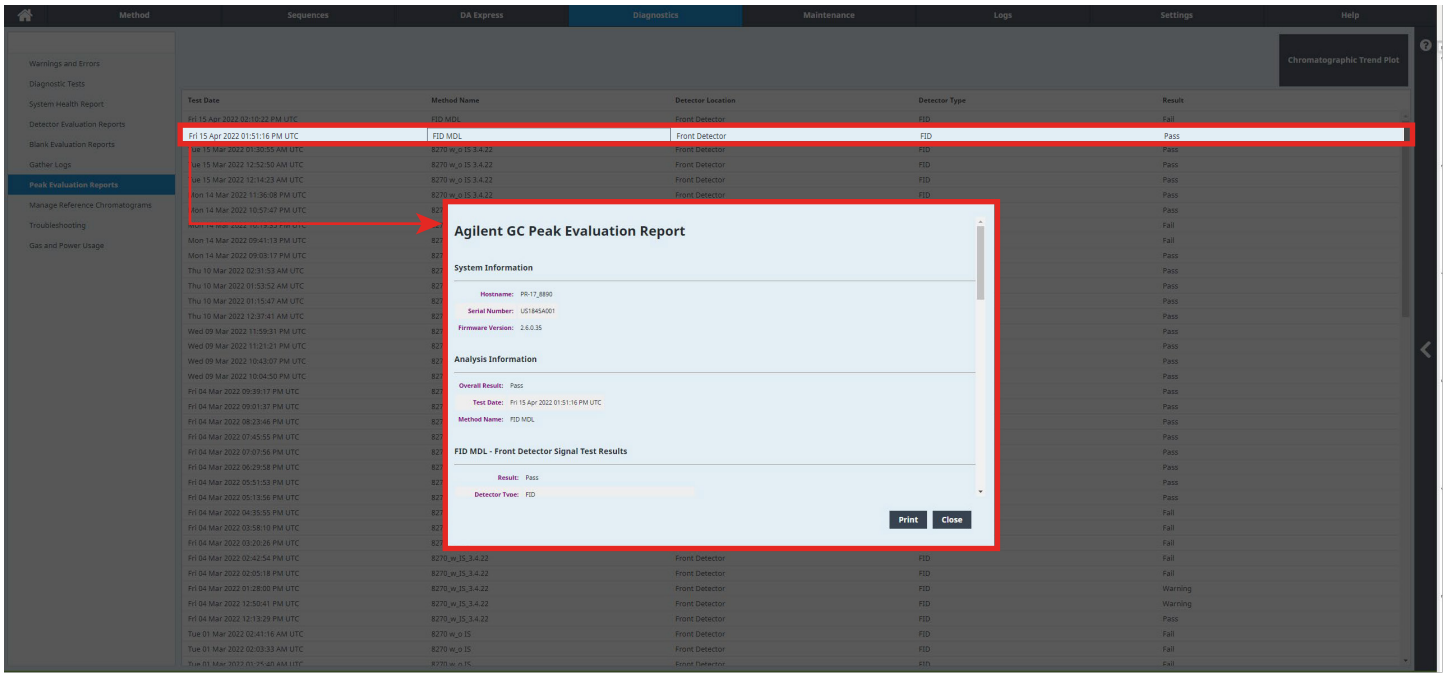


Figure 31. Peak Evaluation reports available from the Peak Evaluation Reports screen under the Diagnostics tab.

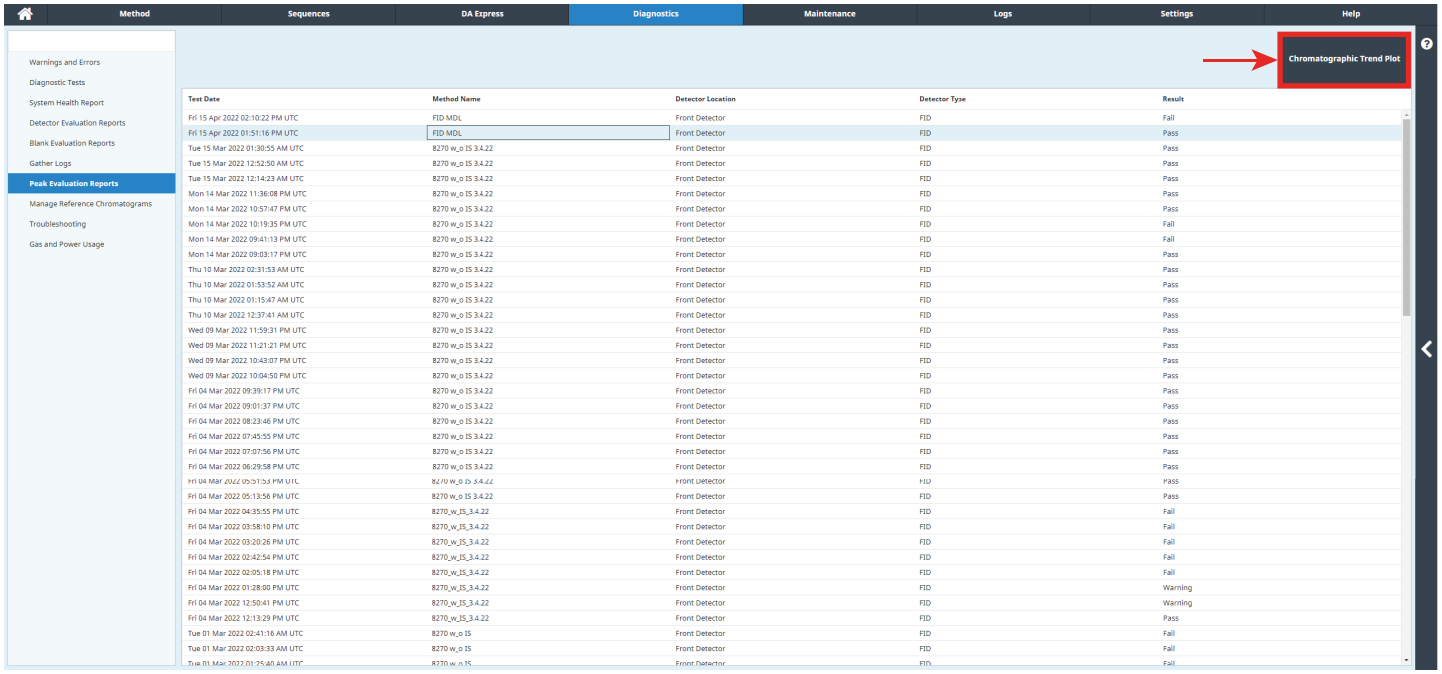


Figure 32. Peak Evaluation chromatographic Trend Plot available from the Peak Evaluation Reports screen under the Diagnostics tab.

The following section will explain the use and setup of Peak Evaluation in a Data System.

Peak Evaluation in the data system

The following section demonstrates the Peak Evaluation workflow in Agilent OpenLab CDS version 2.7 using the Peak Evaluation Setup GC plugin. Use of Peak Evaluation within the data system is only supported on OpenLab CDS software version 2.7. The plugin is installed with the GC driver and requires GC driver version 3.8 or higher. The GC firmware must also be version 2.6 or higher for use of the following workflow. If users have an older version of OpenLab CDS (version 2.6 or earlier), Peak Evaluation will have to be run through the browser interface.

How to initiate a Peak Evaluation within OpenLab CDS

To initiate a Peak evaluation within OpenLab CDS, users must first click the GC Plugins tab at the top of the screen, then click **Peak Evaluation Setup** (see Figure 33).

A pop-up window will then appear, allowing the user to set up Peak Evaluation (see Figure 34).

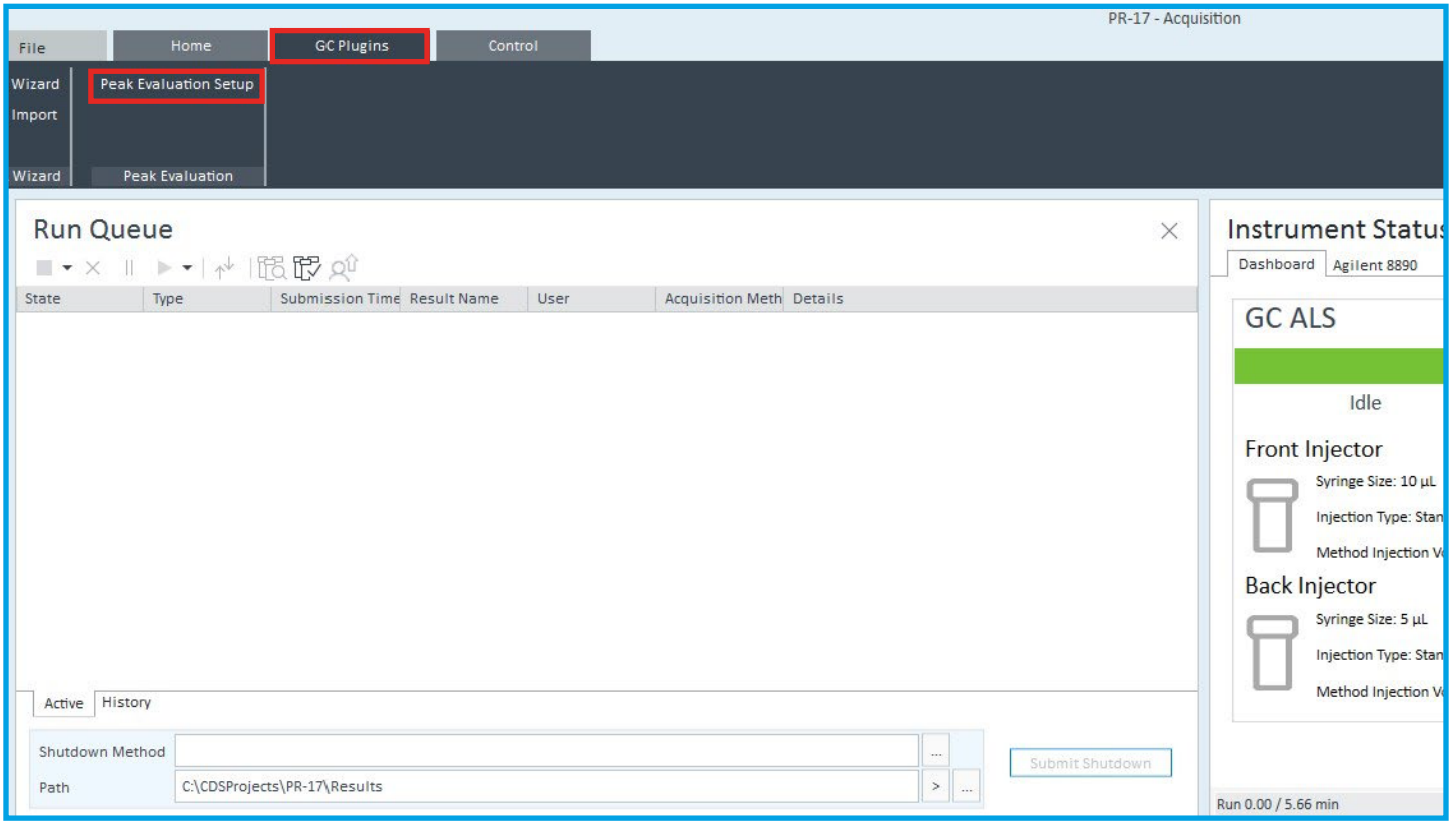


Figure 33. Initiate a Peak Evaluation from the GC Plugins tab at the top of the screen.

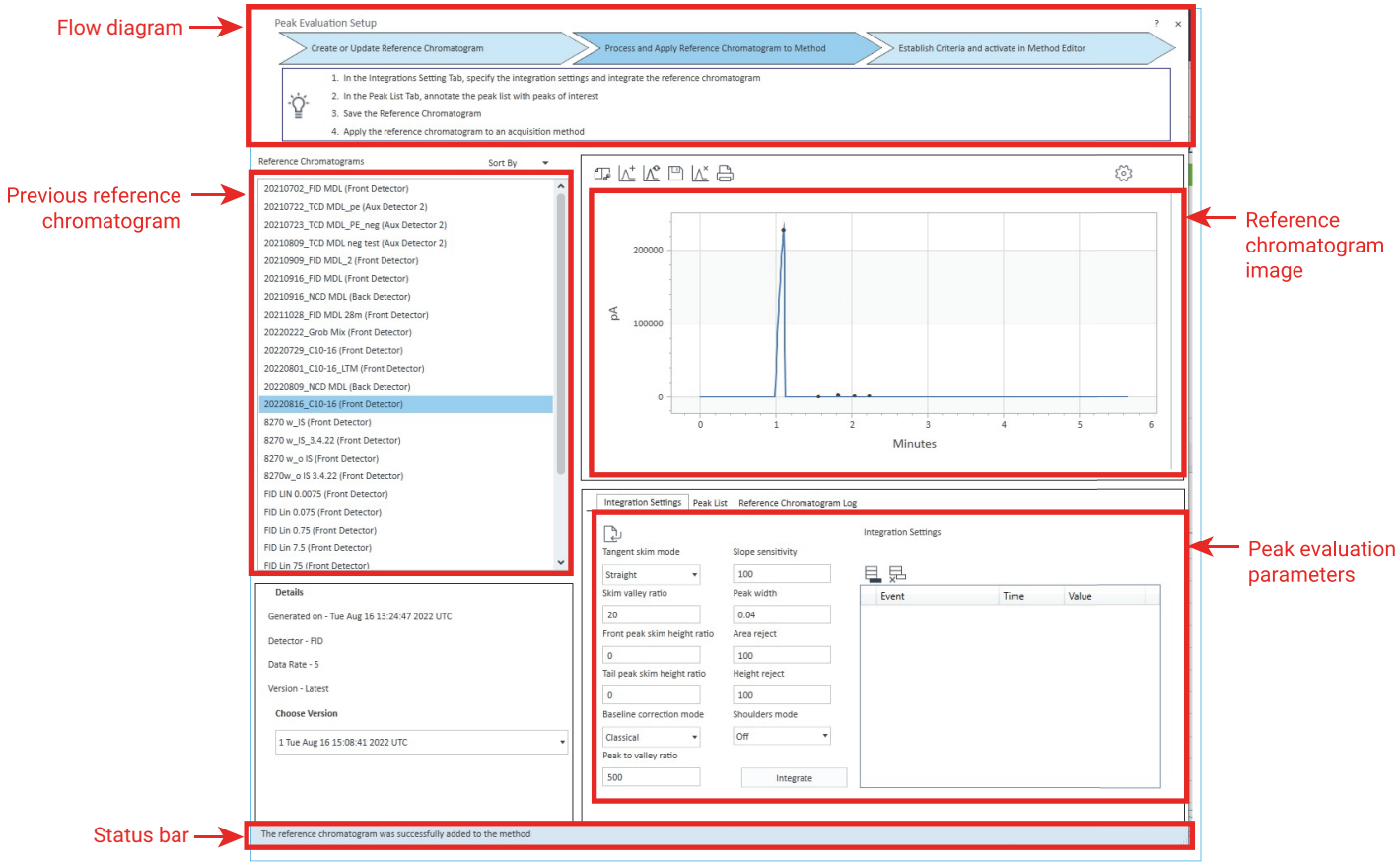


Figure 34. Peak Evaluation Setup pop-up window.

How to set up Peak Evaluation from the GC Plugin tab

Once in the Peak Evaluation Setup window, the user will notice a flow diagram at the top showing the steps for setting up Peak Evaluation in the GC plugin. Peak Evaluation Setup in the plugin is similar to in the Manage Reference Chromatograms screen in the browser interface (see Figure 34). On the left side under Reference Chromatograms, previously collected reference chromatograms can be found. Previously collected reference chromatograms from the browser will also appear in this location. Below the Reference Chromatograms list, details of the above-selected reference chromatogram can be viewed. To the right of the Reference Chromatograms list is an image of the selected reference chromatogram. Below the reference chromatogram image are the tabs Integration Settings, Peak List, and Reference Chromatogram Log. More details about each of these tabs can be found later. At the bottom of the Peak Evaluation Setup window, a status bar to provide alerts while setting up Peak Evaluation can be found. Above the reference chromatogram image are icons allowing the user to perform a variety of tasks (such as transferring the Peak Evaluation to the GC method, saving and deleting reference chromatogram, and so on); see Figure 35 for additional details about these icons.

To create a new reference chromatogram, users will first click the Generate new Reference Chromatogram icon above the chromatogram image (see Figure 35). Another pop-up window will open asking the user to input a variety of parameters that are used to generate a new reference chromatogram (see Figure 36).

As with the browser interface, the following parameters need to be set before collecting the reference chromatogram.

- Select the GC method to be used for generating the reference chromatogram.
- Select the detector signal (should be the same ones listed as those in the GC method).
- Type the reference chromatogram name.
- Select the injection location.
  - This will be Front or Back for ALS injections on the 8890 GC.

1. Apply reference chromatogram to method
2. Generate new reference chromatogram
3. Update reference chromatogram
4. Save and download reference chromatogram to instrument
5. Delete reference chromatogram
6. Print the reference chromatogram's method

Figure 35. Icons above the reference chromatogram image.

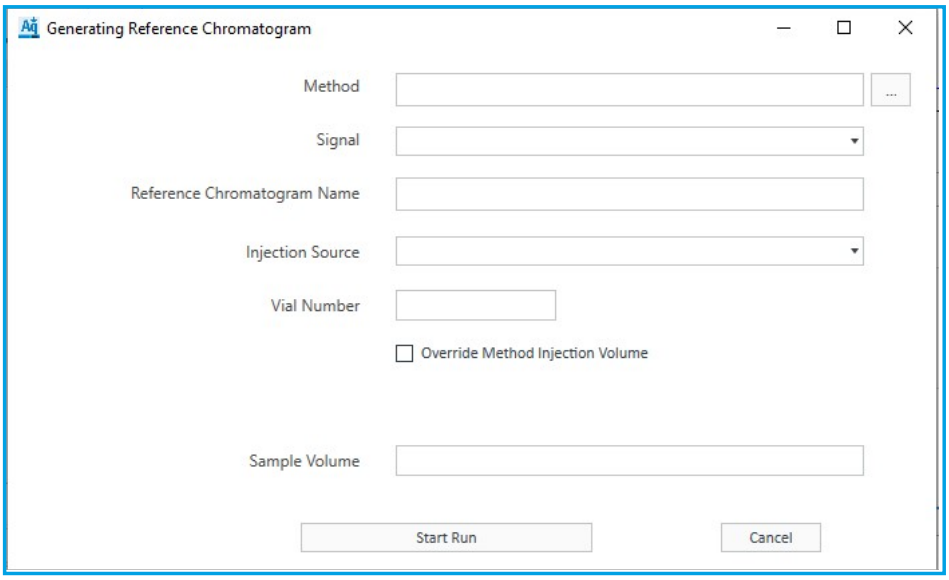


Figure 36. Generate Reference Chromatogram window.

  - A value of 1 will be present on the Intuvo 9000 GC for the injection location because the Intuvo 9000 GC only has a single injection location.
- Select the sample source under Injection Source.
  - Select **Injector** for ALS injections.
  - Select **Valve** if making a valve-based injection.
  - Can also select **Headspace** if an 8697 headspace sampler is installed on the system.
- Type the vial number to make the injection from.
- The user can modify the injected sample volume if desired by selecting the **Override Method Injection** check box.

Finally, click **Start Run** to initiate collection of the reference chromatogram and the instrument will begin collecting the reference chromatogram. Users can monitor the data collection of the reference chromatogram from the real-time plot. The Peak Evaluation Setup window will need to be closed to navigate to difference screens within the data system.

Once collection of the reference chromatogram is complete, users will see a new reference chromatogram name on the left side of the Peak Evaluation Setup window. (Users may need to reopen the Peak Evaluation Setup plugin.) Select the reference chromatogram that was generated from the list of available reference chromatograms. After the reference chromatogram is selected, details of the run will be displayed below the reference chromatogram list. If multiple versions of the reference chromatogram were collected, the version number can be selected in the Details section. To the right of the reference chromatogram, an image of the reference chromatogram that is selected will be displayed. Users can adjust the X- and Y-axes by selecting the plot settings icon in the upper right corner of the chromatogram window (see Figure 35). The chromatogram may also be zoomed in on by holding down the **Shift** key and clicking and dragging the area of interest. Holding down the **Alt** key and left-clicking the plot will zoom out the chromatogram image.

Below the chromatogram image are three tabs: Integration Settings, Peak Lists, and Reference Chromatogram Logs (see Figure 37).

The first tab, Integration Settings, allows the user to input different integration setpoints to determine which peaks are integrated in the reference chromatogram. Integration events can also be set by adding lines to the integration table (see Figure 38).

Within the Peak Evaluation Setup window, users also can import integration settings from a previous Data Analysis processing method (see Figures 39 and 40).

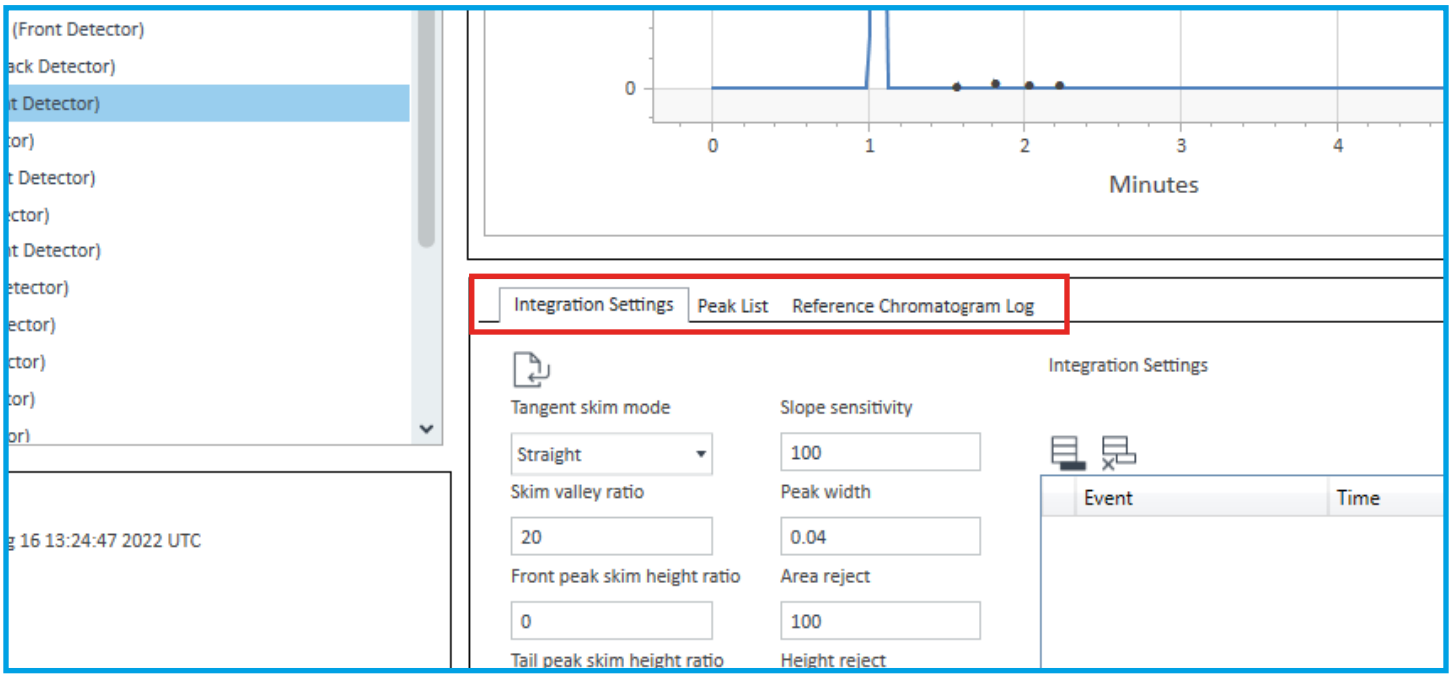


Figure 37. Settings tabs for peak evaluation within the Peak Evaluation Setup window.

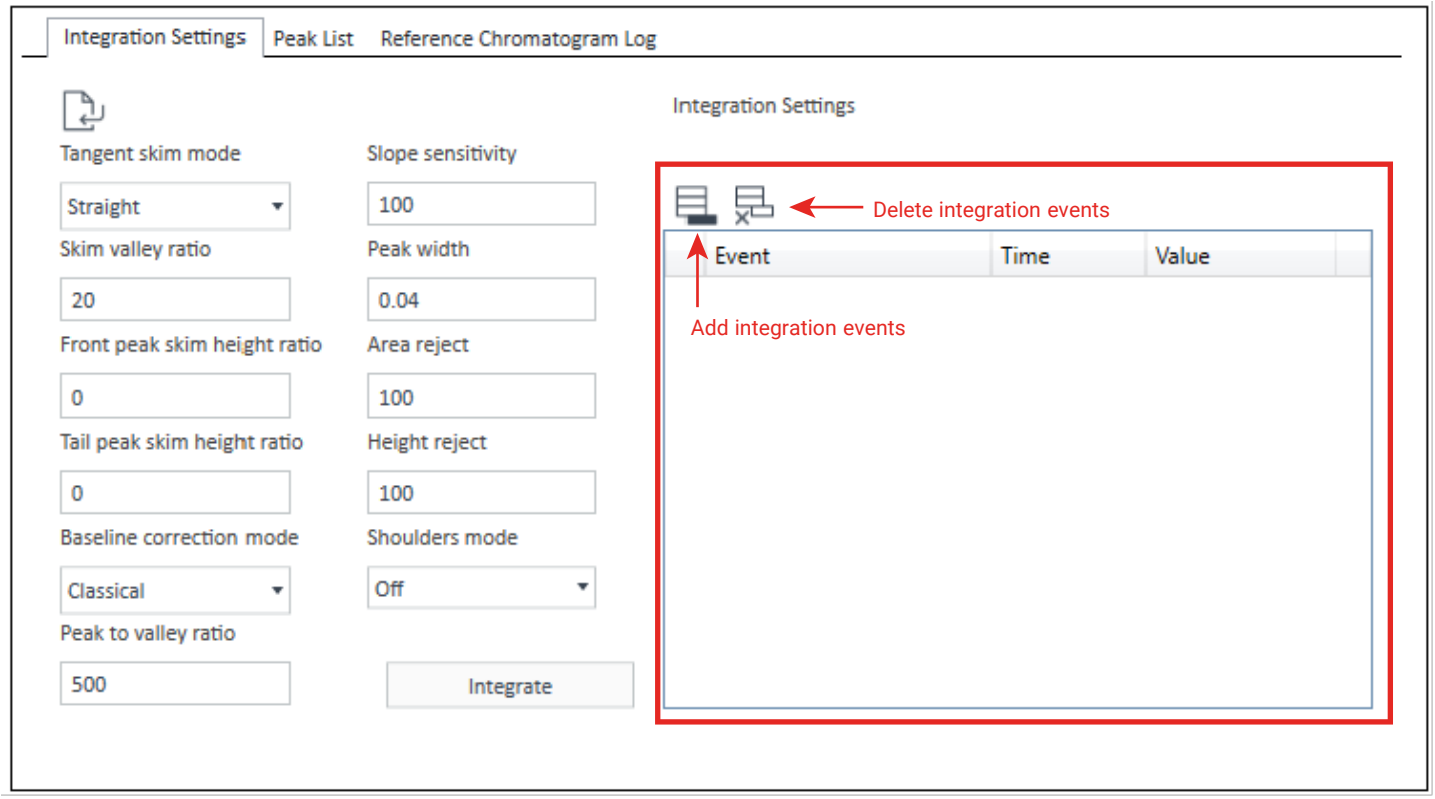


Figure 38. Adding or deleting integration events from the Integration Settings tab.

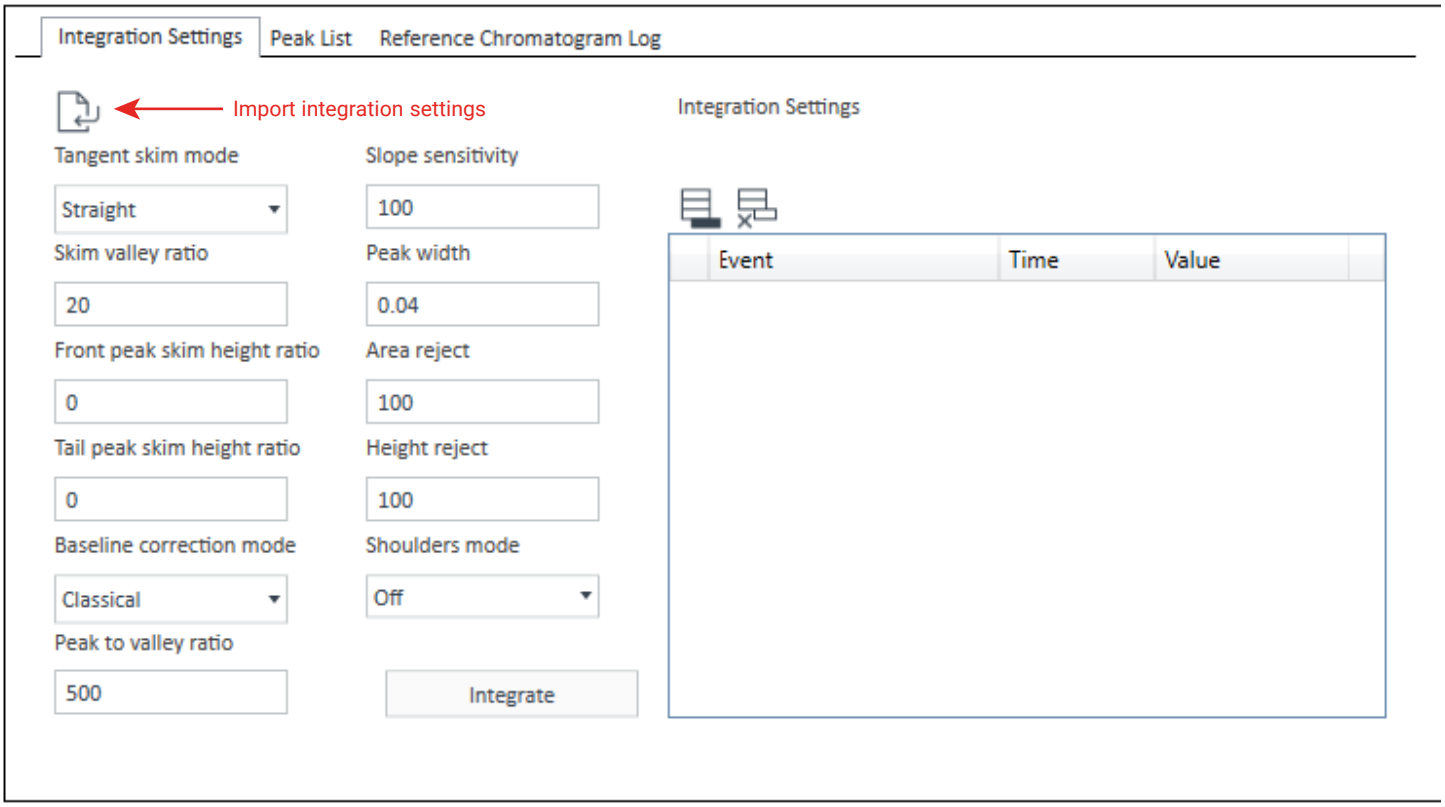


Figure 39. Icon to import Data Analysis processing method integration setpoints.

Import the processing method by clicking the ellipsis icon located near the Processing Method field in the Import Integration Settings window (see Figure 40). Once a processing method is imported, click **Apply and Integrate** to close the window and import the Data Analysis processing method integration parameters to the Peak Evaluation Setup.

After the user has either input or imported the desired integration settings, click **Integrate** to apply these setpoints to the selected reference chromatogram (see Figure 41).

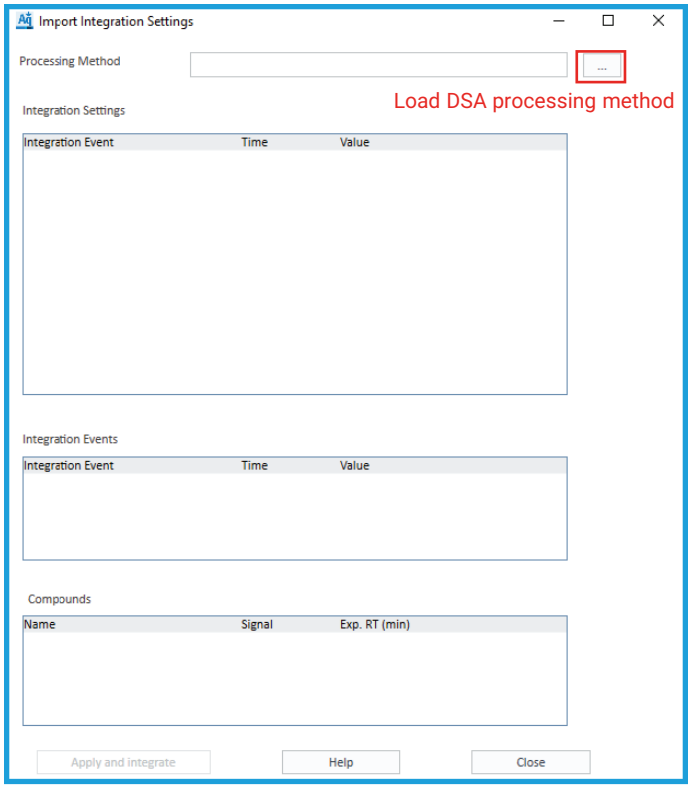


Figure 40. Import integration settings window (for importing processing method from a Data Analysis method).

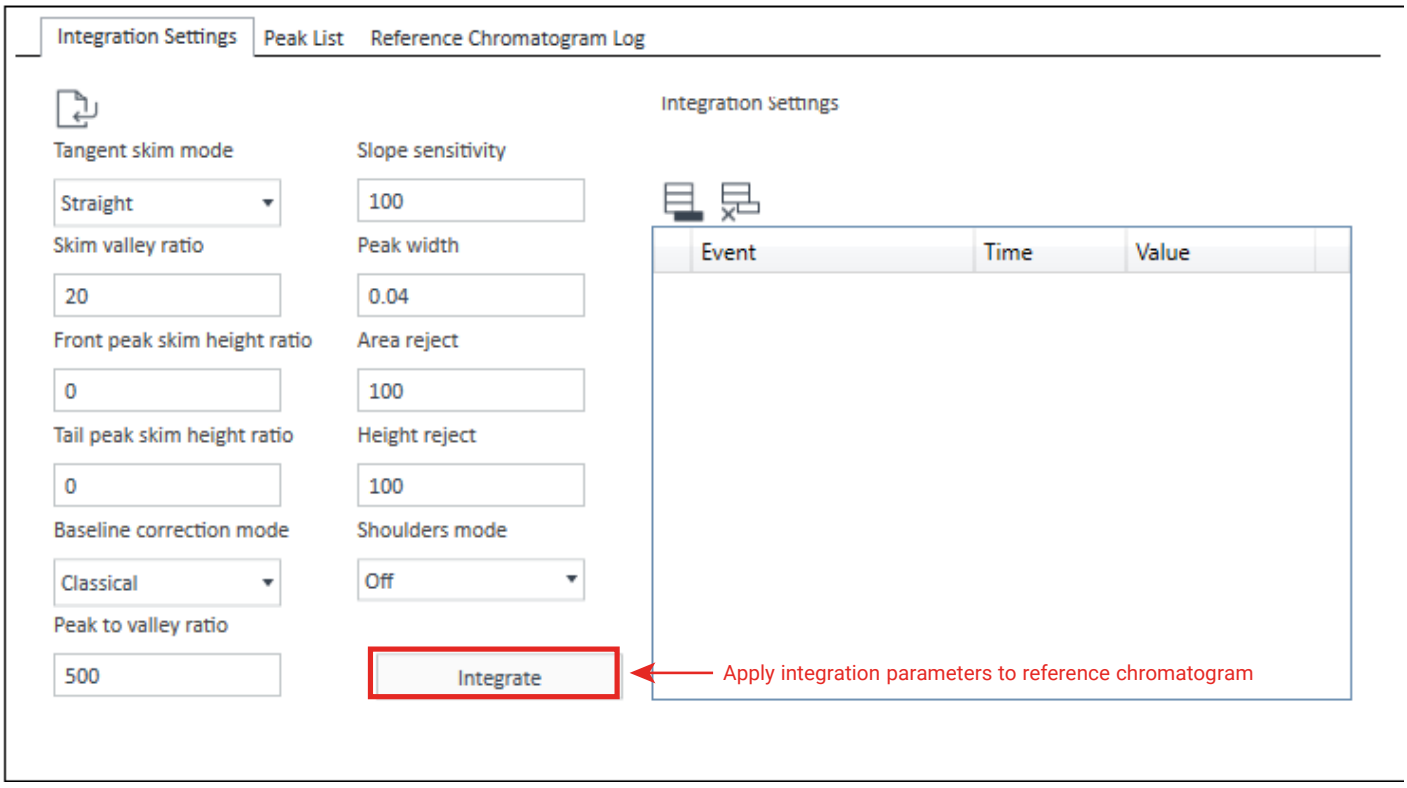


Figure 41. Apply integration parameters to the selected reference chromatogram.

Above each integrated peak in the chromatogram window, a black dot will appear showing that the peak was integrated using the desired integration setpoints (see Figure 42).

After integrating the reference chromatogram, the user may wish to save the integration parameters by clicking **Save**, located above the reference chromatogram image (see Figure 35). This will save the integration setpoints with the reference chromatogram.

Once the integration setpoints have been saved, continue onto the next step by clicking the Peak List tab to define the peaks of interest (see Figure 43).

Within the Peak List tab, the peaks that were integrated in the reference chromatogram will be listed by retention time, with the area displayed in the next column. Users may also name their compounds of interest by typing in the Name column and may type the CAS identification number in the

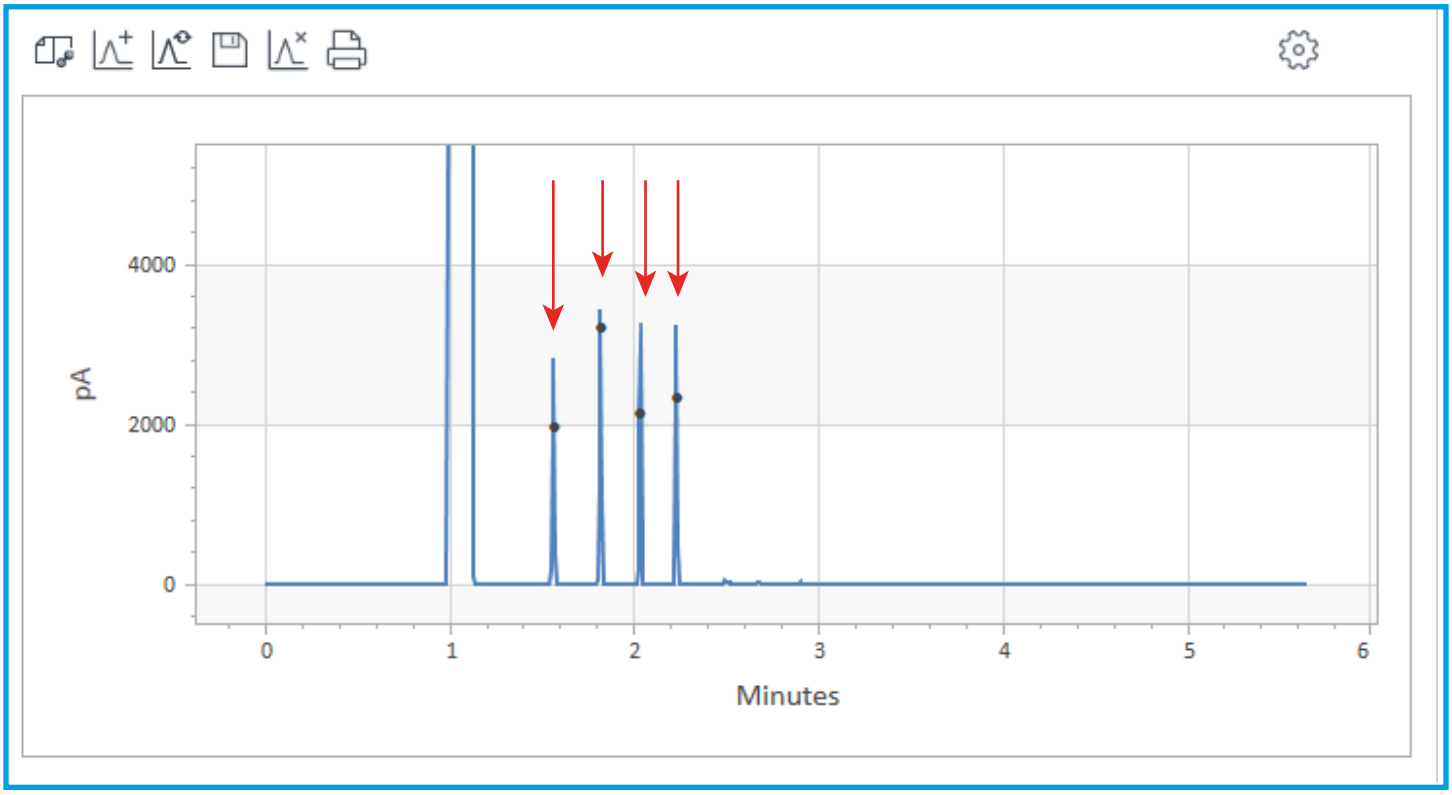


Figure 42. Peaks integrated using the selected integration setpoints.

Integration Settings | Peak List | Reference Chromatogram Log

Retention Time	Area	Name	CAS Id
1.107	1044735.51905614	Default_1.107339	
1.566	2057.69617546079	C10	
1.821	2272.43217881851	C12	
2.040	2354.38255154351	C14	
2.233	2531.58544566273	C16	

Figure 43. Peak List tab showing list of the integrated peaks that are present in the reference chromatogram.

CAS Id column (see the red box in Figure 43). Both fields are optional. The final tab is Reference Chromatogram Log. This tab contains a table with additional information about the reference chromatogram, such as when the reference chromatogram was generated or updated (see Figure 44).

After identifying and naming the compounds of interest, save the reference chromatogram by clicking **Save**, located above the chromatogram image. Next, select the Apply reference chromatogram to method icon (see Figure 35) to transfer the reference chromatogram to a GC method. A pop-up window will appear asking the user to select a method in which it applies the Peak Evaluation setpoints. Once the method is selected and the user clicks **OK**, another pop-up window will appear asking the user to save the method as a new file name. The user must resave the GC method as a new unique file name. OpenLab CDS will not allow the user to overwrite an existing GC method. After the new GC method has been renamed and saved, close the Peak Evaluation Setup window to show the main instrument acquisition page.

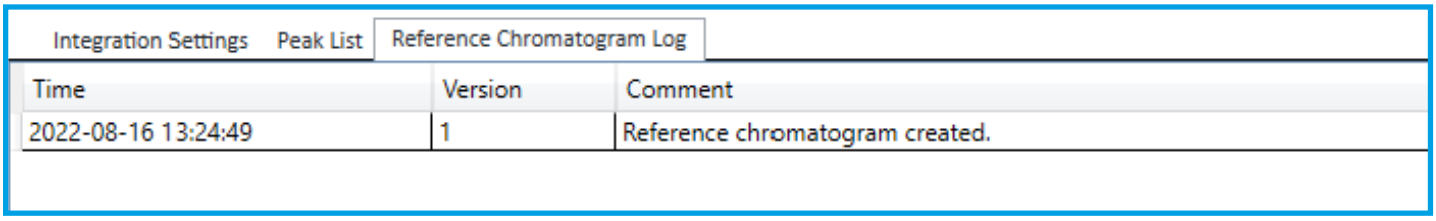


Figure 44. Reference Chromatogram Log tab showing additional information about the selected reference chromatogram.

Establish criteria and activate in method editor

Next, open the new GC method that the reference chromatogram was transferred to. At the top of the screen, click **Method** to view the GC method, then click **Peak Evaluation** under GC Performance on the left side (see Figure 45).

In the Peak Evaluation screen of the GC method editor are three tabs for the user to complete setting up a Peak Evaluation (Setpoints, Peak List, and Limits). The first tab, Setpoints, will allow the user to enable Peak Evaluation and define certain parameters to be used. First, users should select the **Perform Peak Evaluation Test** check box to enable peak evaluation in the GC method (see Figure 46).

Once Peak Evaluation is enabled, the fields below the check box–Action on Failure, Compare Reference Chromatogram with, and Choose Warning Level–will become active, allowing the user to select an option for each. These parameters are the same as those found in the browser interface version of the Peak Evaluation screen (see Figure 47).

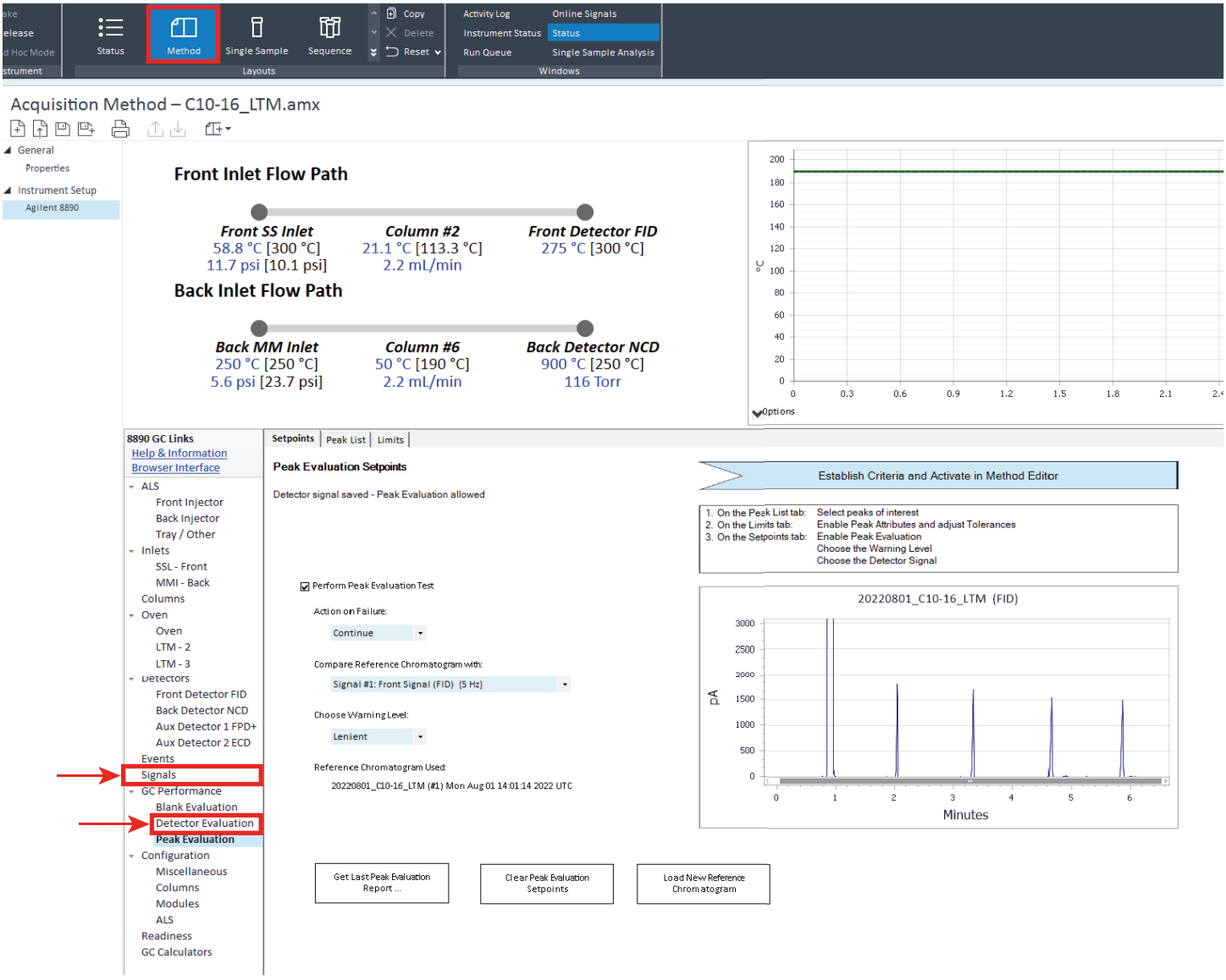


Figure 45. Peak Evaluation from within the GC method.

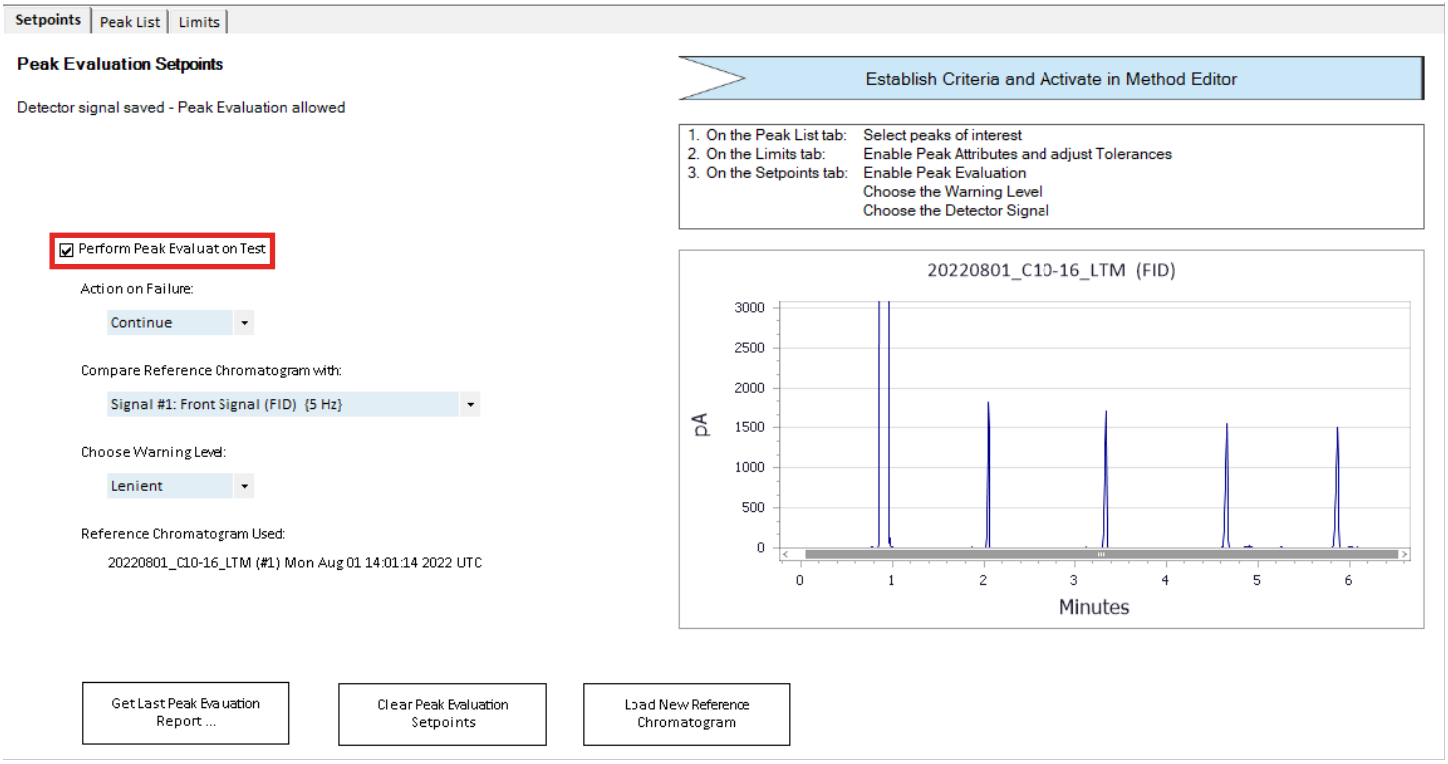


Figure 46. Enabling Peak Evaluation from within the GC method by selecting the **Perform Peak Evaluation Test** check box.

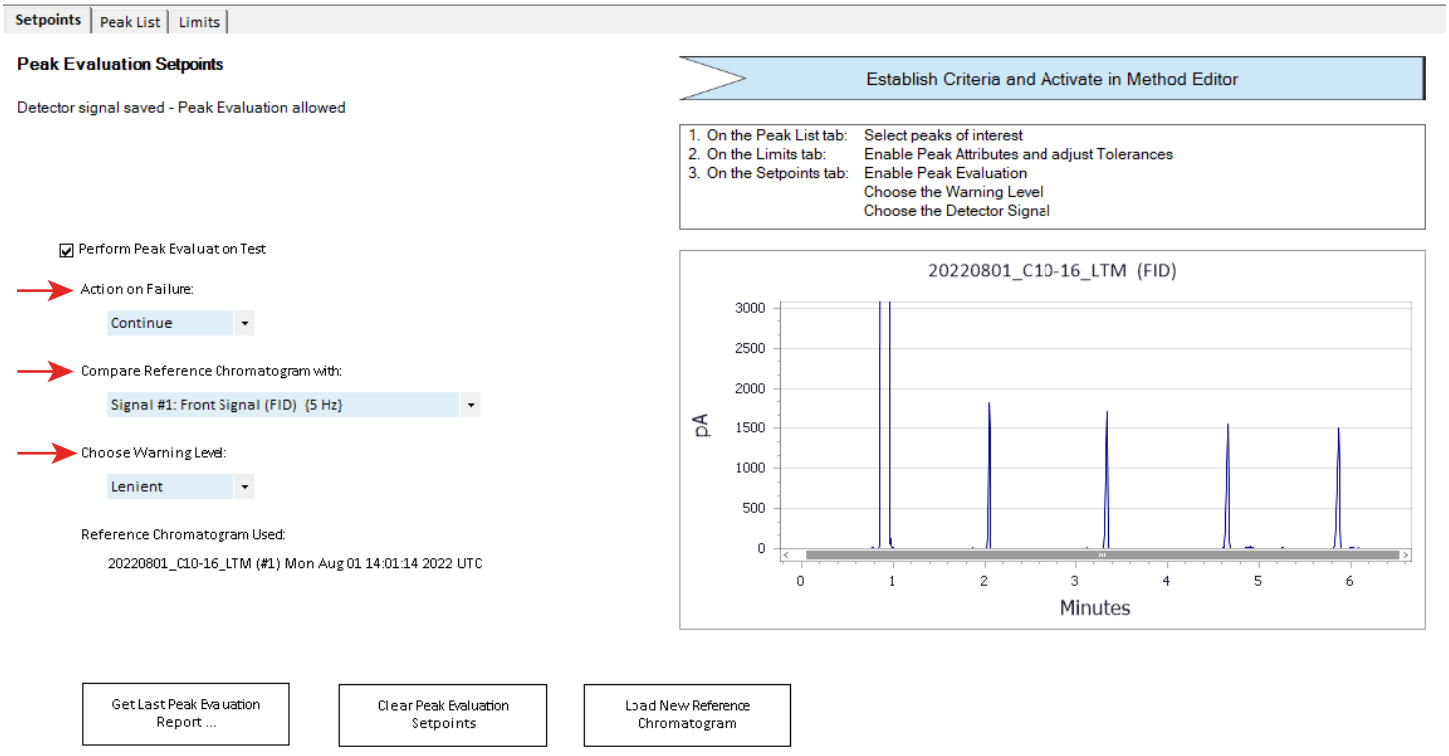


Figure 47. Peak Evaluation parameter setpoints.

For the Action on Failure parameters, users may select what occurs in a sequence if a method in which Peak Evaluation was enabled fails (either Continue or Abort). The next parameter, Compare Reference Chromatogram with, will allow the user to choose the detector signal for Peak Evaluation to compare to (typically this will be the same signal as what the reference chromatogram was collected with). The final parameter the user may modify is Choose Warning Level. Users can either select **None**, **Strict**, or **Lenient** warning levels (see Figure 15 in the browser interface section). After making the above selections, the user should also verify that the chromatogram listed under Reference Chromatogram Used corresponds to the correct reference chromatogram that was transferred over from the Peak Evaluation Setup.

An image of the reference chromatogram is also available on the right side of the screen. Users may zoom in or out of this image as they did previously in the Peak Evaluation setup (**Shift** + click and zoom or **Alt** + left-click). At the bottom of the screen, three buttons are available: **Get the latest Peak Evaluation Report**, **Clear Peak Evaluation Setpoints**, and **Load New Reference Chromatogram** (see Figure 48).

Clicking **Get Latest Peak Evaluation Report** will open a browser session to display the latest peak evaluation report on the screen. Clicking **Clear Peak Evaluation Setpoints** will remove the Peak Evaluation setpoints from the GC method. Clicking **Load New Reference Chromatogram** will show a new pop-up window allowing the user to select a new reference chromatogram to be used in the GC method (see Figure 49). Select the reference chromatogram from the Choose the Reference Chromatogram to be loaded field to view the available reference chromatogram on the instrument (left-hand image in Figure 49). Both reference chromatograms collected in the data system and the browser will be displayed for the user to select. Below the selected reference chromatogram will be details about the selected reference chromatogram. Click **OK** to load the selected reference chromatogram to the GC method or click **Cancel** to close the screen without making any changes.

The next tab, Peak List, contains a list of all the peaks that were found using the integration settings provided during the Peak Evaluation setup (see Figure 50).

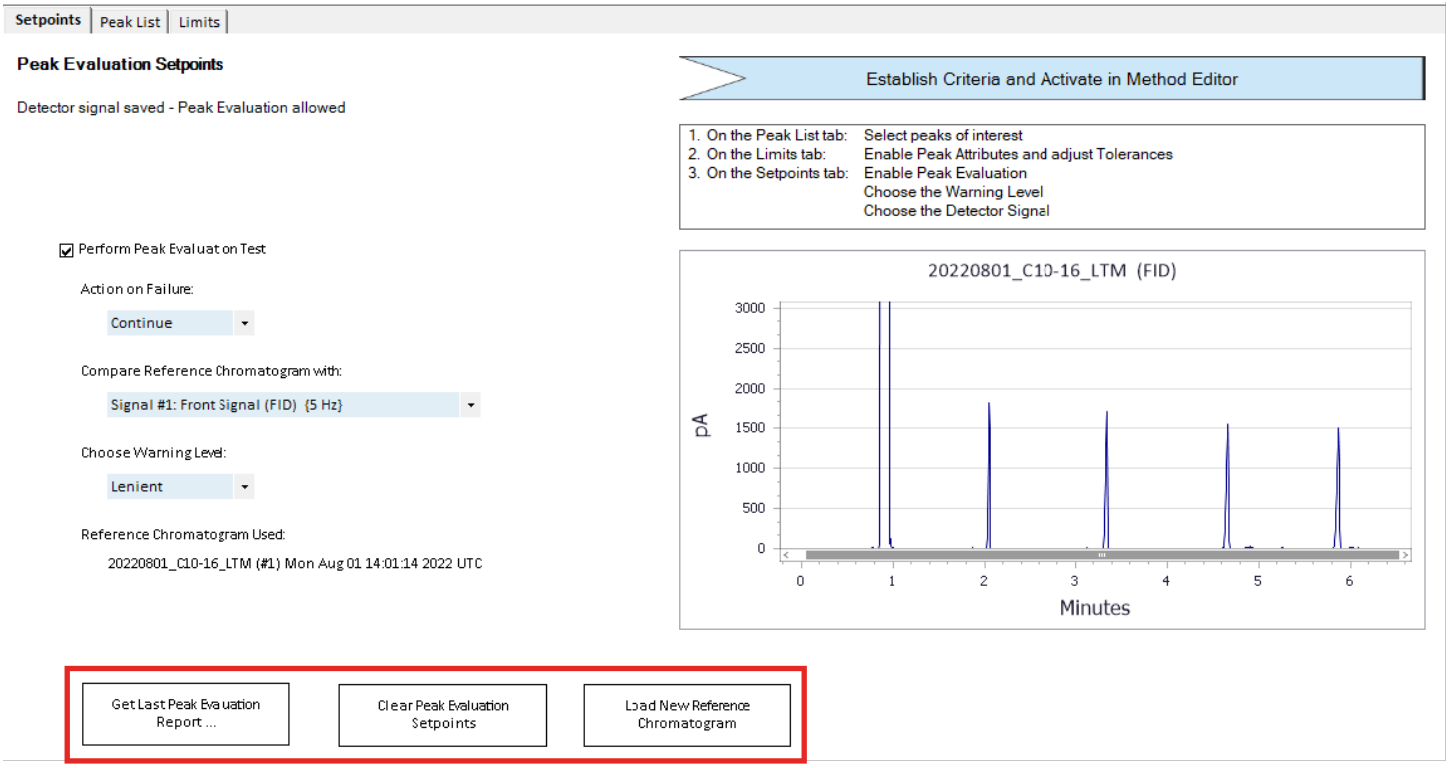


Figure 48. Buttons at the bottom of the Peak Evaluation Setup screen.

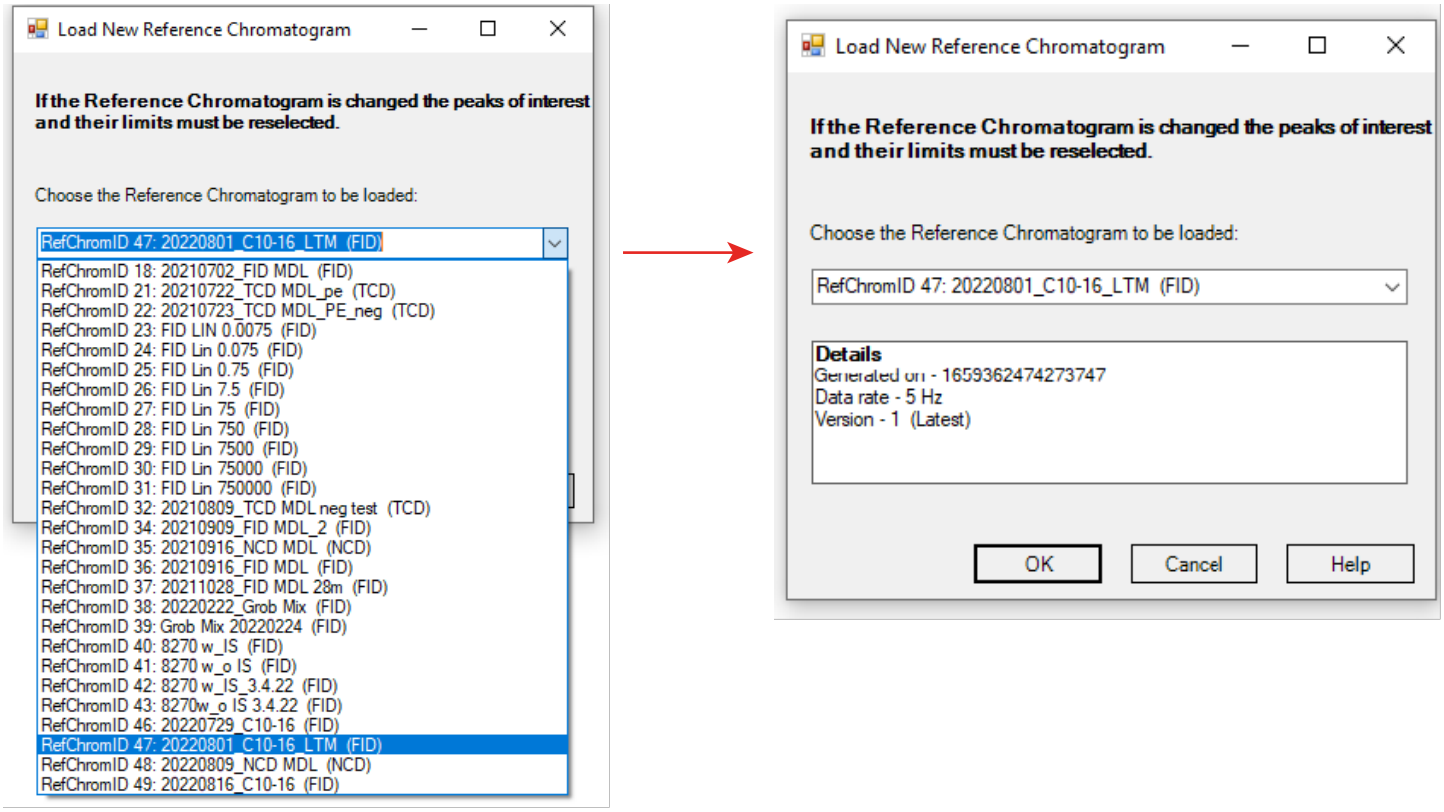
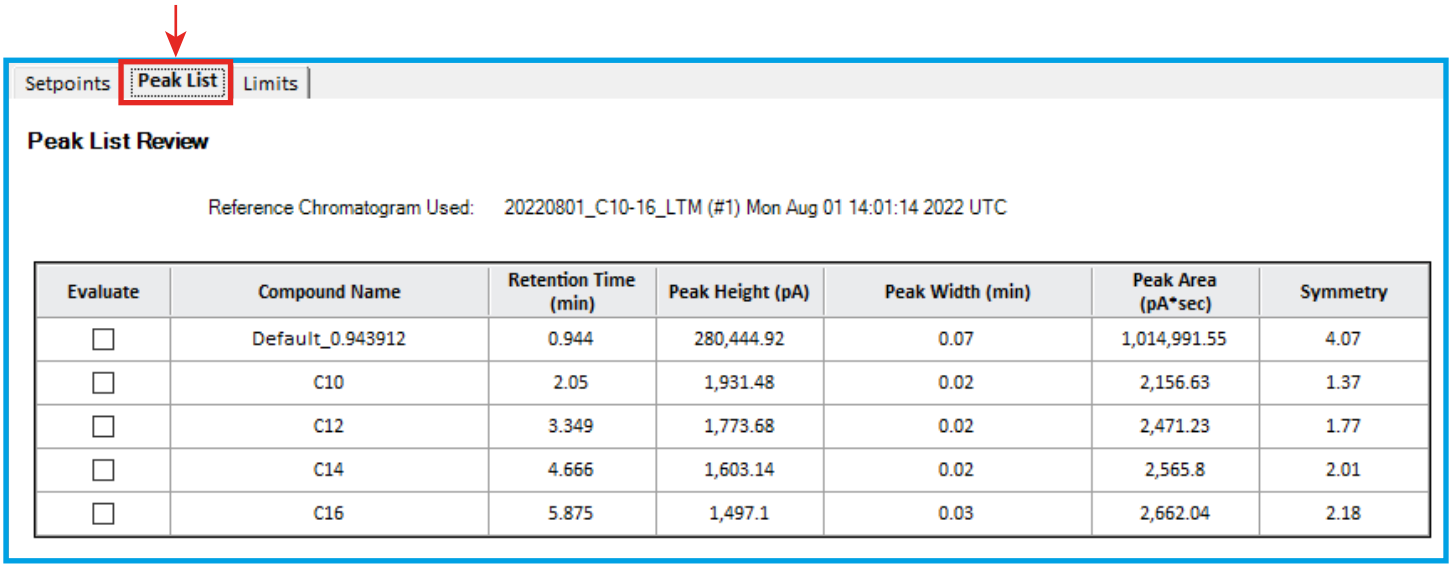


Figure 49. Load New Reference Chromatogram screen.



Evaluate	Compound Name	Retention Time (min)	Peak Height (pA)	Peak Width (min)	Peak Area (pA*sec)	Symmetry
☐	Default_0.943912	0.944	280,444.92	0.07	1,014,991.55	4.07
☐	C10	2.05	1,931.48	0.02	2,156.63	1.37
☐	C12	3.349	1,773.68	0.02	2,471.23	1.77
☐	C14	4.666	1,603.14	0.02	2,565.8	2.01
☐	C16	5.875	1,497.1	0.03	2,662.04	2.18

Figure 50. The Peak List tab within Peak Evaluation Setup in the GC method.

The Peak List tab is where users will determine which peaks to evaluate during the analysis. Users may choose which peaks to evaluate by selecting the check boxes in the Evaluate column next to the compound they wish to monitor. Up to 10 peaks may be selected for evaluation.

The final tab, Limits, allows the user to set limits for the peaks that are being evaluated (see Figure 51).

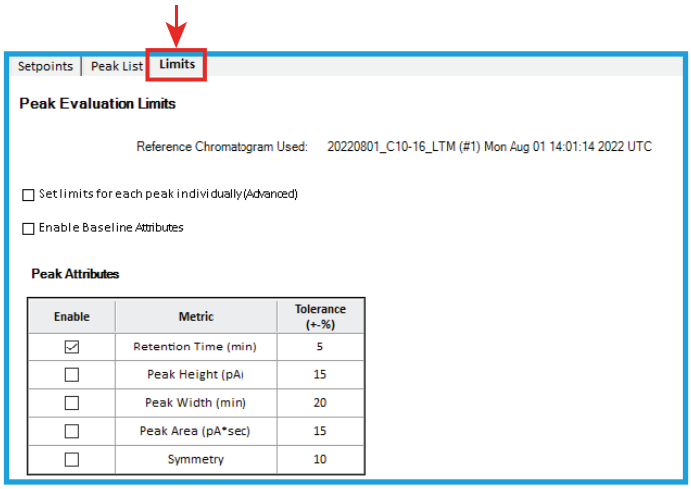


Figure 51. Limits within Peak Evaluation Setup in the GC method.

The parameters in this tab are similar to those found in the browser interface. Users may enable the different peak metrics they wish to monitor by selecting the corresponding check boxes in the Enable column. Global tolerance limits (±%) may also be defined by editing the values in the Tolerance column. Users may also select limits for each peak individually by selecting the **Set limits for each peak individually (Advanced)** check box. This will open a new table allowing the user to select individual peaks (see Figure 52).

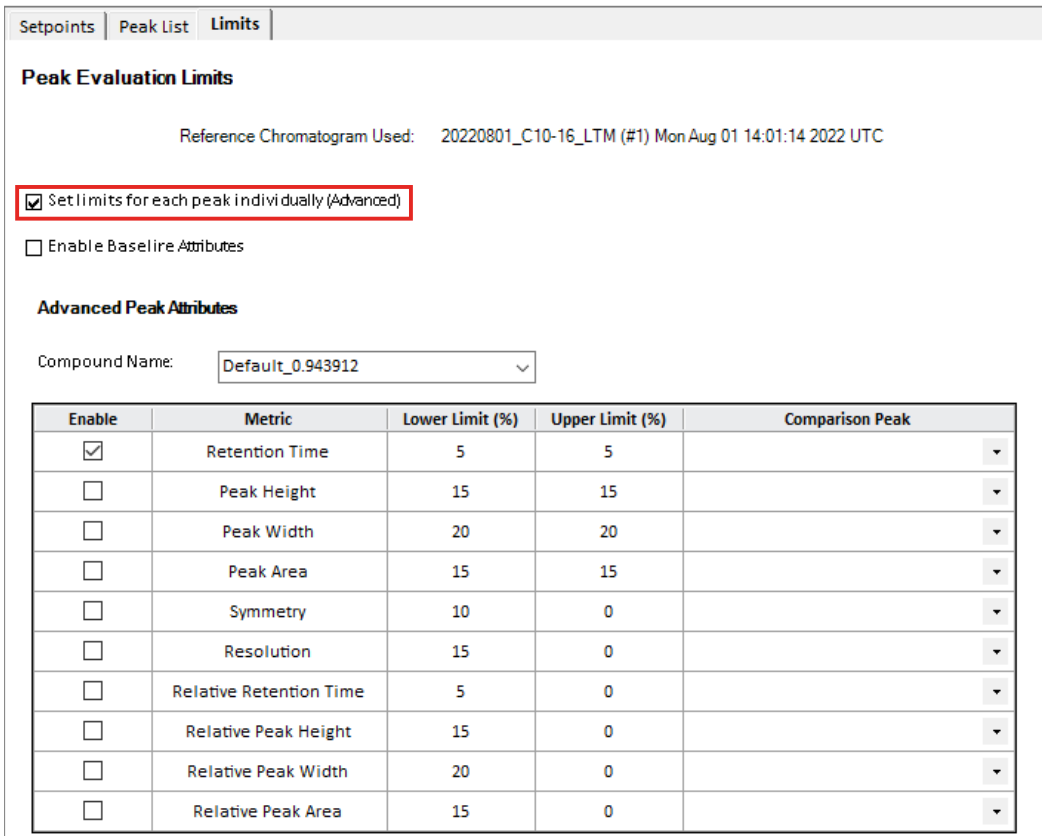
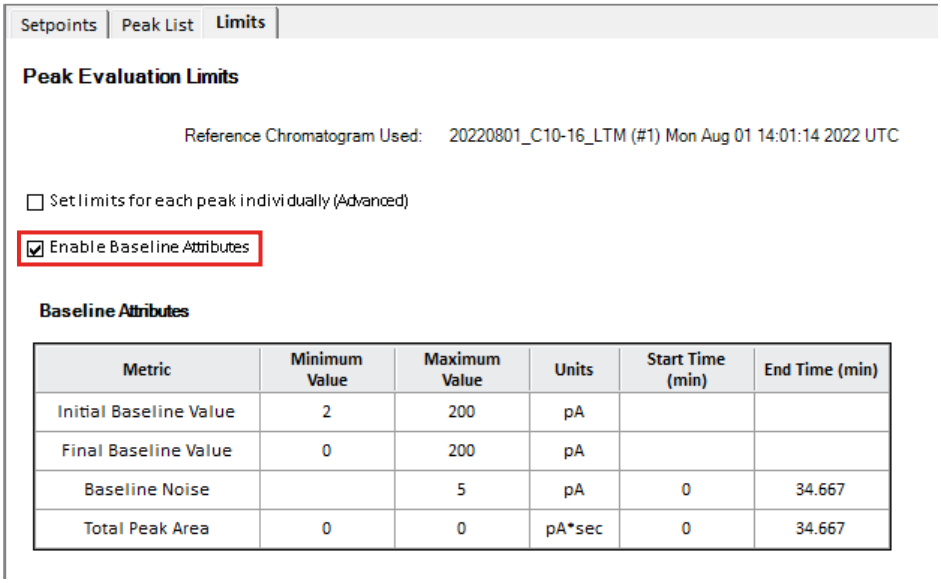


Figure 52. Limits tab with the S**et limits for each peak individually (Advanced)** check box selected.

The user may select the peak of interest from the Compound Name drop-down box. Baseline attributes can also be monitored by selecting the **Enable Baseline Attributes** check box (see Figure 53).

Another table will appear allowing the user to set baseline attributes they wish to monitor in the Peak Evaluation. More details about setting Peak Evaluation limits can be found in the above browser interface section.

After limits are set, save the GC method to save the above Peak Evaluation parameters. When the saved GC method is run (either single injection or a sequence), the evaluation will be performed after each run finishes. After the method was run, users may view the Peak Evaluation results by either clicking **Get Last Peak Evaluation Report** from the Peak Evaluation > Setpoints tab in the method screen in the data system (see Figure 48), or a more comprehensive list of Peak Evaluation reports are available in the browser interface (see previous section).



Metric	Minimum Value	Maximum Value	Units	Start Time (min)	End Time (min)
Initial Baseline Value	2	200	pA		
Final Baseline Value	0	200	pA		
Baseline Noise		5	pA	0	34.667
Total Peak Area	0	0	pA*sec	0	34.667

Figure 53. Limits tab with **Enable Baseline Attribute**s selected.

Example application

The following is an example application showing how Peak Evaluation could be used in a typical laboratory setting. The application below is running a version of EPA 8270 (analysis of semivolatile organic compounds by GC) with an FID using Peak Evaluation to monitor analytes of interest and internal standards as a metric of the instrument's performance and health. Use of Peak Evaluation for standardized methods (such as EPA 8270) is ideal because Peak Evaluation will constantly monitor critical parameters (such as the area of internal standard analytes) for changes when issues may arise causing decreased performance in the instrument. Enabling Peak Evaluation can alert the user if a decrease in analyte area or increase in analyte peak width starts to occur while running a sequence and can interrupt the sequence if desired, thus reducing the amount of time needed to rerun customer samples.

The user will first set up Peak Evaluation as described above but will evaluate the internal standard compounds and/or other analytes of interest. For this example, the internal standard analytes and other analytes of interest were included to be evaluated within Peak Evaluation (additional analytes of 2,4-dinitrophenol and 4,6-dinitro-2-methylphenol were evaluated because of their sensitivity to system activity). Typical integration parameters were used for identifying all the analytes of interest. Integration events were also enabled as not to integrate the solvent peak that elutes at around four minutes (see Figure 54).

Peak Evaluation is then enabled in the GC method, thus allowing for the constant monitoring of the analytes of interest in the 8270 analyses (retention time, area, height, width, and symmetry).

With Peak Evaluation enabled in the GC method, the user will be notified after each run if the Peak Evaluation has passed or failed. This notification will appear in the Warnings and Errors section of the Diagnostics tab on the browser or touch screen interface. After multiple injections were run on the instrument, some of the internal standard analytes (and other analytes of interest) started to show signs of failure (with the peak area and height starting to become reduced), thus Peak Evaluation failed. Once the user selects the failed Peak Evaluation, a pop-up window will appear showing the failed metrics (see Figure 55).

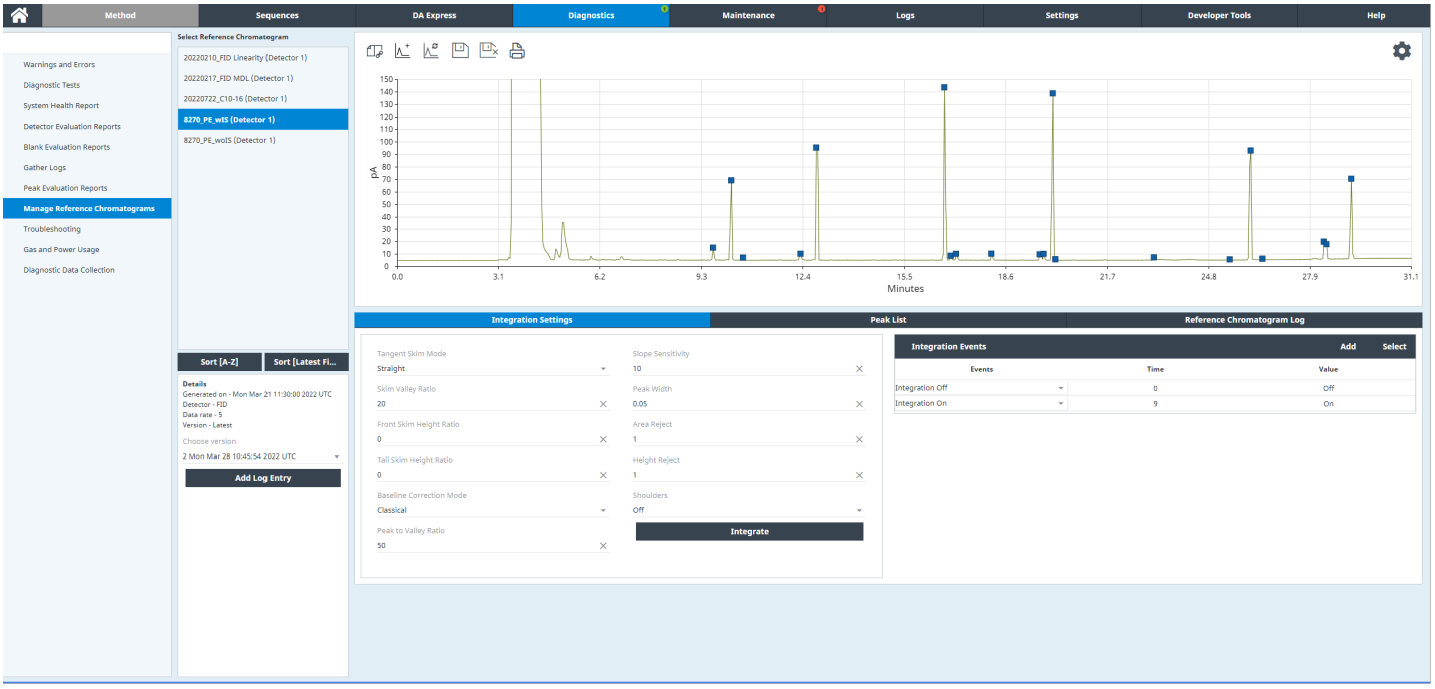


Figure 54. Example Peak Evaluation integration parameters.

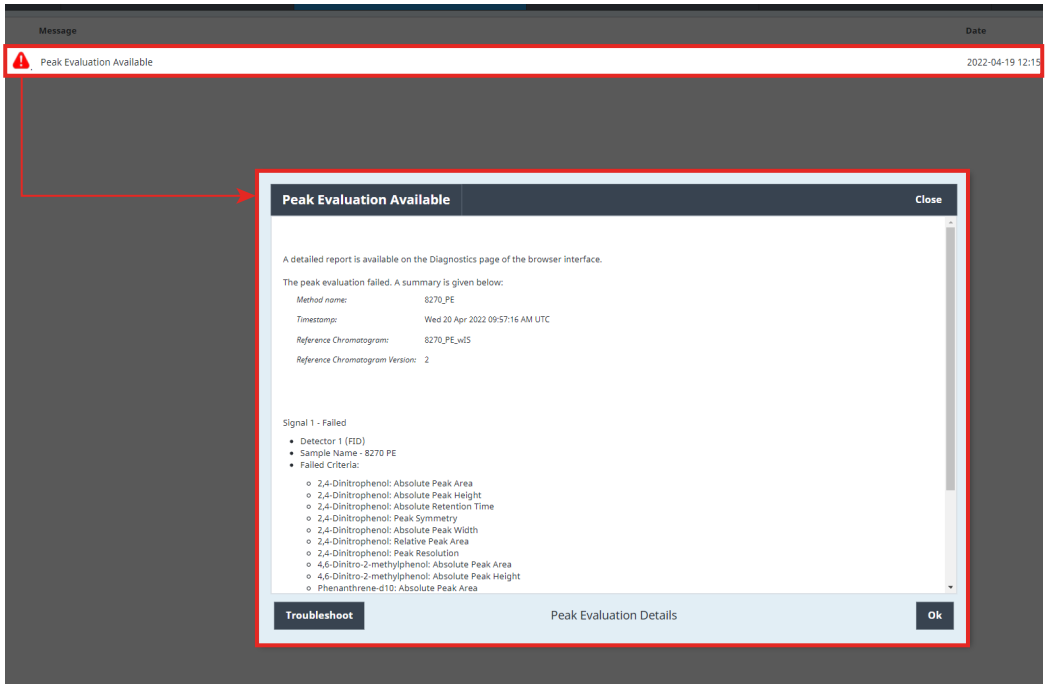


Figure 55. Pop-up window showing failed Peak Evaluation metrics from the browser interface.

User can then choose to initiate troubleshooting–another instrument intelligence feature–from within this pop-up window. Users can also generate a trend plot to see when the area started to drop below the troubleshooting and warning thresholds that were set up in Peak Evaluation (see Figure 56). Note that in Figure 56, the action of Peak Evaluation failure was set to Continue (this can be set in the sequence editor in the browser). Users may also set the action on Peak Evaluation failure to Abort Sequence if critical samples are being run.

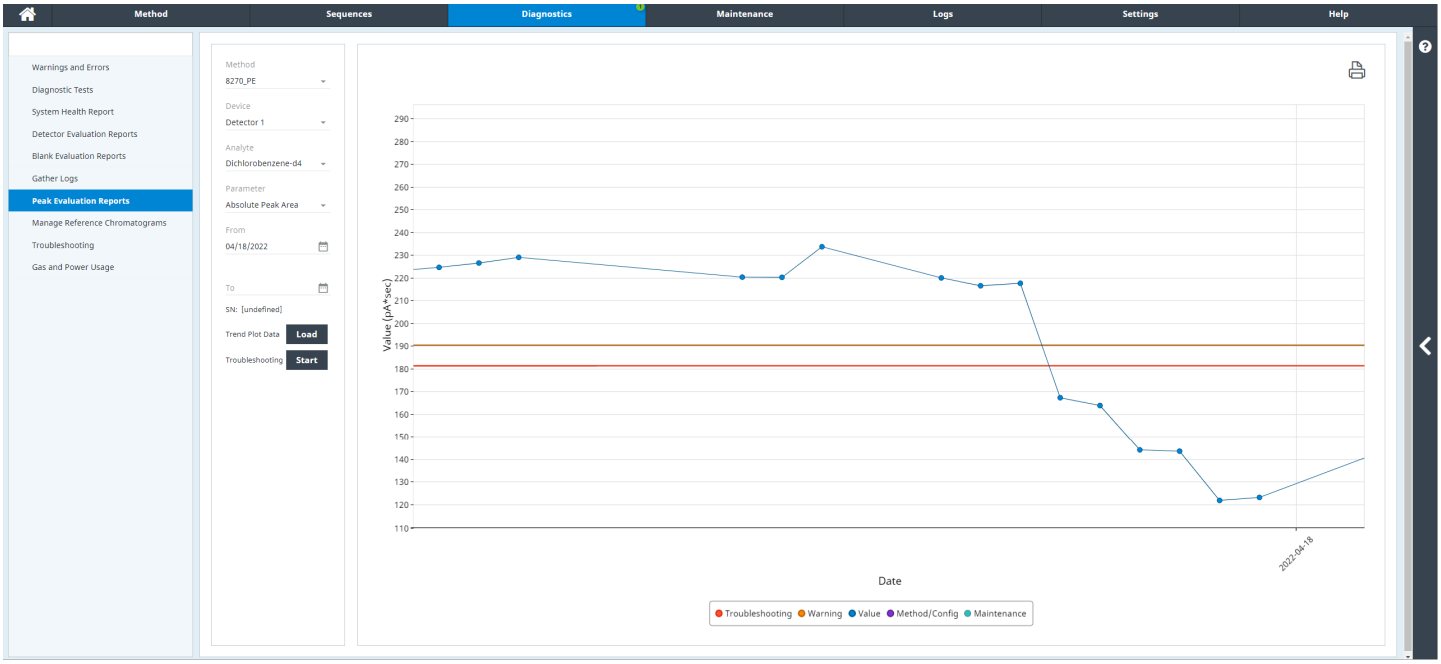


Figure 56. Trend plot showing the 8270 analyte of dichlorobenzene-d4 dropping below the troubleshooting and warning limits set within Peak Evaluation.

In this example, the user goes through troubleshooting and determines that the retention gap at the head of the analytical column needs to be changed. Once the user replaces the retention gap, Peak Evaluation again passes, and the passing results are shown on both the browser and touch screen interface (see Figure 57). The trend plot will again show the areas of the evaluated analytes back between the warning and troubleshooting limits (see Figure 58). Note that on the trend plot, the maintenance marker shows that maintenance was performed on the instrument and the issue was resolved. The user can then continue with the analysis of the 8270 sample.

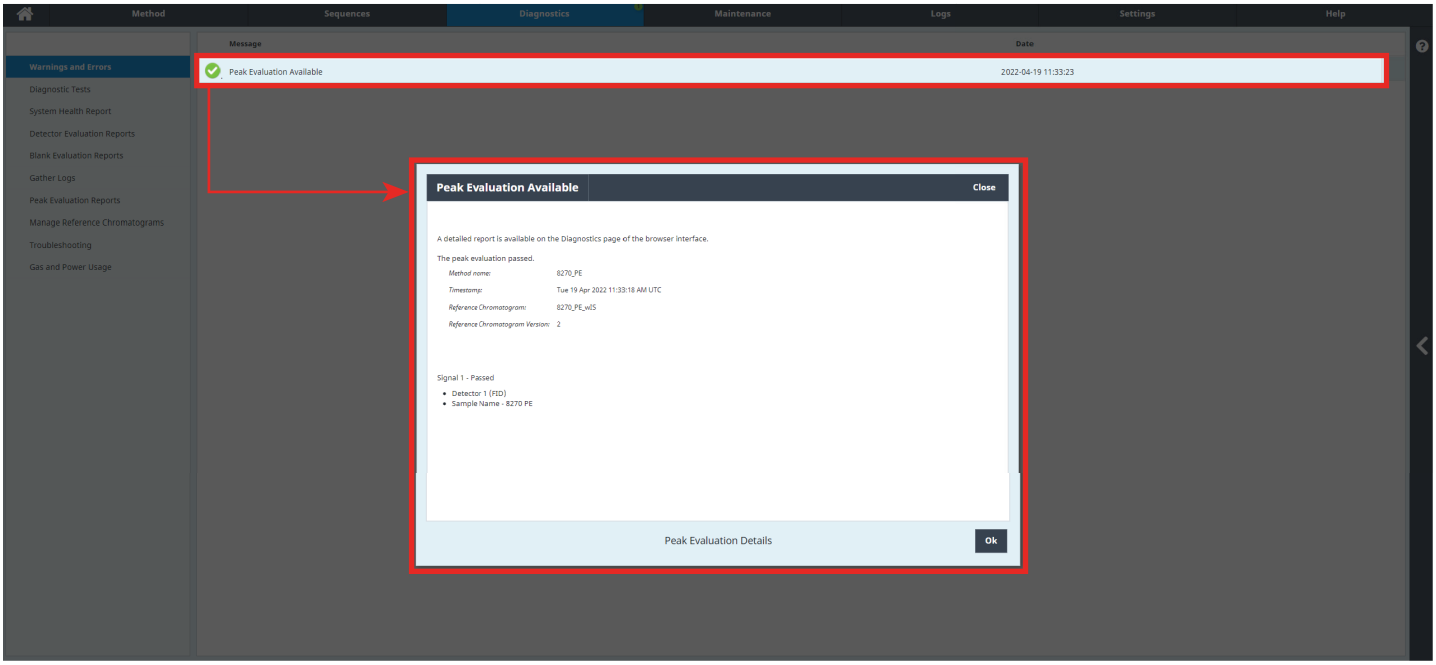


Figure 57. Passing Peak Evaluation after replacing the retention gap before the analytical column.

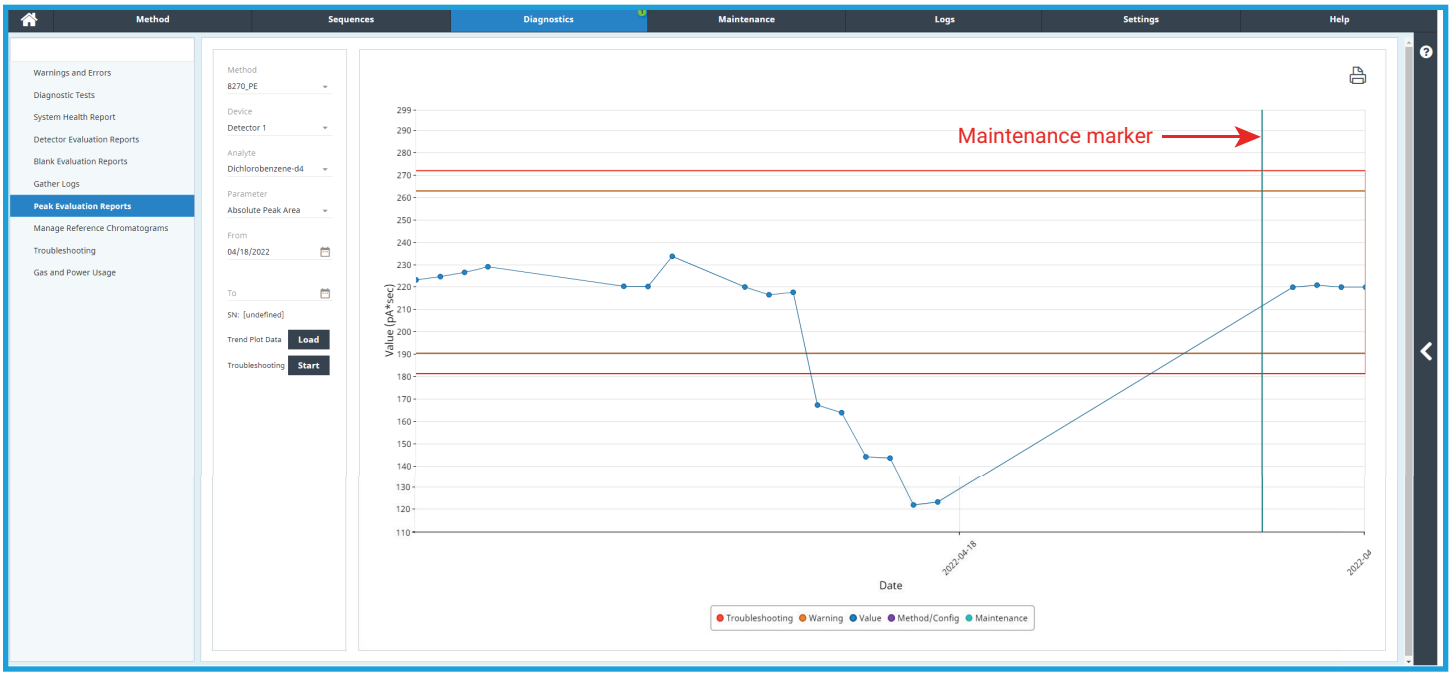


Figure 58. Trend plot showing maintenance was performed to correct the area response of the internal standard dichlorobenzene-d4 in the 8270 mix.

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