GC Intelligence: Trend Plotting

Introduction

The recent GC hardware revisions of the Agilent Intuvo 9000 GC and Agilent 8890 GC have provided an opportunity to enhance the user's day-to-day experience in many ways. Many of these enhancements have allowed the addition of Smart GC features to the instrument, with the addition of a touch screen and browser interface. Some of these new features include integrated diagnostic/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 different aspects and features that are found within the GC Intelligence features of Trend Plotting.

What are Trend Plots?

Trend Plotting is a GC intelligence feature that allows the user to plot many different types of data from the instrument. The types of data from which a trend plot can be generated include diagnostic test results and chromatographic parameter data (such as area and retention time from Peak, Blank, and Detector Evaluations; see the "GC Intelligence: Peak Evaluation" white paper or instrument help for additional information on Peak Evaluation). The ability to plot these parameters allows the user to visually see trends within their data over a user-specified period. This provides the user with better insights into the overall health of the instrument and the analytes they are monitoring. This allows the user to take preventive actions and perform maintenance before the possible loss of valuable samples and time.

How to generate trend plots

Trend plots can be generated from either the touch screen or the browser interface. The browser interface will provide more information and options than what can be found on the touch screen. To generate trend plots from the browser interface, users should navigate to the Diagnostics tab (Figure 1).

– For a diagnostic trend plot, click **Diagnostics Test > Diagnostics Trend Plot** (Figure 2).

– For a chromatographic trend plot, select **Detector Evaluation Report, Blank Evaluation Report**, or **Peak Evaluation Report > Chromatographic Trend Plot** (Figure 3).
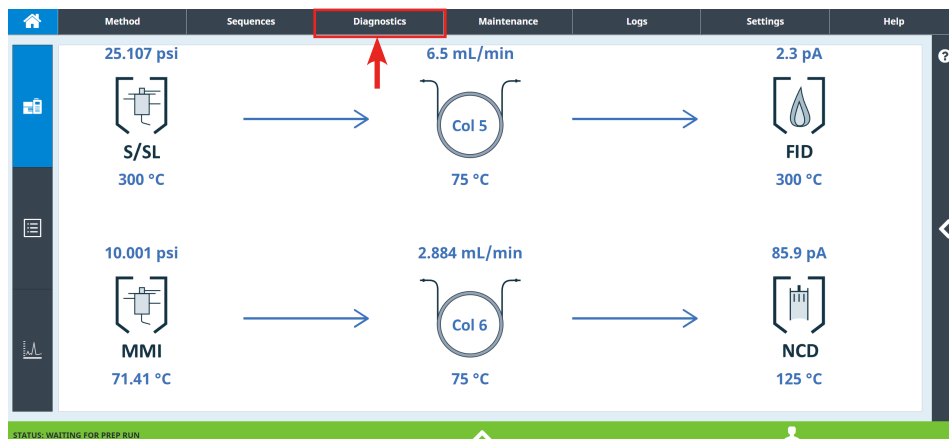

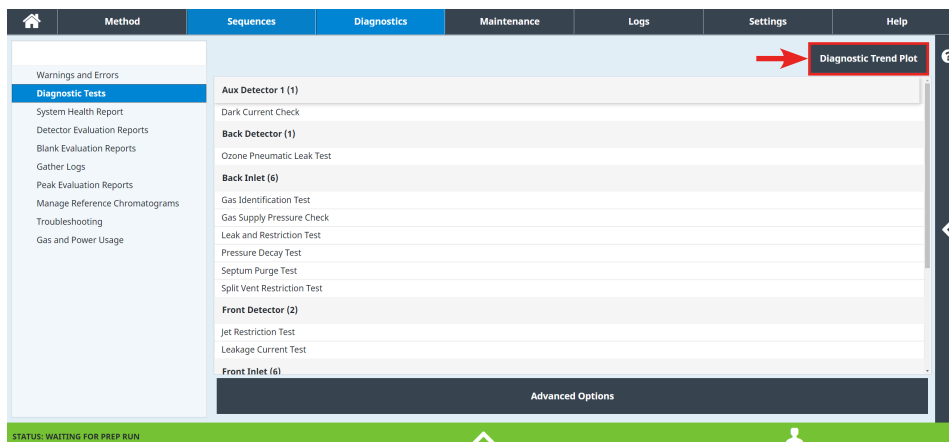**Figure 1.** Generating a trend plot from the browser interface: location of the Diagnostics tab.

Figure 2. Generating a diagnostic trend plot: the **Diagnostic Trend Plot** button.
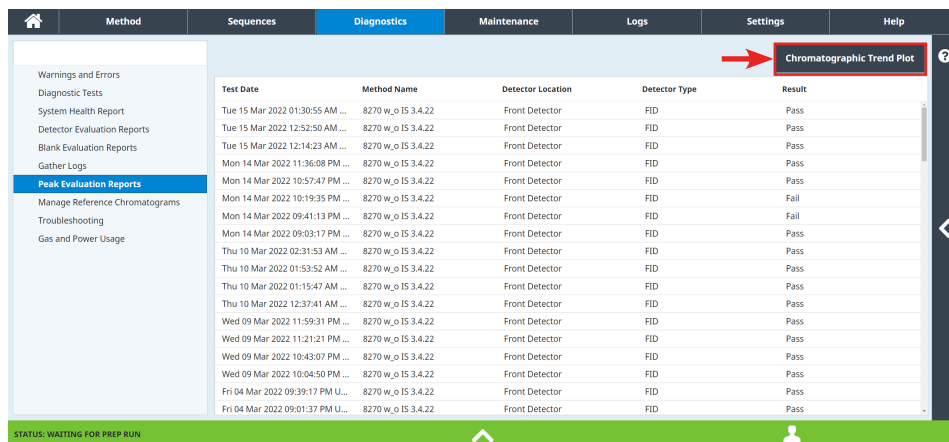

Figure 3. Generating a chromatographic trend plot from the Peak Evaluation Reports window: location of the **Chromatographic Trend Plot** button. A similar option is available from the Detector Evaluation Reports or Blank Evaluation Reports windows.

To generate a diagnostic or chromatographic plot on the touch screen, users should navigate to the Diagnostics tab on the touch screen (Figure 4).

– For a diagnostic trend plot, click **Diagnostic Tests > Diagnostic Trend Plot** (Figures 5 and 6).

– For a chromatographic trend plot, click **Detector Evaluation, Blank Evaluation**, or **Peak Evaluation > Chromatographic Trend Plot** (Figures 7 and 8).
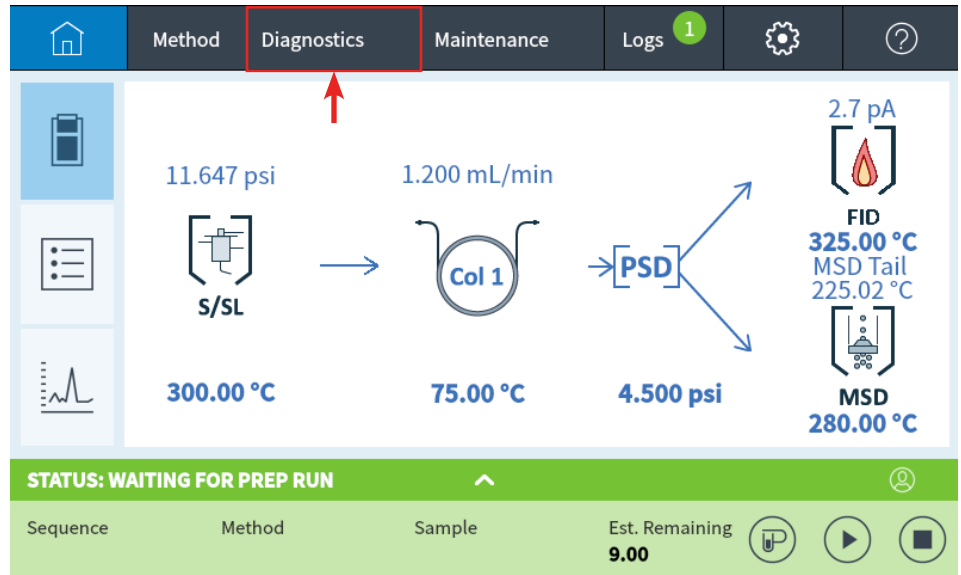

Figure 4. Generating a trend plot from the touch screen interface: location of the Diagnostics tab.
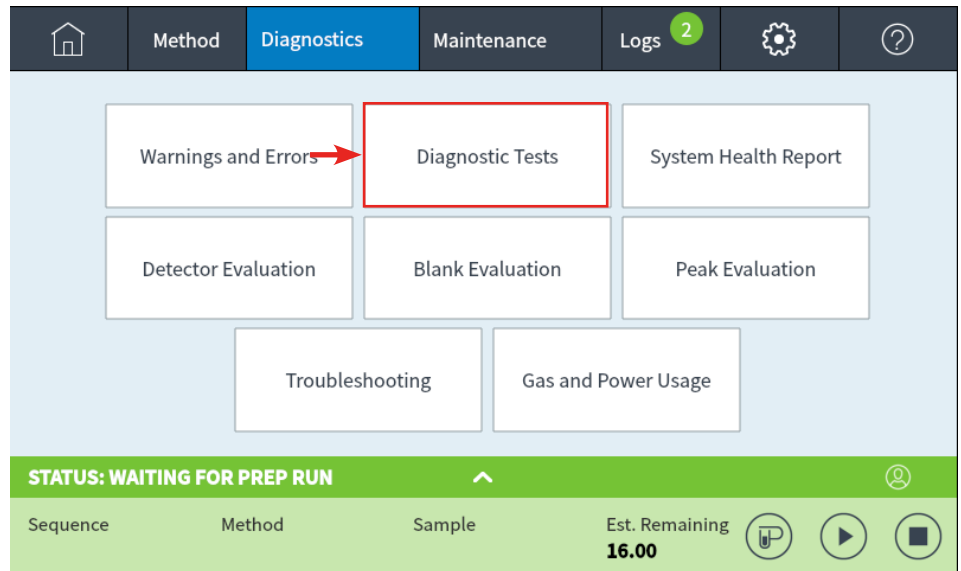

Figure 5. Generating a Diagnostic trend plot from the touch screen interface: location of Diagnostic Tests.

Trend Plot features and highlights

Many features are present within Trend Plotting. All the following features are present on both the browser and touch screen interfaces, unless stated otherwise. Users will be able to specify the date range in which they wish to view both diagnostic and chromatographic data. Many event markers are also visible to the user on the plots to identify when an event may have occurred on the instrument. These event markers might be useful if a user notices a step change in the data. The following are examples of the trend plot markers that may be present. Some of the markers might not be present on the trend plot, depending on the instrument's configuration and if a method or configuration has changed on the instrument.

If the instrument's configuration or the method (which is being used to generate the trend plot) was modified, a configuration/method change marker will be present (purple vertical line). If maintenance was performed on the instrument, a teal vertical line will be shown on the plot. This line is only visible if maintenance was completed using the onboard maintenance procedures, or if the early maintenance feedback "EMF" was reset. Horizontal lines showing the troubleshooting (red) and warning (orange) limits may also be present, depending on the type of trend plot that is generated. If the user is generating a diagnostic plot, the troubleshooting limits are determined by the type of diagnostic test that is being plotted (the pass/fail criteria for the test). The troubleshooting limits for detector evaluation chromatographic plots are also determined by instrument and set to predetermined values. No warning limits will be present on diagnostic or blank/detector evaluation plots. The user is allowed to set both the troubleshooting and warning limits on Peak Evaluation
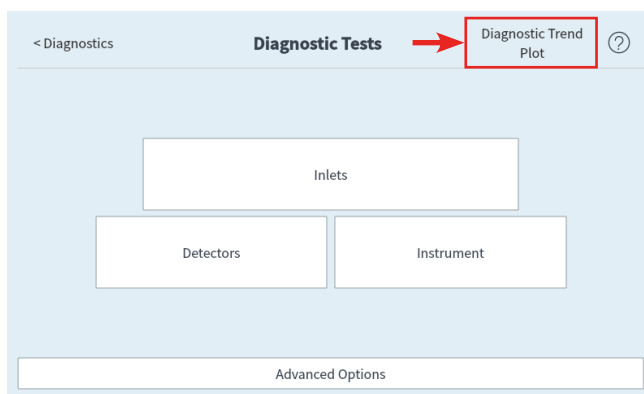

Figure 6. Generating a diagnostic trend plot from the touch screen interface: location of Diagnostic Trend Plot.
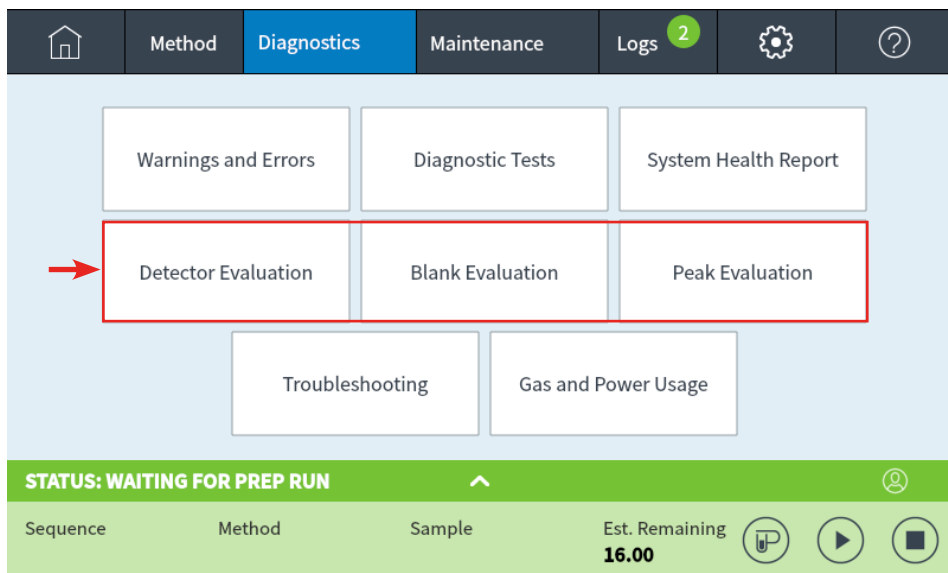

Figure 7. Generating a chromatographic trend plot from the touch screen interface: location of Detector Evaluation, Blank Evaluation, and Peak Evaluation.

Figure 8. Generating a Chromatographic trend plot from the touch screen interface: location of Chromatographic Trend Plot. Note: the example shows location under the Peak Evaluation Report, but Chromatographic trend plots can also be generated from the Detector Evaluation Report and Blank Evaluation Report.

chromatographic plots. The limits for Peak Evaluation are determined when the user configures the pass/fail threshold for Peak Evaluation and the warning limits they wish to use (either strict or lenient). All trend plot markers can be turned on or off in the plot legend (except for the Method/Config marker; this plot marker is defaulted to always be on/visible if this event has occurred on the instrument). Figure 9 for examples of the Trend Plot markers.

Another feature of trend plots is the annotation of individual datapoints. This allows the user to note a change in the data if needed (such as a leak starting to form in the septum or other sample issues). This may be useful to notify other individuals who are also using the instrument of previous issues that may have occurred. Annotation of data points is a feature that is only present on the instrument's browser interface. Figure 10 for an example of adding annotations on the browser interface.

The ability to zoom is also present within the trend plots. This allows the user to enhance an area of the trend plots they want to investigate further (possibly a change in the data). A click-and-zoom feature is available on the browser interface. A zooming feature is available on the touch screen interface (similar to how the real-time plot is zoomed on the touch screen), with zooming only changing to predetermined levels. Figure 11 is an example of the click-and-zoom feature on the browser interface.
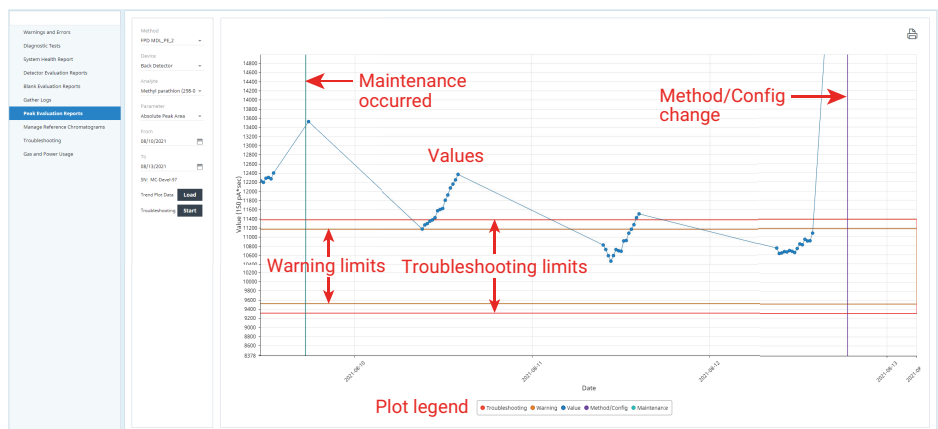

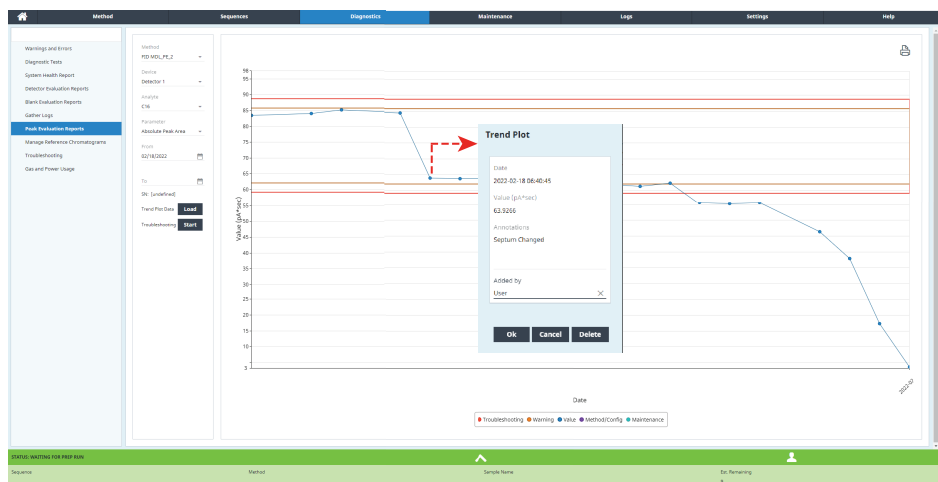**Figure 9.** Legend markers found on diagnostic and chromatographic trend plots.

Figure 10. User ability to add annotations to the trend plot.
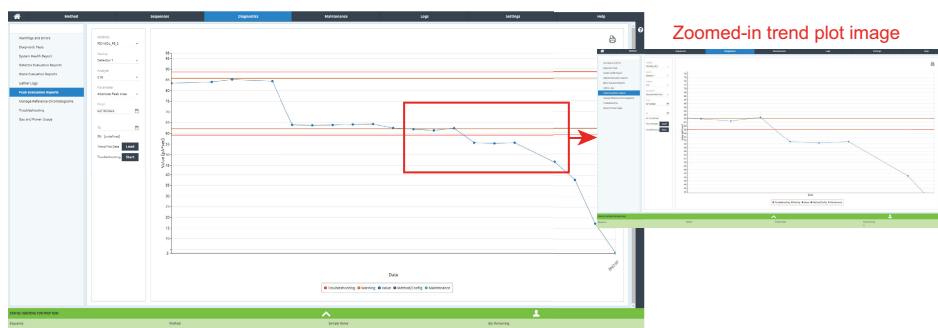

Figure 11. User ability to click and zoom on the trend plot.

5

Within the diagnostic trend plots, users will be able to launch the integrated maintenance routines (Figure 12), if the user determines a maintenance task needs to be performed (for example, if a user notices data starting to drift). Depending on the diagnostic data that is being plotted (inlet, detector, or headspace), the associated maintenance items will be populated when the user launches the integrated maintenance from within the Diagnostic plot. For example, if the inlet tests are being plotted in the diagnostic plot, only inlet maintenance procedures will be shown.

Users will also be able to start the onboard Troubleshooting from within the Chromatographic trend plots (Figure 13). If the GC is failing to meet the passing criteria and more than seven data points are plotted, the GC intelligence will automatically suggest an area of troubleshooting. If not enough data points are plotted, the user can manually start the troubleshooting option.

Another feature is the ability to print the trend plots after they are generated. This feature allows a user to reference back to historical trend plot data as needed (Figure 14). Both launching maintenance/troubleshooting and printing/saving of the trend plots are features that are only available through the browser interface (not available on the touch screen).
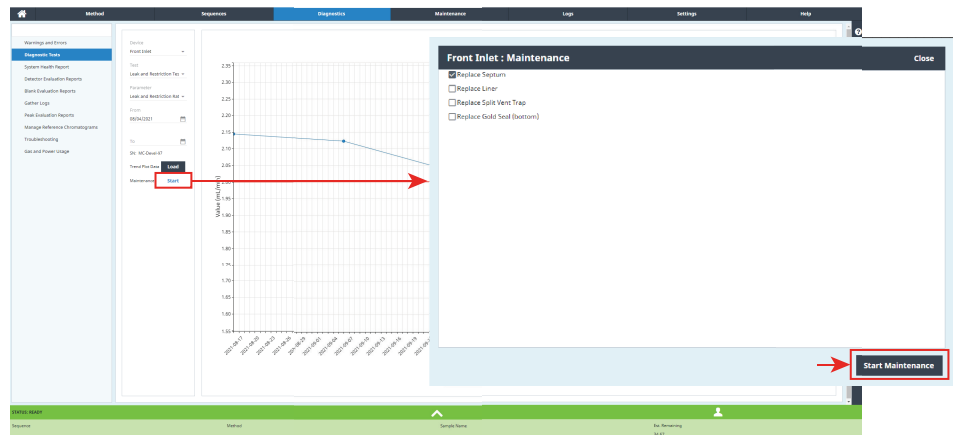

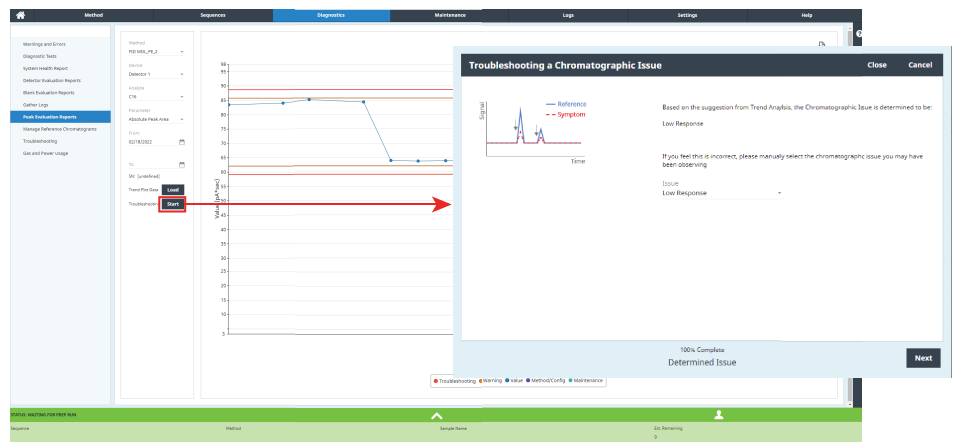**Figure 12.** Starting maintenance from within the diagnostic plot.

Figure 13. Starting troubleshooting from within the chromatographic plot.
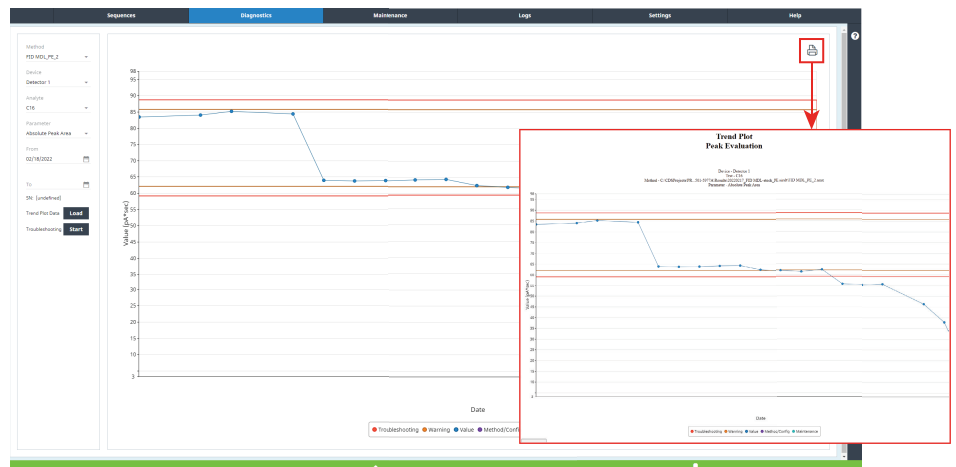

Figure 14. Printing the trend plot.

Example of a Peak Evaluation trend plot

The following example will explain how to set up a trend plot for Peak Evaluation results. All three chromatographic plots (peak, detector, and blank evaluation) are set up by similar means. Therefore, this example of how to set up a trend plot with Peak Evaluation results will serve as an example for all three chromatographic trend plots. The user must have already set up and enabled either a peak evaluation, detector evaluation, or blank evaluation to generate a chromatographic trend plot (to generate a Peak Evaluation trend plot, the user must have already set up and enabled Peak Evaluation on a previously run method). Results from these evaluations are only stored on the instrument and not within a data system that may be connected to the GC. These stored evaluation results on the instrument are then used for generating the corresponding trend plot.

As shown previously, to generate a peak evaluation trend plot, click the Diagnostics tab (Figures 1 and 4) on either the browser or touch screen interface on the instrument. Once under this tab, click **Peak Evaluation Reports** (**Peak Evaluation** on the touch screen), then click **Chromatographic Trend Plot** (Figures 3 and 8). This will open the trend plot screen. On the browser, the trend plot configuration area is located on the left side of the screen. On the touch screen, a configuration window will pop up to configure the trend plot (under **Config** on the touch screen). The parameters in the configuration area will be used to generate the chromatographic trend plot (Figure 15).

The first configuration parameter to be set is to select the Peak Evaluation method that was used during the analysis from the Method drop-down menu. This selected method will be used as a top-level filter for the proceeding configuration parameters. The method chosen can be either a browser- or data system-saved method (both method types will appear in the Method drop-down menu). Figure 16 for an example of the Method drop-down menu in the trend plot configuration area.
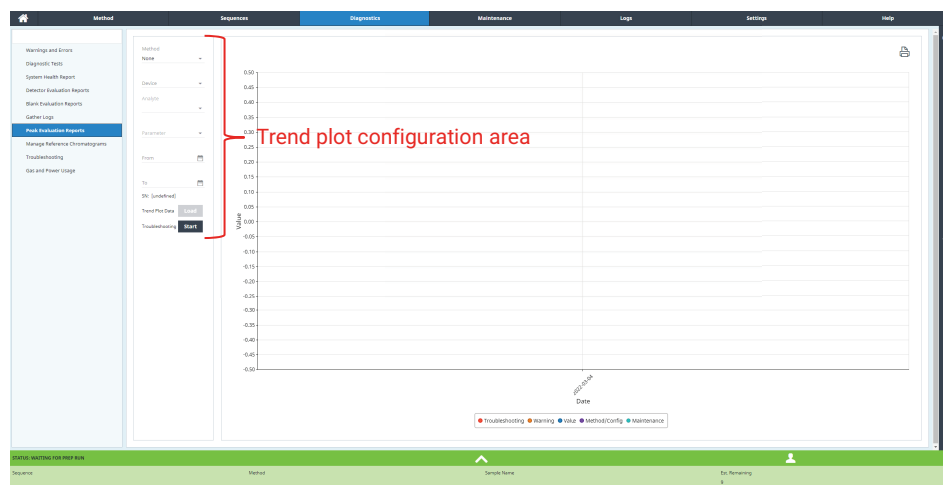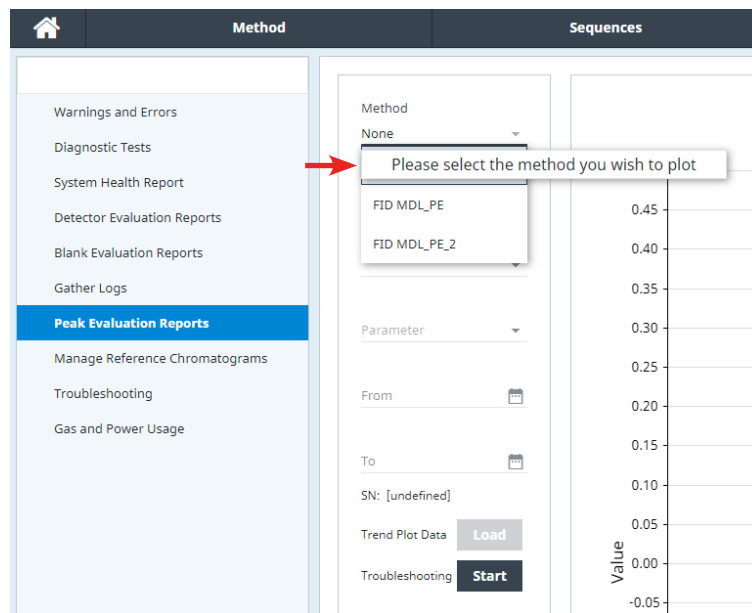

Figure 15. Trend plot configuration area.

Figure 16. Selecting a method from the Method drop-down menu in the trend plot configuration area.

Once the method is selected, the user will select a device from the Device drop-down menu (Figure 17). The device is the detector that was used during collection of the peak evaluation. Generally, there will only be a single detector listed under the Device drop-down menu (for example: Front Detector, Back Detector, or Detector 1), but if the detectors have been moved on the instrument to another position, multiple locations may be present. The best practice is to rename a method if a configuration change occurs on the instrument.
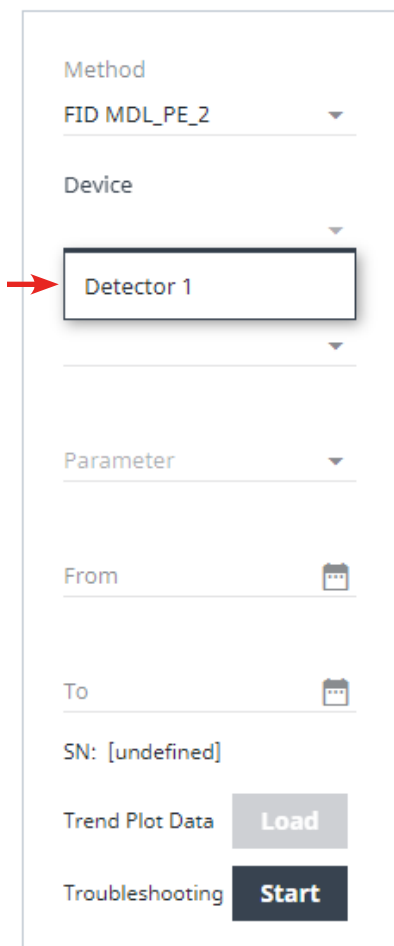

Figure 17. Selecting a device from the Device drop-down menu in the trend plot configuration area.

After selecting a device, the user will select an analyte from the Analyte drop-down menu. The list of analytes will be populated depending on the initially selected method in the first plot configuration parameter. The available analytes will be determined by the type of evaluation that is being plotted (for Blank and Peak Evaluation, the user defines the analytes list, for detector evaluations, the analyte list is predefined by the instrument). Only those analytes that were selected when a peak evaluation was initially set up will appear in the Analyte drop-down menu. If the user has selected to monitor the Baseline Attributes within Peak Evaluation, this will also be listed as Baseline under the Analyte configuration setting. Within Detector Evaluation, the list of analytes in the Analyte drop-down menu will be prepopulated with the associated checkout method analytes for the specified detector. Within Blank Evaluation, Component is listed in the plot configuration instead of Analyte. Users will have the choice of either selecting Baseline or Summary parameters in the Component configuration drop-down menu with a blank evaluation trend plot (see the next section for specific parameters associated with these two blank evaluation components). Figure 18 shows an example of the analyte selection from a Peak Evaluation trend plot.

The next configuration parameter after selecting an analyte/component will be selecting which specific analyte parameter to use in the trend plot. This can be selected from the Parameter drop-down menu. The available analyte parameters will again be prepopulated depending on what the user has set up to monitor within Peak Evaluation (both Absolute and Relative Retention Time, Peak Area, Peak Width, and so on). If the
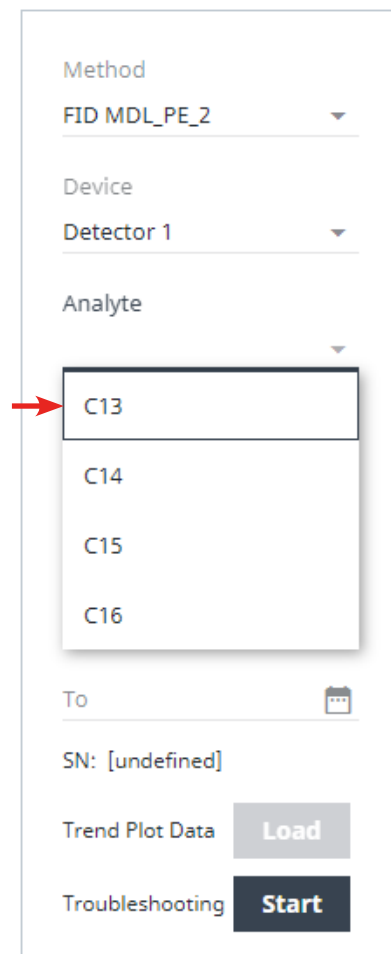

Figure 18. Selecting an analyte from the Analyte drop-down menu in the trend plot configuration area.

user selects Baseline from the analyte plot configuration, the different baseline parameters will be available (Initial/Final Baseline and Noise values). As with the different analyte parameters, the user will only see a Baseline option if it was previously set up in Peak Evaluation. Figure 19 shows an example of the analyte parameter selection from the Parameter drop-down menu.

Detector Evaluation trend plot configuration parameters will have similar items as those present in the Peak Evaluation trend plot. The analytes are predetermined when a user runs Detector Evaluation (which uses the
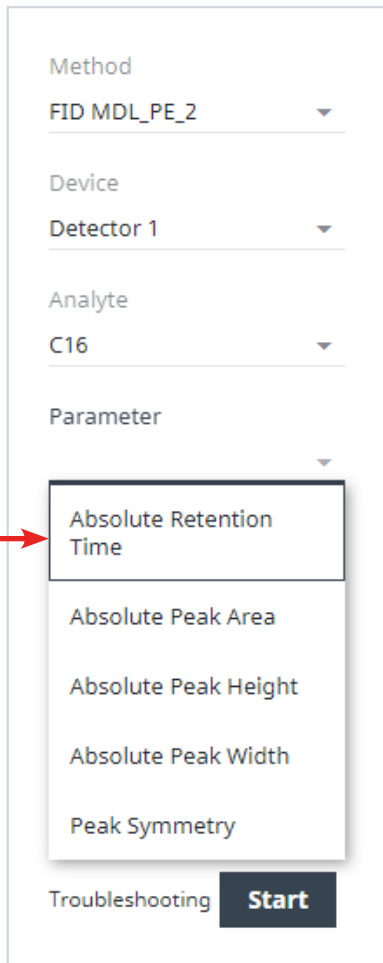
Figure 19. Selecting an analyte parameter from the Parameter drop-down menu in the trend plot configuration area.

Agilent Checkout Sample, so the list of analytes is already predetermined for the evaluation). Therefore, the analyte parameters are also preselected (such as Retention Time, Peak Area, Relative/Absolute Values, and so on). For Blank Evaluation trend plot configuration, if the user selects Baseline under the component plot configurations, different baseline components will be available for the user to select (Baseline Values or Noise). If the user selects Summary, the maximum peak height or total peak area will be available for the user to select.

After selecting the parameter or component, the final plot configuration is the date range. Users will enter the date range they wish to view data for the trend plot parameters they selected previously. On the browser, a calendar will appear, which will allow the user to first select the start date, followed by the selection of the end date range (Figure 20). On the touch screen, the user will have to enter the date range they wish to plot.
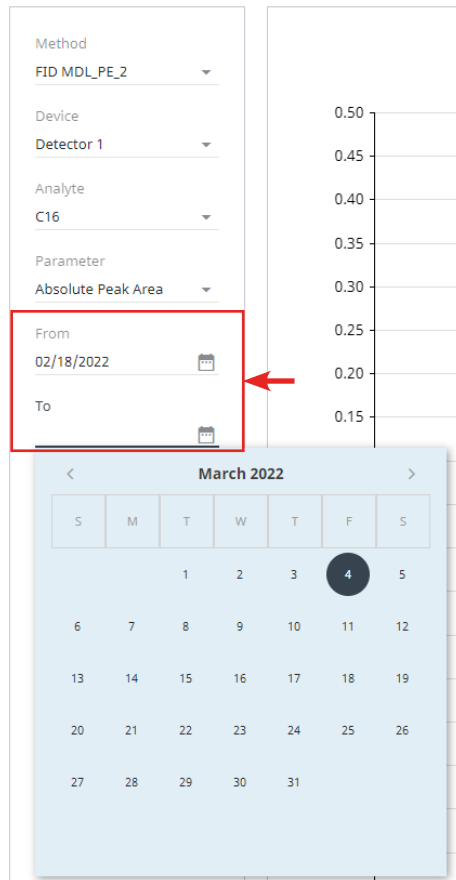

Figure 20. Trend plot configuration date selection.

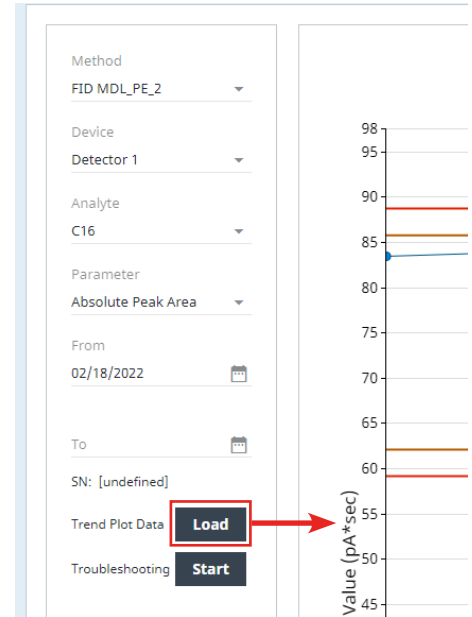After selecting the date range, users will select Load to generate the trend plot (Figure 21).

Figure 21. Loading the trend plot in the trend plot configuration area.

After the trend plot loads, the user will be able to select the plot markers in the plot legend below the trend plot that they wish to turn on/off (except for the Method/Config marker). For the Peak Evaluation plot, the Troubleshooting marker values are the limits the user set up within Peak Evaluation. These values/limits are the threshold that the Peak Evaluation uses to trigger the integrated user-guided Troubleshooting. The Warning marker values for the Peak Evaluation trend plot are taken from the warning level the user set up in Peak Evaluation (strict or lenient limits). Within Detector Evaluation and Blank Evaluation, the troubleshooting and warning limits are automatically determined by the type of evaluation run. These values cannot be modified by the user. Figure 22 shows an example of the plot legend markers that are found within Peak Evaluation.

Other features are available to the user after the Trend Plot is generated, including zooming, printing/saving, and starting the user-guided troubleshooting as needed. Further details of these features are described in the previous section.

The following are all possible selections that the user can make with each chromatographic plot.

Peak Evaluation

- **Method:** Available methods used within Peak Evaluation
- **Device:** Configured detectors on the instrument
  - **8890 GC:** Front, Back, Aux 1, and Aux 2
  - **Intuvo 9000 GC:** Detector 1 (D1) and Detector 2 (D2)
- **Analytes:** Dependent on analytes configured within Peak Evaluation and if Baseline Attribute parameters were set up in Peak Evaluation
- **Parameter:** See Table 1
- **Date:** users can input the date range they wish to view a trend plot

Detector Evaluation

- **Method:** Available methods used within Detector Evaluation
- **Device:** Configured detectors on the instrument
  - **8890 GC:** Front, Back, Aux 1, and Aux 2
  - **Intuvo 9000 GC:** Detector 1 (D1) and Detector 2 (D2)
- **Analytes/Baseline:** Limited to the analytes/baseline attributes that are prepopulated for Detector Evaluation (dependent on the detector being used)
- **Parameter:** See Table 2
- **Date:** Users can input the date range they wish to view a trend plot

Figure 22. Peak Evaluation Trend Plot markers, which can be turned on or off.

Table 1. Parameters selectable from the Parameter drop-down menu within Peak Evaluation.

Absolute	Relative (Defined by User)	Baseline
Retention Time	Retention Time	Initial Baseline
Peak Area	Peak Area	Final Baseline
Peak Width	Peak Width	Baseline Noise
Peak Height	Peak Height	Total Peak Area
Peak Symmetry	Peak Symmetry	
Peak Resolution (Defined by User)		

Table 2. Parameters selectable from the Parameter drop-down menu within Detector Evaluation.

Absolute	Relative (Defined by Detector Evaluation)	Baseline
Retention Time	Retention Time	Initial Baseline
Peak Area	Peak Area	Final Baseline
Peak Height	Peak Height	Baseline Noise
		Total Peak Area

Blank evaluation

- **Method:** Available methods used within Blank Evaluation

- **Device:** Configured detectors on the instrument
  - **8890 GC:** Front, Back, Aux 1 and Aux 2
  - **Intuvo 9000 GC:** Detector 1 (D1) and Detector 2 (D2)

- **Component:** Baseline/Summary

- **Parameter:** See Table 3

- **Date:** Users can input the date range they wish to view a trend plot

Table 3. Parameters selectable from the Parameter drop-down menu within Blank Evaluation.

Baseline	Summary
Initial	Max Peak Height
Final	Total Peak Area
Initial Noise	
Final Noise	

Example of a diagnostic trend plot

The following section demonstrates how to set up a Diagnostic trend plot and the specific features associated with these plots. As with generating the Chromatographic trend plots, click the **Diagnostics** tab on either the browser or touch screen interface. Then, click **Diagnostic Tests**, followed by **Diagnostic Trend Plot** to show the plot configuration (Figures 1 and 4). Once the user is in the Diagnostics tab, click **Diagnostic Tests > Diagnostics Trend Plot** (Figures 2 and 5). This will open the Diagnostic trend plot window. On the browser, the trend plot configuration area will be located on the left side of the screen. On the touch screen, a new window will pop up to configure the trend plot (under Config on the touch screen). The parameters in the configuration area will be used to generate the diagnostic trend plot (Figure 23).
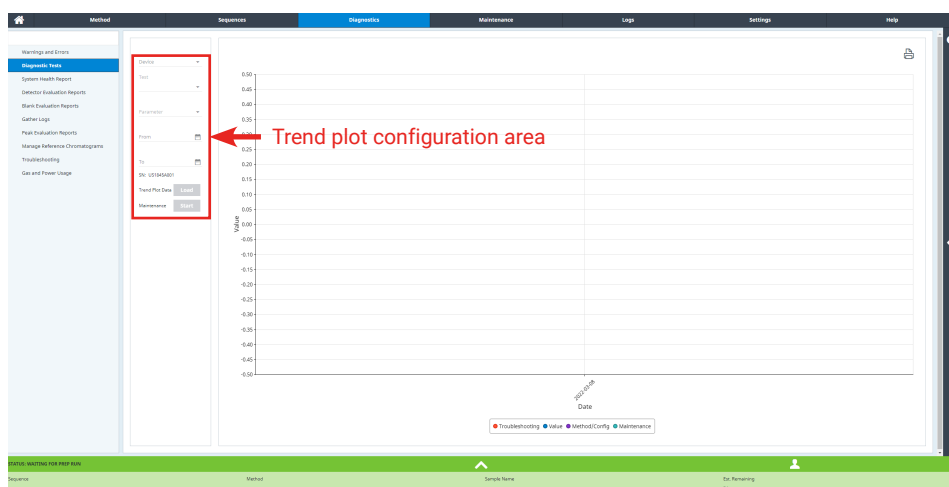

Figure 23. Diagnostic trend plot configuration area.

Similar to the Chromatographic trend plot, users will first select a device from the Device drop-down menu. The devices in this drop-down menu will consist of inlets, detectors, and headspace (if configured on the instrument). The options available to choose under the Device menu will depend on the instrument's configuration (Figure 24).
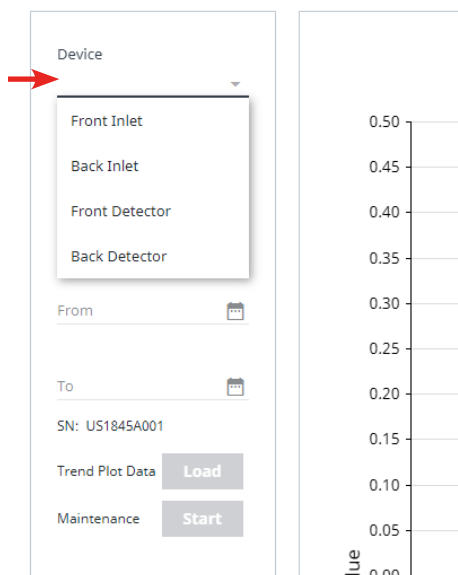

Figure 24. Selecting a device from the Device drop-down menu to generate a diagnostic trend plot.

The next plot configuration parameter that the user can select is the test they wish to plot from the Test drop-down menu. As with the Chromatographic plot, the selection from this list is filtered depending on the device selected previously (for example the inlet test will appear if an inlet was selected in the above device configuration). The different tests listed in the Test drop-down menu are the integrated diagnostic tests that can be run on the instrument (Figure 25).
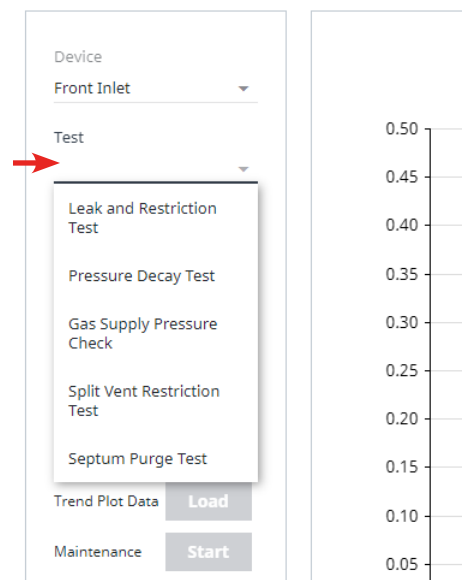

Figure 25. Selecting a test from the Test drop-down menu to generate a diagnostic trend plot.

Once the user selects the test configuration parameter, they will select the test parameter to plot from the Parameter drop-down menu (Figure 26). The test parameters are typically the numerical output/values from each of the integrated diagnostic tests (example: for the automated leak and restriction test, the test parameter is the leak and restriction rate in mL/min). See the end of this section for a detailed list of the possible plot configuration choices.
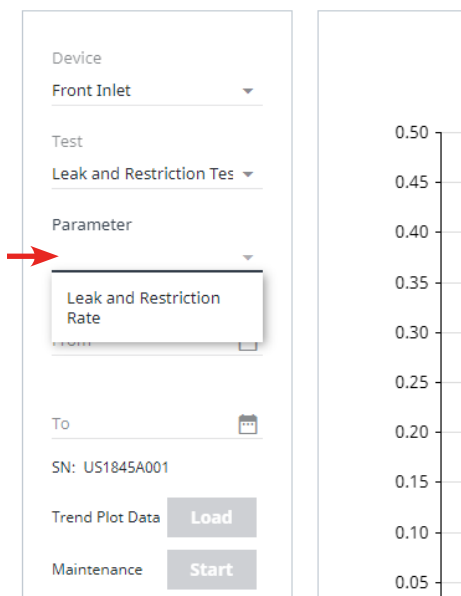

Figure 26. Selecting a parameter from the Parameter drop-down menu to generate a diagnostic trend plot.

The final plot configuration is the date range that the user wishes to generate the Diagnostic plot (Figure 27). The date range is configured in the same manner as previously described.
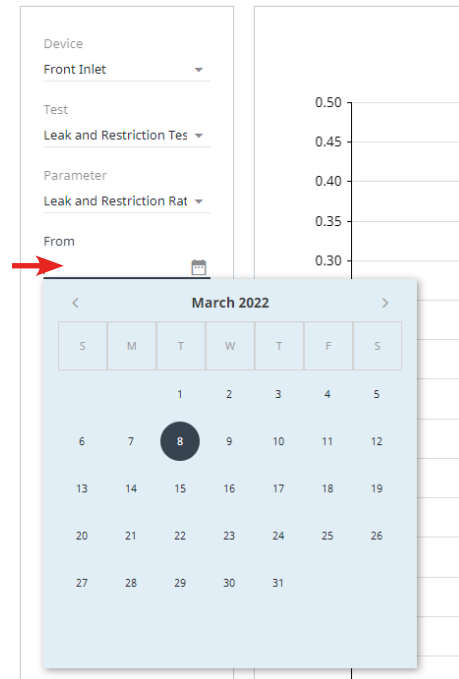

Figure 27. Selecting a date range to generate a diagnostic trend plot.

Once the user sets the date range and selects Load, the Diagnostic trend plot will be generated for the selected plot configuration parameters (Figure 28).
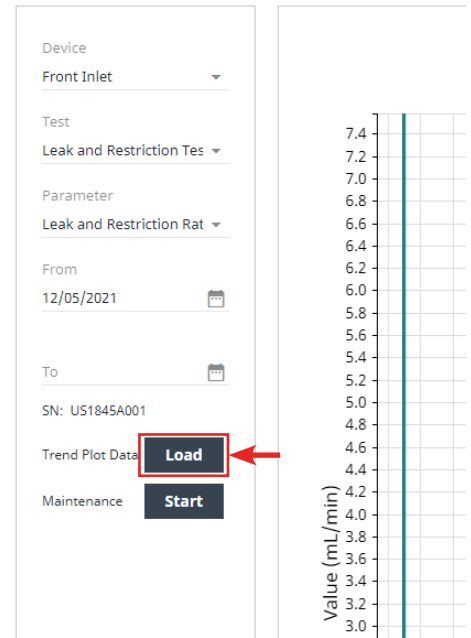

Figure 28. Loading a diagnostic trend plot.

As with the Chromatographic plots, the user may turn on/off the different plot markers from the legend below the plot by selecting the different plot markers (except the Method/Config marker; Figure 29).

The user may also zoom, print, and start the integrated maintenance routines as described in the previous section (Figures 11, 12, and 14).

The following are specific Diagnostic plot configuration parameters that can be selected when configurating a plot.

Diagnostic plot

– **Device:** Configured inlets, detectors, and headspace on the instrument

  – **8890 GC:** Front Inlet, Back Inlet, Front Detector, Back Detector, Aux 1 Detector, and Aux 2 Detector

  – **Intuvo 9000 GC:** Front Inlet, Detector 1, and Detector 2

  – 8697 Headspace

– **Test/parameter:** See Table 4
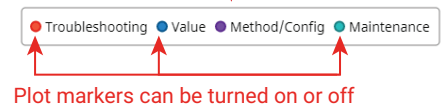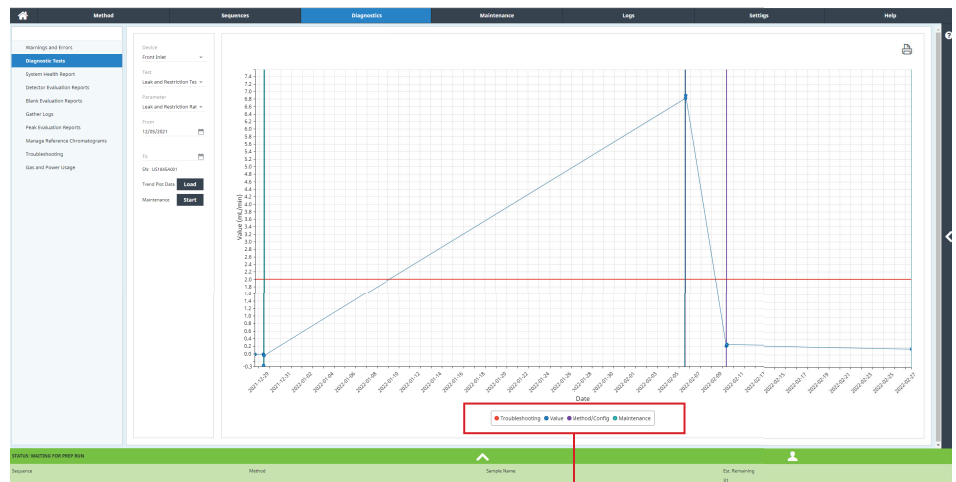
References

1. GC Intelligence | Agilent

Plot markers can be turned on or off

Figure 29. Plot markers can be turned on or off from the Diagnostic trend plot legend.

Table 4. Possible tests to be plotted and their associated parameters.

Test	Parameter
Inlet	
Leak and Restriction Test	Leak and restriction rate
Gas Supply Pressure	Maximum achievable pressure
Pressure Decay Test	Pressure decay
Septum Purge Test	Control error-pressure actual
Split Vent Restriction Test	Split vent backpressure
Detector	
Jet Restriction Test (FID)	Makeup gas flow
Leakage Current Test (FID)	Leakage current
Headspace	
Crossport Leak Test	Crosspoint leak in standby/inject mode
Transfer Line Leak and Restriction Test	Aux pressure
Gas Supply Pressure Test	Maximum achievable pressure
Restriction and Pressure Decay Test	– Restriction in inject mode – Restriction in standby mode – Restriction in vent port – Leak in pre-valve plumbing – Leak in inject mode – Leak in standby mode
User-Vial Leak Test	Average leak rate and suggested leak rate threshold

Agilent
Trusted Answers