Data-driven GC and GC-MS instrument monitoring with SmartStatus intelligent software

Authors

Kenneth M. Free¹, Tim Anderson¹ and Adam Ladak²

¹Thermo Fisher Scientific, USA ²Thermo Fisher Scientific, UK

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Introduction

Rising costs can significantly impact an analytical laboratory's profit margin, and it is crucial to maintain productivity and ensure maximum asset utilization to stay competitive. To balance increased overhead costs, including analytical gases and staff pay, laboratories must ensure that analytical instrumentation consistently produces results, without interruption. Re-analyzing entire runs due to drops in sensitivity, unnecessary downtime, and underutilization of consumables is expensive and time consuming.

Thermo Scientific™ SmartStatus™ instrument tracking can help laboratories realize additional cost savings. This is done by using data-driven insights to accurately determine when to perform maintenance and replace consumables and parts, so that the system consistently runs smoothly for all samples and meets specifications in the initial analysis. This ensures that consumables and parts are replaced on the correct schedule and avoids excess instrument downtime.

SmartStatus instrument tracking is an intelligent instrument health software that allows users to track key aspects of their GC-MS system. It is available as standard on the Thermo Scientific™ TRACE™ 1600 GC series, Thermo Scientific™ Al/AS 1610 liquid autosampler, Thermo Scientific™ ISQ™ 7610 GC-MS series, and the Thermo Scientific™ TSQ™ 9610 GC-MS/MS series. In this technical note, the new SmartStatus instrument tracking capabilities are highlighted with examples of how it can enable analytical laboratories to keep instruments producing consistent results.

SmartStatus software overview

SmartStatus intelligent software, available within Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS), allows monitoring of the entire analytical system including Thermo Scientific™ autosamplers, GC, GC detectors (FID and TCD), and mass spectrometers (MS). Hundreds of key instrument parameters are monitored by SmartStatus software, which provides real-time data and insights informing the user to potential problems before they arise to ensure maximum instrument uptime. This allows users to make informed decisions on which parts of the analytical system require

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attention and when. By performing preventative maintenance using data-driven guidance, optimal instrument performance is sustained day in and day out. Figure 1 shows the SmartStatus software overview page for a TSQ 9610 triple quadrupole MS coupled to a TRACE 1610 GC and Al/AS 1610 liquid autosampler. This overview page allows a user to quickly determine if the system is ready to run or requires attention.

For more information on instrument status, there is a detailed view for each part of the system. This next level view shows how many injections have been performed for the various GC consumables, the lifetime of the MS detector and filament, and

when the last tune was performed. Figure 2 shows an example of the GC and MS parameters and how they are monitored. Each parameter is represented as a counter gauge. As the usage increases, the gauge changes color to quickly notify the user of any maintenance that is required or will be needed soon. This allows users to plan maintenance in advance to fit it around their schedule and workload. SmartStatus instrument tracking can be monitored directly in Chromeleon CDS, and consumables usage can also be monitored directly on the TRACE 1610 GC touch screen through the dedicated instrument health icon, as shown in Figure 3.

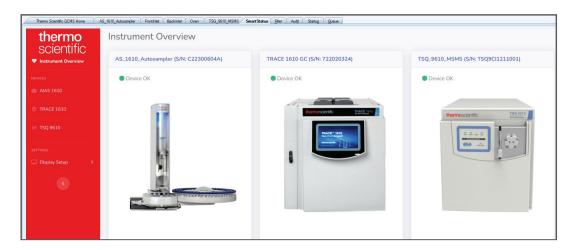


Figure 1. SmartStatus software overview showing that the system does not require maintenance

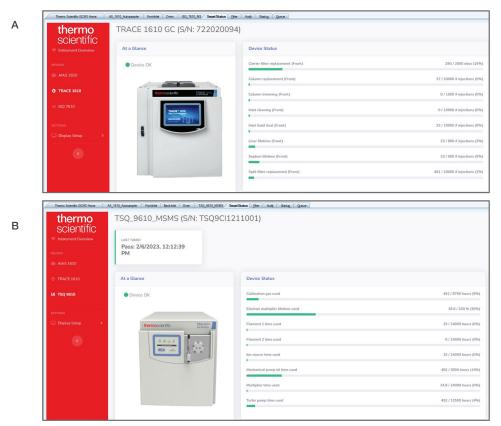


Figure 2. Detailed view of system parameters with counters TRACE 1610 GC (A) and TSQ 9610 MS/MS (B)



Figure 3. Consumables usage tracking on the TRACE 1610 GC touch screen

The ISQ 7610 GC-MS and the TSQ 9610 GC-MS/MS detector lifetime is monitored using a predictive algorithm. This assesses the voltages on the detector and predicts the lifetime remaining on the system so that preventative maintenance can be planned. As the ISQ 7610 GC-MS and TSQ 9610 GC-MS/MS are equipped with the XLXR™ electron multiplier detector as standard, the

lifetime of the detector is several years.¹ By monitoring the detector intelligently, users can avoid unnecessary downtime. Figure 4 shows monitoring of the detector within SmartStatus software.

SmartStatus software customizability

SmartStatus software can be customized to meet the needs of each user, allowing only the parameters that are important to the analysis to be shown. Figure 5 shows a customized list of parameters that are important to track for smooth GC operation. The threshold of each parameter can be set by the user to ensure it reflects their analytical needs. For example, if a user is analyzing samples that have undergone extensive clean up, they may be able to get >500 injections before performing liner maintenance. However, if they are performing analysis of oily samples that have been diluted, the liner may need to be exchanged every 20 injections. Users can set the parameters in an interval that is convenient and matches their needs. This can include injection number or time such as days, weeks, or months. This customizability allows analysts to monitor the parameters in the best way for their workflow. Figure 6 shows the functionality of setting the threshold for parameters, including time scale units.

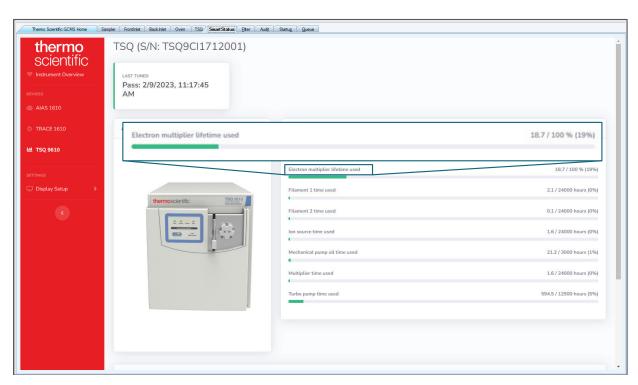


Figure 4. Monitoring the MS detector within SmartStatus instrument tracking

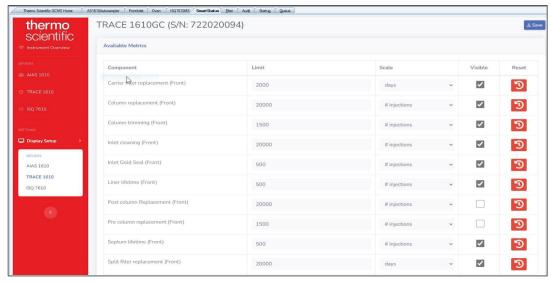


Figure 5. Customized parameters monitoring for GC

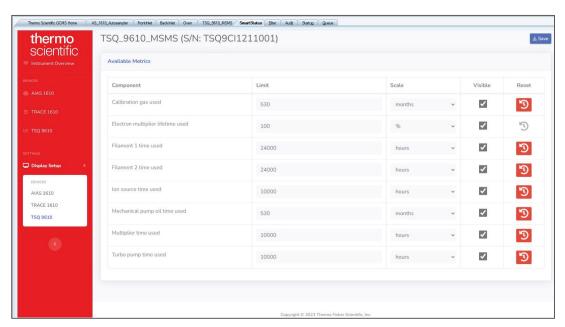


Figure 6. Threshold and time scale customization for MS parameters

Preventative maintenance with SmartStatus software

When a parameter approaches its set threshold, it is quickly brought to the attention of the user. This allows instrument maintenance to be performed before the next batch of samples is analyzed. Preventative maintenance enables the instrument to keep running uninterrupted for longer and ensures quality of results. Figure 7 shows an example of a SmartStatus software alert that can quickly be diagnosed and resolved. Another advantage of SmartStatus software is when different users come to the system, they can quickly see the status of regular consumables. This reduces the unnecessary changing of consumables on a system, potentially reducing operation costs.

This management of the system can contribute to sustainability efforts by optimizing system performance and uptime and reducing the waste of resources.

SmartStatus software can track the entirety of the system in background. If a problem occurs that cannot be easily resolved by the user, a Smart Support file can be sent to a service engineer for detailed diagnosis. Monitored parameters can assist the service engineer to effectively resolve any issues rapidly. This functionality is optional and can be enabled or disabled by the user. Smart Support does not collect any sample data, only instrument parameters, so sample information remains confidential. Figure 8 shows the ability to enable or disable Smart Support by the user.

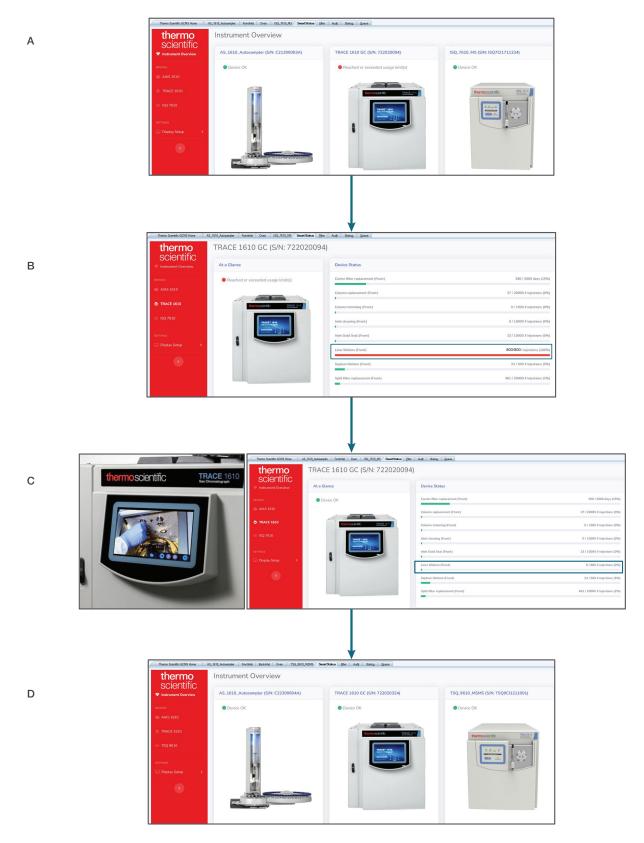


Figure 7. Flow diagram of resolving issue using SmartStatus software. (A) An issue is indicated in red on the status overview page on the TRACE 1610 GC (reads reached or exceeded usage limits). (B) Detailed view on the TRACE 1610 GC clearly shows that the injection liner has reached its set limit of 800 injections (indicated by a full red bar). (C) Maintenance performed on the injection liner using the maintenance video on the TRACE 1610 GC touch screen. The counter is then reset. (D) Once maintenance is performed all devices read "device OK". System is ready to run samples.

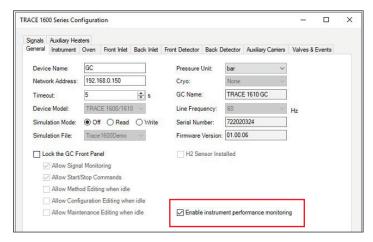


Figure 8. Check box selection of Smart Support controlled by the user

Conclusion

SmartStatus software is intelligent and data-driven, allowing users to make informed decisions on when to perform maintenance on their GC and GC-MS systems. Its features and advantages include:

- At-a-glance system ready status allowing the analyst to act only when needed, removing wastes
- User customizability of monitored parameters, threshold, and time units, which gives users control to monitor the system in a way that fits their needs
- Intelligent preventative maintenance alerts ensuring maintenance to be performed before issues arise, keeping the instrument up and running longer
- Consumable tracking that enables sustainable operation and maximization of the use of each consumable
- Smart Support for rapid remote diagnosis to ensure any instrument issues can be resolved without delay

Utilizing SmartStatus software on the TRACE 1600 series GC, TSQ 9610 GC-MS/MS, and ISQ 7610 GC-MS gives the analyst data-driven insights to make informed decisions that allow laboratories to operate more sustainably by maintain productivity, maximizing consumable usage, and reducing laboratory costs.

Reference

 Thermo Fisher Scientific Technical Note 000421: Extended linear dynamic range with the XLXR detector system on the Thermo Scientific ISQ 7610 single quadrupole GC-MS. https://assets.thermofisher.com/TFS-Assets/CMD/Technical-Notes/tn-000421-gc-mslinear-dynamic-range-xlxr-detector-tn000421-en.pdf



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