Improving Open-Access Mass Spectrometry Reliability Through Automated System Suitability

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Introduction

Open-access mass spectrometry enables 24/7 instrument use by a broad community of scientists, removing the need for specialist training and accelerating routine analysis. However, this model depends on instruments remaining consistently stable, calibrated, and ready for use at all times. We present a system suitability workflow that verifies instrument performance against performance previously established in the laboratory. If a suitability test fails, the operator can ensure that remedial action can be taken to avoid the generation of low-quality or misleading data.

Figure 1. Portable/Field deployable LC-MS.

A workflow using a portable, field deployable, LC-MS (Figure 1) coupled with an integrated environmental sensor module that records temperature, humidity, and other contextual measurements is described. These environmental data streams provide additional diagnostic insight, and metadata for acquired samples. Sample submission, acquisition control, and subsequent data processing are handled seamlessly by SpectralWorks™ RemoteAnalyzer™ software through an intuitive touch-screen and web-based interface that requires minimal user training.

Experimental

Portable LC – SmartLC 200-600nm HPLC UV detector (PolyLC Inc. Columbia USA)

Stationary Phase: PolyHYDROXYETHYL A™
Mobile Phase: 10 mM ammonium formate, pH 3.0, 65% Acetonitrile (Isocratic)
Column: 100 mm x 2.1 mm, 3µm particle size, 60 Å pore size
Flow rate: 0.2 mL/min
UV Detection: 225 nm
Splitter: 100:1 to reduce flow rate to the MS

Field Deployable Ion Trap MS – MTE30 (MassTech Inc, Columbia USA)

Ionization: ESI
Scan Mode: MS Low
Voltage: 2.2 kV
Automatic Gain Control: On
Resolution: 2000
Microscans: 5
Scan Range: *m/z* 140 – 300

System Suitability Sample (SST) – H-Gly-Ser-OH Dipeptide (500 ppm in mobile phase), *m/z* 163

Figure 2 shows the real time instrument telemetry, including system and environmental conditions for the instrument during operation.

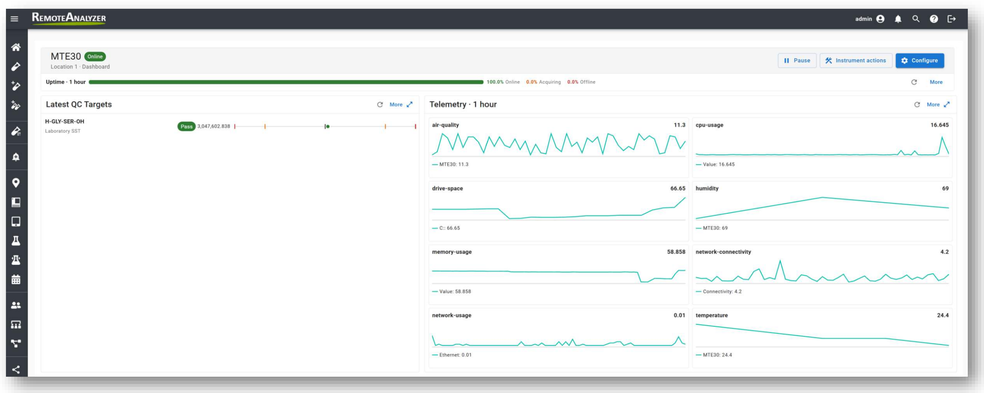

Figure 2. Instrument telemetry and environmental metadata.

System Suitability Samples - Laboratory

To establish the baseline functionality of the system, daily samples (SST) were acquired over a two-week period. This provided the basis for the expected performance in the field.

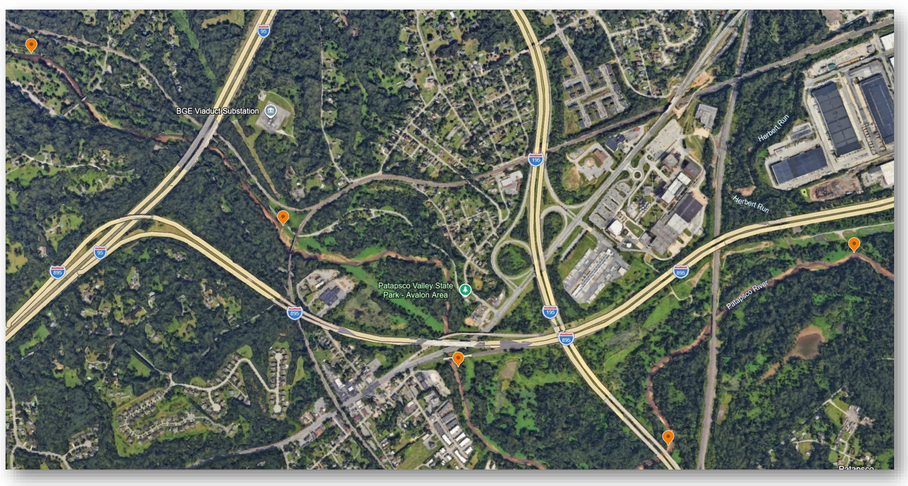

Figure 3. Field sample locations shown in orange.

System Suitability Samples - Field

Five river locations were selected for daily sampling (Figure 3). System Suitability samples were run at the start and end of the working day. The performance of the system in the field was checked immediately against the established performance in the laboratory.

Results

Figure 4 shows the SST results for both the Laboratory and the Field samples. The daily laboratory results from the peak area of the extracted ion chromatogram of *m/z* 163 were used to create a quality control chart for peak areas as well as retention time. Warning (2 x SD) and Action Limits (3 x SD) are shown for the peak areas, with a CV of 22.099%, and an MS peak symmetry consistently over 80% are shown in Figure 5.

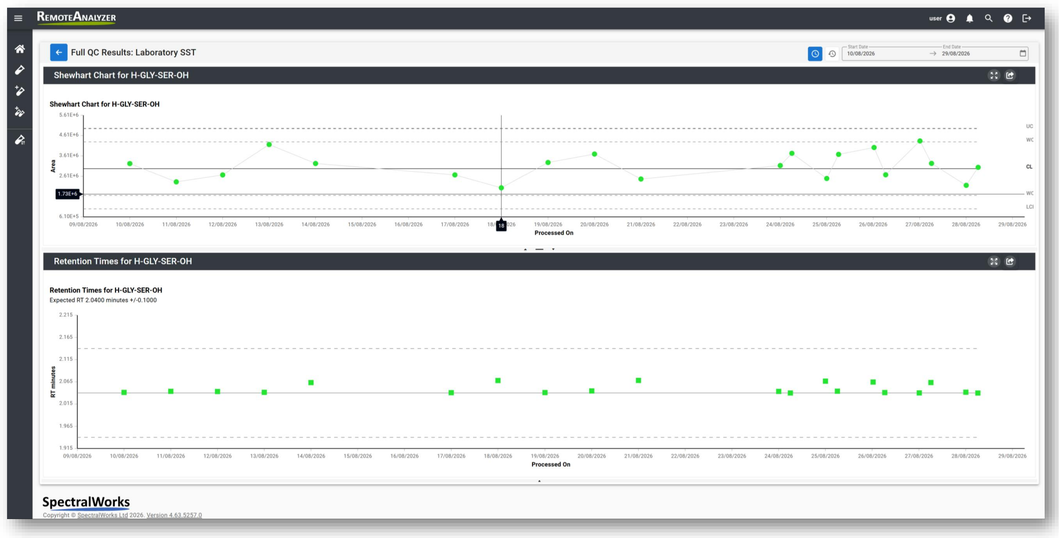

Figure 4. Quality Control Chart for Peak Areas and Retention time.

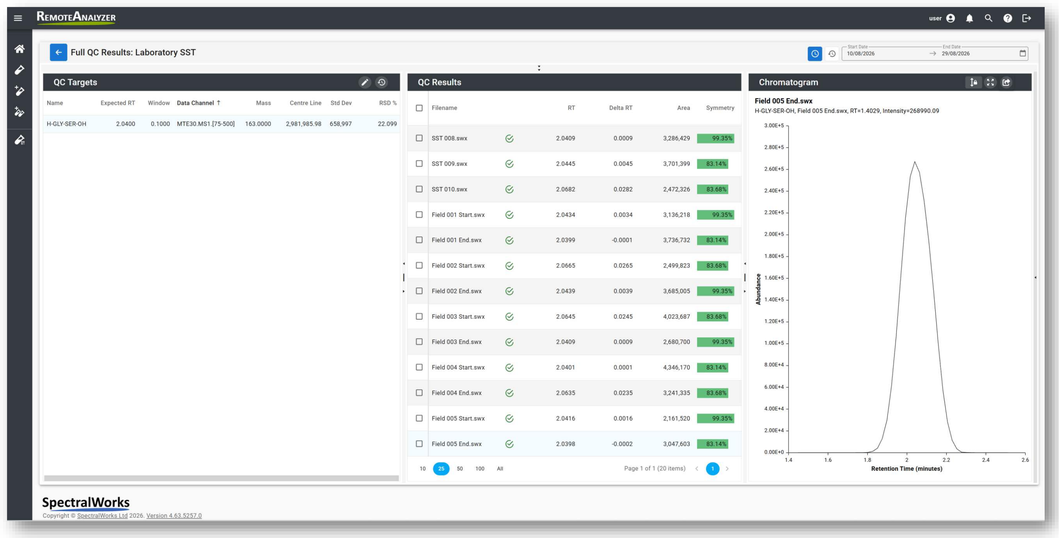

Figure 5. QC Target parameters and QC Results.

Conclusions

Using a simple dipeptide standard, a portable LC-MS platform can support a system suitability workflow to allow non-expert field personnel to effectively monitor instrument performance.

The workflow links established laboratory performance with the challenging conditions in the field. Additional environmental data may prove useful in determining accuracy and validity of field-based data.

Figure 6 shows a typical sample history page which details sample information and conditions that are automatically tracked without user intervention.

Figure 6. Typical Sample History.