

TwinScape™: a digital twin-driven solution for quality management in the modern proteomics laboratory

Data quality management is an emerging topic in proteomics laboratories aimed at ensuring that measurement platforms meet the standards and expectations of researchers who use them.

Introduction

Data quality management is important for users of hyphenated liquid chromatography mass spectrometry (LC-MS) systems because it helps them to ensure the accuracy, reliability, and reproducibility of their results. Such an approach starts with assurance that all components of the LC-MS system are performing as expected and capable of providing deep proteome coverage in a reproducible manner. Bruker TwinScape was developed for this purpose as a digital twin solution that maintains a virtual model of the real-world data acquisition system. It continuously monitors instrument health and serves as a repository for quality control data that together enable “at a glance” assurance of instrument performance before and after the analysis of precious biological samples. When combined with standard reference materials, the Biognosys indexed Retention Time (iRT™) kit containing reference peptides, and Bruker ProteoScope™ software for proteomics data analysis, TwinScape elevates the quality management capabilities of the modern proteomics laboratory and allows longitudinal tracking of data quality for improved results.

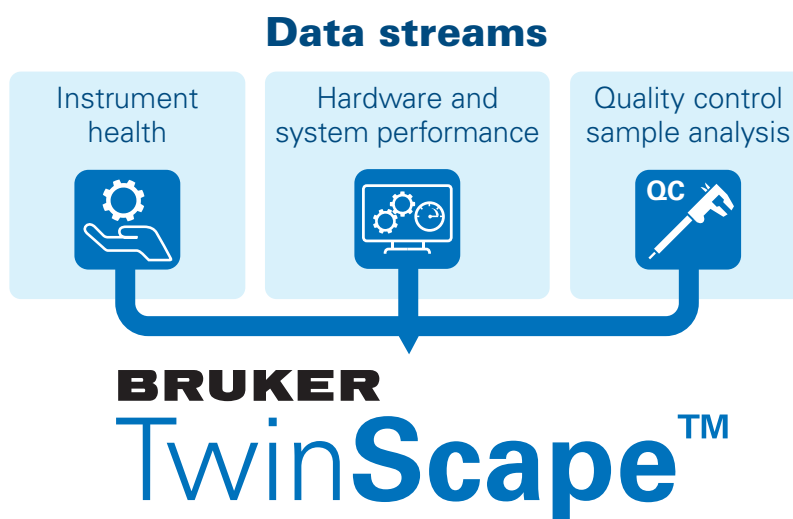


Figure 1
TwinScape combines data from multiple streams, providing users with both a snapshot overview of instrument health and the ability for in-depth analysis of longitudinal performance data.

Methods

The instrument health and performance characteristics of a timsTOF Pro 2 mass spectrometer were monitored using Bruker TwinScape software. System performance was benchmarked by dedicated analyses of K562 (Promega) extract QC samples spiked with the Biognosys iRT peptide standards mixture. Pre-processing of raw data was performed using Bruker ProteoScape and the resulting data was automatically uploaded to TwinScape.

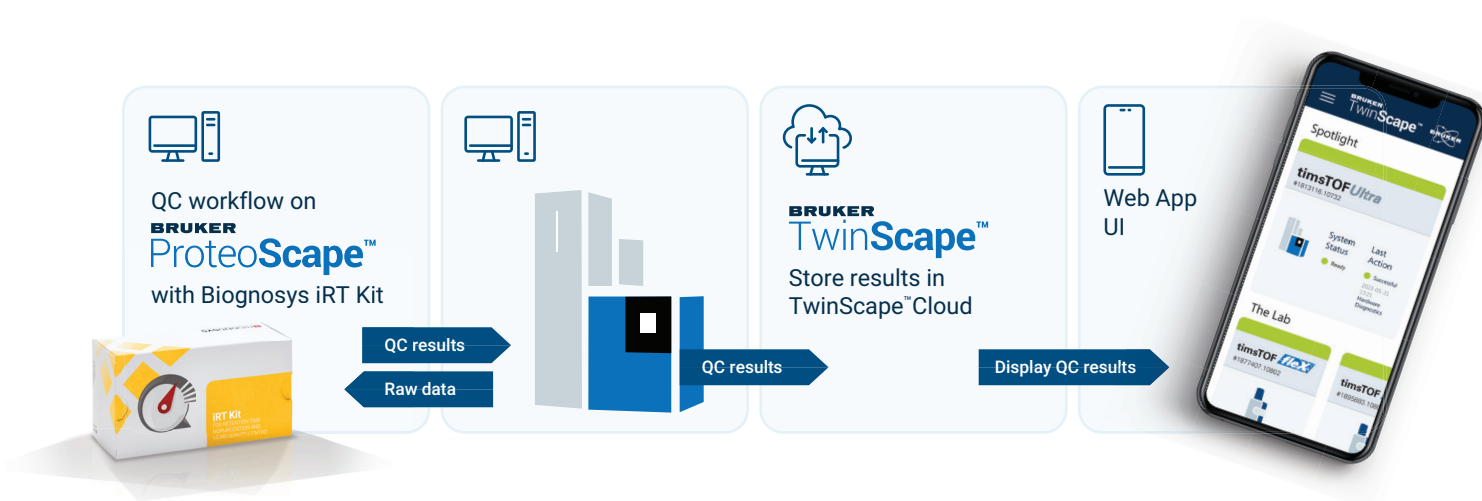


Figure 2

Overview of the quality management workflow integrating Biognosys iRT kit, Bruker ProteoScape data processing and automated upload and monitoring with TwinScape.

Results and discussion

The use of a digital-twin approach provided by TwinScape software, paired with standardized performance benchmarking provided by analysis of standard reference materials and the Biognosys iRT peptide standards kit, enabled the comprehensive review of key data quality factors including total peptide and protein identification rates, as well as iRT peptide specific measurement parameters.

Concurrent metadata and instrument health data acquisition allowed for interpretation of changes in performance metrics. The TwinScape user interface (Figure 3) allows users to visualize timsTOF instrument health at a glance, providing assurance at regular intervals that the system is in good working order. The observation of suboptimal performance and unexpectedly high variation in key quality metrics (Figure 4A) in the absence of instrument health warnings, and despite consistent iRT peptide performance (Figure 4B, 4C), led to a review of quality control materials storage and preparation protocols. After a brief troubleshooting effort, reproducible high performance was observed across QC samples, reflecting the fresh preparation of K562 extract material and revised storage protocol.

As a consequence of longitudinal data quality monitoring, QC processes were therefore modified to enhance laboratory working practices and increase the sensitivity and precision with which further downstream sources of potential error could be observed and identified. Together, the approach provided assurance of instrument performance and enabled reproducible results for omics studies.

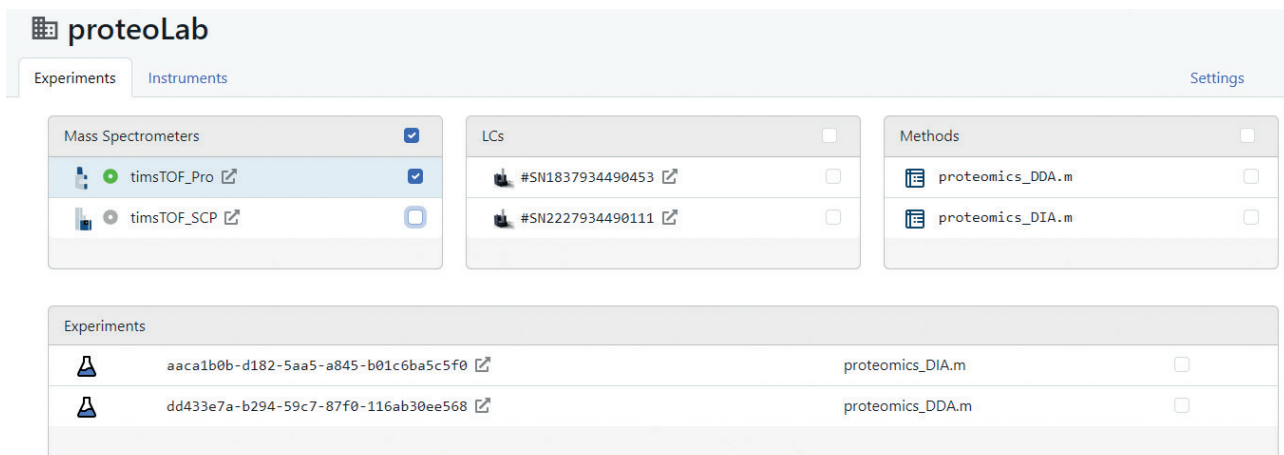


Figure 3 The TwinScope user interface allows for "at-a-glance" assurance of MS instrument health, and allows for filtering of available QC data ("Experiments" panel at bottom) by instrument and method type ("Mass Spectrometers", "LCs", and "Methods" panels at top).

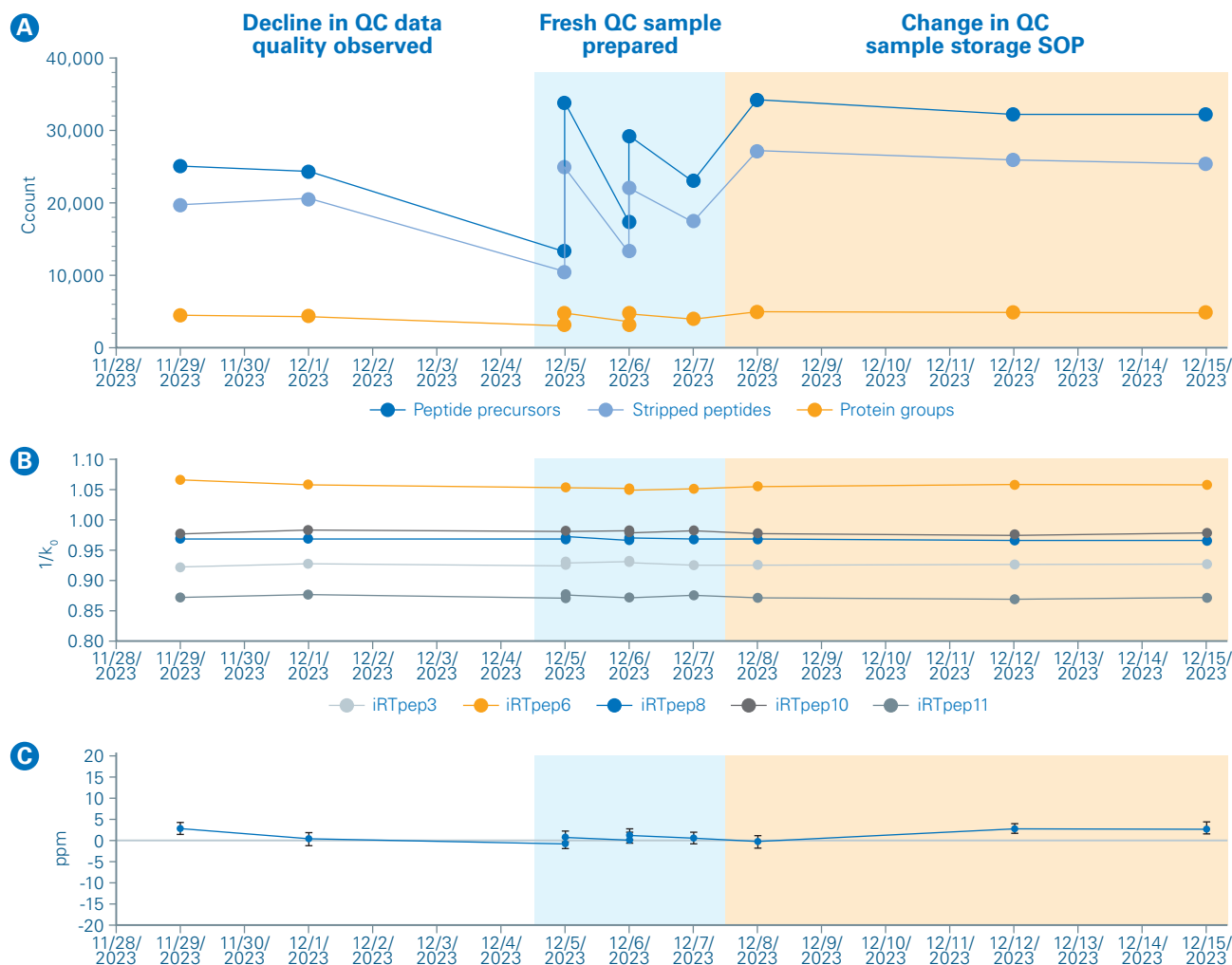


Figure 4 Assessment of key K562 QC performance metrics (number of peptide precursors, stripped peptides, and protein groups) across time revealed a decline of QC data quality (A, left-most plot segment). Simultaneous assessment of iRT peptide measurement performance demonstrated acceptable precision and provided assurance that compromised LC and MS performance was not the underlying cause (B, C). Therefore, the QC materials and preparation protocols themselves were evaluated in a troubleshooting effort (A, middle plot segment) resulting in changes to both that were then implemented, providing reproducible high performance results (A, right-most plot segment).

Conclusion

The digital-twin concept successfully facilitates bioanalytical platform monitoring and data quality assurance when combined with standardised benchmarking materials. When deployed across a modern omics laboratory, TwinScape enables “at a glance” monitoring of instrument health. Where data reproducibility is found to be low in the absence of instrument health warnings, users are directed towards inspection of other variables in the sample preparation workflow. Here, improvements to quality control processes were identified and undertaken as a result of this advanced monitoring capability. In the future, the digital-twin concept may be further developed to deliver additional benefits including enhanced service support as a step towards enabling predictive maintenance. For now, by following quality management guidelines and standards, mass spectrometry users can avoid mistakes, reduce uncertainty, and improve confidence in their data.



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“At NBCC (located at the Lunenfeld-Tanenbaum Research Institute), we support a variety of projects in our Proteomics facility. As such, it’s critical that our instruments are at peak performance and that we always have a pulse on them. The combination of Bruker ProteoScape, TwinScape and the Biognosys iRT kit have become integral for monitoring the instruments in our facility, to ensure everything is operating up to standard. TwinScape is a great place to get an overhead, over-time view of our QC and system performance in simple to view plots. It has been especially useful in helping us go back to ProteoScape to help us pinpoint whether it is a sample, MS or LC problem.”



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