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TwinScape: a digital twin-driven concept for improved timsTOF platform monitoring and data quality assurance

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Introduction:

Data quality management is crucial for users of hyphenated liquid chromatography mass spectrometry (LC-MS) systems, as it ensures the accuracy, reliability, and reproducibility of results. A robust approach to data quality management begins with the assurance that all components of the LC-MS system are operating as expected and are capable of providing deep proteome coverage in a reproducible manner.

Bruker TwinScape has been developed specifically for this purpose, serving as a digital twin solution that maintains a virtual model of the real-world data acquisition system. Through continuous monitoring of instrument health and acting as a repository for quality control data, TwinScape enables swift assessment of instrument performance both before and after the analysis of precious biological samples.

When combined with standard reference materials, such as the Biognosys indexed Retention Time (iRT™) kit containing reference peptides, and Bruker ProteoScape™ software for proteomics data analysis, TwinScape significantly enhances the quality management capabilities of modern proteomics laboratories. It also allows for longitudinal tracking of data quality, ultimately leading to improved results in proteomics analyses.
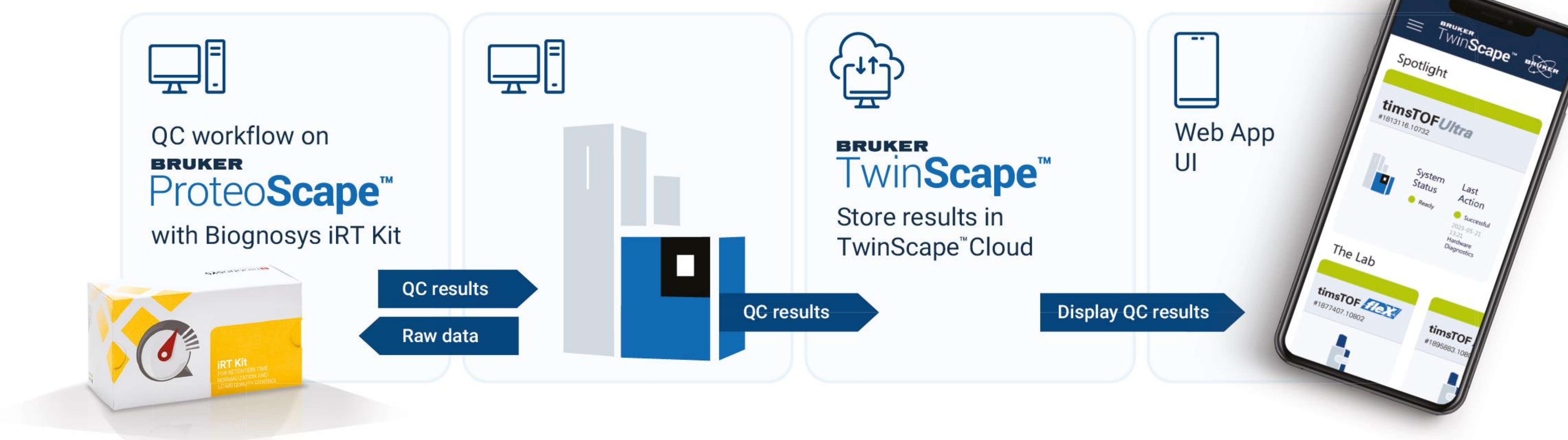
Key Learnings:

- TwinScape facilitates a comprehensive approach to data quality management by maintaining a virtual model of the data acquisition system.
- Integration of standard reference materials like the iRT™ kit enhances data quality and reproducibility.
- Utilization of Bruker ProteoScape™ software enables longitudinal tracking of data quality, thereby improving proteomics results.

Method:

The instrument health and performance characteristics of advanced hyphenated proteomics mass spectrometry systems (typically comprising a nanoElute 2 liquid chromatograph and a timsTOF mass spectrometer) were monitored using Bruker TwinScape software. System performance was benchmarked using the Biognosys iRT peptide standards mixture, and pre-processing of raw data was performed using Bruker ProteoScape.

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

Fig. 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.

Results:

The use of TwinScape software, along with standardized performance benchmarking using standard reference materials and the Biognosys iRT peptide standards kit, enabled a comprehensive evaluation of data quality factors, including peptide and protein identification rates and iRT peptide parameters.

Concurrent acquisition of metadata and instrument health data facilitated the interpretation of performance variations. TwinScape's intuitive interface allowed for easy visualization of timsTOF instrument health, ensuring regular system functionality checks.

Observations of suboptimal performance led to a review of quality control protocols, resulting in reproducibly high performance across samples. Longitudinal data quality monitoring prompted modifications to enhance laboratory practices, ensuring instrument performance assurance and reproducibility in omics studies.
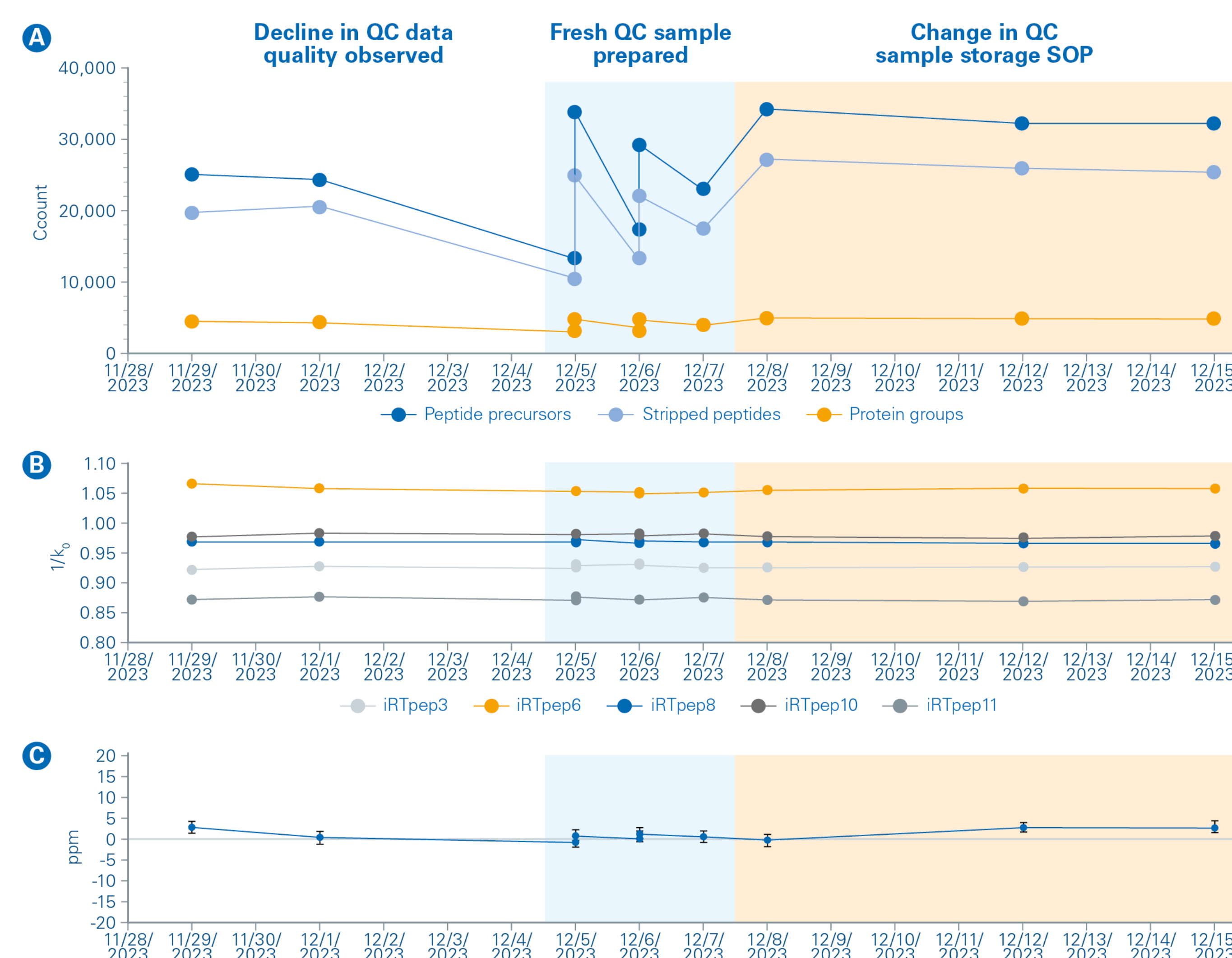

Fig. 2: Assessment of key K562 QC performance metrics (number of peptide precursors, stripped peptides, and protein groups) across time revealed a decline of QC data quality (A, left-most plot segment). Simultaneous assessment of iRT peptide measurement performance demonstrated acceptable precision and 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 effectively supports bioanalytical platform monitoring and data quality assurance.
- Integration with standardized benchmarking materials enhances its efficacy.
- TwinScape enables easy monitoring of instrument health in modern omics laboratories.
- Data-driven prompt to inspect of sample preparation variables.
- Advanced monitoring capabilities identify areas for quality control process improvements.
- Future developments may extend its benefits, potentially including improved service support and predictive maintenance capabilities.

TwinScape: a digital twin-driven concept with Bruker ProteoScape & Biognosys iRT peptides

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