Evaluation of an Integrated LC–MS Quantitation Workflow for Forensic Toxicology Applications

Introduction

Forensic toxicology laboratories require quantitative LC–MS workflows that are reproducible, efficient, and defensible under accreditation and legal scrutiny. Challenges commonly include manual data handling between acquisition and quantitation platforms, inconsistent method setup, and the significant analyst time required for chromatographic review of large multi-analyte datasets. Integrated software environments that consolidate acquisition, optimization, data processing, and review may address these limitations while supporting data integrity requirements.

Objective

The objective of this work was to evaluate the applicability of the waters_connect™ platform with MS Quan for routine screening and quantitative LC–MS workflows typical of forensic toxicology laboratories.

Methods

Representative qualitative screening and quantitative multi-analyte assays were acquired and processed using waters_connect with MS Quan. Method development, MRM optimization, data processing, and review were conducted within the same software environment. Data were assessed using a combination of full manual review and configurable exception-focused review rules reflecting commonly used forensic acceptance criteria (e.g., ion ratios, retention time tolerance, signal-to-noise thresholds, blanks, internal standards, and calibration/QC performance).

Results and Discussion

End-to-end integration of system control, acquisition, quantitation, and reporting eliminated intermediate data transfer steps between software modules, reducing opportunities for transcription and handling errors. Centralized access to instrument tuning and MRM optimization data facilitated consistent method development and transfer, with retention times and dwell times automatically incorporated into acquisition methods.

The workflow-based data processing approach in MS Quan enabled structured review of large datasets containing numerous analytes. Exception-focused review rules automatically highlighted results outside predefined acceptance criteria, allowing analysts to prioritise potential issues while maintaining access to full chromatographic inspection where required. Visualization tools supporting simultaneous review of multiple MRM traces aided rapid identification of carryover, integration, or matrix-related effects across batches.

Automated system suitability assessments (e.g., retention time stability, peak response, ion ratios, and peak shape metrics) provided documented verification of instrument performance prior to case sample analysis. Software features supporting version control, audit trails, user access management, and traceability of analytical changes were available throughout acquisition and processing, aligning with expectations for accredited forensic laboratories.

Conclusion

The integrated waters_connect and MS Quan workflow supported efficient and defensible quantitative LC–MS analysis for forensic toxicology applications. Consolidation of acquisition, optimization, processing, and review within a single environment reduced manual handling

steps and enabled structured, exception-based data review suitable for high-throughput forensic casework.