



TargetLynx Application Manager for Confirmation Analysis

Waters Corporation



For forensic toxicology use only.

Abstract

This application note details on how TargetLynx provides an easy to use and flexible solution to increase laboratory productivity and improve the quality of quantitative LC-MS/MS or GC-MS/MS data.

Introduction

Quantitation using LC-MS/MS is now well established in many forensic, environmental, clinical and veterinary applications. There are often legal, environmental, human health and financial implications arising from the results of quantitative MS analyses. This has led to an increased demand by regulatory and legal authorities for extra confirmatory and quality control checks. Regulatory or statutory methods often require, for example, the monitoring of multiple structurally specific fragment ions, maximum chromatographic peak width and/or retention time. To calculate and check these manually is a labour intensive, time-consuming and subsequently costly task.

TargetLynx automates data acquisition, processing and reporting incorporating a wide range of confirmatory checks allowing samples falling outside user-specified or regulatory thresholds to be easily identified, giving confidence when reporting quantitative results.

TargetLynx is able to rapidly identify and flag samples where, for example:

- Analytes are above a specified concentration
- Analyte confirmatory ion ratios are outside specified limits
- One or more analyte signal-to-noise ratios are below a defined value
- An analyte retention time or relative retention time is outside limits
- The coefficient of determination (r^2) of the calibration curve exceeds a defined value

If the analytical data is required to be used as part of a police investigation or presented in a court of law, it is essential that extensive analytical information is provided to confirm the presence of a suspected drug. TargetLynx is ideal for this application, where the presence of a suspected drug can be confirmed by the presence of a number of different diagnostic ions and MRM transitions. Confirmation analysis using TargetLynx is enhanced as ion ratio measurements and chromatographic retention time information is also incorporated in the analytical procedure.

Drugs of Abuse and Forensic Toxicology

LC-MS/MS is now increasingly used in forensic toxicology laboratories for drugs of abuse confirmation and quantitation applications. LC-MS/MS is typically used for confirmation analysis, following a positive immunoassay analysis that indicates the presence of a class of drugs or specific drug, or when there is evidence present that a drug is likely to be present in a sample.

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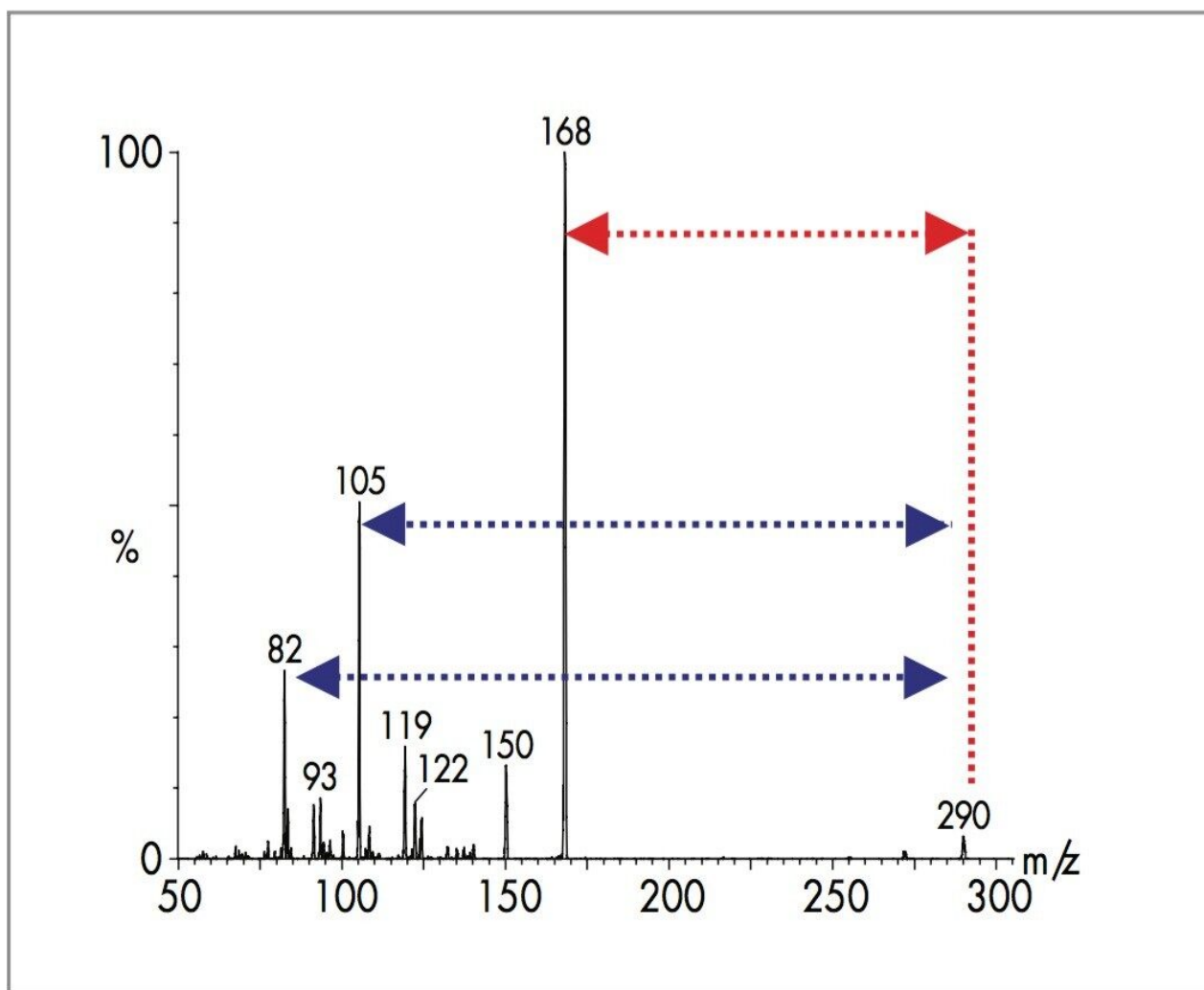


Figure 1. Mass Spectrum of the cocaine metabolite Benzoylecgonine. Transition 290/168 is used for quantitation. Two further MRM transitions 290/105 and 290/82 are monitored for additional confirmation by TargetLynx.

Flexibility and Ease of Use

TargetLynx can be used with LC-MS/MS and GC-MS/MS data. This data can be SIM (Selected Ion Monitoring), MRM (Multiple Reaction Monitoring) or full scan/full spectrum. In the case of full scan/full spectrum data, extracted ion chromatograms are used for quantitation.

Results and Discussion

Customisation and Export of Data

TargetLynx features various reporting options, with reports being printed directly from the Browser file by sample or by compound.

Report formats can be customised and can consist of all or some of the following; the Calibration page, Compound Summary Report, Sample Summary Report, Totals Support, Samples Report, and Audit Report.

In the Calibration page the user can select how the data is displayed, for example 'Show Residuals', 'Show Response Curve' and/or 'Show QC Points'.

The Compound Summary Report, Sample Summary Report, Totals Report, and Samples Report allow the user to display calibration information per compound, report one compound/sample/totals group per page or split and print summary reports per sample.

Data can be exported from the TargetLynx browser as a XML or comma separated text file into a LIMS system.

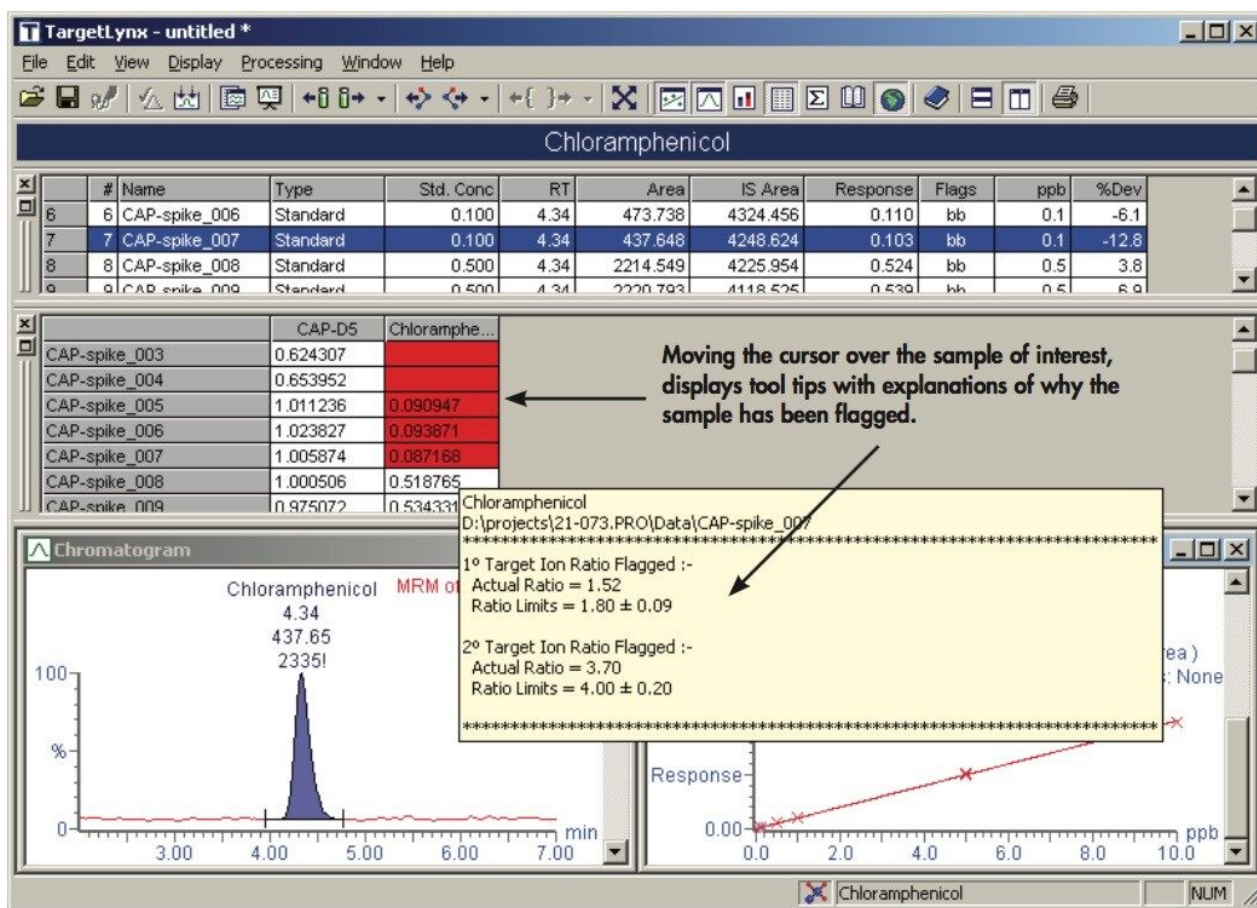


Figure 3. TargetLynx browser – showing results summary with flags, calibration curve and chromatograms.

Conclusion

TargetLynx Application Manager automates data acquisition, processing and reporting incorporating a wide range of confirmatory checks allowing samples falling outside user-specified or regulatory thresholds to be easily identified, giving confidence when reporting quantitative results.

TargetLynx provides an easy to use and flexible solution to increase laboratory productivity and improve the quality of quantitative LC-MS/MS or GC-MS/MS data.

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