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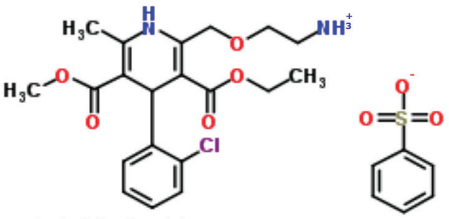
Combining Multiple Acquisition Channels for Analysis of Impurities Using Empower 3 Software

Margaret Maziarz
Waters Corporation, Milford, MA, USA



Empower 3 Chromatography Data Software (CDS) allows users to combine multiple acquisition channels collected during a single injection to generate one result for analysis of impurities.

GOAL

Demonstrate the capabilities of Empower® Software in combining multiple 2D acquisition channels collected during a single injection to create one result for analysis of impurities.

BACKGROUND

Mass spectrometry provides sensitivity, selectivity, and rich-mass information not only to support small-molecule drug development, but also for routine monitoring of low-level impurities in the finished drug products. While different acquisition modes are available with mass spectrometry, the single ion recording (SIR) acquisition mode provides much better sensitivity compared to the total ion chromatogram (TIC) mode. The SIR measures intensity of the single ion of interest and simplifies analysis for the targeted compounds. Often, sample components may have different masses and multiple channels with different SIR values must be collected for one sample injection. These multiple channels must be combined to create one result.

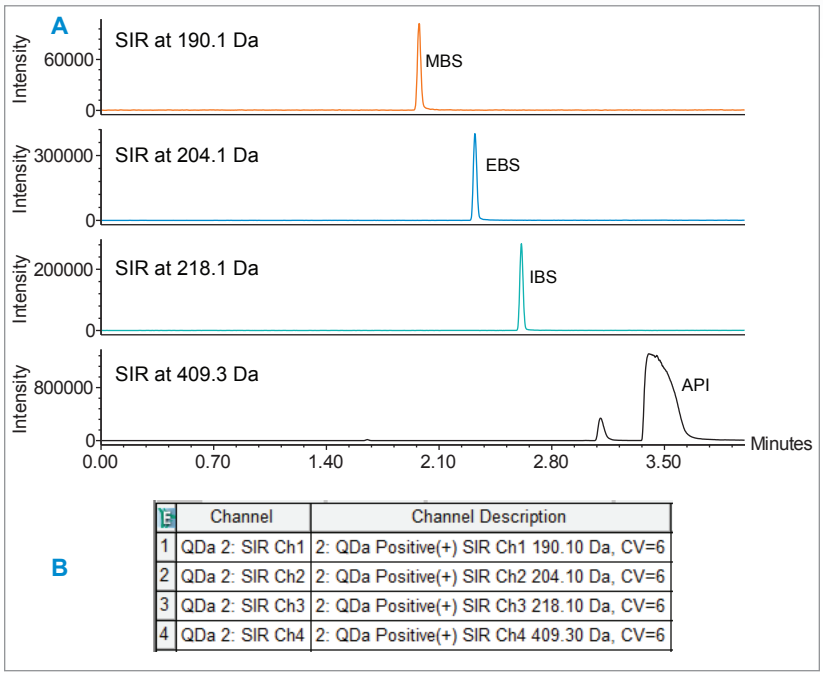


Figure 1. MS Single Ion Recording (SIR) chromatographic data for methyl, ethyl, isopropyl esters of benzenesulfonic acid (MBS, EBS, IBS) and amlodipine besylate API acquired with an ACQUITY QDa Detector (A). MS SIR channels collected for impurity analysis (B).

This technology brief illustrates use of Empower Software for combining multiple MS SIR channels for analysis of potential genotoxic impurities (PGIs). Alkyl esters of benzenesulfonic acid are considered PGIs that can develop during the synthesis of a drug substance and must be accurately measured at low levels to ensure safety of the pharmaceutical products.

THE SOLUTION

Empower Software enables users to combine multiple MS SIR channels acquired for a single injection. To illustrate this capability, we analyzed PGIs of benzenesulfonic acids methyl, ethyl, and isopropyl esters (MBS, EBS, IBS) that have different masses.

A sample solution containing 0.1 mg/mL of amlodipine besylate active pharmaceutical ingredient (API) was spiked with the esters at 0.1% level and analyzed by an ACQUITY® QDa® Detector using previously developed UPLC® method.[1] Four SIR channels were acquired to collect data for the esters and the API (Figure 1). Then, we created a formula-based derived channel to combine the SIR channels (Figure 2) and processed the data. Empower Software generated one chromatographic plot with each ester and API (Figure 3A). The combined data was then used to determine quantity of each impurity in the API sample injection (Figure 3B).

SUMMARY

Empower 3 Software enables users to combine multiple 2D acquisition channels collected for a single injection to generate one sample result.

This capability can be easily adapted by any laboratory that utilizes mass spectrometry and a single ion recording (SIR) acquisition mode for low-level analysis of impurities with different masses. Multiple channels with different SIR values can be combined to determine quantity each impurity in one sample injection. This tool will streamline quantitative analysis protocols during development of the drug substance or release testing of the finished drug products.

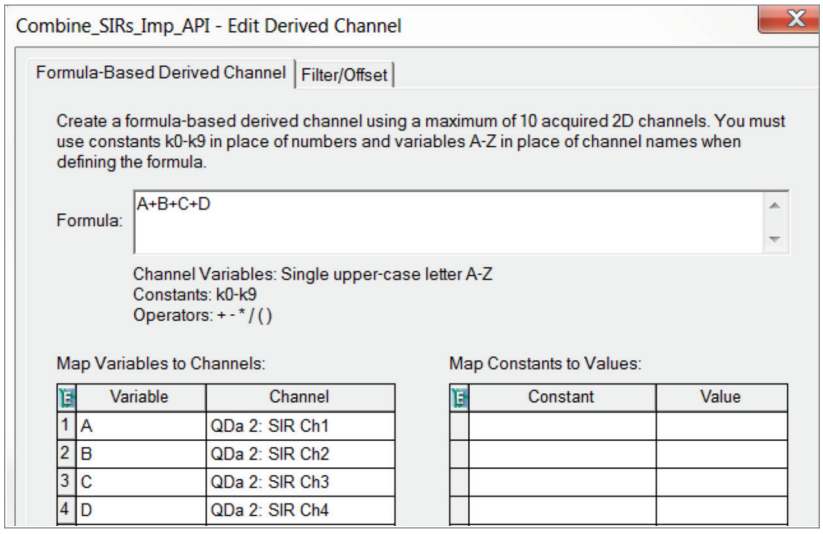


Figure 2. Formula-based derived channel to combine 2D SIR channels for impurity analysis.

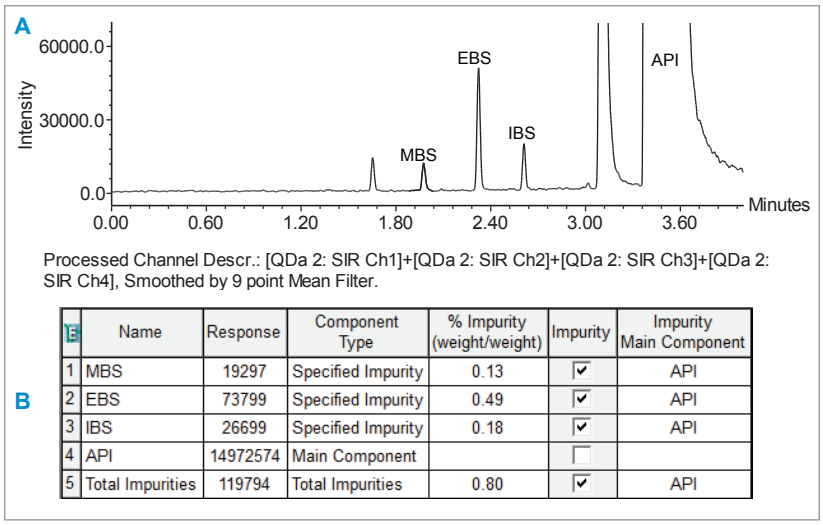


Figure 3. Chromatographic data processed using formula-based derived channel for methyl, ethyl and isopropyl esters of benzenesulfonic (MBS, EBS, IBS) and amlodipine besylate API (A). Results for impurity analysis.

References

1. Maziarz M., Wrona M., Coupling Mass Detection with UV to Improve Method Sensitivity for Esters of Benzenesulfonic Acid in Analysis of Genotoxic Impurities, Waters Application Note, 720005680EN, 2016.

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Waters Corporation
34 Maple Street
Milford, MA 01757 U.S.A.
T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com