Using Your QTRAP® LC/MS/MS System at Full Potential

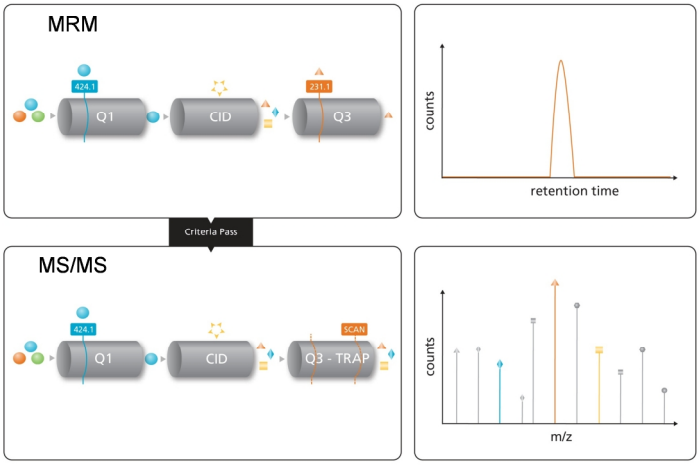
A Quick-Start Guide to Activate and Perform MS/MS Library Searching for Identification and Confirmation MasterView™ and MultiQuant™ Software

Overview

This document outlines the 6 easy steps you can follow to analyze full scan MS/MS spectra (MRM-triggered MS/MS scans collected on a QTRAP® LC/MS/MS system) and compare those results to MS/MS compound libraries to identify and confirm positive peaks in unknown samples.

The benefits of this workflow include:

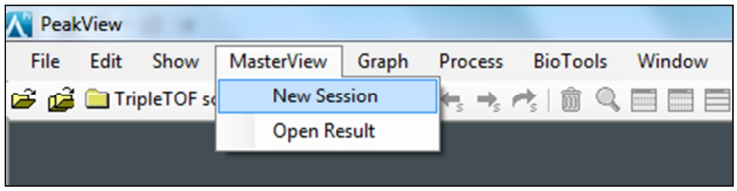
- **Improved selectivity** – multiple fragment ions are detected (beyond just 2 MRM transitions) meaning additional confidence in identification of positive findings
- **Improved sensitivity** – Enhanced MS/MS scans are called 'enhanced' because fragment ions are accumulated in Q3 of your QTRAP®, giving you better signal-to-noise for the detected MS/MS spectra
- **Improved data processing** – dual injection approach with automatic quantitation, identification and confirmation using MasterView™ software and MultiQuant™ software
- **Improved confidence** – ability to automatically calculate ion ratios and compare results to MS/MS mass spectral libraries



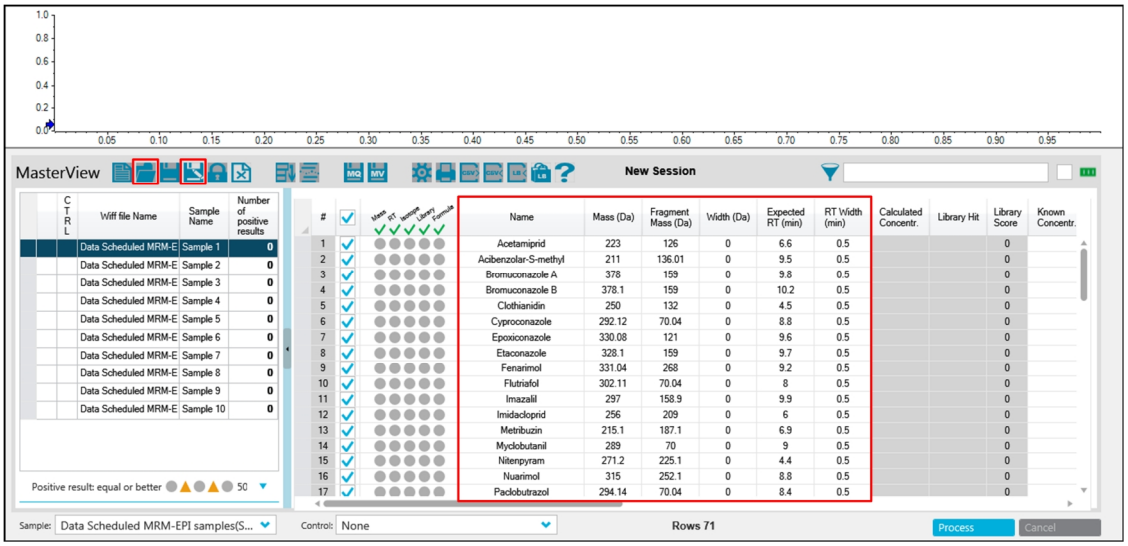
The QTRAP® Software Workflow in MasterView™ Software

Start a new session in MasterView™ and open your sample data file(s)

Select 'New Session' in the MasterView™ menu and select sample(s) to process in the browser window.

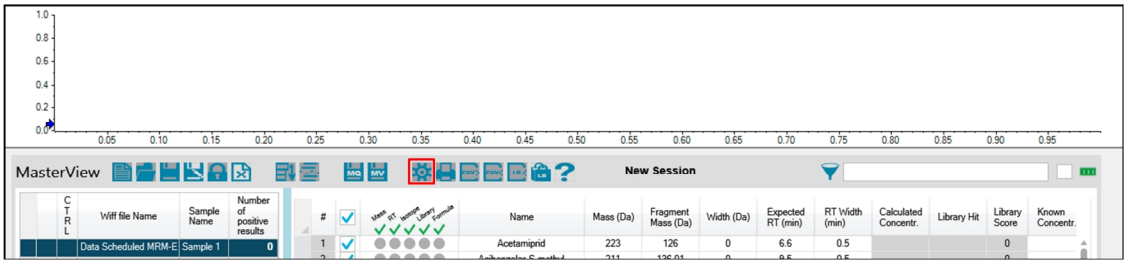


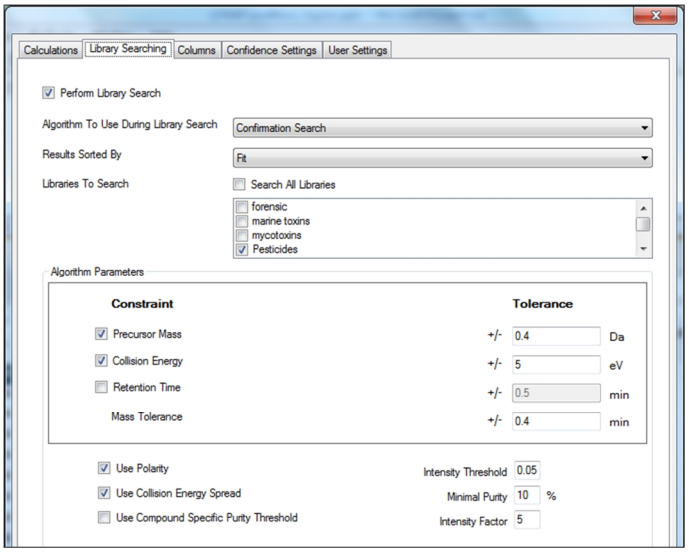
Create a new or open an existing XIC list



- Create a new XIC list by simply copying Name, Mass, Fragment Mass and Retention Time (RT) from your *Scheduled* MRM™ acquisition method into the MasterView™ software.
- The XIC list can be saved and opened for future processing.

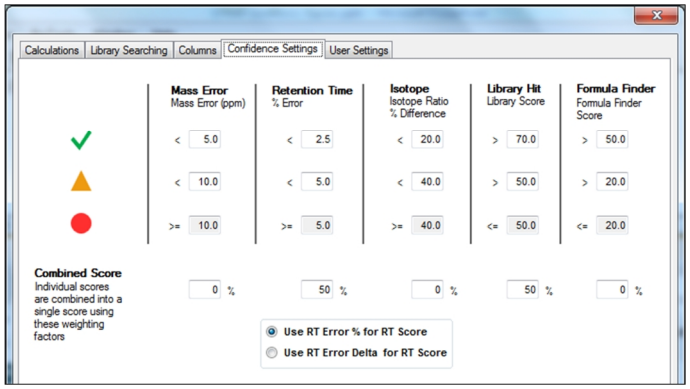
Edit settings for data processing and library searching





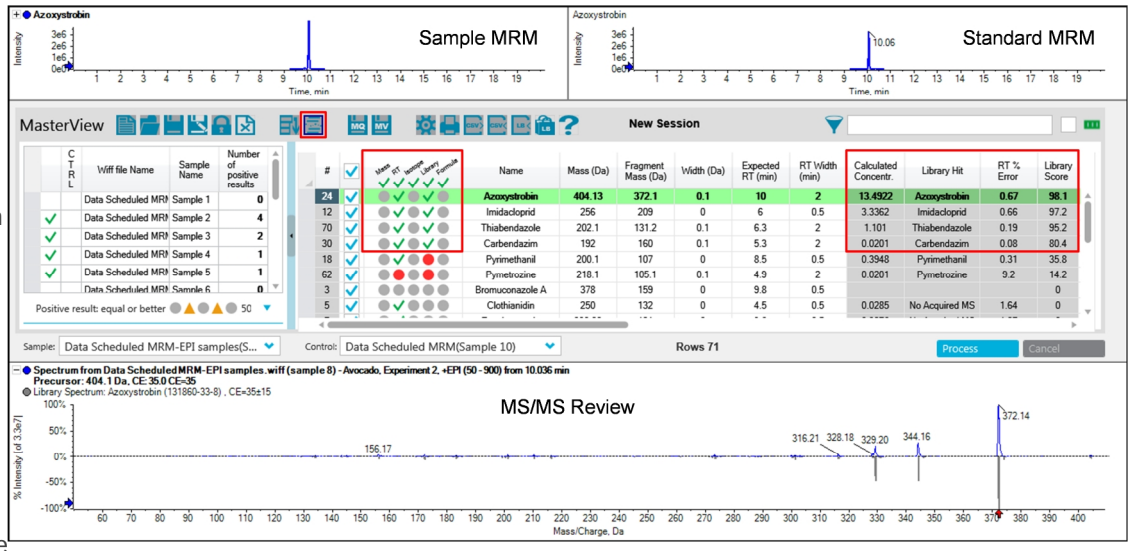
- Data processing settings can be edited by clicking the ‘Settings…’ button at the top of the XIC list
- Define thresholds for intensity and S/N in the calculations tab.
- In the ‘Library Searching’ tab select the libraries to search, the search algorithm, and specify other criteria such as mass tolerance, Collision Energy tolerance, and the use of polarity and Collision Energy Spread when searching

Define confidence settings for compound identification



- Define criteria for compound identification for RT and library searching in the 'Confidence Settings' tab.
- Note: All settings will be saved with the XIC list.

Review qualitative results



- Confidence in identification is visualized using the RT and Library 'traffic light'
- Numeric values can be found in the RT % Error and Library Score column. Any of these columns can be used to sort results.
- The MS/MS spectrum can be visually compared to the library spectrum by clicking the 'Show MS/MS' button.

Data example: Identification of Azoxystrobin, Carbendazim, Imidacloprid, and Thiabendazole in an avocado sample (QuEChERS extract 10x diluted)

Review quantitative results

- Findings in unknown samples are automatically compared against a standard injection of known concentration.
- The MRM transitions can be normalized for easy comparison of peak intensity.
- Results with a concentration higher than the standard are highlighted in green. Results can be filtered using the ‘Display highlighted XIC only’.
- Results can be reported using customizable report templates or can be exported in MultiQuant™ for further processing including the automatic calculation of ion ratios.

Data example: Identification of Carbendazim, Cyprodinil, Fenhexamid, Pyrimethanil, Quinoxyfen, and Trifloxystrobin in a grapes sample (QuEChERS extract 10x diluted), however, only Fenhexamid and Pyrimethanil were present at a concentration higher than 10 µg/kg)

Confirmation of Fenhexamid using a second analysis and automatic ion ratio calculation in MultiQuant™ software

Additional library searching and reporting functionality is available in the LibraryView™ and Cliquid® software.

For additional support on implementing this workflow in your own lab, or for support on other AB SCIEX products, visit our website or email us at support@absciex.com.

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