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

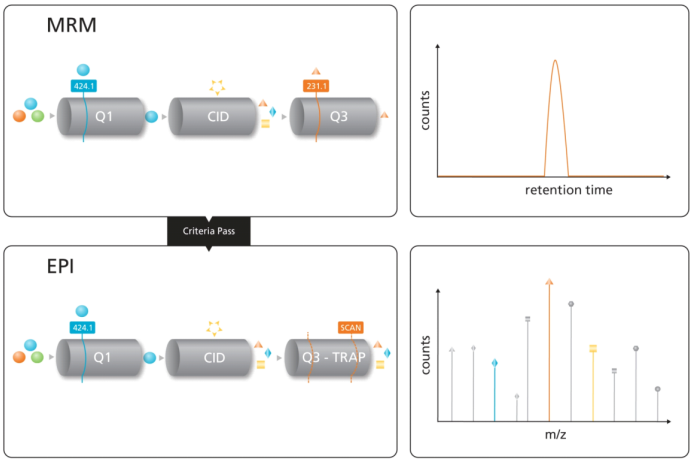
A Quick-Start Guide to Upgrade an MRM Acquisition Method to an MRM-IDA-EPI Acquisition Method in 6 Easy Steps using Analyst® Software

Overview

This document outlines the 6 easy steps to upgrade a basic Multiple Reaction Monitoring (MRM) acquisition method to automatically include Enhanced Production Ion (EPI) scanning to acquire full scan MS/MS spectra for any MRM that was detected in an unknown sample.

The benefits of this workflow include:

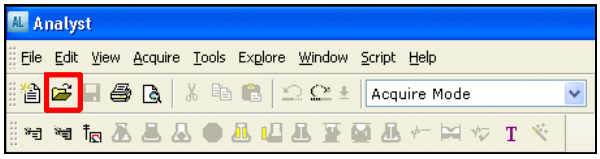
- Improved selectivity – multiple fragment ions are detected (beyond just 2 MRM transitions) meaning additional confidence in identification of positive findings
- Improved sensitivity – EPI scans are called 'enhanced' because fragments are accumulated in Q3 of your mass spectrometer, giving you better signal-to-noise for the detected MS/MS spectra
- Improved data acquisition – EPI spectra are acquired fully automatic using the logic provided by Information Dependent Acquisition (IDA), Dynamic Background Subtraction (DBS), and Dynamic Fill Time (DFT)
- Improved data processing – ability to compare results to MS/MS mass spectral libraries for better identification



The QTRAP® Software Workflow in Analyst® Software

Open your MRM acquisition method in Analyst® software

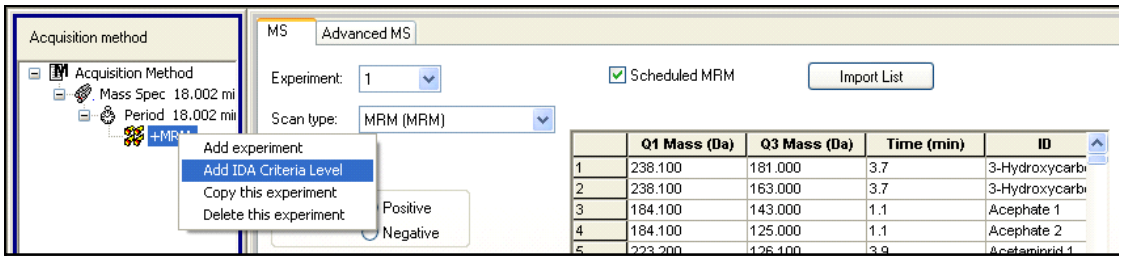
Open any MRM method that contains your list of targeted MRM transitions.

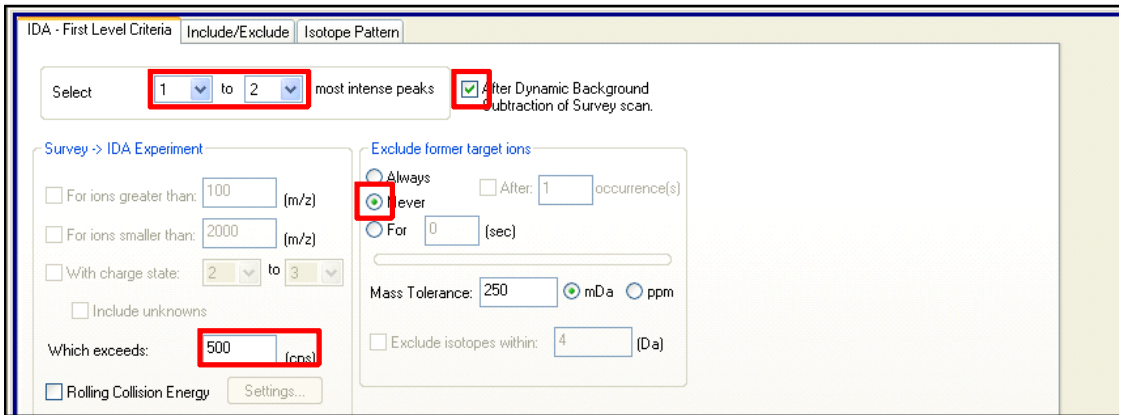


Add IDA criteria

- Right click on your MRM experiment and select 'Add IDA Criteria Level'
- Set-up the criteria by using these recommended settings:

1. Monitor 1 to 2 peaks
2. Activate DBS
3. Set the automatic exclusion to 'Never'
4. Set the IDA threshold to 500 cps (or higher depending on MRM background)

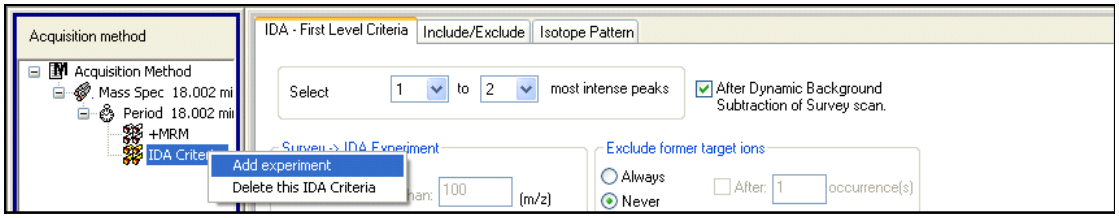


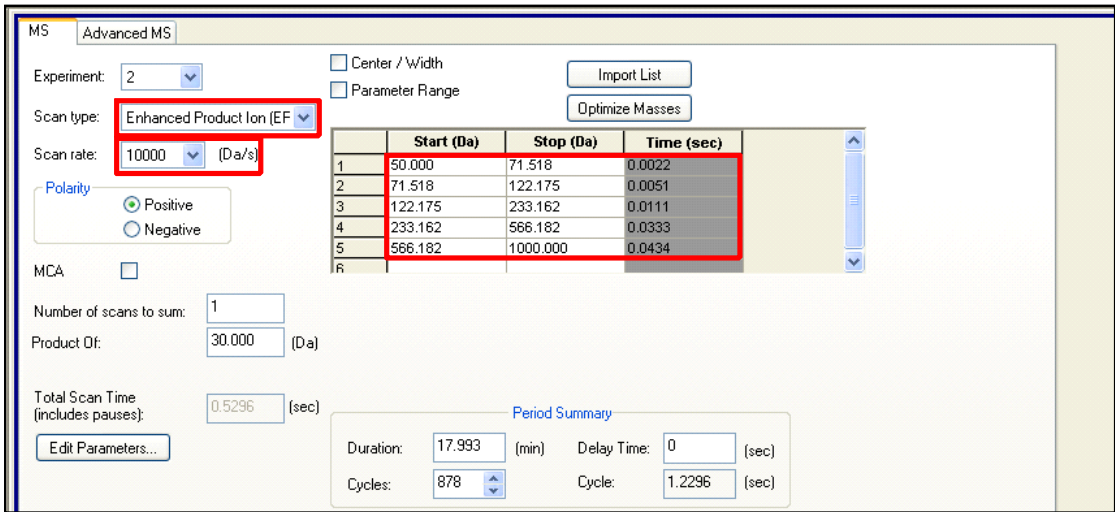


Add EPI experiment

- Right click on your IDA criteria and 'Add Experiment'
- Set-up your EPI scan by:

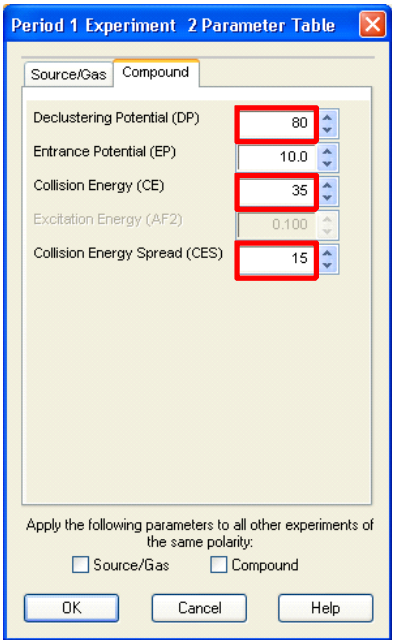
1. Change scan type to 'Enhanced Product Ion'
2. Select a scan rate of 10000 Da/s
3. Specify a mass range to cover all targets of your MRM list, like 50 to 1000



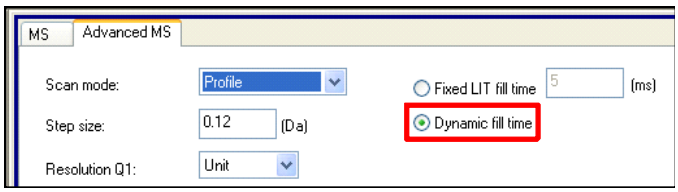


Edit MS and MS/MS parameters

- Set Declustering Potential (DP) to a value near the average DP of all compounds in your MRM list
- Set Collision Energy (CE) to 35 V and Collision Energy Spread (CES) to 15 V for best library search results

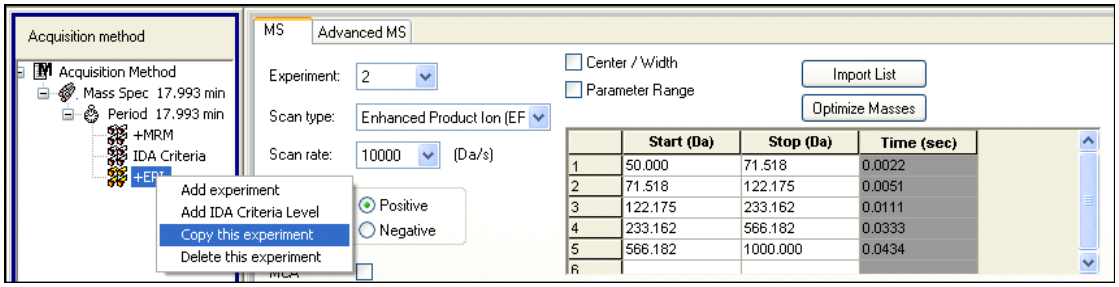


Verify that Dynamic Fill Time (DFT) is active



- Go to the 'Advanced MS' tab and be sure to verify that DFT is active

Duplicate the EPI experiment and save your MRM-IDA-EPI method.



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Headquarters
500 Old Connecticut Path, Framingham, MA 01701 USA
Phone 508-383-7700
www.absciex.com

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