

# Introducing AutoSRM

## MRM Simplicity for High Performance Results

### Overview

The advantages of selected reaction monitoring (SRM) and multiple reaction monitoring (MRM) analyses are often accompanied by some challenges, especially with respect to the adoption of these methods in the laboratory. These challenges can be due to the complexity of the mass spectrometer setup and optimization. Laboratories that want to realize the benefits of MS/MS must overcome some barriers in the tuning, setup and optimization to reduce the lead time to get into routine production.

The Thermo Scientific TSQ 8000 GC-MS/MS system was built with simplicity as a priority. Whether you are starting with a completely new analysis, transferring a method from a single quadrupole GC-MS to a triple quadrupole GC-MS, or porting a known MRM method from another instrument, the TSQ™ 8000 GC-MS/MS system ensures the fastest route to high performance SRM results.

### AutoSRM Studies

AutoSRM is comprised of a three-step process. These steps are called studies:

- Step 1: Precursor Ion Study
- Step 2: Product Ion Study
- Step 3: SRM Optimization Study

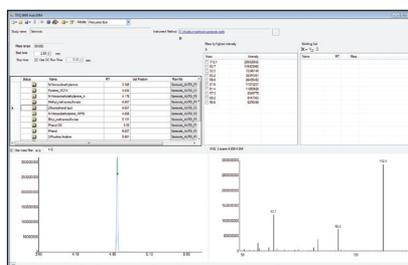
#### Step 1: Precursor Ion Study

The purpose of this first step is to select your precursor ions. To start this study, name your compounds and enter your vial numbers. AutoSRM will signal your TSQ 8000 system to run a full scan analysis on the compounds in your standards.

Along with your chromatographic peak and your product ion spectra, you are presented with a table of the most intense product ion masses to select. If desired, AutoSRM can automatically pick them up for you.

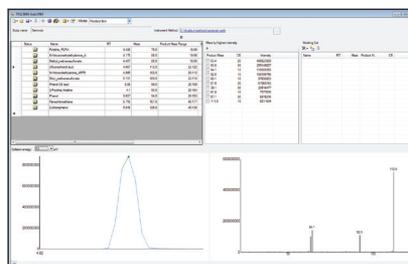
#### STEP 1:

Select your precursor ions from a full scan



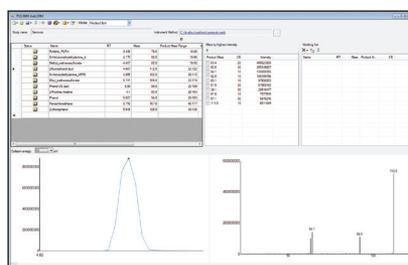
#### STEP 2:

Select your product ions from product ion scans



#### STEP 3:

Optimize the collision energy for selected transitions



AutoSRM Workflow

Figure 1. AutoSRM is the first step in creating an SRM method from scratch. AutoSRM can also be used for SIM method development and to optimize an existing SRM method (for instance with a new collision gas).

## Step 2: Product Ion Study

Now that you have selected your precursor masses, it is time to find your product masses. AutoSRM will signal the TSQ 8000 system to acquire product ion scans of your precursor masses at three collision energies. You are not required to set up any methods, sequences or data layouts to accomplish this. AutoSRM automatically takes care of it. Along with your chromatographic peak and your product ion spectra, you are presented with a table of the most intense product ion masses from which to choose. Again, if you choose, you can have AutoSRM pick for you.

From here you can export your transition list to your instrument method, or you can send your selected transitions to an SRM optimization study for further optimization.

## Step 3: SRM Optimization Study

The final step in SRM development is the SRM optimization step. Now that you have selected your precursor and product masses, AutoSRM will acquire those transitions at multiple collision energies. Because of the fast scanning capabilities of the TSQ 8000 GC-MS system, three transitions per compound, each at 10 unique collision energies, can be analyzed in a single injection. This will give you a well defined maximum for your collision energy, as shown in Figure 2 below.

Once complete, AutoSRM allows the simple creation of the TSQ 8000 instrument method to be ready for routine analysis.

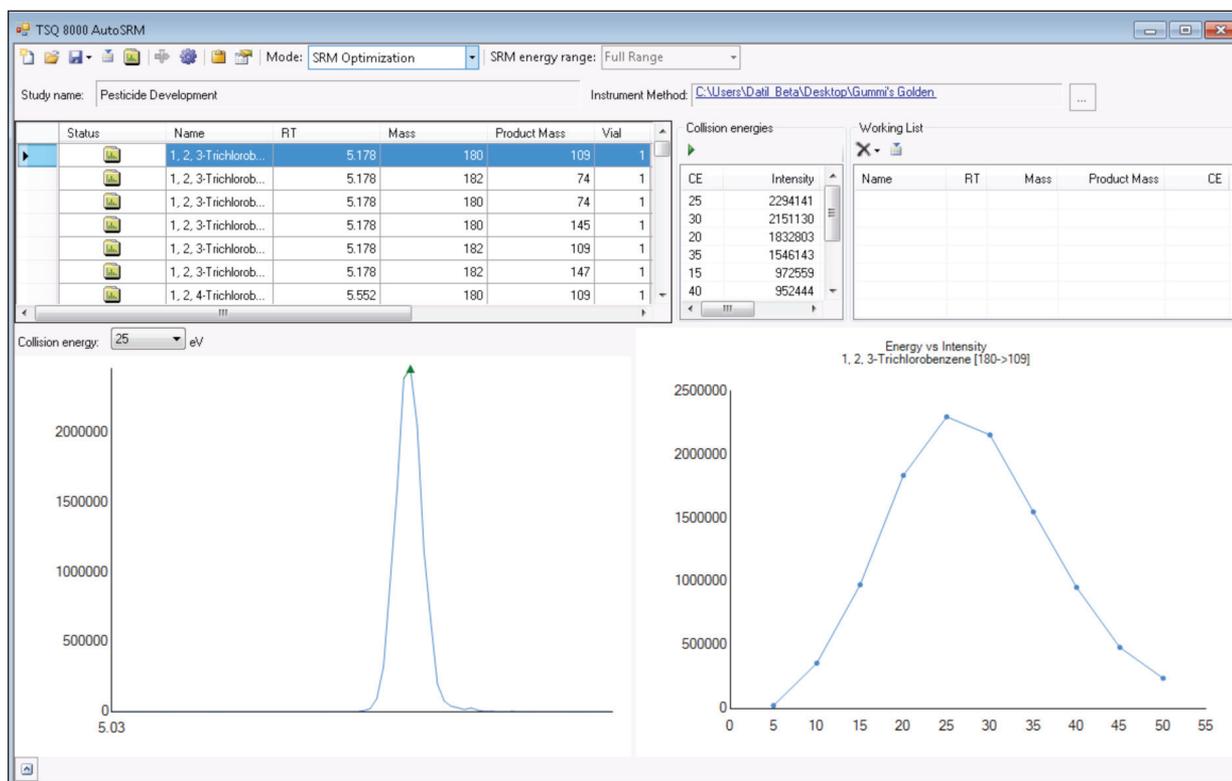


Figure 2. Collision Energy optimization curve for the  $m/z$  180 > 109 transition of 1,2,3-Trichlorobenzene, showing an optimum collision energy of 25 eV. At this point in the process, the optimized SRM transitions can be exported to your instrument method.



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