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SIM Bridge: Simplifying the Transition from Single to Triple Quadrupole Workflows

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AutoSRM, GC-MS, SIM, single quadrupole, SRM, triple quadrupole, TSQ Duo

Many laboratories looking to replace single quadrupole instrumentation understand the benefits a triple quadrupole GC-MS can bring, but believe it is out of their reach—due to cost, regulatory restrictions, operational complexity, or the time needed to get started with productive methods. The Thermo Scientific™ TSQ™ Duo system offers a unique choice when considering a new GC-MS for the lab. It allows analysts to use single quadrupole methods and make the transition to triple quadrupole workflows automatically, on the same system, when appropriate. The transition occurs on a familiar instrument, and using the TSQ Duo as a triple quad is as simple as using it as a single quad, with walk-through method development tools and fully automatic tuning. The TSQ Duo enables laboratories to meet future challenges such as new detection limits, changing client requirements, regulatory updates, and pressures from competing laboratories.

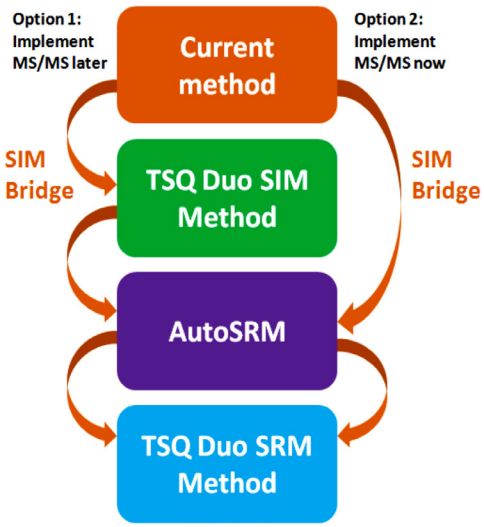

Figure 1. TSQ Duo MS/MS adoption workflow.

Bridging the Gap to Triple Quad Methods

The most complex aspect of adopting triple quadrupole methodology is the creation and implementation of MS/MS methods. To address this problem, the TSQ Duo features SIM Bridge and AutoSRM software capabilities. These integrated tools take the user from a compound list or single quadrupole method to a fully developed, optimized multiple/selected reaction monitoring (MRM/SRM) method on the TSQ Duo system.

The SIM Bridge tool allows the mapping of selected ion monitoring (SIM) methods exported from other sources to the TSQ Duo instrument. Analysts can choose between running a SIM analysis first and MS/MS later, or moving directly to MS/MS methods (Figure 1). After continuing with SIM analysis, the system automatically creates discrete segments in the TSQ Duo SIM method to optimize performance. Once complete, the system is ready to run. At any time, these methods can be submitted to AutoSRM for MS/MS method development to provide optimized methods.

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Alternatively, SIM Bridge can directly submit a SIM method to AutoSRM for immediate development of MS/MS methods.

AutoSRM is a mass spectrometer method development expert, integrated into the GC-MS system. This software walks analysts through the development of fully optimized SRM transitions in a simple and efficient workflow—it offers full MS and MS/MS method development independence, even for the less experienced user.

AutoSRM Using SIM Bridge is Comprised of a Three-step Process:

- Step 1: SIM Bridge import
- Step 2: Product ion study
- Step 3: SRM optimization study

Step 1: SIM Bridge Import

Use SIM Bridge to pull in all compound information including compound name, retention time, and SIM ions from a single quadrupole method.

Step 2: Product Ion Study

Once SIM ions are imported, they become the precursor masses. AutoSRM will signal the TSQ Duo system to acquire product ion scans of the precursor masses at three collision energies. The analyst does not have to set up any methods, sequences, or data layouts; AutoSRM performs those tasks automatically. Along with the chromatographic peak and product ion spectra, SIM Bridge provides a table of the most intense product ion masses from which to choose. Alternatively, AutoSRM can make those selections.

Step 3: SRM Optimization Study

Once precursor-to-product ions have been selected, AutoSRM acquires those ions at multiple collision energies to ensure the best sensitivity possible (Figure 2).

After ion acquisition, AutoSRM allows the very simple creation of a complete MRM instrument method that is ready to use for real sample analysis.

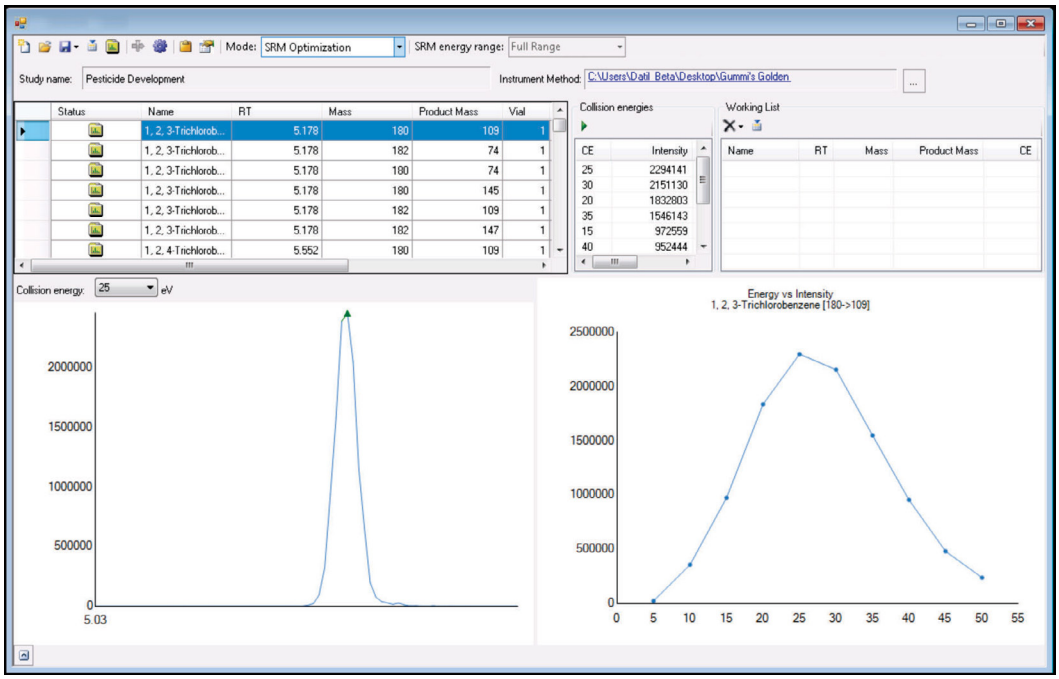

Figure 2. Collision energy optimization curve for the *m/z* 180 › 109 transition of 1, 2, 3-Trichloroethane, showing an optimum collision energy of 25 eV. At this point in the process, the optimized SRM transitions can be exported to your instrument method.

AutoSRM Benefits

The following is a real-life example of SRM method development, illustrating the benefits of SIM Bridge and AutoSRM.

A customer was set to create an MS/MS method for quantitation of 80 targeted compounds, with more than 250 transitions to identify and optimize. With AutoSRM, the method creation and optimization took a total of 24 hours, with a mere 30 minutes of total user interaction with the instrumentation and software. During the remaining time, the instrument was running on its own, under the control of AutoSRM.

User interaction during method development was limited to the initial placement of the sample vial into the autosampler, and importing (via the SIM Bridge) the list of compound names and their retention times (10 min). Once those steps were complete, the first stage of AutoSRM, the precursor ion study, was running on its own. After review of the product ion study results (another 10 min), the next stage—the product ion study—was running again on its own, without any need to manually create a sequence.

Finally, after review of the product ions intelligently selected by AutoSRM based on the set of user-defined criteria (10 min), the selected transitions were optimized for collision energy, again automatically by AutoSRM and unattended by the user.

The result was a ready-to-use GC-MS/MS method, created in 24 hours with only 30 minutes of user interaction. When the customer compared the time and efforts they spent on the analysis using SIM Bridge and AutoSRM to those of another lab, which was not using these tools, the time savings alone was 1:10. In addition to the time-saving benefits, there was no need for tedious manual sequence creation, avoiding the probability of introducing errors while manually typing parameters.

When the same customer needed to add another 12 target analytes to their method a year later, modification of the method (method maintenance) took no more than 24 hours and the entire method, rather than just compounds being added, was re-optimized.

Conclusion

SIM Bridge and AutoSRM, pioneered by Thermo Scientific for GC-MS/MS, represent a significant break-through in method development and maintenance, easily bridging the gap in method transition from single quad SIM to triple quad SRM/MRM.

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