

Thermo Scientific TSQ 8000 GC-MS/MS Method Sync

Introduction

Synchronization of information between various components in the analytical workflow avoids duplication of effort, reduces manual errors, and saves precious time. As shown in the flowchart in Figure 1, the Thermo Scientific TSQ 8000 GC-MS/MS instrument method is designed to be fully integrated with Thermo Scientific TraceFinder software, making it easy to move compound information from method development, to method setup, to batch acquisition. Method Sync enables the user to easily manage complex timed-SRM methods, allowing for a greater focus on acquiring, reviewing, and reporting samples with a smaller focus on maintaining methods.

From Instrument Method to Processing Method

With the TSQ™ 8000 GC-MS/MS system, getting from an instrument method to a full processing method is easy. Within the instrument method, simply export your transition list to a TraceFinder™ Compound Data Store (CDS) file (Figure 2). During this export, you can select which transitions you want to be quantitative and which ones you want to be confirming transitions. After this selection, you can go into the CDS Manager in TraceFinder software, and import your transition list. You can now create your TraceFinder software method, and you can add compounds from the CDS interface to the processing method (Figure 3). The remaining information, such as ion ratios, is updated by associating a data file acquired with the instrument method. All of your target compounds and transitions are now placed within your processing method.

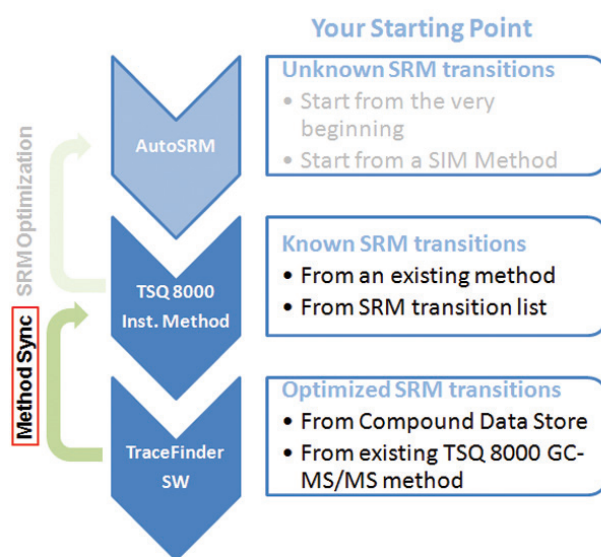


Figure 1. The TSQ 8000 GC-MS/MS instrument method is fully integrated with AutoSRM and TraceFinder software. Method Sync enables TraceFinder software processing method updates to be automatically propagated to the instrument method.

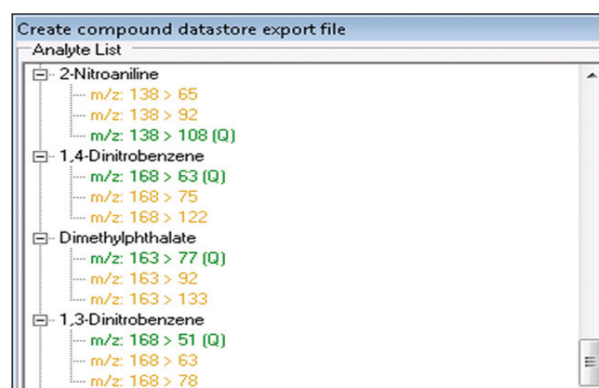


Figure 2. When creating an export file for the TraceFinder Compound Data Store, you are able to select which SRM transitions are for quantitation (shown in green) and which are for confirmation (shown in yellow.)

Automatic Retention Time Update

Since you now have a retention time-based instrument method to acquire your transitions, and a TraceFinder software method to process the data, how do you accommodate the clipping of your column and all your retention times change? If you sync the TraceFinder method with the acquisition method, all you need to do is run a standard and update your retention times in Data Review (Figure 4). Most of these updated retention times will be determined automatically through automatic peak detection. The next time you run the method, the acquisition list will be updated with the new retention times, eliminating most of the manual work previously needed to maintain a complex SRM instrument method. For these complex methods, this can lead to a major time savings in your daily work.

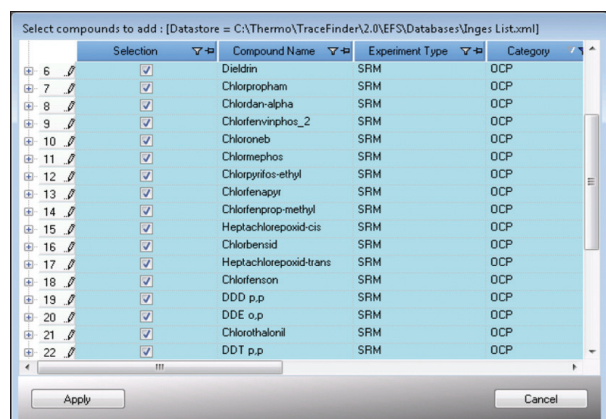


Figure 3. SRM, SIM and full scan rates based on peak width and scans across the peak

Compound-Based Scanning

Having the ability to sync the instrument method and the processing method also allows for easy creation of subsets of acquisition lists from the CDS. For instance, if you have a large multi-residue method available, but you are only interested in the organo-chlorine pesticides instead of the full set for a particular analysis, simply select the category for organo-chlorines when creating a processing method from the CDS. This will not only create a processing method with your selected compounds, but it will also create the corresponding acquisition list, limiting the list to just those compounds. This limited transition list will increase the dwell time of the selected transitions, and thus further increase the sensitivity of the TSQ 8000 GC-MS/MS system.

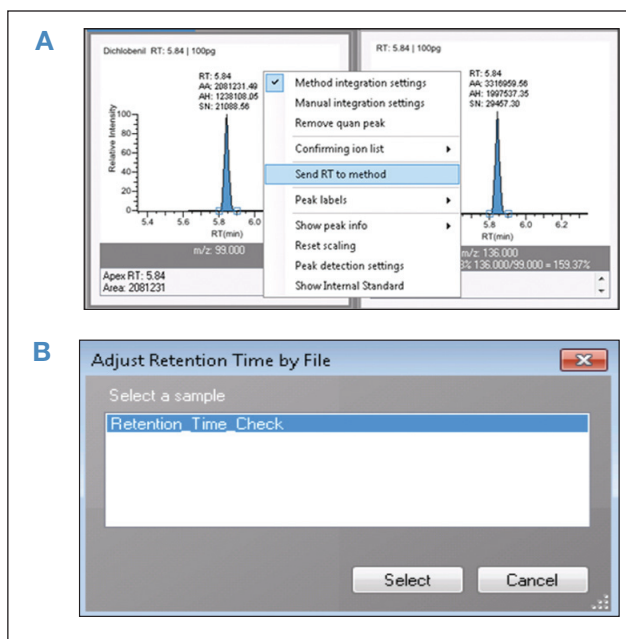


Figure 4. With Method Sync, when you adjust retention times through automatic processing in Data Review, retention times will also be updated in your timed acquisition method. You can update the retention times one at a time while you QC your data in Data Review (a), or adjust retention times en masse from an acquired sample (b).

www.thermoscientific.com

©2012 Thermo Fisher Scientific Inc. All rights reserved. ISO is a trademark of the International Standards Organization. All other trademarks are the property of Thermo Fisher Scientific Inc. and its subsidiaries. This information is presented as an example of the capabilities of Thermo Fisher Scientific Inc. products. It is not intended to encourage use of these products in any manner that might infringe the intellectual property rights of others. Specifications, terms and pricing are subject to change. Not all products are available in all countries. Please consult your local sales representative for details.

Africa-Other +27 11 570 1840
Australia +61 3 9757 4300
Austria +43 1 333 50 34 0
Belgium +32 53 73 42 41
Canada +1 800 530 8447
China +86 10 8419 3588
Denmark +45 70 23 62 60

Europe-Other +43 1 333 50 34 0
Finland/Norway/Sweden
 +46 8 556 468 00
France +33 1 60 92 48 00
Germany +49 6103 408 1014
India +91 22 6742 9434
Italy +39 02 950 591

Japan +81 45 453 9100
Latin America +1 561 688 8700
Middle East +43 1 333 50 34 0
Netherlands +31 76 579 55 55
New Zealand +64 9 980 6700
Russia/CIS +43 1 333 50 34 0
South Africa +27 11 570 1840



Spain +34 914 845 965
Switzerland +41 61 716 77 00
UK +44 1442 233555
USA +1 800 532 4752

AB52300_E 06/12S

Thermo
 SCIENTIFIC
 Part of Thermo Fisher Scientific