

Transferring GC/MSD Methods to a Triple Quadrupole GC/MS System

Technical Overview

Introduction

The ability to transfer and run methods that are created on single quadrupole GC/MSD systems to triple quadrupole instruments allows for a workflow that increases laboratory productivity. Acquisition methods that currently exist on a GC/MSD, when loaded on a triple quadrupole system, may be retention time locked to the original method. The ability to use the same data analysis method without the need for updating retention times enhances productivity.



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Loading a Method from the GC/MSD to the Triple Quadrupole GC/MS

Loading a method that exists on an Agilent GC/MSD, or single quad, to an Agilent Triple Quadrupole GC/MS system, or triple quad, is straightforward. The Agilent MassHunter acquisition home screen (Figure 1) shows an example triple quad method currently loaded on an instrument; in this case, it is Checkout.7000.eiex, but it could be any method that is currently loaded.

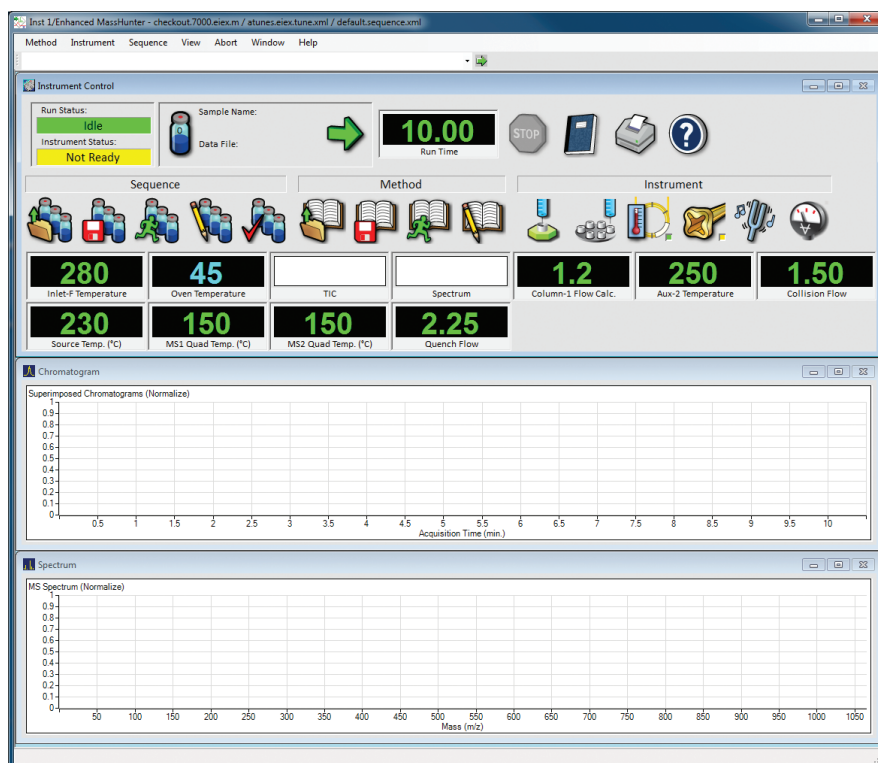


Figure 1. Agilent MassHunter acquisition home screen showing a currently loaded triple quad method prior to loading a single quad method.

The single quad method to be loaded and run is copied and saved to the desired local directory on the triple quad (the default method path is shown in Figure 2). To choose the desired method, **Load Single Quad (597x) Method** is selected, under the Method tab (Figure 3). In our example, we are loading and running a SIM method for 28 PCB congeners.

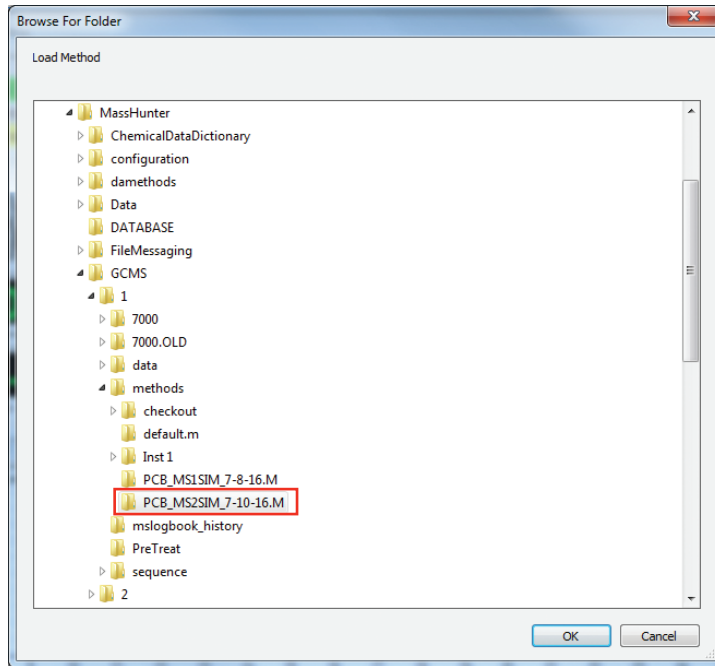


Figure 2. Default method path in the triple quad local directory.

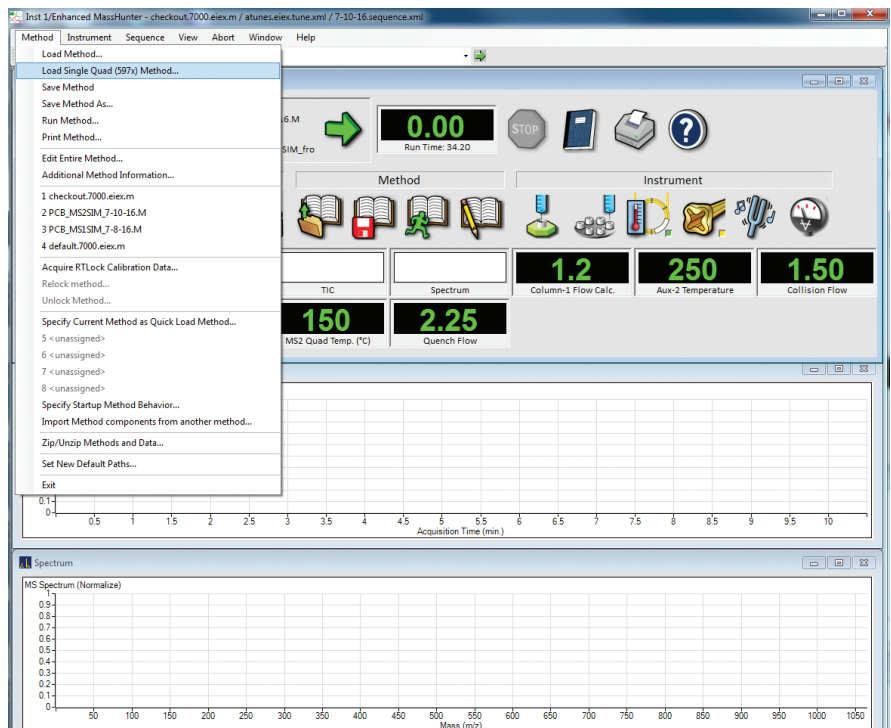


Figure 3. Load Single Quad (597x) Method is selected under the Method tab to choose the desired method.

Method Resolution and Review

Upon loading the method, a text screen appears that lists the differences between the new method and the existing configuration of the triple quad. In the example shown in Figure 4, the method calls for a 5 μ L syringe, but the GC is configured for a 10 μ L syringe. In the method editor screens, change items as required so that the method and GC configuration match. The syringe size is changed under Configuration/ALS (Automated Liquid Sampler). Another possibility is that the inlet position for the triple quad may need to be changed from front to back by accessing the Inlets screen.

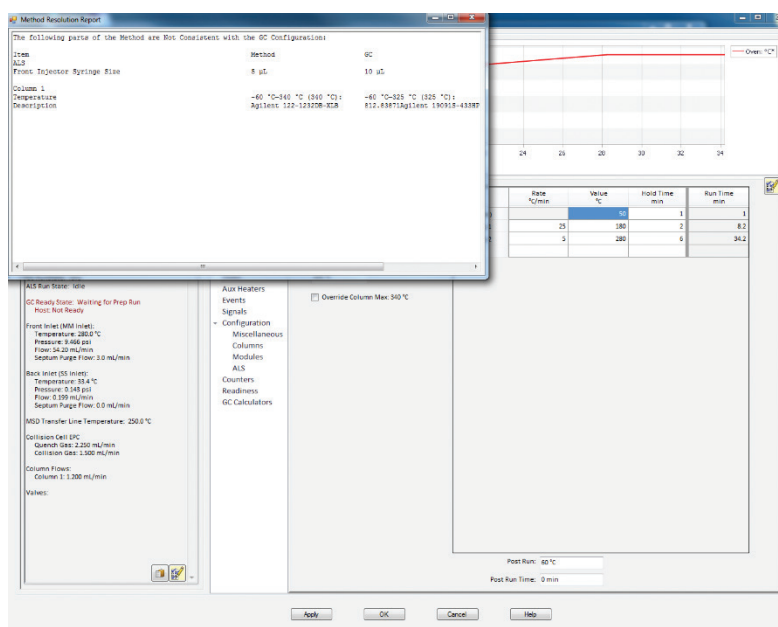


Figure 4. Method Resolution text screen showing that the syringe size is different in the method that was loaded compared to that configured on the triple quad.

Figure 5 shows the MassHunter acquisition home screen with the new method loaded. Next, the source temperature will need to be changed to the correct value, in our example 320 °C and not 230 °C, as was the setting in the previously loaded method.

To do this, open the MS Method Editor (Figure 6) by clicking the quadrupole icon in the home screen. Parameters from the SIM method that were copied from the single quad and loaded on the triple quad appear. Load the desired triple quad tune file, and enter the source temperature to be used for the method.

Save the method, and review all parameters to ensure that they match the original method from the single quad.

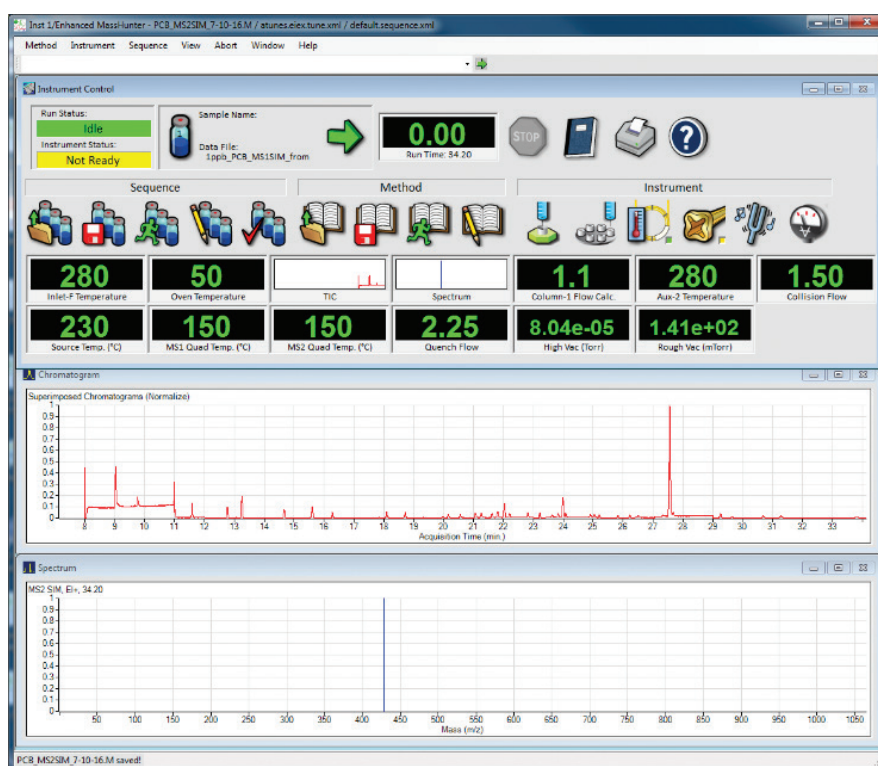


Figure 5. Agilent MassHunter acquisition home screen with a new method loaded.

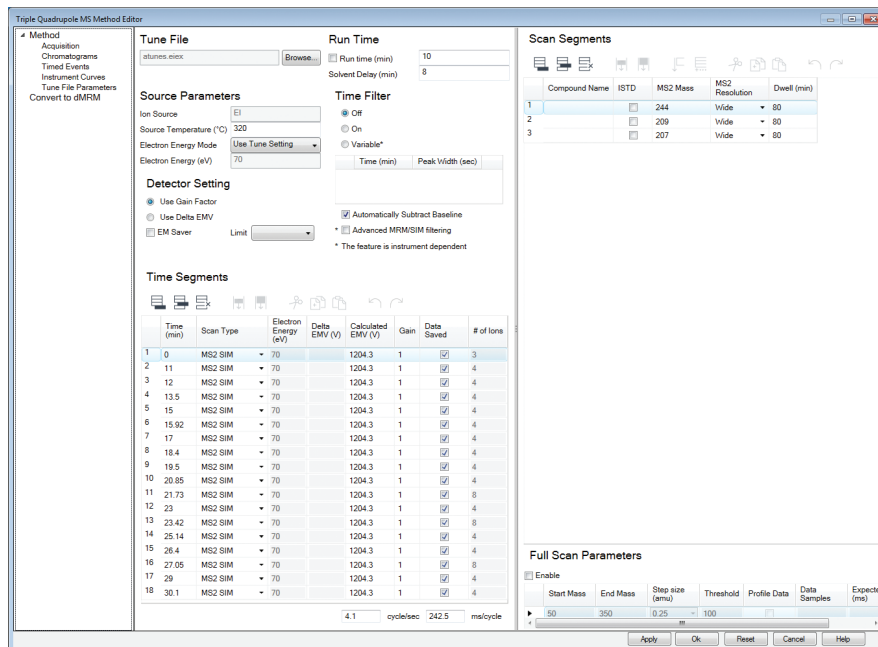


Figure 6. Triple Quadrupole MS Method Editor screen.

If ion sources differ between instruments, a method that was created using one type of source can still be run using another source. However, note that gain adjustments, such as the need to decrease gain, may be necessary to avoid detector saturation of the high efficiency source (HES) as compared with other sources. It is likely that less sample may need to be injected when using the HES versus other sources for the same reason. When using different GC inlets or inlet liners between instruments, the injection parameters may need to be re-optimized if not already determined for a particular inlet and GC liner combination.

Match Retention Times Between Instruments Using Retention Time Locking (RTL)

It may be useful to maintain analyte retention times between analytical instruments. When columns of the same dimensions are used on two or more different Agilent instruments in the laboratory, RTL allows a very close match of retention times. This is accomplished by making approximately five injections at different inlet pressures, developing a retention time (RT) versus column flow calibration curve, and then making the appropriate adjustment to the inlet pressure to create a locked method. This is a fully automated process in MassHunter software, and Agilent publication 5989-8574EN describes the automated process in detail for Agilent ChemStation software. RTL is normally performed after trimming the column or installing a method on a new or different instrument.

Increase Productivity by Using the Triple Quad for SIM and Scan

MassHunter data analysis software handles data files created either on a single quad or triple quad instrument, so there is no need to use a different data analysis program for each platform.

Figure 7 shows the TIC for 28 PCB congeners analyzed by the SIM method on an Agilent 5977B Single Quadrupole GC/MSD along with the TIC obtained using the same method loaded and run on the Agilent 7000D Triple Quadrupole GC/MS system. The method was run on the 7000D Triple Quadrupole GC/MS, then relocked to a RT of 30.71 minutes for PCB209.

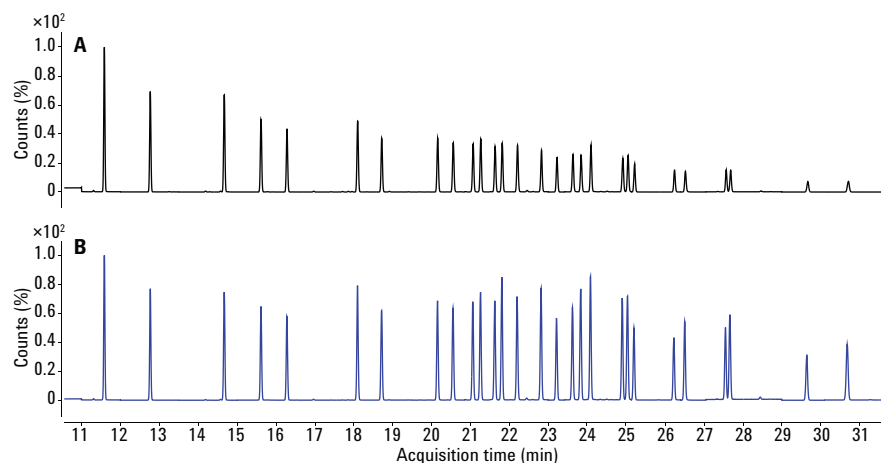


Figure 7. TIC for 28 PCB congeners analyzed by the SIM method on an Agilent 5977B Single Quadrupole GC/MSD (A) with the TIC obtained using the same method loaded and run on an Agilent 7000D Triple Quadrupole GC/MS system (B).

Conclusion

Transferring analytical methods from a single quadrupole GC/MSD system to a triple quadrupole GC/MS/MS instrument is straightforward, and increases laboratory productivity by distributing the workload. Agilent MassHunter data analysis software handles files acquired by both systems, and eliminates the need for a separate data analysis program.

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