MassHunter Forensic Toxicology Triggered MRM Database and Library

Quick Start Guide

For Forensic Use

Agilent Technologies

What is the MassHunter Forensic Toxicology Triggered MRM Database and Library?

The MassHunter Forensic Toxicology Triggered MRM Database and Library contains more than 2800 analytes with up to 10 transitions. This database, when used with the *Familiarization Guide* and *Method Setup Guide*, helps you set up your unique Forensic Toxicology MRM, dMRM, and tMRM analyses by simplifying the method development steps.

Use MRM methods to quickly screen and quantitate a limited number of compounds without prior knowledge of retention times. If you need to maximize instrument dwell time for increased sensitivity, find the retention times (RT) and RT windows, and then update an MRM method to a dMRM method.

Use Dynamic MRM (dMRM) methods to screen and quantitate hundreds of compounds within one run.

If more specificity is required, add secondary transitions to some, or all, of the compounds in a dMRM method to create a Triggered MRM (tMRM) method. Triggered MRM is a data-dependent acquisition mode that lets you collect up to ten MRM transitions per compound. If certain criteria are met, including user-set abundance levels of the Primary MRMs, then the secondary MRMs are acquired. Triggered MRM is particularly beneficial for isobaric compounds and compounds affected by matrix interference.

Each compound in the MassHunter Forensic Toxicology Triggered MRM Database and Library can have multiple primary MRMs, and up to two of these primary MRMs can be specified as Trigger MRMs. Each compound can also have multiple secondary transitions. The database can contain up to ten MRM transitions for each precursor ion. All transitions with the same Compound Name belong to the same compound.
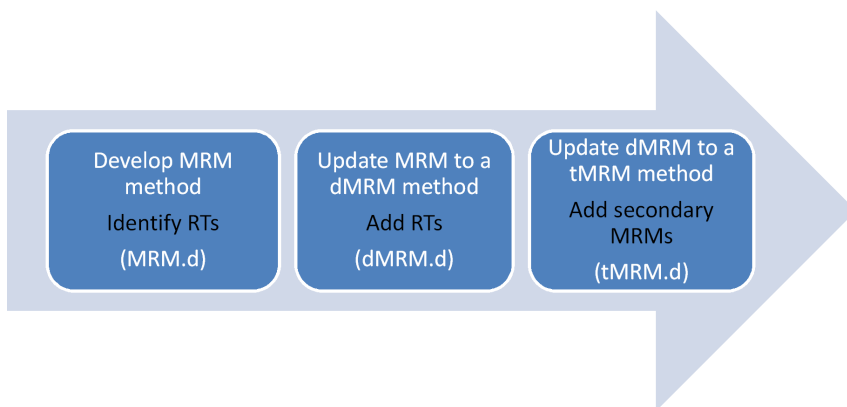
For each analyte, the database also contains optimized fragmentor and collision energy settings for Agilent 6400 Series Triple Quadrupole LC/MS instruments.

Methods can be developed simply by importing target compounds from the database to the MassHunter Data Acquisition program. The database lookup library also includes tMRM reference spectra for compounds in the Forensic Toxicology Comprehensive Test Mix, sold separately.

Workflow Overview

The *MassHunter MRM/dMRM/tMRM Database Familiarization Guide* uses example data and familiarization exercises to illustrate typical MRM, dMRM, and tMRM workflows.

Figure 1 summarizes the workflow, which includes incremental method development from MRM, over to dynamic MRM (dMRM) to triggered MRM (tMRM) methods, including identification of retention times (RT), Trigger parameters, and secondary transitions.

Figure 1 tMRM Method Development Workflow for single standard mix

Single Standard Mix Workflow

The workflow to analyze a single standard mix is:

1 Use the database to create the MRM method for the primary transitions.

2 Establish the Retention Times, and then create a new method using the **Update DMRM Method** command. Save as a DMRM method.

3 Check the dMRM editor for any overlaps and adjust accordingly the dwell time settings and or the Retention Time windows.

4 Acquire data to make sure that the dMRM method is valid.

5 Save the dMRM method as a tMRM method.

6 Add the secondary transitions.

After you have set up methods to analyze a single standard mix, you can adapt the same procedures for your unique multi-component analysis.

Multiple Standard Mix Workflow

To develop a method to analyze multiple standard mixes in one analytical run:

1 Optimize each tMRM method for each standard mix separately. Use the same LC chromatographic method.

2 Combine these tMRM methods. (Copy and paste transition tables of each standard mix tMRM method into a single tMRM method.)

3 Adjust the parameters for the overlapping tMRM transitions for compounds that co-elute.

For ease of use, optimize no more than 50 compounds at a time in each **MRM -> dMRM -> tMRM** workflow. Refer to the *Method Setup Guide* for more information.

Where to find more information

These publications are available on the product installation media and are also installed on your computer.

MRM/dMRM/tMRM Database *Familiarization Guide* Use this guide to learn how to use your tMRM database. The exercises in this guide are based on the LC TOF/Q-TOF/QQQ Pesticide Checkout Mix (optional, sold separately). The example familiarization files are installed with the database.

Method Setup Guide The *Method Setup Guide* lets you easily set up methods for your analysis, based on the Comprehensive Test Mix (sold separately). It also contains instructions to optimize LC and MS acquisition parameters for the Comprehensive Test Mix. Use the instructions in this guide to set up methods for your own samples.

Agilent 6400 Series Triple Quadrupole LC/MS *Familiarization Guide* and *Concepts Guide* Use these guides to learn more about tMRM acquisition.

For more information on Agilent products, go to http://www.agilent.com.

Product Content

Your MassHunter Forensic Toxicology Triggered MRM Database and Library product contains these parts:

- **MassHunter Forensic Toxicology Triggered MRM Database and Library** files
  - MassHunter Forensic Toxicology Triggered MRM Database and Library (**ForTox_TriggeredMRM_B0601**)
  - MassHunter Forensic Toxicology Test Mix Triggered MRM Database (**ForTox_TestMix_TriggeredMRM_B0601**) for use with separately purchased Comprehensive Test Mix
  - Forensic Toxicology Triggered MRM database compound listing
  - *MassHunter Forensic Toxicology Triggered MRM Database and Library Quick Start Guide*
  - *MassHunter Forensic Toxicology Triggered MRM Database and Library Method Setup Guide*
- **Checkout Mix** familiarization files
  - *MassHunter MRM/dMRM/tMRM Database Familiarization Guide*
  - Checkout Mix database and library (**Checkout_TestMix_MRM**)
  - Checkout Mix example method files
  - Checkout Mix example data files
  - Checkout Mix example reports

All user guides are available on the installation media.

Installation

Before you begin

- Check that the following programs are properly installed:
  - MassHunter Data Acquisition B.08.00 or higher
  - MassHunter Quantitative Analysis B.07.01 or higher.
  - MassHunter Qualitative Analysis B.07.01 or higher

Install the MassHunter Forensic Toxicology Triggered MRM Database and Library

1 Insert the installation media into the installation drive.

   If the installation screen does not open, double-click **Start.bat** on the installation media.

2 On the **Installation** page, click **Install**.

3 Click **Complete** to install all databases and supplemental files.

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In This Guide

This Quick Start Guide describes the MassHunter Forensic Toxicology Triggered MRM Database and Library.

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