MassHunter Metabolomics Dynamic MRM Database and Method

For Research Use Only. Not for use in diagnostic procedures.

Quick Start Guide

What is the MassHunter Metabolomics Dynamic MRM Database and Method?

The G6412AA Metabolomics dMRM Database offers a comprehensive solution for targeted analysis of central carbon metabolites. The optimized method provides robust chromatography for over 215 metabolites, including challenging compounds across diverse chemical classes.

The Metabolomics dMRM Database delivers confirmed transitions and retention times for routine metabolite analysis on a triple quadrupole LC/MS system.

Agilent Technologies

This database, when used with the procedures in this guide, helps you set up your unique Metabolomics dMRM analysis by simplifying the method development steps.

Many chromatographic techniques, including reverse phase, normal phase, and HILIC, suffer from poor selectivity, reproducibility, or lack of retention of polar metabolites. The ion-pairing based reverse phase (IP-RP) chromatographic method described here was developed to address these challenges.

The ion-pairing LC/MS method included with the MassHunter Metabolomics Dynamic MRM Database and Method simultaneously analyzes many metabolite functional classes, including amino acids, citric acid cycle intermediates and other carboxylic acids, nucleobases, nucleosides, phosphosugars, and fatty acids.

To provide highly robust and reproducible analysis, the LC/MS method uses a combination of valve-switching and a ternary solvent system to perform on-line back-flushing of the analytical and guard columns after each run. This configuration clears potential matrix contaminants from the column inlet and enables consistent high-quality peak shapes and superior long-term retention time stability.

The MassHunter Metabolomics Dynamic MRM Database and Method has been optimized to provide all of the instrument operating parameters for turn-key data acquisition of over 215 metabolites. The primary transitions, retention times, retention time windows, collision energies, and fragmentor voltages included in the database were developed by Adam Rosebrock and Amy Caudy (University of Toronto), leaders in the metabolomics field, and then validated and curated by Agilent Technologies. Authentic chemical standards were extensively analyzed to optimize these parameters to generate the highest quality results.

The MassHunter Metabolomics Dynamic MRM Database and Method helps minimize method development time for your Metabolomics analysis when used with Agilent recommended LC/MS configuration and accessories.

Each compound in the database includes one or more unique precursor/product ion transitions and their optimized fragmentor and collision energy settings for Agilent 6460/6470 (non-iFunnel) Triple Quadrupole LC/MS instruments only, with an Agilent JetStream Technology source.

The provided optimized acquisition and data analysis methods can be used to immediately generate results. Custom methods can be easily developed by importing transitions and retention times for target compounds from the database into the MassHunter Data Acquisition program.

The detailed *Analysis Guide* and *Method Setup Guide*, along with the included data acquisition and analysis methods, provide instructions from sample preparation to customer report.

Dynamic MRM uses retention-time scheduling of MRM transitions to allow more metabolites to be analyzed in a single run without sacrificing data quality. See the dMRM technical note (p/n 5991-6482), or the Agilent 6400 Series Triple Quadrupole LC/MS *Familiarization Guide* or *Concepts Guide* for more information.

Workflow Overview

The MassHunter Metabolomics Dynamic MRM Database and Method contains optimized acquisition parameters for a set number of endogenous cellular metabolites. However, you can use the Metabolomics dMRM Database with MassHunter Acquisition program to customize the included methods to fit your unique analysis or to create new database entries.

The *MassHunter MRM Database Familiarization Guide* uses example data and familiarization exercises to illustrate typical MRM, dMRM, and tMRM workflows. Figure 1 summarizes the workflow to use with the MassHunter Metabolomics Dynamic MRM Database and Method.
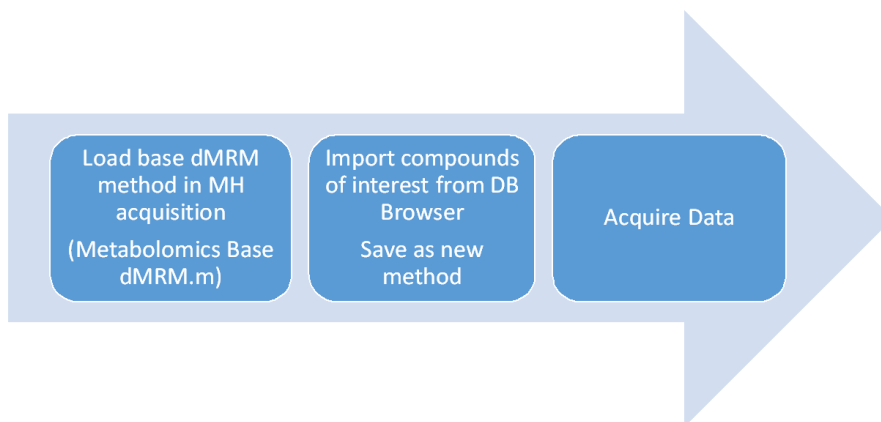
Figure 1   Method Development workflow for Metabolomics Dynamic MRM Database and Method

Product Content

Your MassHunter Metabolomics Dynamic MRM Database and Method product contains these parts:

- **MassHunter Metabolomics Dynamic MRM Database and Method** files
  - Metabolomics dMRM Database (**QQQ_Metabolomics_dMRM_DB**)
  - Metabolomics dMRM Database compound listing
  - *MassHunter Metabolomics Dynamic MRM Database and Method Quick Start Guide*
  - *MassHunter Metabolomics Dynamic MRM Database and Method Method Setup Guide*
  - *MassHunter Metabolomics Dynamic MRM Database and Method Analysis Guide*
- **MassHunter Metabolomics Dynamic MRM Database and Method method files**
  - Metabolomics Base dMRM.m
  - Metabolomics dMRM QuantMethod.m
- **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.

Where to find more information

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

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 Metabolomics Dynamic MRM Database and Method

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.

This page intentionally left blank.

www.agilent.com

In This Guide

This Quick Start Guide describes the MassHunter Metabolomics Dynamic MRM Database and Method.

For Research Use Only. Not for use in diagnostic procedures.

G6412-90000

Agilent Technologies