



MassHunter Mycotoxins and Related Metabolites PCDL

Quick Start Guide

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What is the MassHunter Mycotoxins and Related Metabolites PCDL?

The MassHunter Mycotoxins and Related Metabolites Personal Compound Database and Library (PCDL) lets you screen mycotoxins along with related metabolites in a single LC/MS analysis.

Mycotoxins are toxic secondary metabolites of fungi. They can be found in a variety of food and feed as well as indoor air.



What is the MassHunter Mycotoxins and Related Metabolites PCDL?

Hundreds of mycotoxins and secondary fungal metabolites have so far been identified. About a dozen of these compounds are considered to be a major health risk.

The MassHunter Mycotoxins and Related Metabolites PCDL contains data for compounds that are regulated in food and feed. Analyses of such compounds are essential to ensure food safety in products such as cereals, nuts, fruits, spices, wine, and coffee.

The MassHunter Mycotoxins and Related Metabolites PCDL also includes bacterial metabolites. Bacterial metabolites are relevant to the analysis of environmental samples, such as indoor air and dust.

The Mycotoxins and Related Metabolites PCDL, together with an Agilent TOF or QTOF LC/MS, can be an appropriate supplement to single analyte or analyte-group detection methods to learn about mycotoxins in food and environmental samples.

The MassHunter Mycotoxins and Related Metabolites PCDL lets you screen over 450 analytes with accurate mass database and/or perform a compound library search for over 300 compounds measured with common precursor ions, including ammonium and formate adducts.

Working with your MassHunter PCDL

The MassHunter Mycotoxins and Related Metabolites PCDL as provided by Agilent cannot be changed. You can use the MassHunter Mycotoxins and Related Metabolites PCDL as is to search for compounds. Or you can use the MassHunter Mycotoxins and Related Metabolites PCDL as a master template to create a custom user PCDL. Use MassHunter PCDL Manager with your custom user PCDL to:

- Add, remove and edit the compounds to meet the specific needs of your laboratory and your analyses.
- Add retention times based on standards and/or retention times for compounds you analyze.
- Add your own spectra.

With MassHunter Qualitative Analysis B.07.00 and higher, you can:

- Run a database search or use the Find by Formula algorithm to identify compounds and then send the MS/MS spectra to your custom PCDL.
- Filter spectral noise and correct the product ions to their theoretical accurate mass.

The high mass accuracy of the Agilent tandem quadrupole time-of-flight (Q-TOF) LC/MS instrument provides the capability to screen all compounds in the library that are detected by their exact mass and retention time (if known). Searching the library can then identify the compounds found by comparison to their accurate product ion mass spectra.

Terminology Note

A **PCD** is an accurate mass compound database, which may or may not contain retention times. A **PCDL** contains both an accurate mass compound database and an MS/MS accurate mass spectral database, which is often referred to as a spectral library or library. Agilent provides the MassHunter Mycotoxins and Related Metabolites PCDL data in PCDL format only.

Product Content

Your PCDL product includes these parts:

- **MassHunter Personal Compound Database and Library Manager** software and *Quick Start Guide*
- **MassHunter Mycotoxins and Related Metabolites PCDL** files
 - MassHunter Mycotoxins and Related Metabolites PCDL (**Mycotoxins_AM_PCDL.cdb**)
 - *MassHunter Mycotoxins and Related Metabolites PCDL Quick Start Guide*
 - MassHunter Mycotoxins and Related Metabolites PCDL compound listing
 - technical notes and application notes
- **Checkout Mix** familiarization files
 - *MassHunter PCDL for Qualitative Analysis Familiarization Guide*
 - Checkout Mix PCDL (**Checkout_TestMix_Std.cdb**)
 - Checkout Mix example method files
 - Checkout Mix example data files
 - Checkout Mix example reports

All user guides are available on the installation media.

To acquire data for use with the *MassHunter PCDL for Quantitative Analysis Familiarization Guide*, you also need these parts. You can also use the included Checkout Mix example data to do the familiarization exercises instead.

- ZORBAX LC Column, Eclipse Plus C18, 2.1 mm × 100 mm, 1.8 µm (p/n 959758-902)
- LC TOF/QTOF/QQQ Pesticide Checkout Test Mix (p/n 5190-0469)

Where to find more information

Go to <http://www.agilent.com/> for the most current information on Agilent products.

Installation

Before you begin

- 1 Check that the following programs are properly installed:
 - MassHunter Data Acquisition B.05.00 or higher (if you plan to run the Checkout Mix to acquire data for familiarization exercises)
 - MassHunter Qualitative Analysis B.07.00 or higher
- 2 Install the MassHunter Personal Compound Database and Library Manager (B.07.00 SP1 or higher). Refer to the *MassHunter Personal Compound Database and Library Manager Quick Start Guide*.

Install the MassHunter PCDL

- 1 Place the PCDL disc in your computer drive.

The Contents and Information screen appears. If it does not, double-click **Start.htm** on the installation disc.
- 2 In the Contents and Information screen:
 - a Click **MassHunter Mycotoxins and Related Metabolites PCDL Installation**.
 - b Follow the on-screen instructions to install the PCDL files.

The installation can take from 5 to 10 minutes to complete.
- 3 If you want to run the Checkout Mix or do the familiarization exercises, install the MassHunter PCDL Familiarization Files.

Refer to the *MassHunter PCDL for Qualitative Analysis Familiarization Guide* for details.

Searching and managing the PCDL

To identify compounds and spectrum peaks using MassHunter Qualitative Analysis

Table 1 lists ways to use the MassHunter Qualitative Analysis program to search the PCDL to identify compounds and spectrum peaks.

Table 1 Identifying Compounds

If you want to...	Click...	Refer to online Help topic
Find compounds using the Find by Formula algorithm restricted to formulas within a PCDL (with or without retention times)	Find Compounds by Formula > Find by Formula-Options	Find compounds by formula
Search the database based on information from MS Spectra (with or without retention times)	Identify Compound > Search Database for Compounds	Search database for a compound.
Identify compounds from MS spectrum peaks (with or without retention times)	Identify Compound > Search Database for Spectrum Peaks.	Search database from a spectrum
Search the spectral library based on information from MS/MS spectra	Identify Compound > Search Library for Compounds.	Search accurate mass library for compounds. Search unit mass library for compounds.
Identify compounds from MS/MS spectra	Identify > Search Library for Spectra.	Search accurate mass library for spectra Search unit mass library for spectra

Retention times as a search criterion

- Use retention times with MS data as a search criterion:
 - as **not required** (non-targeted screen)
 - as **optional** providing a targeted and non-targeted screen
 - **required** (targeted screen only)

Managing the PCDL content with PCDL Manager

Use the MassHunter Personal Compound Database and Library (PCDL) Manager to manage the content of your PCDL:

- Create and edit custom PCDLs, including adding proprietary compounds, retention times, and MS/MS spectra.
- Search, browse, and store MS/MS centroid spectra acquired on a Q-TOF instrument.
- Search for compounds in PCDLs, using text, formula, accurate mass, and retention time (optional or required).
- Import mass lists with retention time in the form of a .txt or .csv file.
- Send spectra to your customized PCDL directly from the Qualitative Analysis program to create your own custom library. Choose from options to filter spectral noise and/or to correct the product ions to their theoretical accurate mass.
- Load spectra from either a .CEF file or by copy-and-pasting mass spectra from MassHunter Qualitative Analysis software and search for those spectra in the current PCDL.
- Do private, on-site searches, which keep intellectual property safe.
- Link to web sites for more information on many compounds.

For more information, see the *MassHunter Personal Compound Database and Library Manager Quick Start Guide* and PCDL Manager online Help.

In This Guide

This Quick Start Guide provides an overview of the MassHunter Mycotoxins and Related Metabolites PCDL.

This guide is valid for the B.07.00 revision or higher of the MassHunter Mycotoxins and Related Metabolites PCDL, until superseded.

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Revision A, April 2015



G5883-90000