MassHunter Water Screening PCDL

Quick Start Guide

What is the MassHunter Water Screening PCDL?

The MassHunter Water Screening Personal Compound Database and Library (PCDL) lets you screen a wide range of environmental contaminants in a single LC/MS analysis.

Harmful chemicals that threaten our ecosystem and public health are released to the environment through human, agriculture, and industrial activities. Government regulations exist to closely monitor these contaminants. But toxic effects are often seen only after years of contaminant accumulation in the environment, so the list of monitored compounds constantly changes.

Agilent Technologies

The MassHunter Water Screening PCDL contains data for compounds that are regulated in water bodies across many different geographic regions. Analyses of such compounds are essential to ensure drinking water safety.

The MassHunter Water Screening PCDL includes:

- contaminants of emerging concern, such as pharmaceuticals and personal care products (PPCPs) and their transformation products
- pesticides, veterinary drugs, polar metabolites, cyanotoxins and industrial chemicals and their metabolites and transformation products
- compounds that are present in major water regulations and region-specific lists

Regulations and region-specific lists are included as class tags to allow you to easily narrow down your screening applications. The results can be used to create specific PCDL subsets for your unique analysis criteria. The included regulations are:

- EU Water Framework Directive (EU WFD)
- US Environmental Protection Agency (EPA 521, EPA 535, EPA 539, EPA 1694, EPA 1698, EPA 1699 and EPA Draft CCL 4)
- Chinese region specific lists and regulations (CN-NY-193, CN-NY-235, CN-NY-265, CN-NY-560, Chinese National Food Safety Standard: Maximum Residue Limits for Pesticides in food (GB 2763-2014); CN-EPA screening list, CN-antibiotics list and CN-CDC survey list)
- Japanese region specific lists and regulations:
  - Japanese Positive List System for Agricultural Chemical Residues in Foods (JPL)
  - Japan Drinking Water Quality Standard (JDWQS)

The MassHunter Water Screening PCDL contains compounds that are detectable at trace levels by LC/MS and LC/MS/MS analyses.

For your convenience, a separate PCDL that contains all the compounds from EPA Method 1699 is included. EPA Method 1699 is important to water screening. This method uses HRGC/HRMS to detect pesticides in water, soil, sediment, biosolids and tissue. The PCDL contains some compounds that are compatible with LC-HRMS.

The MassHunter Water Screening 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 contaminants in water.

The MassHunter Water Screening PCDL lets you screen over 1400 analytes with accurate mass database and/or perform a compound library search for over 1000 compounds measured with common precursor ions.

Working with your MassHunter PCDL

You can use the MassHunter Water Screening PCDL as is to search for compounds. Or you can use the MassHunter Water Screening PCDL as a template to create a custom user PCDL in PCDL Manager. But you cannot change the MassHunter Water Screening PCDL as provided by Agilent.

Refer to the *MassHunter PCDL Manager Quick Start Guide* to learn how to create a custom PCDL and:

- 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 time-of-flight (TOF or 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 **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. A database search searches the compound database for precursor ion formula matches. A library search searches the spectral MS/MS library for fragment ion matches.

Product Content

Your PCDL product includes these parts:

- **MassHunter Personal Compound Database and Library Manager** software and *Quick Start Guide*
- **MassHunter Water Screening PCDL** files
  - MassHunter Water Screening PCDL (**Water_AM_PCDL.cdb**)
  - MassHunter EPA Method 1699 Specific Water Screening PCDL (**EPA1699_Water_AM_PCDL.cdb**)
  - *MassHunter Water Screening PCDL Quick Start Guide*
  - MassHunter Water Screening 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.

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 program is properly installed:

- 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 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 PCDLs and supplemental files.

The complete installation can take from 5 to 10 minutes to complete.

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.

To run these algorithms, use the commands from the menu bar. To review the parameters for the algorithms, use the Method Editor window.

Table 1 Identifying Features

If you want to edit the method to..	Select this Method Editor section	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 MS spectral information from compound features (with or without retention times)	**Identify Compounds > Search Database**	Search database for a compound.
Identify compounds from MS spectrum peaks (with or without retention times)	**Identify Compounds > Search Database**	Search database from a spectrum
Search the spectral library based on MS/MS information from compound features.	**Identify Compounds > Search Library**	Search accurate mass library for compounds. Search unit mass library for compounds.
Identify compounds from MS/MS spectra	**Identify Compounds > Search Library**	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 custom PCDLs, specific to your analysis by searching for compound class groups and regulation tags as well as individual compound searches using compound name, formula, mass, CAS registry number or IUPAC name.
- 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.

www.agilent.com

In This Guide

This Quick Start Guide provides an overview of the MassHunter Water Screening PCDL.

This guide is valid for the B.07.00 revision or higher of the MassHunter Water Screening PCDL, until superseded.

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