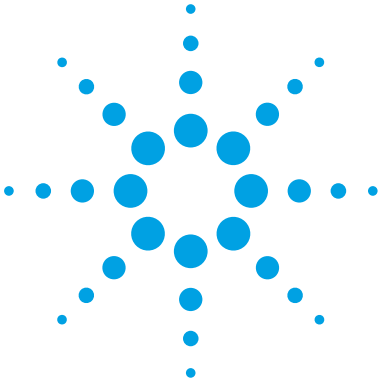

MassHunter Veterinary Drugs PCDL

Quick Start Guide

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Agilent Technologies

What is the MassHunter Veterinary Drugs PCDL?

The MassHunter Veterinary Drugs Personal Compound Database and Library (PCDL) lets you screen 2100 analytes with accurate mass database and/or perform a compound library search for over 1500 compounds.

Veterinary drugs are used as a means to prevent diseases or promote rapid growth in livestock, resulting in drug residues being present in the animal meat and other organs. Several hundred veterinary drugs are available and the levels of veterinary drugs in meat and other foods are regulated with tolerance levels that vary significantly from one drug to another.

The veterinary drug PCDL with accurate mass high resolution time-of-flight (TOF) mass spectrometers enables the analysis of both targets and unknowns. Full-spectrum data acquisition ensures that signals from all ionizing compounds in the sample will be captured. The MassHunter Veterinary Drugs PCDL contains data for compounds that are regulated across many different geographic regions. Analysis of such compounds is essential to ensure food safety.

The MassHunter Veterinary Drugs PCDL includes:

- veterinary drugs, equine drugs, pesticides, and their metabolites and transformation products
- compounds that are present in 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 and region-specific lists are:

- USDA Anal Bioanal Chem 2014

  This novel method streamlines sample preparation, as described in "Validation of a streamlined multiclass, multiresidue method for determination of veterinary drug residues in bovine muscle by liquid chromatography-tandem mass spectrometry"*.
- US Environmental Protection Agency (EPA 521, EPA 535)

* Schneider, M.J., Lehotay, S.J., Lightfield, A.R., *Analytical and Bioanalytical Chemistry (2014)*

- 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, and CN-antibiotics list)
- Japanese Positive List System for Agricultural Chemical Residues in Foods (JPL)

The Agilent application note “Analysis of 122 Veterinary Drugs in Meat Using All Ions MS/MS with an Agilent 1290 / 6545 UHPLC-Q-TOF System” (publication number 5991-6651EN) describes the use of Agilent instruments to replicate the method “USDA Anal Bioanal Chem 2014”.

The accurate mass retention time PCDL (**VetDrugs_AMRT_PCDL**) included with the MassHunter Veterinary Drugs PCDL contains retention times for 104 compounds acquired using the method described in application note “Analysis of 122 Veterinary Drugs in Meat Using All Ions MS/MS with an Agilent 1290/6545 UHPLC Q-TOF System”.

The guide “Conditions for the Estimation of Retention Times for VetDrug_AMRT_PCDL” (**VetDrugs_AMRT_PCDL_System Configuration Guide.pdf**) describes the instrument setup used to collect the 104 retention times found in the **VetDrug_AMRT_PCDL** database.

The MassHunter Veterinary Drugs PCDL, together with an Agilent TOF or QTOF LC/MS, can be an appropriate supplement to single analyte or analyte-group detection methods to analyze veterinary drugs at trace level.

Working with your MassHunter PCDL

You can use the MassHunter Veterinary Drugs PCDL as is to search for compounds. Or you can use the MassHunter Veterinary Drugs PCDL as a template to create a custom user PCDL in PCDL Manager. But you cannot change the MassHunter Veterinary Drugs 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 generated experimentally 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 product ion matches.

Product Content

Your PCDL product includes these parts:

- **MassHunter Personal Compound Database and Library Manager** software and *Quick Start Guide*
- **MassHunter Veterinary Drugs PCDL** files
  - MassHunter Veterinary Drugs PCDL (**VetDrugs_AM_PCDL.cdb**)
  - **VetDrugs_AMRT_PCDL.cdb (**104 retention times acquired using the method described in the application note “Analysis of 122 Veterinary Drugs in Meat Using All Ions MS/MS with an Agilent 1290/6545 UHPLC Q-TOF System”, which is based on the method “USDA Anal Bioanal Chem 2014”)
  - **VetDrugs_Foods_AM_PCDL.cdb** (food safety-related compounds only)
  - **VetDrugs_Equine_AM_PCDL.cdb** (equine drugs only)
  - *MassHunter Veterinary Drugs PCDL Quick Start Guide*
  - MassHunter Veterinary Drugs 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

Where to find more information

All user guides are available on the installation media and are installed on your computer by default.

Application Notes and Publications Find out about your PCDL analysis in the application notes and publications included on the installation media.

MassHunter PCDL for Qualitative Analysis Familiarization Guide Use this guide to learn how to use your PCDL. 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 PCDL.

Method Setup Guide The *Method Setup Guide* lets you easily set up methods for your analysis. It also contains instructions to optimize LC and MS acquisition parameters for the analysis of veterinary drugs. Use the instructions in this guide to set up methods for your own samples.

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

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 several 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 describes how to use the MassHunter Veterinary Drugs PCDL.

This guide is valid for the B.07.01 revision or higher of the MassHunter Veterinary Drugs PCDL, until superseded.

Revision A, August 2016

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