



MassHunter Extractables and Leachables PCDL

Quick Start Guide

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What is the MassHunter Extractables and Leachables PCDL?

The MassHunter Extractables and Leachables Personal Compound Database and Library (PCDL) lets you screen over 1000 analytes with accurate mass database and/or perform a compound library search for over 350 compounds.

Manufacturers of pharmaceuticals, drug packaging components, medical devices and packaged food products are under growing pressure to perform sensitive and accurate analytical studies on extractable and leachable (E&L) compounds. These E&L compounds have the potential to cause undesirable effects on efficacy of drugs and the quality of food. Agilent offers a full range



What is the MassHunter Extractables and Leachables PCDL?

of complementary techniques and software tools for the analysis of small and large molecule E&Ls (volatiles, semi-volatiles, non-volatiles, metals, and oligomeric compounds), including the E&L PCDL for analysis of semi-volatiles and non-volatiles by LC/TOF or Q-TOF.

This product is intended for the detection and identification of potential extractable and leachable compounds that may be found in components of food and drug packaging and medical devices as required by Food, Drug and Cosmetic Act Section 501(a)(3) and Section 502; 21 CFR Part 211.94 (a); and FDA Guidance for Industry Container Closure Systems for Packaging Human Drugs and Biologics (1999). This product is not intended for use in diagnosing, preventing, or treating a human disease.

The MassHunter Extractables and Leachables PCDL includes:

- stabilizers, accelerators, intermediates, residual monomers, phthalates, lubricants, slip agents, photoinitiators, plasticizers, dyes and cosmetic additives
- antioxidants, UV stabilizers and their breakdown or degradation products
- food packaging contaminants and printing ink components and their breakdown or degradation products
- PFCs, PAHs, nitrosamines and silicones

Regulations, region-specific lists, and E&L working group 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:

- US Environmental Protection Agency (EPA 606, EPA 8061A)
- European Union regulations (SWISS Ordinance (SR 817.023.21), (EC) No. 1272/2008 and EU 2005/84/EC)
- ELSIE (The Extractables and Leachables Safety Information Exchange Database)
- PDA JPST RI^{*}. For these entries the risk index (RI) and Cramer class are also specified.
- Agilent Application notes (5991-6348EN; 5990-9510EN; 5991-3441EN and 5991-5490EN)

* Dennis Jenke and Tage Carlson, "A compilation of safety impact information for extractables associated with materials used in pharmaceutical packaging, delivery, administration, and manufacturing systems", *PDA Journal of Pharmaceutical Science and Technology* (2014)

The guide “Conditions for the Estimation of Retention Times for E_n_L_AMRT_PCDL” ([E_n_L_AMRT_PCDL_System Configuration Guide.pdf](#)) describes the LC setup used to collect the retention times for 129 of the compounds found in the **E_n_L_AMRT_PCDL** database.

A subset PCDL (**E_n_L_Dyes_AM_PCDL.cdb**) that contains dyes and compounds used in the manufacturing of dyes is also included for your convenience.

Some compounds, such as PAHs, are only amenable via LC/MS using an APCI source. The following technique tags are included for your convenience.

- APCI amenable
- APPI amenable
- GCMS amenable
- LCMS amenable

Note that all compounds in the **E_n_L_AM_PCDL** are LCMS amenable. Any compound without a technique tag is LCMS and ESI amenable. Compounds with more than one technique tag can be measured using any of the tagged technique. For example, compounds with both the “GCMS amenable” and “LCMS amenable” tags can be measured using either techniques.

The MassHunter Extractables and Leachables PCDL, together with an Agilent TOF or QTOF LC/MS, can be an appropriate supplement to single analyte or analyte-group detection methods to identify extractable and leachable compounds at trace levels.

Working with your MassHunter PCDL

You can use the MassHunter Extractables and Leachables PCDL as is to search for compounds. Or you can use the MassHunter Extractables and Leachables PCDL as a template to create a custom user PCDL in PCDL Manager. But you cannot change the MassHunter Extractables and Leachables 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 Extractables and Leachables PCDL** files
 - MassHunter Extractables and Leachables PCDL (**E_n_L_AM_PCDL.cdb**)
 - **E_n_L_AMRT_PCDL** (compounds found in “Conditions for the Estimation of Retention Times for E_n_L_AMRT_PCDL” (**E_n_L_AMRT_PCDL_System Configuration Guide.pdf**))
 - **E_n_L_Dyes_AM_PCDL.cdb** (dye compounds only)
 - *MassHunter Extractables and Leachables PCDL Quick Start Guide*
 - MassHunter Extractables and Leachables 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.

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.

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.

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www.agilent.com

In This Guide

This Quick Start Guide describes how to use the MassHunter Extractables and Leachables PCDL.

This guide is valid for the B.07.00 revision or higher of the MassHunter Extractables and Leachables PCDL, until superseded.

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