



MassHunter NIST 14 LC/MS/MS PCDL

Quick Start Guide

What is the MassHunter NIST 14 LC/MS/MS PCDL?	1
Working with your MassHunter PCDL	3
Product Content	4
Where to find more information	5
Installation	6
Before you begin	6
Install the MassHunter PCDL	6
Searching and managing the PCDL	7
To identify compounds and spectrum peaks using MassHunter Qualitative Analysis	7
Retention times as a search criterion	8
Managing the PCDL content with PCDL Manager	8

What is the MassHunter NIST 14 LC/MS/MS PCDL?

The NIST 14 MS/MS Database and Library from the National Institute of Standards and Technology (NIST) is a subset of the NIST Standard Reference Database 1A (NIST/EPA/NIH Mass Spectral Library). The NIST 14 MS/MS Database and Library includes annotated lists of over 9,345 compounds, with over 234,000 LC MS/MS spectra. Compound types include metabolites, drugs, phospholipids, sugars, peptides, pesticides, surfactants, those of forensic interest and all di- and tri-peptides.

The MassHunter NIST 14 LC/MS/MS Personal Compound Database and Library (PCDL) provides the content of the NIST 14 MS/MS Database and Library in MassHunter PCDL format.



Agilent Technologies

MassHunter NIST 14 LC/MS/MS PCDL

The MassHunter NIST 14 LC/MS/MS PCDL is provided in four subsets:

- nist_msms_hires (high resolving power spectra)
- nist_msms_lores (spectra acquired under lower resolution conditions)
- nist_msms2_hires (high resolving power spectra of commercially available peptides)
- nist_msms2_lores (low resolution spectra of commercially available peptides)

Each entry includes mass, chemical formula, structure information, and the CAS registry ID.

NIST 14 MS/MS Database and Library

The NIST 14 MS/MS Database and Library and the NIST MS Search Program are included with your PCDL. According to NIST, the NIST 14 MS/MS Database and Library has undergone these evaluation and quality control:

- Each spectrum critically examined by experienced mass spectrometrists.
- Each chemical structure examined for correctness and consistency, using both human and computer methods.
- Spectra of all stereoisomers intercompared.
- Chemical names examined by experts and IUPAC names provided.
- Verified CAS registry numbers.

For details on how the NIST 14 MS/MS Database and Library is curated, see the article “Quality Control for Building Libraries from Electrospray Ionization Tandem Mass Spectra”, available from <http://pubs.acs.org/>.

Working with your MassHunter PCDL

The MassHunter NIST 14 LC/MS/MS PCDL as provided by Agilent cannot be changed. You can use the MassHunter NIST 14 LC/MS/MS PCDL as is to search for compounds. Or you can use the MassHunter NIST 14 LC/MS/MS 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 NIST 14 LC/MS/MS 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 NIST 14 LC/MS/MS PCDL** files
 - **nist_msms_hires.cdb** (accurate mass compound database and accurate mass MS/MS spectral library for small molecules, di- and tri-peptides)
 - **nist_msms_lores.cdb** (accurate mass compound database and unit mass MS/MS spectral library for small molecules, di- and tri-peptides)
 - **nist_msms2_hires.cdb** (accurate mass compound database and accurate mass MS/MS spectral library containing commercially available peptides)
 - **nist_msms2_lores.cdb** (accurate mass compound database and unit mass MS/MS spectral library containing commercially available peptides)
 - *MassHunter NIST 14 LC/MS/MS PCDL Quick Start Guide*
 - MassHunter NIST 14 LC/MS/MS PCDL compound listing
 - technical notes and application notes
- **NIST 14 MS/MS Database and Library** files
 - NIST Format Installer (**setup.exe**)
 - NIST 14 MS/MS Database and Library and MS Search Program
 - MS Search Manual (PDF)
 - Read Me MSMS (text file)
- **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.

Go to <http://www.nist.gov/srd/nist1a.cfm> for the most current information on NIST database and library 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 NIST 14 LC/MS/MS PCDL Installation**.
 - b Follow the on-screen instructions to install the PCDL files.
These files are installed on your computer:
 - **MassHunter\PCDL\nist_msms_hires.cdb**
 - **MassHunter\PCDL\nist_msms2_hires.cdb**
 - **MassHunter\PCDL\nist_msms_lores.cdb**
 - **MassHunter\PCDL\nist_msms2_lores.cdb**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.

www.agilent.com

In This Guide

This Quick Start Guide provides an overview of the MassHunter NIST 14 LC/MS/MS PCDL.

This guide is valid for the B.07.00 revision or higher of the MassHunter NIST 14 LC/MS/MS PCDL, until superseded.

This information is subject to change without notice. Technologies shall not be liable for errors contained herein or for incidental or consequential damages with the furnishing, performance or use of this material. specifically disclaims any warranties for any implied warranties of merchantability or fitness for a particular purpose.

© Agilent Technologies, Inc. 2015

Revision A, April 2015



G4975-90001