ChemVista Library Manager 1.0

Introduction Workbook
Safety Notices

**CAUTION**

A CAUTION notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a CAUTION notice until the indicated conditions are fully understood and met.

**WARNING**

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.
Video Support

This Introduction Workbook has supplemental video support available. Each chapter uses step by step instructions supported by online videos to view and review the material as needed. Scan the code below or use this link to access the videos (https://aglt.co/ChemVistaIntro).
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https://community.agilent.com/
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About this Training Workbook

This Training Workbook provides instructions on the features of ChemVista Library Manager 1.0.

For additional information on the software and detailed instructions on the features not covered in this workbook, refer to the Online Help.

Use the following exercises to experience how to utilize ChemVista Library Manager to import library data, organize via search and list creation, edit structural and compound metadata, and export to desired formats. Example data is provided with the installation of the software to introduce these steps.

How This Training Workbook Works

This training workbook is your introductory guide for the set-up and execution of ChemVista Library Manager 1.0. This workbook is divided into several chapters, each building upon the last, so we recommend that each chapter is completed in succession. During each chapter, lessons are guided step by step.

Instructions look like this:

Tasks or items needed to complete tasks look like this.

If you are expected to enter any information or if something is important, it is set in italicized type like this:

Type Blank One in the field.

If you are expected to press a key on the keyboard or button on the software screen, the key is displayed in bold like this:

press Enter.

Cross references appear in blue:

(For example, Link)
Introduction

Notes and Alerts

Instructions for procedures are presented in a numbered step format:

1. Start the software by clicking the icon on the desktop. The main software window appears.

Notes and Alerts

NOTE

The Note text appears here.

CAUTION

The Caution text appears here.

WARNING

The Warning text appears here.

What This Training Workbook Covers

In this learning experience, the goal is to get up and running using the software as quickly as possible. After completing this learning ChemVista Library Manager event, you will have an introductory level of experience in the use of ChemVista Library Manager 1.0.

This learning experience introduces basic concepts in a learning-by-doing, guided manner. Each chapter uses step by step instructions and is supported by on line videos to view and review the material as needed. Scan the code to the right or use this link to access the videos (https://aglt.co/ChemVistaIntro). At any time if you have a question or get stuck, to find your local sales and support contact, visit the following page using the link below.

• https://www.agilent.com/en/contact-us/page

For technical support, visit the following page:

• https://www.agilent.com/en/support
Requirements

To complete the chapters in this training workbook, you need to have installed the software to the most recent release recommended. The software is found on the install media provided in the install kit, along with specially prepared data sets to load onto the software system before the start of this learning exercise.

Please refer to the Online Help or Installation Guide for further information. As always, feel free to contact Agilent Support for additional assistance.
User Interface and General Navigation

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Launching ChemVista Library Manager

1. After software installation, double-click the ChemVista Library Manager icon or Click Start > All Programs > Agilent Technologies > ChemVista Library Manager.

2. The software splash screen shows the software initialization.

**NOTE**
The splash screen displays the build number of the software, which is needed when contacting support. This information is also available in the File>About section of the software.
User Interface and General Navigation

User Interface

Navigation Ribbon

Ribbon Definitions

**File Tab** - The following commands are available on the File menu.

- Help opens the Online Help file.
- About opens the About Dialog Box
- Exit closes the program.
Home tab - The ribbon has two groups with the following commands and pages:

The Home tab has two groups with the following commands and pages.

- History
  - Back returns to the previous page.
  - Reload reloads the current page, updates values, and resets entered text.
  - Forward goes to the following page.

- Pages:
  - Home
  - Search
  - Import
  - Jobs
  - Lists
  - System
The pages and their basic functionality used for these exercises is reviewed in this section. For further definitions or advanced functionality, refer to the Online Help.

**Home Page**

The Home page is shown when \( \text{Home} \) is clicked on the Ribbon.
User Interface and General Navigation
Home Page

Functionality
The Home page shows overall substance and spectral counts and features the ability to search by name, synonym, CAS, or formula. Enter part or all of the name, synonym, CAS, or formula to search for in the field and press Enter on the keyboard to return results.

Recent lists
Each box represents a different list, up to 12 recently edited lists are displayed. The box displays the name of the list and how many substances are in the list.

Recent jobs
Each box shows jobs that have been started in the last 24 hours.
User Interface and General Navigation

Search Page

Search Page Definition

Click on the Ribbon to show the Search page.

Functionality

This page is used to search within ChemVista by Identifiers, Formulas, Mass, Tags, or Lists and to view the results of a search.
Import Page

Import Page Definition

Click on the Ribbon to show the Import page.

Functionality
This page is used to import data into ChemVista from multiple formats.

Source Types
The type of file to be imported. The options include:

- PCDL (*.cdb)
- PCDL CSV (*.csv)
- MassBank (*.txt)
• SDF (*.sdf)

Refer to the Appendix for more information on file types, sources, and examples.
Jobs Page Definition

Click on the Ribbon to show the Jobs page.

Functionality

This page is used to display information on any data operation (for example, import, add, edit, restore) when created as a job.

NOTE

Any operation that only affects lists (for example creation or editing) does not create a job.
Lists Page Definition

Click the Lists icon on the Ribbon to show the Lists page.

Functionality

From this page, create, remove, or merge lists, which then display in a table. List names are active links that display the substances in each list when clicked.
System Page Definition

Click on the Ribbon to show the System page.

Functionality

From this page clear system data, review registered Data Field definitions, changes, installed source types or review applications settings.

NOTE

These actions should only be done if you understand the effects. Please consult the Online Help for further information.
3 Importing Data

3 Importing Data

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Importing Data

Import Files

Introduction

The following exercises are designed to support the execution of the ChemVista Library Manager features along with video support. The videos are intended to provide visual support for working with the software. We recommend reviewing the video demonstration first, then attempting the processes, using each exercise as a guide. If at any time you have questions or run into an event that is not in alignment with this workbook, please reach out to Agilent Support or your Agilent Consultant.

Import data from PCDL

1. Click **Import** on the Ribbon to navigate to the Import Page.

2. Select **PCDL(*.cdb)** from the Source type drop-down.
3 Importing Data
Import data from PCDL

3 Click Open file(s).

4 Navigate to the folder "\Resources\Example Data\PCDL" and select Checkout_TestMix_Std.cdb and Pesticides_Submix1.cbd.

5 Click Open.
6 Select Create List Upon Import.
7 Enter the name Pesticide List into the List Name field.
8 Enter Checkout Test Mix and Pesticides Submix PCDLs into Description.
9 Select Import selected files to launch the import.

10 Click OK.

NOTE
The PCDL is not saved within the software, the data is imported from the PCDL and stored in the software's internal format.
3 Importing Data
Import data from Mass Bank

11 Review the Status of the import from the System Jobs page to confirm it reads Import complete.

12 Expand the Summary to review the number of substances created and spectra imported.

The MassBank files provided with the installation software are only for instruction purposes. It is advised to obtain updated files from MassBank before performing analysis beyond performing these exercises.

2 Select MassBank (*.txt) from the Source type drop-down.
3 Click Open file(s).
3 Importing Data

Import data from PCDL.CSV

4 Navigate to the folder "Your Directory\Example Data\" and select the MassBank files folder.

5 Click Open.

6 Clear the Create List Upon Import check box.

7 Click Import Select Files to launch the import.

8 Click OK.

9 Expand the Summary to review the number of substances created and spectra imported.

NOTE
The MassBank files are not saved within the software, the data is imported from the files and stored in the software's internal format.

Import data from PCDL.CSV

1 Click Import in the Ribbon to navigate to the Import Page.

2 Select PCDL CSV (*.csv) from the Source type drop-down

3 Click Open file(s).
3 Importing Data
Import data from PCDL.CSV

4 Navigate to the folder "\Your Directory\Example Data\" and select Pesticides_submix1_RT.csv.

5 Click Open.
6 Select the Create List Upon Import check box.
7 Enter the name Pesticide Submix Subset into the List Name field.

8 Select the Apply method label to imported data check box.

9 Enter Agilent Eclipse Plus C18, 2.1 mmx150 mm, 01/2021 into the label field.
10 Click import selected files to launch the import.

Creating a method label is strongly recommended for optimal RT/RI data organization, especially from PCDL and CSV imports. The method label is stored alongside RT/RI data and enhances viewing and downstream use.

11 Click OK.
3 **Importing Data**
Import data from PCDL.CSV

12 Expand the **Summary** to review the number of substances created and spectra imported.

13 Click **Lists** on the Ribbon to view the Substance List pane.

14 View the Substances Lists, noting the two lists created via import display.
This page intentionally left blank.
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Working with Lists

Tag Search

1. Click **Search** on the Ribbon to navigate to the Search Page.
2. Click the **Tags** tab.

**NOTE**
Tags come from rich data that’s included as part of the Agilent PCDL files. They’re parsed from the compound Description and Notes fields and presented as a separate, searchable tag that travels along with the compound information.

3. Enter *pesticide* into the search field, then select it from the auto-generated list.

4. Click **Search** to load the subset in the Search Results window.
Create a Targeting List from Search Results

1. Use the Select All check box to select all compounds in the Search results.

2. Click Add to list.

3. In the Add to new list section of the dialog box, enter the List name "Comprehensive Pesticide List."
Lists
Create a Targeting List from Search Results
Lists
Manage Lists from Lists page

4 Click Create list.

5 Click OK.

Manage Lists from Lists page

1 Click Lists on the Ribbon to navigate to the Lists page.
2 Select the Pesticides Submix Subset and the Comprehensive Pesticide List’s check box.

3 Click Merge.

4 In the Add to List dialog box, select the List drop down and choose Comprehensive Pesticide List.
5 Click Append.
6 Click **OK**.

7 The Substance Lists page refreshes and the Comprehensive Pesticide list displays 47 in Substance count.

<table>
<thead>
<tr>
<th>Name</th>
<th>Last Updated</th>
<th>Substance Count</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pesticide Subset</td>
<td>3/20/2020 5:00 PM</td>
<td>26</td>
<td></td>
</tr>
<tr>
<td>Pesticide List</td>
<td>3/20/2020 5:00 PM</td>
<td>46</td>
<td>Compounds and spectra from the CheckOut Test Mix and Pesticides Submix P221a</td>
</tr>
<tr>
<td>Comprehensive Pesticide List</td>
<td>3/20/2020 5:00 PM</td>
<td>47</td>
<td></td>
</tr>
</tbody>
</table>
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Editing Compounds

Adding Compounds to List

1. Click Search on the Ribbon to navigate to the Search page.
2. Select the Identifiers tab.
3. On the Identifiers tab, select the identifier field CAS.
4. Enter 2886-65-9 in the search field.
5. Click Search.
5 Working with Data
Create a New Substance

6 Select Norfluradiazepam.

7 Click Add to list.
8 Select Comprehensive Pesticide List.
9 Click Append.
10 Click OK.

Create a New Substance

1 Click Lists in the Ribbon to navigate.
2 Click Comprehensive Pesticide Screening list name to view.

3 Click Create substance.

4 Enter the following information:
   • Name: Difenoxuron
   • CAS: 14214-32-5
   • Formula: C16H18N2O3
   • SMILES: COC1C(CC(CC=C(=1)OC1C(CC(CC=C(=1)NC(=O)N(C)C)
   • Mass: 286.13174
Adding any single structural identifier results in the creation of any missing identifiers, including InChI String, InChIKey, MOL text, and a structural image.

5 Click **Commit**. The Systems Jobs pane displays.
Editing Spectra

Add New Spectrum

1. From Systems Jobs page, click View Affected Substances.

2. Click View spectra.

3. Click Create.
4 Add the following information into m/z and Intensity:

<table>
<thead>
<tr>
<th>m/z</th>
<th>Intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>46.065126</td>
<td>19.316</td>
</tr>
<tr>
<td>72.04439</td>
<td>32.018</td>
</tr>
<tr>
<td>123.044056</td>
<td>18.668</td>
</tr>
<tr>
<td>124.051881</td>
<td>1.139</td>
</tr>
<tr>
<td>287.139019</td>
<td>100</td>
</tr>
</tbody>
</table>

5 Edit the Spectral Details with the following information:

- Separation technique: LC
- Mass Analyzer: QTOF
- Ionization Technique: ESI
- Polarity: POSITIVE
- Precursor Type: [M+H]+
- CE: 10
- Precursor ion: 287.1390189076
- MS Level: 2
5 Working with Data
Add New Spectrum

6 Click **Commit**.
7 From Systems Jobs, click **View Affected Substances**.
8 Click **View Spectra** to verify that the data was added.
9 Review the data as needed.
Verifying Spectra

1. Click **Lists** on the Ribbon to navigate to the Lists page.
2. Click **Comprehensive Pesticide List** to view the list of compounds.
3. Sort the list alphabetically by clicking the **Substance Name** column header.

4. Highlight **Bentazone**.

5. Click **View Spectra**.
6. Click **Polarity**.

7. Select **Negative**.

8. View Negative mode spectra and confirm 3 spectra are present.
Update RT

1. From the ribbon, click Back to return to the prior page.
2. Click Browse Methods.
3. Click Select method label or parameters to view the methods available. Click anywhere to close.
4. Click Edit RT /RIs.
5. Type in *Agilent Eclipse Plus C18, 2.1 mmx150 mm, 02/2023* in the Method Label field.
6. Click the RT column header to sort the list.
7 Add additional Retention times in the RT column as needed.

8 Click Commit.

9 To confirm the data is loaded in the software, click Back on the Ribbon.

10 Click Reload on the Ribbon of the Methods page.

11 Select method label or parameters to confirm the method was applied to the list.
6 Exporting Data

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Exporting Data
Exporting a List

1. Select the Select All check box.

2. Click Export to navigate to the Export Page and display options.

3. Confirm that PCDL (*.cbd) is selected for Export As.

4. Click Ionization technique and select ESI.

5. Click Polarity and select Positive.

6. Click Method label and select Agilent Eclipse Plus, C18, 2.1 mmx150 mm, 02/2023.
Exporting Data
Exporting a List

7 Click **Summary Load Statistics** to review summary statistics of the data included in the export.

**CAUTION**
Loading of Summary Statistics may take several minutes if the exported data set is large.

8 Click **Start Export**.

9 Click **OK**.

10 Click **Download output**.

11 In the Save file dialog box, browse to the desired location to save the file.

12 Enter a name for the output and click **Save**.
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Using exported PCDLs in MassHunter data analysis

Exporting PCDLs from Agilent ChemVista enables screening and identification workflows in downstream MassHunter data analysis software. For guidance on using PCDLs in MassHunter Quantitative Analysis, refer to the MassHunter Quant LC/Q-TOF Screener (M6005-10006).

Spectra and RTs can be extracted in MH Qual and sent to a desired PCDL. Once the desired spectra and RTs are in the PCDL, import the PCDL into ChemVista. The import process will use the structural identifiers and meta data to merge data together and eliminate duplicate compounds and will store the new spectra and RTs accordingly. On import, create a method label to keep RTs organized.

Data Format

<table>
<thead>
<tr>
<th>Format</th>
<th>Support File Type</th>
<th>Example Data/Access</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agilent PCDL</td>
<td>.cdb</td>
<td>E:\Resources\Example Data</td>
</tr>
<tr>
<td>CSV</td>
<td>.csv</td>
<td>E:\Resources\Example Data</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E:\Resources\Templates</td>
</tr>
</tbody>
</table>
3rd Party Resources

<table>
<thead>
<tr>
<th>Format</th>
<th>Support File Type</th>
<th>Example Data/Access</th>
</tr>
</thead>
</table>

MassBank (EU)

Spectra from MassBank is viewed on the MassBank web application (https://massbank.eu/MassBank/) and downloaded via the MassBank data repository hosted on GitHub (https://github.com/MassBank/MassBank-data) as .txt files. The data repository is organized in sub-folders according to the contributor or contributing group. Each .txt file contains a single spectral record and there may be many .txt files mapping to the same chemical substance or compound. Downloaded .txt files are imported directly into ChemVista.

MassBank of North America (MoNA)

Spectra from MoNA is viewed and downloaded from the MoNA web application. Spectra are downloaded from MoNA (https://mona.fiehnlab.ucdavis.edu/downloads) in three different formats, but
Appendix
EPA CompTox Chemicals Dashboard

the format supported by ChemVista is the SDF. The SDF download is organized by spectral record, but all entries in the download are contained in a single downloaded file. Downloaded SDFs are imported directly into ChemVista.

Many subset downloads are available from the MoNA downloads page, the following are recommended downloads to supplement Agilent MassHunter data analysis applications:

- All LC-MS/MS QTOF download
- All LC-MS/MS Agilent QTOF download
- All LC-MS/MS Orbitrap download

EPA CompTox Chemicals Dashboard

The EPA CompTox Chemicals Dashboard is a chemical data resource. Data is downloaded from multiple places in four different formats, but the format supported by ChemVista is the SDF (in either v2000 or v3000 MOL format). Data can be downloaded from pre-curated lists of interest ([https://comptox.epa.gov/dashboard/chemical-lists](https://comptox.epa.gov/dashboard/chemical-lists)) as well as from batch searches ([https://comptox.epa.gov/dashboard/batch-search](https://comptox.epa.gov/dashboard/batch-search)) conducted in the Dashboard web application. No spectra are available for download from the Dashboard.

Suggested export filters for MassHunter data analysis

When using third party data in MassHunter workflows, the possibility exists that certain spectra are not compatible with MassHunter data analysis algorithms. For maximum compatibility, the following export filters are recommended:

- MS level = 1 or 2
- Polarity = NEGATIVE and/or POSITIVE
- For optimal library matching, restricting the instrument type to 'QTOF' is recommended.

NOTE

MS Level 2 is for LC-MS/MS and GC-MS/MS; MS Level 1 is for GC-MS.
Forcing a polarity to be selected removes spectra that have errant polarity values from third party sources that would cause issues in data analysis.

Collision Energy (CE) values that are not supported in the PCDL format (e.g., 'Ramp 21.1-31.6 eV') are written out by ChemVista with the value '9999' in the CE field in the exported PCDL.

For maximum compatibility with the PCDL format, the presence of a formula and mass are required for chemical substances to be included in the export. This export option is automatically enforced for PCDL exports. For consistency and compatibility outside of MassHunter workflows, it is recommended to select the same filter when exporting to SDF or MassBank.

Common regex searches for Pattern Search

The Pattern Search option on the Search page in ChemVista supports regular expression (regex) inputs for the selected data field. Some common regex queries that might be helpful are provided below:

<table>
<thead>
<tr>
<th>Regular Expression</th>
<th>Search Conducted</th>
</tr>
</thead>
<tbody>
<tr>
<td>(?i)</td>
<td>When used prior to a search string, makes the search case insensitive (“(?i)pesticide”)</td>
</tr>
<tr>
<td>.</td>
<td>Matches anything</td>
</tr>
<tr>
<td>\d</td>
<td>Matches any digit 0-9</td>
</tr>
<tr>
<td>[a-d]</td>
<td>Matches anything containing any of the letters a, b, c, or d</td>
</tr>
<tr>
<td>[0-9]</td>
<td>Matches anything containing any of the values 0, 1, 2, 3, 4, 5, 6, 7, 8, or 9</td>
</tr>
<tr>
<td>^[0-9][1-9][0-9][0-9][0-9][0-9]</td>
<td>Matches any value between 0 and 999</td>
</tr>
</tbody>
</table>