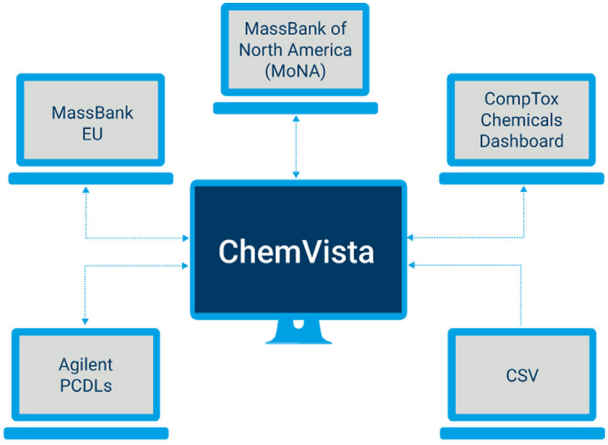
Agilent

# ChemVista Library Manager 1.0

# Introduction Workbook



# Notices

## Document Identification

D0030672
April 2023 Revision A.00

## Copyright



Agilent Technologies, Inc.
5301 Stevens Creek Blvd.
Santa Clara, CA 95051

## Software Revision

This guide is valid for ChemVista Library Manager 1.0 program or higher and compatible ChemVista Library Manager 1.0 programs, until superseded.

## Software Manufacturing

Manufactured for Agilent Technologies
5301 Stevens Creek Blvd
Santa Clara, CA 95051

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**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 on line 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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# Contents

# 1 Introduction

# 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**)

**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

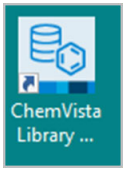
To complete the chapters in this training workbook, you need to have installed the software to the most recent release recommended. The software is found on the install media provided in the install kit, along with specially prepared data sets to load onto the software system before the start of this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

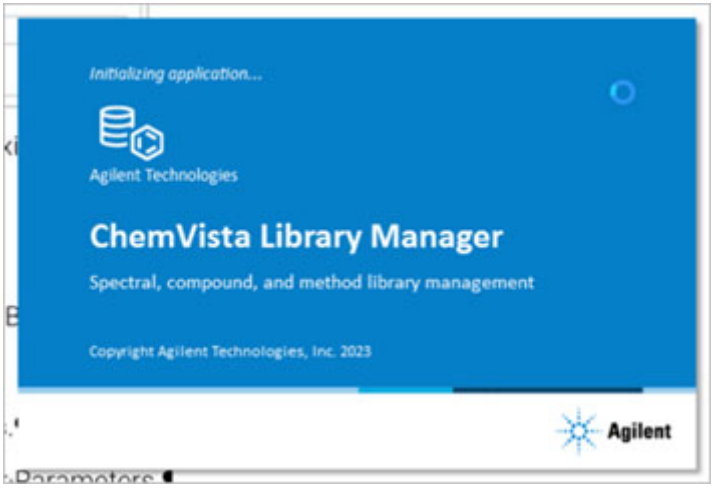
# 2 User Interface and General Navigation

# 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.

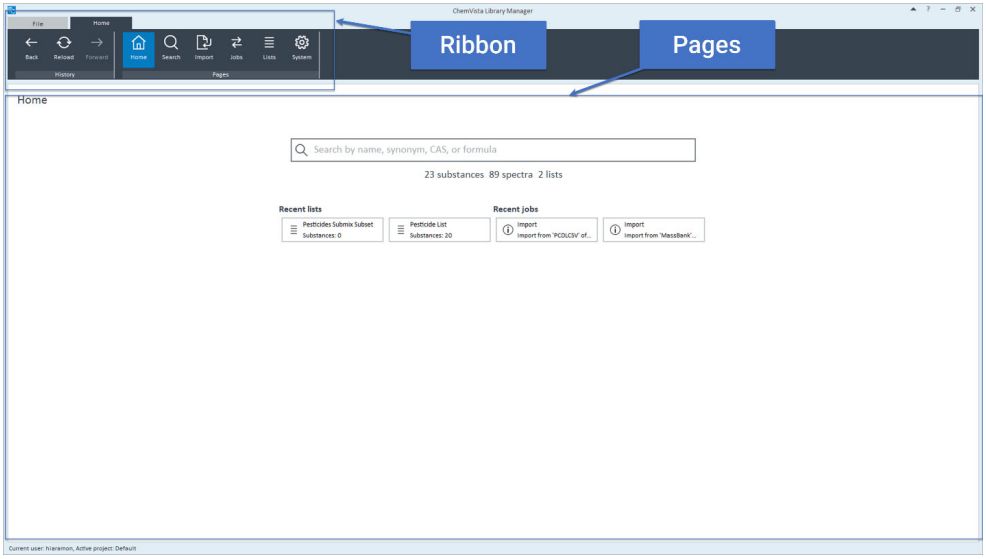



NOTE

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.

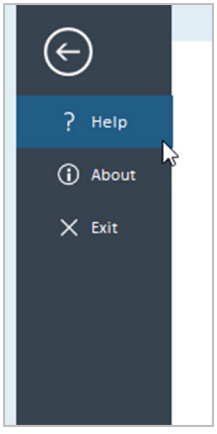
# User Interface

## Navigation Ribbon



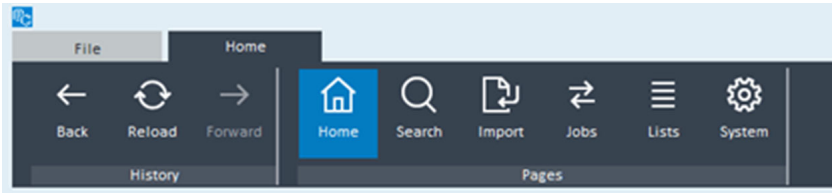

### Ribbon Definitions

**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:



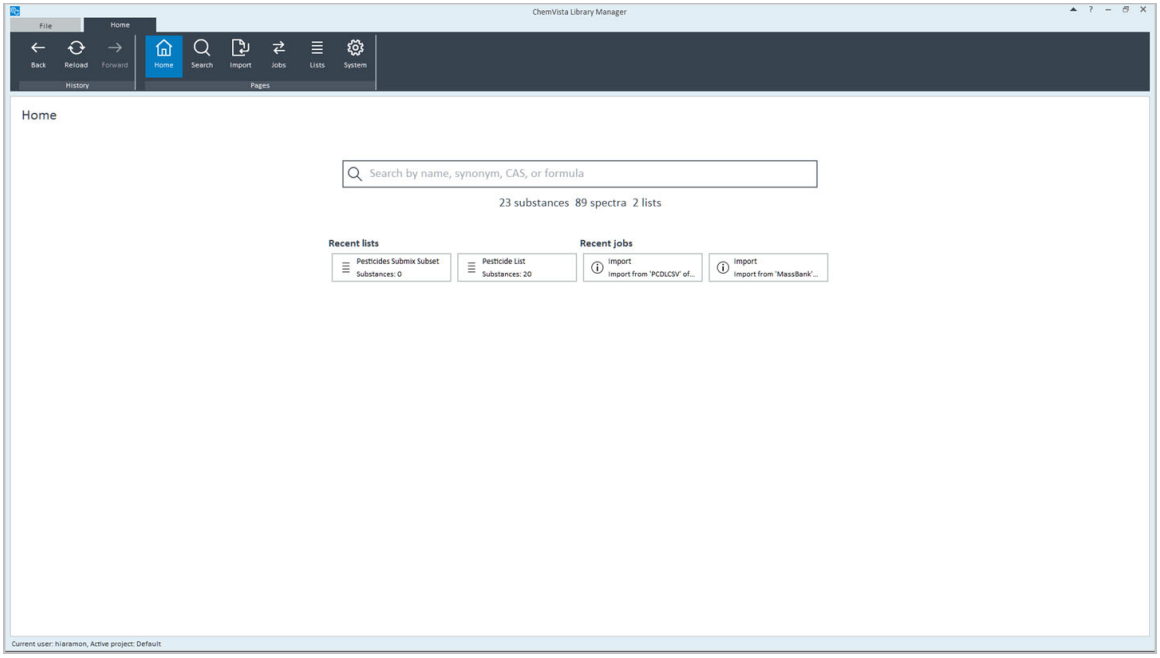

The **Home tab** has two groups with the following commands and pages.

- 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

# Pages

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




### Home Page Definitions

The Home page is shown when 

is clicked on the Ribbon.

### 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.

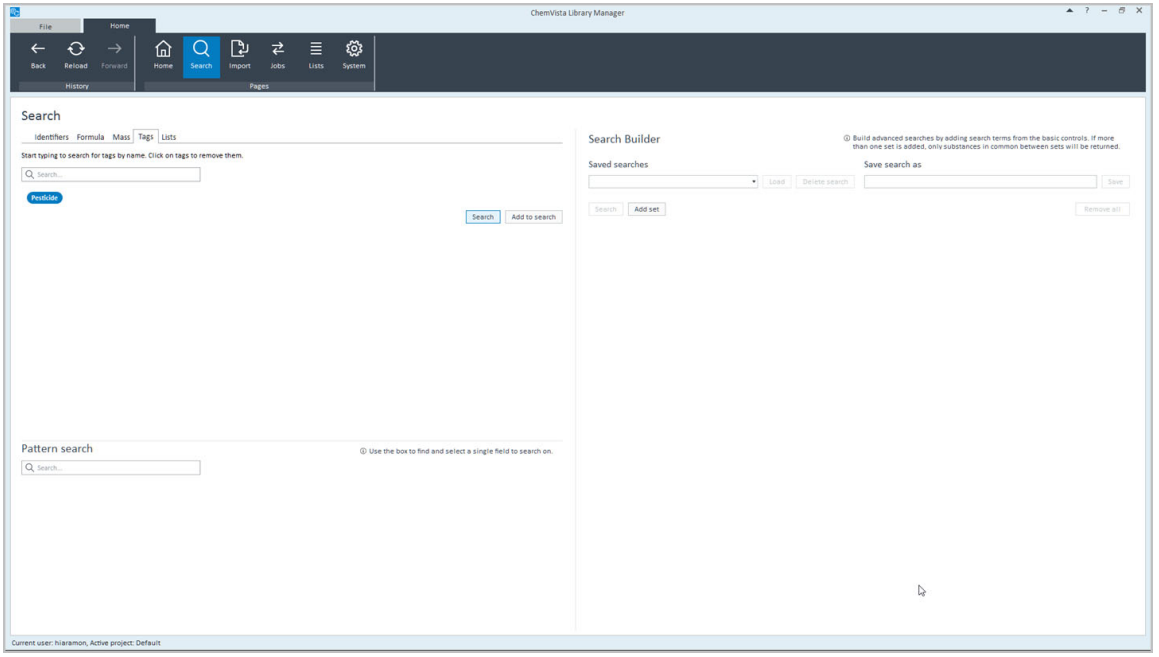
### Recent lists

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.

# Search Page




## Search Page Definition

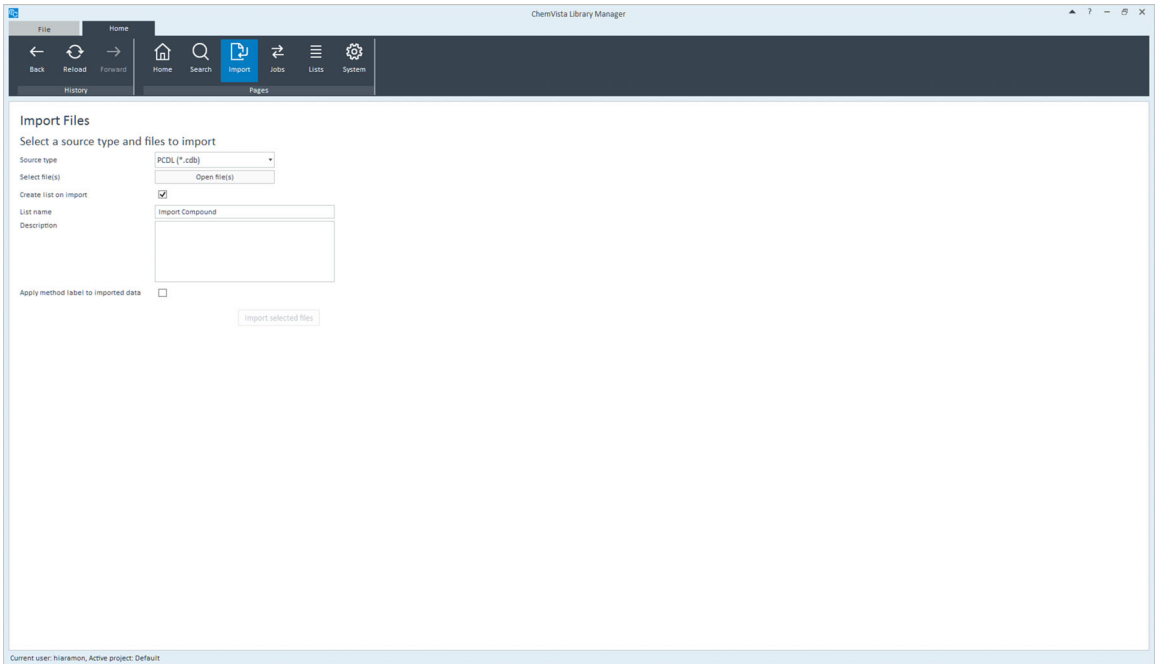
Click 

on the Ribbon to show the Search page.

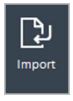
## Functionality

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:

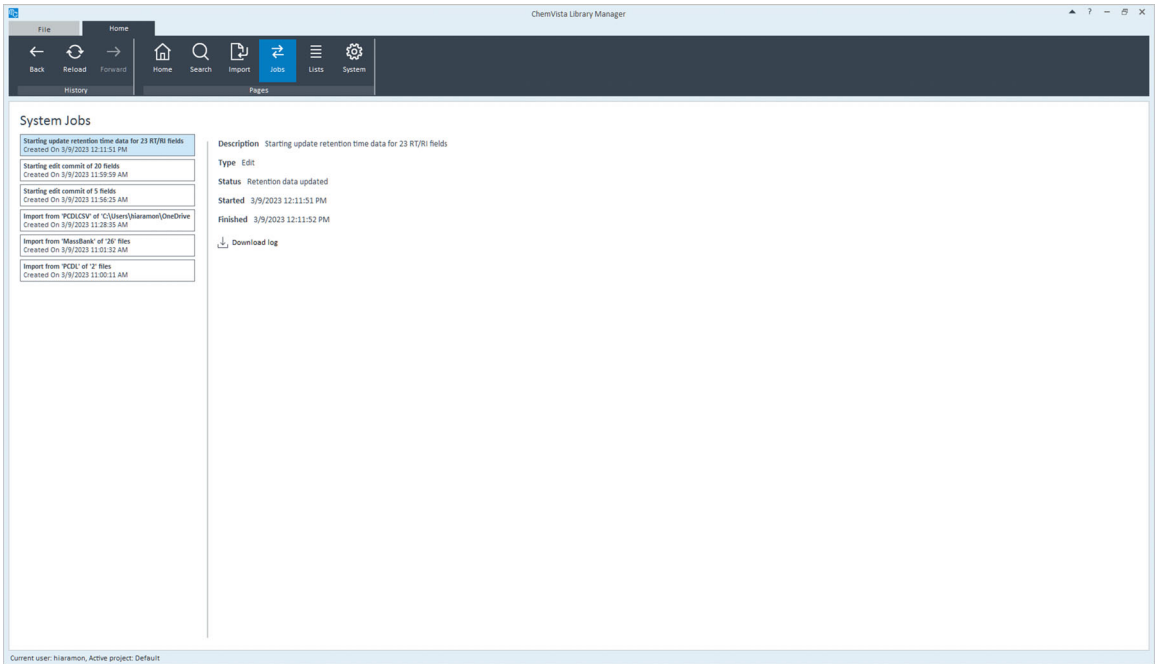
- PCDL (*.cdb)
- PCDL CSV (*.csv)
- MassBank (*.txt)

- SDF (*.sdf)

NOTE

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

# Jobs Page




## Jobs Page Definition

Click 

on the Ribbon to show the Jobs page.

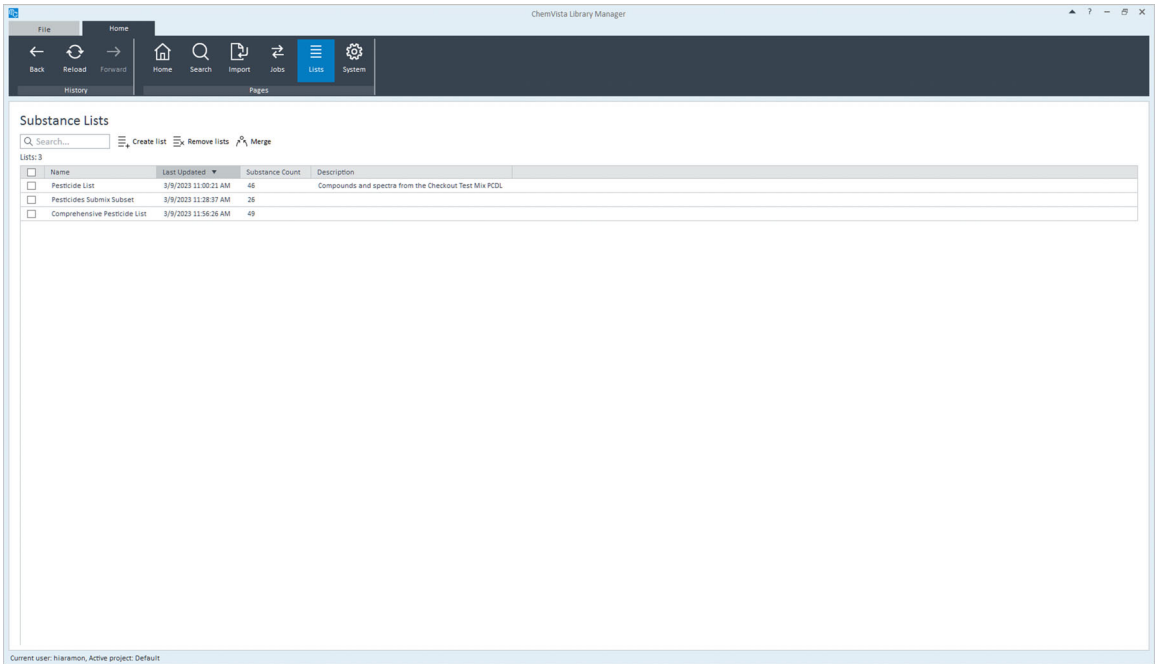
## Functionality

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

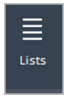
NOTE

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

# Lists Page




## Lists Page Definition

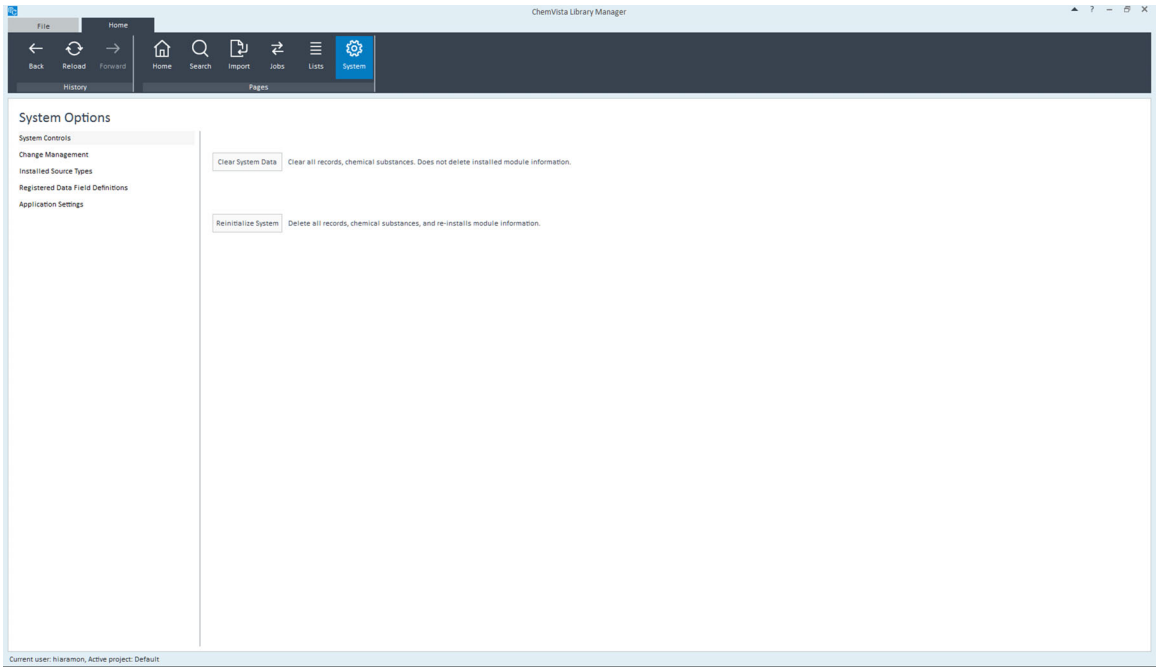
Click 

on the Ribbon to show the Lists page.

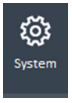
## Functionality

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




## 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

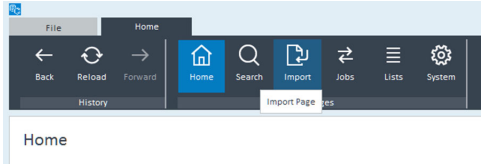
# Import Files

## Introduction

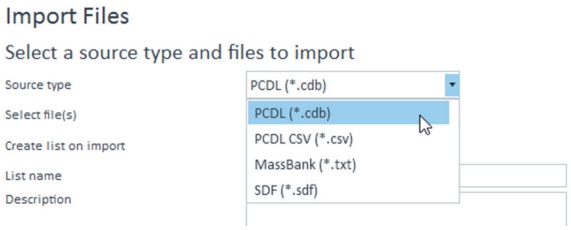
The following exercises are designed to support the execution of the ChemVista Library Manager features along with video support. The videos are intended to provide visual support for working with the software. We recommend reviewing the video demonstration first, then attempting the processes, using 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

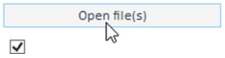
1 Click **Import** on the Ribbon to navigate to the Import Page.



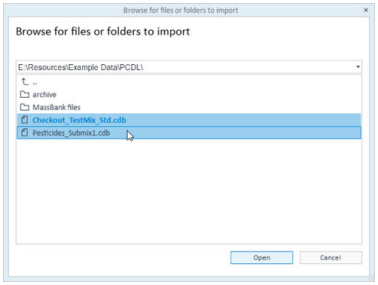

2 Select **PCDL(*.cdb)** from the Source type drop-down.



3 Click **Open file(s)**.




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



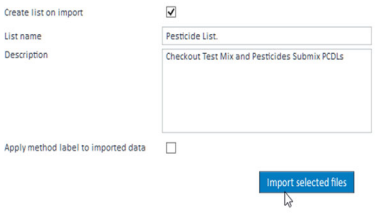

5 Click **Open**.

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.

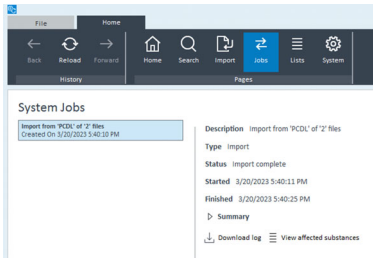



10 Click **OK**.

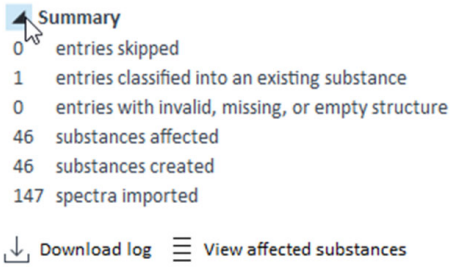
NOTE

The PCDL is not saved within the software, the data is imported from the PCDL and stored in the software's internal format.

**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.




## Import data from Mass Bank

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

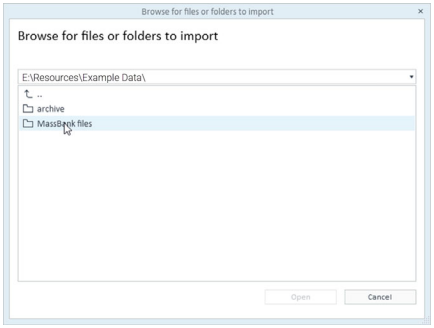
NOTE

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.

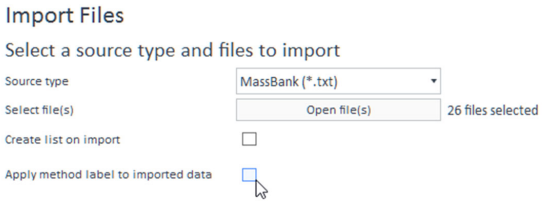
**3** Click **Open file(s)**.

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.

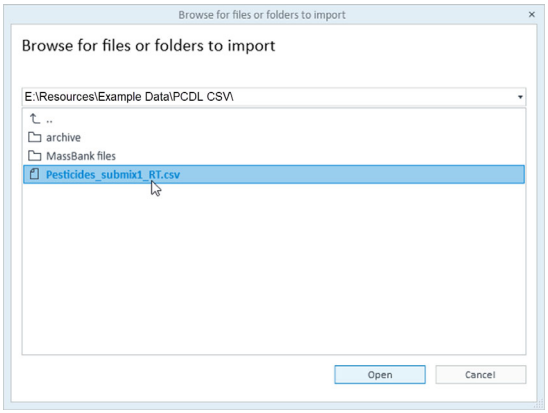
## Import data from PCDL.CSV

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)**.

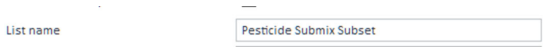
4 Navigate to the folder "\Your Directory\Example Data\" and select **Pesticides_submix1_RT.csv**.



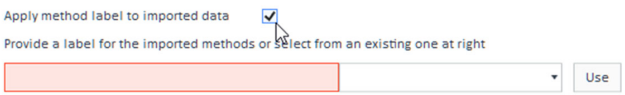

5 Click **Open**.

6 Select the **Create List Upon Import** check box.

7 Enter the name *Pesticide Submix Subset* into the List Name field.

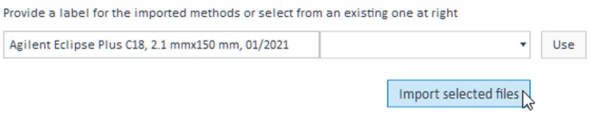



8 Select the **Apply method label to imported data** check box.




9 Enter *Agilent Eclipse Plus C18, 2.1 mmx150 mm, 01/2021* into the label field.

10 Click I**mport selected files** to launch the import.




NOTE

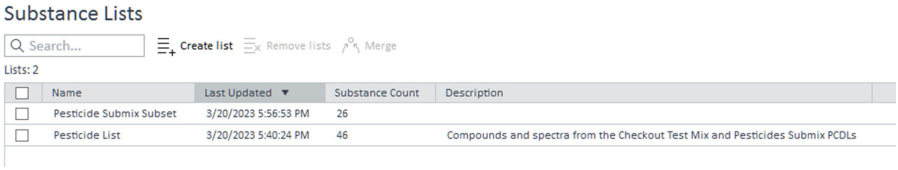
Creating a method label is strongly recommended for optimal RT/RI data organization, especially from PCDL and CSV imports. The method label is stored alongside RT/RI data and enhances viewing and downstream use.

11 Click **OK**.

**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.



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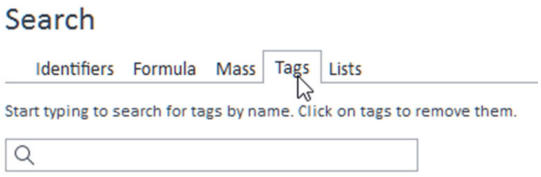
# 4 Lists

# Working with Lists

## Tag Search

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

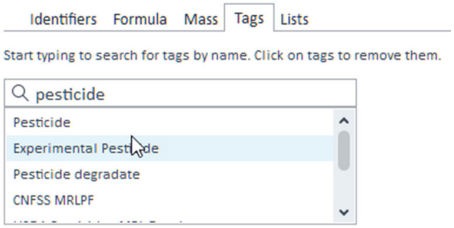
2 Click the **Tags** tab.



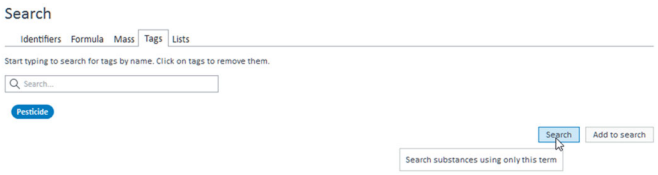

NOTE

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.

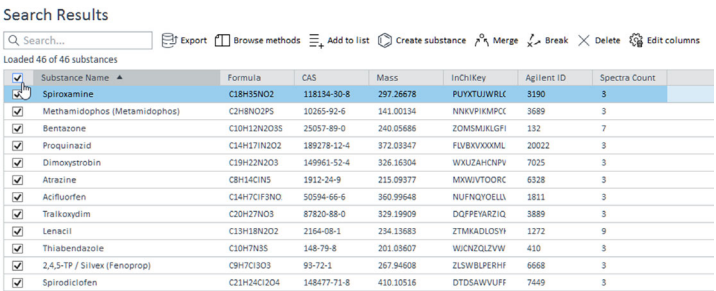


NOTE

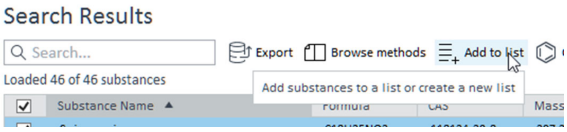
Tags are removed by clicking on the text to clear from the search list.

## Create a Targeting List from Search Results

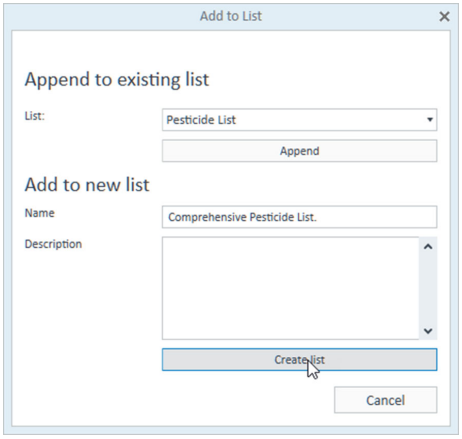
1 Use the **Select All** check box to select all compounds in the Search results.



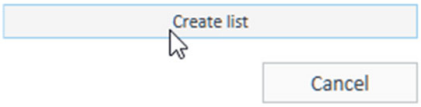

2 Click **Add to list**.




3 In the Add to new list section of the dialog box, enter the List name *Comprehensive Pesticide List*.


Add to List
Append to existing list
List:
Pesticide List
Append
Add to new list
Name
Comprehensive Pesticide List.
Description
Create list
Cancel

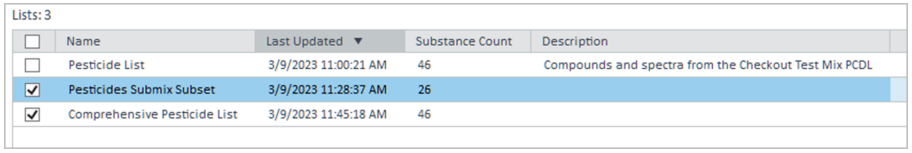
4 Click **Create list**.



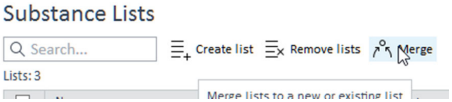

5 Click **OK**.

## Manage Lists from Lists page

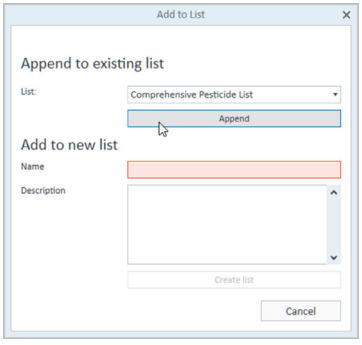
1 Click Lists on the Ribbon to navigate to the Lists page.
2 Select the Pesticides Submix Subset and the Comprehensive Pesticide List's check box.




3 Click **Merge**.

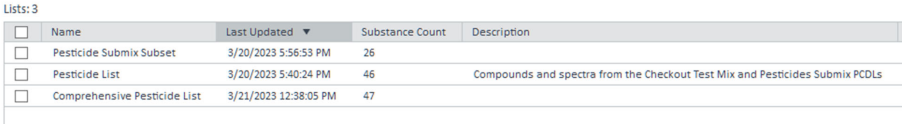



4 In the Add to List dialog box, select the **List** drop down and choose **Comprehensive Pesticide List**.
5 Click **Append**.



6 Click **OK**.

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



Lists: 3

| | Name | Last Updated ▼ | Substance Count | Description |
|---|---|---|---|---|
| ☐ | Pesticide Submix Subset | 3/20/2023 5:56:53 PM | 26 | |
| ☐ | Pesticide List | 3/20/2023 5:40:24 PM | 46 | Compounds and spectra from the Checkout Test Mix and Pesticides Submix PCDLs |
| ☐ | Comprehensive Pesticide List | 3/21/2023 12:38:05 PM | 47 | |

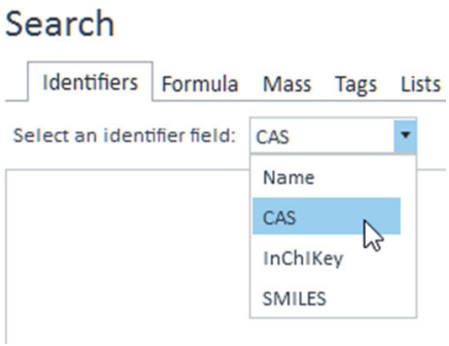
# 5 Working with Data

# Editing Compounds

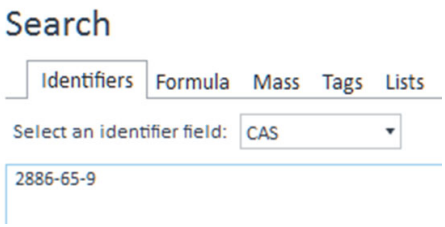
## Adding Compounds to List

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.

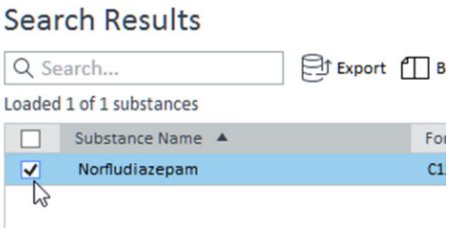



4 Enter *2886-65-9* in the search field.




5 Click **Search**.

6 Select **Norfluradiazepam**.




7 Click **Add to list**.

8 Select **Comprehensive Pesticide List**.

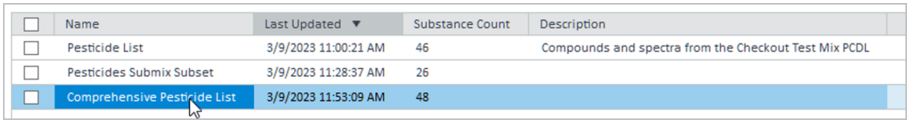
9 Click **Append**.

10 Click **OK**.

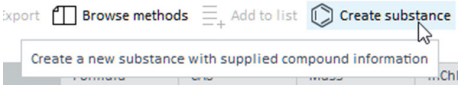
## Create a New Substance

1 Click **Lists** in the Ribbon to navigate.

2 Click **Comprehensive Pesticide Screening** list name to view.

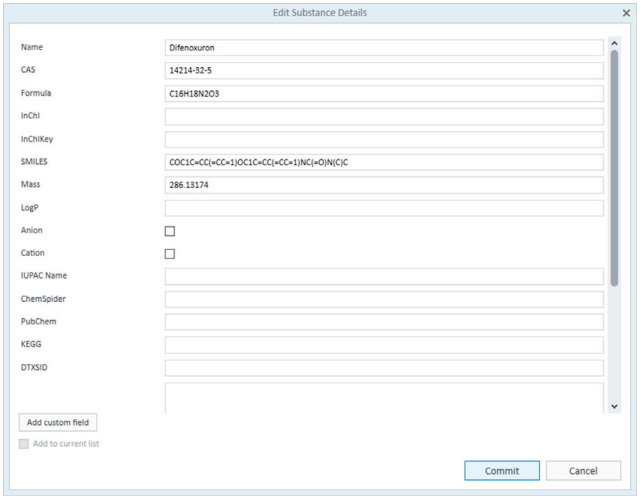



3 Click **Create substance**.




4 Enter the following information:

- Name: *Difenoxuron*
- CAS: *14214-32-5*
- Formula: *C16H18N2O3*
- SMILES: *COC1C=CC(=CC=1)OC1C=CC(=CC=1)NC(=O)N(C)C*
- Mass: *286.13174*




NOTE

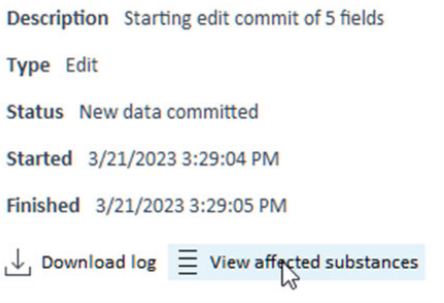
Adding any single structural identifier results in the creation of any missing identifiers, including InChI String, InChIKey, MOL text, and a structural image.

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

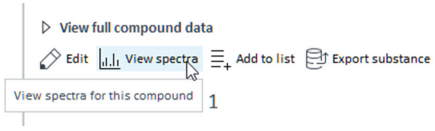
# Editing Spectra

## Add New Spectrum

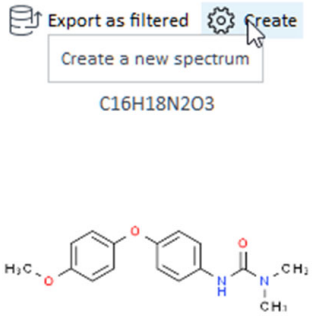
1 From Systems Jobs page, click View Affected Substances.




2 Click **View spectra**.




3 Click **Create**.

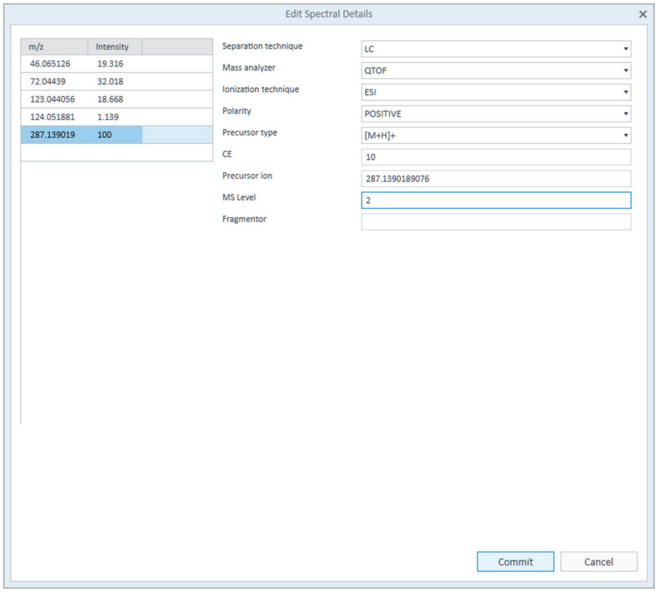


**4** Add the following information into **m/z** and **Intensity**:

| m/z | Intensity |
|---|---|
| 46.065126 | 19.316 |
| 72.04439 | 32.018 |
| 123.044056 | 18.668 |
| 124.051881 | 1.139 |
| 287.139019 | 100 |

**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*

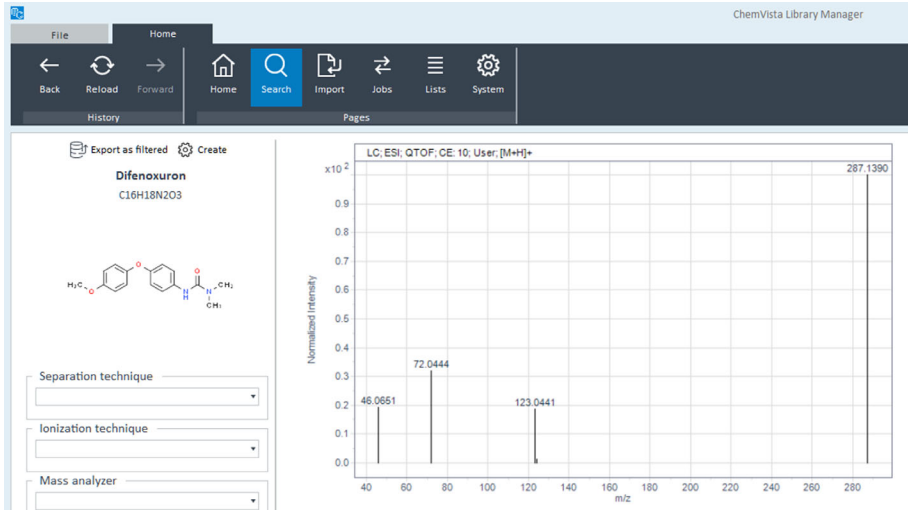



6 Click **Commit**.

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.

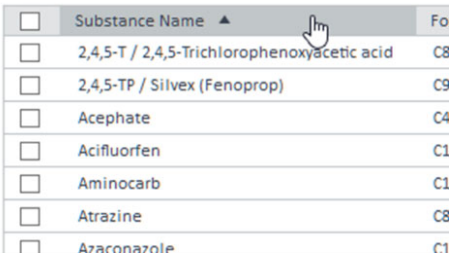


# Verifying Spectra

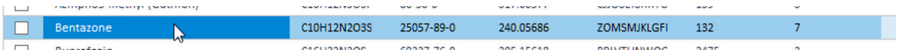
1 Click **Lists** on the Ribbon to navigate to the Lists page.

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**.

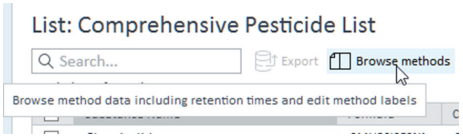

7 Select **Negative**.


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

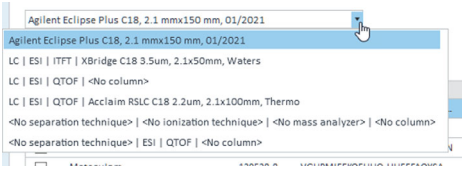
# Update RT

1 From the ribbon, click **Back** to return to the prior page.

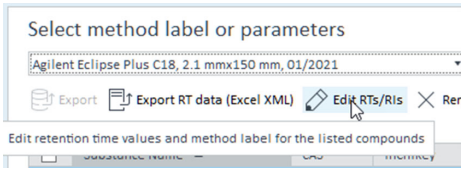
2 Click **Browse Methods**.



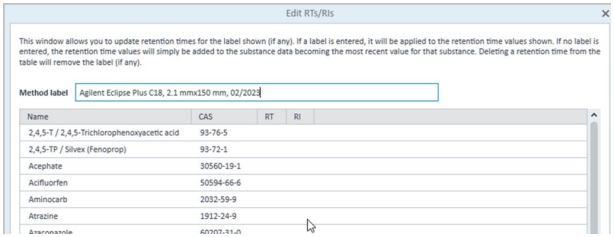

3 Click **Select method label or parameters** to view the methods available. Click anywhere to close.



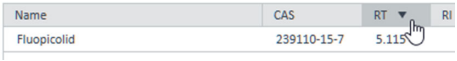

4 Click **Edit RT /RIs**.




5 Type in *Agilent Eclipse Plus C18, 2.1 mmx150 mm, 02/2023* in the Method Label field.



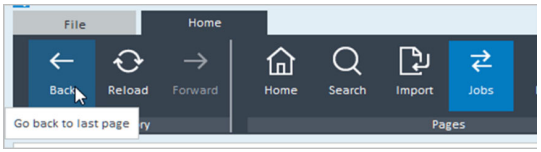

6 Click the **RT** column header to sort the list.



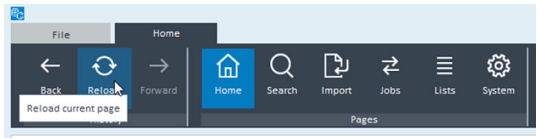
7 Add additional Retention times in the **RT** column as needed.


8 Click **Commit**.

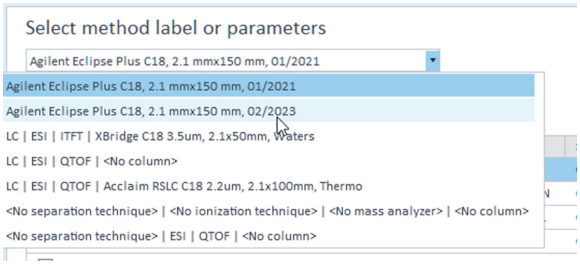
9 To confirm the data is loaded in the software, click **Back** on the Ribbon.




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.

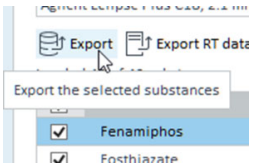


# 6 Exporting Data

# Exporting a List

1 Select the **Select All** check box.

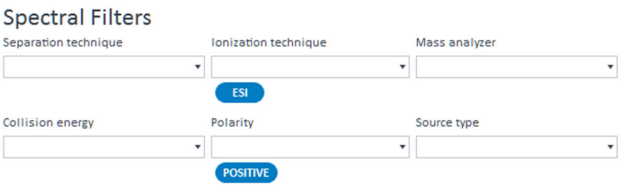

2 Click **Export** to navigate to the Export Page and display options.



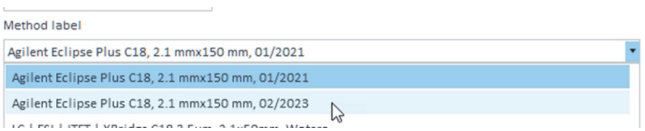

3 Confirm that PCDL (*.cbd) is selected for Export As.


4 Click **Ionization technique** and select **ESI**.

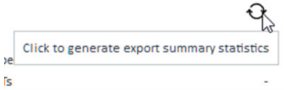
5 Click **Polarity** and select **Positive**.




6 Click **Method label** and select **Agilent Eclipse Plus, C18, 2.1 mmx150 mm, 02/2023**.



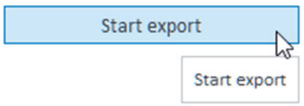
7 Click **Summary Load Statistics** to review summary statistics of the data included in the export.




CAUTION

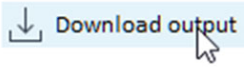
**Loading of Summary Statistics may take several minutes if the exported data set is large.**

8 Click **Start Export**.



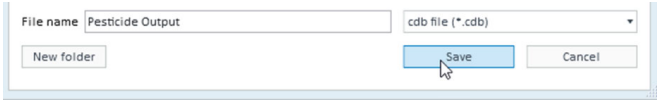

9 Click **OK**.

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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# 7 Appendix

# Tips

## 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

| Format | Support File Type | Example Data/Access |
|---|---|---|
| Agilent PCDL | *.cdb* | E:\Resources\Example Data |
| CSV | *.csv* | E:\Resources\Example Data<br>E:\Resources\Templates |

# 3rd Party Resources

| Format | Support File Type | Example Data/Access |
|---|---|---|
| MassBank EU | *.txt* | E:\Resources\Example Data<br>**https://massbank.eu/MassBank/**<br>**https://github.com/MassBank/MassBank-data** |
| MassBank of North America (MoNA) | *.sdf* | **https://massbank.us/**<br>**https://mona.fiehnlab.ucdavis.edu/downloads** |
| EPA CompTox Chemicals Dashboard | *.sdf* | **https://comptox.epa.gov/dashboard/**<br>**https://comptox.epa.gov/dashboard/chemical-lists** |

## 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

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**) as well as from batch searches (**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.

NOTE

Forcing a polarity to be selected removes spectra that have errant polarity values from third party sources that would cause issues in data analysis.

NOTE

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.

NOTE

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:

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

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D0030672
Revision A.00

April 2023