

MassHunter GC/Q-TOF Personal Compound Database and Library for Pesticides

Familiarization Guide



Agilent Technologies

Notices

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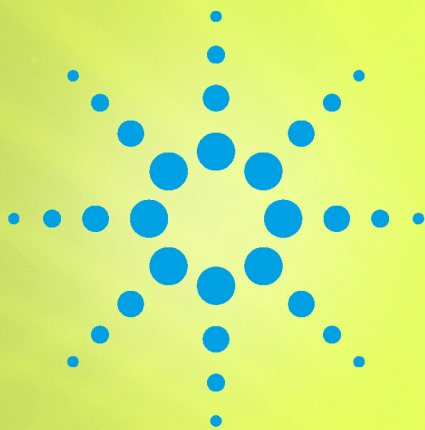
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1 Introduction

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Agilent Technologies

In This Guide

About MassHunter GC/Q-TOF Pesticides PCDL

Before You Begin These Exercises

The Familiarization Guide presents step-by-step exercises to help you learn to use the Agilent MassHunter GC/Q-TOF Pesticides Personal Compound Database and Library (PCDL) with the PCDL Manager program to search for compounds and create a custom PCDL, and with the Agilent MassHunter Workstation Qualitative Analysis and Quantitative Unknowns Analysis B.07.00 Software to identify compounds.

The MassHunter Pesticides PCDL contains an accurate mass Electron Ionization (EI) spectral database, which is often referred to as a *spectral library* or *library*.

With the MassHunter Pesticides PCDL, you can:

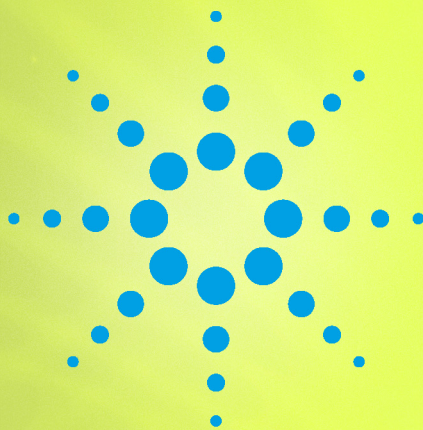
- Screen over 700 pesticides with accurate mass measurement, in a single GC/Q-TOF analysis
- Minimize method development time for your analysis
- Search for compounds using text, formula, exact mass, and retention time
- Store accurate mass spectra, retention time values, and other information for compounds existing in the database at purchase and for compounds added to the database after purchase
- Create subsets of the database, which can contain different lists of compounds with different retention times, allowing the database collection to be tailored to the specific needs of your laboratory

The quadrupole time-of-flight (Q-TOF) instrument provides the capability to screen simultaneously for all compounds in the database that are detected by matching their exact mass spectra and retention time.

The exercises in this guide use the following software programs:

- Agilent MassHunter PCDL Manager B.07.00
- Agilent MassHunter Qualitative Analysis B.07.00
- Agilent MassHunter Quantitative Analysis - Unknowns Analysis B.07.00

See the individual software documentation for more help on installing and using these programs.



2 Familiarization Exercises

- Exercise 1. Search the PCDL 8
- Exercise 2. Create a Custom PCDL in the PCDL Manager 18
- Exercise 3. Use the PCDL to Identify Compounds in Qualitative Analysis 36
- Exercise 4. Use the PCDL to Identify Compounds with Unknowns Analysis 53
- Exercise 5. Create a Custom PCDL from Your Compound Results 62



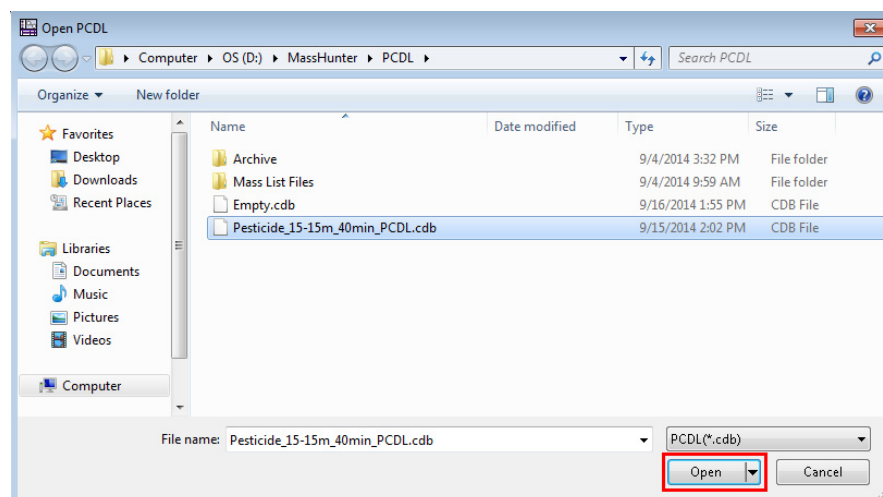
Exercise 1. Search the PCDL

Start the PCDL manager program

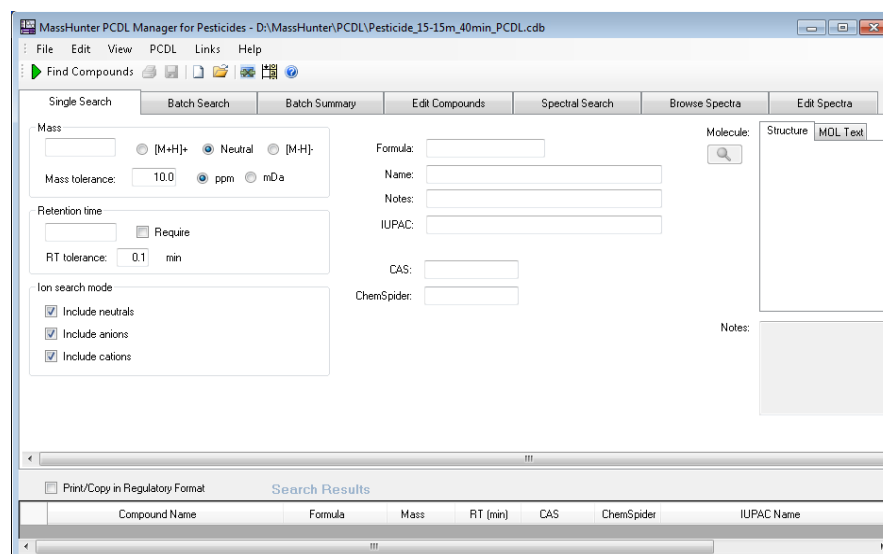
1. Start the **MassHunter PCDL Manager** by double-clicking the desktop icon.
2. From **D:\MassHunter\PCDL**, open the PCDL, **Pesticide_15-15m_40min_PCDL.cdb**.

In this exercise, you will search for compounds in the PCDL.

The MassHunter PCDL Manager lets you edit, search, and create PCDLs. It also lets you search and store spectra acquired on a Q-TOF instrument.



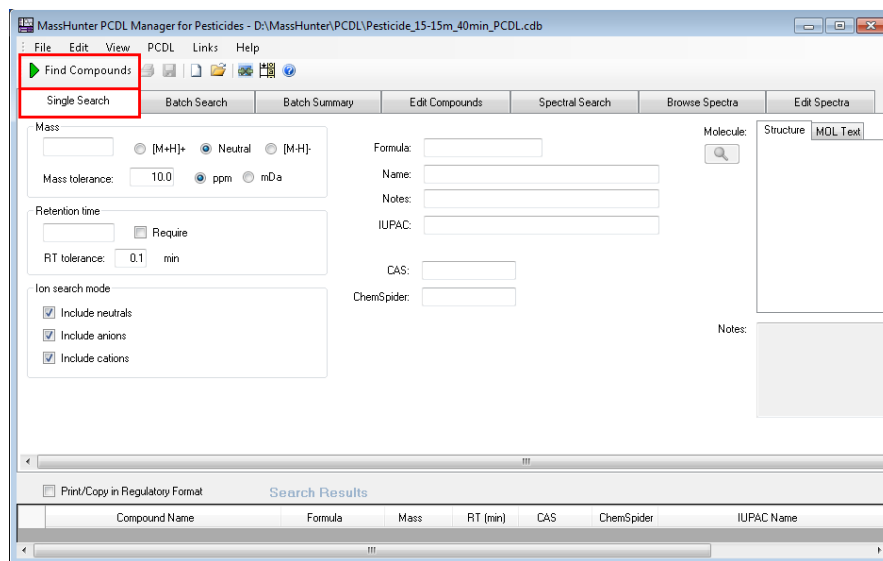
The MassHunter PCDL Manager opens.



Browse compounds in the PCDL

1. Click **Single Search**.
2. Click **Find Compounds**.

Use this procedure to display the entire PCDL and view the information that is contained in the database for the selected compounds.



All compounds in the PDCL are displayed in the **Single Search Results** table.

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	
2-Methylphenol	C7H8O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.098	95-48-7	13835772	2-Methylphenol
4-Methylphenol	C7H8O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.250	106-44-5	13839082	4-methylphenol
2,4-Dimethylphenol (2,4-Xylenol)	C8H10O	122.07316	<input type="checkbox"/>	<input type="checkbox"/>	4.955	105-67-9	13839123	2,4-dimethylphenol
Naphthalene	C10H8	128.06260	<input type="checkbox"/>	<input type="checkbox"/>	5.544	91-20-3	906	Naphthalene
Nitrophenol, 4-	C6H5NO3	139.02694	<input type="checkbox"/>	<input type="checkbox"/>	10.843	100-02-7	955	4-Nitrophenol
Methamidophos (Metamidophos)	C2H8NO2PS	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.885	10265-92-6	3954	O,S-Dimethyl phosphorothioic diisopropylamide
1-Naphthol (Naphthol, 1-)	C10H8O	144.05751	<input type="checkbox"/>	<input type="checkbox"/>	10.508	90-15-3	6739	1-Naphthol
Paradichlorobenzene (Benzene, 1,4-dichloro-)	C6H4Cl2	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.880	106-46-7	13856817	1,4-Dichlorobenzene
1,3-Dichlorobenzene	C6H4Cl2	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.832	541-73-1	13857694	1,3-Dichlorobenzene
Phthalimide	C8H5NO2	147.03203	<input type="checkbox"/>	<input type="checkbox"/>	9.588	85-41-6	6550	1H-isoindole-1-one
Propyl cresol	C10H14O	150.10447	<input type="checkbox"/>	<input type="checkbox"/>	6.705	89-83-8	21105998	Thymol

- Click on a compound in the **Single Search Results** table.

When the structure is included in the PCDL, it is displayed the **Structure** window.

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
2-Phenylphenol (Dithioesters/phenol)	C12H10O	170.07316	<input type="checkbox"/>	<input type="checkbox"/>	10.680	50-43-7	13823012	2-Phenylphenol	1
3,5-Dichloroaniline	C6H3Cl2N	186.97990	<input type="checkbox"/>	<input type="checkbox"/>	8.600	58-43-7	11778	3,5-Dichloroaniline	1
Acenathrin (Rufast)	C26H21FN2O5	541.13239	<input type="checkbox"/>	<input type="checkbox"/>	30.700	101007-06-1	10453290	Cyano[3-phenoxycarbonyl(methyl 3-(1,2,3-tri-1,1,3...]	1
Alachlor	C14H20ClN2O2	269.11826	<input type="checkbox"/>	<input type="checkbox"/>	18.420	15972-60-8	1394	2-Chloro-N-(2,6-dimethylphenyl)-N-methylpyrimidin-4-yl...	1
Azinetyn (Azinetyn)	C9H11N5S	227.12047	<input type="checkbox"/>	<input type="checkbox"/>	18.460	834-12-8	12705	N-Ethyl-N-isopropyl-6-(methylsulfanyl)-1,3,5-triazin-2-amine	1

Search for a single compound

- Click **Single Search**.
- In the **Formula** text box, type **C10H19N5O**.

Use this procedure to search the PCDL for a compound by its formula.

3. Click **Find Compounds**.

All compounds in the PCDL that match the formula are displayed in the **Single Search Results** table.

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Tebuneton	C10H19N5O	225.15886	<input type="checkbox"/>	<input type="checkbox"/>	15.560	33633-04-8	33617	N-Ethyl-6-methoxy-N-(2-methyl-2-propoxyethyl)-3,5-diaza-1,4-dioxane	1
Sebzuneton	C10H19N5O	225.15886	<input type="checkbox"/>	<input type="checkbox"/>	16.630	26293-45-0	30981	N-sec-Butyl-N'-ethyl-6-methoxy-1,3,5-triazine-2,4-diamine	1
Prometon	C10H19N5O	225.15886	<input type="checkbox"/>	<input type="checkbox"/>	15.170	1610-18-0	4759	N,N'-Diisopropyl-6-methoxy-1,3,5-triazine-2,4-diamine	1

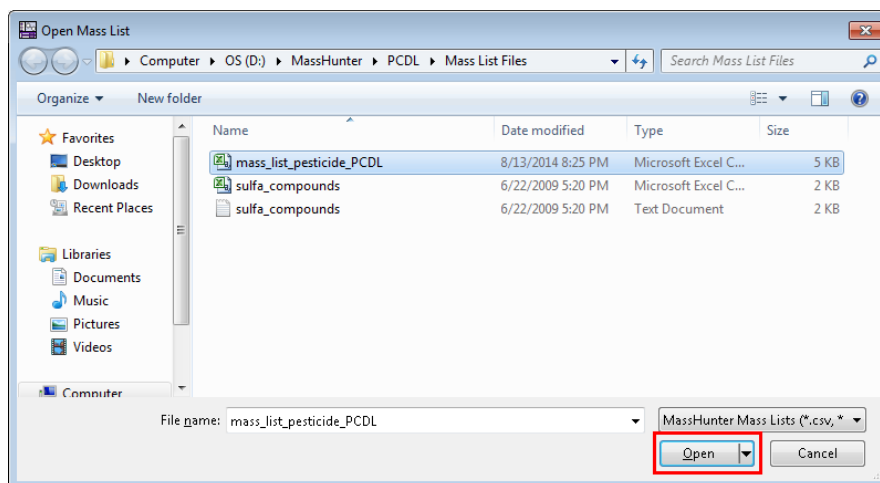
Search for compounds from a mass list

1. Click **Batch Search**.
2. Click **File**.

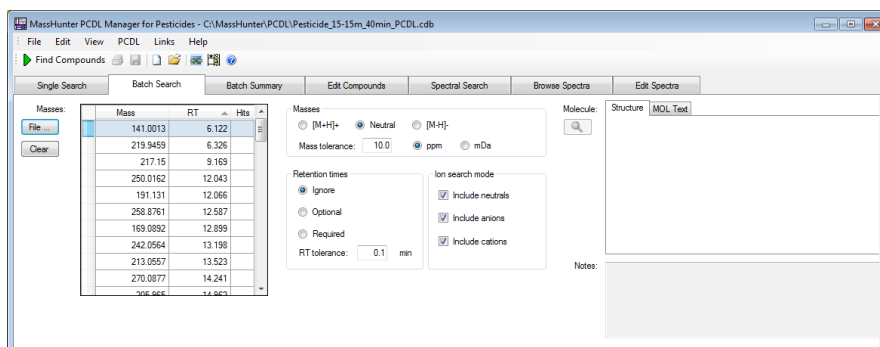
You can search for compounds from mass lists. Use this procedure to open a sample mass list exported from Qualitative Analysis.

Masses	Mass	RT	Hits

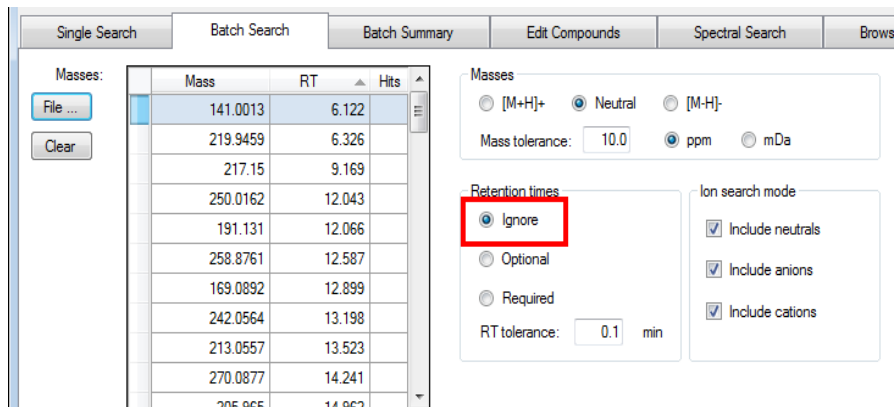
3. From **D:\MassHunter\PCDL\Mass List Files**, open the sample mass list file exported from MassHunter Qualitative Analysis, **mass_list_pesticide_PCDL.csv**.



The mass list opens in the MassHunter PCDL Manager.



4. In the **Retention times** section, select **Ignore**.



5. Click **Find Compounds**.

When the search is complete, the number of hits for each mass appears in the **Hits** column of the mass list table, and the list is automatically sorted to show the masses with the most hits at the top of the list.

Masses:	Mass	RT	Hits
<input type="button" value="File ..."/>	201.0781	15.393	5
<input type="button" value="Clear"/>	294.0327	21.509	3
	225.159	16.816	3
	225.159	15.736	3
	225.159	15.736	3
	225.0824	19.311	2
	279.1471	18.797	2
	241.1361	18.834	2
	241.1361	19.25	2
	317.9537	23.87	2
	279.1367	26.262	2

6. Click on a row in the mass list table to display the compounds found for that mass in the **Batch Search Results** table.

Best	Compound Name	Formula	Mass	Delta	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
<input type="checkbox"/>	Terbutylazine-desethyl	C7H12ON5	201.07812	0.10	<input type="checkbox"/>	<input type="checkbox"/>	13.903	30125-63-4	97278	6-Chloro-N-(2-methyl-2-propenyl)-1,3,5-triazine-2,4...	1
<input type="checkbox"/>	Simazine	C7H12ON5	201.07812	0.10	<input type="checkbox"/>	<input type="checkbox"/>	15.112	122-34-9	5027	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	1
<input checked="" type="checkbox"/>	Sebutylazine-desethyl	C7H12ON5	201.07812	0.10	<input type="checkbox"/>	<input type="checkbox"/>	15.359	37019-18-4	4197234	N-sec-Butyl-6-chloro-1,3,5-triazine-2,4-diamine	1
<input type="checkbox"/>	Fenfuram	C12H11NO2	201.07898	4.38	<input type="checkbox"/>	<input type="checkbox"/>	16.553	24631-80-3	81792	2-Methyl-N-phenyl-3-furamide	1
<input type="checkbox"/>	Carbaryl	C12H11NO2	201.07898	4.38	<input type="checkbox"/>	<input type="checkbox"/>	18.269	63-25-2	5899	1-Naphthyl methylcarbamate	1

7. Click on a compound in the **Batch Search Results** table.

When the structure is included in the PCDL, it is displayed the **Structure** window.

Best	Compound Name	Formula	Mass	Delta	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
<input type="checkbox"/>	Terbutylazine-desethyl	C7H12ON5	201.07812	0.10	<input type="checkbox"/>	<input type="checkbox"/>	13.903	30125-63-4	97278	6-Chloro-N-(2-methyl-2-propenyl)-1,3,5-triazine-2,4...	1
<input type="checkbox"/>	Simazine	C7H12ON5	201.07812	0.10	<input type="checkbox"/>	<input type="checkbox"/>	15.112	122-34-9	5027	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	1
<input checked="" type="checkbox"/>	Sebutylazine-desethyl	C7H12ON5	201.07812	0.10	<input type="checkbox"/>	<input type="checkbox"/>	15.359	37019-18-4	4197234	N-sec-Butyl-6-chloro-1,3,5-triazine-2,4-diamine	1
<input type="checkbox"/>	Fenfuram	C12H11NO2	201.07898	4.38	<input type="checkbox"/>	<input type="checkbox"/>	16.553	24631-80-3	81792	2-Methyl-N-phenyl-3-furamide	1
<input type="checkbox"/>	Carbaryl	C12H11NO2	201.07898	4.38	<input type="checkbox"/>	<input type="checkbox"/>	18.269	63-25-2	5899	1-Naphthyl methylcarbamate	1

- Click **Batch Summary** to view only the best hits from the **Batch Search Results** table.

MassHunter PCDL Manager for Pesticides - C:\MassHunter\PCDL\Pesticide_15-15m_40min_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search **Batch Summary** Edit Compounds Spectral Search Browse Spectra Edit Spectra

Report comments:

Mass list search parameters
Mass list file: C:\MassHunter\PCDL\Mass List Files\mass_list_pesticide_PCDL.csv
Masses: +/- 10.0 ppm Neutral Search: Neutrals Anions Cations

Retention time parameters
RTs: +/- 0.1 min (ignore)

Best mass match results
Total hits: 69 / 69 (100.0%)
Conflicting hits: 0 / 69 (0%)
Single matches: 58 / 69 (84.1%)

Molecule: Structure MOL Text

Notes: Pesticide
Synonyms: sebutylazine-desethyl

Print/ Copy in Regulatory Format

Batch Summary Results: 64 hits (69 total hits, 58 single matches, 69 submitted)

Compound Name	Formula	Mass	Mass	Delta	Anion	Cation	RT (min)	RT meas.	Delta RT	CAS	ChemSpider	IUPAC N
Sebutylazine-desethyl	C7H12ON5	201.07812	201.07810	0.10	<input type="checkbox"/>	<input type="checkbox"/>	15.359	15.393	-0.034	37019-18-4	4197234	N-sec-Butyl-6-chloro-1,3,5
Methiocarb (Mercaptodimethur)	C11H15NO2S	225.08235	225.08240	-0.22	<input type="checkbox"/>	<input type="checkbox"/>	19.155	19.311	-0.156	2032-85-7	15417	3,5-Dimethyl-4-(methylsulfo
Mefenoxam	C15H21NO4	279.14706	279.14710	-0.14	<input type="checkbox"/>	<input type="checkbox"/>	18.643	18.797	-0.154	70630-17-0	9325271	Methyl N-(2,6-dimethylphe
Terbutyn	C10H19NS	241.13612	241.13610	0.08	<input type="checkbox"/>	<input type="checkbox"/>	19.105	19.250	-0.145	886-50-0	12874	N-Ethyl-N-(2-methyl-2-prop

Browse all spectra in the PCDL

- Click **Browse Spectra**.
- Using the default search criteria, click **Find Spectra**.

Use this procedure to search an example library for spectra that match certain parameters, such as mass, formula, name, and RT.

MassHunter PCDL Manager for Pesticides - C:\MassHunter\Pesticide 15-15m 40min PCDL.cdb

File Edit View PCDL Links Help

Find Spectra

Single Search Batch Search Batch Summary Edit Compounds Spectral Search **Browse Spectra** Edit Spectra

Mass
Precursor ion:
Tolerance: 200 ppm mDa

Collision energy
Tolerance: 2.0 eV

Ion polarity: (Any)
Ionization mode: (Any)

Spectral Search Results: 748 hits

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ionization
2,4-Dimethylphenol (2,4-Xylenol)			0	Positive	EI
Nitrophenol 4-			0	Positive	FI

Graphic | Mass List

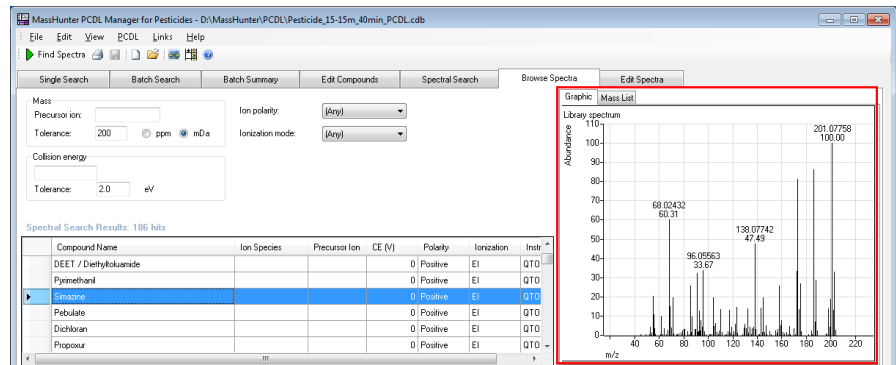
Library spectrum

Abundance

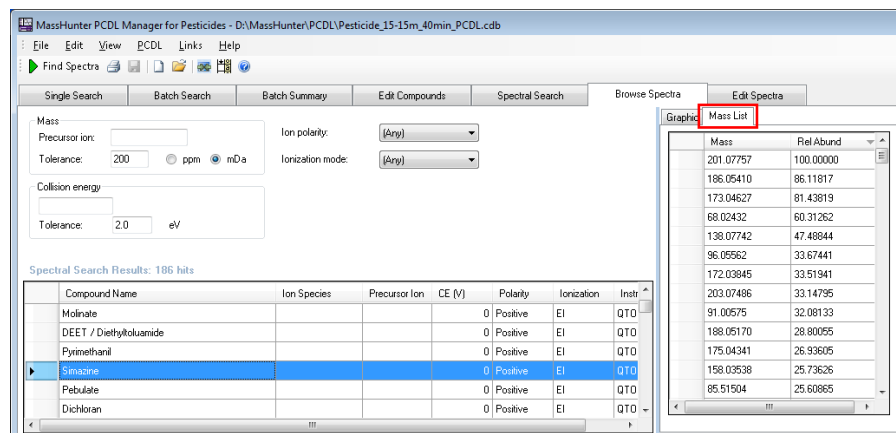
72.98807
100.00

All spectra in the PCDL are displayed in the **Spectral Search Results** table.

- Click on a compound in the **Spectral Search Results** table to view the mass spectrum plot in the **Graphic** window.



- Click **Mass List** to view a list of masses and abundance values for the selected compound.



Search for a specific spectrum

- Click **Single Search**.
- In the **Formula** text box, type **C25H22ClNO3**.

Use this procedure to search for specific spectra in the PCDL.

Single Search | Batch Search | Batch Summary | Edit Compounds | Spectral Search

Mass: [] [M+H]⁺ Neutral [M-H]⁻

Mass tolerance: 10.0 ppm mDa

Retention time: [] Require

RT tolerance: 0.1 min

Ion search mode

Include neutrals

Include anions

Include cations

Formula: **C25H22ClNO3**

Name: []

Notes: []

IUPAC: []

CAS: []

ChemSpider: []

3. Click **Find Compounds**.

All compounds in the PCDL that match the formula are displayed in the **Single Search Results** table.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\Pesticide_15-15m_40min_PCDL.cdb

Find Compounds

Single Search | Batch Search | Batch Summary | Edit Compounds | Spectral Search | Browse Spectra | Edit Spectra

Mass: [M-H]⁺ Neutral [K-H]⁺ Formula: C25H22ClNO3

Mass tolerance: 10.0 ppm mDa Name:

Retention time: Require IUPAC:

RT tolerance: 0.1 min CAS:

Ion search mode: Include neutrals Include anions Include cations ChemSpider:

Structure:

Notes:

Print/Copy in Regulatory Format Single Search Results: 2 hits

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Fenvalerate	C25H22ClNO3	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.100	51630-58-1	3230	(S)-Cyano(3-phenoxyphenyl)methyl (2S)-2-(4-chloro...	1
Efenvalerate	C25H22ClNO3	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.500	68230-04-4	8517510	(S)-Cyano(3-phenoxyphenyl)methyl (2S)-2-(4-chloro...	1

4. Click **Browse Spectra**.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Pesticide_15-15m_40min_PCDL.cdb

Find Spectra | Browse Spectra | Edit Spectra

Mass: Ion polarity: (Any) Tolerance: 200 ppm mDa Ionization mode: (Any) Collision energy: Tolerance: 2.0 eV

Spectra for compound: Fenvalerate

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ionization
Fenvalerate			0	Positive	EI

Graphic: Mass List

Library spectrum

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Fenvalerate	C25H22ClNO3	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.100	51630-58-1	3230	(S)-Cyano(3-phenoxyphenyl)methyl (2S)-2-(4-chloro...	1
Efenvalerate	C25H22ClNO3	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.500	68230-04-4	8517510	(S)-Cyano(3-phenoxyphenyl)methyl (2S)-2-(4-chloro...	1

5. Select the compound **Efenvalerate** and view the mass spectrum plot in the **Graphic** window.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Pesticide_15-15m_40min_PCDL.cdb

Find Spectra | Browse Spectra | Edit Spectra

Mass: Ion polarity: (Any) Tolerance: 200 ppm mDa Ionization mode: (Any) Collision energy: Tolerance: 2.0 eV

Spectra for compound: Efenvalerate

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ionization
Efenvalerate			0	Positive	EI

Graphic: Mass List

Library spectrum

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Fenvalerate	C25H22ClNO3	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.100	51630-58-1	3230	(S)-Cyano(3-phenoxyphenyl)methyl (2S)-2-(4-chloro...	1
Efenvalerate	C25H22ClNO3	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.500	68230-04-4	8517510	(S)-Cyano(3-phenoxyphenyl)methyl (2S)-2-(4-chloro...	1

6. Click **Mass List** to view a list of masses and abundance values.

The screenshot shows the MassHunter PCDL Manager for Pesticides interface. The 'Mass List' window is open, displaying a table of mass values and relative abundances. The table is as follows:

Mass	Rel. Abund.
125.01525	100.00000
181.06479	48.57350
167.06220	44.85603
169.06479	43.65105
225.07843	42.45341
115.05423	37.69688
127.01255	33.22563
141.06988	32.45127
199.06753	29.47695
77.03858	27.57466
197.05971	27.39615
152.00234	24.53469
209.08352	21.23640

Below the mass list, there is a table for 'Spectra for compound: Esfenvalerate' and a main table with columns: Compound Name, Formula, Mass, Anion, Cation, RT (min), CAS, ChemSpider, and IUPAC Name.

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name
Fenvalerate	C ₂₅ H ₂₂ OIN ₃	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.100	51630-58-1	3230	(S)-Cyanol(3-phenoxyphenyl)methyl (2S)-2-(4-chlorophenyl)acrylate
Esfenvalerate	C ₂₅ H ₂₂ OIN ₃	419.12882	<input type="checkbox"/>	<input type="checkbox"/>	35.500	66230-04-4	8517510	(S)-Cyanol(3-phenoxyphenyl)methyl (2S)-2-(4-chlorophenyl)acrylate

Exercise 2. Create a Custom PCDL in the PCDL Manager

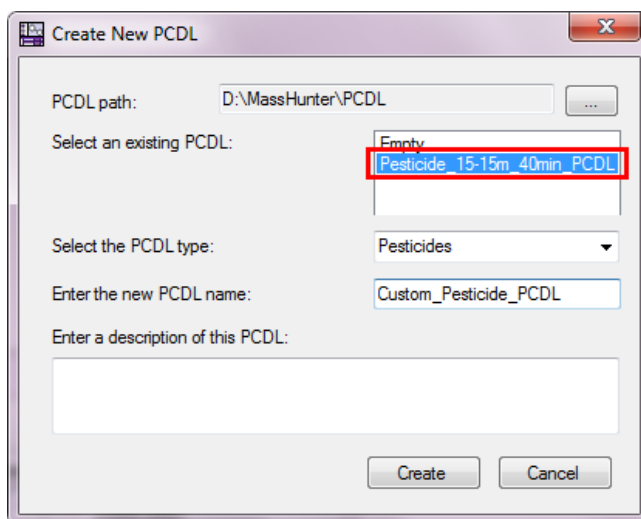
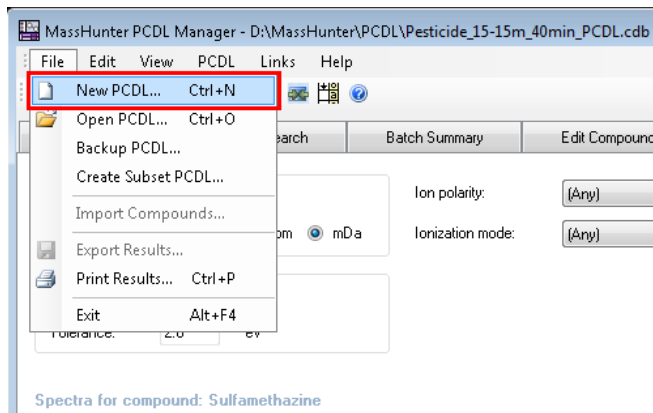
Create a new PCDL

1. Select **File > New PCDL**.

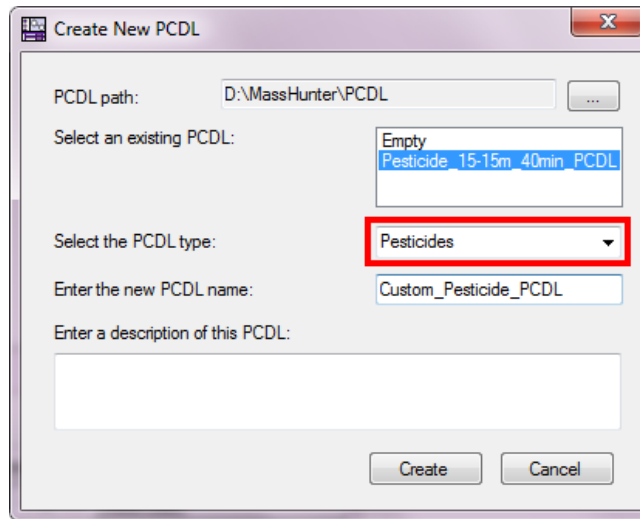
2. Select the existing PCDL, **Pesticide_15-15m_40min_PCDL**.

In this exercise, you will create a custom PCDL that is a subset of the GC/Q-TOF Pesticides PCDL.

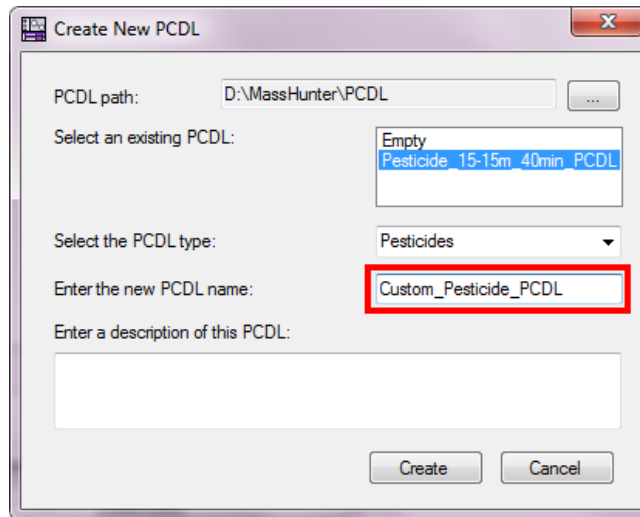
Master PCDLs cannot be edited, but they can be used to create custom PCDLs that can be edited. Use this procedure to create a new custom PCDL.



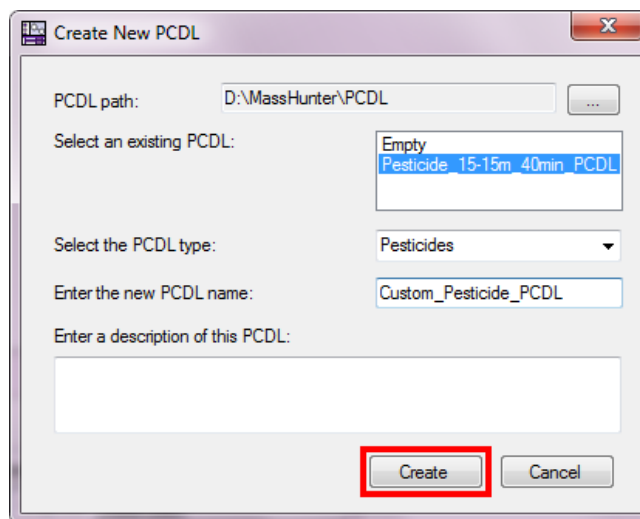
3. Select the PCDL type, **Pesticides**.

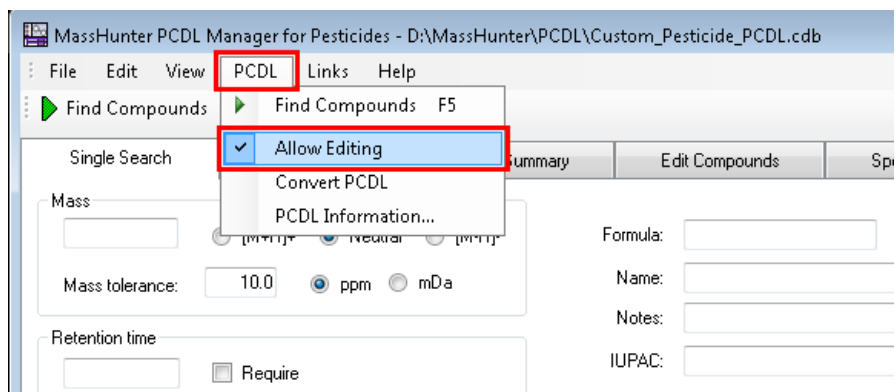


4. Enter the new PCDL name, **Custom_Pesticide_PCDL**.



5. Click **Create**.

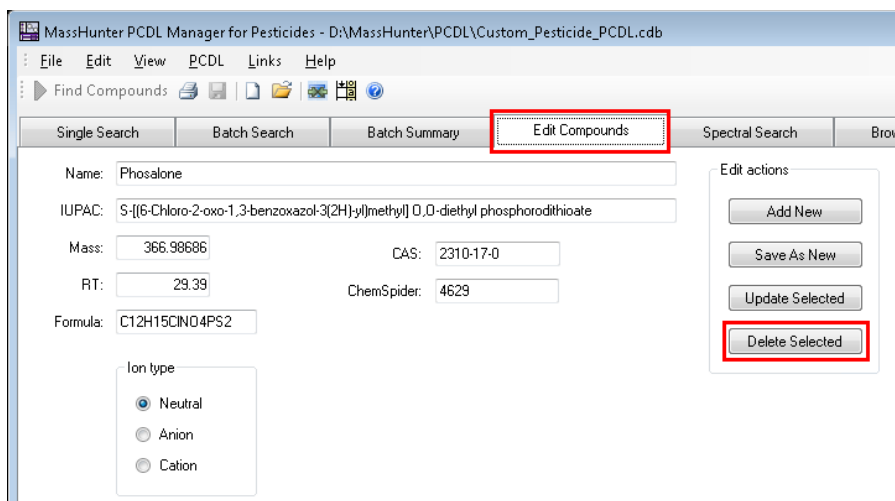
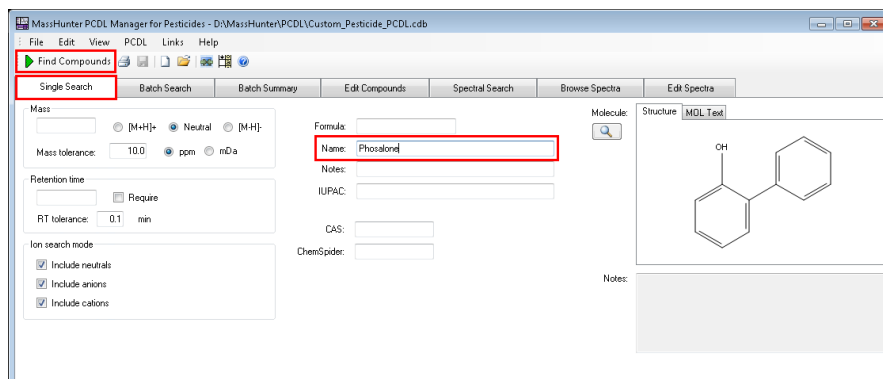


6. Select **PCDL > Allow Editing**.

Delete a specific compound

1. Click **Single Search**.
2. In the **Name** text box, type Phosalone, and then click **Find Compounds**.
3. Click **Edit Compounds**.
4. Click **Delete Selected** and then click **Yes** to confirm.

Use this procedure to search for and delete a specific compound.



Delete a group of compounds

1. Click **Single Search**.
2. Using the default search criteria, click **Find Compounds**.

Use this procedure to delete a group compounds from your custom PCDL based on mass.

All compounds in the PCDL are displayed in the **Single Search Results** table.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Mass: [] [M+H]⁺ Neutral [M-H]⁻ Formula: [] Molecule: Structure MOL

Mass tolerance: 10.0 ppm mDa Name: []

Retention time: [] Require IUPAC: []

RT tolerance: 0.1 min CAS: []

Ion search mode ChemSpider: []

Include neutrals

Include anions

Include cations

Notes: []

Print/Copy in Regulatory Format Single Search Results: 750 hits

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	
2-Methylphenol	C7H8O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.098	95-48-7	13835772	2-Methylpheno
4-Methylphenol	C7H8O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.250	106-44-5	13839082	4-methylpheno
2,4-Dimethylphenol (2,4-Xylenol)	C8H10O	122.07316	<input type="checkbox"/>	<input type="checkbox"/>	4.955	105-67-9	13839123	2,4-dimethylph
Naphthalene	C10H8	128.06260	<input type="checkbox"/>	<input type="checkbox"/>	5.544	91-20-3	906	Naphthalene
Nitrophenol, 4-	C6H5NO3	139.02694	<input type="checkbox"/>	<input type="checkbox"/>	10.843	100-02-7	955	4-Nitrophenol
Methamidophos (Metamidophos)	C2H8NO2PS	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.885	10265-92-6	3954	O,S-Dimethyl p
1-Naphthol (Naphthol, 1-)	C10H8O	144.05751	<input type="checkbox"/>	<input type="checkbox"/>	10.508	90-15-3	6739	1-Naphthol
Paradichlorobenzene (Benzene, 1,4-dichloro-)	C6H4Cl2	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.880	106-46-7	13866817	1,4-Dichlorobe
1,3-Dichlorobenzene	C6H4Cl2	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.832	541-73-1	13857694	1,3-Dichloroben
Phthalamide	C8H5NO2	147.03203	<input type="checkbox"/>	<input type="checkbox"/>	9.588	85-41-6	6550	1H-isoindole-1
Propyl cresol	C10H14O	150.10447	<input type="checkbox"/>	<input type="checkbox"/>	6.705	89-83-8	21105998	Thymol

3. Click **Edit Compounds**.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Name: Boscalid (Nicobifen) Edit actions: Add New Save As New Update Selected Delete Selected

IUPAC: 2-Chloro-N-(4'-chloro-2-biphenyl)tricolonamide Molecule: Structure MOL Text

Mass: 342.03267 CAS: 189425-95-6

RT: 33.36 ChemSpider: 184713

Formula: C18H12Cl2N2O

Ion type: Neutral Anion Cation

Notes: []

Print/Copy in Regulatory Format Single Search Results: 186 hits

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spect
2-Phenylphenol (Orthophenylphenol)	C12H10O	170.07316	<input type="checkbox"/>	<input type="checkbox"/>	10.680	90-43-7	13839012	2-Phenylphenol	1
3,5-Dichloroaniline	C6H5Cl2N	160.97990	<input type="checkbox"/>	<input type="checkbox"/>	8.600	626-43-7	11778	3,5-dichloroaniline	1
Acinathrin (Pufast)	C26H21FN5O5	541.13239	<input type="checkbox"/>	<input type="checkbox"/>	30.700	101007-06-1	10463290	Cyano(3-phenoxycarbonyl)methyl 3-((1Z)-3-((1,1,1,3,3,3-hexafluoroisopropoxy)methyl)propanoate)	1
Alachlor	C14H20ClNO2	269.11826	<input type="checkbox"/>	<input type="checkbox"/>	18.420	15872-60-8	1394	2-Chloro-N-(2,6-diethylphenyl)N-(methoxymethyl)propanamide	1
Ametryne (Ametrex)	C9H17N5S	227.12047	<input type="checkbox"/>	<input type="checkbox"/>	18.460	834-12-8	12705	N-EthylN'-isopropyl-6-(methylsulfonyl)-1,3,5-triazin-2-amine	1

- Click the **Mass** column heading in the **Single Search Results** table to sort the compounds by their mass from lowest to highest.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Br

Name: Boscalid (Nicobifen)

IUPAC: 2-Chloro-N-(4'-chloro-2-biphenyl)nicotinamide

Mass: 342.03267 CAS: 188425-85-6

RT: 33.36 ChemSpider: 184713

Formula: C18H12Cl2N2O

Ion type

Neutral
 Anion
 Cation

Edit actions

Add New
Save As New
Update Selected
Delete Selected

Print/Copy in Regulatory Format Single Search Results: 186 hits

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS
Methamidophos (Metamidophos)	C2H8NO2PS	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.890	10265-92-6
Biphenyl	C12H10	154.07825	<input type="checkbox"/>	<input type="checkbox"/>	8.270	92-52-4
3,5-Dichloroaniline	C6H5Cl2N	160.97990	<input type="checkbox"/>	<input type="checkbox"/>	8.600	626-43-7
Diphenylamine	C12H11N	169.08915	<input type="checkbox"/>	<input type="checkbox"/>	12.730	122-39-4
2-Phenylphenol (Orthophenylphenol)	C12H10O	170.07316	<input type="checkbox"/>	<input type="checkbox"/>	10.680	90-43-7
Molinate	C9H17NOS	187.10308	<input type="checkbox"/>	<input type="checkbox"/>	11.070	2212-67-1
DEET / Diethyltoluamide	C12H17NO	191.13101	<input type="checkbox"/>	<input type="checkbox"/>	11.900	134-62-3
Pyrimethanil	C12H13N3	199.11095	<input type="checkbox"/>	<input type="checkbox"/>	16.160	53112-28-0
Simazine	C7H12ClN5	201.07812	<input type="checkbox"/>	<input type="checkbox"/>	15.110	122-34-9
Deltamethrin	C18H19Cl2O2	295.12220	<input type="checkbox"/>	<input type="checkbox"/>	9.690	1114-71-3

- Select all compounds with masses less than 165.

Print/Copy in Regulatory Format Single Search Results: 186 hits

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS
Methamidophos (Metamidophos)	C2H8NO2PS	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.890	10265-92-6
Biphenyl	C12H10	154.07825	<input type="checkbox"/>	<input type="checkbox"/>	8.270	92-52-4
3,5-Dichloroaniline	C6H5Cl2N	160.97990	<input type="checkbox"/>	<input type="checkbox"/>	8.600	626-43-7
Diphenylamine	C12H11N	169.08915	<input type="checkbox"/>	<input type="checkbox"/>	12.730	122-39-4
2-Phenylphenol (Orthophenylphenol)	C12H10O	170.07316	<input type="checkbox"/>	<input type="checkbox"/>	10.680	90-43-7
Molinate	C9H17NOS	187.10308	<input type="checkbox"/>	<input type="checkbox"/>	11.070	2212-67-1
DEET / Diethyltoluamide	C12H17NO	191.13101	<input type="checkbox"/>	<input type="checkbox"/>	11.900	134-62-3
Pyrimethanil	C12H13N3	199.11095	<input type="checkbox"/>	<input type="checkbox"/>	16.160	53112-28-0
Simazine	C7H12ClN5	201.07812	<input type="checkbox"/>	<input type="checkbox"/>	15.110	122-34-9
Deltamethrin	C18H19Cl2O2	295.12220	<input type="checkbox"/>	<input type="checkbox"/>	9.690	1114-71-3

6. Click **Delete Selected** and then click **Yes** to confirm.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary **Edit Compounds** Spectral Search Browse

Name: 3,5-Dichloroaniline

IUPAC:

Mass: 160.97990 CAS: 626-43-7

RT: 8.6 ChemSpider:

Formula: C₆H₅Cl₂N

Ion type

Neutral
 Anion
 Cation

Edit actions

Add New
Save As New
Update Selected
Delete Selected

Print/Copy in Regulatory Format **Single Search Results: 186 hits**

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS
Methamidophos (Metamidophos)	C ₂ H ₈ NO ₂ PS	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.890	10265-92-6
Biphenyl	C ₁₂ H ₁₀	154.07825	<input type="checkbox"/>	<input type="checkbox"/>	8.270	92-52-4
3,5-Dichloroaniline	C₆H₅Cl₂N	160.97990	<input type="checkbox"/>	<input type="checkbox"/>	8.600	626-43-7
Diphenylamine	C ₁₂ H ₁₁ N	169.08915	<input type="checkbox"/>	<input type="checkbox"/>	12.730	122-39-4
2-Phenylphenol (Orthophenylphenol)	C ₁₂ H ₁₀ O	170.07316	<input type="checkbox"/>	<input type="checkbox"/>	10.680	90-43-7
Molinate	C ₉ H ₁₇ NO ₃	187.10308	<input type="checkbox"/>	<input type="checkbox"/>	11.070	2212-67-1

The selected compounds are removed from your custom PCDL.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary **Edit Compounds** Spectral Search Browse Spectra Edit Spectra

Name: Diphenylamine

IUPAC: N-Phenylaniline

Mass: 169.08915 CAS: 122-39-4

RT: 12.73 ChemSpider: 11003

Formula: C₁₂H₁₁N

Ion type

Neutral
 Anion
 Cation

Edit actions

Add New
Save As New
Update Selected
Delete Selected

Molecule: Structure MOL Text

Nc1ccc(cc1)-c2ccccc2

Notes:

Print/Copy in Regulatory Format **Single Search Results: 186 hits**

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Diphenylamine	C₁₂H₁₁N	169.08915	<input type="checkbox"/>	<input type="checkbox"/>	12.730	122-39-4	11003	N-Phenylaniline	1
2-Phenylphenol (Orthophenylphenol)	C ₁₂ H ₁₀ O	170.07316	<input type="checkbox"/>	<input type="checkbox"/>	10.680	90-43-7	13839012	2-Biphenylol	1
Molinate	C ₉ H ₁₇ NO ₃	187.10308	<input type="checkbox"/>	<input type="checkbox"/>	11.070	2212-67-1	15790	S-Ethyl 1-azepanecarboxylate	1
DEET / Diethyltoluamide	C ₁₂ H ₁₇ NO	191.13101	<input type="checkbox"/>	<input type="checkbox"/>	11.900	134-63-3	4133	N,N-Diethyl-3-methylbenzamide	1
Pyrimethanil	C ₇ H ₁₂ NO ₃	199.11095	<input type="checkbox"/>	<input type="checkbox"/>	16.160	53112-28-0	82783	4,6-Dimethyl-N-phenyl-2-pyrimidinamine	1
Sinazine	C ₇ H ₁₂ NO ₅	201.07812	<input type="checkbox"/>	<input type="checkbox"/>	15.110	122-34-9	5022	6-Chloro-N,N-diethyl-1,3,5-thiazine-2,4-diamine	1
Perbutate	C ₁₀ H ₂₁ NO ₅	203.13439	<input type="checkbox"/>	<input type="checkbox"/>	9.620	1114-71-2	13579	S-Propyl butylethylcarbamothioate	1
Dichloran	C ₆ H ₄ Cl ₂ N ₂ O ₂	205.96498	<input type="checkbox"/>	<input type="checkbox"/>	14.780	99-30-9	7152	2,6-Dichloro-4-nitroaniline	1
Propoxur	C ₁₁ H ₁₅ NO ₃	209.10519	<input type="checkbox"/>	<input type="checkbox"/>	12.580	114-26-1	4775	2-Isopropoxyphenyl methylcarbamate	1
Dichlorodimethylamine	C ₂ H ₇ Cl ₂ N	216.00000	<input type="checkbox"/>	<input type="checkbox"/>	15.200	66300-24-3	10796	1,1-Dichloro-2,2-dimethylhydrazine	1

Add a compound

1. Click **Edit Compounds**.
2. Click **Add New**.

Use this procedure to add a compound to your custom PCDL.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary **Edit Compounds** Spectral Search Browse Spectra Edit Spectra

Name: Isazofos (Miral)

IUPAC: O-(5-Chloro-1-isopropyl-1H-1,2,4-triazol-3-yl) O,D-diethyl phosphorothioate

Mass: 313.04168 CAS: 42509-80-8

RT: 16.89 ChemSpider: 35885

Formula: C9H17ClN3O3PS

Ion type

Neutral
 Anion
 Cation

Edit actions

Add New
 Save As New
 Update Selected
 Delete Selected

Molecule: Structure MOL Text

Notes:

New Compound is added to the table with a mass of 0.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary **Edit Compounds** Spectral Search Browse Spectra

Name: New Compound

IUPAC:

Mass: 0.00000 CAS:

RT: ChemSpider:

Formula:

Ion type

Neutral
 Anion
 Cation

Edit actions

Add New
 Save As New
 Update Selected
 Delete Selected

Molecule: Structure MOL Text

Notes:

Print/Copy in Regulatory Format

Compound Name	Formula	Mass	Mass Submitted	Delta Mass (ppm)	Anion	Cation
New Compound		0.00000			<input type="checkbox"/>	<input type="checkbox"/>

3. Enter the compound information:

Name: Dazomet
Mass: 162.02854
RT: 14.713
Formula: C5H10N2S2
Ion type: Neutral
CAS: 533-74-4

4. Click **Update Selected**.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Br

Name: Dazomet

IUPAC:

Mass: 162.02854 CAS: 533-74-4

RT: 14.713 ChemSpider:

Formula: C5H10N2S2

Ion type

Neutral
 Anion
 Cation

Edit actions

Add New
Save As New
Update Selected
Delete Selected

Print/Copy in Regulatory Format

Compound Name	Formula	Mass	Mass Submitted	Delta Mass (ppm)	Anic
New Compound		0.00000			

The information you entered for the new compound is added to the table and the custom PCDL.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Name: Dazomet

IUPAC:

Mass: 162.02854 CAS: 533-74-4

RT: 14.713 ChemSpider:

Formula: C5H10N2S2

Ion type

Neutral
 Anion
 Cation

Edit actions

Add New
Save As New
Update Selected
Delete Selected

Molecule: Structure MOL Text

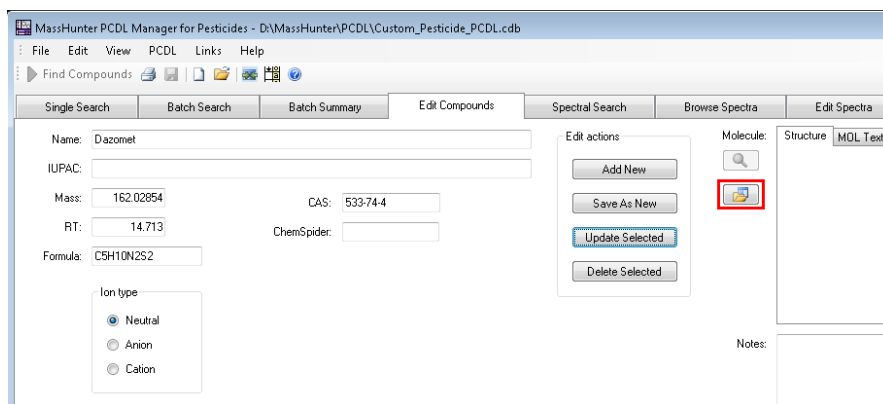
Notes:

Print/Copy in Regulatory Format

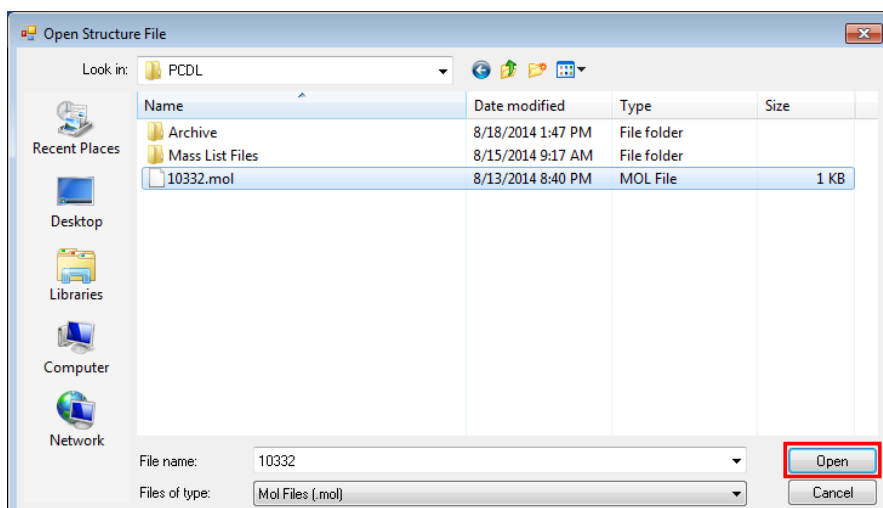
Batch Search Results: 2 hits for Mass: 241.1361 RT: 19.25

Compound Name	Formula	Mass	Delta Mass (ppm)	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Tebutyn	C10H19N5S	241.1...	0.08	<input type="checkbox"/>	<input type="checkbox"/>	19.100	886-50-0	12874	N-Ethyl-N'-(2-methyl-2-propargyl-6-(methylsulfonyl)...	1
Prometryn	C10H19N5S	241.1...	0.08	<input type="checkbox"/>	<input type="checkbox"/>	18.620	7287-19-6	4760	N,N'-Diisopropyl-6-(methylsulfonyl)-1,3,5-triazine-2...	1
Dazomet	C5H10N2S2	162.0...		<input type="checkbox"/>	<input type="checkbox"/>	14.713	533-74-4	10332	3,5-Dimethyl-1,3,5-thiadiazine-2-thione	

5. Click **Open** to the left of the **Structure** window.



6. Navigate to and open **10332.mol**.



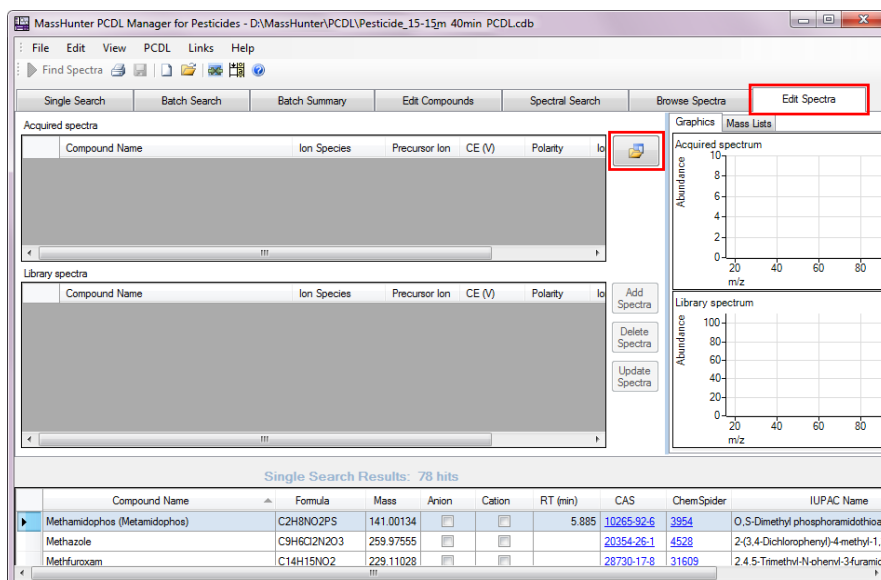
The structure is added to the PCDL and is displayed in the **Structure** window.

Compound Name	Formula	Mass	Mass Submitted	Delta Mass (ppm)	Anion	Cation	RT (min)	RT meas.	Delta RT
New Compound		0.00000			<input type="checkbox"/>	<input type="checkbox"/>			

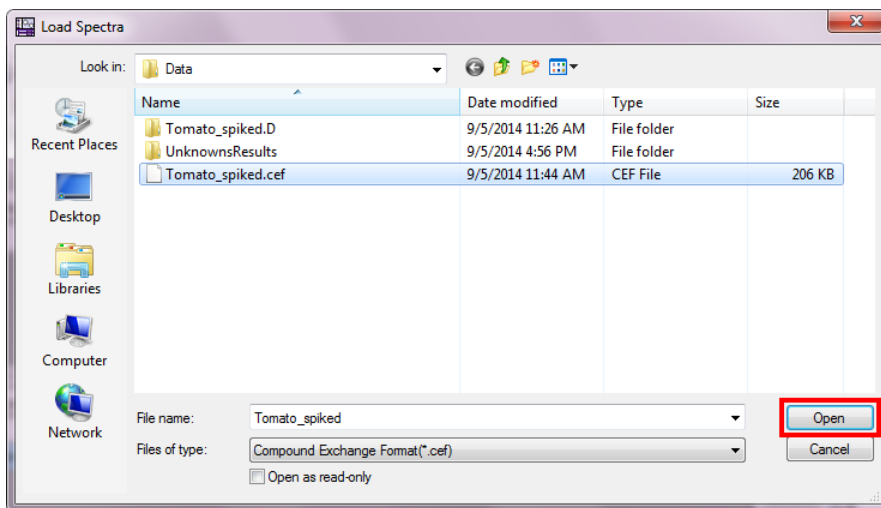
Import Spectra from a CEF file

1. Click **Edit Spectra**.
2. Click **Load Spectra from a CEF file**.

Use this procedure to import spectra from an existing CEF file. For information on exporting spectra and creating a CEF file, see ["Export your results as a CEF"](#) on page 52.



3. Select the CEF file from which to import spectra, and click **Open**.



The imported spectra appear in the **Acquired spectra** table.

The screenshot shows the MassHunter PCDL Manager interface. The 'Acquired spectra' table is highlighted with a red box and contains the following data:

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity
Methamidophos (Metamidophos)			0	Positive
Biphenyl			0	Positive
3,5-Dichloroaniline			0	Positive
Diphenylamine			0	Positive

The 'Library spectra' table below it contains:

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity
Methamidophos (Metamidophos)			0	Positive

At the bottom, a summary table shows the details for Methamidophos (Metamidophos):

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC
Methamidophos (Metamidophos)	C ₂ H ₈ N ₂ O ₂ P ₂ S	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.890	10263-92-6	3954	O,S-Dimethyl phosphor

Modify spectra

1. Click **Single Search**.
2. Using the default search criteria, click **Find Compounds**.

Information about spectra such as ion polarity, ionization mode, and instrument type cannot be edited. You can add, move, or remove spectra from a compound in a custom PCDL or remove small noise peak from spectra in a custom PCDL.

Use this procedure to remove small noise peaks from spectra before or after you add them to your custom PCDL.

All compounds in the PCDL are displayed in the **Single Search Results** table.

The screenshot shows the MassHunter PCDL Manager interface with the 'Single Search' tab selected. The 'Single Search Results' table is highlighted with a red box and contains the following data:

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider
2-Methylphenol	C ₇ H ₈ O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.098	95-48-7	13835772
4-Methylphenol	C ₇ H ₈ O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.250	106-44-5	13839082
2,4-Dimethylphenol (2,4-Xylenol)	C ₈ H ₁₀ O	122.07316	<input type="checkbox"/>	<input type="checkbox"/>	4.955	105-67-9	13839123
Naphthalene	C ₁₀ H ₈	128.06260	<input type="checkbox"/>	<input type="checkbox"/>	5.544	91-20-3	906
Nitrophenol, 4-	C ₆ H ₅ NO ₃	139.02894	<input type="checkbox"/>	<input type="checkbox"/>	10.843	100-62-7	955
Methamidophos (Metamidophos)	C ₂ H ₈ N ₂ O ₂ P ₂ S	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.895	10263-92-6	3954
1-Naphthol (Naphthol, 1-)	C ₁₀ H ₈ O	144.05751	<input type="checkbox"/>	<input type="checkbox"/>	10.508	90-15-3	6739
Paradichlorobenzene (Benzene, 1,4-dichloro-)	C ₆ H ₄ Cl ₂	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.880	106-46-7	13866817
1,3-Dichlorobenzene (Benzene, 1,3-dichloro-)	C ₆ H ₄ Cl ₂	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.832	541-73-1	13857694
Phthalimide	C ₈ H ₅ NO ₂	147.03203	<input type="checkbox"/>	<input type="checkbox"/>	9.588	85-41-6	6550
Propyl cresol	C ₁₀ H ₁₄ O	150.10447	<input type="checkbox"/>	<input type="checkbox"/>	6.705	89-83-8	21105998

3. Click **Edit Spectra**.
4. Click to select a compound from the **Single Search Results** table.

The spectra for that compound are displayed in the **Library spectra** table in the middle of the tab.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra **Edit Spectra**

Acquired spectra

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ion
[Empty]					

Library spectra

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ion
[Empty]					

Single Search Results: 105 hits

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Pyrimethanil	C12H13N3	199.11095			16.160	53112-28-0	82753	4,6-Dimethyl-N-phenyl-2-pyrimidinamine	1
Simazine	C7H12CN5	201.07812			15.110	122-34-9	9027	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	0
Pebulate	C10H21NDS	203.13439			9.620	1114-71-2	13579	S-Propyl butyl(ethyl)carbamothioate	1
Dichloran	CBH4CN2O2	205.96498			14.780	99-30-9	7152	2,6-Dichloro-4-nitroaniline	1
Proxar	C11H15NN3	209.11619			12.590	114-76-1	4775	2-Isononanonebutyl methylcarbamate	1

5. Select the spectrum of interest in the **Library spectra** table.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra **Edit Spectra**

Acquired spectra

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ion
[Empty]					

Library spectra

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ion
Simazine			0	Positive	EI

Acquired spectrum

Library spectrum

6. Click **Mass Lists**.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra **Mass Lists** Edit Spectra

Acquired masses

Mass	Rel Abund
[Empty]	

Library masses

Mass	Rel Abund
201.07757	100.00000
186.05410	86.11817
173.04627	81.43819
68.02432	60.31262
138.07742	47.48844
96.05562	33.67441
172.03845	33.51941
203.07486	33.14795
91.00575	32.08133
188.05170	28.80095
175.04341	26.93605
150.03538	25.73626
85.51504	25.60865

- Click the **Rel Abund** column header if you want the lowest relative abundance values (likely noise peaks) to appear at the top of the table.

Mass	Rel Abund
54.52709	0.00375
77.52420	0.00427
65.50971	0.00594
72.50910	0.00750
71.49867	0.00812
192.00686	0.01058
90.50942	0.01330
152.09335	0.01574
192.99878	0.02181
113.08322	0.02232
168.11153	0.02432
58.01878	0.02704
74.01510	0.03689

- Select the masses to delete by clicking on them in the **Acquired masses** or **Library masses** list. Use **Ctrl+click** or **Shift+click** to select multiple masses.

- Right-click in the **Acquired masses** or **Library masses** list and select **Delete Masses**.

Mass	Rel Abund
201.07757	100.00000
186.05410	86.11817
173.04627	81.43810
68.02432	60.3126
138.07742	47.48844
96.05562	33.67441
172.03845	33.51941
203.07486	33.14795
91.00575	32.08133
188.05170	28.80055
175.04341	26.93605
158.03538	25.73626
85.51504	25.60865

- Click **Update Spectra** to update the selected library compound with a modified library spectrum.

Delete spectra

1. Click **Edit Spectra**.
2. Click to select a compound from the **Single Search Results** table.

Use this procedure to delete spectra from a compound in your custom PCDL.

The spectra for that compound are displayed in the **Library spectra** table in the middle of the tab.

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ionized
Molinate			0	Positive	E1

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Molinate	C ₉ H ₁₇ N ₅ O ₂	187.10308			11.070	2212-82-1	15730	S-Ethyl 1-azepanecarboxoate	1

Mass	Rel Abund
126.09134	100.000
55.05423	56.5205
98.09543	24.5447
63.08553	19.3955
127.09463	7.83375
70.06513	6.51245
187.10254	5.65386
121.09479	5.56905
81.06389	5.06526
56.05529	3.37395
56.07309	3.24767
154.12264	3.00397
68.04949	2.87746

3. Click to select the spectrum of interest in the **Library spectra** table.
4. Click **Delete Spectra**.

Multiple spectra can be selected using **Ctrl+click** or **Shift+click**.

The **Library spectra** table will be updated to show the revised list of spectra for the compound.

Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	Ionized
Molinate			0	Positive	E1

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
Molinate	C ₉ H ₁₇ N ₅ O ₂	187.10308			11.070	2212-82-1	15730	S-Ethyl 1-azepanecarboxoate	1

Save your custom PCDL

Click **Update Selected** to apply the changes to the PCDL.

Use this procedure to save all the changes made to your custom PCDL.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\PCDL\Custom_Pesticide_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Bro

Name: Phosalone

IUPAC: S-[(6-Chloro-2-oxo-1,3-benzoxazol-3(2H)-yl)methyl] O,O-diethyl phosphorodithioate

Mass: 366.98686 CAS: 2310-17-0

RT: 29.39 ChemSpider: 4629

Formula: C12H15ClNO4PS2

Ion type

Neutral

Anion

Cation

Edit actions

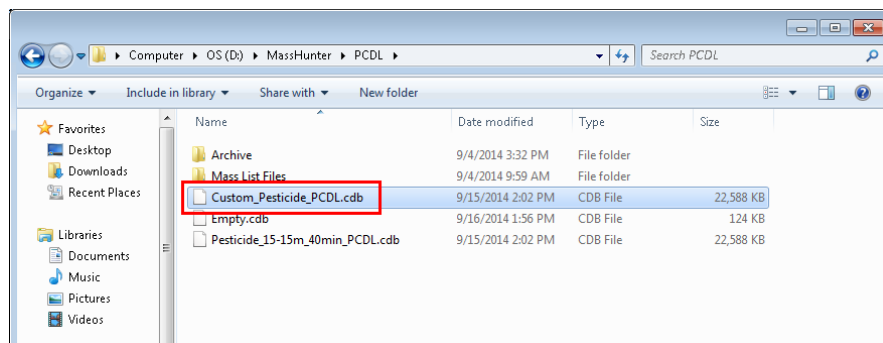
Add New

Save As New

Update Selected

Delete Selected

Your custom PCDL is saved in D:\MassHunter\PCDL and can be used in the PCDL Manager, as well as in the Qualitative Analysis and Unknowns Analysis programs.



Create a PCDL subset

1. Click **Single Search**.
2. Using the default search criteria, click **Find Compounds**.

Use this procedure to create a subset of an existing PCDL using selected compounds.

All compounds in the PCDL are displayed in the **Single Search Results** table.

MassHunter PCDL Manager for Pesticides - D:\MassHunter\Pesticide_15-15m_40min_PCDL.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spect

Mass: [M+H]⁺ Neutral [M-H]⁻ Formula:
 Mass tolerance: 10.0 ppm mDa Name:
 Retention time: Requite Notes:
 RT tolerance: 0.1 min IUPAC:
 Ion search mode CAS:
 Include neutrals ChemSpider:
 Include anions
 Include cations

Print/Clone in Regulatory Format **Single Search Results: 750 hits**

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	
2-Methylphenol	C7H8O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.098	95-48-7	13835772	2-Methylpheno
4-Methylphenol	C7H8O	108.05751	<input type="checkbox"/>	<input type="checkbox"/>	4.250	106-44-5	13839082	4-methylpheno
2,4-Dimethylphenol (2,4-Xylenol)	C8H10O	122.07316	<input type="checkbox"/>	<input type="checkbox"/>	4.955	105-67-9	13839123	2,4-dimethylph
Naphthalene	C10H8	128.06260	<input type="checkbox"/>	<input type="checkbox"/>	5.544	91-20-3	906	Naphthalene
Nitrophenol, 4-	C6H5NO3	139.02694	<input type="checkbox"/>	<input type="checkbox"/>	10.843	100-02-7	955	4-Nitrophenol
Methamidophos (Metamidophos)	C2H8NO2PS	141.00134	<input type="checkbox"/>	<input type="checkbox"/>	5.885	10265-92-6	3954	O,S-Dimethyl p
1-Naphthol (Naphthol, 1-)	C10H8O	144.05751	<input type="checkbox"/>	<input type="checkbox"/>	10.508	90-15-3	6739	1-Naphthol
Paradichlorobenzene (Benzene, 1,4-dichloro-)	C6H4Cl2	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.880	106-46-7	13866817	1,4-Dichlorobe
1,3-Dichlorobenzene	C6H4Cl2	145.96901	<input type="checkbox"/>	<input type="checkbox"/>	3.832	541-73-1	13857694	1,3-Dichloroben
Phthalimide	C8H5NO2	147.03203	<input type="checkbox"/>	<input type="checkbox"/>	9.588	85-41-6	6550	1H-isoindole-1
Propyl cresol	C10H14O	150.10447	<input type="checkbox"/>	<input type="checkbox"/>	6.705	89-83-8	21105998	Thymol

- Select the compounds to include in the subset from the **Single Search Results** table.

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra
2-Methylphenol	C7H8O	108.0571			4.098	95-49-7	13835772	2-Methylphenol	1
4-Methylphenol	C7H8O	108.0571			4.250	106-44-5	13839082	4-methylphenol	1
2,4-Dimethylphenol (2,4-Xylenol)	C8H10O	122.07316			4.955	105-67-9	13839123	2,4-dimethylphenol	1
Naphthalene	C10H8	128.06260			5.544	91-20-3	906	Naphthalene	1
Nitrophenol, 4-	C6H5NO3	139.02694			10.843	100-52-7	955	4-Nitrophenol	1
Methamidophos (Metamidophos)	C2H8NO2PS	141.00134			5.885	10265-92-6	2954	O,S-Dimethyl phosphoramidodithioate	1
1-Naphthol (Naphthol, 1-)	C10H8O	144.05751			10.508	90-15-3	6739	1-Naphthol	1
Parachlorobenzene (Benzene, 1,4-dichloro-)	C6H4Cl2	145.96901			3.880	106-46-7	13866817	1,4-Dichlorobenzene	1
1,3-Dichlorobenzene	C6H4Cl2	145.96901			3.832	541-73-1	13857994	1,3-Dichlorobenzene	1
Phthalimide	C8H5NO2	147.03203			9.588	85-41-6	8550	1H-isoindole-1,3(2H)-dione	1
Propyl cresol	C10H14O	150.10447			6.705	85-53-8	2110598	Thymol	1
Cresol	C7H8O	108.0571			6.194	96-48-0	21106234	2-methyl-5-hydroxy-1-methylpiperidine-2-amine	1

- Right-click in the selected area, and select **Create Subset PCDL**.

Compound Name	Formula	Mass	Anion	Cation
2-Methylphenol	C7H8O			
4-Methylphenol	C7H8O			
2,4-Dimethylphenol (2,4-Xylenol)	C8H10O			
Naphthalene	C10H8			
Nitrophenol, 4-	C6H5NO3			
Methamidophos (Metamidophos)	C2H8NO2PS			
1-Naphthol (Naphthol, 1-)	C10H8O			
Parachlorobenzene (Benzene, 1,4-dichloro-)	C6H4Cl2			
1,3-Dichlorobenzene	C6H4Cl2			
Phthalimide	C8H5NO2	147.03203		
Propyl cresol	C10H14O	150.10447		
Cresol	C7H8O	108.0571		

- Select **Pesticides** from the PCDL type dropdown menu.

The selected rows will be used to create a subset PCDL. The subset PCDL will be loaded.

Select the subset PCDL type: **Pesticides**

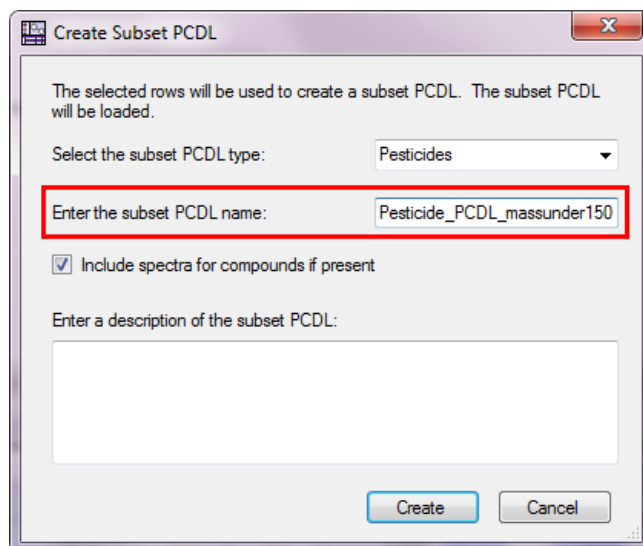
Enter the subset PCDL name:

Include spectra for compounds if present

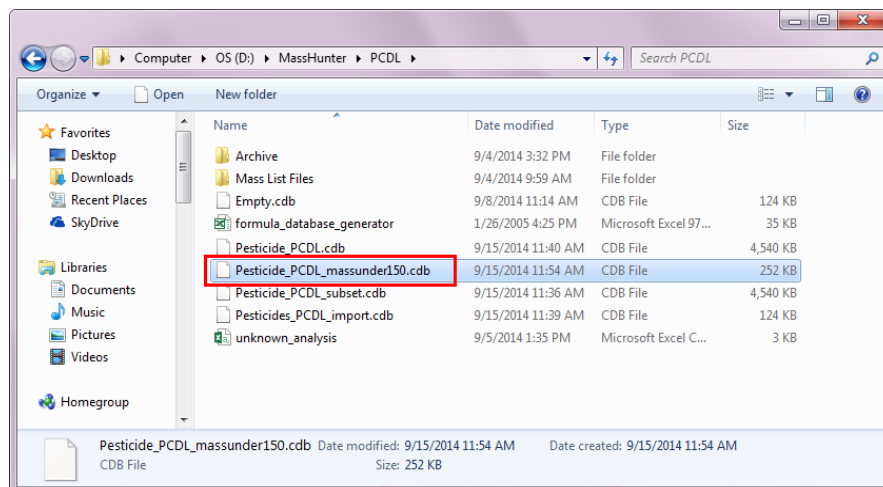
Enter a description of the subset PCDL:

Create **Cancel**

6. Enter a name for the subset PCDL.



The subset library is created in the destination folder.



7. Click **Create**, and then click **Yes** to load the new subset library.

Exercise 3. Use the PCDL to Identify Compounds in Qualitative Analysis

Load data in the Qualitative Analysis program

1. Start the **Agilent MassHunter Qualitative Analysis** program by double-clicking the desktop icon.
2. Navigate to **D:\MassHunter\Data** and open the data file **Tomato_spiked.D**.
3. Load the method **GCQTOF_Pesticide_15-15m_40min_PCDL.m**.

Set the method parameters

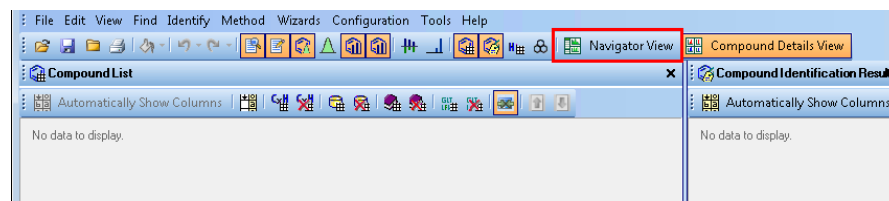
1. Click **Navigator View** in the Method Explorer toolbar.

In this exercise, you will search the PCDL with MassHunter Workstation Software - Qualitative Analysis B.07.00 using the Find by Formula Options.

The Qualitative Analysis program lets you focus on the immediate aspects of data when reviewing chromatographic and mass spectral results.



Use this procedure to define parameters in the Method Editor that are applied to identify compounds in your PCDL.



- In the **Find Compounds by Formula** menu, click **Find by Formula - Options**.

The screenshot shows the software interface with the 'Find Compounds by Formula' menu open. The 'Find by Formula - Options' sub-menu item is highlighted with a red box. The background shows a 'Compound List' table and a 'Chromatogram Results' plot.

Cpd	Name	
1	Methamidophos (Metamidophos)	Cp
2	Biphenyl	
3	3,5-Dichloroaniline	
4	Diphenylamine	
5	2-Phenylphenol (Orthophenylphenol)	Cpd 5:
6	Molinate	
7	DEET / Diethyltoluamide	

Set the formula source options

- Click **Formula Source**.
- Select **Database/Library**.
- Browse for and open the PCDL.

The screenshot shows the 'Method Editor: Find Compounds by Formula - Options' dialog box. The 'Database / Library' radio button is selected and highlighted with a red box. The path 'D:\MassHunter\PCDL\Pesticide_15-15m_40min_PCDL' is entered in the text field below it.

Source of formulas to confirm:

- These formulas:
- Compound exchange file (.CEF):
- Database / Library: D:\MassHunter\PCDL\Pesticide_15-15m_40min_PCDL
- Worklist

Matches per formula:

Maximum number of matches: 1

Automatically increase for isomeric compounds

Values to match:

- Mass
- Mass and retention time (retention time optional)
- Mass and retention time (retention time required)

4. Enter the **Maximum number of matches** and clear **Automatically increase for isomeric compounds**.

If the **Automatically increase for isomeric compounds** option is selected, the isomeric compounds will be grouped as one compound.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Negative Ions | Results | **Result Filters** | Fragment Confirmation

Formula Source | **Formula Matching** | Positive Ions

Source of formulas to confirm:

- These formulas: (type a comma-separated list of formulas, e.g. "C6H6, CH4")
- Compound exchange file (.CEF):
- Database / Library: D:\MassHunter\PCDL\Pesticide_15-15m_40min_PCDL
- Worklist

Matches per formula

Maximum number of matches: 1

Automatically increase for isomeric compounds

Values to match:

- Mass
- Mass and retention time (retention time optional)
- Mass and retention time (retention time required)

Set the formula matching options

1. Click **Formula Matching**.
2. Select a mass range for the extractions of the EIC.

The value selected may depend on whether you are running your acquisition method in high resolution mode or dual gain mode.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Negative Ions | Results | **Result Filters** | Fragment Confirmation

Formula Source | **Formula Matching** | Positive Ions

Match tolerance

Masses: +/- 10.00 ppm

Retention times: +/- 0.350 minutes

Expansion of values for chromatogram extraction

Possible m/z: Symmetric (ppm) +/- 35.0

Limit EIC extraction range

Expected retention time: Symmetric +/- 1.00 minutes

- To limit the EIC extraction range, select **Limit EIC extraction range** and set the expected retention time.

Set the results options

- Click **Results**.
- Select **Delete previous compounds** to remove any previously found compounds.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Negative Ions | Results | Result Filters | Fragment Confirmation

Formula Source | Formula Matching | Positive Ions

Match tolerance

Masses: +/- 10.00 ppm

Retention times: +/- 0.350 minutes

Expansion of values for chromatogram extraction

Possible m/z: Symmetric (ppm) +/- 35.0

Limit EIC extraction range

Expected retention time: Symmetric +/- 1.00 minutes

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Negative Ions | Results | Result Filters | Fragment Confirmation

Previous results

Delete previous compounds

New results

Highlight first compound
 Highlight all compounds

Chromatograms and spectra

Extract EIC

Extract cleaned spectrum Include structure

Extract raw spectrum

Prefer profile for raw spectra, if available

Clip extracted raw spectra

Symmetric (m/z) +/- 5.0000

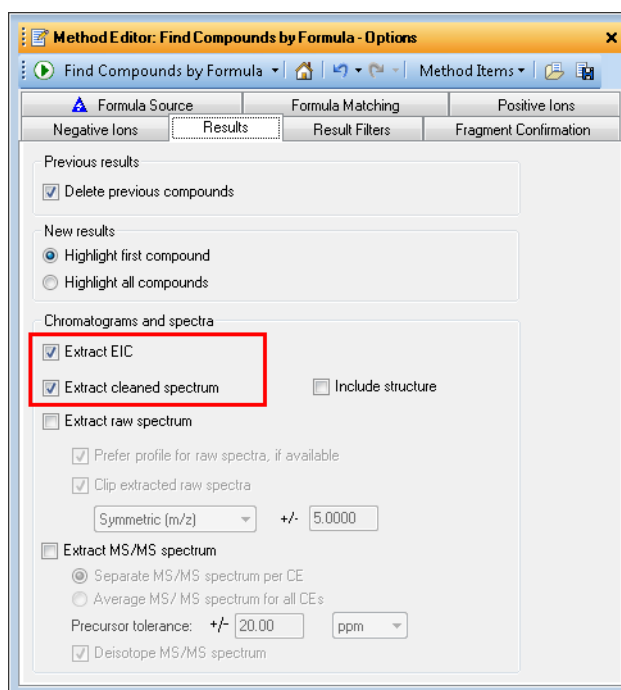
Extract MS/MS spectrum

Separate MS/MS spectrum per CE
 Average MS/MS spectrum for all CEs

Precursor tolerance: +/- 20.00 ppm

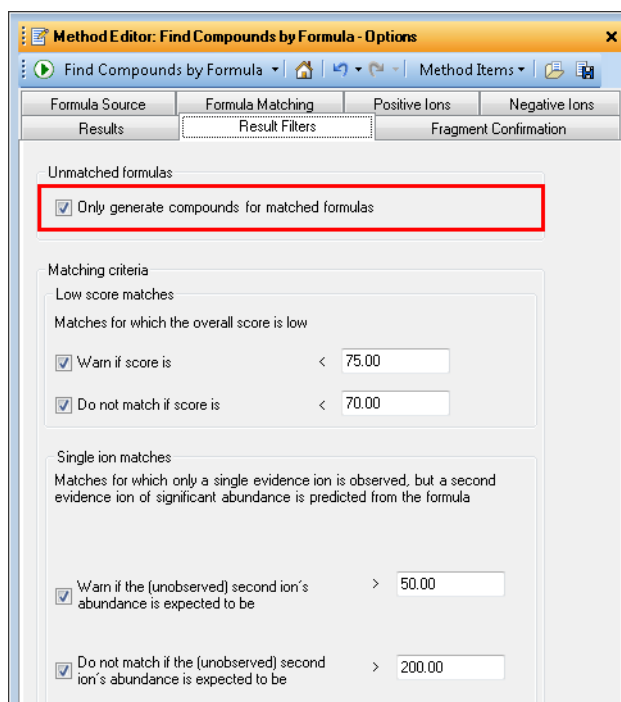
Deisotope MS/MS spectrum

3. Enable **Extract EIC** and **Extract cleaned spectrum**.



Set the result filters options

1. Click **Result Filters**.
2. Select **Only generate compounds for matched formulas**. If not selected, compounds that are not found will also display in the results.



Set the fragment confirmation options

1. Click **Fragment Confirmation**.
2. Select **Confirm with fragment ions** and **Molecular ion optional**.

If not selected, you will be penalized for not having molecular ions or similar compounds.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Formula Source | Formula Matching | Positive Ions
Negative Ions | Results | Result Filters | **Fragment Confirmation**

Search fragment ions

Confirm with fragment ions
 Molecular ion optional

Fragment ion source

Use spectral library only
 Use average fragment spectrum if spectral library not available

Number of most specific ions from spectral library: 5
Number of most specific ions from average fragment spectrum: 7

Fragment ion EIC qualification settings

RT difference +/-: 0.10 min. of expected RT
 S/N ratio >=: 5.00
Coelution score >=: 90

Fragment ion confirmation criteria

Minimum number of qualified fragments: 1
 Minimum percent of qualified fragments: 75

3. Select **Use spectral library only**.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Formula Source | Formula Matching | Positive Ions

Negative Ions | Results | Result Filters | Fragment Confirmation

Search fragment ions

Confirm with fragment ions

Molecular ion optional

Fragment ion source

Use spectral library only

Use average fragment spectrum if spectral library not available

Number of most specific ions from spectral library: 5

Number of most specific ions from average fragment spectrum: 7

Fragment ion EIC qualification settings

RT difference +/-: 0.10 min. of expected RT

S/N ratio >=: 5.00

Coelution score >=: 90

Fragment ion confirmation criteria

Minimum number of qualified fragments: 1

Minimum percent of qualified fragments: 75

4. Enter **7** for the **Number of most specific ions from spectral library**.

A higher number of ions will produce greater specificity and more confidence in the results; however, the higher the number of ions, the longer the program's run time will be.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Formula Source | Formula Matching | Positive Ions

Negative Ions | Results | Result Filters | Fragment Confirmation

Search fragment ions

Confirm with fragment ions

Molecular ion optional

Fragment ion source

Use spectral library only

Use average fragment spectrum if spectral library not available

Number of most specific ions from spectral library: 7

Number of most specific ions from average fragment spectrum: 7

Fragment ion EIC qualification settings

RT difference +/-: 0.10 min. of expected RT

S/N ratio >=: 5.00

Coelution score >=: 90

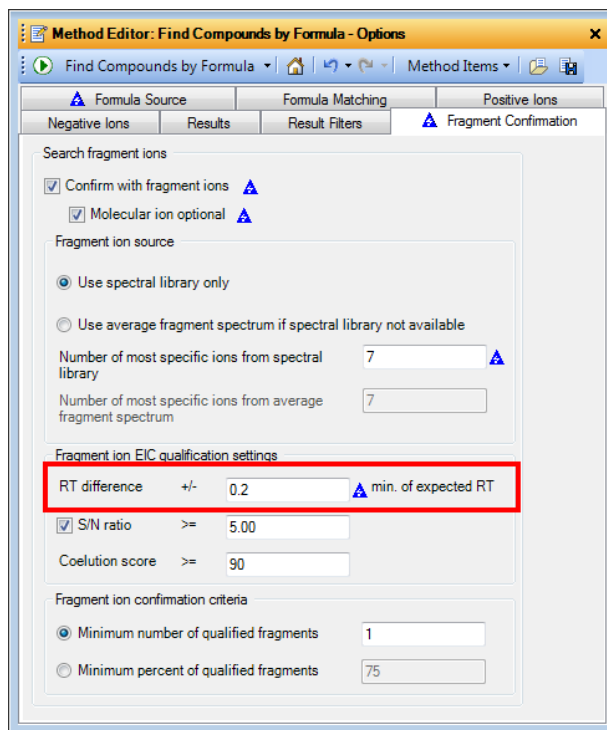
Fragment ion confirmation criteria

Minimum number of qualified fragments: 1

Minimum percent of qualified fragments: 75

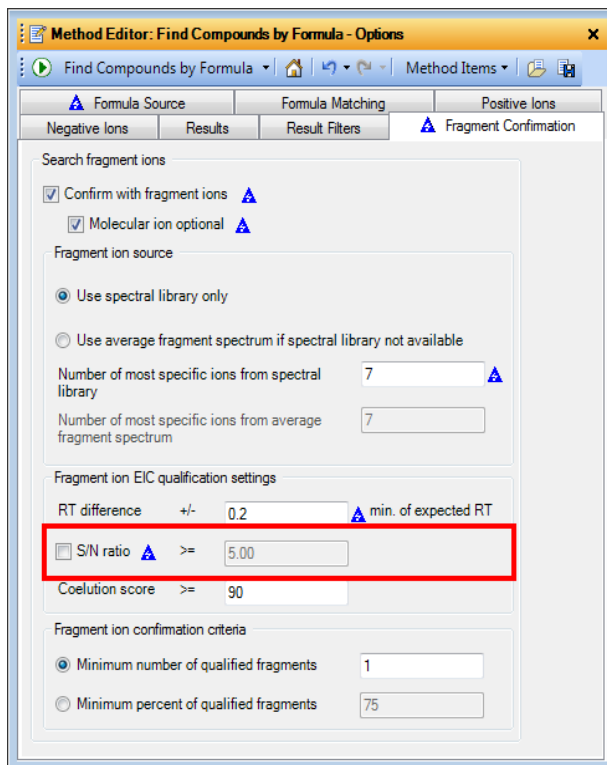
5. Enter **0.2** for the **RT difference**.

The recommended range for this value is 0.1-0.2. The RT difference is the difference that is allowed for the retention time shift of the reference ion. The reference ion is automatically chosen by the MassHunter Qualitative Analysis software.



6. Clear **S/N ratio**.

If selected, there is a high probability of producing false negatives (if the ratio is too low).



7. Enter **80** for the **Coelution score**.

The recommended range for this value is 50-90.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Formula Source | Formula Matching | Positive Ions

Negative Ions | Results | Result Filters | Fragment Confirmation

Search fragment ions

Confirm with fragment ions

Molecular ion optional

Fragment ion source

Use spectral library only

Use average fragment spectrum if spectral library not available

Number of most specific ions from spectral library: 7

Number of most specific ions from average fragment spectrum: 7

Fragment ion EIC qualification settings

RT difference +/-: 0.2 min. of expected RT

S/N ratio >=: 5.00

Coelution score >=: 80

Fragment ion confirmation criteria

Minimum number of qualified fragments: 1

Minimum percent of qualified fragments: 75

8. Select **Minimum number of qualified fragments** and enter **1**.

The recommended starting value is 1-3. This setting requires two qualified fragments: a reference ion and a qualified ion.

Method Editor: Find Compounds by Formula - Options

Find Compounds by Formula | Method Items

Formula Source | Formula Matching | Positive Ions

Negative Ions | Results | Result Filters | Fragment Confirmation

Search fragment ions

Confirm with fragment ions

Molecular ion optional

Fragment ion source

Use spectral library only

Use average fragment spectrum if spectral library not available

Number of most specific ions from spectral library: 7

Number of most specific ions from average fragment spectrum: 7

Fragment ion EIC qualification settings

RT difference +/-: 0.2 min. of expected RT

S/N ratio >=: 5.00

Coelution score >=: 80

Fragment ion confirmation criteria

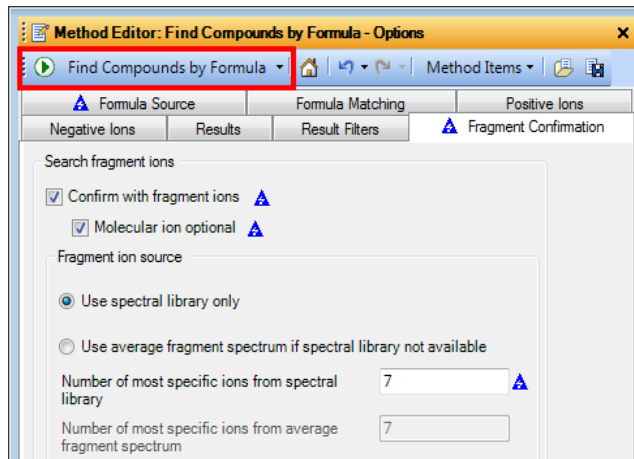
Minimum number of qualified fragments: 1

Minimum percent of qualified fragments: 75

Process and interpret data with All Ions

1. Click **Find Compounds by Formula** in the Method Editor toolbar.

Use this procedure to apply your defined parameters and analyze the Find by Formula results.



2. Click **Compound Details View** in the Method Explorer toolbar to switch views.

Name	Label	Show/Hi	Formula	m/z	Mass	Mass (Tgt)
4-Methylphenol	Cpd 1: 4-Methylphenol	<input checked="" type="checkbox"/>	C7 H8 O	108.0579	108.0584	108.
ethamidophos (Metamidophos)	Cpd 2: Methamidophos (Metamidophos)	<input checked="" type="checkbox"/>	C2 H8 N O2 P S	141.0002	141.0007	141.
1-Naphthol (Naphthol, 1-)	Cpd 3: 1-Naphthol (Naphthol, 1-)	<input checked="" type="checkbox"/>	C10 H8 O			144.
Phthalimide	Cpd 4: Phthalimide	<input checked="" type="checkbox"/>	C8 H5 N O2	147.0329	147.0334	147.
Propyl cresol	Cpd 5: Propyl cresol	<input checked="" type="checkbox"/>	C10 H14 O			150.
Biphenyl	Cpd 6: Biphenyl	<input checked="" type="checkbox"/>	C12 H10	154.0767	154.0774	154.
3,5-Dichloroaniline	Cpd 7: 3,5-Dichloroaniline	<input checked="" type="checkbox"/>	C6 H5 Cl2 N	160.9791	160.9797	160.

3. Click or use the arrow keys to move through the **Compound List** to review one compound a time.

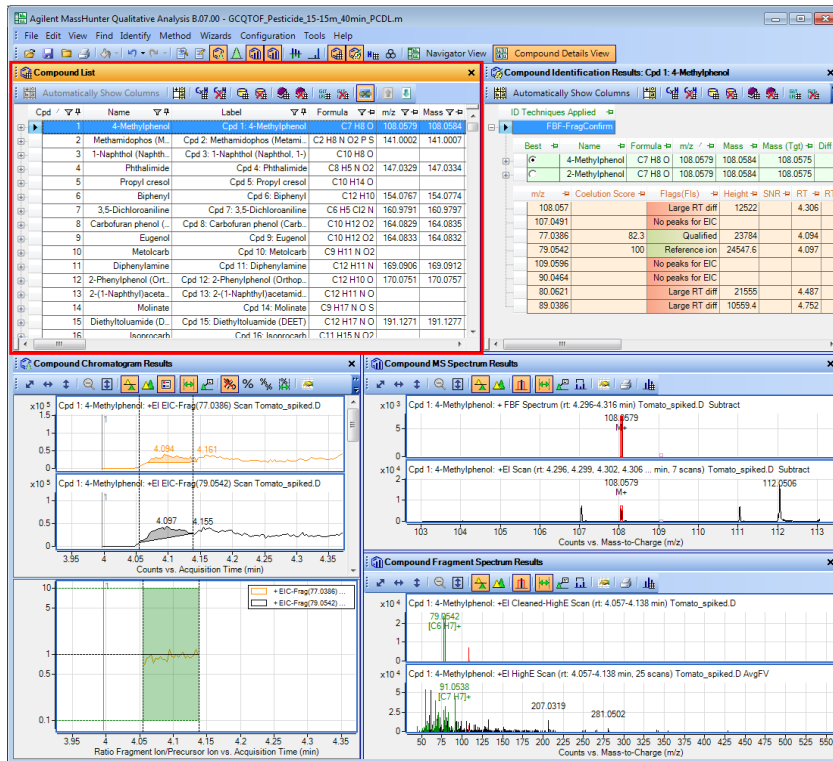
Selecting a compound from the **Compound List** displays the identification results for that compound in the **Compound Identification Results** window.

m/z	Coelution Score	Ref. Ion	Height	SNR	RT	RT Diff	CE
170.0726	100	Qualified	231405.3		10.741	0	
163.0648	98.9	Qualified	216300.7		10.744	0.003	
141.0639	93.5	Qualified	183127.7		10.741	0	
115.0542	94.7	Qualified	119213.2		10.744	0.003	
171.0756	94.2	Qualified	53333.8		10.741	0	
142.0777	93.5	Qualified	57303.1		10.737	0.003	
138.0542	92.3	Qualified	43376.1		10.744	0.003	
168.057	92.5	Qualified	28163.5		10.741	0	
116.0579	90.1	Qualified	16748.4		10.734	0.007	
155.0491	82.8	Qualified	6996.3		10.741	0	
89.0386	90.9	Qualified	23584.1		10.744	0.003	

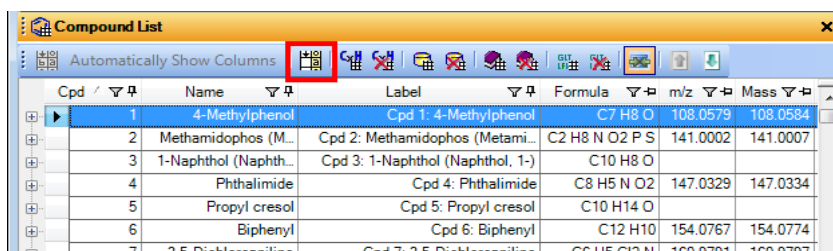
Review the Compound List table

1. Select a compound from the **Compound List** to view the chromatogram results

The **Compound List** table displays information about each compound. Each row in the first level of the table is a different compound. Each column describes a different piece of information about each compound.

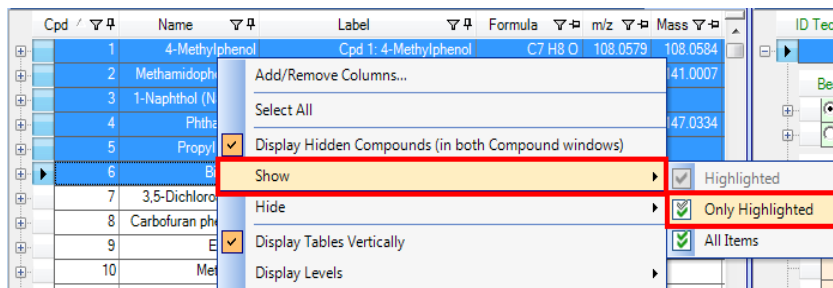


2. If a column is empty, it can be hidden automatically by clicking **Hide any currently empty columns**.



3. Right-click on a compound or group of compounds and select **Show > Only Highlighted**.

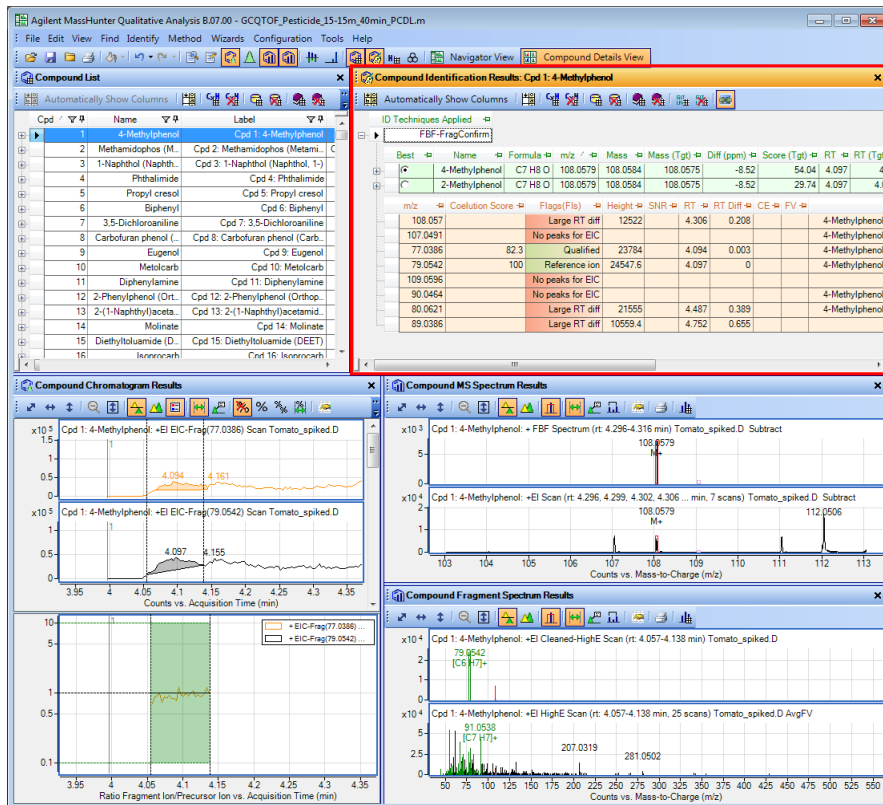
Any compound that was not select will be hidden. When you hide an item in the Compound List table, those items are also hidden in the other windows.



Review the Compound Identification Results table

1. Select a compound from the **Compound List**.

The results from any of the identification algorithms that you run on the selected compound are displayed in the **Compound Identification Results** table.



The first level of this table shows the summary information for all of the identification algorithms that you ran.

Best	Name	Formula	m/z	Mass	Mass (Tgt)	Diff (ppm)	Score (Tgt)	RT	RT (Tgt)	RT Diff	Score	
☑	Methamidophos (Metamidophos)	C ₂ H ₈ N O ₂ P S	141.0002	141.0007	141.0013	4.2	83.04	5.964	5.885	0.079		
			m/z	Coelution Score	Flags (Fls)	Height	SNR	RT	RT Diff	CE	FV	Compound Name
			141.0008	100	Reference ion	15409.7	5.964	0				Methamidophos (Metamidophos)
			94.0052	93.9	Qualified	57249.8	5.971	0.007				Methamidophos (Metamidophos)
			95.0131	88.4	Qualified	49507.2	5.971	0.007				Methamidophos (Metamidophos)
			125.9773	90.3	Qualified	13418.6	5.971	0.007				Methamidophos (Metamidophos)

2. Expand the first level in the table to view the second level.

The second level shows individual scores that were used to create the overall score for an algorithm. This row is present only when a molecular ion is found and reflects Find by Formula results.

Best	Name	Formula	m/z	Mass	Mass (Tgt)	Diff (ppm)	Score (Tgt)	RT	RT (Tgt)	RT Diff	Score	
☑	Methamidophos (Metamidophos)	C ₂ H ₈ N O ₂ P S	141.0002	141.0007	141.0013	4.2	83.04	5.964	5.885	0.079		
				Score (iso. abund)	Score (mass)	Score (MFG, MS/MS)	Score (MS)	Score (MFG)	Score (iso. spacing)	Height	Ion Formula	Species
				92.76	95.65		92.85		4738.4		M+	
			m/z	Coelution Score	Flags (Fls)	Height	SNR	RT	RT Diff	CE	FV	Compound Name
			141.0008	100	Reference ion	15409.7	5.964	0				Methamidophos (Metamidophos)
			94.0052	93.9	Qualified	57249.8	5.971	0.007				Methamidophos (Metamidophos)
			95.0131	88.4	Qualified	49507.2	5.971	0.007				Methamidophos (Metamidophos)
			125.9773	90.3	Qualified	13418.6	5.971	0.007				Methamidophos (Metamidophos)

- Expand the second level in the table to view the third level.

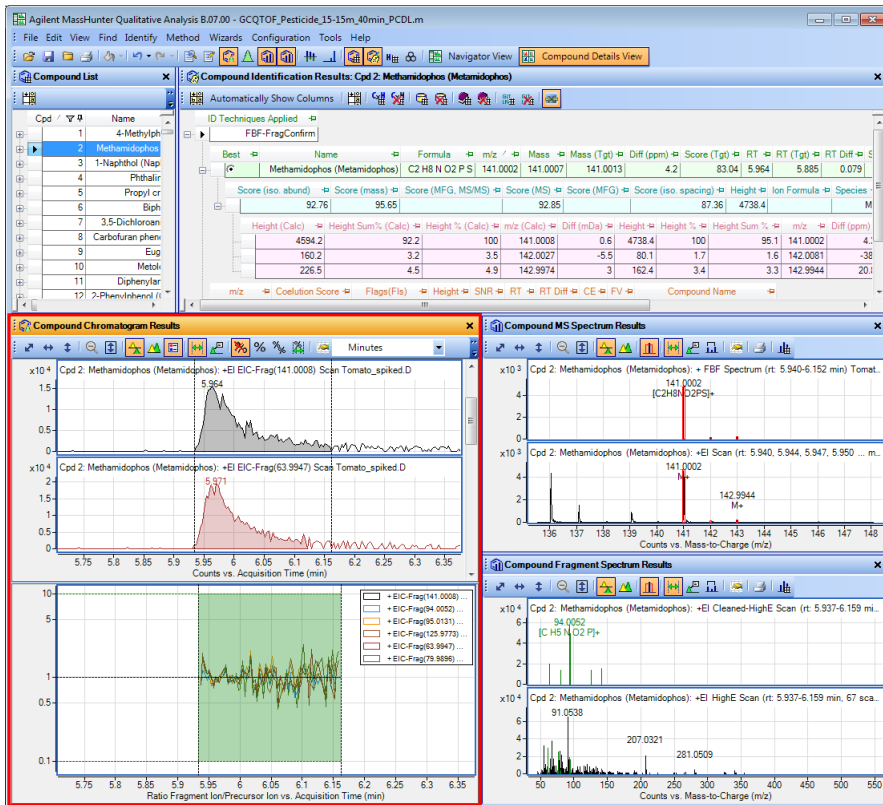
The third level shows height and m/z values (both calculated and actual).

Height (Calc)	Height Sum% (Calc)	Height % (Calc)	m/z (Calc)	Diff (mDa)	Height	Height %	Height Sum %	m/z	Diff (ppm)
4594.2	92.2	100	141.0008	0.6	4738.4	100	95.1	141.0002	4.2
160.2	3.2	3.5	142.0027	-5.5	80.1	1.7	1.6	142.0081	-38
226.5	4.5	4.9	142.9974	3	162.4	3.4	3.3	142.9944	20

Review the Compound Chromatogram Results window

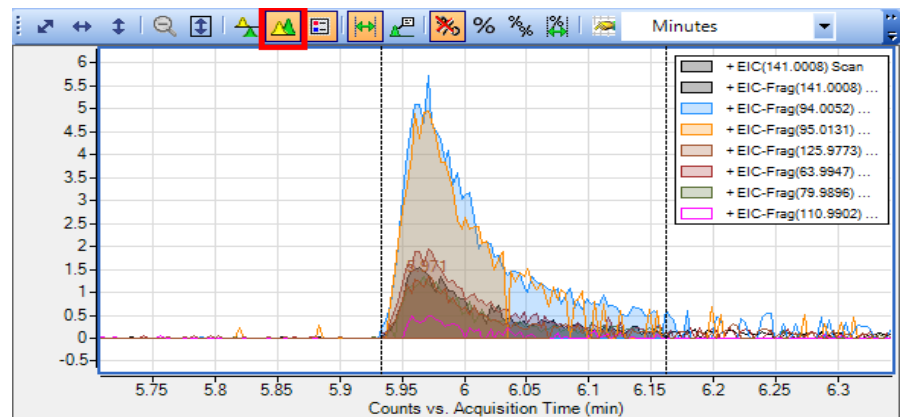
- Select a compound from the **Compound List**.

The **Compound Chromatogram Results** window displays the EICs selected for each ion. Any chromatogram that is part of the selected compound is shown in this window. The start and end of the retention time window are shown as dashed vertical lines. All of the compound chromatograms are automatically extracted when you select the compound in the **Compound List** window.

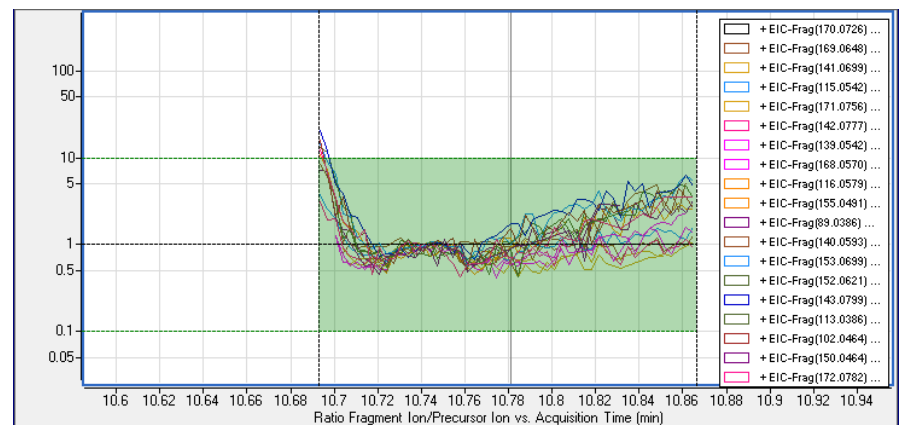


2. Click **Overlaid mode**.

All chromatograms are shown in one graph.



The bottom graph in the Compound Chromatogram Results window is the **Coelution** graph, which displays how closely the Fragment ions coelute with the compound.

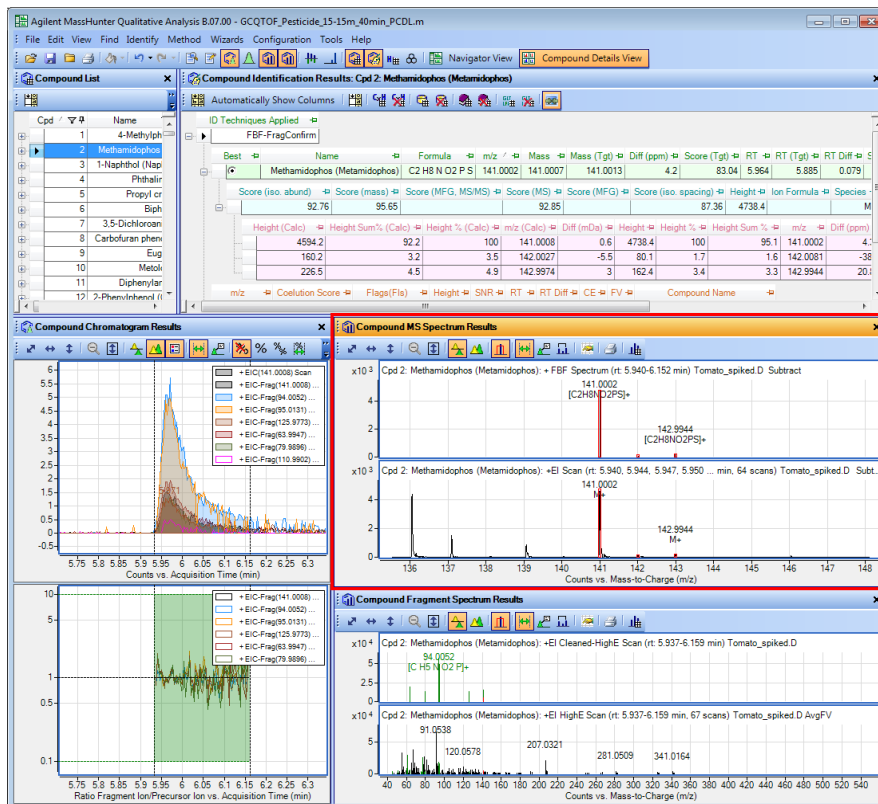


For reference, a black line is shown with the y-value of 1. A value of 1 shows the qualifier ions are exactly coeluting with the reference ion chromatogram. As the ratio approaches 1, the qualifier ion is more closely coeluting with the reference ion.

Review the Compound MS Spectrum Results window

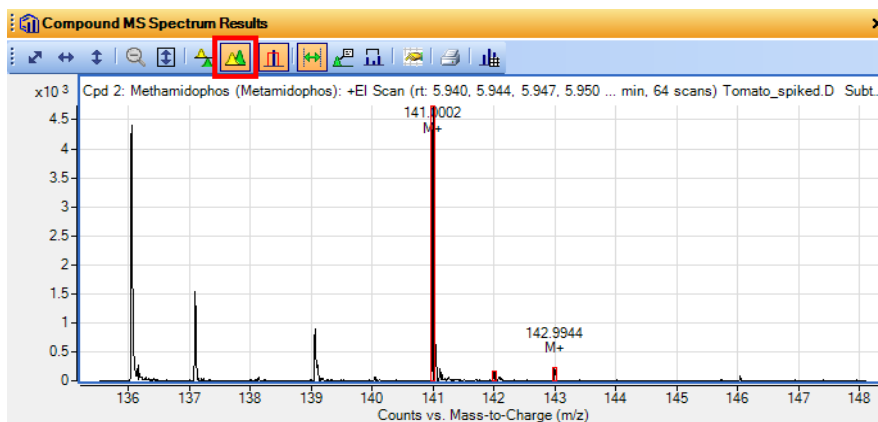
1. Select a compound from the **Compound List**.

The **Compound MS Spectrum Results** window displays MS spectra. If compounds were identified using the Find by Formula algorithm, then the FBF Spectrum is annotated with the formula and the adduct ion. The cleaned (upper) and raw (lower) spectra are shown and the isotopic abundance is also overlaid on the spectrum.



2. Click **Overlaid mode**.

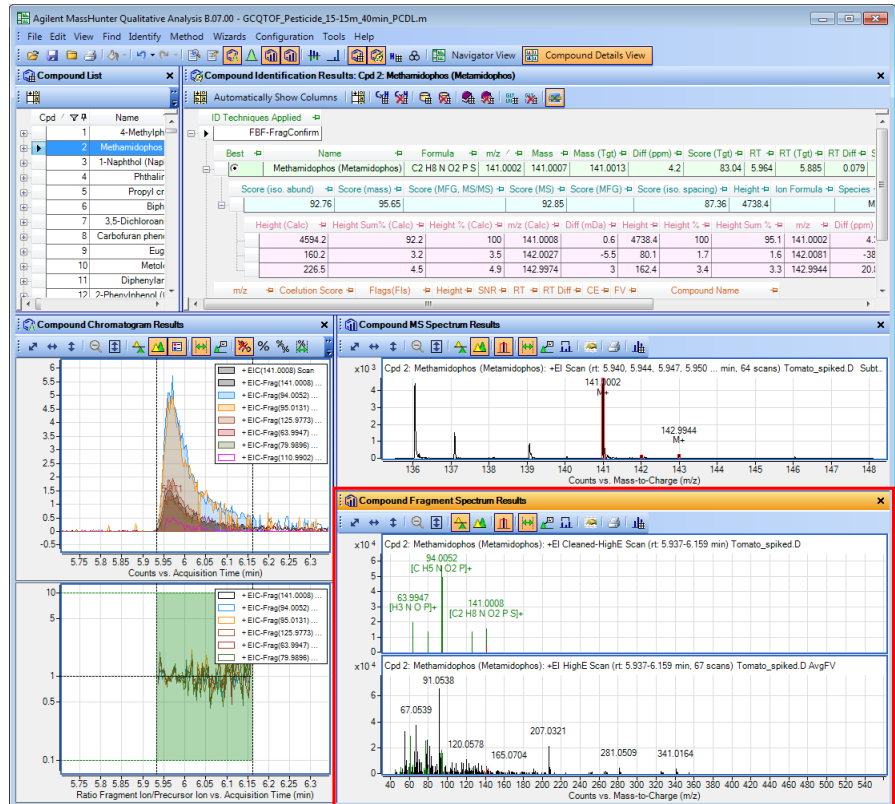
The cleaned MS spectrum and the raw MS spectrum are displayed in one graph.



Review the Compound Fragment Spectrum Results window

Select a compound from the **Compound List**.

The **Compound Fragment Spectrum Results** window displays cleaned (upper) and raw (lower) MS spectra with the ions selected for screening from the PCDL shown in a different color.

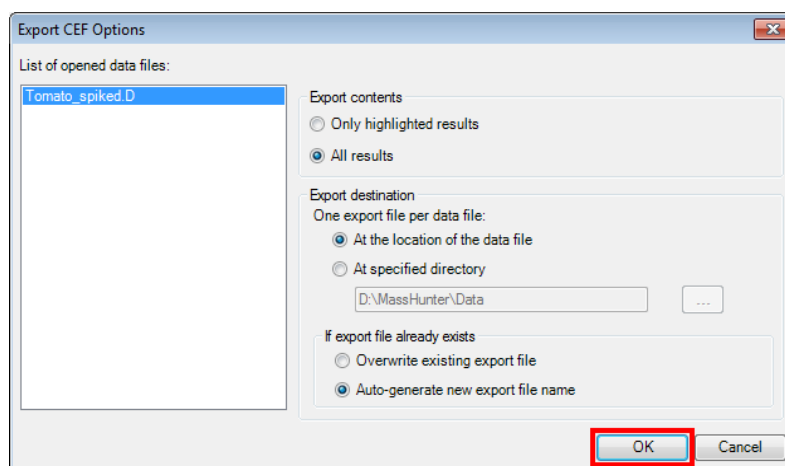
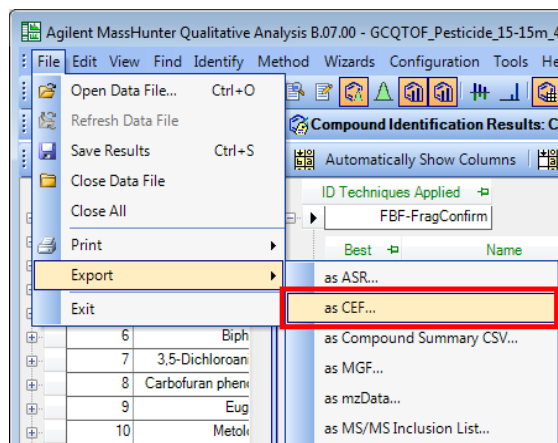


Export your results as a CEF

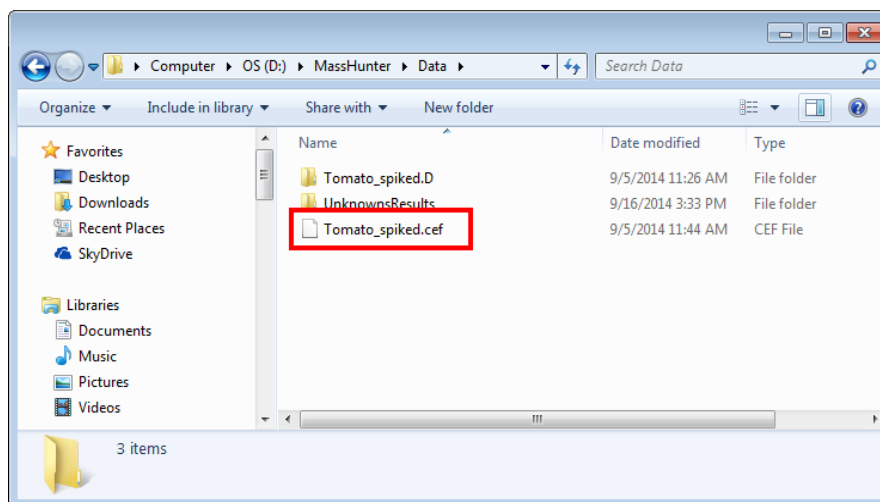
1. Click **File > Export > as CEF**.

2. Specify the **Export CEF options**, and click **OK**.

Use this procedure to export your results to a CEF file for use with other applications.



The CEF file is created in the specified **Export Destination** folder.



Exercise 4. Use the PCDL to Identify Compounds with Unknowns Analysis

Create a new Unknowns Analysis

1. Start **Unknowns Analysis** by double-clicking the desktop icon, or Click **Start > Agilent > Quant Tools > Unknowns Analysis**.
2. Select **File > New Analysis**.
3. Navigate to **Masshunter\Data**, or the folder where the data file to be analyzed is stored. Enter a name for the analysis and click **Open**.

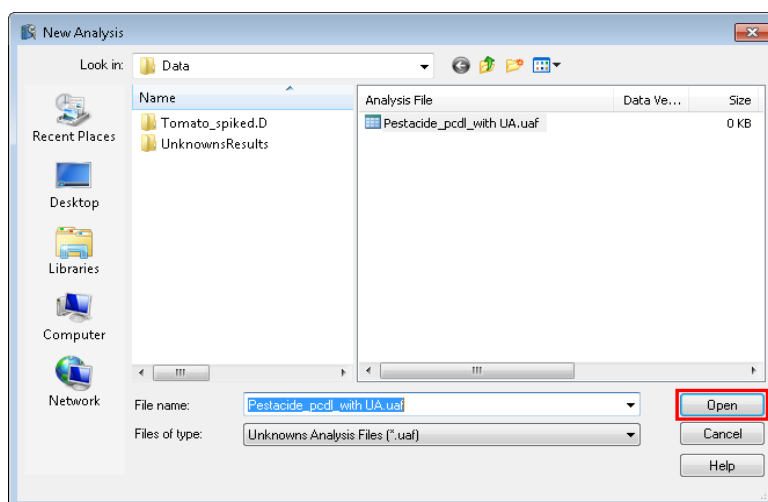
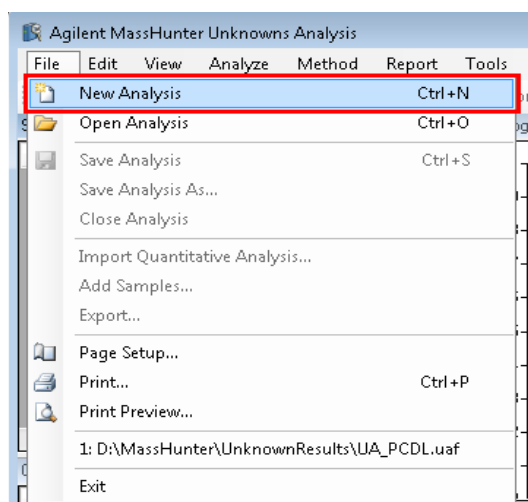
Use the Unknowns Analysis tool uses deconvolution and spectral library matching to identify unknowns, such as compounds that are not on the target list but are in a mass spectral library.

In this exercise, you will identify compounds in the PCDL with Unknowns Analysis.

Use this procedure to create a new Unknowns Analysis file to identify compounds in the PCDL.



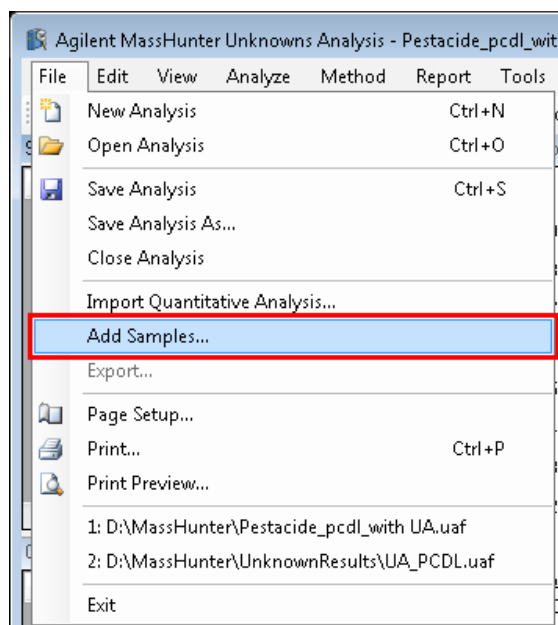
Unknowns Analysis



Add samples to the analysis

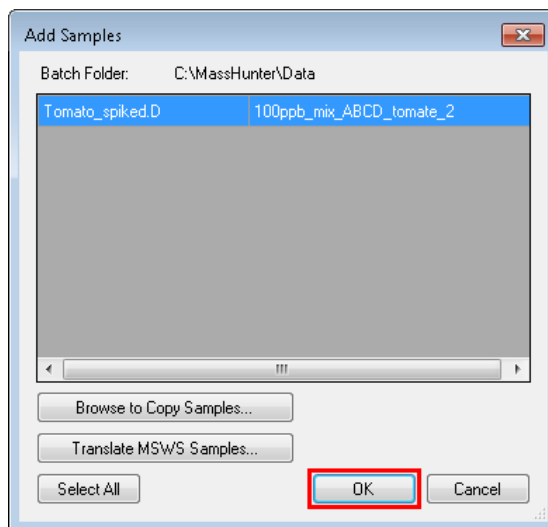
1. Select **File > Add Samples**.

Use this procedure to add samples to include in your analysis.



2. Select the sample file(s) and click **OK**.

If necessary, click **Browse to Copy Samples** to search for and open sample files.



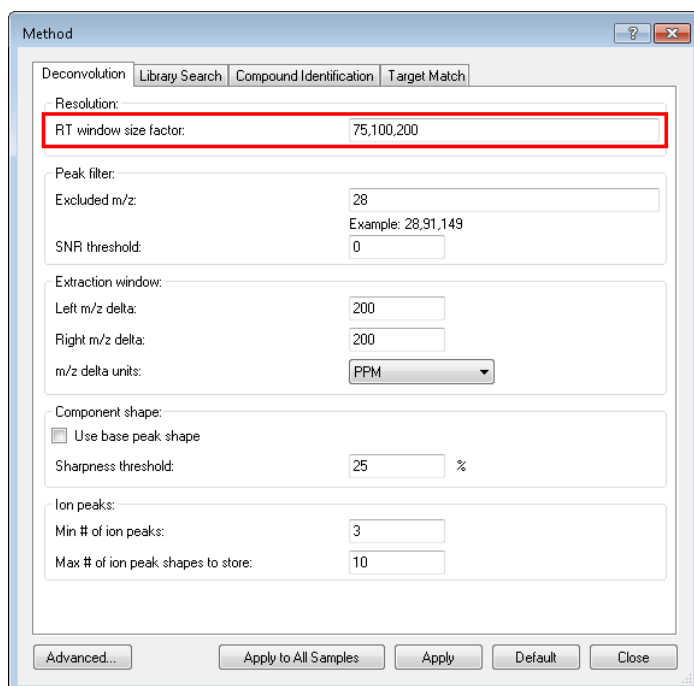
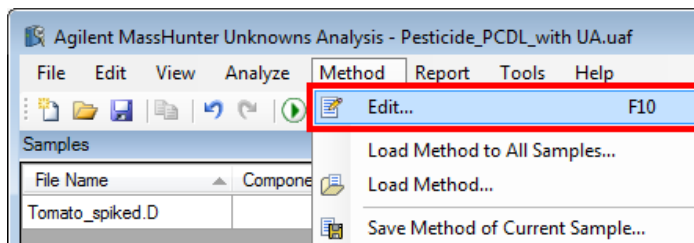
Edit the method

Select **Method > Edit**.

Set deconvolution options

1. Click **Deconvolution**.
2. In the **RT window Size factor** field, enter 75, 100, 200.

Use this procedure to edit the method search options used to identify the unknown compounds.



- In the **Extraction Window** section, enter **200 PPM** for the left and right m/z delta.

The optimum extraction window is 100-200 PPM.

The screenshot shows the 'Method' dialog box with the 'Extraction window' section highlighted by a red box. The settings are as follows:

- Resolution: (empty)
- RT window size factor: 75,100,200
- Peak filter: (empty)
- Excluded m/z : 28 (Example: 28,91,149)
- SNR threshold: 0
- Extraction window:
 - Left m/z delta: 200
 - Right m/z delta: 200
 - m/z delta units: PPM
- Component shape:
 - Use base peak shape
 - Sharpness threshold: 25 %
- Ion peaks:
 - Min # of ion peaks: 3
 - Max # of ion peak shapes to store: 10

Buttons at the bottom: Advanced..., Apply to All Samples, Apply, Default, Close.

Set library search options

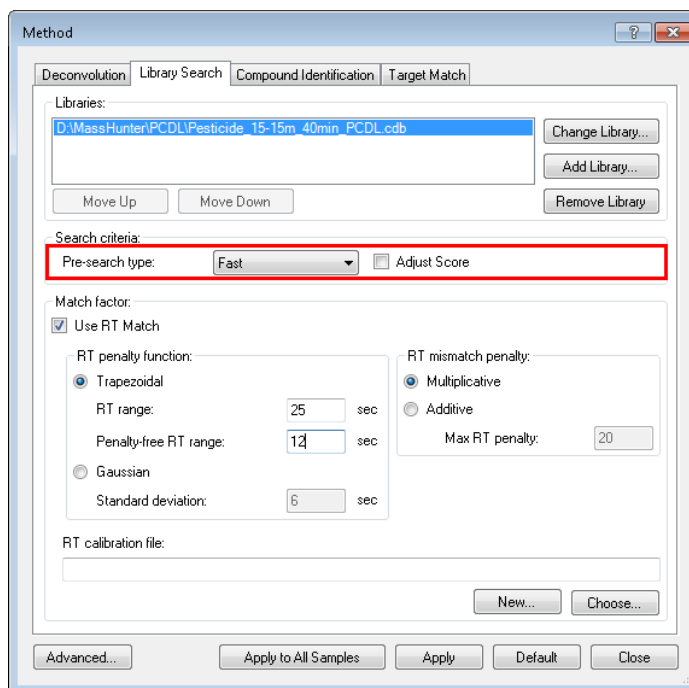
- Click **Library Search**.
- Click **Change Library** and select the PCDL, **Pesticide_15-15m_40min_P-CDL.cdb**.

The screenshot shows the 'Method' dialog box with the 'Library Search' section highlighted by a red box. The settings are as follows:

- Libraries:
 - D:\MassHunter\PCDL\Pesticide_15-15m_40min_PCDL.cdb
 - Buttons: Move Up, Move Down, Change Library..., Add Library..., Remove Library
- Search criteria:
 - Pre-search type: Fast
 - Adjust Score
- Match factor:
 - Use RT Match
 - RT penalty function:
 - Trapezoidal
 - RT range: 25 sec
 - Penalty-free RT range: 12 sec
 - Gaussian
 - Standard deviation: 6 sec
 - RT mismatch penalty:
 - Multiplicative
 - Additive
 - Max RT penalty: 20
- RT calibration file: (empty)

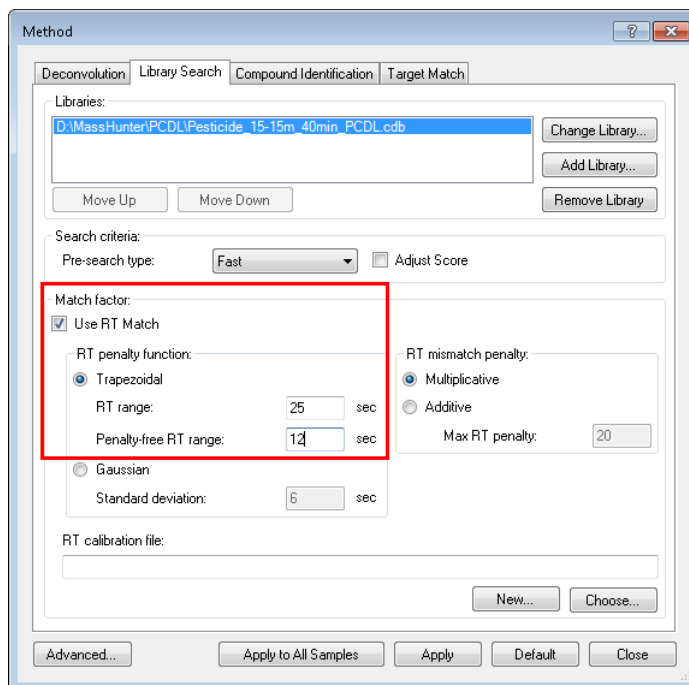
Buttons at the bottom: Advanced..., Apply to All Samples, Apply, Default, Close.

3. Select the **Pre-search type, Fast**.



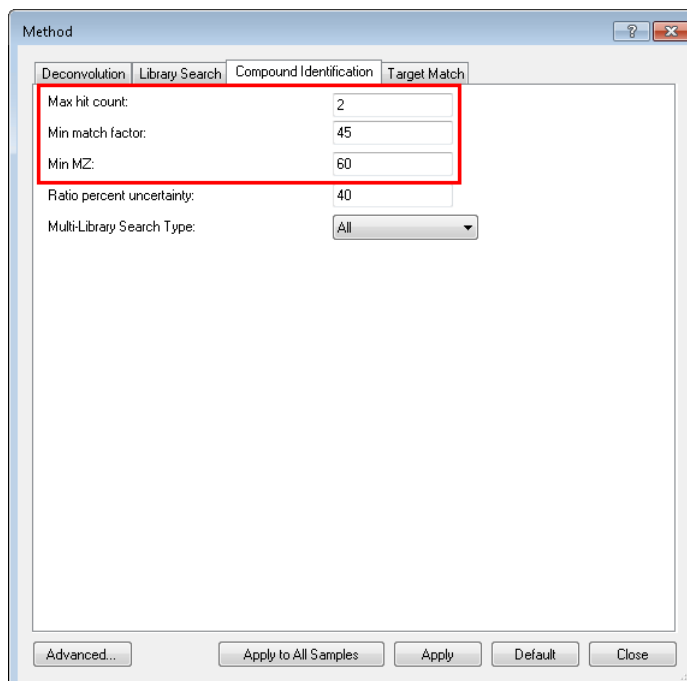
4. In the **Match factor** section, select **Use RT Match**.

5. Enter the following:
RT Range: 25 sec
Penalty-free RT range: 12 sec



Set compound identification options

1. Select the **Compound Identification** tab
2. Enter the following:
Max hit count: 2
Min match factor: 45
Min MZ: 60



Method

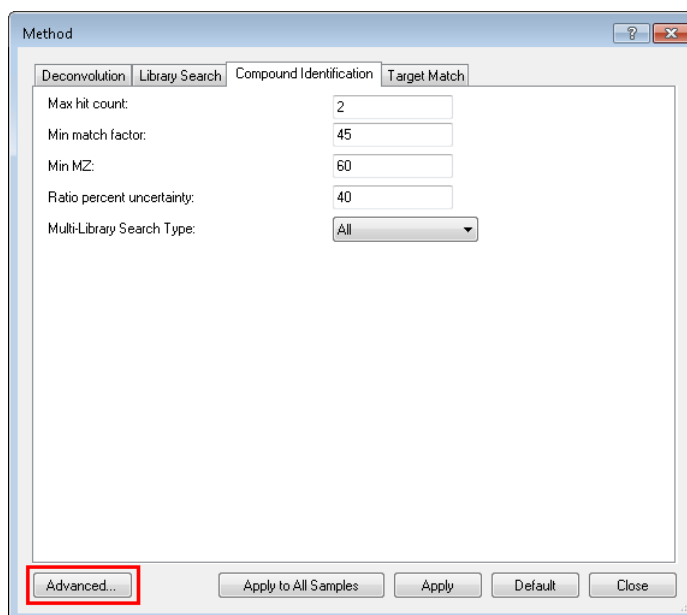
Deconvolution | Library Search | **Compound Identification** | Target Match

Max hit count:	2
Min match factor:	45
Min MZ:	60
Ratio percent uncertainty:	40
Multi-Library Search Type:	All

Advanced... Apply to All Samples Apply Default Close

Set advanced options

1. Click **Advanced**.



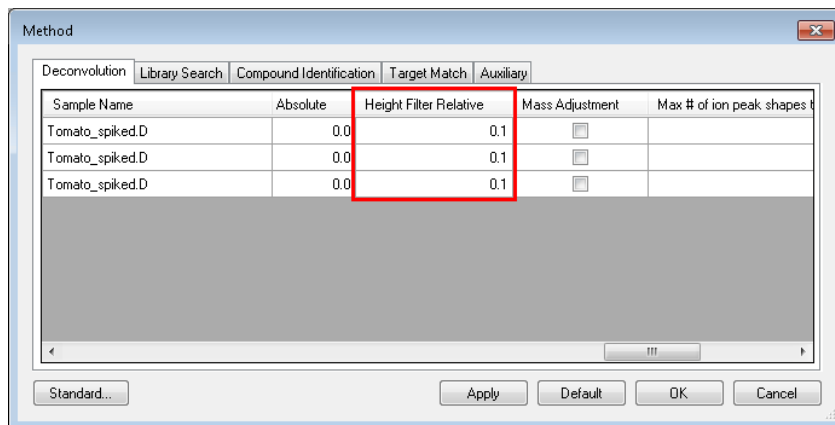
Method

Deconvolution | Library Search | **Compound Identification** | Target Match

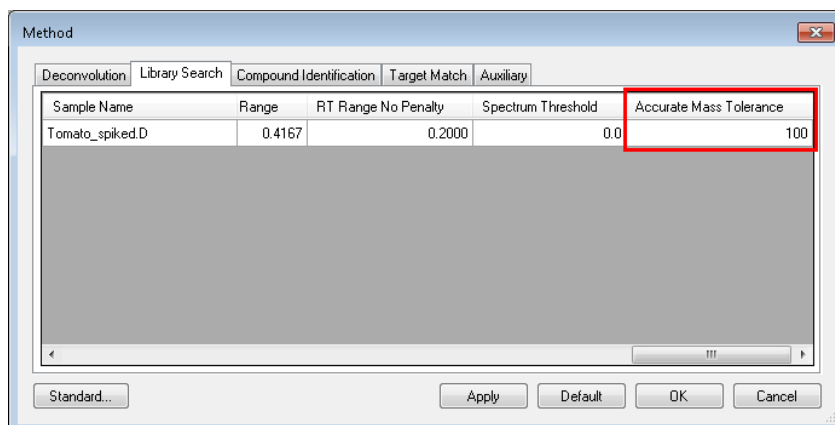
Max hit count:	2
Min match factor:	45
Min MZ:	60
Ratio percent uncertainty:	40
Multi-Library Search Type:	All

Advanced... Apply to All Samples Apply Default Close

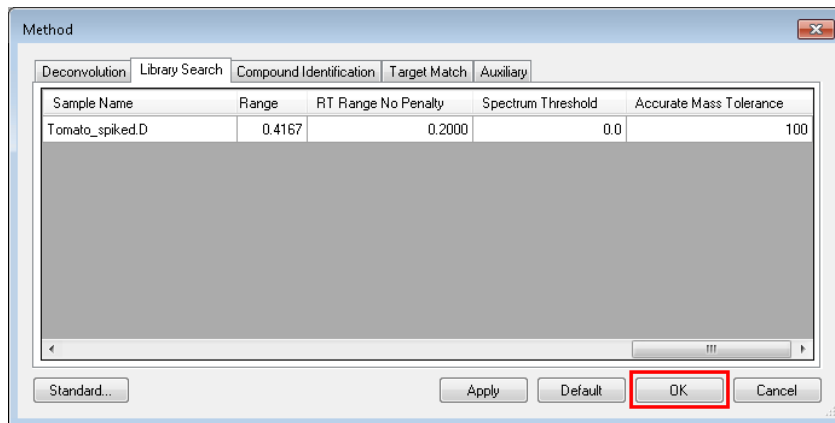
- Click **Yes** to apply changes to all samples.
- Click **Deconvolution**.
- Enter **0.1** for all samples in the **Height Filter Relative** column.



- Click **Library Search**.
- Enter **100** for all samples in the **Accurate Mass Tolerance** column.



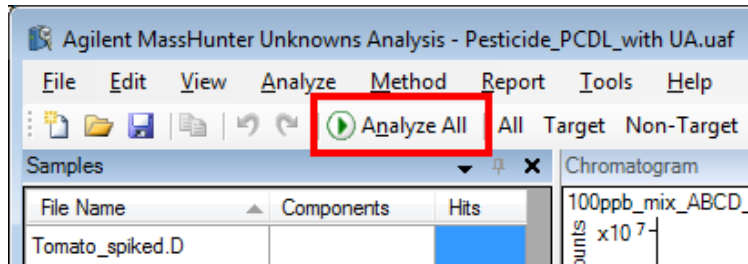
- Click **OK**.



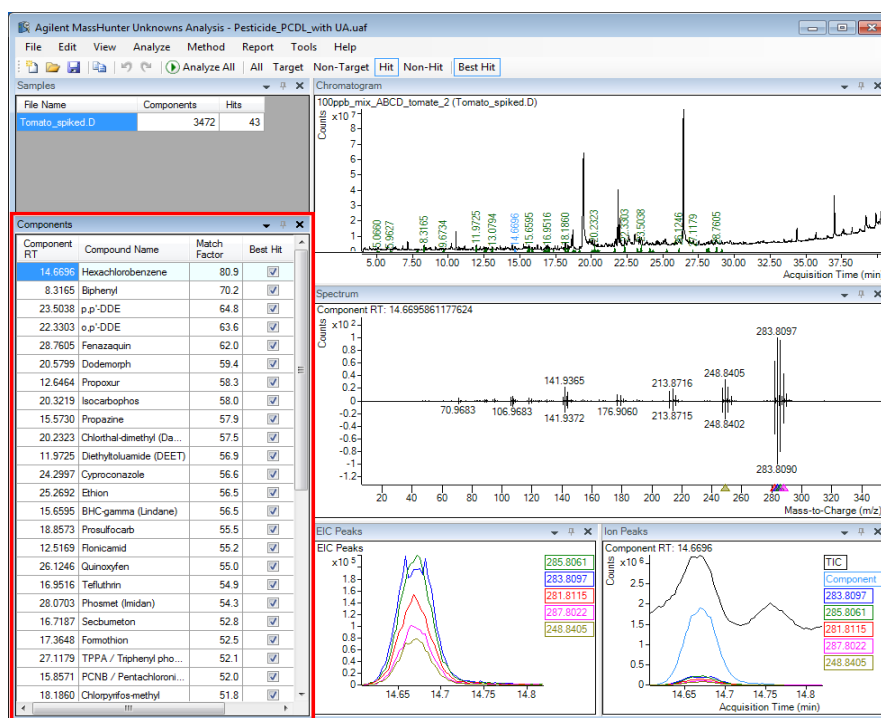
Run the analysis

1. Click **Analyze All**.

Use this procedure to apply your defined methods options and analyze the Unknown Analysis results.

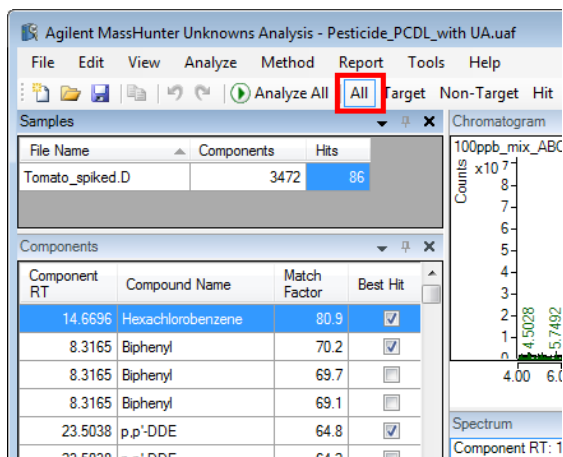


The analysis opens and displays the **Best Hits** in the **Components** table.

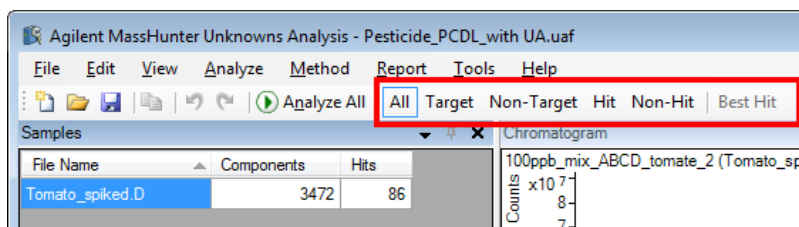


2. Select a component to view the Spectrum and Ion Peaks for the selected component.

3. Click **All** to view all the peaks.



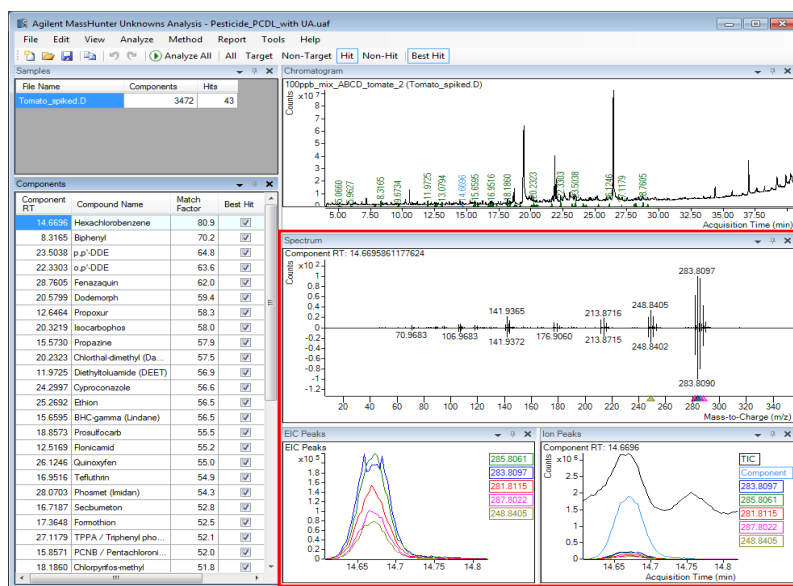
4. Click:
Target to display the peaks that are also in the quantitation batch
Non-Target to display the peaks that are not in quantitation batch
Hit to display the peaks that are also in the library
Non-Hit to display the peaks that are not in the library
Best Hit to display view the best match



5. Select a component from the **Components** table.

6. View the **Spectrum**, **EIC Peaks**, and **Ion Peaks**, for the selected component.

In the **Spectrum** window, the top spectrum is from the component and the bottom spectrum is from the library.



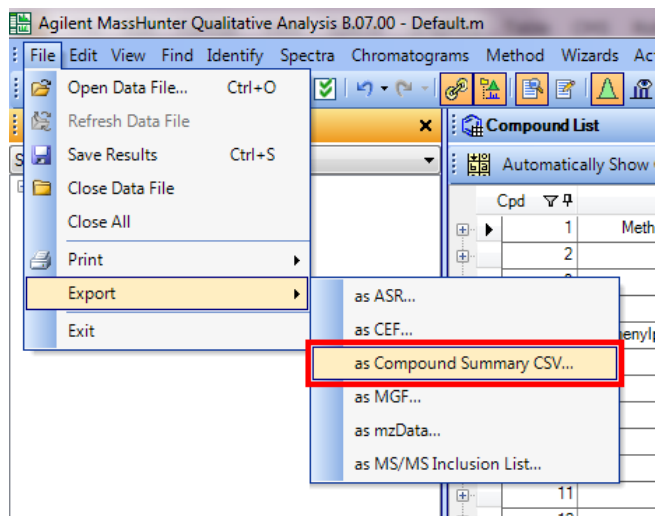
Exercise 5. Create a Custom PCDL from Your Compound Results

Export compound results as a CSV file from Qualitative Analysis

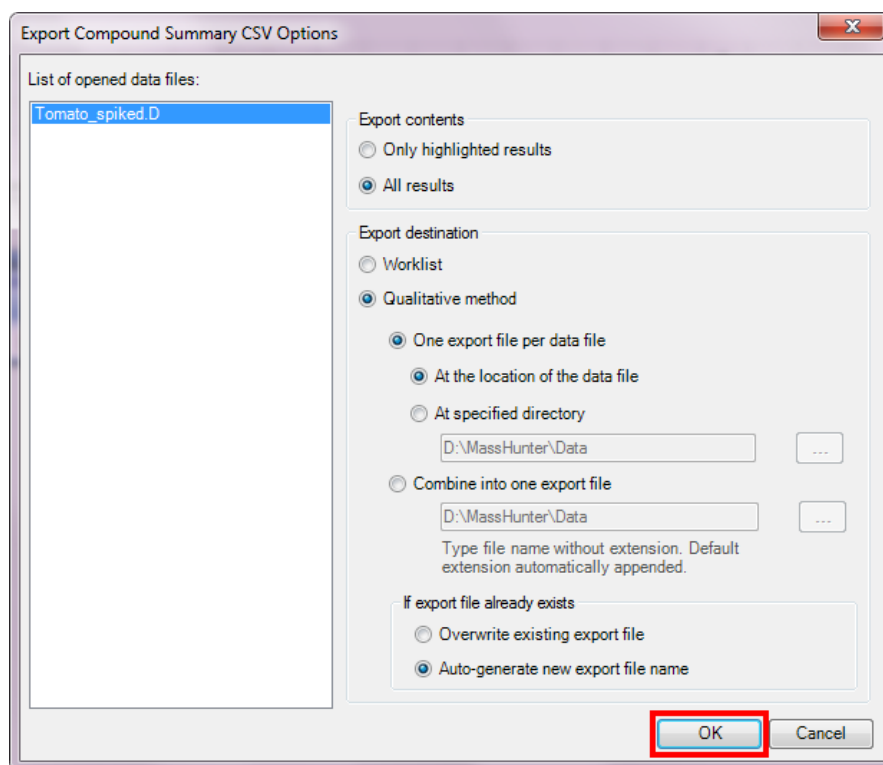
1. Use "Exercise 3. Use the PCDL to Identify Compounds in Qualitative Analysis" on page 36 to identify compounds in Qualitative Analysis.
2. Click **File > Export > as a Compound Summary CSV**.

In this exercise, you will export your compound results from the Qualitative Analysis program or the Unknowns Analysis program and import the compounds into PCDL Manager to create a new custom PCDL containing only the compounds identified in your analysis.

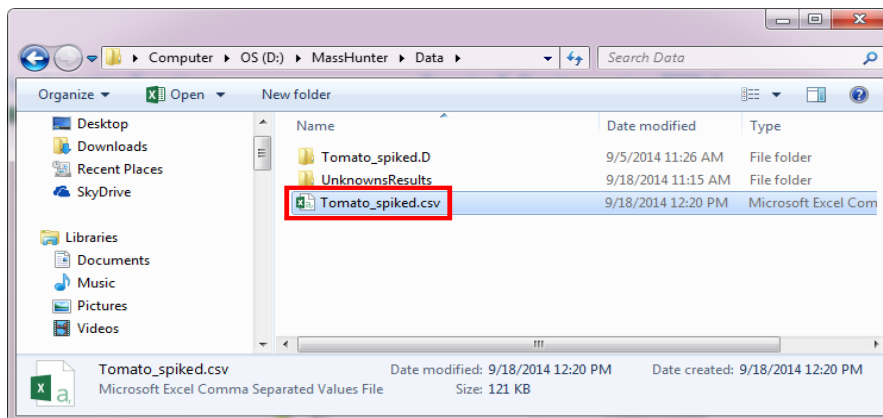
Use this procedure to export your compound results to a CSV file from Qualitative Analysis.



3. Specify the **Export Compound Summary CSV Options**, and click **OK**.



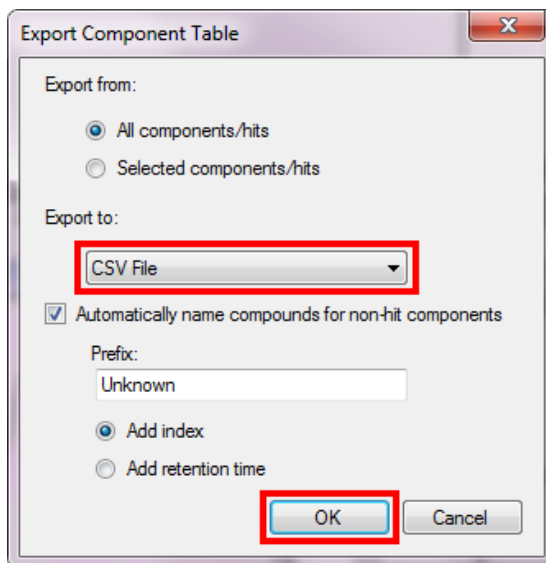
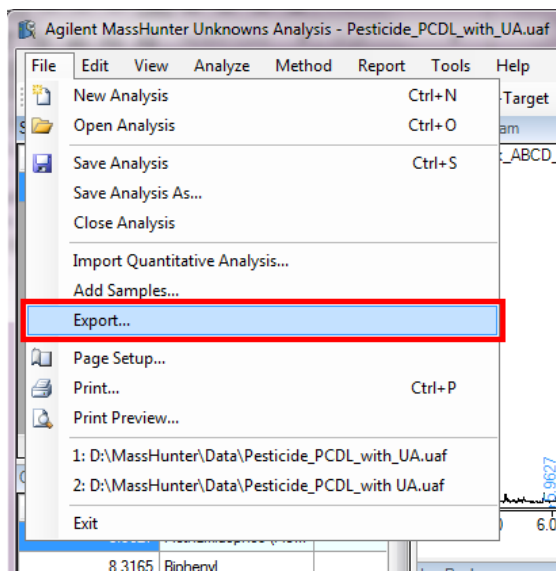
The CSV file is created in the Export Destination folder specified in the Export Compound Summary CSV options.



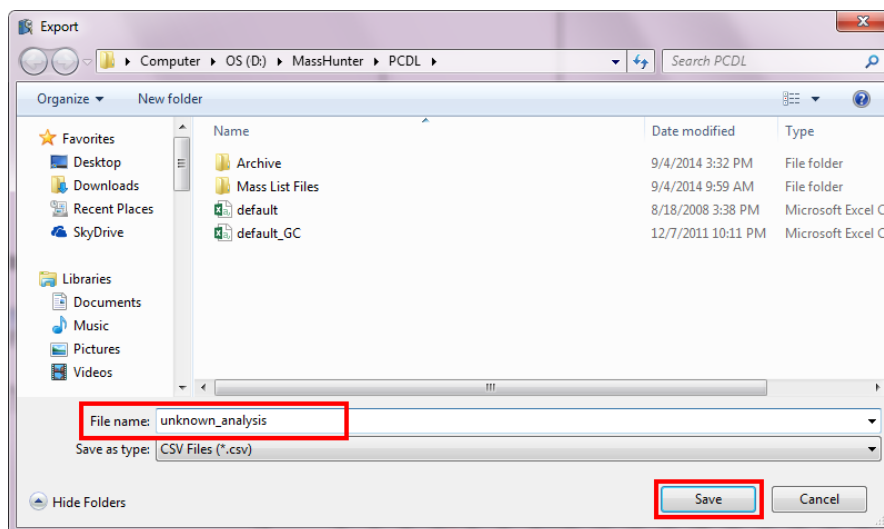
Export compound results as a CSV file from Unknowns Analysis

1. Use "Exercise 4. Use the PCDL to Identify Compounds with Unknowns Analysis" on page 53 to identify compounds in Unknowns Analysis.
2. Click **File > Export**.
3. Select **CSV File** from the **Export to** drop-down menu, and click **OK**.

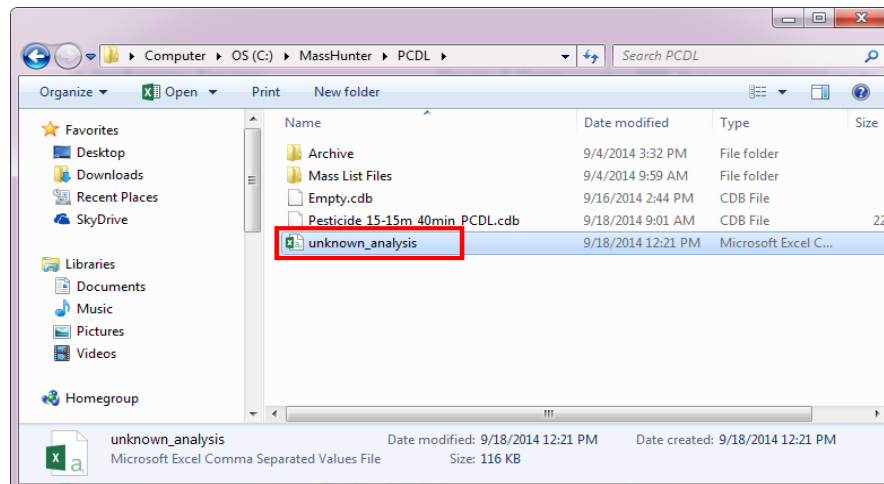
Use this procedure to export your compound results as a CSV file from Unknowns Analysis.



4. Navigate to the folder where you want to save the CSV file.
5. Enter a name for the file, and click **Save**.



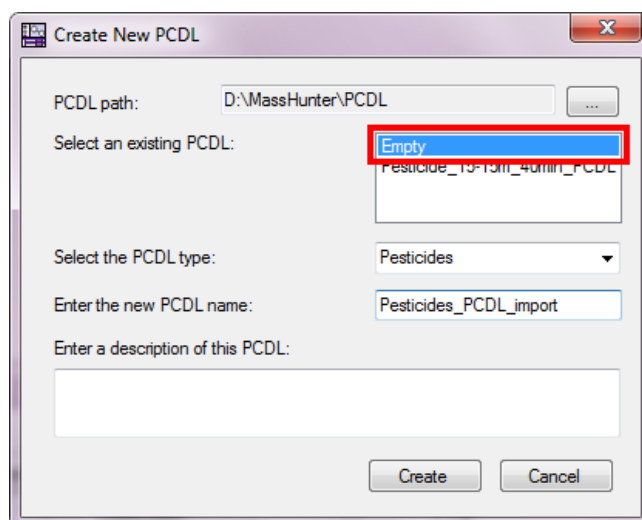
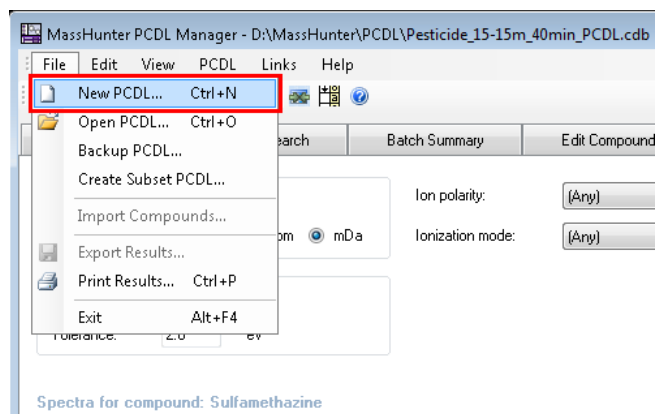
The CSV file is created in the destination folder.



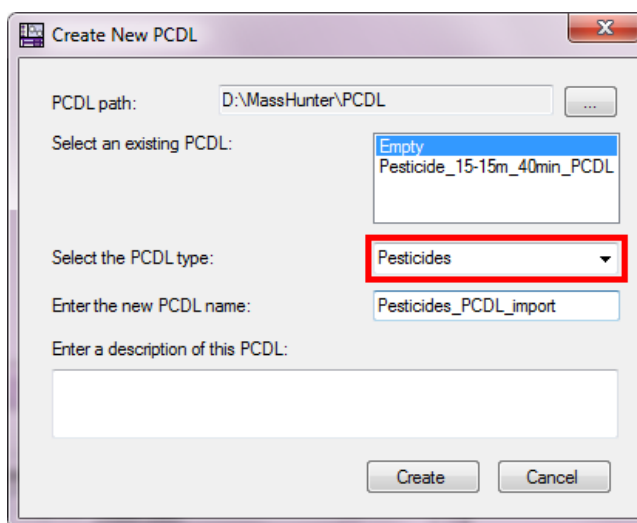
Import compounds from a CSV file into PCDL Manager

1. Start the **MassHunter PCDL Manager** by double-clicking the desktop icon.
2. Click **Cancel** when asked to open a PCDL.
3. Select **File > New PCDL**.
4. Select the existing PCDL, **Empty**.

Use this procedure to create a new PCDL in PCDL Manager by importing compounds from a previously created CSV file.



5. Select the PCDL type, **Pesticides**.



Create New PCDL

PCDL path: D:\MassHunter\PCDL

Select an existing PCDL: Empty
Pesticide_15-15m_40min_PCDL

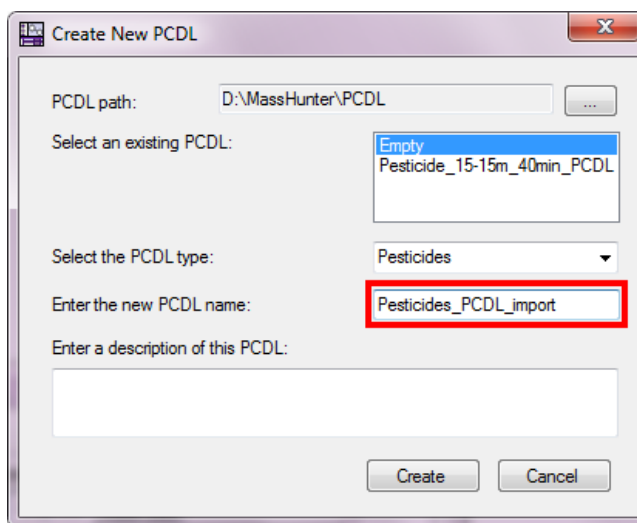
Select the PCDL type: Pesticides

Enter the new PCDL name: Pesticides_PCDL_import

Enter a description of this PCDL:

Create Cancel

6. Enter the new PCDL name, **Pesticide_PCDL_import**.



Create New PCDL

PCDL path: D:\MassHunter\PCDL

Select an existing PCDL: Empty
Pesticide_15-15m_40min_PCDL

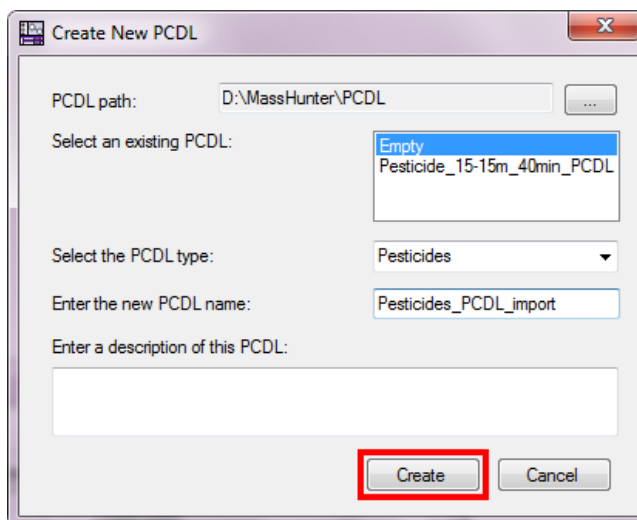
Select the PCDL type: Pesticides

Enter the new PCDL name: Pesticides_PCDL_import

Enter a description of this PCDL:

Create Cancel

7. Click **Create**.



Create New PCDL

PCDL path: D:\MassHunter\PCDL

Select an existing PCDL: Empty
Pesticide_15-15m_40min_PCDL

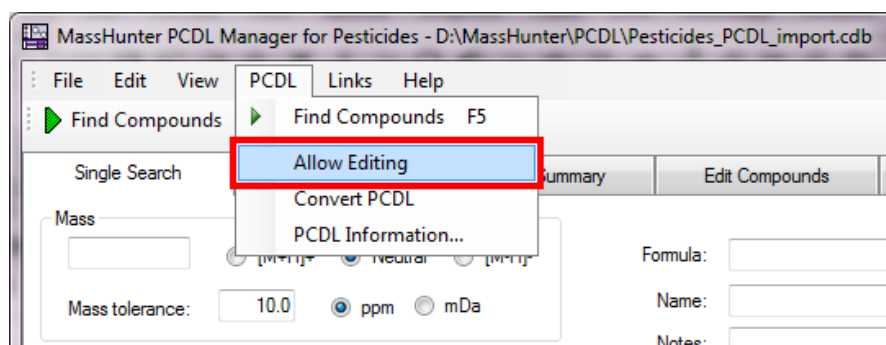
Select the PCDL type: Pesticides

Enter the new PCDL name: Pesticides_PCDL_import

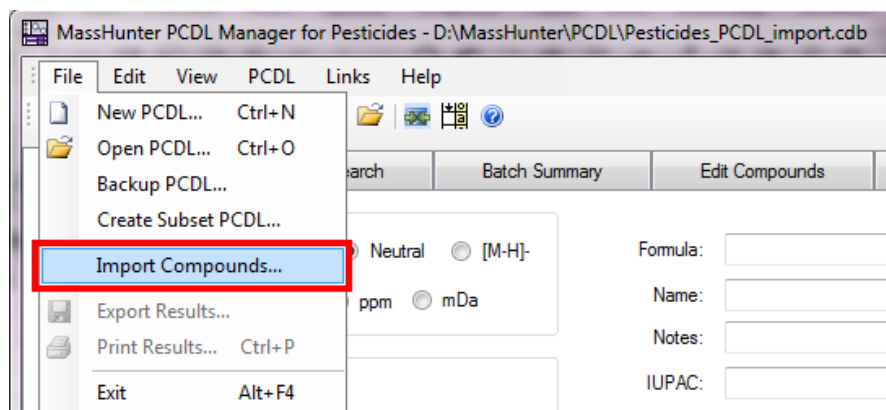
Enter a description of this PCDL:

Create Cancel

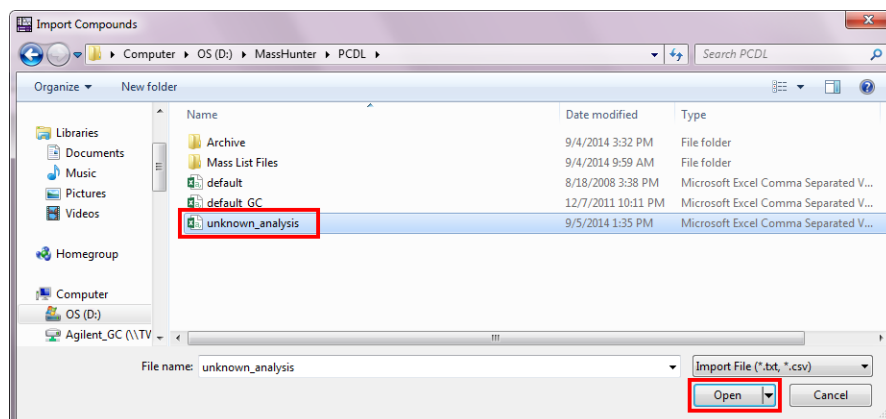
8. Select **PCDL > Allow Editing**.



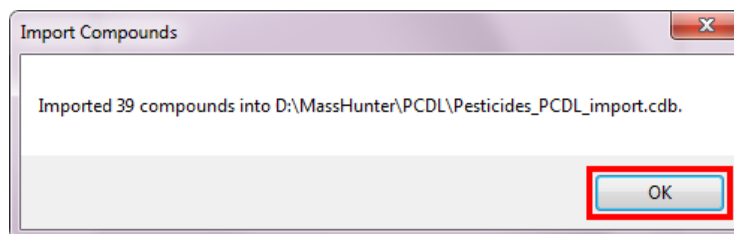
9. Select **File > Import Compounds**.



10. Navigate to and open a .csv file previously created in "Export compound results as a CSV file from Qualitative Analysis" on page 62, or "Export compound results as a CSV file from Unknowns Analysis" on page 64.



11. Click **OK** to confirm the compounds have been imported.



12. Click **Find Compounds** to view a list of all the imported compounds in the **Single Search Results** table.

MassHunter PCDL Manager for Pesticides - C:\MassHunter\PCDL\Pesticides_PCDL_import.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Mass: [M+H]⁺ Neutral [M-H]⁻ Formula:
 Mass tolerance: 10.0 ppm mDa Name:
 Retention time: Require IUPAC:
 RT tolerance: 0.1 min CAS:
 Ion search mode: ChemSpider:
 Include neutrals
 Include anions
 Include cations

Print/ Copy in Regulatory Format

Single Search Results: 65 hits

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name
▶ Methamidophos (Metamidophos)	C2H8NO2PS	141.00134	<input type="checkbox"/>	<input type="checkbox"/>				
Biphenyl	C12H10	154.07825	<input type="checkbox"/>	<input type="checkbox"/>				
DEET / Diethyltoluamide	C12H17NO	191.13101	<input type="checkbox"/>	<input type="checkbox"/>				
Pebulate	C10H21NOS	203.13439	<input type="checkbox"/>	<input type="checkbox"/>				
Propoxur	C11H15NO3	209.10519	<input type="checkbox"/>	<input type="checkbox"/>				
Carbofuran	C12H15NO3	221.10519	<input type="checkbox"/>	<input type="checkbox"/>				
Secbumeton	C10H19N5O	225.15896	<input type="checkbox"/>	<input type="checkbox"/>				
Fonicamid	C9H6F3N3O	229.04630	<input type="checkbox"/>	<input type="checkbox"/>				
Propazine	C9H16ClN5	229.10942	<input type="checkbox"/>	<input type="checkbox"/>				
Tetbutyn	C10H19N5S	241.13612	<input type="checkbox"/>	<input type="checkbox"/>				
Ethoprop (Ethoprophos)	C8H19O2PS2	242.05641	<input type="checkbox"/>	<input type="checkbox"/>				
Prosulfocarb	C14H21NOS	251.13439	<input type="checkbox"/>	<input type="checkbox"/>				
Fomothion	C6H12NO4PS2	256.99454	<input type="checkbox"/>	<input type="checkbox"/>				
Chlorpyrifos	C8H9ClNP3O2	263.00155	<input type="checkbox"/>	<input type="checkbox"/>				





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