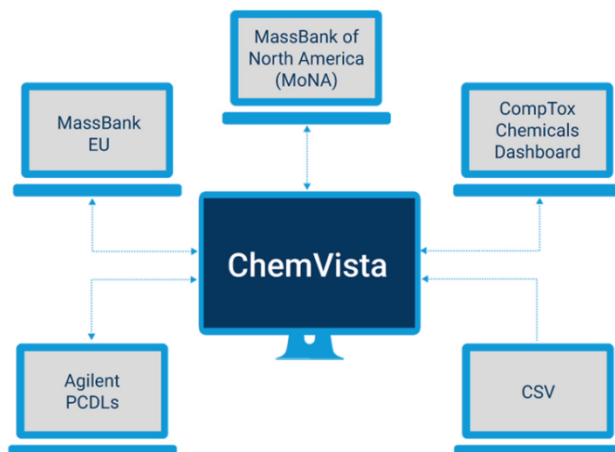


GC/Q-TOF PCDL

User Guide

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Notices

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Software Revision

This guide is valid for the C.01.00 revision or higher of the GC/Q-TOF PCDL program and compatible GC/Q-TOF PCDL programs, until superseded.

Software Manufacturing



Manufactured for Agilent
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In This Book

This book describes the GC/Q-TOF PCDLs. It explains the system configuration and/or method setup information pertaining to subset PCDLs and provides a general data analysis workflow.

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1

Overview

This chapter provides an overview of the GC/Q-TOF PCDL.

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What is the GC/Q-TOF PCDL?

The GC/Q-TOF Personal Compound Database and Library (PCDL) is a collection of accurate mass spectral libraries that let you screen for a wide range of analytes. This document describes configuration and method setup for data acquisition when using Pesticides, Metabolomics, or Natural Product PCDLs. It also provides a generic data analysis workflows.

Software Requirements

The following software is required:

- Agilent MassHunter GC/MS Acquisition software B.10.2
- Agilent MassHunter Qualitative Data Analysis software B.10.0
- Agilent MassHunter Quantitative Data Analysis software B.10.2 or B.11.1
- Use Agilent ChemVista to manage compound and spectral data, including creating subset target lists

Installation file locations

Folder location for files after installation from the Agilent-provided solution disc are described in the following table.

Item	Folder location for files
GC/Q-TOF Metabolomics PCDL (2 .cdb files)	D:\MassHunter\PCDL\GCQTOF PCDLs\Metabolomics
GC/Q-TOF Natural Products PCDL (2 .cdb files)	D:\MassHunter\PCDL\GCQTOF PCDLs\Natural Products
GC/Q-TOF Pesticides PCDL (3 .cdb files)	D:\MassHunter\PCDL\GCQTOF PCDLs\Pesticides

See the *Installation Guide* for more details pertaining to the installed file location. When installed on a PC with a MassHunter home already defined and/or a fixed D:\ drive, files will be installed to the location above.

Glossary

Item	Description
CI	Chemical Ionization
CSL	Cold splitless mode
FAME	Fatty Acid Methyl Esters
EI	Electron Ionization
GC	Gas Chromatography
HSL	Hot splitless mode
MS	Mass spectrometry
PCDL	Personal Compound Database and Library
Q-TOF	Quadrupole Time-of-Flight mass spectrometer
SureMass	Agilent signal processing algorithm for chemical component detection designed specifically for high-resolution profile MS data
RTL	Retention Time Locking

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2

Pesticides PCDL for GC/Q-TOF

This chapter describes the system configuration and recommended data acquisition methods to implement the Pesticide PCDL and Workflow for the GC/Q-TOF solution. Three PCDLs are included for pesticides, each with a different set of RTs based on different gradients with specific GC oven ramps described below.

The GC/Q-TOF system is configured with a midcolumn backflushing setup. After the hardware is properly installed, perform the Retention Time Locking the Data Acquisition Method procedure.

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GC/Q-TOF System Setup

The Agilent 7250 Quadrupole Time-of-Flight GC/Q-TOF MS System is shown in the following figure.



The Agilent 8890 GC system includes:

- Fast oven power supply, where applicable (G3540 Option 002 or 003)
- Split-Splitless or Multimode G3540 Inlet (G3540 Option 112, 150, or 151)
The Split/Splitless inlet (Option 112) only allows for a hot split or splitless injection method. For cold splitless or large volume injection methods, use a Multimode Inlet cooled with air or liquid N₂ (Option 151). If a Multimode Inlet cooled with liquid CO₂ is preferred, choose options 150.
- Mass Spectrometer Detector Interface (G3450-60599)
- Pre-Installed Purged Ultimate Union (G3440-60604)

The Agilent 7693 Series system includes:

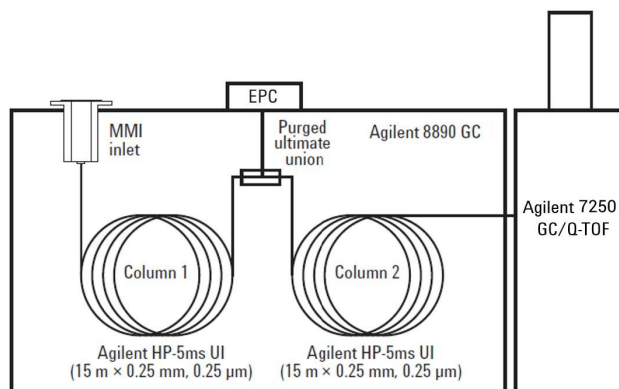
- Agilent 7693A Autoinjector Module (G4513A)
- Agilent 7693A Autosampler Tray Module (G4514A)

Parts and Consumables

Required Parts and Consumables and described in the following table.

Part number	Description	Quantity
19091S-431U	HP-5ms Ultra Inert, 15 m, 0.25 mm, 0.25 μ m, 7-inch cage	2
5183-4757	Agilent septa, bleed and temperature optimized (BTO), nonstick, 11 mm, 50/pk	1
5190-2293	Agilent liner, Ultra Inert, splitless, single taper, glass wool	1
5190-2297	Agilent liner, Ultra Inert, splitless, dimpled, 2 mm id	1
5190-6194	Self-tightening column nut, for Agilent inlet and detector fittings	1
5190-5233	Self-tightening column nut, for Agilent mass spec interface transfer line	1
5181-3323	Ferrule, 0.4 mm id, 15% graphite/85% Vespel, 0.1 to 0.25 column, 10/pk	1
1460-1914	Column hanger	1
G3440-80217	Column install pre-swaging tool, graphite	1

The GC/Q-TOF hardware setup is shown in the following figure.



Data Acquisition Methods

This section describes the HSL and CSL operating conditions.

HSL Operating Conditions

The operating conditions for the two recommended Hot Splitless (HSL) methods are described in the following table.

	Hot splitless, 20 minutes	Hot splitless, 40 minutes
GC		
Columns	Agilent HP-5ms UI, 15 m, 0.25 mm id, 0.25 μ m film (two each)	Agilent HP-5ms UI, 15 m, 0.25 mm id, 0.25 μ m film (two each)
Carrier gas	Helium	Helium
Column 1 flow	1.0 mL/min	1.0 mL/min
Column 2 flow	1.2 mL/min	1.2 mL/min
Injection volume	1 μ L splitless	1 μ L splitless
Inlet liner	4 mm id Ultra Inert Liner Single Taper w wool (p/n 5190-2293)	4 mm id Ultra Inert Liner Single Taper w wool (p/n 5190-2293)
MMI temperature	280 °C	280 °C
Septum purge flow	3 mL/min	3 mL/min
Purge flow to split vent	50 min/min at 1 minute	50 min/min at 1 minute
Gas saver	On, 20 mL/min after 2 minutes	On, 20 mL/min after 2 minutes
Oven temperature program	60 °C for 1 minute 40 °C/min to 170 °C, 0 minutes 10 °C/min to 310 °C, 3 minutes	60 °C for 1 minute 40 °C/min to 120 °C, 0 minutes 5 °C/min to 310 °C, 0 minutes
Run time	20.75 minutes	40.5 minutes
Backflush conditions	5 minutes (post run) 310 °C (oven temperature) 50 psi (Aux EPC pressure) 2 psi (Inlet pressure)	5 minutes (post run) 310 °C (oven temperature) 50 psi (Aux EPC pressure) 2 psi (Inlet pressure)

Pesticides PCDL for GC/Q-TOF

CSL Operating Conditions

	Hot splitless, 20 minutes	Hot splitless, 40 minutes
Retention time locking	Chlorpyrifos-methyl locked to 9.143 minutes	Chlorpyrifos-methyl locked to 18.111 minutes
Transfer line temperature	280 °C	280 °C
Q-TOF MS		
Ionization mode	EI	EI
Source temperature	280 °C	280 °C
Quadrupole temperature	180 °C	180 °C
Mass range	45 to 550 m/z	45 to 550 m/z
Spectral acquisition rate	3-5 Hz, collecting both in centroid and profile modes	3-5 Hz, collecting both in centroid and profile modes
Emission current	5 μ A	5 μ A

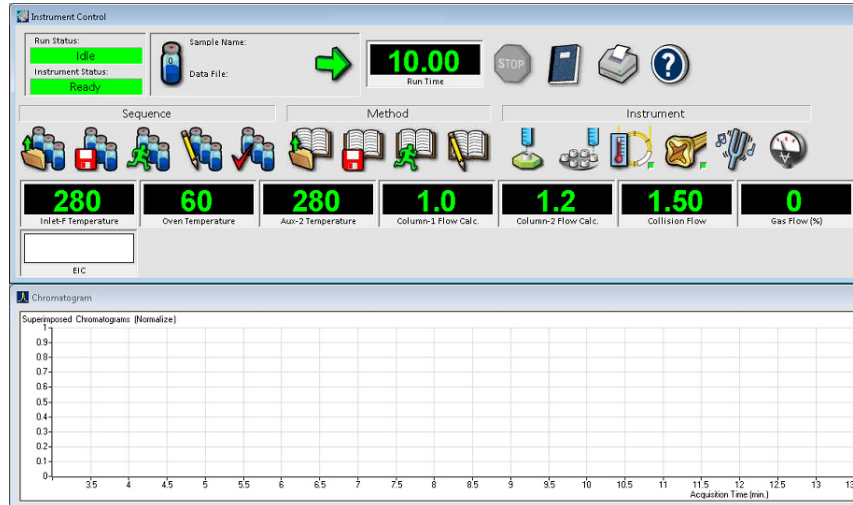
CSL Operating Conditions

Cold Splitless (CSL) mode is also an option to introduce samples. To implement CSL, modify your data acquisition method with the MMI parameters specified in the following table.

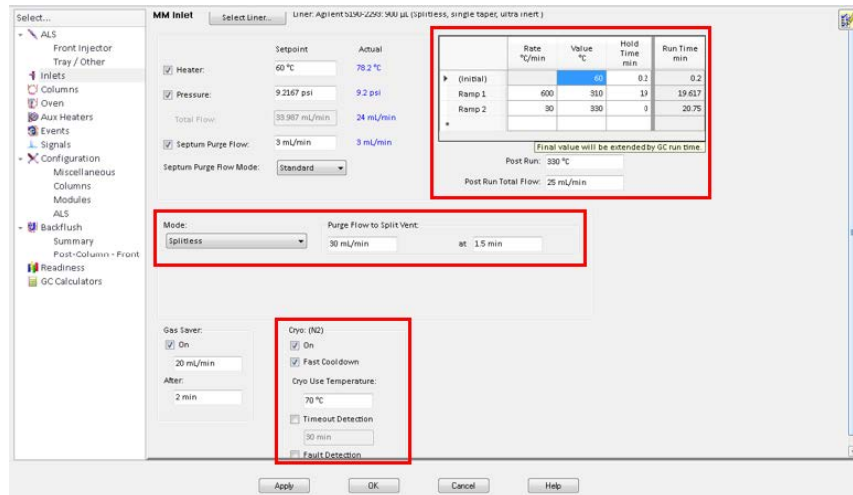
Injection volume	2 μ L Cold splitless
MMI temperature program	60 °C for 0.2 minutes 600 °C/min to 300 °C, hold 330 °C, post run
Purge flow to split vent	30 min/min at 1.5 minutes
Cooling	On Fast cooldown 70 °C, Cyro use temperature

Set up a Cold Splitless Injection Method

- 1 Click **GC Edit Parameters**.



- 2 Enter the **method parameters** as shown in the figure.



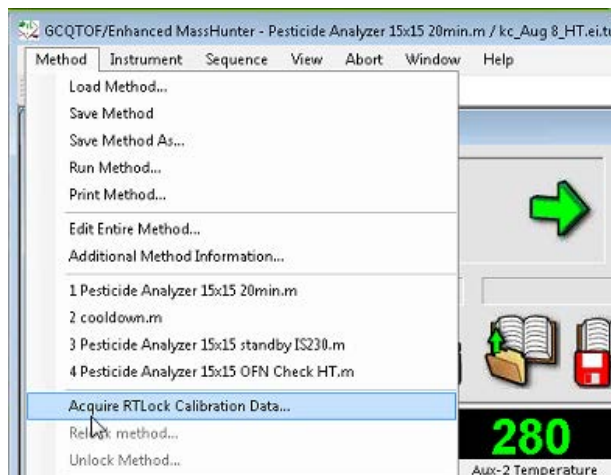
- 3 Click **OK**.
- 4 **Save** your method to a different name.

Retention Time Locking the Data Acquisition Method

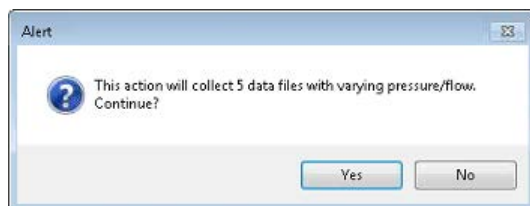
Perform Retention Time Locking (RTL) to Agilent-provided data acquisition methods before your sample analysis. Use the compound Chlorpyrifos-methyl as a locking compound.

Agilent recommends using the pesticide checkout standard (100 µg/mL) for the retention locking process (p/n 5190-0494). The RTL procedure performs several calibration runs and saves the data in your method file. You may choose to acquire only centroid data to reduce the RTL file size. The method must be changed after RTL to acquire Both files (profile and centroid) for your sample analysis.

1 Click **Method > Acquire RTLock Calibration Data.**



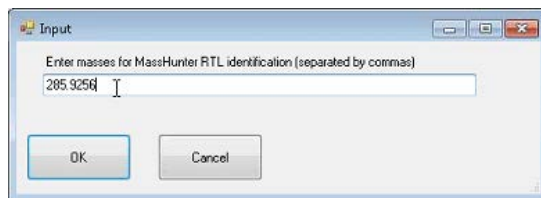
2 Click **Yes.**



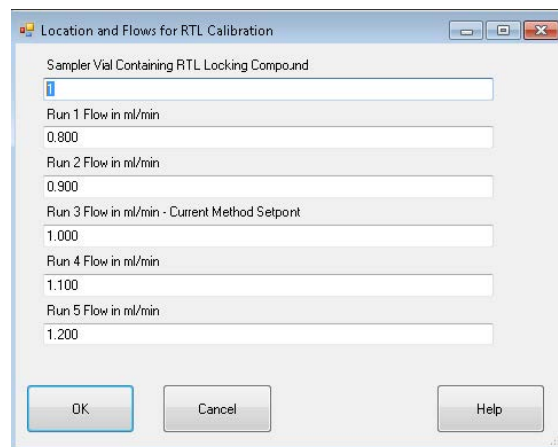
Pesticides PCDL for GC/Q-TOF

Retention Time Locking the Data Acquisition Method

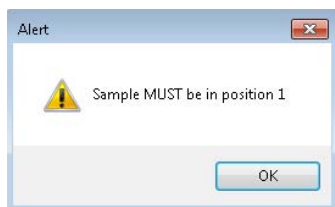
- 3 Enter an accurate mass **value** for the selected ion, and click OK.



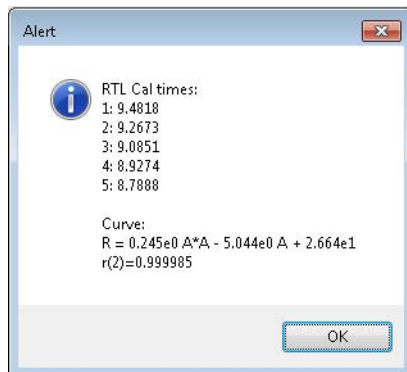
- 4 Ensure your checkout standard is placed in the correct vial position on the autosampler tray, as indicated in the **Sampler Vial Containing RTL Locking Compound** field.



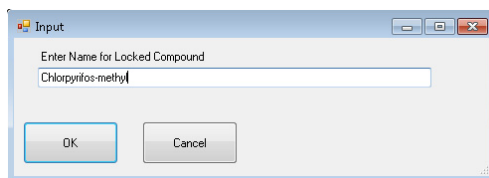
- 5 Click **OK** to start the retention time locking calibration.
- 6 Click **OK**.



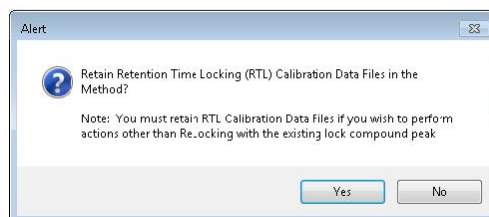
- 7 Once the calibration run completes, click **OK**.



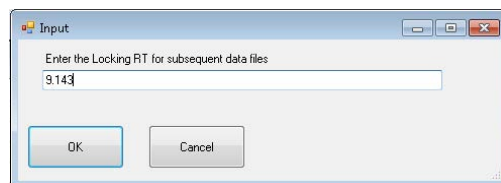
- 8 Enter the **name** of the locking compound, and click **OK**.



- 9 Select whether or not to retain **RTL Calibration Files** in the method. Whether or not you save the original files, the calibration curve will be saved, allowing you to relock your method.



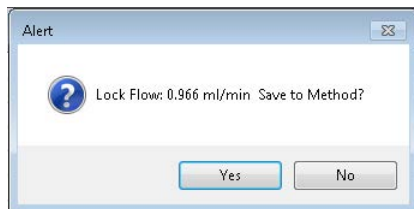
- 10 Enter the target retention **time** of the locking compound, and click **OK**.



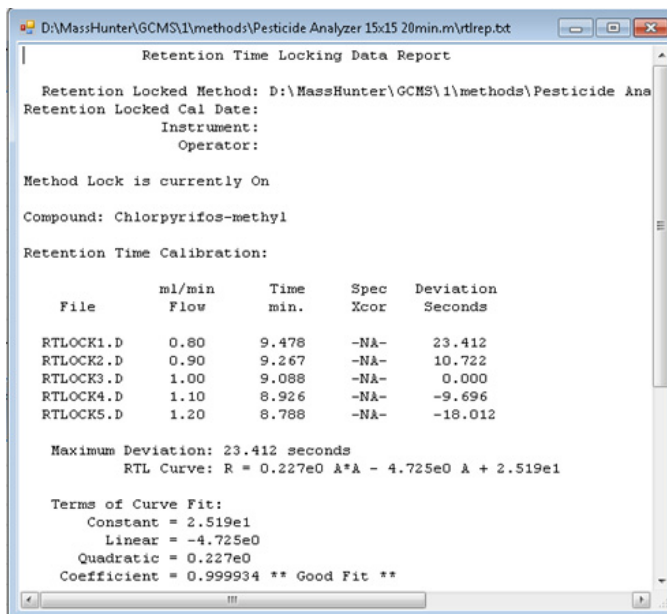
Pesticides PCDL for GC/Q-TOF

Retention Time Locking the Data Acquisition Method

11 Click **Yes** to save the flow to the method.



12 A **Retention Time Locking Data Report** is available to review the RTL results.



The screenshot shows a window titled "Retention Time Locking Data Report" with the following content:

```
Retention Time Locking Data Report
Retention Locked Method: D:\MassHunter\GCMS\1\methods\Pesticide Ana
Retention Locked Cal Date:
Instrument:
Operator:

Method Lock is currently On

Compound: Chlorpyrifos-methyl

Retention Time Calibration:

  File      ml/min   Time   Spec   Deviation
  Flow      min.    Xcor   Seconds

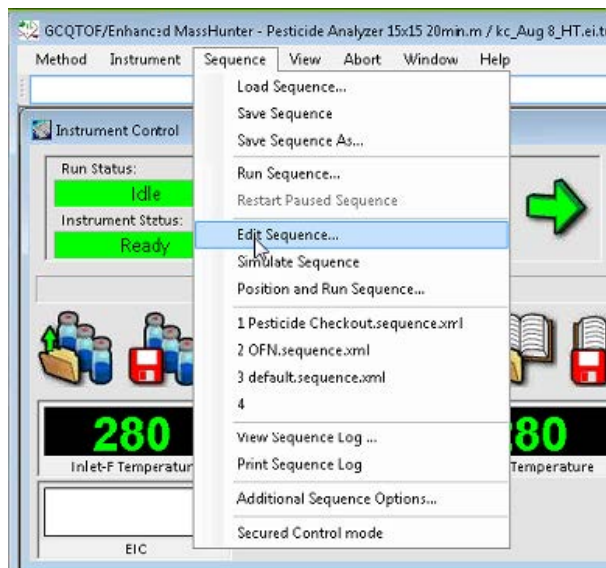
RTLOCK1.D  0.80    9.478  -NA-   23.412
RTLOCK2.D  0.90    9.267  -NA-   10.722
RTLOCK3.D  1.00    9.088  -NA-    0.000
RTLOCK4.D  1.10    8.926  -NA-   -9.696
RTLOCK5.D  1.20    8.788  -NA-  -18.012

Maximum Deviation: 23.412 seconds
RTL Curve: R = 0.227e0 A*A - 4.725e0 A + 2.519e1

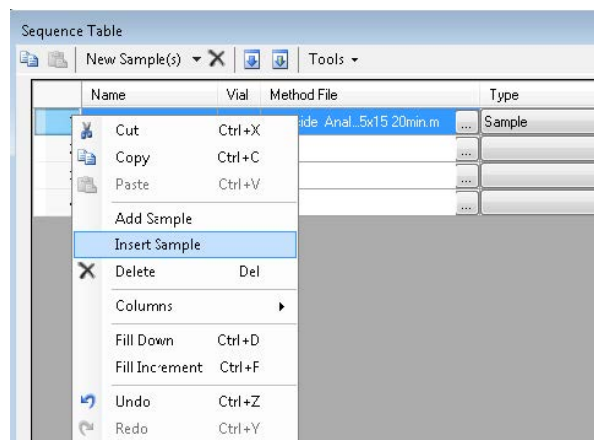
Terms of Curve Fit:
  Constant = 2.519e1
  Linear = -4.725e0
  Quadratic = 0.227e0
  Coefficient = 0.999934 ** Good Fit **
```

Set up an Automatic Mass Calibration in your Sequence

- 1 Click **Sequence > Edit Sequence**.



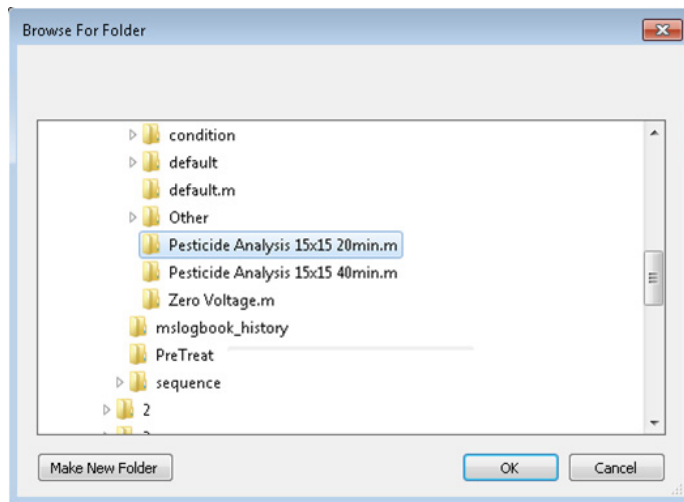
- 2 Right-click in the sequence table and select **Insert Sample**.



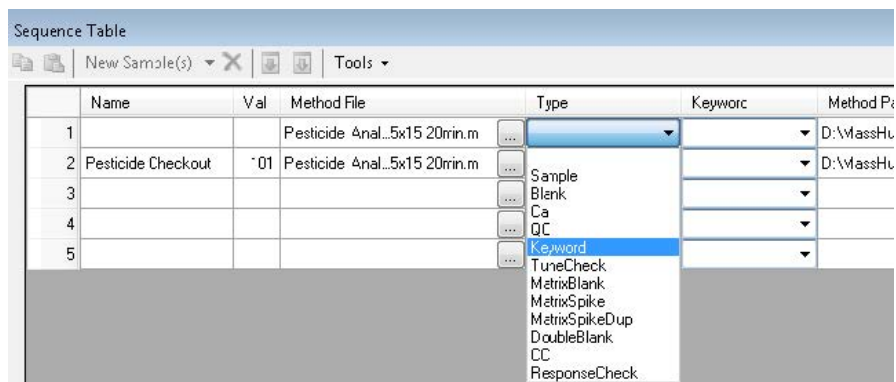
Pesticides PCDL for GC/Q-TOF

Set up an Automatic Mass Calibration in your Sequence

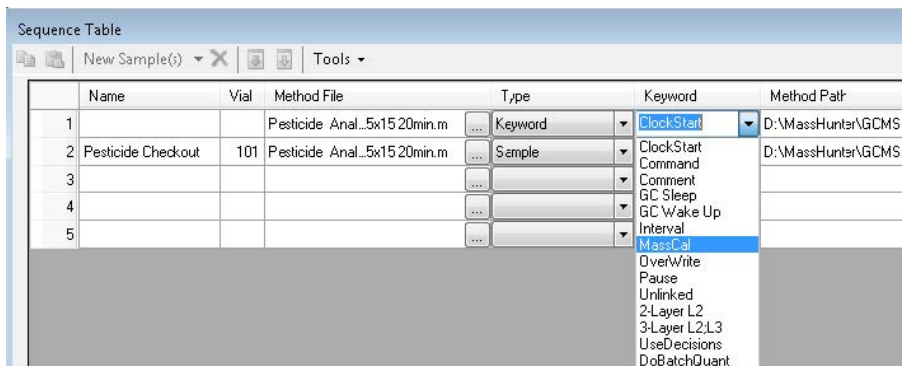
- 3 Select your **method**, and click **OK**. It is important to note that the method loaded for mass calibration should be the one chosen to perform your sample analysis.



- 4 From the **Type** drop-down list, select **Keyword**.



- 5 From the **Keyword** drop-down list, select **MassCal**.



- 6 Click **OK**.

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3

Metabolomics PCDL for GC/Q-TOF

This chapter describes sample preparation, system configuration, and recommended data acquisition methods when using Metabolomics PCDL for GC/Q-TOF. Two PCDLs are included for metabolomics, each with a different set of RI values based on the FAMES and Alkanes indices, respectively.

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Sample Preparation and Derivatization

Biological sample extracts

The preparation of optimal extracts from biological samples is very much dependent on the type of matrix analyzed and the class of compound that is of interest for the study. The exact procedures have to be carefully examined and are not part of this guide.

Metabolites

Metabolites are generally small molecules, and most primary metabolites bear hydrophilic functional groups such as carboxyl, hydroxyl, or amino groups. According to the functional groups, these molecules are often classified into amino acids, carbohydrates, fatty acids and organic acids.

The presence of a variety of hydrophilic functional groups enables cells to use metabolites for a variety of cellular purposes, including transport in the aqueous cellular environment or between compartments and organs.

The presence of these functional groups in extracts of biological samples causes a significant rise in boiling points, rendering most primary metabolites unsuitable for GC separations.

Internal standard

The RTL locking compound should be included in every sample. Examining the locking compound in a data file from an RTL method determines if a re-locking needs to be performed. The retention time or RI is a very important part of the analysis. This measurement is used in combination with the EI spectra to identify a metabolite.

RTL locking compound: Myristic acid d27. RT of the locking standard is 16.752 minutes.

Retention index markers

The FAME markers used for calculating retention indices are not required in a sample. It is required that a FAME marker calibration sample is run and correctly associated with a sample. Acquiring data for FAMEs markers daily can guarantee that a correct RI calibration can be performed.

Fatty acid methyl esters (FAME) are C₈, C₉, C₁₀, C₁₂, C₁₄, C₁₆, C₁₈, C₂₀, C₂₂, C₂₄, C₂₆, C₂₈, and C₃₀ linear chain length. The inclusion of these markers in a sample chromatogram can be used as a QC check. If identical chromatographic conditions as those employed to generate the Agilent Fiehn Library were used, the RT values match.

The *Agilent Fiehn GC/MS Metabolomics Standards Kit* (p/n 400505) contains the RTL locking compound d27 myristic acid, a mix of FAMEs with d27 myristic acid, pyridine as well as MSTFA/1 % TMCS mix.

FAME marker concentrations and RT values are described in the following table.

Name	Concentration	RT (min)
Methyl caprylate C ₈	100 µg/mL	7.812
Methyl perlargonate C ₉	100 µg/mL	9.248
Methyl caprate C ₁₀	100 µg/mL	10.647
Methyl laurate C ₁₂	100 µg/mL	13.25
Methyl myristate C ₁₄	100 µg/mL	15.597
Methyl palmitate C ₁₆	100 µg/mL	17.723
Methyl stearate C ₁₈	50 µg/mL	19.663
Methyl eicosanoate C ₂₀	50 µg/mL	21.441
Methyl docosanoate C ₂₂	50 µg/mL	23.082
Methyl linocerate C ₂₄	50 µg/mL	24.603
Methyl hexacosanoate C ₂₆	50 µg/mL	26.023

Name	Concentration	RT (min)
Methyl octacosanoate C ₂₈	50 µg/mL	27.349
Methyl triacontanoate C ₃₀	50 µg/mL	28.723

Derivatization

The hydrophilic functional groups must be derivatized to remove hydrogen bond formations to increase volatility. This also reduces interaction with the column phase that can cause tailing peaks, poor sensitivity, and poor chromatographic separation. The Agilent Fiehn 2013 GC/MS Metabolomics RTL Library uses a two step derivatization procedure routinely used in most published literature in metabolite profiling by GC/MS.

Key points to consider:

- Thoroughly dry metabolite samples before derivation. Reagents are not compatible with water or protic solvents.
- Use enough reagent to completely derivatize all metabolites.
- Derivatized samples have a 24-hour shelf life.

Before doing a large study, conduct a test to determine the maximum sample size that is completely derivatized with the recommended protocol.

Preparing the biological extract

An aliquot of 5 µL of myristic acid d27 stock solution (0.75 mg/mL) previously diluted 50x is added to the biological extracts. The sample is then evaporated to dryness.

Methoxyamination

Add 10 µL of a 40 mg/mL solution of methoxyamine hydrochloride (Sigma-Aldrich; Cat. No. 226904) in pyridine. This mixture is gently shaken at 30 °C for 90 minutes.

Trimethylsilylation

Add 90 μL of N-Methyl-N- trimethylsilyltrifluoroacetamide with 1% Trimethylchlorosilane (MSTFA +1% TMCS) to the methoxyaminated samples. The mixture is incubated at 37 °C for 30 minutes. The derivatized samples are cooled to room temperature before being transferred into GC vials.

The vials are injected for GC/MS analysis under the conditions given in the “Acquisition Method” section. When analyzing multiple samples, randomize the injection order to reduce the affects of variable reaction times on statistical analysis.

Configuration and Acquisition Method

The following method was used to acquire the retention and spectral data used in the library.

Equipment: Agilent 8890 GC/7250 Q-TOF

GC/Q-TOF Acquisition Parameters are described in the following table.

GC and MS Conditions	Q-TOF (7250)
GC	8890
Column	Agilent J&W DB-5MS UI, 30 m, 0.25 mm, 0.25 μ m, DuraGuard, 10m
Inlet	SSL, 4-mm UI liner single taper
Injection volume	0.5 μ L
Injection mode	Splitless
Inlet temperature	280°C
Oven temperature program	50°C for 0.5 min; 10°C/min to 325°C, 10 min hold
Carrier gas	Helium
Column flow	1 mL/min (The actual flow of the system is determined during the RTL procedure.)
Transfer line temperature	280°C
Quadrupole temperature	150°C
Source temperature	200°C
Electron energy	70 eV
Emission current	5 μ A
Spectral acquisition rate	5 Hz
Mass range	50 to 1200 m/z
Solvent delay	5.90 min



4

Natural Products PCDL for GC/Q-TOF

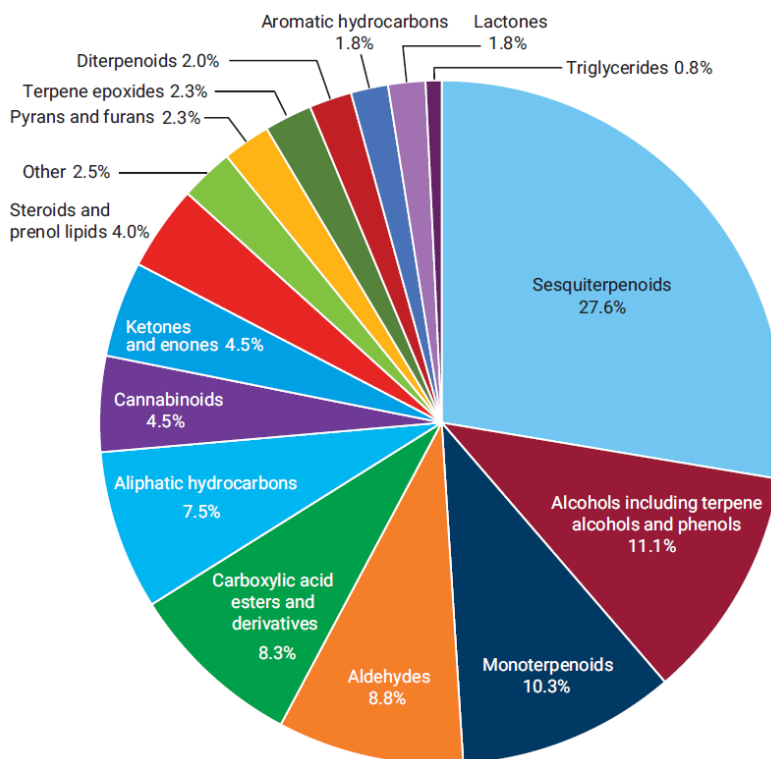
This chapter describes the Natural Products PCDL as well as a recommended data acquisition method. Please note that while this PCDL includes RTs based on the GC method described below, it also includes Kovats RIs for non-polar phase. Additionally, two PCDLs are included: one containing only compounds with spectra and another which includes compounds without spectra.

PCDL Description **32**

Configuration and Data Acquisition Method **33**

PCDL Description

The Natural Products PCDL for GC/Q-TOF is a user-contributed PCDL that has been created from 2D GCxGC hemp CBD oil data and currently includes compound classes shown in the following figure. It is considered user-contributed because it is not solely generated from single standards and contains unidentified compounds with spectra.



Configuration and Data Acquisition Method

Suggested data acquisition parameters are described in the following table.

GC and MS Conditions	Description
MS	Agilent 7250 GC/Q-TOF
GC	Agilent 8890 GC
Inlet	Multimode inlet, 4 mm Agilent Ultra Inert inlet liner, single taper with wool
Inlet Temperature	280 °C
Injection Volume	1 μ L
Columns	Agilent J&W DB-5ms Ultra Inert, 30 m x 0.25 mm, 0.25 μ m (p/n 122-5532UI)
Oven Temperature Program	60 °C for 5 min; 4 °C/min to 300 °C, 7 min hold
Carrier Gas	Helium
Column Flow	1 mL/min constant flow
Transfer Line Temperature	280 °C
Quadrupole Temperature	150 °C
Source Temperature	200 °C
Electron Energy	70 eV
Emission Current	5 μ A
Spectral Acquisition Rate	5 Hz
Mass Range	m/z 40 to 650

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5

Data Analysis Workflows

This chapter describes workflows that are typically used with the accurate mass GC/MS PCDL with GC/Q-TOF data.

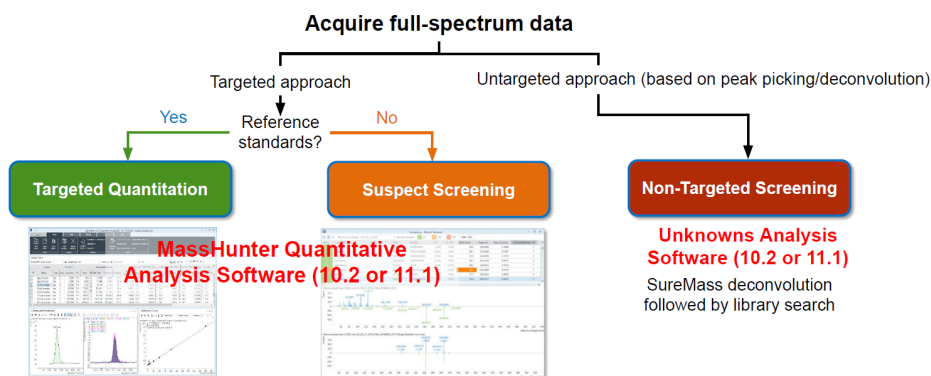
Overview of Target and non-target screening workflows for high-resolution accurate mass GC/Q-TOF	36
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Data Analysis Workflows

Overview of Target and non-target screening workflows for high-resolution accurate mass GC/Q-TOF

Overview of Target and non-target screening workflows for high-resolution accurate mass GC/Q-TOF

The following figure shows the GC/Q-TOF PCDL screening workflow for both targeted and non-targeted approaches.



Managing the PCDL content

Use Agilent ChemVista to manage the content of your PCDL:

- Import your PCDL into the standalone library manager to manage data in a compound-centric fashion. Note that in order to keep derivatized and non-derivatized compound and spectral data properly organized, it may be desirable to turn off or edit the classification feature in ChemVista prior to importing data. This may also apply for stereoisomers where structure information is undefined. See the ChemVista Online Help for more details.

Import Files

Select a source type and files to import

Source type: PCDL (*.cdb)

Select file(s):

Create list on import:

List name:

Description:

Apply method label to imported data:

- Create custom screening lists specific to your analysis by searching for compound class groups and regulation tags as well as searches using compound name, formula, mass, CAS, InChIKey, etc.

Search

Identifiers Formula Mass **Tags** Lists

Start typing to search for tags by name. Click on tags to remove them.

- GB2769-2019
- Pesticide**
- Pesticide degradate
- USDA Pesticides MRL Database

Search

Identifiers Formula Mass **Tags** Lists

Select an identifier field: CAS

13676-82-9
14007-30-8
14868-03-2
15485-05-1
611-99-4
620-92-8
639-44-1
659-22-3
795-43-7
569-58-4
596-27-0
603-41-8
603-44-1

Exact match Non-primary

- Edit and add compounds, retention times, and spectra.

The image shows two overlapping dialog boxes from a software application. The top dialog, titled "Create Substance", contains a form for entering chemical data. The bottom dialog, titled "Edit Spectral Details", contains a table of spectral data and a list of parameters for editing.

Create Substance

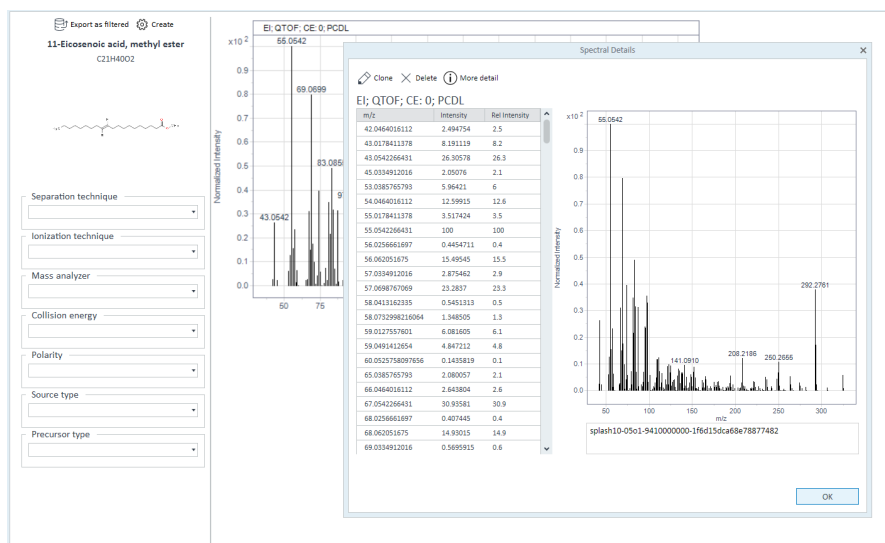
Name: 4,4'-Dihydroxybenzophenone
CAS: 611-99-4
Formula: C
InChI: InChI=1S/C13H10O3/c14-11-5-1-9(2-6-11)13(16)10-3-7-12(15)8-4-10/h1-8,14-15H
InChIKey:
SMILES:
Mass:
LogP:
Anion:
Cation:
IUPAC Name:
ChemSpider:
PubChem:
KEGG:
DTXSID:
Add custom field:
 Add to current list
Commit Cancel

Edit Spectral Details

m/z	Intensity	
73.0649	25.56	
91.0542	53.3	

Separation technique: GC
Mass analyzer: QTOF
Ionization technique: EI
Polarity: POSITIVE
Precursor type: <None>
CE:
Precursor ion:
MS Level:
Fragmentor:
Commit Cancel

- Search, browse, and store spectra acquired on a Q-TOF instrument.

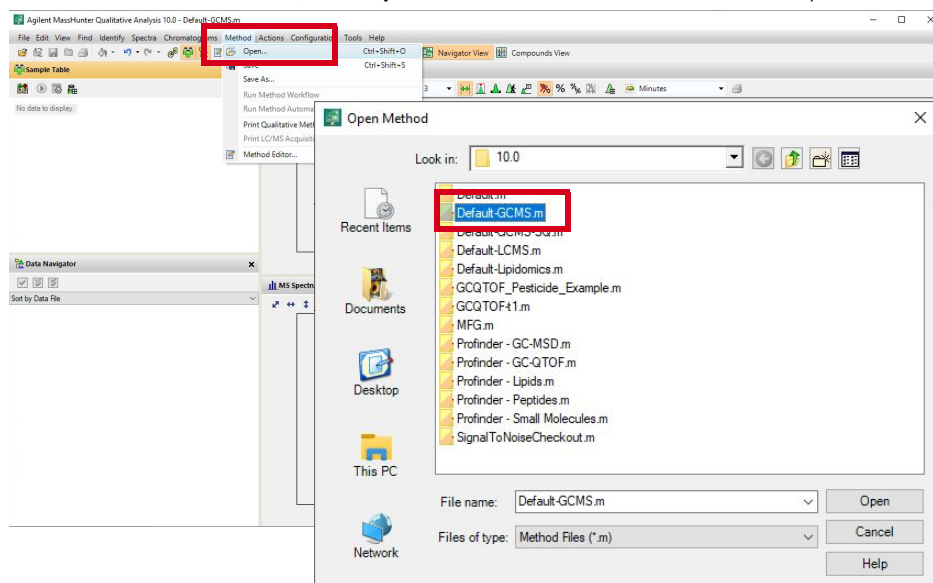


- Merge compounds from your PCDL with compounds and spectra from MassBank, MassBank of North America (MoNA), and the EPA CompTox Chemicals Dashboard. For more information, see the *Agilent ChemVista Introduction Workbook*, introductory videos, and Online Help.
- Send spectra to your customized PCDL directly from the Qualitative Analysis program to create your own custom library. Choose from options to filter spectral noise and/or to correct the product ions to their theoretical accurate mass.
- Import the customized PCDL into Agilent ChemVista.
- Load spectra from either a .CEF file or by copy-and-pasting mass spectra from MassHunter Qualitative.
- For more information, see the *MassHunter Personal Compound Database and Library Manager Quick Start Guide*, *PCDL Manager Online Help*, and *MassHunter Qualitative Analysis Help*.

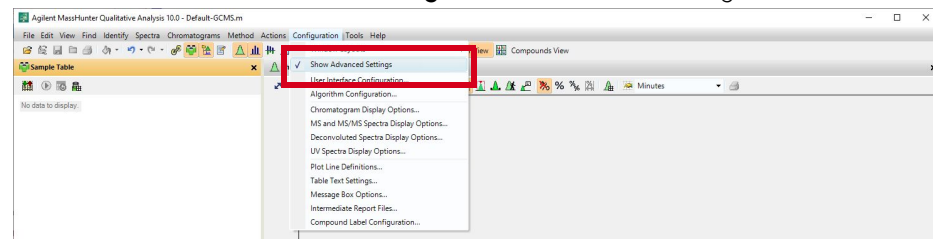
Adding GC/Q-TOF Spectra to a PCDL

Configuring MassHunter Qualitative Analysis 10.0

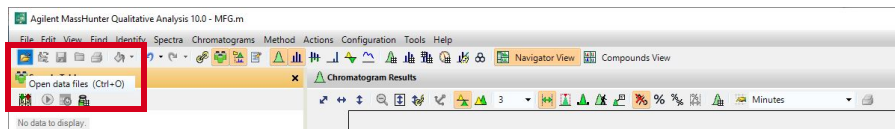
- 1 Acquire data in full spectrum acquisition mode.
- 2 Open **MassHunter Qualitative Analysis** software.
- 3 Under the **Method** tab, click **Open** then click **Default-GCMS.m** and open.



- 4 Make sure **Show Advanced Settings** is checked in the Configuration tab.

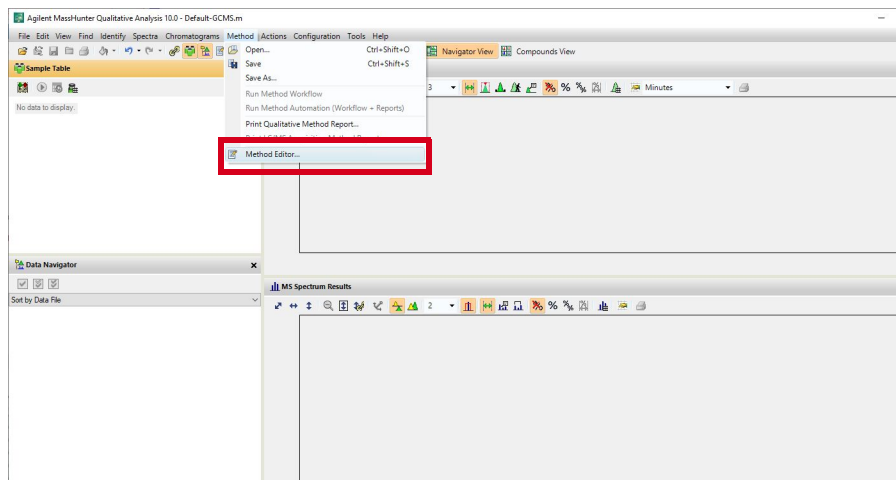


- 5 From the menu bar, load the **data file** (Ctrl+O).

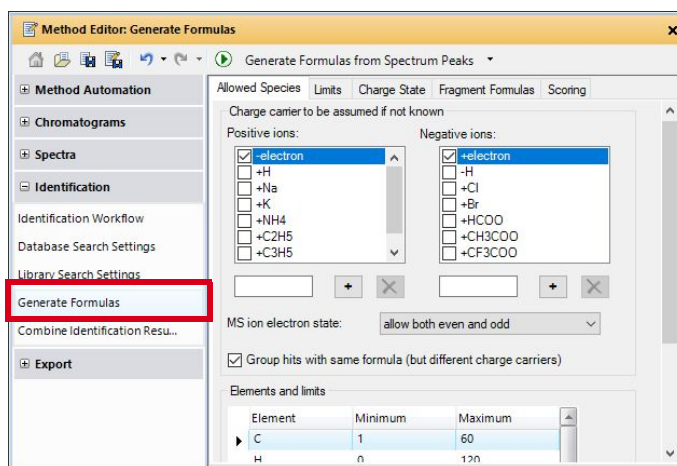


Setting up Molecular Formula Generation with Fragment Formula Annotation Tool in MassHunter Qualitative Analysis Software

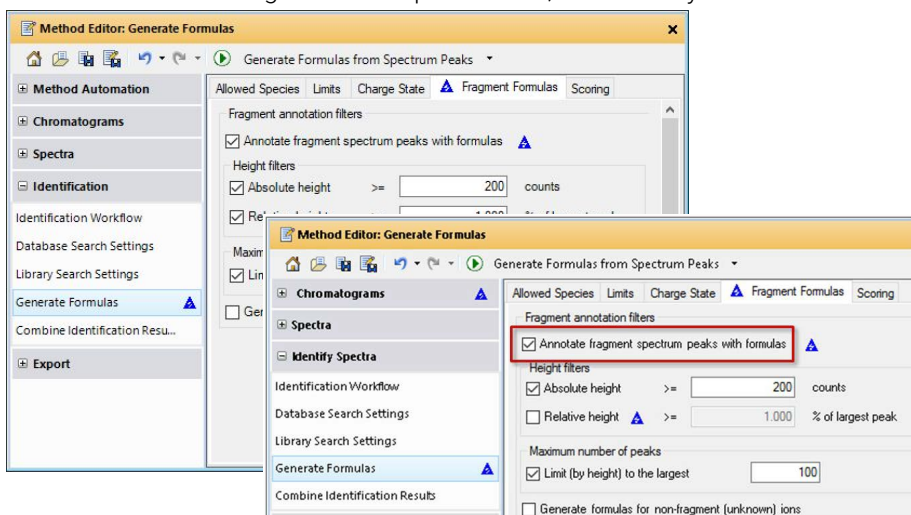
- 1 Under the **Method** tab, click **Method Editor**.



- 2 Navigate to **Generate Formulas** under the **Identification** tab.



- Under the **Fragment Formulas** tab, check **Annotate fragment spectrum peaks with formulas**. Change the filters parameters, if necessary.



Annotation of a Spectrum with Fragment Formulas

- 1 Extract a background subtracted spectrum.
- 2 Right-click on the **spectrum**, and select **Add/Edit Manual Identification** from the right-click menu.

The screenshot displays the Agilent MassHunter Qualitative Analysis 10.0 - MFG.m interface. A 'Method Editor: Generate Formulas' dialog box is open, showing options for 'Fragment annotation filters' such as 'Annotate fragment spectrum peaks with formulas', 'Height filter', and 'Relative height'. In the background, a mass spectrum plot is visible with a right-click context menu open over it. The menu item 'Add/Edit Manual Identification' is highlighted with a red rectangular box.

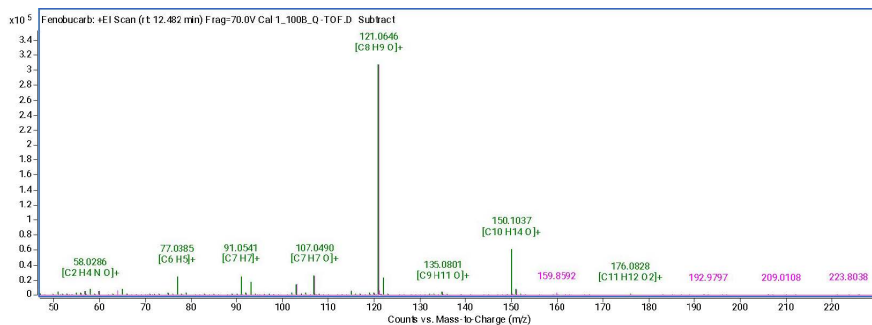
- 3 Enter **formula** and **compound name**. You can add other identifiers such as CAS #. Make sure that the Charge is 1 and M+ is selected in the **ion species** window for EI.

The 'Add/Edit Manual Identification' dialog box is shown with the following fields and values:

- Manual identification results
- Compound name: Fenobucarb
- Molecular formula
- Formula: C12H17NO2
- Charge: 1 (dropdown menu)
- Ion species: M+ (dropdown menu)
- CAS ID: 3766-81-2
- LMP ID: (empty)
- KEGG ID: (empty)
- HMP ID: (empty)
- UniProt ID: (empty)
- Notes: (empty text area)
- Structure: (empty text area)
- Buttons: Load, OK, Cancel

The 'Charge' and 'Ion species' dropdown menus are highlighted with a red rectangular box.

- 4 Check the **Fragment Formula Annotation Results**. All fragments in a spectrum are annotated with formulas which are subsets of a candidate formula for the molecular ion.



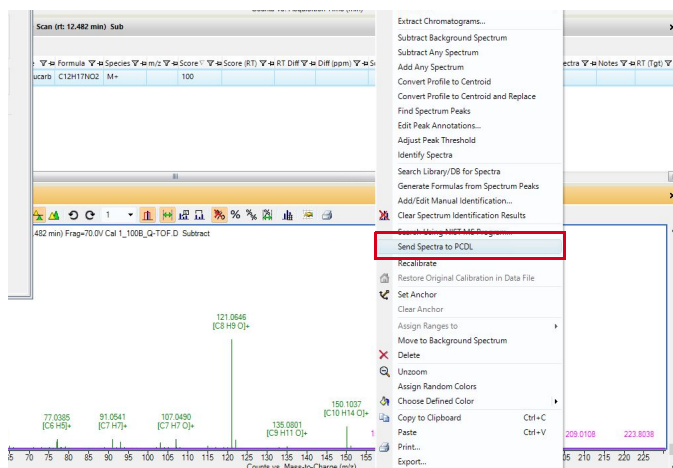
- 5 To edit Fragment Formula Annotation Results, from the right-click spectrum menu select **Edit Peak Annotations**.



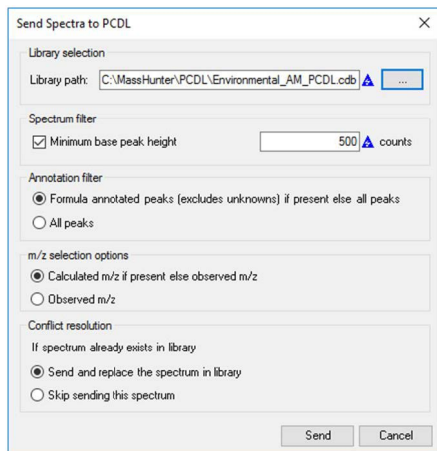
- 6 Species, Formula and Ion Type can be changed. To cancel annotation of an ion, select **Unknown** in the **Ion Type** column.

m/z	Abund	Species	Formula	Formula & to	Diff (ppm)	Ion Type	Loss Formula	Ion
94.0412	630.89	1	M+	C6 H6 O	[C6 H6 O]+	-1.26	Fragment Ion	C6H11NO
94.065	167.4	1	M+	C6 H8 N	[C6 H8 N]+	-1.53	Fragment Ion	C6H9O2
94.0731	1358.9	1	M+	C7 H9	[C7 H9]+	-1.34	Fragment Ion	C5H8NO2
94.0877	156.17							
95.049	579.39	1	M+	C6 H7 O	[C6 H7 O]+	-1.49	Fragment Ion	C6H10NO
95.9162	1329.96	1						
96.0529	127.18	1	M+	C6 H8 O	[C6 H8 O]+	-42.75	Fragment Ion	C6H9NO
96.9241	156.47	1						
97.0109	200.09	1	M+	C8 H	[C8 H]+	37.7	Fragment Ion	C4H16NO2
97.0281	208.75	1	M+	C5 H5 O2	[C5 H5 O2]+	-3.58	Molecular Ion	C7H12N
97.1014	870.25	1	M+	C7 H13	[C7 H13]+	2.31	Confirmed fra	C5H4NO2
97.1094	126.53							
97.9108	237.53							
97.9301	101.8							
98.0367	139.14	1	M+	C5 H6 O2	[C5 H6 O2]+	4.31	Fragment Ion	C7H11N
98.1079	338.4	1	M+	C7 H14	[C7 H14]+	-10.86	Fragment Ion	C5H3NO2
99.1176	273.99	1	M+	C7 H15	[C7 H15]+	7.54	Fragment Ion	C5H2NO2
101.0389	272.12	1	M+	C8 H5	[C8 H5]+	3.25	Fragment Ion	C4H12NO2

- 7 To send Fragment Formula Annotated Spectrum to the PCDL, from the right-click spectrum menu select **Send Spectra to PCDL**.



- 8 Select **Library Path** for the PCDL you want to update. Select **Formula annotated peaks** and **Calculated m/z...** if you would like only theoretical m/z of annotated peaks present in the PCDL.

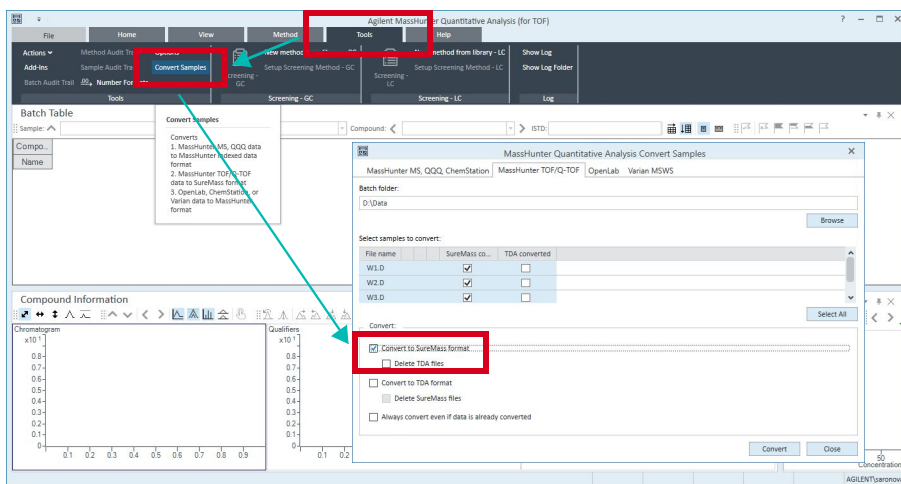


SureMass Overview

SureMass key takeaways:

- Signal processing and feature extraction algorithm for accurate mass data in MassHunter Quant
- Requires profile data
- Allows improvement of mass accuracy and linearity
- Used in suspect screening/target quantitation as well as non-target accurate mass deconvolution (SureMass deconvolution) workflows
- For more information, see the following:
https://www.msconsult.dk/wp-content/uploads/5991-8048EN-High_res_deconvolution_Suremass.pdf

The SureMass Conversion is in both MassHunter Quantitative Analysis Software and Unknowns Analysis (**Tools > Convert Samples > Convert to SureMass format**).



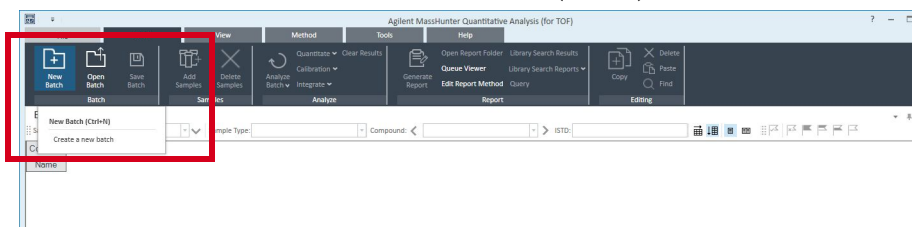
Suspect Screening and Target Quantitation Workflows

Summary of a Typical Workflow for Suspect Screening and Target Quantitation with Large Number of Targets

- 1 Use Agilent ChemVista or PCDL Manager to create a **subset PCDL** for Targets and another for non-targets (everything else).
- 2 Create a new **batch** in MassHunter Quantitative Analysis Software and add samples.
- 3 Create MassHunter Quantitative Analysis Software **method** from **GC library** using a target PCDL subset.
- 4 Set up quantitation **method** for these compounds as you normally do.
- 5 Create **calibration levels**.
- 6 Append **method** from GC Library for non-target compounds.
- 7 Finish setting up MassHunter Quantitative Analysis Software **method**.
- 8 Set up **GC screening method**.
- 9 **Validate** and **run**.

Suspect Screening and Target Quantitation Method Setup

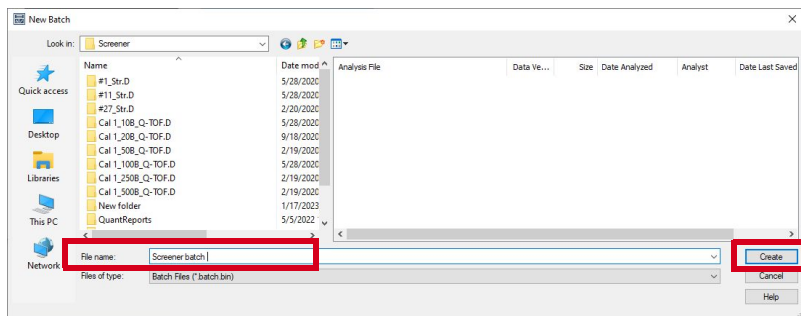
- 1 Open **Quantitative Analysis for TOF**.
- 2 Select **New Batch** and click **Create a new batch** (Ctrl+N).



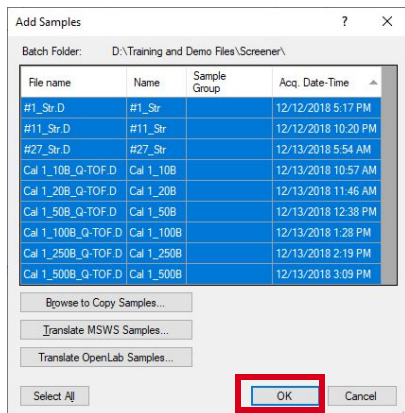
Data Analysis Workflows

Suspect Screening and Target Quantitation Method Setup

3 Name the batch and click **Create**.

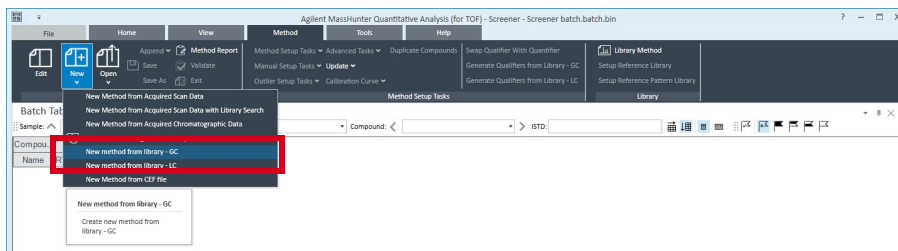


4 Add samples to the batch and click **OK**.

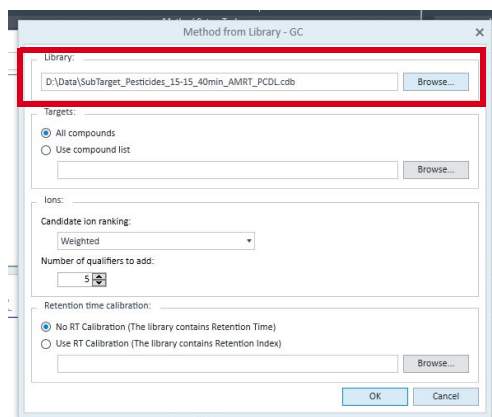


Target Quantitation Method Setup

- 1 Select **New** and click **New method from library-GC**.



- 2 Select the **PCDL library** containing “targets” (compounds for which standards were run for quantitation).



- 3 Choose **ion ranking algorithm** and the number of **qualifier ions**.

- 4 Select **Method > Calibration Curve**, and click **Create levels from Calibration Samples**.

The screenshot displays the Agilent MassHunter Quantitative Analysis interface. The 'Method' menu is open, and the 'Calibration Curve' option is highlighted. A sub-menu is visible, showing 'Create Levels from Calibration Samples' as the selected option. Below the menu, the 'Calibration' table is shown, detailing the levels and concentrations used for the calibration curve.

Level	Conc.	Response
10	10.0000	
20	20.0000	
50	50.0000	
100	100.0000	
250	250.0000	
500	500.0000	

Data Analysis Workflows

Target Quantitation Method Setup

- 5 Select **Append** then click **Append method from Library-GC** to append with non-target compounds (for which no standards for quantitation will be run). This is using a subset PCDL containing spectra of these compounds.

Quantifier Name	TS	Scan	Type	CF	CF Origin	CF Weight
Pyrimethanil		1 Scan	Target	Linear	Ignore	None

Level	Conc.	Response
10	10 0000	
20	20 0000	
50	50 0000	
100	100 0000	
250	250 0000	
500	500 0000	

- 6 Browse and select the **Library**.

Quantifier Name	TS	Scan	Type	CF	CF Origin	CF Weight
Tris (2-Chloro...		1 Scan	Target	Linear	Ignore	None
Tris (3-Chloro...		1 Scan	Target	Linear	Ignore	None
Tolyfluandiol		1 Scan	Target	Linear	Ignore	None
Tetraconazole		1 Scan	Target	Linear	Ignore	None
Terbuthryn		1 Scan	Target	Linear	Ignore	None
TCPSP / Tri-Q		1 Scan	Target	Linear	Ignore	None
TBZ / Thiobe...		1 Scan	Target	Linear	Ignore	None
TBP / Tributy...		1 Scan	Target	Linear	Ignore	None
Simetryn		1 Scan	Target	Linear	Ignore	None
Guinoxxyfen		1 Scan	Target	Linear	Ignore	None

Data Analysis Workflows

Target Quantitation Method Setup

- 7 From **Method Setup Tasks**, click **Compound Setup** to set up the Quant method. Note that many Quant method parameters will be set up in the Screener part of the method.

The screenshot displays the Agilent MassHunter Quantitative Analysis (for TOF) - [New Method] interface. The 'Method Setup Tasks' menu is highlighted in red, and 'Compound Setup' is selected. The 'Method Table' shows a list of compounds with their respective parameters. The 'Sample Information' and 'Compound Information' sections are also visible.

Sample	Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time		
Quantifier	Name	TS	Scan	Type	MZ	RT	Ion Polarity	Criteria
	Pyrimethanil	1	Scan	Target	186.1036	16.156	Positive	Close RT
	Metolazolyl	1	Scan	Target	206.1176	18.636	Positive	Close RT
	Fenofibacarb...	1	Scan	Target	121.0648	12.510	Positive	Close RT
	Ethofencarb...	1	Scan	Target	107.0491	17.341	Positive	Close RT
	Cyprodinil	1	Scan	Target	224.1182	20.903	Positive	Close RT

Sample Information: x10⁷, Signal: chone, Max # of pages: 2

Compound Information: Chromatogram, Qualifiers

5 Compounds (3 total) 0 STD (0 total) | AGLINT@aroma

Data Analysis Workflows

Target Quantitation Method Setup

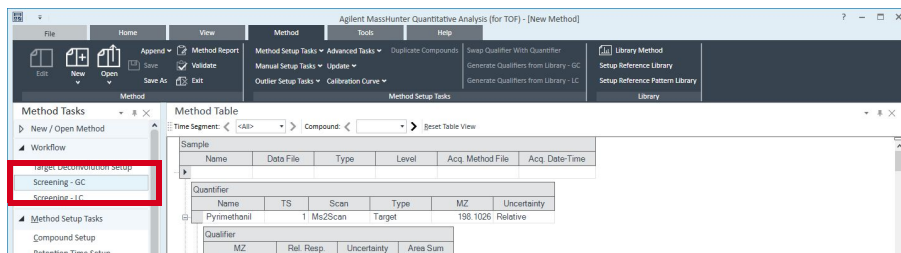
- 8 Click **Globals Setup** and check **SureMass** if you use profile data (recommended).

The screenshot shows the Agilent MassHunter Quantitative Analysis (for TOF) - [New Method] interface. The 'Method Setup Tasks' pane on the left has 'Globals Setup' highlighted with a red box. The 'Method Table' pane shows a list of parameters, with 'SureMass' checked and highlighted with a red box. Below the table are 'Sample Information' and 'Compound Information' sections, each containing a chromatogram plot.

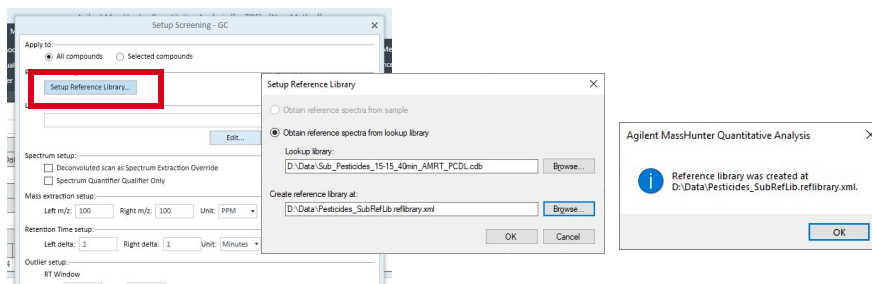
Sample	Name	Data File	Type	Level	Acq. Method File	Acq. Date/Time
Globals						
Bracketing Type			None			
Correlation Window					0.100	
Ignore Peaks Not Found				<input type="checkbox"/>		
Library Method		D:\Data\Lib\Meth.m				
Non Reference Window					70.000	
Non Reference Window Type			Percent			
Reference Library		D:\Data\Pesticides_SubRefLib\reflibrary.xml				
Reference Pattern Library						
Reference Window					80.000	
Reference Window Type			Percent			
Relative ISTD				<input type="checkbox"/>		
SureMass				<input checked="" type="checkbox"/>		

Suspect Screening Method Setup

1 Select Screening-GC.

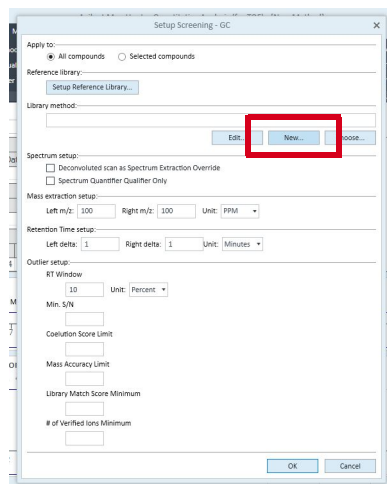


2 Click **Setup Reference Library** and browse for your library. This is based on the complete PCDL, which is your Lookup library.

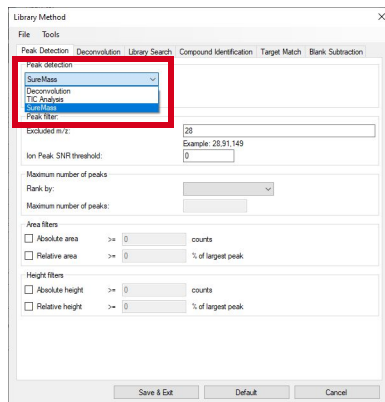


3 Click **OK** at library creation prompt.

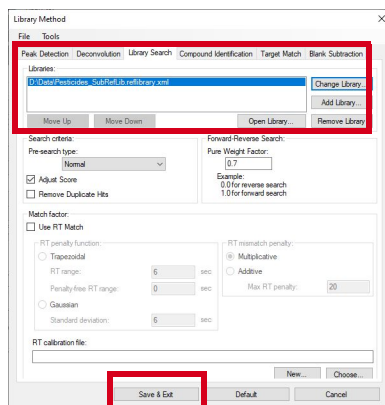
4 Click **New** to create a new library method.



5 Select **SureMass** peak detection.

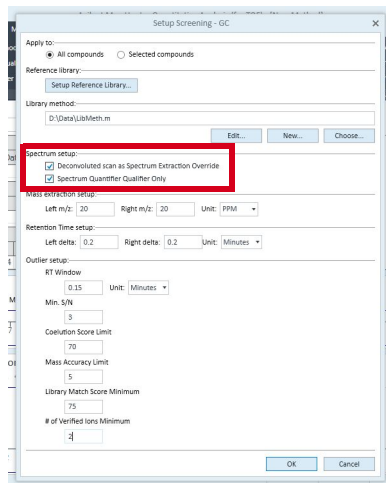


6 Select the newly created **reference library**.



7 Click **Save & Exit**.

8 Check both boxes in **Spectrum setup**.



Deconvoluted scan as Spectrum Extraction Override: Sets which spectrum you want to see on mirror plot. If checked, a deconvoluted spectrum instead of spectrum extracted from the chromatographic region will be shown in mirror plot.

Spectrum Quantifier Qualifier Only: Sets how you want the Library Match Score calculated. If checked, Library Match Score will be based on the selected (quantifier and qualifier) ions.

- 9 Set up **Mass Extraction** and **Retention Time**. (Note: Both m/z and RT windows can be set up in Screener for convenience to avoid Fill Down that takes time for large number of compounds.)

Setup Screening - GC

Apply to: All compounds Selected compounds

Reference library:

Library method: D:\Data\Lib\Meth.m

Spectrum setup: Deconvoluted scan as Spectrum Extraction Override Spectrum Quantifier Qualifier Only

Mass extraction setup: Left m/z: 20 Right m/z: 20 Unit: PPM

Retention Time setup: Left delta: 0.2 Right delta: 0.2 Unit: Minutes

Outlier setup: RT Window: 0.15 Unit: Minutes

Min. S/N: 3

Coelution Score Limit: 70

Mass Accuracy Limit: 5

Library Match Score Minimum: 75

of Verified Ions Minimum: 2

- 10 Set up **Outliers**.

Setup Screening - GC

Apply to: All compounds Selected compounds

Reference library:

Library method: D:\Data\Lib\Meth.m

Spectrum setup: Deconvoluted scan as Spectrum Extraction Override Spectrum Quantifier Qualifier Only

Mass extraction setup: Left m/z: 20 Right m/z: 20 Unit: PPM

Retention Time setup: Left delta: 0.2 Right delta: 0.2 Unit: Minutes

Outlier setup: RT Window: 0.15 Unit: Minutes

Min. S/N: 3

Coelution Score Limit: 70

Mass Accuracy Limit: 5

Library Match Score Minimum: 75

of Verified Ions Minimum: 2

Outliers can be setup in Screener for all compounds for convenience to avoid Fill Down that takes time for large number of compounds.

Outliers can then be adjusted in Quant part of the method for individual compounds if necessary.

Data Analysis Workflows

Suspect Screening Method Setup

These Outliers parameters are recommended for screening for pesticides and environmental contaminants. Other applications may have different settings

11 Exit **Method editor** and click **Yes** to analyze the batch.

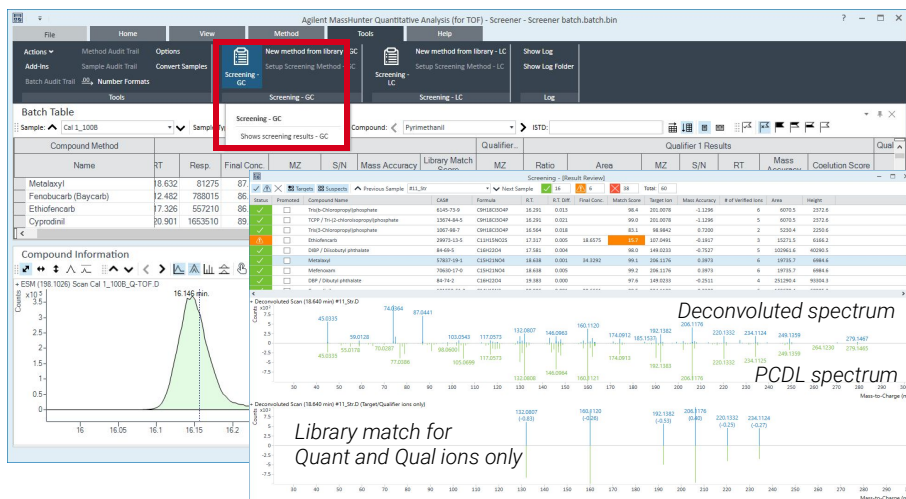
The screenshot shows the 'Method editor' window. The 'Method Table' lists various compounds like Tris(3-Chloro... and Tetryclozole. A dialog box 'Apply Method' is displayed, asking 'Would you like to apply this method to the batch?' with 'Yes', 'No', and 'Cancel' buttons. The 'Yes' button is highlighted with a red box. In the left-hand 'Method Tasks' panel, the 'Exit' button under 'Manual Setup Tasks' is also highlighted with a red box.

12 Wait for analysis to complete.

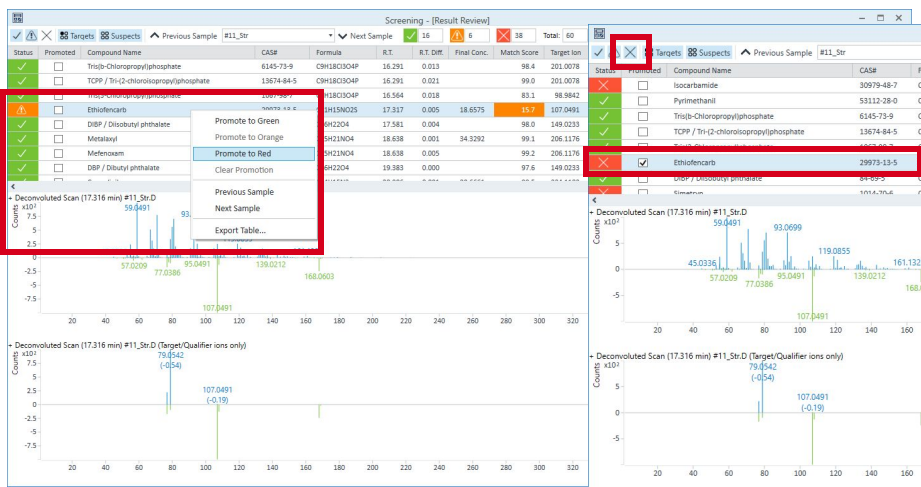
13 View **Target Quantitation Results Table**. You can view detailed results for each compound, including parameters related to the Screener such as Library Match Score and Coelution Score.

The screenshot shows the 'Screener' interface. The 'Batch Table' displays results for compounds like Metolachl, Fenobucarb (Baycarb), Ethionecarb, and Cyprodinil. The 'Library Match Score' and 'Coelution Score' columns are highlighted with red boxes. Below the table, there are three plots: 'Chromatogram' showing a peak at 16.146 min, 'Calibration Curve' showing a linear relationship, and 'Peak Information' showing peak data for 198.1026, 199.1104, 200.1133, 193.0791, 197.0947, and 194.0869.

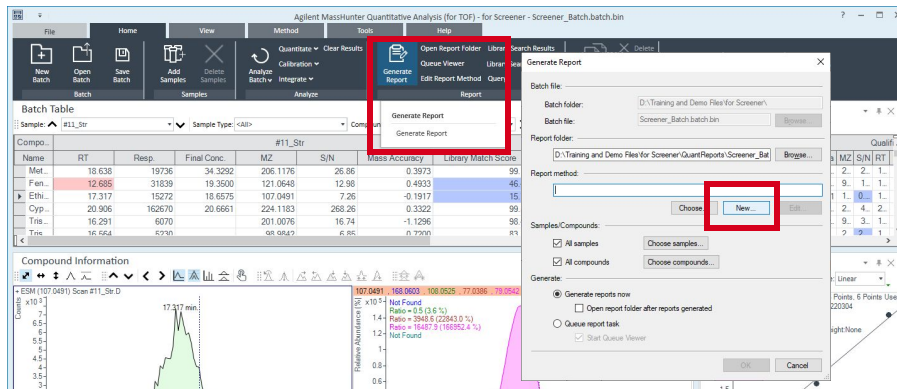
- 14 Click **Screening-GC** to view suspect screening results. The screening window is focused on the compounds identified in samples and only key parameters are displayed.



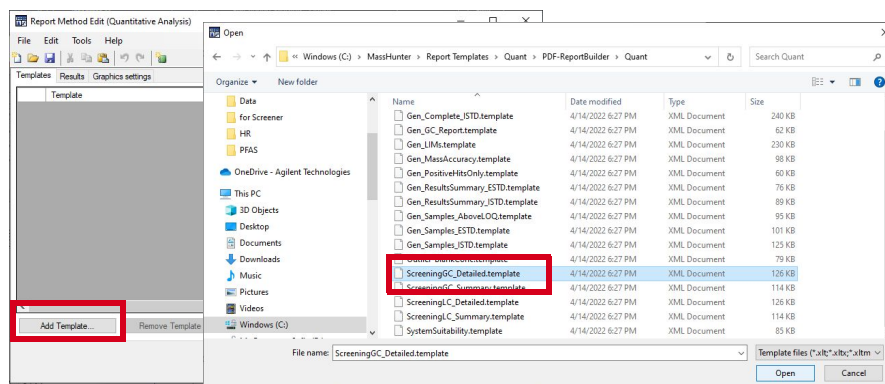
Orange color-labeled compounds are for user's review and can be moved to either "green" (confirmed hits) or "red" (rejected).



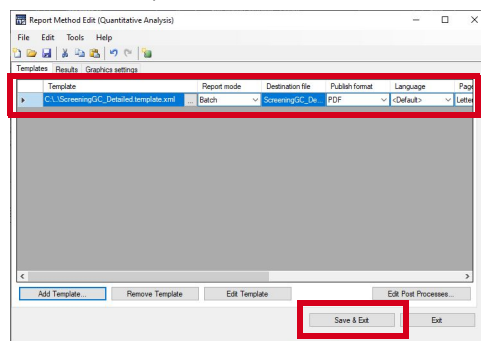
15 To create reports, select **Generate Report** and click **New** under Report method.



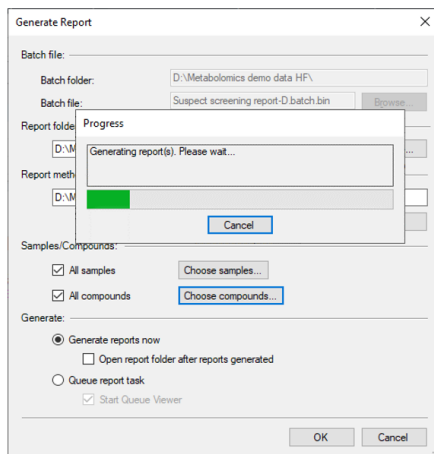
16 Click **Add Template** to select a report template.



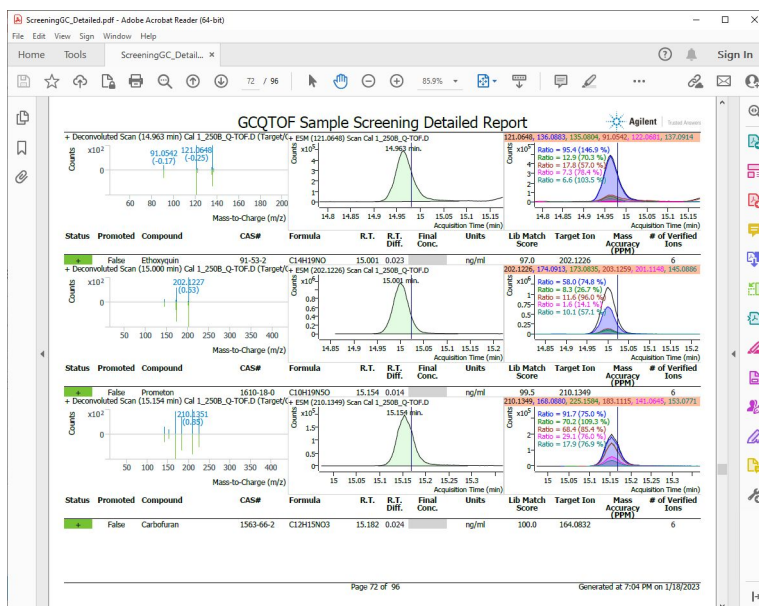
17 Select a template, then click **Save & Exit**.



18 Click **OK** to generate the report.



19 View the detailed report saved in the **Quant Report** folder.



20 You can also generate and view a summary report.

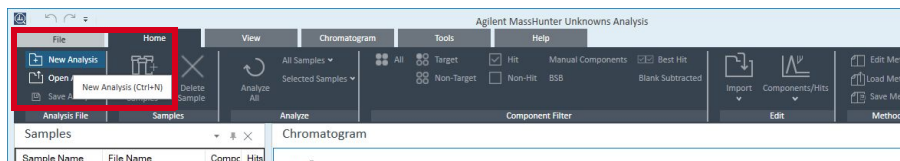
The image shows two overlapping windows. The top window is 'Report Method Edit (Quantitative Analysis)' with a red box highlighting the 'Destination file' field set to 'ScreeningGC_Summary.pdf'. The bottom window is 'ScreeningGC_Summary.pdf - Adobe Acrobat Reader (64-bit)', displaying a 'GC/TOF Sample Screening Summary' report.

Status	Promoted	Compound	CAS#	Formula	R.T. (min)	Area	Height	Final Concentra- tion (ng/ml)	Lib Match	Target Conc (ppm)	Mass on Accuracy	# of Verified Ions	
+	False	2-Methylphenol	95-49-7	C7H10O	4.075	0.023	55498	37270	ng/ml	92.7	108.0070	-3.11	6
+	False	Biphenyl	92-52-4	C12H10	8.241	0.028	181284	85810	ng/ml	90.7	154.0777	-6.27	6
+	False	Methacrylos	62610-77-9	C7H12SO5	16.830	0.029	37836	17340	ng/ml	90.8	207.9504	-0.54	6
+	False	2-Phenylphenol	90-43-7	C12H10O	10.646	0.033	90180	308122	ng/ml	90.4	170.0726	-6.38	5
+	False	3,4,5-Trimethoxyan	2686-89-9	C11H12NO2	14.961	0.017	127476	48811	ng/ml	90.3	119.048	-0.25	6
+	False	Ethionon	91-53-2	C4H11NO	15.001	0.022	277929	1163325	ng/ml	97.0	202.1226	-0.53	6
+	False	Picnoston	1610-18-0	C20H28NO2	15.151	0.014	30132	10339	ng/ml	90.2	210.1349	-0.85	6
+	False	Carbafuran	1563-66-2	C12H12NO2	15.182	0.024	569822	379591	ng/ml	100.0	244.9832	-0.44	6
+	False	Olanopone	8177-88-1	C12H14NO2	15.372	0.021	146469	50369	ng/ml	90.9	204.1619	-0.98	6
+	False	Benzylbenzoate	120-51-4	C14H12O2	15.600	0.016	26860	1985	ng/ml	86.7	105.0335	-1.84	3
+	False	Socarbamide	3009-46-7	C8H10NO2	15.642	0.021	697921	21172	ng/ml	90.5	162.0611	-0.31	5
+	False	Tri(2- Chloroethoxy)phosphate	6145-73-9	C8H18Cl2O4P	16.288	0.009	5986	2216	ng/ml	90.0	201.0078	-0.16	6
+	False	TCPP / Tri-(2- Chloroethoxy)phosphate	13674-84-5	C8H18Cl2O4P	16.288	0.024	5986	2216	ng/ml	90.9	201.0078	-0.16	5
+	False	Tri(2- Chloroethoxy)phosphate	1067-98-7	C8H18Cl2O4P	16.559	0.014	4018	1842	ng/ml	97.9	98.9842	-0.07	2
+	False	DIBP / Diisobutyl phthalate	84-69-5	C16H22O4	17.575	0.009	111463	42919	ng/ml	97.3	149.0233	-0.11	5
+	False	Simefryn	1014-70-6	C8H12NO5	18.249	0.009	852121	313424	ng/ml	90.5	211.1093	-0.38	5
+	False	Carbaryl	63-25-1	C12H11NO2	18.257	0.013	110603	30473	ng/ml	90.2	244.0070	-1.02	6
+	False	Mefenoxam	70630-17-0	C18H21NO4	18.633	0.010	24946	3504	ng/ml	90.1	206.1176	-0.97	6
+	False	Terbufos	896-50-0	C10H19NO5	19.080	0.024	33142	20943	ng/ml	90.9	210.1121	-1.16	6
+	False	DIBP / Diisobutyl phthalate	84-74-2	C16H22O4	19.380	0.001	210508	79218	ng/ml	97.5	149.0233	-0.33	4
+	False	Dichloroethane	87-30-3	C2H4Cl2	19.839	0.001	33397	13998	ng/ml	97.4	125.0566	-0.59	6
+	False	Dichloroamid	927-51-2	C16H17NO	20.054	0.003	148410	53139	ng/ml	90.0	247.8850	-1.05	5
+	False	Isopropyl	38835-51-0	C12H22NO4	20.098	0.011	40146	23070	ng/ml	90.8	200.1252	-1.28	6
+	False	TRZ / Thiazobenzotriazole	149-79-8	C10H7N3S	21.240	0.009	25036	4799	ng/ml	90.1	201.0355	-0.35	5
+	False	Furalaxyl	57996-20-7	C17H19NO4	21.787	0.002	47699	18670	ng/ml	90.2	242.1176	-0.48	6
+	False	Butylid	76019-19-0	C16H18F2NO3	22.743	0.009	24547	17975	ng/ml	90.8	233.0061	-0.51	5
+	False	Isopropylthiane	50512-25-1	C12H18NO2S	22.258	0.008	201179	111204	ng/ml	90.5	188.9675	-0.01	6
+	False	Fluthiaz	85590-19-0	C16H18F2NO3	22.866	0.009	97944	24299	ng/ml	90.4	233.0061	-0.34	6
+	False	Methoprotrene	891-05-5	C11H21NO5	22.937	0.004	42126	19866	ng/ml	90.9	256.1227	-0.87	6
+	False	Bumeth	45481-61-6	C12H24NO5S	23.001	0.009	49715	19416	ng/ml	90.2	273.1618	-1.10	6
+	False	Oxaloxyl	7732-69-3	C14H18NO4	25.113	0.001	17632	8171	ng/ml	90.0	163.0992	-0.76	6
+	False	Benzval	7436-11-4	C8H10NO2	25.096	0.013	89799	33028	ng/ml	90.2	168.1121	-0.75	6
+	False	Piperonal butoxide	51-30-8	C18H20O2	27.226	0.021	85344	31076	ng/ml	90.0	176.8832	-0.97	5
+	False	Piperonate (D 2941)	149877-6-8	C17H20NO3	28.346	0.010	28325	7990	ng/ml	93.0	184.0757	-0.59	6
+	False	DEHP / Di(2-ethylhexyl) phthalate	117-81-7	C24H38O4	29.351	0.028	95859	39530	ng/ml	90.2	149.0233	-0.38	6

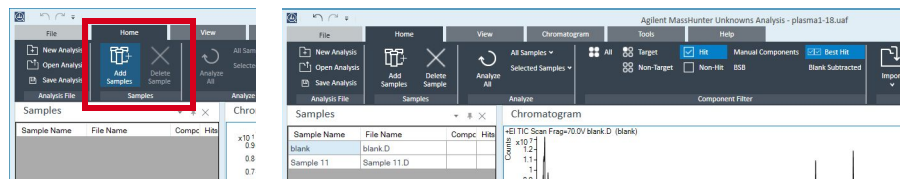
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Generated at 7:13 PM on 1/18/2023

Non-targeted Screening in the Unknowns Analysis Software

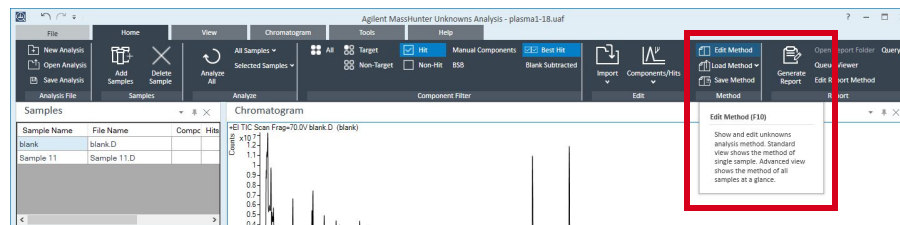
- 1 Click **New Analysis (Ctrl+N)** to create a new **batch**.



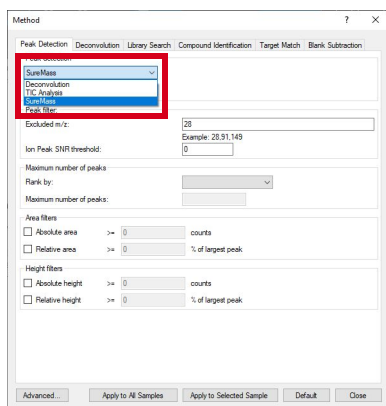
- 2 Click **Add Samples**.



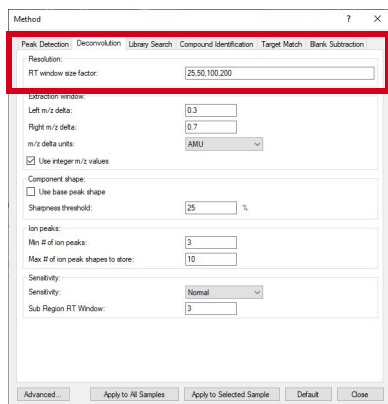
- 3 Click **Edit Method**.



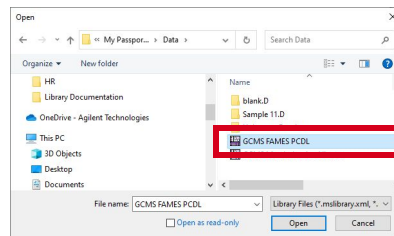
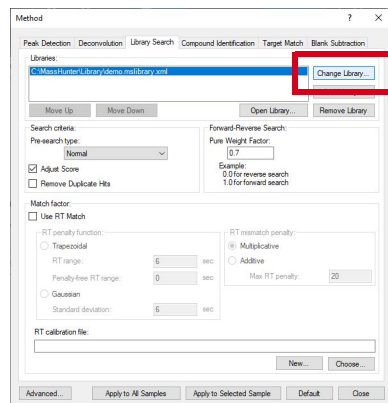
- 4 Under the **Peak Detection** tab, click **SureMass**.

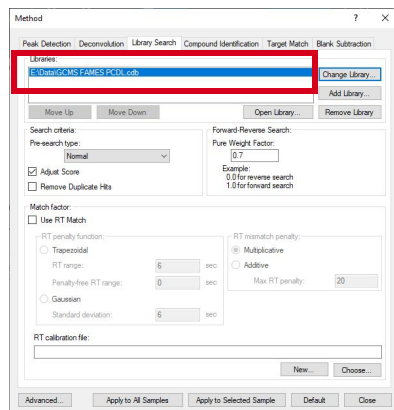
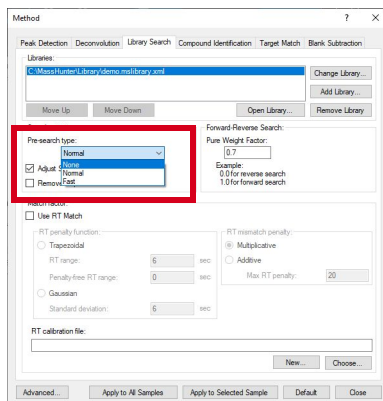


5 Under the **Deconvolution** tab, set the RT window size factor.

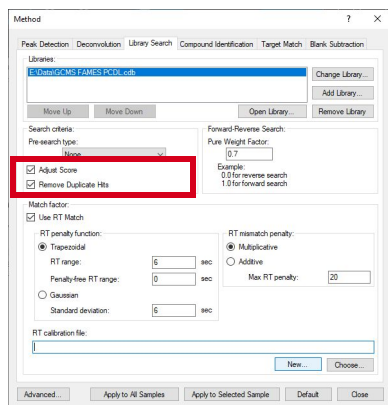


6 Under the **Library Search** tab, click **Change Library** to choose a PCDL library.

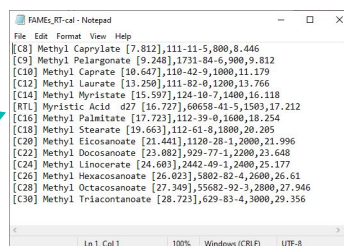
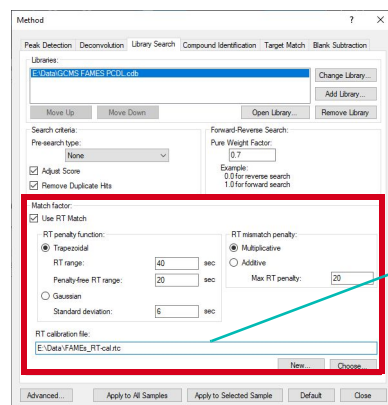


7 Choose a **Library**.8 Use the **Pre-search type** pulldown to choose how fast and accurate you want the search.

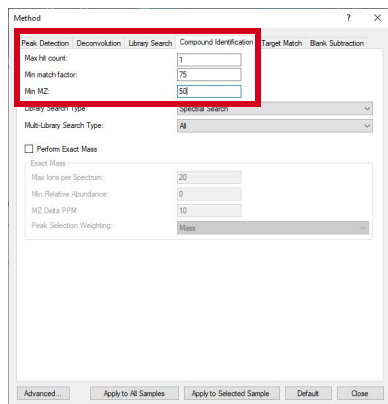
- 9 Check **Adjust Score** to make it similar to NIST scoring, and remove duplicates if you wish.



- 10 Check **Use RT Match** if you want the RT calibration file to match library's RTs. With the calibration file, it will match RTs.



- 11 Under the **Component Identification** tab, set **Min m/z** so that it is no lower than the data acquisition mass range. Also select minimum **Library Match Factor** and **number of hits** per component.



Method

Peak Detection | Deconvolution | Library Search | **Component Identification** | Target Match | Blank Subtraction

Max Hit count: 1

Min match factor: 75

Min MZ: 50

Library Search Type: Spectral Search

Multi-Library Search Type: All

Perform Exact Mass

Exact Mass

Max Ions per Spectrum: 20

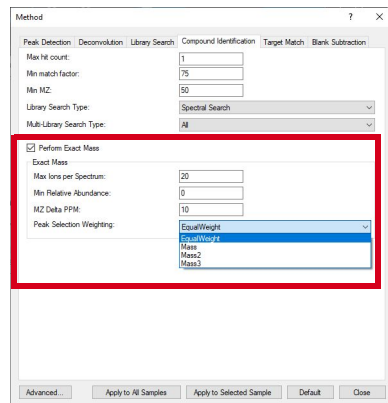
Min Relative Abundance: 0

MZ Delta PPM: 10

Peak Selection Weighting: Mass

Advanced... Apply to All Samples Apply to Selected Sample Default Close

- 12 Click **Perform Exact Mass** box, and select algorithm for ion **Peak Selection Weighting**.



Method

Peak Detection | Deconvolution | Library Search | **Component Identification** | Target Match | Blank Subtraction

Max Hit count: 1

Min match factor: 75

Min MZ: 50

Library Search Type: Spectral Search

Multi-Library Search Type: All

Perform Exact Mass

Exact Mass

Max Ions per Spectrum: 20

Min Relative Abundance: 0

MZ Delta PPM: 10

Peak Selection Weighting: EqualWeight

Library Match

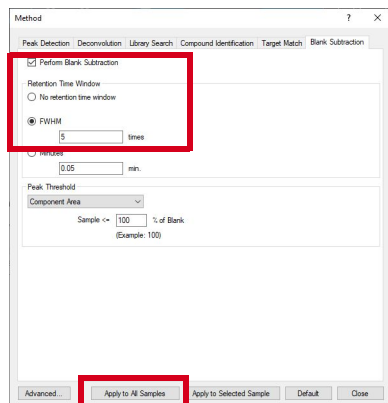
Mass

Mass2

Mass3

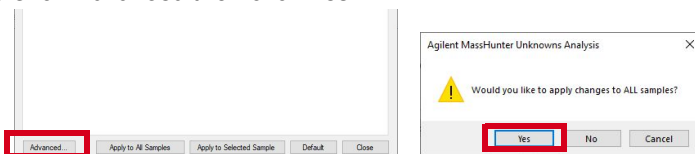
Advanced... Apply to All Samples Apply to Selected Sample Default Close

13 Under the **Blank Subtraction** tab, check **Perform Blank subtraction**.

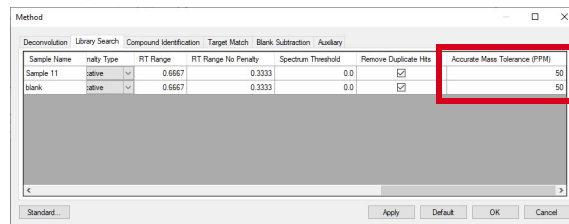


14 Click **Apply to All Samples**.

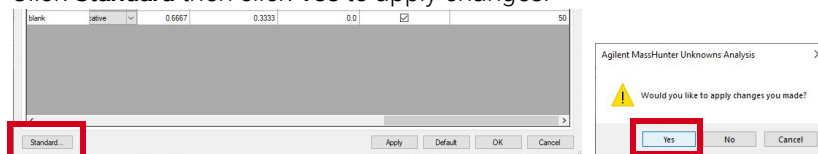
15 Click **Advanced** then click **Yes**.



16 In **Accurate Mass Tolerance (PPM)**, increase the values so very small ions in the deconvoluted spectra do not get discarded due to increased mass accuracy error.



17 Click **Standard** then click **Yes** to apply changes.



18 Select **Blank** sample type for subtraction, then click **Analyze All** to analyze the batch. An **Analyze** window will appear with a progress bar.

The screenshot shows the software interface with the 'Analyze All' button highlighted in red. The 'Type' dropdown menu is also highlighted in red and set to 'Blank'. The 'Analyze All (5)' dialog box is open, showing a progress bar and a table of analysis results for 'Sample Name', 'Peak Detection', 'Library Search', 'Target Match', and 'Blank Subtraction'.

Sample Name	Peak Detection	Library Search	Target Match	Blank Subtraction
blank	100%	7%		
Sample 11	100%	7%		

19 Analysis results will be displayed. Columns can be configured to include Component and Library RI.

The screenshot shows the software interface with the 'Components' table displayed. The table has columns for Component RT, Compound Name, Match Factor, Best Hit, Formula, Component RI, Library RI, and Delta RI. The 'Chromatogram' and 'Spectrum' views are also visible.

Component RT	Compound Name	Match Factor	Best Hit	Formula	Component RI	Library RI	Delta RI
7.2078	2-Hydroxyveridine (1 TMS)	90.6	<input checked="" type="checkbox"/>	CBH13NO5i	709	710	1
7.6878	Hexanoic acid (1 TMS)	90.9	<input checked="" type="checkbox"/>	CBH20O2Si	744	745	1
7.7655	Glycolic acid (2 TMS)	94.3	<input checked="" type="checkbox"/>	CBH20O3Si2	750	748	-2
8.5892	2-Furoic acid (1 TMS)	76.3	<input checked="" type="checkbox"/>	CBH12O3Si	810	806	-4
9.1629	1-Octanol (1 TMS)	76.4	<input checked="" type="checkbox"/>	C11H26Oi	852	854	2
9.5599	Ethanolamine (3 TMS)	82.0	<input checked="" type="checkbox"/>	C11H16NO3Si3	903	903	0
10.1589	Benzoic acid (1 TMS)	95.8	<input checked="" type="checkbox"/>	C10H14O2Si	925	923	-2
10.3449	Caproic acid (1 TMS)	90.6	<input checked="" type="checkbox"/>	C11H24O2Si	939	938	-1
10.4158	Phosphoric acid (3 TMS)	94.7	<input checked="" type="checkbox"/>	CBH27O4PSi3	944	951	6
10.5054	Nicotinic acid (1 TMS)	79.9	<input checked="" type="checkbox"/>	CBH13NO2Si	951	950	-1
11.6454	Nonanoic acid (1 TMS)	97.2	<input checked="" type="checkbox"/>	C12H26O2Si	1036	1037	1
12.2122	Glutaric acid (2 TMS)	88.9	<input checked="" type="checkbox"/>	C11H24O4Si2	1080	1080	0
12.9091	Capric acid (1 TMS)	91.5	<input checked="" type="checkbox"/>	C13H28O2Si	1104	1129	-5
13.0493	L-Phenylalanine acid (2 TMS)	86.6	<input checked="" type="checkbox"/>	C11H23NO3Si2	1194	1192	-2
14.6456	1,2,4-Benzoxetrol (3 TMS)	81.1	<input checked="" type="checkbox"/>	C15H30O3Si3	1276	1268	-7
15.2772	Lauroic acid(1 TMS)	76.4	<input checked="" type="checkbox"/>	C15H32O2Si	1329	1332	3
16.8680	Azelic acid (2 TMS)	95.7	<input checked="" type="checkbox"/>	C15H32O4Si2	1471	1470	-1
17.4412	Myristic acid (1 TMS)	93.2	<input checked="" type="checkbox"/>	C17H36O2Si	1524	1525	1

20 Click **Exact Mass Table** to display **Exact Mass Results**.

The screenshot displays the Agilent MassHunter Unknowns Analysis software interface. The 'Exact Mass Table' is highlighted in the left-hand menu. The main window shows a list of components with their respective match factors, best hit status, and formulas. The 'Ion Peaks' and 'Spectrum' panels are also visible, showing the mass-to-charge ratio (m/z) and relative intensity of the ions.

Component	Match Factor	Best Hit	Formula	Component RI	Library RI	Delta RI
Components at a Glance (1 TMS)	90.6	<input checked="" type="checkbox"/>	CBH13NOSi	709	710	1
7.6876 Hexanoic acid (1 TMS)	90.9	<input checked="" type="checkbox"/>	CBH2002Si	744	745	1
7.7655 Dyoic acid (2 TMS)	94.3	<input checked="" type="checkbox"/>	CBH2003Si2	750	748	-2
8.5592 2-Furanc acid (1 TMS)	78.3	<input checked="" type="checkbox"/>	CBH1203Si	810	806	-4
9.1628 1-Octanol (1 TMS)	76.4	<input checked="" type="checkbox"/>	C11H22OSi	852	854	2
9.8556 Ethanolamine (3 TMS)	82.0	<input checked="" type="checkbox"/>	C11H43NO3Si3	903	903	0
10.1588 Benzoic acid (1 TMS)	95.8	<input checked="" type="checkbox"/>	C10H14O2Si	925	923	-2
10.3449 Caprylic acid (1 TMS)	90.6	<input checked="" type="checkbox"/>	C11H42O2Si	939	938	-1
10.4158 Phosphoric acid (3 TMS)	94.7	<input checked="" type="checkbox"/>	CBH2704PSi3	944	951	6
10.5054 Nicotinic acid (1 TMS)	79.9	<input checked="" type="checkbox"/>	CBH13NO2Si	951	950	-1
11.8464 Nonanoic acid (1 TMS)	97.2	<input checked="" type="checkbox"/>	C12H24O2Si	1036	1037	1
12.2122 Quinic acid (2 TMS)	88.9	<input checked="" type="checkbox"/>	C11H42O4Si2	1080	1080	0
12.9091 Capric acid (1 TMS)	91.5	<input checked="" type="checkbox"/>	C13H48O2Si	1134	1129	-5
13.6948 L-Pyrolutamic acid (2 TMS)	86.6	<input checked="" type="checkbox"/>	C11H23NO3Si2	1194	1192	-2
14.6456 1,2,4-Benzenetriol (3 TMS)	81.1	<input checked="" type="checkbox"/>	C15H30O3Si3	1275	1268	-7
15.2772 Lauric acid (1 TMS)	78.4	<input checked="" type="checkbox"/>	C15H32O2Si	1329	1332	3
16.8850 Azelaic acid (2 TMS)	95.7	<input checked="" type="checkbox"/>	C15H32O4Si2	1471	1470	-1
17.4412 Myristic acid (1 TMS)	93.2	<input checked="" type="checkbox"/>	C17H36O2Si	1524	1525	1

All highlighted ions in the component spectrum and shown in the ExactMass Table correspond to the hit with regards to the accurate mass.

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