Agilent CrossLab
From Insight to Outcome

# Qualitative Analysis Workflows

## MassHunter Qualitative Analysis Webinar Series

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Stephen Harnos
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Agilent

# MassHunter Qualitative Analysis Software B.08.00 SP1

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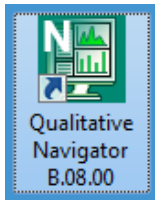
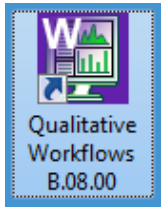
## Navigator and Workflows

### Navigator




- User centric
- Interactive Browsing
  - Walk the Chromatogram
  - Spectrum Preview
- Spectrum ID
  - Library/Database Search
  - Molecular Formula Generator
- No concept of compounds
- No Feature Finding – ‘Find by…’
- What does the chromatography look like? System suitability, S/N, plates…
- What does the spectrum look of each peak look like?
- Can the spectrum be identified by searching a library?

### Workflows




- Compound centric
- Automated Routine Workflows
  - Sample Purity
  - Compound Discovery
  - Compound Identification
- Feature Finding – ‘Find by…’
- No Spectrum Preview
- No ‘User Spectra’
- All Spectra are compound based.
- What compounds can be found and identified?

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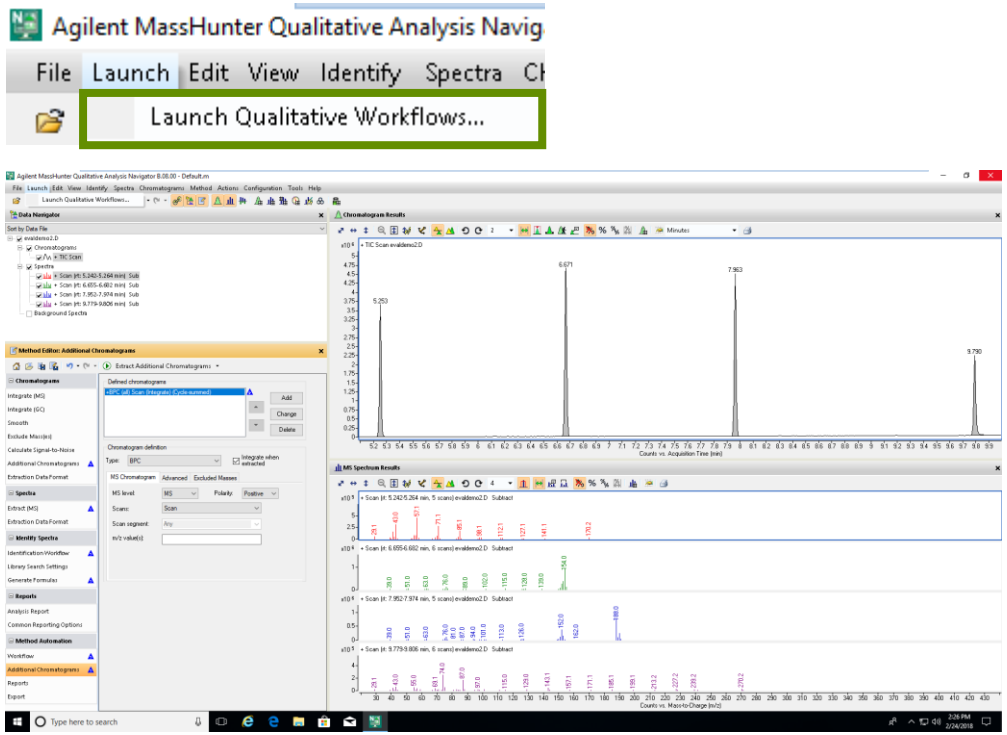
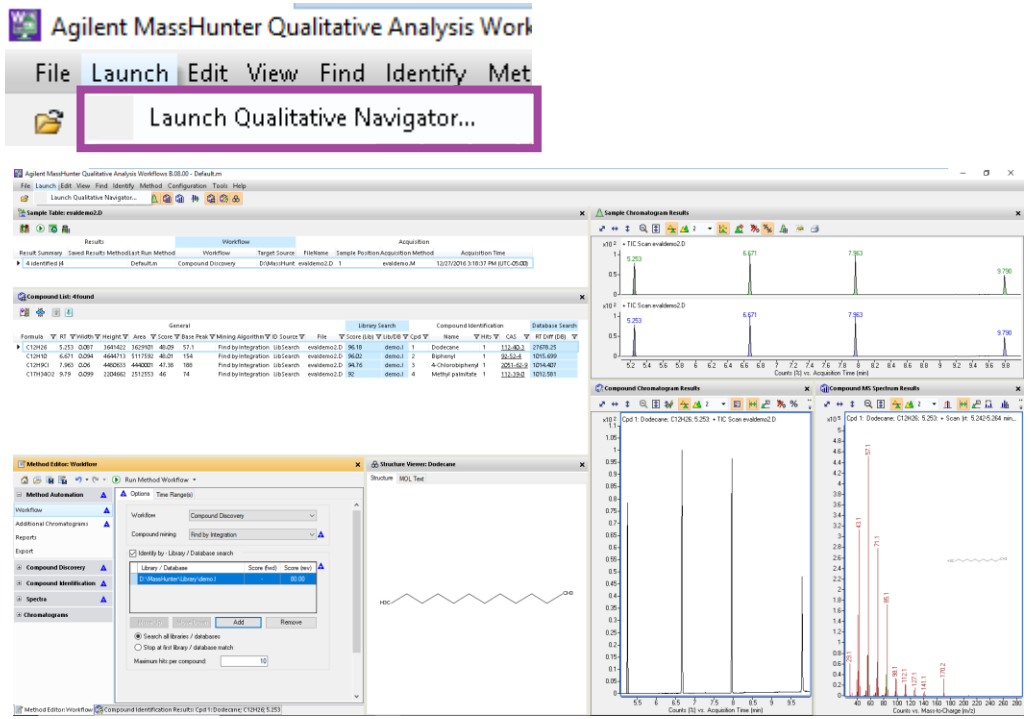
## Navigator and Workflows

### Navigator




File opens in Workflows.
The sample chromatogram(s) extracted.
Spectra not extracted.
Method is NOT passed to other context.

### Workflows




File opens in Navigator.
The sample chromatogram(s) are extracted.
No compound results.
Method is NOT passed to other context.



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# MassHunter Qualitative Analysis Software B.08.00 SP1

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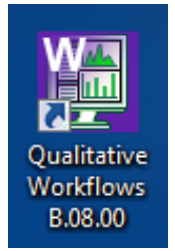
## Topics




### Qualitative Analysis Workflows

### Workflow Definitions

- Target/Suspect Screening
- Compound Discovery
- Sample Purity
- Custom

### Compound Mining Algorithms

- Find by Integration
- Find by Chromatogram Deconvolution
- Molecular Feature Extraction
- Find by Formula

### Compound Identification

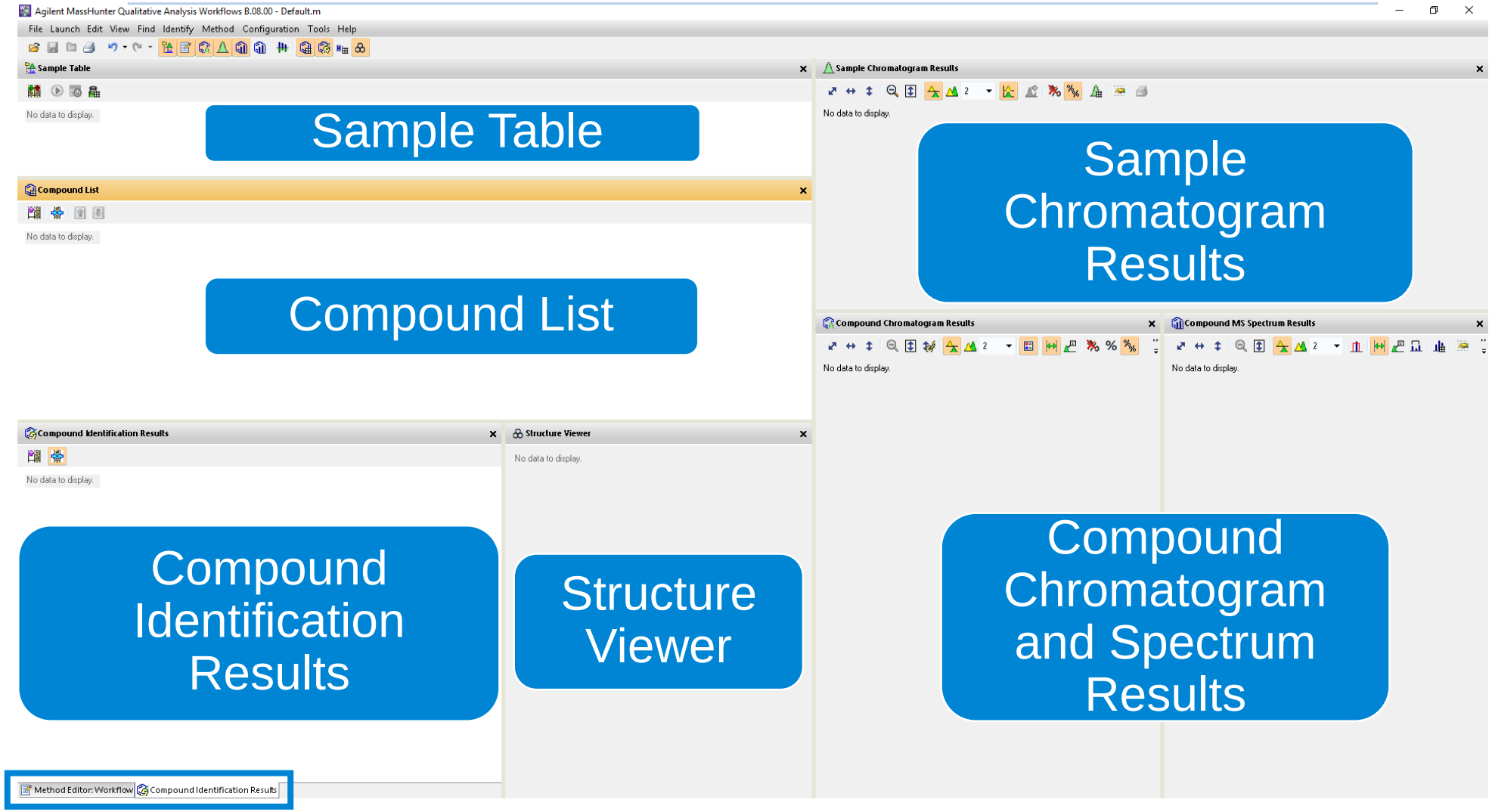
- Library and Databases

### Generating Reports

Basic Qualitative Analysis features were covered in the previous webinar available at [www.agilent.com/en-us/training-events/eseminars/236e](www.agilent.com/en-us/training-events/eseminars/236e)

# MassHunter Qualitative Analysis Software B.08.00 SP1

## Workflows Default Layout




Method Editor is a tab.

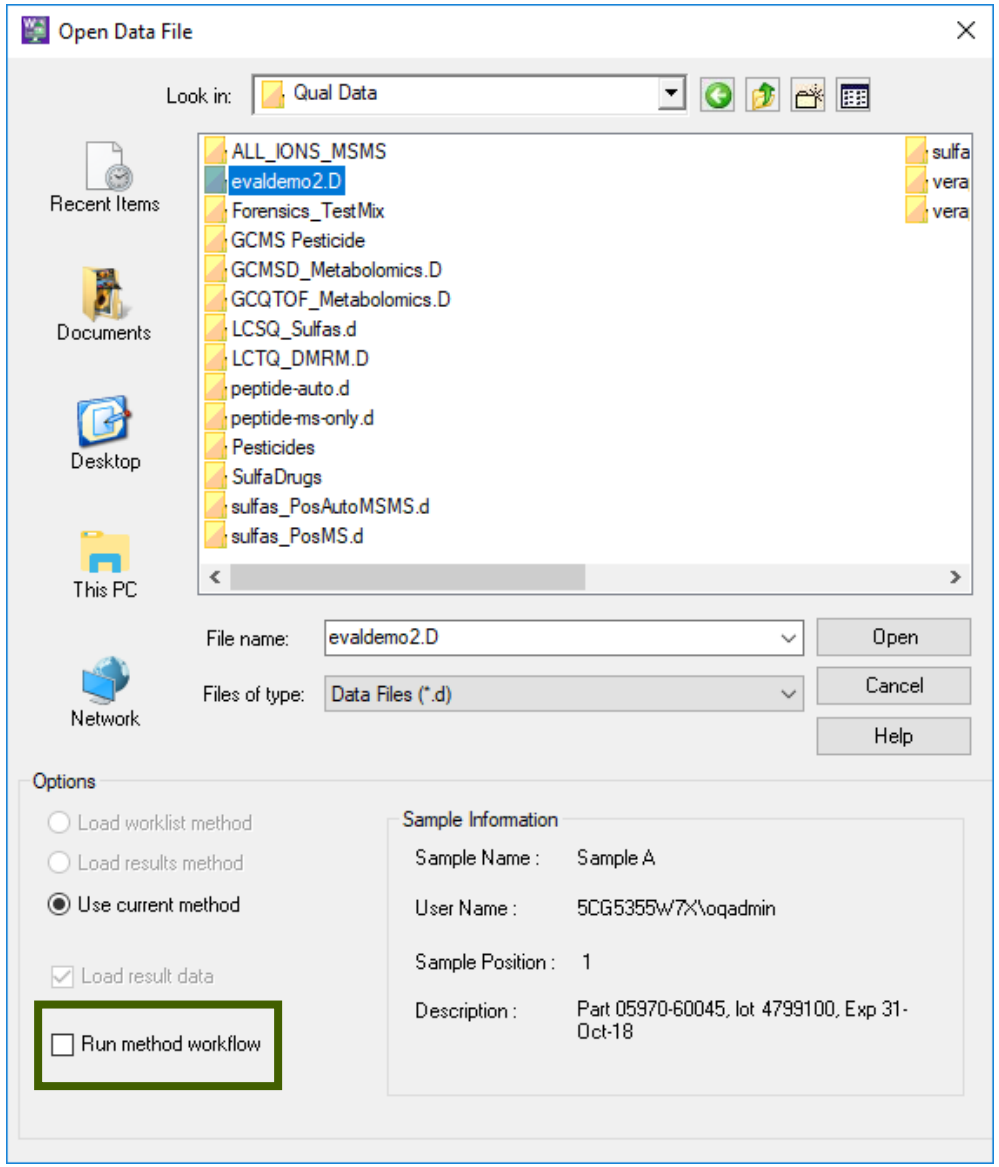
# Workflows

## Open Data File

### Open Data File Dialog Box

- Options
  - Load Worklist Method
  - Load Results Method
  - Use Current Method
- Sample Information

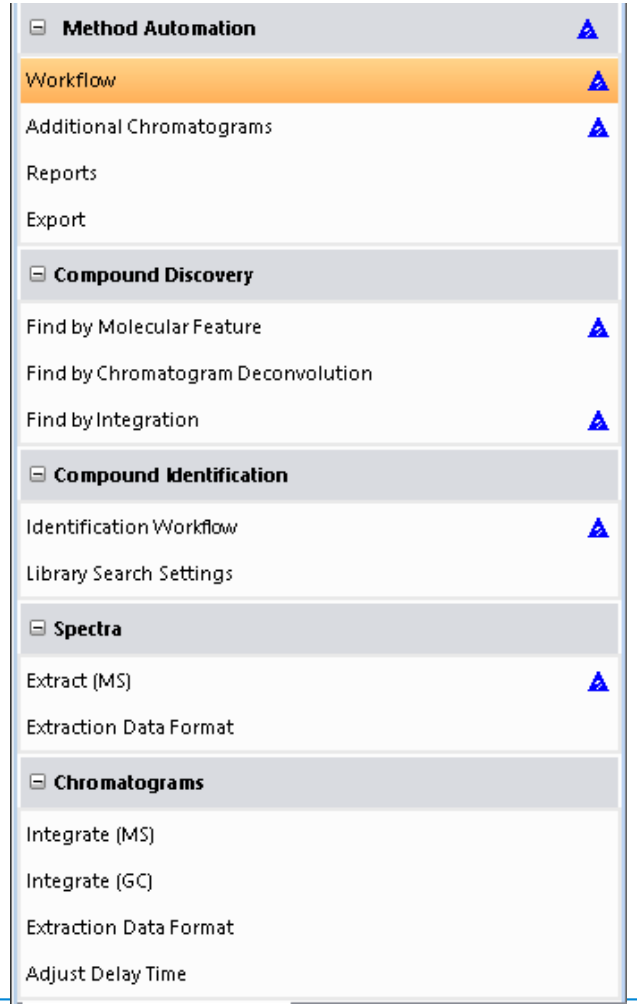
- Load result data
- Run method workflow
  - **NEW FEATURE!**



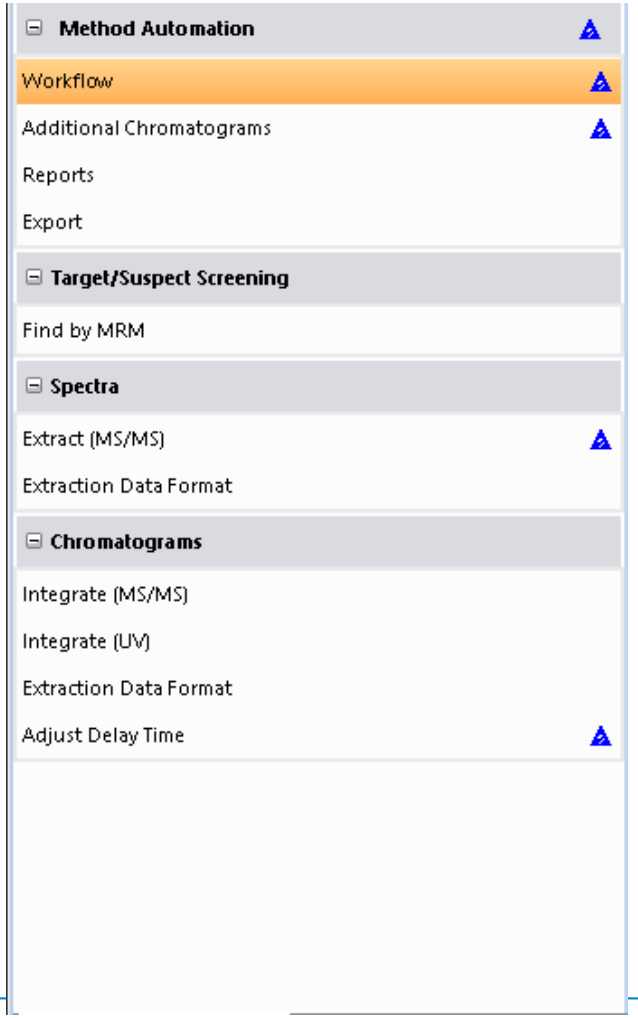
# Method Editor

## Adaptive User Interface– simplifies Method Editor


No Data File Loaded

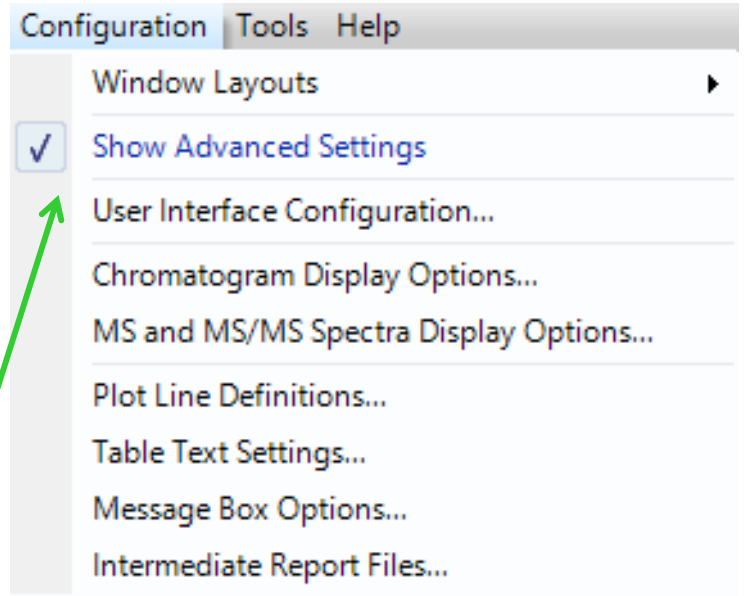



GCMS Data Loaded




LC QQQ dMRM Data Loaded

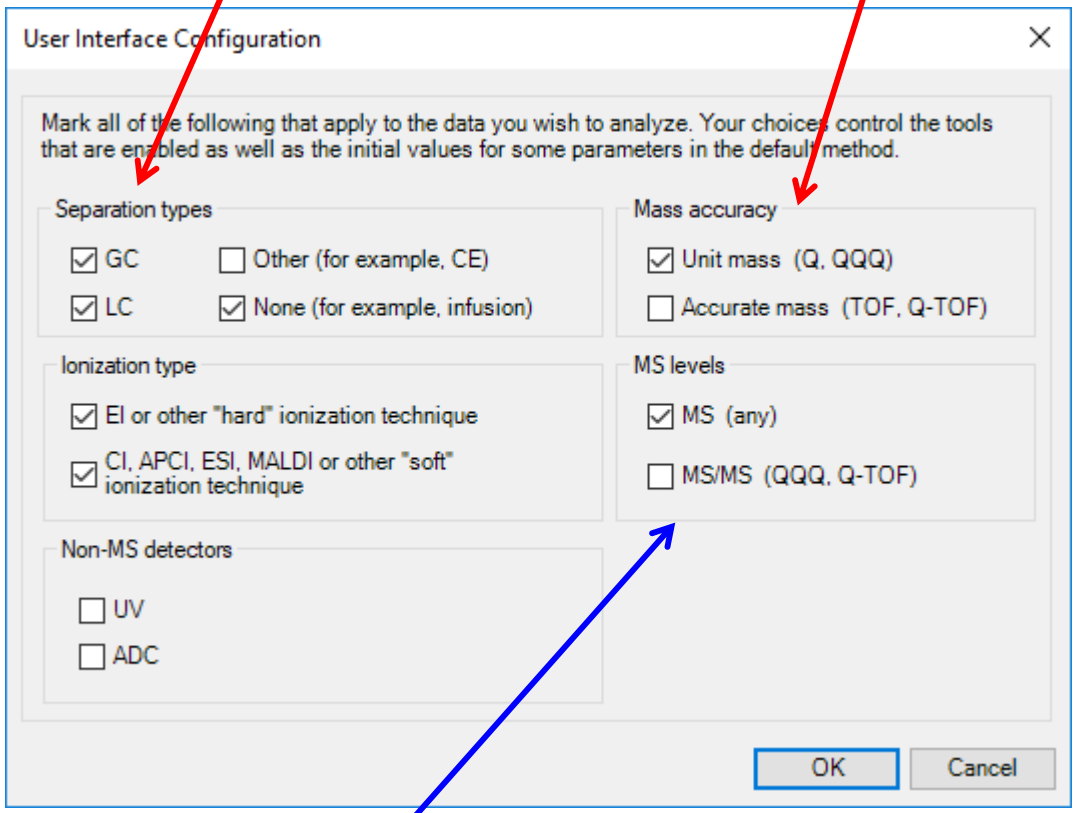
# User Interface Configuration




- Check Show Advanced Settings from the Configuration menu to access the User Interface Configuration.
- Also shows advanced Method Editor features.

Separation types (Check GC or LC)

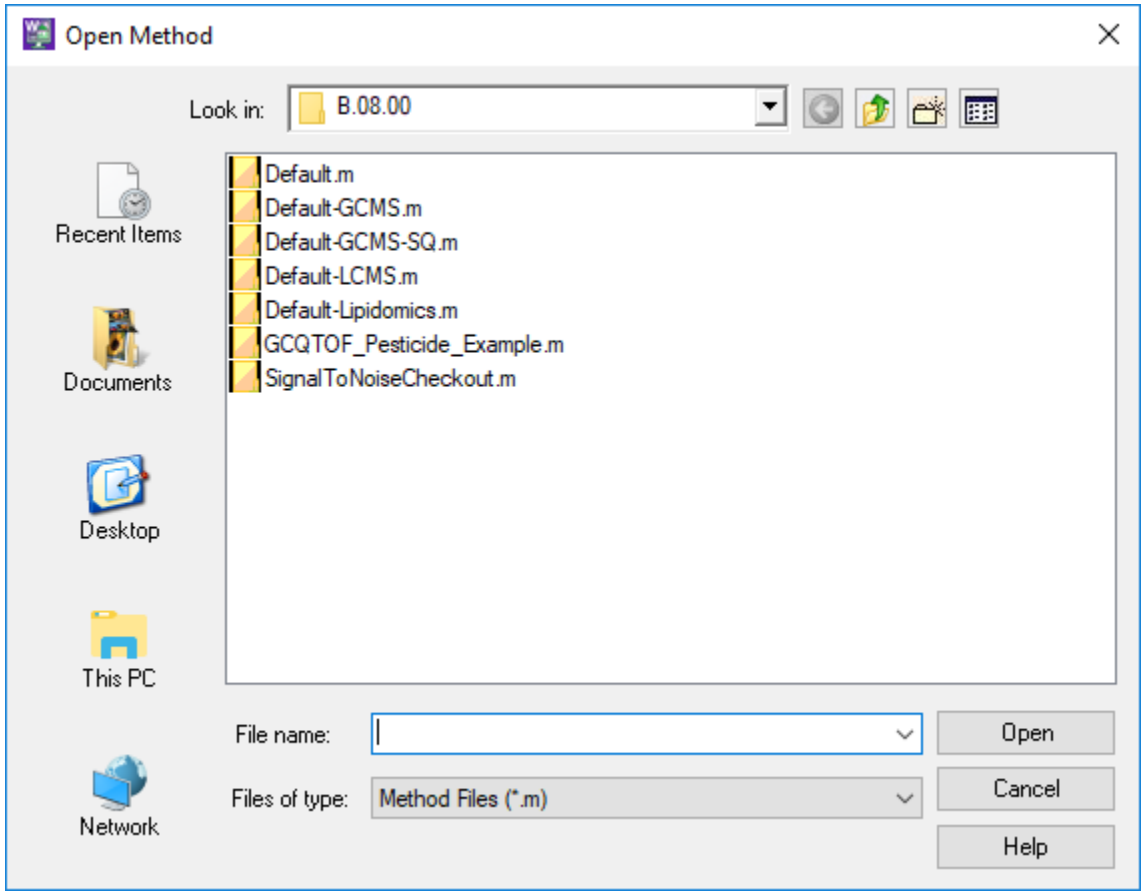
Unit Mass (SQ, TQ)
Accurate Mass (TOF, QTOF)




MS Levels MS or MS/MS

# Qualitative Analysis Methods

## Open Method




### Open Method

- Load the method relevant to the data set.
- Method contains recommended/default parameters.
- Method Editor values can be modified.
- Saves time developing specific values.
- Good starting point.

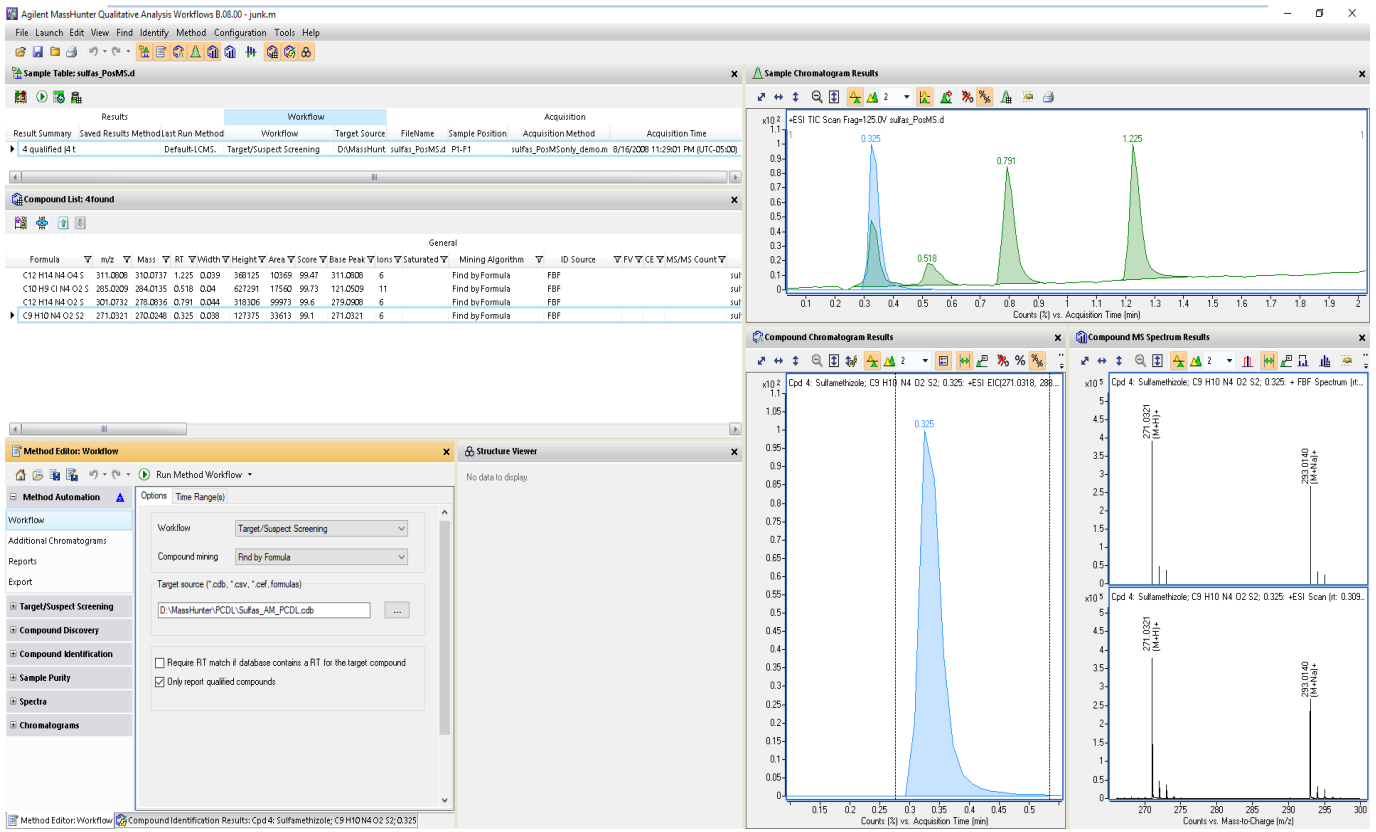
- **Tip: Load the applicable method.**

- Default-GCMS-SQ.M → GCMS and GC QQQ
- Default-GCMS.M →GC QTOF
- Default-LCMS.M → LCMS

# Workflows

## Definition

- Intended for routine and automated analysis.
  - Select a workflow.
  - Select the mining algorithm.
  - Develop method parameters.
- Limited tools for manual spectral extraction.
  - No spectral preview.
  - Manual extraction always creates a compound.
- Double-click on sample in Sample Table to process data files with loaded method.
- Compound report only (no analysis reports).

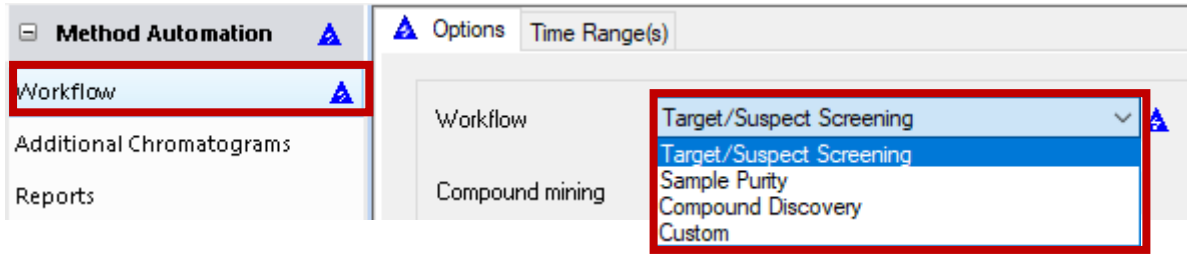


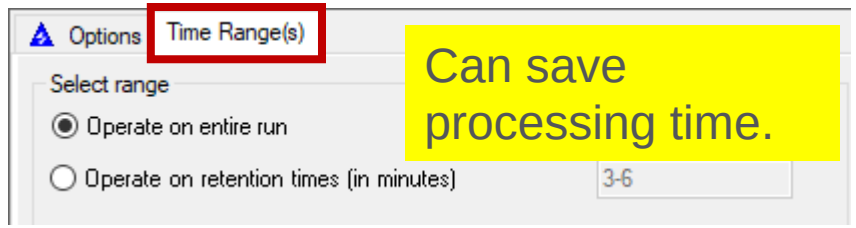
# Workflows

## Definition

A workflow is an automated sequence of steps to complete a task and generate results.

- Workflow is the table of contents.
- All the steps are defined via the Method Editor.
- Default workflows depend upon data set.
- Workflows
  - Target/Suspect Screening
  - Sample Purity
  - Compound Discovery
  - Custom
- The workflow parameters can be saved as part of the Qualitative Analysis Workflows method.



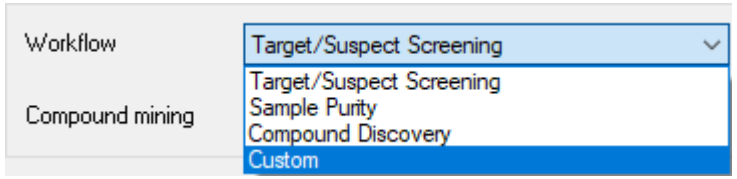



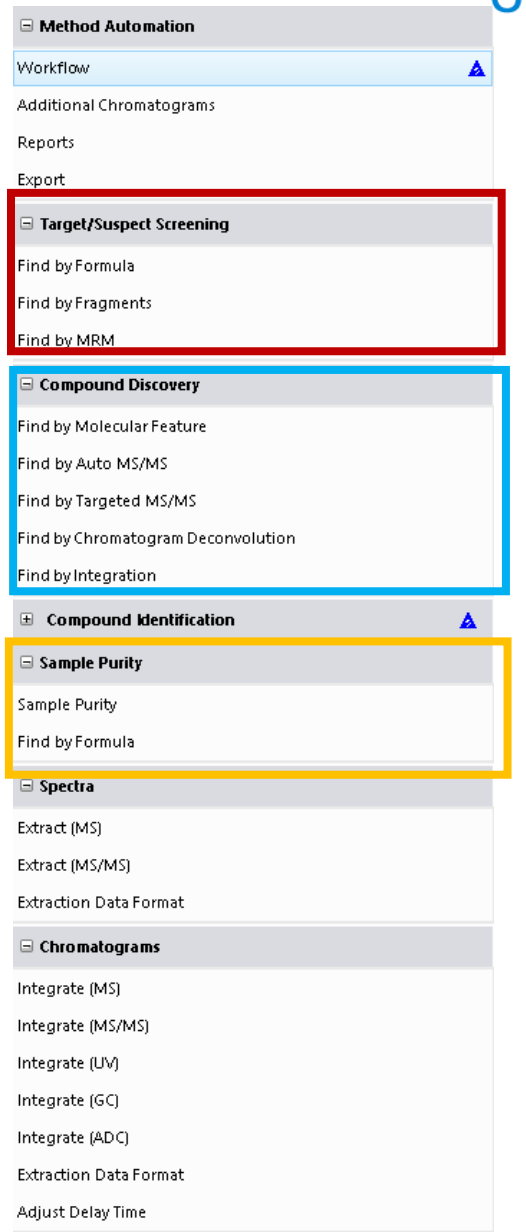
# Workflows

## Method Groupings

The Method Editor groups method sections to match workflows.

- Method Automation via workflows.
- Target/Suspect Screening
- Compound Discovery
- Sample Purity
- Custom
- Compound Identification
- Spectra
- Chromatograms



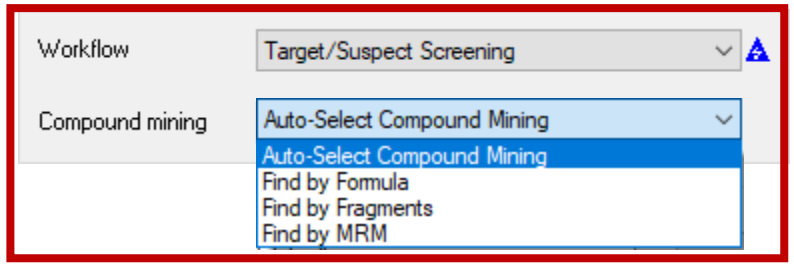



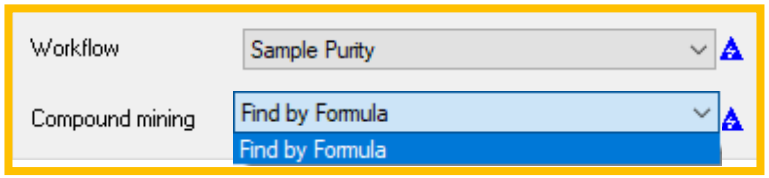
# Compound Mining

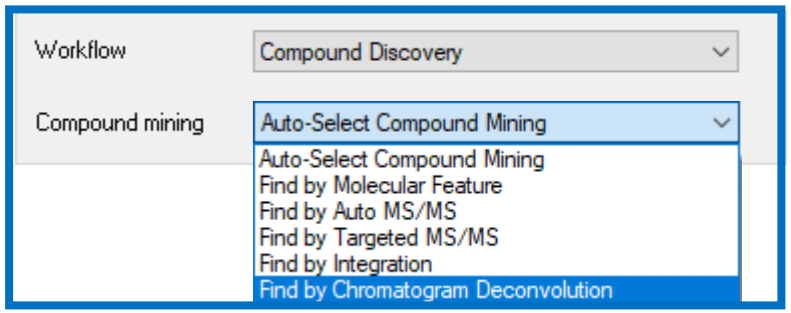
## Definition

Compound Mining defines the algorithm to be run to find compounds.

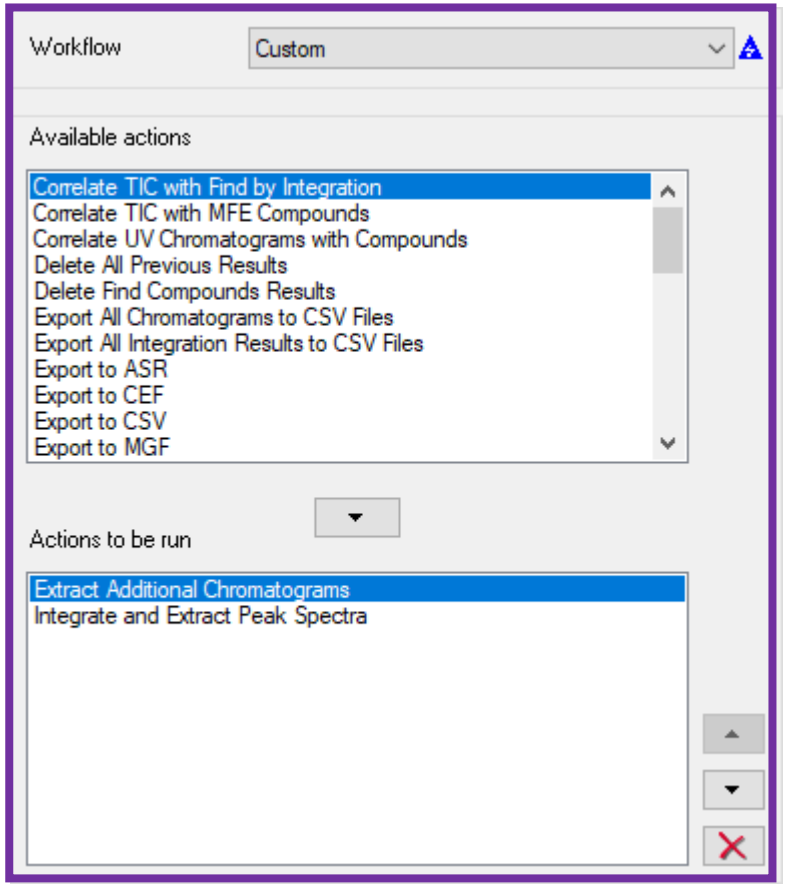
- All the steps are defined via the Method Editor.
- Mining Algorithms depend upon data set selected.
- Mining Algorithms depend upon workflow selected.




All features may not be visible with the Adaptive User Interface.

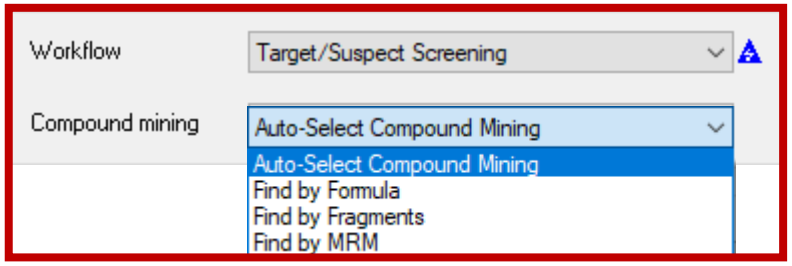


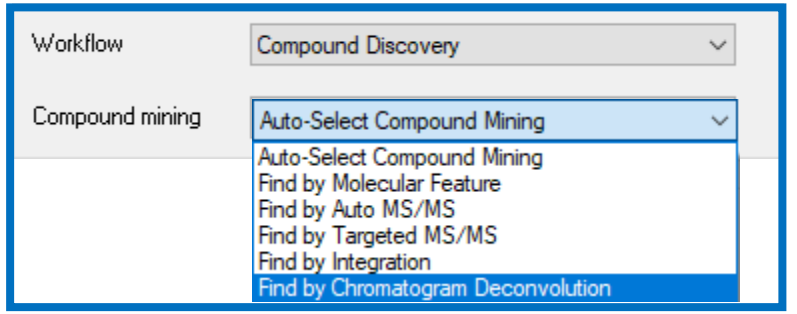
# Compound Mining

## Auto-Select Compound Mining

Auto-Select Compound Mining defines the algorithm to be run to find compounds.

- Based on data set loaded.
- Not always present, for example MRM data.
- Available with only Target/Suspect Screening and Compound Discovery.
- Good starting point.



# Workflows

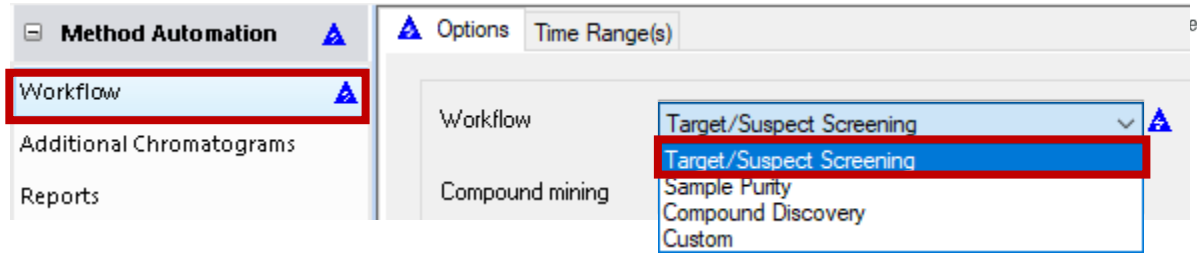
## Target/Suspect Screening

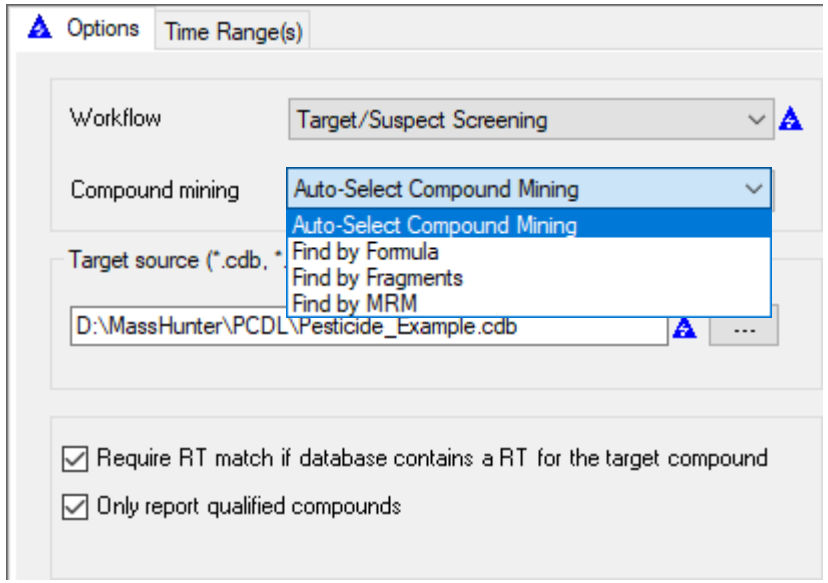
"I know what I want, is it there?

- Useful with accurate mass data (TOF, QTOF).
- Requires a library or a database
  - List of compound formulas (formulae)
  - In the form of cdb, csv, cef files
  - Can enter the neutral mass
- Mining Algorithms (data dependent)
  - Find by Formula
  - Find by Fragment (accurate mass data)
    - Are the fragments logical losses?
  - Find by MRM
    - Used with MRM data (QQQ)

Require RT match

Only report qualified compounds



# Workflows

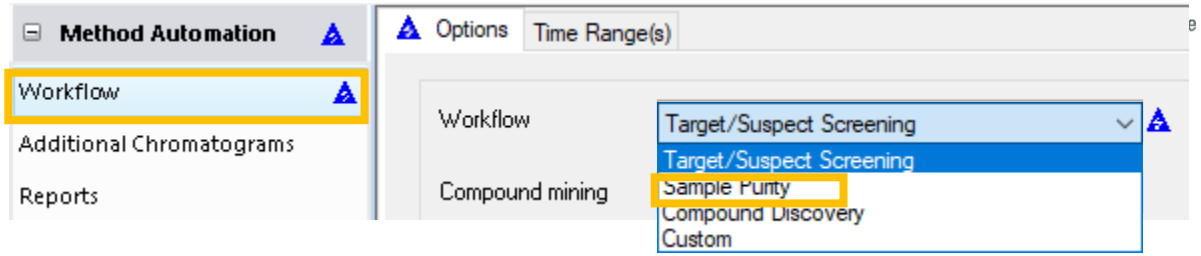
## Sample Purity

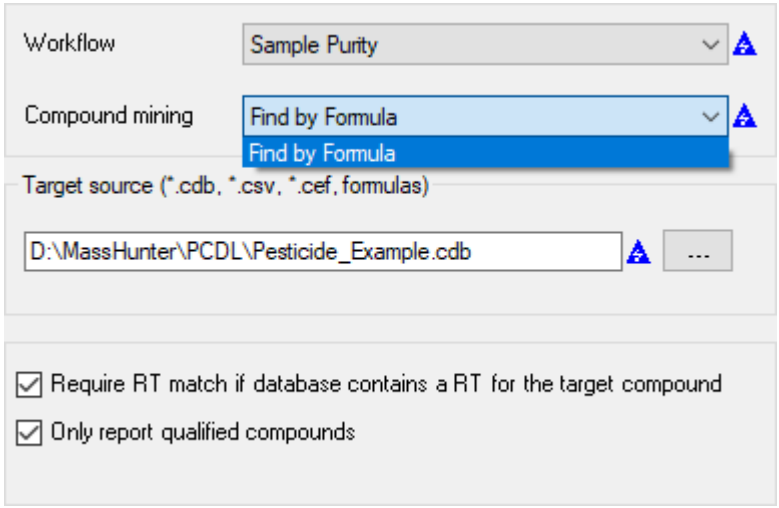
"I know what I want, how pure is it?"

- Uses high resolution data.
- Requires a library or a database
  - List of compound formulas (formulae)
  - In the form of cdb, csv, cef files
- Mining Algorithms (data dependent)
  - Find by Formula
    - Adds sample purity calculations
    - Adds the area percent calculations and report.

Require RT match

Only report qualified compounds



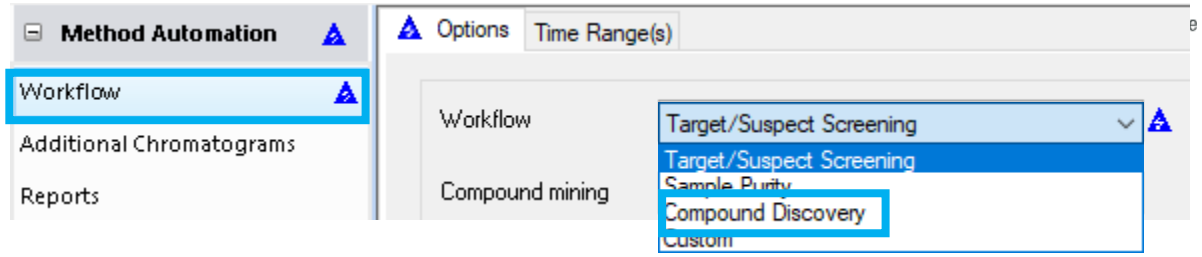



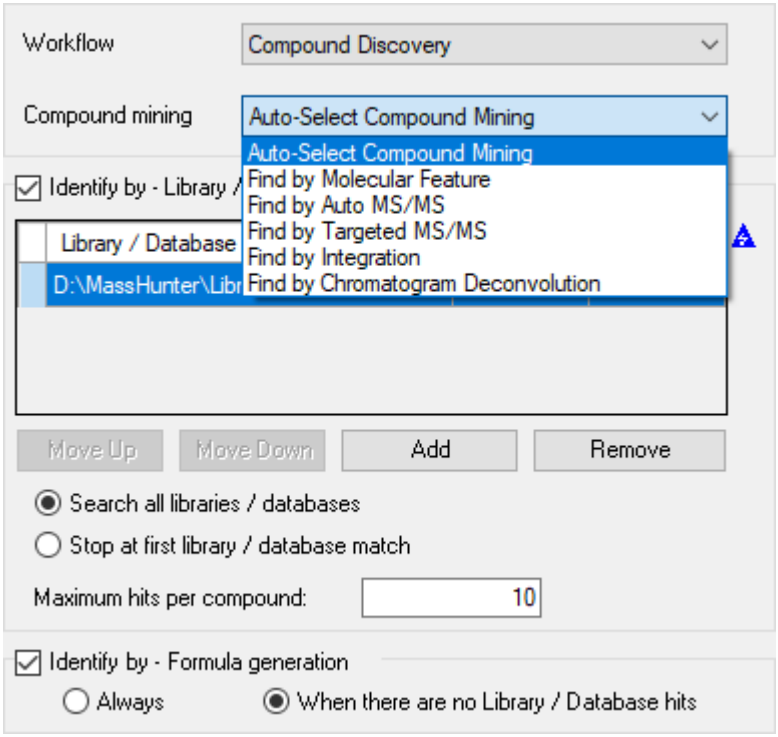
# Workflows

## Compound Discovery

### “I don’t know what I have, find the compounds and identify them”

- Library or database is optional.
  - Usually one database or library is specified.
  - List of compound formulas (formulae)
  - In the form of cdb, csv, cef files
- Compound Mining
  - Auto Select Compound Mining
  - Find by Molecular Feature
  - Find by Auto MS/MS
  - Find by Targeted MS/MS
  - Find by Integration
  - Find by Chromatogram Deconvolution

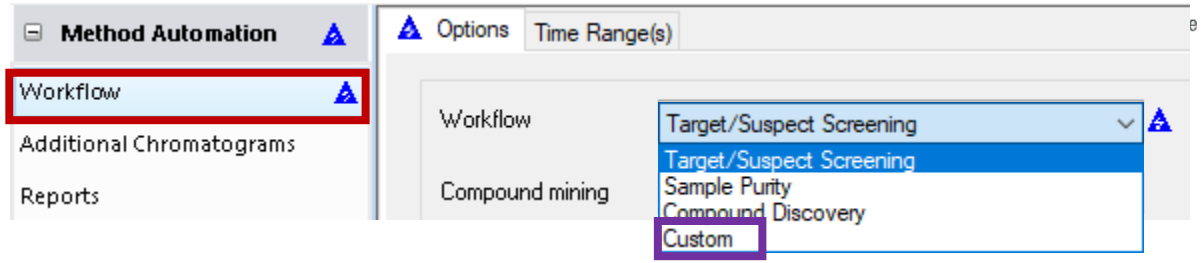


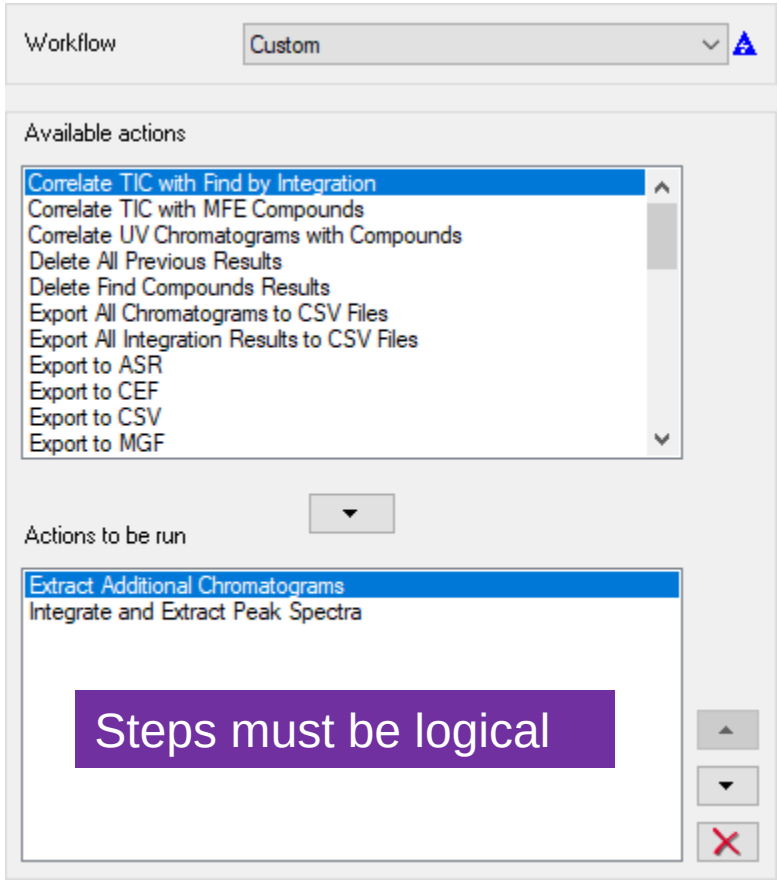
# Workflows

## Custom

"I know what I need to do, generate the compounds!"

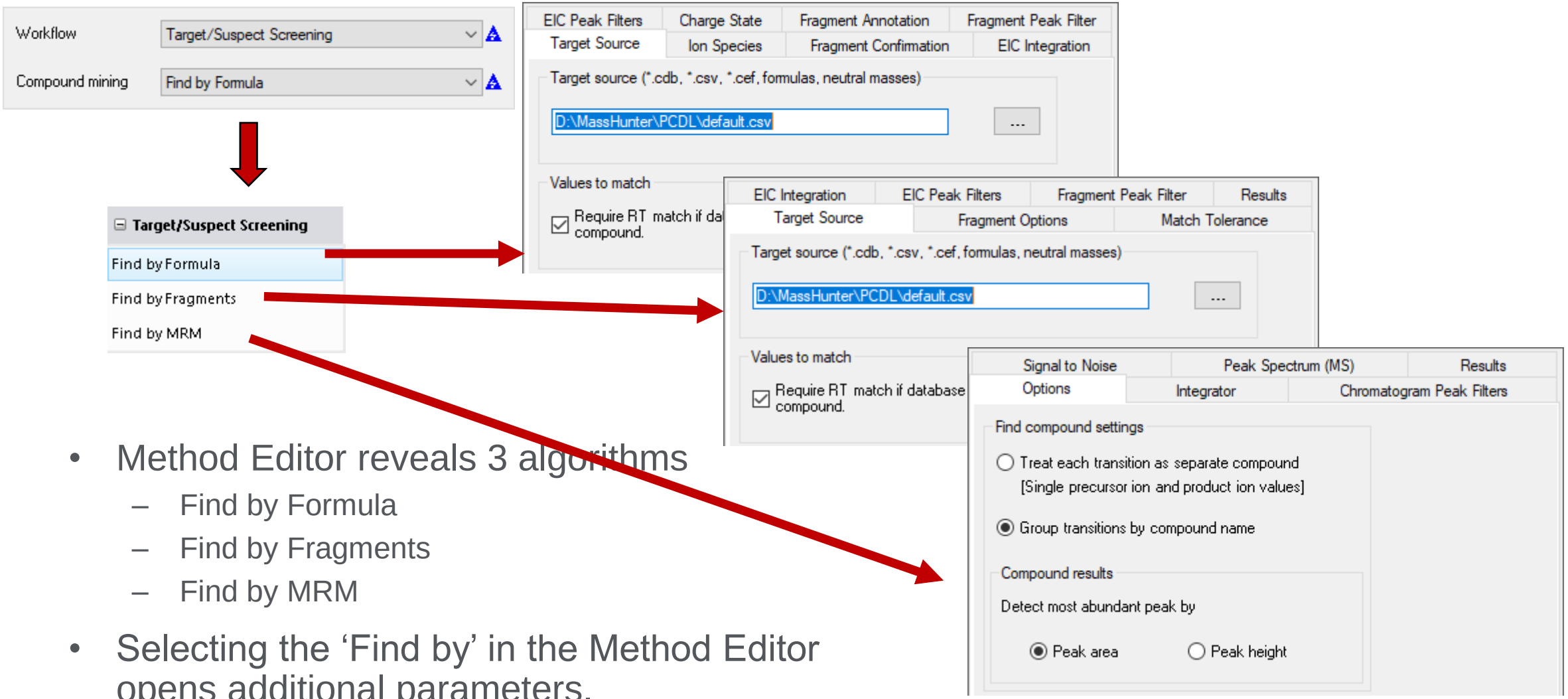



- Selecting Custom provides Available Actions.
- Define and refine the actions in Method Editor.
- Available for all datasets.



# Compound Mining

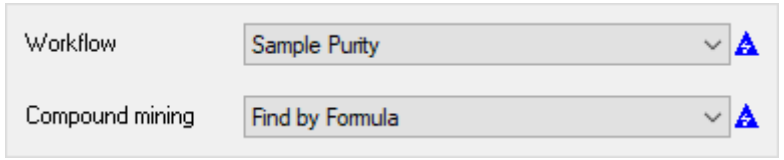
## Target/Suspect Screening Method Editor

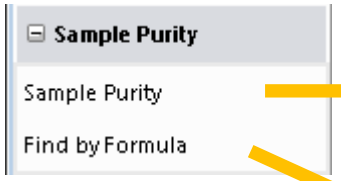


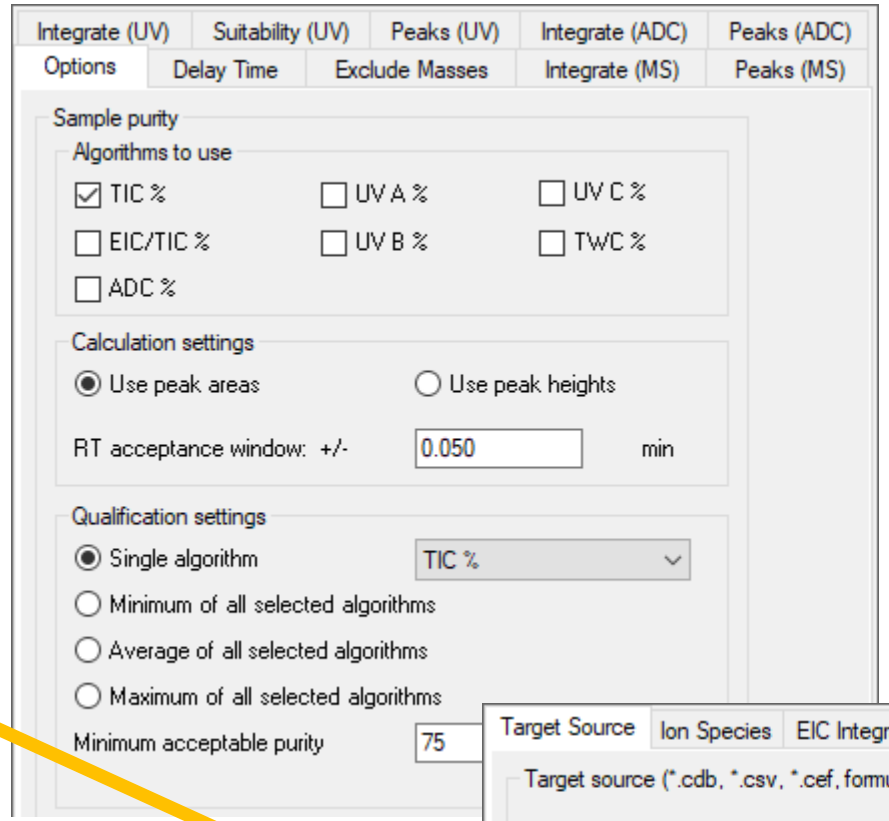

- Method Editor reveals 3 algorithms
  - Find by Formula
  - Find by Fragments
  - Find by MRM
- Selecting the ‘Find by’ in the Method Editor opens additional parameters.

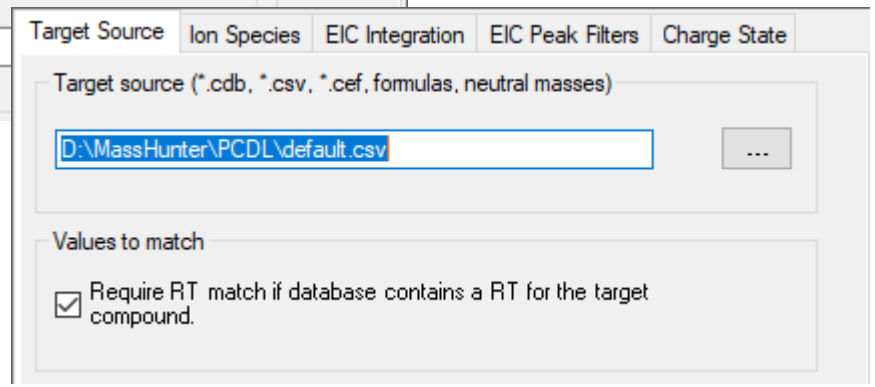
# Compound Mining

## Sample Purity Method Editor



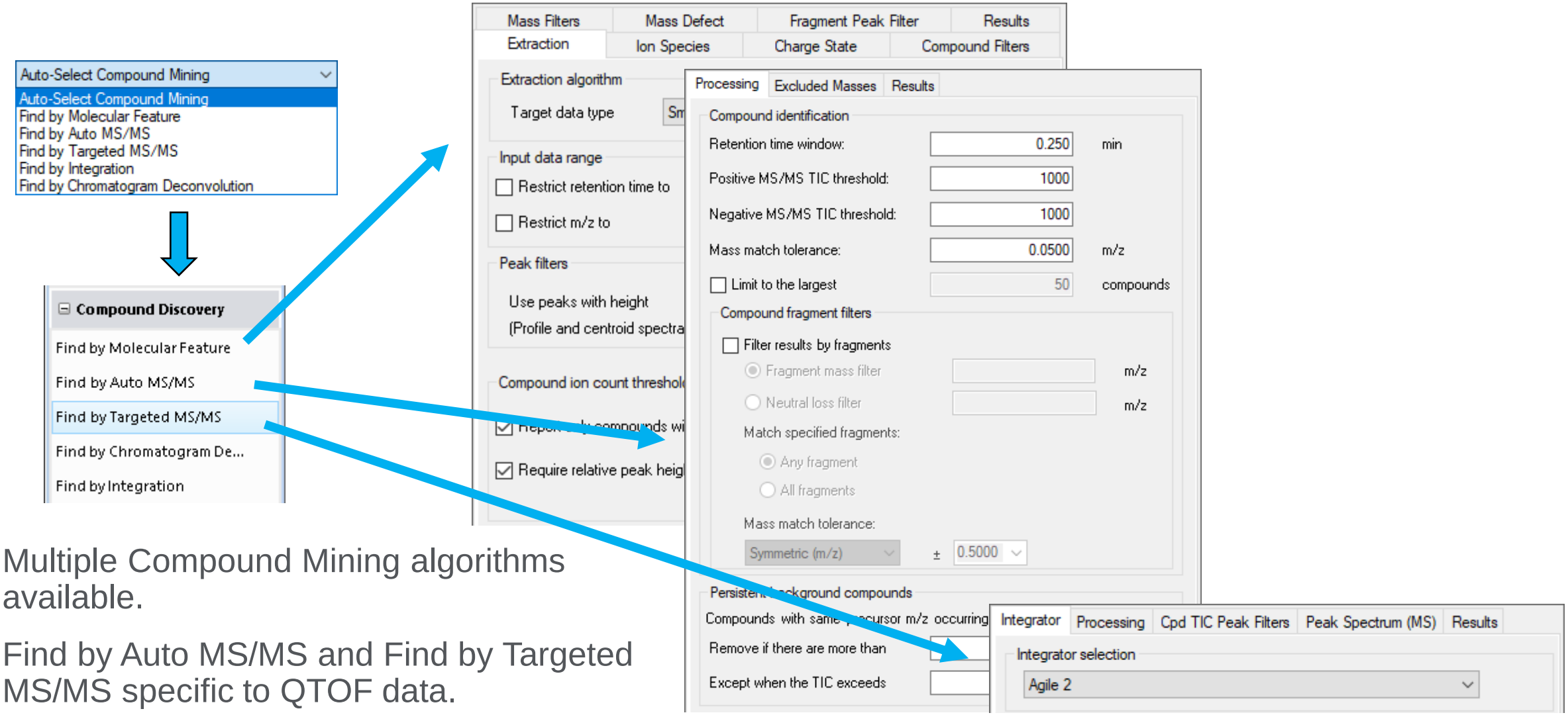




- Only 2 Method Editor choices
- Sample Purity parameters
- Find by Formula
  - Useful for LC/TOF or QTOF data.
  - Requires a formula database.

# Compound Mining

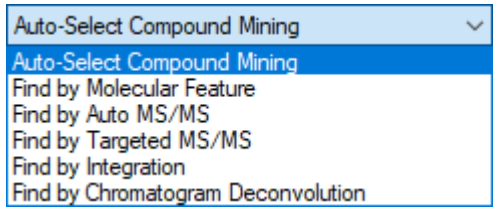
## Compound Discovery Method Editor (1)

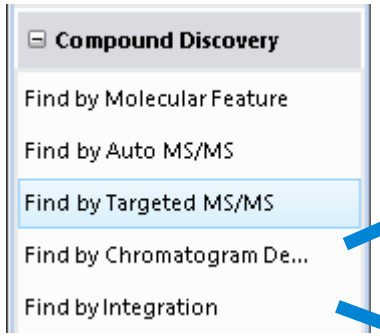


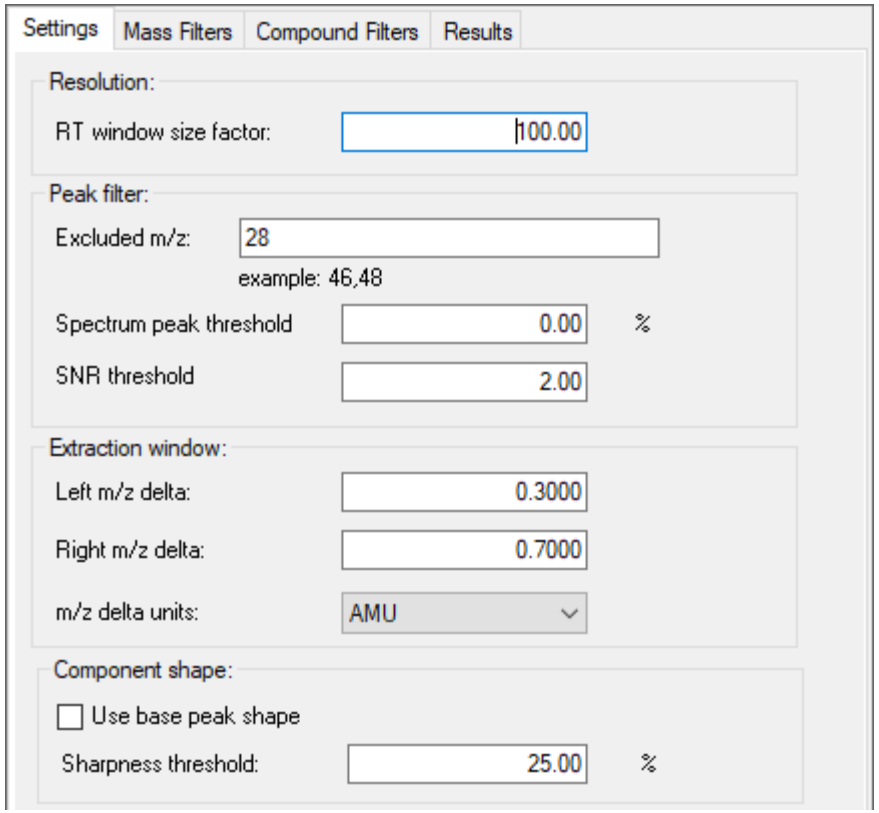

- Multiple Compound Mining algorithms available.
- Find by Auto MS/MS and Find by Targeted MS/MS specific to QTOF data.

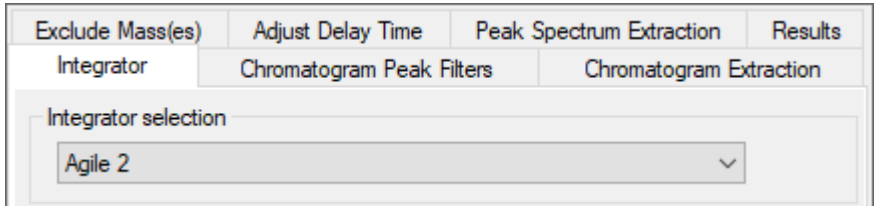
# Compound Mining

## Compound Discovery Method Editor (2)



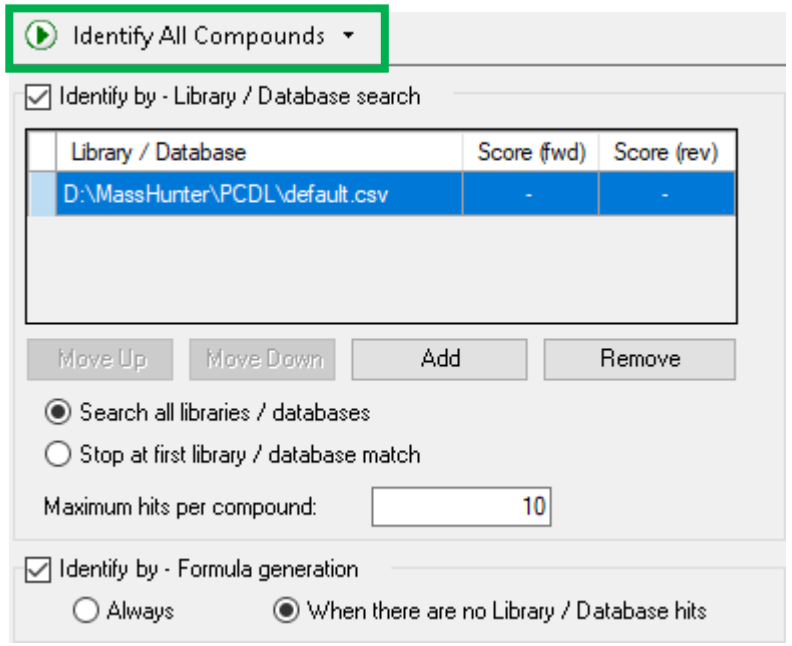



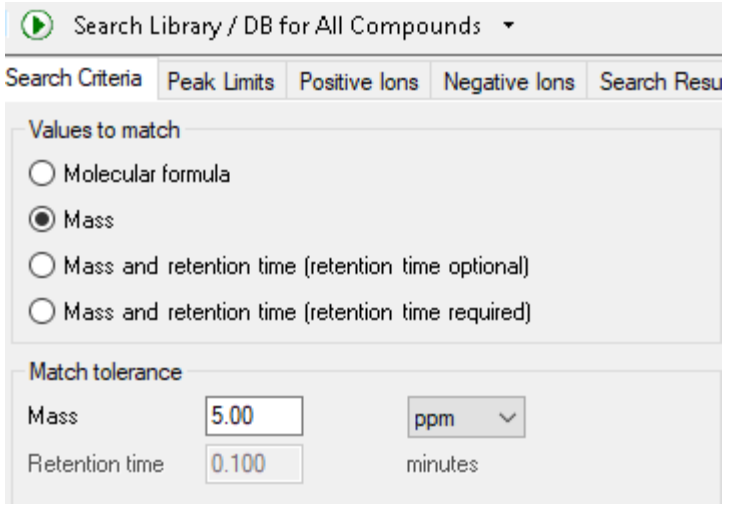



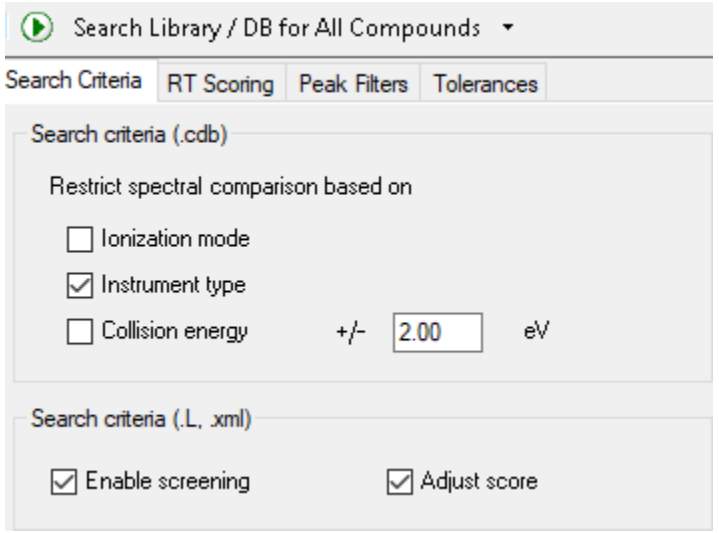

- Find by Chromatogram Deconvolution
  - Similar to Quantitative Analysis and Unknowns Analysis.

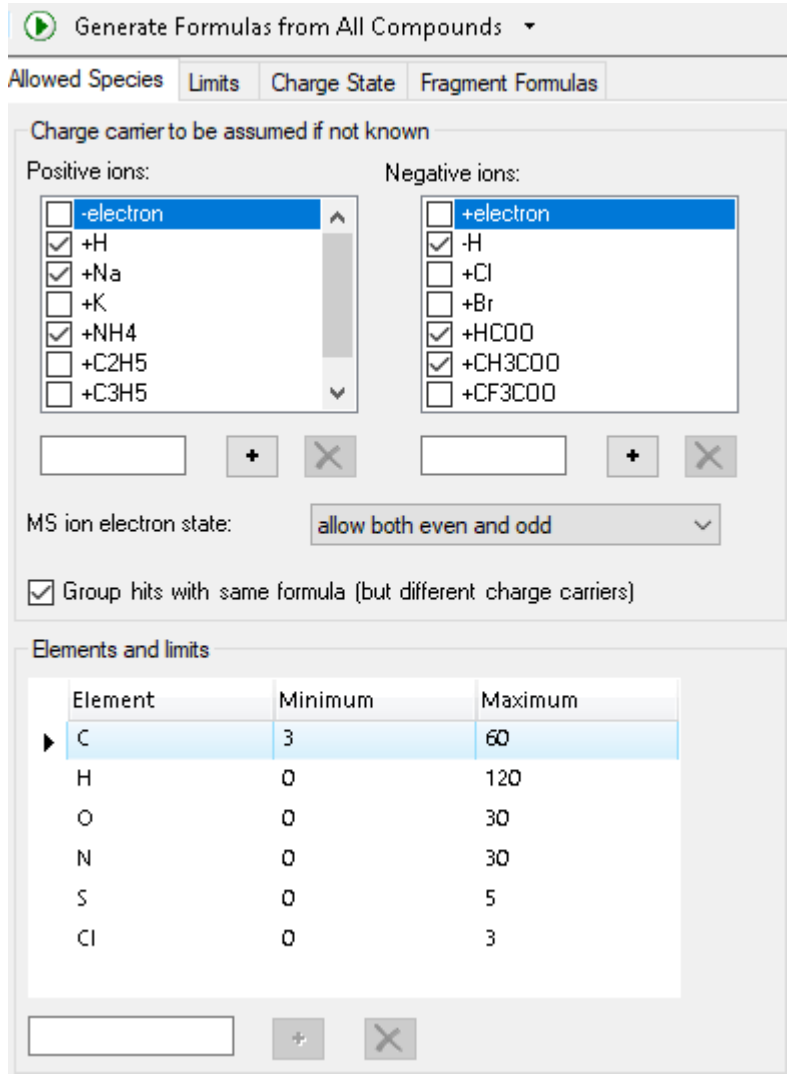
# Compound Identification

## Definition



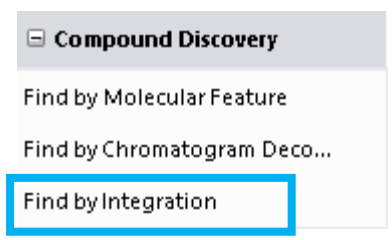



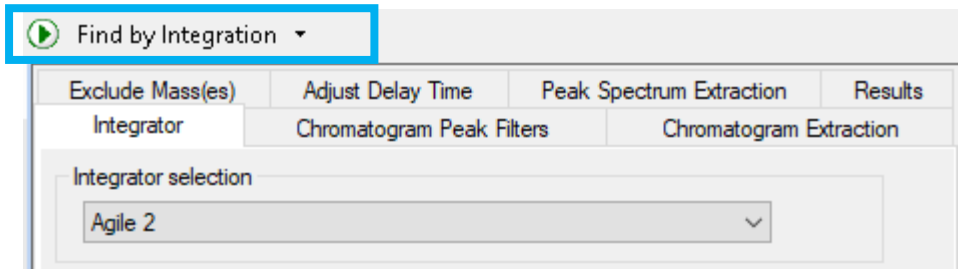

- Component of the Method Editor
  - Establishes database or library to use.

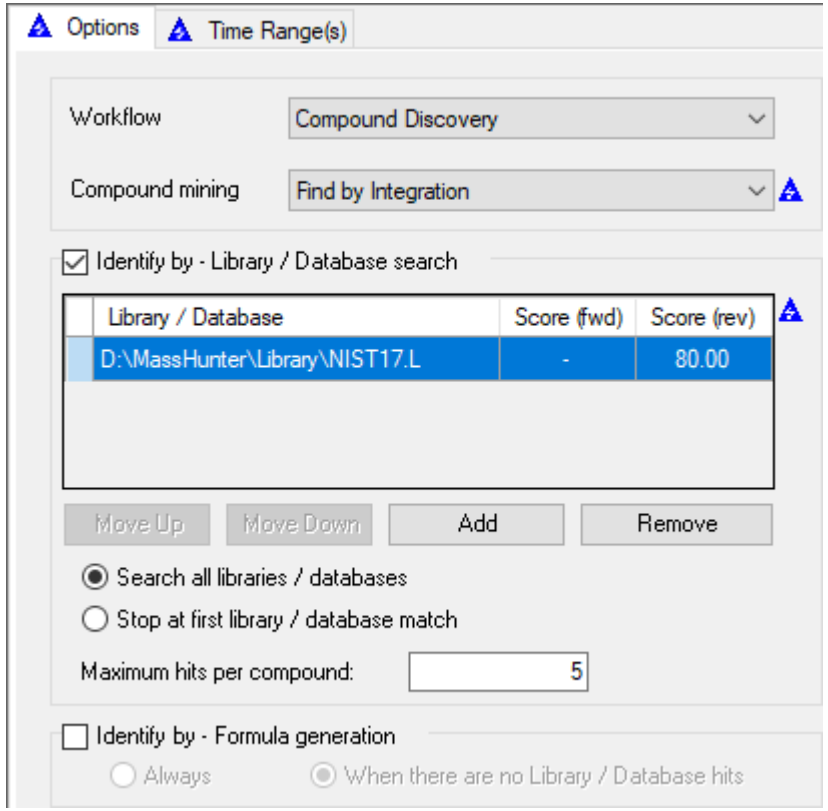
# Find by Integration

## Example

- Load the data file Evaldemo2.D
  - Simple data file.
  - GCMS SQ data.
- Load the method Default-GCMS-SQ.M.
- Set the Workflow to Compound Discovery.
- Select Find by Integration for the Compound Mining.
- Add the NIST17.L.
- Review the Find by Integration parameters.



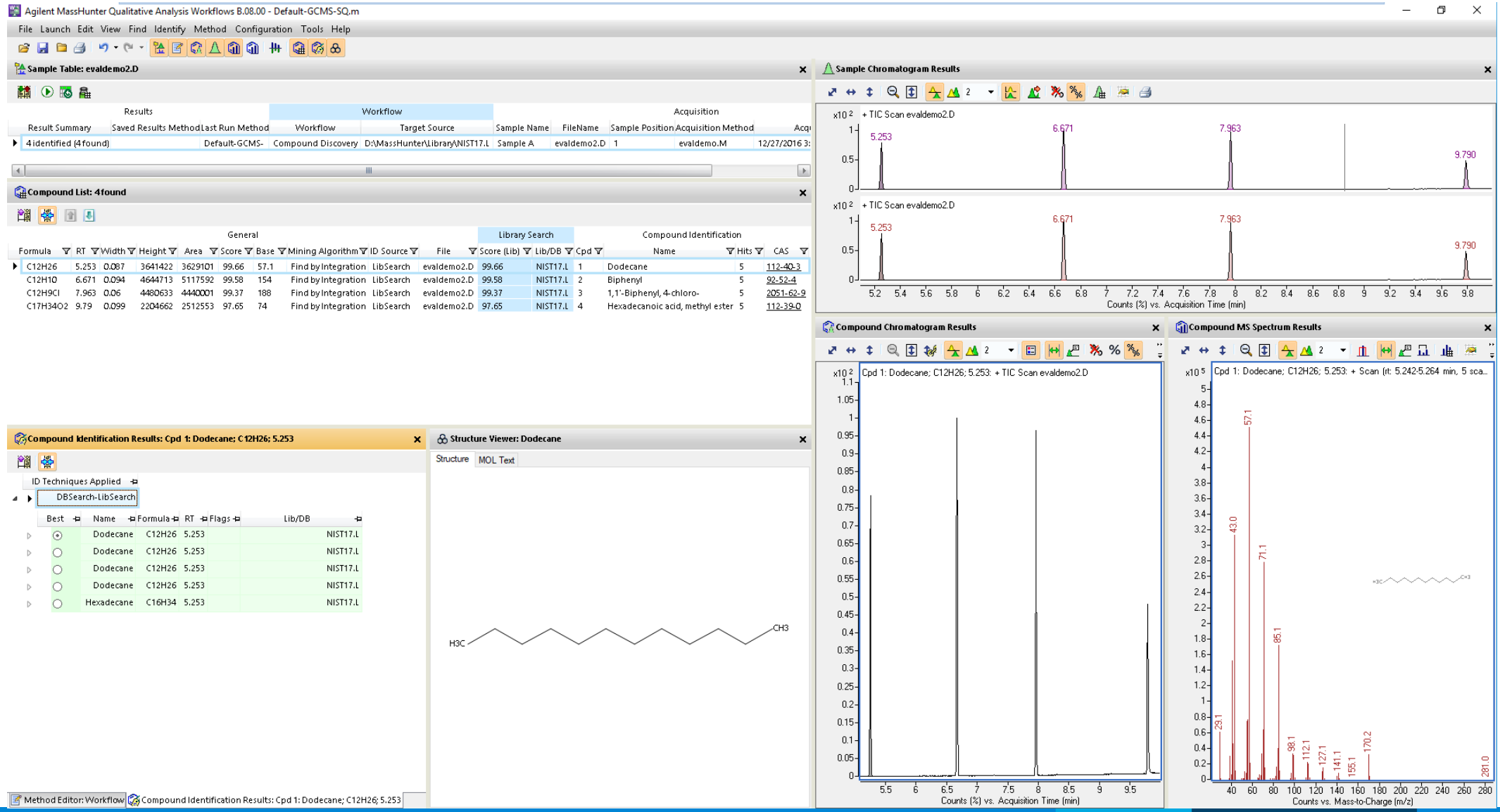




- Run Method Workflow or run icon.

# Find by Integration

## Results



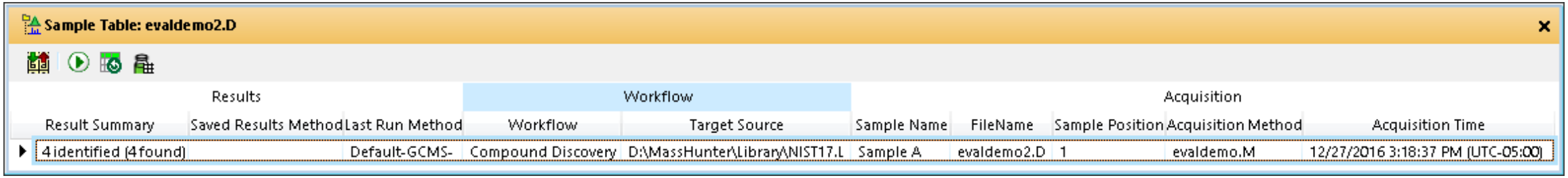
# Let’s take a moment for questions on Workflows and Compound Mining Algorithms

Up Next:

Data Review

# Data Review

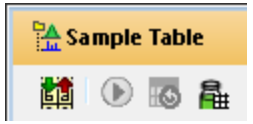
## Sample Table




- Sample Table shows information about the sample.
  - Workflow column shows most recent workflow applied to data file.
- Results
  - Four compounds identified (4 found in library).
  - Saved Results Method.
    - Must be saved and shows Qualitative Analysis parameters.
- Workflow
  - Workflow used and library searched.
- Acquisition

Information about acquisition parameters.

- Toolbar




Add/Remove Columns

Run method workflow

Can run on multiple samples

Reprocess sample

Can reprocess single samples or reprocess with a different workflow.

Sample Information

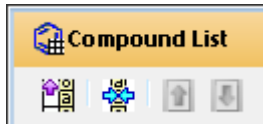
# Data Review

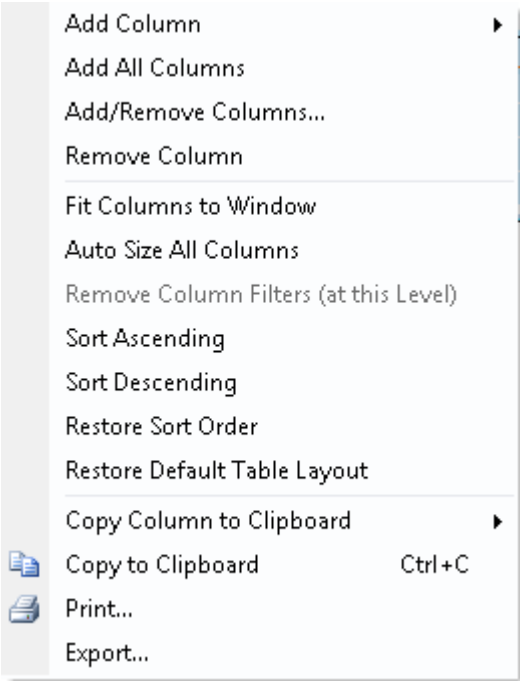
## Compound List

Compound List: 4found

| | General | | | | | | | | | | Library Search | | | Compound Identification | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Formula | RT | Width | Height | Area | Score | Base Peak | Mining Algorithm | ID Source | File | Score (Lib) | Lib/DB | Cpd | Name | Hits | CAS |
| ▶ | C12H26 | 5.253 | 0.087 | 3641422 | 3629101 | 99.66 | 57.1 | Find by Integration | LibSearch | evaldemo2.D | 99.66 | NIST17.L | 1 | Dodecane | 5 | 112-40-3 |
| | C12H10 | 6.671 | 0.094 | 4644713 | 5117592 | 99.58 | 154 | Find by Integration | LibSearch | evaldemo2.D | 99.58 | NIST17.L | 2 | Biphenyl | 5 | 92-52-4 |
| | C12H9Cl | 7.963 | 0.06 | 4480633 | 4440001 | 99.37 | 188 | Find by Integration | LibSearch | evaldemo2.D | 99.37 | NIST17.L | 3 | 1,1'-Biphenyl, 4-chloro- | 5 | 2051-62-9 |
| | C17H34O2 | 9.79 | 0.099 | 2204662 | 2512553 | 97.65 | 74 | Find by Integration | LibSearch | evaldemo2.D | 97.65 | NIST17.L | 4 | Hexadecanoic acid, methyl ester | 5 | 112-39-0 |

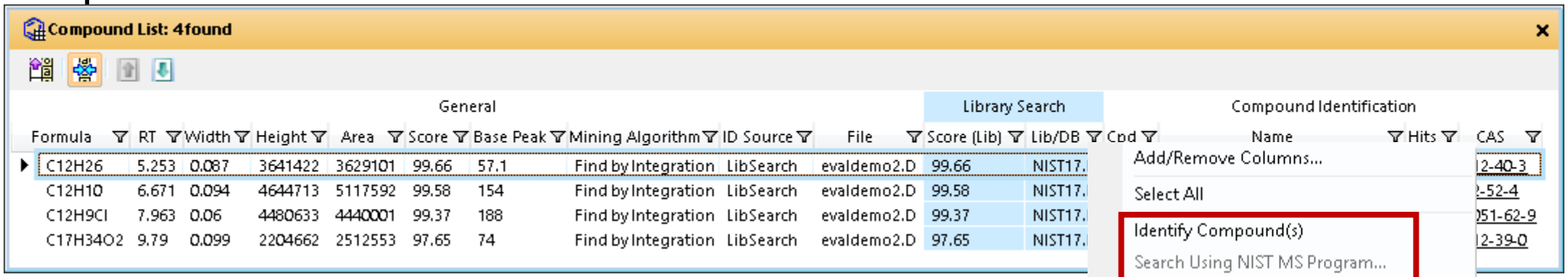
- Compound List shows 4 compounds
- Four compounds identified
- Context menu yields numerous options for formatting
  - Add/Remove Columns
  - Auto Size all Columns
  - Sorting
  - Copying, printing and exporting
- Toolbar
  - Hide any currently empty columns
  - Auto Size All Columns
  - Select previous and next compounds



# Data Review

## Compound List




- Additional options are available in the context menu.
  - Identify Compound(s)
    - Initiates Identification workflow for selected compounds.
  - Search Using NIST MS Program
  - Add/Edit Manual Identification
    - Overwrites current Name column.
  - Send Spectra to PCDL database.
  - Initiate Quantitation
    - Useful with MRM data
    - Launches Quantitative analysis and transfers transitions and collision energies to the quantitation database.

# Compound List

## Super Header vs. Header

Compound List: 5 found

| | General | | | | | | | | | | Library Search | | Compound Identification | | | | Database Search |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Formula | RT | Width | Height | Area | Score | Base Peak | Mining Algorithm | ID Source | File | Score (Lib) | Lib/DB | Cpd | Name | Hits | CAS | RT Diff (DB) |
| ▶ | C12H26 | 5.278 | 0.097 | 325283 | 44275 | 99.39 | 57.1 | Find by Integration | LibSearch | EVALDEMO.D | 99.39 | demo.l | 1 | Dodecane | 1 | 112-40-3 | 27678.225 |
| | C12H10 | 6.431 | 0.159 | 398482 | 69784 | 99.69 | 154.1 | Find by Integration | LibSearch | EVALDEMO.D | 99.69 | demo.l | 2 | Biphenyl | 1 | 92-52-4 | 1015.939 |
| | C12H9Cl | 7.737 | 0.167 | 347841 | 59098 | 99.27 | 188.2 | Find by Integration | LibSearch | EVALDEMO.D | 99.27 | demo.l | 3 | 4-Chlorobiphenyl | 1 | 2051-62-9 | 1014.633 |
| | | 8.947 | 0.109 | 80492 | 15923 | | 253.1 | Find by Integration | | EVALDEMO.D | | | 4 | | 0 | | |
| | C17H34O2 | 9.772 | 0.153 | 373249 | 54842 | 98.89 | 74.1 | Find by Integration | LibSearch | EVALDEMO.D | 98.89 | demo.l | 5 | Methyl palmitate | 1 | 112-39-0 | 1012.598 |

Super Headers can be moved as group.

Compound List: 5 found

| | Compound Identification | | | | General | | | | | | | | | Library Search | | Database Search |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Cpd | Name | Hits | CAS | Formula | RT | Width | Height | Area | Score | Base Peak | Mining Algorithm | ID Source | File | Score (Lib) | Lib/DB | RT Diff (DB) |
| | 1 | Dodecane | 1 | 112-40-3 | C12H26 | 5.278 | 0.097 | 325283 | 44275 | 99.39 | 57.1 | Find by Integration | LibSearch | EVALDEMO.D | 99.39 | demo.l | 27678.225 |
| ▶ | 2 | Biphenyl | 1 | 92-52-4 | C12H10 | 6.431 | 0.159 | 398482 | 69784 | 99.69 | 154.1 | Find by Integration | LibSearch | EVALDEMO.D | 99.69 | demo.l | 1015.939 |
| | 3 | 4-Chlorobiphenyl | 1 | 2051-62-9 | C12H9Cl | 7.737 | 0.167 | 347841 | 59098 | 99.27 | 188.2 | Find by Integration | LibSearch | EVALDEMO.D | 99.27 | demo.l | 1014.633 |
| | 4 | | 0 | | | 8.947 | 0.109 | 80492 | 15923 | | 253.1 | Find by Integration | | EVALDEMO.D | | | |
| | 5 | Methyl palmitate | 1 | 112-39-0 | C17H34O2 | 9.772 | 0.153 | 373249 | 54842 | 98.89 | 74.1 | Find by Integration | LibSearch | EVALDEMO.D | 98.89 | demo.l | 1012.598 |

Sub Headers can be moved with the super header.

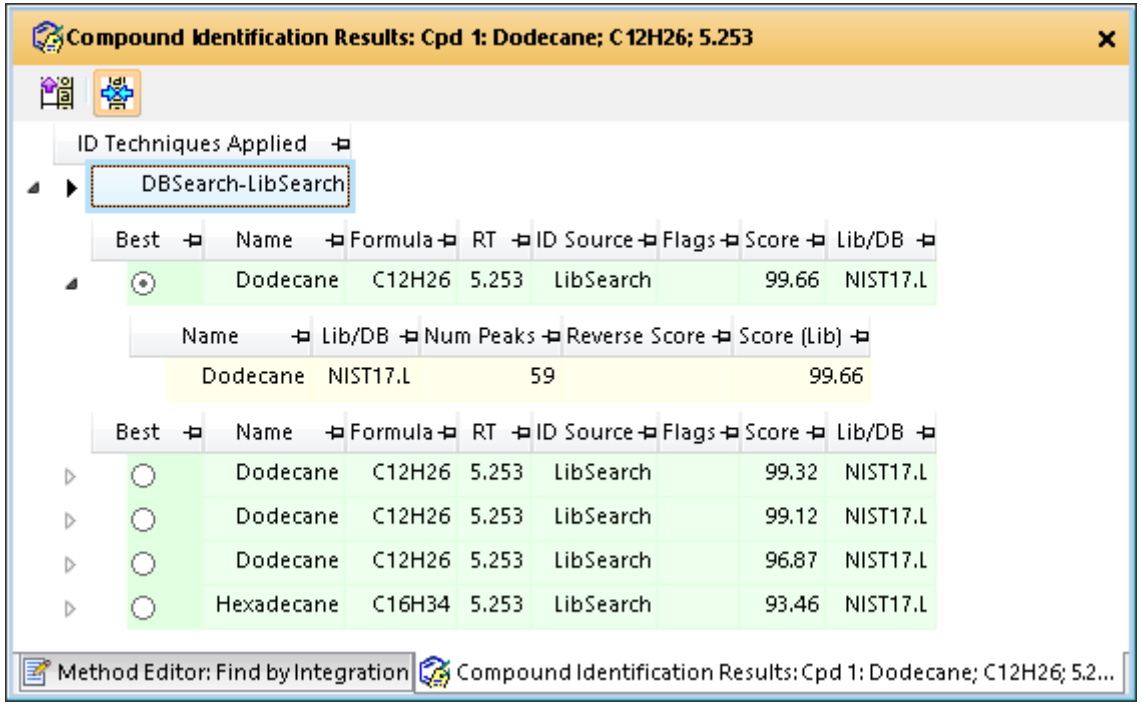
Compound List: 5 found

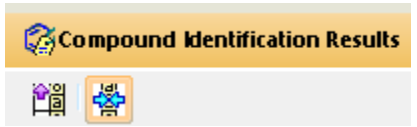
| | General | | | | | | | | | | Library Search | | Compound Identification | | | | Database Search |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Formula | File | RT | Width | Height | Area | Score | Base Peak | Mining Algorithm | ID Source | Score (Lib) | Lib/DB | Cpd | Name | Hits | CAS | RT Diff (DB) |
| ▶ | C12H26 | EVALDEMO.D | 5.278 | 0.097 | 325283 | 44275 | 99.39 | 57.1 | Find by Integration | LibSearch | 99.39 | demo.l | 1 | Dodecane | 1 | 112-40-3 | 27678.225 |
| | C12H10 | EVALDEMO.D | 6.431 | 0.159 | 398482 | 69784 | 99.69 | 154.1 | Find by Integration | LibSearch | 99.69 | demo.l | 2 | Biphenyl | 1 | 92-52-4 | 1015.939 |
| | C12H9Cl | EVALDEMO.D | 7.737 | 0.167 | 347841 | 59098 | 99.27 | 188.2 | Find by Integration | LibSearch | 99.27 | demo.l | 3 | 4-Chlorobiphenyl | 1 | 2051-62-9 | 1014.633 |
| | | EVALDEMO.D | 8.947 | 0.109 | 80492 | 15923 | | 253.1 | Find by Integration | | | | 4 | | 0 | | |
| | C17H34O2 | EVALDEMO.D | 9.772 | 0.153 | 373249 | 54842 | 98.89 | 74.1 | Find by Integration | LibSearch | 98.89 | demo.l | 5 | Methyl palmitate | 1 | 112-39-0 | 1012.598 |

# Data Review

## Compound Identification Results

- Compound Identification Results more detailed information about compounds.
  - Detailed information about identified compound.
- May be tabbed window in default layout.
- Shows 5 library hits.
- Sub level shows additional information about identified compound.
- Context menu yields numerous options for formatting.
  - Add/Remove Columns
  - Auto Size all Columns
  - Sorting
  - Copying, printing and exporting
- Toolbar
  - Hide any currently empty columns
  - Auto Size All Columns

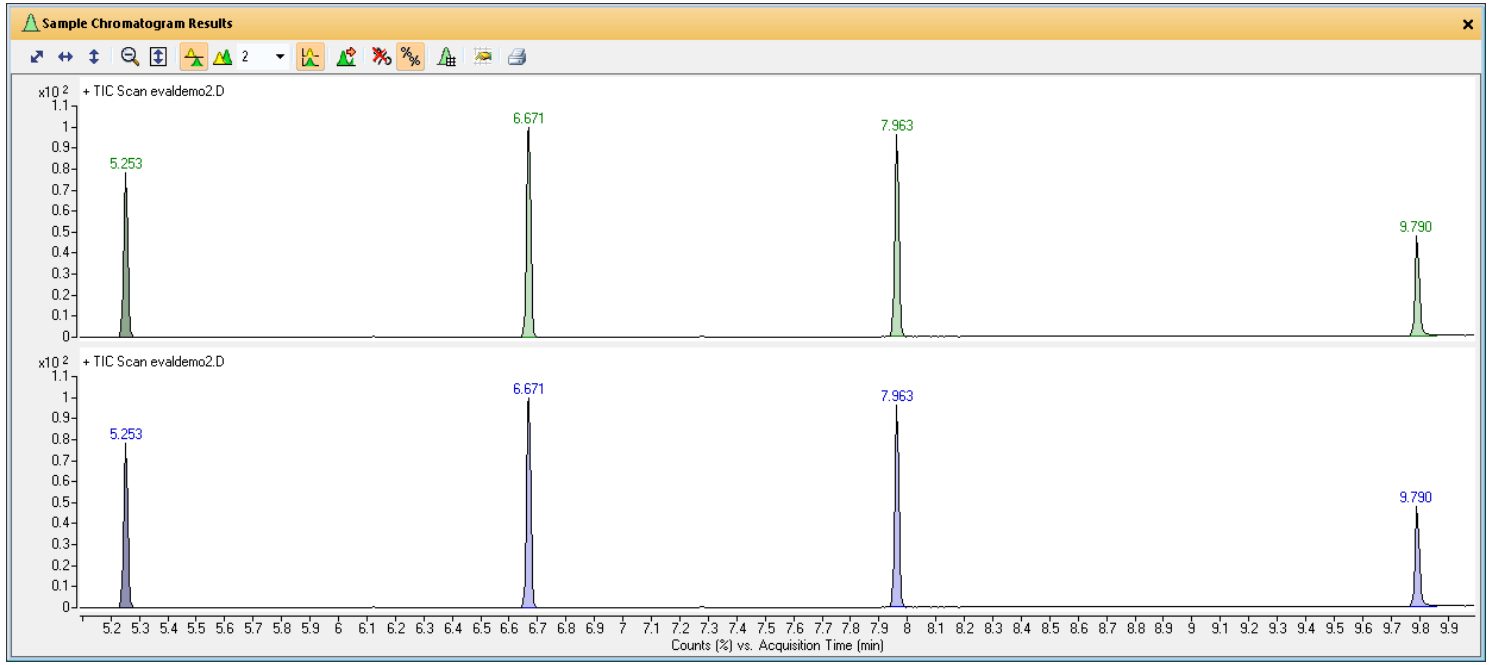


# Data Review

## Sample Chromatogram Results

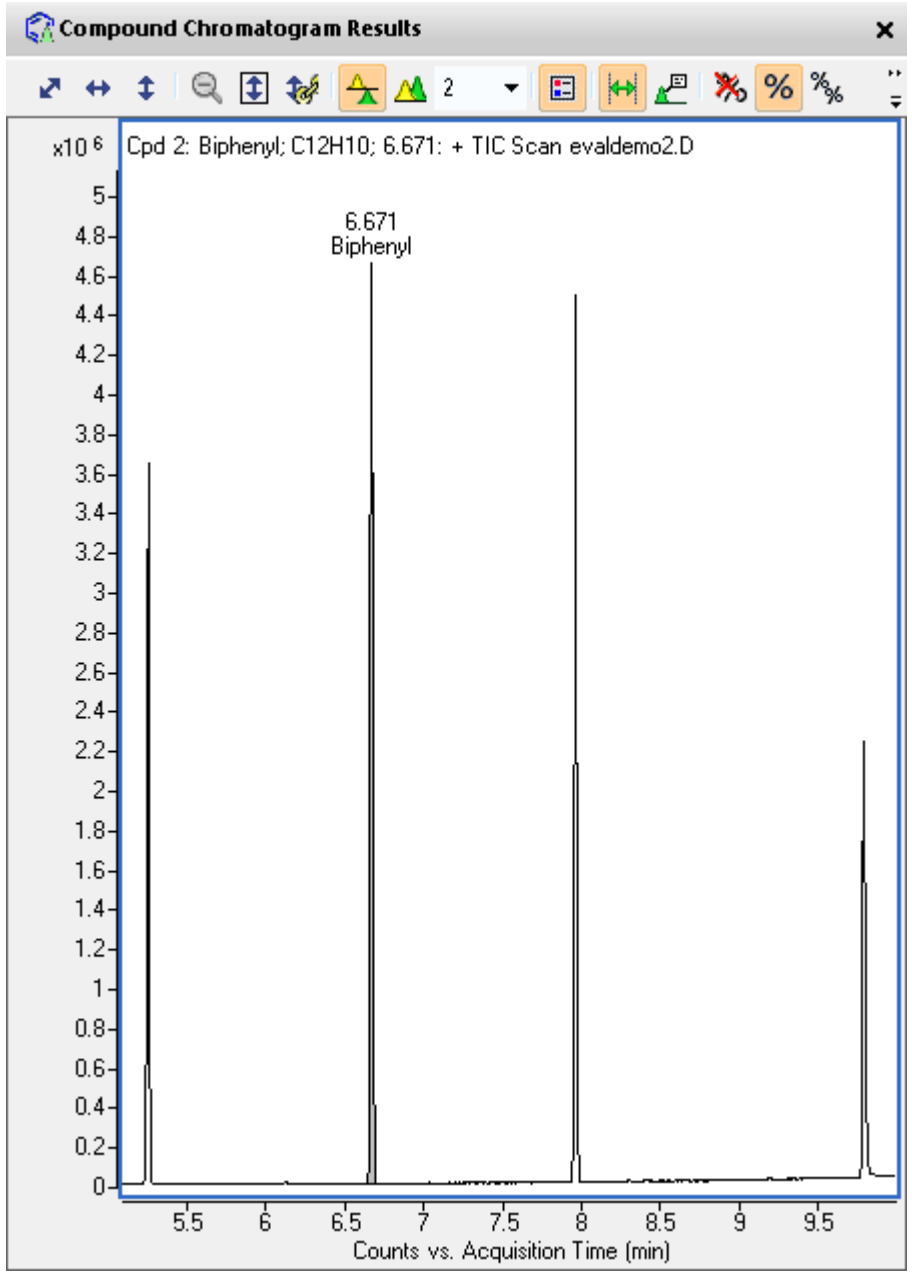
- Sample Chromatogram Results.
  - Can be overlaid or list modes
- Toolbar
  - Autoscale X-axis and Y-axis
  - Autoscale X-axis
  - Autoscale Y-axis
  - Unzoom (multiple levels)
  - Autoscale Y-axis during zoom
  - List mode or overlaid mode
  - Maximum number of panes
  - Compound overlay mode
  - Extract Chromatograms (allows TIC, BPC, EIC, etc. to be extracted.
  - Scale Chromatogram Off
  - Scale to Largest in Each Chromatogram
  - Integration Peak List
  - Chromatogram Display Options
  - Print




# Data Review

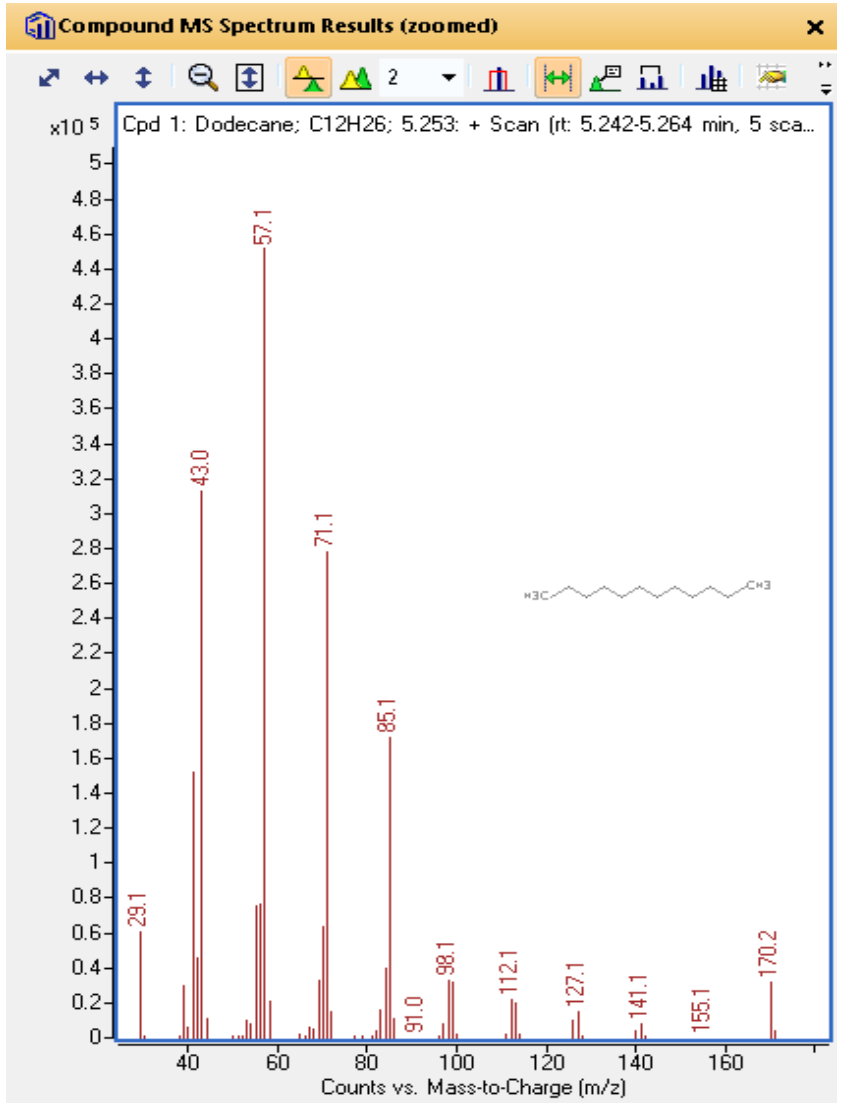
## Compound Chromatogram Results

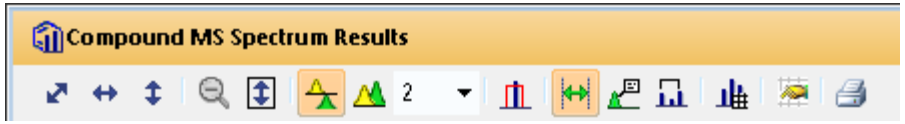
- Compound Chromatogram Results
  - Displays the TCC
  - Can be overlaid or list modes
- Toolbar
  - Autoscale X-axis and Y-axis
  - Autoscale X-axis
  - Autoscale Y-axis
  - Unzoom (multiple times)
  - Autoscale Y-axis during zoom
  - List mode or overlaid mode
  - Maximum number of panes
  - Show Legend in Overlaid Mode
  - Range Select tool
  - Annotation Mouse Tool
  - Scale to Largest in Each Chromatogram
  - Integration Peak List
  - Coelution Plot
  - Chromatogram Display Options
  - Print



# Data Review

## Compound MS Spectrum Results



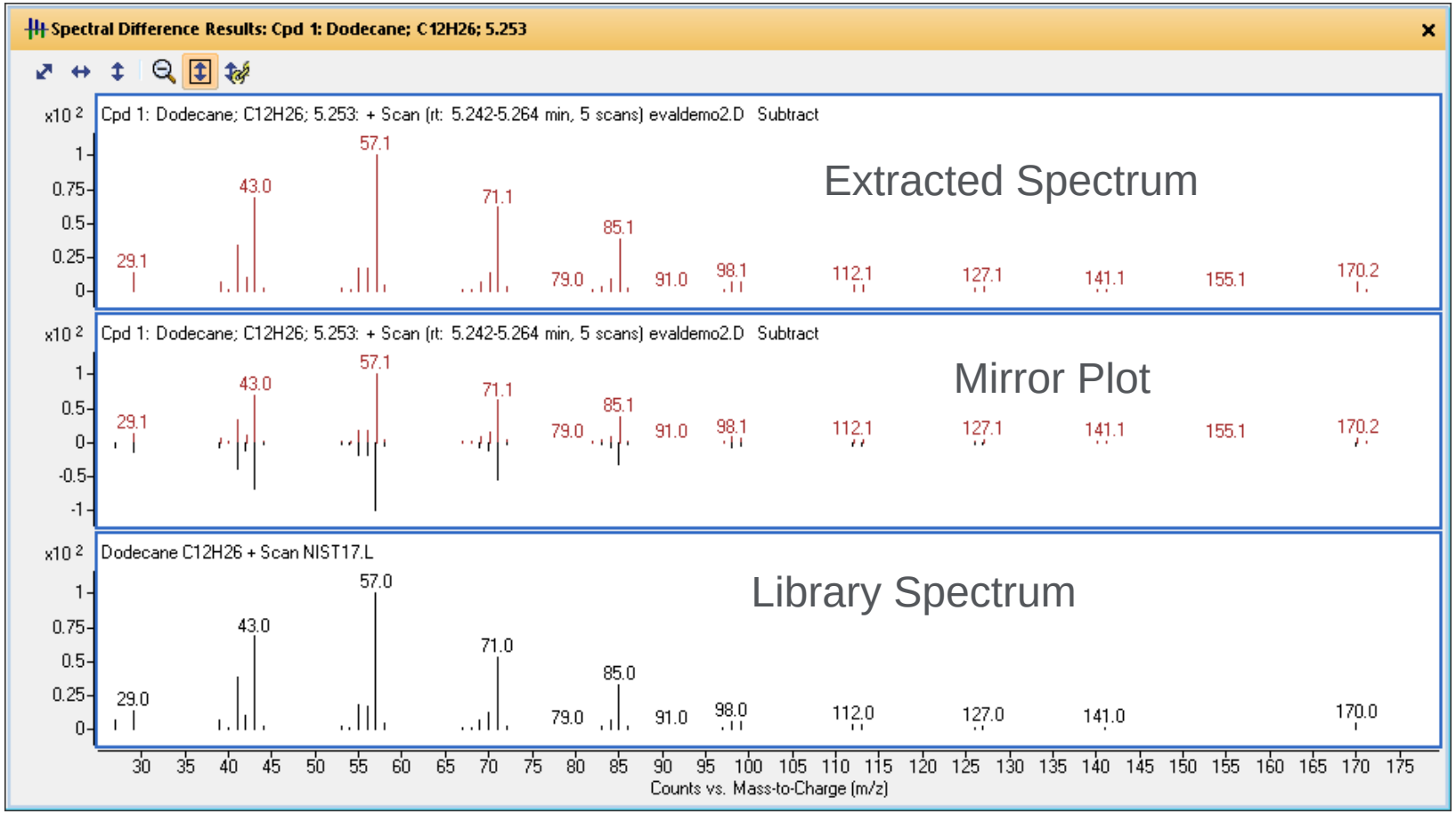




- Compound MS Spectrum Results.
  - Can be overlaid or list modes
- Toolbar
  - Autoscale X-axis and Y-axis
  - Autoscale X-axis
  - Autoscale Y-axis
  - Unzoom (multiple times)
  - Autoscale Y-axis during zoom
  - List mode or overlaid mode
  - Maximum number of panes
  - Show Predicted Isotope Distribution
  - Range Select tool
  - Annotation Mouse Tool
  - Delta Mass Caliper tool
  - Spectrum Peak List
  - Spectrum Display Options
  - Print

# Data Review

## Spectral Difference Results

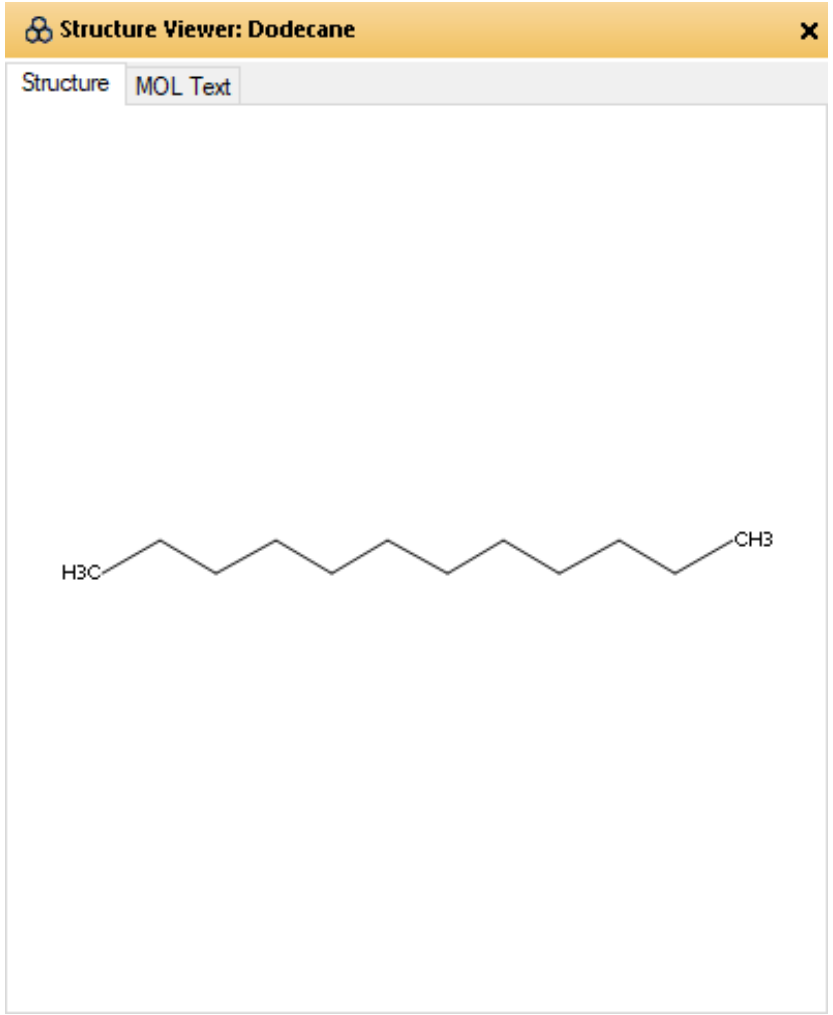
- Spectral Difference Results
- **View > Difference Results** activates this window
- Toolbar
  - Autoscale X-axis and Y-axis
  - Autoscale X-axis
  - Linked Y-axis mode

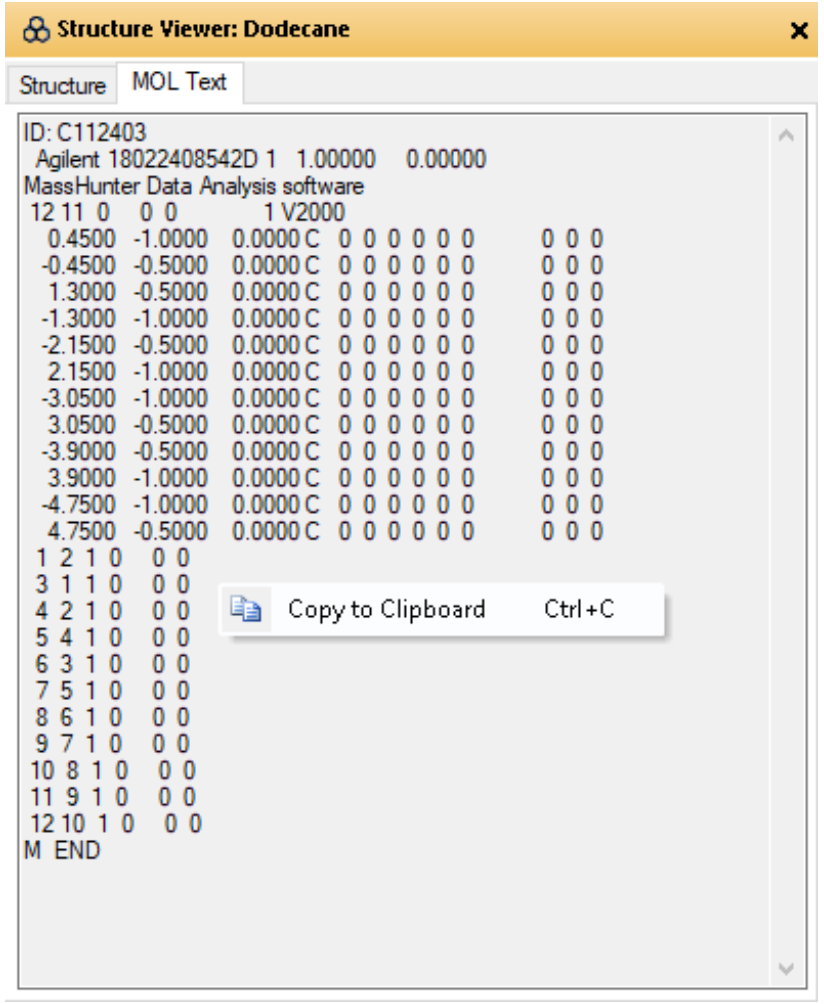


# Data Review

## Structure Viewer

- Composed of two tabs
- Structure tab
- MOL Text
  - Must be available in library
  - Easily copied to clipboard



# Let’s take a moment for questions on Data Review

Up Next:

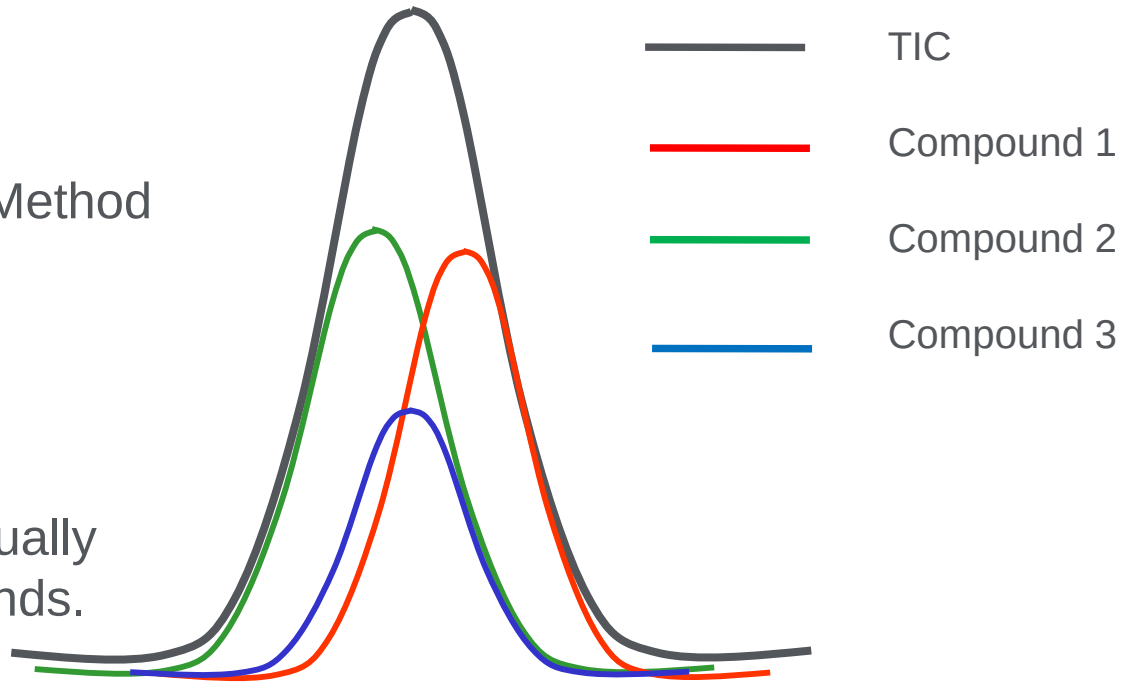
Find by Chromatogram Deconvolution

# Find by Chromatogram Deconvolution

## Case Study

- One of the ‘Find by…..’ algorithms.
- Useful to determine what is in a sample.
- Optional identification through the **Compound Identification > Identification Workflow** in the Method Editor.

One gaussian peak but actually composed of three compounds.



# Find by Chromatogram Deconvolution

## Case Study

An average spectrum is created over the entire or selected RT range.

An EIC is extracted for each mass in the average spectrum.

Each EIC is integrated using the Agile integrator and “EIC peaks” are created.

The “EIC peaks” are grouped together based on common RT and each set of “EIC peaks” become “Compounds”.

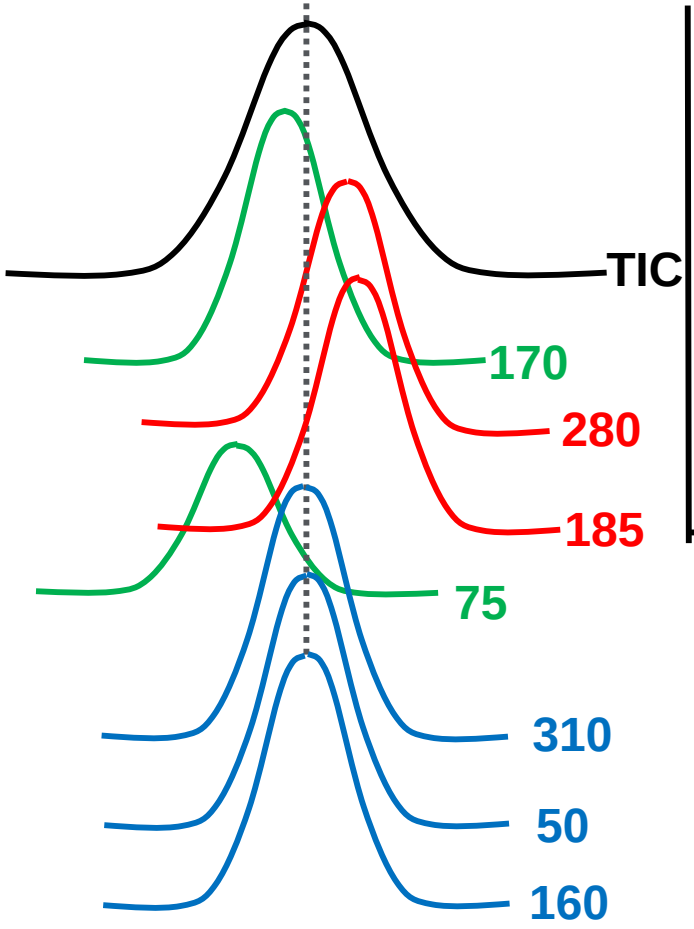
The “EIC peak” shape is used to create a Compound peak shape.

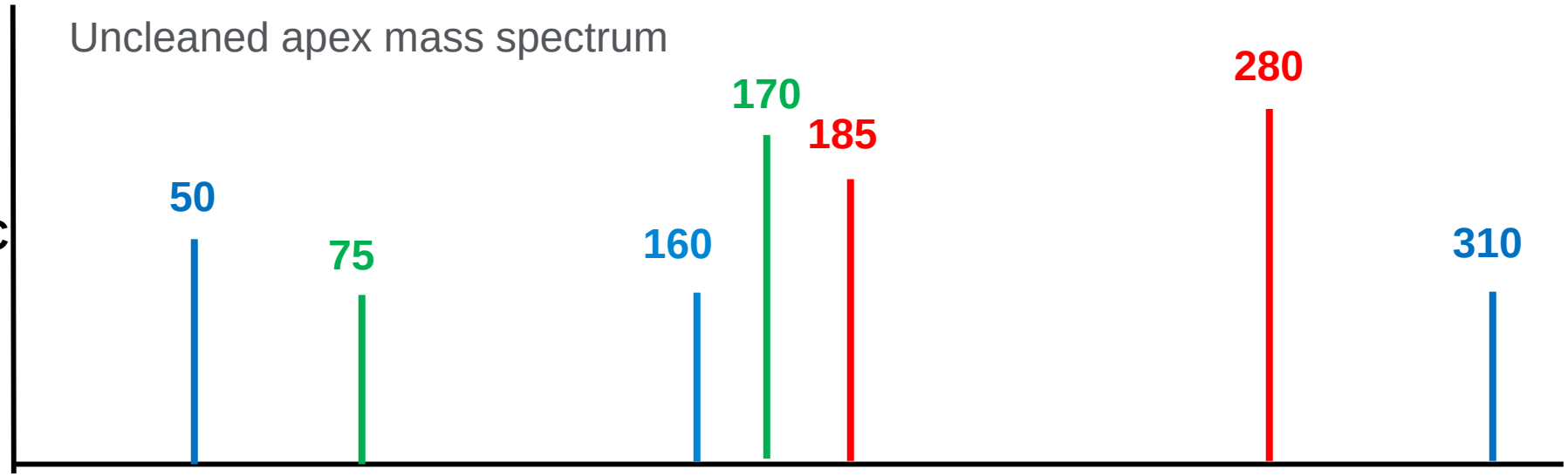
Filters can remove small ions and “compounds” with only a few small ions.

The relative intensity (area) of the “EIC peaks” and the mass of the EIC are used to create a clean spectrum of the Compound.

# Find by Chromatogram Deconvolution

## Case Study




The algorithm creates Extracted Ion Chromatograms (EICs) across a small time range around the apex spectrum RT.

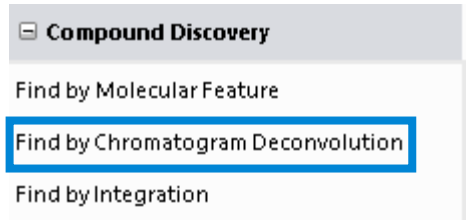
# Find by Chromatogram Deconvolution

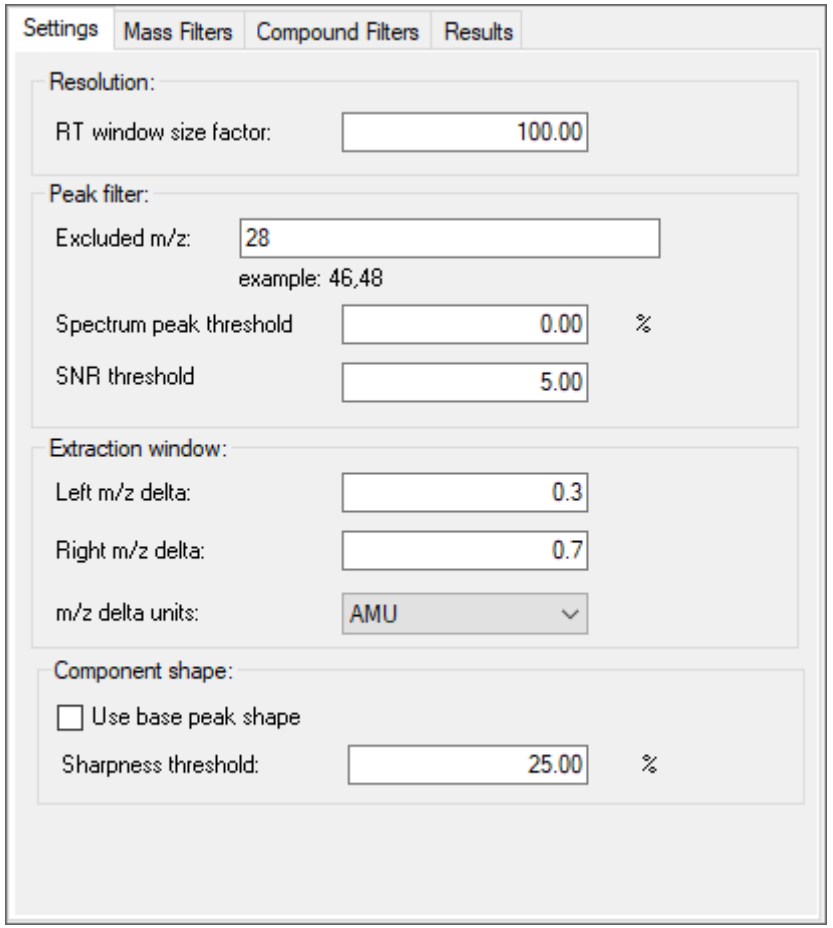
## Case Study

# Find by Chromatogram Deconvolution

## Deconvolution Parameters

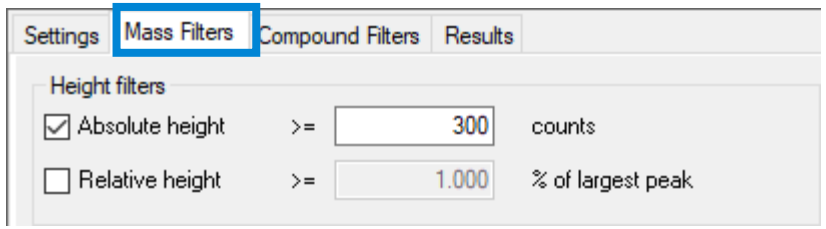
- RT window size factor
  - Key parameter that controls grouping
  - Smaller number → more compounds
  - Possible ‘fake’ compounds
- Excluded m/z
- Spectrum peak threshold
- SNR threshold
- Extraction window
  - Mass defect → -0.3 to +0.7  Low resolution
  - High resolution in ppm.
- Component shape
  - Upper 75% of peak is considered.

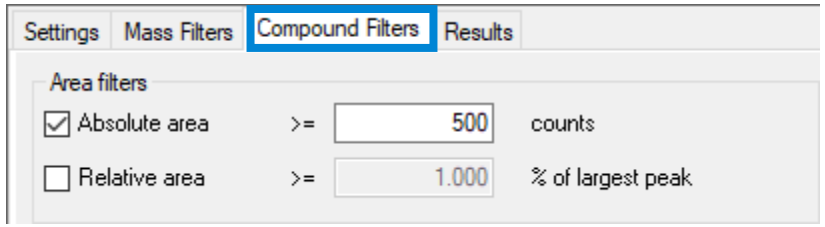


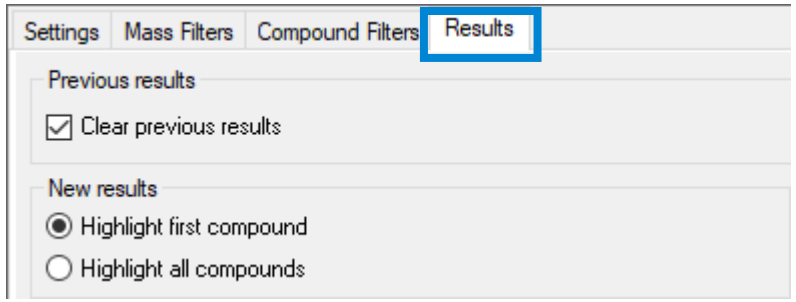



# Find by Chromatogram Deconvolution

## Deconvolution Parameters




•Mass filters are applied after the EICs are organized into compounds.

- Remove small ions from the compounds based on absolute height or relative height of base peak or both.

- Compounds Filters are applied to the compounds based on absolute area or relative area of the largest compound or both.

- Results

- Clear previous results is unchecked allows multiple algorithms to be applied.

# Let’s take a moment for questions on Find by Chromatogram Deconvolution

Up Next:

Molecular Feature Extraction

# Find by Molecular Feature

## Case Study

### MFE (Molecular Feature Extraction)

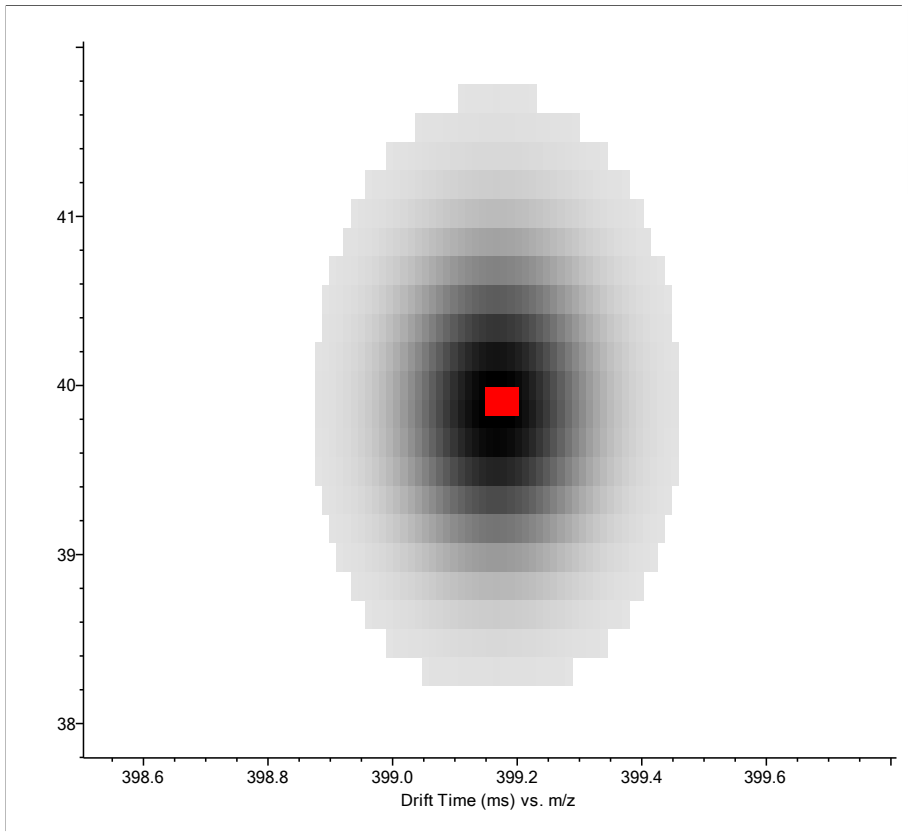
- Untargeted analysis for a unique molecular entity based on three dimensional array of retention time, mass and abundance in GC or LC MS data. Operates on raw scan data.
  - Evaluates the data as a three dimensional array based on retention time, mass and abundance.
  - Removes persistent or slowly changing background.
  - Looks for masses with a common elution profile at approximately the same time.
  - Masses are grouped into compounds.
  - Co-eluting interferences are resolved.
  - Isotopic cluster are determined and grouped (accurate mass).
  - Charge state assignments and molecular adducts are recognized (multi-charged species and ESI).
  - 2D/3D visualization of data.
  - Chemical characterization and identification.

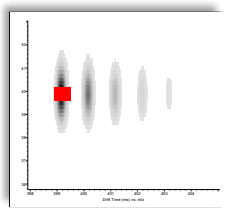
- **NEW FEATURE SUPPORTS UNIT MASS GC/MS CENTROID DATA.**

# Find by Molecular Feature

## Case Study

### MFE (Molecular Feature Extraction)



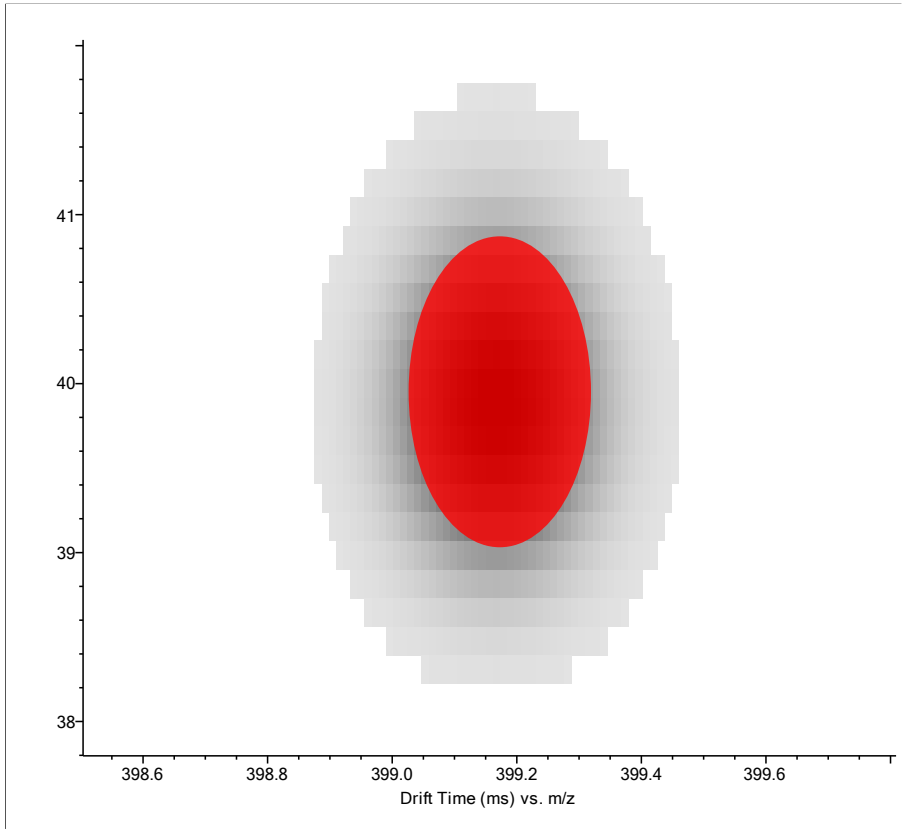



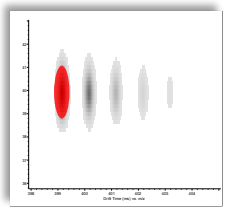
Identify the highest point in the three dimensional array.

# Find by Molecular Feature

## Case Study

### MFE (Molecular Feature Extraction)



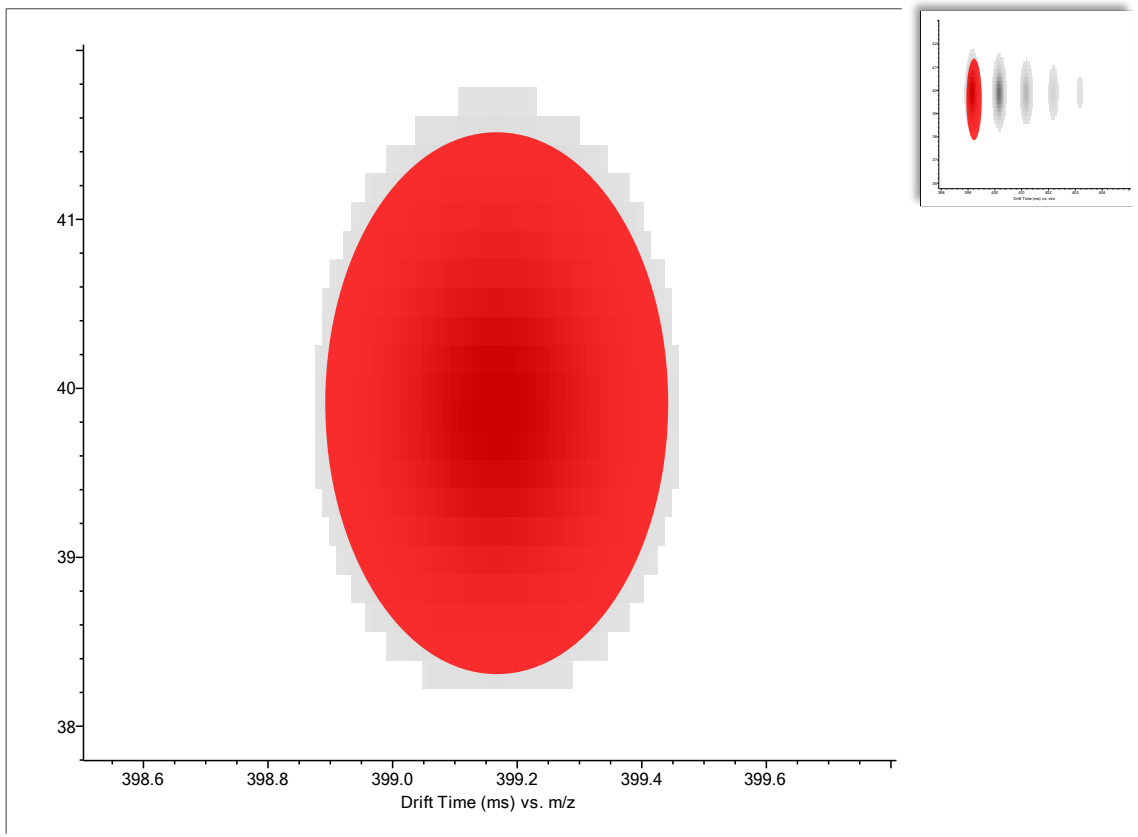
Identify the highest point in the three dimensional array.

Expand the array to include neighboring data points.

# Find by Molecular Feature

## Case Study

### MFE (Molecular Feature Extraction)

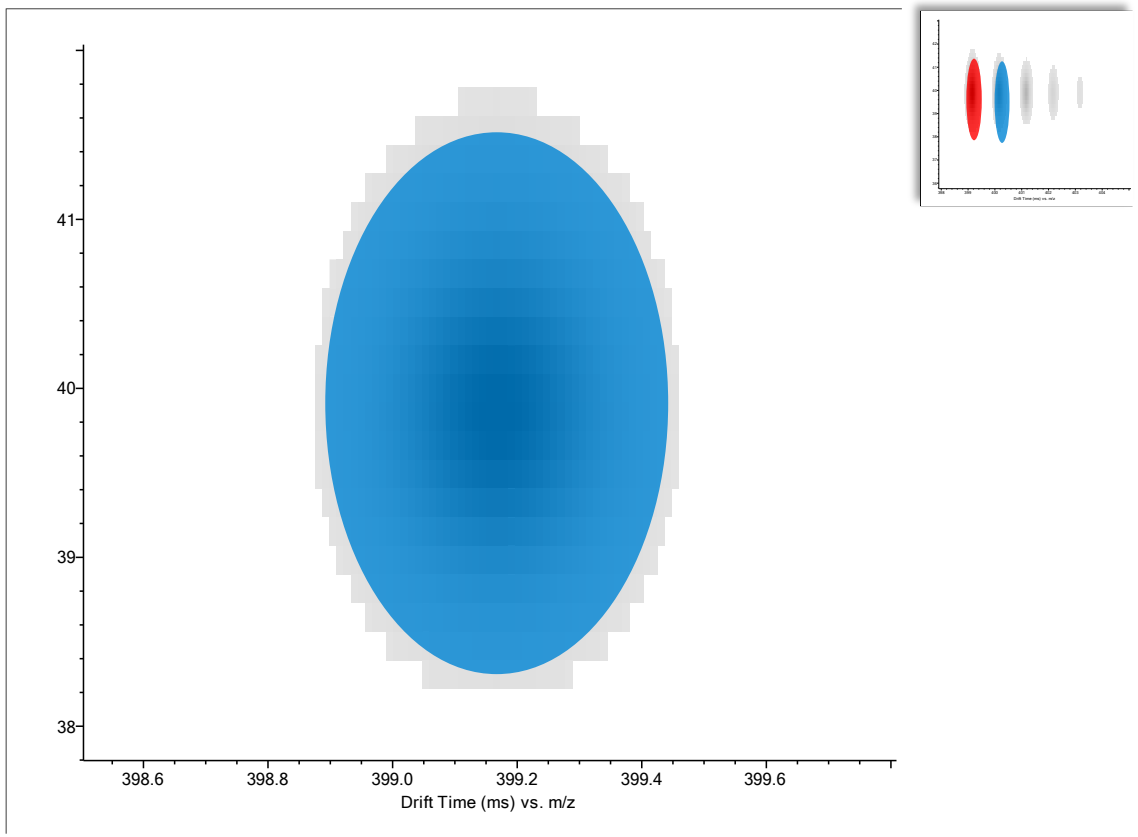



Identify the highest point in the three dimensional array.
Expand the array to include neighboring data points.
Once the bounds of the array have been established, save the 3D peak array.
Resolve co-eluting interferences.
Chemical characterization and subsequent identification.
Reiteratively repeat the process.

# Find by Molecular Feature

## Case Study

### MFE (Molecular Feature Extraction)




Identify the next highest point in the three dimensional array.
After completed, reiteratively process the next highest point in the array.

# Find by Molecular Feature

## Case Study

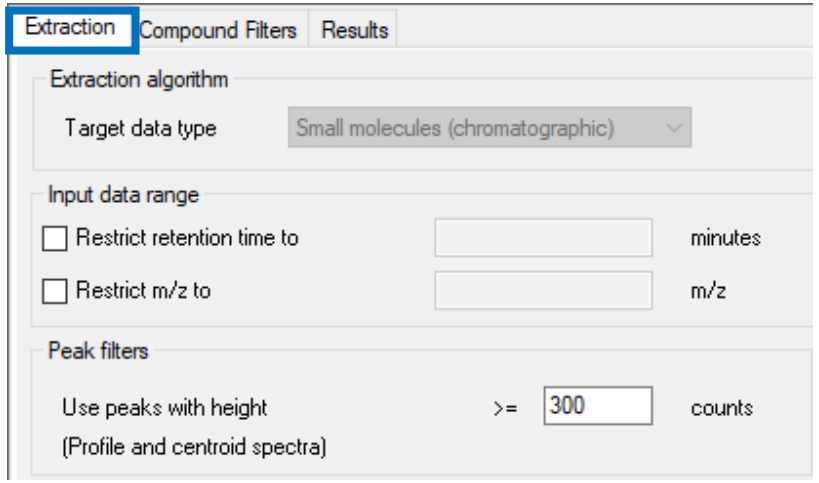
### MFE (Molecular Feature Extraction)

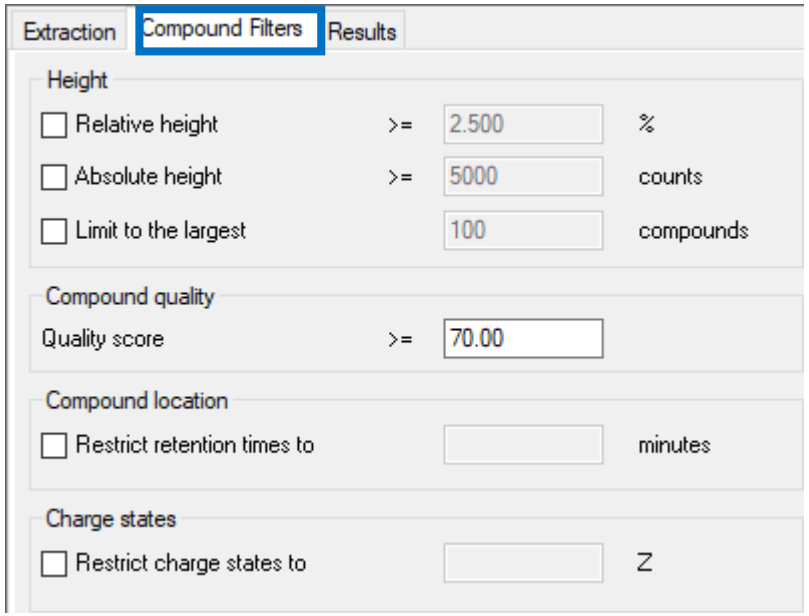
- The algorithm effectively processes the three dimensional array based on retention time, mass and abundance.
- The algorithm does not evaluate the information based on spectra or chromatograms.
- The process is reiteratively applied to the entire data array until no peak remains above background.
- Noise is effectively removed.
- Highly computationally intensive but very effective in identifying compounds.

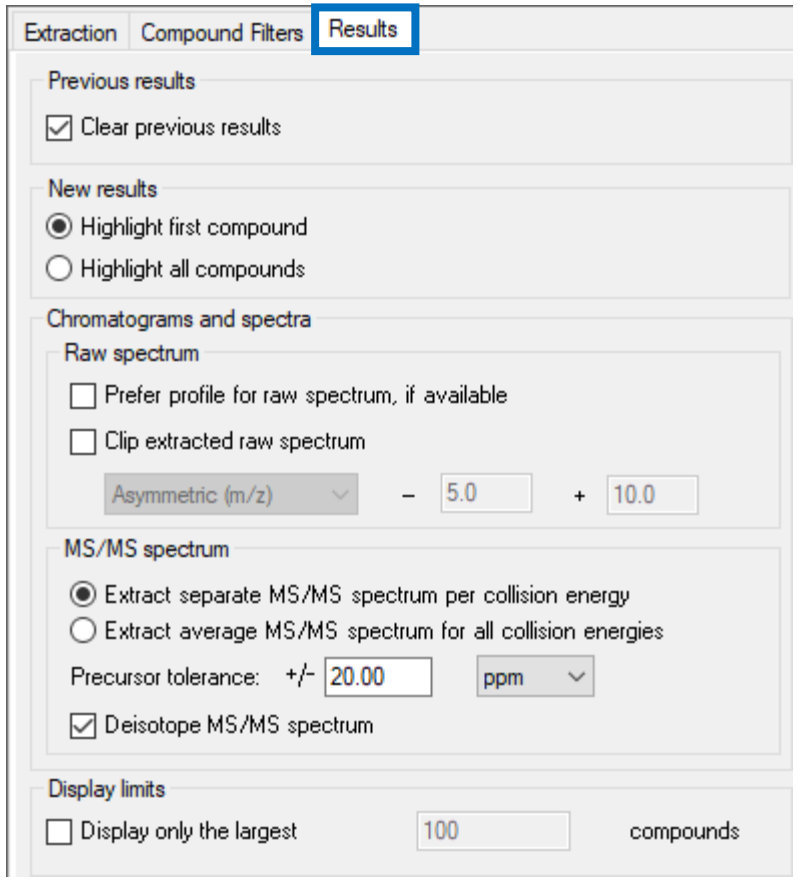
# Find by Molecular Feature

## Parameters (GC/MS)

- **Method Editor > Compound Discovery > Find by Molecular Feature.**
- Composed of 3 tabs.
- Limited to small molecules (chromatographic) for EI GC/MS.
- Quality score is the algorithm's estimation of quality of the feature.
- MS/MS Spectrum for GC QTOF data.



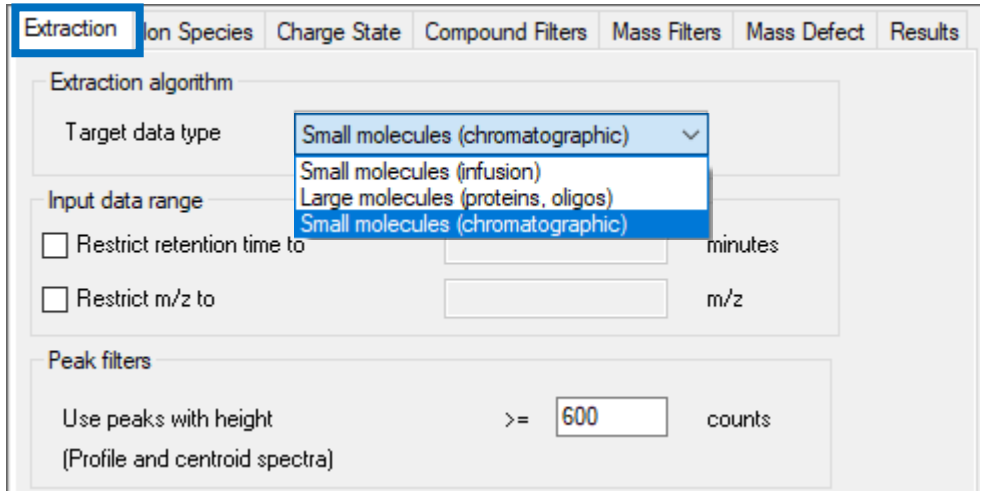



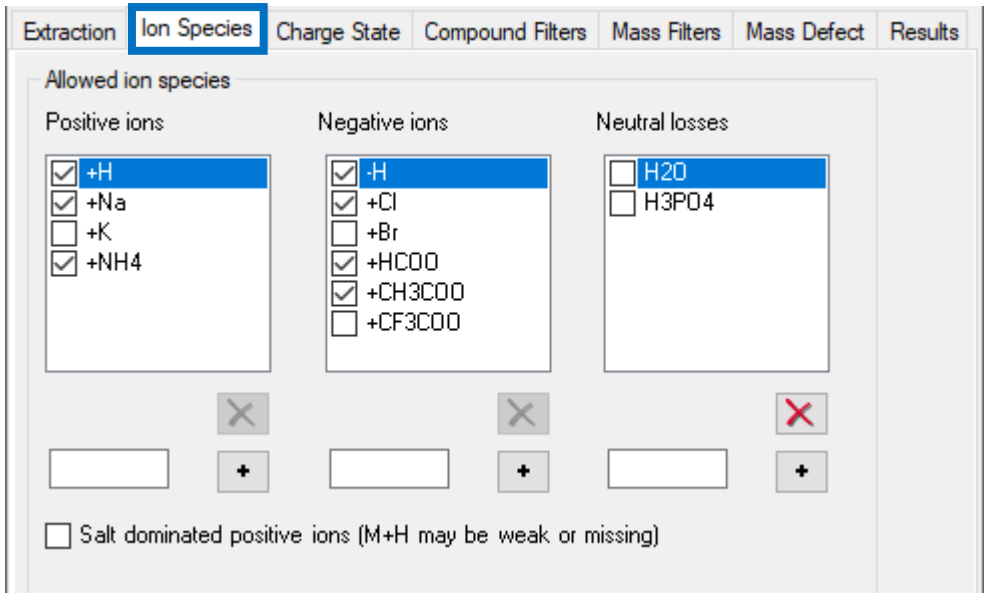
# Find by Molecular Feature

## Parameters (LC/MS) (1)

- Different parameters to accommodate the different data set.
- Composed of multiple tabs.
- Various target data types.
  - Choose applicable to data.



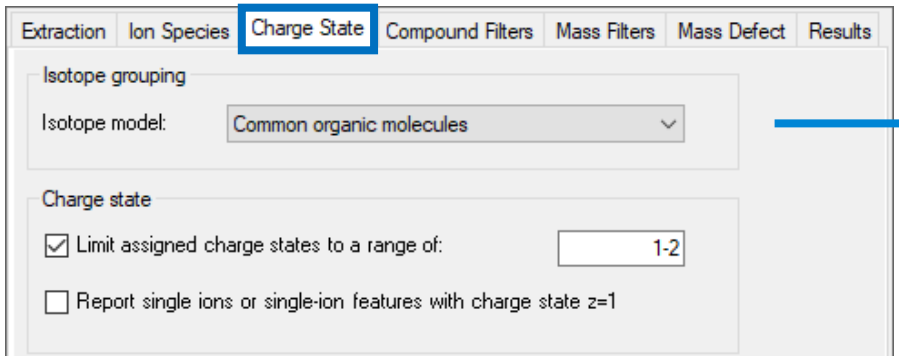

- Ion species
  - Choose expected adducts based on conditions.
  - Can add and delete additional adducts.

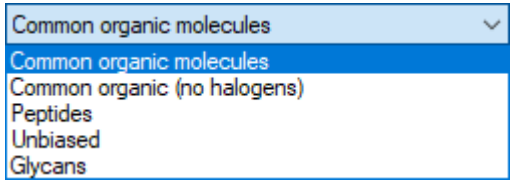


# Find by Molecular Feature

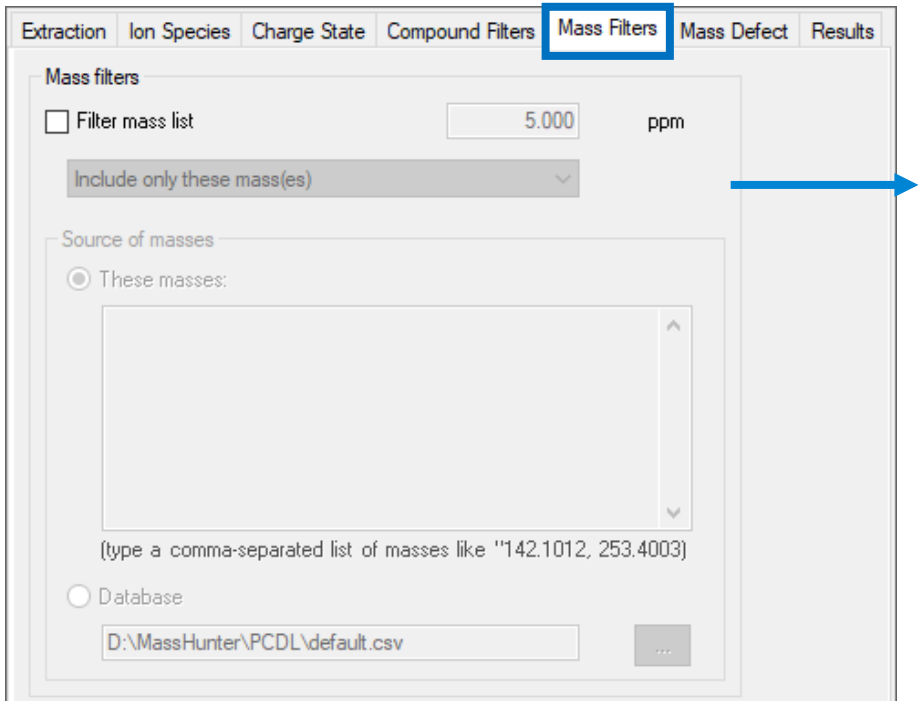
## Parameters (LC/MS) (2)

- Charge State
  - Choice of 5 Isotope models.
  - Choose model appropriate to dataset.
  - Can set a range of charge states.
- Compound Filters same.
- Mass Filters
  - Targeted list.
  - When checked, other items available to refine results.
  - Can also create an exclusion list.



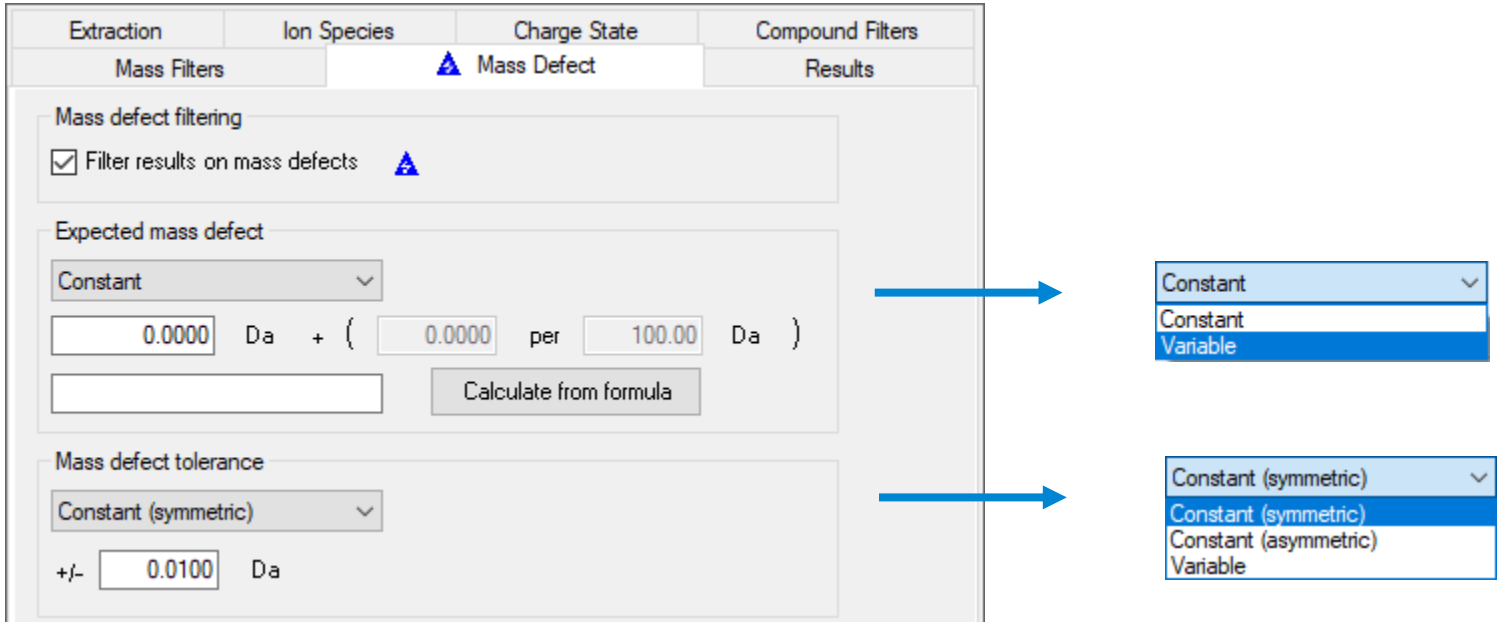

**Tip: If uncertain select unbiased.**




# Find by Molecular Feature

## Parameters (LC/MS) (3)

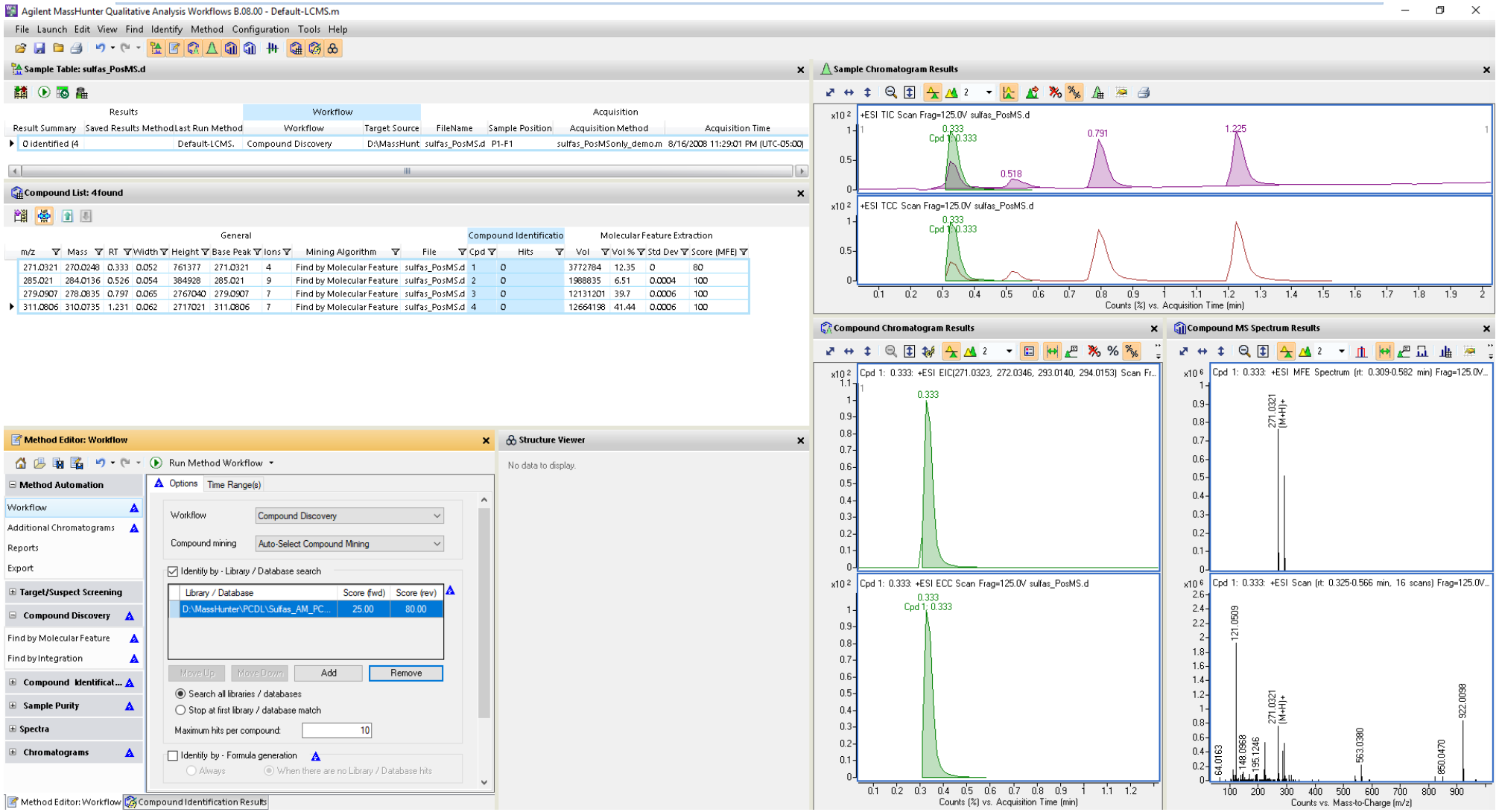
- Mass Defect tab
  - Not applicable to large molecules (proteins, oligos).
  - Useful for halogen containing and hetero atoms.
  - Compounds outside the mass defect tolerance are excluded from the results.




- Results tab is the same as before.

# Find by Molecular Feature

## Results



# Let’s take a moment for questions on Molecular Feature Extraction (MFE)

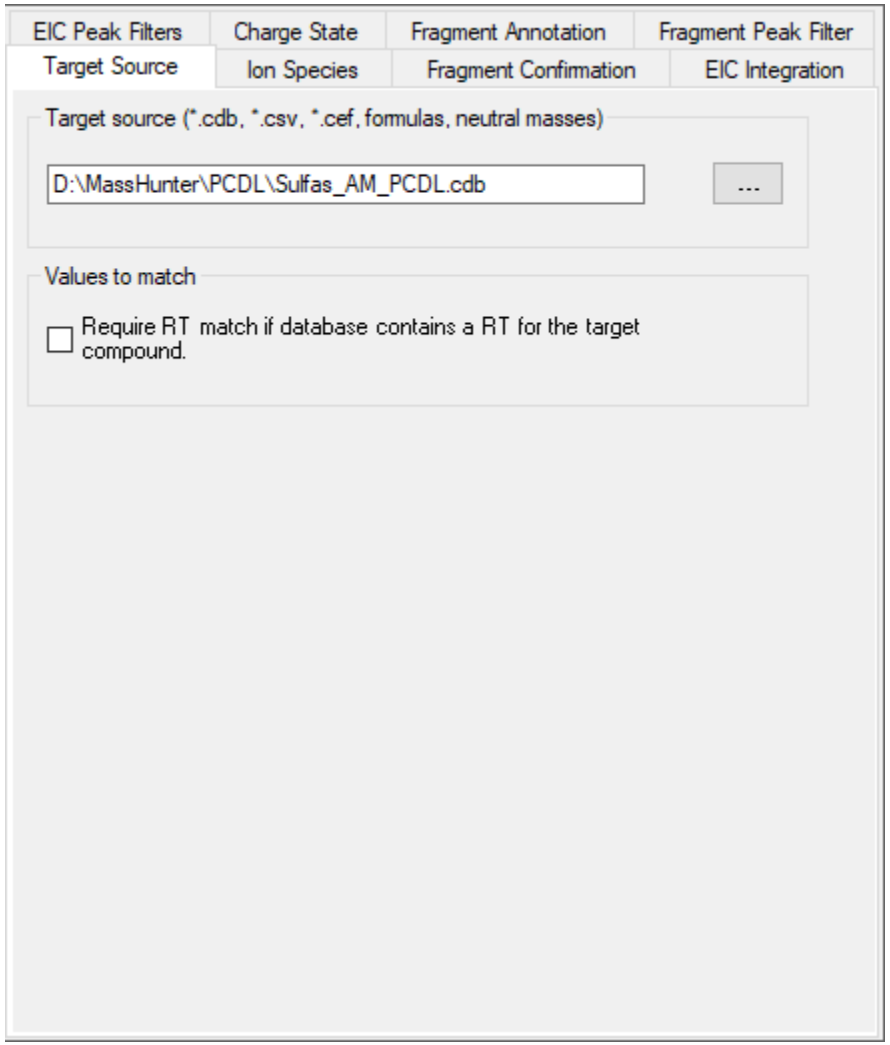
Up Next:

Find by Formula and Compound Identification

# Find by Formula

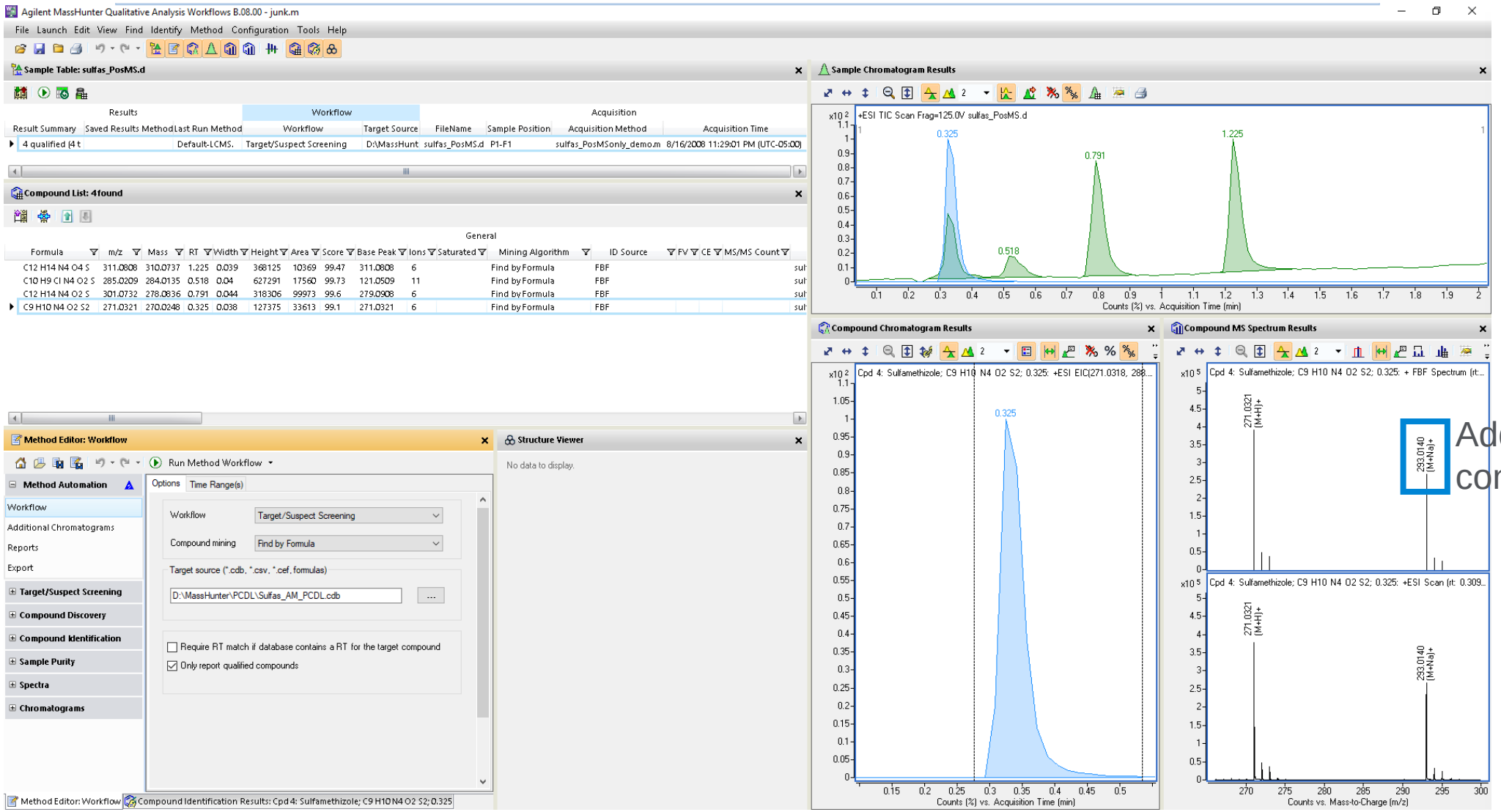
## Parameters (Accurate Mass)

- Find by Formula
  - Targeted analysis.
  - Numerous tabs are available to refine parameters.
  - Requires a target source and optional RT matches.
  - Can confirm fragment ions -> Fragment Confirmation tab.
  - Uses MS scan data but can be used on MS/MS data but ignores MS/MS spectra.



# Find by Formula

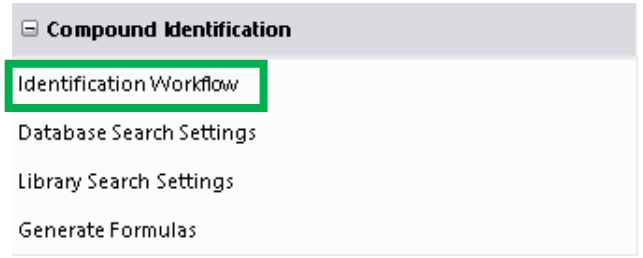
## Results

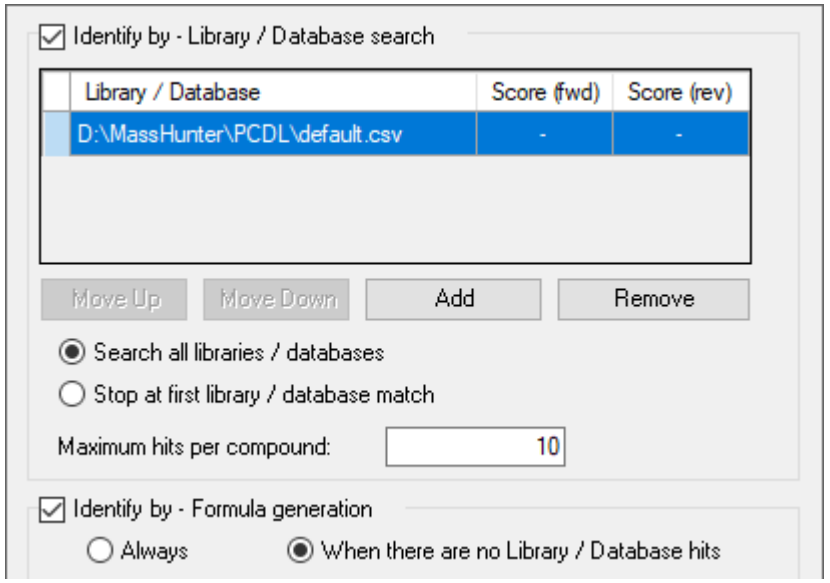



Adduct confirmation

# Compound Identification

## Identification Workflow




## Identification Workflow

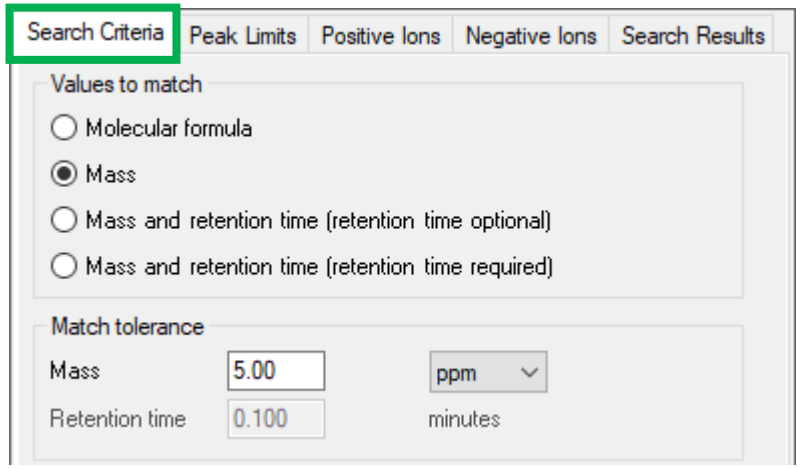
- Identify by Library/Database search
  - Optional search
  - Select numerous libraries.
- Search all libraries / databases
  - Search all libraries or stop when hit is found.

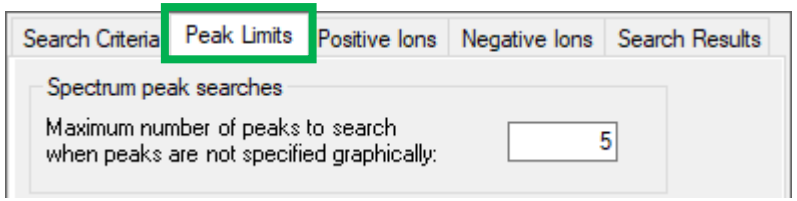
- Identify by Formula Generation
  - Optional generation of formulas

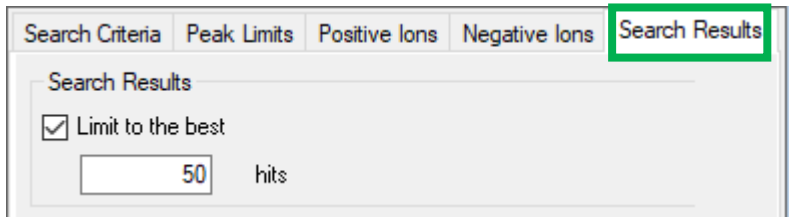
# Compound Identification

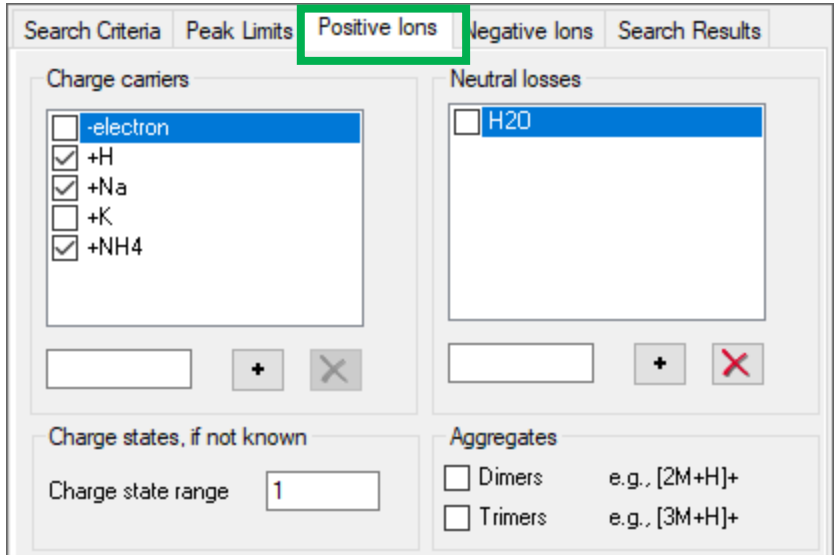
## Database Search Settings

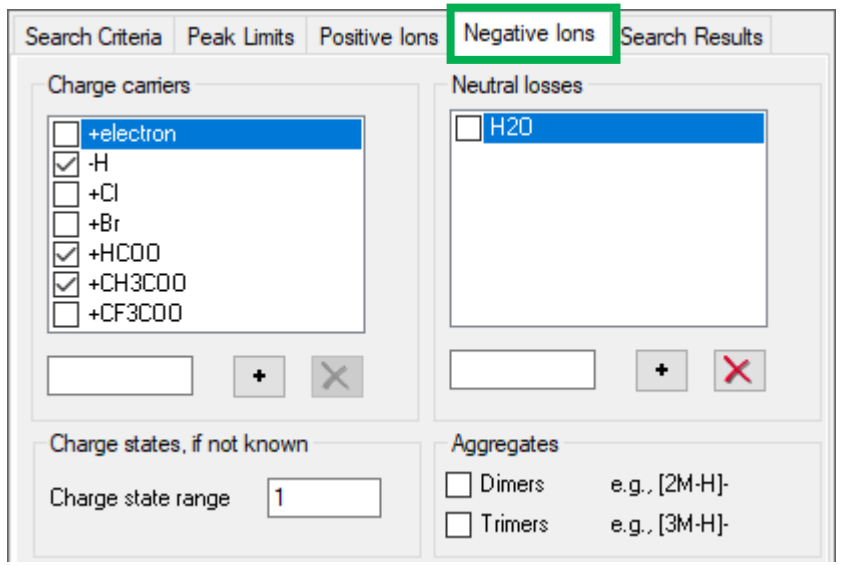

- Numerous tabs
- Define database settings.



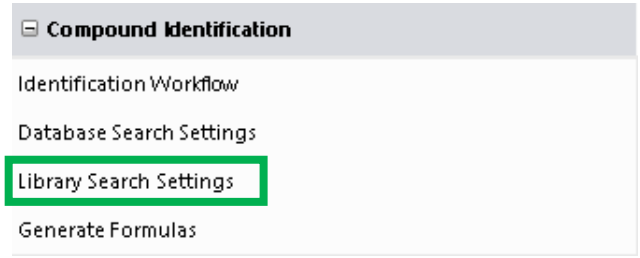



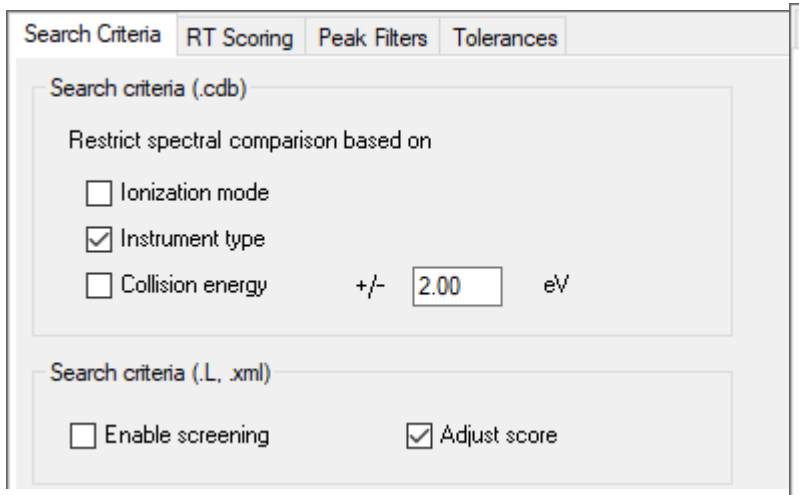
# Compound Identification

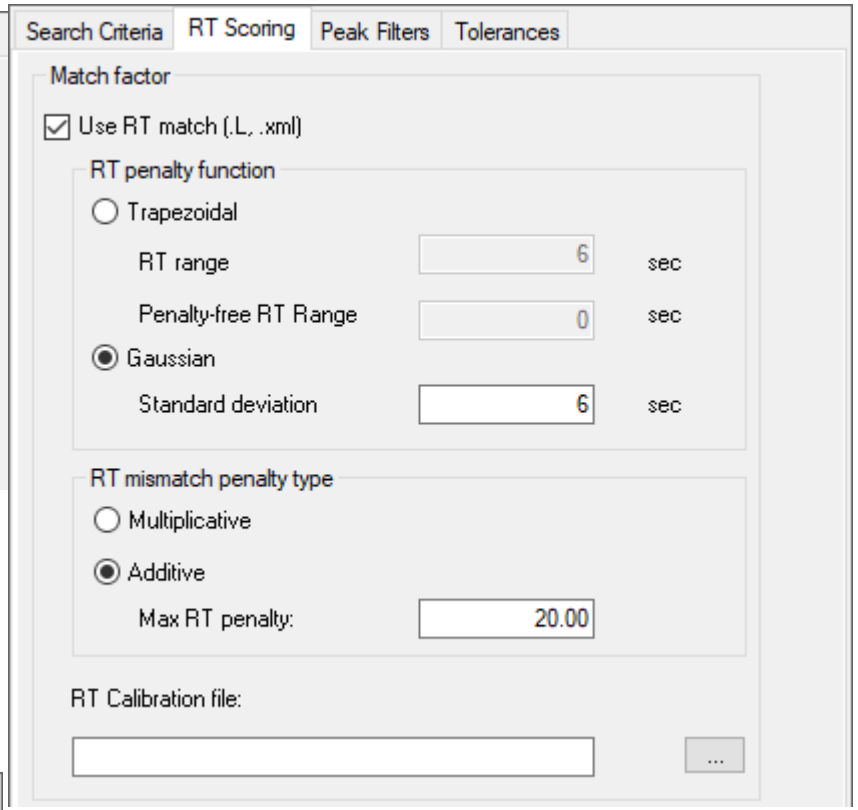
## Library Search Settings

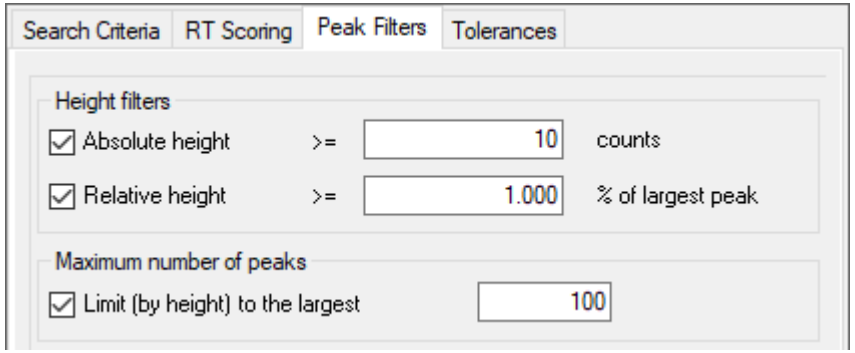



## Library Search Settings

- Search Criteria
  - Adjust Score
- RT Scoring
  - Retention time or retention index.
- Peak Filters
- Tolerances
  - Accurate mass values



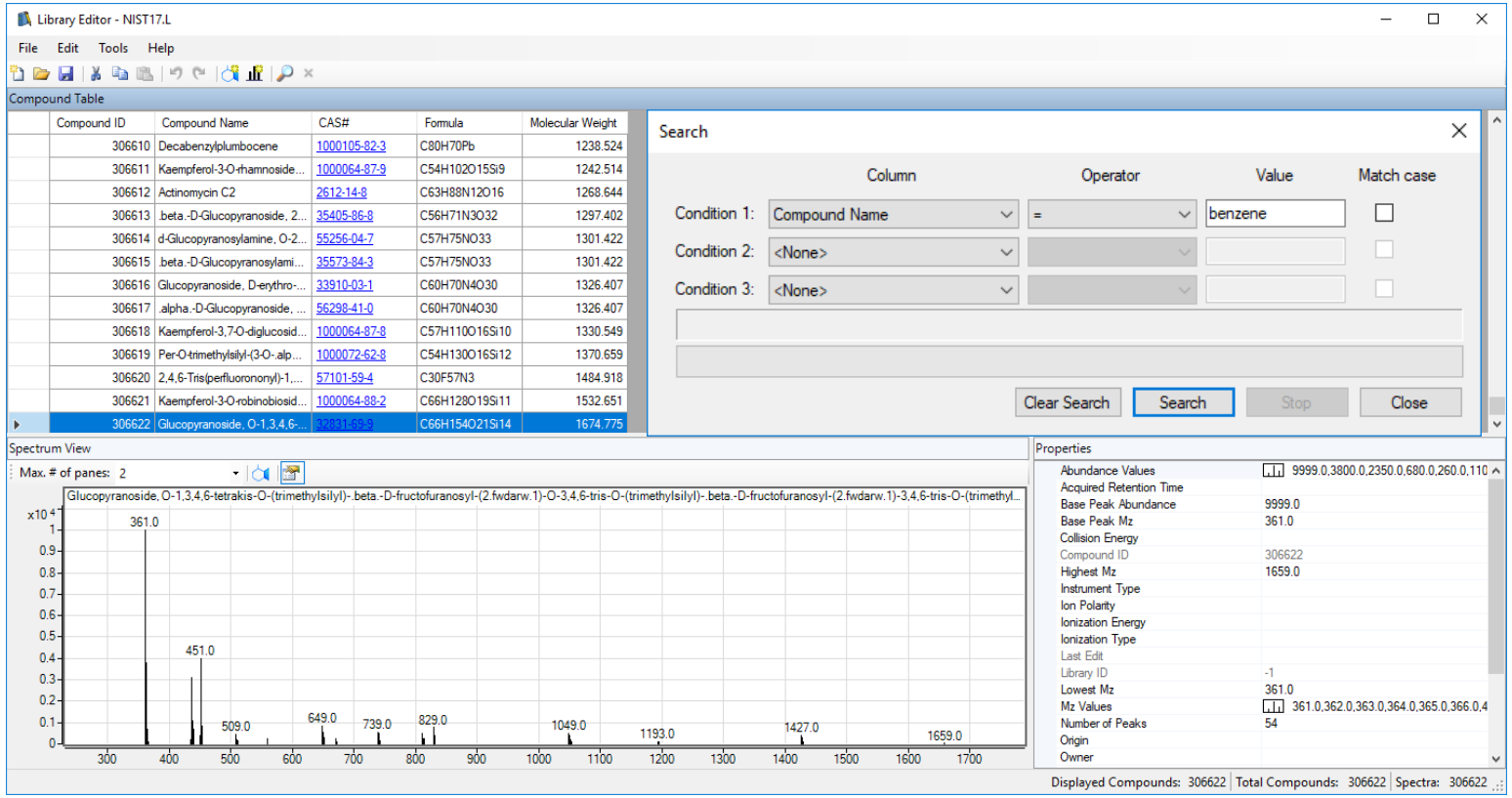



# Database and Library Tools

## Library Editor

- Available from a Desktop icon.
- Installed with Quantitative Analysis.
- Most useful for low resolution data.
  - Most common NIST library.
- Can review and search commercial libraries in .L format.
  - From **Edit > Search**
  - 3 conditional statements
- Can create user generated libraries.
  - Can copy entries from Qualitative Analysis, Quantitative Analysis and Unknowns Analysis.

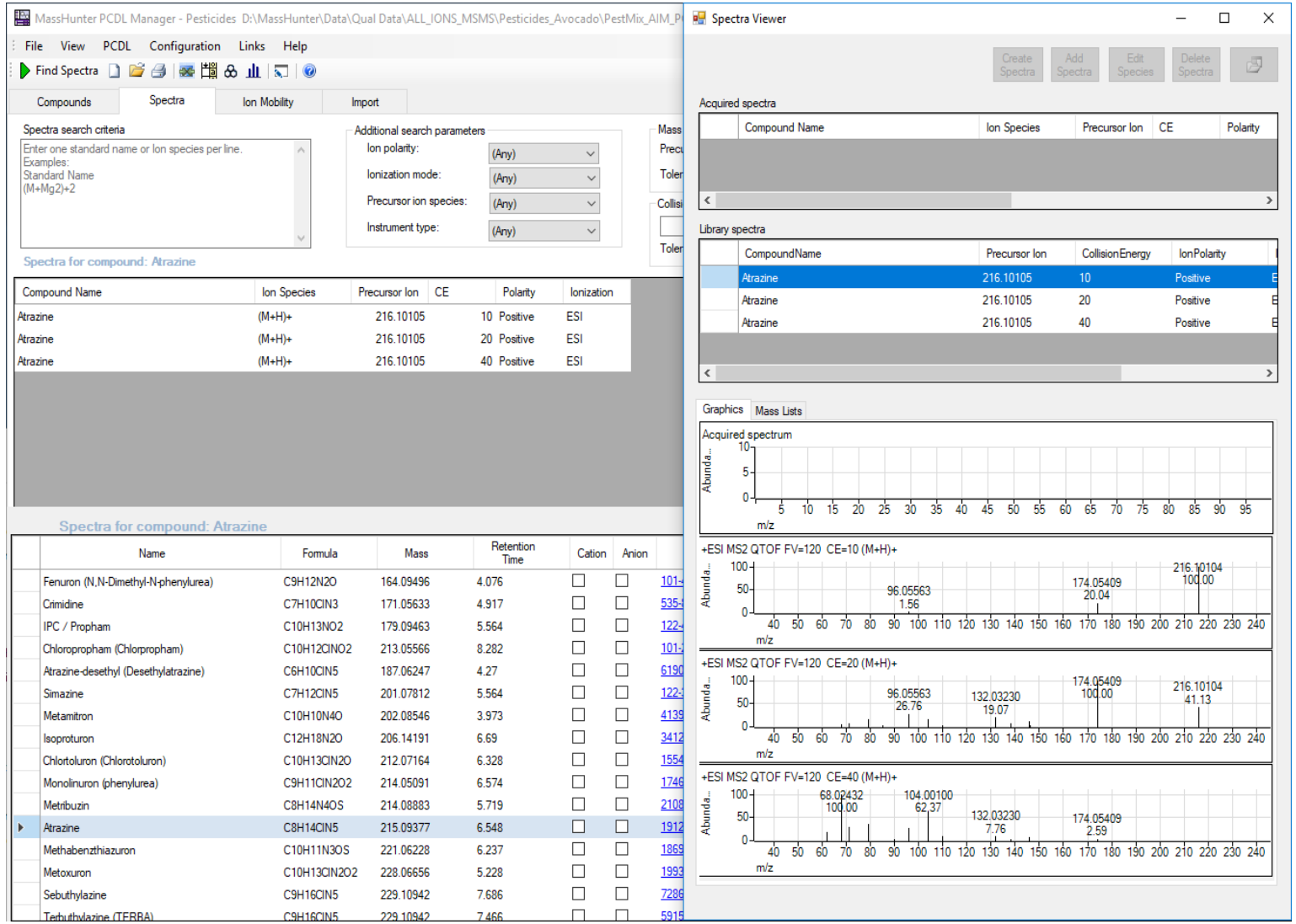


# Database and Library Tools

## PCDL Manager

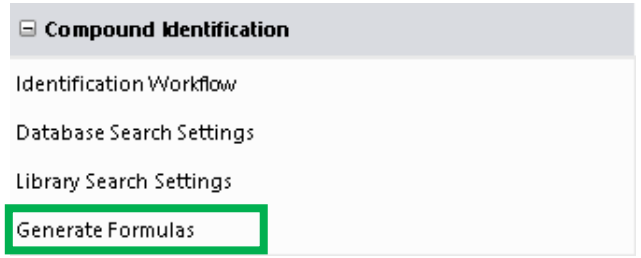
Installed from a stand-alone application

- Useful for high resolution MS/MS data
- Handles both CDB and CDBL
- Can have multiple spectra with various collision energies (CE).
- Works with ion mobility data.



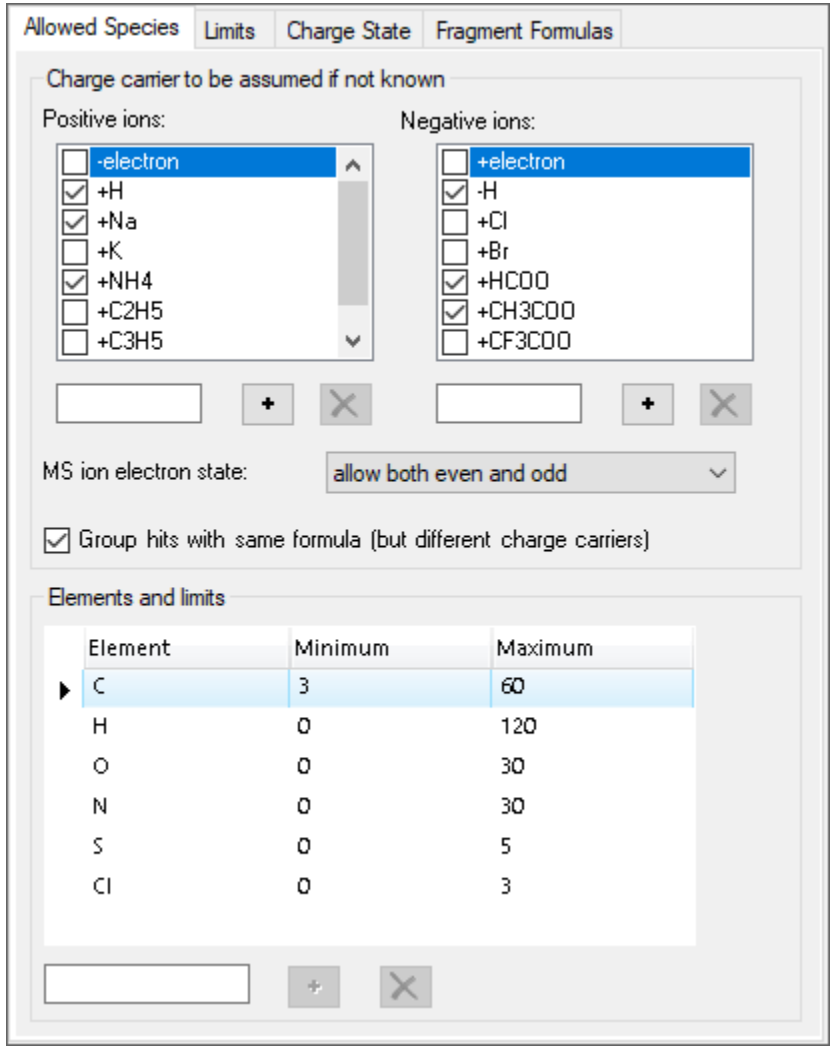
# Compound Identification

## Generate Formulas



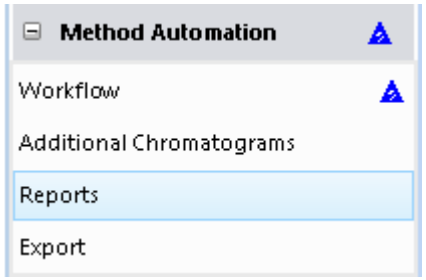

### Generate Formulas

- Allowed Species
  - Elements and limits.
  - Use for narrowing possible hits.
  - Can add elements.



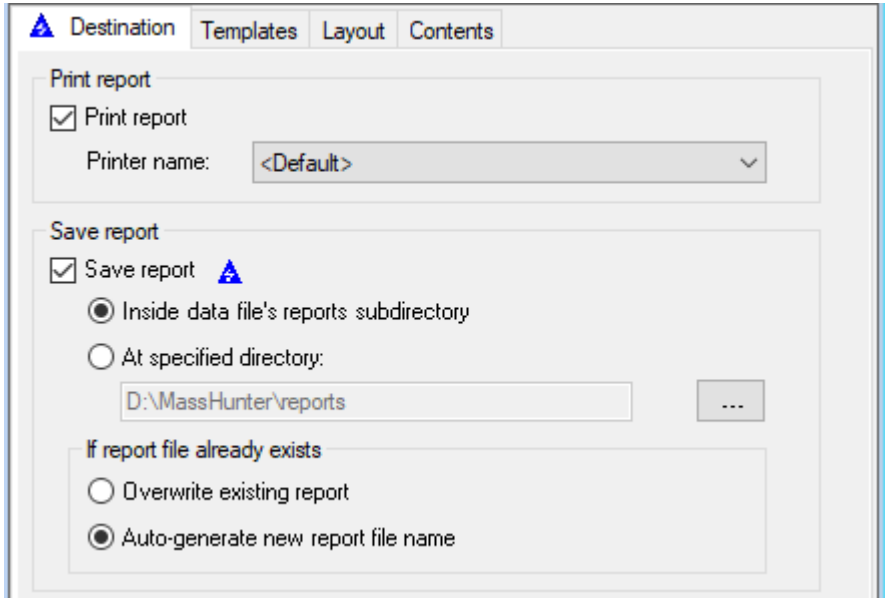
# Reports

## Generating Compound Reports



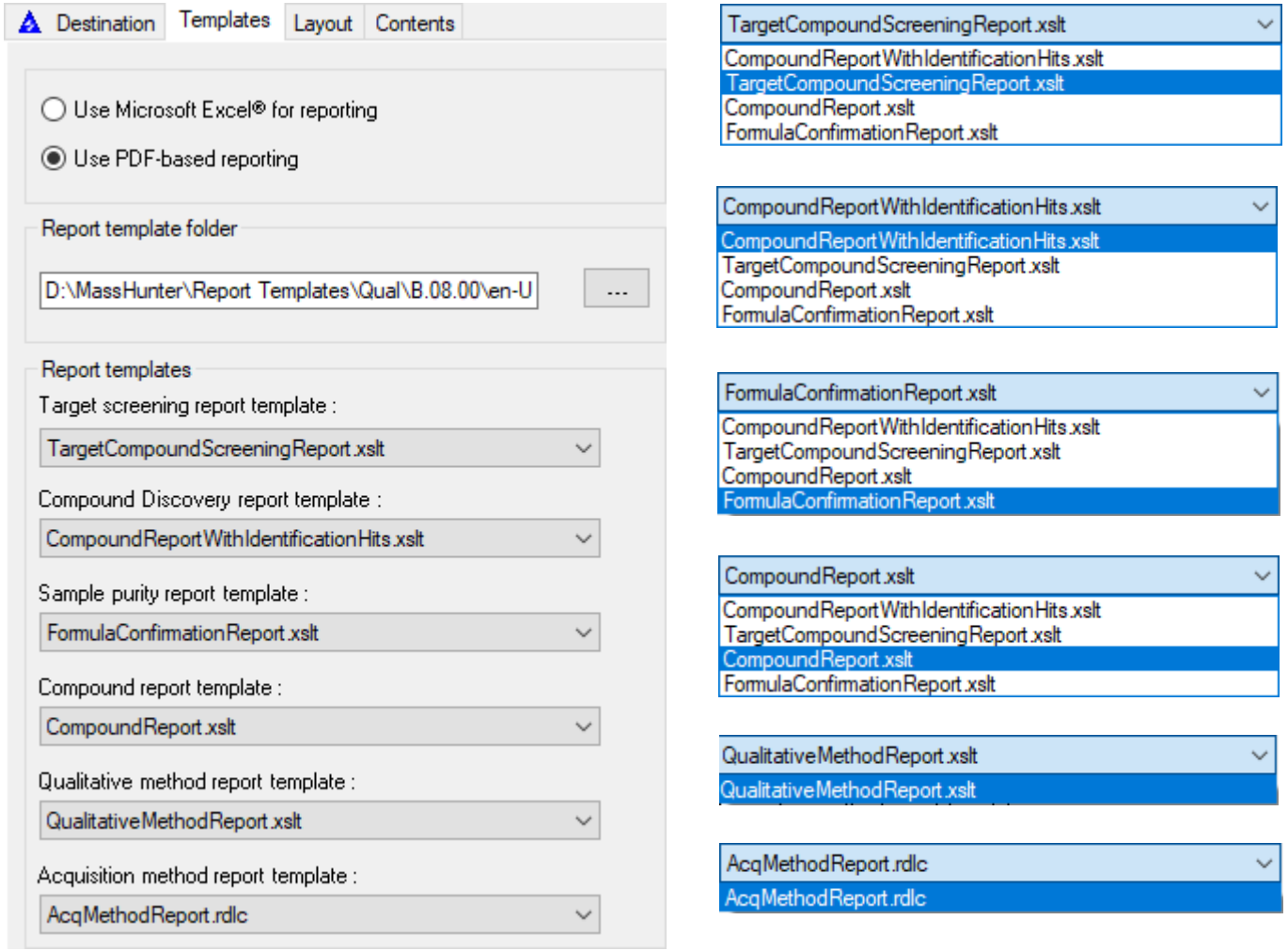

### Method Automation > Reports

- Printed or electronic format available.
- Report can be saved to data file or directory.
- Auto generate file name.



# Reports

## Generating Compound Reports







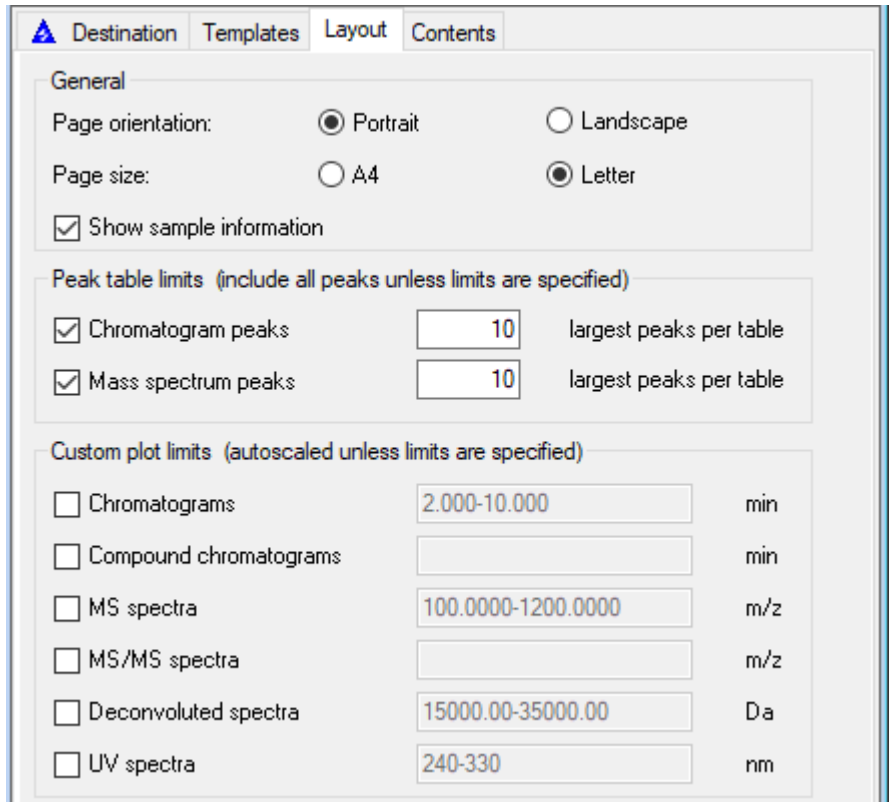
### Templates

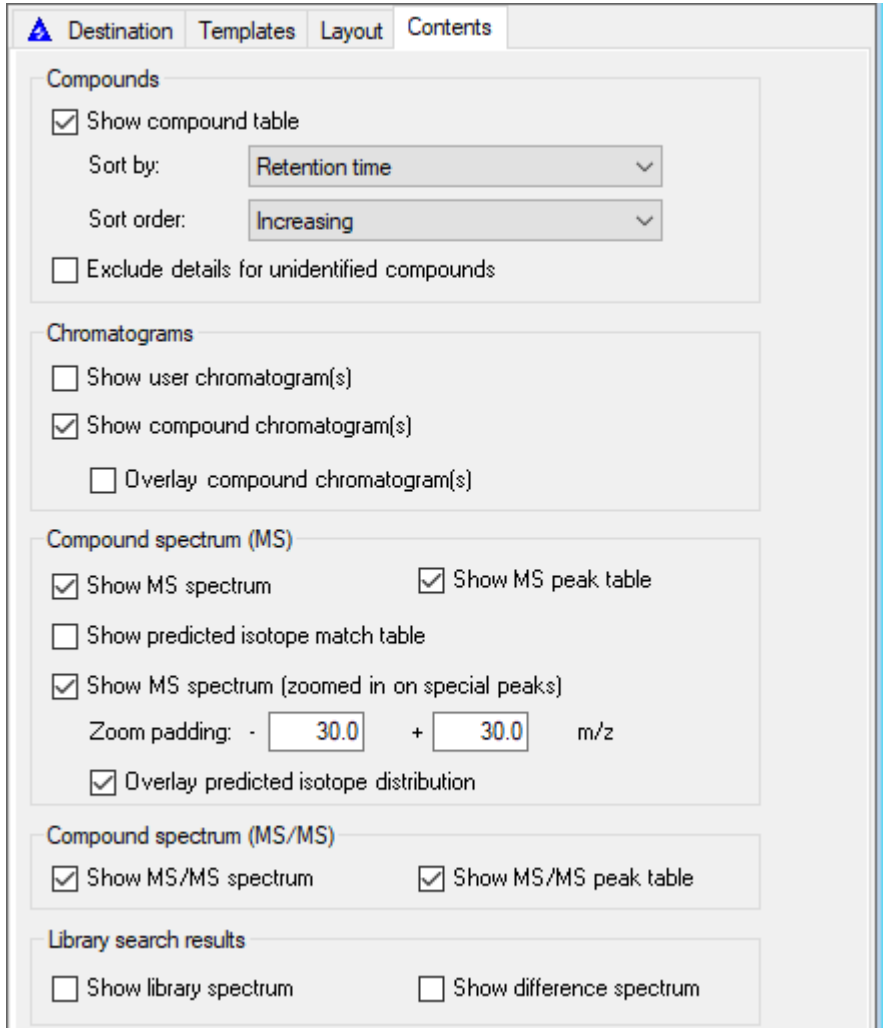
- Excel Reporting or PDF based reporting.
- Various templates are available.
- Organized based on workflows.

- **Tip: Use PDF-based reporting.**

# Reports

## Generating Compound Reports




### Layout & Contents

- Allow further customization of the report.

# Let’s take a moment for questions on Compound Identification and Reporting

Up Next:

Training Resources

# Training Resources

## LCMS Data Analysis Resources DVD

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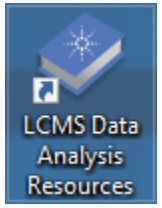


### LC/MS Data Analysis Resource App

B.08.00

**Resources**

Below is a list of resource information for LC/MS Data Analysis.

**Qualitative Analysis Guides**

- Familiarization Guide for LC/MS
- PCDL Manager Quick Start Guide

**Quantitative Analysis Guides**

- Familiarization Guide

**BioConfirm Guides**

- BioConfirm Quick Start Guide
- BioConfirm Familiarization Guide

**Training**

- Qualitative Analysis Training Videos

**Familiarization**

- Qual eFamiliarization for TQ
- Qual eFamiliarization for TOF/Q-TOF
- Quant eFamiliarization



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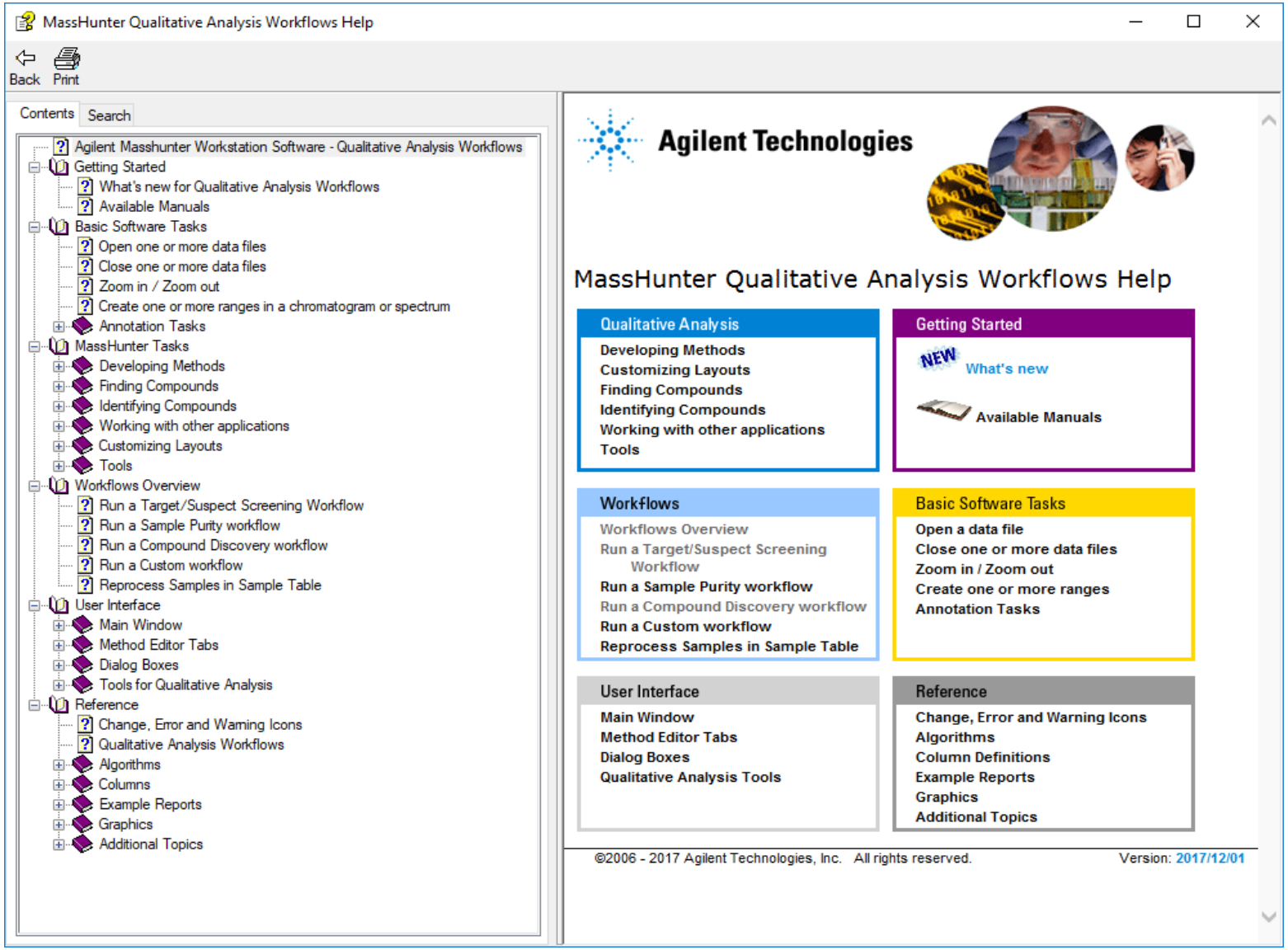
# Training Resources

## Help

- Online Help
- Contents
- Searchable



# Training Resources
## Available Training Resources

Agilent CrossLab
From Insight to Outcome

### Convenient Training

In our classrooms, at your site or online.

From a team of industry experts that deliver a high quality learning experience.

### Classroom Training

Introductory level to in-depth, hands-on for laboratory instrumentation and software.

### Customized On-Site Training

Effective learning environment designed to achieve operational excellence and employ development without the need to travel.

### Online

Offerings from foundation level to expert delivered at your own pace.

# Agilent University

## Access From Home Page

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From Insight to Outcome

### Upgraded customer experience

- Search and find courses that meet your interests and needs in the format they require.

### Introduce new eLearning capabilities

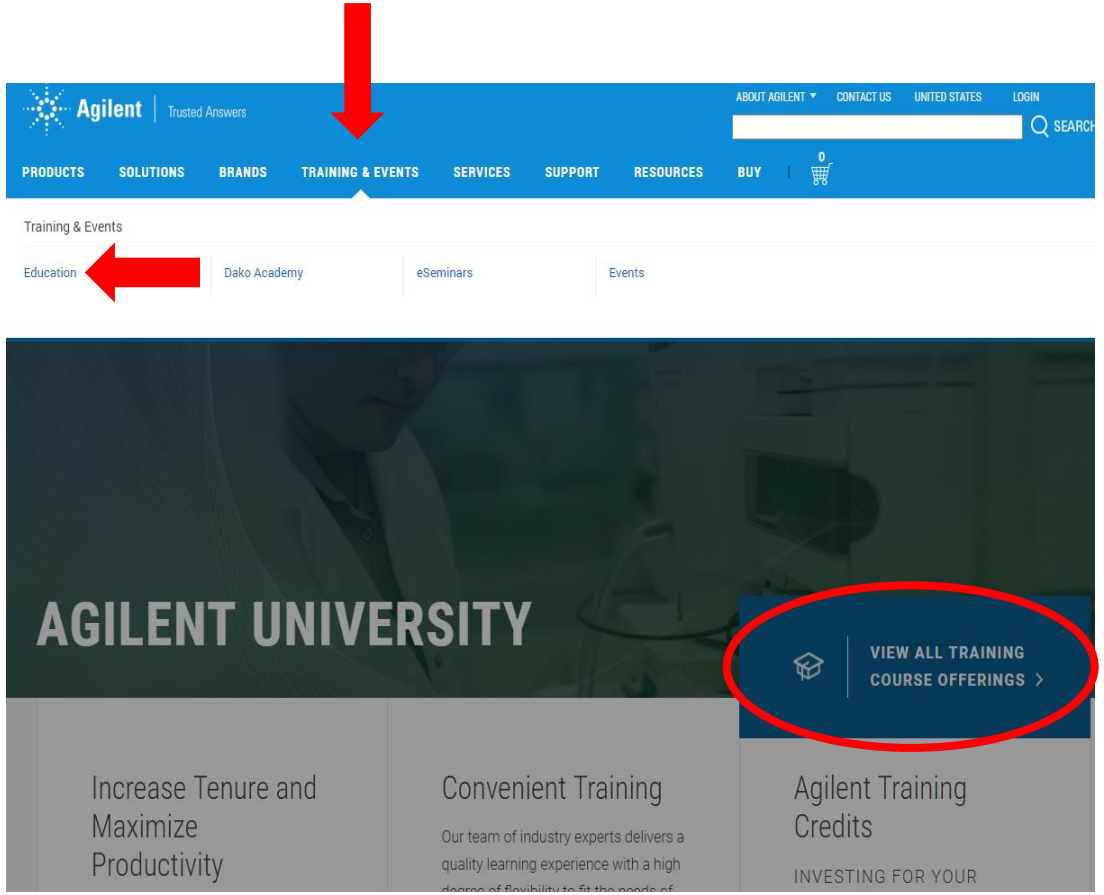
- Recorded and video-based learning
- Virtual online classes

### Expanded portfolio

- Foundational subjects
- Intermediate subjects
- Advanced subjects
- Workflow and applications

### Helping customers

- Educate your employees on Agilent instruments and software.
- From new hires to the most seasoned scientists.



# Agilent Community

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Agilent Community

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Get answers. Share insights. Build connections.

***Collaborate*** *- Ask and answer questions.*

***Connect*** *- Interact with other Agilent users.*

***Discover*** *- Find relevant discussions, documents, and videos.*

***Share*** *- Contribute your insights.*