



# Agilent MassHunter Productivity App

## Quick Start Guide

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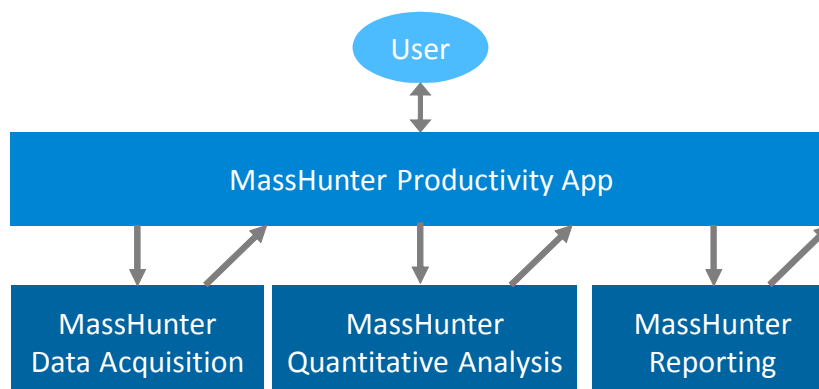
## What is the MassHunter Productivity App?

### MassHunter Productivity App

What is the MassHunter Productivity App?

## MassHunter Productivity App

The MassHunter Productivity App streamlines targeted screening workflows in high-throughput lab environments. The Productivity App sits in a layer above the MassHunter suite of products (**Figure 1**), which gives laboratory technicians a simple interface to submit a sequence of samples, review the results, and create a report.



**Figure 1.** Productivity App structure

Designed specifically for the challenges of a high-throughput lab, the Productivity App offers several features to automate routine or tedious tasks, such as sequence creation, batch analysis, and file management when installed on a MassHunter Data Acquisition system. The Productivity App can also be used on a standalone (offline) computer for data review and reporting only.

## Workflow Overview

The Productivity App is based on a typical technician workflow in a targeted screening laboratory (**Figure 2**). This workflow differs from the MassHunter core in that the sequence and associated analysis parameters must be defined before the run is initiated. Doing so allows the Productivity App to automatically analyze the results immediately following successful acquisition.

After analysis is completed, the results are automatically loaded into the Productivity App for review and reporting. While a sequence is running, the next run can be prepared and any previous results can be reviewed. If acquisition and data review occur on separate computers, the data can be moved to the data review system without a loss of information.



**Figure 2.** Productivity App general workflow

## Where to Find More Information?

You can get more information about the Productivity App in these ways:

**Tooltip** Roll your mouse over any option to get more information on that option.

**Agilent Community** Press **F1** or **?** to visit the **Agilent Community** where you can find answers to your questions or ask a new question. The Agilent Community page for the Productivity App is found at <https://community.agilent.com/masshunter-productivity-app>

**Manager Guide** The *Manager Guide* provides in-depth information about the configuration options available in the Productivity App.

**Reference Guide** The market-specific *Reference Guide* provides information on method settings and the conditions in which the retention times for your database was collected.

**Agilent Web Site** To view support information for the Productivity App and other Agilent products, see <http://www.agilent.com>.

## Understanding the User Interface

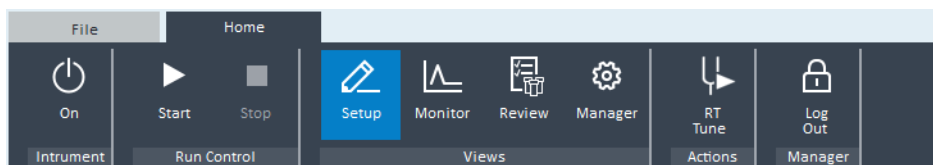
### Where to Find More Information?





# Understanding the User Interface



To start the Productivity App, click the Productivity App icon on your Desktop.

The Productivity App consists of four views. You change from one view to another in the ribbon.



View	Description
 Setup	Create a sequence, select compounds, and set up the analysis parameters
 Review	Filter, search, and tag the analyzed results; generate reports.
 Monitor	View the run progress, the live chromatogram, and the live spectrum.
 Manager	Configure the available methods and control automation options.

## Setup View

The Setup View includes the **Build Sequence** and **Select Compounds** pages. Use these pages to fully define a sequence and a set of analysis parameters before you start the run (from the **Start** button). The numbered topics refer to the numbered sections in **Figure 3** and **Figure 4**.

The screenshot displays the 'Build Sequence' page in the MassHunter Productivity App. The interface is divided into two main sections: 'Build Sequence' (active) and 'Select Compounds'. The 'Build Sequence' section contains a 'Sequence' table with the following data:

Name	Position	Type	Level	Volume	Inj/Sample	Comments	Compound Groups
Blank	p1a1	Blank		As Method	1		+
Double Blank	p1a2	Double Blank		As Method	1		+
Calibration 1	p1a3	Calibration	1	As Method	1		+
Calibration 2	p1a4	Calibration	2	As Method	1		+
Calibration 3	p1a5	Calibration	3	As Method	1		+
Double Blank	p1a2	Double Blank		As Method	1		+
Sample 1	p1b1	Sample		5	1		+ Submix 1
Sample 2	p1b2	Sample		5	1		+
Sample 3	p1b3	Sample		5	1		+ Submix 2
Sample 4	p1b4	Sample		5	1		+
Sample 5	p1b5	Sample		5	1		+
Sample 6	p1b6	Sample		5	1		+
Sample 7	p1b7	Sample		5	1		+ Submix 4
Sample 8	p1b8	Sample		5	1		+
Sample 9	p1b9	Sample		5	1		+

Below the table, there is a checkbox labeled 'Shutdown instrument after run completes'. At the bottom of the window, a status bar shows the instrument configuration: QQQ, HiP Sampler, Binary Pump, and Column Comp. The status is 'Not Ready'.

Figure 3. Build Sequence page

## Understanding the User Interface Setup View

The screenshot shows the MassHunter Productivity App interface. At the top, there's a navigation bar with icons for On, Start, Stop, Setup, Monitor, Review, Manager, RT Tune, and Log Out. Below this is a 'Build Sequence' section with a search bar and a list of submixes (Submix 7, 3, 4, 6, 8, 2, 5, 1). The main area is split into 'Available Compounds (265)' and 'Analysis Setup (265)'. The 'Available Compounds' table has columns for Name, CAS, Formula, and Comments. The 'Analysis Setup' table has columns for Name, Comments, Type, Level, and Concentration (ng/ml). Below this is the 'Selected ISTDs' table with columns for Name and Concentration (ng/ml). At the bottom, there's a status bar with instrument components: QQQ, HiP Sampler, Binary Pump, and Column Comp. The status is 'Not Ready' and the current user is 'admin'.

Figure 4. Select Compounds page


### 1 Create a sequence

You can create a sequence in 4 different ways:

- Manually add and remove samples. Use these buttons:

 or + Add sample... Add samples.

 Insert sample.

 Remove sample. You can also use the **Delete** key to remove one or more samples.

- Import a sequence from CSV:

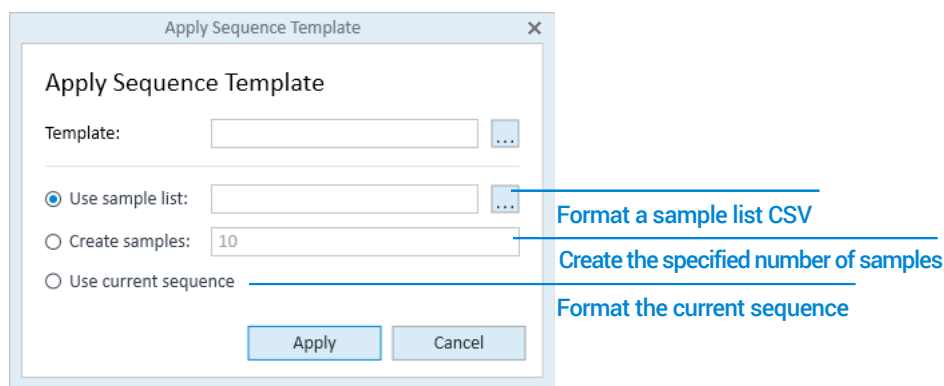
For the required CSV structure, see the example sample list CSV installed at:  
**D:\MassHunter\Documentation\Productivity App.**

## Understanding the User Interface

### Setup View

- Apply a sequence template: 

Sequence templates allow you to apply a preset sequence format to your sequence. The sequence template defines the samples to run at the start and end of a sequence (such as blanks and calibration samples), as well as the non-target samples to run for every X number of target samples (such as blanks and QC samples). You have three ways to use a sequence template to create a sequence.



- Load a saved sequence: 

#### ② Edit the Sequence

Use the sequence table to edit sample information. The sequence editor supports copy (**Ctrl+C**), paste (**Ctrl+V**), and drag-and-drop functions to help you easily work in the editor.

<b>Name</b>	The sample name. Used to create the data file name.
<b>Position</b>	The sample position in the tray. Only positions for the configured tray type are allowed.
<b>Type</b>	The type of sample. Affects how the sample is used during analysis.
<b>Level</b>	The level to which this sample belongs (analogous to a calibration level). Provides a mapping to the compound analysis parameters. Applies only to Calibration, QC, CC, Matrix Blank, and Matrix Spike samples.
<b>Volume</b>	The injection volume. An empty value defaults to the method injection volume.
<b>Inj/Sample</b>	The number of repeat injections for this sample. Use this option to add duplicate rows in the sequence table.
<b>Comments</b>	The sample comments. Included in the analyzed results.
<b>Compound Groups</b>	The compound groups relevant to the sample. When compound groups are added to a sample, the compounds in the group are automatically selected for acquisition. When the results are analyzed, the results in the review page are automatically filtered to show only the compounds from the added compound groups.



## Understanding the User Interface

### Setup View

#### 3 Run a shutdown method

Check this option to automatically run a shutdown method immediately following a successful run. If the manager has set up a shutdown sequence, a sequence table will appear (see below). If not, the shutdown method will run without an injection. With the sequence table, the user can change the sample information, add/remove samples (if allowed by the manager), and restore the sequence to default: ↶.

Shutdown instrument after run completes						
↶	📄	🖨	Runtime: 00:16:00			
Name	Position	Type	Level	Volume	Inj/Sample	Comments
1	Blank 0	p1a1	● Blank		As Method	1

#### 4 Edit selected compounds

Use this table to change the compounds that will be acquired and analyzed, if allowed. This table is irrelevant if the administrator requires all compounds to be acquired. You can edit the selected compounds in the following ways:







- Mark or clear the check box next to the compound:  Metrafenon
- Select or clear all visible compounds. You can filter the visible compounds using either the search bar or the compound group filter buttons directly below the search bar.

Search...				
Group 1		Group 2		
<input checked="" type="checkbox"/>	Name	CAS	Formula	Comments
<input checked="" type="checkbox"/>	1-Naphthalene acet	86-86-2	C12H11NO	
<input checked="" type="checkbox"/>	2,4,5-TP (Silvex)	93-72-1	C9H7Cl3O3	
<input checked="" type="checkbox"/>	Acetochlor	34256-82-1	C14H20ClNO2	

- Open  or merge  a saved compound list with parameters.

#### 5 Specify analysis parameters

Use this table to set up the analysis parameters required by the sequence. The Productivity App will automatically add Calibration and QC groups based on the Calibration and QC groups defined in the sequence. Matrix Spike parameters must be added manually. No CC parameters are available because a CC sample uses the associated Calibration group concentrations.

	<b>Add parameter...</b> Add parameter.
	Remove parameter. You can also use the <b>Delete</b> key to remove one or more parameters.
	Open a saved compound list with parameters.
	Merge a saved compound list with parameters. You have the option to override the current concentrations with those defined in the saved file.
	Remove parameter groups that do not match any groups in the sequence.
	Copy parameters to all visible compounds. You can filter the visible compounds using either the search bar or the compound group filter buttons directly below the search bar.

#### 6 Select ISTD compounds

ISTD compounds and their mapping are defined by the added MassHunter Quantitative Analysis method. If the active method has ISTD compounds, they cannot be individually selected in the list of available compounds. Instead, they are automatically selected if any of the compounds mapped to the ISTD are selected. Once selected, the ISTD concentrations will be enabled for changes.

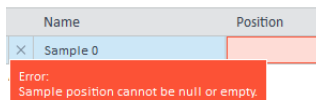
## Understanding the User Interface

### Setup View

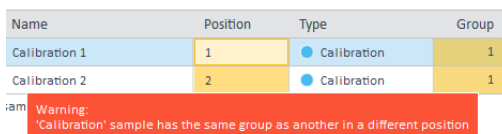
#### Setup Validation

The setup pages have extensive real-time validation behavior designed to help avoid common data entry errors. A red highlight indicates an error while a yellow highlight indicates a warning. If any errors exist in the Setup view, the Start button will be disabled and the button tooltip will explain the errors that prevent the run from starting.

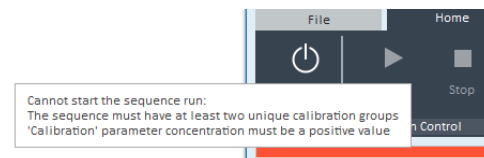
##### Error



##### Warning

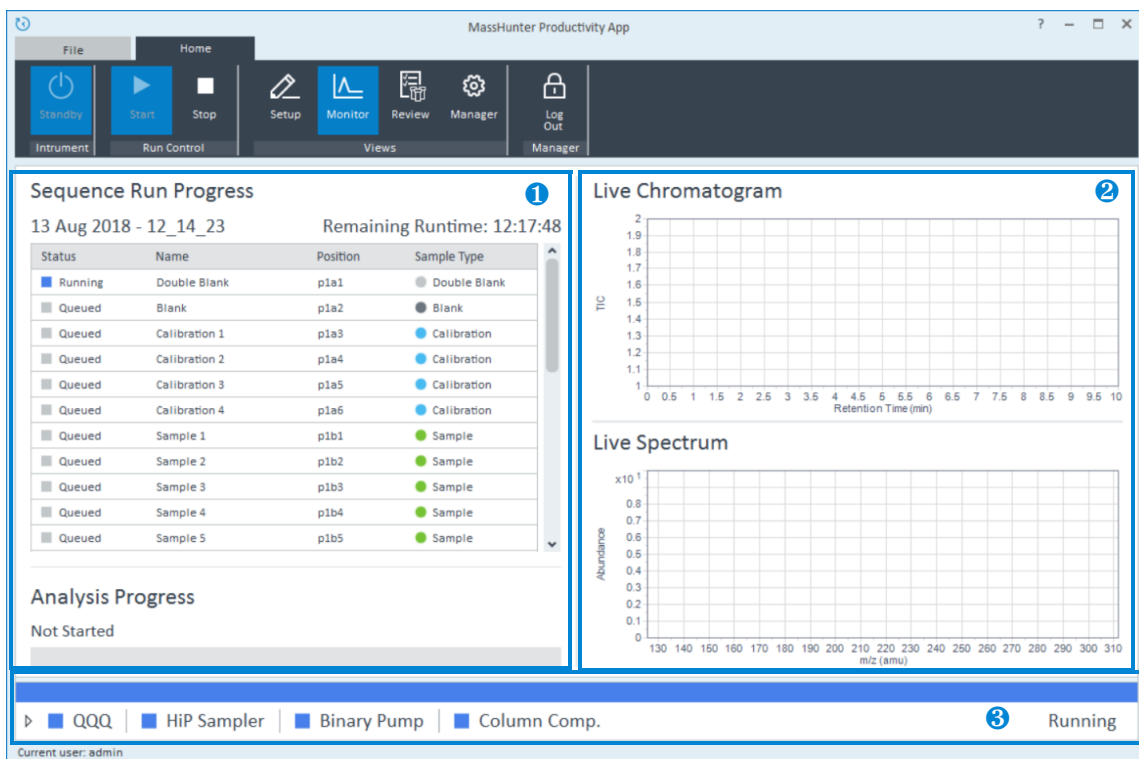


##### Disabled Run Button



### Monitor View

The Monitor View has a single page that allows for monitoring the current sequence run. The numbered topics that follow **Figure 5** refer to the numbered sections in that figure.



**Figure 5.** Monitor View

#### 1 Monitor current sequence run

The sequence run progress table shows every sample injection along with the estimated remaining run time. The analysis progress is displayed below the sequence progress table. If the shutdown sequence is configured to run, the shutdown sequence progress will also be displayed.

#### 2 Monitor real-time data

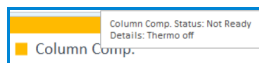
View the live total ion chromatogram (TIC) and live spectrum for the current run.

## Understanding the User Interface

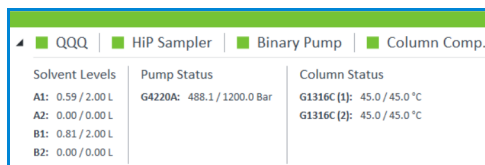
### Monitor View

#### 3 Monitor instrument status

Use this panel to keep track of the overall instrument status and individual device statuses. Hovering over a device status will give additional details:



To view additional system details, expand the status details panel:



The instrument status panel is always visible, regardless of the active page, allowing you to always keep track of the status of your instrument.

## Review View

The Review View includes the **Review Analysis Results**, **Review Control Charts**, and **Create Report** pages. Use these pages to review and edit sequence run results, and to generate reports. The numbered topics that follow **Figure 6**, **Figure 7**, and **Figure 8** refer to the numbered sections in those figures.

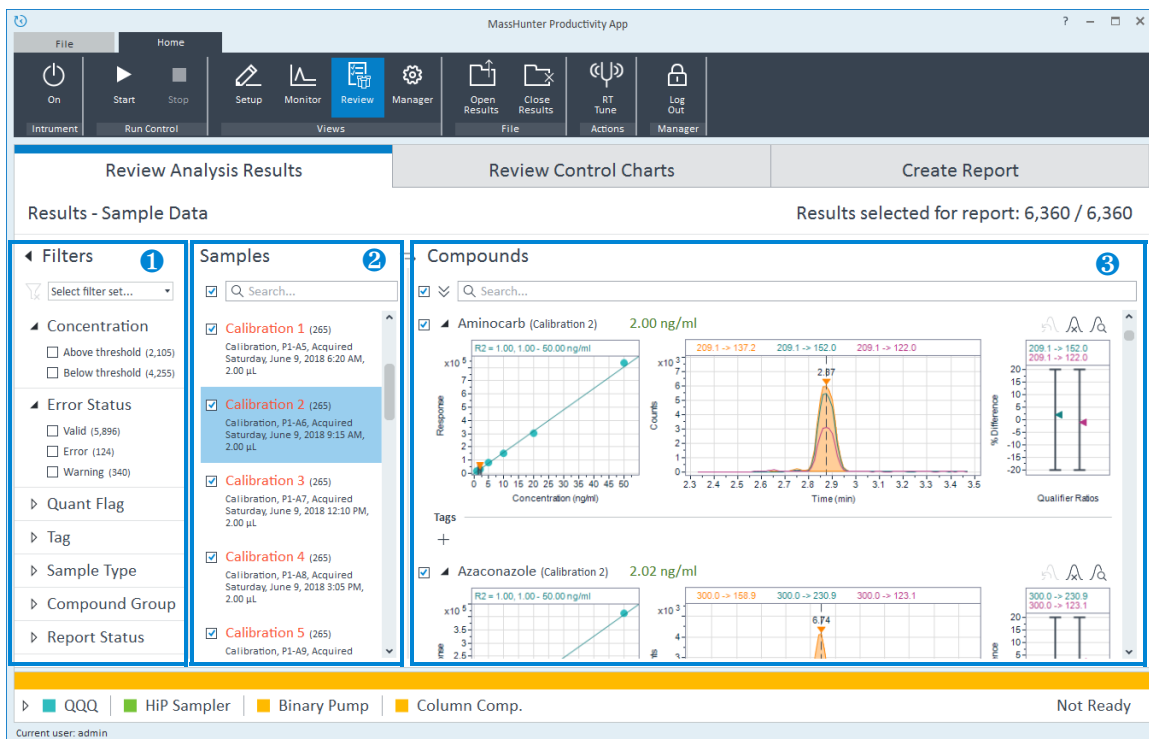


Figure 6. Review Analysis Results page

# Understanding the User Interface

## Review View

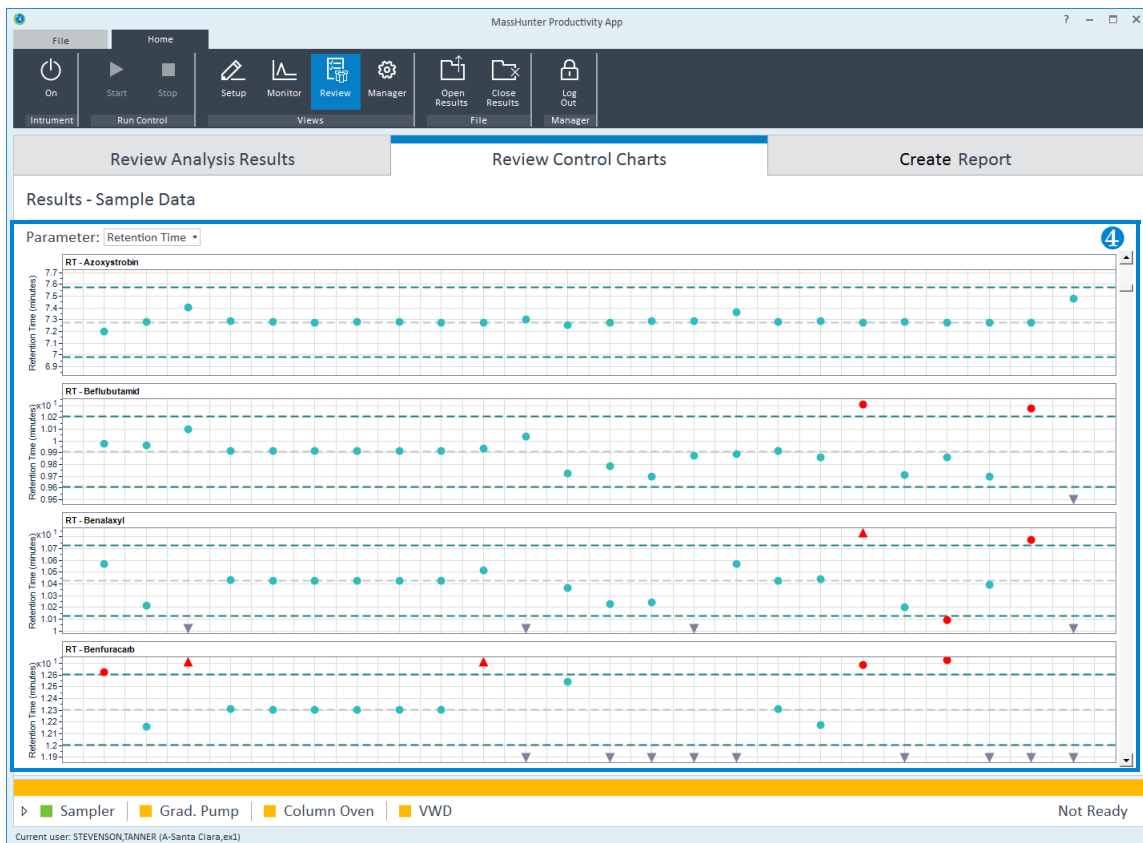


Figure 7. Review Control Charts page

# Understanding the User Interface

## Review View

**Report Options** 5

Method  
Report By Sample

Options  
Report Title  
My Report

Compound Sort Field  
Compound Name

Generate Compound Graphics

**Report Preview** 6

Bookmarks

- Double blank (1\_Double blank.d)
- Blank (2\_Blank.d)
- Double blank (3\_Double blank.d)
- Calibration 1 (4\_Calibration 1.d)
- Calibration 2 (5\_Calibration 2.d)
- Calibration 3 (6\_Calibration 3.d)
- Calibration 4 (7\_Calibration 4.d)
- Calibration 5 (8\_Calibration 5.d)
- Calibration 6 (9\_Calibration 6.d)
- Double blank (10\_Double blank.d)
- Sample 1 (11\_Sample 1.d)
- Sample 2 (12\_Sample 2.d)
- Sample 3 (13\_Sample 3.d)
- Sample 4 (14\_Sample 4.d)
- Sample 5 (15\_Sample 5.d)
- Double blank (16\_Double blank.d)
- QC1 (17\_QC1.d)


Compound	RT	RT Reference	Final Conc.	Units	STD Resp.	Accuracy %	Recovery %	Flags
Abermeth B1a	15.37	15.37	21.81	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range
Ampicillin	2.75	2.75	0.14	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Acetaminophen	3.88	3.88	0.06	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range
Aflatoxin	9.78	10.05	0.38	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Aldicarb	4.67	4.63	0.21	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Amidoxifen	5.35	5.67	0.14	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range, Retention time out of range
Amoxicillin	3.21	2.87	0.15	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Retention time out of range, Qualifier ratio out of range
Anonacelle	6.74	6.74	0.02	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range
Azoxymethionine	5.22	5.00	0.18	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range
Baclofen	(8.53)	8.93	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Adiphen-methyl	(7.03)	7.03	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Azoxymethionine	7.30	7.28	0.00	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range
Benzofuran	10.04	9.91	0.10	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Benzofuran	(10.43)	10.43	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Benzofuran	(12.31)	12.31	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Benzofuran	11.04	10.95	0.26	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Benzofuran	8.57	8.57	16.97	ng/ml	N/A	N/A	N/A	N/A

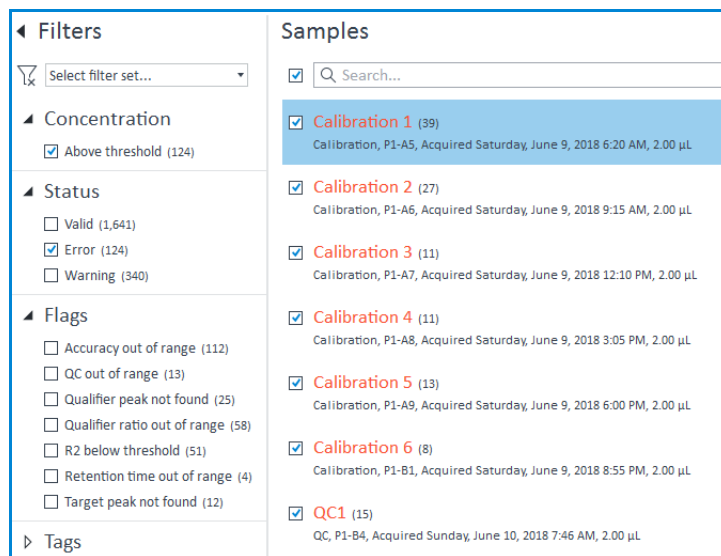
Current user: admin

Figure 8. Create Report page



#### 1 Filter visible results

Use the filter panel to quickly restrict the scope of review. When filtered, the groups of filtered results will update in the middle column. In addition to selecting individual filters, you can select a predefined set of filters to apply at once (if defined by the manager), or you can clear all filters: 



The screenshot shows two panels: 'Filters' and 'Samples'. The 'Filters' panel on the left has a 'Select filter set...' dropdown and several expandable sections: 'Concentration' (with 'Above threshold (124)' checked), 'Status' (with 'Error (124)' checked), and 'Flags' (with several options unchecked). The 'Samples' panel on the right has a search bar and a list of calibration and QC samples, each with a checked checkbox and a count in parentheses. The first sample, 'Calibration 1 (39)', is highlighted in blue.

#### NOTE

The filters do not affect the results selected for reporting. The filters simply change the set of visible results.

The available filters are grouped into the following categories:

#### Concentration

Filter based on whether the result is above or below the concentration threshold defined by the manager. Results from Calibration, QC, and CC samples will always be labeled as **Above Threshold**.

#### Error Status

Filter based on the error status of the result:

- Valid - Results that have no issues (Green)
- Warning - Results that may have issues and might need review (Yellow)
- Error - Results that have issues and require review (Red)

Visit the [Agilent Community](#) for more information about the error statuses.

#### Quant Flags

Filter based on the flags applied to the results by MassHunter Quantitative Analysis. The Productivity App reads in only a limited subset of the available result flags. Visit the [Agilent Community](#) for more information on the flags that are recognized by the Productivity App.

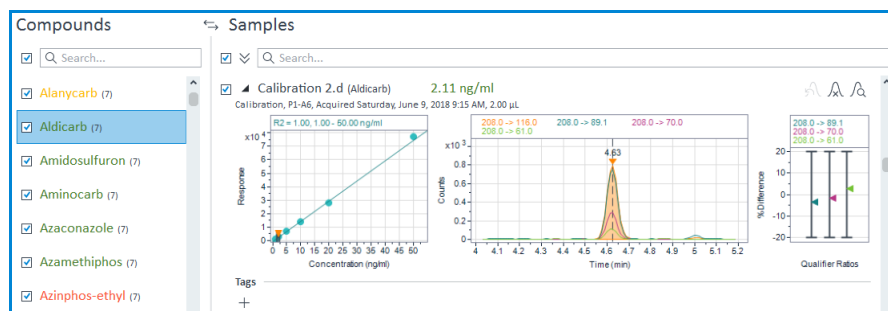
## Understanding the User Interface

### Review View

- Result Tags** Filter based on tags that are not analysis flags.
- Sample Type** Filter based on the type of sample.
- Compound Group** Filter based on the compound group.
- Report Status** Filter based on whether the result is selected or not selected for reporting.

### ② View filtered result groups

The middle column represents all filtered results grouped either by sample (default) or by compound. Click  $\leftrightarrow$  to change between the two.



When you select a group from this list, the results visible in the right-most column will change. To view multiple groups at once, hold the **Shift** (for continuous selection) or **Ctrl** key while you select one or more result groups.

An additional use of this column is to curate the results selected for reporting. Use the check boxes next to the sample or compound name to quickly select or clear an entire set of results for inclusion in the report. Alternatively, you can use the check box next to the search bar to select or clear all visible groups for the report. You can change the visible groups by typing into the search bar.

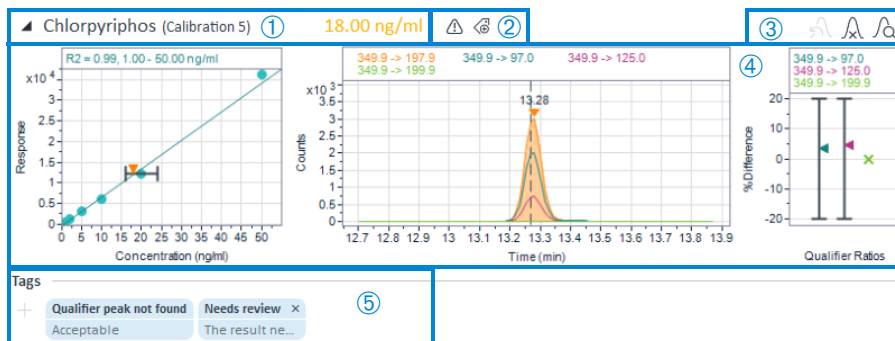
The color of the group name represents the error status of all the results that belong to the group. Any results with an error displays the name in red. Similarly, a yellow name indicates that at least one result has a warning, but no results have an error.






## Understanding the User Interface

### Review View

#### ③ Review and edit results

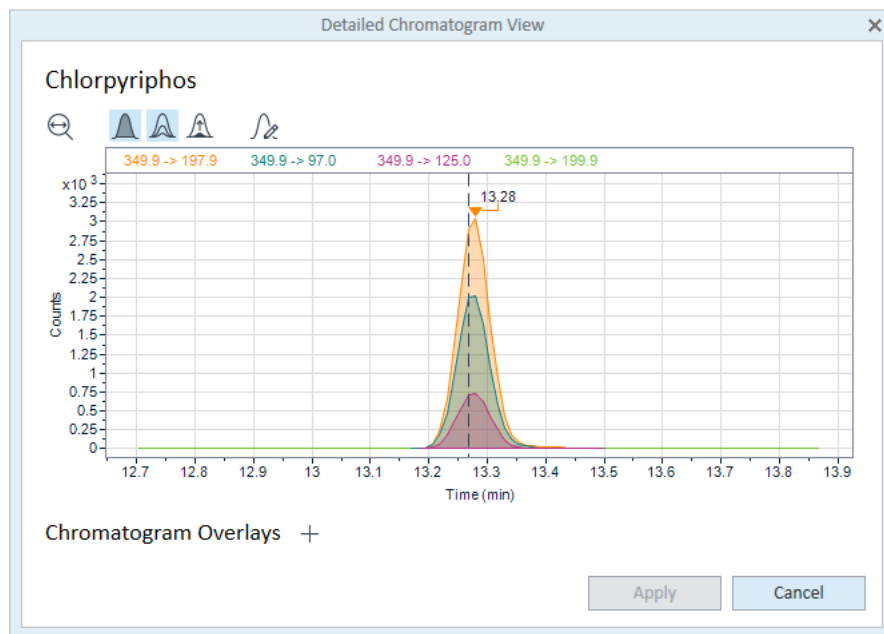
The right-most column displays the result details:




- 1 Quickly view the name of the sample and compound that define the result along with the calculated concentration. Click this area to show or hide the graphs and tags.
- 2 Identify whether flags  or tags  are applied to the result. Hover over the icon to display the added flags or tags, respectively.
- 3 Interact with the result in these ways:
  - Zero the peak: 
  - Undo manual integration: 
  - View the interactive chromatogram window: 

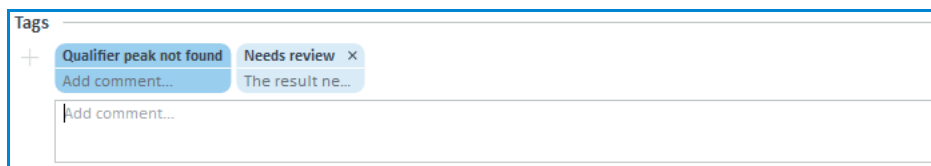
## Understanding the User Interface

### Review View



In this interactive window, you can get a detailed look at the quantifier and qualifier peak integration. If the integration needs modification, you can edit the integration: . Additionally, you can use this window to overlay chromatograms from other samples in the batch.

- 4 View the calibration curve, chromatogram, and qualifier ratio graph images.
- 5 View and edit the result tags. Every tag has an associated comment which can be edited by clicking on a tag. All quant flags are added as tags and cannot be removed. Custom tags that managers create can be manually added by a user and can be removed.

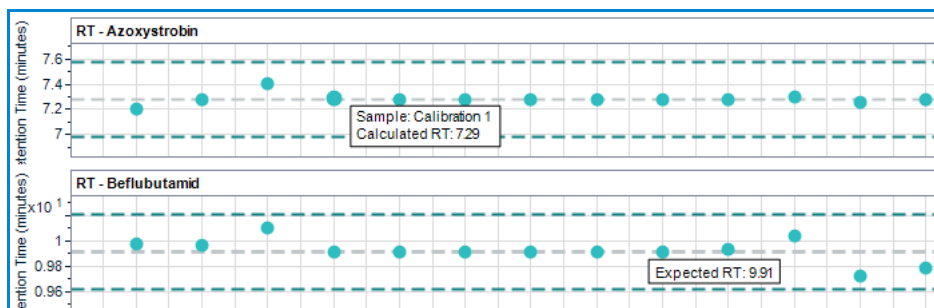


## Understanding the User Interface

### Review View

#### 4 Review control charts

Use this page to review control charts for the opened results. The control charts plot a variable across relevant samples for each compound so that issues can be immediately identified. Four variables are available to plot: Retention Time, QC Concentration Deviation, CC Response Ratio, and ISTD Response.



#### 5 Configure report options

Use this panel to select a report method and configure the method's available options before generating a report. See the *Manager Guide* or visit the [Agilent Community](#) for more information about report method customization.

## ⑥ Review report

Use this panel to view the generated report.

**Report Preview** ①

51 / 130 94% Find: ②

**Bookmarks** ③

- Double blank (1\_Double blank.d)
- Blank (2\_Blank.d)
- Double blank (3\_Double blank.d)
- Calibration 1 (4\_Calibration 1.d)
- Calibration 2 (5\_Calibration 2.d)
- Calibration 3 (6\_Calibration 3.d)
- Calibration 4 (7\_Calibration 4.d)
- Calibration 5 (8\_Calibration 5.d)
- Calibration 6 (9\_Calibration 6.d)
- Double blank (10\_Double blank.d)
- Sample 1 (11\_Sample 1.d)**
- Sample 2 (12\_Sample 2.d)
- Sample 3 (13\_Sample 3.d)
- Sample 4 (14\_Sample 4.d)
- Sample 5 (15\_Sample 5.d)
- Double blank (16\_Double blank.d)
- QC1 (17\_QC1.d)

Compound	RT	RT Reference	Final Conc.	Units	JSTD Resp.	Accuracy %	Recovery %	Flags
Abamectin B1a	15.37	15.37	21.81	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range
Acophate	2.75	2.75	0.14	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Acetamiprid	3.68	3.69	0.06	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range
Alanycarb	9.78	10.05	0.38	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Aldicarb	4.67	4.63	0.21	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Amidosulfuron	5.35	5.67	0.14	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range, Retention time out of range
Aminoacarb	3.21	2.87	0.15	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Retention time out of range, Qualifier ratio out of range
Azacoxazole	6.74	6.74	0.02	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range
Azamethiphos	5.22	5.00	0.18	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range
Aztriphos-ethyl	(8.93)	8.93	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Aztriphos-methyl	(7.03)	7.03	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Azoxystrobin	7.30	7.28	0.00	ng/ml	N/A	N/A	N/A	Qualifier peak not found, Qualifier ratio out of range
Beflubutamid	10.04	9.91	0.10	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Bernaloxyl	(10.43)	10.43	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Benflurocarb	(12.31)	12.31	ND	ng/ml	N/A	N/A	N/A	Target peak not found
Benzoximate	11.04	10.95	0.26	ng/ml	N/A	N/A	N/A	Qualifier ratio out of range, Qualifier peak not found
Bifenazate	8.57	8.57	16.97	ng/ml	N/A	N/A	N/A	

- 1 Refresh the report with updated result selections or report options.
- 2 Save, print, search, and navigate through the report preview.
- 3 Navigate to a specific page in the report.


## Reference

### Glossary

<b>Analysis Parameters</b>	A collection of concentrations that must be defined on a per-run basis for each compound. Examples: Calibration, QC, and Matrix Spike concentrations.
<b>Compound Group</b>	A collection of compounds distinguished by a group name. Compounds can belong to multiple groups.
<b>Level</b>	The identifier that maps an analysis parameter to a sample. It is an extension of calibration levels that additionally applies to QCs, CCs, Matrix Blanks, and Matrix Spikes.
<b>Sequence</b>	The list of samples to be acquired.
<b>Sequence Template</b>	A file that declares the structure of a sequence. It declares the sample types that must be present at the beginning and end, and the sample types that must be repeated for a given number of customer samples in the middle.

## In This Book

This Quick Start Guide gives an overview of the MassHunter Productivity App.

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