

# **Carryover Detection Tutorial**

for the

**MPX<sup>™</sup> Driver Software** 



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# Walk-Up Workspace in Version 2.0 of the MPX<sup>™</sup> Driver Software

The Walk-Up workspace in the MPX<sup>TM</sup> driver software contains the following panes, each providing the user with different access points to MPX<sup>TM</sup> driver software functionality and information related to the system:

- Submitted Batches pane. Refer to Submitted Batches on page 5.
- Samples in Batch pane. Refer to Samples in Batch on page 6.
- Sample Execution History pane. Refer to Sample Execution History on page 7.
- Instrument status pane. Refer to Instrument Status on page 8.
- Notification Messages dialog. Refer to Notification Messages Dialog on page 8.

**Note:** The 🗐 icon that is used to open the Notification Messages dialog is only accessible if messages or warnings were generated during the sample run.

The Walk-Up workspace in the MPX<sup>TM</sup> driver software enables the user to submit batches, modify batch order, and delete selected samples or batches through the MPX<sup>TM</sup> driver software. The user does not have to use the Analyst<sup>®</sup> software to perform these actions.

Refer to:

- Submit a Batch in the Walk-Up Workspace on page 17.
- Change the Batch Order on page 6.

Figure	1-1	Walk-Up	Workspace
--------	-----	---------	-----------

; ods		νp												ow Do I?
ods	Subr	nitt	ted Batches:										0	100
	Status		Time Scheduled	Time Completed	Ratch Name	Batch Out	ur l	Scheduled By	Checkled	Samples C	omoleted Camples	Corrental Canadas	Failed Samples	Rodert
		1	2017/11/27 11:19:42	2017/11/07 11:55:15	Nov 27 Example Carr	vover dab BLT Project	1 485	CIEXDEV/8LT Project	10	1	)	10	0	MPX De
		2	2017/11/27 11:52:55	2017/11/27 11 59:45	Nov 27 Example Carr	vover dab BLT Projec	1 485	CIEXDEVILT Project	1	1		1	0	MPX D
	1	3	2017/11/27 11:52:55	2017/11/27 12:02:04	Nov 27 Example Carr	vover.dab BLT.Projec	1 485	CIEXDEV/8LT Project	1	1		1	0	MPX D
	~	4	2017/11/27 11:55:15	2017/11/27 12:15:50	Nov 27 Example Carr	yover.dab BLT.Projec	t ABS	CIEXDEVIBLT.Project	2	2		2	0	MPX D
	Sam	ple	s in Batch:											100
I	Status		Time Submitted	Time Started	Time Completed	Sample Name	Stree	am Assigned Stream	Barcode	Plate Positio	n Vial Position	Aco, Method	Name	Messa
I	~	1	2017/11/27 12:04:22	2017/11/27 12:06:55	2017/11/27 12:08:56	Blank (re-inject)	2	2		2	15	5500Q Triazines with I	MPX S2A dam	
1	-	2	2017/11/27 12:11:17	2017/11/27 12:13:48	2017/11/27 12:15:49	Unknown 52 (re-inie	ct) 2	2		2	10	5500Q Triazines with I	MPX 52A dam	
	~	1	2017/11/27 11:23:29	2017/11/27 11	25:30 R	inse	1	1 1	2	1				
- 1	~	2	2017/11/27 11:25:38	2017/11/27 11	27:39 R	inse	2	2 2	2	1				
1	1	3	2017/11/27 11:30:19	2017/11/27 11	32.20 C	al 50	1	1 1	2	6				
- 1	1	4	2017/11/27 11:32:35	2017/11/27 11	34.36 C	al 50	2	2	2	6				
1	1	5	2017/11/27 11:37:09	2017/11/27 11	39.10 C	al 10	1	1 3	2	5				
	1	6	2017/11/27 11:39:29	2017/11/27 11	41:30 C	al 10	2	2	2	5				
	1	7	2017/11/27 11:44:04	2017/11/27 11	46.05 8	lank	1	1 2	2	15				
	1.0	8	2017/11/27 11:46:23	2017/11/27 11	48.25 8	lank	2	2	2	15				
				2017/11/27 11	52.54 U	nknown S1	1	1 3	2	11	Above upper o	oncentration limit was o	detected.	
	Å	9	2017/11/27 11:50:53											
	Å	9 10	2017/11/27 11:50:53	2017/11/27 11	55:14 U	nknown S2	2	2 3	2	10	Carryover was	detected.		
		9 10 11	2017/11/27 11:53:53 2017/11/27 11:53:13 2017/11/27 11:57:43	2017/11/27 11 2017/11/27 11	55.14 U 59.44 B	nknown S2 lank (re-inject 1)	2	2 2	2	10 15	Carryover was	detected.		
		9 10 11 12	2017/11/27 11:50:53 2017/11/27 11:53:13 2017/11/27 11:57:43 2017/11/27 12:00:03	2017/11/27 11 2017/11/27 11 2017/11/27 12	55:14 U 59:44 B 02:04 B	nknown S2 lank (re-inject 1) lank (re-inject 1)	2 1 2	2 2 1 2	2 2	10 15 15	Carryover was	detected.		
		9 10 11 12 13	2017/11/27 11:50:53 2017/11/27 11:53:13 2017/11/27 11:57:43 2017/11/27 12:00:03 2017/11/27 12:00:55	2017/11/27 11 2017/11/27 11 2017/11/27 12 2017/11/27 12	55.14 U 59.44 B 02.04 B 108.56 B	nknown S2 lank (re-inject 1) lank (re-inject 1) lank (re-inject)	2 1 2 2	2 2 1 2 2 2	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	10 15 15 15	Carryover was	detected.		
		9 10 11 12 13 14	2017/11/27 11:50:53 2017/11/27 11:53:13 2017/11/27 11:53:13 2017/11/27 12:00:03 2017/11/27 12:00:05 2017/11/27 12:13:48	2017/11/27 11 2017/11/27 11 2017/11/27 12 2017/11/27 12 2017/11/27 12 2017/11/27 12	55:14 U 59:44 8 :02:04 8 :08:56 8 :15:49 U	nknown S2 lank (re-inject 1) lank (re-inject 1) lank (re-inject) nknown S2 (re-inject)	2 1 2 2 2	2 2 1 2 2 2 2 2	2 2 2 2 2	10 15 15 15 10	Cartyover was	detected.		

## **Submitted Batches**

The Submitted Batches pane contains a list of all of the batches that have been submitted. The pane contains one row for each batch submitted, providing the user with information related to the status of the batch, the submission order, the approximate batch start and finish times, the name of the batch, the batch owner, the number of samples contained in the batch, and so on.

Figure 1-2 Submitted Batches Pane

Walk-	Up									H	w Do L.?
Sub	mit	ted Batches:								6	
Status		Time Scheduled	Time Completed	Batch Name	Batch Owner	Scheduled By	Scheduled Samples	Completed Samples	Successful Samples	Failed Samples	Project
	1	2017/11/27 11:19:42	2017/11/27 11:55:15	Nov 27 Example Carryover.dab	BLT.Project	ABSCIEXDEV/BLT.Project	10	10	10	0	MPX Demo
× .	2	2017/11/27 11:52:55	2017/11/27 11:59:45	Nov 27 Example Carryover.dab	BLT.Project	ABSCIEXDEV/BLT.Project	1	1	1	0	MPX Demo
× .	3	2017/11/27 11:52:55	2017/11/27 12:02:04	Nov 27 Example Carryover.dab	BLT.Project	ABSCIEXDEV/BLT.Project	1	1	1	0	MPX Demo
1	4	2017/11/27 11:55:15	2017/11/27 12:15:50	Nov 27 Example Carryover.dab	BLT.Project	ABSCIEXDEV/BLT.Project	2	2	2	0	MPX Demo

### Change the Batch Order

The order of the batches can be changed according to user needs.

**Note:** Only batches that have not been submitted to the Analyst<sup>®</sup> software queue can be moved up and down or deleted in the MPX<sup>™</sup> driver software Walk-Up workspace.

- 1. In the Submitted Batches pane, select the appropriate batch.
- 2. Do one of the following:
  - To move the selected batch and all of the subsequent batches to the top of the list, click the 🔤 icon.
  - To move the selected batch up in the list, one row at a time, click the <u>selected</u> icon.
  - To move the selected batch down in the list, one row at a time, click the 🛂 icon.
  - To delete the selected batch from the list, click the  $\boxtimes$  icon.
  - To delete the selected batch and all of the subsequent batches from the list, click the 😆 icon.

### Status

The **Status** column shows a series of icons indicating the batch status:

lcon	Description
<b></b>	All of the samples in the batch have completed successfully, but at least one sample has a warning message.
	The batch is in progress.
•••	The batch has been submitted, but is waiting to begin.
1	The batch has completed successfully, but at least one sample has failed.
~	All of the samples in the batch have completed successfully, with no warning message.
×	At least one sample in the batch has failed.

## Samples in Batch

The Samples in Batch pane contains a list of all of the samples within a batch. The Samples in Batch pane contains one row for each sample in the selected batch, providing the user with information related to the status of the sample, the submission order, the approximate sample start and finish times, the name of the sample, the assigned

and submission stream, the barcode of the sample, the plate position, and so on. Any RTD<sup>3</sup> Carryover Detection messages related to the sample are shown in the Message column.

#### Figure 1-3 Samples in Batch

Sam	Samples in Batch:								88888			
Status		Time Submitted	Time Started	Time Completed	Sample Name	Stream	Assigned Stream	Barcode	Plate Position	Vial Position	Acq. Method Name	Message
1	1	2017/11/27 12:04:22	2017/11/27 12:06:55	2017/11/27 12:08:56	Blank (re-inject)	2	2		2	15	5500Q Triazines with MPX S2A dam	
<b>~</b>	2	2017/11/27 12:11:17	2017/11/27 12:13:48	2017/11/27 12:15:49	Unknown S2 (re-inject)	2	2		2	10	5500Q Triazines with MPX S2A.dam	
	< 0											

### Status

The Status column shows a series of icons indicating the sample status:

lcon	Description
	The sample is in progress.
•••	The sample is waiting.
<b></b>	The sample has completed successfully, but contains a warning message.
~	The sample has completed successfully.
×	The sample has failed.

### **Sample Execution History**

The Sample Execution History pane contains a complete list of all of the injected samples, Blank sample re-injections, and carryover sample re-injections. The Sample Execution History pane contains one row for each submitted sample, providing the user with information related to the status of the sample, the submission order, the approximate sample start and finish times, the name of the sample, the associated stream number, the plate and vial positions, and so on. Any RTD<sup>3</sup> Carryover Detection messages related to the sample are shown in the Message column.

Figure	1-4	Sample	Execution	Historv

itatus		Time Started	Time Completed	Sample Name	Stream	Assigned Stream	Plate Position	Vial Position	Message
1	1	2017/11/27 11:23:29	2017/11/27 11:25:30	Rinse	1	1	2	1	
	2	2017/11/27 11:25:38	2017/11/27 11:27:39	Rinse	2	2	2	1	
	3	2017/11/27 11:30:19	2017/11/27 11:32:20	Cal 50	1	1	2	6	
1	4	2017/11/27 11:32:35	2017/11/27 11:34:36	Cal 50	2	2	2	6	
1	5	2017/11/27 11:37:09	2017/11/27 11:39:10	Cal 10	1	1	2	5	
1	6	2017/11/27 11:39:29	2017/11/27 11:41:30	Cal 10	2	2	2	5	
<ul> <li>Image: A second s</li></ul>	7	2017/11/27 11:44:04	2017/11/27 11:45:05	Blank	1	1	2	15	
<ul> <li>Image: A set of the set of the</li></ul>	8	2017/11/27 11:46:23	2017/11/27 11:48:25	Blank	2	2	2	15	
	9	2017/11/27 11:50:53	2017/11/27 11:52:54	Unknown S1	1	1	2	11	Above upper concentration limit was detected.
	10	2017/11/27 11:53:13	2017/11/27 11:55:14	Unknown S2	2	2	2	10	Carryover was detected.
<ul> <li>Image: A second s</li></ul>	11	2017/11/27 11:57:43	2017/11/27 11:59:44	Blank (re-inject 1)	1	1	2	15	
<ul> <li>Image: A second s</li></ul>	12	2017/11/27 12:00:03	2017/11/27 12:02:04	Blank (re-inject 1)	2	2	2	15	
1	13	2017/11/27 12:06:55	2017/11/27 12:08:56	Blank (re-inject)	2	2	2	15	
<ul> <li>Image: A second s</li></ul>	14	2017/11/27 12:13:48	2017/11/27 12:15:49	Unknown S2 (re-inject)	2	2	2	10	

### **Instrument Status**

The instrument status panel is shown at the bottom of all of the MPX<sup>™</sup> driver software workspaces. The status panel provides a visual status of the mass spectrometer, LC stream 1, and LC stream 2.

#### Figure 1-5 Instrument Status Panel



#### Table 1-1 Status Icons

lcon	Description
•	Ready
•	Standby
•	Fault

### **Notification Messages Dialog**

The Notification Messages dialog contains a list of all important messages and warnings generated during the sample run. The messages identify issues with the MPX<sup>™</sup>-2 High Throughput System. Users can acknowledge and clear these messages, as required.

1. To access the Notification Messages dialog, click the 🗐 icon in the bottom-right corner of the Walk-Up workspace.

Notification Messages
The system has been running for more than 2 days. Please restart the system.
The system has been running for more than 3 days. Please restart the system.
The system has been running for more than 4 days. Please restart the system.
Aborting LC on stream 2
Sample 13 in Batch 12 paused.
Sample 18 in Batch 12 paused.
Sample 23 in Batch 13 paused.
Clear All

#### Figure 1-6 Notifications Messages Dialog

- 2. To delete the messages, do one of the following:
  - To delete an individual message, click the 😎 icon that is shown at the right of the message.
  - To delete all of the messages, click **Clear All** at the bottom of the Notification Messages dialog.

The Real Time Data Dependent Decision (RTD<sup>3</sup>) Carryover Detection feature enables the user to set a series of Low and High concentration thresholds for various analytes. When the Carryover Detection option is selected, the RTD<sup>3</sup> logic improves sample throughput by minimizing the number of sample re-injections that need to be performed due to sample stream contamination or suspected carryover.

Carryover Detection is designed for high throughput analytical workflows using the same analytical methods on Stream 1 and Stream 2.

After a series of Low and High thresholds have been set in the MPX<sup>™</sup> driver software, the RTD<sup>3</sup> can flag:

- Unknown sample concentration level that exceeds a specified High limit value or a specified Region Height value.
- Blank sample concentration level that exceeds a specified Low limit value.

When an Unknown sample concentration level is below the specified High limit value, the next sample is injected. When an Unknown sample concentration level exceeds the specified High limit value, a Blank sample is automatically injected. For systems equipped with a CTC autosampler, the Blank sample is injected on the other stream. For systems equipped with a Shimadzu autosampler, the Blank sample is injected on the same stream.

For systems equipped with a CTC autosampler, if the Unknown sample concentration level exceeds the Lower limit value and was preceded by a sample with a concentration level that exceeded the High limit value, then Carryover Detection is enabled and the Unknown sample is flagged with the message *Carryover was detected*. The Unknown sample is re-injected at the end of the batch.

When a Blank sample concentration level is below the specified Low limit value, the stream is considered clean and the next sample is injected. When a Blank sample concentration level exceeds the Low limit value, the RTD<sup>3</sup> functionality will inject up to three Blank samples, in succession. If the calculated sample concentration of the third Blank sample still exceeds the Low limit value, then the sample stream stops injecting to prevent carryover contamination of the other samples in the batch.

Because there are small differences in response between the two streams, Carryover Detection does not provide an absolute quantitation value, but rather a rough concentration guide that is useful for flagging suspect samples. For final analytical quantitation and reporting, we recommend that the entire data file be processed using either the MultiQuant<sup>™</sup> software or the Analyst<sup>®</sup> software to confirm the findings.

# Requirements

Carryover Detection can only be performed in the Walk-Up workspace of the MPX<sup>™</sup> 2.0 driver software.

The Carryover Detection function requires the following components:

- An MPX<sup>™</sup> driver software acquisition method (stream 1 or stream 2 only). The method must include an Analyte ID for each MRM transition. Refer to Create the MS Component of a Method in the MPX<sup>™®</sup> driver software *Help*.
- An Analyst<sup>®</sup> software quantitation method. Refer to Create the LC Component of a Method in the MPX<sup>TM®</sup> driver software *Help*.
- A sample batch created using the Analyst<sup>®</sup> software, with a single sample set containing the sample name, location, sample type, and the concentration values for calibration samples. Refer to Create a Batch on page 13.
- A MultiQuant<sup>™</sup> software, version 3.0.2 or later, quantitation method. Refer to Create a Carryover Detection Compatible MultiQuant<sup>™</sup> Software Quantitation Method on page 15. The same MultiQuant<sup>™</sup> software method must be used for both stream 1 and stream 2.

**Note:** Version 3.0.2 of the MultiQuant<sup>™</sup> software is only compatible with the 64-bit version of the Microsoft Windows 7 operating system. Version 3.0.3 of the MultiQuant<sup>™</sup> software is compatible with the 64-bit version of both the Microsoft Windows 7 and the Windows 10 operating systems.

• The **Carryover Detection** check box must be selected on the Submit Batch dialog. This check box is only available for selection if all of the above criteria is met.

### **Carryover Detection Messages**

Message	Description
Above upper concentration limit was detected	The concentration level of an Unknown sample exceeds the specified High limit value.
Above region height threshold was detected	The concentration level of an Unknown sample exceeds the specified Region Height value.
Above lower concentration limit was detected	The concentration level of a Blank sample exceeds the specified Low limit value.
Carryover was detected	The concentration level of an Unknown sample exceeds the specified Low limit value and was preceded by a sample that exceeded the specified High Limit value.

#### Table 2-1 Messages

#### Figure 2-1 Example Messages

Status		Time Started	Time Completed	Sample Name	Stream	Assigned Stream	Plate Position	Vial Position	Message
¥ -	1	2017/11/27 11:23:29	2017/11/27 11:25:30	Rinse	1	1	2	1	Above upper concentration limit was detected.
<ul> <li>Image: A second s</li></ul>	2	2017/11/27 11:25:38	2017/11/27 11:27:39	Rinse	2	2	2	1	Carryover was detected.
¥	3	2017/11/27 11:30:19	2017/11/27 11 32 20	Cal 50	1	1	2	6	Above lower concentration limit was detected.
<ul> <li>Image: A second s</li></ul>	4	2017/11/27 11:32:35	2017/11/27 11:34:36	Cal 50	2	2	2	6	
<ul> <li>Image: A second s</li></ul>	5	2017/11/27 11:37:09	2017/11/27 11 39:10	Cal 10	1	1	2	5	
×	6	2017/11/27 11:39:29	2017/11/27 11:41:30	Cal 10	2	2	2	5	
<ul> <li>Image: A second s</li></ul>	7	2017/11/27 11:44:04	2017/11/27 11 46 05	Blank	1	1	2	15	
× -	8	2017/11/27 11:46:23	2017/11/27 11:48:25	Blank	2	2	2	15	
<b>A</b>	9	2017/11/27 11:50:53	2017/11/27 11:52:54	Unknown S1	1	1	2	11	Above upper concentration limit was detected.
<b>A</b>	10	2017/11/27 11:53:13	2017/11/27 11:55:14	Unknown S2	2	2	2	10	Carryover was detected.
<ul> <li>Image: A second s</li></ul>	11	2017/11/27 11:57:43	2017/11/27 11:59:44	Blank (re-inject 1)	1	1	2	15	
× -	12	2017/11/27 12:00:03	2017/11/27 12:02:04	Blank (re-inject 1)	2	2	2	15	
<ul> <li>Image: A second s</li></ul>	13	2017/11/27 12:06:55	2017/11/27 12:08:56	Blank (re-inject)	2	2	2	15	
<ul> <li>Image: A second s</li></ul>	14	2017/11/27 12:13:48	2017/11/27 12:15:49	Unknown 52 (re-inject)	2	2	2	10	

Refer to Requirements on page 10 for a list of criteria that must be met for Carryover Detection to function as expected.

**Note:** For the Carryover Detection feature to be available in the  $MPX^{TM}$  driver software, the batch must be set up as follows:

• At least one calibrator sample must be identified as a **Standard**.

**Note:** If multiple Standard samples are used, then the same Sample Name can be used for each Standard sample. However, the Vial Position for each sample must be unique.

• At least one negative control sample must be identified as a **Blank**.

**Note:** If multiple Blank samples are used, then the same Sample Name can be used for each Blank sample. However, the Vial Position for each sample must be unique. The RTD<sup>3</sup> (Real Time Data Dependent Decision) feature uses the most recent Blank sample which does not exceed the low concentration limit set by the user. Refer to Define Carryover Detection Limit Values on page 21.

- The **Standard** samples must precede the **Blank** samples in the batch.
- Samples that are to be evaluated by the Carryover Detection feature must be identified as **Unknown**.

**Note:** If multiple Unknown samples are used, then the same Sample Name can be used for each Unknown sample. However, the Vial Position for each sample must be unique.

- Samples identified as **Solvent**, **Double Blank**, or **QC** can be inserted anywhere in the batch. These sample types are ignored by the Carryover Detection feature and are not processed by the RTD<sup>3</sup> method.
- 1. In the Analyst<sup>®</sup> software, make sure that the correct project folder is selected.
- 2. Click **File > New**.

The New dialog opens.

3. Click **Acquisition Batch** and then click **OK**.

The Batch Editor window opens.

- 4. On the **Sample** tab, in the **Set** field, type a name for the set and then click **Add Set**.
- 5. Click Add Samples.

The Add Samples dialog opens.

6. Type the number of samples for the set in the **Number** field and then click **OK**.

The Add Samples dialog closes.

- 7. In the **Acquisition** field, select the acquisition method for the set.
- 8. In the **Quantitation** field, select the quantitation method for the set.
- 9. In the samples table, type the Sample Name, Vial Position, and Data File for each sample in the batch.

**Note:** The information provided in Figure 3-1 is for information purposes only.

#### Figure 3-1 Create Batch—Sample Tab

ample	Locations Quantitation S	ubmit						
Selec	ct Method for Sample Set				Quantitation			
Set:	Stream 1			•	Triazine MPX	Stream1	▼ Quick Q	uant
	Add Set Bemove Add Samples Del Sam	Set ples	Acquisition	n 3 Template ultiple Methods	Editor			
Batch	Script:					Select S	gript	
Batch	Script: Sample Name	Rack Code	Rack Position	Plate Code	Plate Position	Select S Vial Position	oript Data File	Inj.Volume (µl)
Batch	Script: Sample Name Wash	Rack Code	Rack Position	Plate Code	Plate Position	Vial Position	Data File	Inj.Volume (µl) 5.000
Batch	Script: Sample Name Wash Cal 10	Rack Code 3 Drawer 3 Drawer	Rack Position	Plate Code 2x VT54 2x VT54	Plate Position 3	Vial Position	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (µl) 5.000 5.000
Batch	Script: Sample Name Wash Cal 10 Cal 1	Rack Code 3 Drawer 3 Drawer 3 Drawer	Rack Position 1 1	Plate Code 2x VT54 2x VT54 2x VT54	Plate Position 3 3 3	Vial Position	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (μl) 5.000 5.000 5.000
Batch	Script: Sample Name Wash Cal 10 Cal 1 Cal 0.1	Rack Code 3 Drawer 3 Drawer 3 Drawer 3 Drawer	Rack Position 1 1 1	Plate Code 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54	Plate Position 3 3 3 3 3	Vial Position 1 2 3 4	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (μl) 5.000 5.000 5.000 5.000
Batch 1 2 3 4 5	Script: Sample Name Wash Cal 10 Cal 1 Cal 0.1 Blank A	Rack Code 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer	Rack Position	Plate Code 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54	Plate Position 3 3 3 3 3 3 3	Select S Vial Position 1 2 3 4 5	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (µl) 5.000 5.000 5.000 5.000 5.000
Batch 1 2 3 4 5 6	Script: Sample Name Wash Cal 10 Cal 0.1 Blank A High sample A	Rack Code 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer	Rack Position 1 1 1 1 1 1 1	Plate Code 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54	Plate Position 3 3 3 3 3 3 3 3 3 3 3	Select S Vial Position 1 2 3 4 5 6	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (μ)           5.000           5.000           5.000           5.000           5.000           5.000           5.000
Batch : 1 2 3 4 5 6 7	Script: Sample Name Wash Cal 10 Cal 1 Cal 0.1 Blank A High sample A Carryover sample A	Rack Code 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer	Rack Position 1 1 1 1 1 1 1 1 1	Plate Code 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54	Plate Position 3 3 3 3 3 3 3 3 3 3 3 3 3 3	Select S           Vial           Position           1           2           3           4           5           6           7	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (μl)           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000
Batch : 1 2 3 4 5 6 7 8	Script: Sample Name Wash Cal 10 Cal 1 Cal 0.1 Blank A High sample A Carryover sample A Mid sample B	Rack Code 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer	Rack           Position           1           1           1           1           1           1           1           1           1           1           1           1           1           1           1           1	Plate Code 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54	Plate Position 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	Select S           Vial           Position           1           2           3           4           5           6           7           8	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (μl)           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000
Batch 1 2 3 4 5 6 7 8 9	Script: Sample Name Wash Cal 10 Cal 1 Cal 0.1 Blank A High sample A Carryover sample A Mid sample B No carryover sample B	Rack Code 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer 3 Drawer	Rack           Position           1           1           1           1           1           1           1           1           1           1           1           1           1           1           1           1           1	Plate Code 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54 2x VT54	Plate Position 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	Select S           Vial           Position           1           2           3           4           5           6           7           8           9	Data File Jan 10B Stream 1 test\S1 Jan 10B Stream 1 test\S1	Inj.Volume (μl)           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000           5.000

10. Click the **Quantitation** tab.

11. Type the appropriate Quant Type information for each sample in the batch.

**Note:** If multiple Standard, Blank, or Unknown samples are used, then the same Sample Name can be used for each sample but the Vial Position for each sample should be unique.

Set							
Stre	eam 1		Quant Met	nod: Triazin	e MPX Stream	1.qmf	
	Sample Name	Quant Type	Atrazine_d	Ametryn1	Ametryn2	Atrazine1	Atrazine
1	Wash	Solvent	0.000000	0.000000	0.000000	0.000000	0.000000
2	Cal 10	Standard	1.000000	10.000000	10.000000	10.000000	10.000000
3	Cal 1	Standard	1.000000	1.000000	1.000000	1.000000	1.000000
4	Cal 0.1	Standard	1.000000	0.100000	0.100000	0.100000	0.100000
5	Blank A	Blank	1.000000	0.000000	0.000000	0.000000	0.000000
6	High sample A	Unknown	1.000000	0.000000	0.000000	0.000000	0.000000
7	Carryover sample A	Unknown	1.000000	0.000000	0.000000	0.000000	0.000000
8	Mid sample B	Unknown	1.000000	0.000000	0.000000	0.000000	0.000000
9	No carryover sample B	Unknown	1.000000	0.000000	0.000000	0.000000	0.000000
10	Blank B	Blank	1.000000	0.000000	0.000000	0.000000	0.000000

Figure 3-2 Create Batch—Quantitation Tab

12. Click File > Save.

The Save Acquisition Batch dialog opens.

13. Type a **File name** for the batch and then click **Save**.

### Create a Carryover Detection Compatible MultiQuant<sup>™</sup> Software Quantitation Method

The quality of the quantitation method used determines how effectively carryover can be detected. Because the Carryover Detection functionality generates a concentration value for each Unknown and Blank sample, it is important that the concentration be as accurate and reliable as possible so that the appropriate flags can be generated by RTD<sup>3</sup>.

1. If the MultiQuant<sup>™</sup> software is not open, then double-click **MultiQuant** under **Companion Software** on the Navigation bar of the Analyst<sup>®</sup> software.

**Tip!** When using the RTD<sup>3</sup> Carryover Detection feature, use the SignalFinder<sup>TM</sup> algorithm. This algorithm provides a wider linear dynamic range and more accurate quantitation results. In the MultiQuant<sup>TM</sup> software, click Edit > Project Integration Defaults and then select SignalFinder1 from the Integration Algorithm list.

- 2. In the MultiQuant<sup>™</sup> software, click **File > New Quantitation Method**.
- 3. Select the appropriate **Sample** file from the list provided and then click **OK**.

If the required Sample file is not shown, then browse to the appropriate folder and select the file.

- 4. On the **Components** tab, select the check box beside the internal standard, if applicable.
- 5. Select the **Group ID** and the **IS** name from the list provided.
- 6. Verify the **Q1/Q3 Transition** from the list provided and modify, if required.

Component	s Integr	ation & Regression   Outlie	r Settings		
Experimen	t MRM	1 (15 transitions)	-		
Row	IS	Name	Group	IS Name	Q1/Q3
1		Ametryn1	Ametryn	Atrazine_d5	228.2 / 186.2
2		Ametryn2	Ametryn	Atrazine_d5	228.2 / 116.2
3		Atrazine1	Atrazine	Atrazine_d5	216.1 / 174.2
4		Atrazine2	Atrazine	Atrazine_d5	216.1 / 104.2
5		Prometon1	Prometon	Atrazine_d5	226.2 / 142.2
6		Prometon2	Prometon	Atrazine_d5	226.2 / 184.2
7		Prometryn1	Prometryn	Atrazine_d5	242.2 / 158.1
8		Prometryn2	Prometryn	Atrazine_d5	242.2 / 200.2
9		Propazine1	Propazine	Atrazine_d5	230.1 / 146.1
10		Propazine2	Propazine	Atrazine_d5	230.1 / 188.2
11		Simazine1	Simazine	Atrazine_d5	202.1 / 132.1
12		Simazine2	Simazine	Atrazine_d5	202.1 / 124.2
13		Terbutryn1	Terbutryn	Atrazine_d5	242.1 / 186.1
14		Terbutryn2	Terbutryn	Atrazine_d5	242.1 / 68.2
15	1	Atrazine_d5			221.4 / 179.2
16					

#### Figure 3-3 Components Tab

7. On the Integration & Regression tab, type the appropriate values for the integration parameters.

**Tip!** For single point calibrators, type Linear Through Zero in the Fit field. If applicable, for internal standards, type an area value that is approximately 20% to 30% of the average value for the internal standard in the Min. Peak Height field.

8. On the **Outlier Settings** tab, type the appropriate values for the calculated concentration limits.

**Note:** For the RTD<sup>3</sup> functionality, the Lower Limit of Calculated Concentration (LLCC) and the Upper Limit of Calculated Concentration (ULCC) fields are the most important. These values set the concentration limits used by the RTD<sup>3</sup> Carryover Detection feature to assess the Above Lower Concentration Limit and the Above Upper Concentration Limit flagging comments. The LLCC and ULCC values are used when a selected MultiQuant<sup>™</sup> software method is used for carryover detection. The default values in the Carryover Detection pane of the Walk-Up workspace can be modified during batch submission, if required.

#### Figure 3-4 Outlier Settings Tab

Components   Integration & Regre	ession Outlier	Settings			
- I Accuracy for Standards − Max. Accuracy Tolerance for L Max. Accuracy Tolerance for S	LOQ (lowest S	itd): 20 %	Max. Accuracy Toles	ance for QC: 20 %	
I Ion Ratio I Cal Component	culated Concer	ntration Group	Ion Ratio Tolerance (%)	Lower Limit of Calculated Concentration	Upper Limit of Calculated Concentration
Ametryn1		Ametryn		0.05	25
Ametryn2		Ametryn	20	0.05	25
Atrazine1		Atrazine		0.05	25
Atrazine2		Atrazine	20	0.05	25
Prometon1		Prometon		0.05	25
Prometon2		Prometon	20	0.05	25
Prometryn1		Prometryn		0.05	25
Prometryn2		Prometryn	20	0.05	25
Propazine1		Propazine		0.05	25
Propazine2		Propazine	20	0.05	25
Simazine1		Simazine		0.05	25
Simazine2		Simazine	20	0.05	25
Terbutryn1		Terbutryn		0.05	25
Terbutryn2		Terbutryn	20	0.05	25
Atrazine d5		-			

### Submit a Batch in the Walk-Up Workspace

1. In the MPX<sup>™</sup> driver software, in the Workspace pane, click **Walk-Up**.

The Walk-Up workspace opens.

Workspace	Walk-	Up												w Do IL?
• Status	Sub	mit	ted Batches:										0	100
Methods	Chahun		Time Scheduled	Time Completed	Ratch Name	Batch Our	uer .	Scheduled By	Checkded	Samples Co	moleted Semoles	Surrandul Camples	Failed Camples	Broject
sandle the		1	2017/11/27 11:19:42	2017/11/07 11:55:15	Nov 27 Example Cam	vover dab BLT Projec	1 AR5	CIEXDEV/8LT Project	10	10	ordentities seculates	10	0	MPX De
wak-op		2	2017/11/27 11:52:55	2017/11/27 11:59:45	Nov 27 Example Cam	vover dab BLT Projec	A 01	CIEXDEVIELT Project	1	1		1		MPX De
Settings	1	3	2017/11/07 11:52:55	2017/11/27 12:02:04	Nov 27 Example Carry	vover dab BLT Project	1 485	CIEXDEV/8LT Project	1	1		1	•	MPX D
,	- ×	4	2017/11/27 11:55:15	2017/11/27 12:15:50	Nov 27 Example Carry	yover.dab BLT.Projec	t ABS	CIEXDEVIBLT.Project	2	2		2	0	MPX D
Batch														
r the Batch	Sam	nple	s in Batch:										0	100
	Status		Time Submitted	Time Started	Time Completed	Sample Name	Stre	am Assigned Stream	Barcode	Plate Position	Vial Position	Acq. Method	Name	Messa
	~	1	2017/11/27 12:04:22	2017/11/27 12:06:55	2017/11/27 12:08:56	Blank (re-inject)	2	2		2	15	5500Q Triazines with I	MPX S2A dam	
	V	2	2017/11/27 12:11:17	2017/11/27 12:13:48	2017/11/27 12:15:49	Unknown 52 (re-inje	ct) 2	2		2	10	5500Q Triazines with I	MPX S2A dam	
	Sam	nple	Execution His	tory										
	Sam	nple	Execution Hist	tory	Completed	Samole Name	Stream	Assigned Stream	late Position	Vial Position		Messao	se	
	Sam Status	nple	Execution Hist Time Started 2017/11/27 11:23:29	Time ( 2017/11/27 11	Completed	Sample Name	Stream	Assigned Stream F	late Position	Vial Position		Messag	ja	
	San Status	nple	Execution Hist Time Started 2017/11/27 11:23:29 2017/11/27 11:25:30	Time ( 2017/11/27 11 2017/11/27 11	Completed	Sample Name Inse	Stream 1 2	Assigned Stream F	late Position	Vial Position		Messag	p	
	San Status	nple	Execution Hist Time Started 2017/11/27 11:23:29 2017/11/27 11:25:30 2017/11/27 11:30:19	Time ( 2017/11/27 11 2017/11/27 11 2017/11/27 11	Completed 25.30 R 27.39 R 32.29 C	Sample Name Ince Ince al 50	Stream 1 2 1	Assigned Stream F 1 2 2 2 1 2	late Position	Vial Position 1 5		Мезар	je	
	San Status V V	nple	Execution Hist Time Started 2017/11/27 11:23:29 2017/11/27 11:25:38 2017/11/27 11:30:19 2017/11/27 11:32:35	Time ( 2017)11/27 11 2017)11/27 11 2017)11/27 11 2017)11/27 11 2017)11/27 11	Completed 25:30 R 27:39 R 32:20 C 34:36 C	Sample Name Inse Inse al 50 al 50	Stream 1 2 1 2	Assigned Stream F 1 2 2 2 1 2 2 2 2 2 2 2	late Position	Vial Position 1 5 6		Messag	je	
	Sam Status V V	1 2 3 4 5	Execution Hist Time Started 2017/11/27 11:23:29 2017/11/27 11:25:38 2017/11/27 11:30:19 2017/11/27 11:32:35 2017/11/27 11:37:09	Time ( 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11	Completed 25:30 % 27:39 % 32:20 CC 34:36 CC 39:10 CC	Sample Name Inte Inte al 50 al 50 al 10	Stream 1 2 1 2 1	Assigned Stream F 1 2 2 2 1 2 2 2 1 2 1 2 1 2 2 2 1 2 2 2 2	late Position	Vial Position 1 5 5		Messag	je	
	Sam Status V V V	* m ple 1 2 3 4 5 6	Execution His Time Stated 2017/11/27 11:23:29 2017/11/27 11:23:29 2017/11/27 11:30:19 2017/11/27 11:32:35 2017/11/27 11:37:09 2017/11/27 11:39:29	Time ( 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11	Completed 25:30 Ri 27:39 Ri 32:20 Ci 34:36 Ci 34:36 Ci 34:30 Ci	Sample Name Inte al 50 al 10 al 10	Stream 1 2 1 2 1 2 1 2 2	Assigned Stream 8 1 2 2 2 2 1 2 2 2 1 2 2 2 2 2 2 2 2 2 2	late Position	Vial Position 1 6 6 5 5 5		Messag	и	
	Sam Status V V V V V	<pre> + e + + + + + + + + + + + + + + + + + +</pre>	Execution Hist Time Stated 2017/11/27 11:23:29 2017/11/27 11:23:29 2017/11/27 11:32:09 2017/11/27 11:32:09 2017/11/27 11:32:09 2017/11/27 11:32:09 2017/11/27 11:32:09	Tony Time ( 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11	Completed 82530 R0 2530 R0 2739 R0 3229 C1 3436 C1 3436 C1 4430 C1 4605 81	Sample Name inse di 50 di 50 di 10 di 10 di 10 tank	Stream 1 2 1 2 1 2 1 2 1 2 1	Assigned Stream F 1 2 2 1 2 1 2 2 1 1 2 2 2 2 2 2 2 1 2 2 2 2	late Position	Vial Position 1 6 6 5 5 5 5 15		Messag	k	
	Sam Satus V V V V V V V V V V	Imple	Execution His Time Stated 2017/11/27 11:23:20 2017/11/27 11:23:20 2017/11/27 11:32:35 2017/11/27 11:32:35 2017/11/27 11:32:30 2017/11/27 11:32:30 2017/11/27 11:32:30	tory 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11	Completed (2330 R) 2230 R) 3229 C) 3438 C) 34130 C) 4405 B) 4405 B)	Sample Name inse al 50 al 50 al 10 al 10 tank. tank	Stream 1 2 1 2 1 2 1 2 1 2 2 1 2 2	Assigned Stream         I           1         2           2         2           1         2           2         2           1         2           2         2           1         2           1         2           2         1           2         2           2         2	Tate Position	Vial Position 1 6 5 5 5 15 15		Messag	la	
	San Status V V V V V V V	* entropies * entr	Execution Hist Time Stated 2017/11/07 11:23:29 2017/11/07 11:23:29 2017/11/07 11:32:19 2017/11/07 11:32:09 2017/11/07 11:32:09 2017/11/07 11:44:04 2017/11/07 11:46:03	tory Time ( 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 12 2017/11/27 2017/	Completed 25.30 R 22.39 R 32.29 C 39.10 C 39.10 C 46.05 B 46.25 B	Sample Name Inse al 50 al 10 al 10 1	Stream 1 2 1 2 1 2 1 2 1 2 1 2 2 1 2 3 1 2 3	Assigned Stream         8           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         3	late Position	Vial Position 1 6 6 5 5 5 15 15 15 11	Above upper of	Messag ancentration limit was d	je Selected.	
	San Status V V V V V V V V V V	2 3 4 5 6 7 8 9 10	Execution Hist Time Stated 2017/10/27 11:23:20 2017/11/27 11:23:20 2017/11/27 11:23:20 2017/11/27 11:23:20 2017/11/27 11:37:20 2017/11/27 11:37:20 2017/11/27 11:37:20 2017/11/27 11:52:31	tory 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11	Completed 25.30 R 27.39 R 32.20 C 34.34 C 34.34 C 34.34 C 44.05 B 44.25 B 52.54 U	Sample Name inse al 50 al 50 al 10 al 10 al 10 tank roknown \$1 honown \$2	Stream 1 2 1 2 1 2 1 2 1 2 2 1 2 2 1 2 2 2 2	Assigned Stream         F           1         2           2         2           1         2           2         2           1         2           2         2           1         2           1         2           2         2	tate Position	Vial Position 1 6 5 5 5 5 15 15 11 10	Above upper or Carryover was	Messag ancentration limit was d detected.	je Selected	
	Sam Status V V V V V V V V V V V V V V V V V V V	<ul> <li>Imple</li> <li></li></ul>	Execution His/ Time Started 2017/11/27 11:23:29 2017/11/27 11:23:29 2017/11/27 11:32:38 2017/11/27 11:32:35 2017/11/27 11:32:35 2017/11/27 11:34:23 2017/11/27 11:46:23 2017/11/27 11:46:23 2017/11/27 11:46:23 2017/11/27 11:54:33	tory Time 2017/11/27 11 2017/11/27 11	Completed 2530 R 2739 R 2739 R 2739 C 3439 C 3439 C 3439 C 4139 C 4139 C 4139 C 4139 C 45514 U 5514 U	Sample Name inse af 50 af 10 af 10 tank tank reinnum 51 Nanoum 52 ank (tre-inject 1)	Stream 1 2 1 2 1 2 1 2 1 2 1 2 1 2 2 1 2 1 2	Assigned Stream         J           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           1         2           1         2           1         2           1         2	tate Position	Vial Position 1 6 6 5 5 5 15 15 11 10 15	Above upper ci Catryover was	Messag ancentration limit was d detected.	pe delteched.	
	Sam Status V V V V V V V V V V V V V V V V V V V	Imple	Execution Hiss Time Stand Johnney TL2329 2017/11/27 TL2329 2017/11/27 TL2329 2017/11/27 TL3239 2017/11/27 TL3239 2017/11/27 TL3239 2017/11/27 TL3239 2017/11/27 TL3239 2017/11/27 TL3239 2017/11/27 TL523 2017/11/27 TL523	tory 2017/11/27 15 2017/11/27 15 2017/11/27 15 2017/11/27 15 2017/11/27 15 2017/11/27 15 2017/11/27 15 2017/11/27 15 2017/11/27 15 2017/11/27 12 2017/11/27 12	Completed 22.30 R 22.30 R 32.20 C 34.36 C 34.36 C 44.30 C 44.05 B 44.25 B 44.25 B 44.25 U 55.14 U 55.14 U 59.44 B	Sample Name inse inse al 50 al 10 al	Stream 1 2 1 2 1 2 1 2 1 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2 2 1 2	Assigned Stream         F           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2	late Position	Vial Position 1 5 5 5 15 15 11 10 15 15 15 15 15 15 15 15 15 15 15 15 15	Above upper ci Carryover was	Messag ancentration limit was d detected.	je Selected	
	Sans Status V V V V V V V V V V V V V V V V V V V	Imple	Execution His/ Time Stated 30771107 11.23.39 20171107 11.23.39 20171107 11.23.19 20171107 11.23.19 20171107 11.23.19 20171107 11.32.19 20171107 11.32.29 20171107 11.32.29 20171107 11.32.29 20171107 11.32.29 20171107 11.53.13 20171107 11.53.13 20171107 12.08.35	tory 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 11 2017/11/27 12 2017/11/27	Completed 25:30 R) 25:30 R) 32:20 C 33:20 C 33:10 C 45:05 R 46:05 R 46:05 R 46:05 R 46:05 R 46:05 R 46:05 R 46:05 R 46:05 R	Sample Name inte inte af 50 af 50 af 50 af 50 af 10 af 10 tank tank reknown 51 reknown 51 reknown 52 tank (re-inject 1) tank (re-inject 1)	Stream 1 2 1 2 1 2 1 1 2 2 1 2 2 1 2 2 1 2 2 1 2	Assigned Stream         I           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           2         2           2         2           2         2	late Position	Vial Position 1 5 5 5 15 15 11 10 15 15 15 15 15 15 15 15 15 15 15 15 15	Above upper co	Messag ancentration timit was o detected.	je Anteched	
	Sam Status V V V V V V V V V V V V V V V V V V V	<ul> <li>Imple</li> <li></li></ul>	Execution His/ Time Started 307771507 11 23.39 201771107 11 23.39 201771107 11 23.39 201771107 11 23.39 201771107 11 32.39 201771107 11 32.39 201771107 11 32.39 201771107 11 440.23 201771107 11 440.23 201771107 11 45.31 201771107 11 53.13 201771107 11 53.13 201771107 12 50.03 201771107 12 0.03	tory	Completed 223.00 Pk 225.30 Pk 322.00 Ck 34.36 Ck 34.36 Ck 34.35 Ck 44.05 Bk 52.54 Uk 55.14 Uk 55.14 Bk 02.64 Bk 02.64 Bk 02.64 Bk	Sample Name bise bise dise dise dis0 dis0 dis0 dis0 dis0 dis0 dis0 dis0	Stream 1 2 1 2 1 2 1 2 1 2 2 1 2 2 2 2 2 2	Assigned Stream         F           8         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           2         2           2         2           2         2           2         2           2         2	late Position	Vial Position 1 5 5 5 15 15 15 15 15 15 15 15 15 15 1	Above upper of Carryover was	Messag ancentration Bmill was d detected.	je Střected	
	Sans Status V V V V V V V V V V V V V V V V V V V	* mple * 1 2 3 4 5 6 7 8 9 10 11 12 13 14 *	Execution Hiss Time Stated borner(2712)230 2017/11/2712320 2017/11/27113210 2017/11/2711320 2017/11/2711320 2017/11/2711320 2017/11/27114623 2017/11/27114623 2017/11/27114623 2017/11/27114623 2017/11/2712033	tory	Completed 22.30 R) 22.30 R) 32.20 C) 34.36 C) 44.30 C) 44.30 C) 44.05 B) 44.25 B) 44.25 B) 45.514 U) 55.54 U) 55.54 B) 00.56 B) 15.49 U)	Sample Name rise di 50 di 50 di 50 di 10 di 10 dat 10 dat 10 dat 10 dat 10 dat 10 datark knonoun 51 datk (re-inject 1) dark (re-inject) mknovan 52 (re-inject) mknovan 52 (re-inject)	Stream 1 2 1 2 1 2 1 2 1 2 1 2 2 2 2 2 2 2	Assigned Stream         F           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           1         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2           2         2	Tate Position	Vial Position 1 5 5 5 15 15 15 15 15 15 15 15 15 15 1	Above upper or Carryover was	Messag ancentration limit was d detected.	pr	

Figure	3-5	Walk-Up	Workspace
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2. In the Walk-Up section, click **Submit Batch**.

The Submit Batch dialog opens.

Submit Batch			
tep 1: Select a batch	Step 2: Select a QMethod	Step 3: Define limit values	Quant Unit: (none selecte
Project: MPX 👻	Name	Use Name Low	High Region Height
Batch Path: D:\Analyst Data\Projects\MPX\Batch			
June 2017     June 2017     Templates     Freeze.dab     July 20 4 samples.dab     July 10 B1 AAO.dab     July 10 B2 AAO.dab     July 10 B3 AAO.dab     July 10 B1 AAO.dab     July 10 Str1_mixed AAO.dab     July 10 Str1_No IS AAO.dab     July 10 Str2_Nixed AAO.dab			
			Submit

#### Figure 3-6 Submit Batch Dialog

3. Make sure that the correct **Project** is shown and then select the appropriate batch from the list provided.

**Note:** If the batch does not meet the Carryover Detection criteria, then the batch can still be submitted but the Carryover Detection feature will not be invoked. Refer to Requirements on page 10.

#### Figure 3-7 Submit Batch Dialog—Regular Batch

🕎 Submit Batch			
Step 1: Select a batch	Step 2: Select a QMethod	Step 3: Define limit values	Quant Unit: (none selected)
Project: MPX *	Name	Use Name Low	High Region Height
Batch Path: D:\Analyst Data\Projects\MPX\Batch			
<ul> <li>July20 B4 AAO.dab</li> <li>July20 mpx265_str1.dab</li> <li>July20_mpx265_str2.dab</li> <li>July21_simple_str2.dab</li> <li>July21_simple_str2.dab</li> <li>july21_str2long.dab</li> <li>july24_str2long.dab</li> <li>july24_str2long.dab</li> <li>July3 Str1.dab</li> <li>July3 Str1.dab</li> <li>July3 Str2.dab</li> <li>july3 Str2.dab</li> <li>july3 Str2.dab</li> </ul>			
Carryover Detection			
			Submit Cancel

**Note:** If the batch meets the criteria for the Carryover Detection feature, then the **Carryover Detection** check box is automatically selected and a list of available MultiQuant<sup>™</sup> software qmethods is shown.

4. Select the appropriate qmethod from the list provided.

A list of defined limit values that are associated with the selected method is shown. Refer to Define Carryover Detection Limit Values on page 21.

Submit bat	ch							
Step 1: Select	a batch		Step 2: Select a QMethod	Step	3: Define limit va	lues	Quan	t Unit: (none selected)
Project:	МРХ	-	Name	Use	Name	Low	High	Region Height
Batch Path:	D:\Analyst Data\Projects\MPX\Batch		Tri Str 1 and 2_3 IS.qmethod		Bendiocarb_d0			<u>^</u>
			Tri Str 1_2 IS_Row1.qmethod		Fenoxycarb_d0	<u> </u>		
July20	R4 AAO dab	*	Tri Str 1 2 NO IS amethod		Atrazine-d5	-		
July20	mpx265_str1.dab			M	Prometon 1	3	50	
July20	_mpx265_str2.dab				Prometon 2	3	50	
July21	simple_str1.dab				Ametryn 1	3	50	
July21	_simple_str2.dab				Ametryn 2	3	50	
july21	strllong.dab				Atrazine 1	3	50	
o july21	str2long.dab				Atrazine 2	3	50	
o july24	str2long.dab				Prometryn 1	3		1e7
July3 S	itr1.dab				Prometryn 2	3		1e7
o July3 S	itr1_mixed.dab				Propazine 1	3		1e7 0
July3 S	tr2.dab				Propazine 2	3		1e7
a hata e	te? animal data	*			Simazine 1	3		1e7
V Carryov	ver Detection			⊲	I Simarina ?	13	1	11a7 I* ▶
								Submit Cancel

Figure 3-8 Submit Batch Dialog—Carryover Detection Batch

**Note:** All of the transitions contained in the MultiQuant<sup>™</sup> software method are listed. The Low, High, and Region Height values can be modified, if required. Refer to Define Carryover Detection Limit Values on page 21. If the method is being used for the first time, then the original values are shown. If the method has been used in a previous submission, then the values that were used for the previous submission are shown.

5. After all of the required changes have been made, click **Submit**.

The batch is shown in the Submitted Batches pane of the Walk-Up workspace. Any RTD<sup>3</sup> Carryover Detection messages related to the sample are shown in the **Messages** column.

#### Figure 3-9 Samples in Batch

itatus	Time Submitted	Time Started	Time Completed	Sample Name	Stream	Assigned Stream	Barcode	Plate Position	Vial Position	Acq. Method Name	Message
¥ .	2016/11/15 15:43:53	2016/11/15 15:47:56	2016/11/15 15:50:26	Solvent	2	2		3	46	MPX Triazine Stream 2.dam	
× .	2016/11/15 15:53:27	2016/11/15 15:55:44	2016/11/15 15:58:13	Cal 0.1	2	2		3	47	MPX Triazine Stream 2.dam	
× .	2016/11/15 16:01:16	2016/11/15 16:03:32	2016/11/15 16:06:01	Cal 1 ng	2	2		3	48	MPX Triazine Stream 2.dam	
× .	2016/11/15 16:09:05	2016/11/15 16:11:22	2016/11/15 16:13:52	Cal 10ng	2	2		3	49	MPX Triazine Stream 2.dam	
× .	2016/11/15 16:16:53	2016/11/15 16:19:09	2016/11/15 16:21:38	Blank	2	2		3	50	MPX Triazine Stream 2.dam	
	2016/11/15 16:24:42	2016/11/15 16:26:58	2016/11/15 16:29:27	Test 25ng	2	2		3	51	MPX Triazine Stream 2.dam	Above upper concentration limit
× .	2016/11/15 16:32:30	2016/11/15 16:34:46	2016/11/15 16:37:15	No Carryover	2	2		3	52	MPX Triazine Stream 2.dam	
	2016/11/15 16:40:19	2016/11/15 16:42:36	2016/11/15 16:45:05	Check 50ng	2	2		3	53	MPX Triazine Stream 2.dam	Above upper concentration limit
	2016/11/15 16:48:08	2016/11/15 16:50:25	2016/11/15 16:52:55	Carryover Yes	2	2		3	54	MPX Triazine Stream 2.dam	Possible carryover detected.
×	2016/11/15 16:55:57	2016/11/15 16:58:13	2016/11/15 17:00:42	Carryover No	2	2		3	37	MPX Triazine Stream 2.dam	

**Note:** The data (wiff) file that is generated will contain all of the samples in the submitted batch, including any re-injected Blank samples and any re-injected carryover flagged samples.

### **Define Carryover Detection Limit Values**

#### Notes:

- The Carryover Detection limit values must be defined during batch submission in the Walk-Up workspace.
- Although the MultiQuant<sup>™</sup> software allows a maximum of 26 digits in each of the Lower Limit Calculated Concentration and Upper Limit Calculated Concentration fields, a maximum of 7 digits is allowed in the Carryover Detection Limit values table.
- Commas (,) are not supported as decimal separators. If a comma is used, then the MPX<sup>™</sup> driver software ignores the comma and interprets the value as an integer. For example, if 5,01 is typed, then the software interprets this value as 501.
- 1. Make sure that the **Use** check box is selected for each analyte to be evaluated by the Real Time Data Dependent Decision (RTD<sup>3</sup>) feature.

**Note:** By default, the Use check box is selected for all analytes. Users can clear the check box, if required. However, if the Use check box is not selected, then the corresponding analyte will not be evaluated by the RTD<sup>3</sup> carryover detection function. The Use check box cannot be selected for analytes that have been identified as internal standards in the quantitation method (qmethod) file.

#### Figure 3-10 Use Check Box

Use	Name	Low	High	Region Height	
	Bendiocarb_d0				A.
	Fenoxycarb_d0				
	Atrazine-d5				
	Prometon 1	3	50		
V	Prometon 2	3	50		
V	Ametryn 1	3	50		
	Ametryn 2	3	50		
	Atrazine 1	3	50		
V	Atrazine 2	3	50		
1	Prometryn 1	3		1e7	
V	Prometryn 2	3		1e7	
	Propazine 1	3		1e7	U
V	Propazine 2	3		1e7	
V	Simazine 1	3		1e7	
17	Cimarina ?	5		147	Ŧ
4					

2. Set the detection limit values using the guidelines provided. Refer to Table 3-1.

Field	Description
Name	The name of the analyte, as defined in the quantitation method (qmethod) file. This field is automatically populated and cannot be modified.
Low	The lower limit of the calculated concentration used by the RTD <sup>3</sup> Carryover Detection function for the evaluation of <b>Blank</b> samples.
	The Low value is mandatory.
	The Low value can be modified.
	The Low value cannot be less than or equal to zero.
	• The Low value can contain a maximum of five decimal places and seven digits.
	• The Low value must be between 0.00001 and 9999999.
	• The Low value must be less than the High value.

#### Table 3-1 Detection Limit Value Guidelines

Field	Description
High	The upper limit of the calculated concentration used by the RTD <sup>3</sup> Carryover Detection function for the evaluation of <b>Unknown</b> samples.
	• The High value can be modified.
	• The High value cannot be less than or equal to zero.
	• The High value can contain a maximum of five decimal places and seven digits.
	• The High value must be between 0.00001 and 9999999.
	• The High value must be greater than the Low value.
	• If the corresponding Region Height value is provided, then the High value can be left blank.
Region Height	An upper limit defined in counts per second (cps) either alone or in conjunction with the High value.
	• The Region Height window is equivalent to 1.5 times the normal Retention Time window used for the quantitation method (qmethod) analyte integration.
	• The format is scientific notation only, with a maximum of two decimal places and a maximum exponent value of seven.
	• Acceptable formats include values such as: 1e7, 1.0e7, and 9.99e6.

Table 3-1 Detection Limit Value Guidelines (continued)