Standard QC Protocol

Using Standard QC Error Action Functions in ICP-MS MassHunter

Introduction

MassHunter Quality Control (QC) functionality includes the ability to set QC limits and failure flags on many common QC criteria such as internal standard (ISTD) or QC sample recovery and stability, calibration linearity and range, sample measurement precision (CPS, %RSD) and blank concentration. However, unless the optional Intelligent Sequencing software was enabled, it was not possible to set automatic Error Action actions to be executed for a QC failure.

Purpose

The configuring and parameter setup of QC Checks for use in a standard QC Error and Action function in ICP-MS MassHunter Software.

Scope

The protocol outlines the Standard Error Actions in the software and the configuring of parameters using QC checks standards.

Referenced Documents
- Agilent Familiarization Guide G8400-90038
- Agilent Intelligent Sequence Guide G7206-90009

Responsibilities
1. **Users**
    1.1. All Users must obtain training with TRACES Staff prior to system operation. It is the responsibility of the User to ensure they have a good understanding of the instrument and all operation protocols.
    1.2. If additional training sessions are needed it is the responsibility of the User to schedule these with TRACES Staff.

Equipment
- Agilent 7900 ICP-MS
- MassHunter for ICP-MS (v5.2)

'New' QC Checks

The 'new' QC has added the ability to automatically calculate spike recoveries with the addition of two additional sample types, Spike ref and Spike. These new sample types allow the user to set spike amounts for each analyte element and calculate the% spike recovery compared to the unspiked reference sample. Unlike Intelligent Sequencing, no sophisticated filtering of flagging or Error Action based on the relative concentration of the spike-to-spike reference sample is possible.

Configuring FullQuant Outlier with QC Error Action

QC Error Action can be configured from either Instrument Control or Data analysis, depending on whether you are creating a new acquisition batch from scratch, or adding QC Error Action functionality to an existing batch. The steps are the same, though the user interface to select some functions differs slightly. Both methods are demonstrated below.

To open the Batch File you want to configure,

[Open Folder] from the [Batch] group on the [Home] tab in the [ICP-MS MassHunter] window or [ICP-MS Data Analysis] window.

- From the [ICP-MS Data Analysis] window
  Click [Edit] from the [Method] group on the [Home] tab to open the [Method Editor] window.
  Under the Method Development Tasks pane on the left of the screen, click [QC Setup] from the [Advanced Info] group.
  The FullQuant Outlier Setup pane is displayed.

- From the [ICP-MS MassHunter] window
  Click [QC] from the [Acquisition) group in the
  Task Navigator. The FullQuant Outlier Pane is
  displayed.

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The available QC check items are displayed as shown below.

Acq Method	Data Analysis Method	Sample List					

Basic Information	Analyte	Full Quant	Semi Quant	Isotope Ratio	FullQuant Outlier	QC Parameters	Worklist Action

	Method			
Outlier	Minimum Value	Maximum Value	Reference	Error Action
Calibration Curve Fit R	0.95			Ignore and Continue
Relative Standard Error %				Ignore and Continue
Relative Error %				Ignore and Continue
ISTD Recovery % [compared with CalBlk]	80	120		Ignore and Continue
Spike Recovery % [compared with SpikeRef]			Spike Ref	Ignore and Continue
QC Sample Conc Stability % [use 'QC1' Sample]			QC1	Ignore and Continue
QC Sample Conc Stability % [use 'QC2' Sample]			QC2	Ignore and Continue
QC Sample Conc Stability % [use 'QC3' Sample]			QC3	Ignore and Continue
QC Sample Conc Stability % [use 'QC4' Sample]			QC4	Ignore and Continue
QC Sample Conc Stability % [use 'QC5' Sample]			QC5	Ignore and Continue
Count RSD %		5	>= 10000 cps	Ignore and Continue
Blank Conc Level % [use 'BlkVrfy' Sample]		100	BlkVrfy	Ignore and Continue
Out of Calibration Curve Concentration Range %		110		Ignore and Continue

You can enter control limits for each QC item. In most cases they are percentages compared to the Reference value. These entries should be self-explanatory. The blue hyperlinks in the Reference column lead to the Calibration pane, where the actual reference values can be entered for each Reference type as shown below. For example, the reference (expected) value for QC1 is set to 5 ppb for all 4 analytes in the table below. The spike amount is also set to 5 ppb for each analyte. However, there is no requirement for the values to be the same for different analytes.

	Analyte							Level			QC					Blank
	Mass	Name	RT	Curve Fit	Origin	Min Conc.	Units	Spike Amount	Level 1	Level 2	Level 3	QC1	QC2	QC3	QC4	QC5	BlkVrfy
1	75	As(1)	2.792	Linear	Blank offset	<None>	ppb	5	1	5	10	5					
2	75	As(2)	3.658	Linear	Blank offset	<None>	ppb	5	1	5	10	5					
3	75	As(3)	4.293	Linear	Blank offset	<None>	ppb	5	1	5	10	5					
4	75	As(4)	7.140	Linear	Blank offset	<None>	ppb	5	1	5	10	5					

After completing the required reference information in the calibration pane (above), click "FullQuant Outlier" on the Method Development Tasks pane again to return to the previous pane.

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QC Sample Types

The 5 QC sample types (QC1 - QC5) can be used for any QC check that has an expected lower and upper control limit. They can be renamed to reflect their functionality, or to conform to regulatory requirements or standard operating procedures. For example, they could be named CCB, CCV, LCS, etc. To rename them, click the [Edit QC Level Caption] button above the Outlier table.

The following dialog box is displayed allowing you to assign a name to each of the five QC samples. In this example, QC1 was named CCB etc. Click [OK] to accept your changes.
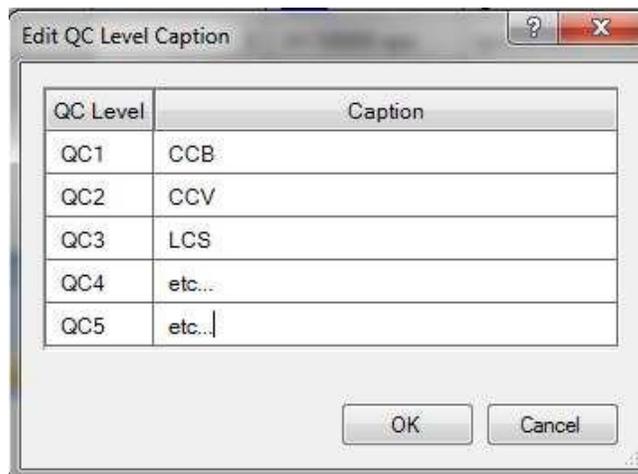
Error Action Options

There are four simple actions that can be automatically executed during sample analysis if a QC check is out of your specified range. These are shown below.
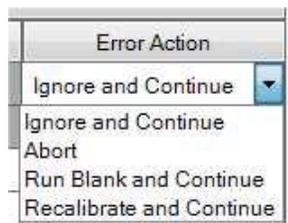
They are mostly self-explanatory with one exception. "Recalibrate and Continue" requires that your sample list is set up in Block Mode, meaning that you have designated a calibration block containing your calibration standards in order.

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This is set up from Instrument Control when creating the sample list for the batch. Click the [Use Block List] button at the top of the Sample List Pane (Sequence).

The sample list layout changes from the default format which shows all samples in the batch in order, to the Block List format which shows the samples grouped into blocks of related sample types. The default (empty) block list is shown below.
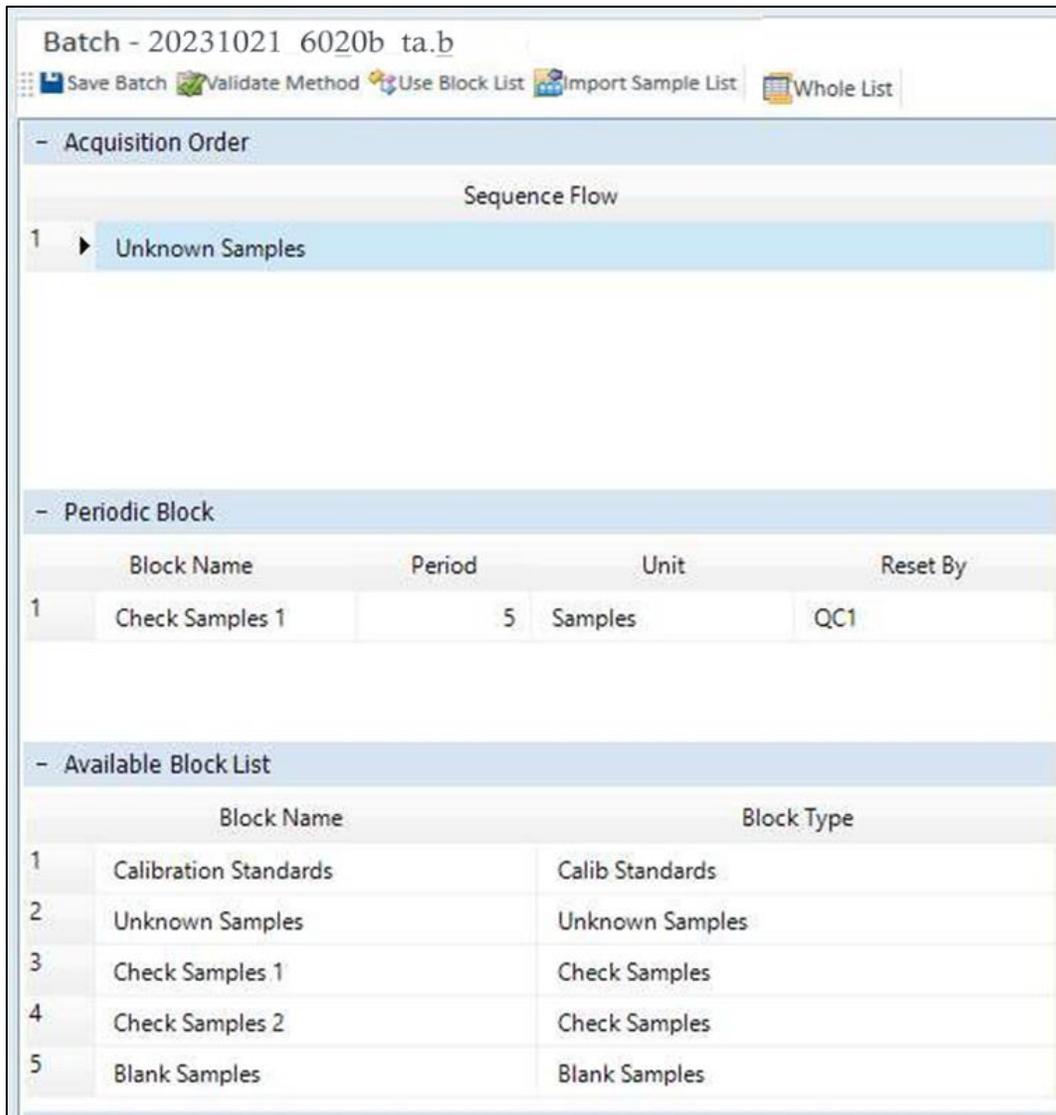
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The list of blocks to be analyzed in order is listed in the top section under Sequence Flow. The default as shown is only the Unknown Samples block. When this block is highlighted as shown, the sequence table displayed to the right contains the samples in this block, as shown below.

To execute the Error Action "Recalibrate and Continue", a calibration block must be defined and added to the Sequence Flow table. To do this, right click anywhere in the Unknown Samples blank area.
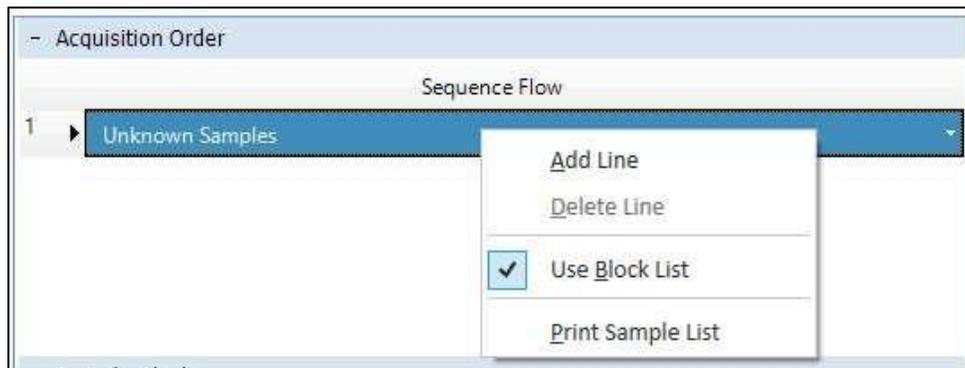
Select [Add Line] from the list. A second line is added to the Acquisition Order list. Click on the first line to enable a pull-down arrow on the right which allows you to select the block type. Select "Calibration Standards" to create a calibration block, which will be the first group of samples to be analyzed. Fill in the table to the right labeled Calibration Standards with your entire calibration set, including the calibration blank, calibration standards, and any additional calibration checks you might want to run automatically if a recalibration occurs, such as an initial calibration blank (ICB) and initial calibration verification (ICV) standard. This entire list is re-run if the Error Action "Recalibrate and Continue" is executed.

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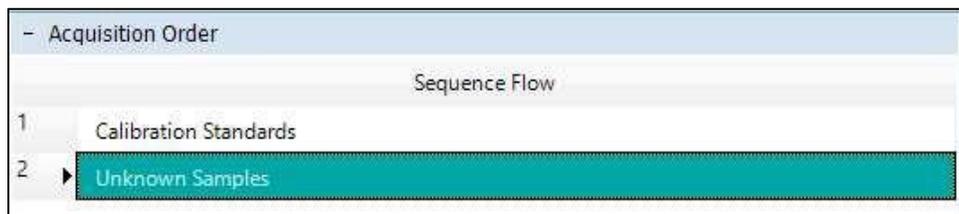
You have now correctly configured QC error action. Save the Batch and add it to the Queue to run it.

*The TRACES Manager will provide full details during hands-on training.