

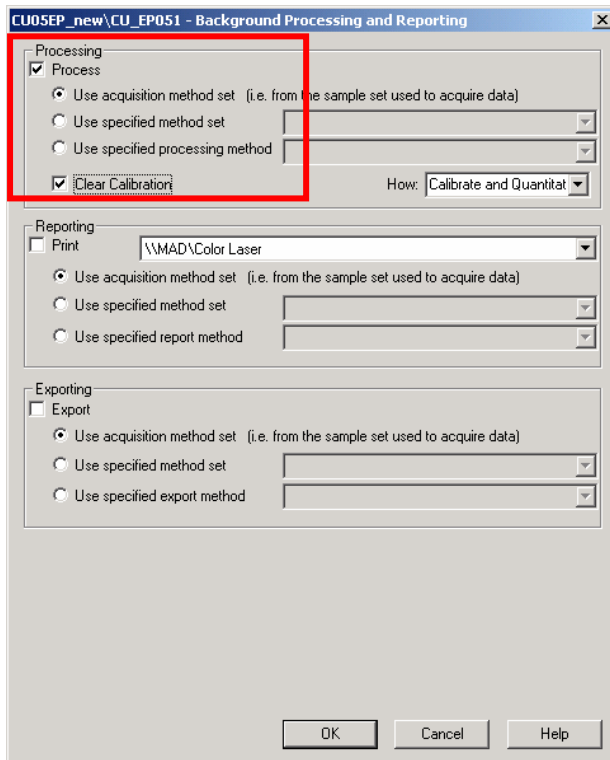
Managing Manually Integrated Results in Result Sets

Empower users really appreciated the ease and traceability of creating manually integrated results, particularly for tricky chromatographic analyses such as impurity profiles. However, using the correct calibration curve and also retrieving the correct result version can prove troublesome if the results are created as standalone individual results. Managing results via Result Sets give huge advantages in easily reviewing data and using the power of complex processing built into the Sample Set, but can you combine these two capabilities?

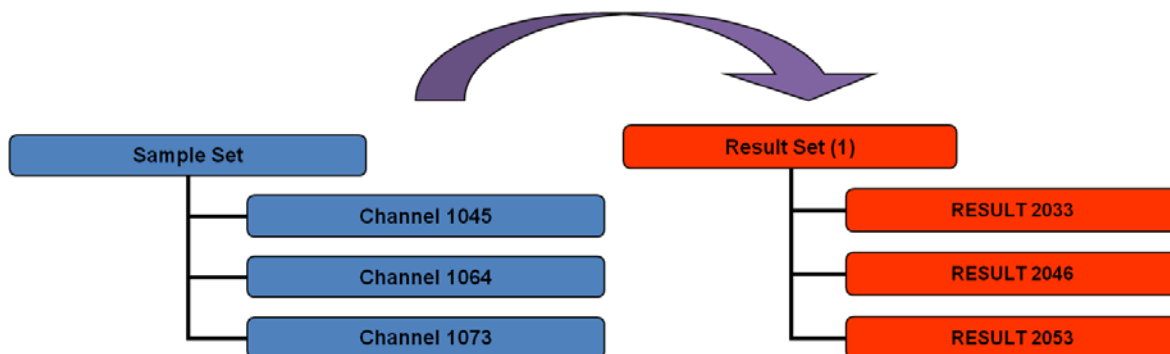
The answer is YES, as long as you know how. It is also important to understand the different procedures to use for SAMPLES and CONTROLS versus the right approach for STANDARDS.

The trick is to begin your evaluation of the automatics integration from the Result Set. After optimizing your processing method to get the best integration for the most chromatograms, save the processing method, ensuring this new method is in the required method sets of your Sample Set. You should be sure that at least the Standards are all correctly identified by this method. This is one adjustment that is difficult to correct manually.

Then create the best Result Set you can, using the Sample Set Process tools and remembering to select the “Using Acquisition Method Set Option” to be sure all special processing instructions are included (eg brackets, multiple methods, PDA or MS extractions, summary calculations).



This will create the Result Set that you are going to review and alter.



From this point the procedure is different depending on the required alterations:

For manually integrating or identifying SAMPLES and CONTROLS:

Select this result set and take into Review.

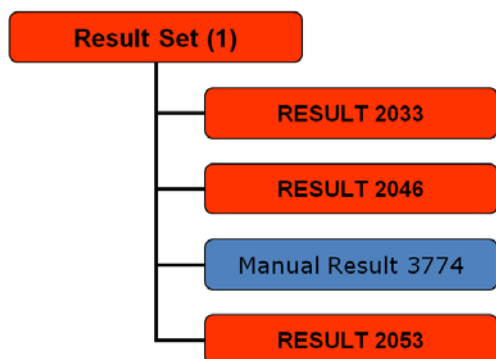
As you step through the chromatograms, review both the integration and the peak identification. If you find a sample or control that needs altering, make the adjustment. Manually integrate the peak then press ONLY QUANTITATE or use the manual identification tool. The results will be immediately updated with the new AMOUNTS.

Do not press the CALIBRATE button during this process as this will affect the calibration curve and you will not be able to Save Result.

NB: if you do not wish the lab to see the new quantitated amounts, use privileges to hide fields like Amount, %Amount, Area and % Area. This prevents analysts “tweaking” results into spec.

After each result is updated to be correct, Save the Result Only using the File Save tool. As you have not altered the calibration curve or the processing method you should not be asked to save those first. If this question comes, or you cannot select the “Save Result” and only the “Save All” options, you must have altered the processing method or the calibration curve accidentally and should cancel and start again for that result.

The new result is inserted into the result set:



Result 3774 is new version of 2046

This can be the FINAL result set. You have both the automatic and the manual version of the result and you will have entered a reason why manual integration was necessary if you have the audit trail switched on. If you print this Result Set it should automatically recognize that there are 2 results for one channel and will only include the most recent version. Hence, in this example, result 2046 was superseded and will not be printed.

If you print from Results you will get 2 versions included.

This can be prevented by setting your table properties to “exclude duplicate results” which is a recent feature in Empower 2.

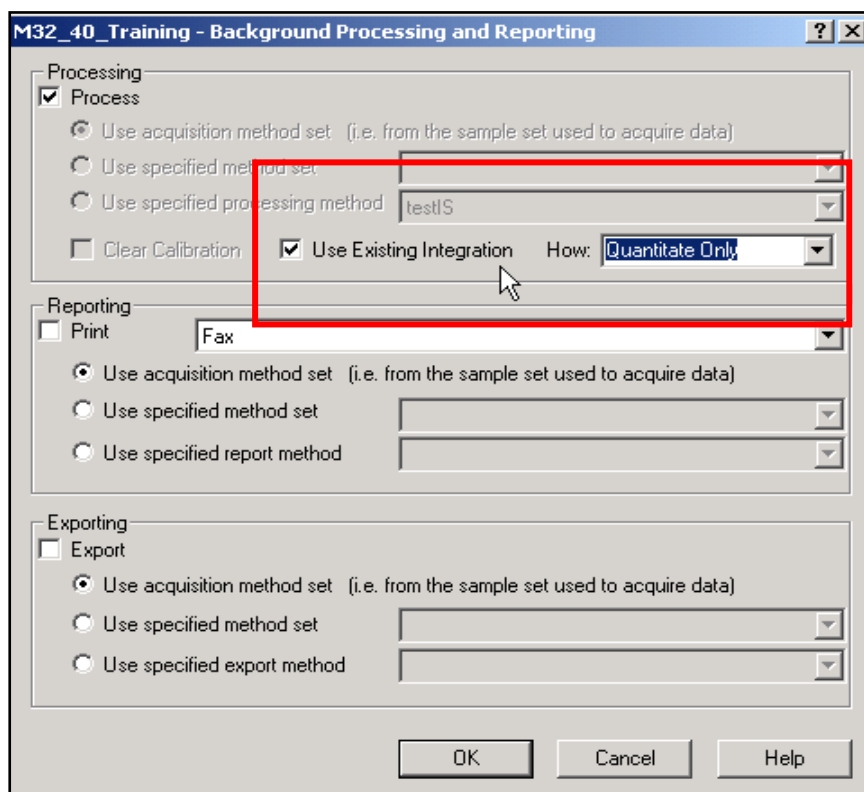
For manually integrating STANDARDS:

For standards the process is a little more involved. This procedure can also be followed if you have to correct both STANDARDS and SAMPLES.

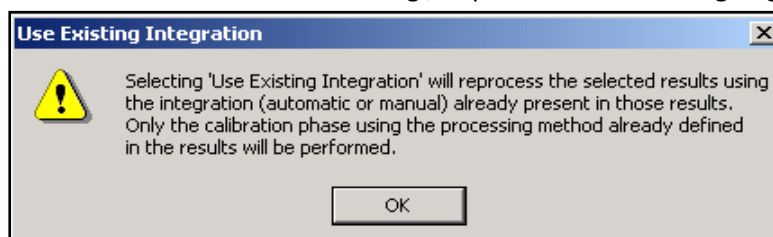
Begin by taking your “best effort” Result Set into Review. Step through the chromatograms and update the Integration ONLY. DO NOT PRESS CALIBRATE or change the processing method at all. Pressing Quantitate is not necessary either as we will perform all Calibration and Quantitation in the next step. Then save the results. I still recommend doing this one at a time as you alter them.

The result set will still have a similar look to the one above, but the manual results will have no peaks identified or Amounts calculated.

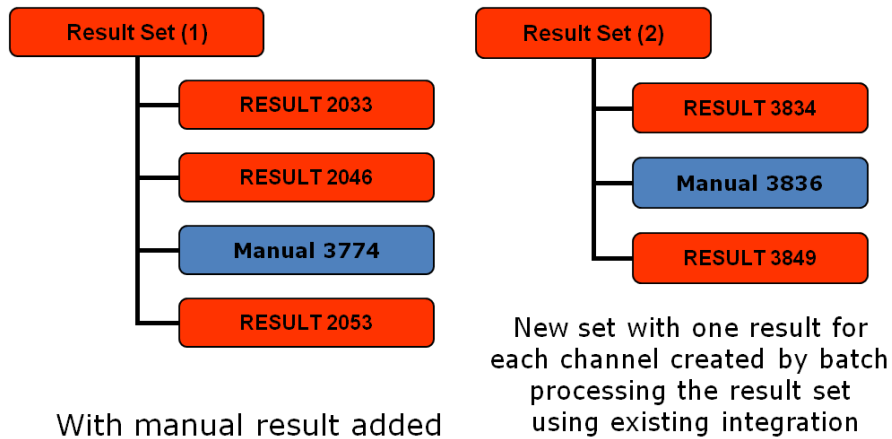
Now we need to process the Result Set again to perform the Calibration and Quantitation. When you batch process a Result Set there is an additional option to choose that is not available when you process from a Sample Set: - “Use Existing Integration” . You should tick this option.



You should choose Calibrate and Quantitate here to ensure the Cal Curve is created and the results calculated. There will be a warning / explanation of what is going to happen:-



New calibration curves will be created based on the Sample Set, Method Set and Processing Method settings. The only step that will be ignored is the integration step. Where two versions of results exist in the original Result Set, only one, the most recent will be processed in the second Result Set:



Result Set 2 then goes forward to your review and approval process.

These two processes can be summarized as follows:-

Samples only

Select the sample set and batch process with the acquisition method set
(Ensure that the correct and optimized processing method has been added to the acquisition method)



Select the result set, take to review



Do not change any of the **standards** or press **CALIBRATE**
(this will invalidate the calibration curve)



Select the samples, make manual changes to the integration



Re-quantitate by clicking on the QUANTITATE Icon



Use Manual Identification if required



File, save, **Result only** and add a reason **WHY** you have manually integrated if prompted



Repeat for each sample, if necessary.

Standards and Samples

Select the sample set and batch process with the acquisition method set
(Ensure that the correct and optimized processing method has been added to the acquisition method set)



Take the result set to Review



Make manual integration changes to both the standards and the samples

(NB: **Do not press CALIBRATE** during this operations

There is no need to calibrate or quantitate standard or samples prior to saving the results).



File, save, **Result only** and add a reason **WHY** you have manually integrated if prompted



Repeat for all standards and samples



Exit Review



Select the Result Set from the project window



Select to Process using the Acquisition Method Set (default setting)



Tick the box to enable “use existing integration”
Calibrate and Quantitate” and tick to “clear calibration”



A new Result Set will be generated

The final result set is now ready for review, electronic sign off, locking channels or printing. It is easy to see which results belong together, which have been manually processed and why. Everything required for compliance is here and you have the right calibration curves associated with the right results. Easy!

If you have any additional comments or suggestions about this article, please let us know in this forum. If you need some extra training or help implementing this procedure in your lab, please call your local Waters support team.