

Procedure to Manually Modify Results in an Empower Result Set when Standards and/or Unknowns Require Manual Peak Identification

This procedure is to be used when you need to manually modify both standard and unknown/control results within an Empower result set.





The process to subsequently calculate summary custom fields is also included.

There is another, similar procedure available: [TECN10195095](#) – Managing Manually Integrated Results in Result Sets. The procedure in [TECN10195095](#) is more straightforward but is to be used if you only need to modify the integration of standards and/or unknowns and you do not need to manually re-identify peaks within standards. The procedure written herein can be used for all combinations of both manual integration and manual peak identification in both standard and unknown/control sample types.

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Manually Processing Empower Data


1. BATCH PROCESS SAMPLE SET AS USUAL: Process your sample set as you normally would to create a result set.
2. MAKE NECESSARY MANUAL CHANGES TO THE STANDARD(S) IN REVIEW
 - a) Bring the result set into Review.
 - b) Modify the standard results as necessary: modify peak integration as necessary and then Calibrate  all standard results you have manually integrated. If you need to manually identify any peaks in the standards, use the Manually Identify tool  to adjust the standard peak's identification. When you manually Identify the standard peaks, the calibration curve(s) is updated. Therefore, DO NOT use the Calibrate button  after you use the Manually Identify tool  as doing so will erase the manual peak identification you have just performed.
 - c) Save the modified results: File > Save > All.


Result: Modified standard results are saved as individual results outside of the result set. An updated calibration curve is created, associated with the processing method, and saved.



Note: Because the calibration curve has been updated, all of the unknowns/controls need to be re-quantitated against the modified curve regardless of whether or not you need to make manual modifications to the unknowns/controls.

3. MAKE NECESSARY MANUAL CHANGES TO THE UNKNOWN(S) RESULTS IN REVIEW AND RE-QUANTITATE ALL UNKNOWN RESULTS:


- a) For each unknown/control result that requires manual integration and/or peak identification changes:

Modify the unknown/control result as necessary in the following order: first modify peak integration as needed within a result, then Quantitate  the manually integrated result. Next, if you need to

manually identify any peaks, use the Manually Identify tool  to adjust the peak's identification.

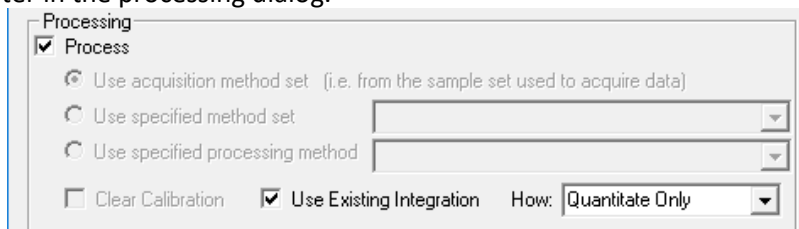
When you manually Identify the unknown/control peaks, the peaks are also quantitated against the current calibration curve. Therefore, DO NOT use the Quantitate button  after you use the Manually Identify tool  as doing so will erase the manual peak identification you have just performed.

- b) For each unknown/control result that **does not** require manual integration and/or peak identification changes:

Click the Quantitate button  to quantitate the result using the standard curve that was modified in Step 2 above. Results that do not require manual modification still need to be re-quantitated against the updated calibration curve.

- c) Save the modified results: File > Save > All.

ALTERNATIVE to Step b), IF you have only made manual changes to integration and you have not re-identified any unknown/control peaks and you do not need to summarize custom fields, you can batch process to re-quantitate the unknowns/controls using 'How: Quantitate only' and enable the 'Use Existing Integration' parameter in the processing dialog.



Final Result: The unknown/control results have been re-quantitated against the updated calibration curve and are saved within the result set and supersede the previous results for the same channels; if manual integration or manual peak identification was performed, those manual changes remain intact. A new result set is NOT created.

Tip: The updated standard results are saved outside of the result set. Be aware that when navigating within the result set, the previous standard results are present and are associated with the previous calibration curve. Because the standards are saved outside of the result set, in order to view the relevant standards and unknowns/controls, you can use a view filter that shows only the latest results for each channel. See the relevant section in this document for information on creating this view filter.

Sample Type	Channel	Channel Id	Sample Set Id	Result Set Id	Date Processed	Result Id	Processing Method
Unknown	VWD.0.0	4781	4732	6397	1/25/2019 5:02:54 PM EST	6428	M1021
Unknown	VWD.0.0	4775	4732	6397	1/25/2019 5:02:35 PM EST	6431	M1021
Standard	VWD.0.0	4741	4732		1/25/2019 5:02:15 PM EST	6430	M1021
Standard	VWD.0.0	4736	4732		1/25/2019 5:02:10 PM EST	6429	M1021
Control	VWD.0.0	4900	4732	6397	1/25/2019 5:00:47 PM EST	6426	M1021
Control	VWD.0.0	4905	4732	6397	1/25/2019 5:00:47 PM EST	6427	M1021
Unknown	VWD.0.0	4876	4732	6397	1/25/2019 5:00:46 PM EST	6422	M1021
Unknown	VWD.0.0	4894	4732	6397	1/25/2019 5:00:46 PM EST	6425	M1021
Unknown	VWD.0.0	4888	4732	6397	1/25/2019 5:00:46 PM EST	6424	M1021
Unknown	VWD.0.0	4882	4732	6397	1/25/2019 5:00:46 PM EST	6423	M1021

Figure 1: Standard results are not included in the result set and therefore have no Result Set ID. The Date Processed for the modified results and calibration curve is updated to the date/time the user pressed File > Save > All.

Summarizing Custom Fields in a Result Set after Results Within the Result Set have been Manually Modified and Saved

- ALTER THE SAMPLE SET TO 'DON'T PROCESS OR REPORT' WITH SUMMARIZE CUSTOM FIELD LINE SET TO 'NORMAL': Bring the Sample Set into Alter Sample. In the Processing column, set all lines to 'Don't Process or Report' EXCEPT for the Summarize Custom Fields line. (You can use Ctrl+D to copy this setting down to all rows.) Set the Summarize Custom Field line to 'Normal'.

Sample Type	Function	Label Reference	Processing
Standard	Inject Controls		Don't Process or Report
Control	Inject Controls		Don't Process or Report
Unknown	Inject Samples		Don't Process or Report
Unknown	Inject Samples		Don't Process or Report
Control	Inject Controls		Don't Process or Report
	Equilibrate		
	Summarize Custom Fields		Normal

- BATCH PROCESS WITH 'QUANTITATE ONLY' TO DETERMINE THE SUMMARY CUSTOM FIELDS: Re-process the result set using 'How: Quantitate only'. It is OK to leave the 'Use Existing Integration' parameter disabled or to enable it (because all injection rows are set to 'Don't Process or Report', this setting has no effect).

Processing

Process

Use acquisition method set (i.e. from the sample set used to acquire data)

Use specified method set

Use specified processing method

Clear Calibration Use Existing Integration How:

Result: The summary custom fields have been determined using unknown/control results *and standard results* within the Result Set. No new results have been created and a new result set is also not created.

Note: *This process is intended for use with summary custom fields that only include Unknown and/or Control sample types. If the summary custom fields include standard results, the standard results included will be the original, unmodified standard results from when the Sample Set was initially processed.*

A *No results produced for this processing job* message will appear in the Message Center. This is accurate, since no new results were created.




All Messages Search Messages E-Mail Queue									
Message Id	Type	Category	Date	Application	User	User Location	Project	Message	
1	61	Error	Processing	11/20/2018 4:40:09 PM EST	Processing Server	System/Administrator	M1021_2017_02	No results produced for this processing job.	

Creating a View Filter to View the Latest Results for each Channel

Use a result view filter that shows the latest results for each channel. Note there is a view filter in the Default project called **Latest Result for Each Channel** that can be copied to your project. It may be useful to add the Channel ID, Sample Set ID and Result Set ID to this view filter, and to remove the ordering on Date Acquired and instead add ordering to the Date Processed field.

Channel Id ()	Sample Set Id ()	Result Set Id ()	Date Processed (Descend)	Result Id ()
				MAX BY Channel Id (CHROM_ID)

Information Useful to Understanding these Procedures

1. When standards within a result set are manually integrated, the new standard results are saved within the existing result set. In order to then update the calibration curve, the standards need to be either manually calibrated  in Review or batch processed with 'Use Existing Integration' and How: 'Calibrate and Quantitate' or 'Calibrate Only.'
2. When standards within a result set are manually identified, they are also calibrated so an updated calibration curve is associated with the processing method. Because they were calibrated, the new standard results are saved as individual results outside of the existing result set.
3. When unknowns/controls within a result set are manually integrated and/or manually identified, the new results are saved within the existing result set.
4. The processing setting of 'Use Existing Integration' does not retain the manual peak identification; when results are batch reprocessed with this setting, the peak identification defined by the processing method is re-applied and manual peak identification is erased.
5. Whenever you batch process or when you apply the Calibrate  or Quantitate  button in Review, the peaks in the results that are processed will be automatically identified based on the processing method used. Any manual peak identification present is erased.
6. If you need to make manual changes to unknowns/controls and you don't need to make any manual peak identification changes, you can make the necessary manual changes in Review, and then batch process the result set with 'Use Existing Integration. If you need to quantitate this data against a standard curve, the appropriate standard curve must be associated with the processing method you are using.
7. If you need to manually identify unknown/control peaks and quantitate them against a modified calibration curve, you will need to make all necessary manual changes in Review (make integration changes first and then manually identify the peaks) AND you will need to Quantitate each result, even the ones that don't require manual integration or peak identification changes. This is only true if you modified the calibration curve.