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System Policies and Privileges for Processing Data in Empower Software with Data Integrity in Mind

Explore how Empower Chromatography Data Software System Policies and privileges can be used to control what users can or cannot do when processing data, particularly when working in the Review window

INTRODUCTION

With increased scrutiny around Data Integrity, it is important for Quality Units and Regulators to understand the Empower™ Software capabilities for processing data and the need for varied levels of flexibility. There is a perception that analysts may use Processing Method parameters or manual integration to 'polish results' and cause otherwise out of specification (OOS) samples to pass laboratory test requirements, such as assays and impurity methods. In order to fully ascertain what is happening in the laboratory, both the Quality Unit and Regulators should be fully aware of how an organization utilizes the Review window to optimize Processing Method parameters. This white paper will walk through the current system policies and privileges in Empower 3Software that effect what analysts can and cannot do when processing data, focusing on the use of Review.

SYSTEM POLICIES

System policies control the behavior of Empower Software for the whole application. They also control certain aspects of how all users accessing the system interact with the software. The Empower system administrator can set rules governing user accounts, log in procedures, full audit trail default settings, data processing techniques, result sign-off requirements, and date formats. System Policies help define the peak detection and integration techniques, and calculations that Empower uses to process data.

There are several general data processing system policies which effect processing data:

- **Calculate % deviation of point from curve** – changes the formula for calculating % deviation.

- **Allow Interactive System Suitability when acquiring in RUN ONLY mode** – Interactive System Suitability, such as Stop on Fault, can be triggered when in Run Only mode. It is recommended to operate in the Run and Process mode so that all result(s) will be saved in a regulated environment.

There are also system policies which control the use of the Apex Track Algorithm:

- **Allow the use of Apex Track integration** – Enables the use of the Apex Track algorithm in the Empower database.

- **Default settings used when creating new projects**
  - Enable Apex Track Integration – Sets the default for new projects.
  - Default Integration Algorithm – Sets the default for new Processing Methods.

There is also one critical policy which adds a control for users working in Review:

- **Prompt user to save manual changes made in Review** – If a user exits from Review after creating a result(s) they will be prompted to save the result(s). In Figure 1 the message reads, "Do you wish to save all modified results?" If users save results at this point, it will automatically save the last version of all results and any related changes (i.e. calibration curves or methods).
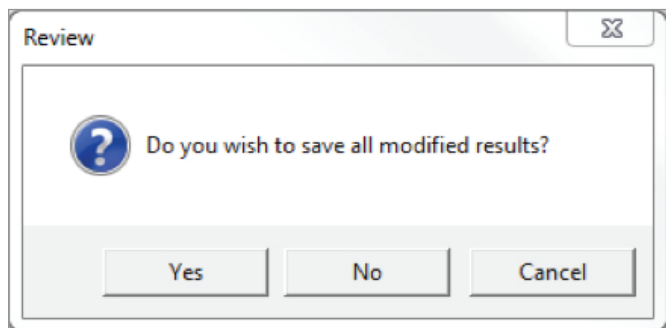

Figure 1. Save results message when exiting from Review.

Any results saved in the Review window in this manner will automatically be labeled as manual results regardless of whether manual integration was used.

PROCESSING METHOD PRIVILEGE OPTIONS

Empower Software allows users to operate under a set of defined privileges that collectively define an overall user type. It is possible for an individual user to be able to log in with a different user type, with a different set of privileges, if they have to perform a specific task. Depending on the tasks performed, the system administrator can assign or remove the privileges associated with a user type. In order to properly validate Empower it is extremely useful to understand how these privileges operate and to document the privileges that laboratory users need to perform their work.

The privileges associated with processing methods have a significant effect on what users can do in the Review window:

- **Lock Methods** – A locked method can be used to generate results, however, it cannot be modified.

- **Unlock Methods** – This privilege allows a user to unlock a method for editing purposes. This privilege should most likely be given to lab managers or group leaders.

- **Delete Processing Methods** – This privilege should only be granted to a high level administrator. It should be noted that any processing methods associated with existing results will not be deleted.

- **Save Processing Method** – Allows the user to create new processing methods and/or modify existing processing methods. This allows users to modify ALL parameters in any section of the processing method. It is important to note that the more detailed privileges described below have no effect if this privilege is granted (Figure 2).

If the Save Processing Method privilege is NOT granted, the ability to modify a processing method depends on whether or not any of the next three privileges are granted. This enables an administrator to grant access to only specific parameters in the processing method.

- **Modify Integration Parameters** – Allows the user to modify peak detection and integration parameters on the Integration tab, such as peak width and detection threshold. This privilege is required for users to optimize integration and account for day-to-day variation in peak shape.

- **Modify Component Times** – Allows the user to modify the expected retention times of named peaks on the Components tab. This privilege is required for users to account for day-to-day variation in retention times and ensure correct peak identification.

- **Modify Component Constants/Default Amounts** – Allows the user to modify the CConst fields on the Components tab. This may be required to modify constants used to capture values such as Label Claim or Moisture Content, when these values periodically require updating. This also allows the user to modify existing Default Amounts.
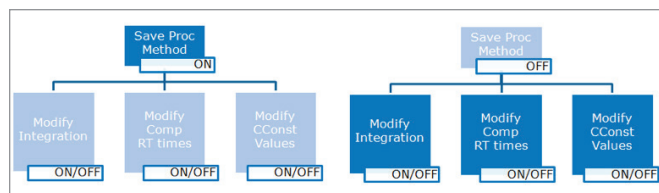

Figure 2. Hierarchy of Processing Method privileges. The bold color indicates which privileges are in effect.

There are instances, when working with Impurity methods for example, where it becomes necessary to modify integration parameters and component times due to complex chromatography. Collectively these privileges allow a company to tailor a user's ability to modify specific parts of the processing method.

REVIEW WINDOW PRIVILEGE OPTIONS

The privileges associated with calibration and quantitation have a significant effect on how far through the workflow of processing data and generating results is possible in Review. These are also used to limit the calculated peak values viewable in Review prior to data processing.

- **View Quantitation Peak Fields in Review** – Allows the user to view the following fields in the Review window peaks table: Area, % Area, Height, % Height, Amount, % Amount, Response, and Concentration. Users not assigned this privilege cannot view these fields nor will they be visible in the properties of the peak table.

- **View Numerical and Textual Results in Review** – Allows the user to view all numerical and textual results in Review. Users not assigned this privilege will only see an integrated 2D chromatogram. These users can perform batch processing or manual processing and Empower will recalculate the results, however, only the integrated chromatogram will be visible.
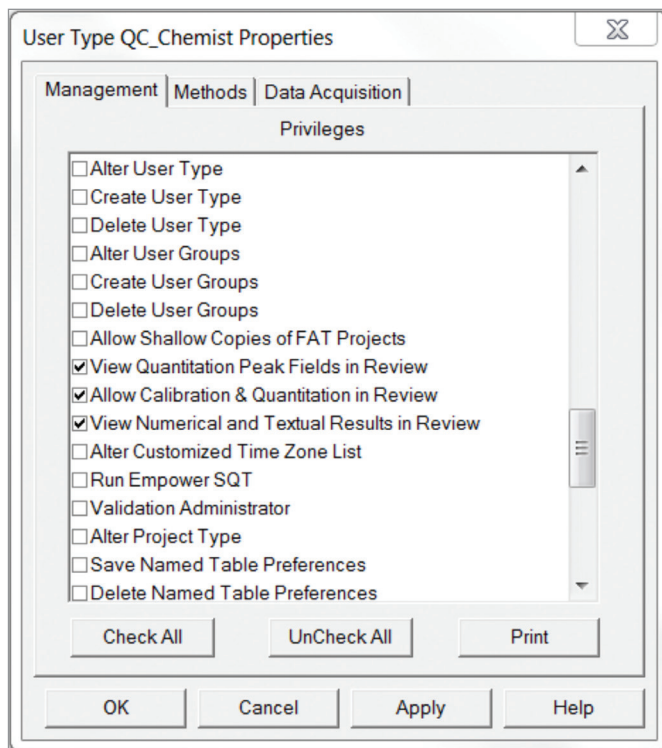

Figure 3. Privileges associated with actions in Review.

- **Allow Calibration and Quantitation in Review** – Allows the user to calibrate and quantitate data in the Review window. Users not assigned this Privilege cannot calibrate and quantitate data in Review. They cannot add, insert, delete or modify points on the calibration curve, individual-point table, or delete points on the calibration curve plot. Disallowing this privilege removes the ability of a user to see peak/component identification or any component-specific processing values in the peaks table or plot for any unsaved live data they are working with in Review (Figure 3).

There are several possible scenarios resulting from an analyst being assigned these privileges for working in Review. Here are some examples:

- Analyst has the Allow Calibration & Quantitation in Review privilege
  - The analyst can use the Integrate, Calibrate and Quantitate tools in Review.
  - If the analyst has the View Numerical and Textual Results in Review privilege but not the View Quantitation Peak Fields in Review privilege.
    - The peak quantitation fields such as Area and Amount fields are not displayed
    - However, limits set in System Suitability will be effective and will indicate pass/fail. Additionally any component-specific tailored calculations will be calculated and displayed.
  - If the analyst does not have the View Numerical and Textual Results in Review privilege (regardless of whether the analyst has the View Quantitation Peak Fields in Review privilege),
    - No peak fields, peak labels, spectra or calibration curves will be displayed
- Analyst does not have the Allow Calibration and Quantitation in Review privilege
  - Allows use of the Integrate tool but not the Calibrate or Quantitate tools.
    - The analyst will only have the ability to optimize the integration graphically

- If the analyst has the View Numerical and Textual Results in Review privilege and the View Quantitation Peak Fields in Review privilege.

  - When a result is brought into Review all peak fields will be displayed

  - When a channel or injection is brought into Review and 'Integrated'

    - Area and % Area fields can be viewed

    - Amounts and other component specific fields are not generated

- If the analyst has the View Numerical and Textual Results in Review privilege and does not have the View Quantitation Peak Fields in Review privilege.

  - Area and % Area fields cannot be viewed

  - Amounts and other component specific fields are not generated

- If the analyst does not have the View Numerical and Textual Results in Review privilege (regardless of whether the analyst has the View Quantitation Peak Fields in Review privilege,)

  - No peak fields, peak labels, spectra or calibration curves will be displayed

Purposeful management of these two privileges can allow an analyst to optimize a Processing Method in the Review window, with a view to using that method to batch process results, but limit the information they can create or view while performing that optimization.

	Allow Calibration and Quantitation in Review	Do Not Allow Calibration and Quantitation in Review
View Numerical and Textual Fields in Review ✔ View Quantitation Peak Fields in Review ✔	■ All available peak fields can be viewed	■ For Results: — All peak fields can be viewed ■ For Channels: — Peak fields including Area and % Area fields can be viewed — Component specific peak fields will be empty
View Numerical and Textual Fields in Review ✔ View Quantitation Peak Fields in Review ✖	■ All peak fields except Area, Area%, Amount, and % Amount can be viewed ■ Other component-specific peak fields can be viewed	■ All peak fields except Area, and % Area can be viewed ■ Component-specific peak fields will be empty
View Numerical and Textual Fields in Review ✖ View Quantitation Peak Fields in Review ✖	■ Peak fields cannot be viewed	■ Peak fields cannot be viewed

Figure 4. Privilege Matrix controlling which peak fields can be calculated and viewed in the Review application.

SAVING RESULTS PRIVILEGE OPTIONS

Typically processing of samples to create results will be performed using batch processing. This ensures consistency and is much more efficient than processing through the Review window. Batch processing is required to achieve more sophisticated quantitation practices such as bracketing, summary custom fields, or using multiple processing methods for defined samples in the Sample Set.

The privileges associated with saving results can have a limiting effect on what analysts can do in Review:

- **Save Results** – Allows the analyst to batch process as well as save results while working in Review. Analysts not assigned this privilege cannot save results in any part of Empower.

- **Save Results and Calibration in Review** – This allows the analyst to save results while working in Review. Analysts not assigned this privilege can batch process; however, they cannot save any results while in the Review window.

SAVING MANUAL RESULTS IN RESULTS SETS

If data requires manual peak identification or manual integration, analysts may need to process and save results in Review. After bringing a Result Set into Review, analysts may perform manual integration and quantitate samples. Saving this result will add it to the Result Set. It is important to note that this does not apply when standards are calibrated in Review.

This privilege is required if a company perceives a need to Save All results created in Review and leverage the system policy described at the beginning of this white paper.
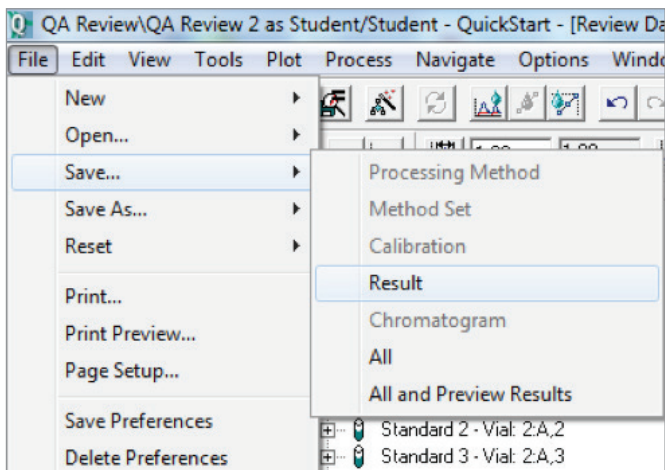

Figure 5. Manually saving results in Review.

An alternative control might be to have analysts save only manual integration in the Review window. This allows manual integration of both samples and standards. Analysts could then batch process with the Use Existing Integration feature to quantitate a Result Set that retains the manually integrated peaks for both samples and standards.
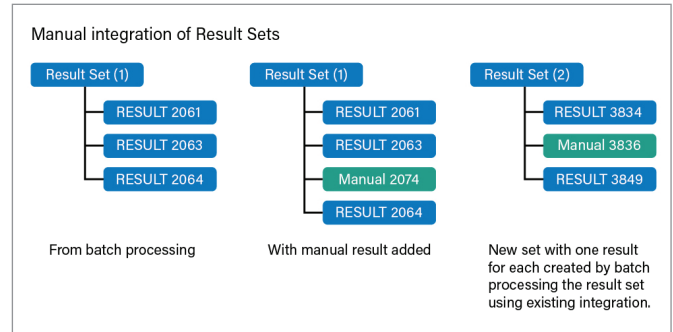

Figure 6. Saving a manual result into a Result Set and batch reprocessing a Result Set containing manually integrated chromatograms, with Use Existing Integration.

Knowing how these privileges impact processing of chromatographic data in the Review window helps laboratory supervisors better understand how data is generated by analysts. Concerns exist about an analyst's ability to fine tune the integration of peaks in a sample to bring failing results into specification. However, this would only be possible for samples which are very close to specification without creating obviously 'incorrect' integration.

For example, viewing a set of data as shown in an Empower control chart (Figure 7), the five results closest to the lower control limit may have been integrated into a passing state.
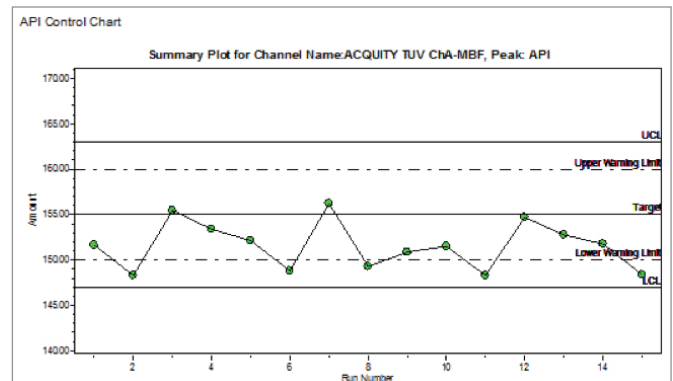

Figure 7. Control chart illustrating batch results exceeding warning limits yet passing specification.

Control charts are easily generated within Empower reports and provide laboratory supervisors a visual tool to look for trends in results.

COMBINING PRIVILEGES TO MANAGE HOW USERS INTERACT WITH DATA IN REVIEW

Figure 8 is an example of how privileges might be assigned depending on job function within an organization.
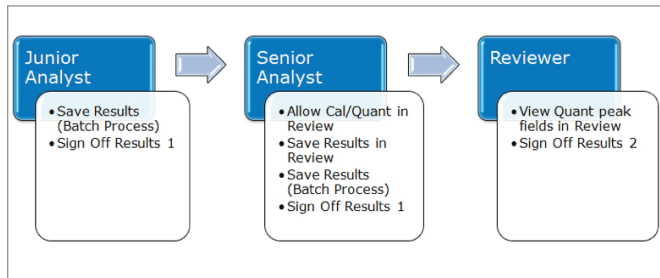

Figure 8. Example of tailored User Types.

Remember that a user who normally logs in as a Senior Analyst, may need to switch roles by logging out and logging in again in a Review role.

ADDITIONAL CONSIDERATIONS FOR DATA INTEGRITY

Locking channels from further processing

There are two further privileges associated with locking channels: Lock Channels and Unlock Channels.

Once results have been generated the associated channels can be locked so that users cannot generate any further results. In a Quality Control (QC) laboratory it is common for a channel to be locked once the result has been signed off. If a result is deemed inaccurate the channel can be unlocked for further processing by a user with the privilege to do so.

- A user can view the information associated with a locked channel.

- Allow Lock Channels after Sign-off 2 is a system policy that, when enabled, would allow a channel to be locked after Sign-off 2 in the Sign-off dialogue box.

Recording the reason "why?" for saving results

- Empower automatically records what actions were performed in the various audit trails and the user needs to document why they were performed.

- Users are typically expected to enter reasons why changes were made to project level objects such as methods, and system level objects such as chromatographic systems. It is important that these reasons reflect 'why' changes were made rather than 'what' changes were made. In regulated laboratories this is likely to be a requirement. In non-regulated laboratories it is not a requirement; however, these reasons add value by giving extra details about activity in Empower and could be seen as good practice.

- For example, when an analyst processes a Sample Set, the selection of the reason why is done in the Background Processing and Reporting dialogue box (Figure 9).
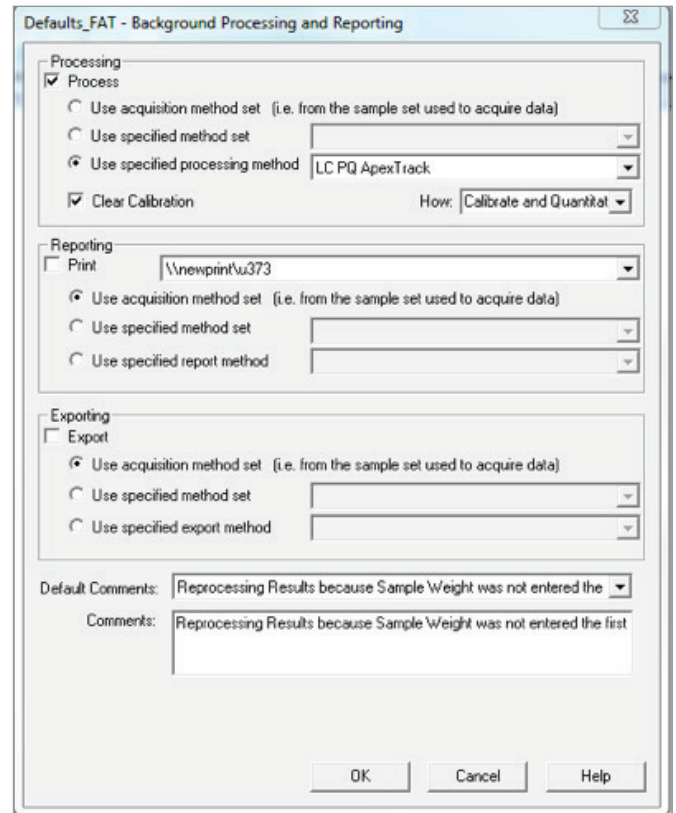

Figure 9. Background Processing and Reporting dialogue box showing the reason 'why' in the Comments box.

The reason why a Sample Set was processed would then appear in the Project Audit Trail and the Result Audit Viewer (Figure 10).

Figure 10. Reason why a result was reprocessed in the Result Audit Viewer.

There are two approaches to entering these comments – in an unrestricted manner or a restricted manner. Unrestricted allows the user to enter the reason why as free text. Restricted entry requires the user to select a predefined reason from a list. These predefined reasons are called Default Strings. It is important to make sure the Default Strings reflect the reason why an action was performed. Default Strings are created in Configuration Manager and can be created by any senior user with the privilege to do so.

SUMMARY

Regulators have concerns that laboratory staff could be operating with privileges that allow too much flexibility, or system policies which are set in an inappropriate way, allowing the opportunity to pass samples which do not meet specifications. It is important for both Regulators and Quality Units to understand software configuration and how it impacts the laboratory workflow as well as the data.

- It is important to understand how Empower System Policies can limit data processing.

- User types can be setup with very granular privileges to constrain how analysts create results in Review.

- Once results have been generated the associated channels can be locked so that users cannot generate any further results.

- Reviewer user types can be set up with unique privileges to suit their role which would allow them to view metadata and sign results, but not create or modify results.

- Empower automatically records what was done in the various audit trails and users should apply comments to document why it was done.

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