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CUSTOM FIELDS FOR ASSAY CALCULATIONS IN FOOD

INTRODUCTION

This White Paper discusses how Waters® Empower® 3 Software can increase workflow efficiency and reduce errors using custom calculations in Food assay. Calculations tailored to your application, such as percent difference, can be created, without relying on external calculations or specialized software packages.
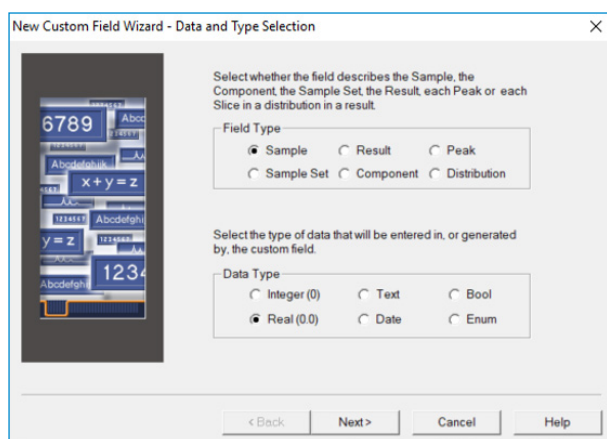

Figure 1. Create custom fields calculations using the Custom Field Wizard

USER-FRIENDLY WIZARD

Empower 3 has a user-friendly wizard to assist you in the creation of custom calculations. The wizard provides options such as: type of calculation (peak or result), type of data (real numbers or Boolean logic), type of sample the calculation will apply to (standards, samples, controls), and the type of peaks the calculations will apply to (individual peaks, and/or grouped peaks).

ELIMINATE MANUAL CALCULATIONS AND TRANSCRIPTION ERRORS

Creating custom calculations in Empower 3 simplifies workflow by eliminating the need to export information to a separate program. All custom calculations will be automatically processed when the raw data is processed. Furthermore, it eliminates transcription errors if the user is manually entering information into a separate program or if the calculations are being made in a laboratory notebook.

INCREASE WORKFLOW EFFICIENCIES

The flexibility of custom calculations in Empower 3 allows for multiple fields to be evaluated with a single formula. In addition, calculations can be created to summarize all outcomes, allowing users to determine quickly whether the batch is suitable for release or requires out of specifications investigation.

WHAT KIND OF CUSTOM CALCULATIONS CAN EMPOWER CREATE?
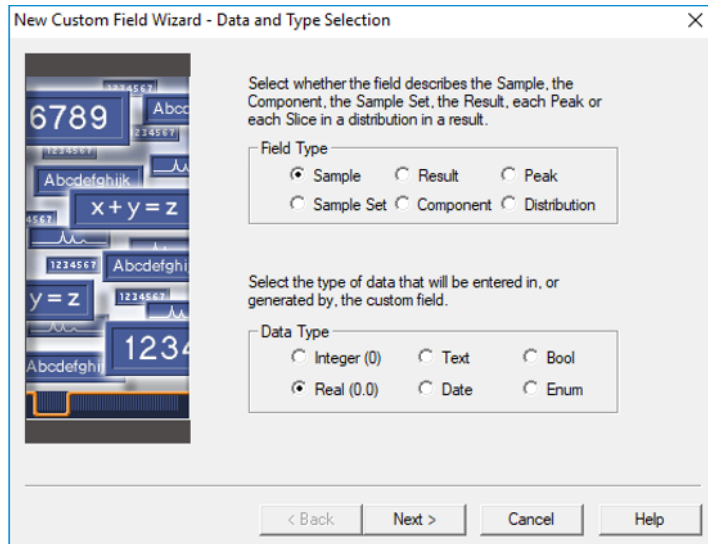
FIELD TYPE:

Which field does this custom field describe?

- Sample: Describes samples, vials, and sample parameters
- Sample Set: Describes sample set, used for information that is the same for the entire set of data
- Peak: Performs a mathematical calculation pertaining to a peak
- Result: Performs a mathematical calculation pertaining to a result-level parameter
- Component: Allow the input of analyte information
- Distribution: Performs a mathematical calculation pertaining to a distribution slice-level parameter for GPC/V data

DATA TYPE:

What kind of data will be entered in, or generated by this custom field?

- **Integer (0):** Whole number (without fractional parts)
- **Text:** Alphanumeric entry
- **Bool (Boolean):** The Boolean data type allows for the translation of a mathematical question into 2 possible answers upon processing
- **Real (0.0):** Floating-point number entry (can contain a fraction)
- **Date:** Date entry by the user or from an external source (for example, a LIMS system)
- **Enum (Enumerated):** The Enumerated data type allows creation of a drop-down list or translate a mathematical question into 3 or more possible answers.

EXAMPLES OF CUSTOM CALCULATIONS AND THEIR FIELD TYPES AND DATA TYPES:

Common Custom Fields Examples	Field Types	Data Types
Sample Lot Number	Sample	Integer / Text
Sample Storage Conditions (Drop-down List)	Sample	Enumerated
Sample Set SOP Number	Sample Set	Integer / Text
Column Used for Sample Set Run (Drop-down List)	Sample Set	Enumerated
Analyte Label Claim	Component	Real
Assay Calculations	Peak	Real
Assay Calculations (Pass / Fail)	Peak	Boolean

CALCULATION OF PERCENT DIFFERENCE IN EMPOWER FOR FOOD

Percent Difference is commonly calculated in the Food industry. This calculation allows users to compare two independent measurements and determine how much the measurements differ. Empower 3 custom calculation can help you calculate Percent Difference and subsequently compare calculated Percent Difference against the maximum acceptable Percent Difference.
The below custom fields are set up using Aspartame as an example.

First, a field, *Target Amount* was created to allow users to input the target amount of Aspartame expected in the food sample. The second field, *Calculated Percent Difference* has a formula that calculates the percent difference based on the calculated amount and *Target Amount*.

Subsequently, a third field compares the *Calculated Percent Difference* against the maximum acceptable percent different for Aspartame. This Boolean logic field, *Aspartame Percent* Difference, reports a pass if the *Calculated Percent Difference* falls below the threshold. Custom calculations eliminate misinterpretation of the results and are fully automated.

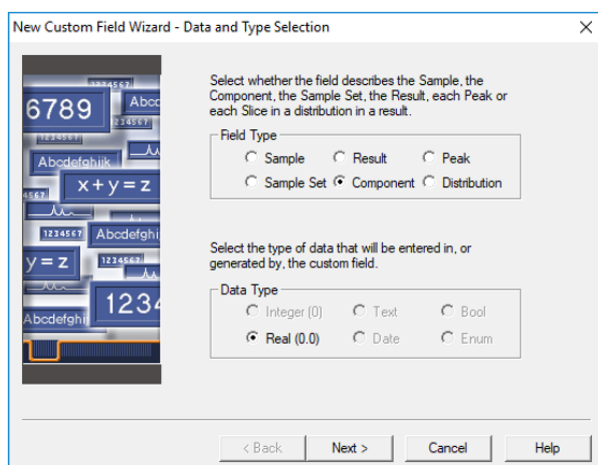## CUSTOM FIELD 01
TARGET_AMOUNT

- **Aim:**
  The Percent Difference calculation is performed on Samples. Target_Amount allow users to enter a Target Amount for the samples so that Empower can compare the Target Amount with the Amount calculated in Empower.

- **Formula:**
  This is a user-entered field.

- **Creating This Custom Field:**
 Custom Field 1: Target_Amount

Step
01

From the Configuration Manager window, start the New Custom Field Wizard by right-clicking on a project to view its properties, and choose "New" in the Custom Fields tab in the Properties dialog. Since we need a real number input that is component-specific, select "Component" and "Real" as the Field Type and Data Type, respectively.
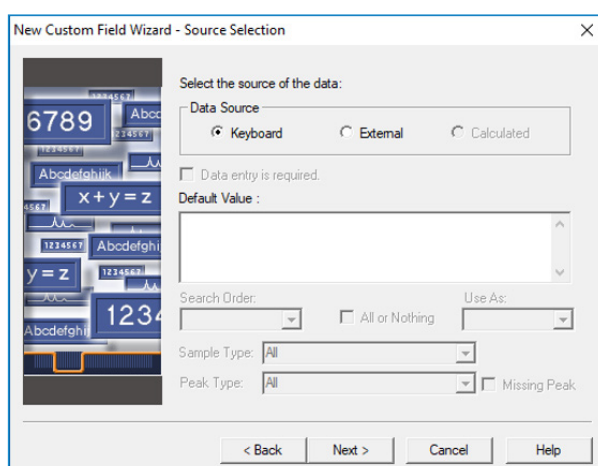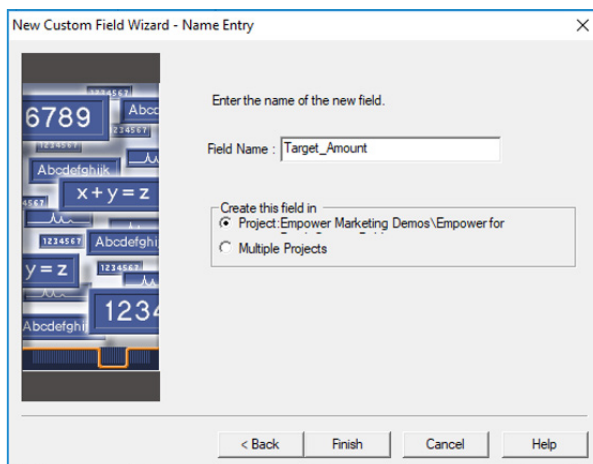
Step
02

The next dialog is the Source Selection dialog. In this dialog, The Data Source is chosen as "Keyboard" because the user will enter this information via the computer keyboard.
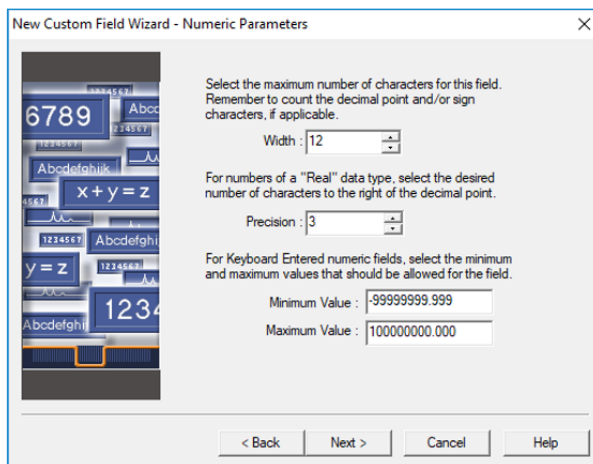
Step

03

The next dialog allows you to determine how many precision and characters you can enter for this field. By a precision of 3, this means the field can accommodate up to 3 decimal places.

Step

04

Finally, the Name Entry dialog appears, which allows you to name the custom field. The name you choose is displayed for this field in the Run Samples window, on reports, and throughout the software. In this case, we will name it Target_Amount.
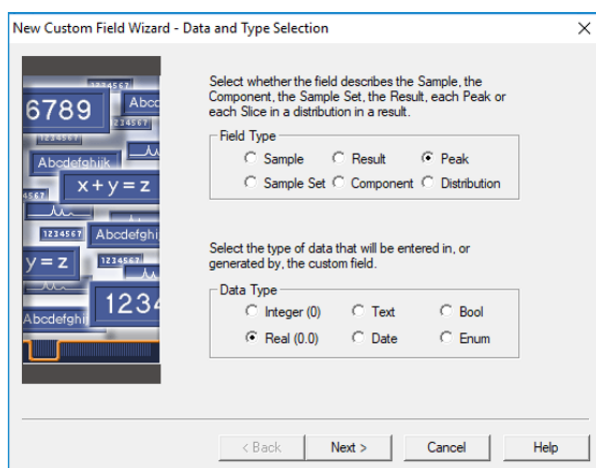
CUSTOM FIELD 02
PCT_DIFFERENCE

- **Aim:**

  The Percent Difference calculation is performed on Samples. Empower compares the Target Amount with the Amount calculated in Empower and divide the difference by the Target Amount.

- **Formula:**

  Pct_Difference = ABS(Target_Amount-Amount)/Target_Amount*100

- **Creating This Custom Field:**

Step
01

In the same way, access the New Custom Field Wizard from the Configuration Manager window. The field type is Peak as this calculation is performed for each integrated peak. As the field is expected to generate a Real number, the Field Type is "Peak" and Data Type is "Real" respectively.
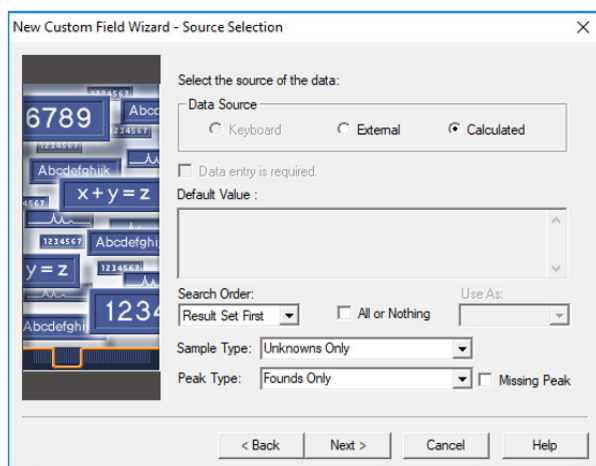
Step
02

The next dialog is the Source Selection dialog. In this dialog, The Data Source is chosen as "Calculated" as Empower will be performing a calculation. The user can specify the Sample Type and Peak Type that this calculation will be generated for. As the Percent Difference calculation is only required for known peaks found in samples, "Unknowns Only" is chosen as the Sample Type and "Founds Only" is selected for the Peak Type.
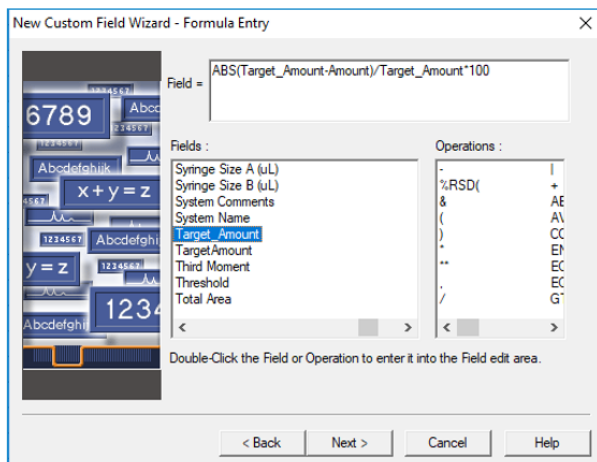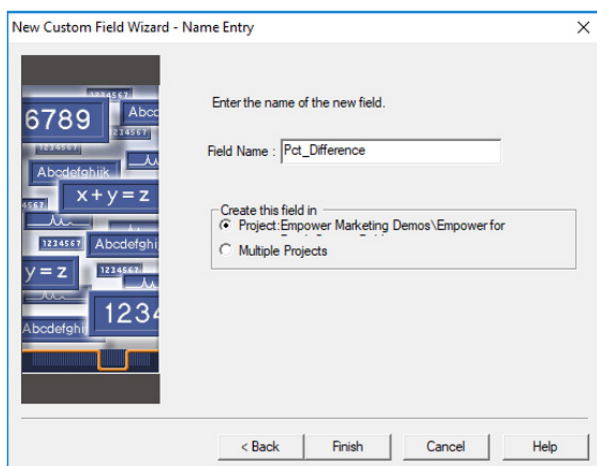
Step

03

The next dialog is the Formula Entry dialog. Here, Percent Difference is calculated by taking the absolute value of the difference between Target_Amount and Amount divided by the Target_Amount, then multiplied by 100. The formula is entered into the Field Edit box at the top of the dialog. Beneath the Field Edit box, there are a list of available Fields and Operations. The user can double click the Field and Operation to enter it into the Field Edit box.
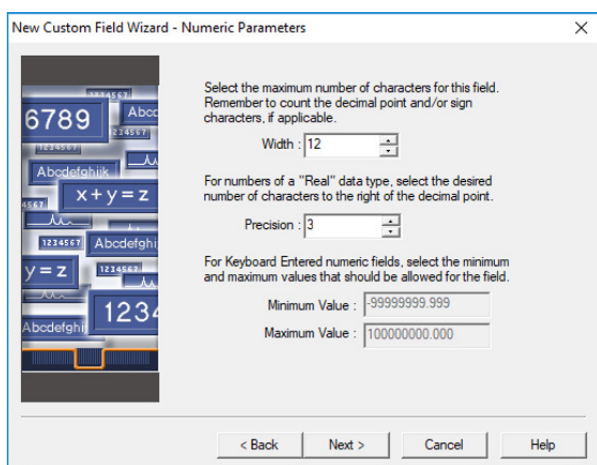
Step

04

The next dialog allows you to determine the precision and number of characters you can enter for this field.

Step

05

Finally, the Name Entry dialog appears, which allows you to name the custom field. In this case, we will name it Pct_Difference.

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CUSTOM FIELD 03
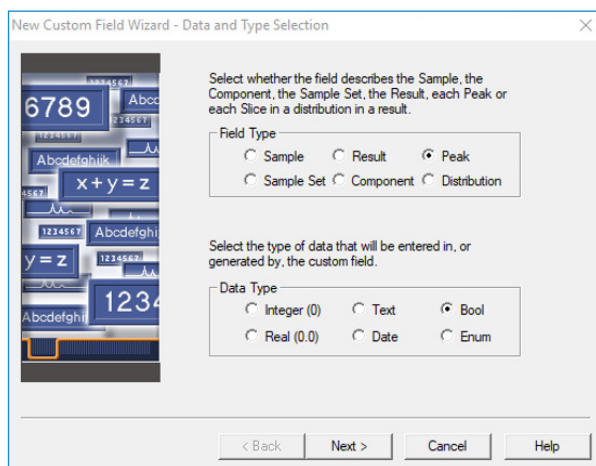## PCT_DIFFERENCE_DECISION_ASP

■ **Aim:**

The user would like to compare the Percent Difference Calculated (Pct_Difference) with a set maximum threshold of 15% for Aspartame. The Target Amount for Aspartame is 85.

■ **Formula:**

Pct_Difference_Decision_Asp = LT(Pct_Difference,15)

■ **Creating This Custom Field:**

Step
01

In the same way, access the New Custom Field Wizard from the Configuration Manager window. The field type is Peak as this calculation is performed for each integrated peak. As the user would like Empower to give 2 possible answers to a Boolean question, "Peak" and "Boolean" is selected in the Field Type and Data Type areas, respectively.
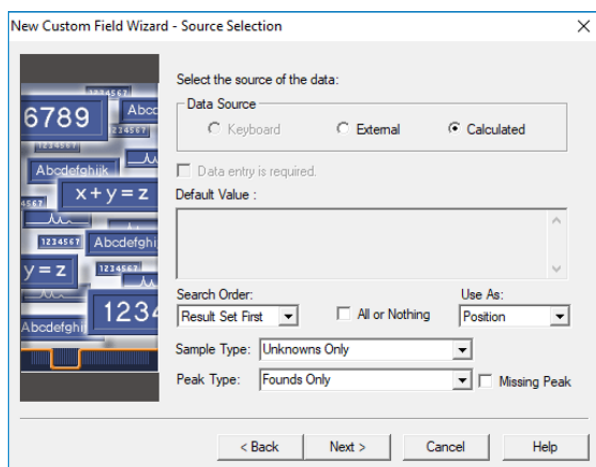
Step
02

The next dialog is the Source Selection dialog. In this dialog, The Data Source is chosen as "Calculated" as Empower will be performing a calculation. Similar to Pct_Difference, "Unknowns Only" is chosen as the Sample Type and "Founds Only" is selected for the Peak Type.

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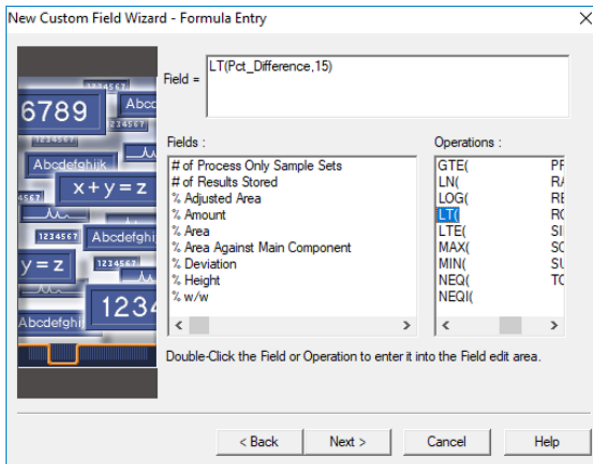
The next dialog is the Formula Entry dialog. This is a Boolean logic field. LT means Less Than. This formula asks Empower to compare the Pct_Difference field with a fixed threshold of 15.
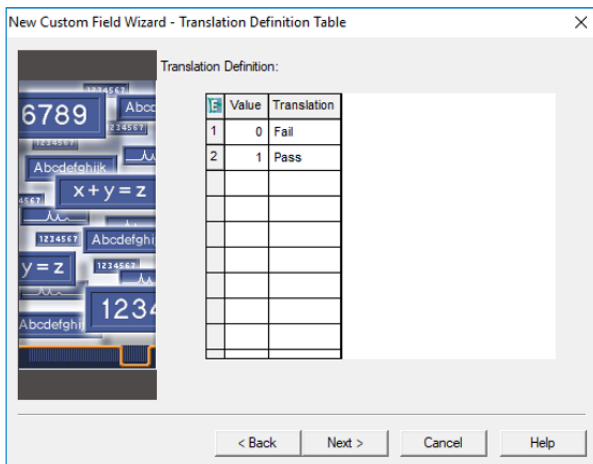
If Pct_Difference is less than 15, this field is True and returns a value of 1. This is then translated into a "Pass". Conversely, if Pct_Difference is 15 or more, this field is False and returns a value of 0. This is then translated into a "Fail".

Finally, the Name Entry dialog appears, which allows you to name the custom field. Here, we name it Pct_Difference_Decision_Asp.

To illustrate the functionality of the custom fields, enter the Target_Amount for Aspartame in the Component Editor. The Target Amount for Aspartame is 85.

Subsequently, process the sample set and the custom calculations will be automatically generated.

Pct_Difference_Decision_Asp Example: Soft Drink Sample B [Aspartame – Pass]

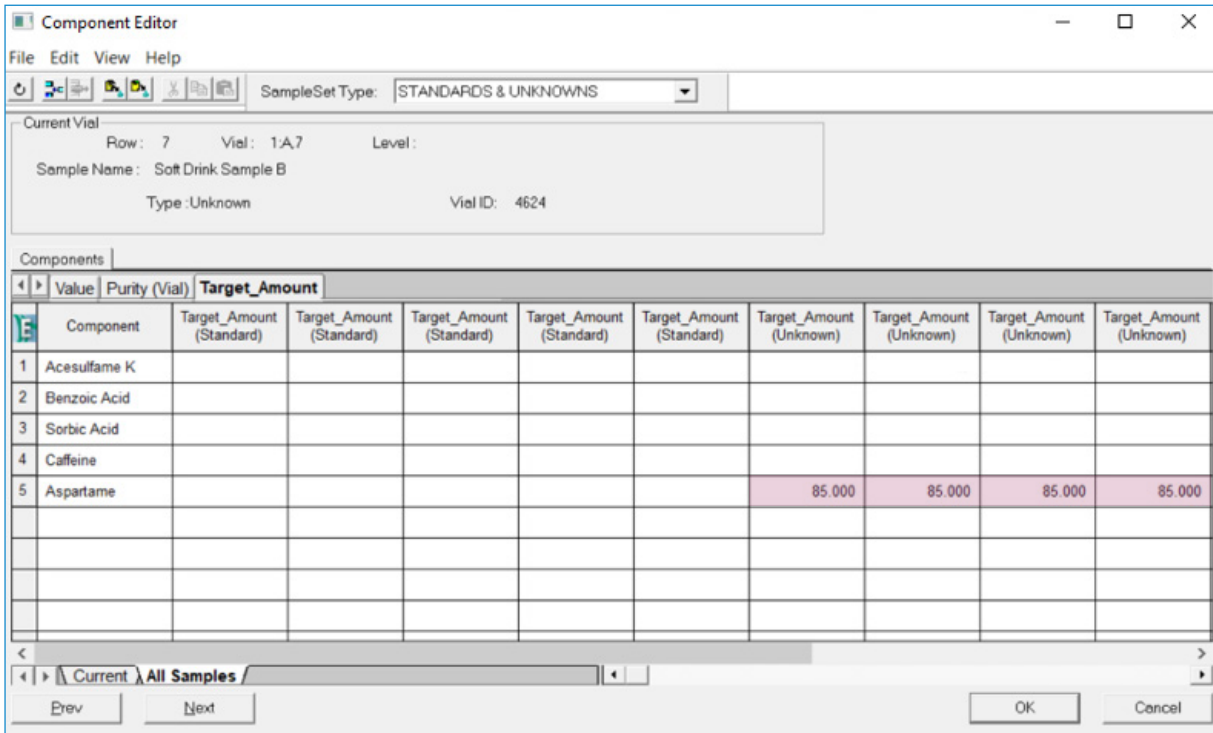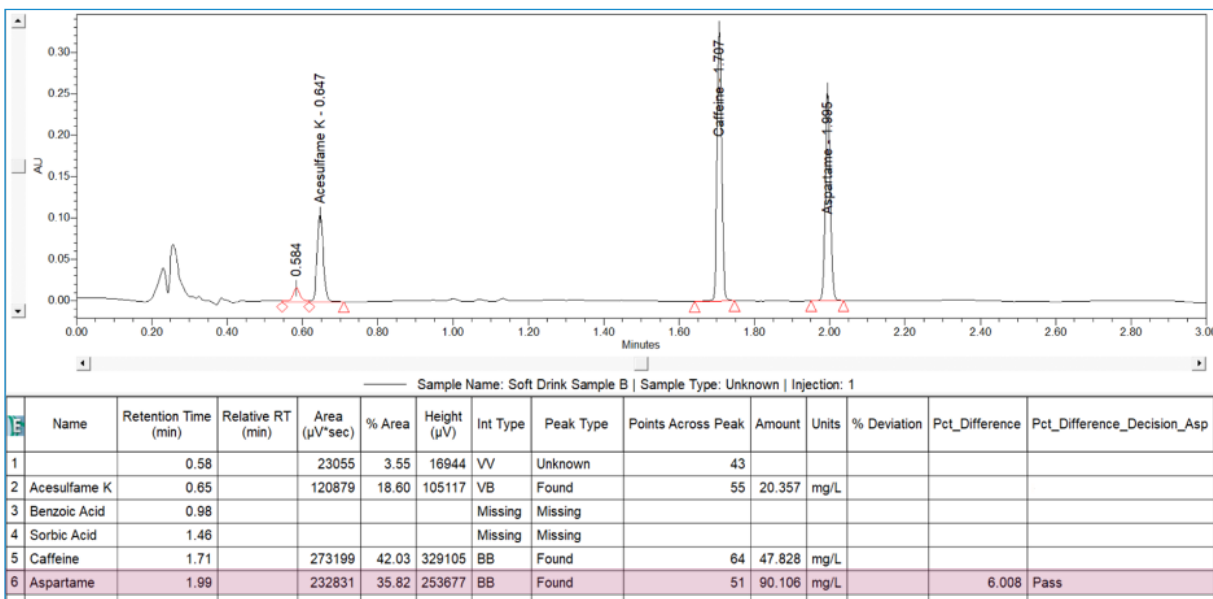|	Name	Retention Time (min)	Relative RT (min)	Area (µV*sec)	% Area	Height (µV)	Int Type	Peak Type	Points Across Peak	Amount	Units	% Deviation	Pct_Difference	Pct_Difference_Decision_Asp
1		0.58		23055	3.55	16944	VV	Unknown	43					
2	Acesulfame K	0.65		120879	18.60	105117	VB	Found	55	20.357	mg/L			
3	Benzoic Acid	0.98					Missing	Missing						
4	Sorbic Acid	1.46					Missing	Missing						
5	Caffeine	1.71		273199	42.03	329105	BB	Found	64	47.828	mg/L			
6	Aspartame	1.99		232831	35.82	253677	BB	Found	51	90.106	mg/L		6.008	Pass

Figure 2. The Review window demonstrating the custom fields calculations of Pct_Difference and Pct_Difference_Decision_Asp

Aspartame Percent Difference

	Sample Name	Inj	Peak Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Aspartame Percent Difference (Range: 0 - 15%)
1	Soft Drink Sample A	1	Aspartame	1.999	53.018	mg/L	85.000	37.625	Fail
2	Soft Drink Sample A	2	Aspartame	1.997	53.430	mg/L	85.000	37.142	Fail
3	Soft Drink Sample B	1	Aspartame	1.995	90.106	mg/L	85.000	6.008	Pass
4	Soft Drink Sample B	2	Aspartame	1.990	90.382	mg/L	85.000	6.331	Pass
5	Soft Drink Sample C	1	Aspartame	1.994	90.566	mg/L	85.000	6.549	Pass
6	Soft Drink Sample C	2	Aspartame	1.991	91.348	mg/L	85.000	7.469	Pass
7	Soft Drink Sample D	1	Aspartame	1.992	78.614	mg/L	85.000	7.513	Pass
8	Soft Drink Sample D	2	Aspartame	1.992	78.009	mg/L	85.000	8.224	Pass

Table 1. A tailored report showing Aspartame passing or failing the Percent Difference tolerance.

Empower's custom calculations functionality can be greatly expanded with the use of generic peak names and constants. This allows custom calculations to become highly flexible, allowing users to compare multiple peaks against different thresholds. Subsequently, Boolean calculations enables Empower to generate batch release decision based on multiple outcomes. These formulae can even be used across various analytical assays that requires the same calculations.

SOFT DRINK BATCH RELEASE REPORT

Sample Name: Soft Drink Sample A

	Sample Name	Inj	Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Acesulfame K Percent Difference (Range: 0-10%) Aspartame Percent Difference (Range: 0 - 15%)	Batch Release Decision
1	Soft Drink Sample A	1	Acesulfame K	0.645	62.236	mg/L	48.000	29.657	Fail	Out of Specifications
2	Soft Drink Sample A	1	Aspartame	1.999	53.018	mg/L	85.000	37.625	Fail	
3	Soft Drink Sample A	2	Acesulfame K	0.643	63.042	mg/L	48.000	31.337	Fail	Out of Specifications
4	Soft Drink Sample A	2	Aspartame	1.997	53.430	mg/L	85.000	37.142	Fail	

Sample Name: Soft Drink Sample B

	Sample Name	Inj	Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Acesulfame K Percent Difference (Range: 0-10%) Aspartame Percent Difference (Range: 0 - 15%)	Batch Release Decision
1	Soft Drink Sample B	1	Acesulfame K	0.647	20.357	mg/L	48.000	57.589	Fail	Out of Specifications
2	Soft Drink Sample B	1	Aspartame	1.995	90.106	mg/L	85.000	6.008	Pass	
3	Soft Drink Sample B	2	Acesulfame K	0.646	20.016	mg/L	48.000	58.301	Fail	Out of Specifications
4	Soft Drink Sample B	2	Aspartame	1.990	90.382	mg/L	85.000	6.331	Pass	

Sample Name: Soft Drink Sample C

	Sample Name	Inj	Name	RT	Amount	Units	Target Amount	Calculated Percent Difference (%)	Acesulfame K Percent Difference (Range: 0-10%) Aspartame Percent Difference (Range: 0 - 15%)	Batch Release Decision
1	Soft Drink Sample C	1	Acesulfame K	0.646	50.358	mg/L	48.000	4.914	Pass	Batch Release
2	Soft Drink Sample C	1	Aspartame	1.994	90.566	mg/L	85.000	6.549	Pass	
3	Soft Drink Sample C	2	Acesulfame K	0.643	50.106	mg/L	48.000	4.388	Pass	Batch Release
4	Soft Drink Sample C	2	Aspartame	1.991	91.348	mg/L	85.000	7.469	Pass	

Table 2. A tailored report showing Empower comparing Percent Difference with different thresholds for Acesulfame K and Aspartame. Both Acesulfame K and Aspartame have to pass threshold for the batch to be released. Empower can evaluate the response of the outcome of both fields and only generate a Batch Release Decision if both Acesulfame K and Aspartame pass their threshold.

CONCLUSION

Empower 3 Software provides the tailored calculation tools necessary for final result calculations, without the time, cost, or potential errors associated with manual calculations, or the use of spreadsheet calculations from exported chromatography data files. Its flexibility allows users to achieve their calculation objectives with minimal custom fields. The ability to evaluate multiple fields at a time allows users to make everyday decisions effectively, eliminating misinterpretation.

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