CDS Solutions

Key Features:

- Highly customizable CDS providing application specific tools

- Automated calculation functionality results in fewer transcription errors and increased productivity

- CDS traceability function enables access to details of all previous analyses, including custom calculation results

Empower® 3 Software: Automated Custom Calculations

Empower® 3 Automates Custom Calculations

With Waters® Empower® 3 Software, you can perform custom calculations, such as percent purity without relying on external calculations or specialized software programs.
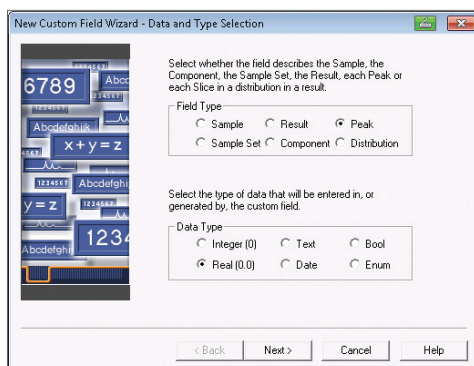

Figure 1. The Empower® 3 Software wizard assists you in creating custom calculations.
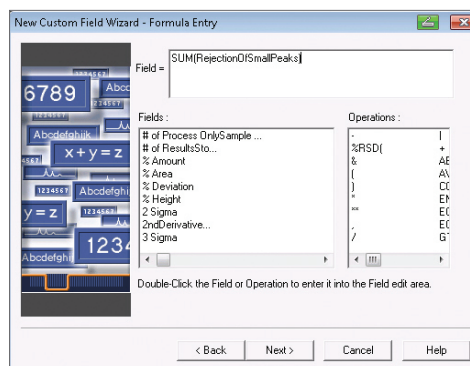

Figure 2. With Empower® 3 Software, you do not need to export data to other programs for custom calculations.

PerkinElmer®

For the Better

Purity Calculations

Chromatographic purity determinations from incoming raw material are frequently performed by industrial and pharmaceutical organizations before the material is released to production. The purity calculation measures the percent area of the active component in the mixture.

Frequently, a batch of incoming raw material is accepted if the peak area of an active component exceeds a certain percentage, typically 95%, from the total peak areas obtained. Difficulties arise when deciding which peaks qualify for inclusion in the total peak area calculation.

Some measurement protocols require that only peaks with areas greater than 0.05% of the total peak area be included in the final calculation. In this situation, peaks whose areas are less than 0.05% of the total must be eliminated before the final percent purity calculation can be determined.

Empower® 3 Software provides custom calculation tools that minimize the time, cost, and potential errors associated with manual calculations, and it eliminates the need to use spreadsheet calculations from exported chromatography data files.

Accomplish Your Objectives Faster with Empower® Software

How can a chromatography data system eliminate from the final purity calculation all "minor peaks" whose areas are less than 0.05% of the total peak area? Empower® 3 custom calculations contains various field types and formulae that can be used to help you to get the right answer faster.

Using the various calculation features of Empower® 3 Software, a variety of fields are created to accomplish the objectives. The first field tests the percent area for each peak against the 0.05% area rejection threshold. When the calculated area for an individual peak is greater than 0.05% of the total peak area, the formula returns that component's peak area. When the component's peak area is less than or equal to the 0.05% area threshold, the custom field removes the component from further calculations. Next, the peaks above the 0.05% threshold are summed so that an adjusted percent area can be determined.

A final field uses Boolean logic to determine if the percent area of the active component is greater than 95%; if so, the component is indicated as 'passed.'

Figure 3 shows the results of these calculations as they appear in an Empower® 3 report. This table compares the original areas and percent areas prior to the Empower® 3 custom calculation (blue box) with those after the 0.05% area rejection calculations (red box). The field that determines if the active component passes; is greater than 95% of the total area, is also shown.

? The routine test for impurities in our pharmaceutical manufacturing plant involves calculating the percent area of active versus minor contaminants in a batch of incoming raw material. Unfortunately, a simple percent area calculation is not possible. We must first remove all peaks with less than 0.05% of the total area before the final calculation is made. Must we rely on other software packages, such as Microsoft Excel, to perform these series of calculations on our collected data?

✓ "Custom calculations" have traditionally been performed using specialized software programs. Few chromatography software programs provide tools that assist you in reducing raw data to the format you need to make critical decisions, such as whether to accept or reject a particular lot of material.

	Peak Name	Retention Time	Area	% Area	Area after 0.05% Area Rejection	Percent Purity (% Area After 0.05% Area Rejection)	Pass if >95%
1		2.630	3889.200	0.04431	Area < 0.05%	Area < 0.05%	
2		2.866	8653.135	0.09859	8653.135	0.09867	
3		2.965	12310.866	0.14026	12310.866	0.14038	
4		4.670	3571.200	0.04069	Area < 0.05%	Area < 0.05%	
5	Imp A	5.648	79955.794	0.91095	79955.794	0.91172	
6		5.970	6396.810	0.07288	6396.810	0.07294	
7		6.655	8273.794	0.09426	8273.794	0.09434	
8		6.983	7996.032	0.09110	7996.032	0.09118	
9	Imp B	7.899	34906.201	0.39769	34906.201	0.39803	
10	Imp C	9.138	43687.802	0.49774	43687.802	0.49817	
11	Active	10.482	8567563.540	97.61153	8567563.540	97.69457	Pass

Peak Purity Results with 0.05% Area Rejection

Figure 3. Empower® 3 Software's percent purity custom calculation report.

Summary

Empower® 3 Software provides the custom 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. Empower® 3 Software's wizard technology helps you generate user definable calculation criteria to produce validated results without the need to qualify and maintain specialized application software.