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 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.
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 contain 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.

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.