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Empower 3 Software ApexTrack Integration Algorithm

Effective detection and efficient integration of peaks

ApexTrack™ is a powerful integration algorithm that forms the foundation of Waters® Empower® 3 Software integration package. ApexTrack effectively detects and integrates shouldered peaks, providing more reliable detection of low-level peaks on noisy or sloping baselines. Peak detection using ApexTrack's curvature approach is much more sensitive than the slope criteria used in traditional integration, and requires less manual integration and fewer adjustments of integration parameters.

BETTER PEAK DETECTION

Peaks which elute close to one another can very in height. Such variations in height and resolution present integration challenges. The ApexTrack algorithm effectively addresses these difficulties by using the second derivative of the chromatogram to detect peaks. Peak detection based on the second derivative can detect peaks of all sizes, including coeluted peaks and those on sloping or drifting baselines.

SHOULDERED PEAKS AND GAUSSIAN SKIMMING

ApexTrack easily detects even the most subtle peak shoulders with a Detect Shoulders integration event (Figure 1). The addition of the Gaussian Skim integration event replaces vertical drop lines with Gaussian skims, where appropriate.

The figures below show three different examples of peaks containing shoulders in a progression. From left to right: optimized traditional integration, ApexTrack integration with default parameters and Detect Shoulders event; ApexTrack integration with default parameters, and Detect Shoulders Gaussian Skim events.

These examples show that the ApexTrack algorithm simply and effectively integrates shoulders, whether in simple clusters with defined shoulders, or in complex clusters with subtle shoulders. Shoulders are detected whether they are located on the front or the tail of the parent peak.

Figure 1. Peaks containing shoulders integrated using traditional integration and ApexTrack integration.
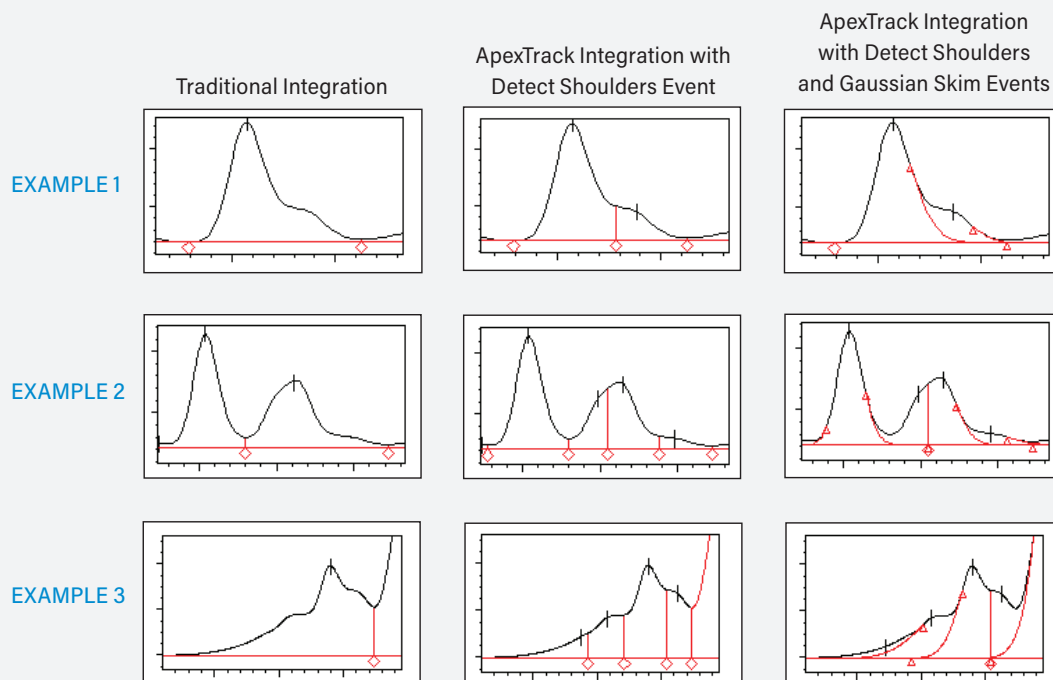
NEGATIVE PEAKS

With ApexTrack often times additional timed events are not needed thus simplyfing the processing method and reducing the time required for method development (Figure 2).
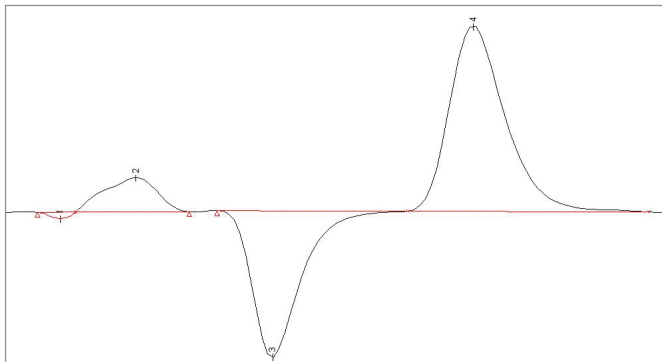

Figure 2. Negative peaks integrated with ApexTrack integration.

FASTER METHOD DEVELOPMENT FOR OPTIMAL PEAK DETECTION

ApexTrack automatically determines the proper peak width and threshold parameters to use for optimal peak detection. These critical parameters are obtained directly from your data. Using automatic parameters can significantly reduce your method development times. The ApexTrack processing parameters that control peak detection and baseline placement are independent of each other. This is not the case with other integration packages. The ApexTrack algorithm lets you accurately control both the sensitivity and baseline placement, because these parameters do not affect one another. This means that changing the parameter that affects the peaks' baseline placement does not affect the sensitivity, or the number of peaks detected (and vice-versa). This greatly reduces the time required to develop the method and the need to manually integrate peaks.

TRADITIONAL INTEGRATION VERSUS APEXTRACK INTEGRATION

Figures 3 and 4 examples compare optimized traditional integration to ApexTrack integration with default parameters. It's easy to see that difficult chromatograms are more effectively and efficiently integrated when using ApexTrack.
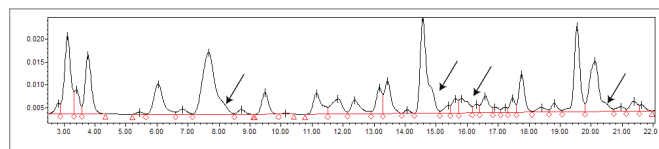

Figure 3. Complex chromatogram integrated using traditional integration; integration parameters optimized and Tangential Skim events enabled. Arrows indicate undetected shoulders.
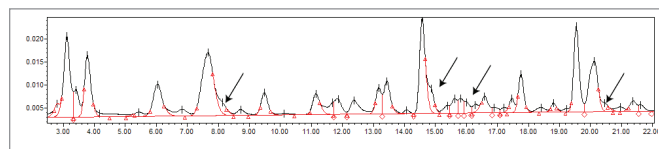

Figure 4. Complex chromatogram integrated using ApexTrack integration; integration parameters set at default with Detect Shoulders and Gaussian Skim events enabled.

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