Agilent MSD Productivity ChemStation G1701 & G1710

EasyID Resolution, Tailing, and Degradation

Agilent Technologies

Notices

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Introduction

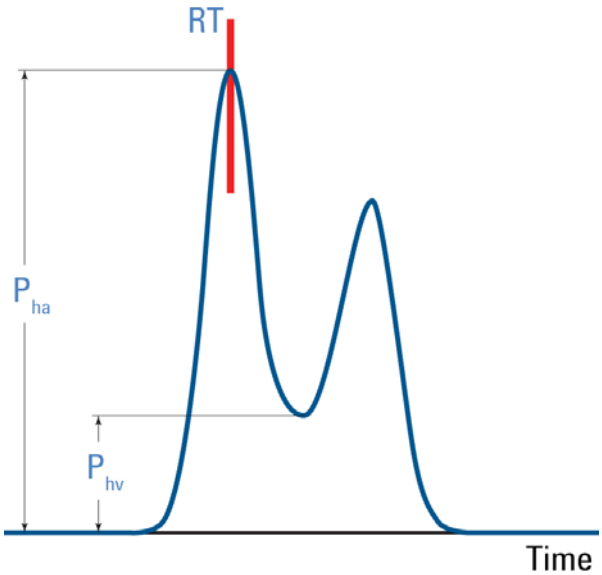
This document describes the calculations used by EasyID for finding Peak Resolution and Tailing in the Agilent MSD Productivity ChemStation. EasyID is a tool for updating the retention times in a quantitation database on a *compound-by-compound* basis.

With a quantitation method and data file loaded, EasyID is started by selecting EasyID from the View menu (Tools menu if Enviromental Data Analysis mode). This displays the Quick EasyID window. In the Quick EasyID window, double click on a compound entry to display a chromatogram of that compound in window #6.

This resolution calculation has its origin in the EPA method 8280B which uses a resolution suitability requirement to determine the separation of critical isomer pairs. This requirement specifies that the % valley as calculated here must be at or below 25%.

Evaluate Resolution

To display the resolution between adjacent peaks in the chromatogram, select Evaluate Resolution from the ChromEval menu. The software asks for you to select the two peaks used for calculating resolution by manually integrating them. Integrate these peaks manually by drawing a baseline (right-click and drag) under each peak. The software calculates the resolution and displays it as a valley percentage next to the peak.

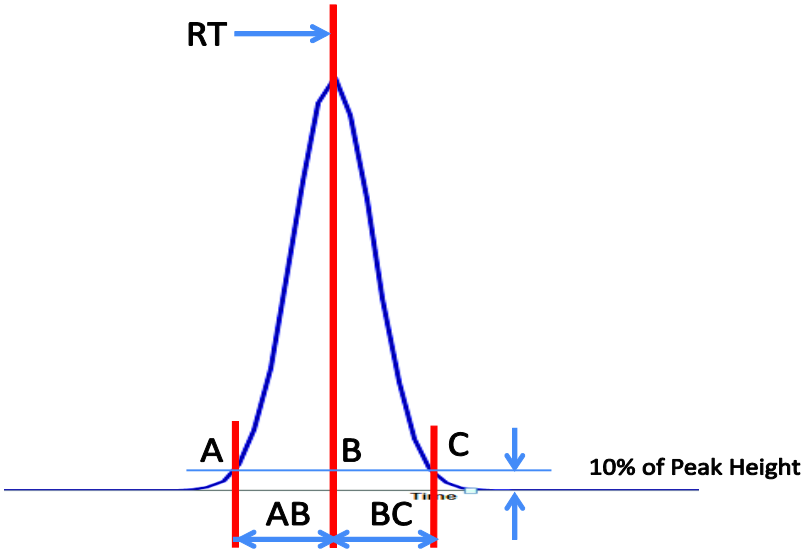


$$\%\,Valley = \frac{P_{\mathrm{hv}}}{P_{ha}} * 100$$

Where: P_{hv} = baseline height of the valley between the peaks;
P_{ha} = baseline peak height to the apex.

Evaluate Tailing

In EasyID, Tailing uses the calculation for the Asymmetry factor (see definition below) and not the more common tailing calculation as used in a USP System Suitability method. It is a measure of peak symmetry. For a perfectly symmetric peak, the peak tailing factor = 1. In EasyID, to display the Tailing for a peak, select Evaluate Tailing from the ChromEval menu. The software asks for you to select the peak by manually integrating it. Integrate this peak manually by drawing a baseline under the peak. The software calculates the tailing and displays it next to the peak. The values used for calculating tailing are displayed in the status line at the bottom of the screen.



$$Tailing = \frac{BC}{AB}$$

Where: B = Retention time at the peak apex.
C = RT of peak end at 10% of peak height;
A = RT of peak start at 10% of peak height;

Asymmetry factor

The asymmetry factor is a measure of peak tailing. It is calculated when a user selects Evaluate Tailing in EasyID. It is defined as the distance from the center line of the peak to the back slope divided by the distance from the center line of the peak to the front slope, with all measurements made at 10% of the maximum peak height. The asymmetry factor of a peak will typically be similar to the tailing factor for the same peak, but the two values cannot be directly converted.

Evaluate Degradation

To display the Degradation between a primary peak and a peak containing a degradation compound of the same primary peak compound, select Evaluate Degradation from the ChromEval menu. The software asks for you to select the two peaks used for calculating degradation by manually integrating them. Integrate these peaks manually by drawing a baseline (right-click and drag) under each peak, starting with the Primary peak. The software calculates Degradation and displays it as a Degradation percentage next to the primary peak.

Degradation is calculated as a percent area ratio of the degradation peak to the primary peak.

$$Degradation = \frac{D}{P} \times 100$$

Where: D = Degradation peak area
P = Primary peak area

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