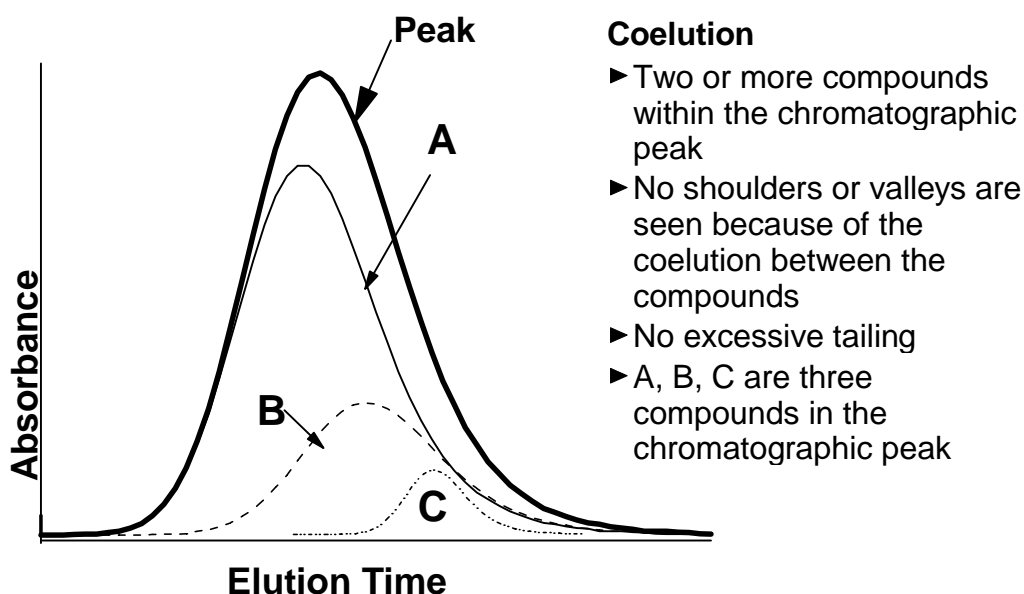


Waters 996 Photodiode Detector: Peak Purity I

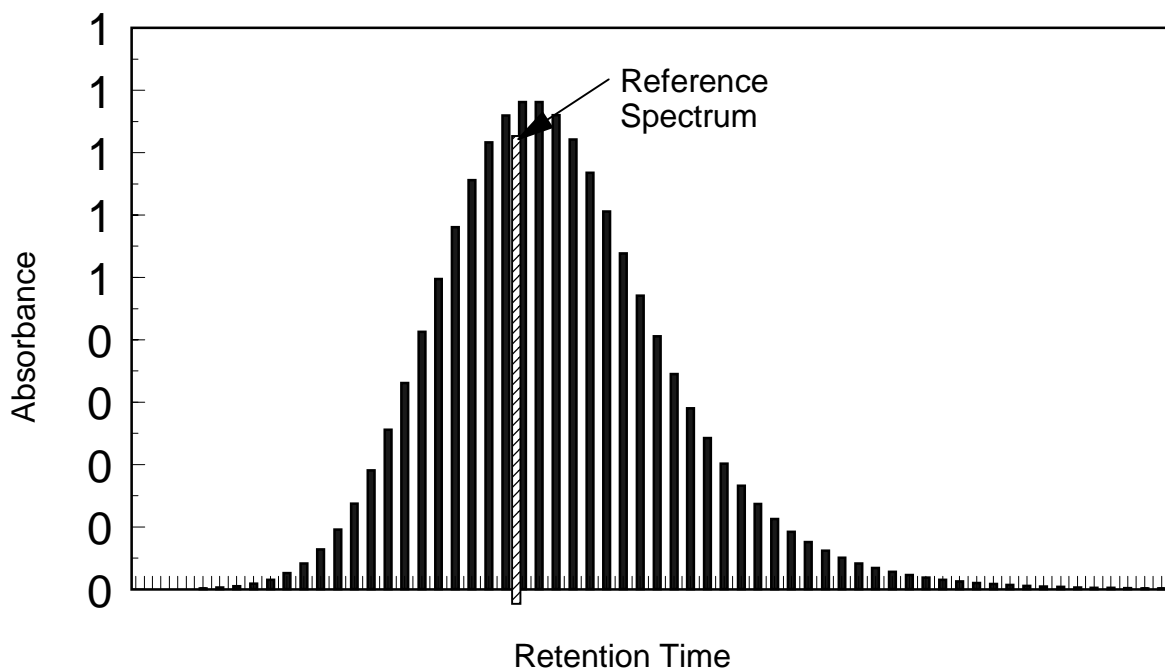
What is peak purity analysis?



Peak purity analysis is designed to detect the presence of an impurity that is coeluting with the analyte peak. For impurity detection with a single wavelength UV/visible detector, one must see a shoulder, valley or excessive tailing to suspect the presence of an impurity. The absence of these features on the chromatographic peak are not an assurance of peak purity. The impurity was not "seen" because the chromatographic resolution is too low, less than $R=0.3$, or the impurity concentration is quite low. A photodiode array detector can provide additional information using the acquisition of spectra to determine "peak purity".

Peak purity analysis incorporates Waters Millennium® software and data from the Waters 996 Photodiode Array detector to detect the presence of coeluting impurities. The spectral uniqueness of each compound is used to indicate when there are two or more components present in the peak.

Peak purity analysis



Peak Purity is an analysis of absorbance spectra across the peak to determine if they are all similar or there are differences. If there are spectral differences, it implies there are two or more compounds eluting in that chromatographic peak each being spectrally different.

The Millennium peak purity algorithms analyze each spectrum in the peak. If data is collected at one point per second and the peak is 20 seconds wide, 20 spectra will be analyzed. All spectra in the peak are compared to the apex spectrum, which is used as an internal reference point.

A photodiode array detector is used to determine peak "purity" by determining spectral homogeneity across the peak. This is sometimes referred to as peak homogeneity. It is **never proof of chemical purity** because:

1. The impurity must be spectrally different from the analyte.
2. There must be some chromatographic resolution between the analyte and the impurity.
3. The impurity must be present above the limit of detection.

To prove chemical purity, the sample must be analyzed several different ways using different techniques such as LC-MS, IR, NMR, wet chemistry.

PDA peak purity or homogeneity is used to help with chromatographic methods development and as an indication that a peak may not be a single compound.