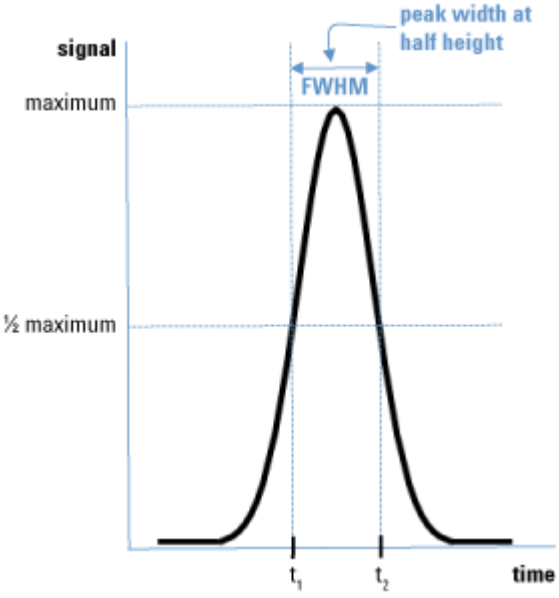
Enough Data Points across a LC peak

How many Data Points to be acquired across an LC peak.

When you acquire data from an LC detector of any type, make sure the data acquisition rate is appropriate for the narrowest chromatographic peak. If you acquire too many points across the peak, data files will be larger and unwieldy, resulting in slower data analysis. This is particularly true of diode array detectors and mass spectrometers, where you can acquire a full spectrum for each data point. If you acquire too few data points across a peak, you risk irreproducible quantitation and incorrect reporting of retention time.

Typically, you need to acquire a minimum of eight to ten data points across an LC peak to define its shape and to enable reproducible quantitation based on the area under the peak. To expose subtle peak-shape features that may result from co-elution, you should try to acquire 15 to 20 points across the peak.

To simplify method setup, Agilent acquisition software asks you to type the half-height peak width of the narrowest peak in the chromatogram. Then the software automatically selects the appropriate data rate, so that narrow peaks are well characterized. By doing this, you need only to input an easily measurable parameter, and you do not need to worry about the details of the detector settings.



To measure the peak width at half height, estimate the signal height at the top of the peak and at the baseline and calculate the mean of the two values – the signal halfway up the peak. Then draw a horizontal line at this value, to determine the peak width at half height in seconds or minutes.

This approach of using half-height peak width, also called full width at half maximum (FWHM), is especially useful with mass spectrometric detectors, which typically have more parameters that affect the data rate. By simply inputting the half-height peak width, the acquisition software (Agilent ChemStation or Agilent MassHunter Workstation software) can compensate and optimize to ensure the best acquisition rate.

With the increased use of Rapid Resolution LC and short columns with sub-two-micron particles, narrow peaks are becoming more important. Half-height peak widths can be less than one second, and the latest generation of detectors with data rates that are 40 Hz and greater are a necessity. As LC manufacturers push to even faster gradients and narrower peaks, data rates over 100 Hz could be needed for peaks that are 100 ms wide.

Acquisition of the correct number of data points across an LC peak is an important consideration in any LC lab. You can get more information on this topic by listening to an Agilent podcast, or by reading two Application Notes that illustrate fast data acquisition rates:

- “Agilent 1200 Series Rapid Resolution LC system and the Agilent 6210 TOF MS – Highest data content with highest throughput,” 5989-4505EN

- “Performance of the Agilent 1200 Series diode-array detector SL using different detector cells and different data rates up to 80 Hz,” 5989-5033EN

www.chem.agilent.com

Printed in USA August 7, 2007

Agilent Technologies