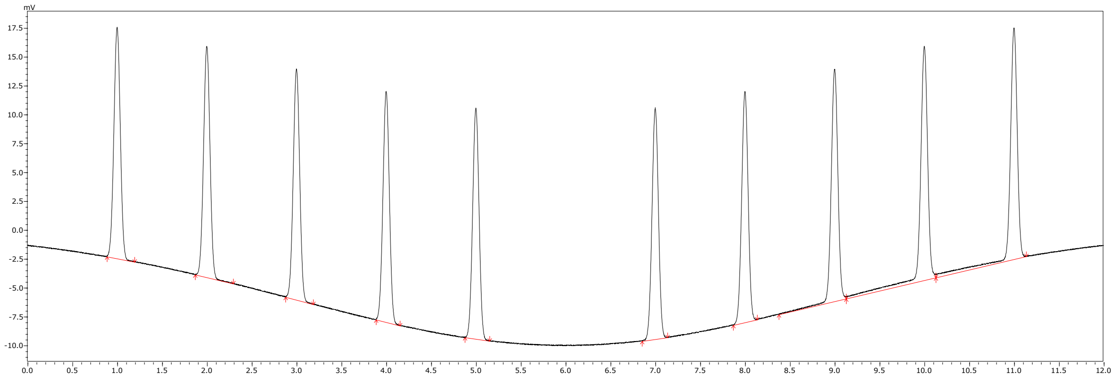
Part 1: Adjusting Noise Estimation and Peak Detection Sensitivity

In the browser, clicking [Quant Browser] - [Layout] - [Open Browsing File] and opening the "Smile.lcq" file loads the following data into the "Smile.lcm" method file.

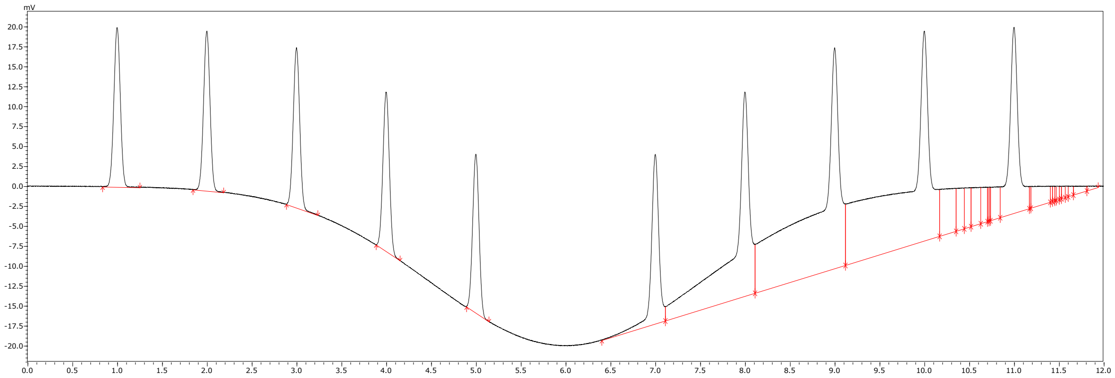
Smile_10000_txt.LCD, Smile_20000_txt.LCD, Smile_40000_txt.LCD

Initially the Chromatopac algorithm is used for processing.

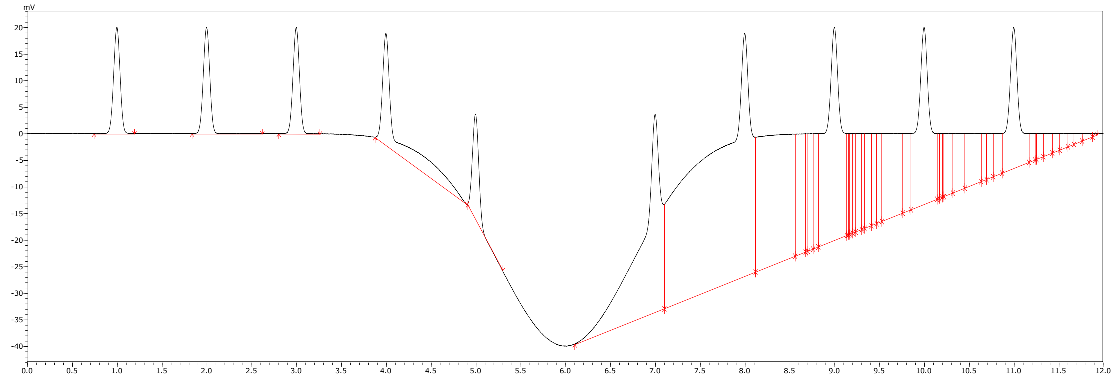
Smile_10000_txt.LCD



Smile_20000_txt.LCD

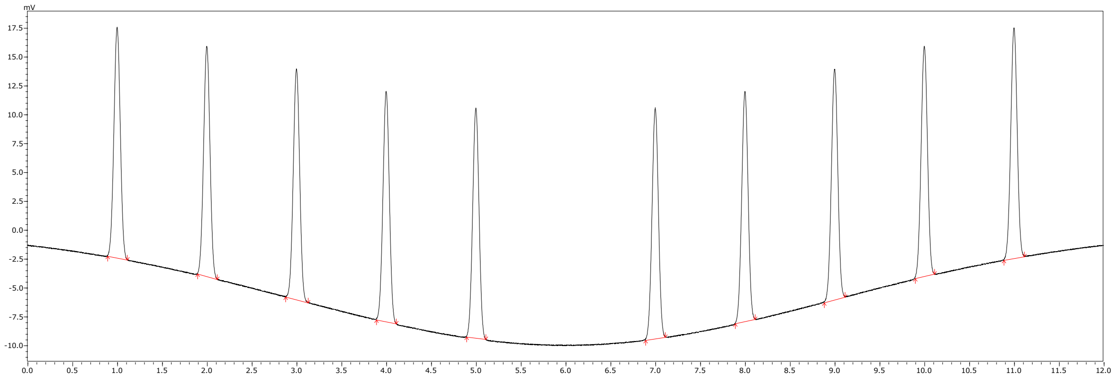


Smile_40000_txt.LCD

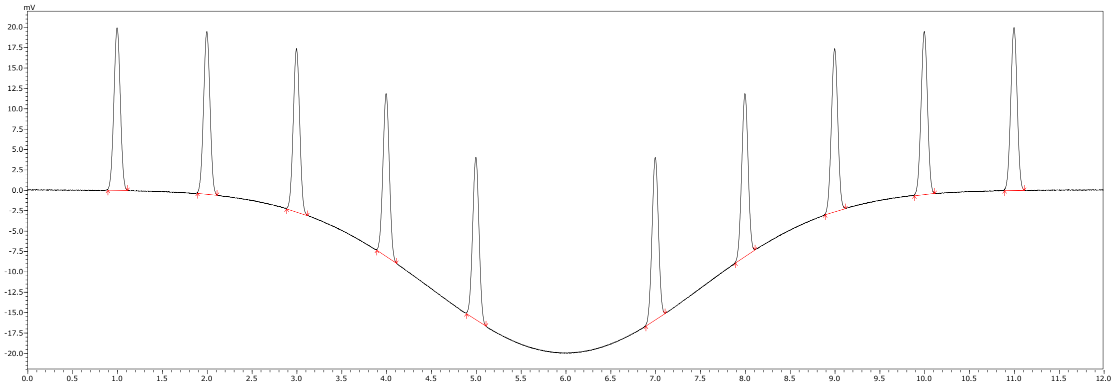


Select [i-PeakFinder] at [Algorithm] on the [Integration] tab page in the method view.

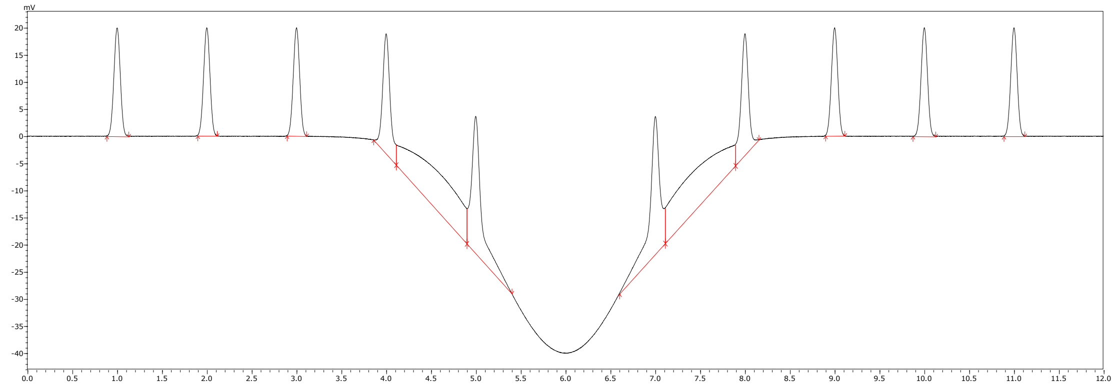
Smile_10000_txt.LCD



Smile_20000_txt.LCD



Smile_40000_txt.LCD



The automatic baseline estimation function functions to correctly process even baselines with a certain amount of undulations. This is one of the key features of i-PeakFinder.

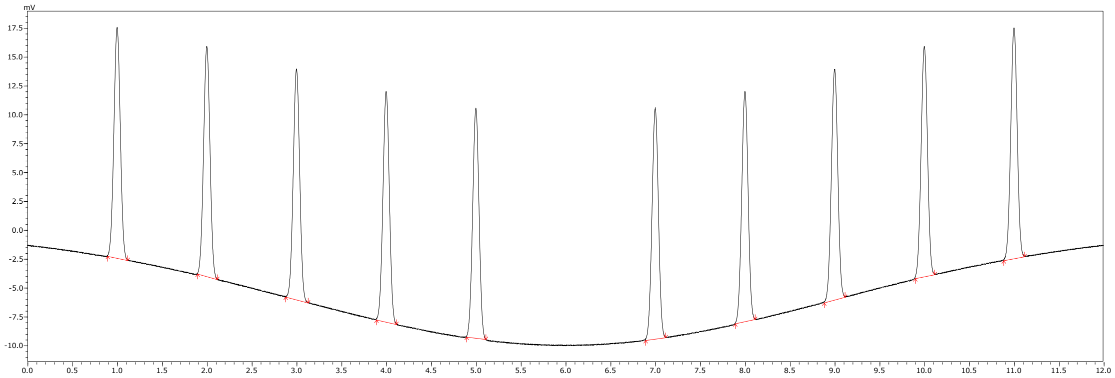
For larger undulations that exceed the automatic baseline estimation range, adjust the parameter settings.

Successively increase the [Detection Threshold] (S/N criteria value) setting. In this case, the chromatogram is processed properly with a setting of 100.

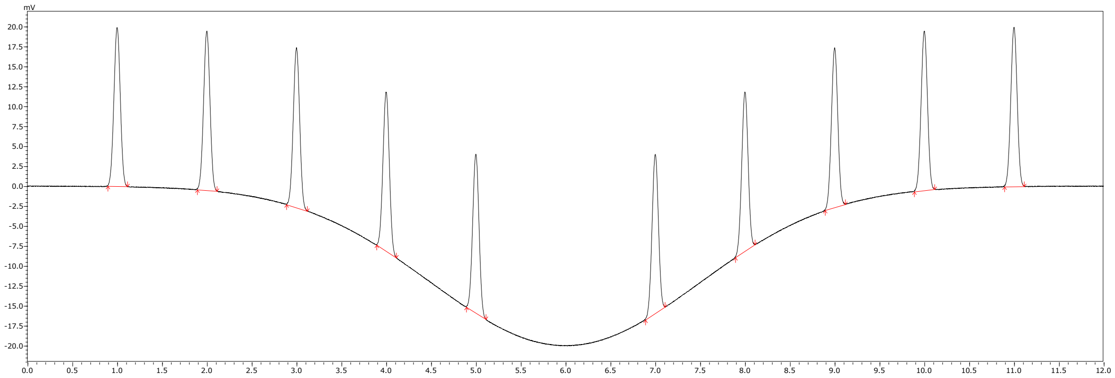
Alternatively, select the baseline area with large bends (i.e. high noise) in the [Integration Advanced Settings] - [Peak Detection] - [Noise Estimation Range] field, so that a larger N value is used for determining S/N. In this case, the chromatogram is processed properly with a setting of 4.2 to 4.8.

(Specify a somewhat large value for this parameter, which is used to determine S/N criteria, because of the low noise level in the artificial data.)

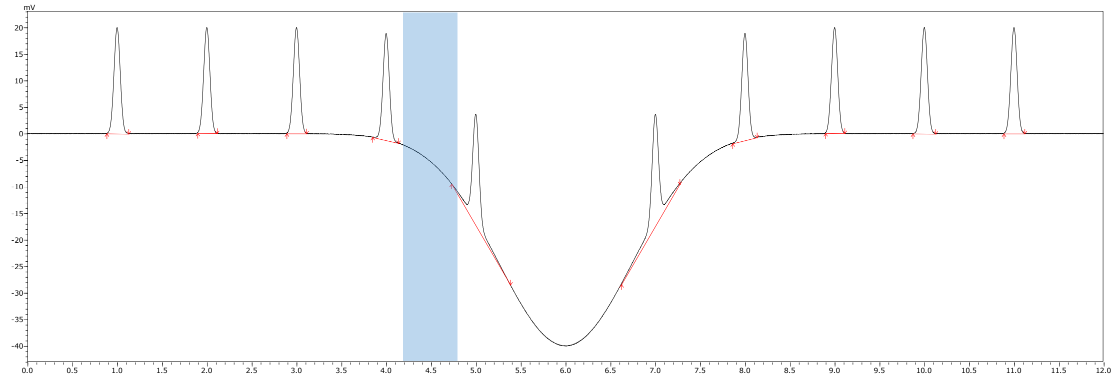
Smile_10000_txt.LCD



Smile_20000_txt.LCD



Smile_40000_txt.LCD



If the undulating areas of baselines with large undulations are specified in [Noise Estimation Range], then noise is estimated based on the undulation frequency, so that the corresponding [Detection Threshold] setting is applied appropriately.

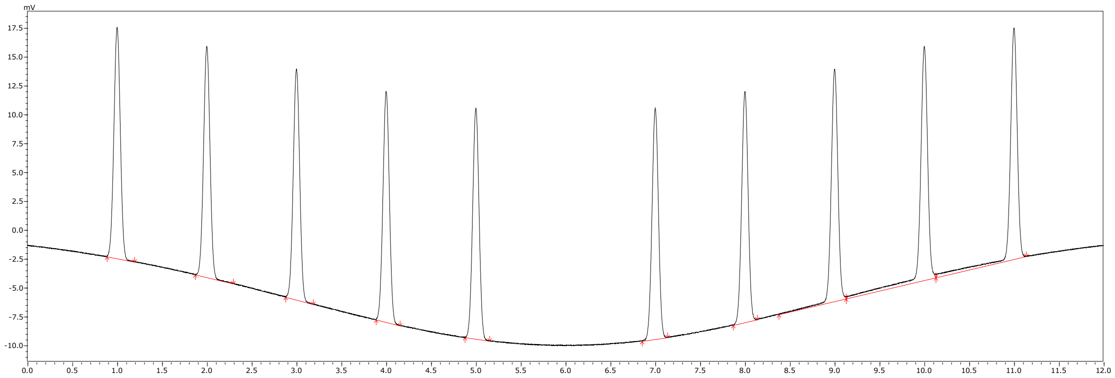
Part 2: Bending the Peak-Baseline

In the browser, clicking [Quant Browser] - [Layout] - [Open Browsing File] and opening the "Smile.lcq" file loads the following data into the "Smile.lcm" method file.

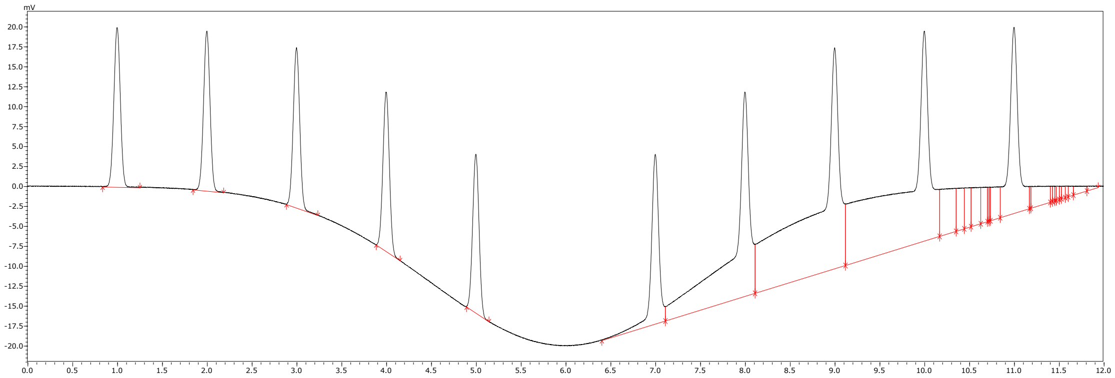
Smile_10000_txt.LCD, Smile_20000_txt.LCD, Smile_40000_txt.LCD

Initially the Chromatopac algorithm is used for processing.

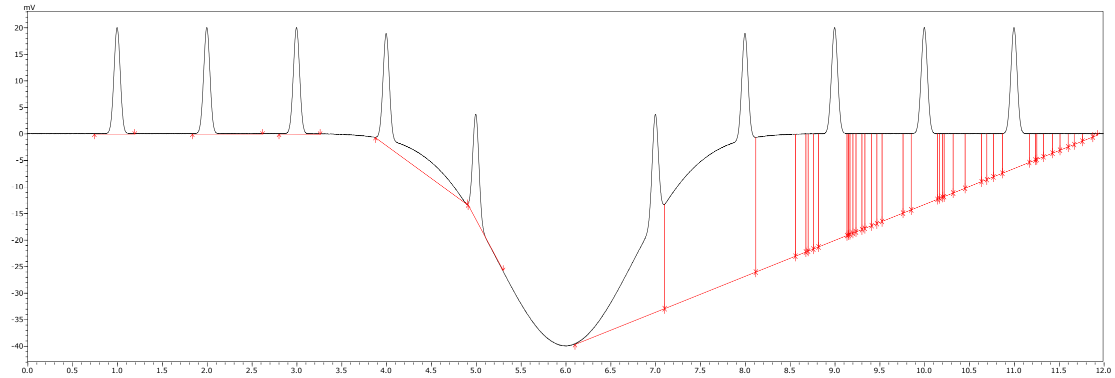
Smile_10000_txt.LCD



Smile_20000_txt.LCD

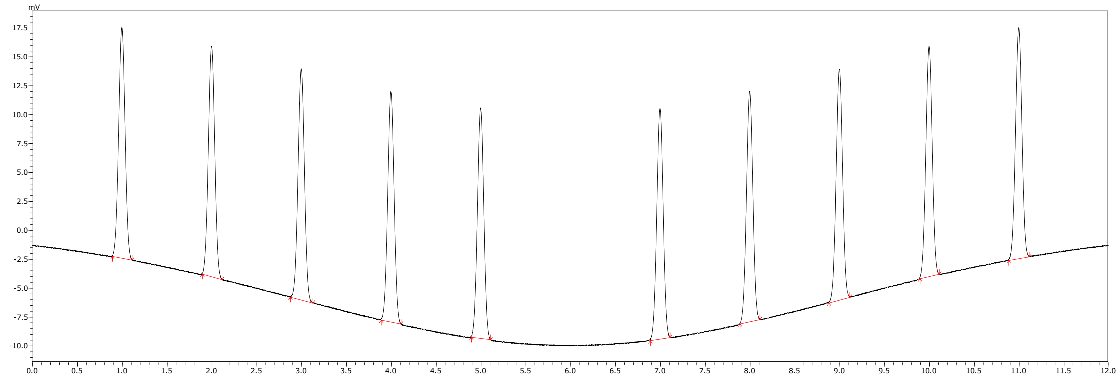


Smile_40000_txt.LCD

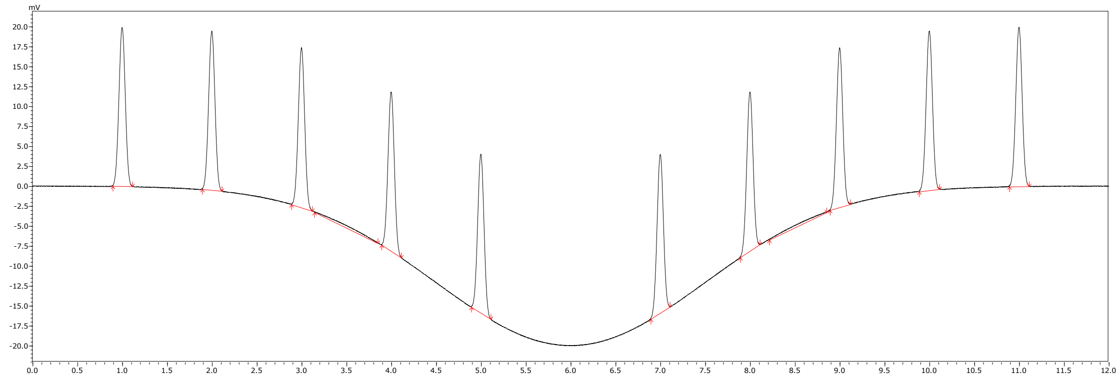


In the method view, click [Integration] - [Algorithm] - [i-PeakFinder] and then set [Baseline Type] - [Baseline Length] to 0.1 min, so that it is less than the peak width.

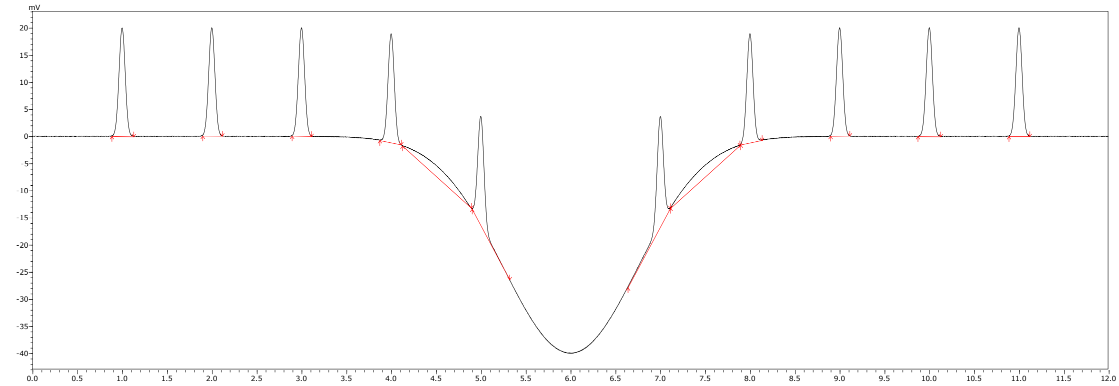
Smile_10000_txt.LCD



Smile_20000_txt.LCD



Smile_40000_txt.LCD

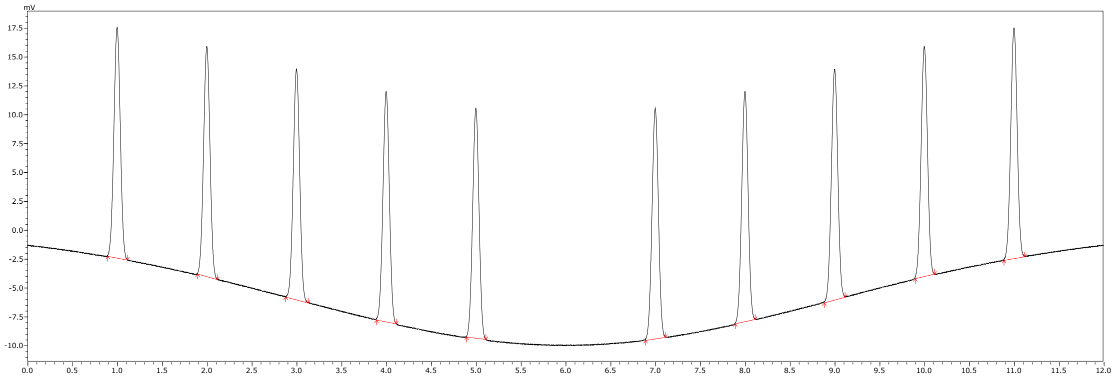


Though there are still some short broad areas remaining as false peaks* between peaks, the desired peaks are detected correctly.

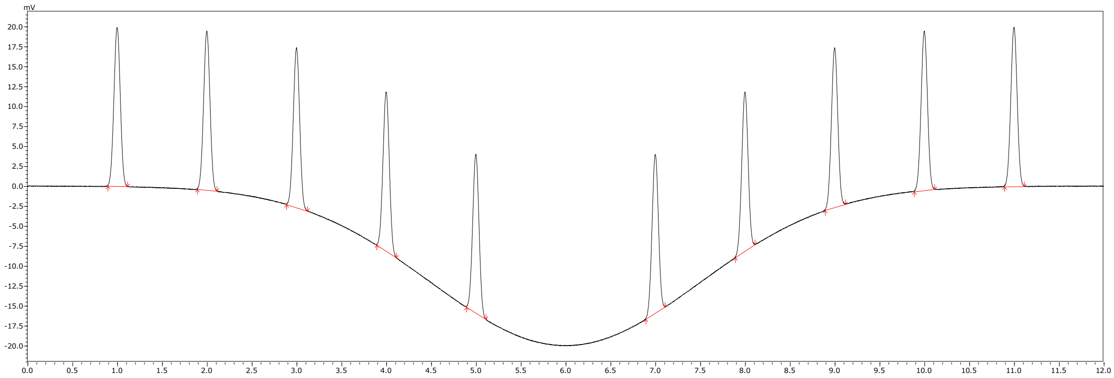
*: Bulges in the baseline misidentified as a peak

Eliminate false-peak areas by using a [Min. Aspect] filter or other such means.
In this case, good results can be obtained by setting [Min. Aspect] to 10000.

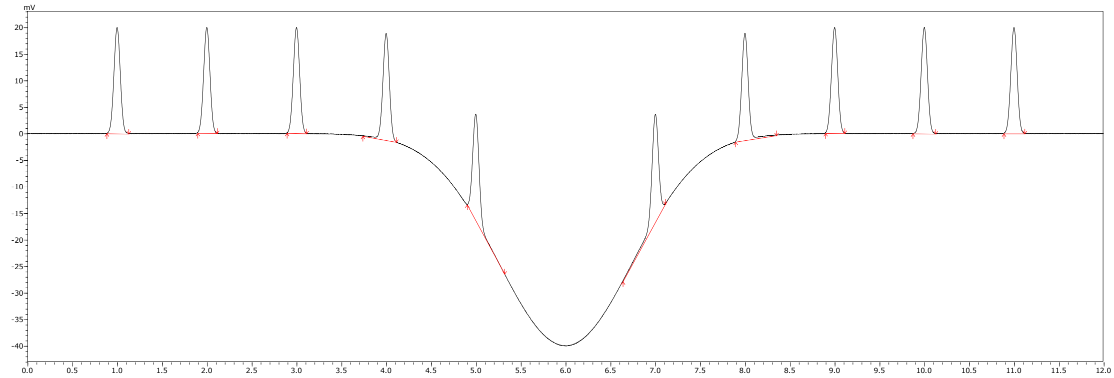
Smile_10000_txt.LCD



Smile_20000_txt.LCD



Smile_40000_txt.LCD



Because the process can be performed artificially, care is required to make sure it is used appropriately, but the process is intuitive and easy to use.

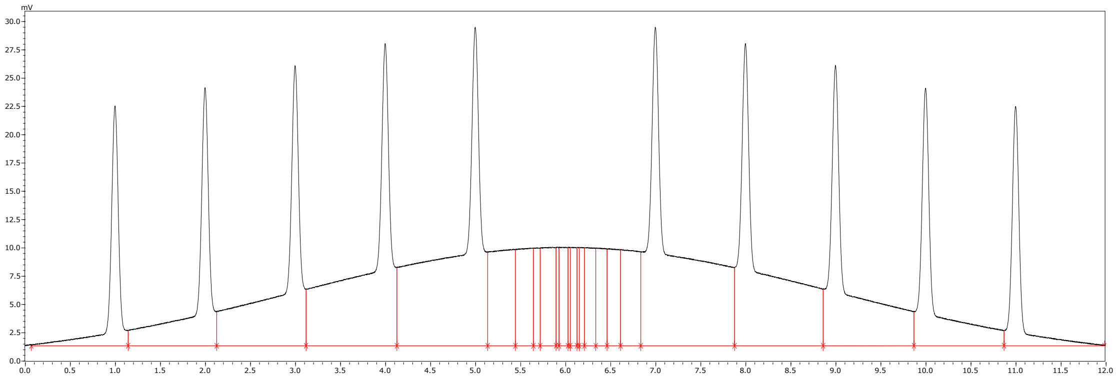
Part 3: Using Maximum Half Height Width to Designate a Large Bulge as Baseline

In the browser, clicking [Quant Browser] - [Layout] - [Open Browsing File] and opening the "Angry.lcq" file loads the following data into the "Angry.lcm" method file.

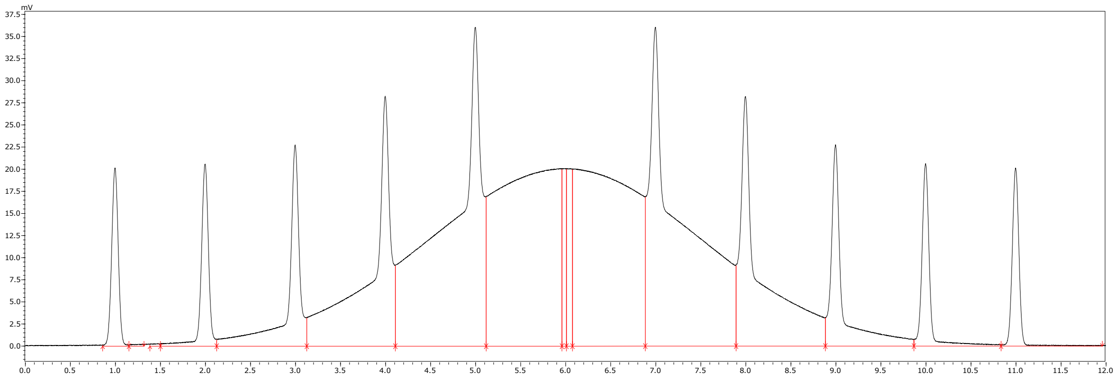
Angry_10000_txt.LCD, Angry_20000_txt.LCD, Angry_40000_txt.LCD

Initially the Chromatopac algorithm is used for processing.

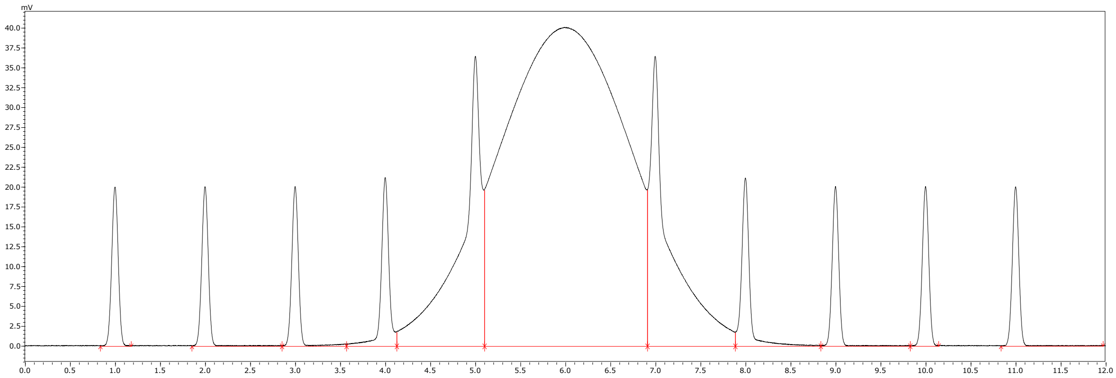
Angry_10000_txt.LCD



Angry_20000_txt.LCD

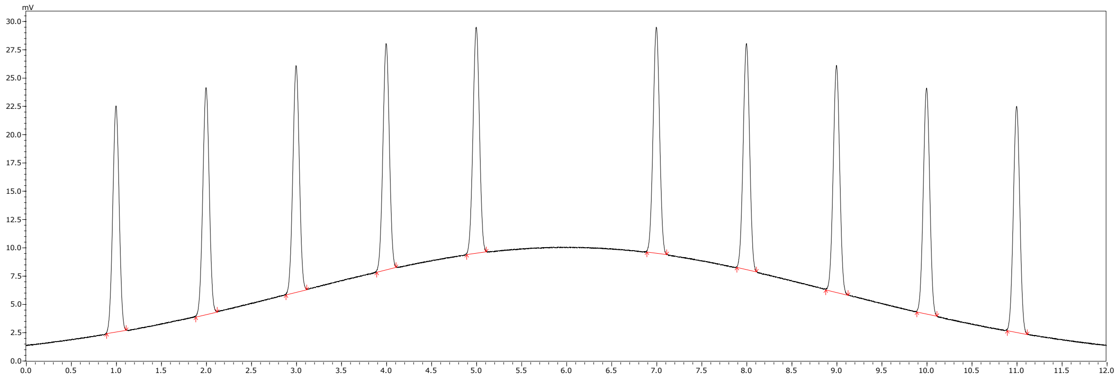


Angry_40000_txt.LCD

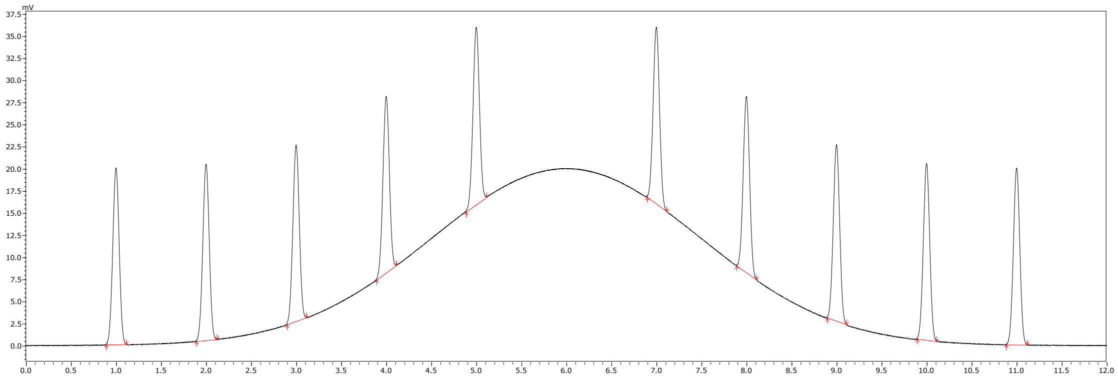


Select [i-PeakFinder] at [Algorithm] on the [Integration] tab page in the method view.

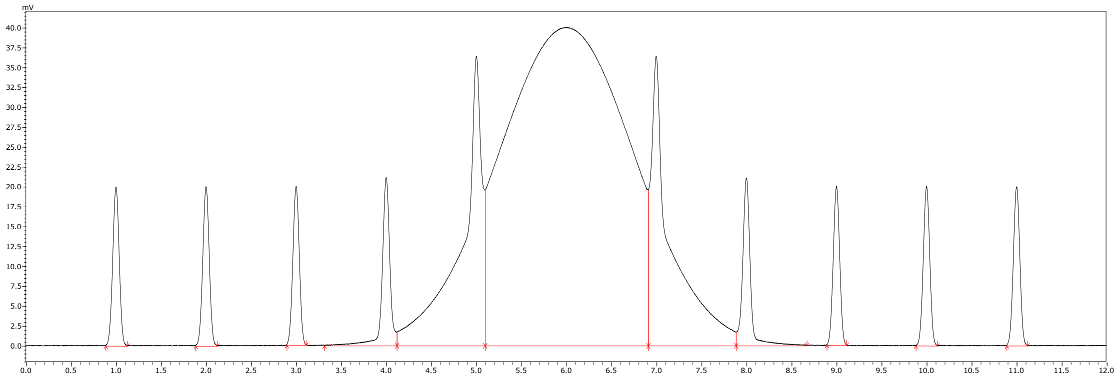
Angry_10000_txt.LCD



Angry_20000_txt.LCD



Angry_40000_txt.LCD

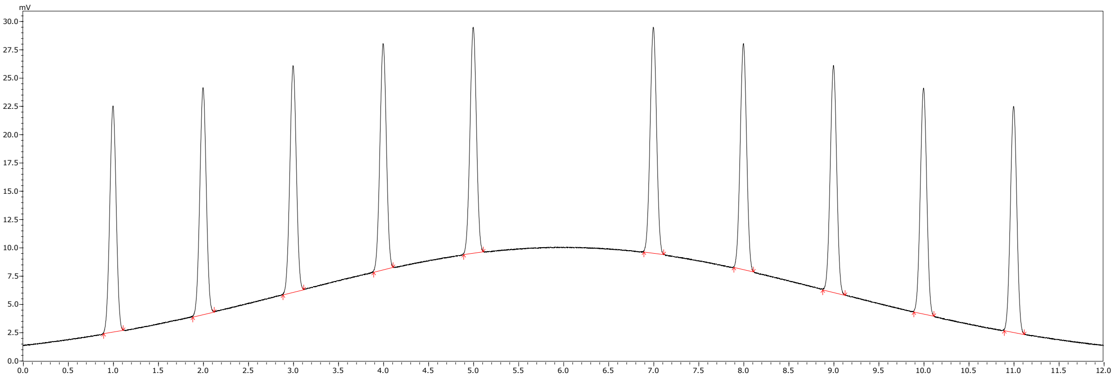


In this case as well, the automatic baseline estimation function functions to correctly process even baselines with a certain amount of undulations.

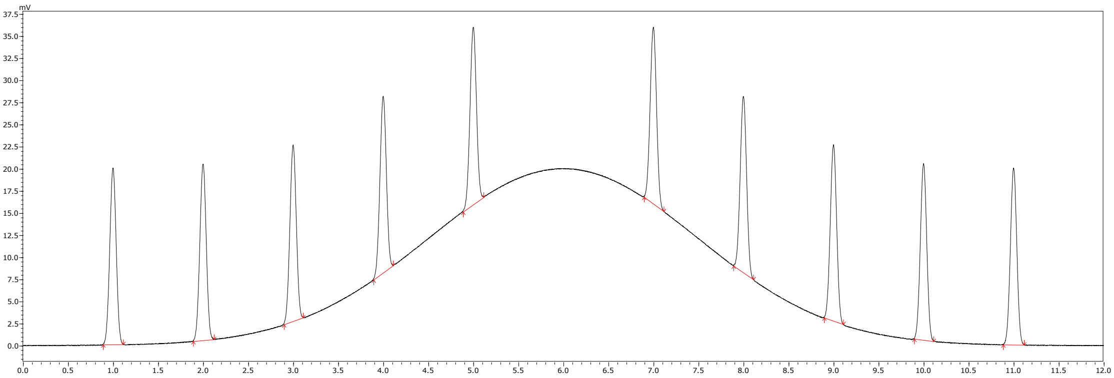
For larger undulations that exceed the automatic baseline estimation range, adjust the parameter settings.

In the [Integration Advanced Settings] - [Peak Detection] - [Maximum Half Width] field, specify a half height width that is a little greater than necessary for the peaks to be detected. In this case, the chromatogram is processed properly with a setting of 5 sec.

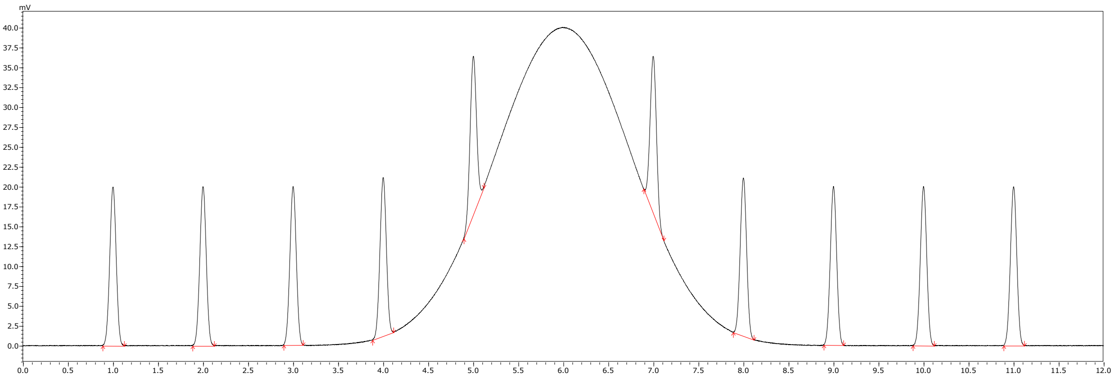
Angry_10000_txt.LCD



Angry_20000_txt.LCD



Angry_40000_txt.LCD



A large undulation (bulge) in the center plot line was incorrectly detected as a peak, but its half height width was greater than the [Maximum Half Width] setting, so the peak was eliminated and included in the baseline to obtain the desired results.

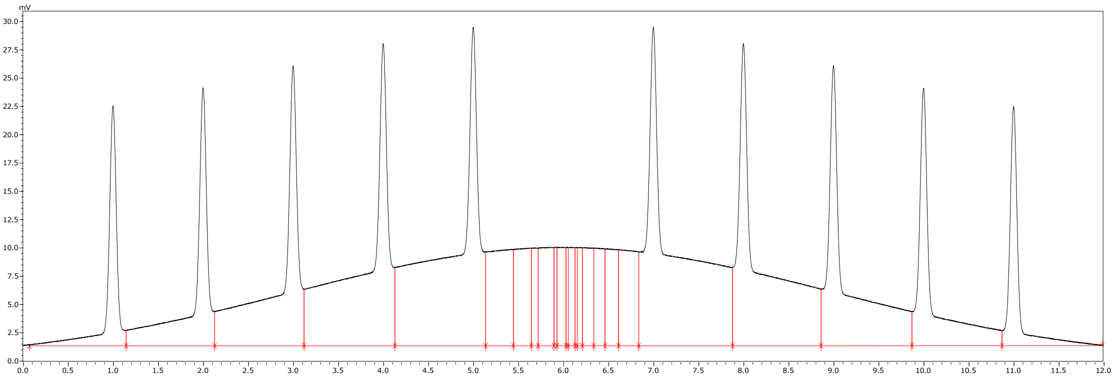
Part 4: Types of Analysis Where Results Are Not Permitted to Track the Baseline

In the browser, clicking [Quant Browser] - [Layout] - [Open Browsing File] and opening the "Angry.lcq" file loads the following data into the "Angry.lcm" method file.

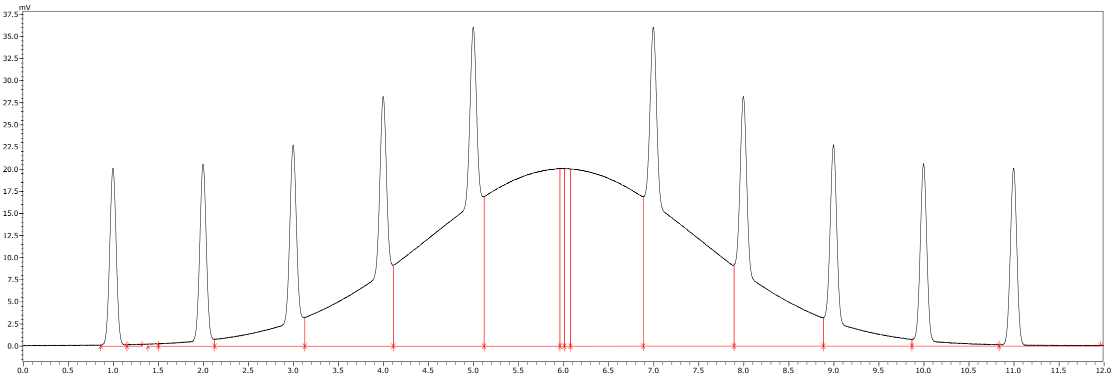
Angry_10000_txt.LCD, Angry_20000_txt.LCD, Angry_40000_txt.LCD

Initially the Chromatopac algorithm is used for processing.

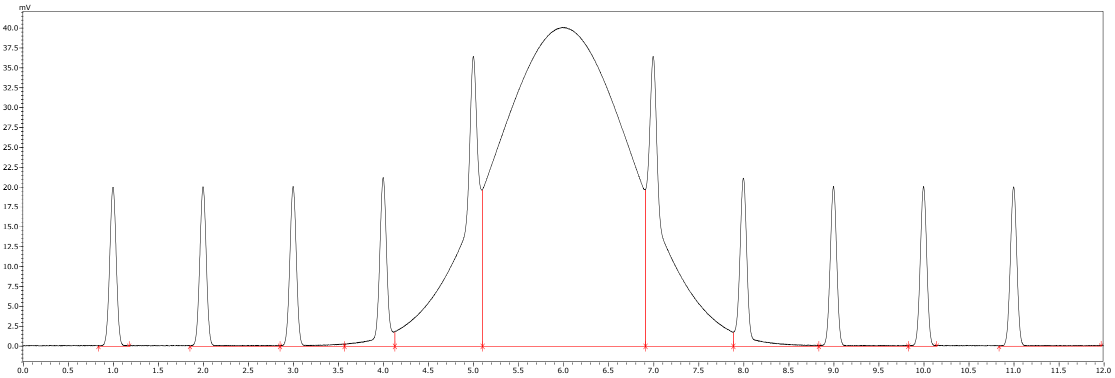
Angry_10000_txt.LCD



Angry_20000_txt.LCD

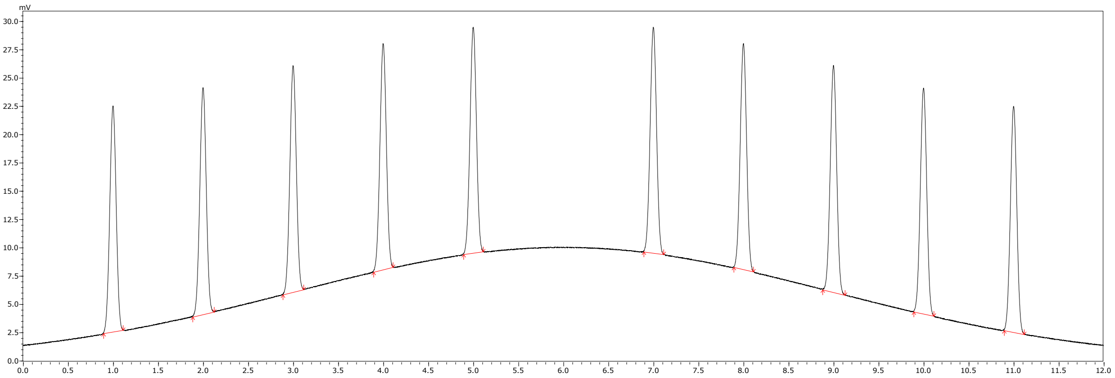


Angry_40000_txt.LCD

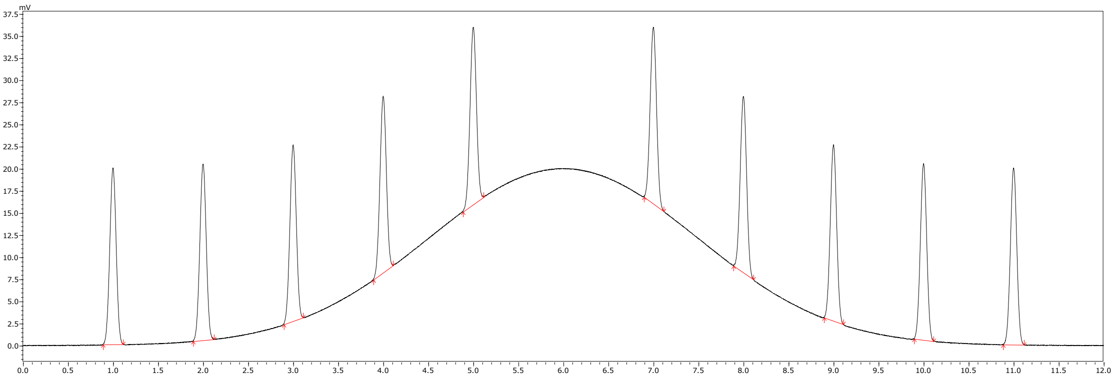


Select [i-PeakFinder] at [Algorithm] on the [Integration] tab page in the method view.

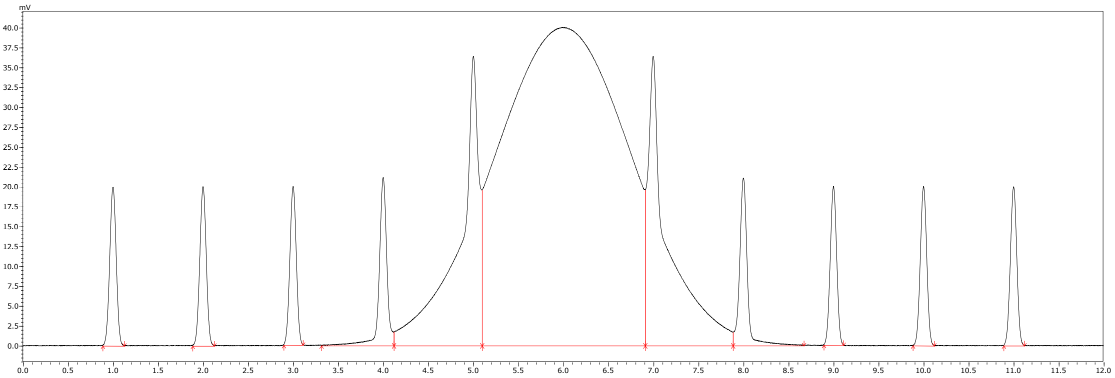
Angry_10000_txt.LCD



Angry_20000_txt.LCD



Angry_40000_txt.LCD

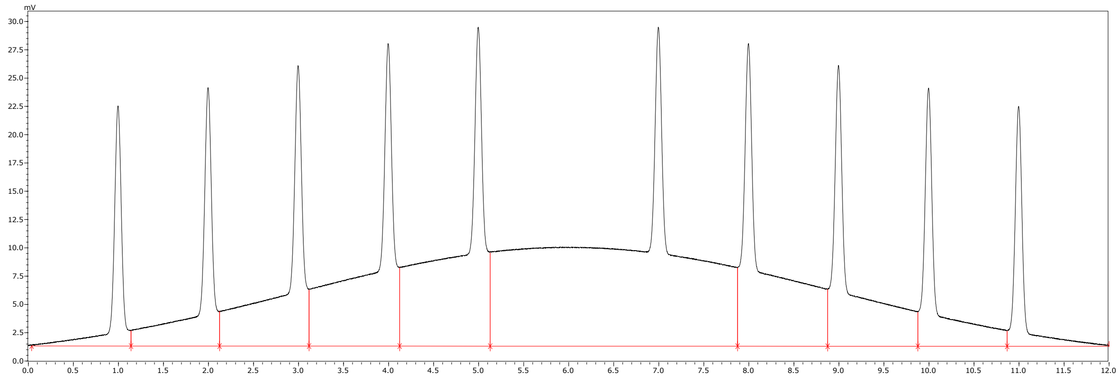


Again, the automatic baseline estimation function functions to correctly process even baselines with a certain amount of undulations, but for some applications, more correct data can be obtained without baseline estimation.

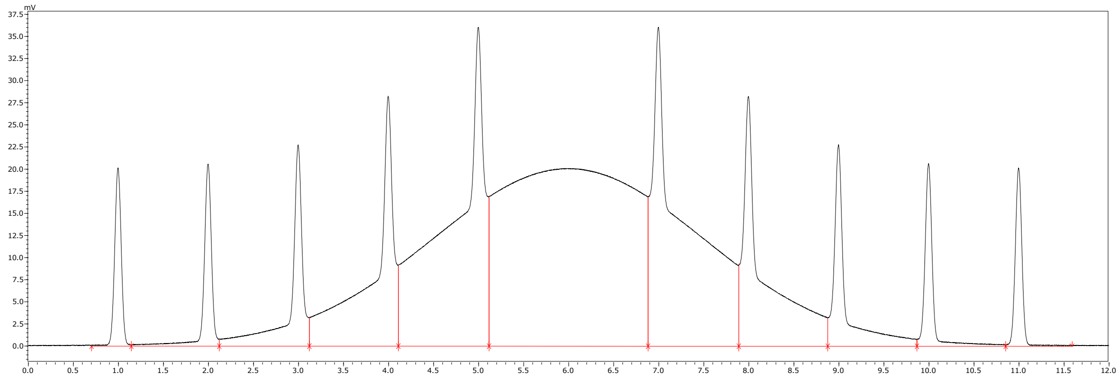
Examples include GC analysis of hydrocarbons, distillation GC analysis, and so on.

Set [Baseline Type] to [Vertical Division].

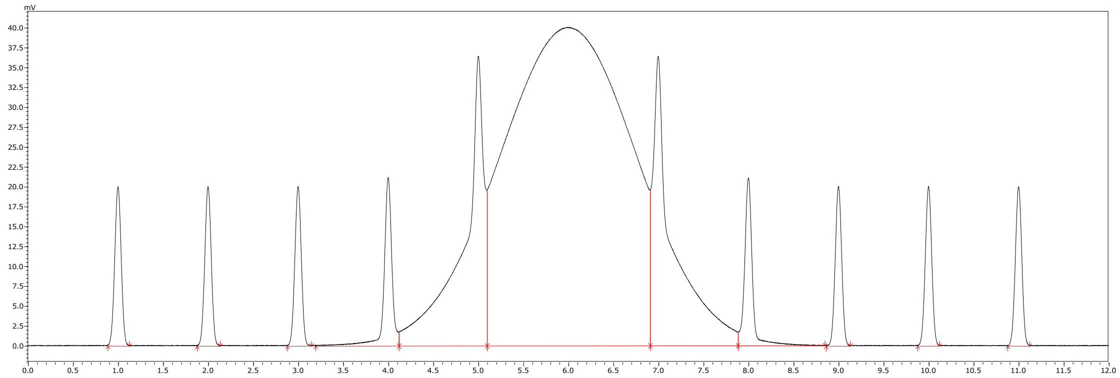
Angry_10000_txt.LCD



Angry_20000_txt.LCD



Angry_40000_txt.LCD

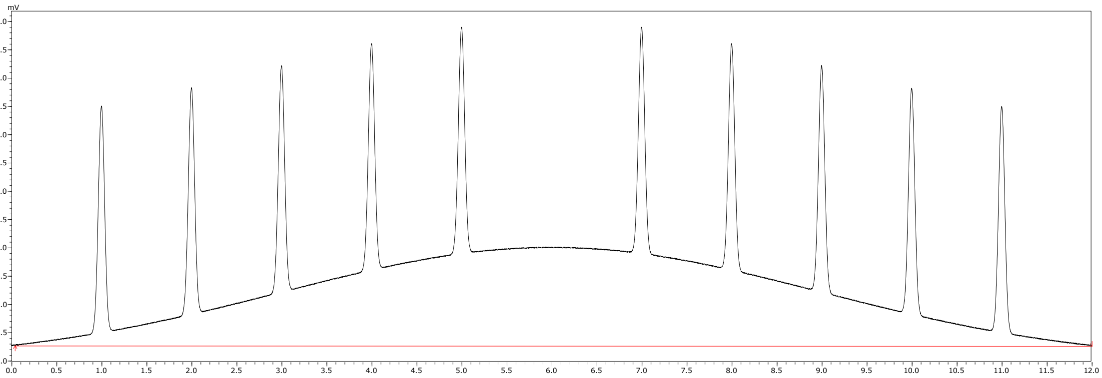


In addition, some applications calculate the entire area as one peak.

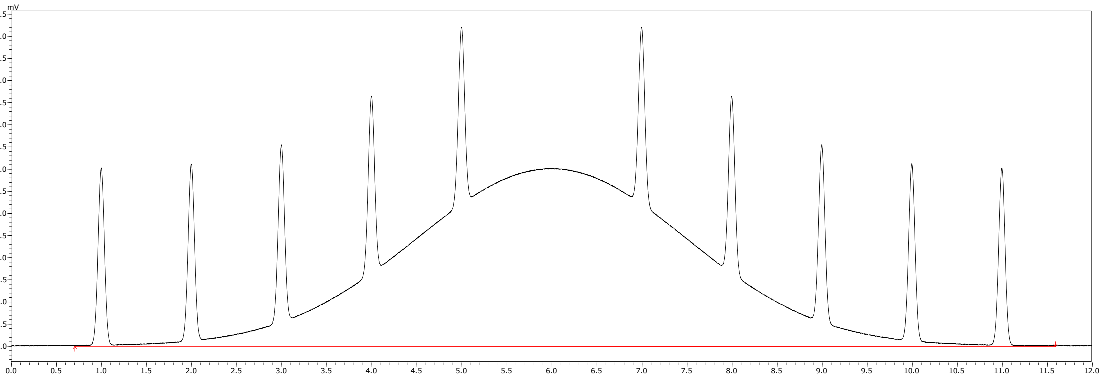
In the [Integration Advanced Settings] - [Peak Detection] - [Minimum Half Width] field, specify a half height width that is greater than necessary for the area to be detected as one peak.

Given the 12 min total width of the chromatogram, specify a 4 min value, which is about one third the total, or 240 sec.

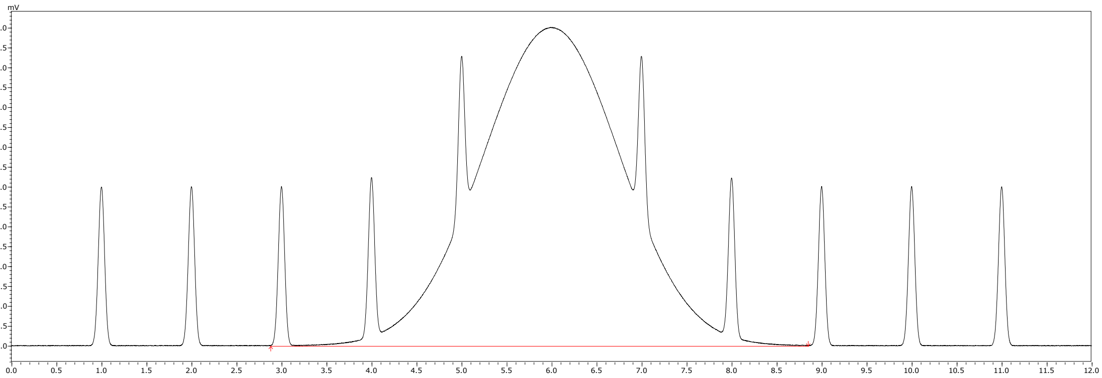
Angry_10000_txt.LCD



Angry_20000_txt.LCD



Angry_40000_txt.LCD



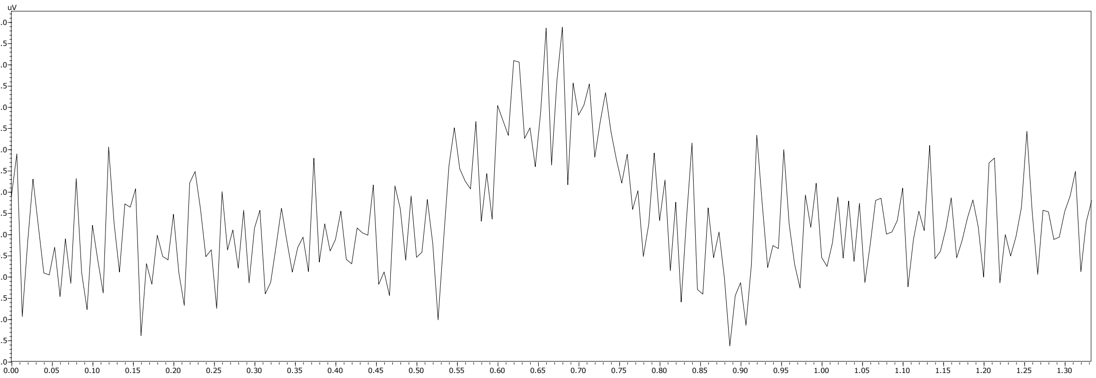
Part 5: Detecting Peaks at Risk of Being Buried in Noise

In the browser, clicking [Quant Browser] - [Layout] - [Open Browsing File] and opening the "gauss_quant.lcq" file loads the following data into the "gauss_quant.lcm" method file.

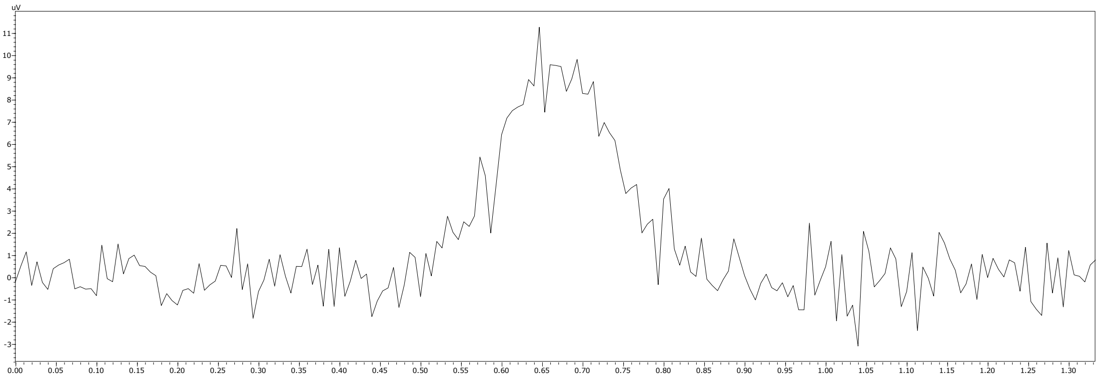
gauss_snr_3.1.gcd, gauss_snr_10.1.gcd, gauss_snr_20.1.gcd, gauss_snr_50.1.gcd, gauss_snr_100.1.gcd

Initially the Chromatopac algorithm is used for processing.
Since the chromatogram includes short peaks, set the minimum area to 10 count, rather than specifying a minimum height setting.

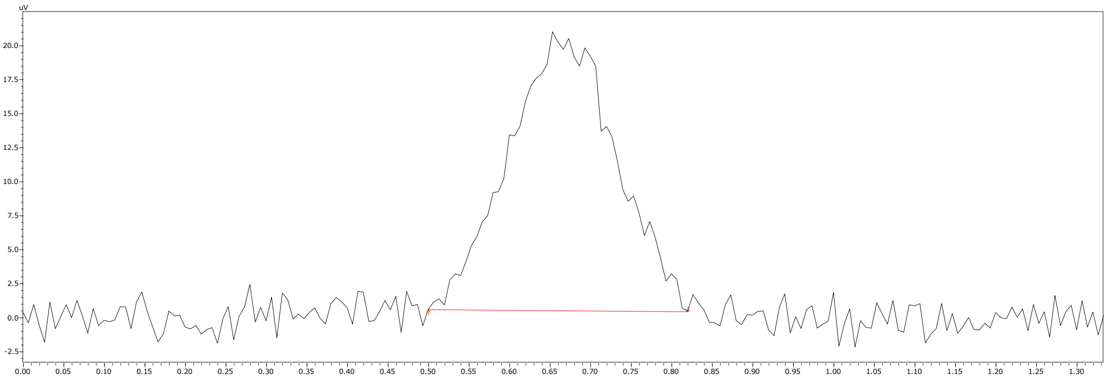
gauss_snr_3.1.gcd



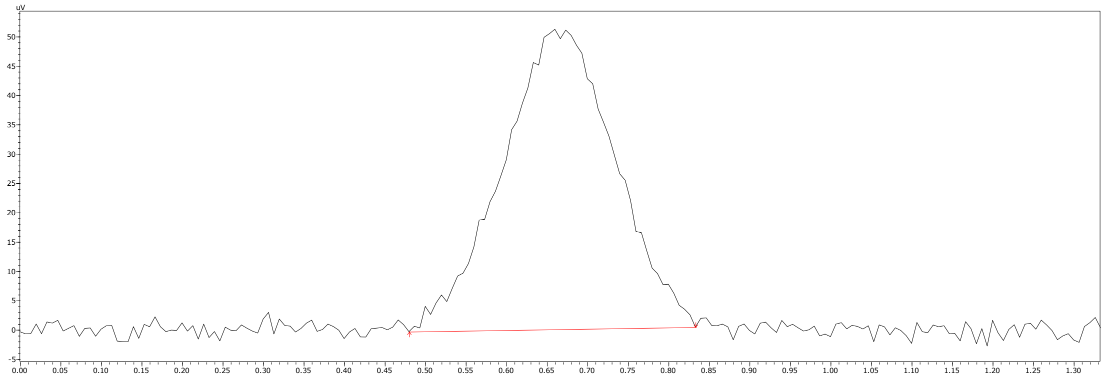
gauss_snr_10.1.gcd



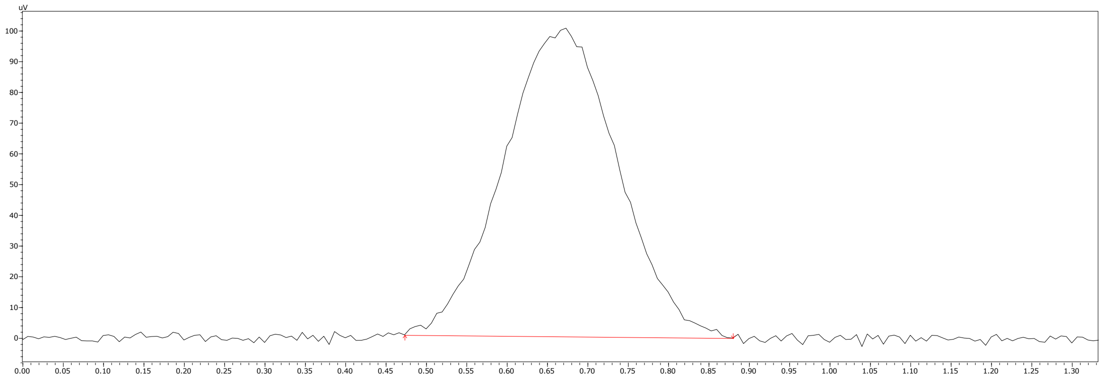
gauss_snr_20.1.gcd



gauss_snr_50.1.gcd



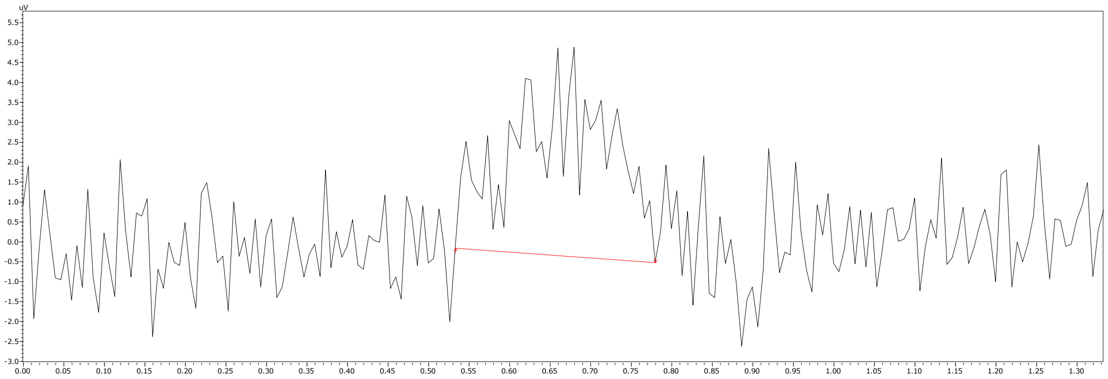
gauss_snr_100.1.gcd



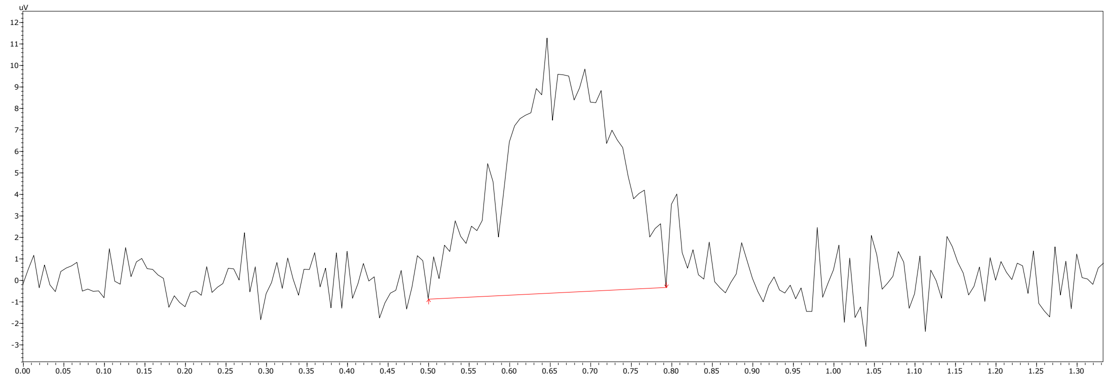
In the low concentration sample, peaks were buried in noise and not detected.

Select [i-PeakFinder] at [Algorithm] on the [Integration] tab page in the method view. In this case, some peaks were only about double the height of the noise. Therefore, set [Detection Threshold] to 2 or, just like for the Chromatopac algorithm, clear the [Min. Height] checkbox and set [Min. Area] to 10, so that shorter peaks are not deleted.

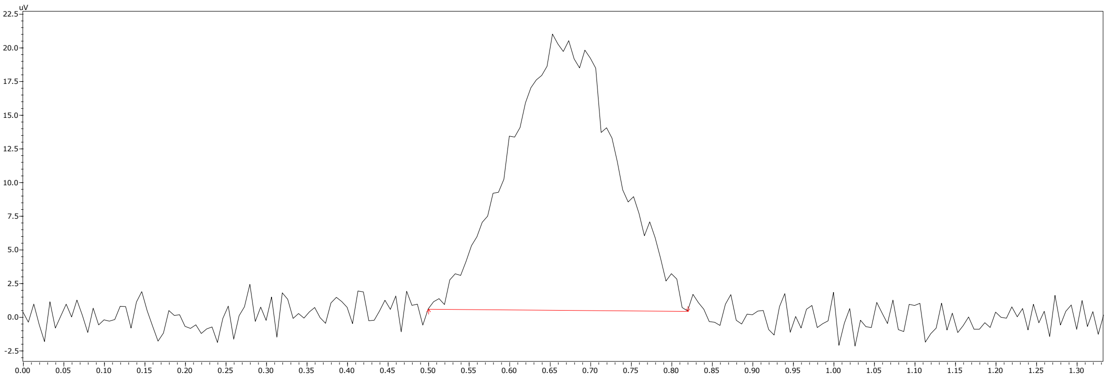
gauss_snr_3.1.gcd



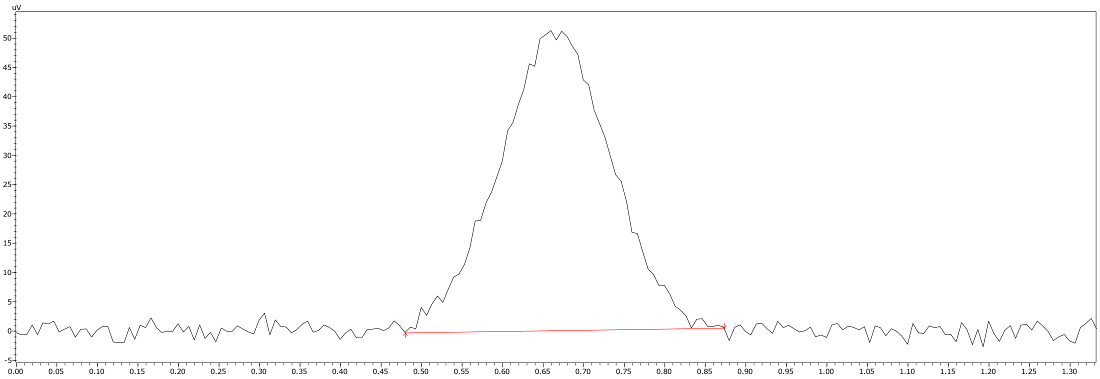
gauss_snr_10.1.gcd



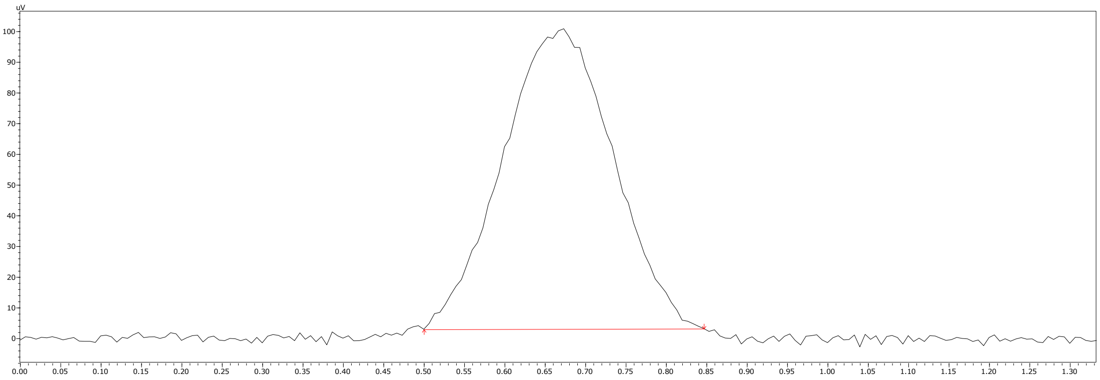
gauss_snr_20.1.gcd



gauss_snr_50.1.gcd



gauss_snr_100.1.gcd



Peaks are now detected properly even in the low concentration sample.

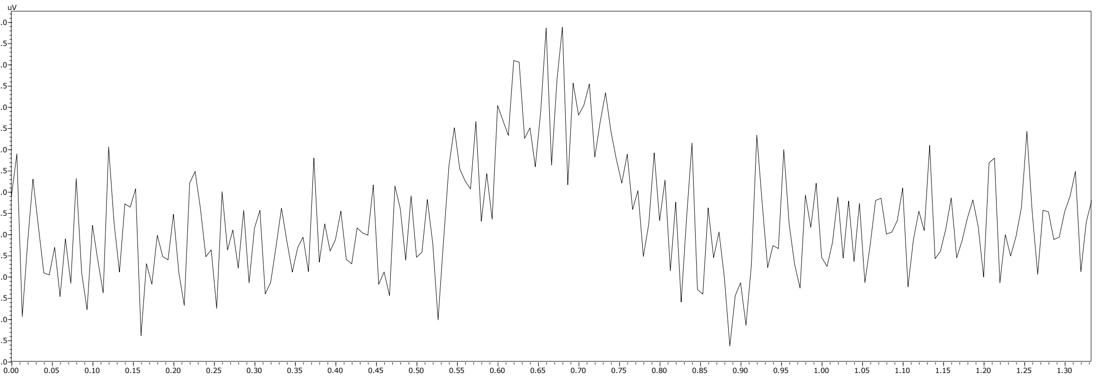
Part 6: Unifying Multiply-Divided Peaks Based on Default LCMS Parameter Settings

In the browser, clicking [Quant Browser] - [Layout] - [Open Browsing File] and opening the "gauss_quant.lcq" file loads the following data into the "gauss_quant.lcm" method file.

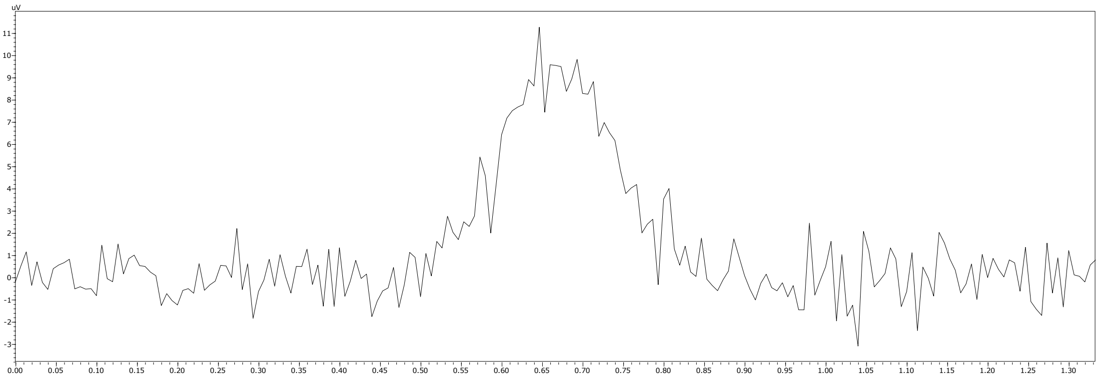
gauss_snr_3.1.gcd, gauss_snr_10.1.gcd, gauss_snr_20.1.gcd, gauss_snr_50.1.gcd, gauss_snr_100.1.gcd

Initially the Chromatopac algorithm is used for processing.
Since the chromatogram includes short peaks, set the minimum area to 10 count, rather than specifying a minimum height setting.

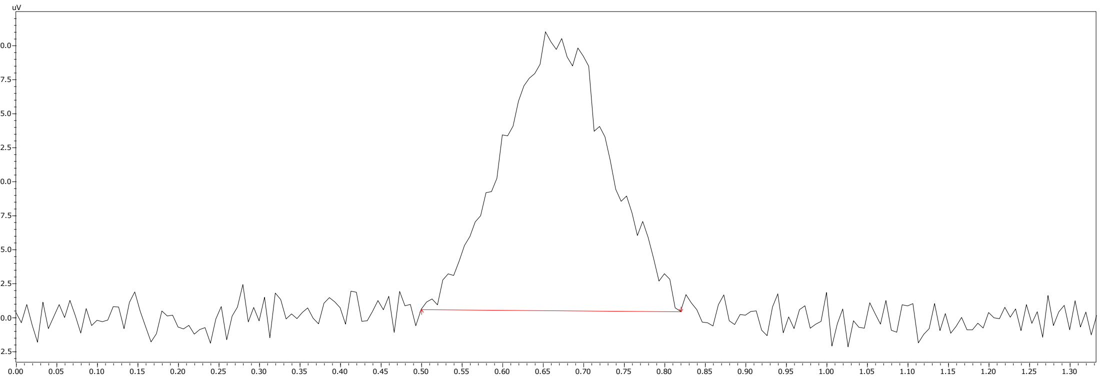
gauss_snr_3.1.gcd



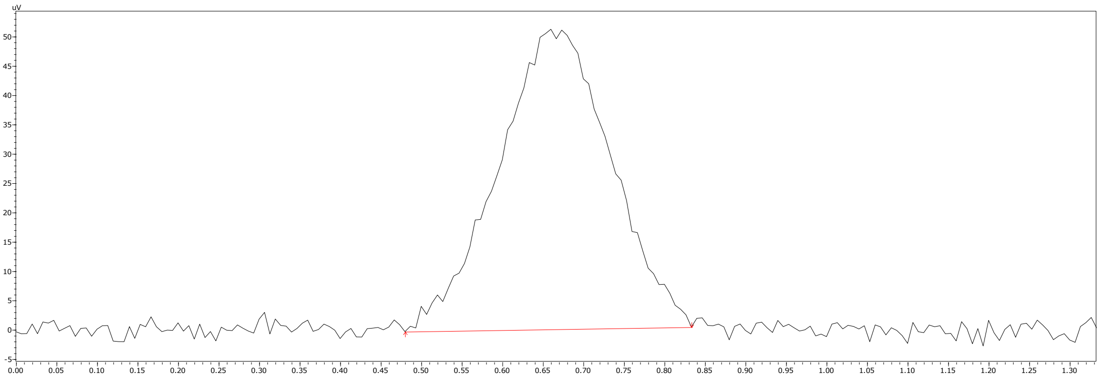
gauss_snr_10.1.gcd



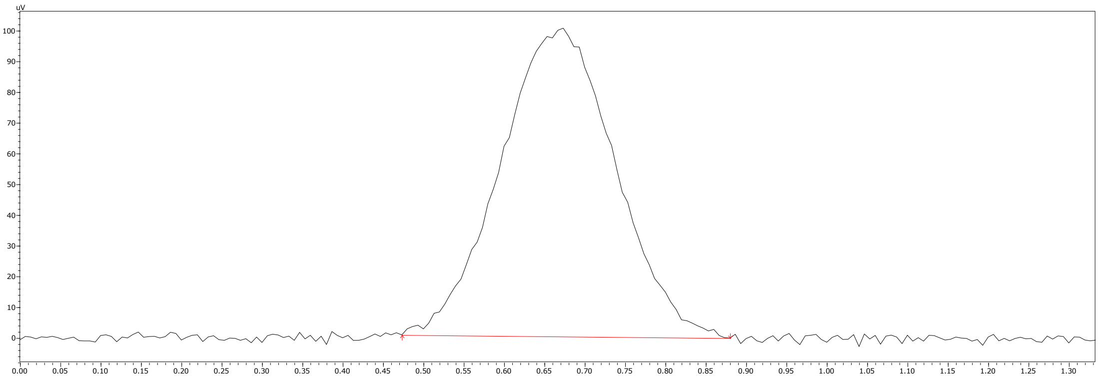
gauss_snr_20.1.gcd



gauss_snr_50.1.gcd



gauss_snr_100.1.gcd



In the low concentration sample, peaks were buried in noise and not detected.

Select [i-PeakFinder] at [Algorithm] on the [Integration] tab page in the method view.

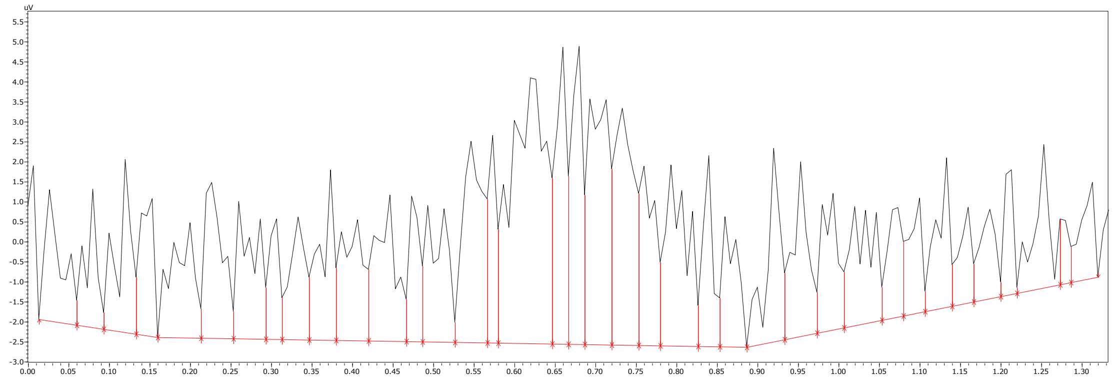
[Detection Threshold] = 0

Set [Integration Advanced Settings] - [Peak Detection] - [Noise Estimation Range] to 0 to 0 min*

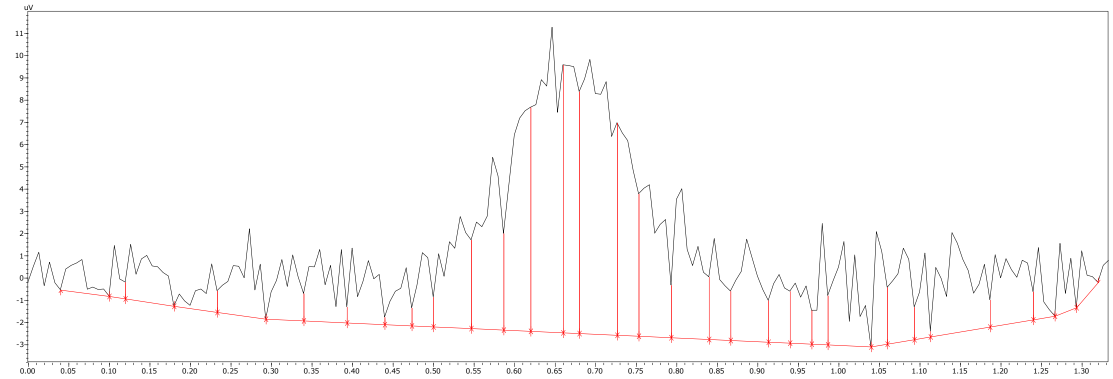
and set [Integration Advanced Settings] - [Peak Detection] - [Peak Baseline Height] to 0.1.

*: That results in fixing the minimum noise estimation level at 1 μV, so that even the smallest peaks are detected.

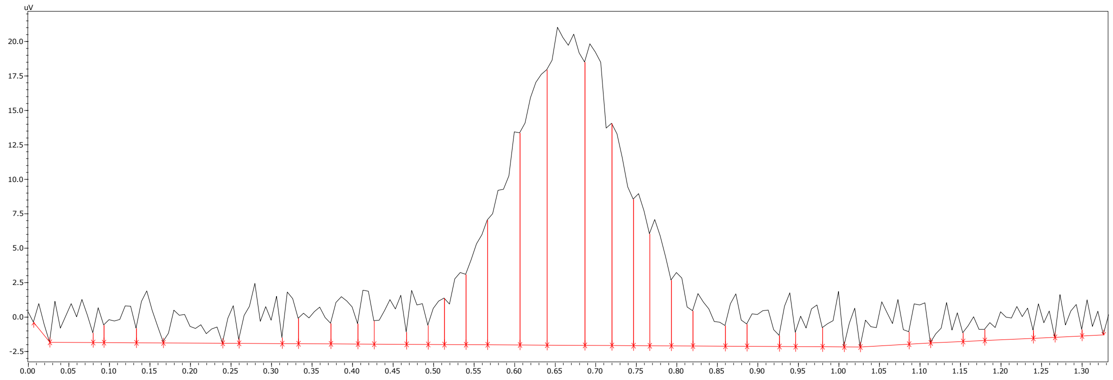
gauss_snr_3.1.gcd



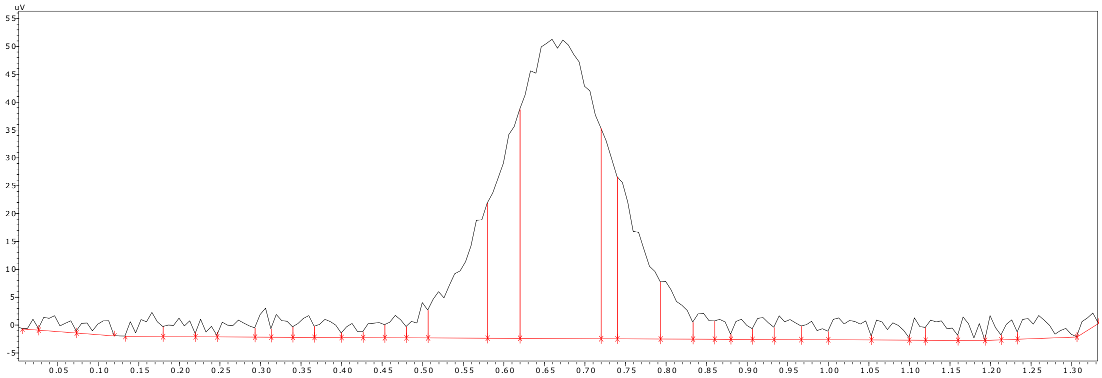
gauss_snr_10.1.gcd



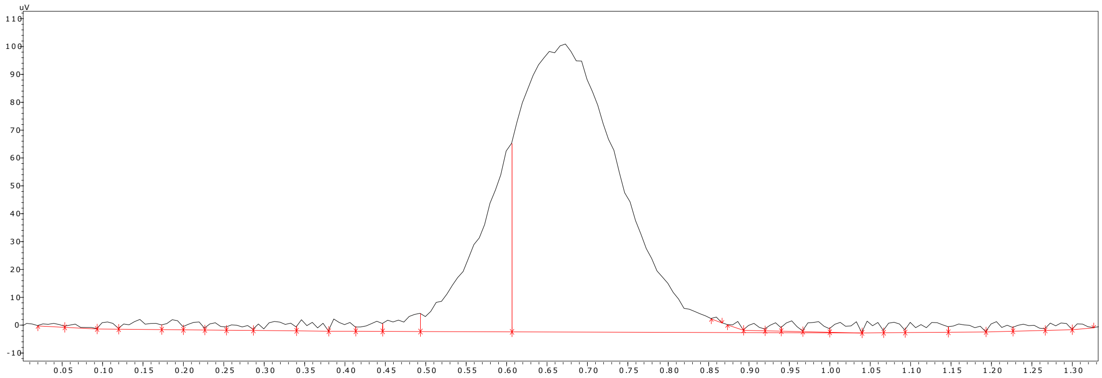
gauss_snr_20.1.gcd



gauss_snr_50.1.gcd



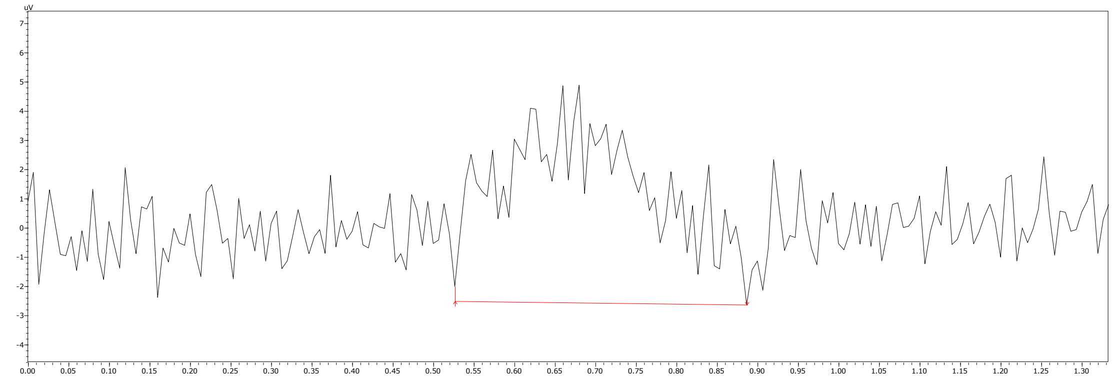
gauss_snr_100.1.gcd



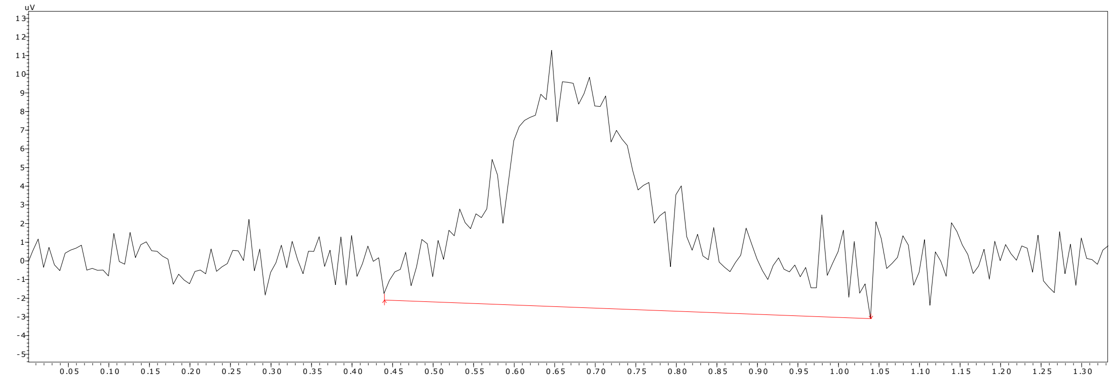
After initially detecting even tiny peaks (noise), then use the procedure below to unify the peaks into a single peak.

Set [Integration Advanced Settings] - [Peak Detection] - [Minimum Half Width] to 3 and set [Integration Advanced Settings] - [Peak Filter] - [Max. Peaks] to 1.

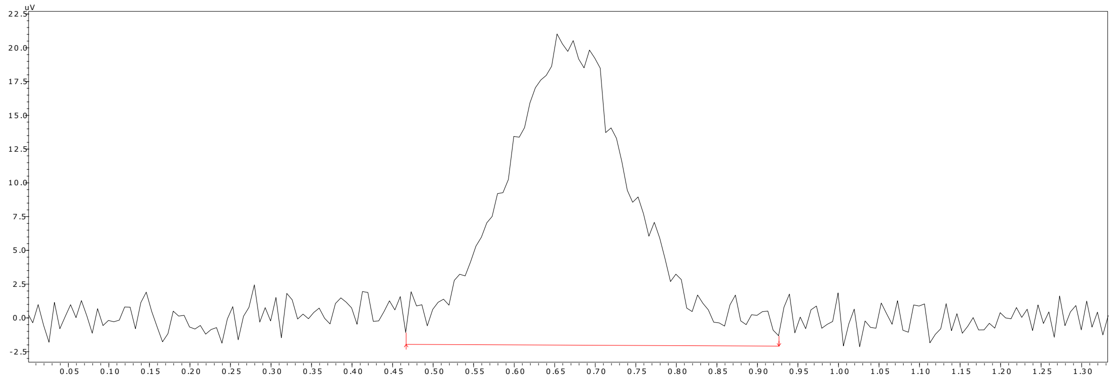
gauss_snr_3.1.gcd



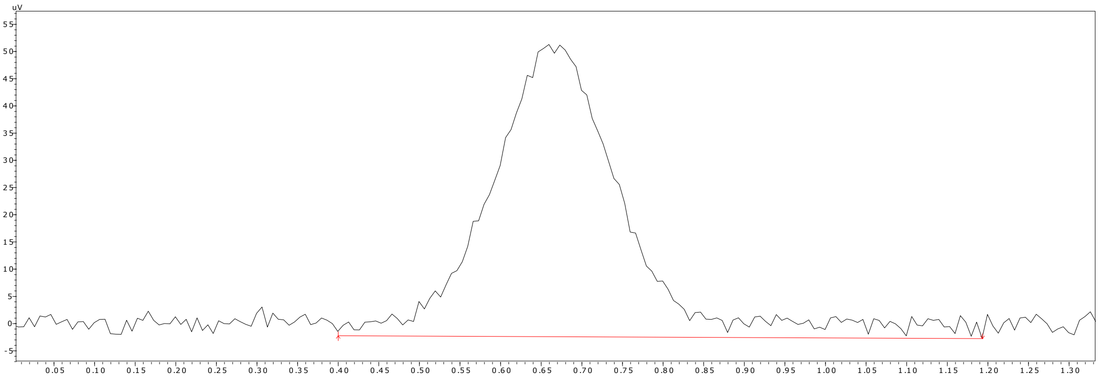
gauss_snr_10.1.gcd



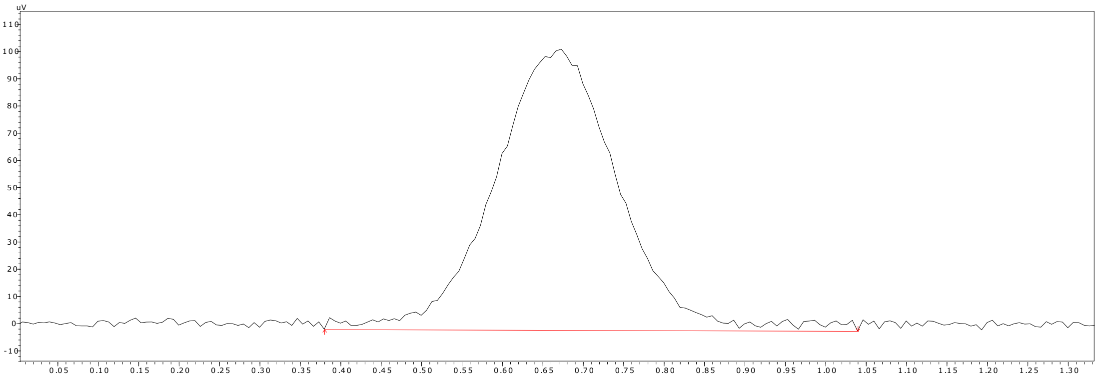
gauss_snr_20.1.gcd



gauss_snr_50.1.gcd



gauss_snr_100.1.gcd



If high noise prevents automatically detecting the peaks as a single peak, this method can be used to unify them into a single peak.