

LabSolutions

# **i-PeakFinder** (New Peak Integration)

## **Instruction Manual**

### Guide to Adjusting Parameters

Read this manual thoroughly before you use the product.

Keep this manual for future reference.

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# Introduction

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Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing this product.

This manual describes the operation for this product. Read this manual thoroughly before using the product and operate the product in accordance with the instructions in this manual.

Keep this manual for future reference.

## IMPORTANT

- If the user or usage location changes, ensure that this Instruction Manual is always kept together with the product.
- If this manual or a product warning label is lost or damaged, immediately contact your Shimadzu representative to request a replacement.

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# 1. i-PeakFinder

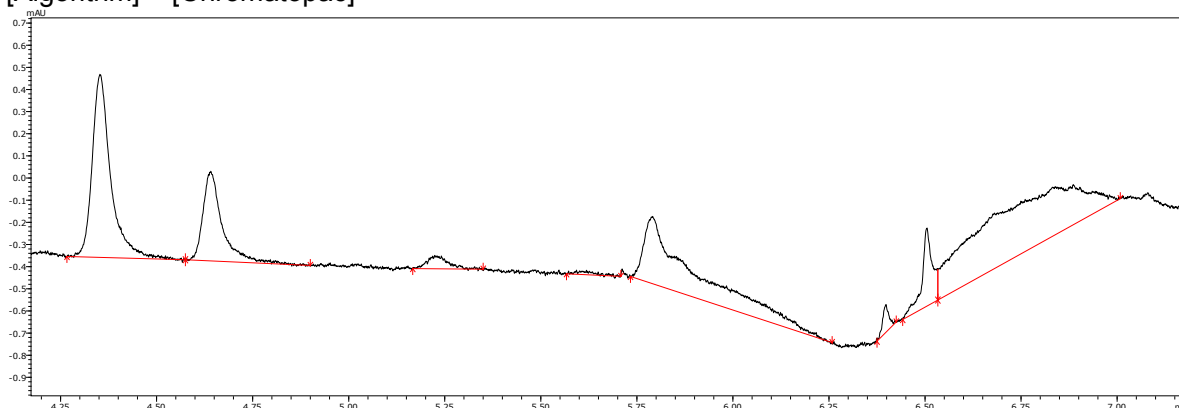
i-PeakFinder is a new peak integration algorithm for LabSolutions LC/GC/LCMS chromatograms.

Parameter settings can be changed to modify the default processing methods used by i-PeakFinder. This guide describes which parameters, or combinations thereof, are effective for making adjustments to i-PeakFinder processes.

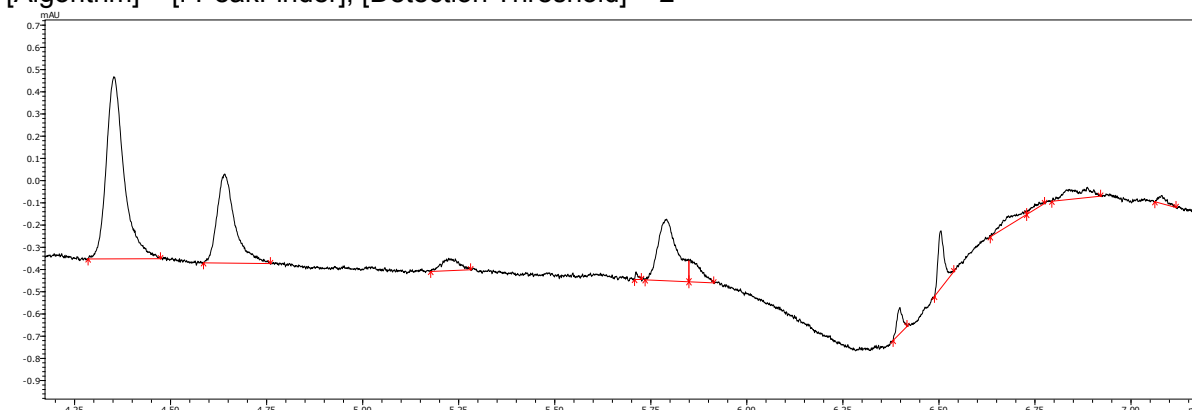
## 1.1 When to Use i-PeakFinder

- **When the Baseline Is Undulating or When Shoulder Peaks Are Detected**

[Algorithm] = [Chromatopac]



[Algorithm] = [i-PeakFinder], [Detection Threshold] = 2

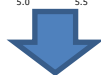
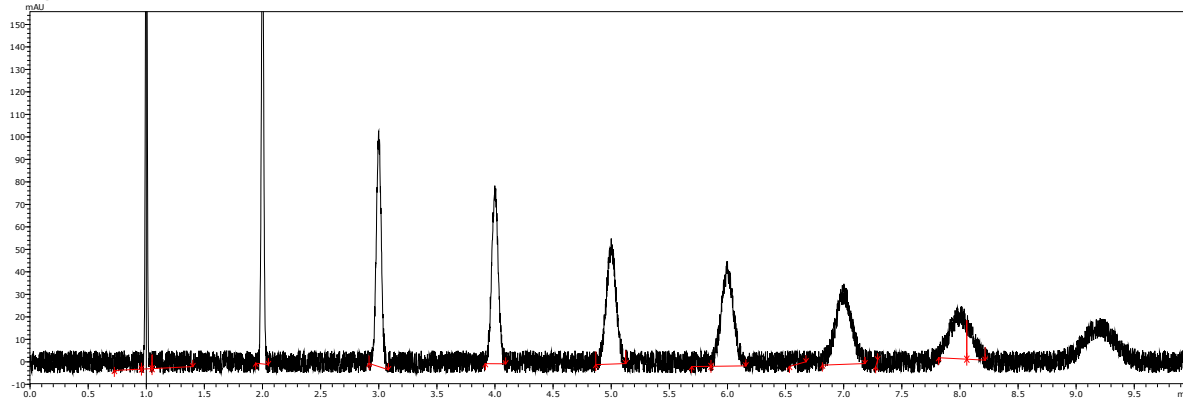


Existing peak integration algorithms used to detect peaks based on parameters equivalent to slope generally require using a time program for analysis, because baseline undulations (changes in baseline slope as a function of time) also result in varying the degree of initial rise and fall of peaks as a function of time.

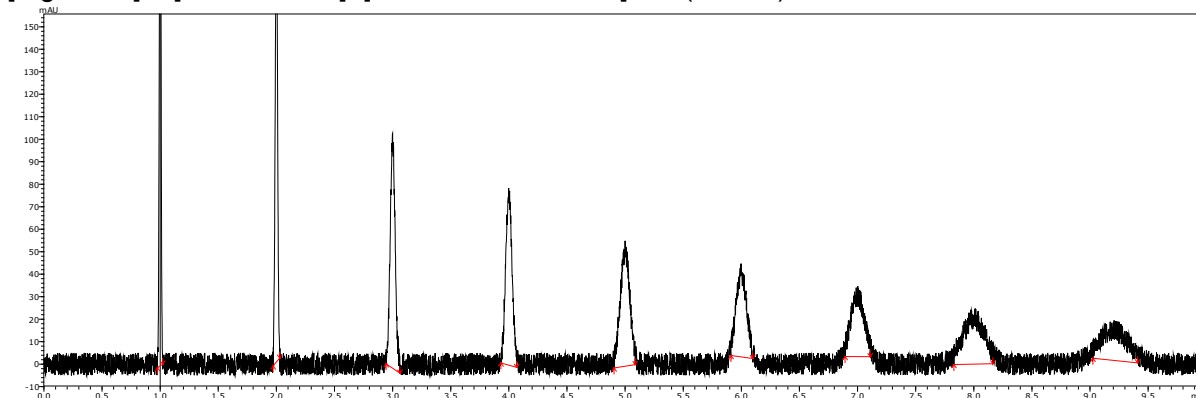
Because i-PeakFinder can also detect shoulder peaks, as can be seen from peak integration results near the center area, it is also useful for applications that require more accurate peak separation, such as for analyzing impurities.

- **When Peaks Are Buried in Noise or When Peak Widths Vary**

[Algorithm] = [Chromatopac], SLOPE = 100000



[Algorithm] = [i-PeakFinder], [Detection Threshold] = 5 (default)

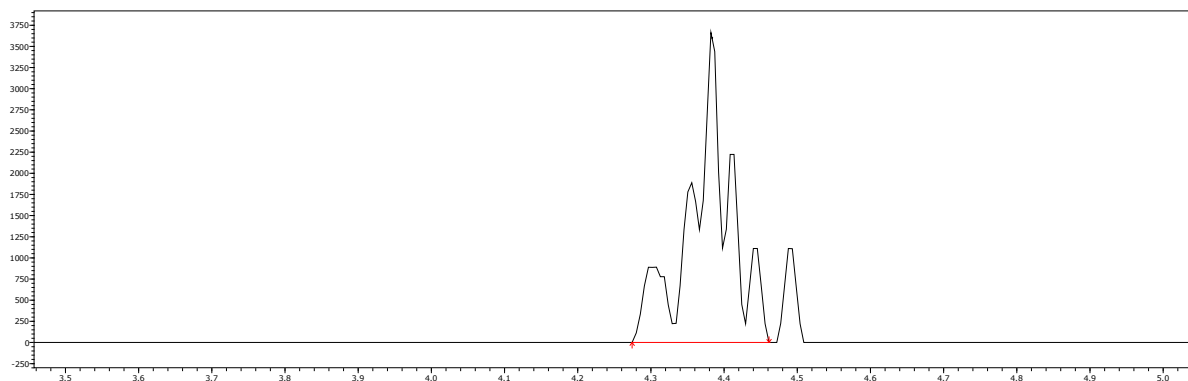


Due to its superior ability to detect peaks with low S/N ratios, i-PeakFinder is able to correctly process chromatograms even when peak widths vary within the chromatogram or when the noise level suddenly increases.

- **When Peak Distortion Is Large or When Peaks Are Divided**

[Algorithm] = [i-PeakFinder], [Minimum Half Width] = 20

→ See [Example: LCMS Chromatograms with Peak Profiles Divided into Multiple Segments.](#)



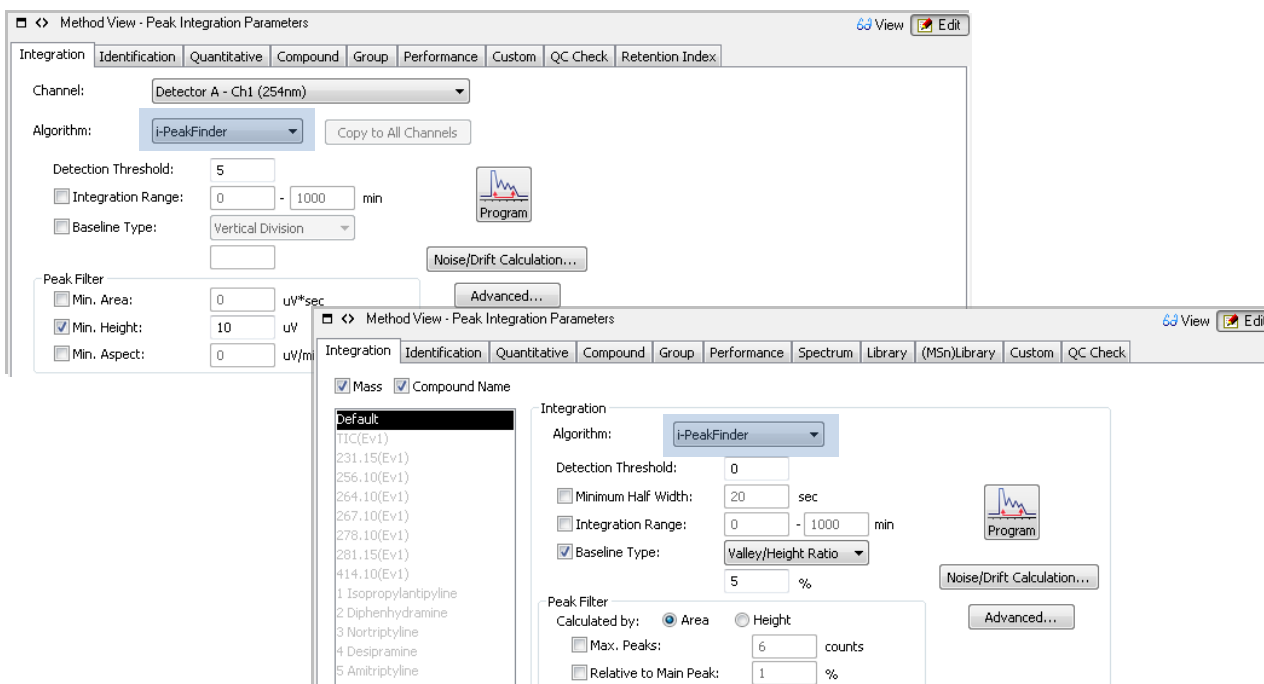
In this example, both algorithms result in multiple peaks, given default parameter settings. However, to unify peaks into a single peak, the Chromatopac algorithm requires manually integrating each peak, whereas the i-PeakFinder algorithm only requires changing a single set of parameter settings for all peaks.



## 1.2 Using i-PeakFinder

i-PeakFinder can be specified on the [Integration] tab page either in the Method View or in the [Peak Integration Parameters] dialog box.

Start by selecting [i-PeakFinder] in the [Algorithm] pull-down menu.



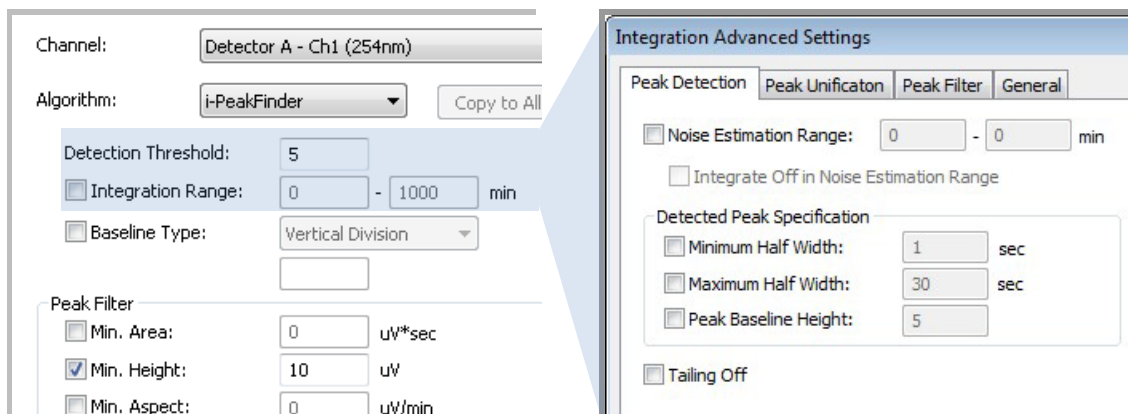
Infrequently used settings are specified in the [Integration Advanced Settings] window, which is displayed by clicking the [Advanced] button on the right side of the window.

Respective settings are organized based on application and arranged in roughly the order processes are performed.

### Peak Detection Parameters

Parameters for peak detection include the following.

[Detection Threshold], [Minimum Half Width]\*, [Integration Range], and all parameters on the [Peak Detection] tab page in the [Integration Advanced Settings] window

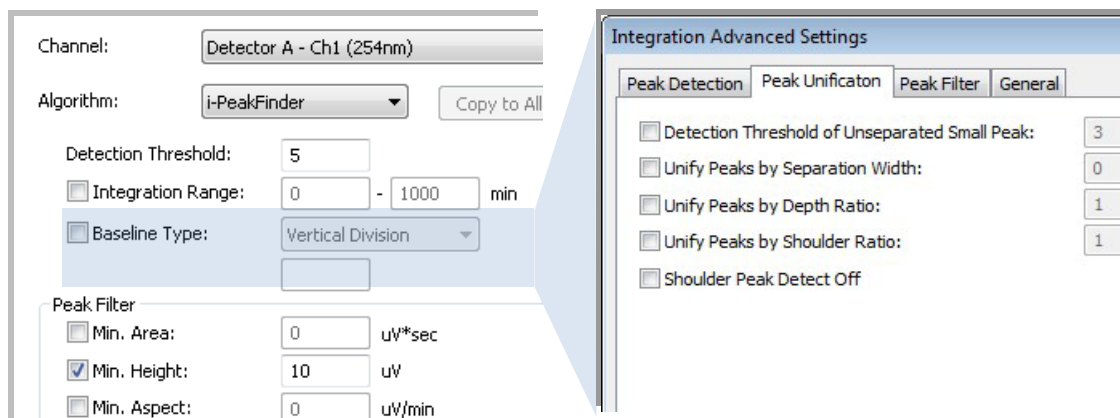


\* For LCMS. For LC or GC, the parameter is specified in the [Integration Advanced Settings] window.

## Baseline Type and Peak Unification Parameters

Parameters for peak unification include the following.

[Baseline Type], and all parameters on the [Peak Unification] tab page in the [Integration Advanced Settings] window

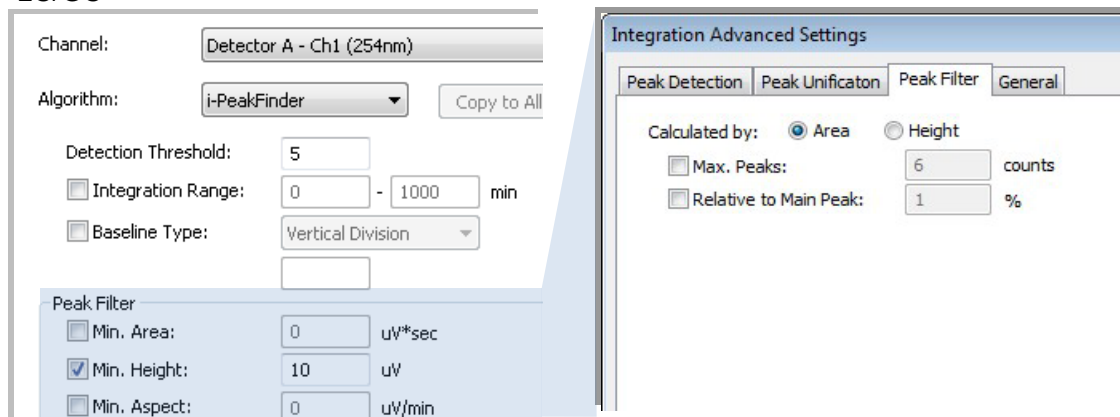


## Peak Filter

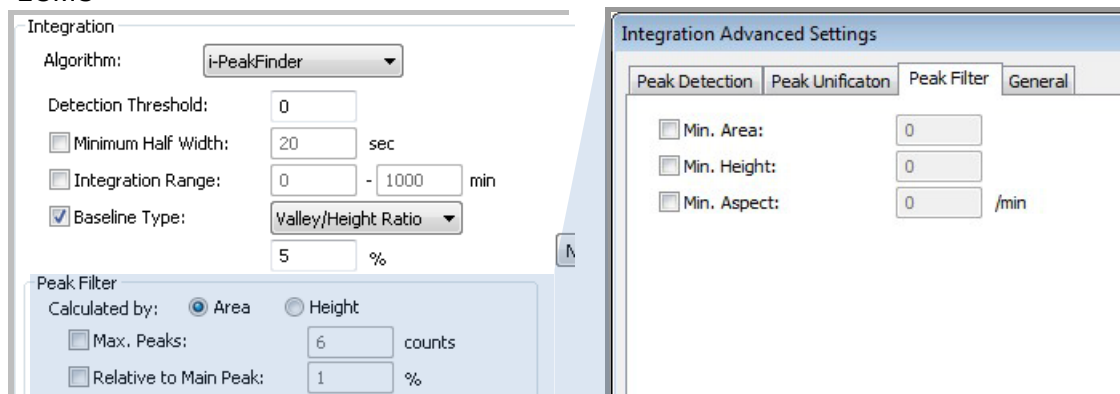
Parameters for peak filtering include the following.

All parameters on the [Peak Filter] tab page, and all parameters on the [Peak Filter] tab page in the [Integration Advanced Settings] window

### LC/GC



### LCMS



## 2. Adjusting the Baseline

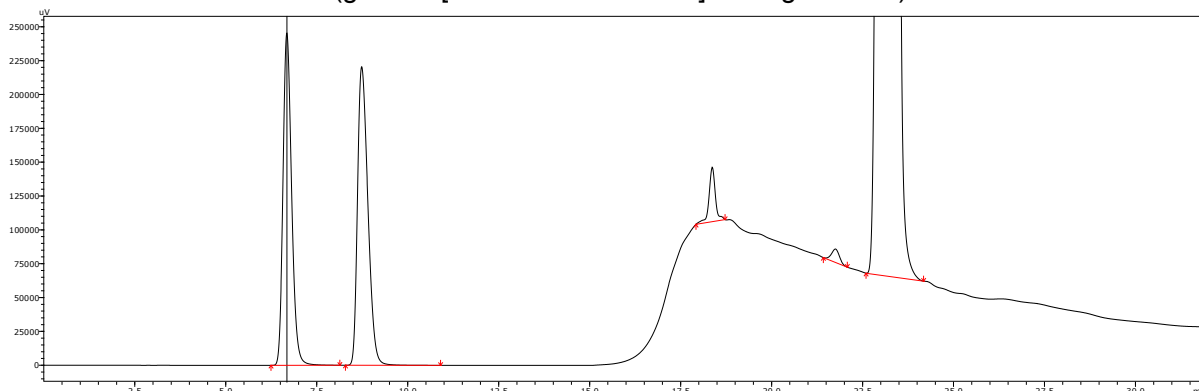
The baseline depends significantly on the peak detection status. This chapter describes how to adjust the baseline and what to do if the baseline cannot be adequately adjusted due to the peak detection status.

### 2.1 Adjusting the Baseline

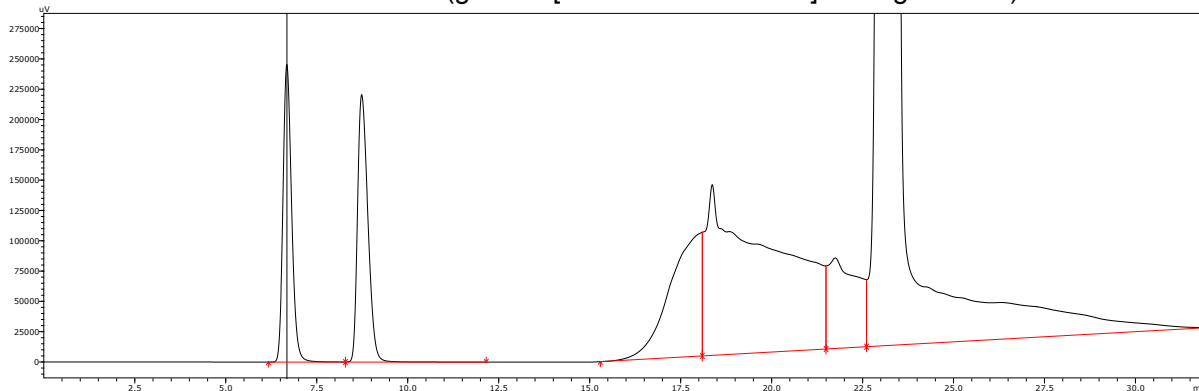
i-PeakFinder adjusts for undulations and other baseline variations by automatically estimating the chromatogram baseline and noise level.

For many chromatograms, this feature can be used to obtain correct results automatically by simply specifying the detection sensitivity based on the required number of peaks.

With baseline estimation (given a [Detection Threshold] setting of 1000)

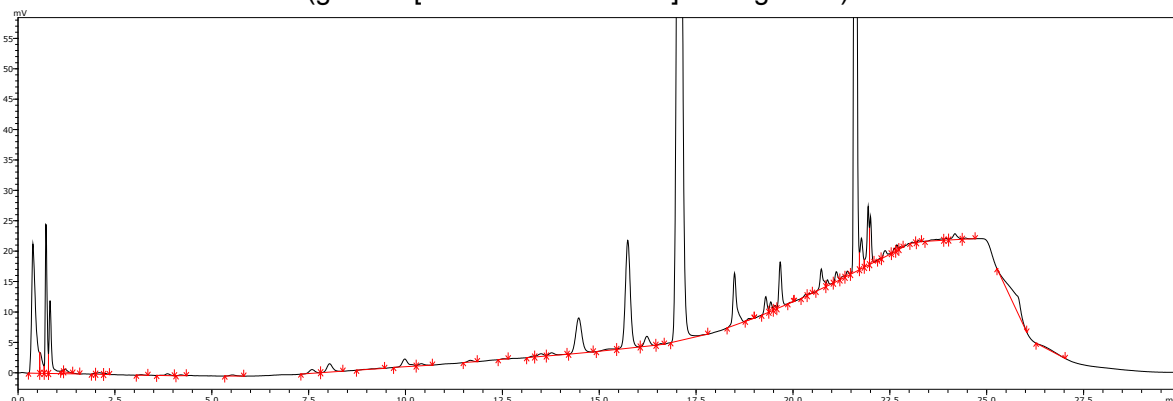


With baseline estimation disabled (given a [Detection Threshold] setting of 1000)



By simply adjusting the [Detection Threshold] setting, even the chromatograms above can be automatically processed without any problem by using the parameter settings changed as described in [Example:](#) in 2.3 Baseline Type Parameter.

With baseline estimation (given a [Detection Threshold] setting of 30)



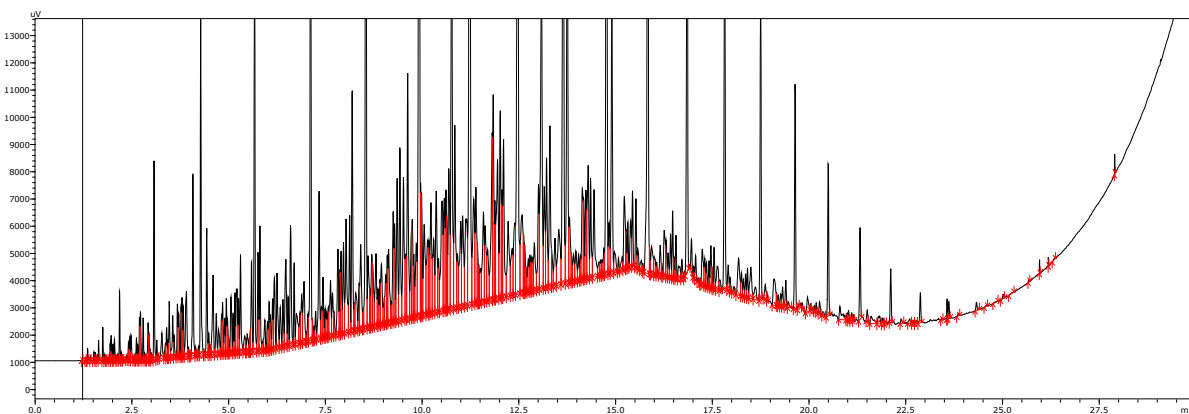
However, in cases where large baseline undulations prevent successful estimation or for types of analytical methods that would produce better peak integration results with estimation disabled, good results can be obtained by specifying peak integration parameter settings.

In this chapter, examples are used to describe how to obtain appropriate results.

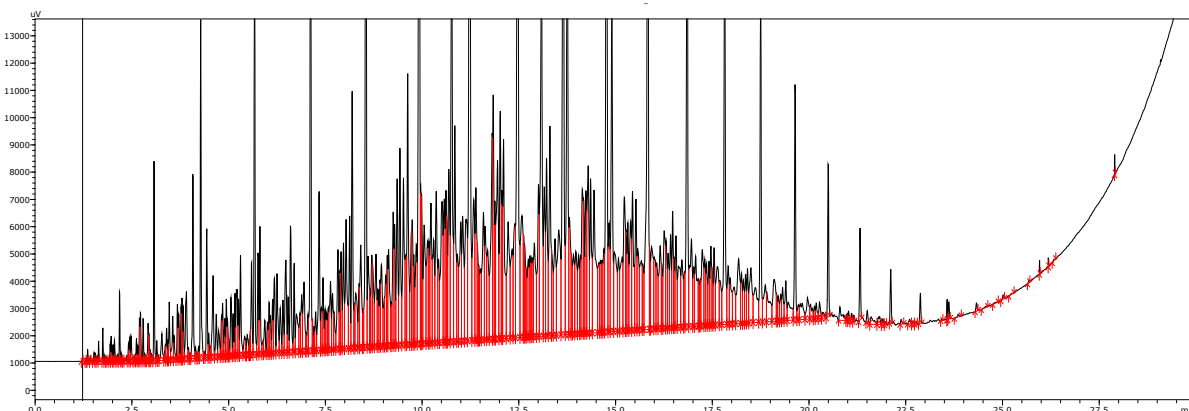
### Example: Chromatograms of Hydrocarbons Analyzed by GC with and Without Baseline Estimation

For this analysis, better results were obtained by disabling baseline estimation.

With baseline estimation



With baseline estimation disabled

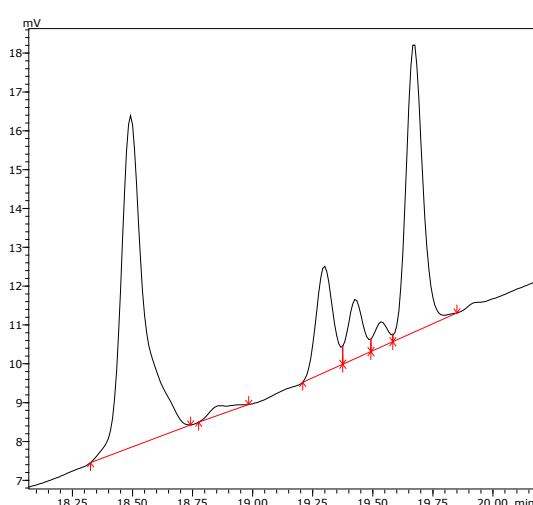


## 2.2 Fused Peaks and Baseline-Resolved Peaks

If a series of fused = unseparated peaks are detected, then the adjacent peaks are divided vertically and, in general<sup>i</sup>, the peak-baseline is formed by a straight line between the starting point of the first peak and the ending point of the last peak in that group of peaks.  
(Fused peaks that satisfy certain specific conditions can also be processed with tailing process.)

If a group of peaks is separated, baseline segments are formed between the peaks and the overall baseline is formed by connecting those baseline segments together.

### Baseline-Resolved Peaks (Left) and Fused Peaks (Right)



For chromatograms separated into peaks and baseline segments based on peak detection parameters (baseline resolution), such as [Detection Threshold] or [Minimum Half Width], the baseline segments are always used to form the overall baseline, regardless of the Baseline Type Parameter described below<sup>ii</sup>.

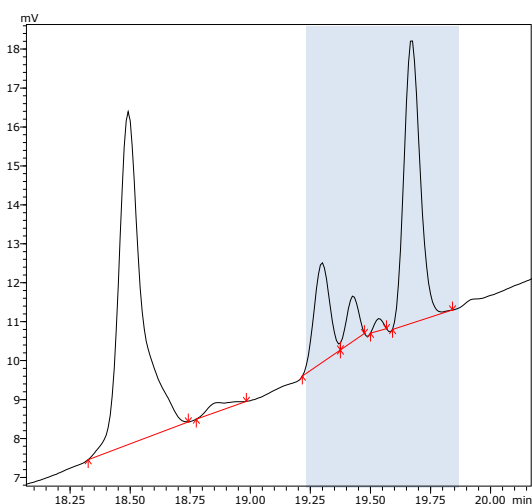
If the baseline is not tracked adequately by the baseline estimation function or the level of tracking needs to be adjusted, then consider first adjusting peak detection parameters so that an appropriate baseline area forms between peaks (i.e. refine baseline estimation for detecting the desired peaks).

→ See [Example: .](#)

Conversely, to ensure fused peaks (vertical division), such as in the case of the GC analysis of hydrocarbons mentioned above, peak detection parameters must be adjusted so that no baseline segments form between an uninterrupted series of detected peaks.

→ See [Example: Chromatograms of Hydrocarbons Analyzed by GC.](#)

## 2.3 Baseline Type Parameter



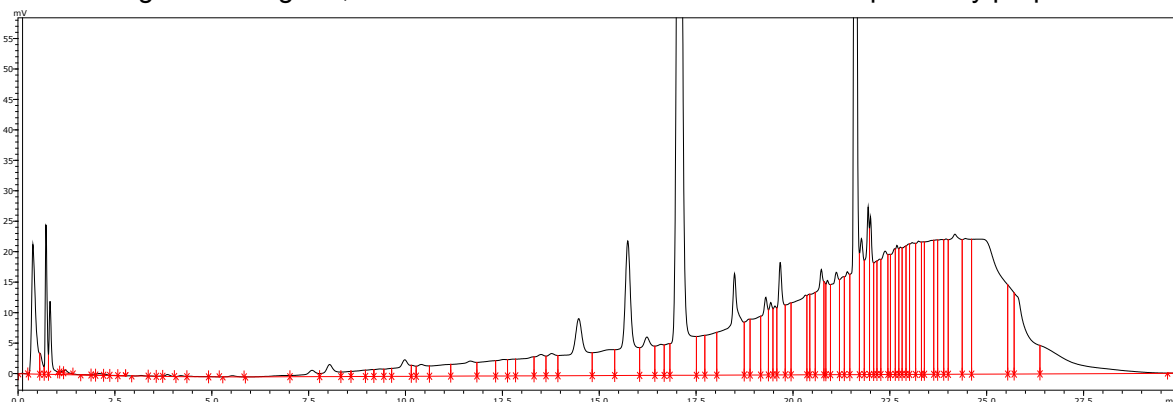
Baseline estimation forms a straight peak-baseline through groups of fused and vertically divided peaks, except if the peak-baseline crosses the chromatogram plot line, in which case it is always bent downward to avoid the plot line.

In contrast, the peak-baseline can also be bent upward<sup>iii</sup> by specifying peak height or baseline length criteria, unless [Vertical Division] is specified in the [Baseline Type] setting.

The level of peak-baseline bending can be adjusted even if baseline segments did not form after the adjustments above.

**Example: Processing of HPLC Gradient Curve in Under-estimated Baseline**

In the following chromatogram, baseline estimation was disabled<sup>iv</sup> for explanatory purposes.



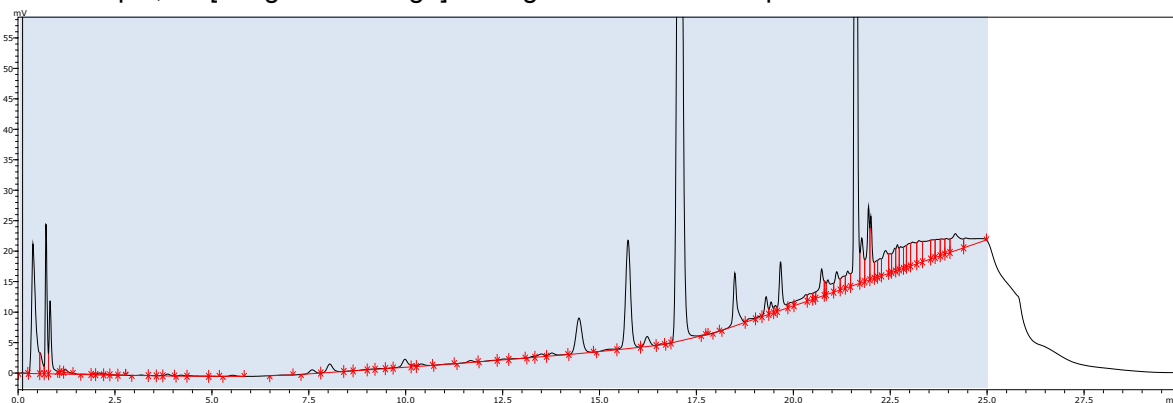
### 1 Specify parameters that does not result in misidentifying the baseline as a peak

For chromatograms with upward baselines (baselines that initially rise and then fall), the baseline bulges can sometimes be misidentified as peaks. Therefore, if there are no necessary peaks after the down slope, it is easier to use the [Integration Range] setting to exclude that section.

If that is not possible, the misidentification can probably be eliminated by using the [Maximum Half Width] setting to exclude false peaks\* greater than the required peak half width. (See 17 on page [Maximum Half Width])

\*: Bulges in the baseline misidentified as a peak

In this example, an [Integration Range] setting of 0 to 25 min is specified.

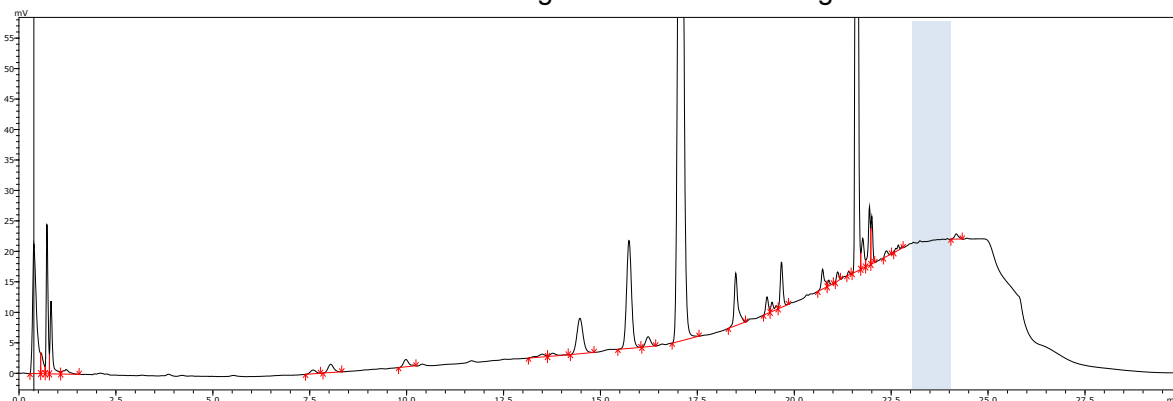


### 2 Specify peak detection parameters that result in baseline segments (standard method)

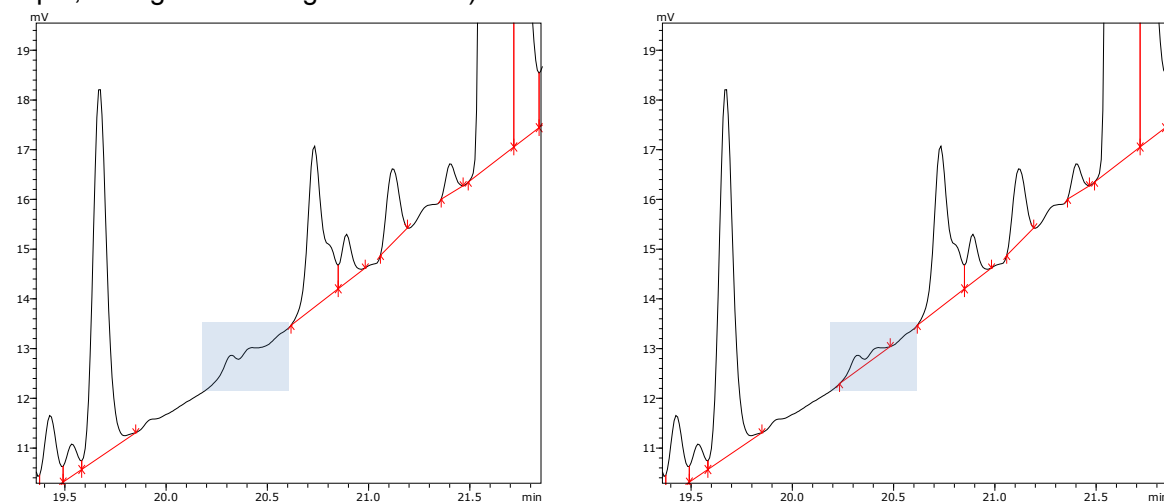
Normally, the [Detection threshold] setting is adjusted, which involves dividing the chromatogram plot line into peaks and baselines based on an S/N ratio as the threshold value. However, if possible, adjustments to [Detection threshold] can be minimized or eliminated by setting [Noise estimation range] to the non-peak area which the user feels to have the highest noise level, so that the user can set the noise value in the S/N ratio as desired.

Because the noise estimation function estimates the noise based on the chromatogram signal frequency, if an area of the baseline with a gentle bend is specified, a low noise component can be estimated based on that bend.

In this example, the baseline area range between 23 and 24 minutes is specified, near the shouldered baseline area where the chromatogram has finished rising.



If necessary, make minor adjustments<sup>v</sup> to the [Detection Threshold] setting. (In the following example, change the setting from 5 to 3.)

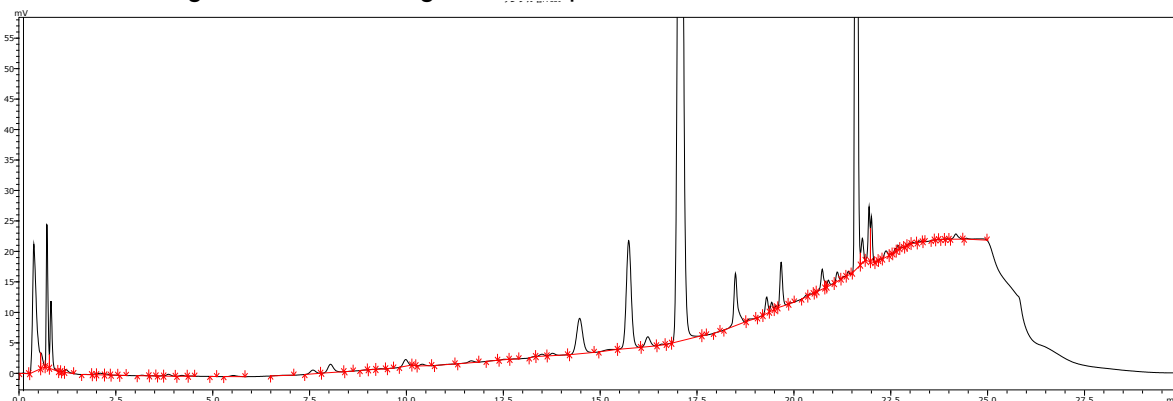


## 2 Bend the fused peak-baseline upward during baseline processing (alternative method)

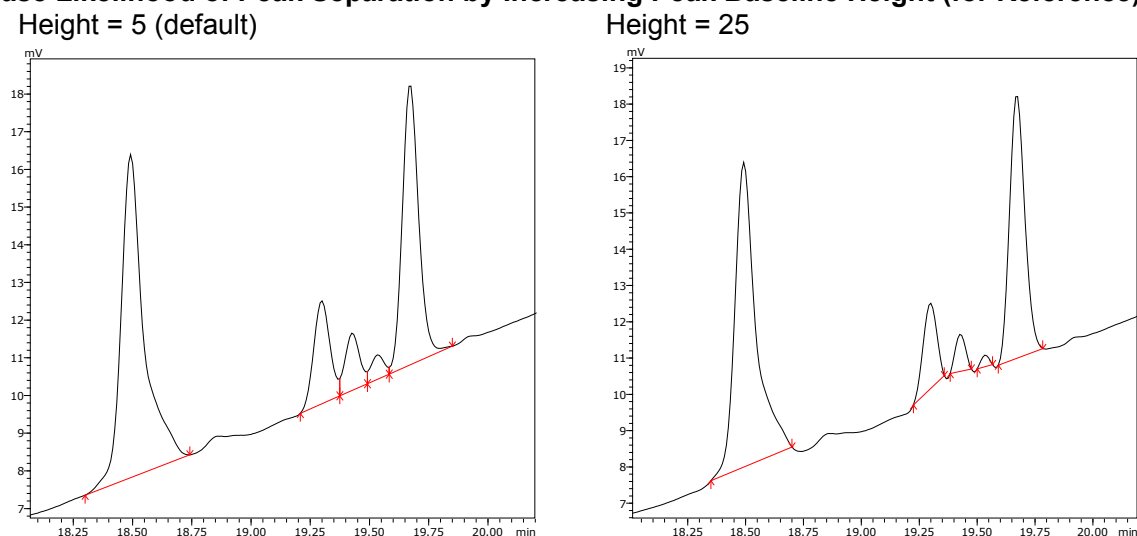
This method involves moving the peak-baseline for the fused peaks so that it more closely matches the chromatogram plot line shown after 19 minutes in the chromatogram in step 1 above (straight peak-baseline corresponding to vertically divided peaks).

The level of baseline bend can be specified in the edit box that is enabled by selecting the [Baseline Type] checkbox and clicking [Baseline Length] and [Valley/Height Ratio] in the pull-down menu.

In this example, [Baseline Length] was set to 0.5 minutes, so that any straight areas of fused peak-baseline longer than that setting are bent upward.



### Increase Likelihood of Peak Separation by Increasing Peak Baseline Height (for Reference)



The [Peak Baseline Height] setting (on the [Peak Detection] tab page in the [Integration Advanced Settings] window) determines the height of peak starting and ending points based on the specified multiple of noise standard deviations. Increasing the setting raises the peak-baseline position, which shortens the length of leading and trailing ends.

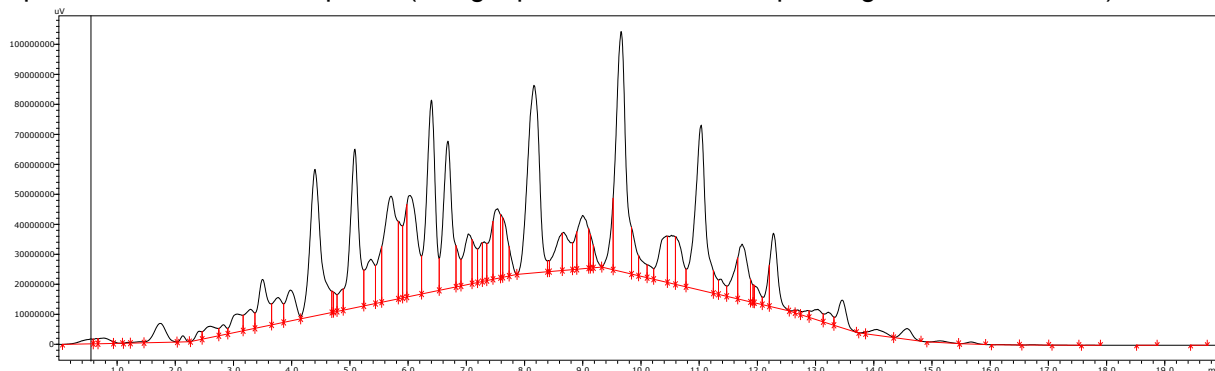
That results in peaks with narrower bases and increases the likelihood of peak separation which means peak-baseline separation between peaks. This technique can be especially effective when used in conjunction with the method described above.

Because the result is determined based on the standard deviation of noise, a relatively modest initial setting should probably be specified for chromatograms with a high noise level, whereas a significantly large initial value should be specified for chromatograms with low noise.

#### Example: Chromatograms of Hydrocarbons Analyzed by GC<sup>vi</sup>

With default settings, the baseline estimation function is enabled, but the peak-baseline automatically tracks the chromatogram plot line.

Consequently, basically the completely opposite settings to the settings described in [Example:](#) are specified to induce fused peaks (straight peak-baseline corresponding to vertical division).

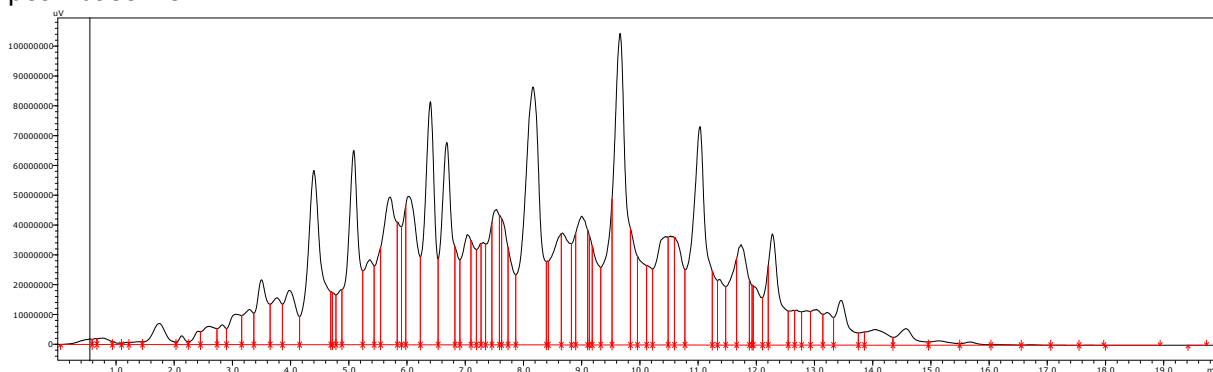


#### 1. Disabling Baseline Estimation (and Simultaneously Decreasing the Peak Baseline Height)

If [Vertical Division] is selected for [Baseline Type], the baseline estimation function is disabled and [Peak Baseline Height] is set to 0.01 automatically. (The [Tailing Off] checkbox is also enabled.)



In this chromatogram, peaks are detected so continuously that the default [Detection Threshold] setting of 5 results in almost all peaks being unseparated, so that vertical division results in a straight peak-baseline.

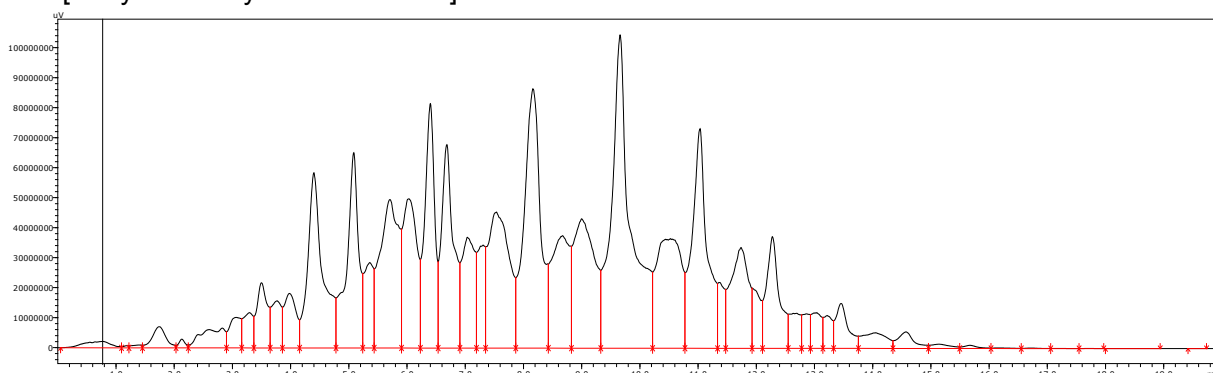


## 2. Obtaining the Desired Peak Profile

Given the excessive peak division in this example, adjust the division level.

To adjust the separation level for the group of peaks without destroying the unseparated status, use the settings on the [Peak Unification] tab page ([Integration Advanced Settings] window) to resolve the state of excessive division based on the characteristics between adjacent peaks.

For this example, [Unify Peaks by Separation Width] was set to 1.2, [Unify Peaks by Depth Ratio] to 1, and [Unify Peaks by Shoulder Ratio] to 2.



### Caution: Perform a Trial to Confirm Results Are Acceptable Before Using the Peak Detection Function to Unify Fused Peaks

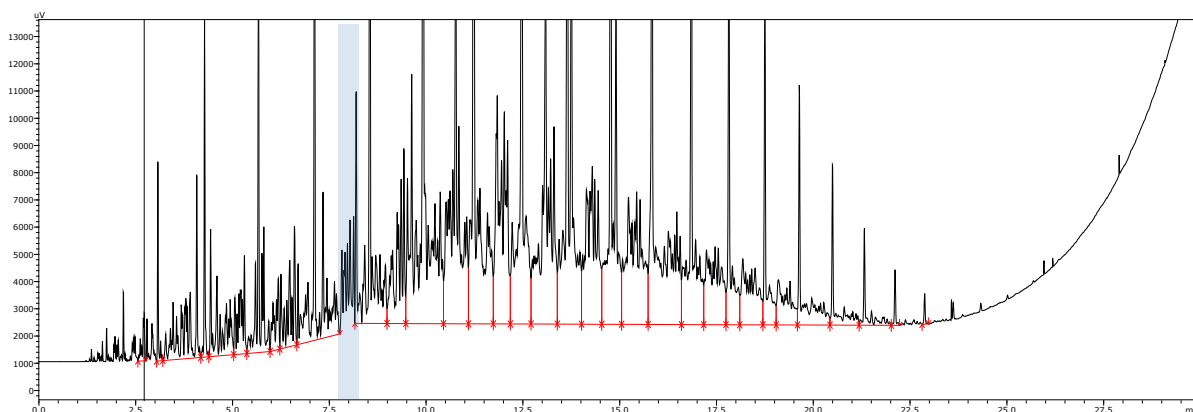
Attempting to determine the division level using the peak detection function (reducing the peak detection sensitivity by either increasing the [Detection Threshold] setting value or setting a [Minimum Half Width] value) will result in baseline segments between peaks or at the end of the group of peaks, so that the overall peak-baseline is bent or elevated.

It is important to understand that, unlike the peak unification function, which simply merges adjacent peaks, the peak detection function separates the peak and baseline area from the plot line of the chromatogram. (That results in unifying the peaks.)

(For an explanation of the differences between peak detection parameters and peak unification parameters, see the next chapter.)

The chromatogram used for this explanation was adequate for unifying the peaks to achieve the level of division shown above, but it can sometimes produce results like those shown in the example below.

(For this example, the [Minimum Half Width] setting is 10.)



### Using Peak Integration to More Reliably Ensure the Peak-baseline Does Not Bend (for Reference)

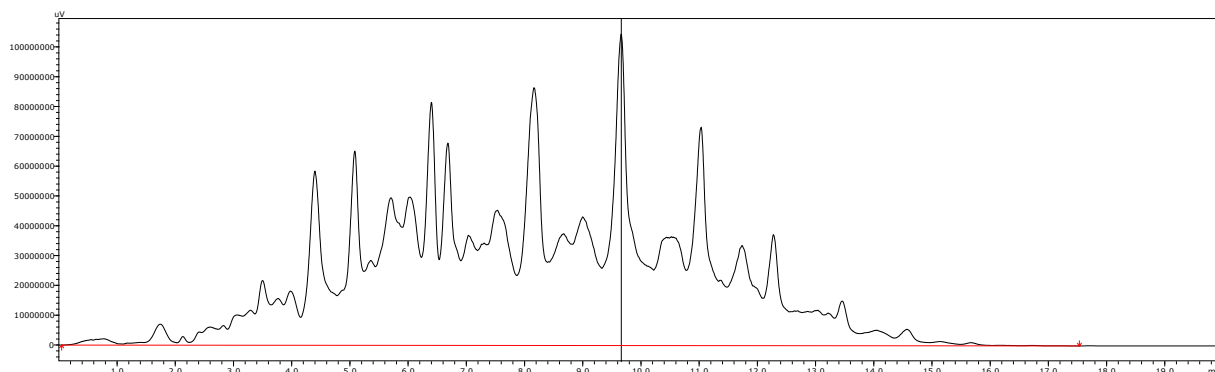
If the peak-baseline is bent in step 1, then the peak detection sensitivity value must be increased (by decreasing the [Detection Threshold] setting), so that there is no separation between peaks.

Setting [Detection Threshold] to 0 results in all noise spikes, regardless of their width, being detected as peaks and maximizes the likelihood of peaks being unseparated. However, to obtain more robust results, specify the [Noise Estimation Range] range (on the [Peak Detection] tab page in the [Integration Advanced Settings] window) to zero (from 0 to 0 minutes, for example).

Doing so disables the noise estimation function, with noise assumed to be at the minimum 1  $\mu\text{V}$  level. That minimizes the N value for [Detection Threshold], which is the S/N ratio threshold value, and maximizes the sensitivity accordingly.

Of course, that tends to cause excessive peak division, but peaks can be unified again later, according to the procedure described in step 2, above, or, for applications such as distillation GC analysis, for example, temporary excessive division will not affect final results, because all the peaks are eventually unified into one peak.

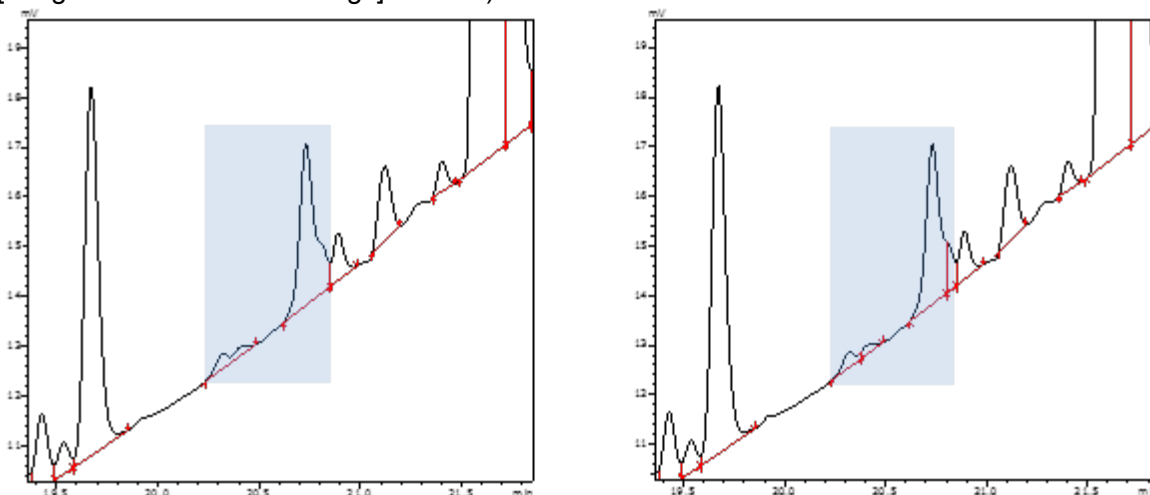
In this case, a [Minimum Half Width] setting of 50 was specified for the chromatogram in step 2. (Instructions for using the [Minimum Half Width] setting is provided below.)



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## Chapter Endnotes

- i Unseparated peaks that satisfy certain specific conditions can also be processed with tailing process.
- ii If [Baseline Type] is set to [Vertical Division], then peak detection parameters are preset internally to reduce the likelihood of forming baseline areas.
- iii This is referred to as valley-to-valley or base-to-base peak-baseline resolution. The software uses a time program command name "Base to Base On/Off" to switch the base-to-base mode ON or OFF.
- iv Selecting the [Peak Baseline Height] checkbox on the [Integration Advanced Settings] - [Peak Detection] tab page disables baseline estimation and enables baseline adjustment based on specifying a peak-baseline height. In this example, the explanation assumes a setting of 5.
- v The [Detection Threshold] setting is also applied to bulges within peaks (noise and undulations), but if the peak detection sensitivity is increased ([Detection Threshold] setting value is decreased) to detect those increases as peaks, it could affect how the peak-baseline is drawn in some cases. For such cases, it is also possible to increase only the shoulder peak detection sensitivity by adjusting the [Detection Threshold of Unseparated Small Peak] setting (on the [Peak Unification] tab page in the [Integration Advanced Settings] window).



- vi Basically the same approach is also used for LCMS, with the settings as described below.
  - [Peak Baseline Height] = 0.01 (this setting also disables the baseline estimation function)
  - [Detection Threshold] = 0
  - [Noise Estimation Range] = Range of zero
 However, because the [Tailing Off] checkbox is cleared in default settings, [Valley/Height Ratio] is set to 5, rather than setting [Baseline Type] to [Vertical Division], which would collectively perform the [Tailing Off] checkbox. In addition, several default settings are specified for newly created methods on the [Peak Unification] tab page.



## 3. Detecting and Unifying Peaks

Though already addressed in the previous chapter, this chapter describes when to use the peak detection function and peak unification function and how to determine when to use those functions and peak filters.

### 3.1 Peak Detection

Peak detection is functionality used to separate chromatograms into peak and non-peak (baseline) areas. Note that the functionality<sup>vii</sup> is also used to detect baseline areas.

Peak detection includes both functionality that uses information based on the signal intensity direction (peak S/N ratio) and functionality that uses information based on the time direction (peak half height width).

After detecting peaks, it automatically determines the starting and ending points of the peaks based on the specified multiple of either the estimated baseline or estimated noise height, which are used to determine the characteristic values of peaks and the remaining baseline areas.

### 3.2 Peak Detection Sensitivity and Estimated Noise Range

#### [Detection Threshold]

Given the S/N ratio used as the threshold value, this parameter is used to determine the baseline by treating plot line bulges with a signal intensity greater than the threshold value as a peak and those with a lower signal intensity as noise.

#### [Noise Estimation Range]

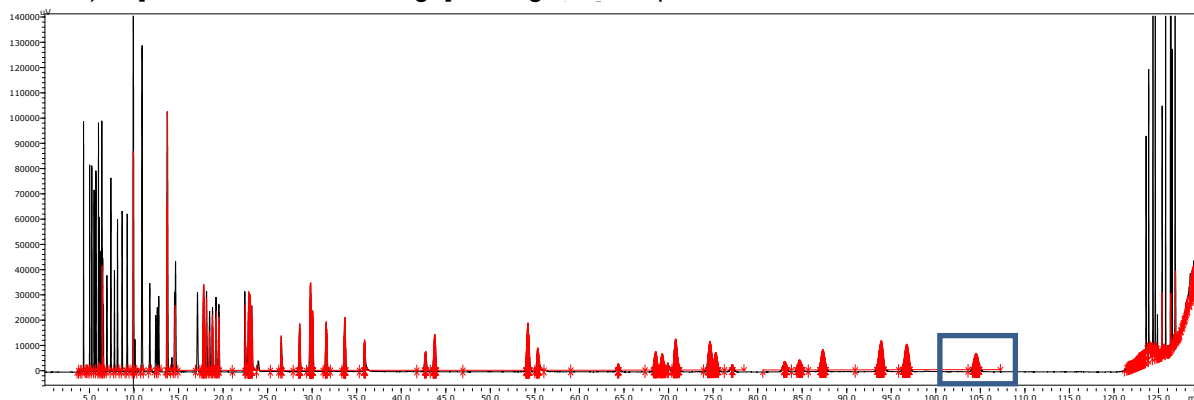
The noise value in the S/N ratio is automatically estimated by default, but this parameter allows the user to fix the estimated noise level with this time range based on a user-specified plot line, which has noise. (Normally it is baseline.)

Consequently, it can be set to a value more similar to the value the user desires, even when specifying a [Detection threshold] setting.

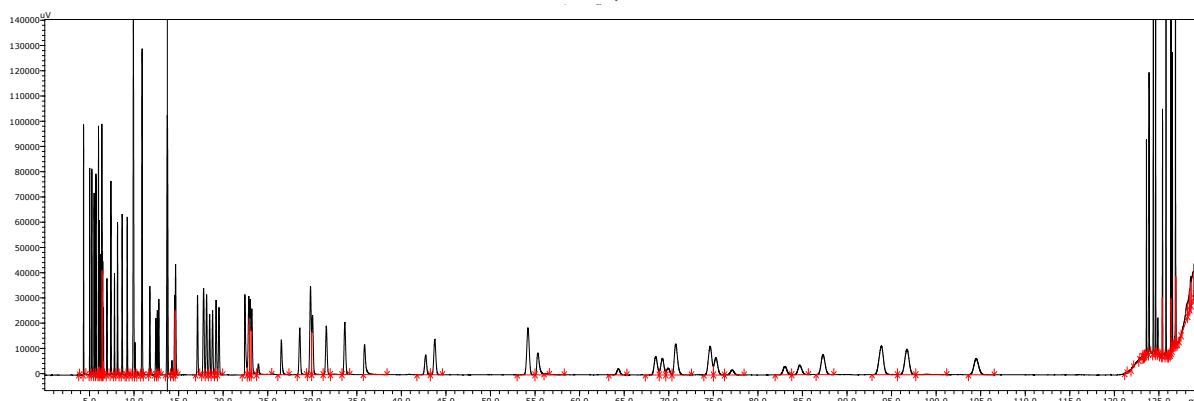
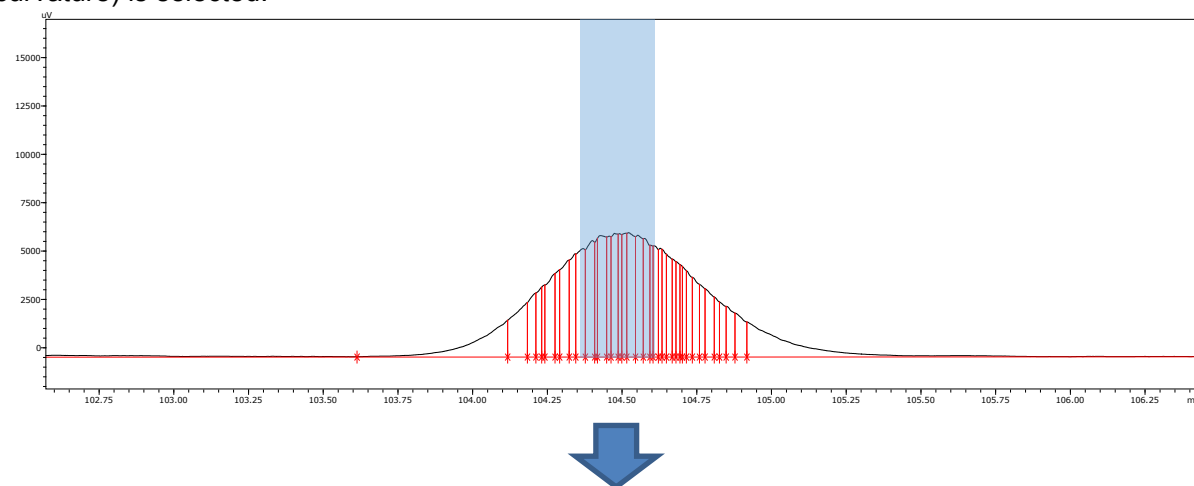
#### **Example: Chromatograms with High Noise Near Peak Tops and Excessive Peak Division**

The [Noise Estimation Range] setting is normally set to target the highest noise range over the baseline areas, but if the noise is higher for peaks than the baseline areas, then the range can also be set based on noise over peak areas.

Usually, the process can be performed based only on the [Detection Threshold] setting, but in this case, due to the excessive peak division by noise within the blue box (where the peaks appear like a red blur), a [Noise Estimation Range] setting can be specified for that area.



The [Noise Estimation Range] was specified near the peak tops of the excessively divided peaks (104.35 to 104.6 min). To avoid the overall peaks from being detected as noise, the flattest possible point (with minimal curvature) is selected.



After looking down the overall chromatogram and confirming that the required peaks are detected, make any necessary fine adjustments using the [Detection Threshold] or other settings.

Due to the narrow peaks in the beginning and end of this chromatogram and the broader peaks in the center, attempting to resolve the excessive peak division using the [Minimum Half Width] or peak unification function described below will affect other peaks. Therefore, if the procedure described here is not successful, consider using the time program mode to process only the range required.

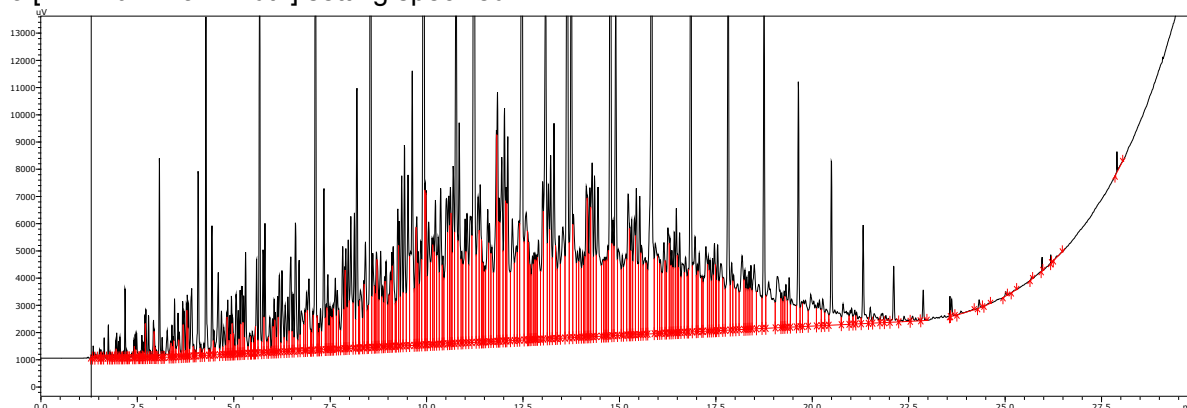
### 3.3 Minimum Half Height Width and Maximum Half Height Width

#### [Minimum Half Width]

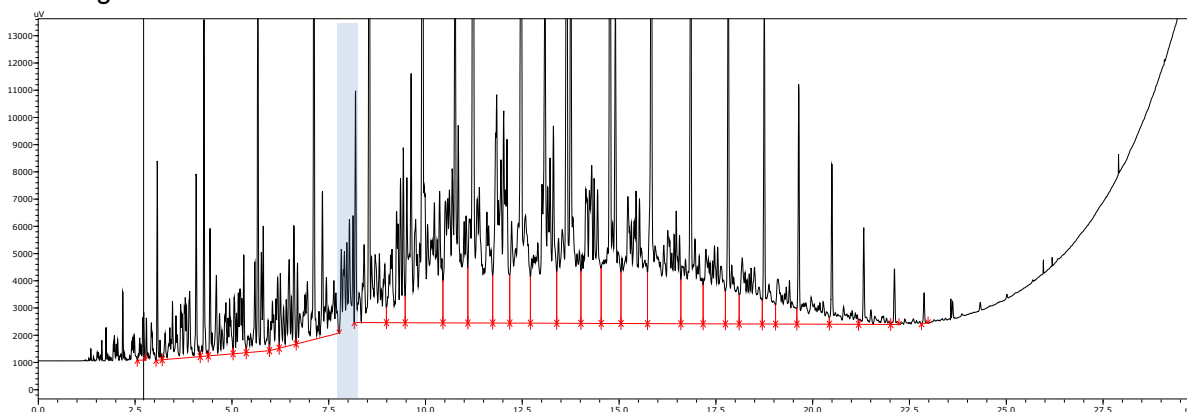
This setting specifies that any plot line bulges narrower than this setting are not detected as peaks. As the level of chromatogram smoothing is gradually increased, so that bulges become broader and lower, this setting determines whether undulations satisfy the specified width, until their height eventually falls below the [Detection Threshold] setting.

The function successively identifies each bulge that satisfies the specified conditions as a peak and treats the rest as baseline. It functions similarly to the function that unifies adjacent fused peaks until they reach the specified half height width, but it differs from the peak unification function that any area that is not successively identified as a peak based on satisfying the specified conditions is treated as the baseline.

#### No [Minimum Half Width] setting specified



Bulges are successively identified as peaks based on a [Minimum Half Width] setting of 10 and any remaining areas are treated as the baseline.

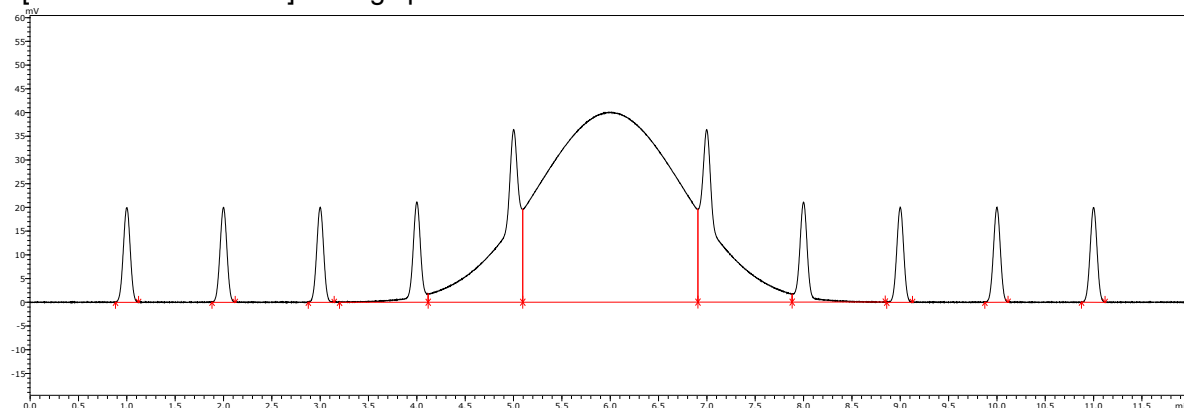


#### [Maximum Half Width]

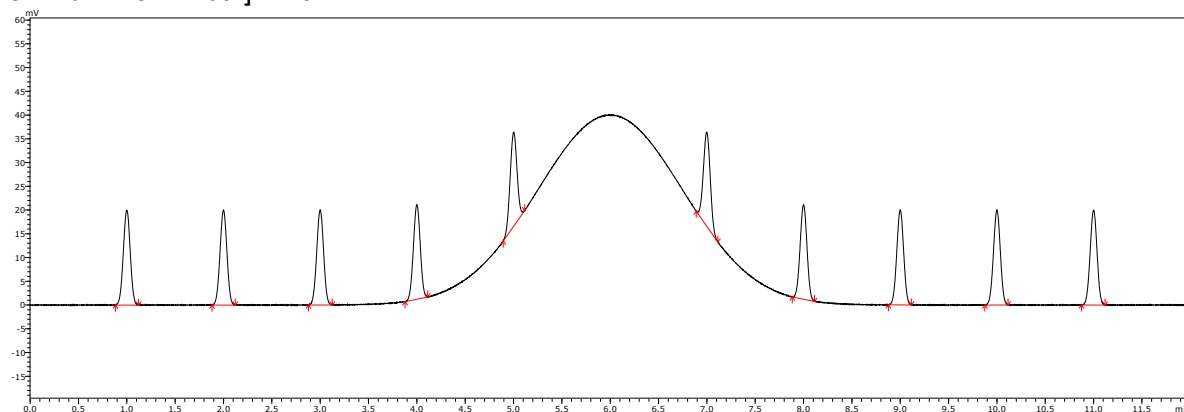
This setting is used to identify any bulges wider than this setting as upward baselines, rather than peaks.

If the baseline estimation function is functioning, it is possible to approximately track the baseline, but if it does not track properly, non-peaks can be reliably changed to baseline by specifying a [Maximum Half Width] setting based on assuming plot line undulations and bulges are peaks.

No [Maximum Half Width] setting specified



[Maximum Half Width] = 20



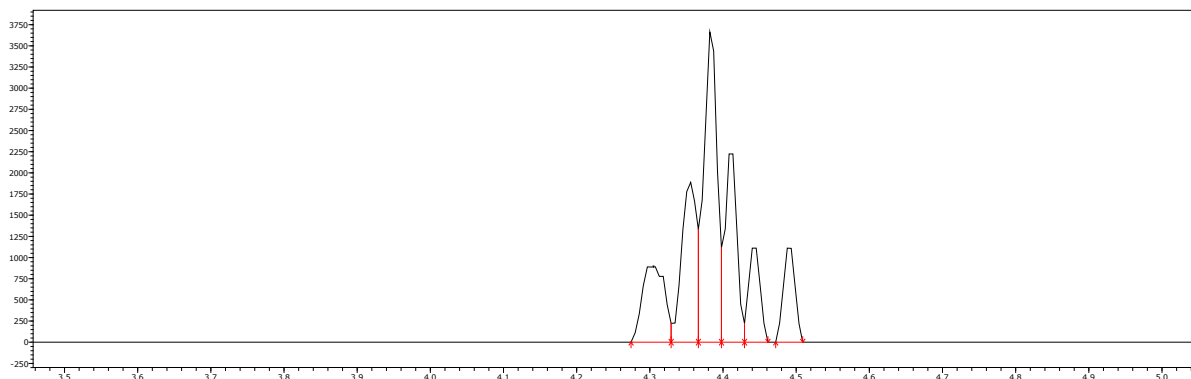
### Example: LCMS Chromatograms with Peak Profiles Divided into Multiple Segments<sup>viii</sup>

For LCMS, other than adjusting the [Minimum Half Width] setting, parameter settings for this procedure are already configured by default, but in this case each process step is performed for explanatory purposes.

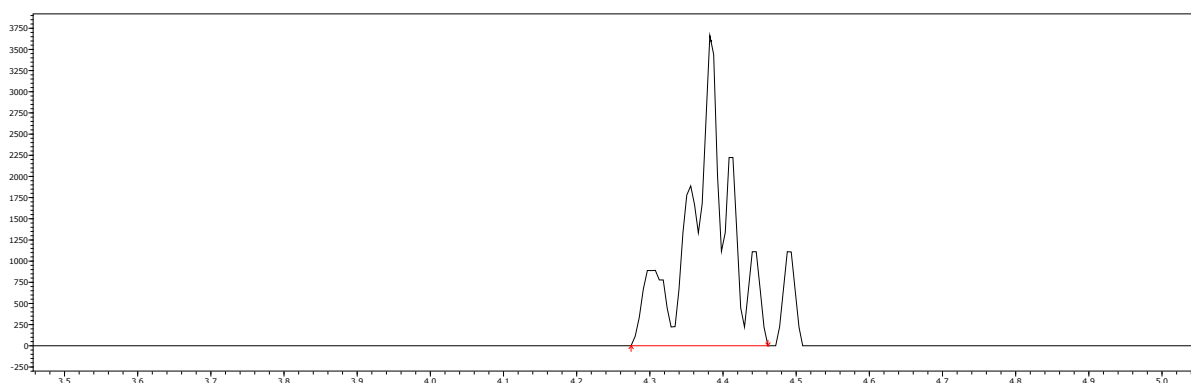
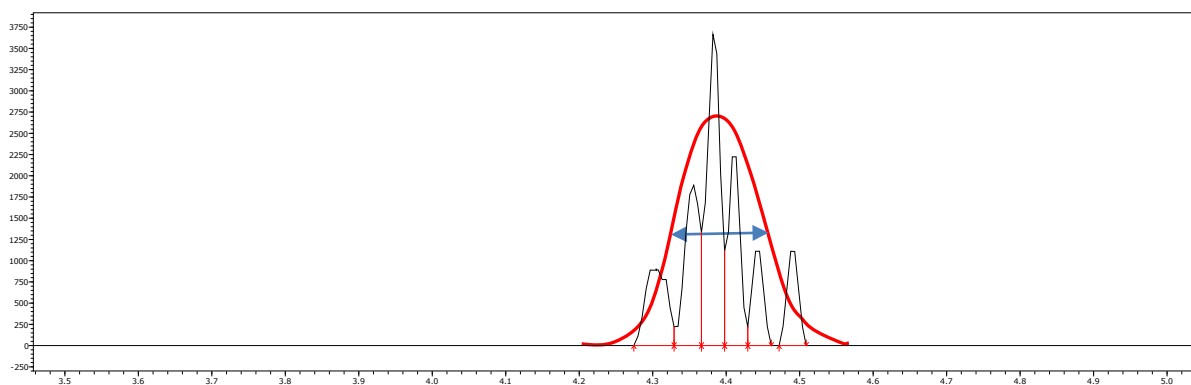
For LCMS quantitative peak integration, profiles such as those shown in the figures below are often obtained. Therefore, roughly the same approach is used as described above in [Example: Chromatograms of Hydrocarbons Analyzed by GC](#), except that in the GC example, [Baseline Type] is set to [Vertical Division], assuming peaks are not processed with tailing process. Therefore, other than specifying whether or not to process peaks with tailing, the LCMS settings are the same as for GC.



- To maximize peak detection, set [Noise Estimation Range] to 0 to 0 min (which fixes estimated noise at the minimum value of 1  $\mu\text{V}$ ) and set [Detection Threshold] to 0.
- By setting [Peak Baseline Height] to 0.01, detection of adjacent unseparated peaks (a straight fused peak-baseline involving vertical division) can be induced, while also disabling the baseline estimation function.



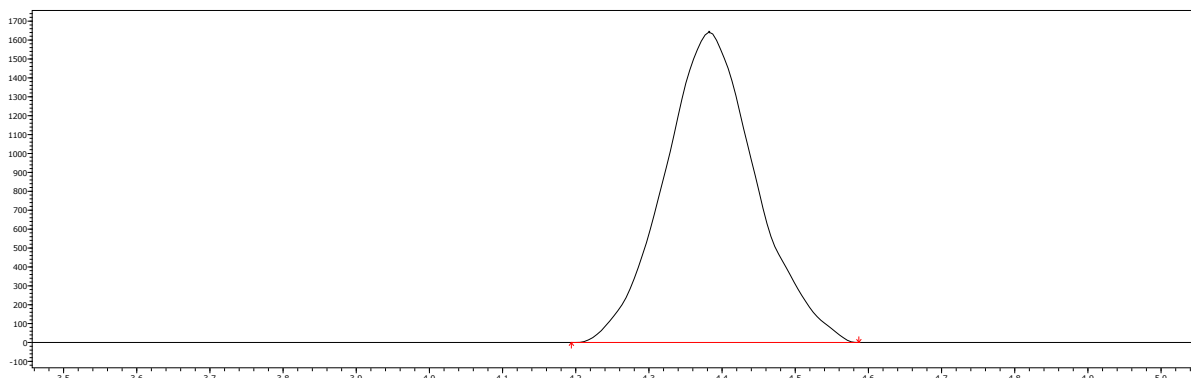
If multiply-divided peaks are presumed to be one peak, specify the half height width as the [Minimum Half Width] setting.



Because i-PeakFinder does not plot a peak-baseline that intersects with the chromatogram plot line, the bulge in the plot line near 4.49 min (on the far right) was not included in the peak. Nevertheless, it resulted in detecting a single peak roughly in the desired location.

If detecting all bulges as a single peak and including it in the peak area value is desired, then use the smoothing process. This can be understood by imagining a moving average, where the smoothing process preserves the peak area value. Consequently, it can usually be used without any problem.

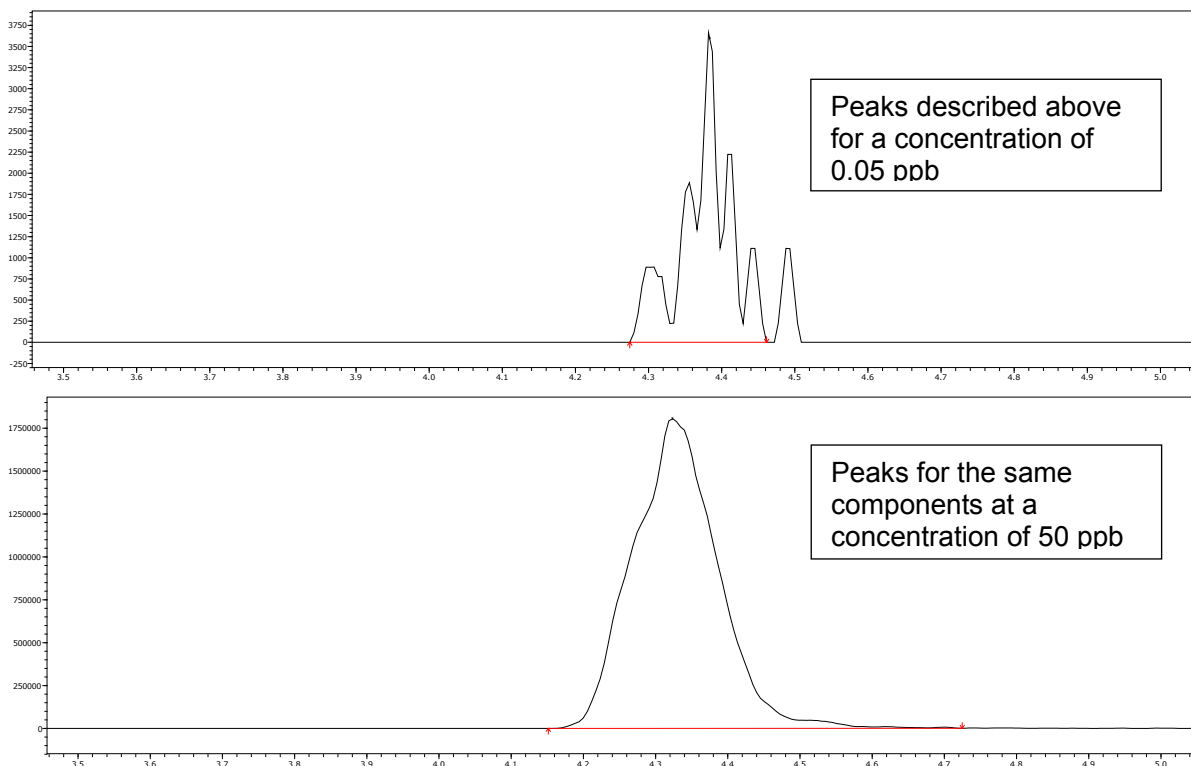
In this case, [Method] is set to [Standard(Priority width)], [Counts] to 1, and [Width] to 10 in smoothing settings.



For this procedure, [Minimum Half Width] was set to 8 sec, which is the half height width determined from this figure. However, because [Detection Threshold] is set to 0 (so that the peak is detected regardless of the smoothing level), the same result can be achieved even if a larger [Minimum Half Width] value (the approximate value that does not match the target peak profile) is set.

The setting simply needs to be large enough (the default setting for LCMS is 20) to prevent accidentally including any separate peaks located in the same area. This approach can significantly reduce the amount of trouble normally involved in specifying peak integration settings individually for each target peak.

Note, however, that whether or not the cluster of bulges in the multiply-divided plot line should be treated as one peak is determined as shown in the figures below.



When preparing calibration curves, if the [Minimum Half Width] value is approximated (on the high side) based on peaks from a high concentration sample used as a standard sample for calibration curve preparation, then calibration points on the low-concentration end can also be determined accurately.

### 3.4 Peak Baseline Height

#### [Peak Baseline Height]

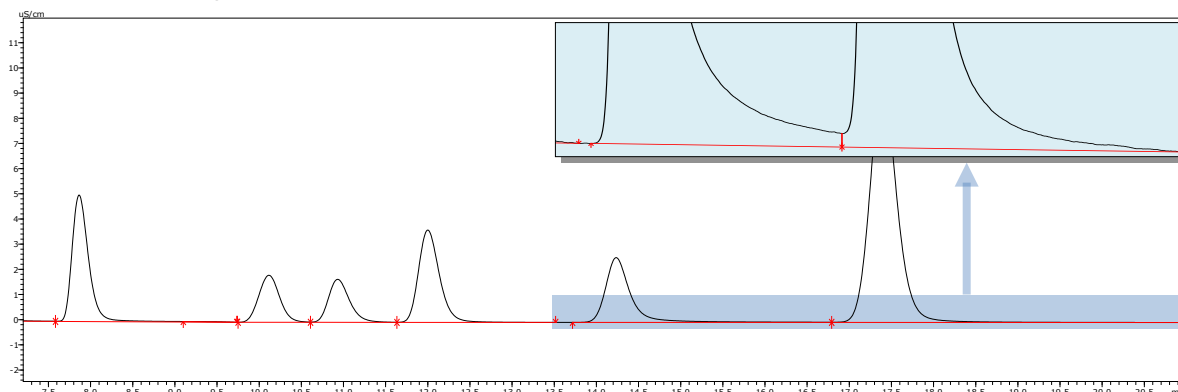
After i-PeakFinder detects a peak top, the starting and ending points are determined as the points where the deviation of chromatogram at the rising and falling of the peak becomes less than the specified multiple of standard deviations for the estimated noise (specified in [Peak Baseline Height]).

Therefore, chromatograms with high noise levels have the characteristic of higher peak-baselines and chromatograms with low noise result in lower peak-baselines.

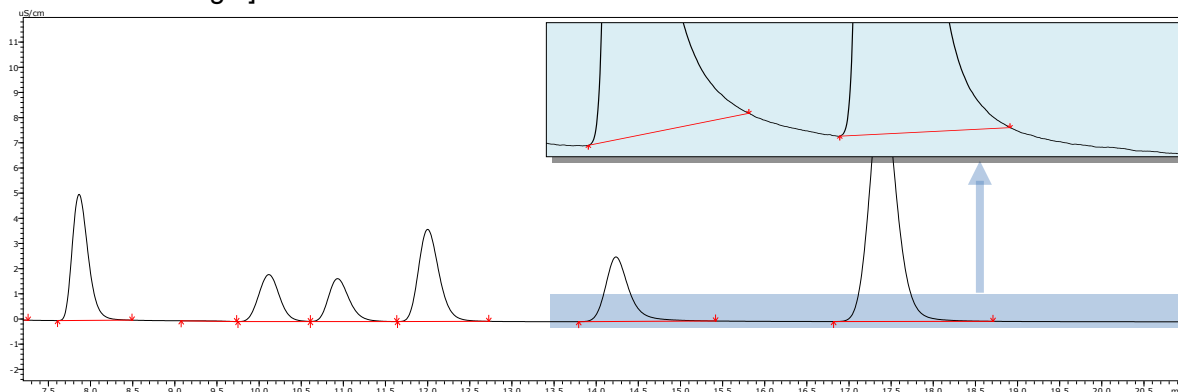
However, specifying this setting disables the automatic baseline estimation function.

In the chromatograms below, the noise level is extremely low, given the size of peaks, but actually magnifying the peak base area shows tailing. Even though default settings result in correctly plotting the peak-baseline, if the peak-baseline appears to be too long at that scale, it can be adjusted with the [Peak Baseline Height] setting.

[Peak Baseline Height] = 5 (default)

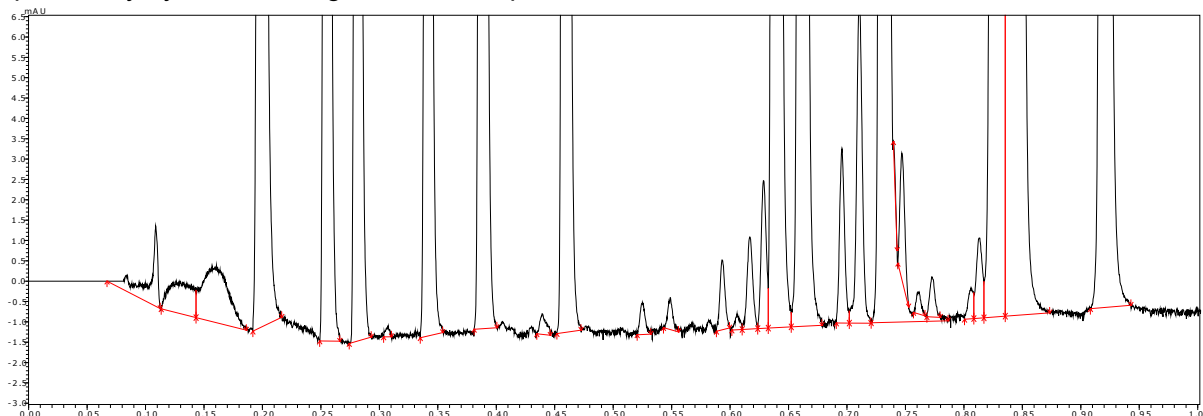


[Peak Baseline Height] = 200

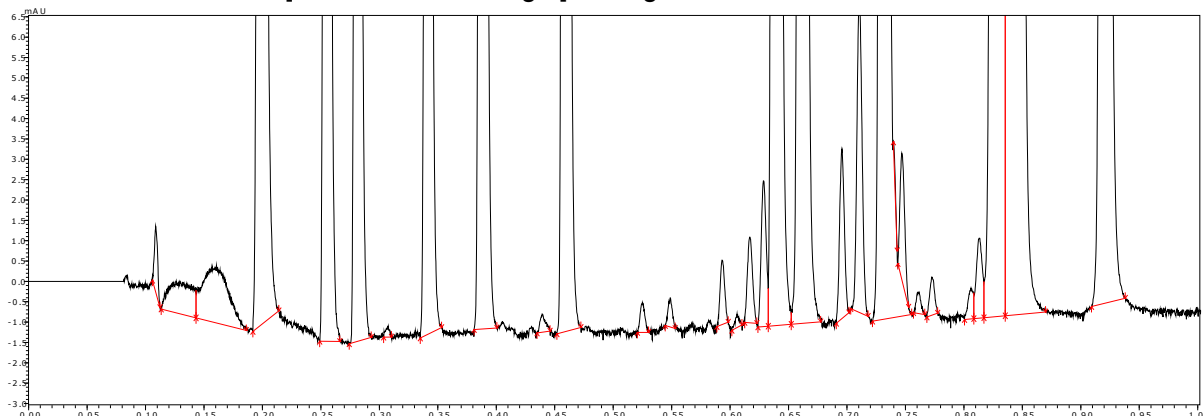


### Example: Ensuring Area Repeatability by Raising the Peak-baseline Slightly

If the baseline undulates, includes noise spikes, or otherwise does not stabilize at a given level<sup>ix</sup>, specifying a higher peak-baseline that avoids those unstable areas can help ensure adequate area repeatability by not including the unstable peak base area.

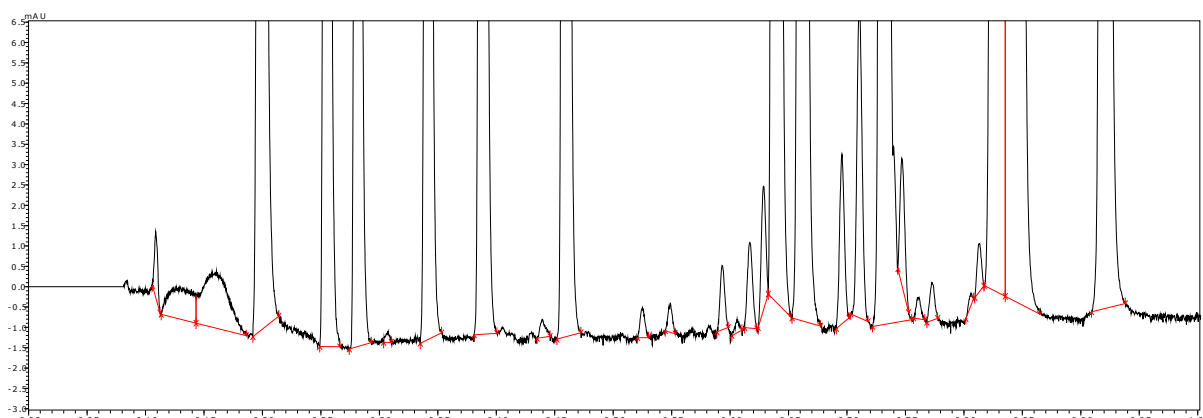


In this case, the default [Peak Baseline Height] setting of 5 was increased to 20.



Noise can cause variability in the status of fused or baseline-resolved adjacent peaks. Therefore, corrective measures should be implemented accordingly, such as by specifying [Baseline Length] for a [Baseline Type] setting, for example, that results in separation that is closer to baseline resolution and by disabling detection for shoulder peaks and other factors that the presence of which tends to be detected with relative variability.

In this case, the peak profile was stabilized by selecting the [Shoulder Peak Detect Off] checkbox and setting [Unify Peaks by Depth Ratio] to 5 (explained in the next section), and by setting [Valley/Height Ratio] to 1 for [Baseline Type] to adjust the peak-baseline in the baseline-resolved direction.



### 3.5 Unifying Peaks

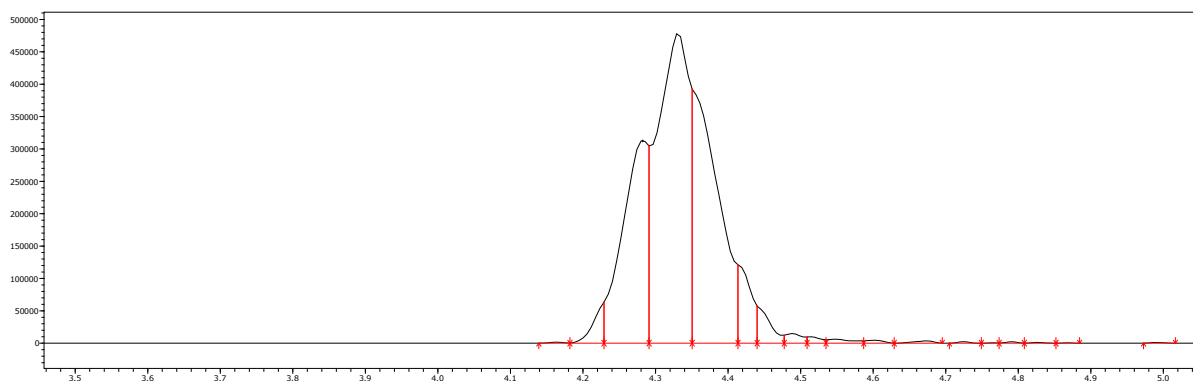
This function merges detected adjacent peaks (with some exceptions) into a single peak. This requires that peaks are detected, so it must be used after peak detection.

#### Example: Chromatograms with Peak Distortion for LCMS Quantitative Peak Integration

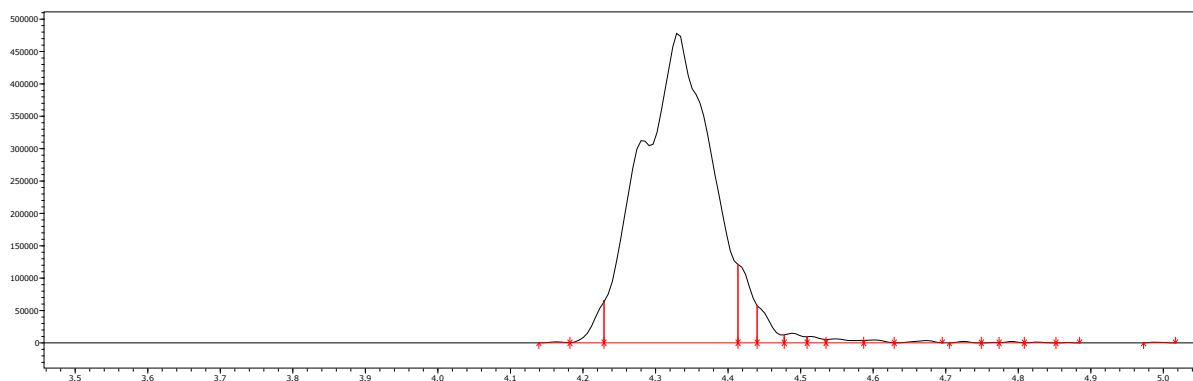
Given peaks for the same components as described above in [Example: LCMS Chromatograms with Peak Profiles Divided into Multiple Segments](#), but with sample concentration increased slightly from 0.05 ppb to 10 ppb, the peak separation was not to the extent of being divided, but that tendency still remained, making the peak profile not very well shaped.

For LCMS, the peak unification setting is specified by default, so that peaks can be processed even if the [Minimum Half Width] setting is not appropriate.

In this case, the following explains how to use that approach by specifying each successive step.

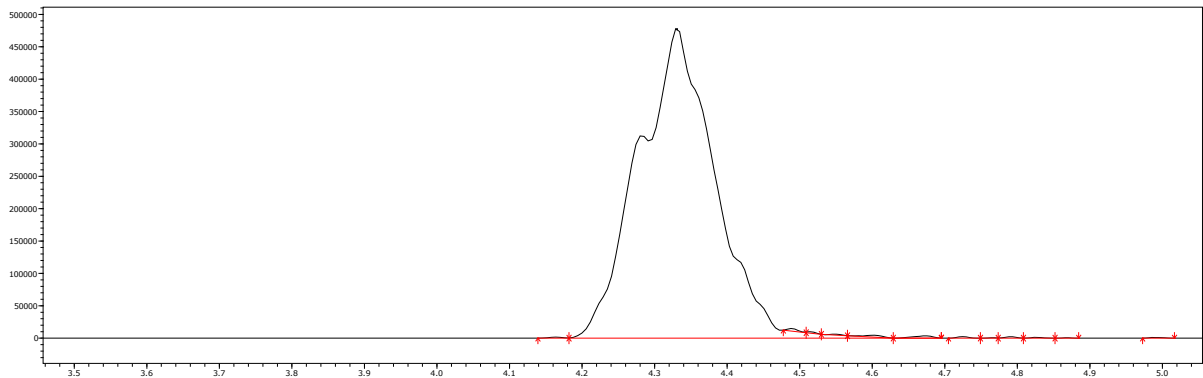


Given the above, 0.8 was specified for the [Unify Peaks by Separation Width]<sup>x</sup> setting. This unified the peaks within the specified separation factor, with the highest peak in the center.



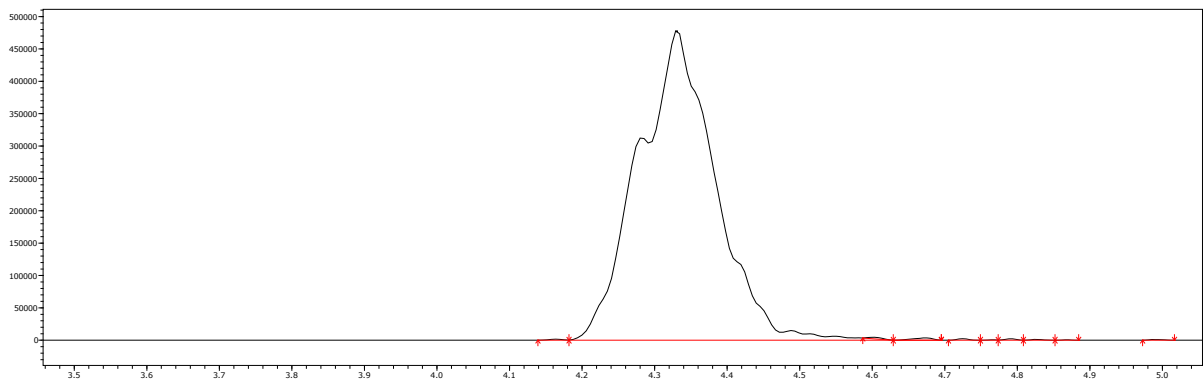
Next, the [Shoulder Peak Detect Off]<sup>xi</sup> checkbox was selected (to switch OFF the function).

This shows the shoulder peaks on the peak base area unified.



There are small peaks remaining on the right side of the peak base, but an enlargement of the peak shows a valley, indicating that it is not a shoulder peak. That is why it was not unified in the process above.

However, this area can be unified, if desired, by setting [Unify Peaks by Depth Ratio] to 20. (The default setting for LCMS is 5.)

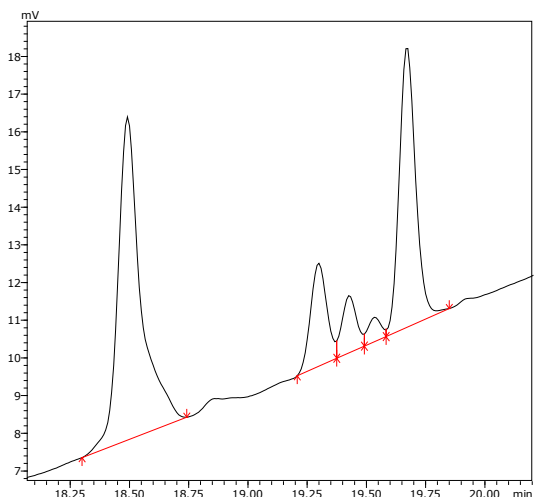


### 3.6 Peak Filters

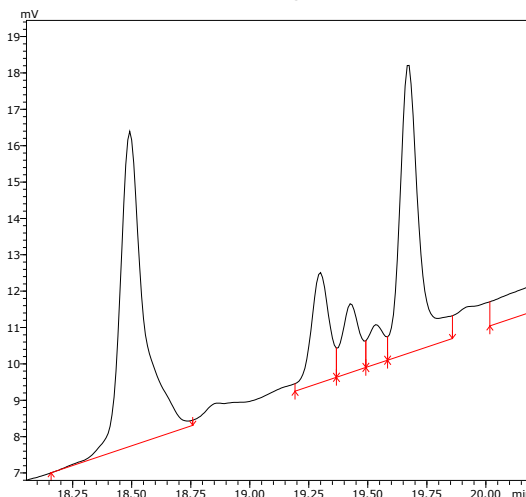
This function is used to eliminate detected peaks and return them to the baseline.

Just like the peak detection function, it can be used to retain large peaks and avoid detecting small baseline bulges as peaks, but because peak filtering is used as the final step, after peak detection and peak unification, simply deleting the peaks can prevent affecting the baseline confirmed up to that point.

Result of peak detection function

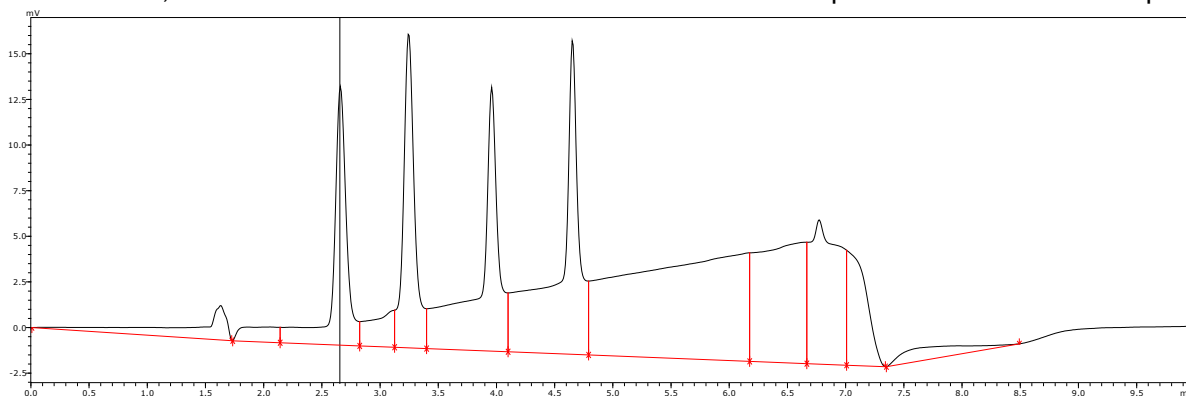


Result of peak filtering function

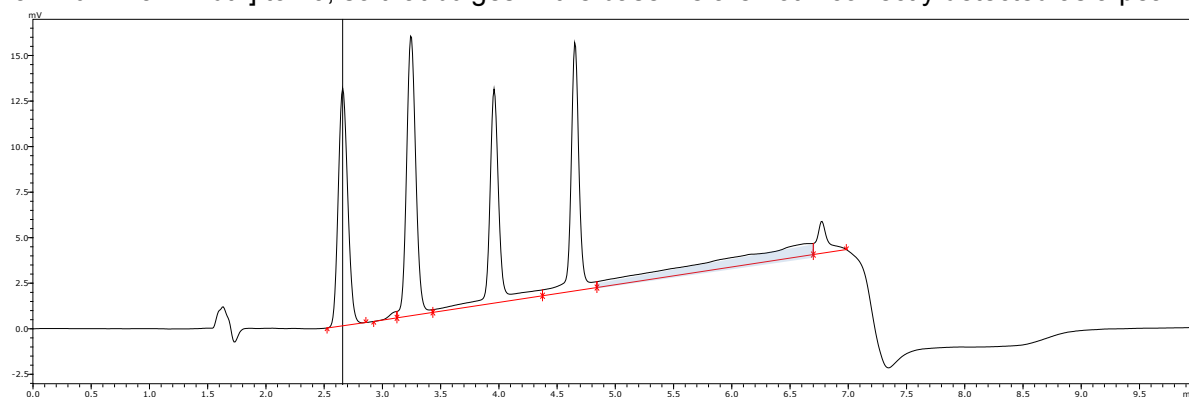


#### Example: Process for When a Downturn at the Peak End Point Due to Baseline Undulations Causes a Long Narrow Region That Is Detected as a Peak

In some cases, baseline undulations can cause an area that is not a peak to be detected as a peak.



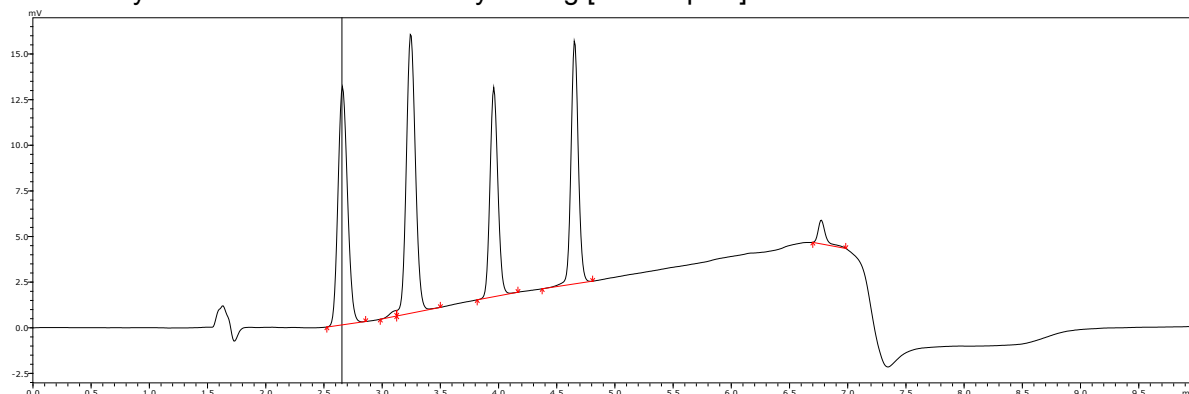
To avoid effects from the negative peak near 1.7 min, set [Integration Range] from 2 min and set [Maximum Half Width] to 10, so that bulges in the baseline are not incorrectly detected as a peak.



The [Maximum Half Width] setting is disabled if a bulge in the baseline does not have the characteristics of a peak (i.e. does not have a half height width area). Consequently, broad short areas can remain incorrectly detected as peaks.

In such cases, try setting the [Peak Filter] - [Min. Aspect] setting to a somewhat larger value, such as 1000 or 10000, and then determine the setting based on that result.

Unnecessary areas can be eliminated by setting [Min. Aspect] to 1000.





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## Chapter Endnotes

vii This function is used to determine the peak-baseline by determining whether the tail of the main peak is treated at baseline, with corresponding peaks treated as tailing peaks, based also on whether or not tailing processing is specified, or whether the baseline is determined assuming the tailing peaks are simply fused rider peaks.

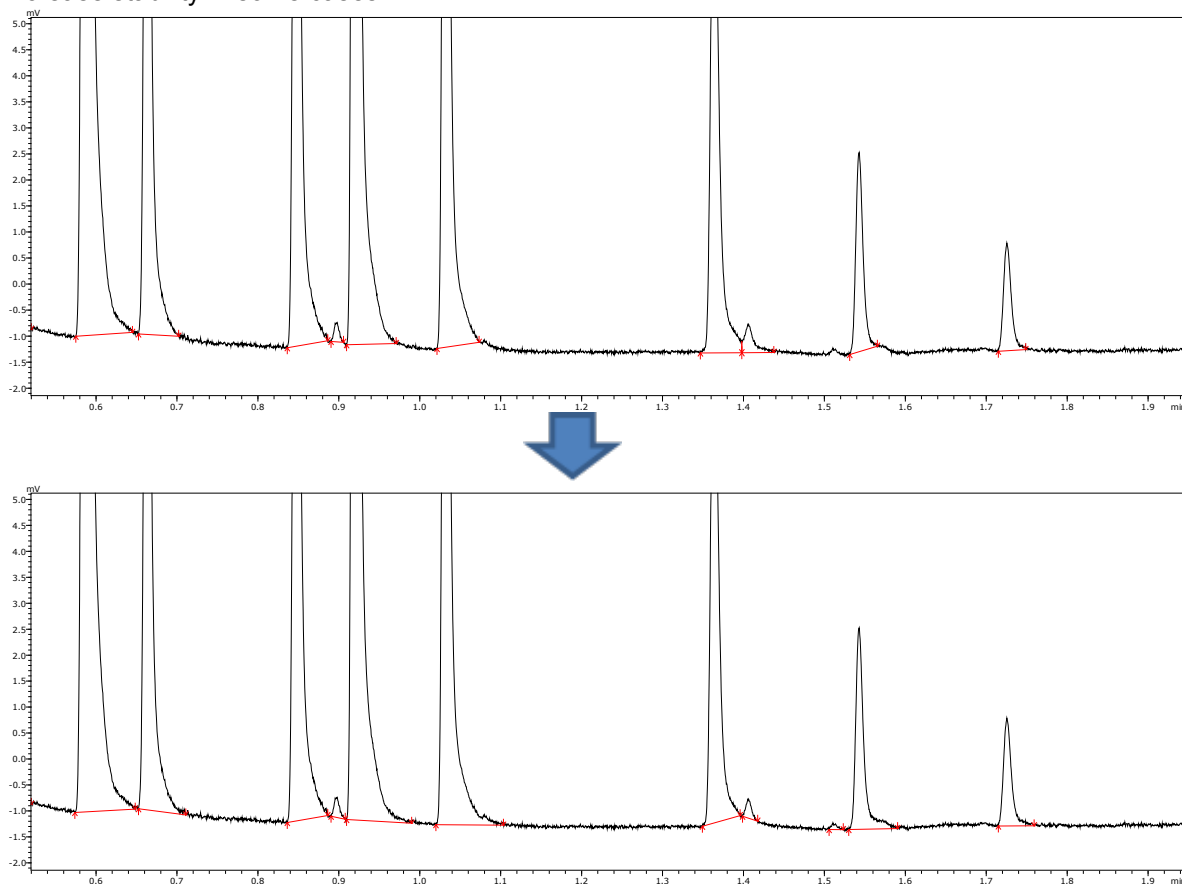
viii Basically the same approach is also used for LCMS, with the settings as described below.

- [Peak Baseline Height] = 0.01 (this setting also disables the baseline estimation function)
- [Detection Threshold] = 0
- [Noise Estimation Range] = Range of zero

However, because the [Tailing Off] checkbox is cleared in default settings, [Valley/Height Ratio] is set to 5, rather than setting [Baseline Type] to [Vertical Division], which would collectively perform the [Tailing Off] checkbox.

In addition, several default settings are specified for newly created methods on the [Peak Unification] tab page.

ix Conversely, if the baseline noise is constant, and peaking tailing is long, lowering the peak-baseline height can increase stability in some cases.



x This is the only peak unification function that unifies peaks based on the resolution, but does not have a prerequisite of peaks being adjacent.

xi To reduce the detection level of shoulder peaks, rather than not detecting them at all, the detection level can be adjusted by selecting the [Unify Peaks by Shoulder Ratio] checkbox and specifying the tangent line height ratio (in terms of percent) for shoulder peaks on the main peak. Conversely, it is also possible to increase the detection level by resetting the [Detection Threshold] setting or increase only the shoulder peak detection sensitivity with the [Detection Threshold of Unseparated Small Peak] setting (on the [Peak Unification] tab page in the [Advanced] window).