Waters
THE SCIENCE OF WHAT'S POSSIBLE.™

Empower System Suitability

Quick Reference Guide

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General information

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Updated information

Refer to the Waters website (www.waters.com) and click **Support** > **Support Documents and Downloads** for updates to this document.

Compliance recommendations

Any time you install, change, or uninstall software or system modules in a regulated environment, Waters recommends that you follow your organization's approved change control procedure.

You should assess the impact of the changes described in the release notes on the qualification status and validation for the intended use of your system, including any impact on personnel, methods, laboratory workflows, or connected equipment, and scale your activities accordingly.

Antivirus considerations

Some real-time virus scanners mistake normal data acquisition and instrument control for virus activity, and thus interfere with proper operations. Full-system scans and live updates can be network-intensive, disk-intensive, and CPU-intensive, and they can also interfere with normal

data acquisition. Schedule scans and updates for idle times when data acquisition does not occur.

Certain antivirus program features such as "intrusion prevention", "tamper protection", and "heuristic analysis" can also interfere with normal operation. If you observe issues with the software, review and verify the antivirus logs. It may be necessary to white-list any affected components.

Related documentation

You can find related product information and documentation on the Waters website, www.waters.com.

Documentation for base product

Waters Licenses, Warranties, and Support Services (71500029510): Provides software license and warranty information, describes training and extended support, and explains how Waters handles shipments, damages, claims, and returns.

Empower Getting Started Guide: Provides an introduction to the Empower software. Describes the basics of how to use Empower software to acquire data, develop a processing method, review results, and print a report. Also covers basic information for managing projects and configuring systems.

Empower Data Acquisition and Processing Theory Guide: Provides theories pertaining to data acquisition, peak detection and integration, and quantitation of sample components.

Empower Installation, Configuration, and Upgrade Guide: Describes Empower software installation, including the stand-alone Personal workstation, Workgroup configuration, and the Enterprise client/server system. Discusses how to configure the computer and chromatographic instruments as part of the Empower System. Also covers the installation, configuration, and use of acquisition servers, such as the LAC/E modules, the busLAC/E card, and interface cards, used to communicate with serial instruments.

Empower online Information System: Describes all Empower windows, menus, menu selections, and dialog boxes for the base software and software options. Also includes reference information and procedures for performing all tasks required to use Empower software. Included as part of the Empower software.

Empower System Administrator's Guide: Describes how to administer the Empower Enterprise client/server system and Workgroup configuration.

Empower Release Notes: Contains last-minute information about the product. Describes product features and enhancements, helpful tips, installation and configuration considerations, and changes since the previous version. Also provides supplementary information about specific Empower software releases.

Documentation for software options

Empower PDA Software Getting Started Guide (71500031503): Describes the basics of using the Empower PDA option to develop a PDA processing method and review PDA results.

Empower Gas Chromatography Getting Started Guide (71500044403): Describes how to use the Empower GC option to develop a GC processing method and review the GC results.

Empower GPC Software Getting Started Guide (71500031303): Describes how to use the Empower GPC option to develop a GPC processing method and review GPC results.

Empower GPCV Software Getting Started Guide (71500031403): Describes how to use the Empower GPCV option to develop a GPCV processing method and review the GPCV results.

Empower Light Scattering Software Getting Started Guide (71500043903): Describes how to use the Empower Light Scattering option to develop a light scattering processing method and review light scattering results.

Empower AutoArchive Software Installation and Configuration Guide (71500044207): Describes how to install and configure the Empower AutoArchive option, which is available for Empower Personal installations.

Related documentation for the System Suitability option

Technical notes require a Total Assurance Plan number to access the additional content. Recommended technical notes include:

Signal-to-Noise Values in Empower 3 (TECN134884650): Describes how Empower 3 calculates the Signal-to-Noise (s/n) ratio as compared with the USP, EP, and JP s/n definitions.

Using Interactive System Suitability in Empower 2 (TECN10115982): Describes the Interactive System Suitability features that were introduced in Empower 2. Describes how you can calculate user-defined summary statistics from multiple results and test the values against System Suitability in real time.

Interactive System Suitability: Using 'Reinject on Fault' function (TECN1852298): Describes the Reinject on Fault setting for Interactive System Suitability.

Additional eLearning courses are available for purchase on the Waters website. Recommended eLearning courses include:

Empower 3: Intermediate Empower Custom Fields - Limits Tab and Acceptance Criteria (750001023): This module covers the Limits tab in the Empower processing method. It utilizes Acceptance Criteria functionality by the creation of inter-sample and inter-sample summary custom fields to determine the Acceptance Criteria specifications.

Empower 3: Advanced Empower Custom Fields - Boolean Custom Fields (750001025): This module is an in-depth view of Boolean type custom fields with examples.

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1 Overview

1.1 Empower System Suitability software overview

System Suitability software is used to monitor and ensure system performance over time, and it is a supporting component to other method validation techniques. System Suitability software enables confirmation that both the system and the method are functioning within the predefined limits, and it is essential for laboratories that use GMP, GLP, or other regulatory protocols.

1.2 System Suitability and Empower software

System Suitability is fully integrated into Empower software and provides testing capabilities to ensure that your chromatography system is working within acceptable limits. As described by the pharmacopoeias supported by Empower, suitability testing is the concept that the electronics, equipment, analytical operations, and samples analyzed constitute an integral system. System suitability is the mechanism by which that integral system is proven fit for purpose prior to and throughout sample analysis.

With the Empower System Suitability software option, you can implement system testing for all of your chromatography applications. System Suitability performs statistical calculations on results and summarizes the information in graphical or tabular format. System Suitability calculates the following and other peak values:

- Resolution
- Tailing and symmetry factor
- Plate count
- Peak height and width
- Signal-to-noise

With System Suitability, you can set limits and acceptance criteria on the calculated peak values. By setting limits and acceptance criteria, you can fault the values that are out of range or outside the acceptance criteria. You can produce reports that show the statistical accuracy and reproducibility of your chromatographic system data. Your reports can also include control charts that monitor user-specified error and warning parameter limits on the individual components in a chromatogram. Empower software bases its system suitability tests on standard laboratory calculations, including *The United States Pharmacopeia*[1], *The European Pharmacopoeia*[2], *The Japanese Pharmacopoeia*[3], and *The Chinese Pharmacopoeia*[4] guidelines and calculations.

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[1] *United States Pharmacopeia (2023). General Chapter, <621> Chromatography. USP-NF. Rockville, MD: United States Pharmacopeia. DOI:* https://doi.org/10.31003/USPNF_M99380_06_01

[2] *The European Pharmacopoeia, 11th Edition; European Directorate for the Quality of Medicines & HealthCare; 2022.*

[3] *The Japanese Pharmacopoeia, 18th Edition; Committee on the Japanese Pharmacopoeia; 2021.*

1.3 What is system suitability testing?

System Suitability testing provides a means of verifying that an entire chromatographic system is working within acceptable limits. Empower System Suitability software monitors your chromatographic system automatically and provides a tabular and graphical summary of system performance based on parameters and limits you set up within Empower software. If all the monitored values fall within the specified relative standard deviation (RSD) criteria or other criteria that you define, your system is suitable for use. Empower software produces reports showing statistical accuracy and reproducibility of the chromatographic system data.

System Suitability enables users to track and review the following:

- System performance
- Reproducibility
- Plots and trends
- Reports and data processing

1.3.1 System performance

System Suitability software monitors system performance, enabling users to confirm that the system and method are functioning within predefined limits.

To monitor your system's ability to separate components, System Suitability software calculates the following chromatographic fields:

- Plate number or plate count (*N*)
- Symmetry or tailing (*T*)
- Resolution (*R*)
- Relative resolution
- Selectivity (α)
- Capacity factor (k')

1.3.2 Reproducibility

System Suitability enables Empower software to measure system reproducibility by analyzing the consistency of the separation from injection to injection using the following peak parameters (among others):

- Area
- Resolution

[4] *The Chinese Pharmacopoeia, 11th Edition; Chinese Pharmacopoeia Commission; 2020.* Applicable starting with Empower 3.7.0.

- Retention time
- Response

1.3.3 Tracking and plotting trends

System Suitability allows Empower software to track and plot trends in the performance of a chromatography system. For example, to detect column aging, you can track and plot trends for plate count values from the results of sample sets acquired over time.

1.3.4 Processing and reporting

You create processing and report methods that include parameters, limits, acceptance criteria, and report groups from System Suitability because it is a completely integrated part of Empower software.

System Suitability parameters, limits, and acceptance criteria are part of a processing method. You set them during method development in the Empower Review window. For details, see the "Using System Suitability" topic in the *Empower online Information System*.

System Suitability report groups and fields are part of a report method. You can create System Suitability report methods in the Report Publisher window, or you can use one of the report methods included in the System Suitability default project. For details, see the "Interpreting System Suitability Data Plots in Reports" topic in the *Empower online Information System*.

After System Suitability processing and report methods are created, you can run and report System Suitability analysis on a set of samples during data acquisition. You can also combine processing and reporting on multiple sets of samples after data acquisition.

1.4 Using System Suitability

You use Empower System Suitability software to determine if a system is suitable to acquire, process, and report data by testing separation criteria and reproducibility criteria.

You begin by activating the system suitability option in the project. You then set system suitability processing parameters and reporting parameters. The processing parameters define the calculations to use and the range of allowable peak values. The reporting parameters define the reports used to monitor the results. After setting the processing and reporting parameters, save the associated methods in a method set. For details, see the "Defining System Suitability Processing Method Parameters" or "Specifying System Suitability system and separation efficiency parameters" topic in the *Empower online Information System*.

After you set processing parameters, create the methods necessary to monitor your system, and report the system suitability data, you can begin using System Suitability software to test your system.

1.4.1 Verifying System Suitability

To verify that the system is suitable for acquiring and processing samples, perform the actions described in the *Empower online Information System* topics "Acquiring data from multiple samples" and "Viewing chromatographic data."

If System Suitability fields are not generated, type `System Suitability, troubleshooting` on the *Empower online Information System* Search tab to access the “System Suitability Troubleshooting” and "Verifying System Performance" topics.

1.4.2 Suitability Limits

Suitability Limits, a user-defined method of monitoring the suitability of a system to run your method, is available with the System Suitability option. Suitability Limits are properties that can be applied to data using a specific Processing Method. Suitability Limits report error and warning parameters on the individual peak components within a chromatogram.

You can define System Suitability limits as a range of allowable values for each component involved in system suitability testing. By using Suitability Limits, you can enter absolute criteria that define allowable values with respect to one or more constant values. For example, an allowable peak value may be defined as greater than zero and less than ten in order for the peaks to pass suitability testing. The System Suitability Limits that you set are used to determine the limits shown as minimum and maximum values in summary charts, and the limits also define faulted, out-of-range values in Review or Reports. Faulted values appear in a different color and font in the tabular data in Review and in the printed reports.

You identify the components and set the limits for the appropriate fields in the Components table and the Suitability Limits table using the Components tab and the Limits tab in Processing Method. To define a Suitability Limit, you must click a row in the Suitability Components table and use the available fields to define the peak components. Table 1–1: Suitability Limits table columns (Page 12) describes the properties of the Suitability Limits table. If you want to copy the specified limits to other components in the processing method, select **Copy All Limits** or **Copy Selected Limits** on the Options menu.

Table 1–1: Suitability Limits table columns

Field	Description
Field Name	Specifies the peak fields to which System Suitability limits are to be applied. Selecting a field from this list allows you to set System Suitability limits for that field in the Peaks table.
Target	Specifies the target value for the peak field. The target value provides a visual reference point on a summary plot for the value you want to achieve. Entries: Greater than or equal to the Lower Error and Warning Limits and less than or equal to the Upper Error and Warning Limits. Default: Blank

Table 1–1: Suitability Limits table columns (continued)

Field	Description
Lower Error Limit (LCL)	Specifies the Lower Error Limit (LCL) used for faulting peak field values less than this minimum value and for display in a summary plot. Entries: -999999999.999 to 9999999999.999. Default: Blank
Upper Error Limit (LCL)	Specifies the Upper Error Limit (UCL) used for faulting peak field values greater than this maximum value and for display in a summary plot. Entries: -999999999.999 to 9999999999.999. Default: Blank
Lower Warning Limit (LWL)	Specifies the Lower Warning Limit value for display in a summary plot. Entries: -999999999.999 to 9999999999.999. Default: Blank **Tip:** Ensure that the Lower Warning Limit is set within the specified Lower and Upper Limits.
Upper Warning Limit (UWL)	Specifies the Upper Warning Limit value for display in a summary plot. Entries: -999999999.999 to 9999999999.999. Default: Blank **Tip:** Ensure that the Upper Warning Limit is set within the specified Lower and Upper Limits.
Error %	A number field with a range of 0 to 100, a precision of 2, and a blank default value. This field is enabled only when the target field contains a value. When you enter a number in the Error % field or change the Target value while there is an Error % value, the Lower Error Limit (LCL) and the Upper Error Limit (UCL) are calculated by these formulas: LCL = Target - [Target x (Error %) / 100] UCL = Target + [Target x (Error %) / 100] If you modify the LCL or UCL, the Warning % is cleared.
Warning %	A number field with a range of 0 to 100, a precision of 2, and a blank default value. This field is enabled only when the target field contains a value. When you enter a number in the Warning % field or change the Target value while there is a Warning % value, the Lower Warning Limit (LWL) and the Upper Warning Limit (UWL) are calculated by these formulas: LWL = Target - [Target x (Warning %) / 100] UWL = Target + [Target x (Warning %) / 100] If you modify the LCL or UCL, the Warning % is cleared.
Ignores Blank Values	Specify whether to fault a blank value when these is a Lower Error Limit: • If enabled and you enter a Lower Error Limit, the corresponding peak field is not faulted if it is blank. • If disabled and you enter a Lower Error Limit, the corresponding peak field is faulted if it is blank.
Check Limits	Specify when the limits defined in this row of the table will be checked.

Table 1–1: Suitability Limits table columns (continued)

Field	Description
	• Always • During Calibration • During Quantitation • During Custom Summary

For more details about setting limits and acceptance criteria, see the "System Suitability Limit fields" and "Verifying system performance" topics in the *Empower online Information System*.

Restriction: You can set only one type of limit condition for a given field. If you set upper and lower limits on a particular field in the Suitability Limits table, you cannot set relative criteria limits on that same field in the Acceptance Criteria table.

1.4.3 Acceptance criteria

Acceptance Criteria are another method of monitoring the reproducibility of a chromatogram by way of testing relative limits. Acceptance Criteria define the range of allowable component values with respect to another component value or formula. Like Suitability Limits, you apply Acceptance Criteria to data using a specific Processing Method.

To set Acceptance Criteria, navigate to the Limits tab in Processing Method and locate the Acceptance Criteria table at the bottom of the window. Select a row in the table and use the available columns to define the Acceptance Criteria for that peak. You specify Acceptance Criteria by selecting the component and adding a formula using the Formula Editor. Table 1–2: Acceptance Criteria table columns (Page 14) describes the properties of the Acceptance Criteria table.

Table 1–2: Acceptance Criteria table columns

Field	Description
Field Name	The name of the field that you want to fault if this acceptance criterion is not met.
Left Side	Click to open the custom Formula Editor. Hold the Ctrl key and click to enter a formula directly in the cell. **Tip:** For the first click of a new session, a message appears giving you the option to use the Formula Editor or to Ctrl+click. The message appears only once after you click in any of the formula cells.
Operation	The operator to use in the formula. You can select from a list of Boolean comparison operators.

Table 1–2: Acceptance Criteria table columns (continued)

Field	Description
Right Side	The right side of the formula. You can edit this cell just as you would edit the Left Side cell. The value of this cell is also used as the Target when a value is specified for the % of Target field.
Precision	The precision is used when comparing the left and right side values. The Left Side and Right Side values are rounded to this number of decimal places when displayed in the field.
Warning/Error	When setting this value to Warning, the field on which you set limits is not faulted, even if it fails to pass the limit criteria. When it is set to Error, the field on which you set limits is faulted when it does not pass the limit criteria.
% of Target	When you specify a range using the RANGE function, you can use this field to describe the range. Example: Range is between "right side - (right side × % of target)" and "right side + (right side × % of target)". Assume the right side as 1000 and % of target as 10. The range is then between 1000 - (1000 × 10%) and 1000 + (1000 × 10%). The value of the assessed field must be greater than or equal to 900 and less than 1100.
Ignore Blank Values	Select this check box to exclude blank values from suitability testing. If any of the fields that are part of the criterion, assessed field, Left Side, or Right Side are blank, the corresponding peak field does not get faulted for this criterion. Clear this check box when a blank value in any of the fields that are part of the criterion should cause a fault for the corresponding peak field.
Check Relative Limits	Specify when to verify limit criteria. • Always • During Calibration • During Quantitation • During Custom Summary

For more details about setting limits and acceptance criteria, see the following topics in the *Empower online Information System*:

- "System Suitability Limit fields"
- "Verifying system performance"
- "Including user-defined formulas in result calculations"

1.4.4 Interactive System Suitability

Interactive System Suitability is a function in the base Empower software that detects faults during data acquisition and allows you to select the mode for responding to a fault. The System Suitability option is not required to use Interactive System Suitability. You can enable Interactive System Suitability from the modes drop-down list in Run Samples. This selection provides you with fault detection similar to that provided in the System Suitability option. Table 1–3: Interactive System Suitability options (Page 16) describes the options provided with Interactive System Suitability.

Table 1–3: Interactive System Suitability options

Option	Description
Continue on Fault	Continues to make injections and/or acquire data even if a Fault condition occurs during processing (default).
Reinject on Fault	Stops acquiring data and repeats the current injection if a Fault condition occurs during processing. Injections are repeated as many times as you specify in Customize Defaults. If the reinjection also results in a Fault, acquisition stops.
Stop on Fault	Stops acquisition when a Fault condition occurs during processing.
Next Sample on Fault	Skips to the next sample when a Fault condition occurs during processing.
Next Sample Set on Fault	Skips to the next sample set when a Fault condition occurs during processing.

To assess acquired data for faults, Empower must process your data. When using Interactive System Suitability, you must provide a processing method within the method set used during acquisition. Waters recommends that you acquire data using Run and Process or Run and Report mode. If you acquire using Run Only mode, Empower processes the data to determine if faults are present, but processed results are not saved to the Empower database. For more information on Interactive System Suitability, see the "New Sample Set Method Wizard - Describe Run Time Options" and "Monitoring analysis performance results interactively" topics in the *Empower online Information System*.

1.5 Troubleshooting

System Suitability allows you to perform troubleshooting procedures on a chromatography system by viewing peak data based on your procedure's requirements. Examples of peak data you can use for troubleshooting procedures include:

- Retention time (R_t)
- Resolution (R_s)

- Capacity factor (*k'*)
- Selectivity (*α*)
- Column efficiency (plate number or plate count, *N*)
- Symmetry factor or tailing (*T*)
- Baseline noise and drift
- Signal-to-noise ratio (*s/n*)
- Statistical peak moments

To quickly determine whether your system is performing correctly, create a report for a sample set that includes the overall percent RSD for selected fields. If the replicate system suitability injections in your sample set vary by more than a user-defined value, such as 2%, you can examine data from each injection until you locate the problem.

For details, see the following topics in the *Empower online Information System*:

- “System Suitability Limit Fields”
- “Modifying System Suitability Report Group Properties”
- “Creating a Report Method Interactively”

Alternatively, type `System Suitability, troubleshooting` on the *Empower online Information System* Search tab to access the “System Suitability Troubleshooting” and "Verifying System Performance" topics.

2 Enabling System Suitability

This chapter contains instructions for enabling Empower System Suitability software. System Suitability is a software option in Empower, and it is enabled by activating a System Suitability Option license using the Waters Licensing Wizard on the workstation or server where Empower software resides.

You can use the System Suitability default project as a template for testing your chromatographic system. To use the System Suitability default project, you must restore the default project from the example projects media included with your purchase of Empower, or you can download the default project from the Waters online marketplace (https://marketplace.waters.com). Contents of the System Suitability default project (Page 19) summarizes the contents of the System Suitability default project.

2.1 System Suitability and Empower installations

To use Empower System Suitability, you must enable the Empower System Suitability software. You can install System Suitability on a Personal stand-alone workstation, an Enterprise client/server system, or a Workgroup system.

You can only activate a System Suitability option license on one instance of Empower at a time. To enable a previously used license on a different instance of Empower, you must first deactivate it on the initial instance of Empower.

Restriction: You cannot enable a System Suitability option license for an Enterprise client/server or Workgroup node on a Personal stand-alone workstation, nor can you enable a System Suitability option license for a Personal stand-alone workstation on an Enterprise client/server or Workgroup node.

2.2 Activating System Suitability software option

System Suitability is a software option for Empower that you enable using the Waters Licensing Wizard.

Prerequisite: Empower base software is installed and activated.

To enable the System Suitability option, you must create a license activation file using the Waters License Activation Center page (https://www.waters.com/activate/licenseintro.htm).

To activate the System Suitability option on an Empower Personal workstation, follow the instructions in the topic "Activating Empower software licenses and options", in the chapter "Installing an Empower Personal workstation" of the *Empower Installation, Configuration, and Upgrade Guide*.

To activate the System Suitability option on an Empower Enterprise or Workgroup server, follow the instructions in the topic "Activating Empower licenses on a server", in the chapter "Installing an Empower Enterprise or Workgroup server" of the *Empower Installation, Configuration, and Upgrade Guide*.

Note: If you must transfer the license from one installation of Empower to another, you must deactivate it from the original computer before you activate it on another computer. To deactivate the license on another computer, see Deactivating the System Suitability software option (Page 19).

2.3 System Suitability and specific projects

After you enable System Suitability using the procedures in this section, the System Suitability software option is available for all projects. You can enable or disable System Suitability for specific projects. For details on enabling or disabling an option for a specific project, see the "Modifying project properties" topic in the *Empower online Information System*.

2.4 Restoring the System Suitability default project

After you enable System Suitability software, you can restore the System Suitability default project from the sample projects media. You can use the System Suitability default project as a template for testing your chromatographic system. The project name is SysSuit_Default.

For details on restoring a project, see the “Restore Project Wizard - Start Software page” topic in the *Empower online Information System*.

2.4.1 Contents of the System Suitability default project

The System Suitability default project contains:

- Four sample sets, each containing six raw data files
- Four results sets, each containing six results files
- A processing method with System Suitability enabled and typical parameter settings
- Report methods

2.5 Deactivating the System Suitability software option

To activate the System Suitability option on another installation of Empower, you must deactivate it from its current installation. To deactivate System Suitability, use the Waters Licensing Wizard (see the *Empower Installation, Configuration, and Upgrade Guide*).

Note: To avoid rendering the System Suitability license unusable, deactivate the option before uninstalling Empower software. If you do render the licenses and options unusable, contact Waters Technical Support for assistance.

To deactivate System Suitability, log on to the Waters Licensing Wizard and click **Deactivate licenses**. On the Deactivate licenses page, select the System Suitability license to create a deactivation file. After you create a deactivation file, you must register the deactivation file on the Waters License Activation Center page (https://www.waters.com/activate/licenseintro.htm) before it can be enabled on another computer.

3 System Suitability Equations

3.1 System Suitability results

Table 3–1: System Suitability results based on pharmacopoeia (Page 21) summarizes all Empower System Suitability results using the terminology from The European Pharmacopoeia, The Japanese Pharmacopoeia, The United States Pharmacopeia, and The Chinese Pharmacopoeia. To obtain the results in Table 3–1: System Suitability results based on pharmacopoeia (Page 21), select **EP**, **JP**, **USP**, **ChP**, or **All** from the **Suitability** tab of the Processing Method window. See the “Specifying System Suitability system and separation efficiency parameters” topic in the *Empower online Information System*.

Table 3–1: System Suitability results based on pharmacopoeia

Options				
European Pharmacopoeia (EP)	**Japanese Pharmacopoeia (JP)**	**Chinese Pharmacopoeia (ChP)[a]**	**United States Pharmacopoeia (USP)**	**All**
Results				
Capacity factor (k')	Capacity factor (k')	Capacity factor (k')	Capacity factor (k')	Capacity factor (k')
Selectivity	Selectivity	Selectivity	Selectivity	Selectivity
Resolution	Resolution	Resolution [b]	Resolution [b]	Resolution
—	—	—	USP Resolution	USP Resolution
—	—	ChP Resolution	—	ChP Resolution
—	—	—	USP Resolution (HH)	USP Resolution (HH)
—	—	ChP (HH) Resolution	—	ChP (HH) Resolution
—	—	—	—	Asym @ 4.4
—	—	—	—	Asym @ (4.4)^2
—	—	—	—	Asym @ 10
—	—	—	—	Asym @ (10)^2
—	—	—	—	Asym
Symmetry Factor	Symmetry Factor	Symmetry Factor [b]	Symmetry Factor [b]	Symmetry Factor

Table 3–1: System Suitability results based on pharmacopoeia (continued)

Options				
European Pharmacopoeia (EP)	**Japanese Pharmacopoeia (JP)**	**Chinese Pharmacopoeia (ChP)[a]**	**United States Pharmacopoeia (USP)**	**All**
Results				
—	—	—	USP Tailing	USP Tailing
—	—	ChP Tailing Factor	—	ChP Tailing Factor
Plate Number [b]	Plate Number [b]	Plate Number [b]	Plate Number [b]	Plate Number [b]
—	—	—	USP Plate Count	USP Plate Count
—	—	ChP Plate Count	—	ChP Plate Count
—	—	ChP Plate Count (HH)	—	ChP Plate Count (HH)
EP Plate Count	—	—	—	EP Plate Count
—	JP Plate Count	—	—	JP Plate Count
—	JP14 Plate Count	—	—	JP14 Plate Count
—	—	—	—	2 Sigma
—	—	—	—	3 Sigma
—	—	—	—	4 Sigma
—	—	—	—	5 Sigma
Relative Resolution [b]	Relative Resolution [b]	Relative Resolution [b]	Relative Resolution [b]	Relative Resolution [b]
Rel. Resol.[c d e]	Rel. Resol.[c d e]	Rel. Resol.[f d e]	Rel. Resol.[g d e]	Rel. Resol.[h d e]
—	—	—	—	Width @ Baseline
—	—	Width @ Tangent (Resolution)	Width @ Tangent (Resolution)	Width @ Tangent (Resolution)
—	—	Width @ Tangent (Plate Count)	Width @ Tangent (Plate Count)	Width @ Tangent (Plate Count)
—	—	—	—	Width @ 4.4%
Width @ 5%	Width @ 5%	Width @ 5%	Width @ 5%	Width @ 5%
—	—	—	—	Width @ 10%
—	—	—	—	Width @ 13.4%
—	—	—	—	Width @ 32.4%
Width @ 50%	Width @ 50%	Width @ 50%	Width @ 50%	Width @ 50%

Table 3–1: System Suitability results based on pharmacopoeia (continued)

Options				
European Pharmacopoeia (EP)	**Japanese Pharmacopoeia (JP)**	**Chinese Pharmacopoeia (ChP)[a]**	**United States Pharmacopoeia (USP)**	**All**
Results				
—	—	—	—	Width @ 60.7%
f @ 5%	f @ 5%	f @ 5%	f @ 5%	f @ 5%
s/n	s/n	s/n	s/n	s/n
EP s/n	—	—	—	EP s/n
—	JP s/n	—	—	JP s/n
—	—	—	USP s/n	USP s/n
—	—	ChP s/n	—	ChP s/n
EP Noise (Plot Units)	—	—	—	EP Noise (Plot Units)
—	JP Noise (Plot Units)	—	—	JP Noise (Plot Units)
—	—	—	USP Noise (Plot Units)	USP Noise (Plot Units)
—	—	ChP Noise (Plot Units)	—	ChP Noise (Plot Units)
Start p/v	Start p/v	Start p/v	Start p/v	Start p/v
End p/v	End p/v	End p/v	End p/v	End p/v
Zeroth Moment	Zeroth Moment	Zeroth Moment	Zeroth Moment	Zeroth Moment
First Moment	First Moment	First Moment	First Moment	First Moment
Second Moment	Second Moment	Second Moment	Second Moment	Second Moment
Third Moment	Third Moment	Third Moment	Third Moment	Third Moment

Table 3–1: System Suitability results based on pharmacopoeia (continued)

Options				
European Pharmacopoeia (EP)	Japanese Pharmacopoeia (JP)	Chinese Pharmacopoeia (ChP)[a]	United States Pharmacopoeia (USP)	All
Results				
Fourth Moment	Fourth Moment	Fourth Moment	Fourth Moment	Fourth Moment

a. Starting with Empower 3.7.0.

b. Starting with Empower 3.8.0.

c. EP and JP Rel. Resol. are calculated using the formula for Resolution.

d. In versions prior to Empower 3.8.0, the Rel. Resol. field appears as Relative Resolution in the Chinese, Korean, and Japanese languages.

e. Starting with Empower 3.8.0, this field is called Legacy Relative Resolution in the Chinese, Korean, and Japanese languages. The formula for this calculation has not changed and depends on the Pharmacopoeia setting as described in these footnotes.

f. ChP Rel. Resol. is calculated using the formula for the ChP Resolution.

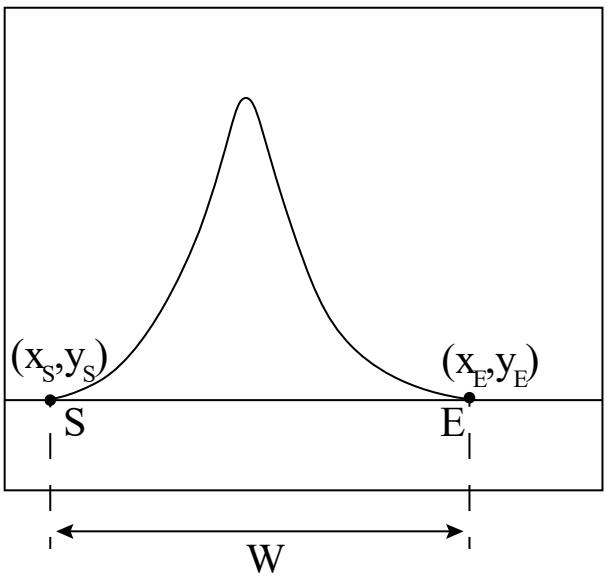
g. USP Rel. Resol. is calculated using the formula for USP Resolution (HH).

h. When selecting All pharmacopoeia, the Rel. Resol. is calculated using the formula for USP Resolution.

3.2 Calculating peak width at baseline

Width at baseline (Width @ Baseline) is the peak width at the baseline of the peak, as determined by the processing method. Figure 3–1: Width @ Baseline (Page 24) describes the width at baseline calculation.

Figure 3–1: Width @ Baseline



$W = x_E - x_S$

W = Width @ Baseline

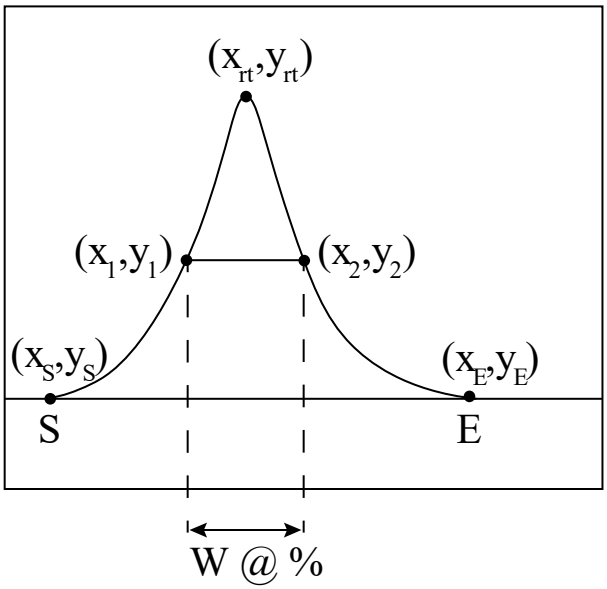
x_E = The x value corresponding to the rightmost point on the peak, or end time

x_S = The x value corresponding to the leftmost point on the peak, or start time

3.3 Calculating width at percent of peak height

Empower System Suitability software uses the equation in Figure 3–2: Calculation of width at percent of peak height (Page 25) to calculate width at percent of peak height used in several System Suitability equations referenced in this section.

Figure 3–2: Calculation of width at percent of peak height



Width (W) @ % = (x_2 - x_1)

Where:

y_2 = (% / 100) × (y_{rt} - y_E) + y_E

y_1 = (%/100) × (y_{rt} - y_S) + y_S

x_1 = Interpolated x-value at y_1

x_2 = Interpolated x-value at y_2

3.3.1 Peak integration type labels

The peak integration type restricts the method of calculating width at percent of peak height. The Peaks table (in the Review Main window and the Results window) displays the field Int Type with a two-character label that describes the way a peak was integrated. For a complete listing, see

the “Integration Type Labels in the Peaks Table” topic in the *Empower online Information System* and the *Empower Data Acquisition and Processing Theory Guide*.

Peaks are identified as follows:

- BB = Baseline to Baseline
- BV = Baseline to Valley
- VB = Valley to Baseline
- VV = Valley to Valley
- EE = Exponential to Exponential
- TT = Tangential to Tangential
- BG = Baseline to Gaussian Skim

You create manual integrations when you draw or adjust a baseline or when you move a drop line. Manual integration is noted in the Int Type field by lowercase letters (b, v, t, and e). For example:

- bV = Manual Baseline to Valley
- vV = Manual Valley to Valley
- bb = Manual Baseline to Manual Baseline

3.3.2 Restrictions to calculation of width at percent of peak height

All fields for peak width at percent height are calculated for baseline-resolved peaks (BB) but not for skimmed peaks (such as GB or BG). Some or all fields for peak width at percent height can be calculated for peaks that are not resolved at the baseline (BS, SB, BR, and RB), depending on the height of the start and end points.

System Suitability does not perform any calculation that requires a peak width if the peak width at the percentage of height cannot be calculated. There are three use cases where the width cannot be calculated:

- For BV or bv when the *y* value at the end time of the peak is greater than the *y* value at the percent height at the start of the peak.
- For VB or vb when the *y* value at the start time of the peak is greater than the *y* value at the percent height at the end of the peak.
- For VV or vv when the *y* value at either the start or end of the peak is greater than the percent height at the retention time of the peak. The percent height at the retention time of the peak is calculated as (% / 100) × (y_{rt} - y_{rtb}), where y_{rt} is the *y* value at the retention time and y_{rtb} is the *y* value at the baseline for the same retention time.

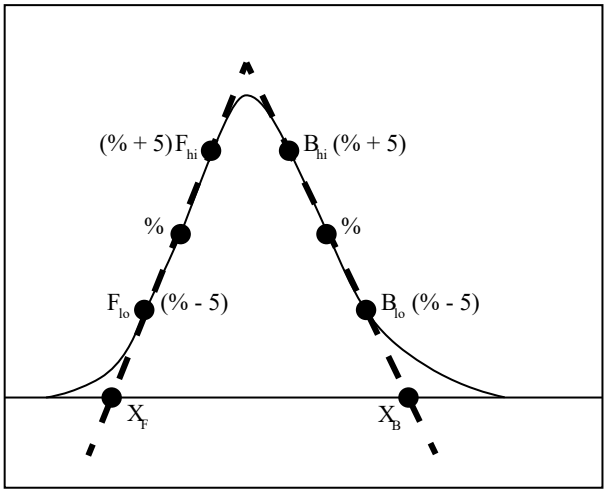
3.4 Calculating peak width at tangent using traditional integration

Empower System Suitability software calculates peak width at tangent to determine the width (*W*) when calculating Width @ Tangent (Resolution) and the Width @ Tangent (Plate Count) (Figure 3–3: Calculation of peak width at tangent (Page 27)). Empower uses the peak width at tangent in subsequent calculations such as the USP Resolution, USP Plate Count, ChP Resolution, and ChP Plate Count.

Restriction: Peak width at tangent is calculated only if the peak widths at both the tangent percent plus five and the tangent percent minus five can be calculated.

Requirement: To complete the peak width at tangent calculation, System Suitability software requires an intersection of the tangent lines with the baseline.

Figure 3–3: Calculation of peak width at tangent



$$Width\ at\ tangent_{Traditional} = x_B - x_F$$

Where:

X_B = The *x* value of the point where the baseline intersects a line drawn between the points B_{hi} and B_{lo}

X_F = The *x* value of the point where the baseline intersects a line drawn between the points F_{hi} and F_{lo}

B_{hi} =The interpolated point on the back side of a peak at (% + 5) × the height of the peak

B_{lo} = The interpolated point on the back side of a peak at (% - 5) × the height of the peak

F_{hi} = The interpolated point on the front side of a peak at (% + 5) × the height of the peak

F_{lo} = The interpolated point on the front side of a peak at (% - 5) × the height of the peak

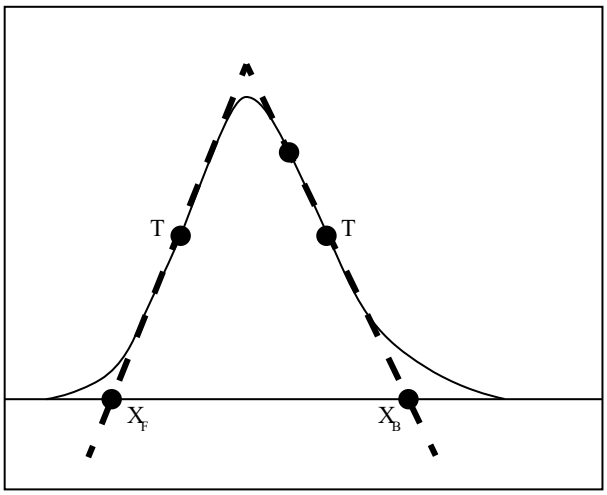
% = The percentage of peak height at which you are calculating the tangent (for example, 50% or 61%), specified in the processing method

Recommendation: Whenever possible, use ApexTrack instead of traditional integration to automatically calculate the peak width at tangent. ApexTrack's Auto Peak Width algorithm ensures that the width at tangent is calculated correctly.

3.5 Calculating peak width at tangent using ApexTrack integration

If the Peak Width field is left blank when processing the data, System Suitability software calculates Width @ Tangent (Resolution) and Width @ Tangent (Plate Count) values using the tangents at the peak's inflection points, as defined by the ApexTrack algorithm (Figure 3–4: Width at tangent using ApexTrack integration (Page 28)). ApexTrack uses an Auto Peak Width algorithm to determine the optimum peak width value. This algorithm automatically positions the inflection points correctly to ensure that the width at tangent is calculated correctly.

Figure 3–4: Width at tangent using ApexTrack integration



Width at tangent $_{ApexTrack} = x_B - x_F$

Where:

T = Inflection point of peak, as determined by the ApexTrack algorithm

x_B = The *x* value of the point where the baseline intersects a line drawn tangent to the inflection point on the back of the peak

x_F = The *x* value of the point where the baseline intersects a line drawn tangent to the inflection point on the front of the peak

Tip: Empower reports an S29 processing code for peaks when the width at tangent was calculated using ApexTrack to determine inflection points.

Correct identification of the peak's inflection points is required. The peak inflection points are identified based on the user-entered value for peak width in the processing method. For peaks with an Int Type of BB and with a user-identified peak width in the processing method that is not appropriate for identifying inflection points, Empower re-calculates the peak's inflection points

using a peak width that is appropriate for the peak. To recalculate the inflection points, ApexTrack uses the data between the peak's start and end times after the peak is re-smoothed using an internally determined correct peak width.

Tip: Empower reports an S53 processing code for all peaks where the inflection points were recalculated using an internally determined peak width.

In an ApexTrack result, some manual changes to peaks have the potential to position the peak start, end, or both such that the inflection points that were originally calculated for the peak no longer fall within the peak. When this occurs, the ApexTrack result no longer reports the second derivative apex or inflection width. When this occurs, peak type processing code I37 is used, and the peak is referred to as a Traditional peak in an ApexTrack result. Traditional peaks in an ApexTrack result do not have values for the fields 2nd derivative apex and inflection width in the Peaks table. When this occurs, Width @ Tangent (Resolution) and Width @ Tangent (Plate Count) values are determined using the Traditional integration approach.

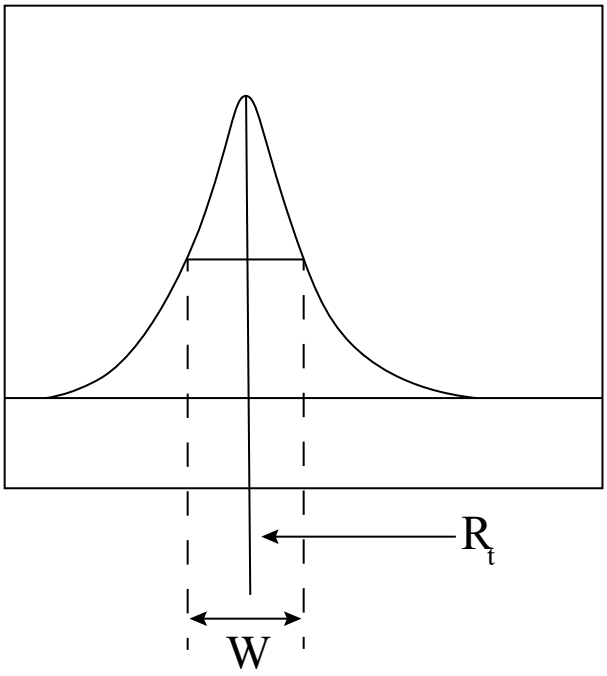
3.6 Plate number (plate count) equations

Plate number (plate count) calculations determine column efficiency. Starting with version 3.8.0, Empower software calculates the Plate Number for all pharmacopoeia choices. This section includes figures that describe the equations used to calculate the following values:

- Plate Number (Figure 3–5: Plate Number, EP Plate Count, JP Plate Count, and ChP Plate Count (HH) (half height) equation (Page 30))
- EP Plate Count (Figure 3–5: Plate Number, EP Plate Count, JP Plate Count, and ChP Plate Count (HH) (half height) equation (Page 30))
- JP Plate Count (Figure 3–5: Plate Number, EP Plate Count, JP Plate Count, and ChP Plate Count (HH) (half height) equation (Page 30))
- USP Plate Count (Figure 3–6: USP Plate Count and ChP Plate Count equation (Page 30))
- ChP Plate Count (Figure 3–6: USP Plate Count and ChP Plate Count equation (Page 30))
- ChP Plate Count (HH) (Figure 3–5: Plate Number, EP Plate Count, JP Plate Count, and ChP Plate Count (HH) (half height) equation (Page 30))
- 5 Sigma (Figure 3–7: 5 Sigma equation (Page 31))
- 4 Sigma (Figure 3–8: 4 Sigma equation (Page 32))
- 3 Sigma (Figure 3–9: 3 Sigma equation (Page 32))
- 2 Sigma (Figure 3–10: 2 Sigma equation (Page 33))
- Asymmetry (Asym) (Figure 3–11: Asym equation (Page 34))[1]
- JP14 Plate Count (Figure 3–12: JP14 Plate Count equation (Page 35))

[1] Foley, J.P.; Dorsey, J.G. Equations for calculation of chromatographic figures of merit for ideal and skewed peaks. Anal. Chem. **1983**, 55, 730-737. DOI: 10.1021/ac00255a033

Figure 3–5: Plate Number, EP Plate Count, JP Plate Count, and ChP Plate Count (HH) (half height) equation



$$N = 5.54\left(\frac{R_t}{W}\right)^2$$

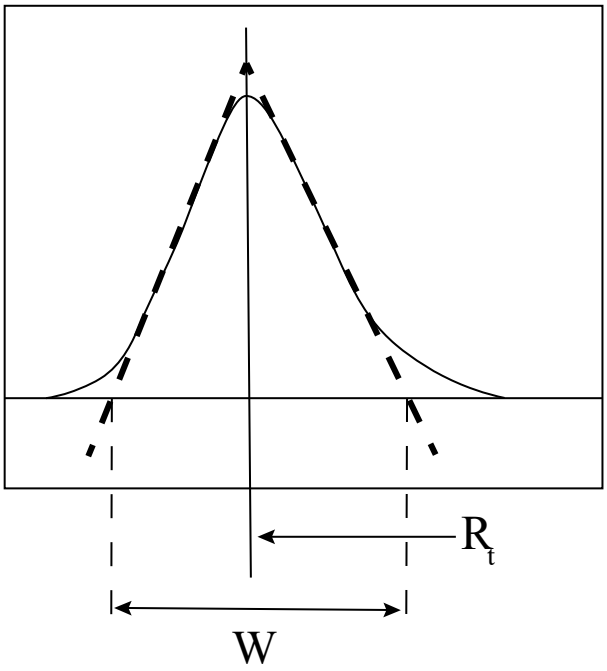
Where:

N = Plate number or count (the number of theoretical plates in a chromatographic column)

R_t = Retention time

W = Peak width at 50% of peak height

Figure 3–6: USP Plate Count and ChP Plate Count equation



$$N = 16\left(\frac{R_t}{W}\right)^2$$

Where:

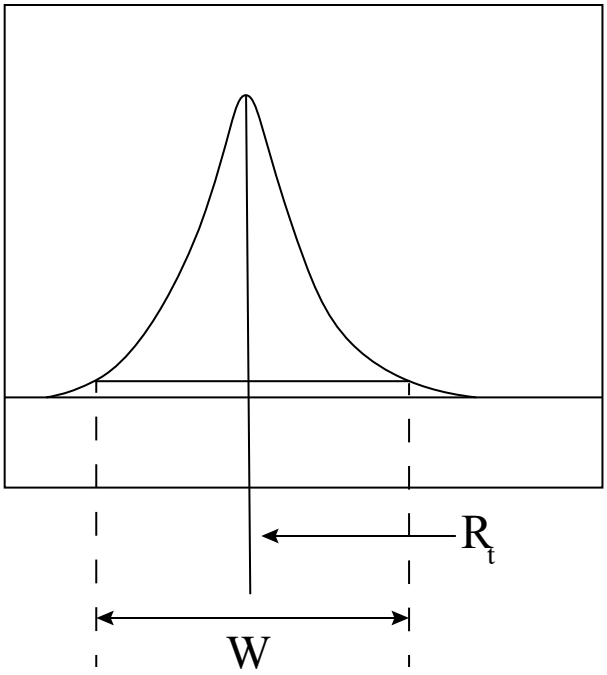
N = Plate count (the number of theoretical plates in a chromatographic column)

R_t = Retention time

W = Peak width at baseline determined by tangents drawn at the inflection points (for Apex Track integration) or to a % of Peak Height

% = 61% if Pharmacopoeia choice is **USP** or **ChP**, or the Tangent Percent specified by the user if the Pharmacopoeia choice is **All**

Figure 3–7: 5 Sigma equation



$$N = 25\left(\frac{R_t}{W}\right)^2$$

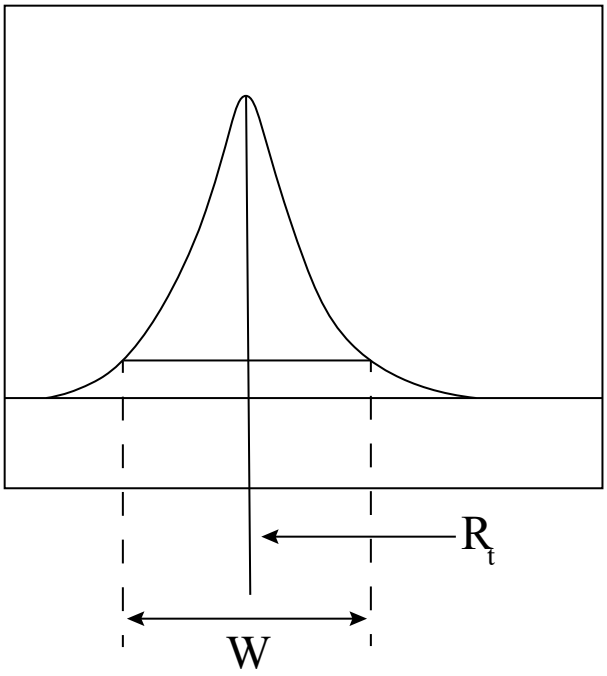
Where:

N = 5 Sigma

R_t = Retention time

W = Peak width at 4.4% of peak height

Figure 3–8: 4 Sigma equation



$$N = 16\left(\frac{R_t}{W}\right)^2$$

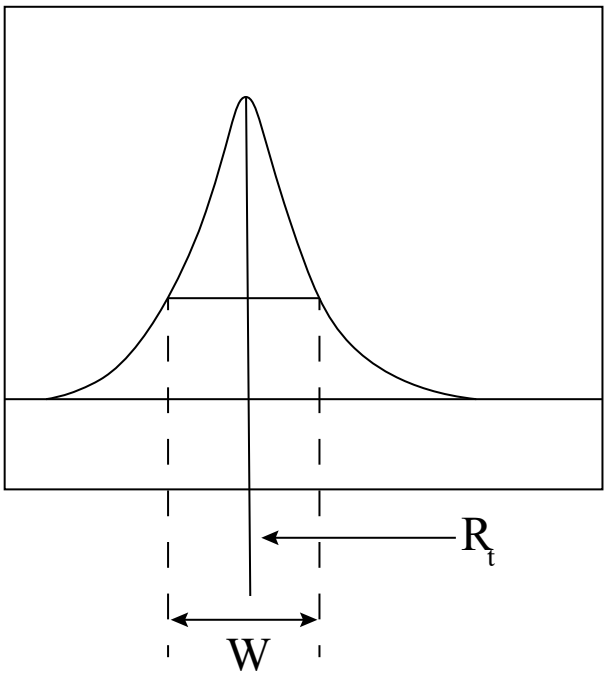
Where:

N = 4 Sigma

R_t = Retention time

W = Peak width at 13.4% of peak height

Figure 3–9: 3 Sigma equation



$$N = 9\left(\frac{R_t}{W}\right)^2$$

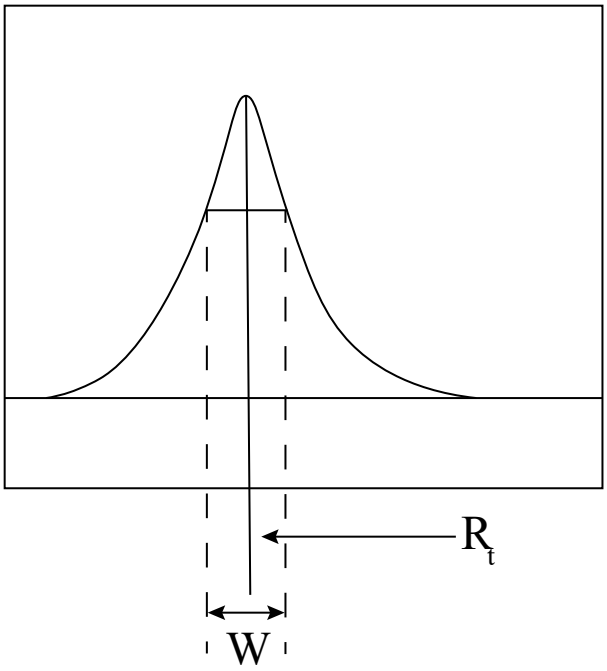
Where:

N = 3 Sigma

R_t = Retention time

W = Peak width at 32.4% of peak height

Figure 3–10: 2 Sigma equation



$$N = 4\left(\frac{R_t}{W}\right)^2$$

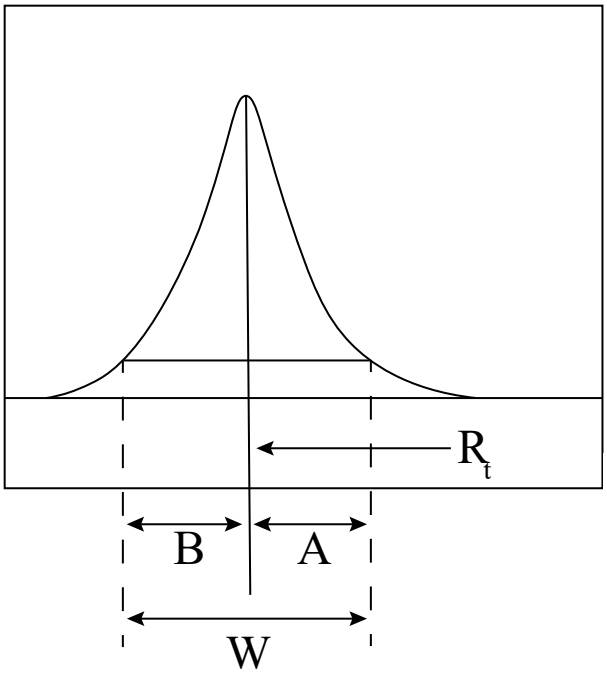
Where:

N = 2 Sigma

R_t = Retention time

W = Peak width at 60.7% of peak height

Figure 3–11: Asym equation



$$N = \frac{41.7\left(\frac{Rt}{W}\right)^2}{\left(\frac{A}{B} + 1.25\right)}$$

Where:

N = Asym

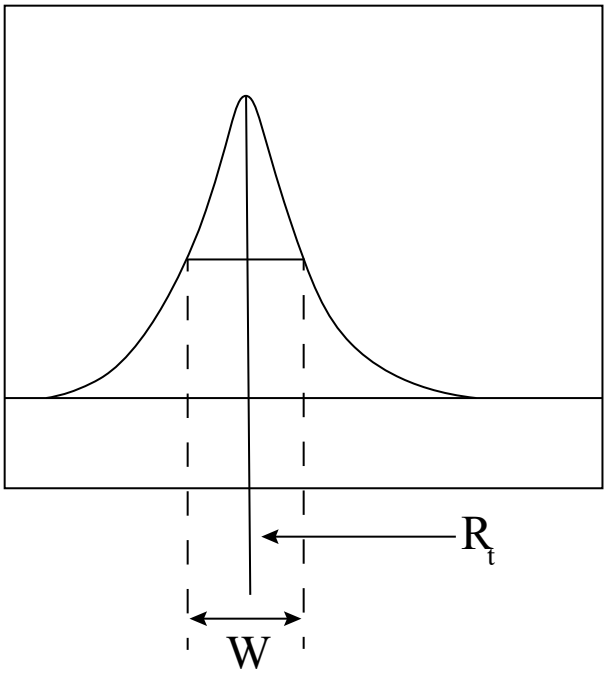
R_t = Retention time

W = Peak width at 10% of peak height

A = Time from retention time (R_t) to width end point at 10% of peak height

B = Time from width start point at 10% of peak height to retention time (R_t)

Figure 3–12: JP14 Plate Count equation



$$N = 5.55\left(\frac{R_t}{W}\right)^2$$

Where:

N = Plate count (the number of the theoretical plates in a chromatographic column)

R_t = Retention time

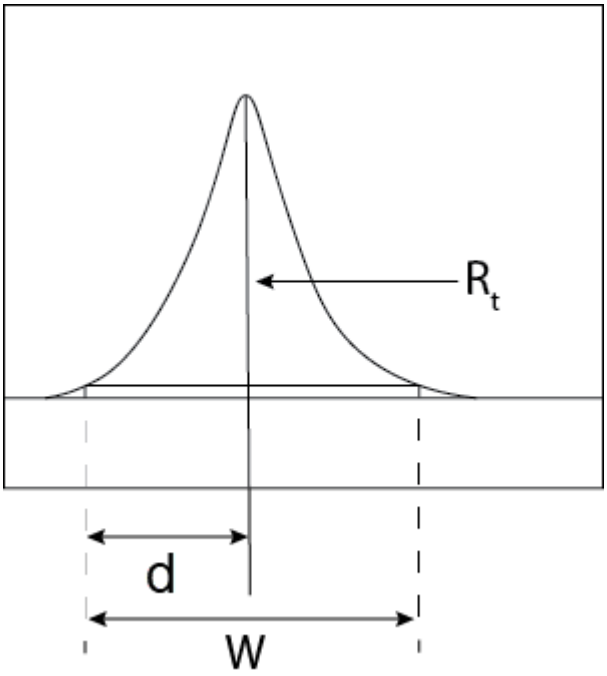
W = Peak width at 50% of peak height

3.7 Symmetry factor or tailing equations

This section contains figures that describe the equations used to calculate the asymmetry of a peak. Starting with version 3.8.0, Empower software calculates the value in the Symmetry Factor field for all pharmacopoeia choices. These figures illustrate the following tailing equations:

- Symmetry Factor (Figure 3–13: Symmetry Factor, USP Tailing, and ChP Tailing Factor equation (Page 36))
- USP Tailing (Figure 3–13: Symmetry Factor, USP Tailing, and ChP Tailing Factor equation (Page 36))
- ChP Tailing Factor (Figure 3–13: Symmetry Factor, USP Tailing, and ChP Tailing Factor equation (Page 36))
- Asymmetry $(10\%)^2$ (Asym @ (10)^2) (Figure 3–14: Asym @ (10)^2 equation (Page 37))
- Asymmetry (10%) (Asym @ 10) (Figure 3–15: Asym @ 10 equation (Page 38))
- Asymmetry $(4.4\%)^2$ (Asym @ (4.4)^2) (Figure 3–16: Asym @ (4.4)^2 equation (Page 39))
- Asymmetry (4.4%) (Asym @ 4.4) (Figure 3–17: Asym @ 4.4 equation (Page 39))

Figure 3–13: Symmetry Factor, USP Tailing, and ChP Tailing Factor equation



$$T = \frac{W}{2d}$$

Where:

T = Symmetry or tailing factor

W = Peak width at 5% of peak height

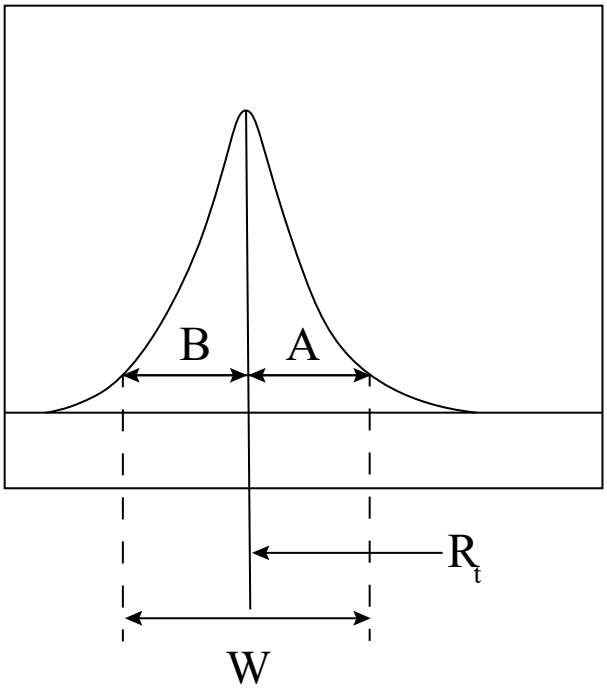
R_t = Retention time

d = Time from width start point at 5% of peak height to R_t

The symmetry factor is the same measurement as the USP tailing and ChP tailing factors. The symmetry or tailing factor, *T*, establishes the maximum permissible asymmetry of the peak. For pharmaceutical purposes, *T* is defined as the distance between the leading edge and tailing edge of the peak at a width of five percent of the peak height divided by twice the distance, *d*, between the peak maximum and the leading edge of the peak at five percent of peak height. For a symmetrical peak, *T* is 1.0, and the value of *T* increases as tailing becomes more pronounced.

Note: The value of *d* is reported in the f @ 5% field.

Figure 3–14: Asym @ (10)^2 equation



$$As_{10}{}^{2} = \left(\frac{A}{B}\right)^{2}$$

Where:

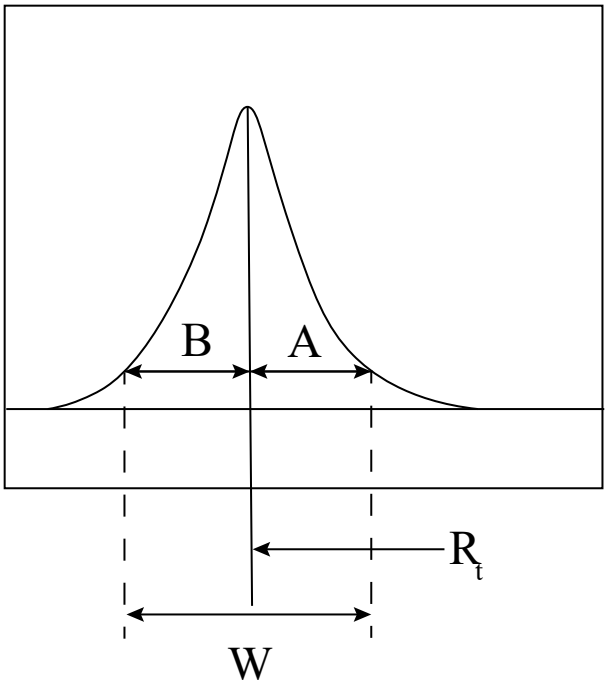
As_{10^2} = Asym @ (10)^2

R_t = Retention time

A = Time from R_t to width end point at 10% of peak height

B = Time from width start point at 10% of peak height to R_t

Figure 3–15: Asym @ 10 equation



$$As_{10} = \frac{A}{B}$$

Where:

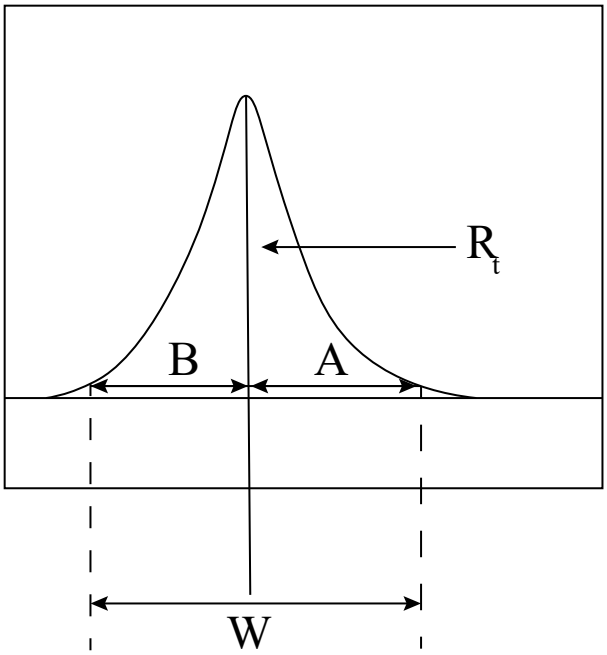
As_{10} = Asym @ 10

R_t = Retention time

A = Time from R_t to width end point at 10% of peak height

B = Time from width start point at 10% of peak height to R_t

Figure 3–16: Asym @ (4.4)^2 equation



$$As_{4.4}{}^{2} = \left(\frac{A}{B}\right)^{2}$$

Where:

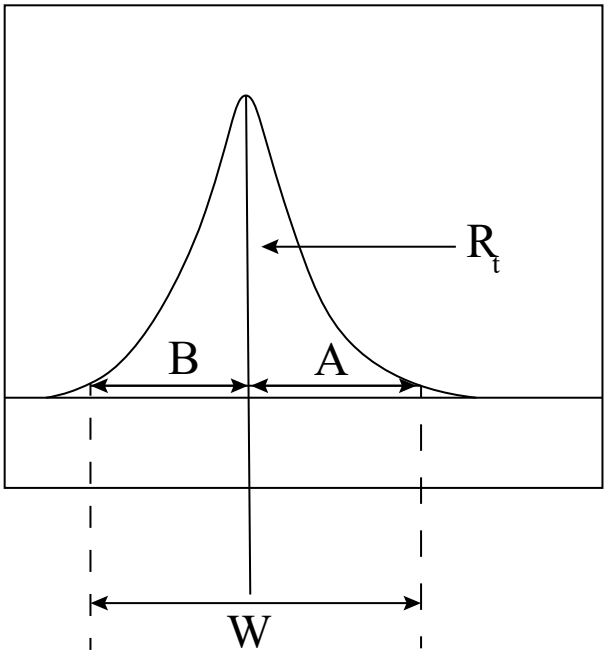
$As_{4.4^2}$ = Asym @ (4.4)^2

R_t = Retention time

A = Time from R_t to width end point at 4.4% of peak height

B = Time from width start point at 4.4% of peak height to R_t

Figure 3–17: Asym @ 4.4 equation



$$As_{4.4} = \frac{A}{B}$$

Where:

$As_{4.4}$ = Asym @ 4.4

R_t = Retention time

A = Time from R_t to width end point at 4.4% of peak height

B = Time from width start point at 4.4% of peak height to R_t

3.8 Resolution equations

Resolution between peaks is measured to ensure that the system has the resolving power to separate closely eluting components of a mixture. Starting with version 3.8.0, Empower software calculates the value in the Resolution field for all pharmacopoeia choices.

System Suitability software measures resolution between an integrated peak and the preceding integrated peak. Relative resolution is measured between named peaks and their referenced peaks when a relative resolution reference peak is specified in the processing method. Starting with version 3.8.0, Empower software calculates the new Relative Resolution field for all pharmacopoeia choices using the Resolution equation.

The theoretical calculation of Resolution is 2.0 times the difference between the retention times of two adjacent peaks divided by the sum of the width of the peaks. Theoretically, the peak width used in the Resolution formula should be the width of the peak at baseline. However, this peak width cannot be calculated for overlapping peaks. This peak width can be approximated by either the tangent width or the peak width at 50% of peak height multiplied by a constant value of 1.7. For most pharmacopoeias and when using the peak width at 50% peak height, the 2.0 in the numerator divided by the 1.7 in the denominator is simplified to a single multiplier, 1.18.

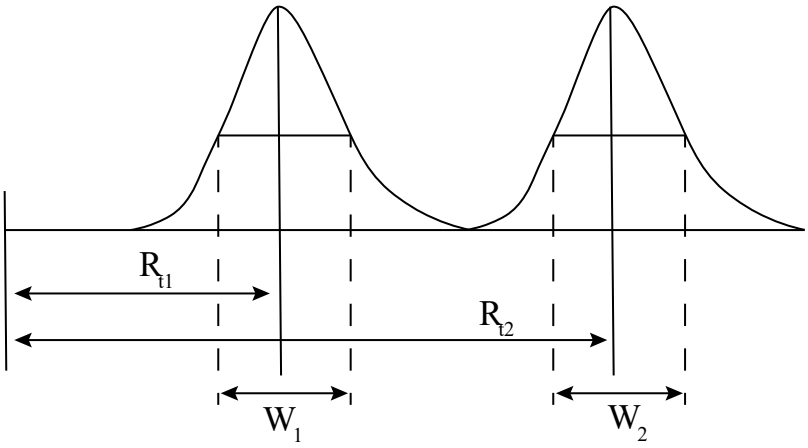
The different resolution equations implemented in Empower System Suitability software use the approximate peak widths and constants specified by The United States Pharmacopeia (USP), The European Pharmacopoeia (EP), The Japanese Pharmacopoeia (JP), and The Chinese Pharmacopoeia (ChP) as follows:

- The Resolution and USP Resolution (HH) (half height) equations use peak widths at 50% of peak height, but replace the 2.0 constant value in the numerator and the 1.7 constant value in the denominator by a single constant multiplier of 1.18 (Figure 3–18: Resolution, Relative Resolution, and USP Resolution (HH) (Page 41)).
- The USP Resolution and ChP Resolution equations use the baseline peak width calculated using lines tangent to the peak multiplied by a constant of 2.0 (Figure 3–19: USP Resolution and ChP Resolution equation (Page 42)).
- The ChP Resolution (HH) (half height) equation uses the peak widths at half-height multiplied by a constant value of 2.0/1.7 (Figure 3–20: ChP Resolution (HH) equation (Page 43)).

Resolution is calculated for both named and unnamed peaks, where the appropriate peak width can be calculated. Resolution is not calculated for skimmed peaks.

Note: Resolution is calculated between a peak and its preceding peak; hence, it is never calculated for the first peak in a chromatogram because there is no preceding peak to use in the calculation.

Figure 3–18: Resolution, Relative Resolution, and USP Resolution (HH)



$$R = \frac{1.18(R_{t2} - R_{t1})}{(W_2 + W_1)}$$

Where:

R = Resolution (EP and JP) and USP Resolution (HH)

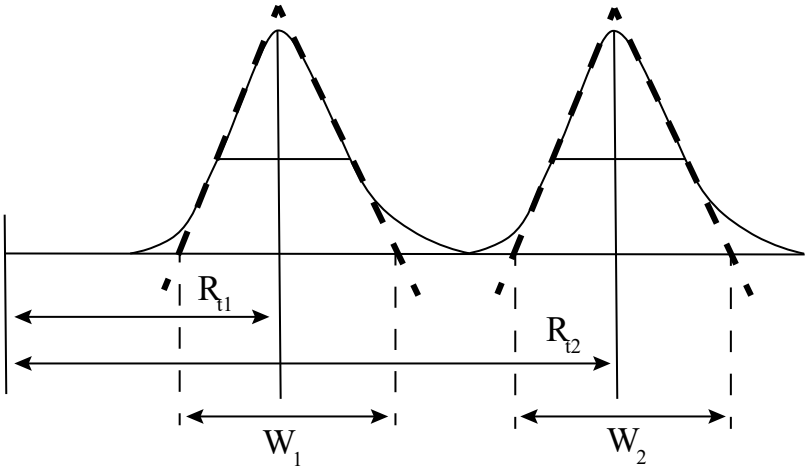
R_{t1} = Retention time of the first peak

R_{t2} = Retention time of the second peak

W_1 = Width of the first peak at 50% peak height

W_2 = Width of the second peak at 50% peak height

Figure 3–19: USP Resolution and ChP Resolution equation



$$R = \frac{2.0(R_{t2} - R_{t1})}{(W_2 + W_1)}$$

Where:

R = USP Resolution and ChP Resolution

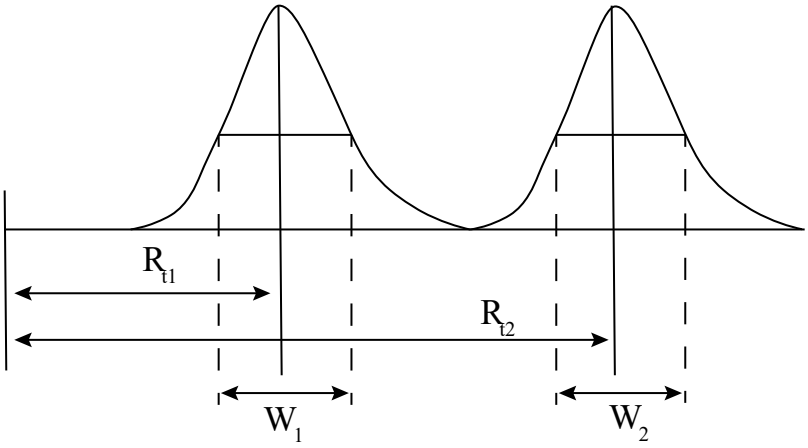
R_{t1} = Retention time of the first peak

R_{t2} = Retention time of the second peak

W_1 = Width of the first peak at the baseline between lines tangent to the inflection points (for Apex Track integration) or to a % of Peak Height (50% if the pharmacopoeia choice is **USP** or the user-specified *%* if the pharmacopoeia choice is **All**)

W_2 = Width of the second peak at the baseline between lines tangent to the inflection points (for Apex Track integration) or to a % of Peak Height (50% if the pharmacopoeia choice is **USP** or the user-specified *%* if the pharmacopoeia choice is **All**)

Figure 3–20: ChP Resolution (HH) equation



$$R = \frac{2.0(R_{t2} - R_{t1})}{1.7(W_2 + W_1)}$$

Where:

R = ChP Resolution (HH)

R_{t1} = Retention time of the first peak

R_{t2} = Retention time of the second peak

W_1 = Width of the first peak at 50% peak height

W_2 = Width of the second peak at 50% peak height

3.9 K Prime (capacity factor, *k'*) equation

K Prime (capacity factor, *k'*) is a measurement of the retention time of a sample molecule relative to the column dead volume. Figure 3–21: K Prime equation (Page 43) describes the capacity factor (*k'*) equation.

Figure 3–21: K Prime equation

$$k' = \frac{R_t - V_O}{V_o}$$

Where:

k' = K Prime

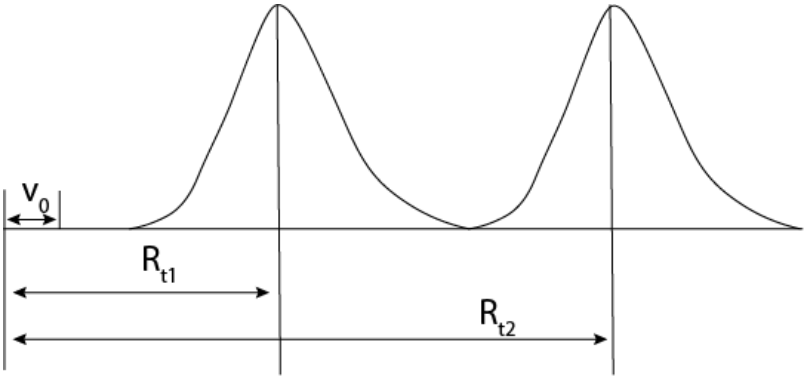
R_t = Retention time

V_0 = Void volume time

3.10 Selectivity (α) equation

Selectivity (α) measures the relative retention of two peaks in a chromatogram (the ratio of two K Prime values). Figure 3–22: Selectivity equation for peak at Rt2 (Page 44) describes the equation used to compute selectivity.

Figure 3–22: Selectivity equation for peak at Rt_2



$$\alpha = \frac{K\ Prime_2}{K\ Prime_1} = \frac{R_{t2} - V_0}{R_{t1} - V_0}$$

Where:

α = Selectivity (also called alpha)

Rt_1 = Retention time of the first peak

Rt_2 = Retention time of the second peak

V_0 = Void volume time

Note: Selectivity is never measured for the first peak in a chromatogram because a preceding peak is not available to use in the calculation.

3.11 Noise and drift

3.11.1 Detector noise and drift

On the Noise and Drift tab, you can specify a start time, stop time, and segment width over which to average. A best fit line is calculated for the points between the start and stop times inclusively, and noise is calculated from this line. To obtain valid noise and drift values, the time interval must be free of component peaks.

3.11.1.1 Detector noise

Detector noise is calculated for the given time range. Residuals are calculated for each data point based on the distance of the point from the best fit line. These residuals are then squared and averaged. The resulting noise is the square root of the average.

3.11.1.2 Average detector noise

Detector noise is calculated over user-specified segments. Average detector noise is the average of the resulting noise for all of the segments.

3.11.1.3 Peak-to-peak noise

The peak-to-peak noise is the difference between the maximum residual and minimum residual from the best fit line. This calculation reduces the impact of drift on the noise calculation.

Note: The EP, JP, ChP, and USP s/n calculations use Peak to Peak Noise.

3.11.1.4 Average peak-to-peak noise

A best fit line is calculated for each user-specified segment. The difference between the maximum residual and minimum residual is calculated for each segment. The displayed noise value is the average difference of all segments.

3.11.1.5 Detector drift

Detector drift is calculated when the detector noise values are calculated. A best fit line to the noise region is created over user-specified start and end times. The slope of this best fit line is the Detector Drift. This line is used to calculate detector noise and drift.

3.11.2 Baseline noise and drift measurements

Empower software calculates baseline noise and baseline drift from a segment of the baseline between the Baseline Start time and the Baseline End time. To obtain a valid noise calculation, the baseline interval must be free of component peaks.

3.11.2.1 Baseline noise

The software calculates baseline noise based on the maximum voltage change over a 30-second or 30-point interval. The reported baseline noise value is an average of a number of intervals as determined by the % Run Time Over Which to Average parameter.

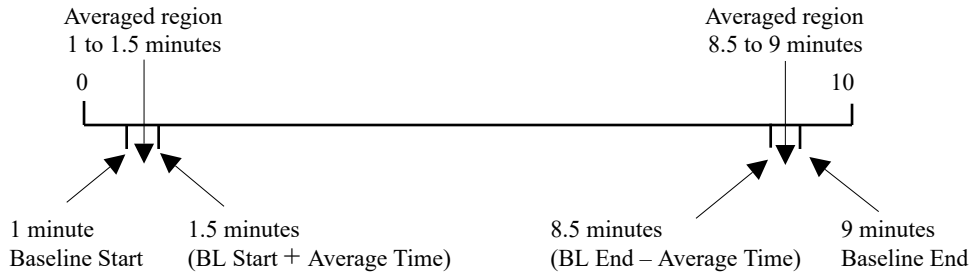
To determine the intervals, the software begins counting seconds or points from the Baseline Start time and the Baseline End time toward the middle of the chromatogram. Any points left over after the last full interval are not included in the calculation.

Table 3–2: Conditions used to average regions (Page 46) identifies the specific conditions used to average the regions shown in the example in Figure 3–23: Percent of run time to average (Page 46).

Table 3–2: Conditions used to average regions

Condition	Setting
Total Run Time	10 minutes
% of Run Time to Average	5%
Average Time	0.5 minute (5% of 10 minutes)
Baseline Start	1 minute
Baseline End	9 minutes
Baseline Noise Minimum	30 seconds

Figure 3–23: Percent of run time to average



A maximum change in millivolts (low to high) is calculated for each interval by subtracting the highest voltage in the interval from the lowest voltage, and then the millivolt change values for all intervals are averaged and reported as the noise value.

If the averaged region contains fewer than 30 seconds when the Baseline Noise Minimum is equal to 30 seconds or fewer than 30 points when the Baseline Noise Minimum is equal to 30 points, noise is reported as a blank.

3.11.2.2 Baseline drift

Baseline drift is the comparison of the millivolt (mV) readings at Baseline Start and Baseline End. To calculate drift, the software subtracts the millivolt value at the Baseline Start time from the millivolt value at the Baseline End time.

3.12 Signal-to-noise ratio (s/n)

Empower calculates a peak's signal-to-noise ratio (s/n) using one of two methods. One method is based on the equation defined by the pharmacopoeias (Figure 3–24: Pharmacopoeia signal-to-noise equation (Page 47)).

Figure 3–24: Pharmacopoeia signal-to-noise equation

$$s/n = \frac{2H}{h}$$

Where:

s/n = Signal-to-noise ratio

H = Height of the peak measured from the maximum of the peak to the extrapolated baseline of the signal observed over a distance equal to 20 times the width at half height

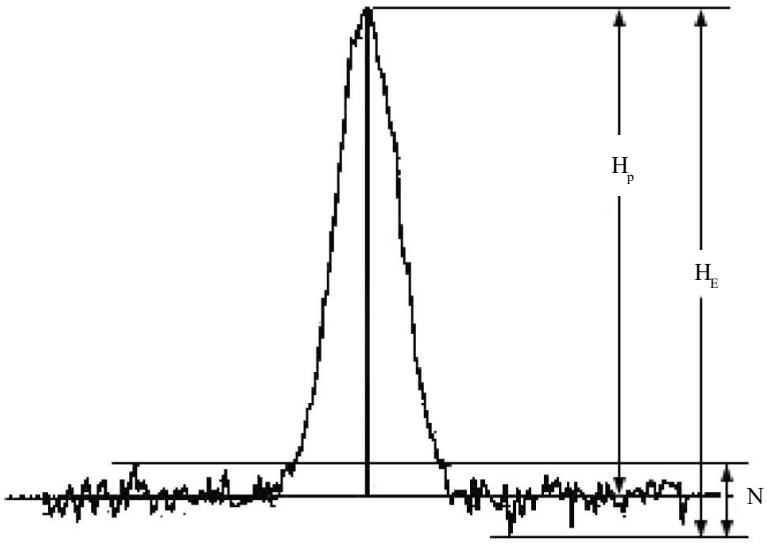
h = Range of the noise in a chromatogram obtained by the injection of a blank observed over a region equal to 20 times the width at half-height of the peak in the chromatogram obtained with the prescribed reference solution and, if possible, situated equally around the peak of interest

3.12.1 Signal-to-noise values for pharmaceutical applications

Empower uses a different measurement for peak height than the pharmacopoeias (Figure 3–25: Height comparison between Empower and Pharmacopoeia (Page 47)). The four pharmaceutical signal-to-noise values are USP S/N, EP S/N, JP S/N, and ChP S/N. Peak height as defined by the pharmacopoeias is the difference in height from the peak apex to the middle of the noise. Peak Height as measured by Empower using ApexTrack or traditional peak integration is defined as the peak apex to the lowest signal in the baseline, and it is reported in microvolts (µV).

Because the difference between the pharmacopoeia and Empower peak height calculations is equal to one-half of peak-to-peak noise, the System Suitability option calculates signal-to-noise using the derived formula described in Figure 3–26: Pharmacopoeia signal-to-noise equation for Empower peak height (Page 48).

Figure 3–25: Height comparison between Empower and Pharmacopoeia



Where:

H_P = Peak height from the apex to the middle of the noise as described by the diagrams presented in the pharmacopoeias

H_E = Empower height field, which is measured from the peak apex to the lowest signal point in the baseline

N = Peak to Peak Noise calculated for the noise interval

Note: If using a blank, the noise interval is set by the multiplier times the peak's width at half height and is centered on the retention time of the peak.
If not using a blank, the noise interval is set by the start and end times on the Noise and Drift tab.

Figure 3–26: Pharmacopoeia signal-to-noise equation for Empower peak height

$$s/n = \frac{2\left[H - \left(0.5 \times \frac{N}{S}\right)\right]}{\frac{N}{S}}$$

Where:

s/n = Signal-to-noise ratio

H = The Empower height field that is measured from the peak apex to the lowest signal point in the baseline

N = If using a blank, the Peak-to-Peak Noise value calculated for the region in the blank and stored in the Empower peak fields USP Noise, EP Noise, JP Noise, or ChP, or the Empower result field Peak-to-Peak Noise if calculated using a section of the same chromatogram

S = The scaling factor that converts plot units to height (µV) units (for example, a UV detector uses AU as plot units, and the Scale to µV is 1×10^{-6} Plot Units/µV)

When calculating the noise values for the pharmacopoeia signal-to-noise values, you can choose to use a blank chromatogram and calculate a separate Peak to Peak Noise value for each peak in the chromatogram centered around the retention time of the peak.

To calculate signal-to-noise using the pharmacopoeias, select **Calculate USP, EP, JP, and ChP s/n** on the Suitability tab of processing method. When not using a blank, you must use the Noise and Drift tab to specify the start time, stop time, and segment width to calculate the noise.

If you are using a blank injection, you must also select **Use noise centered on peak region in blank injection** on the Suitability tab. When you select this option, the software calculates a noise value for each peak using peak-to-peak noise determined from the same region in the blank injection. This region is centered around the peak's retention time and has a width that is equal to the peak's width at half-height multiplied by the half-height multiplier for the USP, EP, JP, or ChP noise region value. You can edit the half-height multipliers, and the default multipliers are provided in Table 3–3: Pharmacopoeia half-height multipliers (Page 48).

Table 3–3: Pharmacopoeia half-height multipliers

Selected pharmacopoeia	Half-height multiplier default value
USP	5

Table 3–3: Pharmacopoeia half-height multipliers (continued)

Selected pharmacopoeia	Half-height multiplier default value
EP	5
JP	20
ChP	5

Empower can use one or more blank injections to calculate the noise. For each blank injection in the sample set, select the **Blank** check box in Run Samples, Sample Set Method Editor, or the Alter Sample table. The noise value when there are multiple blank injections in a sample set is the average of the noise values calculated for all the earlier blank injections.

Note: Both the injection and the blank injection must have the same sample matrix.

3.12.2 Signal-to-noise ratio for non-pharmaceutical applications

Empower software additionally supports the calculation of the signal-to-noise ratio based on the calculated peak height and a user-specified noise value. This signal-to-noise ratio is calculated using the following formula:

Figure 3–27: s/n Equation

$$s/n = \frac{H}{N/S}$$

Where:

s/n = Signal-to-noise ratio (the non-pharmaceutical signal-to-noise value)

H = The absolute value of the height of the peak

N = The result's noise (in the value as specified by the user)

S = The scaling factor, which is either 1000 if the Noise Value for s/n is Baseline Noise or the Scale to µV value if the Noise Value for s/n is set to one of the other noise values

To calculate signal-to-noise using this equation, select the desired Noise Value for s/n from the drop-down list on the Suitability tab of the processing method. For more information on the noise calculations available in Empower, see Baseline noise (Page 45).

3.13 Statistical moments for peaks

Empower System Suitability software calculates the statistical moments for all peaks.

The statistical moments describe the peak behavior in relation to Gaussian peak shape, and you can use them to identify poor system performance.

The statistical peak moment fields are visible in the Peak tables of Review and QuickStart, and you can add them to table report groups and peak view filters in both the Project window and QuickStart.

A checkbox labeled Calculate Peak Statistical Moments is located at the bottom of the SysSuit tab in the Process Method window. When selected, the statistical moments are calculated as a part of the system suitability processing. Users can specify limits for the peak moments on the Limits tab of the processing method.

Table 3–4: Peak moment fields (Page 50) describes the peak moments that Empower System Suitability software can calculate. Peak moments are calculated for all peaks using a summation of all time and height values of each data point within the peak. For all equations, *t* is the time of the data point within the peak, *h* is the peak height for that data point, and *dt* is the time difference between the data point and the next data point within the peak.

Table 3–4: Peak moment fields

Name	Description	Formula
Zeroth moment	Area under the peak	$M_0 = \sum h \times dt$
First moment	Average retention time, equal to the retention time of a Gaussian peak	$M_1 = \frac{1}{M_0}\sum t \times h \times dt$
Second moment	Variance, measures the lateral spreading	$M_2 = \frac{1}{M_0}\sum (t - M_1)^2 \times h \times dt$
Third moment	Vertical peak symmetry and departure from Gaussian shape	$M_3 = \frac{1}{M_0}\sum (t - M_1)^3 \times h \times dt$
Fourth moment	Peak excess or vertical flattening	$M_4 = \frac{1}{M_0}\sum (t - M_1)^4 \times h \times dt$

3.14 Statistical quantity equations

These figures describe equations used to calculate the following statistical quantities:

- Mean (X_{mean}) (Figure 3–28: Mean (xmean) equation (Page 51))
- Standard deviation (*SD or Std. Dev.*) (Figure 3–29: Standard deviation (S) equation (Page 51))
- Relative standard deviation (% RSD) (Figure 3–30: Relative standard deviation (% RSD) equation (Page 51))

Figure 3–28: Mean (x_{mean}) equation

$$X_{mean} = \frac{\sum_{i=1}^{n} (X_i)}{n}$$

Where:

x_{mean} = Arithmetic mean of all observations

x_i = One observation

n = Number of observations

Figure 3–29: Standard deviation (S) equation

$$S = \sqrt{\frac{\sum_{i=1}^{n} (X_i - X_{mean})^2}{n-1}}$$

Where:

S = Standard deviation

x_{mean} = Arithmetic mean of all observations

x_i = One observation

n = Number of observations

Figure 3–30: Relative standard deviation (% RSD) equation

$$\%RSD = \frac{100}{X_{mean}} \sqrt{\frac{\sum_{i=1}^{n} (X - X_{mean})^2}{n-1}}$$

or

$$\%RSD = 100 \times \frac{S}{X_{mean}}$$

Where:

% RSD = Relative standard deviation in %

x_{mean} = Arithmetic mean of all observations

x_i = One observation

n = Number of observations

S = Standard deviation