Agilent

Agilent GPC/SEC Software for OpenLab CDS

User Manual

Notices

Document Information

Document No: D0134790 Rev. A.00
Edition: 03/2026

Copyright

Software Revision

This guide is valid for revision 2.0 and above of the GPC/SEC Software for OpenLab CDS.

Warranty

The material contained in this document is provided "as is," and is subject to being changed, without notice, in future editions. Further, to the maximum extent permitted by applicable law, Agilent disclaims all warranties, either express or implied, with regard to this manual and any information contained herein, including but not limited to the implied warranties of merchantability and fitness for a particular purpose. Agilent shall not be liable for errors or for incidental or consequential damages in connection with the furnishing, use, or performance of this document or of any information contained herein. Should Agilent and the user have a separate written agreement with warranty terms covering the material in this document that conflict with these terms, the warranty terms in the separate agreement shall control.

Technology Licenses

The hardware and/or software described in this document are furnished under a license and may be used or copied only in accordance with the terms of such license.

Restricted Rights Legend

U.S. Government Restricted Rights. Software and technical data rights granted to the federal government include only those rights customarily provided to end user customers. Agilent provides this customary commercial license in Software and technical data pursuant to FAR 12.211 (Technical Data) and 12.212 (Computer Software) and, for the Department of Defense, DFARS 252.227-7015 (Technical Data - Commercial Items) and DFARS 227.7202-3 (Rights in Commercial Computer Software or Computer Software Documentation).

Safety Notices

CAUTION

A **CAUTION** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in damage to the product or loss of important data. Do not proceed beyond a **CAUTION** notice until the indicated conditions are fully understood and met.

WARNING

A WARNING notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a WARNING notice until the indicated conditions are fully understood and met.

Contents

In This Guide...

This manual covers the following products:

- GPC/SEC Software for OpenLAB CDS (G7860AA)
- Advanced GPC/SEC Software for OpenLab CDS (G7861AA)

Terms and Abbreviations

Table 1: Terms and Abbreviations used in this document

Term	Description
AIC	Agilent Instrument Controller – part of a distributed Client/Server system
CDS	Chromatography Data System
Da	Dalton, equal to g/mol
FRM	Flow rate marker
GPC	Gel Permeation Chromatography
LS	Light scattering
M_n	Number average molecular weight
M_v	Viscosity average molecular weight
M_w	Weight average molecular weight
M_z	z-average molecular weight
MW	Molecular weight
R_g	Radius of gyration
R_h	Hydrodynamic radius
RT	Retention time
SEC	Size Exclusion Chromatography

1 Introduction

This chapter gives an introduction to the software and describes the features of the conventional and advanced GPC/SEC software add-on.

About the GPC/SEC Software for OpenLab CDS

This Agilent Technologies GPC/SEC software is an easy-to-install add-on for OpenLab CDS, allowing you to perform GPC/SEC application-specific calibrations and calculations on data acquired with OpenLab CDS.

Agilent provides the GPC/SEC add-on with two different license options, allowing basic or advanced workflows (see Product Details of G7860AA on page 9 and Product Details of G7861AA on page 10). The advanced license type also includes the basic software operations and functionalities.

The GPC/SEC add-on using the basic or advanced license option is compatible with the OpenLab workstation and network-based solutions. Being fully integrated into the OpenLab CDS platform, HPLC- and GPC/SEC-specific evaluations can be performed on the same set of data files. This GPC/SEC software uses existing workflows, method processing options, data storage, reporting, and compliance options supplied by the OpenLab CDS platform.

This online help is intended to familiarize you with the available features, evaluation options and the final reporting of GPC/SEC-specific results based on the purchased GPC/SEC add-on versions.

About the GPC/SEC Software for OpenLAB CDS (G7860AA)

The standard GPC/SEC software for OpenLab CDS includes a data analysis module for conventional GPC/SEC calibration and calculation options. Thus, e.g. the GPC/SEC-specific column calibration can be created based on a set of narrow standards or using a well-characterized broad sample (Broad Hamielec or Integral approach). The G7860AA add-on allows to process any signal from a concentration detector collected or imported into an OpenLab CDS project to unveil the molecular weight distribution and molecular weight average values of biomolecules and synthetic macromolecules.

Product Details of G7860AA

- Only concentration detector signals (UV, RID or ELSD) can be processed for GPC/SEC specific calibrations and calculations.

NOTE

The Agilent Infinity MDS RI detector (G7801A) is a recently supported concentration detector for the data acquisition part of the OpenLab CDS. Acquired MDS RI signals can be used for data evaluation with the GPC/SEC Software.

- Only conventional calibration approach supported (three column calibration methods available: Narrow standard calibrants, Broad Hamielec, or Broad Integral method).
- Available GPC/SEC results and plots: GPC/SEC-typical distribution and calibration plot, molecular weight averages values, and calculation of molecular weights at specific percentage area fractions.
- Important: no support and control of Agilent 1260 Infinity Multi-Detector Suite (MDS) LS detectors (G7803A, G7808A, and G7809A) or Agilent 1260 Infinity II Multi-Angle Light Scattering (MALS) Detector (G7885A).

About the Advanced GPC/SEC Software for OpenLab CDS (G7861AA)

The Advanced GPC/SEC Software for OpenLab CDS is a data analysis module which combines basic GPC/SEC software options and functionalities of the G7860AA product with the new advanced light scattering (LS) calibration and calculation options. Besides concentration detector signals, the advanced add-on allows to process Agilent LS detector signals when acquired with the OpenLab CDS.

The G7861AA GPC/SEC add-on comes with new Agilent 1260 Infinity Multi-Detector Suite and Agilent 1260 MALS Detector drivers added to the data acquisition part of the OpenLab CDS platform enabling data collection of these advanced LS detectors (only G7803A, G7808A, G7809A and G7885A).

With the newly added advanced GPC/SEC processing method and LS-specific calculation options, the determination of accurate molecular weights without the need for column calibration is possible. Combining an Agilent LS detector with a concentration detector, the collected data can unveil the accurate bulk molecular weight of a compound and allows furthermore the detection of aggregates.

Complementing the Agilent MDS LS detector, the supported dynamic light scattering (DLS) option in the advanced add-on provides insight into hydrodynamic size information of synthetic and bio-macromolecules.

Product Details of G7861AA

- Full control of the Agilent Infinity MDS RI detector (G7801A) and Agilent LS detectors (MDS Dual Angle LS and 1260 Infinity II MALS Detector) by new driver package for the OpenLab CDS platform.
- Conventional calibration and calculation options included.
- New LS-specific calibration and calculation options allow to determine absolute molecular weights (M_w).
- Collected LS detector signals can be used for detection of aggregates.
- Included DLS options allow the determination of accurate R_h values.
- Available GPC/SEC results and plots: advanced LS plot (partial Zimm plot), bulk molecular weight (M_w), bulk radius of gyration (R_g) and bulk hydrodynamic radius (R_h) values.

Instrument Control and Data Collection

The GPC/SEC add-on, identified as G7860AA (basic license and functionalities) and G7861AA (advanced license with full functionalities), serve primarily as data analysis modules within the OpenLab CDS platform.
The standard add-on does not modify the platform's data acquisition capabilities, while the advanced add-on introduces recent light scattering (LS) detector drivers. These drivers enable instrument control and LS data collection for the first time within OpenLab CDS. This advancement supports specific LS detectors such as the Agilent 1260 Infinity Multi-Detector Suite (MDS) and the Multi-Angle Light Scattering (MALS) Detector.

GPC/SEC operates as an isocratic liquid chromatography (LC) technique, applicable in both organic and aqueous environments, utilizing specialized GPC/SEC columns for separation. Therefore, any LC system compatible with OpenLab CDS and capable of isocratic operation can be employed.

Typical concentration detectors used in GPC/SEC include:

- Refractive Index Detector (RID), including the Agilent Infinity MDS RI (G7801A)
- UV Detectors: Multiple Wavelength (MWD), Variable Wavelength (VWD), and Diode Array Detector (DAD)
- Evaporative Light Scattering Detector (ELSD)
- Third-party detectors connected by analog-to-digital devices

Supported advanced LS detectors:

The advanced GPC/SEC add-on (G7861AA) supports specific LS detectors:

- Agilent 1260 Infinity Multi-Detector Suite (MDS) detectors (G7803A, G7808A or G7809A)
- Agilent 1260 Infinity II Multi-Angle Light Scattering (MALS) Detector (G7885A)

Detector choice depends on the specific application requirements. Both add-ons can process chromatograms collected through the OpenLab CDS data acquisition component or imported into OpenLab CDS projects, depending on detector signal types.

Basic Theory of GPC/SEC and Advanced LS Detection Methods

Introduction to GPC/SEC

The interest in gel permeation chromatography (GPC), which is also known as size exclusion chromatography (SEC), has dramatically increased since its introduction by Moore [1] and others as a powerful characterization tool for natural and synthetic macromolecules. Quality assurance and control, even during the production and processing stage increase in significance, to retain international competitive ability. Also, in academic and industrial polymer research, the exact knowledge of molecular weights and their distribution are of great importance. However, support for users by evaluation of the GPC/SEC data has not found the necessary interest in the past. The improvement of the GPC/SEC Software has not kept in step with the improvement and re-development of PC and HPLC components. Therefore, it still happens to this day that GPC/SEC elugrams have to be evaluated manually. Through the increasing automation of polymer analytics, GPC/SEC software today should be flexible and powerful at the same time and simplify the workload of the user, thereby making effective use of the powerful and expensive hardware.

GPC/SEC is characterized by a series of specific marginal conditions, which partly differentiate considerably from the conditions of liquid chromatography (LC):

- different calibration procedure for transformation of elution volume into molar masses
- different separation mechanism: diffusion-controlled exclusion chromatography instead of adsorption equilibration
- basically, different requirements to the system parameters which determine the reproducibility, measurement and evaluation accuracy
- varied time bases: measurement time, peak width etc.
- varied analysis goals: molecular weight specification instead of qualitative or quantitative analysis

1 J.C. Moore, J. Polym. Sci., A2, 835 (1964)

- multi-detection operation in the GPC/SEC suggests parallel evaluation of all used detectors
- evaluation procedure should automatically process volume correction between the different detectors, so that only one calibration relation will be needed for all connected detectors

Basics of GPC/SEC Analysis

In contrast to gas chromatography (GC) and high pressure liquid chromatography (HPLC), the separation mechanism of gel permeation chromatography (GPC) is not based on a distribution equilibration but on volume exclusion chromatography [2]. The separation in GPC/SEC results from the hydrodynamic volume (V_h) of the sample molecule [3] which can be directly determined from the quasi-elastic light scattering by measurement of the diffusion coefficients. The separation in the GPC/SEC is based on the molecular size and not on the molecular weight of the sample molecule.

Macro porous polymer gels (particles) are mostly used as column material in GPC/SEC. The diffusion of a molecule between the mobile phase and pore is the basis for separation mechanism and performance. Since for smaller molecules more pores are accessible, these will be retained longer and consequently elute later than the higher molecular fractions. Unfortunately, the GPC/SEC does not present an absolute method; i.e. the retention times (in GPC/SEC terminology called elution volume, V_e) have no direct relation to the molecular weight of the investigated substance and depend on the measurement conditions (type of columns, mobile phase (eluent), type of polymer, etc.). Therefore, an accurate calibration is required using the same analytical conditions. Under optimum conditions it is possible to determine molecular weights quickly, economically, and reliably, with an accuracy that does not differ from other absolute methods (osmosis, light scattering). In contrast to this, the conventional GPC/SEC approach (column calibration) does not have high demands on the sample preparation. Besides the molecular weight information, GPC/SEC also unveils the molecular weight distribution, which influences many physical and physico-chemical properties of macromolecular samples and therefore it is of great interest.

2 P. Flodin, Dissertation, Uppsala, 1962

K.H. Altgelt, J.C. Moore, in: Cantow (Ed.), Polymer Fractionation, New York, 1966

3 Z. Grubisic, R. Rempp, H. Benoit, J. Polym. Sci., B5, 753 (1967)

M.J.R. Cantow, R.S Proter, J.F. Johnson, J. Polym. Sci. A-1, 5, 987 (1967)

Calibration Methods

Only with proper calibration the measured elution volume (V_e) of sample can be transformed into molar masses. The calibration can be carried out in various ways:

- Narrow Standard Calibration Method on page 14
- Universal Calibration Method on page 14
- Broad Standard Calibration Method on page 16
- Broad Integral Calibration Method on page 17

Narrow Standard Calibration Method

The use of polymer standards with narrow molecular weight distribution is the simplest and most accurate way to assign molecular weight to elution volume. For this it is best to use M_p values (molecular weight at peak maximum) for the calibration set-up, because those values are the only molecular weight that can clearly be identified in the elugram. If the weight-average molecular weights (M_w) are used, then the calibration function should be iterated until the used M_w values will be received again by re-calculation.

Independent of the used procedure, the user always has to select a fit function which should fit optimally the measured calibration points (plotting molecular weight versus elution volume). Since the calibration function in GPC/SEC is typically not linear or only slightly curved, it may be difficult to fit this dependence by a simple function (linear). The typical strong S-shaped curvature of GPC/SEC calibration curves often require the selection of higher order fit functions, like 3rd or 5th order polynomial fits. Based on the calibration points and selected fit function, the software transforms the recorded elution volume (V_e) information into molecular weight information.

Universal Calibration Method

Since for some polymers no polymer standards are available, very early possibilities were studied to convert existing calibrations to other types of polymers. This method developed by Benoit et al. [4] assumes that the property which determines the elution behavior in GPC is the hydrodynamic volume (V_h) of the polymer under investigation. Since V_h should be proportional to the product of intrinsic viscosity, [η], and molecular weight, M, it follows that for two polymers eluting at the same elution volume:

4 H. Benoit, Z. Grubisic, P. Rempp, D. Decker, J.-G. Zilliox; J. Chim. Phys, 63, 1507 (1966)

$$[\eta]_1 M_1 = [\eta]_2 M_2$$

valid at the same elution volume using the Mark-Houwink relation:

$$[\eta] = K \times M^{\alpha}$$

the molecular weight of the polymer type (1) can be converted into the molecular weight of polymer type (2):

$$\lg M_2 = \frac{1}{1+a_2} \lg \frac{K_1}{K_2} + \frac{1+a_1}{1+a_2} \lg M_1$$

It is apparent that the Mark-Houwink constants must be known for both polymers in the respective eluent under separation conditions. Unfortunately, this is not the case for frequently used GPC eluents (e.g., THF, DMF). For the determination of the intrinsic viscosities solution viscometry measurements are necessary. However, the determination of intrinsic viscosities for some polymers is difficult in some solvents (e.g., PMMA in THF).

In such cases a trick may help. Instead of doing viscometry measurements of polymer standards with known weight-average molecular weight (M_w), GPC characterizations are performed. Using the known Mark-Houwink constants, [η] $M(V_p)$ is calculated from the molecular weight calibration curve of the polymer. Thus, it is possible to determine intrinsic viscosities of polymers by GPC/SEC. Plotting log [η] vs. log M of the polymers investigated by GPC the Mark-Houwink coefficients can be calculated from slope and intercept.

NOTE

The Mark-Houwink relation is valid only above a certain molecular weight, which depends on polymer type (approx. 10,000 to 20,000 Da). Below this limit, the Mark-Houwink coefficients are dependent on the degree of polymerization. In this case the log [η] vs log M plot deviates from the straight line to higher viscosities. The reason for this behavior is based on a structural change of the macromolecule which usually changes from a wormlike to a Gaussian coil behavior with increasing molecular weight.

The universal calibration presents a very useful calibration method; its validity should be checked for the used polymer type (literature, combination of direct calibration with universal calibrated samples). Special attention should also be paid in the molecular weight section below approx. 20,000 Da.

Broad Standard Calibration Method

The broad calibration procedure is based on papers of Mahabadi and O'Driscoll [5], Weiss and Cohn-Ginsberg [6], and Mori [7], which use the dependence of the GPC/SEC separation on the hydrodynamic volume, to calibrate reliable and flexible with broad standards. The procedure described here has no limitations (e.g., only linear calibration function, calibrations only with (inaccurate) M_n and M_w) and even permits deduction of the Mark-Houwink coefficients of the polymers under investigation. Since this calibration method is based on the universal calibration approach, its requirements have to be considered as well.

Requirements for creating such a broad calibration are:

- Existence of a base calibration curve (Index: 1, see equation below), which will be used for the characterization of the pore size distribution of the column set used.

NOTE

The so-called broad *Hamielec* calibration uses a linear calibration curve as a base of processing the broad calibration. The 1st order polynomial is automatically applied and cannot be changed.

- One or more broad polymer standards or well-characterized samples (Index: 2) with known average molecular weight values (M_n and/or M_w) and/or intrinsic viscosity values [η], which must be available (valid for all broad calibration procedures!).

According to the theory of universal calibration for each elution volume it is assumed that all samples have the same hydrodynamic volume independent of the type of polymer. The molecular weight on the other hand is different; however, a transformation can be carried out, which depends on the stiffness of the main chains of the considered polymer. For each elution volume the following equation holds true:

5 H. K. Mahabadi, K.F. O'Driscoll; J. Appl. Polym. Sci., 21, 1283 (1977)

6 A. R. Weiss, E. Cohn-Ginsberg; J. Polym. Sci. Part B, 7, 379 (1969)

7 S. Mori; Anal. Chem., 53, 1813 (1981)

$$M_2 = A \times M_1 B$$

where A and B are constants, which must be optimized through the mean values of the broad samples.

In order to do so, A and B are iterated and the molecular weight averages are calculated from the chromatograms and the calibration curve. These molecular weight averages are compared with the reference values. This process will be optimized with an algorithm until the calculated and reference molecular weights agree sufficiently exact.

Broad Integral Calibration Method

The broad integral calibration is a special method that uses existing chromatograms and the integral (cumulative match) molecular weight distribution of one or more broad standards or well-characterized samples to generate a calibration curve. However, in contrast to the calibration methods mentioned before a base calibration is not needed.

This method requires the use of a broad standard(s) or sample(s):

- with a large dispersity value
- with a known table detailing the % cumulative Weight Fractions and either Log Molecular Weight or Molecular Weight values

NOTE Using multiple broad standards offers the possibility to extend the area of calibration reliability.

Once the broad integral calibration option is selected in the software (see specific GPC/SEC processing methods) the integral table must be entered and the user must select the default curve fit, which will be applied to the calibration data points.

NOTE Only 1st to 5th order polynomial fit functions are available for the GPC/SEC add-on for OpenLab CDS.

Introduction to Light Scattering

Light Scattering refers to the process in which light from an incident polarized laser beam is scattered in all directions when it interacts with a molecule or particle. Light scattering is an everyday occurrence and was first described by Lord Rayleigh in the late 1800's. An example of light scattering is the scattering of sunlight by particles in the atmosphere: the sky is blue because shorter visible wavelength radiation (blue light) is scattered more strongly by the gas molecules in air than light of longer wavelengths (red light). There are two general techniques for the measurement of physical properties of polymers (synthetic polymers and natural polymers such as proteins and polysaccharides), and particles.

Static Light Scattering

Also known as Rayleigh scattering or classical light scattering - the intensity of the scattered light from the sample dissolved in the solvent. This difference between the two measurements can be used to determine the average molecular weight and R_g (radius of gyration). To complete the molecular weight determination, the concentration of the compound of interest is required (typically obtained from a refractive index detector or an absorbance detector). Static Light Scattering is described in section Static Light Scattering on page 20.

Dynamic Light Scattering

Also known as Quasi- elastic scattering, Photocorrelation Spectroscopy, or Beat Spectroscopy - the fluctuations of the intensity of the scattered light is used to determine the diffusion coefficient of the molecules as they move in solution (Brownian motion). The Stokes- Einstein equation is used to determine R_h (the hydrodynamic radius of the molecule). Dynamic Light Scattering is described in section Measuring Rh using Dynamic Light Scattering on page 25.

Static and Dynamic measurements can be made on a sample in a cuvette or in a flowing stream such as that found in gel permeation chromatography (GPC). In flowing streams, measurements are made on each elution slice using a unique light scattering design and very fast digital signal processors.

Physical Basis of Light Scattering

Light consists of perpendicular electric and magnetic fields that oscillate in a direction that is perpendicular to the direction of propagation of the light as shown in Light Scattered by a Molecule. When light strikes a molecule, the electrons will experience a force due to the electric field and will move slightly. This movement will induce an oscillating dipole moment that will radiate light in all directions at the oscillating frequency. This radiated light is the scattered light that is detected and processed as described below.

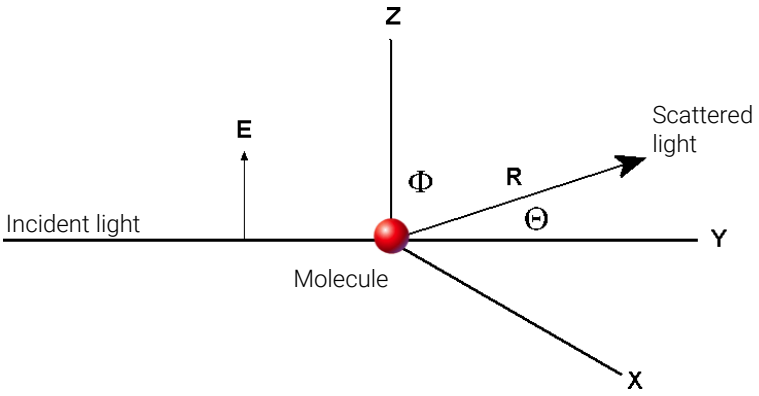


Figure 1: Light Scattered by a Molecule

Light Scattered by a Molecule describes the spatial arrangement of the incident light and scattered light in the light scattering experiment. The light is polarized in the vertical direction, thus the electric field will oscillate in the Z direction and the magnetic field will oscillate in the X direction.

A diode laser, which is a monochromatic source of light that can be focused to a very small point in the centre of the sample cell, is used in the light scattering system. Typical sources include a semiconductor laser that can provide 20 to 30 mW at 685 nm and another, which provides 100 to 150 mW at 800 nm. The scattered light is collected at a given angle and orientation (e.g. 15° or 90°) from the incident radiation, and is used to deduce the desired molecular properties.

Static Light Scattering

Measuring the Molecular Weight

NOTE

Agilent Technologies systems include polarized laser light sources, the equations presented in this chapter will be slightly different than those presented in discussions of light scattering when non-polarized sources are used.

The electric dipole moment that is induced is shown in equation 1:

$$\vec{p} = \alpha \vec{E} \quad (1)$$

where:

p	is the dipole moment
α	is the polarizability
E	is the electric field

The polarizability can be related to measurable parameters via equation 2:

$$A = M_w \left(\frac{dn/dc}{2 \cdot \pi \cdot N_A} \right) \quad (2)$$

where:

M_W	is the molecular weight
N_A	is Avogadro's number (6.02×10^{23} molecules per mol)
dn/dc	is the change in the index of refraction as a function of the change in concentration. It is considered to be a constant for any specified solvent-solute pair under constant operating conditions.

The oscillating dipole will radiate light in all directions at the oscillating frequency. This is the origin of scattered light. If a single molecule has dimensions that are small with respect to the wavelength of the incident light, the intensity of the light can be defined by equation 3:

$$I_S = \frac{\left[4 \cdot \pi^2 \cdot M_W \cdot \sin^2 \Phi \cdot (dn/dc)^2 \cdot I_0\right]}{N_A^2 \cdot \lambda_0^4 \cdot R^2} \quad (3)$$

where:

I_S	is the intensity of the radiated light
I_o	is the intensity of the incident light
λ_o	is the wavelength of light in a vacuum
Φ	as defined in Light Scattered by a Molecule
R	Radius of molecule in solution

If we collect light from a volume V of a solution with a concentration c (gm/mL), the intensity of scattered light can be found by multiplying equation 3 by the number of molecules in the volume V.

The number of molecules can be expressed by

$$N_A \cdot c \cdot \frac{V}{M_W}$$

Now if we solve for M_W, we obtain equation 4:

$$M_W = \frac{\left[N_A^2 \cdot \lambda_0^4 \cdot R^2 \cdot I_S\right]}{4 \cdot \pi^2 \cdot M_W \cdot \sin^2 \Phi \cdot c \cdot (dn/dc)^2 \cdot I_0 \cdot V} \quad (4)$$

Collecting all the constants and instrumental parameters into an overall instrumental constant, A, we obtain equation 5:

$$M_W = \frac{[I_S]}{A \cdot c \cdot (dn/dc)^2 \cdot I_0} \quad (5)$$

Equation 5 can be used to measure the molecular weight M_w of small molecules at any scattering angle Θ. It should be noted, however, that larger molecules scatter less light at high values of Θ than at low angles because of interference effects caused by the fact that light scattered from one part of the molecule travels a different distance from another part of the molecule, and is not in phase

with light scattered. This phenomenon can be quantified by defining the light scattering form factor (equation 6). A more detailed discussion of the form factor is presented in section The Form Factor on page 24.

$$P(\Theta) = \frac{\textit{scattering intensity at angle } \Theta}{\textit{scattering intensity at angle } \Phi} \quad (6)$$

It should be noted that P(Θ) can be written as a series as shown in equation 7:

$$P(\Theta) = 1 - \frac{1}{3}(q^2 \cdot R_g^2) + \ldots \quad (7)$$

q	$4\pi * n * \sin(\Theta/2)/\lambda_o$
R_g	is the radius of gyration of the molecule
n	is the index of refraction of the liquid
λ_o	is the wavelength of light in a vacuum

For scattering at 15° and 90°, equation 7 can be expressed as equations 8 and 9, respectively.

$$P(\Theta) = 1 - 26.3\left(\frac{R_g \cdot n}{\lambda_0}\right)^2 \quad (8)$$

$$P(\Theta) = 1 - 0.0897\left(\frac{R_g \cdot n}{\lambda_0}\right)^2 \quad (9)$$

Table 2 Values of P as a function of molecular weight on page 23 shows values of P for 15° and 90° degrees as a function of molecular weight. These values assume that the molecules are random coils.

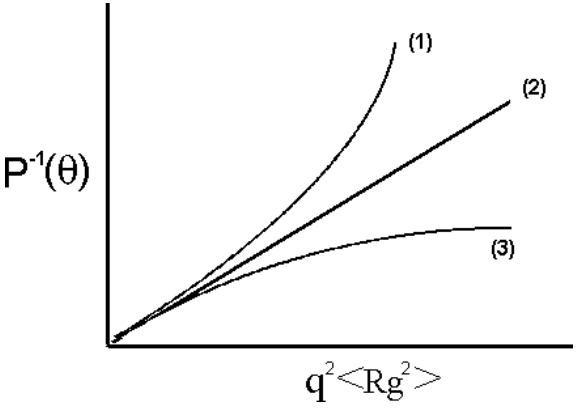
Table 2: Values of P as a function of molecular weight

M_W	R_g (approx.) nm	P(90°)[1]	P(15°)[1]
5×10^3	2.3	0.9993	1.0000
5×10^4	7	0.9993	0.9928
5×10^5	23	0.9993	0.9976
5×10^6	70	[2]	0.9880
5×10^7	230	[2]	0.7622

[1] Value of P(90°) and P(15°) for λ_o = 685 nm, n = 1.5

[2] Values depend on shape

If the value of P(Θ) found in equation 7 is below 0.7, higher order components become important. In this case, P(Θ) depends on R_g and also on the shape of the molecule as shown in Values of p-1 as a function of q².



Values of $P^{-1}(\Theta)$ as a function of $q^2<R_g^2>$ for various particle shapes

1	Sphere
2	Gaussian Coils
3	Rods

It is clear that all three molecular shapes yield the same value of P(Θ) when $q^2<R_g^2>$ is less than approximately 1. As the value of P(Θ) increases, the shape of the molecule clearly influences the light scattering intensity.

The Form Factor

The form factor at a particular angle is the ratio of the signal at that angle when compared to the signal expected at the theoretical angle of 0° (where there is no form factor) as indicated by equation 6. The importance of the form factor is that small molecules (e.g. those which have a radius that is < 10 nm, which is small when compared to the wavelength of the incident light) are studied, generate comparable signals at all angles, while large molecules generate signals that are smaller at higher angles and larger at small angles.

Characteristics of Low-Angle (15°) Light Scattering

Low-angle light scattering data is collected at a 15° angle to the incident beam and is typically used for determination of the molecular weights of large molecules. This measurement angle is especially useful for the study of proteins with molecular weight of greater than $1 \cdot 10^6$ Da and for random coils with molecular weight between $2 \cdot 10^6$ Da and about $1 \cdot 10^7$ Da. In addition, 15° data is also used with 90° data to measure R_g, the radius of gyration of molecules over a limited range of sizes (12 – 150 nm) using static light scattering analysis.

Right-Angle Light Scattering

Right-angle light scattering data is collected at a 90° angle to the incident beam and is typically used with static light scattering analysis to measure the molecular weight of smaller molecules such as proteins with a molecular weight below $1 \cdot 10^6$ Da, random coils with molecular weight below $2 \cdot 10^5$ Da and for lower molecular weight non- spherical coil polymers. In addition, it is used with dynamic light scattering analysis to measure R_h, the hydrodynamic radius of molecules and particles from 1 to 1000 nm.

$$[\eta] = \lim_{c \to 0} (\eta_{sp}/c)$$

Measuring Rh using Dynamic Light Scattering

Basics of Dynamic Light Scattering

The fundamental measurement for dynamic light scattering is the fluctuation of the intensity of the scattered light. This data is analyzed as described to yield the diffusion of the molecules or particles moving under Brownian movement.

When polarized laser light is scattered, the scattered light is at the same wavelength as the incident beam. However, it should be noted that when the light is monitored over extremely short time increments (in the microsecond time regime), a Doppler shift occurs and the frequency of the light appears to be changing. As the particle moves toward the detector, the frequency increases, and as it moves away the frequency decreases. The amount of the increase (decrease) of the change in the frequency is related to the diffusion rate of the scattering molecule in the solvent.

While the diffusion coefficient could be obtained from the frequency spectrum, it is easier to measure the small intensity fluctuations and then compute the autocorrelation function. The autocorrelation function is related to the frequency spectrum by the Fourier transform (i.e. the data processing is performed in the time domain rather than the frequency domain.

From an experimental perspective, the intensity of the scattered light is detected by counting the photons scattered via an avalanche photodiode, an electronic device that emits a pulse every time a photon passes through its detector. This high sensitivity detector sees a time varying signal rather than a relatively constant (in batch mode) or slowly varying “total intensity“ signal.

It should be noted that even when measurements are taken in flow mode, the sample can be considered as slowly varying. This is due to the time frame of the scattered light measurement, relative to the rate of elution of the light scattering molecules from the column.

The photon counting measurement is performed over a very short period of time to record the very rapid diffusion that is taking place. Small particles or biomolecules diffuse quickly with the scattered light showing rapid small fluctuations while larger particles such as protein aggregates, nanoparticles, polymers, etc., diffuse more slowly, resulting in lower frequency fluctuations.

The Autocorrelator

The autocorrelation function of these short interval counts is computed by an autocorrelator, which is a special purpose proprietary parallel computer that has been specially designed by Agilent Technologies. The correlator uses 256 channels that can be distributed over a maximum "channel space" of 1024 channels. Each channel can be considered as a separate "bucket" in which the emitted photons are counted during the sample period (which is in the order of a few *i* s). The 1024 channel spaces occupy a total "time- space" of 1024 equal sampling times that can be set by the operator according to the size and shape of the molecule of interest. Counts are collected in up to 256 of these channel spaces, which are arranged logarithmically throughout the total channel space by the software, the higher density being at the start.

The autocorrelator function over the 1024 channel space is computed by correlating the counts in each of the channels. Observation of the correlation function provides information that is useful to optimize the analysis. In addition, the display indicates the fraction of the sample with the indicated particle size.

Using Diffusion Coefficient to Determine Rh

R_h, the hydrodynamic radius of the compound of interest can be determined using the Stokes- Einstein equation (equation 10):

$$Rh = \frac{k \cdot T}{6 \cdot \pi \cdot v \cdot D} \quad (10)$$

where:

k	is Boltzman's constant
T	is the temperature of the eluent
v	is the viscosity of the sample
D	is the Diffusion coefficient calculated from the autocorrelation function

2 Licensing

This chapter gives an introduction about the licensing types for the GPC/SEC software. It also describes how to obtain and install a license.

About the Licensing of the GPC/SEC Software for OpenLab CDS

The GPC/SEC data analysis license comes bundled with the GPC/SEC data analysis software; no separate data acquisition license is needed. License management is handled through the OpenLab CDS Control Panel, starting with a standard 60-day trial license. To continue using GPC/SEC add-ons beyond this period, you must create a customer-specific license file (.lic) in SubscribeNet, download it, and install it.

Agilent offers two license types for the GPC/SEC Software for OpenLab CDS:

- Basic (G7860AA): Conventional column calibration workflow and basic operations and functionalities.
- Advanced (G7861AA): Includes all basic features plus advanced LS workflows for light-scattering calibrations, bulk molecular weight and hydrodynamic size calculations.

A single license provides one seat for GPC/SEC analysis on a Workstation or Client configured for GPC/SEC. Without a valid license:

- You cannot perform GPC/SEC data processing.
- The OpenLab CDS software only allows you to review GPC/SEC results.

If a valid license is only available for the basic GPC/SEC software add-on (G7860AA), you cannot access advanced LS data processing.

The licenses for the GPC/SEC software add-ons (G7860AA and G7861AA) ensure controlled access to advanced data processing features within the OpenLab CDS environment.

Supported Configurations

The following instances are supported for installation:

- **Workstation Installation**

  All concurrent OpenLab CDS Data Analysis instances on the PC can use the GPC/SEC software.

- **Client/Server Installation**

  The server provides a pool of GPC/SEC data analysis licenses on a “first come, first served” basis.
- **Agilent Instrument Controller (AIC) Installation**

  For unattended automatic GPC/SEC processing, install the GPC/SEC software and license on the AIC.

License file

A license file contains your software license. It is a collection of product, instrument, and add-on licenses (or activation keys). Information in the license file defines the number of instruments and other options that may be used concurrently with your system.

The license file is installed to your OpenLab CDS Workstation. The license file is bound to this computer, and cannot be moved to another workstation without regenerating the license in SubscribeNet.

License types

The licenses or activation keys in the license file can either be shared or counted:

Shared licenses System computers and other components can have shared, or add-on, licenses — because they share a core license.

Counted licenses These licenses are part of the GPC/SEC Software for OpenLab CDS floating licensing strategy. They are not permanently assigned to any one component. Instead they are automatically assigned to components, such as AICs and instruments, while the components are starting up. The licenses are automatically returned when the component is closed. The license management program controls license issuance and retrieval.

In this case, the only requirement is that a component is licensed while running. You only need enough licenses for all components running concurrently, rather than for each installed component.

Get a license

NOTE

During this process you will have to enter the MAC address of your license server. For workstations, this is the local computer. For client/server systems, this is the server.

Generate, download, and install a license with SubscribeNet

In case you do not have internet access, skip to the section Other ways to obtain a license on page 33.

If you are a new user who has not registered with SubscribeNet, continue with the section *New Users*.

If you have registered with SubscribeNet, skip to the section *Users registered with SubscribeNet*.

Preparations You will need:

- The authorization code label provided in the lavender envelope containing your Software Entitlement Certificate. If you have not received a lavender envelope for your product, contact your vendor or internal support.
- The URL for SubscribeNet from the Software Entitlement Certificate.
- The MAC address, and host name of the computer where the Control Panel is running.

  To retrieve your MAC address from a computer where GPC/SEC Software for OpenLab CDS is already installed, open the Control Panel and browse to the Administration > Licenses section. Use the Copy MAC Address or Save MAC Address function to obtain the MAC address for license generation.

NOTE If any changes are made to the computer name or domain reference after the license is installed, remove the license, and create a new license in SubscribeNet, download and install it .

NOTE If the network adapter that provides the MAC address used during license creation is removed from the machine, your license will no longer be valid. A new license will need to be generated with a currently available MAC on the license server.

New Users

1 Go to https://agilent.subscribenet.com/control/agil/AgilRegisterToAccount to register the product with SubscribeNet.

2 On the registration page, enter the authorization code from the label and complete the profile information (required fields are marked with *).

The email address you enter will become your login ID.

3 Click Submit. The system will generate and display an account name for you.

SubscribeNet will send a welcome email with your login ID and password.

4 Log in to SubscribeNet using your login ID and password.

Once you log in, you can use the online user manual link for help with any questions you have.

5 Select Generate or View licenses from the left navigation bar.

6 Follow the prompts to generate your new license. You will be prompted for the HOST NAME of the computer.

Enter the server hostname. Do not include any DNS suffix (*domain.com*) references in the entered machine name.

7 When the system generates the license, view its details, then click Download License File. Save the license file to your computer and to a backup location (such as a portable storage device).

Use your login ID and password when you revisit the Agilent SubscribeNet site to regenerate a license file, add new authorization codes, or further configure the license for your system.

Users registered with SubscribeNet

1 If you already have a SubscribeNet account, use https://agilent.subscribenet.com/.

Lost your SubscribeNet password? Use https://agilent.subscribenet.com/control/agil/password to have it emailed to you.

2 Select the SubscribeNet account associated with this authorization code, if you have more than one account.

3 From the SubscribeNet navigation pane, select Register Authorization Code.

This will allow you to enter your new authorization code and make available the new license entitlements.

4 Select Generate or View licenses from the left navigation bar.

5 Follow the prompts to generate your new license. You will be prompted for the HOST NAME of the computer.

Enter the server hostname. Do not include any DNS suffix (*domain.com*) references in the entered machine name.

6 When the system generates the license, view its details, then click Download License File. Save the license file to your computer and to a backup location (such as a portable storage device).

Use your login ID and password when you revisit the Agilent SubscribeNet site to regenerate a license file, add new authorization codes, or further configure the license for your system.

Check for software updates

After registering your authorization codes in SubscribeNet, check for software updates released for your products. If updates are available, open the ReadMe files and follow the instructions.

Other ways to obtain a license

If you are unable to generate a license, contact your nearest Agilent technical support office. A representative will tell you how to submit an OpenLab License Generation Form in your location.

Offline licensing

If an internet connection is not available in your laboratory:

You or your local on-site service engineer will collect the necessary information from you to allow Agilent to create a license account on your behalf. For phone support in your region, call the sales and service number for your region. See the Appendix for contact information.

Required Customer Information for Agilent License Support:

The following information must be provided to Agilent in order to enable us to create a licensing account on your behalf.

1 Collect Account Information:

Your account name will be your company name and Lab name separated by a comma. Employee information provided here will be used to define the first administrator of your account for future access to the system as required. Please prepare the following pieces of information prior to contacting your local Agilent sales and service center in order to expedite service:

- Company Name
- Lab/Department Name
- First Name
- Last Name
- E-mail address
- Job Title
- Phone #
- Address, City, State/Province, Postal Code, Country

2 Collect Authorization Code(s):

The authorization code is an alpha-numeric code provided on a label which is enclosed in a lavender envelope. If you have received more than one code you must provide all codes to ensure that all ordered licenses are granted to your account.

3 Receiving your license:

Once the above information is provided Agilent will then work on your behalf to generate a license file through SubscribeNet. The license file will either be sent to your shipping address (on a CD), or your local FSE will deliver it in person (usually on USB media). Once your license is received follow the below section on “Install your License” to finish installing your license on your system(s).

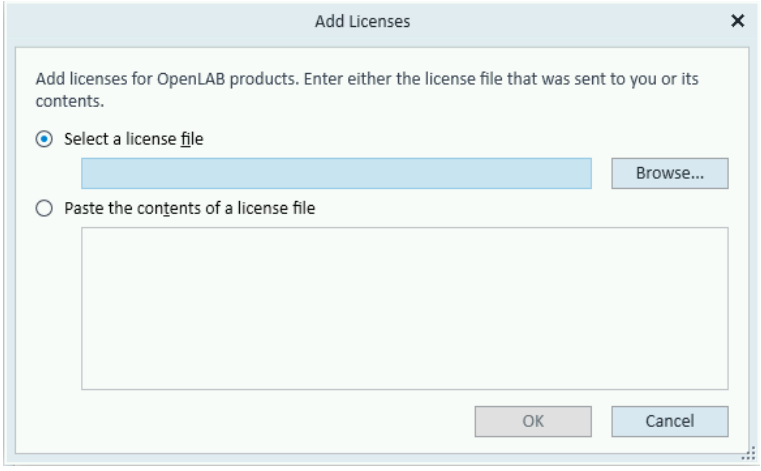
Install your license

The license must be added to your system using the Control Panel.

1 Start the **Control Panel** shortcut on the desktop or go to **Start** > (**All apps** >) **Agilent Technologies** > **Control Panel** .

2 Navigate to **Administration** > **Licenses** .

3 In the ribbon, click **Add License** + .



4 Choose to install the license by:

- Using the license file option to browse to and open the license file (.lic) saved from the license generation process in SubscribeNet.
- Selecting the License Text option and copying the license text from a text file received into the provided field.

5 Click **OK**.

The **Administration** interface in the Control Panel will now display the status of installed licenses.

NOTE A full restart is required in order for any license to have an immediate effect.

License Enforcement

The GPC/SEC data analysis license only protects GPC/SEC processing in OpenLab CDS Data Analysis. You can still process data using other methods, control instruments, acquire data, and generate reports without this license.

When the GPC/SEC Data Analysis License Is Available

If a valid license is available, you can:

- Create and modify GPC/SEC methods
- Perform and review column calibrations (basic features)
- Perform and review LS system calibrations (advanced features)
- Process and reprocess injections to generate conventional and/or advanced GPC/SEC results (basic and advanced features required)
- Review existing conventional or advanced GPC/SEC results (basic or advanced features required)

When the GPC/SEC Data Analysis License Is Not Available

Without a valid license:

- GPC/SEC data processing is disabled; the software acts only as a results reviewer.
- Sections of the GPC/SEC processing method are locked.
- You can view existing calibrations and results, but cannot process new data or save changes to the calibration.
- Attempting to process or reprocess injections will result in error messages (see examples below) and empty results windows.
- You can still process data using other methods if no GPC/SEC analyses are present in the results set.

Error Messages

Without a valid license, an error message will be displayed in the following cases:

- If you load an existing processing method or create a new processing method (Method type = 'GPC/SEC'):
  Error Agilent GPC Analysis license is not available. GPC processing is disabled!
- If you load a results set that contains GPC/SEC analyses (GPC/SEC processing method, column calibration, processed injections):
  Error Agilent GPC Analysis license is not available. GPC processing is disabled
- If you try to reprocess sample injections containing GPC/SEC analyses:
  Injection processed (with errors)

3 Getting Started

This chapter outlines the requirements in the GPC/SEC software and provides a summary of the steps required for a successful analysis.

Sample Preparation

Gel Permeation Chromatography (GPC) and Size Exclusion Chromatography (SEC) require careful sample preparation to ensure accurate and reproducible polymer analysis. This chapter outlines best practices for preparing samples, considerations for concentration, and the use of advanced detection methods.

Sample Preparation and Handling

Optimal samples for GPC/SEC are pure liquids or solids free from salts, residual solvents, and contaminants. Samples must be representative, fully soluble, and chemically stable throughout dissolution and analysis. It is critical to avoid using ultrasonic treatment or strong heating, as they can degrade polymer chains due to mechanical or thermal stress.

To minimize system peaks caused by eluent aging or contamination, use the same eluent for both the chromatographic system and sample preparation. When switching to fresh eluent, refresh the sample preparation solvent accordingly.

High molecular weight polymers require extended dissolution times for complete solubilization. For samples above 20 kg/mol, a minimum of four hours is suggested with gentle shaking to aid dissolution. For very high molecular weight samples (> 500 kg/mol), overnight dissolution before injection is advised.

To remove particulates, we recommend filtering the sample before injection. Polytetrafluoroethylene (PTFE) syringe filters with a 0.45 µm cutoff are typical, while a 1.0 µm cutoff filter is preferable for very high molecular weight samples to prevent clogging.

Concentration Recommendations

Sample concentration depends on polymer type, molecular weight distribution, and molecular weight. Higher molecular weight samples require lower concentrations to avoid high solution viscosity and pore overloading effects in the columns. These effects can distort separation by restricting molecular diffusion based on hydrodynamic size.

A general guideline is to prepare samples with molecular weights exceeding 1,000,000 at concentrations below 0.5 mg/mL. Broadly distributed samples can tolerate higher concentrations compared to narrowly distributed ones.

Advanced Detection Methods: Light Scattering and Viscometry

When using molar-mass-sensitive detectors such as light scattering (LS) or viscometers, precise knowledge of sample concentration is essential for accurate molecular weight calculations. We recommend weighing both the sample and the added eluent accurately. For volatile solvents, tightly cap the vial after adding the eluent to minimize evaporation and concentration errors. Record the mass of the added solvent, and calculate its volume using known density values (for example, THF density = 0.899 g/cm^3 at room temperature).

Using these measurements, you can then perform exact concentration calculations in the vial. For the system or column calibration using Agilent pre-weighed standards, the exact sample mass is provided in the certificate accompanying the standards.

This comprehensive approach to sample preparation and concentration control ensures reliable and reproducible GPC/SEC results, particularly when combined with advanced detection technologies.

To calculate the exact concentration in the vial use the following equations:

$$V(solvent) = \frac{m(solvent)}{\rho\,(solvent)}$$

$$c\,(sample) = \frac{m\,(sample)}{V\,(solvent)}$$

NOTE If Agilent standards (pre-weighed standards) are used to run the system calibration or a column calibration, the exact sample mass (*m (sample)*) can be found on the provided certificate.

System Preparation

This guide is designed for users of the OpenLab CDS platform, specifically for LC applications. Before working with the GPC/SEC software add-on, it's recommended to complete the interactive curriculum available in the OpenLab Help and Learning Online. This curriculum covers essential topics for operating your Agilent LC system with OpenLab CDS.

Key Curriculum Topics

- User Interface Navigation: Learn to use the Control Panel and Acquisition interfaces, including instrument launching and custom layout creation.
- LC Acquisition Methods: Understand how to modify, save, and download acquisition methods for instrument control.
- Run Submission: Discover how to submit single sample analyses and manage the run queue.
- Data Analysis: Explore processing methods, result packages, integration, compound identification, and calibration.
- Reporting: Learn to reprocess data, generate reports, and use report templates for single sample reports and template modifications.

Once you're comfortable with the basics, use the GPC/SEC specific Online Help for guidance on the basic and advanced workflows. Access this help directly via the GPC/SEC software by pressing F1 in the relevant windows.

Set up Instrument and Detectors in OpenLab CDS

Prerequisites

- Before you can start to configure the instruments, you need to prepare a corresponding OpenLab CDS project. Then you can add instruments that are assigned to the new project. For detailed information on how to create a new project and add instruments, refer to OpenLab Help and Learning Online.

After an instrument has been added to the Control Panel, it must be configured for its specific hardware components.
In order to configure an instrument, the instrument must be turned on and connected to the same network as your Agilent Instrument Controller or Workstation. The modules and instruments of the LC system are configured through Auto Configuration, whereas, the advanced MDS or MALS detectors must be manually added and then configured.

To configure an MDS or MALS detector, follow the next steps:

Configure the MALS Detector

1 In the Available modules list, select the MALS (G7885A) to move it to the Configured modules list.

2 To manually configure the LS detector, double-click the detector.

3 In the dialog, enter the device name and IP address.

4 Select the Retrieve Info button to read serial and firmware details.

5 Confirm your instrument configuration and select OK to close the dialog.

Configure the MDS Detector

1 In the Available modules list, select the appropriate MDS detector (1260 MDS DLS, 1260 MDS LS or 1260 MDS RI) to move it to the Configured modules list.

2 To manually configure the detector, double-click the detector.

3 In the dialog, enter the device name and check the Type ID.

4 Under Signal Acquisition > Collect LS angles, select the desired angle.

5 Confirm your instrument configuration and select OK to close the dialog.

Prepare Users

The GPC/SEC software provides specific privileges that are automatically created during installation.

The following GPC/SEC specific privileges are added to certain default roles provided within the OpenLab CDS platform. Assign the following roles to the relevant users.

Role	Privileges
Everything	• Edit GPC/SEC Parameter: Users are allowed to view and edit GPC/SEC parameters in the processing method. • Create and Modify GPC/SEC Calibration: Users are allowed to create/ modify column or system calibrations. • Do GPC/SEC Data Analysis: Users are allowed to perform GPC/SEC data analysis.
Chemist	• Edit GPC/SEC Parameter: Users are allowed to view and edit GPC/SEC parameters in the processing method. • Create and Modify GPC/SEC Calibration: Users are allowed to create/ modify column or system calibrations. • Do GPC/SEC Data Analysis: Users are allowed to perform GPC/SEC data analysis.
Technician	• Do GPC/SEC Data Analysis: Users are allowed to perform GPC/SEC data analysis.

In the Administration pane of the OpenLab CDS Control Panel, you can create custom roles, groups, and users with GPC/SEC specific privileges. For more information on creating custom roles, groups, and users, see OpenLab Help and Learning Online.

Configure Data Analysis Project in the OpenLab Control Panel

Projects used for advanced GPC/SEC data processing must meet specific requirements. Follow the steps below to ensure that all settings are complete.

Prerequisites

- To be able to carry out the procedure as described, you need the privilege **Project Management** > **Manage project or project group**. Privileges are configured in the Control Panel.
- An OpenLab CDS project has already been created in OpenLab Control Panel (for details, refer to OpenLab Help and Learning Online and search for "Add a project").

1 In the Control Panel, select the relevant project.

2 IIf required, change the Audit Trail Settings (for details, refer to OpenLab Help and Learning Online and search for "Audit Trail Settings"). If relevant, select **Automatically enable audit trail** for method and sequence.

3 In the **Home** ribbon tab, click **Add GPC/SEC Parameters**.

✓ The following sample custom parameters are added, which are required for advanced GPC/SEC analysis (used by the advanced GPC/SEC processing method on page 135).

Name	Type	Default Value	Mandatory	Description
GPC/SEC Cal. Std.	Text	no	yes	Flag indicating whether the injection (which should be a Cal. Std.) should be used for the column calibration of conventional GPC/SEC analysis (when using advanced GPC/SEC processing method).
GPC/SEC LS Cal. Std.	Text	no	yes	Flag indicating whether the injection (which should be a Cal. Std.) should be used for the system calibration of advanced GPC/SEC analysis.
Concentration (g/L)	Numeric		no	The sample concentration used for system calibration and advanced sample analysis. It can be used for the the full sample or only for the monomer, as both cases can be handled within the advanced GPC/SEC processing method.
dn/dc (mL/g)	Numeric		no	Refractive index increment used for system calibration and advanced sample analysis.
UV ext. coeff. ((mg/mL)$^{-1}$(cm)$^{-1}$))	Numeric		no	UV extinction coefficient (also known as ε) used for system calibration and advanced sample analysis.

Name	Type	Default Value	Mandatory	Description
Molar mass (Da)	Numeric		no	The molar mass used for system calibration.
Eluent RI	Numeric		no	Refractive index of the eluent used for system calibration and advanced sample analysis.
MH K ((10e-5) dL/g)	Numeric		no	The Mark-Houwink K parameter used for column calibration and conventional sample analysis (when using advanced GPC/SEC processing method).
MH alpha	Numeric		no	The Mark-Houwink Alpha parameter used for column calibration and conventional sample analysis (when using advanced GPC/SEC processing method).

NOTE

These sample custom parameters can also be edited manually, for example to set default values.
Do not change the spelling and capitalization of the names. They should remain unchanged, as they are used for the advanced GPC/SEC analysis.

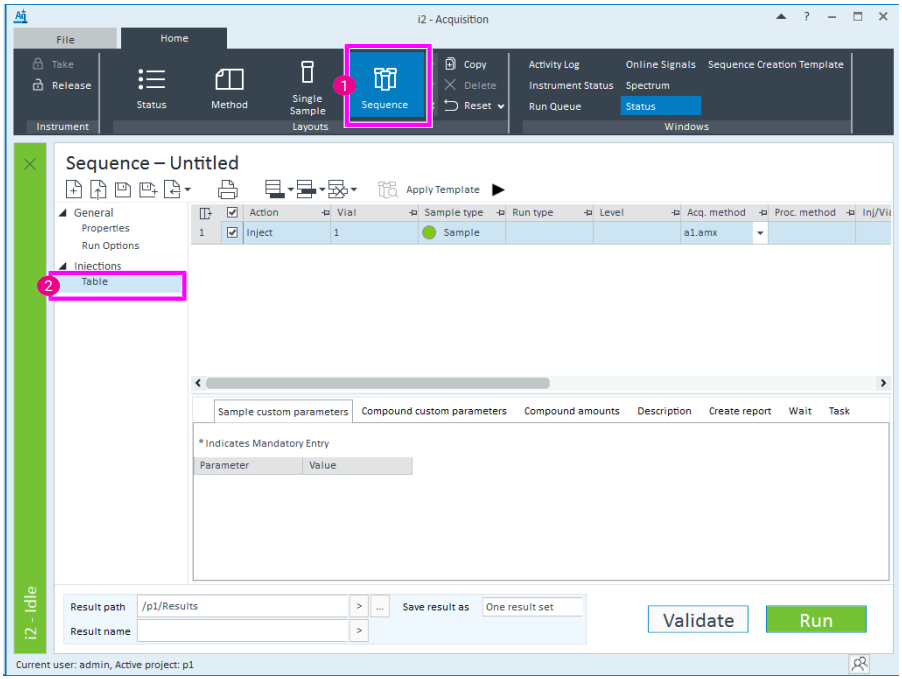
A chemist or technician will fill in the values for each calibration standard and sample when preparing the sequence in the Acquisition client. The values can also be added or edited directly in the Data Analysis client when working on the data in the Injection List (for details, refer to OpenLab Help and Learning Online and search for "Injection List"). For information on creating Sample Custom Parameters, refer to OpenLab Help and Learning Online (search for "Sample Custom Parameters").

Run a Sequence

A sequence automates the analysis of multiple samples. The samples to be analyzed are listed in the Sequence table.

For details on the techniques how to create/complete a sequence table, refer to OpenLab Help and Learning Online.

1 Click **Sequence**, and then click **Table**.

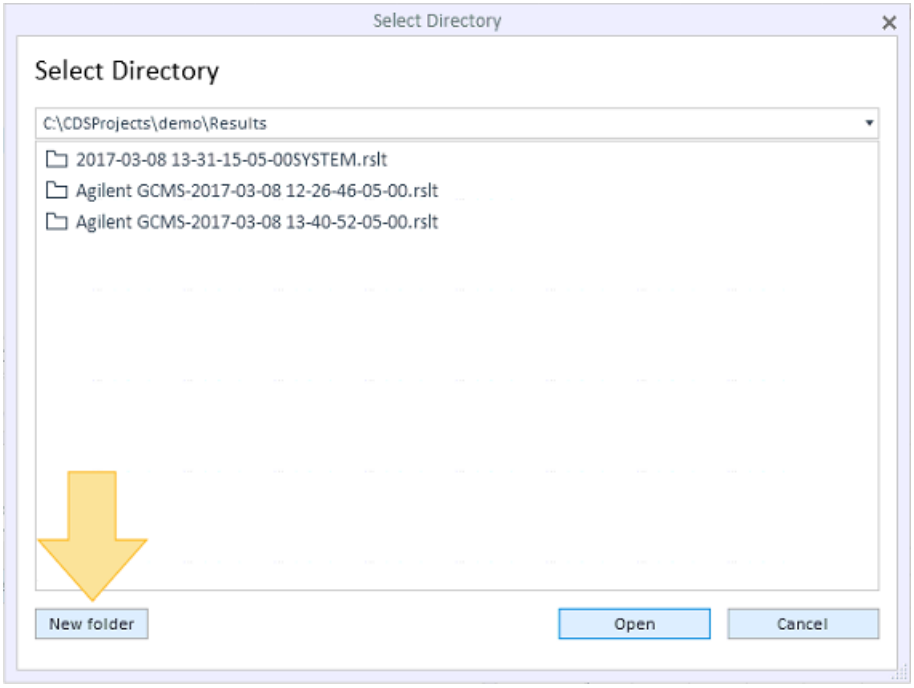


2 Complete the Sequence table using one or more of the following techniques:

- Complete the Sequence table manually.
- Scan barcodes from sample tray
- Reuse and modify a saved sequence
- Import or drag a CSV, TSV, or sequence file into the Sequence table.
- Use a sequence creation template.
- Create a Dual Simultaneous sequence

3 Select the rows to submit as part of the run. By default, all rows are selected.

4 To save your results to a sub-folder inside your **Results** folder, change the **Result path** by clicking **Browse** ... and creating a new folder. You cannot save your results to an existing .rslt folder.



5 The **Result name** defaults to the last filename used for this instrument and project. Enter a filename by typing in the field or using the token › button. If left blank, the instrument name and local date & time is used for the filename.

6 Select **Save result as**:

- One result set to save the data acquired for all sample injections in the sequence within a single result set. For example:

  ResultSetName: A1, B1, A2, B2, A3, B3, A4, B4, A5, B5
- **Separate single injections** to save each sample injection in the sequence as an individual result set. When using this option, result set names will be based on the value of the **data file** column for each sequence row. For example:

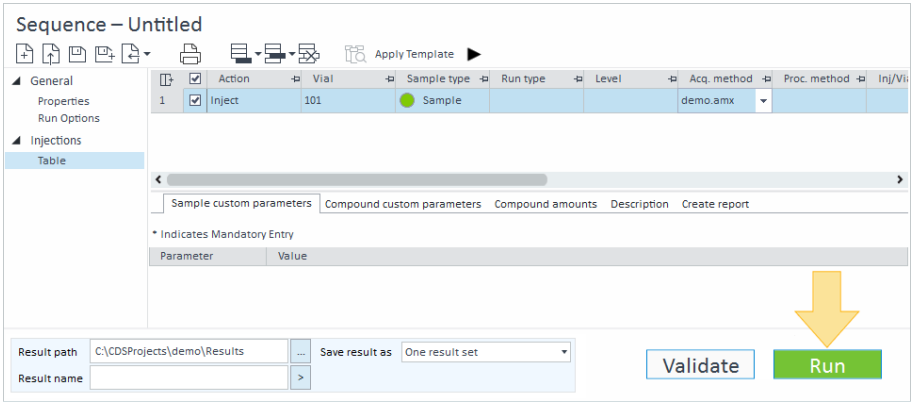
  DataFileName: A1

DataFileName: B1

DataFileName: A2

DataFileName: B2

7 Click **Run**. If this is a new "Untitled" sequence, the sequence file is saved as the instrument name + the local date and time. Submitted sequences are placed in the **Run Queue**, where you can stop or pause a run, or edit a sequence. A result folder (.rslt) is created when the run is added to the **Run Queue**.



NOTE Always include standards for calibration. For details, refer to advanced LS workflow or conventional column calibration workflow.

Create a Processing Method

Processing methods are used in the data analysis context. They contain the information and parameters needed to process the data and to generate results.

For the GPC/SEC data processing three different default processing methods are available:

- GPC/SEC (includes only conventional data processing, column calibration options)
- GC/LC Quantitative + GPC/SEC (includes only conventional data processing, column calibration options)
- GC/LC Quantitative + GPC/SEC + LS Bulk (includes conventional and advanced LS data processing)

Method Creation Workflow

1 In Data Processing view, select the Processing ribbon tab, and select New Method from the ribbon.

2 Select the appropriate method based on your GPC/SEC data.

3 In the method, define the standard parameters (available in section Integration Events, System Suitability, Reports, Tools).

4 For a standard GPC/SEC analysis:

   a Go to Processing Method > GPC/SEC > GPC/SEC Conventional > General tab.

   b Specify signal to use, flow rate correction, and Mark-Houwink values.

5 For an advanced GPC/SEC analysis:

   a Go to Processing Method > GPC/SEC > GPC/SEC General, select Advanced LS Bulk as analysis type, and define the detectors.

   b Go to GPC/SEC Advanced > General tab, and define the Peak Identification Time Window to identify peaks as a GPC compound

NOTE Only identified GPC compounds will be shown in the GPC/SEC LS Results window.

6 Save the method once all parameters are set.

For more details, refer to section Working with GPC/SEC Processing Methods on page 108.

Calibrate the System

Set up Conventional Column Calibration

All GPC/SEC processing methods, whether conventional or advanced LS workflows are used, require a calibration of the system.

1 Go to **Processing Method** > **GPC/SEC** > **GPC/SEC Conventional** > **Column Calibration** tab.

2 Select the calibration type (**Narrow Standard**, **Broad Hamielec** or **Broad Integral**).

3 Choose curve fitting and set the Mark-Houwink values if needed.

4 Save the processing method.

5 Link calibrant injections and provide necessary information for calibration tables.

6 Go to **GPC/SEC** > **GPC/SEC Conventional** > **Peak Identification** tab and set up the table.

7 Save the processing method.

For more details, refer to section Workflow for a GPC/SEC Column Calibration on page 121.

Set up Advanced LS Calibration

Align Detector Signals

Before you begin the system calibration, perform the alignment of the detector signals:

1 Go to Processing Method > General > Signals > Alignment tab.

   a Adjust the delay (retention time) of the detectors in order to align their signals in the Chromatograms window.

   b In the Alignment tab, select Calculate delay from RT.

   c Reprocess All.

NOTE

This inter-detector delay correction aligning the concentration detector signal with the LS detector signals is essential for all further LS calculation steps.

For more details, refer to Perform the Detector Signal Alignment on page 147.

Create System Calibration

To generate a system calibration, use a narrow calibrant and proceed with the following steps:

1 In the Injection List window, provide the required sample parameter.

2 Go to Processing Method > GPC/SEC > GPC/SEC Advanced > General tab, and define the expected retention time window for peak identification under Peak Expected Retention Time.

3 Ensure sample parameters are correct.

4 Reprocess the injections to create the system calibration.

5 Save the processing method.

For more details, refer to section Generate the System Calibration on page 148.

Additional Resources

- OpenLab Help and Learning Online
- *OpenLab CDS Workstation Installation and Configuration (CDS_v2.8_WorkstationGuide_en.pdf, D0028022)*
- Agilent GPC/SEC Software for OpenLab CDS Online help with chapters on workflows, processing methods, and reporting.

4 User Interface Reference

This chapter describes the user interface of the GPC/SEC software add-on. The software components used for data analysis, results review, and report generation are described in detail.

GPC/SEC Data Review

GPC/SEC Results

You can access the GPC/SEC Results window via the Home ribbon tab.

The tabs of the window are explained below.

Peak Results Tab

The Peak Results tab contains the GPC/SEC results table of the selected injections. It lists the GPC/SEC results calculated by peak. Each line of the table represents a peak, each column represents a value calculated on the peak.

You can choose the columns that are shown in the GPC/SEC peak results table. For example, the following columns are available:

Peak#	Index of the peak according to its retention time.
Sample name	Sample name of the injection as entered in the sequence.
Signal description	Name of the signal on which the peak is integrated.
RT (min)	Retention time of the peak. It corresponds to the time at the peak apex.
Data file	Name of the data file if source system is file based.
Method	Name of the method used to analyze the data (processing method).
Results set	The name of the results set. The result set contains the results of a sequence that has been run. It consists of raw data, acquisition method, data analysis method, results, and used report templates.
Mp (g/mol)	The calculated molecular weight at peak maximum of the processed sample peak in g/mol (= Da, Dalton).
Mn (g/mol)	The calculated *number average* molecular weight of the processed sample peak in g/mol (= Da, Dalton).
Mw (g/mol)	The calculated *weight average* molecular weight of the processed sample peak in g/mol (= Da, Dalton).
Mz (g/mol)	The calculated z-average molecular weight of the processed sample peak in g/mol (= Da, Dalton).

Mz+1 (g/mol)	The calculated (z+1)-average molecular weight of the processed sample peak in g/mol (= Da, Dalton).
Mv (g/mol)	The calculated *viscosity average* molecular weight of the processed sample peak in g/mol (= Da, Dalton).
PD	The polydispersity of the peak calculated as M_w/M_n.
FRM name	The flow rate marker peak name. This is an optional correction for flow variation using standard internal marker.
FRM RT (min)	Retention time of the flow rate marker peak. It corresponds to the time at the peak apex. This is an optional correction for flow variation using standard internal marker.
FRCF	The calculated flow rate correction factor. This is an optional correction for flow variation using standard internal marker.
K ((10e-5) dL/g)	The Mark-Houwink K value for the sample.
Alpha	The Mark-Houwink Alpha value for the sample.

Functions Available

- Order on the active column
- Resize the displayed columns
- Reorder the displayed columns

The following commands are available on the right-click menu:

Table 3: Context menu commands

Command	Description
Choose columns ...	Displays the **Choose Columns** dialog.
Numeric precision ...	If relevant, displays the **Numeric Precision** dialog.
Copy to Clipboard	Copies the displayed information and the calibration data points table to the clipboard as a tab separated text.
Export to file...	Saves the displayed information to a file. You can choose between the following file formats: • Comma separated value (*.CSV) • Excel worksheet (*.XLS) • Word document (*.DOC) • PDF file (*.PDF)

GPC Column Calibration Tab

The GPC Calibration Details tab shows the generated GPC/SEC column calibration details.

The following values are displayed:

Administration information	
Calibration type	The column calibration type. Either **Narrow Standard**, **Broad Hamielic**, or **Broad Integral**.
Signal	Name of the signal used to create the column calibration.
Calibration Mark-Houwink parameters	
K ((10e-5) dL/g)	The Mark-Houwink K value for the column calibration.
Alpha	The Mark-Houwink Alpha value for the column calibration.
Curve fit	
Order of curve fit	The polynomial curve fit order.
Curve fit equation	The equation of the calibration curve.
Curve fit statistics	
Residual sum of squares	The sum of the squares of residuals. This is a measure of the discrepancy between the data and the curve. A small RSS indicates a better fit of the calibration curve to the data points.
Coefficient of determination	A statistical measure of how close the data is to the fitted curve.
Linear correlation coefficient	The correlation coefficient r measures the strength and direction of the linear relationship between the data values. The value will always be between +1 and -1. For a GPC/SEC column calibration, values should be tending to -1.
Corrected sum of squares	The sum of the squared differences of the assigned MW from the overall mean.
Standard Y error estimate	The standard error estimate of the residuals.
FRM information	
FRM name	The flow rate marker name.
FRM RT (min)	The retention time in minutes of the flow rate marker.
FRM source	The data source chromatogram for the flow rate marker.
Calibration limit information	
High MW limit RT (min)	The retention time in minutes for the high MW limit of the calibration.
Low MW limit RT (min)	The retention time in minutes for the low MW limit of the calibration.

High limit MW (g/mol)	The high limit MW value of the calibration in g/mol (= Da, Dalton).
Low limit MW (g/mol)	The low limit MW value of the calibration in g/mol (= Da, Dalton).

Functions Available

The following commands are available on the right-click menu:

Table 4: Available commands

Command	Description
Copy to Clipboard	Copies the displayed information and the calibration data points table to the clipboard as a tab separated text.
Export to file...	Saves the displayed information and the calibration data points table to the file.

MW Ranges Tab

The MW Ranges tab contains the calculated percentages of material within the specific MW ranges specified in the processing method. It lists the MW ranges as applied to each peak. Each line of the table represents a MW range.

M+ denotes the actual maximum molecular weight specified in the method for a sample.

M- denotes the actual minimum molecular weight specified in the method for a sample.

You can choose the columns that are shown in the MW ranges table. For example, the following columns are available:

Peak#	Index of the peak according to its retention time.
Sample name	Sample name of the injection as entered in the sequence.
Signal description	Name of the signal on which the peak is integrated.
Data file	Name of the data file if source system is file based.
Method	Name of the method used to analyze the data (processing method).
Results set	The name of the results set. The result set contains the results of a sequence that has been run. It consists of raw data, acquisition method, data analysis method, results, and used report templates.
Method high limit MW (g/mol)	The value of the high limit for the instance in the MW ranges table in the processing method. The MW value is specified in g/mol (= Da, Dalton).
High limit MW (g/mol)	The actual value of the high limit for the instance in the MW ranges table in the processing method. The MW value is specified in g/mol (= Da, Dalton).
Method low limit MW (g/mol)	The value of the low limit for the instance in the MW ranges table in the processing method. The MW value is specified in g/mol (= Da, Dalton).
Low limit MW (g/mol)	The actual value of the low limit for the instance in the MW ranges table in the processing method. The MW value is specified in g/mol (= Da, Dalton).
Percent MW	The calculated percentage of the sample for the instance of the MW range.
MW Range Name	The optional text label defined for the MW Range in the processing method.

Functions Available

- Order on the active column

- Resize the displayed columns
- Reorder the displayed columns

The following commands are available on the right-click menu:

Table 5: Context menu commands

Command	Description
Choose columns ...	Displays the **Choose Columns** dialog.
Numeric precision ...	If relevant, displays the **Numeric Precision** dialog.
Copy to Clipboard	Copies the displayed information and the calibration data points table to the clipboard as a tab separated text.
Export to file...	Saves the displayed information to a file. You can choose between the following file formats: • Comma separated value (*.CSV) • Excel worksheet (*.XLS) • Word document (*.DOC) • PDF file (*.PDF)

Percentage Fractions Tab

The Percentage Fractions tab contains the calculated molecular weights at specific percentage area fractions of a sample peak. It lists the percentage fractions as applied to each peak. Each line of the table represents a fraction.

You can choose the columns that are shown in the percentage fractions table. For example, the following columns are available:

Peak#	Index of the peak according to its retention time.
Sample name	Sample name of the injection as entered in the sequence.
Signal description	Name of the signal on which the peak is integrated.
Data file	Name of the data file if source system is file based.
Method	Name of the method used to analyze the data (processing method).
Results set	The name of the results set. The result set contains the results of a sequence that has been run. It consists of raw data, acquisition method, data analysis method, results, and used report templates.
High fraction percent	The high fraction percentage specified in the method.
High fraction RT (min)	The actual retention time in minutes at the high fraction percentage specified in the method.
MW at high fraction (g/mol)	The actual slice MW at the retention time at the high fraction percentage specified in the method. The value is specified in g/mol (= Da, Dalton).
High fraction Mn (g/mol)	The calculated M_n average for the high fraction percentage specified in the method. The value is specified in g/mol (= Da, Dalton).
High fraction Mw (g/mol)	The calculated M_w average for the high fraction percentage specified in the method. The value is specified in g/mol (= Da, Dalton).
Low fraction percent	The low fraction percentage specified in the method.
Low fraction RT (min)	The actual retention time in minutes at the low fraction percentage specified in the method.
MW at low fraction (g/mol)	The slice MW at the retention time at the low fraction percentage specified in the method. The value is specified in g/mol (= Da, Dalton).
Low fraction Mn (g/mol)	The M_n average calculated for the low fraction percentage specified in the method. The value is specified in g/mol (= Da, Dalton).
Low fraction Mw (g/mol)	The M_w average calculated for the low fraction percentage specified in the method. The value is specified in g/mol (= Da, Dalton).

Functions Available

- Order on the active column
- Resize the displayed columns
- Reorder the displayed columns

The following commands are available on the right-click menu:

Table 6: Context menu commands

Command	Description
Choose columns ...	Displays the **Choose Columns** dialog.
Numeric precision ...	If relevant, displays the **Numeric Precision** dialog.
Copy to Clipboard	Copies the displayed information and the calibration data points table to the clipboard as a tab separated text.
Export to file...	Saves the displayed information to a file. You can choose between the following file formats: • Comma separated value (*.CSV) • Excel worksheet (*.XLS) • Word document (*.DOC) • PDF file (*.PDF)

Export GPC/SEC Results

The results of a processed injection can be exported as a simple ASCII file which can be loaded directly into Excel and provides access to the full GPC results and slice by slice data of the processed peak(s) within the injection.

1 From the **Home** ribbon tab, click on the **GPC/SEC Results** window to enable the **GPC/SEC Results** tab on the ribbon bar.

2 From the **GPC/SEC Results** ribbon tab, select **Export to file ...**.

3 In the dialog box, navigate to the desired folder and save the data.

GPC/SEC Distributions

You can access the **GPC/SEC Distributions** window via the **Home** ribbon tab.

It shows the GPC/SEC distribution and cumulative plots for the selected injection. If you did not pin any injections in the injection tree, only the distribution and cumulative plot of the focused injection is shown. If you pin several injections in the injection tree, you can compare multiple distribution and cumulative plots with the distribution and cumulative plots for the focused injection.

Plot Content

Plot Content	Plot of dw/dLog(M) -v- Log MW The Cumulative Area (%) is plotted on the 2nd Y-axis by selecting the button  . The color of the plot is linked to the color of the source injection
Y1-Axis	Scale: Linear Title: dw/dLog(M)
Y2-Axis	Scale: Linear Title: Area (%)
X-Axis	Scale: Log Title: Fitted MW (g/mol) Units: 1 ex
Legend	Displays the injection name and filename of the source injection(s)

Functions Available

The following GPC/SEC-specific items are available:

Button	Function
	Display the Distribution plot(s) and associated cumulative plot(s).
	Auto scales the plot.

Table 7: Available commands

Command	Description
Zoom	To zoom into a specific section of the distribution plot, drag the mouse over the required section while holding down the left mouse button. To zoom out, select the **Auto scale plot** toolbar button (top left), or double-click the plot using the left mouse button.
Right-click menu options	Allows you to export the plot as a graphic. You can copy the plot to the clipboard or save it as a file (*.EMF or *.PNG file format available).

GPC/SEC Calibrations

You can access the GPC/SEC Calibrations window via the Home ribbon tab.

It shows the GPC/SEC calibrations used to analyze the selected injection. If you did not pin any injections in the injection tree, only the calibration used to analyze the focused injection is shown. If you pin several injections in the injection tree, you can compare multiple calibrations with the calibration used to analyze the focused injection.

Plot Content

Plot Contents	Plot of Log MW -v- RT corrected (min) that contains the data points and calculated line of fit. The color of the line is linked to the color of the source injection.
Y-Axis	Scale: Log Title: MW (g/mol) Units: 1 ex
X-Axis	Scale: Linear Title: Retention time (min) Units: Minutes
Legend	Displays the sample name and filename of the injection analysed by the calibration.

Functions Available

The following GPC/SEC-specific items are available:

Button	Function
	Displays the properties dialog for the GPC/SEC calibration axes scaling.
	Auto scales the plot.

Properties Dialog

The options available in this dialog allow you to define the axes limits for the GPC/SEC calibration plot.

Table 8: Plot scaling

Option	Description
MW Axis custom scaling	Check-box to enable/disable MW axis custom scaling (Y-axis).
Minimum/Maximum	Enter a value to set the minimum and maximum MW axis limits [g/mol or Daltons].
RT axis custom scaling	Check-box to enable/disable RT axis custom scaling (X-axis).
Minimum/ Maximum	Enter a value to set the minimum and maximum RT axis limits [g/mol or Daltons].

Table 9: Available commands

Command	Description
Zoom	To zoom into a specific section of the distribution plot, drag the mouse over the required section while holding down the left mouse button. To zoom out, select the **Auto scale plot** toolbar button (top left), or double-click the plot using the left mouse button.
Tooltip	When the mouse cursor is over a data point in the calibration plot, a tool tip displays the following information: • The retention time (min) of the data point. • The MW (g/mol) assigned to the data point. • The sample name of the source chromatogram. • The filename of the source chromatogram. The values are taken from the GPC/SEC column calibration used to process the sample of the selected (active) injection. The **Retention Time** value displayed is the value displayed in the **RT corrected** column of the GPC calibration points tab of the method.
Right-click menu options	Allows you to export the plot as a graphic. You can copy the plot to the clipboard or save it as a file (*.EMF or *.PNG file format available).

GPC/SEC LS Results

You can access the **GPC/SEC LS Results** window via the **Home** ribbon tab.

The tabs of the window are explained below.

Peak Results Tab

The Peak Results tab contains the GPC/SEC LS results table for the selected injection, provided that its sample type is set to **Sample** and it has been reprocessed using the advanced GPC/SEC processing method (see Advanced GPC/SEC Processing Method on page 82).
Each line of the table represents a GPC Compound (for details, refer to About the GPC Compound Concept on page 139).
The table is empty for other sample types or if no GPC compound was found in the selected injection.

The peak selection is synchronized with the peak selection in the Chromatograms and the Injection Results windows.

You can choose the columns that are shown in the GPC peak results table and their position. The following columns are available:

Peak#	Index of the peak according to its retention time.
Name	Name of the GPC compound on page 139. Empty if the GPC compound is not identified.
Signal description	Name of the signal where the main integrated peak of the GPC compound was found.
RT (min)	Retention time of the main peak. It corresponds to the time at the main peak apex.
Bulk MW (g/mol)	The bulk molecular weight calculated in g/mol (Dalton).
Bulk Rg (nm)	The bulk radius of gyration in nm. Only available if the GPC compound contains peaks of at least two LS angle signals and the slope of the fit of those (in the LS Results window) is positive.
dn/dc (mL/g)	The parameter **dn/dc** entered as sample custom parameter.
Calculated dn/dc (mL/g)	The value of **dn/dc** calculated for the selected GPC compound using the entered **Concentration** parameter.
Concentration (g/L)	The parameter **Concentration** entered as sample custom parameter.
Calculated Concentration (g/L)	The value of the **Concentration** calculated for the selected GPC compound using the entered **dn/dc** parameter.

Recovery(%)	The percentage recovery based on the calculated **Concentration**.
UV Ext. Coeff ((mg/mL)-1(cm)-1)	The UV extension coefficient entered as sample custom parameter.
Calculated UV Ext. Coeff ((mg/mL)-1(cm)-1)	The value of the **UV extension coefficient** calculated using the entered or calculated **dn/dc** and **Concentration** parameters.

A cell is empty when a value is not available (for example, when an entered parameter is missing or a calculated value could not be derived). When a value is not used for LS analysis, it is displayed in a grayed-out cell. This can be the case, for example, for the columns **Concentration**, **dn/dc** and **UV Ext. Coeff.**, where both entered and calculated values are displayed.

Functions Available

- Order on the active column
- Resize the displayed columns
- Reorder the displayed columns

The following commands are available on the right-click menu:

Table 10: Context menu commands

Command	Description
Choose columns ...	Displays the **Choose Columns** dialog.
Numeric precision ...	If relevant, displays the **Numeric Precision** dialog.
Copy to Clipboard	Copies the displayed information and the calibration data points table to the clipboard as a tab separated text.
Export to file...	Saves the displayed information to a file. You can choose between the following file formats: • Comma separated value (*.CSV) • Excel worksheet (*.XLS) • Word document (*.DOC) • PDF file (*.PDF)

System Calibration Results Tab

The **System Calibration Results** tab displays the calibration parameters and the detector constants used to perform the LS data analysis. The information is also displayed in **System Calibration Results** tab of the advanced Processing Method (see System Calibration Results tab on page 87).

Export GPC/SEC LS Results

The results of a processed injection can be exported as a simple ASCII file which can be loaded directly into Excel and provides access to the full GPC/SEC results and slice by slice data of the processed peak(s) within the injection.

1 From the Home ribbon tab, click on the GPC/SEC LS Results window to enable the GPC/SEC LS Results tab on the ribbon bar.

2 From the GPC/SEC LS Results ribbon tab, select Export to file ....

3 In the dialog box, navigate to the desired folder and save the data.

LS Results Plot

You can access the **LS Results Plot** window via the **Home** ribbon tab.

It shows the LS results plot demonstrating a partial Zimm plot for the selected injection. Depending on the acquired LS detector signals, the plot displays a different number of data points, reflecting the number of selected detection angles. If required, you can select the detection angles for the LS data processing (in the Processing method, section **GPC/SEC Advanced** > **LS Detector** tab).

NOTE

The MALS detector (G7885A) provides up to 20 angles and the MDS Dual Angle LSD (G7803A, G7808A, and G7809A) provides two angles which can be used for advanced LS data processing.

In the graph, where K*c/ R(θ) vs. $\sin^2(\theta/2)$ is plotted, the bulk MW can be obtained from the intercept with the Y-axis and the radius of gyration (R_g) from the slope of the angular dependence plot.

Functions Available

The following GPC/SEC-specific items are available:

Button	Function
	Auto scales the plot.

Table 11: Available commands

Command	Description
Zoom	To zoom into a specific section of the distribution plot, drag the mouse over the required section while holding down the left mouse button. To zoom out, select the **Auto scale plot** toolbar button (top left), or double-click the plot using the left mouse button.
Right-click menu options	Allows you to export the plot as a graphic. You can copy the plot to the clipboard or save it as a file (*.EMF or *.PNG file format available).

GPC/SEC Compound Details

You can access the **GPC/SEC Compound Details** window via the **Home** ribbon tab.

It displays the selected peak or GPC compound with concentration and LS signals overlaid. The graph plots the response against retention time for all selected signals. The integration limits (integrated area) of the selected peak are shown in gray for the selected signals. It is possible to display **slice MW** and **Rh results** in this graph (see Display Options). A tooltip shows the current value for each slice.

NOTE

Only the Agilent Bio MDS Dual Angle LSD provides a DLS option (G7809A) which allows R_h signal acquisition.

For more information on GPC compounds, refer to About the GPC Compound Concept on page 139.

Functions Available

The following GPC/SEC-specific items are available:

Button	Function
	Scaling option: All signals same scale (per pane) If the graphs are shown separately, each graph is scaled individually to its own signal maximum. If shown as an overlaid graph, the signals use the same scale.
	Scaling option: Relative full scale Each signal is displayed using its own signal maximum (100%).
	Show/Hide slice MW results. Displayed on the right side in logarithmic scale.
	Show/Hide R_h results.
	Show/Hide Slice MW Cursor.
	Auto scales the plot.

Table 12: Available commands

Command	Description
Zoom	To zoom into a specific section of the distribution plot, drag the mouse over the required section while holding down the left mouse button. To zoom out, select the **Auto scale plot** toolbar button (top left), or double-click the plot using the left mouse button.
Right-click menu options	Allows you to export the plot as a graphic. You can copy the plot to the clipboard or save it as a file (*.EMF or *.PNG file format available).

GPC/SEC Processing Method

This section describes:

- The GPC/SEC-specific additions to the processing method
- The GPC/SEC parameters and their function

The GPC/SEC software provides a GPC/SEC-specific processing method type based on the method type GC/LC Area Percent and supports:

- Integration and Area% / Height% calculation
- Signal alignment
- Blank subtraction for GC, LC, A/D data
- System suitability
- GPC/SEC column calibration
- Calculation of molecular weight averages & distribution plot
- Calculation of % Material within specific MW ranges
- Calculation of MW information at specific % Fractions
- Custom calculation
- Reporting

The GPC/SEC parameters are accessed from the GPC/SEC section of the processing method which is added to the bottom of the processing method section. The parameters are displayed in two sub sections:

- GPC/SEC Conventional
- GPC/SEC Column Calibration

All GPC/SEC parameters are stored as part of the data analysis processing method.

Conventional GPC/SEC Processing Methods

Two conventional processing methods are installed with the GPC/SEC software add-on and can be applied to data obtained without GPC LS detectors.

- GPC/SEC
- GC/LC Quantitative + GPC/SEC

NOTE

The sections shown here are specific to the methods GPC/SEC and GC/LC Quantitative + GPC/SEC.
They will therefore only be displayed if you have loaded these methods, regardless of whether you are using the standard or advanced software add-on.

Both conventional processing methods consist of sections used in the standard data analysis . These sections are:

- General
- Integration Events
- Compounds
- System Suitability
- Reports
- Tools

Section GPC/SEC contains parameters for:

- GPC/SEC Conventional on page 74
- GPC/SEC Column Calibration on page 117

NOTE

Methods based on an GPC/SEC add-on version older than 2.0 can also be used with 2.0. Only the naming of the sections have changed.

GPC/SEC Conventional

General

General	
Signal	Under Signal, select the signal type that will be used to generate a GPC/SEC calibration and for the GPC/SEC analysis. The GPC/SEC calibration and analysis must use the same signal.

Flow Rate Correction		
Use flow rate correction	This option allows samples to be corrected for variation in flow rate using the standard marker method. To use flow rate correction, you must include a "marker component" in your samples.	
FRM name	Specify the name of the flow rate marker component.	
Expected RT	When processing samples, the system will expect a marker peak at the expected retention time +/- half the RT window value.	
RT window	When processing samples, the system will expect a marker peak at the expected retention time +/- half the RT window value.	
Sample Mark-Houwink Parameters		
K ((10e-5) dL/g)	The Mark-Houwink K value used for all samples (non-calibrants).	
alpha	The Mark-Houwink alpha value used for all samples (non-calibrants).	

Column Calibration

Calibration Type		
Column calibration type	Select the type of column calibration you wish to generate:	
	Narrow Standard	Requires a series of Narrow Standards of known M_p.
	Broad Hamielic	This method utilizes a Broad Standard with known M_n and M_w. The Hamielic method assumes that the calibration is linear. The software performs a trial and error search such that the calculated values of **Mn** and **Mw** match those documented for the Standard. The *Maximum Number of Searches* (iteratons), together with a *Tolerance Value* for **Mn** and **Mw**, expressed as a percentage of those Molecular Weights need to be defined in the Broad Hamielic Parameters tab.
	Broad Integral	Requires a characterized Standard with known MW at specific Wt%.
Polynomial curve fit	Defines the polynomial curve fit order that will be applied to the column calibration. For a Broad Hamiliec calibration a 1st order polynomial is automatically applied and cannot be changed.	
Cal. Std. Mark-Houwink Parameters		
K ((10e-5) dL/g)	The Mark-Houwink K value used for all calibrant samples.	
alpha	The Mark-Houwink alpha value used for all calibrant samples.	

Peak Identification

This tab is specific to the Narrow Standard calibration option.

Peaks that are not given a molecular weight will not be used for identification and for the generation of the column calibration.

The following columns for the Peak Identification table are available:

RT (min)	Retention time of the peak. It corresponds to the time at the peak apex.
Mp (g/mol)	The user assigned peak MW in g/mol (= Da, Dalton).
Peak RT window (min)	The window in minutes around the expected retention time that defines the range in which the peak will be identified.
Sample name	The sample name of the sample from which the data point has been added.
Signal	The detector signal name of the sample from which the data point has been added.
Source chromatogram	The source chromatogram of the injection from which the data point has been added.
Source Chromatogram data sequence	The data sequence containing the source chromatogram.
Source Chromatogram project	The name of the project containing the source chromatogram data sequence.
Use point	Defines if the point is to be included in the calculation of the line of fit of the GPC/SEC calibration.

Choose the Displayed Columns in the Table

1 Click the Column Chooser symbol in the top left corner of the window.

The Choose columns dialog opens.

2 Select the columns that you want to be displayed.

3 Click OK.

Context Menu Options

The right-click context menu offers the following options:

- To copy the table to the clipboard, select Copy to Clipboard.

- To export the table, select **Export to file...**. You can choose between the following file formats:
  - Comma separated value (*.CSV)
  - Excel worksheet (*.XLS)
  - Word document (*.DOC)
  - PDF file (*.PDF)
- To add peaks from the currently focused injection, select **Add peaks from chromatogram**.
- To manually add a peak, select **Add peak**.
- To delete a selected peak, select **Delete selected peak(s)**.

Broad Hamielec Parameters

The **Broad Hamielec** method utilizes a **Broad Standard** with known M_n and M_w. The Hamielic method assumes that the calibration is linear. The software performs a trial and error search such that the calculated values of M_n and M_w match those documented for the standard (see certificate). The maximum number of searches or iterations together with a tolerance value for M_n and M_w, expressed as a percentage of those molecular weights need to be defined.

Target Tolerance	The target tolerance is expressed as a percentage of the known molecular weights.
Max iterations	The maximum number of iterations to use in the search process determining the best calibration line to achieve the target M_n and M_w values within the defined target tolerance.
Target Mn average	The target M_n values of the calibrant sample to be used.
Target Mw average	The target M_w values of the calibrant sample to be used.

Broad Integral Setup

A **Broad Integral** calibration involves the use of a single well characterized **Broad Standard** i.e. with a large dispersity value to ideally calibrate the whole separation range of the utilized column or column set. The standard to be used must have a table detailing the % cumulative weight fraction and either log molecular weight or molecular weight values supplied by the manufacturer of the standard.

Slice MW (g/mol)	The slice molecular weight in g/mol (= Da, Dalton) for the corresponding percentage weight fraction.
Percentage weight	The percentage weight fraction of the MW slice.

Context Menu Options

The right-click context menu allows you to add new broad integral slices or delete existing slices. In addition, you can paste an existing table from another program such as Excel or export the table by copying to the clipboard or save it as a file. You can choose between the following file formats:

- Comma separated value (*.CSV)
- Excel worksheet (*.XLS)
- Word document (*.DOC)
- PDF file (*.PDF)

MW Ranges

Enable the option **Calculate MW ranges** to generate a MW range report for each peak processed in a sample chromatogram.

Any number of MW ranges can be defined in the table. A new MW range can be added by using the right-click context menu. In addition, the current ranges can be copied to the clipboard or selected ranges can be deleted.

M+ denotes the actual maximum molecular weight specified in the method for a sample.

M- denotes the actual minimum molecular weight specified in the method for a sample.

If you define a range as **M+** to **M-** then this is a way of reporting the maximum and minimum molecular weights of each sample.

High MW limit (g/mol)	The high limit MW value is specified in g/mol (= Da, Dalton).
Low MW limit (g/mol)	The low limit MW value is specified in g/mol (= Da, Dalton).
MW Range Name	An optional text label that provides a way to identify specific MW ranges in a report.

Percentage Fractions

The option **Calculate percentage fractions** allows the calculation of molecular weights at specific percentage area fractions of a sample peak.

Use the right-click context menu of the table to add, copy or delete values for the percentage fractions:

High fraction %	The high percentage fraction.
Low fraction %	The low percentage fraction.

The percentage values for the high and low fractions do not need to be the same.

GPC/SEC Column Calibration

The tabs in the GPC/SEC Column Calibration section show information of the calibration.

GPC Calibration Points on page 79	Displays the current column calibration data points table and associated parameters.
GPC Calibration Plot on page 80	Comprises of a read-only plot of the data displayed in the GPC calibration points tab.
GPC Calibration Details on page 81	Displays details about the column calibration data and how it was derived.

GPC Calibration Points

In the GPC Calibration Points tab, you can choose the columns that are shown in the GPC/SEC calibration points table. For example, the following columns are available:

RT corrected (min)	Retention time of the peak in minutes corrected for changes in the flow rate. If use flow rate correction is off in the method, then this value is the same as the value in the corresponding RT actual field.
RT actual (min)	The actual uncorrected retention time of the peak in minutes. It corresponds to the time at the peak apex.
Assigned MW (g/mol)	• Narrow Standard The MW value in g/mol (= Da, Dalton) corresponding to the RT value of the peak nearest to the entry in the Peak Identification table. • Broad Hamielec The MW value in g/mol (= Da, Dalton) corresponding to the start and end points of the calculated line of fit. • Broad Integral The slice MW for the individual fractions.
Log MW	The logarithm to the base 10 of the assigned MW value.
Sample name	Sample name of the injection as entered in the sequence.
Source Chromatogram	The source chromatogram of the injection from which the data point has been added.
Source Chromatogram data sequence	The data sequence containing the source chromatogram.
Source Chromatogram project	The name of the project containing the source chromatogram data sequence.

Signal	Name of the signal on which the peak is integrated.
Percent error	The percent ratio between the predicted and actual MW values.
Residual	The difference between the actual MW value and the predicted MW value.
Predicted MW (g/mol)	The predicted MW in g/mol (= Da, Dalton) of the data point calculated from the calibration curve.
FRM RT (min)	The flow rate marker retention time in minutes if flow rate correction is being used.

Export Calibration Points

The context menu of the GPC Calibration Points window offers the possibility to export the table. You can copy the table content to the clipboard or save it as a file. You can choose between the following file formats:

- Comma separated value (*.CSV)
- Excel worksheet (*.XLS)
- Word document (*.DOC)
- PDF file (*.PDF)

GPC Calibration Plot

The **GPC Calibration Plot** tab shows the generated GPC/SEC column calibration.

Zooming and Scrolling

To zoom into a specific section of the calibration plot, you can simply drag the mouse over the required section while holding down the left mouse button. To scroll the graph, hold the right mouse button down and drag.

To zoom out, double-click the plot using the left mouse button or right-click with the right mouse button and select the **Auto scale** menu item from the context menu.

Tooltip

When the mouse cursor is over a data point in the calibration plot, a tool tip displays the following information:

- The retention time (min) of the data point.

- The MW (g/mol) assigned to the data point.
- The sample name of the source chromatogram.
- The filename of the source chromatogram.

The values are taken from the current GPC/SEC column calibration displayed in the GPC calibration points tab of the method.

The Retention Time value displayed is the value displayed in the RT corrected column.

Export GPC Calibration Plot

The right-click context menu allows you to export the plot as a graphic. You can copy the plot to the clipboard or save it as a file.

GPC Calibration Details

The GPC Calibration Details tab shows the generated GPC/SEC column calibration details.

The following values are displayed:

Administration information	
Calibration type	The column calibration type. Either Narrow Standard, Broad Hamielic, or Broad Integral.
Signal	Name of the signal used to create the column calibration.
Calibration Mark-Houwink parameters	
K ((10e-5) dL/g)	The Mark-Houwink K value for the column calibration.
Alpha	The Mark-Houwink Alpha value for the column calibration.
Curve fit	
Order of curve fit	The polynomial curve fit order.
Curve fit equation	The equation of the calibration curve.
Curve fit statistics	
Residual sum of squares	The sum of the squares of residuals. This is a measure of the discrepancy between the data and the curve. A small RSS indicates a better fit of the calibration curve to the data points.
Coefficient of determination	A statistical measure of how close the data is to the fitted curve.

Linear correlation coefficient	The correlation coefficient r measures the strength and direction of the linear relationship between the data values. The value will always be between +1 and -1. For a GPC/SEC column calibration, values should be tending to -1.
Corrected sum of squares	The sum of the squared differences of the assigned MW from the overall mean.
Standard Y error estimate	The standard error estimate of the residuals.
FRM information	
FRM name	The flow rate marker name.
FRM RT (min)	The retention time in minutes of the flow rate marker.
FRM source	The data source chromatogram for the flow rate marker.
Calibration limit information	
High MW limit RT (min)	The retention time in minutes for the high MW limit of the calibration.
Low MW limit RT (min)	The retention time in minutes for the low MW limit of the calibration.
High limit MW (g/mol)	The high limit MW value of the calibration in g/mol (= Da, Dalton).
Low limit MW (g/mol)	The low limit MW value of the calibration in g/mol (= Da, Dalton).

Export GPC Calibration Details

The right-click context menu allows you to export the calibration details. You can copy the calibration details to the clipboard or save it as a text file.

Advanced GPC/SEC Processing Method

The GPC/SEC software add-on with advanced functionalities (G7861AA) comes pre-installed with the method GC/LC Quant + GPC/SEC + LS Bulk.

NOTE

The sections shown here are specific to the method GC/LC Quant + GPC/SEC + LS Bulk.
They will therefore only be displayed if you have loaded this method.

The method consist of sections used for the standard data analysis (for more information on the displayed parameters, refer to OpenLab Help and Learning Online, search for "Working with processing methods" in the core Data Analysis). These sections are:

- General

  More details about the displayed parameters are described below in chapter General on page 83.
- Integration Events
- Compounds
- System Suitability
- Reports
- Tools
- GPC/SEC

  This section is specific for GPC/SEC data analysis. More details about the displayed parameters are described below in chapter GPC/SEC on page 84.

General

The **General** section of the processing method is displayed for all three GPC/SEC specific processing methods. But only when working with the advanced **GC/LC Quant + GPC/SEC + LS Bulk** method, you must define a specific signal alignment.

NOTE

The parameters available in section **Properties** and **Signals** are used in standard data analysis of the OpenLab CDS. For more information on the displayed parameters, refer to OpenLab CDS core functionality.

Properties

Info	Displays general information about the method.
Global	Select the ChemStation or EZChrom integrator.

Signals

Scaling	Select if you want to use fixed chromatogram scaling.
Alignment	The **Alignment** tab is important for advanced LS data processing. In the **Use delay** column, select the utilized concentration detector (e.g. RID or UV) and the LS detector and provide the retention time at peak maximum (Vp) for the identified peak in both detectors. **NOTE:** Use a narrow standard to determine the inter detector delay. If you use conventional GPC/SEC analysis (column calibration), you can ignore the **Alignment** tab.
Smoothing	Set the **Global Signal Settings** and select the check boxes to override global signal parameters for specific signals.
Blank Substraction	Set the parameters for injections with blank subtraction applied.
Reference Chromatogram	Displays the reference Chromatogram table.

GPC/SEC

Section **GPC/SEC** contains parameters for:

- GPC/SEC General on page 84
- GPC/SEC Conventional on page 74, similar to conventional GPC/SEC methods
- GPC/SEC Column Calibration on page 79, similar to conventional GPC/SEC methods
- GPC/SEC Advanced on page 85

GPC/SEC General

Section **GPC/SEC General** contains parameters for:

Analysis Type	
Select the type of analysis that will be applied to generate GPC/SEC results.	
Conventional	Select this option to apply the column calibration approach.
Advanced LS Bulk	Select this option to apply light scattering (LS) calibration and calculations.
Detectors	
Concentration Detector	From the drop-down list, select the used concentration detector.
LS Detector	From the drop-down list, select the used LS detector. If the loaded data does not contain an LS detector signal, only **None** is available.

For more information, refer to GPC/SEC General on page 137.

GPC/SEC Advanced

This specific method configuration contains parameters for advanced LS calculations.

The following tabs are displayed:

- General
- LS Detector
- System Calibration Results

General tab

System Calibration Settings

Peak Expected Retention Time	Enter a value for the expected retention time [min] of the peak used in the system calibration process.
Absolute Time Window	Enter a value for the absolute time window [min] used to identify the peak for the system calibration.
Relative Time Window	Enter a value for the relative time window [%] used to identify the peak for the system calibration.
Use all compounds concentration area	If enabled, the detector constant for concentration detectors (typically RID or UV) is calculated based on the sample concentration entered in the **Injection List** window and the identified peaks in the **Chromatograms** window. This is particularly important for calibrants that produce multiple peaks, where all peak areas must be considered to accurately determine the monomer peak concentration. This monomer concentration is then used to calculate the correct detector constant. **NOTE:** For example, the BSA (bovine serum albumin) calibrant – commonly used in aqueous applications – typically produces a chromatogram with at least three peaks (monomer, dimer, and higher-order species). While the total peak area reflects the overall sample concentration (as entered in the injection list), the detector constant is calculated based solely on the monomer peak concentration. This is determined using the **Use all compounds concentration area** option.

GPC Compounds

Absolute Time Window	Enter a value for the absolute time window [min] used to generate GPC compounds out of integrated peaks in the concentration and LS signal chromatograms. The entered value will be applied on the retention time of the main peak (typically, this is the peak in the concentration signal) used to find matching peaks in other signals (typically, in the LS signals). For more details, refer to section About the GPC Compound Concept on page 139. The identified GPC compounds consequently show up in the **Peak Results** table of the **GPC/SEC LS Results** window.
Relative Time Window	Enter a value for the relative time window [%] used to generate GPC compounds out of integrated peaks in the concentration and LS signal chromatograms. The entered value will be applied on the retention time of the main peak (typically, this is the peak in the concentration signal) used to find matching peaks in other signals (typically, in the LS signals). For more details, refer to section About the GPC Compound Concept on page 139.

Analysis Settings

Used to calculate the sample concentration or sample property parameters, such as dn/dc value or UV extinction coefficient of a GPC compound. The prerequisite is that concentration values or the sample property parameters are entered in the **Injection List** window.
The results are shown in the **GPC/SEC LS Results** window. The comparison of the calculated concentration with your entered sample concentration allows to calculate the sample recovery of an eluted compound.

Concentration	Select the option to calculate the sample property parameters. **NOTE:** Depending on the selected concentration detector (RID, UV), your entered concentration in the Injection List window will be used to calculate the sample property parameters (dn/dc value (RID) or UV ext. coeff (UV detector)).
Sample Property (dn/dc, UV Ext Coeff)	Select the option to calculate the sample concentration. **NOTE:** Your entered dn/dc value (RID) or UV ext. coeff. (UV detector) in the Injection List window will be used to calculate the sample concentration.

LS Detector tab

The LS Detector tab allows a selection of LS detection angles used for advanced result calculation. For more information, refer to LS Detector tab on page 142.

System Calibration Results tab

Verify the parameters and the determined detector constants that are used for the advanced calculation of GPC/SEC LS results.

Acquisition Parameter	
Flow Rate	The flow rate of the collected data.
Calibration Parameters	
Concentration (g/L)	Concentration of the sample (entered in the **Injection List** window).
Molar Mass (Da)	Molecular weight of the sample (entered in the **Injection List** window).
dn/dc (mL/g)	dn/dc of the sample (entered in the **Injection List** window).
UV Extinction Coefficient ((mg/mL)-1(cm)-1)	UV extinction coefficient of the sample (entered in the **Injection List** window).
Eluent RI	Eluent refractive index (dimensionless) (entered in the **Injection List** window).
Detector Constants	
Displays the calculated detector constant for the concentration detector and the advanced LS detector. Depending on the used LS detector, a different number of entries will be displayed. For each detection angle, the user can review the calculated constant and the normalization coefficient (value in brackets). **NOTE:** The 90° detection angle is always used as reference (normalization factor set to 1) to calculate the normalization factors for all other angles. This normalization is essential because it strongly affects the determination of the radius of gyration (R_g) and calculation of results. **NOTE:** The displayed detector constants and normalization coefficients are based on the system calibration which must be performed with a narrow and well-characterized calibrant with known molecular weight (certified by light scattering measurements). For the normalization, it is required that the selected calibrant is an isotropic scatter (molecular weight below 120 kDa).	

GPC/SEC Reporting

The following section describes the GPC/SEC additions to the OpenLab Reporting module.

- Additions to existing report items
- Addition of GPC/SEC specific report items
  - GPC/SEC column calibration specific items
  - GPC/SEC analysis specific items

Additions to Existing Report Items

The following data analysis **Method Information** report items have been updated to provide GPC specific information:

- Data Analysis Method Information Multi Column
- Single Data Analysis Method Parameter
- Single Data Analysis Method Table Row

The Data Analysis Method Information Multi Column Item

The following GPC/SEC-specific parameters are output at the end of the data analysis method report.

- GPC/SEC Method Parameters
- MW Ranges Table
- Percentage Fractions Table
- GPC/SEC Column Calibration
- GPC/SEC Calibration Data Points Table
- Peak Identification Table (Narrow Standard calibration)
- Broad Hamielec Parameters (Broad Hamielec calibration)
- Broad Integrals Table (Broad Integral calibration)

The Single Data Analysis Method Parameter Item

This report item allows the selection of a single parameter for display.

The following sections are added to this item.

- Method Parameters
  - GPC/SEC Column Calibration
  - GPC/SEC Method Parameters

The Single Data Analysis Method Parameter Item

This report item allows the selection of a single table row for display.

The following sections are added to this item.

- Method parameters
  - GPC/SEC Column Calibration
  - GPC/SEC Method Parameters

GPC/SEC-Specific Report Items

GPC/SEC-specific report items are provided which comprise of a series of tables and plots. The GPC/SEC report items can be found in the GPC/SEC node in the Reporting view under Report Items.

The added items can be divided into:

- GPC/SEC Column Calibration Specific Items
  - GPC Column Calibration Details Table
  - GPC Calibration Points Table
  - Single GPC Calibration Plot
  - GPC Calibration Plot Overlaid
- GPC/SEC Analysis-Specific Items
  - Peak Results Table
  - Peak Results Summary Table
  - MW Ranges Table
  - MW Ranges Summary Table
  - Percentage Fractions Table
  - Percentage Fractions Summary Table
  - Peak Results Table – First Peak
  - Peak Results Summary Table – First Peak
  - MW Ranges Table – First Peak
  - MW Ranges Summary Table – First Peak
  - Percentage Fractions Table – First Peak
  - Percentage Fractions Summary Table – First Peak
  - GPC Time Slice Table
  - Single GPC Distribution Plot
  - GPC Distribution Plot Overlaid
- Advanced LS-Specific Items
  - GPC/SEC LS Results Table
  - GPC/SEC System Calibration Results

GPC/SEC Column Calibration Specific Items

GPC Column Calibration Details Table

Provides a two-column table (<parameter name>, <value>) which provides the following information:

- Method name
- Residual sum of squares
- FRM RT (min)
- Calibration type
- Coefficient of determination
- FRM source
- Signal
- Linear correlation coefficient
- High MW limit RT (min)
- K ((10e-5) dL/g)
- Corrected sum of squares
- Low MW limit RT (min)
- Alpha
- Standard Y error estimate
- High limit MW (g/mol)
- Order of curve fit
- FRM name
- Low limit MW (g/mol)

Customization Available

The items and the order in which they are displayed are fixed.

The format of individual items in the table cannot be customized.

GPC Calibration Points Table

Provides the following parameters for each calibration data point:

- RT corrected (min)
- Sample name
- Residual
- RT actual (min)
- Source chromatogram
- Source chromatogram data sequence
- Source chromatogram project
- Predicted MW (g/mol)
- Assigned MW (g/mol)
- Signal
- FRM RT (min)
- Log MW
- Percent error

Customization Available

The items and the order in which they are displayed can be changed.

The properties of each parameter column can be customized.

Single GPC Calibration Plot

Provides a GPC Calibration Plot which contains a plot of Log MW (g/mol) vs Retention Time (min).

If this item is used in a Single Injection report, the output will consist of a plot of the GPC calibration used to process the injection.

If this item is used in a Sequence Summary report, the output will consist of a separate calibration plot, one for each injection in the sequence summary.

Customization Available

Table 13: Plot properties

Option		Description
Show grid lines		Select the check-box to display the axes gridlines in the calibration plot.
Show legend		Select the check-box to display the name of the injection on the top left corner of the plot.
Show calibration points		Select the check-box to display the individual calibration data points in the calibration plot. Define the following properties:
	Color	The color of the calibration data points.
	Point size	The point size of the calibration data points.
	Point shape	The point shape of the calibration data points.
Show calibration line		Select the check-box to display the calculated line of fit in the calibration plot. Define the following properties:
	Color	The color of the calibration line.
	Line weight	The thickness of the calibration line.

The options available in this dialog allow you to define the axes limits for the GPC Calibration plot item.

Table 14: Plot scaling

Option	Description
MW Axis custom scaling	Check-box to enable/disable MW axis custom scaling (Y-axis).
Minimum/Maximum	Enter a value to set the minimum and maximum MW axis limits [g/mol or Daltons].

Option	Description
RT axis custom scaling	Check-box to enable/disable RT axis custom scaling (X-axis).
Minimum/ Maximum	Enter a value to set the minimum and maximum RT axis limits [g/mol or Daltons].

GPC Calibration Plot Overlaid

Provides a GPC Calibration Plot which contains overlaid plots of Log MW (g/mol) vs Retention Time (min).

If this item is used in a Single Injection report, the output will consist of a single plot of the GPC/SEC calibration used to process the injection.

If this item is used in a Sequence Summary report, the output will consist of a single plot contain an overlay of all the GPC/SEC calibrations, one from each selected injection in the sequence summary.

Customization Available

Table 15: Plot properties

Option		Description
Show gridlines		Select the check-box to display the axes gridlines in the calibration plot.
Injection Colors		Defines the color of the calibration line and the data points for each individual injection # (1- 8).
Show calibration points		Select the check-box to display the individual calibration data points in the calibration plot. Define the following properties:
	Point size	The point size of the calibration data points.
	Point shape	The point shape of the calibration data points.
Show calibration line		Select the check-box to display the calculated line of fit in the calibration plot.
	Line weight	Defines the thickness of the calibration line.

The options available in this dialog allow you to define the axes limits for the GPC/SEC Calibration plot item.

Table 16: Plot scaling

Option	Description
MW Axis custom scaling	Check-box to enable/disable MW axis custom scaling (Y-axis).
Minimum/Maximum	Enter a value to set the minimum and maximum MW axis limits [g/mol or Daltons].
RT axis custom scaling	Check-box to enable/disable RT axis custom scaling (X-axis).
Minimum/ Maximum	Enter a value to set the minimum and maximum RT axis limits [g/mol or Daltons].

GPC/SEC Analysis Specific Items

Peak Results Table / Peak Results Summary Table

The tables provide the following parameters for each processed peak:

- Peak#
- Sample name
- Data file
- Signal description
- Method
- Results set
- RT (min)
- M_p (g/mol)
- M_n (g/mol)
- M_w (g/mol)
- M_z (g/mol)
- M_{z+1} (g/mol)
- M_v (g/mol)
- PD
- FRM name
- FRM RT (min)
- FRCF
- K ((10e-5) dL/g)
- Alpha

Usage	Description
Single Injection Report	If this item is used in a Single Injection report, the output will consist of a table containing the calculated MW Averages for the selected processed injection.
Sequence Summary Report	If a **Peak Results Table** is used in a Sequence Summary report, the output will consist of a separate table containing the calculated MW Averages, one table for each selected injection in the sequence summary. If a **Peak Results Summary Table** is used in a Sequence Summary report, the output will consist of a single table containing the calculated MW Averages for all selected injections in the sequence summary.

First Peak Tables

Only the results of the first peak will be reported.

Customization Available

Double-click the table to customize the column properties (for example, add/remove columns, change the style, etc.).

MW Ranges Table / MW Ranges Summary Table

The tables provide the following parameters for each processed peak:

- Peak#
- Sample name
- Data file
- Signal description
- Method
- Results set
- Method high limit MW (g/mol)
- High limit MW (g/mol)
- Method low limit MW (g/mol)
- Low limit MW (g/mol)
- Percent MW
- MW Range Name

Usage	Description
Single Injection Report	If this item is used in a Single Injection report, the output will consist of table containing the calculated MW ranges for the selected processed injection.
Sequence Summary Report	If a **MW Ranges Table** is used in a Sequence Summary report, the output will consist of a separate table containing the calculated MW ranges, one table for each selected injection in the sequence summary. If a **MW Ranges Summary Table** is used in a Sequence Summary report, the output will consist of a single table containing the calculated MW Ranges for all selected injections in the sequence summary.

First Peak Tables

Only the results of the first peak will be reported.

Customization Available

Double-click the table to customize the column properties (for example, add/remove columns, change the style, etc.).

Percentage Fraction Table / Percentage Fraction Summary Table

The items provide the following parameters for each processed peak:

- Peak#
- Sample name
- Data file
- Signal description
- Method
- Results set
- High fraction percent
- High fraction RT [min)
- MW at high fraction (g/mol)
- High fraction M_n (g/mol)
- High fraction M_w (g/mol)
- Low fraction percent
- Low fraction RT (min)
- MW at low fraction (g/mol)
- Low fraction M_n (g/mol)
- Low fraction M_w (g/mol)

Usage	Description
Single Injection Report	If this item is used in a Single Injection report, the output will consist of a table containing the calculated Percentage Fractions for the selected processed injection.
Sequence Summary Report	If a **Percentage Fraction Table** is used in a Sequence Summary report, the output will consist of a separate table containing the calculated Percentage Fractions, one table for each selected injection in the sequence summary. If a **Percentage Fraction Summary Table** is used in a Sequence Summary report, the output will consist of a single table containing the calculated Percentage Fractions for all selected injections in the sequence summary.

First Peak Tables

Only the results of the first peak will be reported.

Customization Available

Double-click the table to customize the column properties (for example, add/remove columns, change the style, etc.).

GPC Time Slice Table

The items provide the following parameters for each processed peak:

- Peak#
- Sample name
- Data file
- Signal description
- Method
- Results set
- RT (min)
- Response
- Area (mV.s)
- Slice MW
- LogM
- dw/dLogM
- Cum Area
- Norm Area

If this item is used in a Single Injection report, the output will consist of a table containing the GPC time slice values for the selected processed injection(s).

Customization Available

Double-click the table to customize the column properties (for example, add/remove columns, change the style, etc.).

Single GPC Distribution Plot

Provides a GPC Distribution Plot which contains a plot of

- dw/dLogM vs Fitted MW (g/mol)
- Area (%) vs Fitted MW (g/mol)

Usage	Description
Single Injection Report	If this item is used in a Single Injection report, each distribution plot from an injection will be displayed on a separate plot in the report.
Sequence Summary Report	If this item is used in a Sequence Summary report, the output will consist of a separate distribution plot, one for each selected injection in the sequence summary.

Customization Available

Table 17: Plot properties

Option	Description
Show grid lines	Select the check-box to display the axes gridlines in the calibration plot.
Show legend	Select the check-box to display the name of the injection on the top left corner of the plot.
Distribution	Define the following properties:
Color	The color of the GPC Distribution plot.
Line weight	The thickness of the GPC Distribution plot.
Show cumulative plot	Select the check-box to display the Cumulative plot on the second Y-axis. Define the following properties:
Color	The color of the Cumulative plot.
Line weight	The thickness of the Cumulative plot.

The options available in this dialog allow you to define the axes limits for the Single GPC Distribution Plot.

Table 18: Plot scaling

Option	Description
Fitted MW axis custom scaling	Select the check-box to enable fitted MW axis custom scaling (X-axis).
Minimum/Maximum	Enter a value to set the minimum and maximum MW axis limits [g/mol or Daltons].

Option	Description
dw/dLogM axis custom scaling	Select the check-box to enable dw/dLogM axis custom scaling (Y1-axis).
Minimum/ Maximum	Enter a value to set the minimum and maximum dw/dLogM axis limits.
Percentage area axis custom scaling	Select the check-box to enable Percentage area axis custom scaling (Y2-axis).
Minimum/ Maximum	Enter a value to set the minimum and maximum Percentage area axis limits (%).

GPC Distribution Plot Overlaid

Provides a GPC Distribution Plot Overlaid which contains overlaid plots of

- dw/dLogM vs Fitted MW (g/mol)
- Area (%) vs Fitted MW (g/mol)

Usage	Description
Single Injection Report	If this item is used in a Single Injection report, all the distribution plots from an injection will be displayed on one plot in the report.
Sequence Summary Report	If this item is used in a Sequence Summary report, all the distribution plots from all selected injections will be displayed on one plot in the report.

Customization Available

Table 19: Plot properties

Option	Description
Show grid lines	Select the check-box to display the axes gridlines in the calibration plot.
Show legend	Select the check-box to display the name of the injection on the top left corner of the plot.
Injection Colors	Define the color of the GPC Distribution plot (and cumulative plot if selected) for each individual injection # (1- 8).
Distribution	Define the following properties:
Color	The color of the GPC Distribution plot.
Line weight	The thickness of the GPC Distribution plot.
Show cumulative plot	Select the check-box to display the Cumulative plot on the second Y axis. Define the following properties:

Option		Description
	Color	The color of the Cumulative plot.
	Line weight	The thickness of the Cumulative plot.

Table 20: Plot properties

Option		Description
Show grid lines		Select the check-box to display the axes gridlines in the calibration plot.
Show legend		Select the check-box to display the name of the injection on the top left corner of the plot.
Injection Colors		Define the color of the GPC Distribution plot (and cumulative plot if selected) for each individual injection # (1- 8).
Distribution		Define the following properties:
	Line weight	The thickness of the GPC Distribution plot.
Show cumulative plot		Select the check-box to display the Cumulative plot on the second Y-axis. Define the following properties:
	Line weight	The thickness of the Cumulative plot.

The options available in this dialog allow you to define the axes limits for the GPC Distribution Plot Overlaid.

Table 21: Plot scaling

Option	Description
Fitted MW axis custom scaling	Select the check-box to enable fitted MW axis custom scaling (X-axis).
Minimum/Maximum	Enter a value to set the minimum and maximum MW axis limits [g/mol or Daltons].
dw/dLogM axis custom scaling	Select the check-box to enable dw/dLogM axis custom scaling (Y1-axis).
Minimum/ Maximum	Enter a value to set the minimum and maximum dw/dLogM axis limits.
Percentage area axis custom scaling	Select the check-box to enable Percentage area axis custom scaling (Y2-axis).
Minimum/ Maximum	Enter a value to set the minimum and maximum Percentage area axis limits (%).

Advanced LS-Specific Items

The available LS-specific report items report the GPC/SEC results based on the advanced LS calibration and calculations.

- GPC/SEC LS Results Table
- GPC/SEC System Calibration Results

Report Type Selection Guide

The following tables outline the GPC/SEC report items and their use in the three different report types.

Table 22: GPC/SEC column calibration specific report types

GPC/SEC Column Calibration Specific Items	Injection	Sequence	Cross Sequence
GPC Column Calibration Details Table	✔	-	-
GPC Calibration Points Table	✔	-	-
Single GPC Calibration Plot	✔	-	-
GPC Calibration Plot Overlaid	✔	✔	✔

Table 23: GPC/SEC analysis specific report types

GPC/SEC Analysis Specific Items	Injection	Sequence	Cross Sequence
Peak Results Table	✔	-	-
Peak Results Summary Table	-	✔	✔
MW Ranges Table	✔	-	-
MW Ranges Summary Table	-	✔	✔
Percentage Fractions Table	✔	-	-
Percentage Fractions Summary Table	-	✔	✔

GPC/SEC Analysis Specific Items	Injection	Sequence	Cross Sequence
Peak Results Table – First Peak	✔	-	-
Peak Results Summary Table – First Peak	-	✔	✔
MW Ranges Table – First Peak	✔	-	-
MW Ranges Summary Table – First Peak	-	✔	✔
Percentage Fractions Table – First Peak	✔	-	-
Percentage Fractions Summary Table – First Peak	-	✔	✔

The following table contains recommendations for report types for different requirements:

What is required?	Recommendation for	
	Report Type	GPC/SEC Report Item
A detailed report per injection.	Injection Report	
A single report that provides a summary for the selected injections in a sequence in a project.	Single Sequence Summary	Summary table and overlaid plot
A single report that provides a summary for the selected injections across a number of sequences in a project.	Cross Sequence Summary	Summary table and overlaid plot

The Default Report Templates Supplied

A series of report templates that are specific to GPC and SEC applications are installed as part of the product installation. The report templates are installed to the central location for default report templates.

The report templates consist of two sets, one designed for typical GPC applications and the other for SEC applications.

Each template set is supplied in A4 and Letter paper sizes

The filenames of the template in the two sets supplied are:

Table 24: GPC Report Templates

GPC report type	Description	Template filename
Sample Analysis Injection		
Concise	Provides details on a per sample injection basis	GPC_Sample_Analysis
		GPC_Sample_Analysis_Letter
Full		GPC_Sample_AnalysisLong
		GPC_Sample_AnalysisLong_Letter
Sequence Summary		
Concise	Provides summary reports for a series of injections in the same sequence	GPC_SeqSummary
		GPC_SeqSummary_Letter
Full		GPC_SeqSummaryLong
		GPC_SeqSummaryLong_Letter
Cross Sequence Summary		
Concise	Provides summary reports for a series of injections across sequences	GPC_CrossSeqSummary
		GPC_CrossSeqSummary_Letter
Full		GPC_CrossSeqSummaryLong
		GPC_CrossSeqSummaryLong_Letter
Column Calibration Report		
	Provides the column calibration used for the selected injection	GPC_Calibration
		GPC_Calibration_Letter

Table 25: SEC Report Templates

SEC report type	Description	Template filename
Sample Analysis Injection	Provides details on a per sample injection basis	SEC_Sample_Analysis SEC_Sample_Analysis_Letter
Sequence Summary	Provides a summary report for a series of injections in the same sequence	SEC_SeqSummary SEC_SeqSummary_Letter
Cross Sequence Summary	Provides a summary report for a series of injections across sequences	SEC_CrossSeqSummary SEC_CrossSeqSummary_Letter
Column Calibration Report	Provides the column calibration used for the selected injection	SEC_Calibration SEC_Calibration_Letter

5 Working with the GPC/SEC Software

This chapter describes in detail conventional and advanced workflows using the GPC/SEC software add-on (for example, setup of processing methods, data analysis, results review, etc.).

Workflow for Data Analysis

Once data is available to process in a project, the workflows for performing GPC/SEC analyses can be broadly summarized into the following:

1. Defining a processing method.
2. Generating a GPC/SEC column calibration (conventional approach) or system calibration (LS advanced approach) linked to the processing method.
3. Reviewing the results of the GPC/SEC column calibration or system calibration depending on application.
4. Processing injections using the calibrated and saved processing method.
5. Reviewing the results of the processed injections.

Working with GPC/SEC Processing Methods

Processing Methods in GPC/SEC Data Analysis

Processing methods are used in the data analysis context. They contain the information and parameters needed to process the data and to generate results.

For the GPC/SEC data processing three different default processing methods are available:

- GPC/SEC (includes only conventional data processing, column calibration options)
- GC/LC Quantitative + GPC/SEC (includes only conventional data processing, column calibration options)
- GC/LC Quantitative + GPC/SEC + LS Bulk (includes conventional and advanced LS data processing)

These default GPC/SEC processing methods can be used as a starting point to create your individual processing method for the standard and/ or advanced GPC/SEC data processing.

Workflow

1 According to the detection type, use the appropriate processing method (for information how to create a new processing method, refer to OpenLab Help and Learning Online).

   a Select a conventional GPC/SEC method for data obtained with only concentration detectors. For more information, see Conventional GPC/SEC Processing Methods on page 111.
   OR

   b Select the advanced GPC/SEC method for data obtained with light scattering detectors. For more information, see Advanced GPC/SEC Processing Method on page 135.

2 Provide the data processing parameters.

a Define the parameters used for a the standard data analysis (such as Integration Events, System Suitablity, Reports, Tools). For further information on how to work with processing methods, refer to OpenLab Help and Learning Online.

3 Define the parameters, specifically for the GPC/SEC analysis.

a Define the general GPC/SEC parameters:

Signal to use	Multiple detector signals can be collected for injections at the same time, but only one concentration detector signal can be processed by the GPC/SEC software add-on at any one time generate GPC/SEC results. E.g. the refractive index (RI) signal from a RI / UV combination or a single UV signal from multiple UV signals. To process sample injections, the detector signal used to generate a GPC/SEC column calibration must be present in the sample injections. For a conventional processing method located under: **GPC/SEC** > **GPC/SEC Conventional** > **General** tab For an advanced processing method: **GPC/SEC** > **GPC/SEC General** **NOTE:** Advanced LS data analysis requires selecting a concentration detector and an LS detector (including all acquired detection angle signals), which will be processed to generate GPC/SEC LS results.
Flow Rate Correction	Optional. This option allows injections to be corrected for variation in flow rate using the standard marker method. To use flow rate correction, a "marker component" must be included in the samples. For a conventional processing method located under: **GPC/SEC** > **GPC/SEC Conventional** > **General** tab For an advanced processing method:**GPC/SEC** > **GPC/SEC Conventional** > **General** tab
Universal Calibration (Mark-Houwink)	Optional. This calibration method can be used to account for different polymer types between the calibrant(s) used to generate a GPC/SEC column calibration and the polymer samples to be evaluated. Define the Mark-Houwink parameters K and α (alpha) for both calibrants and sample polymer types. The default values provided are for Polystyrene in THF at ambient temperature. For a conventional processing method located under: **GPC/SEC** > **GPC/SEC Conventional** > **General** tab:

b For conventional data processing, define the column calibration type to generate the **Column Calibration** located under **GPC/SEC** > **GPC/SEC Conventional** > **Column Calibration** tab. Depending on the method, certain parameters must be defined:

Column Calibration Type/ Column Calibration Parameters	Narrow Standard	Broad Hamielec	Broad Integral
Polynomial Curve Fit	Select the order of fit	Not applicable	Select the order of fit
Cal.Std. Mark Houwink parameters	Optional	Optional	Optional
Peak Identification Tab on page 113	Define this table	Not applicable	Not applicable
Broad Hamielic parameters table on page 114	Not applicable	Define this table	Not applicable
Broad Integral parameters table on page 115	Not applicable	Not applicable	Define this table

c Optional: Specify the option you wish to apply for post-analysis of integrated peaks:

MW Ranges **GPC/SEC** > **GPC/SEC Conventional** > **MW Ranges**	Enable this option and define the values for the MW limits. This will calculate the percentage of material within the specific MW ranges of an integrated peak.
Percentage Fractions **GPC/SEC** > **GPC/SEC Conventional** > **Percentage Fractions**	Enable this option and define a value [%] for the high and low fraction. This will calculate the molecular weights at specific percentage area fractions of an integrated peak.

For more details on the parameters, see section GPC/SEC Conventional on page 112.

4 Save the processing method once all parameters have been defined.

NOTE

Ensure all processing parameters are defined prior to processing injections either to calibrate or evaluate samples. If any changes are made to the processing method after for example, generating a GPC/SEC column calibration, then changes to the processing method will make the GPC/SEC column calibration inconsistent with the processing method and any processed injections will be marked as inconsistent. The injections of the GPC calibrants will need to be reprocessed to regenerate the GPC/SEC column calibration.

Conventional GPC/SEC Processing Methods

Two conventional processing methods are installed with the GPC/SEC software and can be applied to data obtained without GPC LS detectors.

- GPC/SEC
- GC/LC Quantitative + GPC/SEC

NOTE

The sections shown here are specific to the methods GPC/SEC and GC/LC Quantitative + GPC/SEC.
They will therefore only be displayed if you have loaded these methods, regardless of whether you are using the GPC/SEC software with standard or advanced functionalities.

Both conventional processing methods consist of sections used in the standard data analysis (for more information on the displayed parameters, refer to OpenLab Help and Learning Online). These sections are:

- General
- Integration Events
- Compounds
- System Suitability
- Reports
- Tools

Section GPC/SEC contains parameters for:

- GPC/SEC Conventional on page 112
- GPC/SEC Column Calibration on page 117

NOTE Methods based on an GPC/SEC add-on version older than 2.0 can also be used with 2.0. Only the naming of the sections have changed.

GPC/SEC Conventional

General

General	
Signal	Under **Signal**, select the signal type that will be used to generate a GPC/SEC calibration and for the GPC/SEC analysis. The GPC/SEC calibration and analysis must use the same signal.
Flow Rate Correction	
Use flow rate correction	This option allows samples to be corrected for variation in flow rate using the standard marker method. To use flow rate correction, you must include a "marker component" in your samples.
FRM name	Specify the name of the flow rate marker component.
Expected RT	When processing samples, the system will expect a marker peak at the expected retention time +/- half the RT window value.
RT window	When processing samples, the system will expect a marker peak at the expected retention time +/- half the RT window value.
Sample Mark-Houwink Parameters	
K ((10e-5) dL/g)	The Mark-Houwink K value used for all samples (non-calibrants).
alpha	The Mark-Houwink alpha value used for all samples (non-calibrants).

Column Calibration

Calibration Type		
Column calibration type	Select the type of column calibration you wish to generate:	
	Narrow Standard	Requires a series of Narrow Standards of known M_p.

	Broad Hamielic	This method utilizes a Broad Standard with known M_n and M_w. The Hamielic method assumes that the calibration is linear. The software performs a trial and error search such that the calculated values of **Mn** and **Mw** match those documented for the Standard. The *Maximum Number of Searches* (iteratons), together with a *Tolerance Value* for **Mn** and **Mw**, expressed as a percentage of those Molecular Weights need to be defined in the Broad Hamielic Parameters tab.
	Broad Integral	Requires a characterized Standard with known MW at specific Wt%.
Polynomial curve fit	Defines the polynomial curve fit order that will be applied to the column calibration. For a Broad Hamiliec calibration a 1st order polynomial is automatically applied and cannot be changed.	
Cal. Std. Mark-Houwink Parameters		
K ((10e-5) dL/g)	The Mark-Houwink K value used for all calibrant samples.	
alpha	The Mark-Houwink alpha value used for all calibrant samples.	

Peak Identification

This tab is specific to the **Narrow Standard** calibration option.

Peaks that are not given a molecular weight will not be used for identification and for the generation of the column calibration.

The following columns for the Peak Identification table are available:

RT (min)	Retention time of the peak. It corresponds to the time at the peak apex.
Mp (g/mol)	The user assigned peak MW in g/mol (= Da, Dalton).
Peak RT window (min)	The window in minutes around the expected retention time that defines the range in which the peak will be identified.
Sample name	The sample name of the sample from which the data point has been added.
Signal	The detector signal name of the sample from which the data point has been added.
Source chromatogram	The source chromatogram of the injection from which the data point has been added.
Source Chromatogram data sequence	The data sequence containing the source chromatogram.

Source Chromatogram project	The name of the project containing the source chromatogram data sequence.
Use point	Defines if the point is to be included in the calculation of the line of fit of the GPC/SEC calibration.

Choose the Displayed Columns in the Table

1 Click the Column Chooser symbol in the top left corner of the window.

The **Choose columns** dialog opens.

2 Select the columns that you want to be displayed.

3 Click **OK**.

Context Menu Options

The right-click context menu offers the following options:

- To copy the table to the clipboard, select **Copy to Clipboard**.
- To export the table, select **Export to file...**. You can choose between the following file formats:
  - Comma separated value (*.CSV)
  - Excel worksheet (*.XLS)
  - Word document (*.DOC)
  - PDF file (*.PDF)
- To add peaks from the currently focused injection, select **Add peaks from chromatogram**.
- To manually add a peak, select **Add peak**.
- To delete a selected peak, select **Delete selected peak(s)**.

Broad Hamielec Parameters

The **Broad Hamielec** method utilizes a **Broad Standard** with known M_n and M_w. The Hamielic method assumes that the calibration is linear. The software performs a trial and error search such that the calculated values of M_n and M_w match those documented for the standard (see certificate). The maximum number of searches or iterations together with a tolerance value for M_n and M_w, expressed as a percentage of those molecular weights need to be defined.

Target Tolerance	The target tolerance is expressed as a percentage of the known molecular weights.
Max iterations	The maximum number of iterations to use in the search process determining the best calibration line to achieve the target M_n and M_w values within the defined target tolerance.
Target Mn average	The target M_n values of the calibrant sample to be used.
Target Mw average	The target M_w values of the calibrant sample to be used.

Broad Integral Setup

A **Broad Integral** calibration involves the use of a single well characterized **Broad Standard** i.e. with a large dispersity value to ideally calibrate the whole separation range of the utilized column or column set. The standard to be used must have a table detailing the % cumulative weight fraction and either log molecular weight or molecular weight values supplied by the manufacturer of the standard.

Slice MW (g/mol)	The slice molecular weight in g/mol (= Da, Dalton) for the corresponding percentage weight fraction.
Percentage weight	The percentage weight fraction of the MW slice.

Context Menu Options

The right-click context menu allows you to add new broad integral slices or delete existing slices. In addition, you can paste an existing table from another program such as Excel or export the table by copying to the clipboard or save it as a file. You can choose between the following file formats:

- Comma separated value (*.CSV)
- Excel worksheet (*.XLS)
- Word document (*.DOC)
- PDF file (*.PDF)

MW Ranges

Enable the option **Calculate MW ranges** to generate a MW range report for each peak processed in a sample chromatogram.

Any number of MW ranges can be defined in the table. A new MW range can be added by using the right-click context menu. In addition, the current ranges can be copied to the clipboard or selected ranges can be deleted.

M+ denotes the actual maximum molecular weight specified in the method for a sample.

M- denotes the actual minimum molecular weight specified in the method for a sample.

If you define a range as M+ to M- then this is a way of reporting the maximum and minimum molecular weights of each sample.

High MW limit (g/mol)	The high limit MW value is specified in g/mol (= Da, Dalton).
Low MW limit (g/mol)	The low limit MW value is specified in g/mol (= Da, Dalton).
MW Range Name	An optional text label that provides a way to identify specific MW ranges in a report.

Percentage Fractions

The option Calculate percentage fractions allows the calculation of molecular weights at specific percentage area fractions of a sample peak.

Use the right-click context menu of the table to add, copy or delete values for the percentage fractions:

High fraction %	The high percentage fraction.
Low fraction %	The low percentage fraction.

The percentage values for the high and low fractions do not need to be the same.

GPC/SEC Column Calibration

The tabs in the GPC/SEC Column Calibration section show information of the calibration.

GPC Calibration Points on page 117	Displays the current column calibration data points table and associated parameters.
GPC Calibration Plot on page 118	Comprises of a read-only plot of the data displayed in the GPC calibration points tab.
GPC Calibration Details on page 119	Displays details about the column calibration data and how it was derived.

GPC Calibration Points

In the GPC Calibration Points tab, you can choose the columns that are shown in the GPC/SEC calibration points table. For example, the following columns are available:

RT corrected (min)	Retention time of the peak in minutes corrected for changes in the flow rate. If use flow rate correction is off in the method, then this value is the same as the value in the corresponding RT actual field.
RT actual (min)	The actual uncorrected retention time of the peak in minutes. It corresponds to the time at the peak apex.
Assigned MW (g/mol)	• Narrow Standard The MW value in g/mol (= Da, Dalton) corresponding to the RT value of the peak nearest to the entry in the Peak Identification table. • Broad Hamielec The MW value in g/mol (= Da, Dalton) corresponding to the start and end points of the calculated line of fit. • Broad Integral The slice MW for the individual fractions.
Log MW	The logarithm to the base 10 of the assigned MW value.
Sample name	Sample name of the injection as entered in the sequence.
Source Chromatogram	The source chromatogram of the injection from which the data point has been added.
Source Chromatogram data sequence	The data sequence containing the source chromatogram.
Source Chromatogram project	The name of the project containing the source chromatogram data sequence.
Signal	Name of the signal on which the peak is integrated.
Percent error	The percent ratio between the predicted and actual MW values.

Residual	The difference between the actual MW value and the predicted MW value.
Predicted MW (g/mol)	The predicted MW in g/mol (= Da, Dalton) of the data point calculated from the calibration curve.
FRM RT (min)	The flow rate marker retention time in minutes if flow rate correction is being used.

Export Calibration Points

The context menu of the GPC Calibration Points window offers the possibility to export the table. You can copy the table content to the clipboard or save it as a file. You can choose between the following file formats:

- Comma separated value (*.CSV)
- Excel worksheet (*.XLS)
- Word document (*.DOC)
- PDF file (*.PDF)

GPC Calibration Plot

The GPC Calibration Plot tab shows the generated GPC/SEC column calibration.

Zooming and Scrolling

To zoom into a specific section of the calibration plot, you can simply drag the mouse over the required section while holding down the left mouse button. To scroll the graph, hold the right mouse button down and drag.

To zoom out, double-click the plot using the left mouse button or right-click with the right mouse button and select the Auto scale menu item from the context menu.

Tooltip

When the mouse cursor is over a data point in the calibration plot, a tool tip displays the following information:

- The retention time (min) of the data point.
- The MW (g/mol) assigned to the data point.
- The sample name of the source chromatogram.

- The filename of the source chromatogram.

The values are taken from the current GPC/SEC column calibration displayed in the GPC calibration points tab of the method.

The Retention Time value displayed is the value displayed in the RT corrected column.

Export GPC Calibration Plot

The right-click context menu allows you to export the plot as a graphic. You can copy the plot to the clipboard or save it as a file.

GPC Calibration Details

The GPC Calibration Details tab shows the generated GPC/SEC column calibration details.

The following values are displayed:

Administration information	
Calibration type	The column calibration type. Either Narrow Standard, Broad Hamielic, or Broad Integral.
Signal	Name of the signal used to create the column calibration.
Calibration Mark-Houwink parameters	
K ((10e-5) dL/g)	The Mark-Houwink K value for the column calibration.
Alpha	The Mark-Houwink Alpha value for the column calibration.
Curve fit	
Order of curve fit	The polynomial curve fit order.
Curve fit equation	The equation of the calibration curve.
Curve fit statistics	
Residual sum of squares	The sum of the squares of residuals. This is a measure of the discrepancy between the data and the curve. A small RSS indicates a better fit of the calibration curve to the data points.
Coefficient of determination	A statistical measure of how close the data is to the fitted curve.
Linear correlation coefficient	The correlation coefficient r measures the strength and direction of the linear relationship between the data values. The value will always be between +1 and -1. For a GPC/SEC column calibration, values should be tending to -1.
Corrected sum of squares	The sum of the squared differences of the assigned MW from the overall mean.

Standard Y error estimate	The standard error estimate of the residuals.
FRM information	
FRM name	The flow rate marker name.
FRM RT (min)	The retention time in minutes of the flow rate marker.
FRM source	The data source chromatogram for the flow rate marker.
Calibration limit information	
High MW limit RT (min)	The retention time in minutes for the high MW limit of the calibration.
Low MW limit RT (min)	The retention time in minutes for the low MW limit of the calibration.
High limit MW (g/mol)	The high limit MW value of the calibration in g/mol (= Da, Dalton).
Low limit MW (g/mol)	The low limit MW value of the calibration in g/mol (= Da, Dalton).

Export GPC Calibration Details

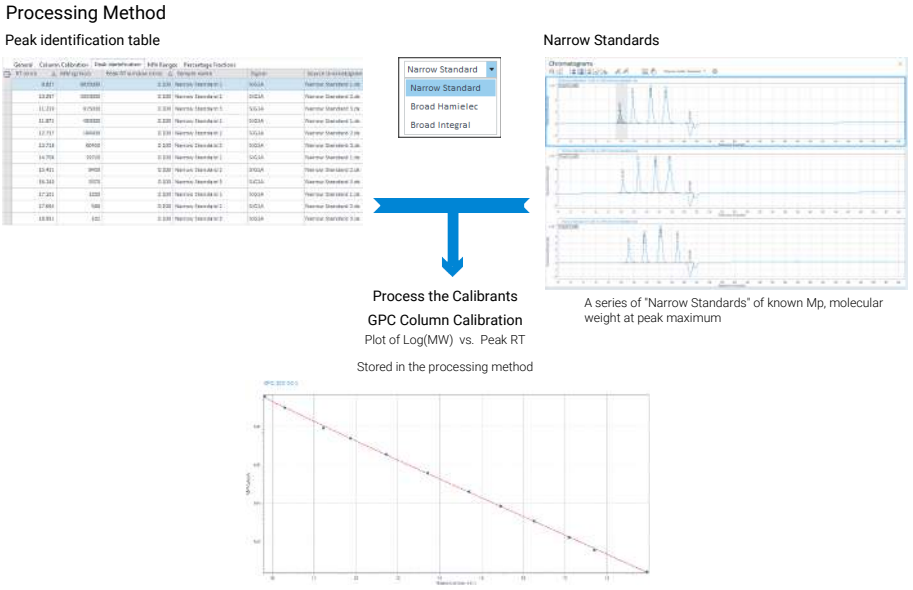
The right-click context menu allows you to export the calibration details. You can copy the calibration details to the clipboard or save it as a text file.

Workflow for a GPC/SEC Column Calibration

Instruction steps to generate a GPC/SEC column calibration:

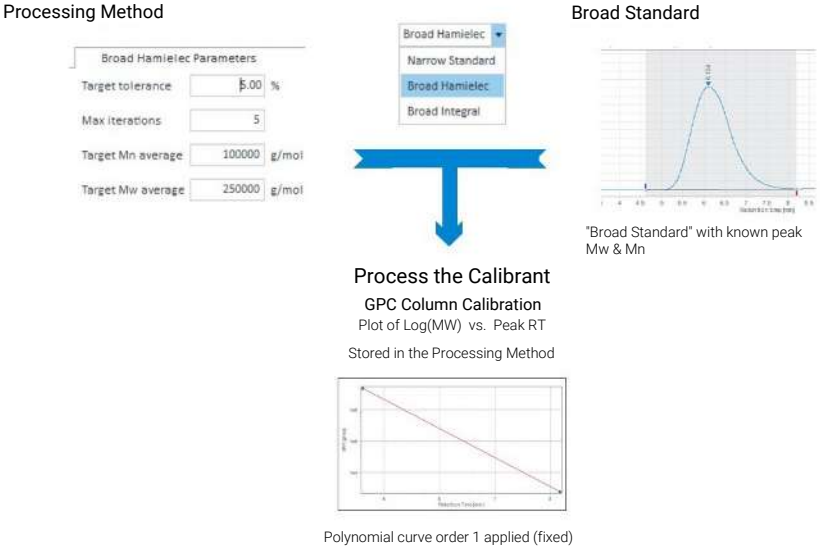
1 Set up the GPC/SEC processing method:

- For a Narrow Standard column calibration: Set up the Peak Identification on page 113 table. For each of the calibrant, enter the expected retention time of the peak maximum and its associated M_p (supplied by the certificate of analysis of the calibrants).



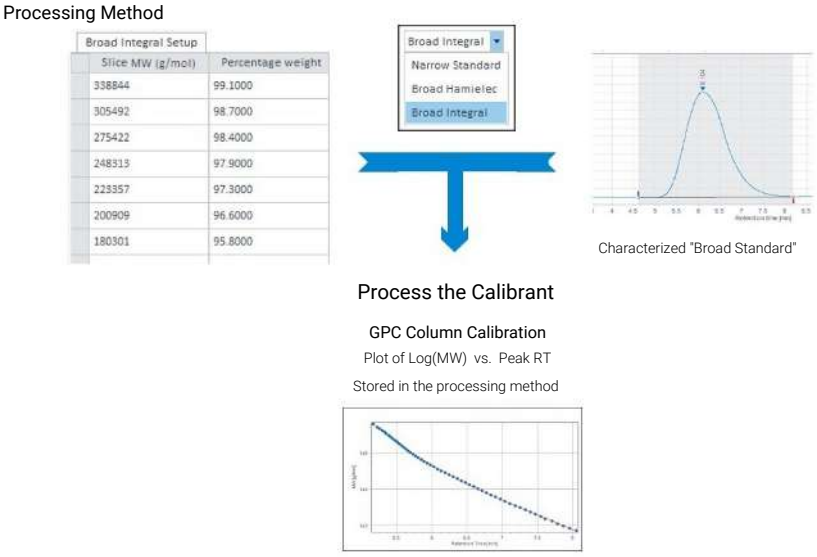
OR

- For a Broad Hamielec column calibration: Set up the Broad Hamielec parameters on page 114 table. For each of the calibrant, enter the target tolerance, the maximum number of search iterations, and the target M_n average and target M_w average (supplied by the certificate of analysis of the calibrants).



OR

- For a Broad Integral column calibration: Set up the Broad Integral Setup on page 115 table. For each of the calibrant, enter the cumulative weight fraction (%) and the slice molecular weight (g/mol) (supplied by the certificate of analysis of the calibrants).



2 Generate the column calibration.

3 Review the generated column calibration.

4 Fine-tune the column calibration parameters.

Set up a GPC/SEC Processing Method for Narrow Standard Column Calibration

Define the following parameters:

Location: Processing Method > GPC/SEC > GPC/SEC Conventional > General tab

1 Select the default concentration detector signal to use (typically UV or RID).

2 Decide if you want to use flow rate correction.

3 If using the Universal Calibration option, enter the Mark-Houwink Parameter for the utilized calibrant.

Location: Processing Method > GPC/SEC > GPC/SEC Conventional > Column Calibration tab

1 Select Column calibration type Narrow Standard.

2 Select the fit function in the field Polynomial curve fit that will be applied to the calibration data points.

NOTE

The GPC/SEC Software add-on supports linear and polynomial regression models. Typically, linear regression (select 1) or 3rd and 5th order polynomial fit functions are used in the GPC/SEC column calibration approach.

3 If using the Universal Calibration option, enter the Mark-Houwink Parameter for the utilized calibrant.

4 Save the processing method.

5 Ensure the calibrant injections to be used are linked to the GPC/SEC processing method to be calibrated.

Set up the Peak Identification Table

There are two ways defining the parameters in the Peak Identification table.

Set up Parameters using a Set of Calibrants

The method requires a set of injections of the narrow standards that are to be used under these conditions. The injections need to be either integrated using the automated integrator to identify the calibrant peaks or, defined using the manual integration tool.

Peak Identification for the Calibrant Set:

1. Select the Chromatogram view and define the start and end of each peak and the software will determines the peak maxima of each calibrant. The peak start and end do not need to be defined exactly as it is only the retention time at the peak maximum that is required for each peak.

2. If using flow correction, ensure the expected peak maximum of the flow marker component has been defined in the GPC/SEC Conventional > General tab of the processing method.

Peak Identification for each Calibrant:

1. Under Method view > GPC/SEC Conventional section, select the Peak Identification tab.

2. Ensure the first calibrant is selected in the run list and right-click in the Peak Identification tab area.

3. Select Add peaks from chromatogram from the right-click menu.

   The peaks identified in the injection will be added to the Peak Identification table of the processing method.

4. Assign the M_p for each peak to be used.

   It doesn't matter if peaks identified in the chromatogram are added to the Peak Identification table that are not from the Narrow Standards. These peaks can be either deleted from the final Peak Identification table or ignored. Any peaks in the table which have not been assigned M_p value are ignored by the system when generating a GPC/SEC column calibration.

5. Define the Peak Identification Window.

The criteria for peak identification is:

- The expected retention time of the peak +/- [(The Retention Time window)/2].
- The default value is 0.1 minute giving a default window of +/- 3 seconds.

6 Repeat the process for each subsequent narrow standard calibrant.

Manually Enter Parameters From a Set of Calibrants

The method requires a predetermined table of the expected peak retention times and their associated M_p values.

For the Calibrant Set:

1. In the Processing Method view, select the GPC/SEC > GPC/SEC Conventional > Peak Identification tab.
2. Enter the retention time of the peak maximum of each calibrant peak and its associated M_p value.
3. In Peak Identification window, define the following criteria:
   - The expected retention time of the peak =
   - +/- [(Retention Time window) / 2].

   The default value is 0.1 minute giving a default window of +/- 3 seconds.
4. Once the peak identification table has been completed, save the processing method.
5. If not already done so, ensure the injections are linked to the processing method.

Set up a GPC/SEC Processing Method for Broad Hamielec Column Calibration

Define the following parameters:

Location: Processing Method > GPC/SEC > GPC/SEC Conventional > General tab

1 Select the default concentration detector signal to use (typically UV or RID).

2 Decide if you want to use flow rate correction.

3 If using the Universal Calibration option, enter the Mark-Houwink Parameter for the sample.

Location: Processing Method > GPC/SEC > GPC/SEC Conventional > Column Calibration tab

1 Select Column calibration type Broad Hamielec.

2 If using the Universal Calibration option, enter the Mark-Houwink Parameter for the sample.

NOTE

The GPC/SEC Software add-on supports only linear regression for the Broad Hamielec column calibration approach. The Polynomial curve fit field is grayed out and 1 is automatically used when selecting Broad Hamielec.

3 Save the processing method.

Set up the Broad Hamielec Parameters Table

1 Select the Broad Hamielec Parameters table and define the following:

- The target M_n average and M_w average in g/mol from the certificate of analysis of the calibrant
- The target tolerance
- The maximum number of search iterations.

2 Save the processing method.

3 Ensure the calibrant injection to be used is linked to the processing method to be calibrated.

Set up a Processing Method for Broad Integral Column Calibration

Define the following parameters:

Location: Processing Method > GPC/SEC > GPC/SEC Conventional > General tab

1 Select the default concentration detector signal to use (typically UV or RID).

2 Decide if you want to use flow rate correction.

3 If using the Universal Calibration option, enter the Mark-Houwink Parameter for the sample.

Location: Processing Method > GPC/SEC > GPC/SEC Conventional > Column Calibration tab

1 Select Column calibration type Broad Integral.

The Polynomial curve fit parameter and Broad Integral Setup table are displayed.

2 Select the fit function in the field Polynomial curve fit that will be applied to the calibration data points.

NOTE

The GPC/SEC Software add-on supports linear and polynomial regression models. Typically, linear regression (select 1) or 3rd and 5th order polynomial fit functions are used in the GPC/SEC column calibration approach."

3 If using the Universal Calibration option, enter the Mark-Houwink Parameter for the sample.

4 Save the processing method.

Defining the Broad Integral Table

This Broad Integral Setup tab consists of a grid containing Slice MW (g/mol), Percentage Weight data pairs.

1 Edit the Integral table (% Cumulative Weight Fraction and Slice Molecular Weight) and enter the values supplied on the certificate of analysis for the calibrant.

If the integral table is available as a text file with the format:

```
<Slice MW value 01 <tab> <Percentage Weight value 01>
<Slice MW value 02 <tab> <Percentage Weight value 02>
...
<Slice MW value N <tab> <Percentage Weight value N>
```

a Copy the text file to the Windows clipboard.

b Right-click the **Broad Integral Setup** grid to open the context menu and select **Paste**. The table is added below the current last row of the existing table. Any rows without the tab separator are ignored.

c Alternatively, to manually enter the data table, open the context menu and select **Add broad integral**.

d To delete a row, select the row, open the context menu, and select **Delete selected broad integral(s)**.

2 Save the processing method.

3 Ensure the calibrant injection to be used is linked to the processing method to be calibrated.

Generate the GPC/SEC Column Calibration

1 Select the **Injection List** window and ensure the **Sample Type** is set to **Cal. Std.** for the injections to be used to generate the GPC/SEC column calibration.

2 For the first of the calibrant injections to be used, ensure the **Run Type** is set to **Clear all calibration**.

3 In the **Run List**, select all the calibrants.

4 Select **Reprocess selected injections**.

✓ For a Narrow Standard column calibration, any peaks identified in each of the calibrants injections that match the peak retention time values in the **Peak Identification** table are assigned with the associated M_p from the Peak Identification table and added to the **GPC/SEC Column Calibration** section.

Processing Completed

On completion of processing all **Cal. Std.**, the data points are added to the GPC Calibration Points table and the curve fit defined in the method applied to the data points.

The column calibration has now been created and can be reviewed.

Review the Generated GPC/SEC Column Calibration

1 In the Processing Method, under GPC/SEC > GPC/SEC Column Calibration, review the calibration on the following tabs.

A column calibration generated using the Hamielec method will consist of a straight-line fit with two data points indicating the retention time limits of the calibrant used.

GPC Calibration Points	Displays the current column calibration data points table and associated parameters.
GPC Calibration Plot	Comprises of a read only plot of the data displayed in the GPC Calibration Points Tab.
GPC Calibration Details	Displays details about the column calibration data and how it was derived.

Fine-Tune GPC/SEC Column Calibration Parameters

For the generated column calibration (applies only to Narrow Standard and Broad Integral column calibration), the following modifications may be necessary:

- Change to the curve fit
- Deselection of calibration data points
- Addition or deletion of a data point
- Change to the MW of a data point
- Change to the Mark-Houwink K and Alpha parameters
- Change to the flow rate marker retention time

If the generated Broad Hamielec column calibration requires modification, edit the parameters in the Broad Hamielec parameters table and reprocess the calibrant.

To regenerate the calibration with the new parameters, all changes must be applied to the processing method and the calibrants must be reprocessed.

Advanced GPC/SEC Processing Method

For data analysis obtained with light scattering detectors, the GPC/SEC software add-on with advanced functionalities (G7861AA) comes pre-installed with the method GC/LC Quant + GPC/SEC + LS Bulk. This advanced processing method includes standard data analysis (conventional) and the advanced options for the essential GPC LS detector calibration and LS specific calculation options to determine the bulk molecular weight (M_W) and size information (R_h) from collected LS and DLS data, respectively.

NOTE The acquisition of R_h signals and the calculation of bulk R_h values is only possible for MDS Dual Angle LS detectors with DLS option (only for G7809A).

NOTE The sections shown here are specific to the method GC/LC Quant + GPC/SEC + LS Bulk.
They will therefore only be displayed if you have loaded this method.

The method consist of sections used for the standard data analysis (for more information on the displayed parameters, refer to OpenLab Help and Learning Online). These sections are:

- General:

  The Alignment tab in section Signals is only specific for advanced LS data processing. Here, you determine the inter detector delay between the used concentration detector (for example, RID or UV) and the used LS detector. For more information, refer to General on page 135.
- Integration Events
- Compounds
- System Suitability
- Reports
- Tools

General

The General section of the processing method is displayed for all three GPC/SEC specific processing methods. But only when working with the advanced GC/LC Quant + GPC/SEC + LS Bulk method, you must define a specific signal alignment.

NOTE The parameters available in section **Properties** and **Signals** are used in standard data analysis of the OpenLab CDS. For more information on the displayed parameters, refer to OpenLab CDS core functionality.

Properties

Info	Displays general information about the method.
Global	Select the ChemStation or EZChrom integrator.

Signals

Scaling	Select if you want to use fixed chromatogram scaling.
Alignment	The **Alignment** tab is important for advanced LS data processing. In the **Use delay** column, select the utilized concentration detector (e.g. RID or UV) and the LS detector and provide the retention time at peak maximum (Vp) for the identified peak in both detectors. **NOTE:** Use a narrow standard to determine the inter detector delay. If you use conventional GPC/SEC analysis (column calibration), you can ignore the **Alignment** tab.
Smoothing	Set the **Global Signal Settings** and select the check boxes to override global signal parameters for specific signals.
Blank Substraction	Set the parameters for injections with blank subtraction applied.
Reference Chromatogram	Displays the reference Chromatogram table.

GPC/SEC

Section **GPC/SEC** contains parameters for:

- GPC/SEC General on page 137
- GPC/SEC Conventional on page 112, similar to conventional GPC/SEC methods
- GPC/SEC Column Calibration on page 117, similar to conventional GPC/SEC methods
- GPC/SEC Advanced on page 137

GPC/SEC General

This specific method configuration is only displayed if you have activated the advanced functionalities of the GPC/SEC add-on (G7861AA) and are working with the GC/LC Quant + GPC/SEC + LS Bulk method.

Analysis Type	
Select the type of analysis that will be applied to generate GPC/SEC results.	
Conventional	Select this option to apply the column calibration approach.
Advanced LS Bulk	Select this option to apply light scattering (LS) calibration and calculations.
Detectors	
Concentration Detector	From the drop-down list, select the used concentration detector.
LS Detector	From the drop-down list, select the used LS detector. If the loaded data does not contain an LS detector signal, only None is available.

NOTE If the Conventional analysis type is used, you can only select a concentration detector signal (typically RID or UV) and the LS detector option is grayed out. Only one concentration detector signal can be used to process the data.

NOTE If you wish to perform advanced LS calculation to determine the absolute bulk molecular weight (M_W) of a compound, the collected data must include a concentration detector signal and LS detector signals.

GPC/SEC Advanced

This specific method configuration is only available for the advanced GPC/SEC add-on (G7861AA) and the following method GC/LC Quant + GPC/SEC + LS Bulk.

If you are using the standard GPC/SEC add-on (G7860AA), you can load the advanced Bulk method GC/LC Quant + GPC/SEC + LS Bulk and also link it to a data set, however only the conventional method parameters can be edited. The GPC/SEC Advanced method section is read-only.

General tab

The General tab provides parameter for advanced LS calibration and calculations and is only available when working with the advanced GC/LC Quant + GPC/SEC + LS Bulk method:

System Calibration Settings	
Peak Expected Retention Time	Enter a value for the expected retention time [min] of the peak used in the system calibration process.
Absolute Time Window	Enter a value for the absolute time window [min] used to identify the peak for the system calibration.
Relative Time Window	Enter a value for the relative time window [%] used to identify the peak for the system calibration.
Use all compounds concentration area	If enabled, the detector constant for concentration detectors (typically RID or UV) is calculated based on the sample concentration entered in the Injection List window and the identified peaks in the Chromatograms window. This is particularly important for calibrants that produce multiple peaks, where all peak areas must be considered to accurately determine the monomer peak concentration. This monomer concentration is then used to calculate the correct detector constant. **NOTE:** For example, the BSA (bovine serum albumin) calibrant – commonly used in aqueous applications – typically produces a chromatogram with at least three peaks (monomer, dimer, and higher-order species). While the total peak area reflects the overall sample concentration (as entered in the injection list), the detector constant is calculated based solely on the monomer peak concentration. This is determined using the Use all compounds concentration area option.
GPC Compounds	
Absolute Time Window	Enter a value for the absolute time window [min] used to generate GPC compounds out of integrated peaks in the concentration and LS signal chromatograms. The entered value will be applied on the retention time of the main peak (typically, this is the peak in the concentration signal) used to find matching peaks in other signals (typically, in the LS signals). For more details, refer to section About the GPC Compound Concept on page 139. The identified GPC compounds consequently show up in the Peak Results table of the GPC/SEC LS Results window.
Relative Time Window	Enter a value for the relative time window [%] used to generate GPC compounds out of integrated peaks in the concentration and LS signal chromatograms. The entered value will be applied on the retention time of the main peak (typically, this is the peak in the concentration signal) used to find matching peaks in other signals (typically, in the LS signals). For more details, refer to section About the GPC Compound Concept on page 139.
Analysis Settings	

Used to calculate the sample concentration or sample property parameters, such as dn/dc value or UV extinction coefficient of a GPC compound. The prerequisite is that concentration values or the sample property parameters are entered in the **Injection List** window. The results are shown in the **GPC/SEC LS Results** window. The comparison of the calculated concentration with your entered sample concentration allows to calculate the sample recovery of an eluted compound.	
Concentration	Select the option to calculate the sample property parameters. **NOTE:** Depending on the selected concentration detector (RID, UV), your entered concentration in the Injection List window will be used to calculate the sample property parameters (dn/dc value (RID) or UV ext. coeff (UV detector)).
Sample Property (dn/dc, UV Ext Coeff)	Select the option to calculate the sample concentration. **NOTE:** Your entered dn/dc value (RID) or UV ext. coeff. (UV detector) in the Injection List window will be used to calculate the sample concentration.

About the GPC Compound Concept

Advanced LS data processing requires the identification of GPC compounds, which are used as the base for the advanced LS result calculations. With the help of the **Peak Identification Time Window**, the advanced GPC/SEC software add-on searches for matching peaks in the concentration detector signal and LS detector signals assigning them to the same sample molecule (the same GPC compound). Advanced LS result calculations can only be done for samples showing peaks in both, concentration and LS signals within the provided time window.

NOTE Before you start with data processing and peak identification, you must first perform the Detector Signal Alignment on page 147 to determine the inter detector delay.

Theory

In general, a GPC compound is a list of matching peaks generated from collected data including a concentration detector signal (typically RI or UV) and LS detector signals. A GPC compound is generated out of an integrated peak in a sample chromatogram. In the processing method, in section **GPC/SEC** > **GPC/SEC Advanced** > **General** tab > **GPC Compounds**, you define the **Peak Identification Time Window** (for more information about Peak Identification, refer to OpenLab Help and Learning Online).

The sum of both, the absolute and relative time window, is applied to the retention time of the detected main peaks in the sample chromatogram (see listed RT values in results table, RT information at peak maximum).
If a main peak is first detected in the concentration signal, the specified time window is applied to all LS signals to find matching peaks within it. For each integrated peak in the concentration signal (main peaks), a GPC compound is generated. If a certain LS peak matches with the specified time window of the concentration detector peak, the LS peak will be identified as the same GPC compound. In this case, the LS results, for example the bulk M_w value, will be calculated.

NOTE

The identified GPC compounds are automatically listed in the GPC/SEC LS Results table. The LS results, such as the bulk M_w value, are displayed when both the concentration and LS signal information for the selected sample peak are available.

If a main peak is first detected in one of the LS signals, the specified time window is applied to the concentration signal and other LS signals to find matching peaks within it. An identified peak match will be assigned to the same GPC compound and, consequently, the LS results will be calculated and displayed.

If no peak match is identified between concentration and LS signals, the detected peak (either LS peak or concentration detector peak) will be identified as a new GPC compound and is added to the GPC/SEC LS Results table. However, advanced LS calculations are not performed for such identified GPC compounds missing one of the required signal information.

Examples

The following figure illustrates the GPC Compound concept.

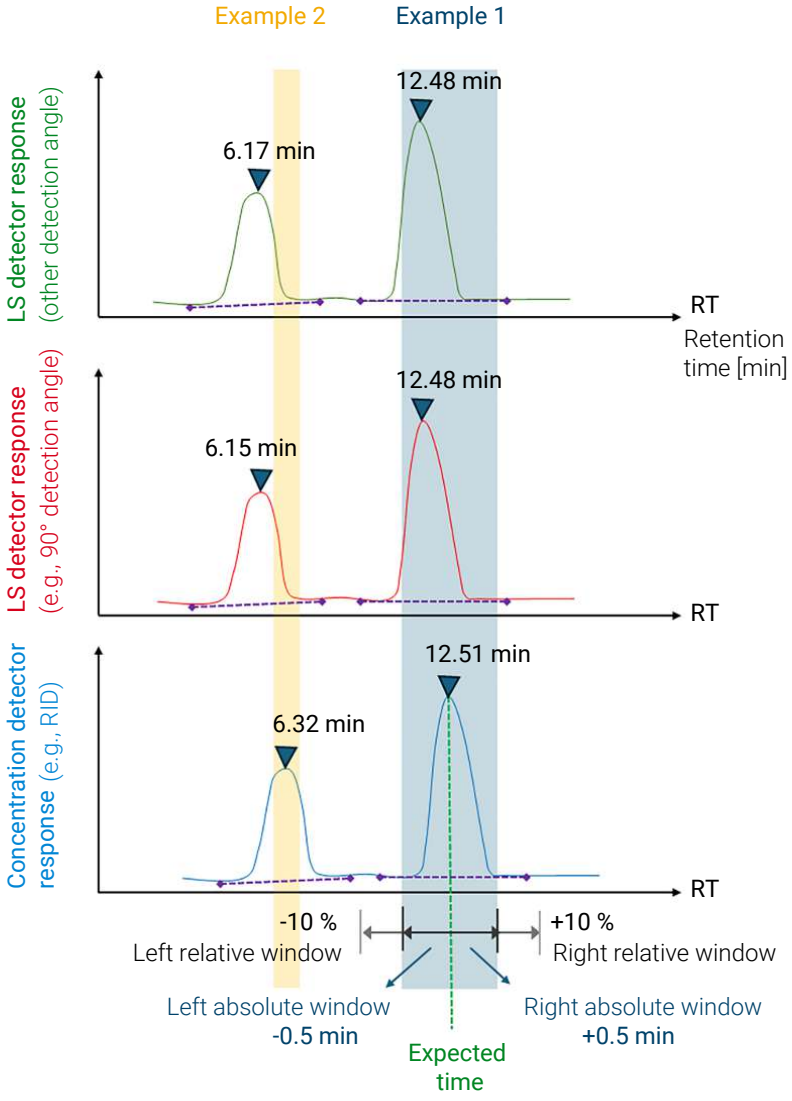


Figure 2: GPC compound concept

In **Example 1** (see figure above), the provided retention time window is high enough resulting in a peak match between the concentration detector and LS detector signals. Thus, the LS peaks are identified as the same GPC compound

that was already identified in the concentration detector chromatogram. In this case, the advanced LS calculations will be carried out. For the main peak detected at 12.5 min in the concentration signal, the bulk M_w value will be calculated and displayed in the GPC/SEC LS Results table.

In Example 2 (see figure above), the provided retention time window is not sufficient to generate a peak match, and consequently, a new GPC compound for the LS peaks is identified. As a result, the advanced LS calculations will not be carried out missing the concentration information for the identified LS peaks. The same applies to the main peak at 6.32 min in the concentration signal. For the latter, the bulk M_w value will not be calculated because there is only a concentration peak identified and no LS information available.

Solution for Example 2: If you increase the retention time window for the main RI peak around 6.32 min, this will likely result in a peak match between the concentration detector and required LS detector signals generating the same GPC compound for both signals.

LS Detector tab

In this tab, you select the desired LS detection angles used for sample analysis and LS result calculations.

Depending on used LS detector, a different number of detection angles can be displayed. The MALS detector (G7885A) will show a selection of 20 angles whereas the MDS Dual Angle LS detector will provide two angles for sample analysis.

NOTE

Under certain circumstances, for example to improve signal quality, it may be beneficial to disable certain detection angles in order to improve data processing. Especially low angles are very sensitive to impurities (particles, dust, etc.) within the mobile phase leading to a high noise and low signal/noise ratios.

System Calibration Results tab

Verify the parameters and the determined detector constants that are used for the advanced calculation of GPC/SEC LS results.

Acquisition Parameter	
Flow Rate	The flow rate of the collected data.
Calibration Parameters	
Concentration (g/L)	Concentration of the sample (entered in the Injection List window).

Molar Mass (Da)	Molecular weight of the sample (entered in the **Injection List** window).
dn/dc (mL/g)	dn/dc of the sample (entered in the **Injection List** window).
UV Extinction Coefficient ((mg/mL)-1(cm)-1)	UV extinction coefficient of the sample (entered in the **Injection List** window).
Eluent RI	Eluent refractive index (dimensionless) (entered in the **Injection List** window).
Detector Constants	
Displays the calculated detector constant for the concentration detector and the advanced LS detector. Depending on the used LS detector, a different number of entries will be displayed. For each detection angle, the user can review the calculated constant and the normalization coefficient (value in brackets). **NOTE:** The 90° detection angle is always used as reference (normalization factor set to 1) to calculate the normalization factors for all other angles. This normalization is essential because it strongly affects the determination of the radius of gyration (R_g) and calculation of results. **NOTE:** The displayed detector constants and normalization coefficients are based on the system calibration which must be performed with a narrow and well-characterized calibrant with known molecular weight (certified by light scattering measurements). For the normalization, it is required that the selected calibrant is an isotropic scatter (molecular weight below 120 kDa).	

Workflow for Advanced GPC/SEC LS Data Analysis

Workflow overview and instruction steps to generate advanced GPC/SEC LS results:

1. Load your GPC/SEC Data on page 144.
2. Set up the advanced GPC/SEC processing method on page 145.
3. Perform the Detector Signal Alignment on page 147.
4. Generate the System Calibration on page 148.
5. Review results of the System Calibration on page 150.
6. Fine-tune the System Calibration results on page 151.
7. Reprocess Sample Injections on page 152.
8. Review the LS specific results on page 157.

Load your GPC/SEC Data

To load either a complete sequence or single samples, go to the **Data Selection** screen, and select **Home** > **Load Data**.

To import data for GPC/SEC data analysis, go to the **Data Selection** screen and select **Import/Export** > **Import Raw Data**.

For more details about how to load or import data for data processing, refer to OpenLab Help and Learning Online (search for "Loading and Finding Data" and "Import Data").

Set up the Advanced GPC/SEC Processing Method

For advanced LS data processing and calculations, use the GC/LC Quantitative + GPC/SEC+LS Bulk processing method. This default method is the only method that includes method configuration items for the advanced LS data analysis (such as bulk M_w determination, bulk R_g, etc.).

NOTE

The selected method configuration determines which sections of the method are visible and can be edited in the Processing Method window.

1. In the Data Processing view, select the Processing ribbon tab.
2. To create a new processing method, click New Method.
3. Select the advanced processing method GC/LC Quantitative + GPC/SEC+LS Bulk.
4. Confirm with Create method.

5 Provide the standard data processing parameters.

a Define the parameters as used for the standard data analysis (general properties, integration events, compounds, system suitability, reports, tools) in OpenLab CDS. These parameters correspond to core functionalities of OpenLab CDS.

b Set up peak integration. This is important because only identified peaks will be considered for the advanced LS calculations and the essential system calibration. Integration parameters can be set up in several ways. For further details, refer to OpenLab Help and Learning Online (search for "Integrator Events").

NOTE

To manually add integration events in the sample chromatogram for all selected signals at once, right-click into the desired position of the chromatogram and select **Add integration event** > **Integration**. Set the integration flags close to the peak of interest. On the left side select integration on and right side of the peak select integration off.

c If you need support with identifying sample peaks, especially in the LS signals (MLS, LSD), select the **Integration Optimizer** to run the wizard.

d To utilize the manual integration, click in the **Chromatograms** window. This allows you to set the baseline for each peak individually.

6 Define the GPC/SEC-specific parameters, specifically for the *advanced LS analysis*.

a In the **GPC/SEC General** section, select **Advanced LS Bulk** as **Analysis Type** and under **Detectors** select the utilized concentration detector (typically RID or UV detector) and the LS detector (e.g. MLS1 or LSD1).

b Under **GPC/SEC Advanced** > **General**, enter a time window to identify peaks as a GPC compound.

NOTE

Only identified compounds will be shown in the **GPC/SEC LS Results** window (Peak Results table).

c Under **GPC/SEC Advanced** > **General**, define the System Calibration Settings and enter the expected peak retention time of the calibrant used for the system calibration. For more details, see Generate the System Calibration on page 148.

d Under **GPC/SEC Advanced** > **LS Detector**, deselect detection angles, if required (see also LS Detector tab on page 142).

Perform the Detector Signal Alignment

1 In the Processing Method, under **General** > **Signals**, select the **Alignment** tab.

2 To generate the essential signal alignment, select the advanced LS detector (for example MLS1) and the concentration detector (for example RID1).

3 For both detectors, provide the retention time information at peak maximum taken from the acquired LS calibrant chromatogram (run a narrow standard).

4 Click **Calculate delay from RT**.

5 In the **Home** ribbon tab, click **Reprocess All** to apply the signal alignment.

NOTE After reprocessing the retention time of the concentration, the detector signal is corrected to align perfectly with the LS detector signal. This inter-detector delay correction is essential for all further LS calculation steps.

NOTE Repeat the signal alignment after changing the concentration detector, changing column(s), changing capillary connections (changes of length and/or inner diameter affect the inter detector delay), or changing the acquisition flow rate.

Generate the System Calibration

Prerequisites

- For system calibration and data processing, you are using an LS calibrant with a narrow distribution (low PDI) and a known weight-average molecular weight (M_w certified by light scattering).
- In the **Injection List** window, provide the following sample parameter:

NOTE

Ensure that you enter the correct values, because these parameters are taken into account for the advanced LS calculations to determine values such as the absolute bulk M_w. The concentration in particular must be very accurate and you need to wait for the calibrant and samples to dissolve completely before starting the data acquisition part. Depending on the molecular weight, complete dissolution can take several hours.

1 In the **Home** ribbon tab, open the **Injection List** window.

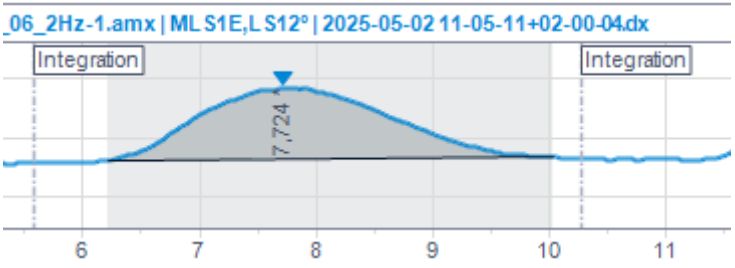
2 Select the respective sample line and ensure that the **Sample type** column is set to **Cal.Std.**.

3 Ensure that the **GPC/SEC LS Cal.Std.** column is set to **yes**. Otherwise, the system calibration will not be performed.

4 Ensure that the **System Calibration Settings** are configured correctly.

   a In the **Processing Method**, select **GPC/SEC** > **GPC/SEC Advanced** and select the **General** tab.

   b In the **Chromatograms** window, examine the peak integration of the calibrant. Note down the retention time information (RT at peak maximum) used to define the **System Calibration Settings**.



c Enter the **Peak Expected Retention Time** according to the value found in the chromatogram.

d Provide a value for the **Absolute Time Window** and **Relative Time Window**, otherwise the system calibration will not be performed successfully and no peak will be identified.

NOTE Take the peak maximum from the sample chromatogram for the LS narrow standard and enter the obtained value in the field **Peak Expected Retention Time**. Otherwise, if both fields are left with the default value 0 min, the system calibration will not calculate results for the detector constants.

5 Once all parameters have been entered correctly in the Injection List table, click **Reprocess All** in the **Home** ribbon tab.

The system calibration is created and can be reviewed.

NOTE Also for samples that are analyzed after system calibration, enter the above sample parameters in the respective column of the **Injection List** table (in the **Home** ribbon tab, open the **Injection List** window).

Review Results of the System Calibration

Once the system calibration is final, you can review the results under Processing Method > GPC/SEC > GPC/SEC Advanced > System Calibration Results tab.

1 The tab lists general information like injection volume, flow rate and the wavelength of the used LS detector. Under Calibration Parameter, the entered sample parameters (in the Injection List) are listed. Carefully review the entered values. If modifications are required, consult the injection list table and provide the correct sample parameter. Afterwards, reprocess the calibrant and review the new results for the system calibration.

2 Under Detector Constants, review the calculated detector constants for the selected concentration detector and the advanced LS detector. Depending on the used LS detector a different number of detection angles and their calculated constants are displayed. For further details, refer to section LS Detector tab on page 142.

3 If all results are correct, save the modified processing method for further use.

   a In the Processing ribbon tab, click Save Method As.

   b Select a file path.

   c Enter a file name for the modified method.

   d Click Save.

NOTE

Repeat the system calibration whenever you use a different:

- concentration detector (also for UV when a different wavelength is used),
- LS detector (or after repair: exchange of laser diode, cell, etc.),
- mobile phase (eluent).

Fine-tune the System Calibration Results

If the generated system calibration requires modifications, these changes need to also be made to the processing method and the calibrant used for system calibration.

These changes include, for example:

- Deselection of detection angles for the LS detector used, due to signal quality issues
- Correction of sample properties, due to inaccurate sample concentration, dn/dc value, UV extinction coefficient or eluent refractive index provided
- Selection of a different concentration detector, if more than one concentration detector was used for data collection
- Wrong peak assignment

To regenerate the system calibration with the new set of parameters, you need to reprocess the sample.

Reprocess Sample Injections

Once a GPC/SEC processing method has been calibrated, injections can be processed using this method. The procedure to process a sample injection is the same regardless of the method of calibrating the system.

NOTE

The GPC/SEC processing method needs to be fully defined before you perform the GPC/SEC column calibration.
Any change to the processing method after the GPC/SEC column calibration has been generated will make the calibration inconsistent with the processing method. Any processed injections will be marked as inconsistent. In this case, you must recreate the column calibration.

NOTE

The LS advanced data and sample processing requires a detector calibration (system calibration). If the system calibration is not valid or was not successfully performed before sample analysis is carried out, the processed injections will be marked as inconsistent, and no results can be reviewed.

Always use a narrow and well-characterized calibrant with known M_w (certified by LS) and ensure that the selected calibrant is an isotropic scatter (M_w below 120 kDa) to correctly determine the normalization coefficients for all detection angles. A correct determination of the normalization coefficients is the basis for the calculation of sample bulk R_g values (radius of gyration) from the angular dependency plot.

Each injection can be processed in turn or all injections in a sequence can be processed automatically.

Sample Processing Workflow

Preparations

- The GPC/SEC processing method exists and either a GPC/SEC column calibration (conventional approach) or the system calibration (LS advanced approach) was generated.

1 In the injection tree, select the injection to be processed.

2 Select **Reprocess selected injections**.

✓ The GPC/SEC results are calculated for each integrated peak in the defined signal of the selected injection.

✓ Based on the approach, you can review the GPC/SEC-specific results in different result windows.

Reviewing Data and Results

Review Results from a Single Injection

1 From section Layouts of the Home ribbon tab, select the GPC/SEC view.

2 From section Windows of the Home ribbon tab, select the desired result window.

3 From the run list of the navigation tree, select the processed injection.

✓ The results will be displayed in the window.

Review Results from a Series of Single Injection

1 From section Layouts of the Home ribbon tab, select the GPC/SEC view.

2 From section Windows of the Home ribbon tab, select the desired result window.

3 In the navigation tree, select the processed injections to be compared using the Pin function (the processed injections can be from the same or different results sets).

✓ The results of the pinned injections are now displayed in the results windows.

Review Calibration Results

The review of the calibration results is part of the Processing Method and is highly recommended. If required, you can fine-tune your calibration results.

Conventional Calibration Review

In the processing method, under GPC/SEC > GPC/SEC Column Calibration, you can review the calibration points, plots, and details. If needed, adjust the curve fit, data points and MW information, Mark-Houwink parameters and flow rate marker settings. All changes must be applied to your processing method and the calibrants need to be reprocessed. Save modified methods for future use.

For more details, refer to section Review the Generated GPC/SEC Column Calibration on page 134.

Advanced LS Calibration Review

In the processing method, under GPC/SEC > GPC/SEC Advanced > System Calibration Results tab, you can review the results, such as the injection volume, flow rate, wavelength and calibration parameters. If needed, adjust sample parameters, detector selection and LS detection angles. All changes must be applied to your processing method and the calibrants need to be reprocessed. Save modified methods for future use.

For more details, refer to section Review Results of the System Calibration on page 150.

Review Conventional GPC/SEC Results

To access the conventional GPC/SEC results for the processed injections, go to the **Home** ribbon tab, and select either **GPC/SEC** or **Results** from the **Layouts** section. Alternatively, you can select **GPC/SEC Results** from the **Windows** section.

The following GPC/SEC windows for conventional result review exist:

- GPC/SEC Results on page 55
- GPC/SEC Distributions on page 63
- GPC/SEC Calibrations on page 65

Review Advanced LS-Specific Results

To access the advanced LS results for the processed injections, go to the **Home** ribbon tab, and select **GPC/SEC** from the **Layouts** section. Alternatively, you can select **GPC/SEC LS Results** from the **Windows** section.

The following advanced GPC/SEC windows exist:

- GPC/SEC LS Results on page 67
- LS Results Plot on page 70
- GPC/SEC Compound Details on page 71

Reporting

Create Results Report

Use the OpenLab CDS Reporting tool to generate and modify GPC/SEC specific reports. The **Reporting** view can be accessed via the navigation pane in OpenLab CDS Data Analysis.

1 In Data Analysis, save your results.

2 Select the **Reporting** view.

3 In the **Home** ribbon tab, under **Layouts**, select **Editor**.

4 Select data for template development.

5 In the **Report Templates** section, double-click a report template to load it.

The section lists all report templates of the currently selected directory. If templates are missing, navigate to the desired directory, and refresh the list of templates.

6 To preview the report template, select the **Report Preview** window.

7 As **Reporting** option (in the **Home** ribbon tab), select the preferred reporting format and generate the final report.

NOTE

GPC/SEC report templates are available in the default directory under **C:\CDSProjects\GPC\Report Templates**. You can modify templates according to your requirements.

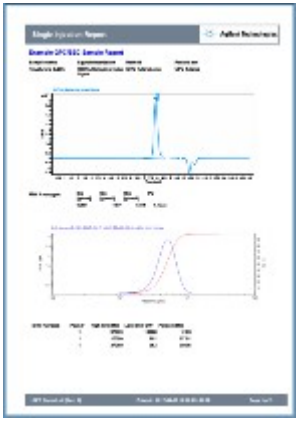
A series of report templates that are specific to GPC and SEC applications are installed as part of the product installation. For details, refer to The Default Report Templates Supplied on page 104.

Information about the GPC/SEC-specific report items, refer to section GPC/SEC Reporting on page 88.

Using a Single Injection Report Type

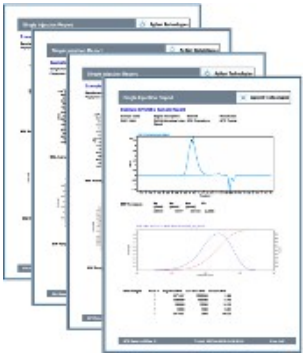
Single Injection Selected

This will produce a single report for the selected injection.



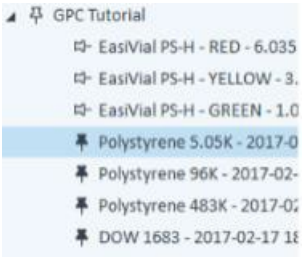
Series of Injections Selected in a Single Sequence

This will produce a separate report for each of the selected injections.

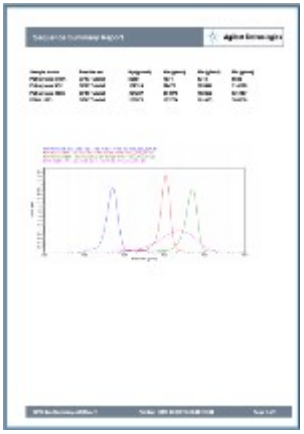


Using a Single Sequence Summary Report Type

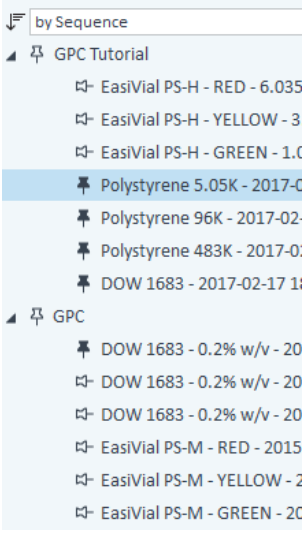
Series of Injections Selected in a Single Sequence



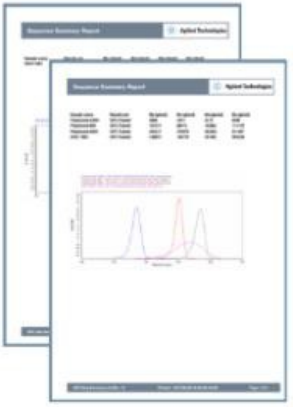
This will produce a single report with each of the selected injections overlaid and combined into one report.



Series of Selected Injections Across Sequences

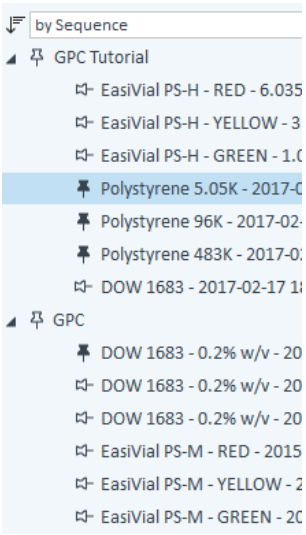


This will produce a separate report for each of the sequences combining the selected injections per sequence.

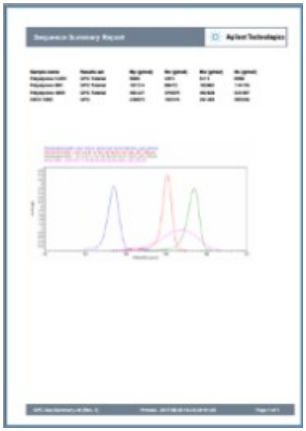


Using a Cross Sequence Summary Report Type

Series of Injections Selected Across Sequences



This will produce a single report with all selected injections from all sequences overlaid and combined in one report.



Share Data Between Systems

Exporting Data

The standard export features provided by OpenLab are available within the various GPC specific windows and grids, allowing:

- Graphics (Chromatograms, calibrations & distribution plots) to be exported to the standard graphic formats (EMF (*.emf) and PNG (*.png)).
- The contents of tables and grids to be exported to various standard file formats. (CSV File (*.csv), Excel Workbook (*.xls), Word document (*.doc) and PDF File (*.pdf)).

In addition, an option is available which allows the GPC results of a processed injection to be exported as a simple ASCII file. The generated ASCII file can be loaded directly into Excel and provides access to the full GPC results and slice by slice data of the processed peak(s) within the injection.

Processing Method

The parameters defined in a processing method can be exported to the standard file formats using a suitable report template containing the Data Analysis Method Information Multi Column report item accessed from the Method Information section.

6 Compliance

This chapter describes the features that enable the GPC/SEC software to be used in a compliant environment.

Storage of Parameters and Results

The GPC/SEC-specific processing parameters, column calibrations, GPC/SEC results and report templates are all stored within the OpenLab CDS system.

- The GPC/SEC-specific processing parameters and column calibration are stored as part of the processing method.
- The GPC/SEC results generated from an injection are stored as part of the results of a processed injection.

Auditing

The GPC/SEC software hooks into the following OpenLab audit processes:

- The processing method audit trail
- The injection audit trail
- The result set audit trail

Logs

You can access the GPC/SEC software logs in the OpenLab CDS Control Panel. Open the Administration pane > Diagnostics and navigate to section Logs.

Format of the Log

The log file uses the same format as the other OpenLab log files.

Content of the Log

The content uses the same format as the other OpenLab log files.

Diagnostics

General

Diagnostic information about the GPC/SEC software is accessible from the Diagnostics section of the Administration section accessed from the OpenLab Control Panel.

Installed Components

No GPC/SEC-specific information is shown in this area.

7 Appendix

Additions to the OpenLab Platform

GPC/SEC-specific processing method types	GPC/SEC-specific processing method types are added to the method options. • GPC/SEC (includes only conventional data processing, column calibration options) • GC/LC Quantitative + GPC/SEC (includes only conventional data processing, column calibration options) • GC/LC Quantitative + GPC/SEC + LS Bulk (includes conventional and advanced LS data processing)
GPC/SEC processing parameters	The GPC/SEC-specific processing parameters are accessed from the GPC/SEC-specific method sections. Depending on the selected processing method, the GPC/SEC- specific section contains the following subsections: • GPC/SEC General • GPC/SEC Conventional • GPC/SEC Column Calibration • GPC/SEC Advanced
Storage of GPC/SEC parameters	The GPC/SEC-specific processing parameters are stored as part of the method.
Storage of GPC/SEC column calibration	A GPC/SEC column calibration generated from injections is stored as part of the method used. Only one GPC/SEC column calibration can exist for the method.
Addition of GPC/SEC-specific windows in the **GPC/SEC** Layout of the **Home** ribbon tab:	
GPC/SEC Results window	This view comprises of the following tabs: • Peak Results • GPC Column Calibration • MW Ranges • Percentage Fractions
GPC/SEC LS Results window	This view comprises of the following tabs: • Peak Results • System Calibration Results
GPC/SEC Distributions window	This view comprises of a plot of the Molecular weight distribution plot(s) for the selected processed injection(s).
GPC/SEC Calibrations window	This view comprises of a plot of the column calibration plot(s) for the selected processed injections.
LS Results Plot window	This window shows the LS results plot demonstrating a partial Zimm plot for the selected samples.

GPC/SEC Compound Details window	This window displays the selected peak or GPC compound with concentration and LS signals overlaid. It is possible to display slice MW and Rh results in this graph.
Reporting	Additions of GPC/SEC-specific information to the processing method report items. Additions of GPC/SEC-specific report items. A series of report templates are supplied with the software, which have been designed to cater for the common types of output, required from the software.
Compliance Features	Audit logs Privileges

Standard Functions & Options Available

The standard features provided by OpenLab CDS are available within the GPC/SEC specific windows and grids.

Graphics

- Zoom
- Last Zoom
- Auto Scale
- Copy to Clipboard
- Export to file

Grids/Text

Ability to:

- Order on the active column
- Re size the displayed columns
- Re order the displayed columns

Content Specific Right-Click Menu

For example:

- Choose Column
- Numeric Precision
- Copy to Clipboard
- Export to File

Save As Dialog

- Displays the standard OpenLab Save As dialog.
- Standard available types dependent of the type of data to be saved.

About Software Installation

Before You Begin

Prerequisites

- If you plan to upgrade from a previous version of OpenLab CDS, refer to the documentation supplied with the OpenLab platform. In particular:
  - The chapter *Upgrade OpenLab CDS* of the *OpenLab CDS Workstation Installation and Configuration (CDS_v2.8_WorkstationGuide_en.pdf, D0028022)*.
  - The chapter *Upgrade OpenLab CDS* of the *OpenLab CDS Workstation Plus Installation and Configuration (CDS_v2.8_WorkstationPlusGuide_en.pdf, D0028021)*.
- GPC/SEC software version 1.6 or earlier should be uninstalled before upgrading to OpenLab CDS 2.8.
- OpenLab CDS must be installed and configured before installing the GPC/SEC software.
- GPC/SEC software 2.0 is compatible with OpenLab CDS version 2.8 (FP 2) and above.
- Prepare an account with administrative privileges to run the installation.
- A user that is part of the administrators group must install the software.
- You need the hostname of your OpenLab Server. If you are required to enter your user credentials when starting OpenLab, then you will require these credentials as part of the installation process.
- If you use Trend Micro as an antivirus software, turn off Web Reputation to allow the installation of all components.

Both workgroup and domain installation are supported.

Recommendation

Use a domain account if you are in a domain.

NOTE No Silent Installation option is provided for the software.

Software Installation Workflow

Software Upgrade

Uninstall the previous GPC/SEC software version before installing the new version.

Before installing the GPC/SEC software v2.0, you must install or upgrade to OpenLab CDS 2.8 (Feature Pack 2).

Compatibility of OpenLab CDS with GPC/SEC Software

Only GPC/SEC software v2.0 is compatible with OpenLab CDS version 2.8 (Feature Pack 2).

Older versions of the GPC/SEC software which are compatible with previous versions of OpenLab CDS are shown in the following table. They are available from the Agilent SubscribeNet. Please contact your Agilent sales representative for further details.

Table 26: Software versions and compatibilities

OpenLab CDS	GPC/SEC Software
Ver. 2.8	Version 2.0 Version 1.7
Ver. 2.7	Version 1.6
Ver. 2.6	Version 1.5
Ver. 2.5	Version 1.4
Ver. 2.3 & 2.4	Version 1.3
Ver. 2.2	Version 1.0

Please be aware that the Agilent 1260 Infinity MDS driver has a different execution path than the Agilent WinGPC (G7890AA/AB/AC/AD) or Agilent GPC/SEC software (G7850AA).

If the Agilent WinGPC or Agilent GPC/SEC software is already installed, the MDS driver for the GPC/SEC Add-on for OpenLab CDS cannot be installed and executed on this PC.

Installation Workflow Overview

Prepare and Check	
• OpenLab CDS platform compatible • OpenLab CDS platform is installed and configured	For details, see Table 26 Software versions and compatibilities on page 172.
Install	
• Run the Installation • Run the software verification • Post Installation	For details, see Software Verification on page 174.
Get License	
• Obtain license via SubscribeNet • Install your license	For details, see Licensing on page 27.
Configure	
GPC/SEC software specific components, such as: • Instruments • Projects • Privileges	For details, see System Preparation on page 42.

Software Verification

To confirm everything has been installed correctly, run the Software Verification Tool.

1 Select Start > Agilent Technologies > Software Verification Tool.

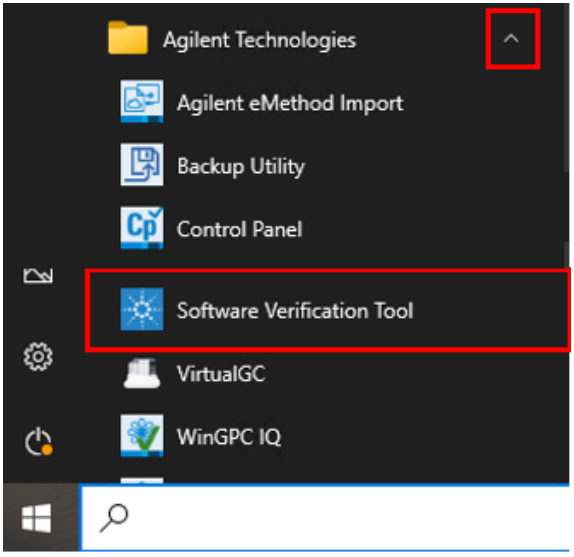


Figure 3: Software Verification Tool

2 Select the report options required and the post qualification actions.

3 Select the **OpenLab CDS** component and click **Qualify**.

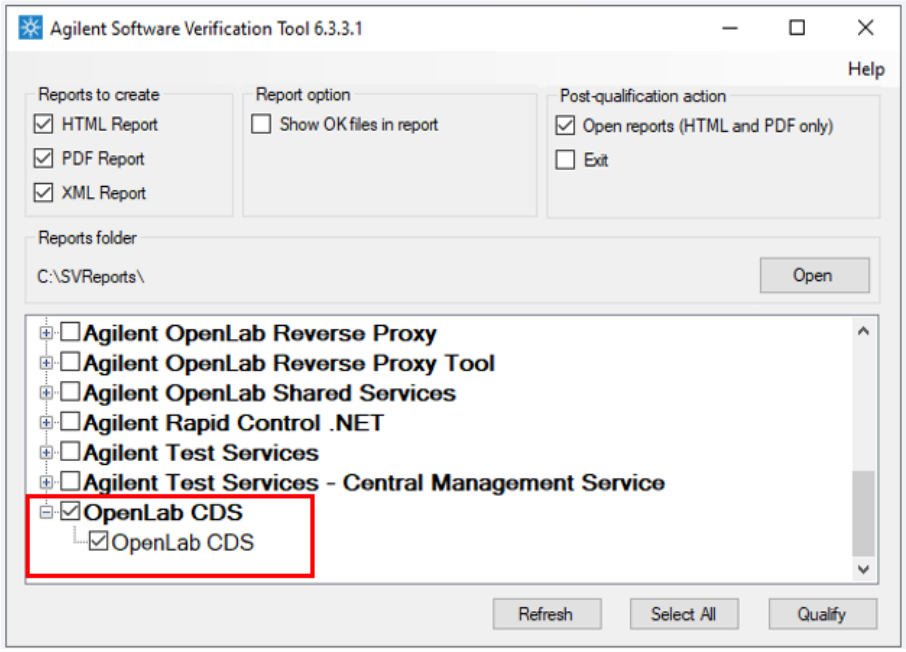


Figure 4: Available components

✓ The GPC/SEC Software is checked as part of the OpenLab CDS component and is reported as an entry in the verification report.

ID	Description
10548	Agilent OpenLab CDS - Agilent GPC/SEC Software

Figure 5: Details

Driver Verification Using Software Verification Tool

After installing the MALS and MDS drivers, it is important to verify that the installation was successful.

- **Run the Software Verification Tool**

Follow the instructions to start the Software Verification Tool, see Software Verification on page 174.

- **Verification Report**

  The tool will check the GPC/SEC software and confirm that the MALS and MDS drivers are installed as part of the OpenLab CDS components. The results will be listed in the verification report.

ID	Description
10549	Agilent OpenLab CDS - Agilent MALS
10556	Agilent OpenLab CDS - Agilent MDS

Figure 6: Verification report

Refer to the chapter Software Verification on page 174 for additional details on running the verification tool.

Troubleshooting

GPC/SEC Functionalities Not Available

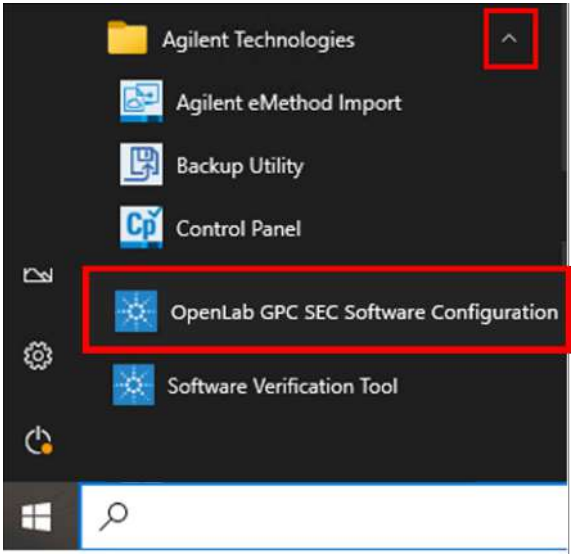
The GPC specific privileges have not been added to the OpenLab Shared Services. This means all GPC/SEC specific functionalities and software options are disabled within OpenLab CDS Data Analysis. The GPC/SEC specific method types exist but the GPC/SEC nodes and tabs within the method are read only.

Solution

Run the **OpenLab GPC SEC Software Configuration** application to register the GPC specific privileges (you will need the hostname of your OpenLab Server and your OpenLab user credentials).

1 Close OenLab CDS Data Analysis.

2 Select **Start** > **Agilent Technologies** > **OpenLab GPC SEC Software Configuration**.



3 In the OpenLab Configuration dialog, enter one of the following strings for the hostname of your OpenLab Server:

- The IP address of the workstation, starting with 192.x.x.x.

  OR

- The IP address of the localhost, 127.0.0.1

  OR

- Enter **localhost** as shown in next figure.

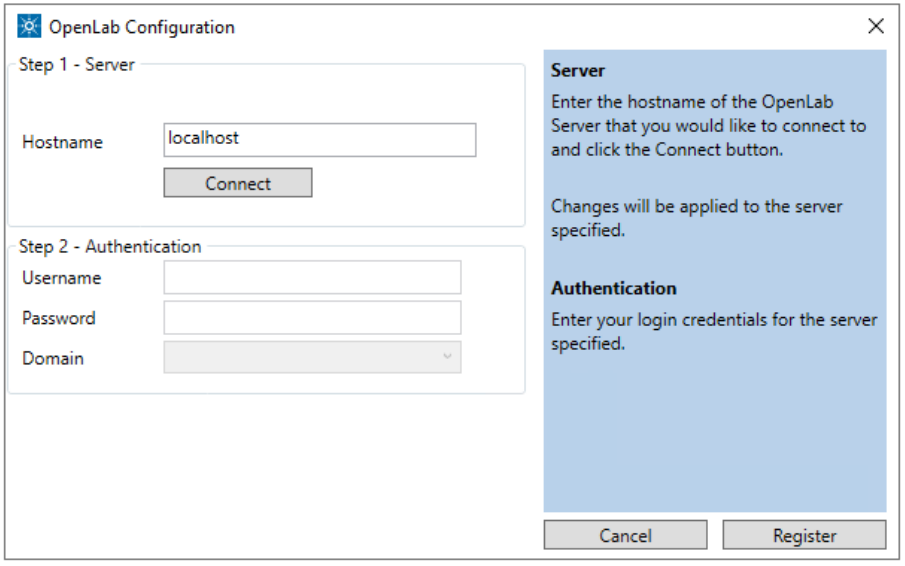


Figure 7: OpenLab Configuration window

4 Click **Connect** to enable the input boxes for the user credentials.

5 (Optional) Under **Step 2 – Authentication**, if you are required to enter your user credentials when starting OpenLab CDS, enter your login credentials.

6 Click **Register** to complete the process.

✓ After the registration process has succeeded, the following dialog opens:

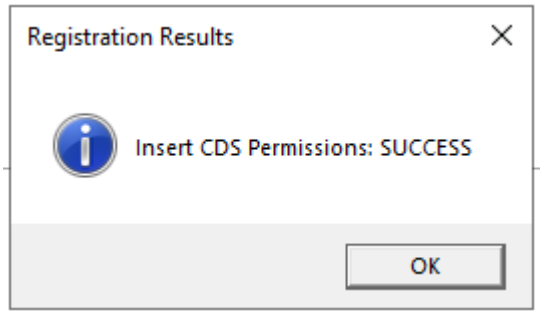


Figure 8: Registration Results window

In This Book

This manual contains detailed information about the Agilent GPC/SEC Software for OpenLab CDS with basic functionalities (G7860AA, conventional data processing) and advanced functionalities (G7861AA, advanced LS data processing including conventional workflows). The manual describes the following:

- Introduction
- Licensing
- Getting Started
- User Interface Reference
- Working with the GPC/SEC Software
- Compliance

www.agilent.com

Edition: 03/2026

Document No: D0134790 Rev. A.00

Agilent