Agilent OpenLAB Data Analysis

Comparison and Advice for CDS Users

Agilent Technologies

Notices

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Software Revision

This guide is valid for revision A.01.02 of Agilent OpenLAB Data Analysis.

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In This Guide...

This guide describes the main differences between OpenLAB CDS ChemStation Edition or OpenLAB CDS EZChrom Edition and OpenLAB Data Analysis.

Table 1 Terms and abbreviations used in this document

Term	Description
ChemStation	OpenLAB CDS ChemStation Edition
EZChrom	OpenLAB CDS EZChrom Edition
ACAML	Agilent Common Analytical Markup Language

1 Introduction

This chapter provides an overview of the OpenLAB Data Analysis software.

2 Methods

This chapter describes the different types and display modes of methods, and the connection between methods and data.

3 Calibration

This chapter contains information on the displayed calibration curve. It also describes the different calibration parameters and how they are used in OpenLAB Data Analysis.

4 Amount Calculation

This chapter describes the availability and usage of multipliers and dilution factors.

5 Integration Results

This chapter describes the integrator and integration tools used in OpenLAB CDS ChemStation Edition and OpenLAB CDS EZChrom Edition.

Contents

1 Introduction

This chapter provides an overview of the OpenLAB Data Analysis software.

About OpenLAB Data Analysis

Current Features of OpenLAB Data Analysis

With OpenLAB Data Analysis, Agilent introduces a new data analysis package that brings you a unique data analysis experience! This release is specially designed for data analysis in chemical and petrochemical laboratories and Hydrocarbon Processing Industry.

OpenLAB Data Analysis features intuitive operation, easy sample review and fast reprocessing of large sets of chromatographic data:

- OpenLAB Data Analysis was designed for ease of use. It comes with a "flat" and intuitive user interface.
- Microsoft-style function ribbons provide fast access to the main functions.

  An improved data selection tree allows fast access to your data. You can select data from multiple folders, load complete result sets, or select single samples.
- Improved data navigation with a new data viewing concept allows overlaying and comparing hundreds of signals. You can work with both LC and GC instruments at the same time and use multiple methods and data sets in parallel.
- You can scale automatically to a specific peak, ignore main peaks, or scale to the baseline. You will no longer need to zoom per sample.
- You can design your own layout and organize your screen to meet your workflow-specific needs. Four predefined configurable layouts help you to match your screen layout with the task you are performing.
- OpenLAB Data Analysis provides very fast reprocessing (more than 10 times faster than OpenLAB CDS).
- OpenLAB Data Analysis introduces a unique one-click peak integration tool for fast review.
- OpenLAB Data Analysis works with data from EZChrom and ChemStation Edition, allowing you to use the same integration, calculation, calibration and reporting across your laboratory.

- OpenLAB Data Analysis includes both the EZChrom and ChemStation Integrator for backwards compatibility and flexibility to use the same integration across your laboratory.
- You can import the compounds from existing ChemStation and EZChrom methods.
- OpenLAB Intelligent Reporting is fully integrated. You can create sample reports, sequence summary reports, and cross-sequence summary reports.
- The Peak Explorer allows you to easily review and compare large amounts of data.

Planned Features of OpenLAB Data Analysis

Some features planned for future revisions of OpenLAB Data Analysis:

- Support of MS, CE or UV-spectral data
- System Suitability Calculation
- Full migration of EZChrom/ChemStation methods into processing methods for OpenLAB Data Analysis
- Seamless integration of automated processing with OpenLAB Data Analysis during acquisition (currently only via macros/commands)
- Compliance with regulations like GLP or 21 CFR Part 11

OpenLAB Data Analysis and ChemStation/EZChrom

OpenLAB Data Analysis is a single data analysis product for LC and GC data that can be used together with either OpenLAB CDS ChemStation Edition or OpenLAB CDS EZChrom Edition. It evaluates the raw data and the ACAML (=Agilent Common Analytical Markup Language) files generated by those systems. ACAML files are generated by OpenLAB CDS A.01.01 or higher. To receive an ACAML file that you can use with OpenLAB Data Analysis, you must first reprocess the data with OpenLAB CDS A.01.01 or higher.

The workflows covered by OpenLAB Data Analysis range from a review of the acquired data and result processing to reporting. Reporting is achieved with the Intelligent Reporting module that is also available in OpenLAB CDS ChemStation and EZChrom Editions.

2 Methods

This chapter describes the different types and display modes of methods, and the connection between methods and data.

Overview

Table 2 Overview of differences for methods

Description	ChemStation	EZChrom	Data Analysis
Method content	Data acquisition parameters Data analysis parameters	Data acquisition parameters Data analysis parameters	Data analysis parameters
Types of methods	Master methods Sequence methods Data file methods	Master methods Result set methods	Master methods Result set methods
Possibility to discard reprocessed results without saving	No	No	Yes
Connection between method and data	Calculate or reprocess data with any method	Reprocess data with any method	Reprocess data only with a linked method.

Method Content

In ChemStation and EZChrom, methods contain information on both acquisition parameters and data analysis parameters. As OpenLAB Data Analysis is a tool for reviewing and reprocessing data, the methods in OpenLAB Data Analysis do not contain any acquisition parameters; they contain only the data analysis parameters. They are therefore called *processing methods* and have the file extension .pmx.

Data analysis parameters can be categorized as follows:

- General properties (such as ChemStation integrator or EZChrom integrator)
- Integration events
- Identification parameters (such as compound name and expected retention time)
- Calibration parameters (such as the amounts per compound and calibration level)
- Report generation parameters (such as report template name and report export settings)

In ChemStation, you enter identification and calibration parameters in one single table. In EZChrom, identification and calibration parameters are configured in the same table, but compound groups are set in a separate table. In OpenLAB Data Analysis, identification and calibration parameters are shown in separate sections of the method. You can configure compound groups in the **Identification** section.

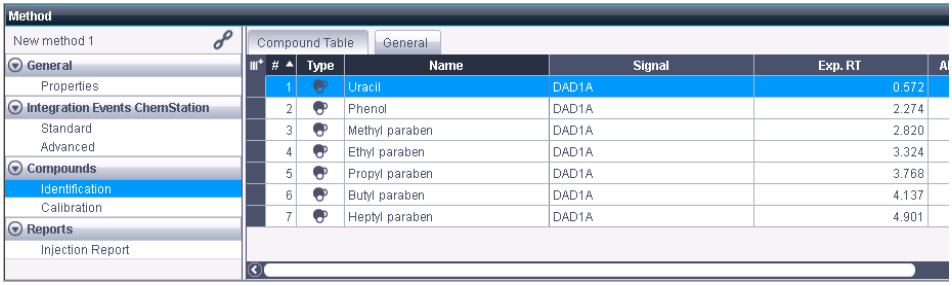

Figure 1 OpenLAB Data Analysis **Method** window: I**dentification** section

Method Types

In ChemStation, there are three different types of methods, depending on the context in which a method is used:

- *Master methods* are not directly associated with any result set or data file and can be used as templates or directly for processing of injections.
- *Sequence methods* are located in the result set and take effect when you start a sequence run, reprocess a sequence, or generated a report.
- *Data file methods* reflect the data analysis parameters used to generate the current data; they are automatically updated after each result generation (that is, after each data acquisition, recalculation, reprocessing, or report generation).

In OpenLAB Data Analysis and EZChrom, there are two types of methods:

- *Master methods* are located in a directory that is independent of the data. They are not linked to any specific result set.
- *Result set methods* are located in the corresponding result set folder.

With OpenLAB Data Analysis, if you link a method to an injection that is part of a result set, a copy of the method file is automatically created in the result set folder. The copy in the result set folder is used to process the injections in the result set.

If you want to reprocess data in OpenLAB Data Analysis, you need a processing method created in OpenLAB Data Analysis (.pmx file), and you must link this method to the specific injection or injections. Each injection can have its own linked method.

After editing a result set method, you can use the **Update Master Method** function in OpenLAB Data Analysis to overwrite the master method.

Discarding Results Without Saving

When you review the data, you typically change the method parameters and recalculate or reprocess the data. With ChemStation and EZChrom, this recalculation automatically modifies the results that are stored in the file system.

With OpenLAB Data Analysis, you can reprocess the data or generate a report without saving the results. Saving the results is a separate step that you must perform explicitly after reprocessing.

3 Calibration

This chapter contains information on the displayed calibration curve. It also describes the different calibration parameters and how they are used in OpenLAB Data Analysis.

Overview

Table 3 Overview of differences in calibration

Description	ChemStation	EZChrom	OpenLAB Data Analysis
Displayed calibration curve	As stored in the method	As stored in the method	As it has been available during processing of the current injection
Parameters for updating the calibration table	Sample Type	Run Type	Sample Type Run Type
Individual Points	No	Yes	Yes
Curve calculation	From average per level	From individual calibration points	From average per level or from individual calibration points

Updating the Calibration Table

Calibration Table

The calibration table specifies conversions of peak areas or heights into the required amount. During an analysis, the amounts entered for each compound are used to calculate the amounts for the samples. The type and amount of information required for creating a calibration table varies with the type of calculation procedure desired.

The following information is needed to create a calibration table:

- the retention time for each peak
- the amount of each compound per calibration level

In ChemStation: Sample Type, Response Factor

In ChemStation, you can set the following parameters in the sequence table:

- **Sample Type**: only the sample type **Calibration** causes an update of the calibration table.
- **UpdateRF**:

  With **Replace**, you delete existing information for the response factor in the current calibration level and replace it with the new data.

  With **Average**, you keep the existing data for a calibration level and build the weighted average with the new data.

  With **Interval**, you can create cyclic recalibrations where the calibration is automatically repeated after a given number of samples, and average values are built.

  With **Bracket**, you can create cyclic recalibrations where the quantitative reports for an unknown sample are calculated using the average between the two calibration sets injected before and after the sample.
- **UpdateRT**: you can choose whether you want to update the retention time, build an average with existing values, or do nothing at all.

All parameters take effect only for the calibration level given in the current row of the sequence table.

In EZChrom: Run Type

In EZChrom, you set the Run Type in the sequence table. The run type can be used for other purposes as well, but it also determines how the application updates the calibration table.

You can use the following run types:

- **Clear All Calibration**: All calibration points for all calibration levels are deleted before the new calibration data (response factor) is saved.
- **Clear Calibration at Level**: All calibration points for the given calibration level are deleted before the new calibration data (response factor) is saved.

In OpenLAB Data Analysis: Sample Type and Run Type

You set the information relevant for recalibration in the sequence table of your OpenLAB CDS system, or in the **Injection List** window in OpenLAB Data Analysis. OpenLAB Data Analysis uses the following parameters:

- **Sample Type**: Similar to ChemStation, only the sample type **Cal. Std.** causes an update of the calibration table.
- **Run Type**: similar to EZChrom, you can choose between **Clear All Calibration**, **Clear Calibration at Level**, or a blank run type. A blank run type means that a new individual calibration point is added to the specific level, and the average of all individual points per level is calculated. You can only edit the run type if the sample type is **Cal. Std.**.
- The sample types **Sys Suit**, **Control**, **Spike**, and **Blank** are not used in OpenLAB Data Analysis. They behave the same as **Sample**.

When you load data in OpenLAB Data Analysis, the application evaluates the parameters given by a ChemStation or EZChrom sequence, and transforms them into the most suitable settings in the OpenLAB Data Analysis injection list. The tables Table 4 on page 19 and Table 5 on page 19 show parameter transformations.

If you used intervals or bracketing in ChemStation, all individual resulting injections will be listed in the **Injection List** window, and for each calibration standard an average calibration point will be built. The quantitative reports for unknown samples are calculated using the current calibration curve. The calculation model of bracketing as in ChemStation is not supported in OpenLAB Data Analysis.

Table 4 ChemStation data in OpenLAB Data Analysis

ChemStation Sample Type	ChemStation Update RF	Data Analysis Sample Type	Data Analysis Run Type
Sample	n/a	Sample	n/a
Control Sample	n/a	Control	n/a
Blank	n/a	Blank	n/a
Calibration	Average	Cal. Std.	(blank)
Calibration	Replace	Cal. Std.	Clear Calibration at Level
Calibration	Bracket	Cal. Std.	(blank)
Calibration	Delta	Cal. Std.	(blank)
Calibration	No update	Cal. Std.	(blank)

Table 5 EZChrom data in OpenLAB Data Analysis

EZChrom Run Type	Data Analysis Sample Type	Data Analysis Run Type
Clear Calibration at Level	Cal. Std. (if cal. level > 0)	Clear Calibration at Level
Clear all Calibration	Cal. Std. (if cal. level > 0)	Clear all Calibration

Calibration Curve Display

Data of the Displayed Curve

The calibration curve builds up during processing a sequence. If there are several calibration standards in your sequence, the calibration curve equation for calculating a compound amount will change slightly during processing. The final calibration curve and equation are then saved in the method used for processing.

ChemStation and EZChrom always show the final calibration curve as it is stored in the method. That is, if you review a specific sample, you still see the final calibration curve including all calibration points - even though this curve was not entirely applicable at the point in time when the compound amounts for this specific sample have been calculated.

OpenLAB Data Analysis shows the calibration curve as it has been available at the time of processing the injection. If you review a sample after processing the entire sequence, you will still see the calibration curve as it has been available at that point in time. If calibration points have been added after processing this specific sample, these calibration points are not yet included in the calibration curve and equation.

Individual Calibration Points

ChemStation does not display individual calibration points. If you have several injections for the same calibration level, and you calculate an average response factor, ChemStation builds the average value of all calibration points for this level. The individual calibration points of the calibration level are not stored. Therefore you always see only one calibration point per level, no matter how many calibration standards you use.

EZChrom always uses individual calibration points for the curve calculation.

In OpenLAB Data Analysis, you can define whether the application uses average values or individual calibration points to calculate the curve. If

required, you can disable individual calibration points. The curve is then recalculated. Disabled calibration points are shown in red in the calibration curve.

The following figure shows the calibration curve for a calibration standard in OpenLAB Data Analysis. The yellow square marks the given amount for the compound at this calibration level, and the measured area. In this example, the amount is 5 mg. The dotted line shows the calculated amount, that is, if the amount was calculated for an unknown sample with the same measured area.

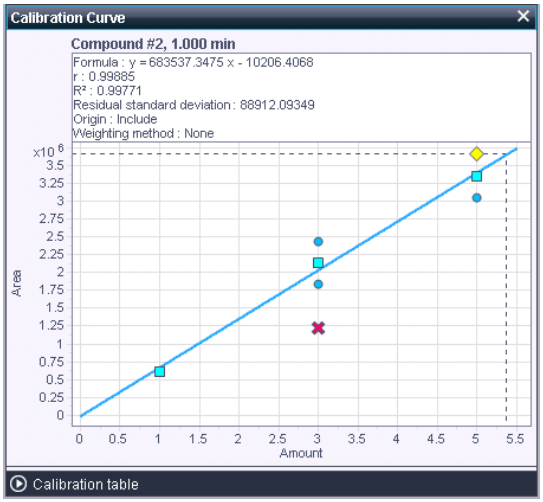

Figure 2 Calibration curve for a calibration standard in OpenLAB Data Analysis

- Blue squares: average calibration points (not shown if you use individual points for curve calculation)
- Yellow diamond: point corresponding to the selected injection. The compound area and the calculated amount for the selected injection are drawn with a dashed line.
- Blue circles: points corresponding to other calibration samples in the same sequence.
- Red cross: point has been disabled and is ignored for calculations.

4
Amount Calculation

This chapter describes the availability and usage of multipliers and dilution factors.

Overview

Table 6 Overview of differences in amount calculation

Description	ChemStation	EZChrom	OpenLAB Data Analysis
Number of multipliers and dilution factors	1 multiplier 1 dilution factor	5 multipliers 5 dilution factors	5 sample multipliers 1 compound multiplier 5 dilution factors
Where to specify sample amount, multipliers and dilution factors	Sequence Table **Specify Report** dialog	Sequence Table Result Set Table	Injection List: Sample multipliers and dilution factors Method (**Calibration** section): Compound multiplier
Concentration calculation	Amount * Multipliers * Dil. factors	Amount * Multipliers / Dil. factors	Setting in the Method (**Calibration** section)
Result value after applying multipliers and dilution factors to the amount calculated using the calibration curve	Compound amount	Compound amount	Concentration

Multipliers and Dilutions Factors

In ChemStation, you can provide a dilution factor and a multiplier in the sequence table. When the application calculates the compound amount, the amount will be multiplied with these factors before the final result is returned. In EZChrom and in OpenLAB Data Analysis, you can provide up to five dilution factors and five multipliers. In OpenLAB Data Analysis, you can in addition provide a specific multiplier for each compound.

In ChemStation, you can provide these settings in the sequence table, but you can also override them by constant values in the **Specify Report** dialog. In OpenLAB Data Analysis, you set the factors and multipliers for the sample in the **Injection List** window. The compound-specific multiplier is set in the **Calibration** section of the method.

In OpenLAB Data Analysis, the **Injection Results** window displays results for both *Amount* and *Concentration*. The amount is achieved by simply applying the calibration equation, no multipliers or factors are taken into account. The concentration is the result of multiplying the amount with all available factors and multipliers. You provide the amount unit and concentration unit in the processing method under **Compounds**/**Calibration**.

For example, you have dissolved 10 mg of a sample in 2 L of a solvent. You provide the concentration unit mg/L, and use the multiplier 0.5 to get the correct concentration relating to 1 L of solvent.

Reporting Settings

There are different ways of calibration – you can use internal or external standards (ISTD or ESTD), and you can relate the compound amount to the amount of all identified peaks (NORM%) or to the entire sample amount as entered in the sequence table or injection list (ESTD% or ISTD%).

In ChemStation, you can provide information related to the calibration type at two places:

- In the sequence table, you enter the values for sample amount, multipliers, and dilution factors.
- Under **Specify Report**, you select a suitable report template. In addition, you can override the sample amount, multipliers, and dilution factors by constant values for all injections in the entire sequence table.

In OpenLAB Data Analysis and in EZChrom, there is only one place where you can provide sample amount, sample multipliers and sample dilution factors.

In OpenLAB Data Analysis, you find the settings for the sample in the **Injection List** window. In addition, you can set a compound-specific multiplier in the **Calibration** section of the method. In the **Reports** section of the method, you select the suitable report template. There are no other settings related to calibration in the **Reports** section of the method.

5
Integration Results

This chapter describes the integrator and integration tools used in OpenLAB CDS ChemStation Edition and OpenLAB CDS EZChrom Edition.

Integrator and Integration Tools

OpenLAB Data Analysis includes the same integration algorithms as available in both OpenLAB CDS ChemStation Edition and OpenLAB EZChrom Edition. It supports all the initial and timed events from ChemStation or EZChrom in the Data Analysis method.

Agilent has conducted an extensive number of tests comparing integrator results from Data Analysis and ChemStation to ensure compatibility between the results from the two software packages. The tests include a variety of different signal types and peak forms. Differences that have been observed in these tests are in general below 0.1 %of the peak area/height, due to minor improvements in accuracy of the integrator algorithms.

For the ChemStation integrator, somewhat larger differences may occur:

- when using a high value for the Slope Sensitivity in connection with classic Baseline Correction
- for "aborted" peaks where the run time of the chromatogram ends before end of the peak

In addition to the automated integrators, OpenLAB Data Analysis provides a completely new one-click manual integration tool making use of intelligent tools like attractors to the chromatogram baselines, thus allowing for fast adjustment of peak integration results.

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In This Book

This guide describes the main differences between OpenLAB CDS ChemStation Edition or OpenLAB CDS EZChrom Edition and OpenLAB Data Analysis:

- Methods
- Calibration
- Amount Calculation
- Integration Results

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