Agilent OpenLAB Data Analysis

Getting Started

Agilent Technologies

Notices

Manual Part Number

M8370-90001 B

Edition

9/2014

Printed in Germany

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This product may be used as a component of an in vitro diagnostic system if the system is registered with the appropriate authorities and complies with the relevant regulations. Otherwise, it is intended only for general laboratory use.

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 installation of OpenLAB Data Analysis, the required configuration steps, and the main workflows. Read this manual if you want to install OpenLAB Data Analysis or if you want to use it to analyze your data.

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 Installation

This chapter describes how to install OpenLAB Data Analysis either as an add-on to OpenLAB CDS or as a standalone application. For details about the installation of OpenLAB CDS, refer to the CDS installation guides.

3 OpenLAB Control Panel Configuration

This chapter describes the project configuration that is needed as a preparation to work with OpenLAB Data Analysis.

4 Working with OpenLAB Data Analysis

This chapter describes general and specific functions of OpenLAB Data Analysis. It introduces the user interface and includes information on basic data and method handling. The specific features include descriptions of advanced display options, calibration and integration settings.

5 OpenLAB CDS Configuration for Automated Usage

You can configure ChemStation or EZChrom so that they use OpenLAB Data Analysis by default. This chapter describes the required configuration in ChemStation or EZChrom.

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 Installation

This chapter describes how to install OpenLAB Data Analysis either as an add-on to OpenLAB CDS or as a standalone application. For details about the installation of OpenLAB CDS, refer to the CDS installation guides.

Install OpenLAB Data Analysis as Add-on or Standalone Application

NOTE Before installation, you should verify that the configuration of your workstation computer meets all requirements. On our bundle systems, the workstation computers are already configured for optimum performance with OpenLAB Data Analysis. If you are not using a bundle computer, please configure your computer as described in the corresponding installation guide included on disc 1.

If you have not installed OpenLAB Data Analysis together with OpenLAB CDS, you can install OpenLAB Data Analysis as an add-on to OpenLAB CDS or as a standalone application.

NOTE OpenLAB Data Analysis is not supported for installations with ECM or Data Store as central data storage.

1 Run the Master Installer.

2 From the **Master Installer** screen, select **Installation**.

3 Select **OpenLAB Data Analysis**.

4 The **OpenLAB Data Analysis Installation Wizard** opens. Read the terms of the **License Agreement**. The Master Installer provides a printable PDF of the license agreement under the **Resources** option of the main menu.

5 Select **I agree with the terms and conditions**. You cannot proceed with installation unless you agree to these terms.

6 Click **Next** to proceed to the **Installation Folder** screen.

7 If you already have installed OpenLAB CDS on your PC, OpenLAB Data Analysis will be installed as an add-on.

   a To run an installation verification as part of this installation, select **Run Software Verification**. The Software Verification Tool provides documentary evidence that your system has been built and installed correctly. You can run the Software Verification Tool at a later time if you prefer.

b Click **Next** to proceed to the **OpenLAB Shared Services Settings for Registration** screen.

c Enter the server name and authentication provider.

d Click **Test Connection ...** to run a connectivity check.

The system will display a **Connection succeeded** message if the check is successful.

e Continue with step 10.

8 If you have not installed OpenLAB CDS on your PC, OpenLAB Data Analysis will be installed as a standalone application.

a You can use the default folder, type a new folder name or browse to the directory where you want to install OpenLAB Data Analysis.

b To run an installation verification as part of this installation, select **Run Software Verification**. The Software Verification Tool provides documentary evidence that your system has been built and installed correctly. You can run the Software Verification Tool at a later time if you prefer.

c Click **Next**.

d Select the required installation type.

NOTE An installation on a networked workstation is only supported in combination with OpenLAB CDS EZChrom Edition. For this type of installation, only the Enterprise path without Advanced File Security (AFS) is supported as storage.

9 If you have selected **Networked Workstation**:

a Click **Next**.

b In the **OpenLAB Shared Services Settings for Registration** screen complete the **Server name** field.

c Select the authentication provider as set in the OpenLAB Control Panel.

d When you type in the **Server name**, the **Test Connection...** button will be activated. You can test connectivity for this server before completing the rest of this screen.

e Select **Next**. The system will perform a connectivity check for the server.

If the connectivity test fails, verify that the server name was entered correctly, without spaces, and select **Next** to run the test again. If the test is still unsuccessful, you can:

- Enter a new server and try another test.
- Call internal support for assistance if you cannot connect to a server.

When a connectivity test has run successfully, the system will proceed to the **Additional items** screen.

f In the **Additional Items** screen, **Enterprise path** is selected. The enterprise path has been configured during the installation of the OpenLAB Shared Services server.

10 Click **Next** to proceed to the **Summary** screen.

11 Click **Start** to begin installation.

12 When the installation is finished, click **Next** to proceed to the **Installed Features** screen.

13 Click **Finish** to close the installation wizard.

3
OpenLAB Control Panel Configuration

This chapter describes the project configuration that is needed as a preparation to work with OpenLAB Data Analysis.

About Projects

A project is a pointer to a set of directories that store related methods, data, and templates. You can combine several projects to a project group and configure the directories for the entire group. Project groups can be used to arrange projects to match your organization.

You configure projects in the OpenLAB Control Panel.

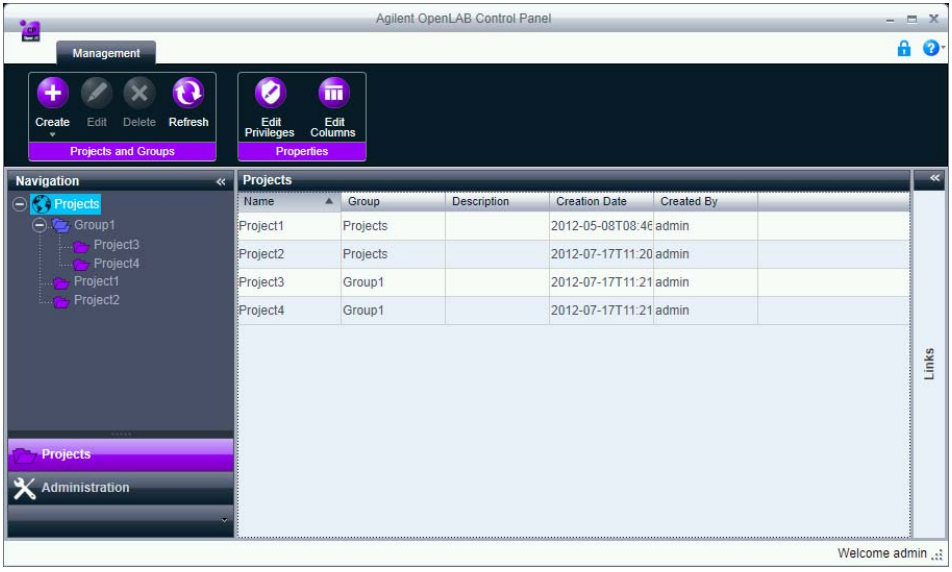


Figure 1 OpenLAB Control Panel

There are different types of projects:

- EZChrom projects
- Reporting projects
- OpenLAB Data Analysis projects (also required for ChemStation users)

The required project type depends on the installed software. For each type of project you can provide different attributes. You select the type when you create a new project.

Create a Project for OpenLAB Data Analysis as a Standalone Application

This procedure describes how to create an OpenLAB Data Analysis project if you have no OpenLAB CDS ChemStation or EZChrom Edition installed on your PC.

1 Start OpenLAB Control Panel.

2 Select the **Projects** page.

3 In the navigation pane, select the **Projects** root node, or navigate to the project group where you want to create your project.

4 In the **Projects and Groups** ribbon group, click **Create > Create Project**.

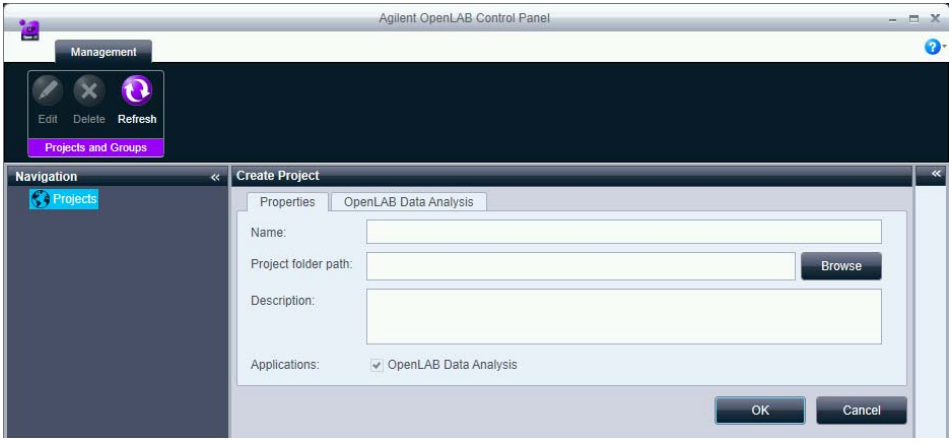


Figure 2 Creating a project in OpenLAB Control Panel

5 In the **Name** box, type a name for the project.

6 In the **Project folder path** box, type the path of the folder where all of your project data are located, or click **Browse** and navigate to and select the folder. This folder is typically a superordinate folder with subfolders for data, methods, and report templates.

NOTE After saving the project, you cannot change the project folder path again.

7 In the **Description** box, type a description of the project.

8 Select the **OpenLAB Data Analysis** tab, and provide the information required for OpenLAB Data Analysis.

   a Enter a valid path under **Data path**. In OpenLAB Data Analysis, you will be able to load only data that is located in this folder or its subfolders.

   b Enter a valid path under **Method path**. This path will be used as a default path for selecting method files in OpenLAB Data Analysis, but you can also open methods from any other location.

   c Enter a valid path under **Template path**. This path will be used as a default path for selecting report templates in OpenLAB Data Analysis, but you can also load report templates from any other location. You can copy default report templates from disc 7 (\Disk7\Report Templates) to the location of the template path.

9 Click **OK**.

Create a Project for ChemStation with OpenLAB Data Analysis

ChemStation itself does not require the configuration of projects in OpenLAB Control Panel. However, if you want to analyze ChemStation data with OpenLAB Data Analysis, you must configure OpenLAB Data Analysis projects. We recommend creating one OpenLAB Data Analysis project for each ChemStation instrument and setting the paths on the **OpenLAB Data Analysis** tab to the data subfolder of your instrument folder (for example, C:\Chem32\1) and creating a method folder for the OpenLAB Data Analysis processing methods. The report templates are located in an instrument-independent folder.

The following procedure describes how you can automatically create a project for each configured ChemStation instrument.

Prerequisites

Before creating the projects, you should already have configured all ChemStation instruments. For details on instrument configuration, see *Agilent OpenLAB CDS ChemStation Edition - Instrument Configuration Guide*.

1. Start OpenLAB Control Panel.
2. Select the **Projects** page.
3. In the navigation pane, select the **Projects** root node, or navigate to the project group where you want to add a project.
4. Right-click the node, and select **Create Projects for ChemStation Instruments** from the context menu.

   Under the selected node, the system will create one OpenLAB Data Analysis project for each configured ChemStation instrument.

   The project names correspond to the instrument names. The data and method paths of the projects correspond to the paths used for the instruments. The template path is not specific to an instrument; it will be the same path for all projects.

For example, if you installed Instrument 1 on **C:\Chem32\1**, a project with the following properties would be created:

- **Name**: Instrument 1
- **Project folder path**: C:\Chem32\1
- **Data path**: C:\Chem32\1\DATA
- **Method path**: C:\Chem32\1\METHODS
- **Template path**: C:\Chem32\REPSTYLE

As an alternative, you can create a project that includes the data paths for all instruments. This allows you to load data from all instruments. For example, the project path for such a project could be C:\Chem32, and the data path also C:\Chem32.

Create a Project for EZChrom with OpenLAB Data Analysis

If you use EZChrom, you must configure EZChrom projects in OpenLAB Control Panel. For details, refer to the OpenLAB Control Panel online help. The following procedure describes how to create an EZChrom project with additional information for OpenLAB Data Analysis.

1 Start OpenLAB Control Panel.

2 Select the **Projects** page.

3 In the navigation pane, select the **Projects** root node, or navigate to the project group where you want to create your project.

4 In the **Projects and Groups** ribbon group, click  **Create > Create Project**.

5 In the **Name** box, type a name for the project.

6 In the **Project folder path** box, type the path of your project folder, or click **Browse** and navigate to and select the folder. This folder contains subfolders, for example, for methods, results, and sequences (for example C:\Enterprise\Projects\Project1). For a networked workstation, the Enterprise path is the Project folder path.

NOTE After saving the project, you cannot change the project folder path again.

7 In the **Description** box, type a description of the project.

8 Select both, the **EZChrom** and the **OpenLAB Data Analysis** check box.

9 Select the **EZChrom** tab and provide the information required for EZChrom. For details, refer to the online help.

10 Select the **OpenLAB Data Analysis** tab, and provide the information required for OpenLAB Data Analysis.

a Enter a valid path under **Data path**. In OpenLAB Data Analysis, you will be able to load only data that is located in this folder or its subfolders.

NOTE Use the same path as under **Results** in the **EZChrom** tab (for example C:\Enterprise\Projects\Project1\Results).

b Enter a valid path under **Method path**. This path will be used as a default path for selecting method files in OpenLAB Data Analysis, but you can also open methods from any other location.

c Enter a valid path under **Template path**. This path will be used as a default path for selecting report templates in OpenLAB Data Analysis, but you can also load report templates from any other location. You can copy default report templates from disc 7 (\Disk7\Report Templates) to the location of the template path.

11 Click **OK**.

Edit Existing EZChrom Projects

If you installed OpenLAB Data Analysis as an add-on to EZChrom Edition, you may have existing EZChrom projects in OpenLAB Control Panel. The following procedure describes how you must configure these projects to use them with OpenLAB Data Analysis.

1 Start OpenLAB Control Panel.

2 Select the **Projects** page.

3 In the navigation pane, navigate to your existing EZChrom project.

4 Click **Edit** in the ribbon.

5 Select the **OpenLAB Data Analysis** check box.

6 Select the **OpenLAB Data Analysis** tab, and provide the information required for OpenLAB Data Analysis.

   a Enter a valid path under **Data path**. In OpenLAB Data Analysis, you will be able to load only data that is located in this folder or its subfolders.

NOTE Use the same path as under **Results** in the **EZChrom** tab (for example C:\Enterprise\Projects\Project1\Results).

   b Enter a valid path under **Method path**. This path will be used as a default path for selecting method files in OpenLAB Data Analysis, but you can also open methods from any other location.

   c Enter a valid path under **Template path**. This path will be used as a default path for selecting report templates in OpenLAB Data Analysis, but you can also load report templates from any other location. You can copy default report templates from disc 7 (\Disk7\Report Templates) to the location of the template path.

Create Project Shortcuts

You can create a desktop shortcut for each OpenLAB Data Analysis project in OpenLAB Control Panel. With this shortcut you can launch OpenLAB Data Analysis directly without starting OpenLAB Control Panel first. The paths for the corresponding project are automatically applied.

1 In OpenLAB Control Panel, select the **Projects** page.

2 Navigate to the project for which you want to create a desktop shortcut.

3 Click **Create Desktop Shortcut**  .

A shortcut is created on your desktop with the name of the project in OpenLAB Control Panel.

4
Working with OpenLAB Data Analysis

This chapter describes general and specific functions of OpenLAB Data Analysis. It introduces the user interface and includes information on basic data and method handling. The specific features include descriptions of advanced display options, calibration and integration settings.

Optional: Preparation of Example Data

To play through the manual and reproduce the examples described in the following chapters, OpenLAB Data Analysis is delivered with results sets as example data.

1 Navigate to Demo_Data\Getting_Started_Guide on disc 7.

2 Copy the example data files to your local data folder which you have provided in the project settings in OpenLAB Control Panel under **Data path**.

   For example, with ChemStation the data path could be C:\Chem32\1\Data.

Starting the Application

If you have created a shortcut for your project, you can double-click the shortcut to open the project directly. Alternatively, you can open any project from OpenLAB Control Panel as described below.

1 Start OpenLAB Control Panel.

2 From the navigation pane, select the **Projects** page.

3 Navigate to your OpenLAB Data Analysis project.

4 Click  **Start Data Analysis**.

Introduction to the User Interface

Terms Used to Describe User Interface Elements

Screen terms related to the ribbon

The *ribbon* is a toolbar element which is always shown on the top of the application window. It is a combination of a classic menu with an application toolbar. The ribbon contains two different types of *ribbon tabs*. The first type is always visible (e.g. **Home**) and allows access to functions which are present independently of the selected object in the application. The other type (*contextual tab*) appears only if you select a specific user interface element.

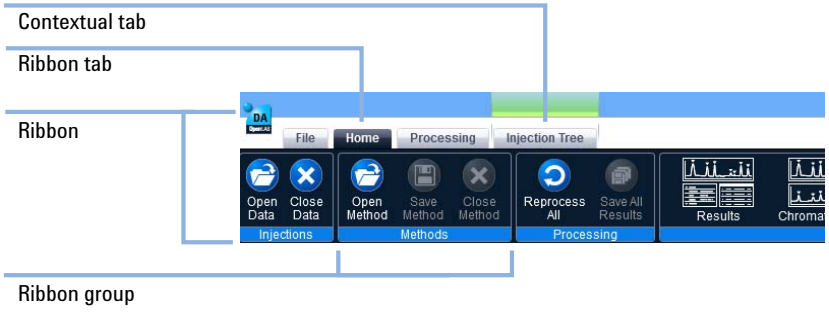


Figure 3 The ribbon

Screen terms related to the navigation pane

The *navigation pane* is the area at the left of the application. It consists of a title bar, a *navigation tree* that may contain additional sections, and the *view* selection buttons. Additional sections are, for example, the *signal selector* and the *method selector*. The layout and purpose of the navigation tree depend on the selected view. Under **Data Processing** the navigation tree is called *injection tree* and contains all loaded data.

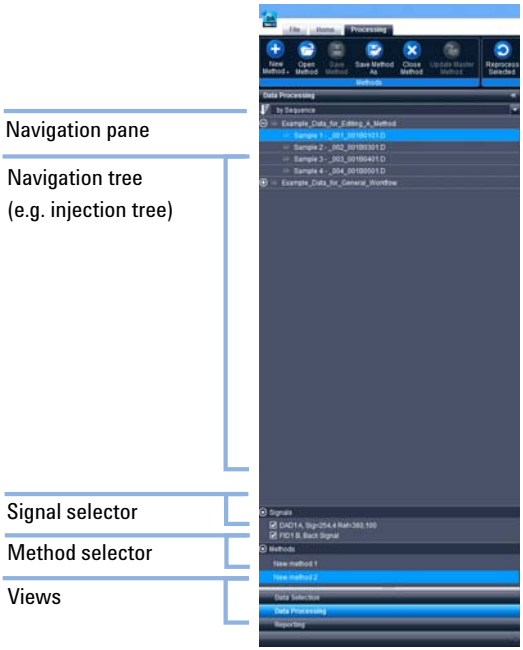


Figure 4 The navigation pane

Screen terms related to the workspace

The *workspace* is the area in the user interface where the different *windows* are shown. A window can have a specific *toolbar*.

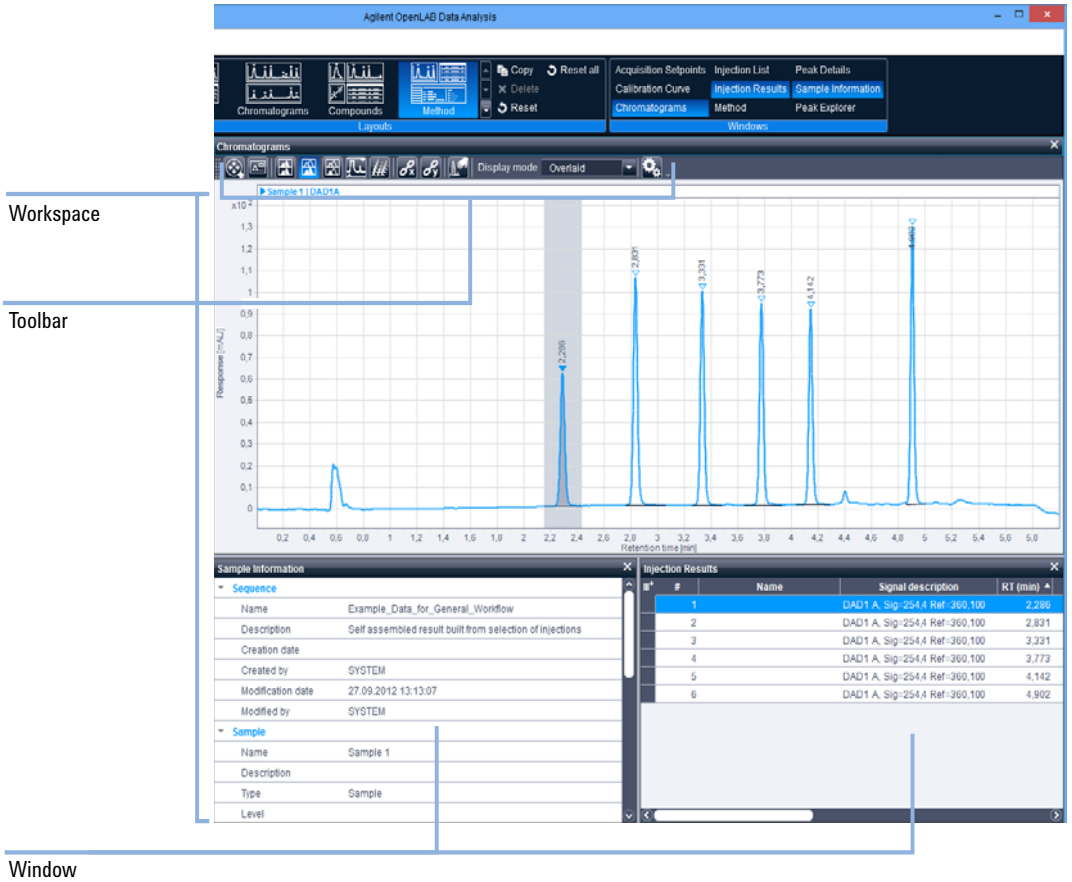


Figure 5 The workspace

Selecting an Injection

There are different kinds of selecting an injection from the injection tree:

- Blue highlighting: If you have selected one or more injections, all injections highlighted in blue can be reprocessed (see "To Link and Reprocess the Data" on page 44).

  The last selected injection has a light blue highlighting and is called *focused injection*. The data related to the focused injection are shown in the corresponding windows.

  Injections highlighted in blue are referred to as *selected injections*.

- With pin: Independently of the blue highlighting, you can pin injections in the injection tree. Injections with a vertical pin are referred to as *pinned injections*. Injections with a horizontal pin are *unpinned*. The **Chromatograms** window displays all pinned injections plus the focused injection (see "Reviewing Chromatograms" on page 35). Pinned injections will continuously be displayed, even if you change the focused injection.

The following figure shows the different kinds of injection selection.

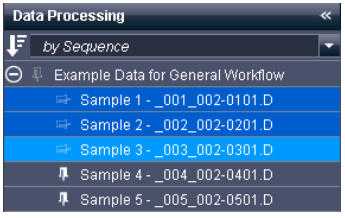


Figure 6 Selecting an injection

Working with Layouts

The application provides several preconfigured layouts for different user tasks. Layouts define which windows are shown in your workspace and how they are positioned. You can adjust these layouts, or set them back to the factory default.

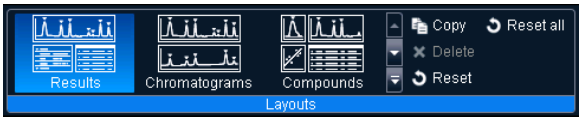


Figure 7 **Layouts** ribbon group

To Adjust a Layout

1 In the ribbon, select the layout that you want to adjust.

2 Customize your workspace to suit your requirements.

The layout is automatically saved after each workspace modification.

If you log in to OpenLAB Data Analysis with a user name and password, the changed layout is saved specifically for your user.

To Create a Custom Layout

1 In the **Layouts** ribbon group, select and adjust one of the default layouts, for example **Results**.

2 To save your layout for later reuse, click **Copy**.

Your custom layout is now listed in the ribbon, for example **Results1**.

To Reset a Layout

1 To reset a specific layout, select the layout in the ribbon, and click **Reset**.

2 To reset all layouts, click **Reset all**.

Customizing your Workspace

In OpenLAB Data Analysis, you can change the visibility, position and size of all windows. If you change a layout, the application will remember the new layout. When you start the application the next time, your changes will still be active.

To Show or Hide a Window

1 To hide a window, simply click the cross at the top right of the window. Alternatively, you can click the button corresponding to this window in the **Windows** ribbon group.

2 To show a window, click the button corresponding to this window in the **Windows** ribbon group.

3 To display a tabbed window, find the window where the required tab is shown, and select that tab.

To Resize a Window

1 Point the mouse between two windows.

2 When the pointer becomes a double-headed arrow, drag the pointer to move the split line.

To Modify the Position of a Window

1 Grab the window heading and move it to a new position.

NOTE If you want to move a tabbed window, grabbing the window heading will move the entire window including all tabs. To move individual tabs out of a window, you must grab the tab label.

As soon as you move the window, the possible new positions are indicated by arrows. When you move the window over an arrow icon, the corresponding new location for the window is highlighted in blue.

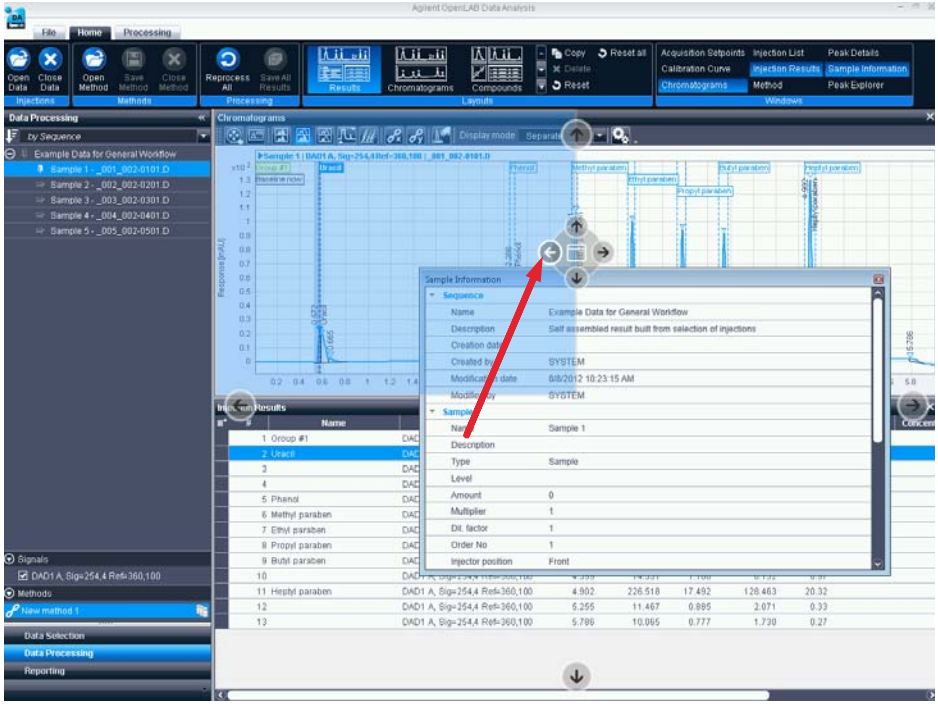
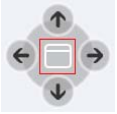


Figure 8 Positioning a window

2 If you want to position a window as a new tab to an existing window, move it over the existing window and then over the middle of the central arrows icon.



General Workflow

This section gives you an overview of the basic tasks in OpenLAB Data Analysis.

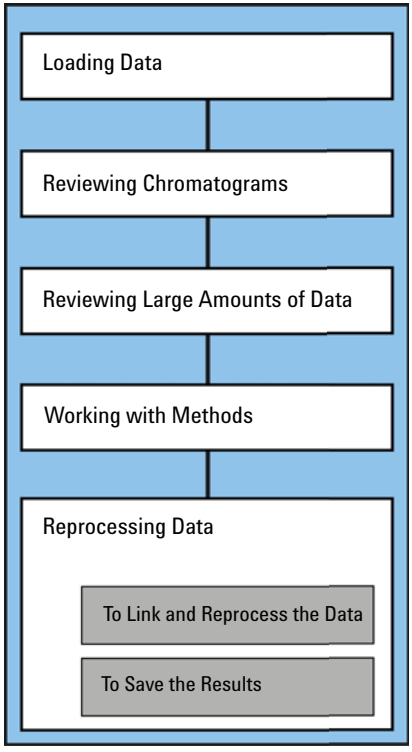


Figure 9 Basic tasks

The section *Loading Data* explains how to load a result set or single sample. In *Reviewing Chromatograms*, you learn how to review chromatograms of selected injections and how to receive details on specific peaks. The section *Reviewing Large Amounts of Data* shows how to easily review and compare large amounts of data by using the Peak Explorer. *Working with Methods* includes an explanation of what a method is and how to create and save a method. The section *Reprocessing Data* explains how to link and reprocess your data. After reprocessing the data, you can save your results.

Loading Data

In the **Data Selection** view, you can select either result sets or single samples, and load the associated data. If you have already loaded data, the following procedures will add the result sets or single samples to the data that is already available in the **Data Processing** view.

1 Select the **Data Selection** view.

The data selection tree shows the folder structure of the data path given in the OpenLAB Data Analysis project in OpenLAB Control Panel. The tree can contain the following items:

- (folders): A folder can contain other folders, result sets or single runs. If it contains result sets, they are shown as subnodes in the tree. If the folder contains single runs, the respective data files are listed in the **Injection List** window.
- (result sets): The contained data files are listed in the **Injection List** window. You can only load the entire result set; loading parts of a result set is not supported.

2 To load a result set:

a Navigate to the required result set and select it.

b In the ribbon, click **Load Data**.

OR

Double-click on result set in the navigation tree.

3 To load a single sample:

a Navigate to the folder containing the corresponding data files, and select the required injections in the **Injection List** window.

b In the ribbon, click **Load Data**.

The selected result sets or injections are loaded, and the application switches to the **Data Processing** view. The data is added to other data that you may have loaded before. If there are processing methods linked to the data, the methods are automatically loaded together with the data. The methods are then listed in the method selector.

Injections with the ending *.D* are ChemStation generated samples, injections with the ending *.dat* are EZChrom generated.

NOTE To reproduce the examples that are described in the following sections, load the result set **Example_Data_for_General_Workflow**. This result set is delivered as example data with OpenLAB Data Analysis.

Reviewing Chromatograms

The following sections describe how to work with chromatograms and receive details on specific peaks.

To Review the Chromatogram of a Single Injection

1 Load the relevant result set or single sample. The following examples use the result set **Example_Data_for_General_Workflow**.

2 In the injection tree, highlight or pin the injection of which you want to review the chromatogram.

3 If the **Chromatograms** window is not shown, choose **Chromatograms** from the **Layouts** ribbon group.

Your OpenLAB Data Analysis window should look similar to the following figure.

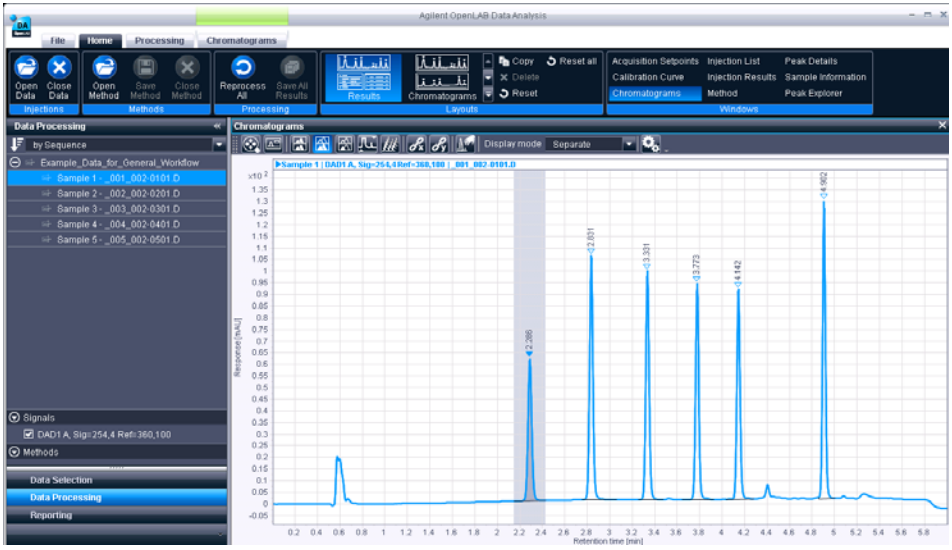


Figure 10 **Chromatograms** layout

The peak tops are labeled with the retention times.

In case of a multisignal injection, several signals may be displayed. The **Chromatograms** window shows all signals that you selected in the **Signal selection** area in the navigation pane.

The color of the signals is automatically determined by the application.

4 If you want to display only one signal, clear the check boxes for the other signals in the **Signal selection** area of the navigation pane.

The **Chromatograms** window now shows the chromatogram of your choice. (To adjust the view in the **Chromatograms** window, for example by zooming or using custom scaling, see "Adjusting the View in the Chromatograms Window" on page 47)

To Review the Results for a Specific Peak

1 Display the chromatogram containing a specific peak in the **Chromatograms** window.

2 Select the **Results** layout from the **Layouts** ribbon group.

Your workspace now consists of three windows - **Chromatograms**, **Sample Information** and **Injection Results** - as in the following figure:

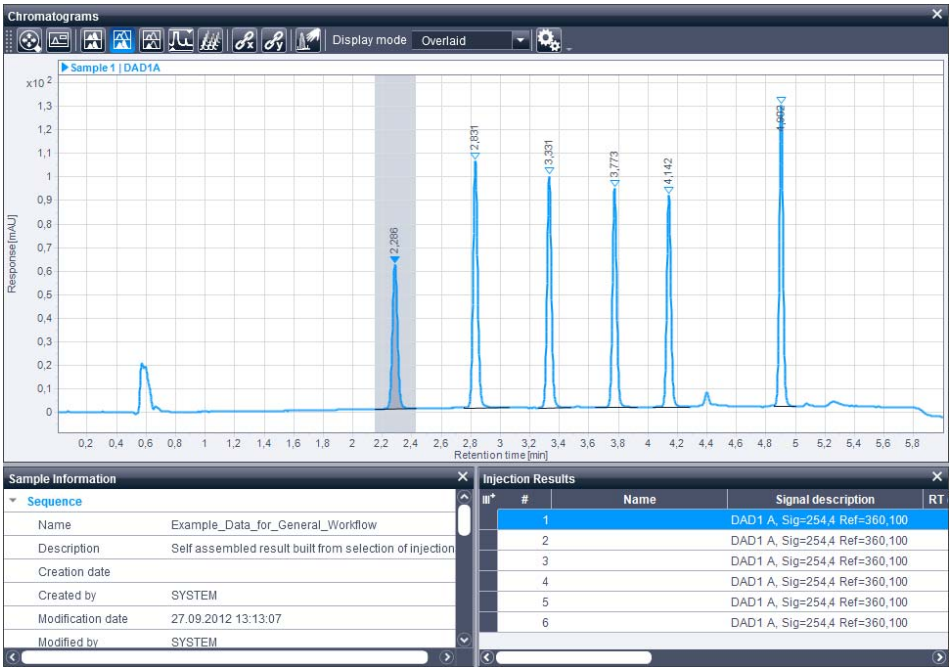


Figure 11 **Results** layout

3 Click on a specific peak in the **Chromatograms** window to see more details on this peak in the **Injection Results** window.

The line corresponding to the peak is highlighted in the **Injection Results** window. Within the **Injection Results** window, you can switch between peaks by clicking on the different lines.

The highlighting of the peak is always synchronized between all windows.

If you have run a data analysis in ChemStation or EZChrom, the **Injection Results** window contains these results, for example **Area** or **Height**.

Reviewing Large Amounts of Data

This section describes how to easily review and compare large amounts of data by using the Peak Explorer.

NOTE To reproduce the examples that are described in the following sections, load the result set **Example_Data_for_Peak_Explorer**. This result set is delivered as example data with OpenLAB Data Analysis.

To Show the Peak Explorer

1 To show the Peak Explorer, click **Peak Explorer** in the **Windows** ribbon group.

2 For this example, open the **Chromatograms** window as well, close all other windows and deactivate the signal **DAD1 B**.

To Choose the Injections Shown in the Peak Explorer

The Peak Explorer shows the peaks of all pinned injections, that is, all injections with a vertical pin in the Injection Tree. If you have loaded multiple samples or result sets, you can compare the data for all of them.

A blue line highlights all bubbles belonging to the focused injection. A blue circle highlights the selected peak of this injection. These selections are synchronized with the injections or peaks selected in other windows.

If there is no pinned injection at all, the application shows all injections of every loaded result set and single sample.

About the Peak Explorer

The Peak Explorer diagram shows the pinned injections of all loaded sequences in a bubble chart, with one diagram for each selected signal:

- The y-axis shows the loaded injections, ordered as in the injection tree.
- The x-axis shows the retention times of all injections.
- The bubble size represents a value related to the peak size. You can choose the value from the drop-down list in the Peak Explorer toolbar. When using, for example, the peak width as an indicator for the bubble size, you can graphically spot peaks with a bad integration. With the toolbar buttons, you can also choose if you want to see identified peaks, not identified peaks, or both, in the diagram.

The bubbles are displayed in different colors:

Identified peaks

Not identified peaks

The application allows you to quickly detect an unexpected peak.

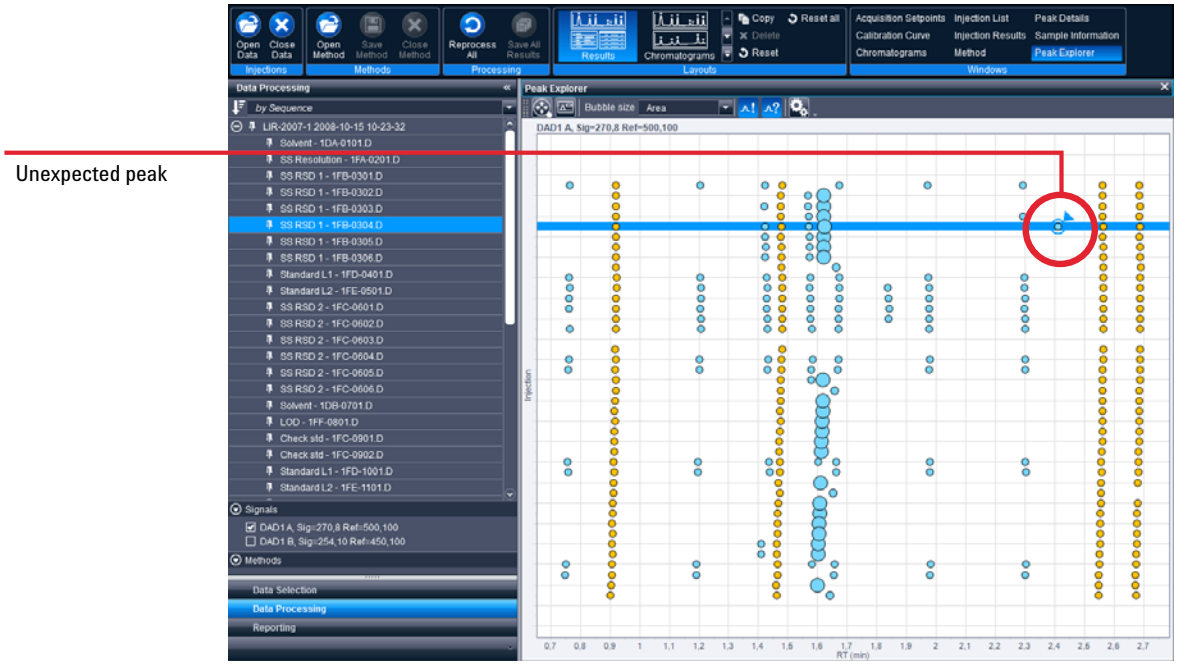


Figure 12 Peak Explorer: detecting an unexpected peak

In the **Chromatograms** window you can detect that the compound does not have a constant retention time, but you cannot see whether the variation in retention times is a systematic shift or a random distribution. When zooming in the Peak Explorer, a systematic shift becomes visible.

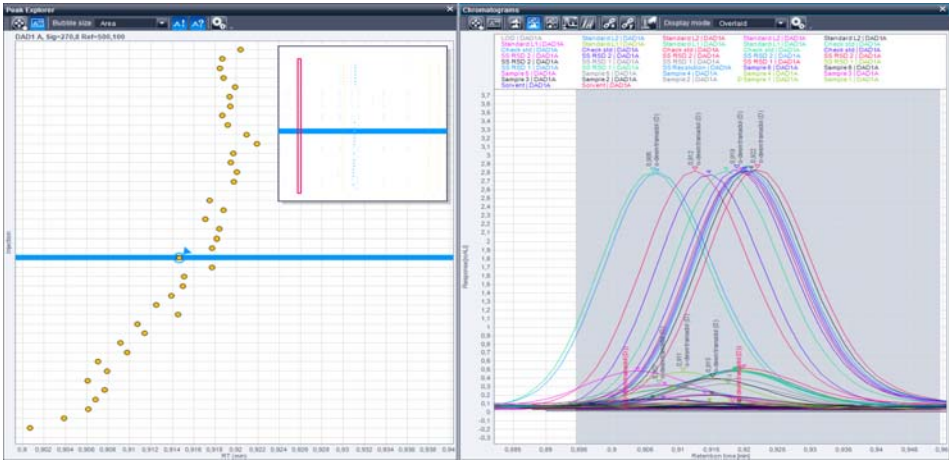


Figure 13 Peak Explorer: detecting a systematic shift

Working with Methods

A method contains all the information and parameters which you need to process the data and generate results.

For example, in the **Compounds** section, you can find settings for compound identification and calibration. The **Identification** node includes the peak name, signal and expected retention time, for example. The **Calibration** node is needed to create a calibration curve by setting parameters like amount unit and the number of levels (for more details see "To Edit Compound Identification Parameters" on page 57 and "To Edit Calibration Parameters" on page 59).

In **Reports** you can specify the **Report template** and **Report destination** (for more details on how to generate a report see "Generating a Report" on page 80).

It is possible to work with empty or incomplete methods, but a method must be saved at least once before you can link it to certain data. When linking data to a method, the data is reprocessed automatically.

To Create a New Method

1 In the ribbon, select the **Processing** tab.

2 Click **New Method**.

The application switches to the **Method** layout. Input fields for the properties of the new method are shown in the **Method** window.

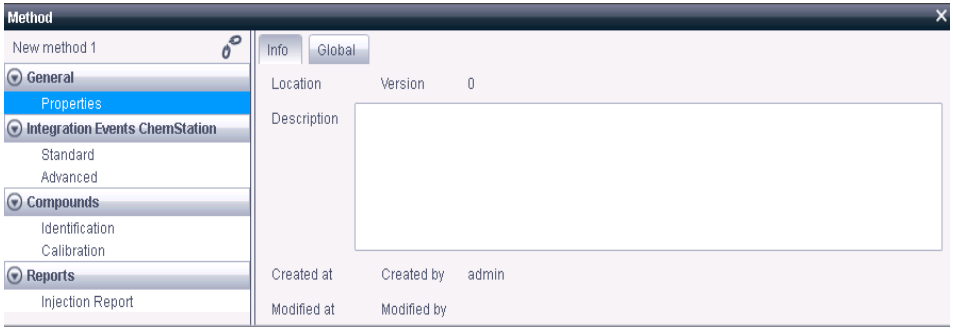


Figure 14 **Method** window

The new method is automatically added to the method selector in the navigation tree.

Adjacent to the method name, a link symbol shows if this method is linked to an injection:

: This method is linked to the focused injection.

: This method is *not* linked to the focused injection.

3 In the **Info** tab, enter a description for the new method.

The method name is determined by the file name when saving the method.

4 In the **Global** tab, you can select the integrator. For this example, choose the **ChemStation integrator**.

The properties under the **Integration Events** section are default parameters.

For more details on **Integration Events** and **Compounds** refer to "Editing a Method with a 2-Level-Calibration" on page 52.

To Save a Method

If you have created a new or changed an existing method and have not saved the changes, the method is marked with a pencil symbol  .

1 Select the **Processing** ribbon tab.

2 Click  **Save Method As** in the **Methods** ribbon group.

The **Save As** dialog opens.

3 Navigate to the path where you want to store the method. Alternatively, you can click in the field with the path name, and edit the path name directly.

The drop-down list shows the recently used paths. By default, the application shows the method path that you specified in the project settings in OpenLAB Control Panel.

4 Enter a file name.

5 Click **Save**.

To save changes to an existing method:

1 Select the **Processing** ribbon tab.

2 Click  **Save Method** in the **Methods** ribbon group.

Reprocessing Data

To Link and Reprocess the Data

When linking data to a method, this data is reprocessed automatically. Reprocessing means that you apply all method parameters to your data.

1 Click on the injection to select it. You can select multiple injections by holding the **Ctrl** key or a range of injections by holding the **Shift** key while clicking.

The selected data files are highlighted in blue in the injection tree.

2 In the method selector, right-click the method that you want to link to the selected data files, and select **Link selected injections to selected method** from the context menu.

OR

Select the relevant method in the method selector. Right-click the selected data files, and select **Link selected injections to selected method** from the context menu.

The data is linked to the method and is reprocessed.

The link symbol is shown in front of all selected data files. If you select an injection, the corresponding method will show the link symbol.

If the data has been reprocessed successfully, your injection tree should look like the following figure:

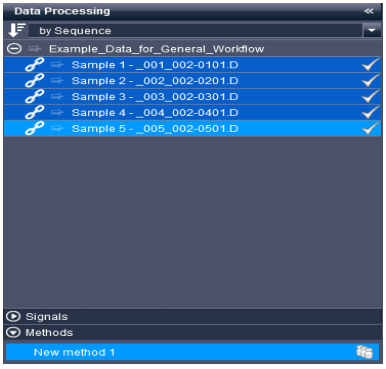


Figure 15 Navigation pane

If the reprocessed data files belong to a result set, the application copies the processing method into the result set directory. The copied method is added to the list of methods in the method selector and marked with a result set symbol  .

3 If you make changes in your method, and would like to see those changes in your data, you can reprocess your data manually:

   a In the ribbon, select the **Processing** tab.

   b In the ribbon, click  **Reprocess Selected**.

   OR

   Right-click the data files and select **Reprocess selected injections** from the context menu.

Each of the selected data files (highlighted in blue) is reprocessed using the method linked to it. Different data files can have different methods assigned.

New results are automatically calculated and can be reviewed directly in OpenLAB Data Analysis. For result sets, the processing method is automatically copied to the result set folder.

The following symbols may be shown for the reprocessed data files:

-  The data file has successfully been reprocessed, but has not been saved.
-  Warnings occurred during reprocessing. Move the mouse over the symbol to get more details.
-  The data file could not be reprocessed. There is no method linked to the data file, or an incorrect method is used. Move the mouse over the symbol to get more details.
-  Reprocessing has been stopped, or an error occurred.
- * Manual integration or manual identification has been applied to the data.

To Save the Results

1 If the results are correct, you can save the results by clicking  **Save All Results**.

After saving, the checkmarks next to the samples disappear in the injection tree.

Methods that are linked to the injections of a result set will be saved together with the results. Other methods (not linked, or linked to single samples) must be saved individually.

2 Optional: If you want to discard the modifications, simply close the data and the method without saving them. In the **Home** ribbon tab, click  **Close Data**.

Linked methods will be closed automatically.

If a method is not linked to data, you can close the method by selecting the **Processing** ribbon tab and clicking  **Close Method**.

Using Specific Features

Adjusting the View in the Chromatograms Window

This section describes how to change the view of a chromatogram by zooming, changing the visible window area and choosing between different display modes. It also contains how to show and hide the zoom overview window, and to use custom scaling.

NOTE To reproduce the examples that are described in the following sections, load the result set **Example_Data_for_General_Workflow**. This result set is delivered as example data with OpenLAB Data Analysis.

To Zoom In and Out of a Graph

If you change the original view of a chromatogram, your settings will also be applied to further chromatograms.

1 Move the mouse over the area of interest within the **Chromatograms** window.

2 Use the mouse wheel to zoom in or out. Scroll down to zoom out, or scroll up to zoom in.

The system will magnify or demagnify the area around the position of the mouse cursor.

3 Alternatively, you can select the area of interest which you want to zoom in to. Hold the mouse down and pull a square over the area of interest.

The **Chromatograms** window now shows the selected area.

4 To zoom out step by step, double-click the graph.

5 To reset your zooming actions, click  in the **Chromatograms** toolbar.

The **Chromatograms** window shows the original scale of the chromatogram.

To Move Along the X- and Y-Axis

If you change the original view of a chromatogram, your settings will also be applied to further chromatograms.

1 To move the x- or y-axis, move the mouse over one of the axes until it turns into a double-headed arrow.

2 Hold the left mouse button and move the axis left and right, or up and down.

NOTE If you use the right mouse button, you will scale the x- or y-axis.

3 To reset your changes, click  in the **Chromatograms** toolbar.

To Show and Hide the Zoom Overview Window

1 To show an overview window of the entire, unenlarged or custom scaled chromatogram and the location of the zoom area, click  in the **Chromatograms** toolbar.

The overview window appears within the **Chromatograms** window.

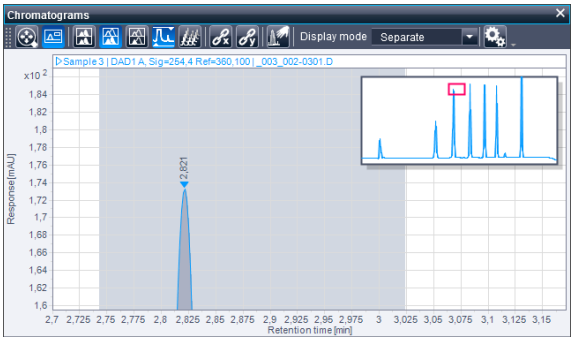


Figure 16 Zoom overview window

2 To hide the overview window, click  again.

To Turn Custom Scaling On/Off

If you have data with a large solvent peak and want to ignore this peak in your **Chromatograms** view, follow these steps.

1 Load your data.

NOTE To reproduce the example that are described in this section, load the result set **Example_Data_for_Editing_a_Method**. This result set is delivered as example data with OpenLAB Data Analysis.

2 In the **Chromatograms** window, click  in the chromatograms toolbar to turn custom scaling on.

Figure 17 Custom scaling off

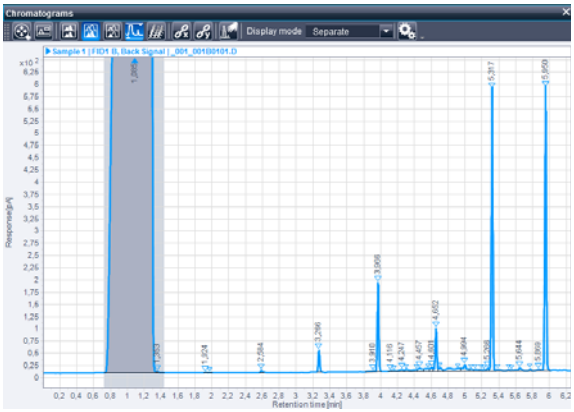


Figure 18 Custom scaling on

The scale of the graph in the **Chromatograms** window changes automatically.

If more than one chromatogram is displayed, custom scaling will be applied to all chromatograms.

3 To change custom scaling settings, click  to open the **Chromatogram Properties** window.

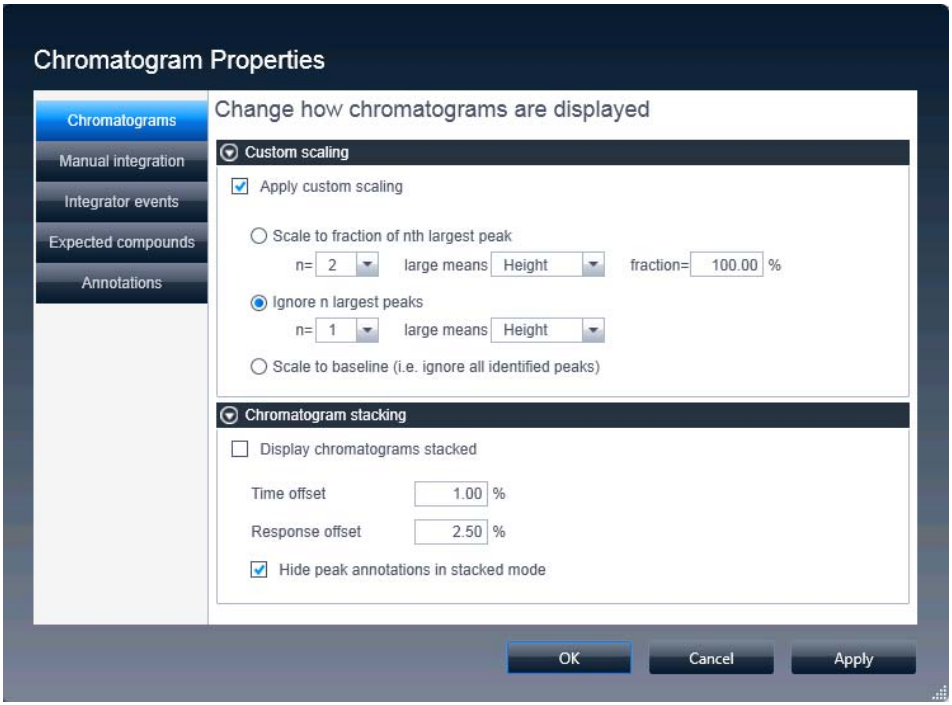


Figure 19 Custom scaling settings

You can choose between

- **Scale to fraction of nth largest peak**
- **Ignore n largest peaks** and
- **Scale to baseline (i.e. ignore all identified peaks)**.

For example, when you leave the default setting, the first largest peak (here the solvent peak) will be ignored.

4 Click **OK** to apply and close the **Chromatogram Properties** window.

5 To turn custom scaling off, click  again.

Editing a Method with a 2-Level-Calibration

This section gives you an overview of how to edit a method and to perform a 2-level-calibration.

Generally, editing a method and performing a calibration includes the following steps:

- Open the relevant data.
- Create a new method and save it as file.
- Link the injections to the method.
- Edit the integration events to decide what peaks should be integrated.
- Edit the compound parameters for identification and calibration.
- Edit the injection list to define sample parameters.
- Review calibration results in the injection results table and the calibration curve.
- Save your results and method for later reuse.

Data and Method Preparation

1 Load the relevant result set.

NOTE

To reproduce the examples that are described in the following sections, load the result set **Example_Data_for_Editing_a_Method**. This result set is delivered as example data with OpenLAB Data Analysis.

2 Create a new method and save it as file (see "Working with Methods" on page 41).

3 Link the method to the data (see "To Link and Reprocess the Data" on page 44).

To Edit Integration Events

If your data shows a lot of small, irrelevant peaks that you would like to exclude from your analysis, you can edit the **Integration Events** within your method.

1 Select the **Method** layout in the **Home** ribbon tab.

2 In the **Method** window, select the **Integration Events** section, and the **Standard** node.

3 Within the shown table, you can change parameters like **Slope sensitivity**, **Peak width** and **Area reject** by changing the **Value**.

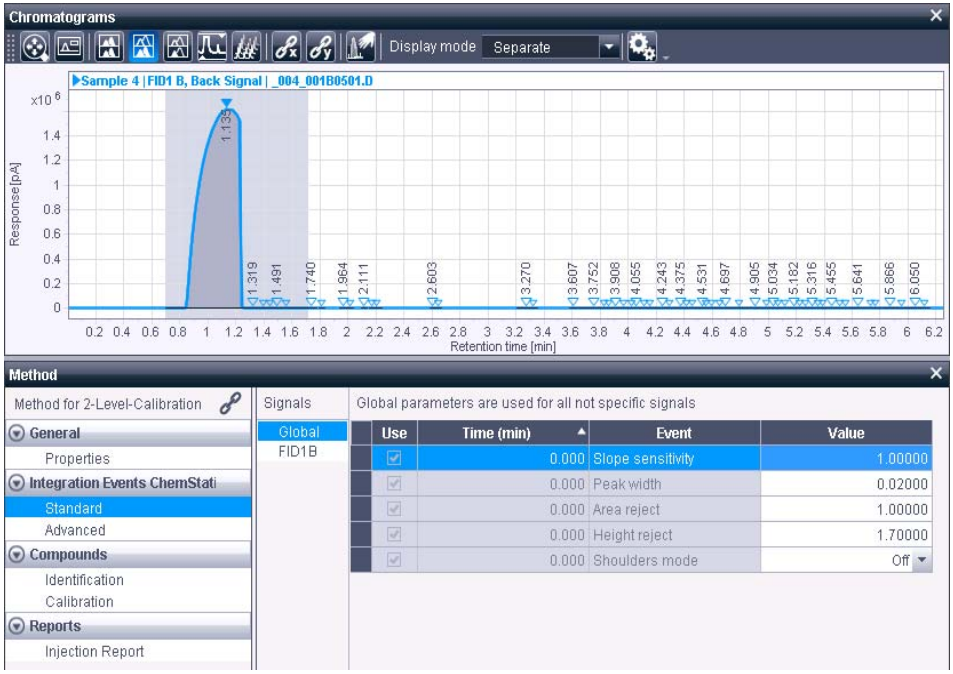


Figure 20 Sample 1 before editing integration events

4 The **Height reject** event, for example, sets the height of the smallest peak of interest. In Sample 1 of the example data, edit the **Height reject** event by changing the **Value** from **1.7** to **45.0**.

5 To apply the height reject to all samples, select all samples and reprocess the data.

When using the example data, in the **Chromatograms** window, there should now only be five other peaks apart from the solvent peak. All other smaller peaks are now being suppressed, as shown in the following figure.

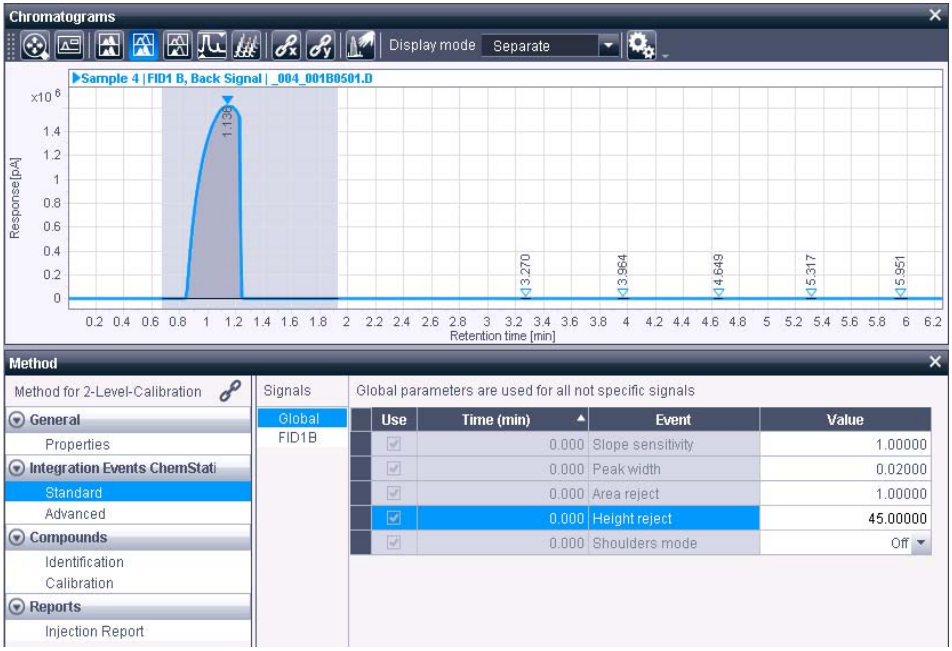


Figure 21 Sample 1 after editing integration events

To Edit Timed Integration Events

In **Sample 1-3** of the example data, the end of the solvent peak is not clearly defined (light gray area), see the following figure.

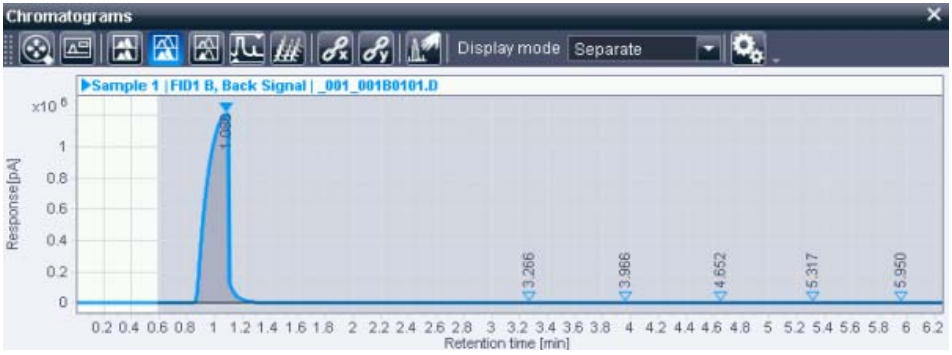


Figure 22 Sample 1 of example data without timed events

1 To determine an end for the solvent peak range, you can add two timed events. Right-click beneath the table, and select **Add integration event** from the context menu.

   Repeat this step to receive two new rows to the **Integration Event** table.

2 Under **Events**, select **Integration** from the drop-down list for both rows.

3 Under **Value**, set **Off** for the first new integration event and **On** for the second new event.

4 Under **Time [min]**, set the time, where the solvent peak should end (Integration Off), for example **1.400**, and a time to turn integration back on, for example **1.800**.

5 Reprocess the data.

   The chromatogram should now look similar to the following figure.

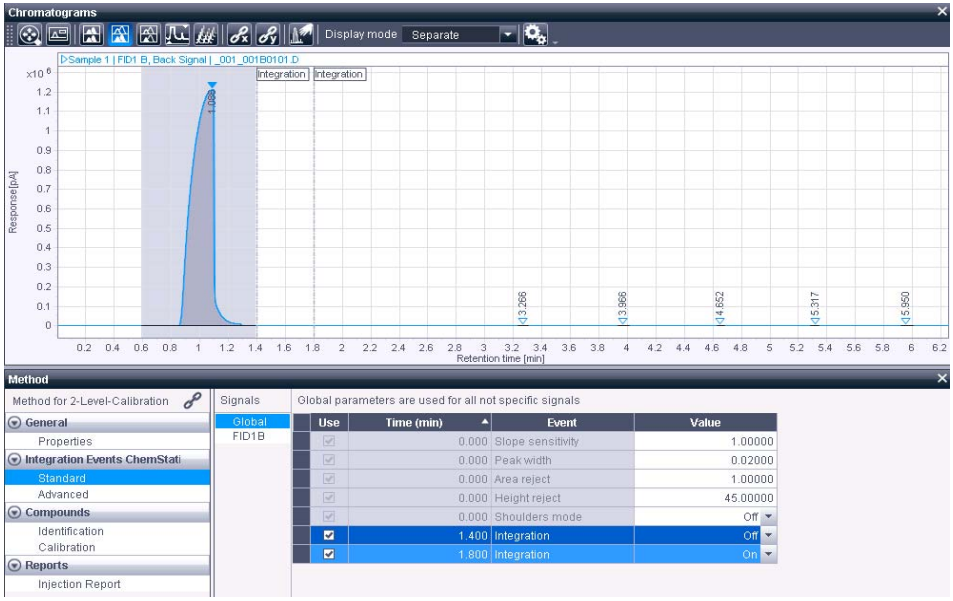


Figure 23 Sample 1 of example data with timed events

To Edit Compound Identification Parameters

The expected compounds are stored in a compound table as part of the method. The following procedure describes how you add one or more peaks from the chromatogram as new compounds to the compound table.

Preparations

To have a better view at the relevant peaks, turn custom scaling on (see "To Turn Custom Scaling On/Off" on page 49).

If you only receive an unintended enlarged view of the baseline after turning custom scaling on, select the option **Scale to fraction of nth largest peak** in the **Chromatogram Properties** window, and scale to the second largest peak.

1 In the **Method** window, select the **Compounds** section, and the **Identification** node.

   You can see the empty **Compound Table** within the **Method** window.

2 In the **Chromatograms** window, select the required peak or peaks corresponding to the compounds you want to add.

   To select multiple peaks, hold the **Ctrl** key while clicking the peaks. To select a range of peaks, hold the **Shift** key while clicking the peaks.

3 Right-click the selected peak, and choose **Add peak as compound to method** from the context menu. If you selected multiple peaks, the command is **Add multiple peaks as compound to method**.

   The corresponding information is added to the compound table of the selected method. By default, the compound parameters are set as follows:

   - **Type**: Different icons are used for the compound types:

      for a single compound

      for a named group

      for a timed group

   - **Name**: **peak@RT**
   - **Signal**: the signal from which you selected the peak
   - **Exp.RT**: the retention time of the selected peak of the current chromatogram used to build the compound table

For the example data, add all five peaks as compound to the method apart from the solvent peak.

4 Type a name in the **Name** column for each relevant peak.

For the example data, name the five peaks **Compound 1** to **Compound 5**.

The names appear as peak annotations for expected compounds as in the following figure.

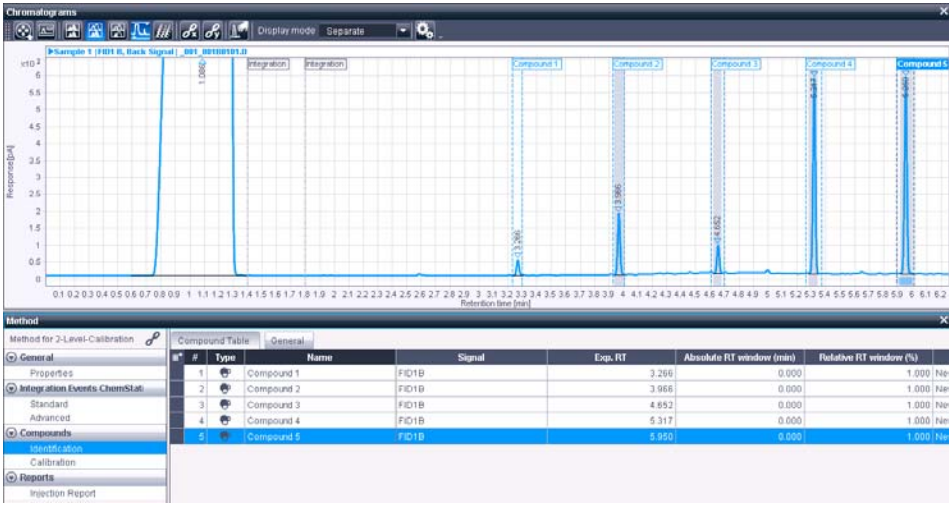


Figure 24 Expected compounds

5 Select all samples and reprocess the data.

In each sample, all defined peak names appear next to the retention times in the **Chromatograms** window as in the following figure.

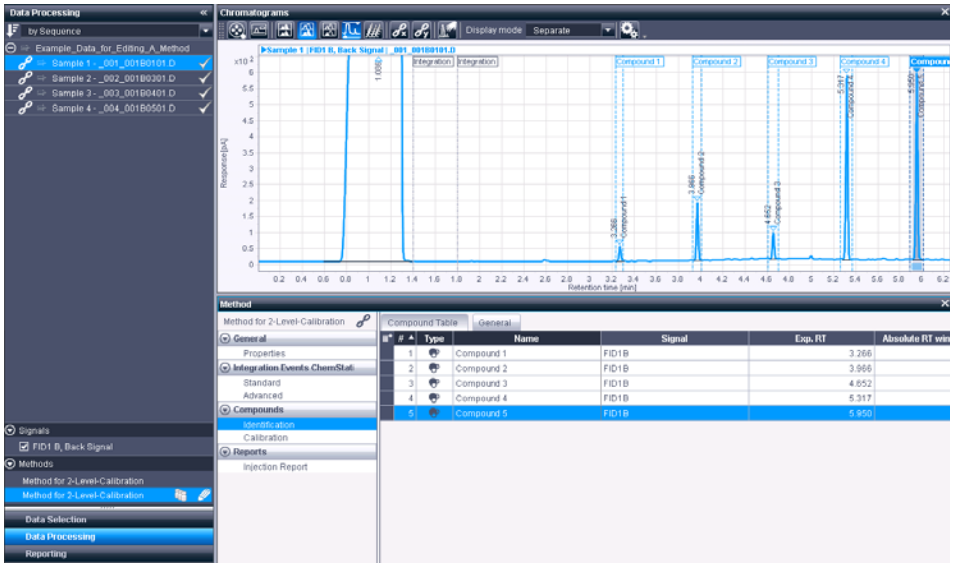


Figure 25 Compound identification

To Edit Calibration Parameters

The following procedure describes what parameters to set to perform a calibration for a compound, in this example *Compound 5*, the highest peak of the example data. The following steps can also be performed with Compound 1 to 4.

1 In the **Method** window, select the **Compounds** section, and the **Calibration** node.

  Compound **Type** and **Name** have been applied to the calibration compound table.

2 Indicate the **Amount unit**, for example **mg** for the example data.

  The amount unit is equivalent to the x-Axis naming of the calibration curve.

3 Indicate the **Concentration unit**, for example **µg/mL** for the example data.

  The concentration will be calculated after calibration and shown in the **Injection Results** window.

  To receive the correct concentration, multipliers must be set in the **Injection List** window (see "To Edit the Injection List" on page 61).

4 Choose if the **Response** used to calibrate and quantify the compound is **Area**, **Height**, **Area%** or **Height%**.

For the example data, choose **Area**.

5 For this example, set the **Mode** to **Curve** and the **Curve model** to **Linear**.

6 In the **Origin** column, you can choose from four options:

- **Ignore**: The origin is not used. At least two calibration points are needed.
- **Include**: A virtual point (0;0) is taken into account to calculate the equation of the calibration curve. At least one calibration point is needed.
- **Force**: The calibration curve is forced to the origin. The curve equation is y = ax. At least one calibration point is needed.
- **Connect**: The curve is connected to the origin by a linear segment from the lowest calibration level point. At least two calibration points are needed.

For the example data, choose **Ignore**.

7 For the example data, set **1** for the compound **Multiplier**.

For details on calculation, refer to *Agilent OpenLAB Data Analysis - Reference Guide*.

8 For a 2-level-calibration, we need to define two levels for calibration.

For Compound 5 of the example data, set **10** for **Level 1** and **20** for **Level 2**. Leave level 3 to 5 empty.

If you want to change the number of levels, select the **General** tab and set a different number in the **Number of levels** text box. For this example, you can deactivate level 3 to 5 and set **2** for the **Number of levels**.

To Edit the Injection List

The last step for the calibration is to define the sample parameters if this has not been done in ChemStation or EZChrom.

1 To view the **Injection List** window, select the **Injection List** from the **Windows** ribbon group.

2 In the **Injection List** window, define the sample type of each injection. For a 2-level-calibration, you need two calibration standards.

For the example data, set sample type **Cal. Std.** for Sample 1 and 2 and leave **Sample** for Sample 3 and 4.

3 In **Run type** you can either leave the empty space, which means the calibration point will stay in the calibration curve after reprocessing. Or you can choose between **Clear all calibration** or **Clear calibration at level** to remove certain calibration points.

For the example data, leave the empty space.

4 Under **Level**, define which calibration standard equals which level that you have set in the calibration parameters of your method.

For the example data, set levels **1** for Sample 1 and **2** for Sample 2.

5 In **Multiplier 1-5** and **Dil. factor 1-5** set the correct value to calculate the concentration of your sample.

For example, the solvent is 100 mL. When 10 mg are dissolved in 100 mL, to receive µg/mL you must multiply with 1000/100 = 10.

For the example data, set **10** for **Multiplier 1** in Sample 3 and 4.

Injection List

Ord. #	Inj. #	Name	Sample type	Run type	Level	Injection date	Modification date	Amount	ISTD Amt 1	ISTD Amt 2	ISTD Amt 3	ISTD Amt 4	ISTD Amt 5	Multiplier 1	Multi
1	1	Sample 1	Cal. Std.		1	02/14/2012 04:56 PM	09/06/2013 11:08...	0.000						1.00000	
2	1	Sample 2	Cal. Std.		2	02/14/2012 05:19 PM	09/06/2013 11:08...	0.000						1.00000	
3	1	Sample 3	Sample			02/14/2012 05:30 PM	09/06/2013 11:08...	0.000						10.00000	
4	1	Sample 4	Sample			02/14/2012 05:42 PM	09/06/2013 11:08...	0.000						10.00000	

Figure 26 Injection list

6 All columns with a grey background display meta data that can be reviewed but not changed, for example **Injection date** or **Modification date**.

To Review the Calibration Results

The injection results and calibration curve can now be reviewed.

1 Reprocess all injections.

In this example, warning symbols are still shown next to the calibration standards (**Sample 1** and **Sample 2**) because a calibration curve has only been defined for *Compound 5*. *Compounds 1 to 4* are still missing input. You can repeat the previously described procedures for these compounds as well. Then after reprocessing, checkmarks should appear instead of the warning symbols.

2 Review the **Injection Results** window.

You can find the **Amount** and **Concentration** results of your configured compounds by selecting the relevant samples in the injection tree or the **Injection List** window.

For Compound 5 of the example data, the amount of Sample 3 is **12.278 mg** and the concentration is **122.780 µg/mL**. The amount of Sample 4 is **17.246 mg** and the concentration is **172.457 µg/mL**.

3 To review the calibration curve of your expected compounds, click on **Calibration Curve** in the **Windows** ribbon group or select the **Compounds** layout.

4 Select your samples to review the corresponding calibration curve in the **Calibration Curve** window.

For Compound 5 of the example data, the results in Sample 4 should look like the following figure.

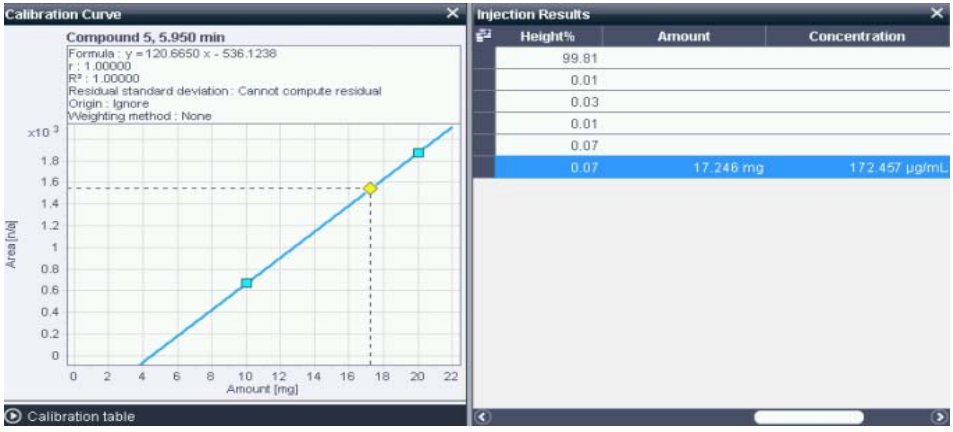


Figure 27 Calibration results for Compound 5 in Sample 4 of the example data

In the **Calibration Curve** window, the light blue squares are the two calibration levels. The yellow diamond is the compound of the selected sample.

The **Injection Results** window shows the **Amount** and calculated **Concentration** results.

To Save Results and Methods

1 Save your results (see "To Save the Results" on page 46).

The method linked to the injections of your result set is automatically saved together with the results.

2 If you want to use your edited method for other data, you can update the master method.

a Click  **Update Master Method**

A dialog opens. If a master method exists, the exact paths of the master method and result set method are shown. If no master method exists, a new one will be created.

b Click **Yes**.

Manual Integration

This section describes how you can interactively change the integration of your chromatogram by using manual integration.

Generally, manual integration includes the following steps:

- Open the relevant data and method.
- For manual integration, the data must be linked to a method.
- Display the chromatogram, and zoom into the area of interest.
- Activate manual integration.
- Move the mouse cursor over the area of the baseline where you want to change the integration.
- Depending on the position of the mouse cursor, the system will offer the corresponding manual integration tool.
- When the required manual integration tool is active, use the mouse to draw a new baseline or drag an existing baseline point to a new position.
- The data is automatically reprocessed. An asterisk (*) is appended to the file name in the injection tree to indicate the manual integration.

Data and Method Preparation

1 Load the relevant data.

NOTE To reproduce the examples that are described in the following sections, load the result set **Example_Data_for_Manual_Integration**. This result set is delivered as example data with OpenLAB Data Analysis.

2 Create a new method (see "To Create a New Method" on page 42) or load an existing method. To load a method:

   a Click  **Open Method** in the **Processing** ribbon tab.

   b Browse to the result set directory (for example, if you use ChemStation: C:\Chem32\1\Data\Example_Data_for_Manual_Integration) and select the method.

   c Click **Open**.

NOTE To reproduce the examples that are described in the following sections, load the method **Manual_Integration.pmx**. This method is delivered as part of the example data with OpenLAB Data Analysis.

3 Link the method to the data (see "To Link and Reprocess the Data" on page 44).

4 Display the chromatogram in the **Chromatograms** layout, and zoom in the area of interest.

For the example data, zoom to the retention time between about *7.0* and *9.0* min as in the following figure.

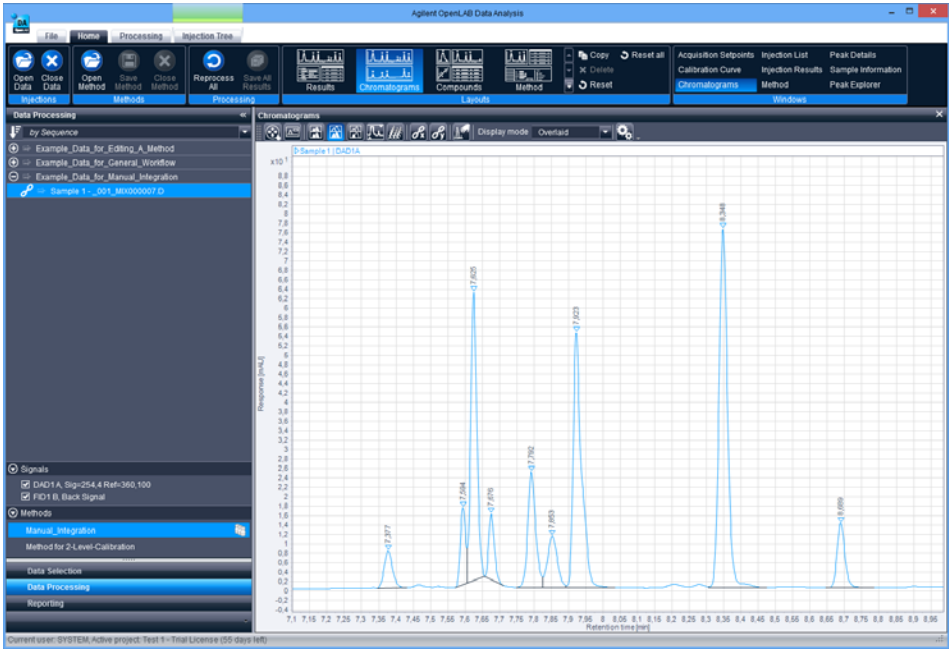


Figure 28 Data preparation for manual integration

To Enable or Disable Tools

You can enable or disable the single manual integration tools. By default, all tools are enabled.

1 To check which tools are enabled, click  in the **Chromatograms** toolbar.

The **Chromatogram Properties** dialog opens.

2 Select the **Manual integration** page.

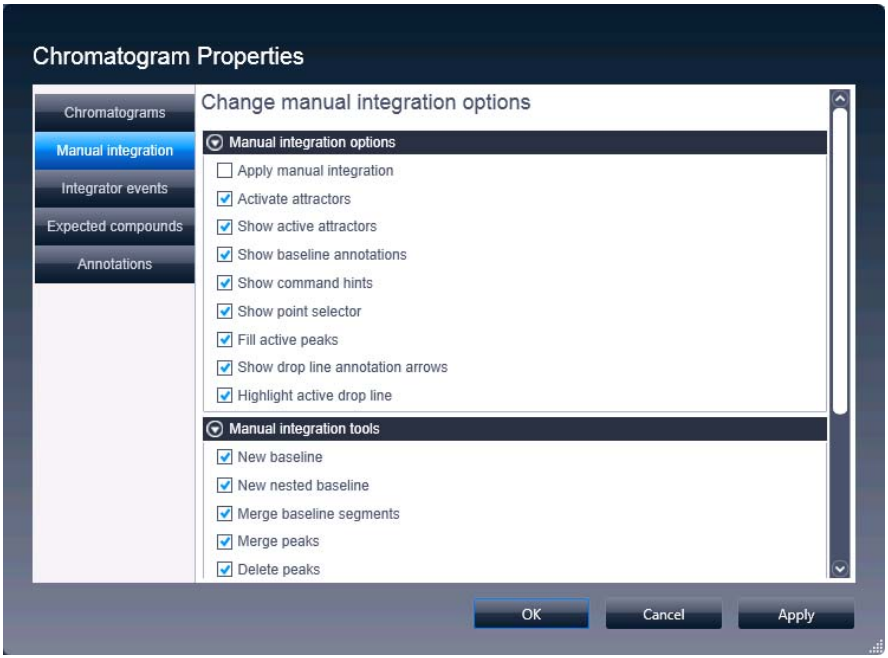


Figure 29 **Manual integration** page in the **Chromatogram Properties** dialog

Under **Manual integration options**, you can define the general behavior of manual integration tools. For example, you can choose whether you want to use attractors (see "Attractors" on page 67) or whether you want to see command hints when using the tools.

Under **Manual integration tools**, you can enable or disable each single manual integration tool.

To Activate Manual Integration

1 Click the Manual Integration icon in the **Chromatograms** toolbar.

The Undo and Redo icons appear.

Attractors

Many of the manual integration tools interact with so-called attractors. Attractors are usually visible on the signal and at baseline points of the adjacent elements. They are indicated by four small arrows. When the cursor approaches an attractor, it will automatically snap to the attractor. This allows to position new elements directly on the signal or directly attached to adjacent baseline segments.

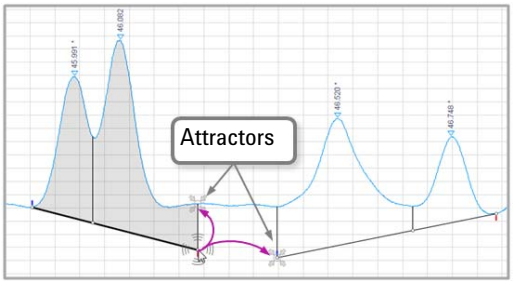


Figure 30 Attractor examples when moving a baseline point

Figure 31 Active Attractor with snapped in cursor

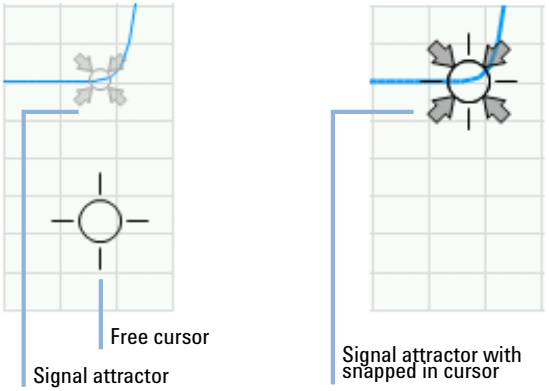


Figure 32 Attractor example when creating a new baseline

Integration Wheel

The manual integration allows modification of baseline points in various ways. To clarify the possibilities, see the following figure. The example shows the result of an automatic integration. As you can see there are several baseline segments. Some of them are associated with a single peak, others contain multiple peaks.

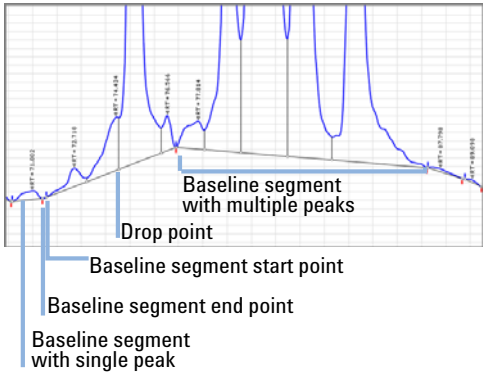


Figure 33 Baseline points

A baseline point can be part of one or two individual peaks or baseline segments. Depending on the type of baseline point, there exist multiple options of what to do with this single baseline point:

- *Move left baseline point*

  The baseline point is moved so that the whole left baseline segment including all its associated peaks is modified. The right baseline segment is not modified by this action.

- *Move right baseline point*

  The baseline point is moved so that the whole right baseline segment including all its associated peaks is modified. The left baseline segment is not modified by this action.

- *Move common baseline point*

  The baseline point is moved so that both baseline segments and all of their associated peaks are modified.

- *New connected baseline*

  A new baseline segment is created that directly starts at the active baseline point. The end point of the new segment can be freely positioned.

To allow easy selection of the possible options, the so-called *Integration Wheel* is used. The Integration Wheel appears automatically when you move the mouse close to a baseline start/end point or to the connection point of a drop line with a baseline segment. The Integration Wheel consists of several colored segments. Each of these segments is associated with a specific action that is possible for the active baseline point. For example, the following figure shows the Integration Wheel for a baseline point shared by two baseline segments.

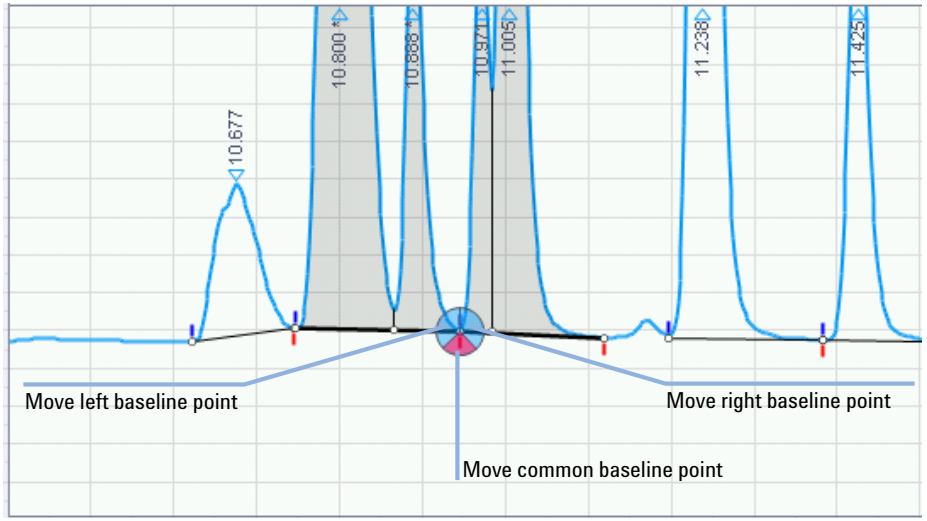
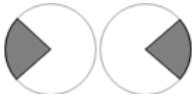


Figure 34 Integration Wheel for a common baseline point

In this specific example the Integration Wheel consists of three segments – one for each of the three possible options. The colors of the segments are linked with the associated action. The following tools can be offered by the Integration Wheel:

Segment	Integration Tool
	*Move baseline point* Modifies the whole baseline segment and all its associated peaks.
	*Move common baseline point* Modifies both (left and right) baseline segments and all of their associated peaks.
	*New connected baseline* Allows creation of a new baseline segment that starts directly at the baseline point.

Depending on the type of baseline point (for example, end point of a baseline segment, drop point on a baseline segment etc.), the integration tools offered within the Integration Wheel will vary. The system automatically offers the tools which are appropriate to use for the selected baseline point.

New Baseline

The **New Baseline** tool is automatically activated when you move the mouse cursor below the signal in an area where no peak is integrated. In this case, the cursor will change to a crosshair symbol.

Prerequisites For the example data, zoom between *7.3* and *7.5* min.

1 Move the mouse cursor below the signal in an area where no peak is integrated.

   The **New Baseline** tool is automatically activated. The cursor changes to a crosshair symbol.

2 Click with the left mouse button, and drag the appearing baseline to a new position.

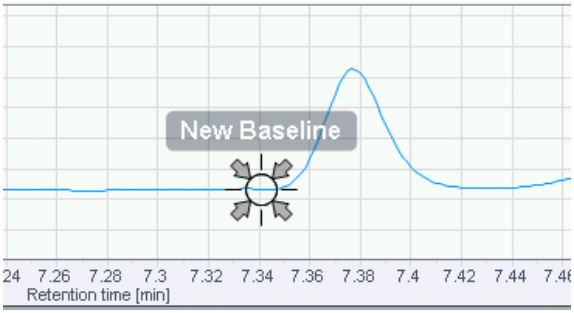


Figure 35 **New Baseline** tool with snapped in cursor

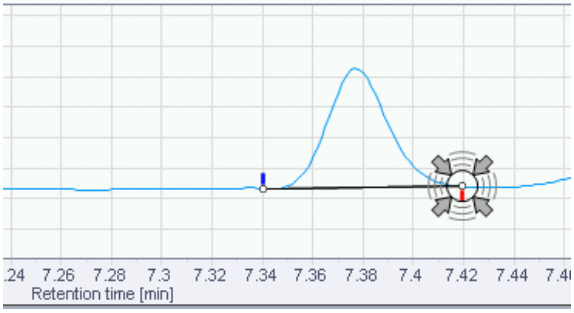


Figure 36 Active attractor with snapped in cursor

The new peak is now integrated.

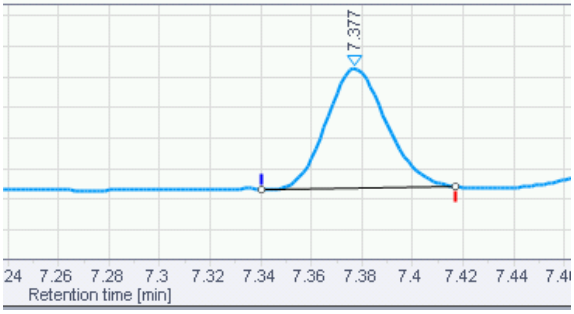


Figure 37 New integrated peak

The integrated peak is labeled with its retention time.

NOTE

You can construct the new baseline segment freely at any position within areas that do not contain peaks. However, it is often required that the baseline segment starts or ends directly at the signal. To achieve this, you can make use of the *signal attractor* (see "Attractors" on page 67).

New Nested Baseline

With the **New Nested Baseline** tool you can integrate shoulder or rider peaks. The shoulder and rider peaks are always associated with so-called nested baseline segments. These are segments that are defined within a parent peak. The **New Nested Baseline** tool works the same way as the **New Baseline** tool, but the dragging range is limited to the region of the associated peak.

Prerequisites For the example data, zoom between *8.3* and *8.5* min.

1 Move the mouse cursor within a peak, in a range where no other nested segments are defined.

   The **New Nested Baseline** tool is activated. The dragging range is limited by the parent peak and by already existing nested baseline segments.

2 Click with the left mouse button, and drag the appearing baseline to a new position.

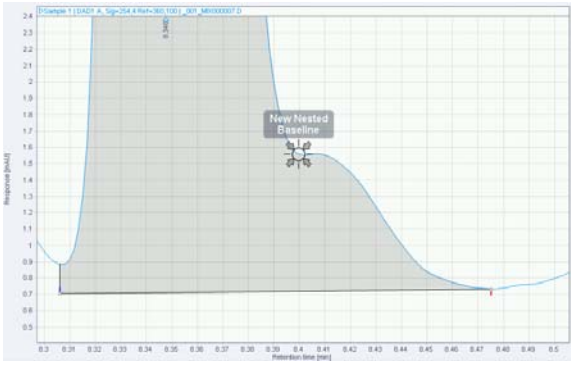


Figure 38 New **Nested Baseline** tool with snapped in cursor

Figure 39 Defining the end point of the new nested baseline

The new rider or shoulder peak is now integrated.

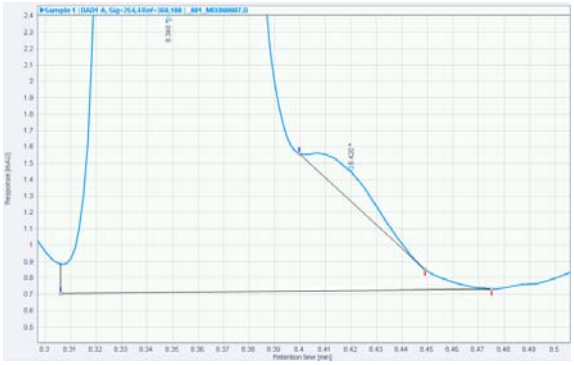


Figure 40 New integrated rider peak

The integrated rider peak is labeled with its retention time.

Merge Peaks

Prerequisites For the example data, zoom between *7.7* and *8.0* min.

1 Move the mouse cursor to a position above a drop line.
The **Merge Peaks** tool is activated.

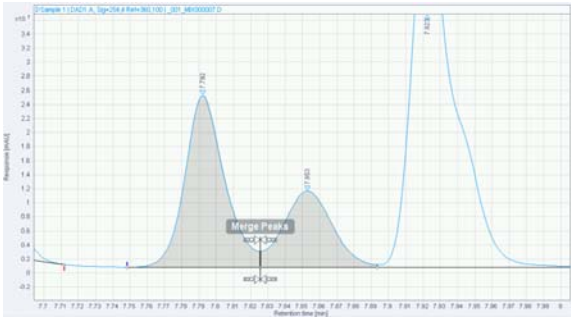


Figure 41 **Merge Peaks** tool activated

2 Click with the left mouse button to merge the highlighted peaks.

Split Peaks

Prerequisites For the example data, zoom between *7.7* and *8.1* min.

1 Move the mouse cursor above the signal of an integrated peak. The **Split Peaks** tool is shown.

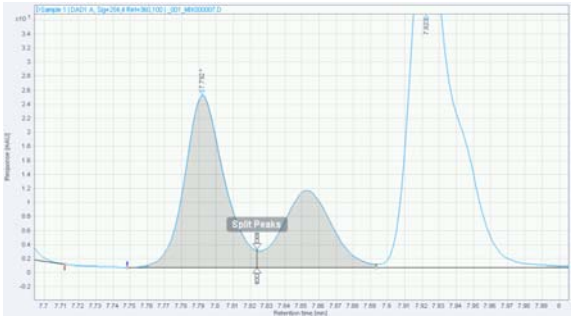


Figure 42 **Split Peaks** tool activated

2 Click with the left mouse button to split the peak at the position indicated by the drop line.

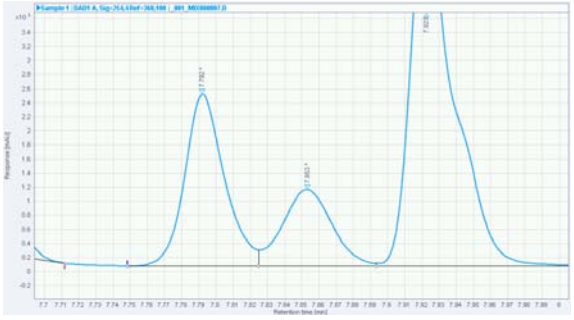


Figure 43 Split peak

Move Baseline Point

This procedure describes how you can modify a baseline point that indicates the intersection of a drop line with the baseline. This so-called *drop point* is part of a baseline segment and has no blue or red markers. Moving a drop point splits the baseline segment into two parts.

Prerequisites For the example data, zoom between *7.7* and *8.1* min.

1 Move the mouse cursor over the drop point.

The Integration Wheel is shown with the blue **Move Baseline Point** tool only.

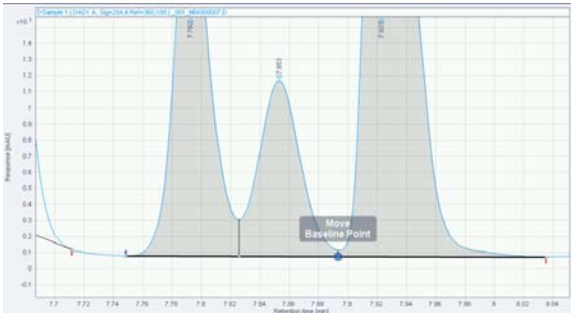


Figure 44 **Move baseline point** tool

2 Click the Integration Wheel, and move the baseline point to its new position.

The baseline segment will be split into two parts. Each baseline segment has a blue start point and a red end point .

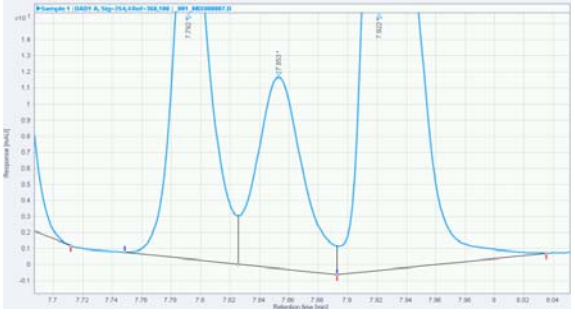


Figure 45 Moving a baseline point

Move Common Baseline Point

This procedure describes how you can modify a baseline point that is shared by two baseline segments. Moving a common baseline point affects both the baseline segments to the left and to the right of the baseline point.

Prerequisites For the example data, zoom between *7.7* and *8.1* min.

1 Move the mouse cursor over the baseline point.

The Integration Wheel is shown.

2 Move the mouse over the red section of the Integration Wheel.

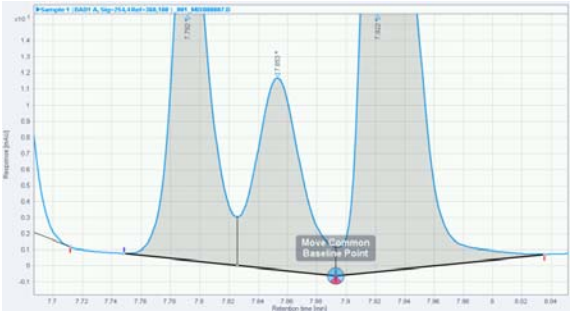


Figure 46 Integration Wheel with highlighted **Move Common Baseline Point** tool

3 Click the red section and drag the common baseline point to its new position.

Delete Peak

1 Move the mouse cursor over the area of an integrated peak.

2 Right-click in the peak area, and select **Delete peak** from the context menu.

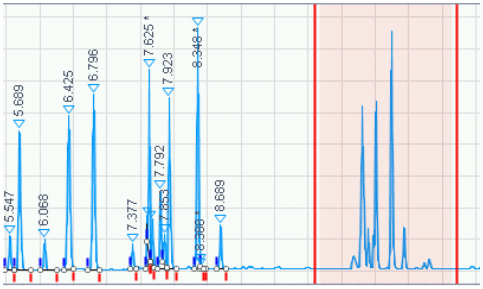
The baseline for this peak is deleted, and the peak is not integrated any more.

Delete Peaks in a Time Range

1 Press and hold the **Shift** key.

2 Click and drag the mouse over the time range where you want to delete the peaks.

While dragging, the relevant time range is highlighted in red.



To Clear Corrections

1 To undo all manual integrations, select **Clear corrections** in the **Processing** ribbon tab.

2 Process your data.

All manually changed integrations of your chromatogram will be removed.

Generating a Report

This section describes how to generate a report automatically and manually. If a report is generated manually, you can save the report for later review.

To Generate Reports Automatically

You can configure a method so that a report is automatically created after reprocessing each injection.

NOTE

When reprocessing the data, make sure the check box **Create reports** in the **Processing** ribbon tab is selected.

Especially when reprocessing a large number of injections, automatic report generation can reduce the processing performance. In this case, it is recommended to use the **Reporting** view for report generation (refer to "To Generate a Report Manually" on page 82).

1. If the **Method** window is hidden, click **Method** in the **Home** ribbon tab to show the window.
2. Under **Methods** in the navigation pane, select the method you want to edit, for example the method **Method for 2-Level-Calibration**.

3 In the **Method** window, select the **Reports** section, and then the **Injection Report** node as in the following figure.

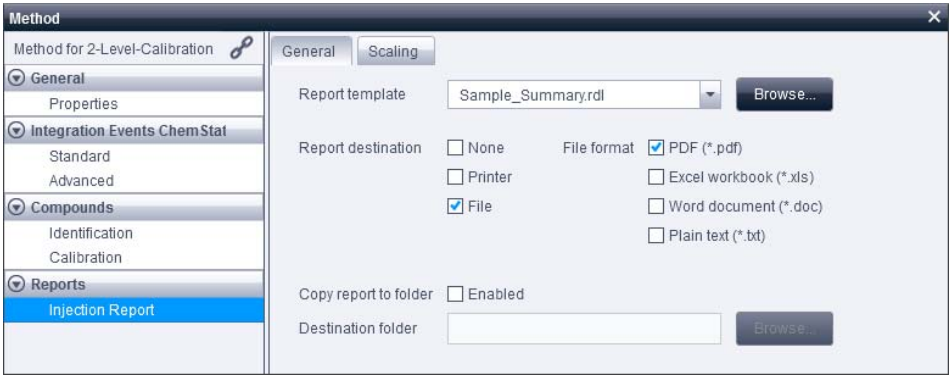


Figure 47 Generating a report automatically

4 Select one of the default templates from the **Report template** drop-down list, or click **Browse...** to select a specific template from another location.

5 Under **Report destination**, select **Printer**, **File**, or both.

You can send the report files directly to the printer, save them as a file, or use both options at the same time. If you save the report as a file, select a suitable file format. The report files will be saved in the data file folder corresponding to the injection data.

6 Optional: To save copies of the reports in an additional location, select **Copy report to folder** and provide a folder name under **Destination folder**.

7 Link the method to one or more data files.

The report files are automatically generated.

To Generate a Report Manually

1 Select the **Reporting** view.

2 Select the data that you want to report.

   a The **Injections** section of the navigation tree lists all currently loaded injections. If you want to consider other data: Load the corresponding data files (see "Loading Data" on page 34).

   b Select the relevant data either by clicking the names so that they are highlighted, or by pinning them.

   For example, select **Example_Data_for_General_Workflow**.

   If you do not select any data, the report will be created using demo data.

3 Load a report template.

   a The **Report Templates** section lists all report templates in the currently selected directory. If required, navigate to a different directory.

   You can find a set of default templates at the following locations:

   - Program Files\Agilent Technologies\OpenLAB Data Analysis\Bin\Reporting\IntelligentReporter\DefaultTemplates
   - Program Files (x86)\Agilent Technologies\OpenLAB Data Analysis\Bin\Reporting\IntelligentReporter\DefaultTemplates
   - On disc 7 of the installation DVDs: \Disk7\Report Templates\

   b Double-click the report template, for example SequenceSummary_Standard.rdl.

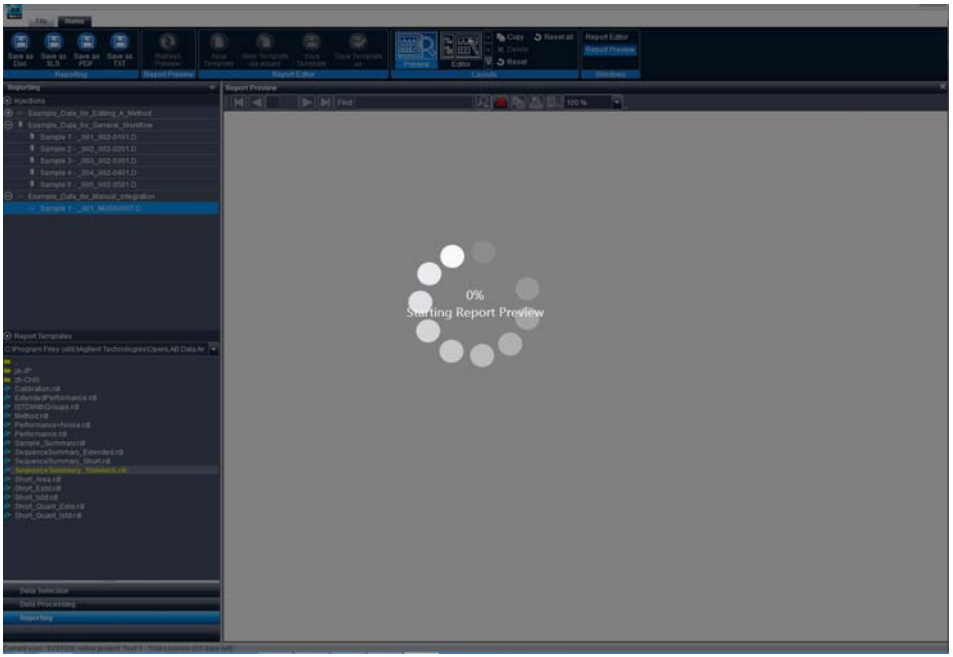


Figure 48 Generating a report manually

A report will be created based on the selected report template and the selected data. The report template used to create the report is shown.

NOTE The **Performance+Noise** report only works with data processed by ChemStation or EZChrom. When reprocessing data in OpenLAB Data Analysis, the required peak performance parameters are not calculated.

4 If you have created a report manually, you need to save the report for later review.

a In the ribbon, click on one of the save buttons  corresponding to the required format. You can choose among the formats DOC, XLS, PDF, or TXT.

A **Save As** dialog opens.

NOTE TXT files do not contain pictures. Chromatograms, calibration curves, spectra, and charts are not available in this format.

b Specify the file name and location for the report, and click **Save**.

5 OpenLAB CDS Configuration for Automated Usage

You can configure ChemStation or EZChrom so that they use OpenLAB Data Analysis by default. This chapter describes the required configuration in ChemStation or EZChrom.

Configuring ChemStation for Automated Processing with OpenLAB Data Analysis

ChemStation methods contain both data acquisition parameters and data analysis parameters. In each ChemStation method, you can call a processing method from OpenLAB Data Analysis instead of the ChemStation-specific data analysis.

Copying the ChemStation Macro File

Copy Disk7\CDS_Automatic_Processing\ChemStation\da_processing.mac to Chem32\Core.

Editing the ChemStation Method

Repeat these steps for each ChemStation Method. You can find example methods for ChemStation on disc 7 under the following paths:

- CDS_Automatic_Processing\ChemStation\Example_GC.M
- CDS_Automatic_Processing\ChemStation\Example_LC.M

These methods already use a Run Time Checklist as described below, you must only adjust the path to the .pmx file. You can use these methods as a starting point for developing your own method.

1 Load your ChemStation method.
   a Select **View > Method and Run Control**.
   b Select **Method > Load Method**.
   c Select the method to be edited. (Method files have a .m extension.)
   d Click **OK**.
2 Select **Method > Run Time Checklist...**.

3 Select the **Pre-Run Command / Macro** check box, and enter the following string in the input field:

loadmacro "da_processing.mac"

4 Clear the **Standard Data Analysis** check box.

The standard data analysis is performed directly in ChemStation. If you use an OpenLAB Data Analysis method, this section is irrelevant.

5 Make sure the **Customized Data Analysis Macro** check box is cleared as well.

6 Select the **Post-Run Command / Macro** check box, and enter the following string in the input field:

da_postrun "<.pmx file path>"

For example, if you are working with ChemStation, the file path could look like the following:

da_postrun "C:\Chem32\1\Method\example.pmx"

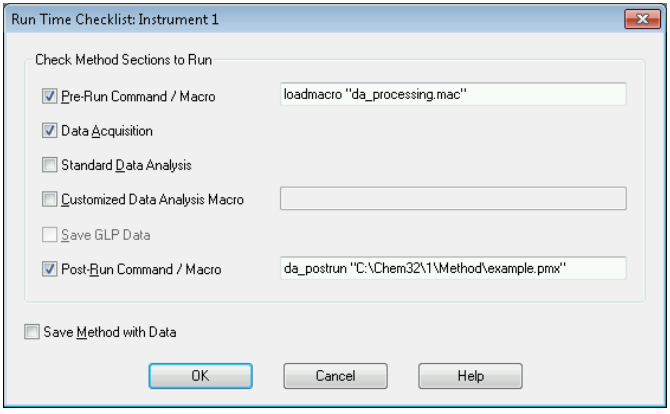


Figure 49 Run Time Checklist for using an OpenLAB Data Analysis method

7 Save your settings.

When you use this method in ChemStation, the OpenLAB Data Analysis method will automatically be used for analyzing the data.

Configuring EZChrom for Automated Processing with OpenLAB Data Analysis

Repeat these steps for each EZChrom method.

1. Load your EZChrom method.
2. Click **Method > Advanced**.
3. In the **Advanced Method Options** dialog, select the **Files** tab.
4. Select the **After export** check box.
5. Click the Browse icon and navigate to the file iDAProcessing.exe, or enter the path and filename directly.

   Typically, this file is located under C:\Program Files\Agilent Technologies\OpenLAB Data Analysis\Bin\iDAProcessing.exe.
6. Under **Additional parameters** in the **After export** section, enter the path and file name of the required OpenLAB Data Analysis method (.pmx file).

NOTE Use double qoutes for the path to the method.

For example, if you are working with EZChrom, the file path could look like the following:

"C:\Enterprise\Projects\Project1\Method\example.pmx"

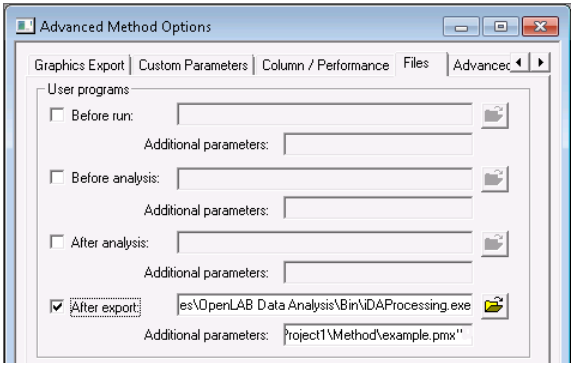


Figure 50 Advanced method options for using an OpenLAB Data Analysis method

7 Save your settings.

When you use this method in EZChrom, the OpenLAB Data Analysis will automatically be used for analyzing the data.

6
Appendix

Invalid Characters for File or Path Names

The following table lists the invalid characters for file or path names in ChemStation and EZChrom. These names are used, for example, for storing data, methods, or report templates.

- X denotes an invalid character.
- - denotes a valid character.

Table 2 Invalid characters

Character	ChemStation	EZChrom
< (less than)	X	X
: (colon)	X	X
> (greater than)	X	X
" (double quote)	X	X
/ (forward slash)	X	X
\ (backslash)	X	X
| (vertical bar or pipe)	X	X
? (question mark)	X	X
* (asterisk)	X	X
; (semicolon)	X	-
& (ampersand)	X	-
' (quote)	X	-
@ (at sign)	X	-
% (percent)	X	-
Blank space	X	-
[(bracket open)	X	-
] (bracket close)	X	-
+ (plus)	X	-
. (dot)	X	-

Uninstallation of OpenLAB Data Analysis

If you have installed OpenLAB Data Analysis as a stand-alone application, that is, there is no OpenLAB CDS ChemStation or EZChrom Edition running on your system, you can uninstall OpenLAB Data Analysis as described in the following.

If OpenLAB Data Analysis is running together with OpenLAB CDS, an uninstallation of OpenLAB CDS will also remove OpenLAB Data Analysis. For more information on the uninstallation of OpenLAB CDS, refer to the OpenLAB CDS installation manual.

1 In the Master Installer, select **Maintenance** from the side bar menu.

2 Select **OpenLAB Uninstallation**.

An uninstallation wizard opens.

3 In the **Shared Components** screen: If any other Agilent products are installed, clear the **Uninstall Software Verification** check box.

4 Click **Next**.

In the **Summary** screen, there is a list of the components you want to uninstall.

5 Select **Start** to start the uninstallation.

If you want to abort the uninstallation, select **Cancel**. If you want to change any settings, select **Back**.

All listed components are automatically uninstalled, one after another.

6 When the uninstallation has finished, click **Finish** to close the uninstallation wizard.

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In This Book

This guide describes the installation of OpenLAB Data Analysis, the required configuration steps, and the main workflows. Read this manual if you want to install OpenLAB Data Analysis or if you want to use it to analyze your data.

The manual describes the following:

- Introduction
- Installation
- OpenLAB Control Panel Configuration
- Working with OpenLAB Data Analysis
- OpenLAB CDS Configuration for Automated Usage
- Appendix

Printed in Germany
9/2014

M8370-90001
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