



Quick Start Guide

Chromeleon 7

Thermo Scientific Chromeleon

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1 Introduction

1.1 About this Document

The Quick Start Guide is designed to provide a quick reference to starting to work with Chromeleon. It is recommended that you review the Quick Start Guide thoroughly before working with Chromeleon.

The Quick Start Guide has two parts:

Using Chromeleon	Guidance in starting a simple analysis, processing the data, and reporting the results.
Appendix: Chromeleon Overview	An overview of the Chromeleon interfaces and common features.

This Quick Start Guide is provided "as is". Every effort has been made to supply complete and accurate information and all technical specifications and programs have been developed with the utmost care. However, Thermo Fisher Scientific assumes no responsibility and cannot be held liable for any errors, omissions, damage, or loss that might result from any use of this manual or the information contained in it.

1.2 Other Documentation

Chromeleon is provided with other documents that will help you to learn more about the software. Their scope is described in the *Document Overview*, which is delivered in printed form with the Chromeleon installation media, but also available in electronic form on the installation disk in the *Documents* folder.

2 Using Chromeleon

2.1 Overview

Every analysis using Chromeleon follows the same 6 basic steps:

1. Start Chromeleon
2. Start the Instrument
3. Create a Sequence
4. Acquire Data
5. Process Data
6. Review and Report Results

This Quick Start Guide provides enough information to perform each of these 6 steps as part of a simple analysis. For more advanced use of Chromeleon, including performing more complex analyses, please refer to Chromeleon Help or the Chromeleon User Guide.

Note: It is assumed that Chromeleon has been installed and at least one instrument has been connected and configured. For details on installation, connecting and configuring instruments see the Installation Guide.

2.2 Starting Chromeleon

To start the Chromeleon software either:

- Double click the **Chromeleon 7** icon on the desktop:



- Use the Windows Start menu:

Select **Start > All Programs > Chromeleon 7 > Chromeleon 7**

The Chromeleon Console window opens. If user management is active, you will be prompted to log in to the software; enter the credentials provided by your Chromeleon administrator to proceed.

2.3 Starting an Instrument

To start and monitor an instrument you must:

- Make sure the Instrument Controller service is running
- Establish a connection
- Start and monitor the instrument

2.3.1 Making sure the Instrument Controller Service is Running

The Chromeleon Instrument Controller Service handles instrument communications, control, and data acquisition. It runs in the background as a Windows service on any PC to which instruments are physically connected. Its status is represented by an icon in the Notification Area of the Windows Taskbar.

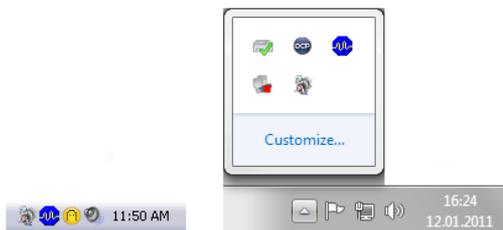


Figure 1 : Notification Area of Windows Taskbar for Windows XP and Windows 7

-  Instrument Controller Service is stopped
-  Instrument Controller Service is running

If the Instrument Controller Service is stopped, start it by following these steps:

1. Right-click the **Chromeleon tray icon** in the notification area of the Windows task bar.
2. Click **Start Chromeleon Instrument Controller**.

Tip: If the Chromeleon tray icon is not visible on the task bar, click Start, point to Programs (or All Programs, depending on the operating system) and Chromeleon 7, and click Services Manager.

Note: You can configure the Chromeleon Instrument Controller Service to automatically start every time the computer is switched on. See the Controlling Instruments and Modules section of the Chromeleon Help for more information.

2.3.2 Establishing a Connection

Before you can control an instrument, communication must be established between the Modules and the Chromeleon Instrument Controller. This is referred to as “Connecting the Modules”.

To connect the chromatography modules follow these steps:

1. In the **Console**, choose the **Instruments** category and click your instrument’s name in the Navigation Pane.
2. Select the ePanel tab for the required module in the Work Area (for example **Pump**).
3. On the **ePanel**, click **Connect**.

Note: The ePanel sets are generated automatically to support modules from a specific instrument series (e.g., UltiMate 3000, ICS-5000). When combining modules from these instruments, ePanels for some modules may not be displayed automatically. See “Managing ePanel Sets and ePanels” in Chromeleon Help for details on manually adding ePanels to a set.

2.3.3 Starting and Monitoring the Instrument

To start the instrument modules follow these steps:

1. In the **Console**, choose the **Instruments** category. Select the instrument by clicking its name in the Navigation Pane.
2. In the Work Area select the **ePanel tab** for the required module.
3. Use the controls on the **ePanel** to issue instrument commands (for example setting the wavelength of a UV/VIS detector or starting mobile phase flow on a pump).

You can monitor instrument parameters and outputs such as the detector signal output or pump pressure from the module's **ePanel**.

Note: Most common commands are available from the ePanels. If you need to execute a command that is not available you can access all available instrument commands from a dialog that is accessible via the commands button  **Command** in the Instruments toolbar.

Tip: For certain instruments, Chromeleon provides procedures for automatically starting or shutting down a chromatography system, or setting it into standby mode. These procedures are referred to as Smart Startup, Smart Shutdown, and Smart Standby, respectively. For details of which instruments can be controlled in this way and how to use this functionality see “Smart Startup, Smart Shutdown, and Smart Standby” in Chromeleon Help.

2.4 Creating a Sequence

A sequence determines how a group of injections should be processed. The injection list is the primary element of the sequence. The list groups injections in the order in which they will be processed and includes injection variables (name, type, etc.) that characterize each injection.

Sequences can be created in the **Console** or by using an **eWorkflow**. eWorkflows are simple but powerful tools for creating sequences based on pre-defined templates and rules. For more information on creating and using eWorkflows see “Creating eWorkflows” in Chromeleon Help.

You create a sequence using the Sequence Wizard within the **Console**. But first, the following files should be prepared:

- Instrument Method
- Processing Method
- Report Template

2.4.1 Creating an Instrument Method

1. In the **Console**, on the **Create** menu, click **Instrument Method**.
2. If you have multiple instruments, select the instrument for which you want to create the Instrument Method and click **Next**.
3. Complete all wizard steps and click **Finish**.

The created Instrument Method opens in the Chromatography Studio.

4. Review the Instrument Method by selecting the module views in the navigation pane. Edit settings, if required.

5. Save the Instrument Method using the **Save** icon  in the Quick Access Toolbar and specify a location and object name.
6. Close the Chromatography Studio.

2.4.2 Creating a Processing Method

1. In the **Console**, on the **Create** menu, click **Processing Method**.
2. Select one of the predefined layouts and click **Next**
3. Enter a name, select a file location and optionally enter a comment.
4. Click **Finish** to save the Processing Method and close the wizard.

The new Processing Method opens in the Chromatography Studio.

2.4.3 Creating a Report Template

1. In the **Console**, on the **Create** menu, click **Report Template**.
2. Select one of the predefined templates and click **Next**.
3. Select a file location and enter a file name.
4. Click **Finish** to save the Report Template and close the wizard.

2.4.4 Creating a Sequence

To create a sequence using the Sequence Wizard within the **Console**:

1. In the Console, on the **Create** menu, click **Sequence**.
2. If you have multiple instruments, select the instrument for which you want to create the sequence and click **Next**.
3. Complete the Injection Configuration fields for the injections:

Pattern for Injection Name: Specify how injections will be named. This is a free text field to which the codes #n #p #i and #r can be added. (Click the  button to the right of the **Pattern for Injection Name** field to see definitions for these codes)

Number of Vials: Specify the total number of vials in the analysis.

Injections per Vial: Specify the number of injections per vial in the analysis.

Start Position: Specify the sequence start position of the sequence for the analysis. This specifies the position of the first vial in the autosampler. The wizard automatically increments for the following vials.

Injection Volume: Specify the injection volume.

4. Click **Next**.

Note: When you are creating a sequence using the wizard, you can only add injections with type Unknown. Once the sequence is created, you can modify the Injection Types and Positions.

5. Select **Methods and Reporting Preferences**: For each field use the  button to navigate to and select the file you want to use. When all fields are completed click **Next**.
6. Enter a comment for the sequence (optional) and click **Finish**.

The Save dialog opens.

7. Specify where to save the sequence, enter a file name and click **Save**.
8. If necessary, change the injection names, Injection Types, Injection Positions, and other entries. For an overview of Injection Types refer to section 3.3.1.2.

The sequence is now visible in the Chromeleon Console's **Navigation Pane**.

2.5 Acquiring Data

2.5.1 Starting an Analysis

Once the sequence has been created and the instrument is ready you can start data acquisition.

2.5.1.1 Check the Instrument is Ready

1. In the **Console**, choose the **Instruments** category. Select the instrument by clicking its name in the Navigation Pane.
2. In the Work Area select the **ePanel** tab for the required module. To check the baseline for example, select the detector's **ePanel** and switch on data acquisition by clicking the **Monitor Baseline** button.

When you are satisfied that the instrument is ready for analysis, start the sequence.

2.5.1.2 Starting the Sequence

1. Select the **Data** category in the Console.
2. In the Navigation pane select the sequence you want to run by clicking on it.

The Sequence then opens in the **Work Area**.

3. Click the  button to start the sequence.

The sequence is added to the Queue. If the Queue is not running, it will start (Figure 2).

#	Name	Type	Positio	Volume [µl]	Instrument Method	Proce
1	7 Anion Standard 1	Unknown	1	20.0	ICS-3000 - AS14A Production Test Chromatogram	AS14
2	7 Anion Standard 2	Unknown	2	20.0	ICS-3000 - AS14A Production Test Chromatogram	AS14
3	7 Anion Standard 3	Unknown	3	20.0	ICS-3000 - AS14A Production Test Chromatogram	AS14

Figure 2: Running Sequence

Note: The Chromeleon Queue can be used to schedule multiple sequences ready to perform consecutive analyses. See “Managing Queues” in Chromeleon Help for information on using Queues.

Tip: Chromeleon contains tools (Smart Startup) which let you start sequences automatically when the instrument parameters (such as baseline drift), are suitable for analysis. Smart Shutdown, and Smart Standby can be used to shut down or flush instruments at the end of analysis. For details of which instruments can be controlled in this way and how to use this functionality see “Smart Startup, Smart Shutdown, and Smart Standby” in Chromeleon Help

2.5.2 Monitoring an Ongoing Analysis

During analysis it is useful to monitor the detector signal and other instrument parameters (such as pressure and temperature).

To monitor an ongoing analysis:

1. In the **Console**, choose the **Instruments** category and click your instrument’s name in the Navigation Pane.
2. Select the ePanel for the detector in the Work Area.

The detector signal is displayed.

Note: The settings of other modules can be monitored on their respective ePanels.

2.6 Processing Data

After chromatographic data has been acquired, it can be processed. Chromeleon has many tools to simplify or speed up data processing tasks, such as **SmartPeaks**, but only the most common processing steps will be described in this Quick Start Guide.

All processing steps are performed in the **Studio**. To open the Studio from the Console, double click any object in a sequence, or on the sequence itself, or click the Studio  **Studio** button.

Note: When you make a change in the Processing Method, the results for all injections in the sequence which use that Processing Method are recalculated instantaneously. There is no need to “reprocess” the sequence or manually update results.

2.6.1 Reviewing Chromatograms and Data

Once data for all samples in a sequence has been acquired it is useful to review the chromatograms and peak data before reporting the results. (Often, peak detection, integration and calibration settings need to be modified before results are reported. See Integration, Identification, Calibration and Quantitation 2.6.1.2 for details on these tasks).

2.6.1.1 Viewing Data

1. Open the first injection of the sequence in the **Chromatography Studio** by double clicking on an injection in the Data view of the Chromeleon Console's Work Area.

The Chromatography Studio opens.

2. Open the **Data Processing Category** and in the Navigation Pane select the injection you want to view.

The data for that injection is displayed in the Work Area, using the default Preset view.

Tip: There are several Views in Chromeleon which can be selected from the Presets menu of the ribbon. You can also create new Views and store these to be used again. See "Create New View Settings" in Chromeleon Help for details on setting up custom Views.

3. You can navigate through the data by:
 - Using the **Previous**  and **Next**  **Injection** buttons in the **Navigation** group of the **Data Processing Home** Ribbon tab or
 - Selecting Injections in the **Navigation Pane** or
 - Double-clicking the component or injection you want to evaluate in the Integration/Summary Table of the **Interactive Results table** (Figure 3).

A	B	C	D	E
Sample No.	Sample Name	Ret. Time min	Area mAU*min	Height mAU
Pro-OH	Pro-OH	Pro-OH	Pro-OH	Pro-OH
6	Linearity 2	4.527	0.6847	6
7	Linearity 3	n.a.	n.a.	
8	Linearity 3	4.523	0.6851	6
9	Linearity 3	n.a.	n.a.	
10	Linearity 4	4.512	0.7401	7
11	Linearity 4	n.a.	n.a.	
12	Linearity 4	n.a.	n.a.	
13	Linearity 5	4.507	0.7847	12
14	Linearity 5	4.507	0.7402	11
15	Sample	n.a.	n.a.	
16	Sample	n.a.	n.a.	
17	Sample	4.475	0.9297	12
Average:		4.516	0.7906	8.3
Total Area:		0.2808	10.0938	21

Figure 3: Selection in interactive results table

Tip: You can use the pins  in the Navigation Pane to overlay chromatograms from different injections or channels.

2.6.1.2 Integration, Identification, Calibration and Quantitation Peaks

This section covers:

- Peak Detection and Integration
- Peak Identification
- Calibration and Quantitation

2.6.2 Detecting and Integrating Peaks

For correct quantification or qualification of a chromatogram all required peaks must be detected and correctly integrated. To achieve this you can either:

- Create a new set of Detection Parameters or
- Modify an existing Processing Method

For the purposes of this guide it is assumed that the user will first create a new set of Detection Parameters and then modify these to improve the integration and peak detection.

2.6.2.1 Creating a New Set of Detection Parameters Peaks

This section gives information on how to set up a new Processing Method and use the **Cobra™ Peak Detection Wizard** to determine the initial integration settings for a chromatogram. For more information about creating Processing Methods see section 2.4.2.

1. Open the sequence in the Chromatography Studio (by double-clicking an injection in the Console) and open the **Data Processing** category.
2. Select the Chromatogram by clicking somewhere in the Chromatogram Plot area.

3. Click the **Processing** contextual Ribbon tab and activate the Cobra™ Peak Detection Wizard by selecting the **Cobra Wizard**  in the **Detection Parameters** group.

The Cobra Wizard opens.

Tip: While using the Cobra wizard, you can zoom in to the chromatogram by holding the control (Ctrl) key and zooming in using the mouse.

4. Select the area of the Chromatogram to be integrated.

If the section selected contains negative peaks (for example solvent peaks), you can specify that these are ignored during Cobra Peak Detection by checking the **Consider Void Peak** check box. Otherwise leave this check box cleared.

Click **Next**.

5. Either:

- Select the **Use Auto Range** option (default), or
- Manually enter a baseline range to be used to determine the noise.

Click **Next**.

6. Either:

- Select the **Use Auto Smoothing Width** option (default), or
- Select the narrowest peak in the chromatogram in order to define the Cobra smoothing width used for peak detection.

Click **Next**.

7. Either:
 - Select **Use Auto Minimum Area** (default), or
 - Select the smallest peak in the chromatogram that you want to be detected (the minimum area will be set to 90% of the area of the selected peak).

Click **Next**

8. Use the drop down **Channel** menu to select the channel, and the **Injection Type** field to specify which data the integration settings will apply to.
9. Click **Finish**.
10. Click the Chromeleon icon  and select **Save > Save** from the menu to save the updated processing method.

The **Cobra™ Peak Detection Wizard** determines the best initial integration settings for a chromatogram. For simple chromatograms, where all peaks are well resolved, these settings will be ideal. For complex chromatograms or where peaks are only partially resolved the addition of further detection parameters may be required.

2.6.2.2 Modifying an existing Processing Method

2.6.2.2.1 Insert a New Detection Parameter

To insert a new Detection Parameter, follow these steps:

1. Click in the chromatogram plot.
2. Click the **Processing** contextual Ribbon tab.
3. If not already shown, display the Detection Parameters in the chromatogram, by clicking **Detection Parameters**  in the **Detection Parameters** group.
4. Click the drop down arrow on the **Insert**  ribbon button.

5. Select the appropriate Detection Parameter from the list.

The most frequently needed parameters are listed here. If you need other Detection Parameters, select **Other Parameter**.

For a list and further details on all Chromeleon Detection Parameters see “Detection Parameters (Overview)” in Chromeleon Help.

6. Move the cursor to the location in the chromatogram where you want to insert this parameter and click.

The new Detection Parameter is placed in the chromatogram and peak integration is automatically updated.

Detection Parameters have a tag which shows details of the parameter and a vertical dashed line which shows the exact point of the Detection Parameter in the chromatogram.

2.6.2.2.2 Moving, Modifying and Deleting Detection Parameters

1. Click in the chromatogram plot.
2. Click the **Processing** contextual Ribbon tab.
3. If not already shown, display the detection parameters in the chromatogram, by clicking Detection Parameters  in the **Detection Parameters** group.
4. In the **Pointer / Zoom** group ensure that the **Automatic**  tool is selected.

5. Then:

To Move a Detection Parameter:

- Drag and drop the Detection Parameter to the required location (you can drag a Detection Parameter by its tag or line).

To edit the value of a Detection Parameter:

- Double click the tag and select a new setting from the drop down list.

To change the type of Detection Parameter:

- Right click on the Detection Parameter and select **Edit Detection Parameter**.

The **Edit Cobra Detection Parameter** dialog box opens.

- Select a new Detection Parameter type from the Parameter Name field and set any Parameter Values needed.
- Click OK to save the change and close the **Edit Cobra Detection Parameter** dialog box.

To delete a Detection Parameter

- Right click on the Detection Parameter and select **Delete Detection Parameters**.

2.6.2.2.3 Integrate Unresolved Peaks

Partially resolved peaks can be difficult to integrate. The SmartPeaks™ integration assistant helps you to integrate these peaks:

1. Click in the chromatogram plot.
2. Click the **Processing** contextual Ribbon tab.
3. Select the **SmartPeaks** tool  from the **Detection Parameters** group.
4. Use the cursor to drag a rectangle in the chromatogram around the area that contains the partially resolved peaks.

The **SmartPeaks: Select Alternative** dialog box opens (Figure 4).

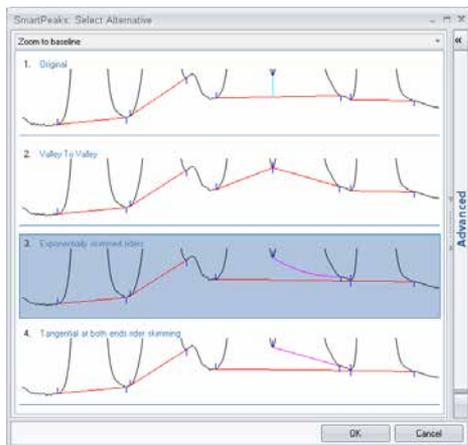


Figure 4: SmartPeaks: Select Alternative dialog box

Tip: For more options you can click the Advanced tab in the SmartPeaks: Select Alternative dialog box. For details of how to use these settings see “SmartPeaks: Select Alternative” in Chromeleon Help.

5. Select the preferred peak detection and click **OK**.
6. The Detection Parameters in the Processing Method are now updated and the new Detection parameters are shown in the chromatogram.

2.6.3 Identifying Peaks

Once peaks have been detected and satisfactorily integrated they can be used for reporting or results calculations. It is useful when reporting, to name components in a chromatogram. It is essential when performing Calibration and Quantification that at least the calibration peaks in a chromatogram are named.

The process of assigning a name to a component is called Identification. The names and expected retention times of named components are stored in a Chromeleon Component Table.

The following sections describe how to:

- Create a Component Table
- Update the expected retention times and windows.

2.6.3.1 Creating a Component Table

There are three ways to create a Component Table:

- Via the Component Table Wizard
- Interactively in the Chromatogram Pane
- Via the Component Table (Processing Method)

2.6.3.1.1 Via the Component Table Wizard

To create a component table by using the Component Table wizard:

1. Click in the Chromatogram Plot.
2. Click the **Processing** contextual Ribbon tab.
3. If not already shown, display the Peak Windows in the chromatogram, by clicking Peak Windows () in the **Component Table** group.
4. Click the **Component Table** button ().

The Component Table Wizard dialog box opens.

The 5 page wizard guides you through the process of naming components. On the first 4 pages you specify whether to keep existing components (adding new components to the existing), the time range over which to consider components, and a minimum area below which components are ignored. On the final page you can name all found components, modify the retention time and peak window and add comments.

5. Click **Finish** to save the Component Table updates and close the Component Table Wizard.

The chromatogram view in the Chromatography Studio Work Area is automatically updated to display the new Component Windows.

2.6.3.1.2 Interactively in the Chromatogram Pane

To add a component from the Chromatogram plot:

1. Click in the chromatogram plot.
2. Click the **Processing** contextual Ribbon tab.
3. Activate the **Peak Windows** option and the **Add Component** option in the **Component Table** group.
4. Drag a rectangle around the peak you want to add to the component table.

The peak is added to the component table with a generic name (for example **Component 1**) and the Peak Window is visible in the chromatogram plot.

5. Double-click the Peak Window tag and enter the component name.

2.6.3.1.3 Via the Component Table (Processing Method)

To create a component table in the processing method:

1. Click the **Data Processing Home** Ribbon tab.
2. In the **Panes** group, click **Processing Method** to display the Processing Method.

Tip: You can maximize screen space by hiding the other panes and view the Processing Method only.

3. In the Processing Method, select the **Peak Table** tab.
4. Click the **Click here to add a new component** link at the bottom of the Peak Table.

A **Create new Component** dialog box opens.
5. Type the name of the component in the name field and click **Create**.

A new component is created and displayed in the Peak Table.
6. Update the component retention time and window in the **Ret. Time** and/or **Window** columns of the Peak Table.

Tip: Over a period of time, peak retention times may drift from their expected values. Because of this, it is sometimes useful to set wide peak windows in the Component Table. When peak retention time drift is too large for this method to compensate, you can use the retention time of a previous peak for peak identification. For details on correcting for Retention Time drift see "Identify Peaks" in Chromeleon Help.

2.6.3.2 Updating Retention Times and Windows

You can modify the retention time and width of Peak Window by modifying the properties in the Peak Table or by dragging and dropping the Peak window on the Chromatogram plot.

2.6.4 Calibration

Calibration is applied only to Standards in the sample sequence. A calibration curve is constructed for each component, using the area or height and amount or concentration for the corresponding peak.

This section takes you through the steps required to perform a simple external standard calibration (using a single component standard at multiple concentrations). Chromeleon supports various methods of calibration including internal standards and standard addition. For information on using these methods of calibration see “Calibration and Amount Calculation” in Chromeleon Help.

To perform a simple calibration in Chromeleon you will need to:

- Specify which injections are Calibration Standards
- Create Calibration Levels and assign these to the Calibration Standards
- Enter the Calibration Amounts for Calibration Standards
- Review the calibration curve

2.6.4.1 *Specifying which Injections are Calibration Standards*

Calibration standards are marked as such in the injection sequence:

1. Click the **Injection List** Category in the Chromeleon Chromatography Studio window.
2. For each Calibration Standard injection click in the **Type** field and select **Calibration Standard** from the drop down list of types.

2.6.4.2 *Creating and Assigning Calibration Levels*

1. Click the **Injection List** Category in the Chromeleon Chromatography Studio window.
2. Click in the **Level** cell for the first calibration standard and select **Create new level**. The value 01 is added. Assign this level to all injections of this calibration standard.
3. Repeat Step 2 for all calibration levels.

2.6.4.3 *Entering Calibration Amounts*

1. Click the **Data Processing** Category in the Chromeleon Chromatography Studio window.
2. In the **Panes** group of the **Data Processing Home** Ribbon tab, click **Processing Method**.
3. In the Processing Method, select the **Amount Table** Tab.
4. Enter the standard amount for each level of the Calibration Component in the appropriate field (Level "01", Level "02", etc).

Calibration curves are updated automatically when you make changes to Calibration standards.

2.6.4.4 Viewing Calibration curves

You can view the calibration curve(s) (Figure 5) in the Data Processing Category of the Chromatography Studio:

1. Click the **Data Processing** Category in the Chromeleon Chromatography Studio window.
2. Go to the **Data Processing Home** Ribbon tab.
3. Either:
 - Select a preset work area layout which contains a calibration pane from the **Presets** group or
 - Select **Calibration Plot** in the **Panes** group

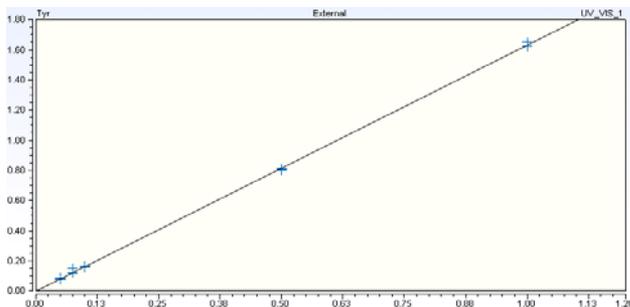


Figure 5: A Calibration Curve

Tip: You can view the calibration curve for each component of a multi-component standard by double clicking the component in the calibration table, selecting the peak in the chromatogram, or by using the   **Component** buttons in the ribbon.

2.7 Review and Report Results

Once data has been acquired and Calibration performed you can Review and Report results.

You can create Report Templates, which output results and other data in any format and layout you require, or use one of Chromeleon's default templates. This Quick Start Guide gives information on using the default templates only; for information on modifying reporting templates or creating new templates see "Designing Reports" in Chromeleon Help.

To review and report results you must first associate a template with the sequence. Once you have done this you can then:

- Review the results
- Print results
- Export a report

In Chromeleon you can create an Electronic Report which can include worksheets comprising of chromatograms, tables, charts, calibration curves, and other instrument or results values. These Electronic Reports can be subjected to an Electronic Signature process for approval. For more information on creating and using Electronic Reports and the Electronic Signatures functionality "Electronic Reports" in Chromeleon Help.

2.7.1 Reviewing Results

The results can be reviewed by clicking the appropriate tab at the bottom of the Work Area of the Report Template.

You can navigate through the sequence by:

- Use the **Previous** and **Next** buttons in the **Navigation** group of the **Home** Ribbon tab.
- Selecting the injection and/or channel you want to view in the Navigation pane.

2.7.2 Printing Results

When printing results, you can:

- Print the currently selected injection only.
- Print the entire sequence.

Both processes will be described in the following sections.

2.7.2.1 *Printing Results for a Single Injection*

To print the results for the currently selected injection:

1. Select the **Report Designer** category from the Chromatography Studio.
2. In the Navigation Pane select the injection you want to print out.
3. On the Studio Menu, select **Print** to open the **Print...** dialog.
4. From the **Print...** dialog box:
 - Select **Apply to Current Injection**.
 - Select the **Printer** you want to use.
 - Select the **Sheets** to be printed for the current injection.

The results for the current injection are now printed.

2.7.2.2 **Print Results for the Entire Sequence**

To print results for the entire sequence, follow the steps for “ Printing Results for a Single Injection” but in the **Print...** dialog box:

- Select **Apply to Current Sequence**.
- When selecting the **Sheets** to be printed you can click the **Down Arrow**  in the Condition column to manage information specific to the sequence rather than individual injections (such as Overview, Calibration Details and Summary Information).

Tip: To print several injections from a sequence, first select the injection row or rows you want to print, right-click, and then click **Print**.

3 Appendix: Chromeleon Overview

3.1 Introduction

Chromeleon is a Chromatography Data System that allows you to control chromatography instruments and evaluate, process, report, and backup data.

The software consists of two major parts:

Instrument Controller Service	The Instrument Controller Service handles communication with and data acquisition from the connected instruments.
Client	The Client provides a user interface for instrument control accessing, processing, and presenting chromatographic data.

Chromeleon has several other software components

Services Manager: Shows the status of the Chromeleon Instrument Controller Service and provides a user interface to control this service. The status of all other Chromeleon services is also displayed.

Instrument Configuration Manager: Allows configuration of Instruments connected to the Instrument PC.

Administration Console: Central access point for administrative tasks, like:

1. **License Manager:** Provides tools for managing licenses for Chromeleon stations and users.
2. **Scheduler:** Provides tools for scheduling data transfer.
3. **User Database:** Provides tools for managing system policies, users and roles, access privileges, and operational privileges.

4. **Global Policies:** Provides settings for global Chromeleon policies.
5. **Discovery:** Central repository with information about the available Instruments and Data Vaults.
6. **Local Machine:** Provides tools for managing local Chromeleon 7 Data Vaults (Create, Mount and Dismount) and Chromeleon 6 Datasources (Mount and Dismount) and offers possibility to change the Chromeleon Domain Controller.

3.2 Instrument Controller Service

The Chromeleon Instrument Controller Service handles all real-time instrument processes (communications, control, and data acquisition). It runs in the background as a Windows service on PCs to which instruments are physically connected. Its status is represented by an icon   in the Notification Area of the Windows Taskbar (Figure 6).



Figure 6: Notification Area of Windows Taskbar for Windows XP and Windows 7

You can Add, Configure, or Delete Instruments and Modules, connect to instruments, and track changes made to instruments from the Instrument Configuration Manager.

3.3 Chromeleon Client

The Chromeleon Client provides the user interface for all frequently used chromatography tasks (instrument operation, data analysis, and data management).

The Chromeleon Client is comprised of two windows:

Chromeleon Console:	The main Chromeleon window in which you can control instruments, navigate through all data and use or manage eWorkflows.
Chromatography Studio:	A separate window that is launched from the Console, in which you can work with data and objects related to a selected sequence. Here you can view and optimize all aspects of the data, modify instrument methods and processing methods, define and generate reports, and manage spectral libraries.

3.3.1 Chromeleon Console

When you start Chromeleon 7, the Console is the first window to appear. The Console window has three major parts.

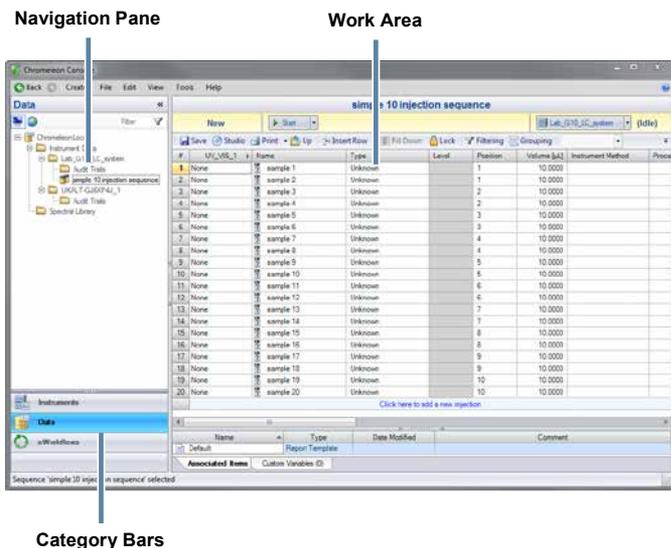


Figure 7: Chromeleon Console

1. **Category Bars:** Use the category bars to switch between the three categories: Instruments, Data, and eWorkflows (Figure 8).



Figure 8: Category Bars

2. **Navigation Pane:** Here you can navigate the objects related to the selected category.

3. **Work Area:** This area shows the content of objects selected in the Navigation Pane. Here you can work on Chromeleon objects.

There are three additional parts for user interaction:

The **Filter Toolbar** offers different views of the list in the Navigation Pane:

- a.  Local: Items available on the local Chromeleon station.
- b.  Global: Items available on the Chromeleon Domain.
- c.  Custom: Filter based on text input.

The **Menu Bar** is always present.

The **Sequence Toolbar** is available when a Sequence is selected in the Navigation Pane.

Finally there are two parts for status information:

The **Sequence Control Bar** indicates the sequence status (New, Running, Complete, Interrupted, Incomplete) and provides relevant actions for the sequence.

Note: When a sequence is configured to be electronically signed, additional statuses are available.

The **Status Bar** shows general information such as the currently logged on user.

3.3.1.1 Instruments

The Instruments Category gives access to all instruments on the network (this might be limited by user privileges).

In the Instruments Category the Navigation Pane shows the configured instruments. The Work Area gives details about the Instrument selected in the Navigation Pane.

From the Work Area you can review instrument status and make changes to instrument parameters. Across the top of the work area a series of ePanel tabs are displayed. These give access to further instrument information and the Audit Trail, Startup, and Queue ePanels.

Note: When you select an instrument from the Navigation Pane which is currently offline a message is displayed in the Work Area.

3.3.1.2 Data

The Data Category provides access to all data stored in each connected Data Vault (, container for all data).

Note: Chromeleon 6 Datasources  are visible in Chromeleon 7. It is not possible to make changes in these Datasources, but data can be copied from them to Chromeleon 7 Data Vaults.

Chromatography data can be accessed and organized from the Navigation Pane. The Work Area shows the content of the selected object and allows you to edit the object.

A Data Vault can contain the following objects:

1.  **Folder:** A container for objects. Use folders to organize data in a Data Vault.
2.  **Sequence:** A collection of **injections** that belong together. A typical sequence contains an Instrument and Processing Method, a Report Template, and a View Settings file.
3.  **Instrument Method:** A collection of timed commands for an instrument to perform during a chromatographic analysis.
4.  **Processing Method:** A collection of parameters (including parameters for peak detection and calibration) which are used when evaluating chromatograms.
5.  **Report Template:** A file which defines how data is displayed, printed, or exported. A Report Template can also contain calculations. When applied to a sequence (to view, print, or export the results) the outcome is referred to as a Report.
6.  **Electronic Report:** An electronic version of the results of a sequence.
7.  **View Settings:** The definition of how data is presented on screen.
8.  **Spectral Library:** A collection of spectra used for peak identification.
9.  **Query:** A Data Vault search.
10.  **Instrument Audit Trails:** A log of instrument events such as system settings, executed commands, and error messages.

A sequence is a collection of injections that are analyzed and processed together in series. Each injection is represented by a row in the sequence (replicate injections are represented with multiple rows). Injections can have one of the following **Injection Types**:

1.  **Unknown:** A sample for which the quantity, presence, or absence of components is to be determined during the analysis.
2.  **Calibration Standard:** A sample with known concentration(s) of component(s). Calibration Standards are used in the construction of calibration curves.
3.  **Check Standard:** A sample with known component concentration(s). Check Standards are used to verify a calibration.
4.  **Blank:** An injection used to characterize the background signal (baseline), and/or to ensure that unwanted components are not detected. Blank “injections” can be made without an actual injection taking place.
5.  **Matrix:** The sample matrix. The peak areas in the Matrix can be subtracted from the corresponding peak areas in all the other injections in the sequence.
6.  **Unspiked:** An Unknown sample to be analyzed with the Standard Addition method.
7.  **Spiked:** An Unknown sample to be analyzed with the Standard Addition method, with known amounts of components added.

3.3.1.3 eWorkflows

eWorkflows are electronic procedures for automating laboratory processes related to a chromatographic analysis.

An eWorkflow contains a set of templates (such as Instrument Methods, Processing Methods, Report Templates, View Settings, and/or Spectral Libraries) and a set of rules. The rules define, for example, the sequence layout (such as the maximum number of Unknown injections allowed between Calibration Standards), and the list of instruments in the network that are suitable for the analysis. When you start an eWorkflow, it will create a sequence with predefined associated files and a well-defined structure.

The list of available eWorkflows is visible in the Navigation Pane. An overview of the instruments (including their status) that can be used with the selected eWorkflow is displayed in the Work Area. From here you can launch a eWorkflow and will be guided in creating an appropriate sequence.

3.3.2 Chromatography Studio

In the Chromatography Studio you can edit all objects related to the selected sequence:

- Injection List
- Instrument Methods
- Processing Methods
- View Settings
- Report Templates
- Electronic Reports
- Spectral Libraries.

When you open a sequence from the Console, the Chromatography Studio (Figure 9) is opened.

Note: When you open an object outside the context of a sequence, only the corresponding category of the Studio will be available.

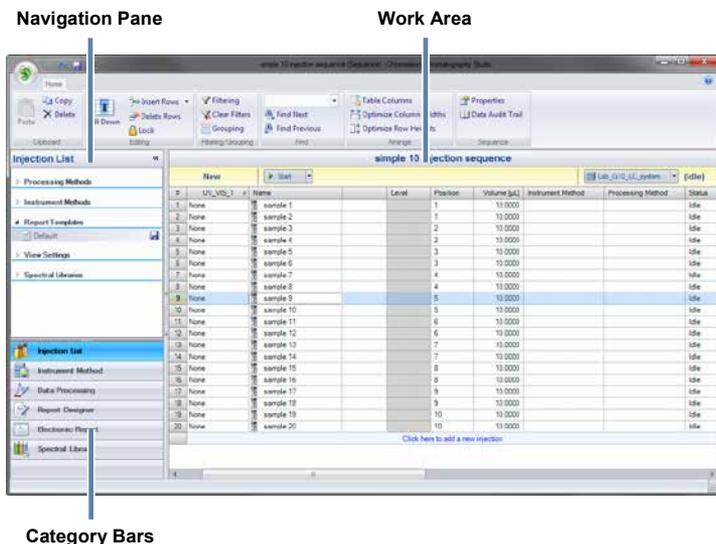


Figure 9: Chromatography Studio

The Chromatography Studio is structured similarly to the Chromeleon Console, and consists of the following major parts:

1. **Category Bars:** These switch the display between the six categories; Injection List, Instrument Method, Data Processing, Report Designer, Electronic Report and Spectral Library.

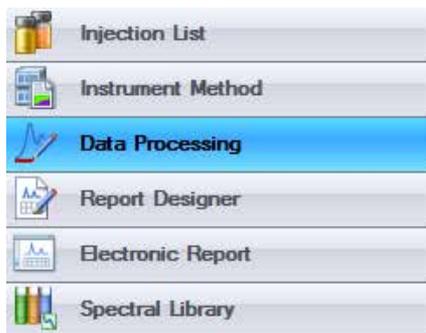


Figure 10: Categories

2. **Navigation Pane:** An area in which you can navigate through the objects available in the selected category.
3. **Work Area:** The content changes according to the selected category.

There are two additional parts for user interaction:

Ribbon: The menu tool for main commands in the Studio. Commands are organized in groups, which are collected together under tabs. To reduce clutter, some tabs are only shown when needed.

Studio Menu: To access the Studio Menu, click the Chromeleon icon  in the top left corner of the Chromatography Studio

Window. From this menu you can access related to general tasks, such as printing, exporting, and saving.

3.3.2.1 *Injection List*

From the Injection List category, you can edit, print and export the Injection List.

The Navigation pane gives an overview of all files used in the sequence. The work area displays further details about each injection, such as the type of sample (for example Calibration Standard) and the Injection Status.

Note: You can also edit the Injection List directly in the Console. If a Sequence is open in both the Console and the Studio, changes made in either window are automatically made in the other, so that copies of the Sequence stay synchronized.

3.3.2.2 *Instrument Method*

The Instrument Method category lets you edit Instrument Methods.

The Navigation Pane lists the Instrument Methods in the sequence and provides an overview of the instrument's modules. The Work Area lets you edit the Instrument Method.

3.3.2.3 *Data Processing*

In the Data Processing category, you can view chromatography results, edit the Processing Method, and manually integrate chromatograms.

The Navigation Pane gives an overview of all injections, channels, processing methods and view settings used in the sequence. Chromatographic results are shown in the Work Area.

You can customize the panes displayed (such as Chromatogram, Interactive Results, Calibration Plot, and Processing Method) on the Ribbon by selecting or hiding each in the **Panes** group of the **Data Processing Home** tab of the Ribbon (Figure 11).

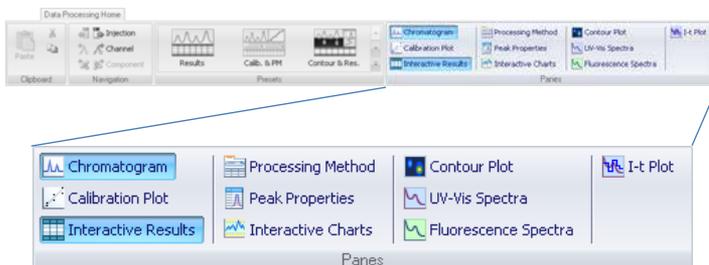


Figure 11: Pane Selection in Ribbon

Tip: The Presets group (left of the Panes group in the Data Processing Home Ribbon tab) provides shortcuts to display typical combination of Panes.

3.3.2.4 Report Designer Category

In the Report Designer category, you can view reports and edit Report Templates.

The Navigation Pane shows a list of all channels, injections and report templates available in the sequence. In the Work Area you can view and modify the report.

3.3.2.5 Electronic Report

In the Electronic Report category, you can create and manage electronic reports. This is an electronically captured snapshot of the results.

The Navigation Pane shows a list of all injections and sheets available in the electronic report and the electronic report itself. The

Work Area shows the electronic report, or, when no electronic report is available, the option to create one.

3.3.2.6 *Spectral Library*

The Spectral Library view of the Chromatography Studio provides tools for managing and comparing UV-Vis spectra extracted from 3D Field data.

3.3.2.7 *Menus*

Chromeleon 7 Studio commands are accessible via the Ribbon or Studio Menu. To access the Studio Menu click the Chromeleon

icon .

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