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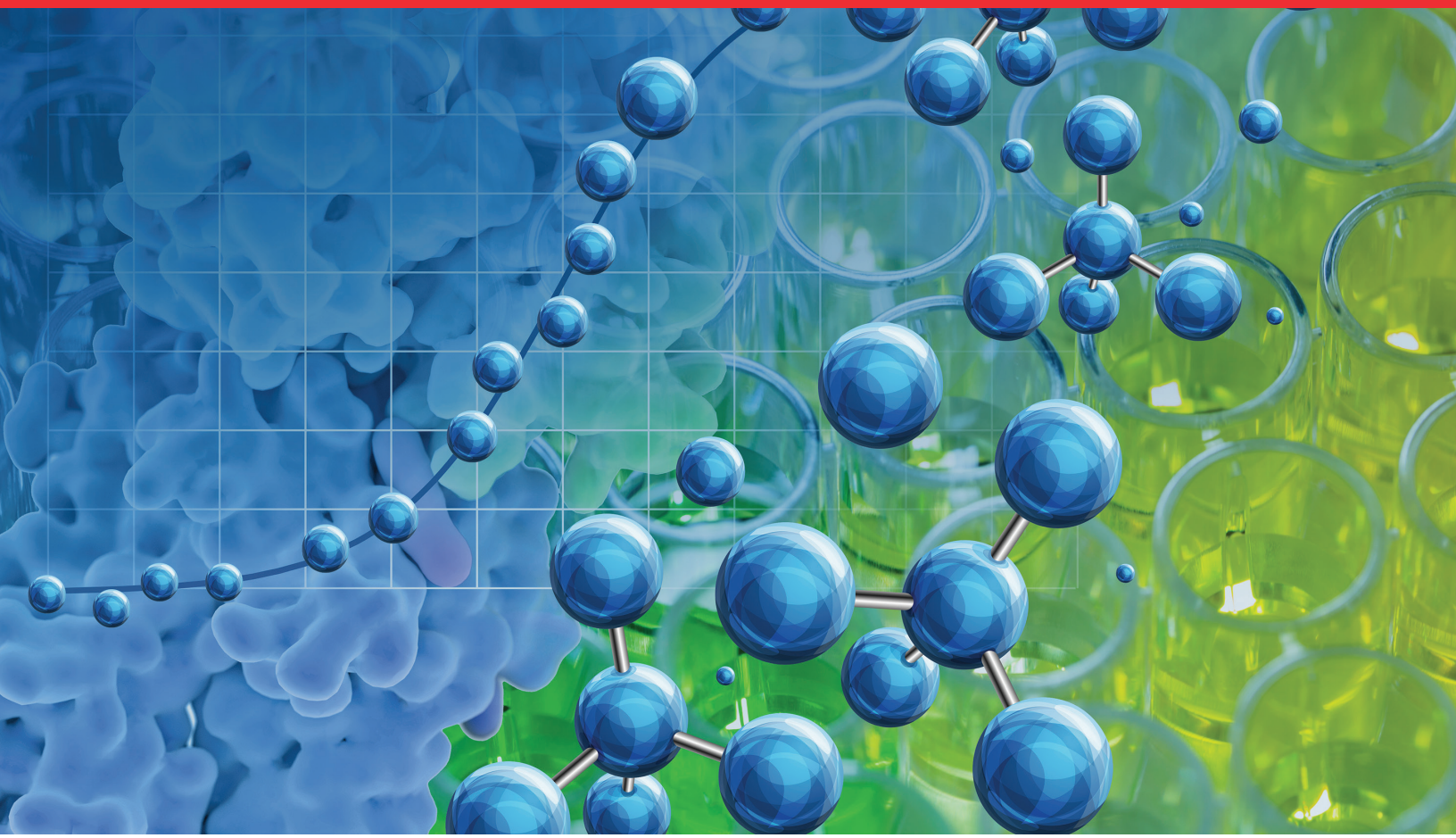

Watson LIMS Gateway for Chromeleon CDS

Installation Guide

Version 1.2

ThermoFisher SCIENTIFIC

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Preface

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- Related Documentation
- Special Notices
- Contacting Us

Related Documentation

Watson includes Help, manuals, and guides as PDF files.

❖ **To view the Watson product manuals**

Navigate to the Manuals folder on the Watson installation media.

❖ **To open the Help**

With the Watson client running, you can access Help from the main menu, choose **Help**, and then click **Contents**.

Special Notices

Make sure that you follow the precautionary statements presented in this guide. The special notices appear in boxes.

Special notices include the following:

CAUTION Highlights information necessary to prevent damage to software, loss of data, invalid test results, or information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need.

❖ **To contact Technical Support**

Email support.informatics@thermofisher.com

Web http://support.thermoinformatics.com/contacts

❖ **To contact Customer Service for ordering information**

Web http://www.thermoscientific.com/informatics

❖ **To suggest changes or provide feedback on the documentation**

Send an email to the Documentation Manager: sidinf.documentation@thermofisher.com.

Introduction

This manual provides instruction for the installation and usage of the Thermo Scientific™ Watson LIMS™ Gateway for Thermo Scientific™ Chromeleon™ CDS.

The gateway uses the Chromeleon SDK to accomplish the following tasks:

- Send analytical run sequence data from Watson to create a sequence in Chromeleon
- Import analysis result data from a processed Chromeleon sequence to a Watson study for a selected analytical run

The gateway transfers information between Watson and Chromeleon without the use of intermediary files.

Contents

- Operating System Requirements
- Prerequisites

Operating System Requirements

Any operating system that supports your installed version of Watson LIMS and Chromeleon CDS is acceptable.

Prerequisites

This manual assumes the following:

- Watson LIMS has been installed and is functioning.
- Chromeleon 7.2 SR5 (or later) software has been installed on the same machine where Watson is installed.

The instructions in this manual use the validation material provided with the installation material of this interface. Be sure to use the validation material to familiarize users with the interface, whether or not it will be used for actual operational qualification.

Installing the Gateway

❖ **To install the gateway**

1. Double-click the file `ChromeleonGateway.msi` to run the installer.
2. If you want to generate an installation log file, complete the following steps:
   a. Open a Command Prompt window.
   b. Change directory to the folder that contains the `ChromeleonGateway.msi` file.
   c. Enter the command **msiexec -i ChromeleonGateway.msi /l log.txt**
3. When prompted, enter the path where your Watson application file `Watson.exe` is installed. Click **Next** to install the Chromeleon gateway to the entered path.

   Note To function correctly, the Chromeleon gateway application must be installed on the same computer and in the same folder where the Watson application is installed.

   The executable file modifies the system registry in the background to add the gateway information. There is no visible change or user confirmation required.
4. When the installation completes, a message appears and the gateway is ready for configuration.

Configuring Watson to Use the Gateway

You must configure a new instrument interface in Watson for the Chromeleon gateway. The instrument interface serves as a link between Watson and the gateway. You can create multiple instrument interfaces.

❖ To configure the gateway

1. In Windows Explorer, locate the file `ChromeleonGateway.exe.config` and open it in Notepad.
2. Locate the following section in the file:

```
<appSettings>
   <add key="DebugMode" value="false" />
   <add key="DataVaultServers" value=""/>
   <add key="DataVaults" value=""/>
   <add key="InstrumentConnectionTimeoutInMilliseconds"
value="20000" />
</appSettings>
```

3. Edit the following values to match your Chromeleon configuration:

   DebugMode – Set to "false" to suppress debug logging of the Watson LIML produced by the gateway.

   DataVaultServers – Enter the names of specific data vault servers to be searched for eWorkflows/sequences. If left blank, all servers on the Chromeleon domain will be searched. Separate multiple entries with commas.

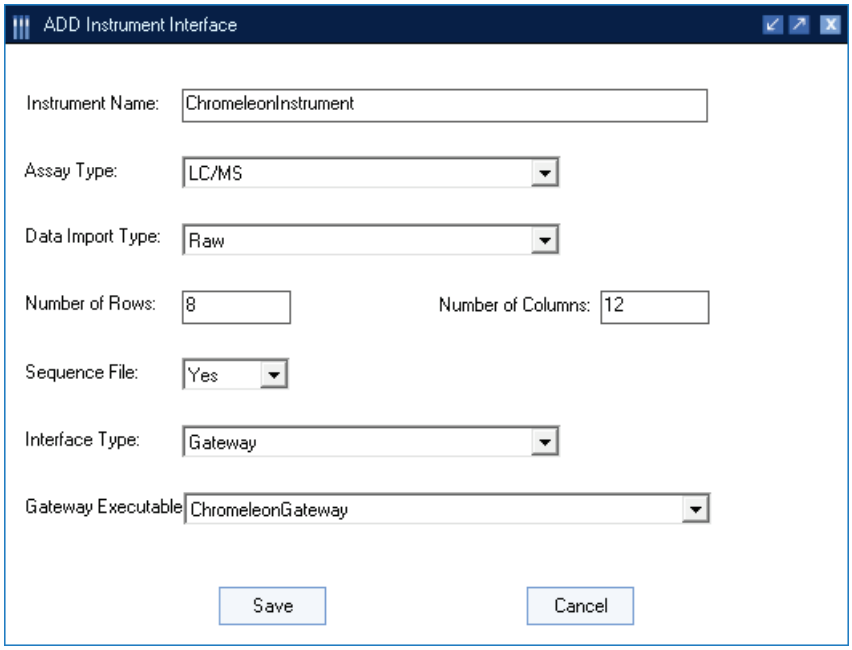
   DataVaults – Enter the names of specific data vaults to which searches will be limited. If left blank, all data vaults on the specified data vault servers, which may be filtered by the previous parameter, will be searched. Separate multiple entries with commas.

   InstrumentConnectionTimeoutInMilliseconds – If the instrument is slow to respond, you can change the connection timeout.

4. Save the changes.
5. Start the Watson application. Log on using a system administrator account.
6. From the **Options** menu, select **Instrument Interfaces**.

7. Click **Add** to create a new entry. The Add Instrument Interface form appears.

Figure 3-1. Add Instrument Interface form



8. Enter the following information:
   - **Instrument Name:** ChromeleonInstrument
   - **Assay Type**: HPLC or LC/MS
   - **Data Import Type:** Raw
   - **Number of Rows:** <Number of Rows on the plate> (Not Used)
   - **Number of Columns:** <Number of Columns on the plate> (Not Used)
   - **Sequence File:** Yes
   - **Interface Type:** Gateway
   - **Gateway Executable:** ChromeleonGateway
9. Save the changes. The interface is now available for use.

Using the Gateway

This chapter contains procedures that describe how to set up an assay, generate a sequence, and import results using the new gateway.

Contents

- Setting up the Assay
- Generating the Sequence
- Importing Results

Setting up the Assay

❖ **To set up the assay to use the new gateway**

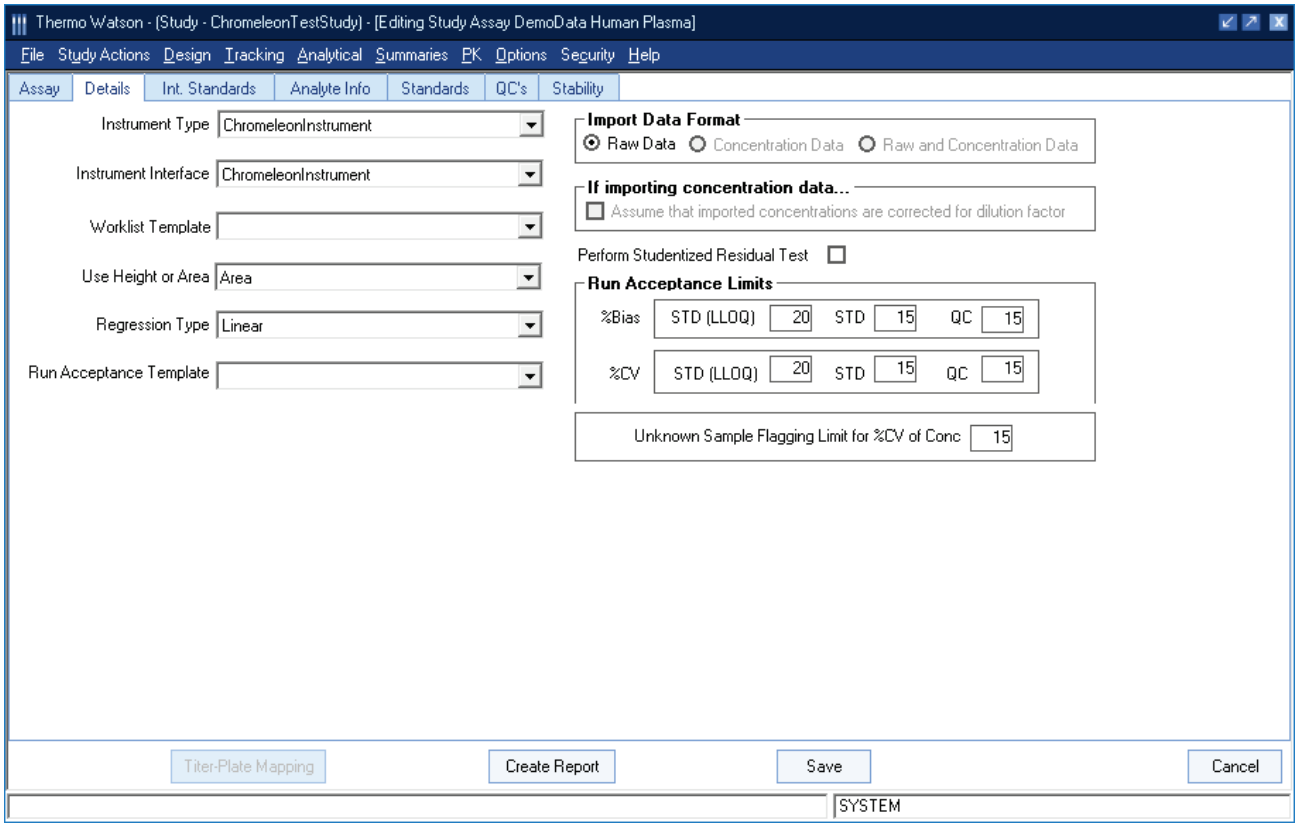
1. From the Analytical menu, choose **Update Assays.**
2. Select **Study Assay** or **Analytical Run Assay**, depending on what you need.

   The Assay Information form appears, populated with a list of assays.
3. Select the assay that you want to edit and click **Edit**.

   The Edit Assay form appears.

4. Click the **Details** tab.

Figure 4-1. Edit Assay form



5. From the **Instrument Type** list, select the name of the new instrument interface that you created.
6. From the **Instrument Interface** list, select the name of the new instrument interface that you created.
7. In the **Import Data Format** area, select the data type to import to set up the assay.

   The options available in the Import Data Format area vary based on what you chose for the Data Import type when you configured Watson manually.

Generating the Sequence

A Watson analytical run that is configured to exchange data with Chromeleon displays two forms that collect information before sending the analytical run data to Chromeleon.

❖ To complete a sequence

1. In Watson, open the validation study **Chromeleon Interface Validation**.
2. From the Analytical menu, select **Analytical Run Actions**.

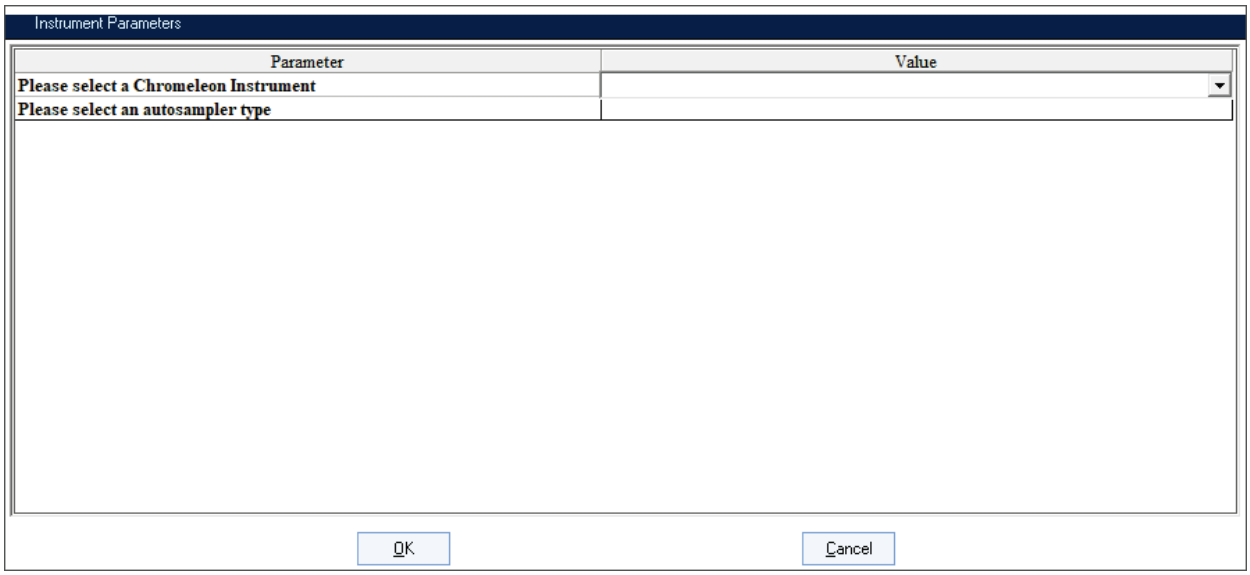
The View Analytical Run form appears.

3. Select the run that you want to create a sequence file for and click **Sequence File**.
4. If Chromeleon User Mode is enabled and user credentials are required, the Chromeleon logon screen appears. Log on to Chromeleon.

Figure 4-2. Chromeleon Logon

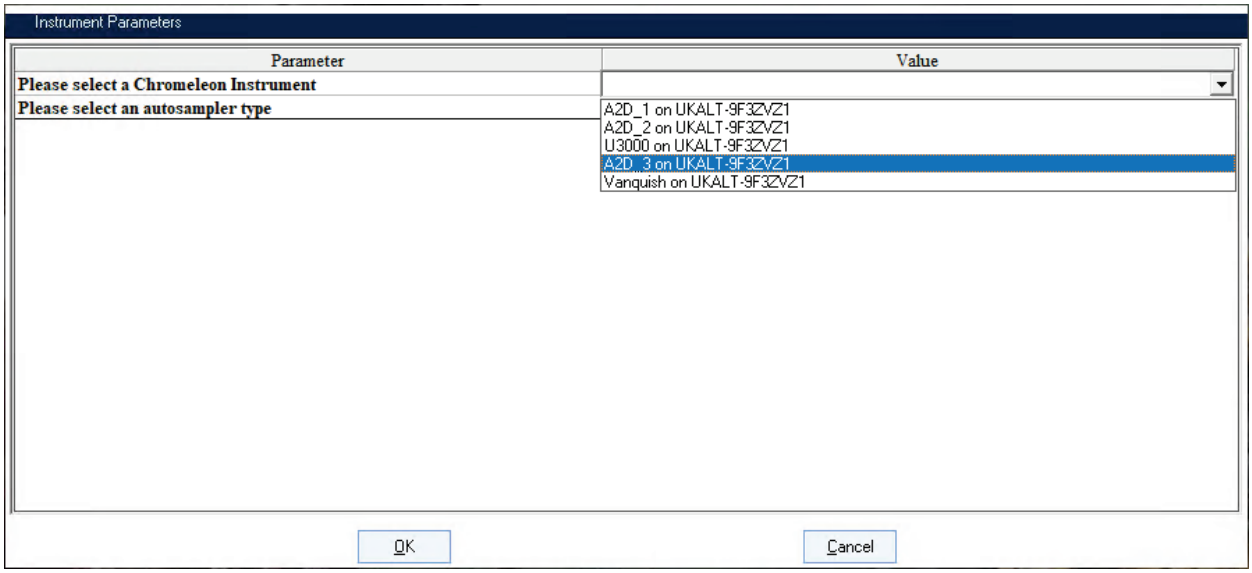
5. If logon is successful, the Instrument Parameters form appears.

Figure 4-3. Instrument Parameters form for Chromeleon Instrument



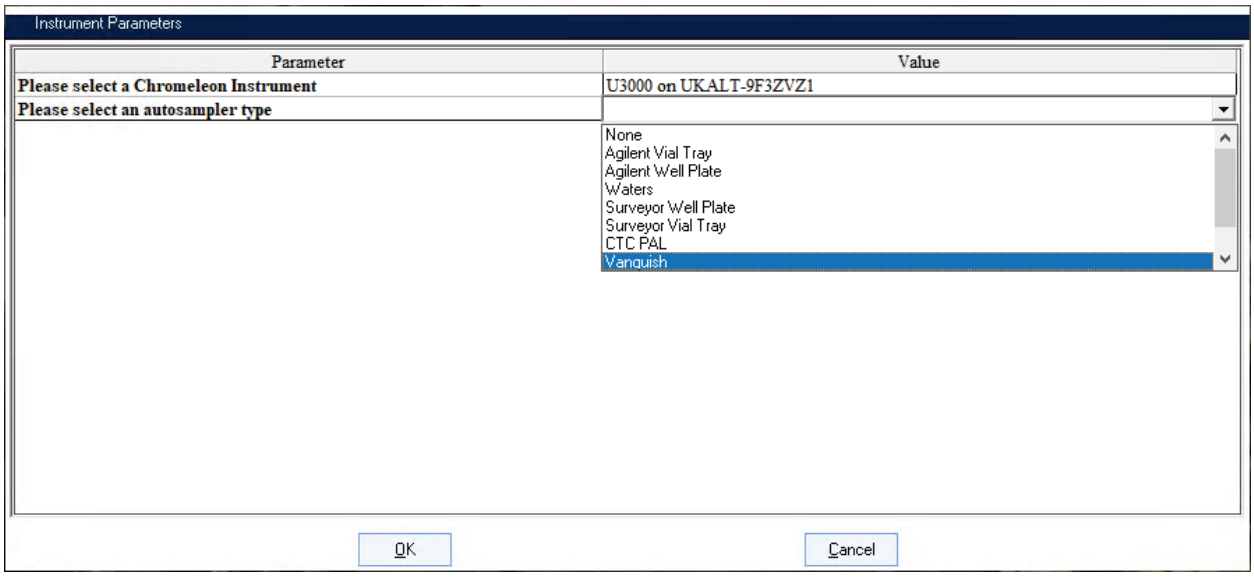
6. For the **Chromeleon Instrument** parameter, click the Value list and select an existing instrument. The list of instruments is acquired by requesting a list of instruments from Chromeleon. If no instruments have been configured in Chromeleon, you will see a message stating "No instruments available."

Figure 4-4. Instrument Parameters – select a Chromeleon Instrument



7. For the **autosampler type** parameter, click the Value list and select an existing autosampler. The list of autosamplers is populated from the `ChromeleonAutoSamplerFormats.xml` file, which is installed in the Watson folder with the gateway. For further information about this XML file, which is also used to map Watson sample positions to Chromeleon sample positions, refer to Configuring Autosampler Entries in this manual.

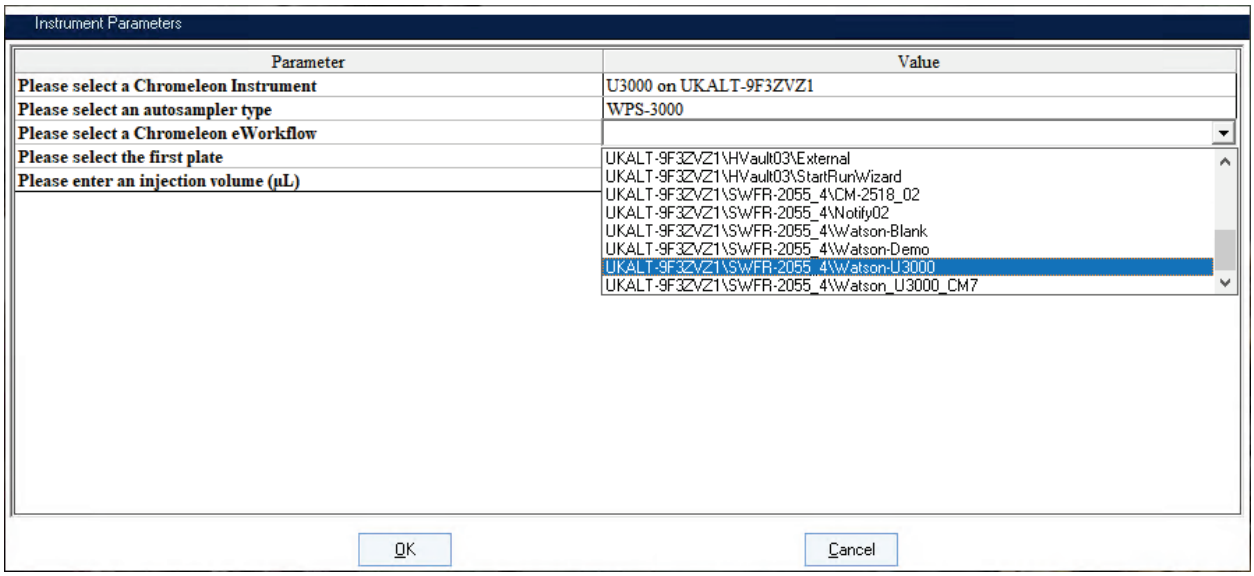
Figure 4-5. Instrument Parameters – select an autosampler type



The Instrument Parameters form updates, and additional parameters appear.

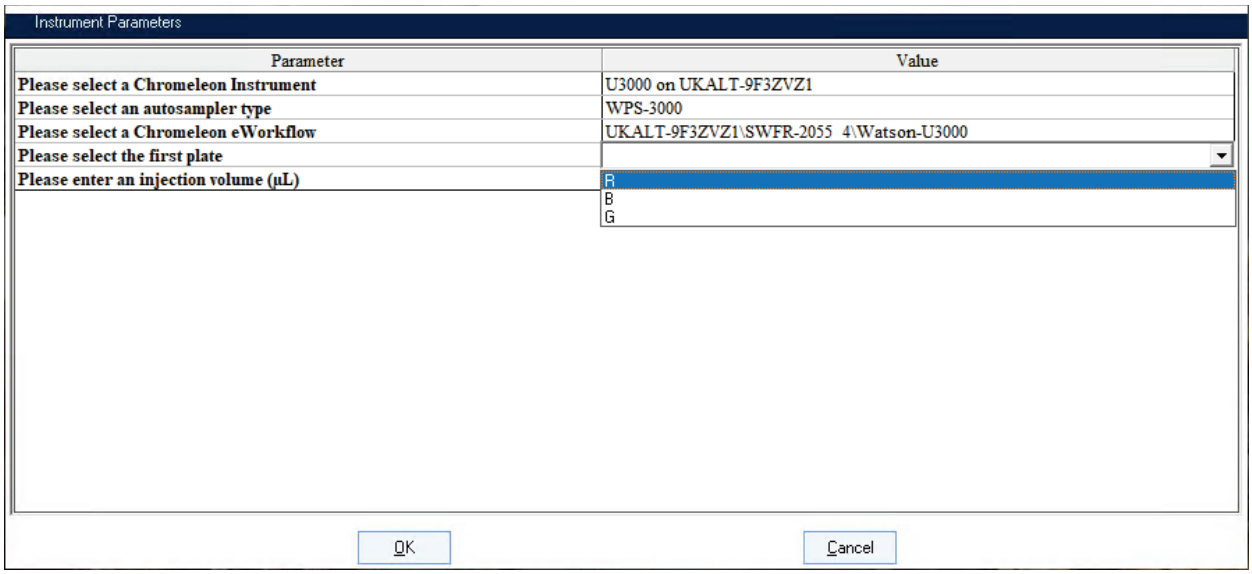
8. For the **Chromeleon eWorkflow** parameter, click the Value list and select an existing eWorkflow. The list of eWorkflows is provided by Chromeleon. If no eWorkflows have been provided, you will see an error stating "No eWorkflows available." If you have configured eWorkflows in Chromeleon but they are not shown in the Value list, make sure that your eWorkflows are defined in the same data vault servers and/or data vaults that were selected in `ChromeleonGateway.exe.config`. Also make sure that the eWorkflows are assigned to the Instrument you selected in step 6.

Figure 4-6. Instrument Parameters – select a Chromeleon eWorkflow



9. If the autosampler type selected in Step 7 has defined plates, choose the plate to start on. For the **first plate** parameter, click the Value list and select a plate from the available options. If there are no plates, this parameter is not shown.

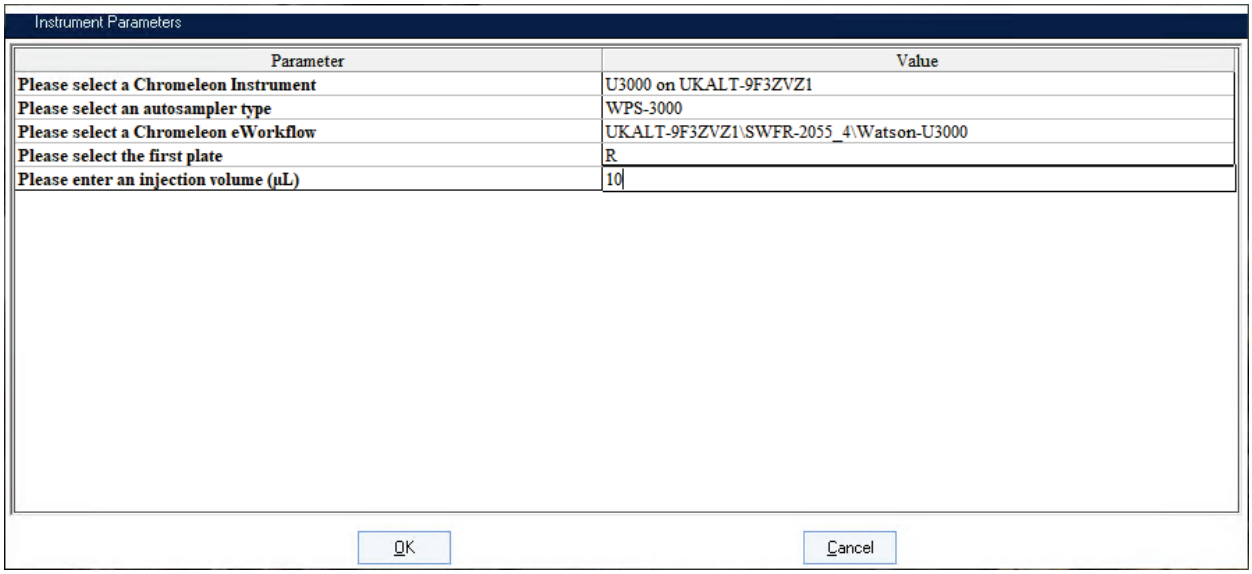
Figure 4-7. Instrument Parameters – select the first plate



In the example shown in Figure 4-7, if **B** is selected, this would be used as the first plate, then **G** would be used for the second plate for mappings.

10. For the **injection volume** parameter, click the Value list and enter the injection volume to be applied to every sample in Chromeleon.

Figure 4-8. Instrument Parameters – enter an injection volume



11. Click **OK**.

    The gateway uses the form data to create a sequence in Chromeleon. A message appears confirming successful submission of the sequence operation.

12. Open Chromeleon to verify that the sequence has been created as expected.

Note that the sequence contains two custom sequence variables:

- **Watson Study** – contains the Watson Study name
- **Watson Run** – contains the Watson Run value

These custom variables enable the sequence to be associated with the originating Watson study when retrieving results.

13. Start the acquisition of the sequence in Chromeleon.

Importing Results

A Watson analytical run that is configured to exchange data with Chromeleon displays one form to collect information before connecting to Chromeleon to import data for an analytical run.

Note In the Chromeleon sequence, when RT is zero due to N/F or N/A, the value (0) for peak area or peak height is skipped and not stored in Watson.
When RT is non-zero, meaning the actual analyte RT is within the expected window and peak area or height is N/F, stores a value of 0 in Watson.

❖ To import results

1. From the Analytical menu, choose **Analytical Run Actions**.

   The Analytical Run Actions form appears with a list of runs.

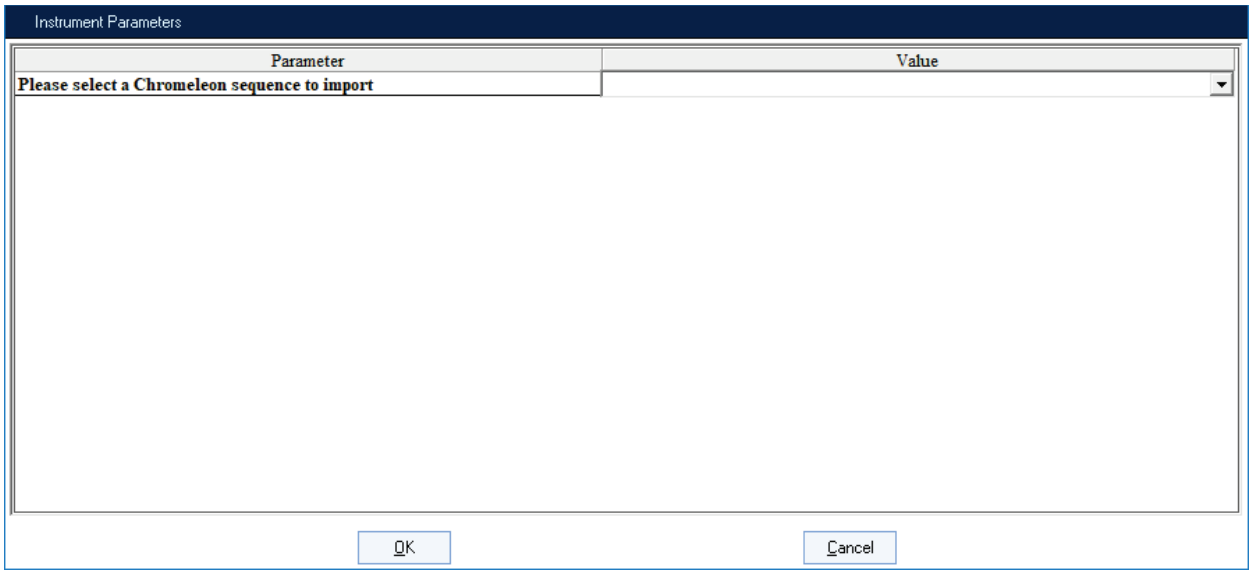
2. Select the run that you want to import and click **Import.**

3. If Chromeleon User Mode is enabled and user credentials are required, the Chromeleon logon screen appears. Log on to Chromeleon.

Figure 4-9. Chromeleon Logon

If logon is successful, the Instrument Parameters form appears.

Figure 4-10. Import Parameters – select a Chromeleon sequence

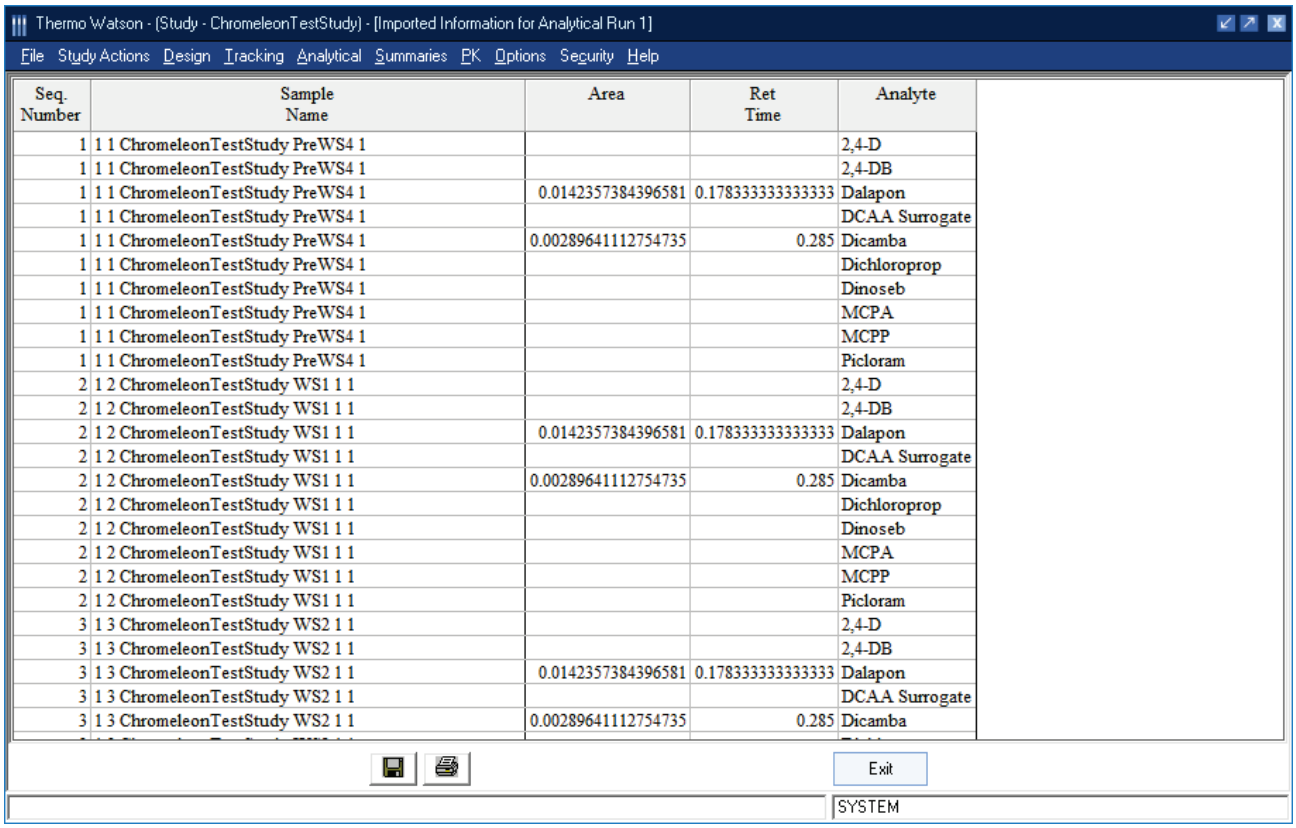


4. For the **Chromeleon sequence** parameter, click the Value list and select an existing sequence. The list of sequences is acquired from Chromeleon. Only sequences that were exported from the current Watson study and run will be displayed. If sequences are present in Chromeleon but they are not displayed in the Value list, make sure that your sequences are defined in the same data vault servers and/or data vaults that were selected in `ChromeleonGateway.exe.config` and that they were created from the selected analytical run.

5. Click **OK**.

The gateway imports the data into Watson. If it is successful, the results appear in a report grid in Watson.

Figure 4-11. Imported results report



Seq. Number	Sample Name	Area	Ret Time	Analyte
1	1 1 ChromeleonTestStudy PreWS4 1			2,4-D
1	1 1 ChromeleonTestStudy PreWS4 1			2,4-DB
1	1 1 ChromeleonTestStudy PreWS4 1	0.0142357384396581	0.178333333333333	Dalapon
1	1 1 ChromeleonTestStudy PreWS4 1			DCAA Surrogate
1	1 1 ChromeleonTestStudy PreWS4 1	0.00289641112754735	0.285	Dicamba
1	1 1 ChromeleonTestStudy PreWS4 1			Dichloroprop
1	1 1 ChromeleonTestStudy PreWS4 1			Dinoseb
1	1 1 ChromeleonTestStudy PreWS4 1			MCPA
1	1 1 ChromeleonTestStudy PreWS4 1			MCPP
1	1 1 ChromeleonTestStudy PreWS4 1			Picloram
2	1 2 ChromeleonTestStudy WS1 1 1			2,4-D
2	1 2 ChromeleonTestStudy WS1 1 1			2,4-DB
2	1 2 ChromeleonTestStudy WS1 1 1	0.0142357384396581	0.178333333333333	Dalapon
2	1 2 ChromeleonTestStudy WS1 1 1			DCAA Surrogate
2	1 2 ChromeleonTestStudy WS1 1 1	0.00289641112754735	0.285	Dicamba
2	1 2 ChromeleonTestStudy WS1 1 1			Dichloroprop
2	1 2 ChromeleonTestStudy WS1 1 1			Dinoseb
2	1 2 ChromeleonTestStudy WS1 1 1			MCPA
2	1 2 ChromeleonTestStudy WS1 1 1			MCPP
2	1 2 ChromeleonTestStudy WS1 1 1			Picloram
3	1 3 ChromeleonTestStudy WS2 1 1			2,4-D
3	1 3 ChromeleonTestStudy WS2 1 1			2,4-DB
3	1 3 ChromeleonTestStudy WS2 1 1	0.0142357384396581	0.178333333333333	Dalapon
3	1 3 ChromeleonTestStudy WS2 1 1			DCAA Surrogate
3	1 3 ChromeleonTestStudy WS2 1 1	0.00289641112754735	0.285	Dicamba

Configuring Autosampler Entries

You can customize positional formats for autosampler values. The provided sample file `ChromeleonAutoSamplerFormats.xml` (installed in the Watson folder with the gateway) contains comments to identify the permitted entries and their purposes.

Edit the sample file with a text editor such as Notepad. More advanced editors might leave problematic hidden characters in the file. You can edit, remove, or add existing entries, but you must have at least one entry in the file. At a minimum, we recommend that you include a simple ~NSEQ~ entry.

The autosampler XML file transmitted from Watson contains four values:

- Plate number
- Row number
- Column number
- Sequence number

These values can be formatted in five different ways:

- Raw/unformatted
- Padded to two digits
- Padded to three digits
- Set to an alphabetic equivalency (1=A, 2=B …26=Z)
- Mapped to a plate identifier (for plate number only)

The available formats are represented as follows:

FormatValue identifiers for plate number values:	
~NPLATE~	= Numeric Plate ID Unpadded
~NPLATE2~	= Numeric Plate ID Padded to 2 digits
~NPLATE3~	= Numeric Plate ID Padded to 3 digits
~APLATE~	= Alphabetic Plate ID
~UPLATE~	= Plate identifier

FormatValue identifiers for row number values:	
~NROW~	= Numeric Row D Unpadded
~NROW2~	= Numeric Row ID Padded to 2 digits
~NROW3~	= Numeric Row ID Padded to 3 digits
~AROW~	= Alphabetic Row ID

FormatValue identifiers for column number values:	
~NCOL~	= Numeric Column ID Unpadded
~NCOL2~	= Numeric Column ID Padded to 2 digits
~NCOL3~	= Numeric Column ID Padded to 3 digits
~ACOL~	= Alphabetic Column ID

FormatValue identifiers for the sequence number:	
~NSEQ~	= Numeric Sequence/Order ID Unpadded
~NSEQ2~	= Numeric Sequence/Order ID Padded to 2 digits
~NSEQ3~	= Numeric Sequence/Order ID Padded to 3 digits
~ASEQ~	= Alphabetic Sequence/Order ID

The sample file `ChromeleonAutoSamplerFormats.xml` contains the following entries:

```
<Parameters>
   <AutosamplerList>
      <Autosampler ItemName="None" FormatValue="" />
      <Autosampler ItemName="Agilent Vial Tray" FormatValue="~NSEQ~" />
      <Autosampler ItemName="Agilent Well Plate" FormatValue="~NPLATE~:~AROW~~NCOL~" />
      <Autosampler ItemName="Waters" FormatValue="~NPLATE~:~AROW~~NCOL~" />
      <Autosampler ItemName="Surveyor Well Plate" FormatValue="~NPLATE~:~AROW~~NCOL~" />
      <Autosampler ItemName="Surveyor Vial Tray" FormatValue="~AROW~:~NCOL~" />
      <Autosampler ItemName="CTC PAL" FormatValue="Tray~NPLATE2~:~NSEQ~" />
      <Autosampler ItemName="Vanquish" FormatValue="~UPLATE~:~AROW~~NCOL~">
         <UPLATE PLATENUM = "1" TEXT = "R"/>
         <UPLATE PLATENUM = "2" TEXT = "B"/>
         <UPLATE PLATENUM = "3" TEXT = "G"/>
         <UPLATE PLATENUM = "4" TEXT = "Y"/>
      </Autosampler>
    <Autosampler ItemName="Vanquish with Charger" FormatValue="~UPLATE~:~AROW~~NCOL~">
      <UPLATE PLATENUM = "1" TEXT = "R"/>
      <UPLATE PLATENUM = "2" TEXT = "B"/>
      <UPLATE PLATENUM = "3" TEXT = "G"/>
      <UPLATE PLATENUM = "4" TEXT = "CH01"/>
      <UPLATE PLATENUM = "5" TEXT = "CH02"/>
      <UPLATE PLATENUM = "6" TEXT = "CH03"/>
      <UPLATE PLATENUM = "7" TEXT = "CH04"/>
      <UPLATE PLATENUM = "8" TEXT = "CH05"/>
      <UPLATE PLATENUM = "9" TEXT = "CH06"/>
      <UPLATE PLATENUM = "10" TEXT = "CH07"/>
      <UPLATE PLATENUM = "11" TEXT = "CH08"/>
      <UPLATE PLATENUM = "12" TEXT = "CH09"/>
      <UPLATE PLATENUM = "13" TEXT = "CH10"/>
      <UPLATE PLATENUM = "14" TEXT = "CH11"/>
      <UPLATE PLATENUM = "15" TEXT = "CH12"/>
      <UPLATE PLATENUM = "16" TEXT = "CH13"/>
      <UPLATE PLATENUM = "17" TEXT = "CH14"/>
      <UPLATE PLATENUM = "18" TEXT = "CH15"/>
      <UPLATE PLATENUM = "19" TEXT = "CH16"/>
      <UPLATE PLATENUM = "20" TEXT = "CH17"/>
      <UPLATE PLATENUM = "21" TEXT = "CH18"/>
      <UPLATE PLATENUM = "22" TEXT = "CH19"/>
      <UPLATE PLATENUM = "23" TEXT = "CH20"/>
    </Autosampler>
      <Autosampler ItemName="WPS-3000" FormatValue="~UPLATE~~AROW~~NCOL~">
         <UPLATE PLATENUM = "1" TEXT = "R"/>
         <UPLATE PLATENUM = "2" TEXT = "B"/>
         <UPLATE PLATENUM = "3" TEXT = "G"/>
      </Autosampler>
    </AutosamplerList>
    <AppParameters>
    </AppParameters>
</Parameters>
```

❖ To add a new autosampler entry

1. Insert a new line between the `<AutosamplerList>` and `</AutosamplerList>` tags.
2. The FormatValue can be any combination of the formats listed in the tables, as well as alphanumeric values. The name will appear in the Select Autosampler list when you generate a sequence.
3. For autosamplers that use plate identifiers, for example, the Vanquish autosampler, UPLATE can be used to map the plate number in `Watson` to a specified plate identifier. One or more `<UPLATE>` elements can be added under an `<Autosampler>` element to define the mappings.
4. To format a plate position for "Vanquish" given the following data:

   Plate = 1

   Row = 2

   Column = 3

   Sequence = ""

   The instrument software would display the results as this string:

   R:B3