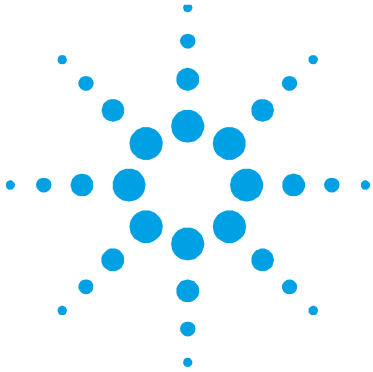

Sample Scheduler for OpenLAB

Guide for former Galaxie Scheduler users

Agilent Technologies

Notices

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This guide is valid for version 2.0 of Sample Scheduler for OpenLAB.

This version is compatible to version 2.1 SR1 of OpenLAB CDS.

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Contents

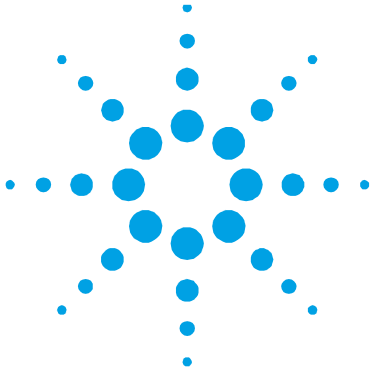
In this Guide

Sample Scheduler for OpenLAB was designed to facilitate the replacement of Galaxie solution (Galaxie CDS /Galaxie Scheduler) by the *OpenLAB CDS* solution.

As the Scheduler is strongly linked to the CDS it works with, some features or behaviors can differ from one solution to the other.

This document details these differences or limitations.

New features have also been added to the Sample Scheduler for OpenLAB (ex: sequence of analyses), to know more about these features, please refer to both *Sample Scheduler for OpenLAB Installation & Configuration User's guide* and *Sample Scheduler for OpenLAB Online Help*.



1. Scheduler Deployment

Both Scheduler applications use a database, and work in Client/server configuration.

As the Client/Server management is different in both solutions, the deployment has been adapted to the CDS solution.

Galaxie Scheduler Deployment

Galaxie Scheduler deployment fits the Galaxie CDS Client/server:

- Scheduler database (Firebird) and the Scheduler engine (Run Manager) are installed on the Galaxie server computer.
- Scheduler client is installed on a Galaxie client computer which can be or not an acquisition server.

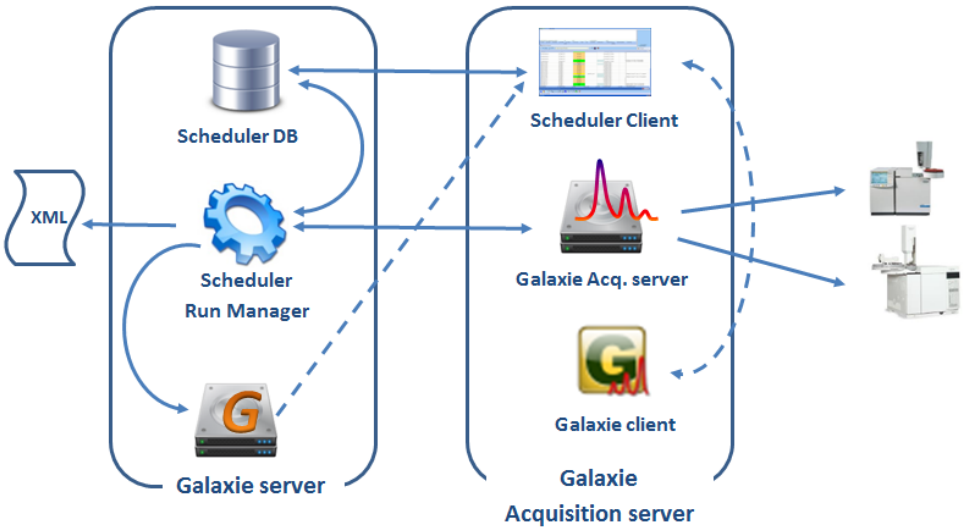


Figure 1 Galaxie Scheduler

Table 1 Galaxie Scheduler

Galaxie server computer	Galaxie client computer
The Scheduler engine (Run Manager): • Scans the LIMS folder to detect XML commands and checks their validity • Sends XML command parameters in Database • Manages analysis execution: Communicates with Galaxie Acquisition server • Checks Galaxie credentials: User (user profile)/ Project/ Group.	The Scheduler client : • Displays analyses according to Galaxie credentials: User (user profile)/ Project/ Group • Opens chromatograms in Galaxie client

Sample Scheduler for OpenLAB Deployment

Sample Scheduler for OpenLAB deployment can be distributed over several computers, all with OpenLAB CDS installed.

- The database is a SQL server database. It can be installed on any computer.
- The Galaxie Scheduler Run Manager is replaced by two agents:
  - Sample Scheduler agent, installed on a computer where OpenLAB CDS is installed, is aimed to manage analysis execution.
  - Sample Scheduler LIMS agent, installed on any computer where OpenLAB CDS is installed, scans the LIMS command folder to detect XML commands and check their validity

The Scheduler client is replaced by Sample Scheduler for OpenLAB client that can be installed on any computer where OpenLAB CDS is installed.

Sample Scheduler Agent, Sample Scheduler LIMS Agent and Scheduler client can be installed on the same computer.

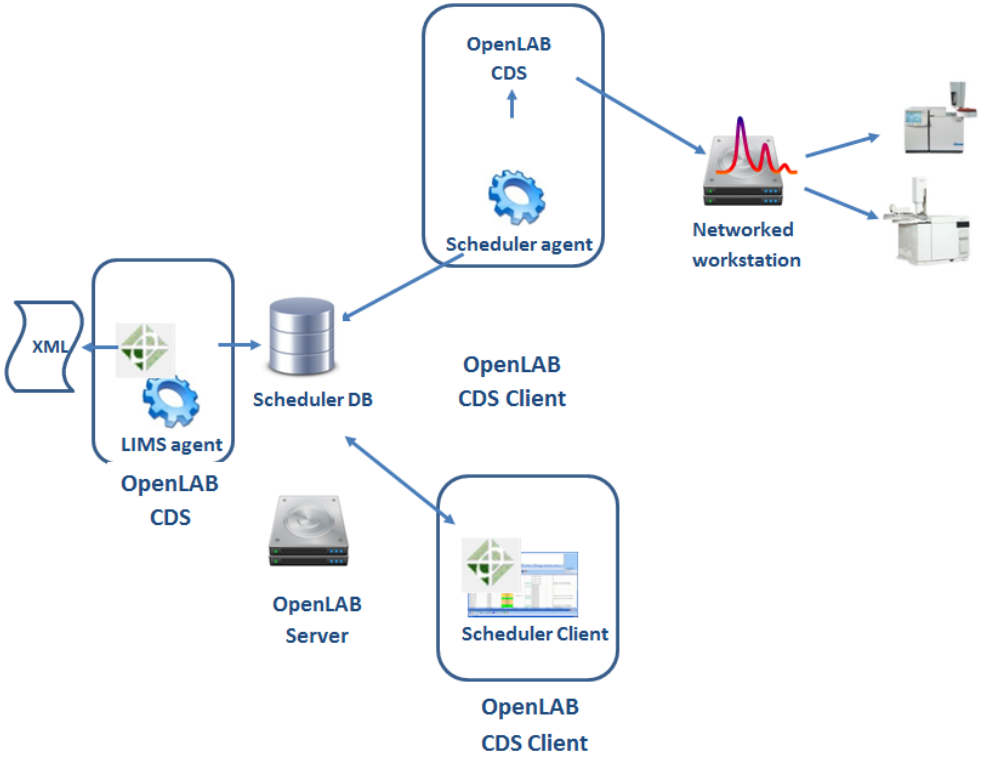
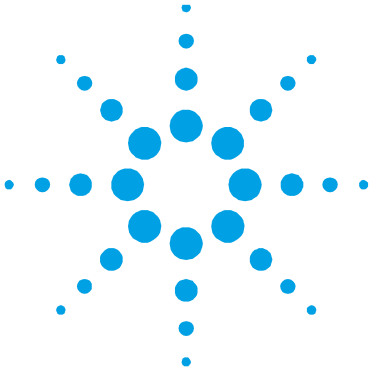


Figure 2 Sample Scheduler for OpenLAB



2. Scheduler Configuration

Galaxie Scheduler Configuration

Galaxie Scheduler configuration is performed through the SCHV2_Param.ini file which lists:

- General scheduler configuration parameters: database computer name, LIMS commands folder, general behavior etc.
- Default values attributed to an analysis if not defined in the XML command: initial state, vial position...
- Authorized Scheduler actions in client: Stop analysis, Quick start...

The Galaxie Scheduler client Layout is saved by user in two files:

- SCHV2_Client_ExperimentQueueGridsettings.ini
- SCHV2_Client_TaskDetailsGridsettings.ini files

Those three .ini files are available only from Galaxie server computer.

Sample Scheduler for OpenLAB Configuration

Sample Scheduler for OpenLAB Configuration parameters are stored in a SQL server database. They are displayed in a dedicated interface (Scheduler Configuration), *available from any computer where Sample Scheduler client is installed*. The access to Sample Scheduler for OpenLAB Configuration is limited to the Sample Scheduler Administrators, as assigned in OpenLAB CDS Control panel (Is an administrator - Sample Scheduler). A quick access is available from the Start menu.

The Sample Scheduler for OpenLAB Client layout is saved by the user in the SQL database.

Comparison between Galaxie Scheduler and Sample Scheduler for OpenLAB Configuration parameters

The list of configuration parameters has increased in Sample Scheduler for OpenLAB regarding to Galaxie Scheduler, due to the addition of new features.

This chapter handles only the comparison of the common parameters.

The following table lists the parameters configured in the Galaxie Scheduler Configuration file **SCHV2_Param.ini** and the corresponding parameters in Sample Scheduler for OpenLAB.

Table 2 Database

Galaxie Scheduler	Sample Scheduler for OpenLAB
Server name	N/A
Server port	N/A
Server timeOut	N/A

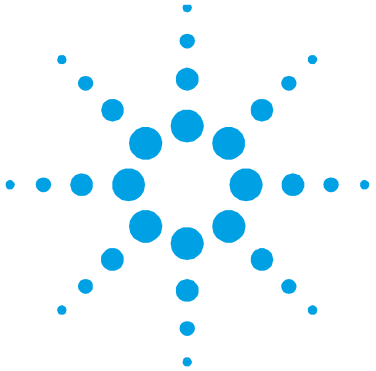
Table 3 Server

Galaxie Scheduler	Sample Scheduler for OpenLAB	Comments
LoggingLevel	N/A	
LoggingByProcess	N/A	
KeepLog	N/A	
MemCheck	N/A	
CustomGUI	N/A	
QuickStart	N/A	The rights to perform the action are defined in the OpenLAB role (in OpenLAB Control panel). In Sample Scheduler for OpenLAB, the rights are assigned by user and not for the entire application as it is the case in Galaxie Scheduler.
Restart	N/A	
Merge	N/A	
StopSystem	N/A	
ChangeSystemMethod	N/A	
AutomaticRefreshPeriod	System Configuration/Client/Automatic refresh period	
Run Queue State Colors	System Configuration/Client/State color: state	
	Analysis variable i: name displayed in Client. Defined for all users.	Corresponds to E_Custom variables in Galaxie Scheduler. The name assigned to E_Custom variable is defined in SCHV2_Client_ExperimentQueueGridsettings.ini by user.

Table 4 License

Galaxie Scheduler	Sample Scheduler for OpenLAB	Comments
Licenses #	N/A	Sample Scheduler for OpenLAB license defined in OpenLAB Control Panel.

NOTE Additional configuration parameters have been added for Sample Scheduler for OpenLAB. Refer to the *Sample Scheduler for OpenLAB Installation & Configuration guide* to know more.



3. XML command scheme

In both Galaxie Scheduler and Sample Scheduler for OpenLAB, the LIMS generates analysis orders thanks to XML commands. These commands contain the information and the acquisition parameter values used to perform the analysis.

In Sample Scheduler for OpenLAB an additional feature is proposed, to collect directly the analysis orders in the LIMS database thanks to SQL queries. This feature allows the Sample Scheduler to support LIMS that are not able to generate XML commands. Refer to the Sample Scheduler for *OpenLAB Installation & Configuration User's guide* for more information.

XML command

The XML command structure must match an XML scheme that establishes the XML validity rules. When a command is generated by the LIMS, it is checked by the Scheduler to ensure that, among others criteria, the parameters required by the CDS to perform the acquisition are assigned a value.

If the validity rules are satisfied, the XML is accepted and an analysis is generated in the Scheduler Client.

If the validity rules are not satisfied, the XML command is trashed. No analysis is generated in the Scheduler Client.

Galaxie Scheduler is able to recover a value in the Galaxie method for all the acquisition parameters required by Galaxie CDS (ex: vial, injection volume, description, multiplier...). When no value is assigned to an acquisition parameter in the XML command, the one defined in the method is used. It is the reason why the XML commands generated by the LIMS can contain only a few information to be considered valid.

In the case of Sample Scheduler for OpenLAB, no acquisition parameter can be retrieved from the method, except the injection volume. As the acquisition parameters are required by the OpenLAB CDS to perform an acquisition, and that all the LIMS are not able to assign a value for all of them, it has been given to the system administrator the possibility to configure the list of mandatory parameters fitting his LIMS capabilities in the Scheduler Configuration. By this way we avoid too many commands to be rejected. The Sample Scheduler XML scheme has then been modified to fit this list of mandatory parameters, and also to match the OpenLAB CDS architecture. The XML structure has been defined to look like Galaxie XML Scheme as much as possible.

NOTE The XML scheme (.XSD) is provided by the Sample Scheduler for OpenLAB Setup. It is available in the <Sample Scheduler for OpenLAB>/Documentation folder.

Table 5 XML scheme

Galaxie Scheduler XML parameters	Sample Scheduler for OpenLAB XML parameters
<Experiment>	
TypeCommand [CANCEL]	Other XML scheme to be used
	Template
Experiment ID*	Sample Name * / **
	Identifier*
Group**	-
Project**	Project**

Table 5 XML scheme

User**	User**
Injection Number	Replicates
Initial State**	State**
E_Custom1 to E_Custom5	AnalysisVariable1 to AnalysisVariable5
+ <Task> section	+ <Tasks> section
<Task>	**<Tasks>/<Task>**
-	ResultName**
-	Processing Methodname
MethodFullFileName*	(InstrumentName/MethodName)
OptionalMethodList / MethodFullFileName	(InstrumentName/MethodName) x N CanUseMethodInjectionVolume
-	InstrumentVariable1 to
T_Custom1 to T_Custom10	InstrumentVariable10
+ <Injector> section	+ <Injection sources> section
<Injector>	**<Towers>/<Tower>**
-	InjectionSource
RunName**	-
+ <Sample Info> section	+ <Sample info> section
+ <Calibration> section	+ <Calibration> section
+ <InternalStandard> section	+ <InternalStandard> section
<SampleInfo>	**<SampleInfo>**
Description / Line	Description / Line
RackNumber	-
AutoSamplerPosition	Vial
-	UseMethodInjectionVolume
InjectionVolume	InjectionVolume
InjectionVolumeUnit	InjectionVolumeUnit
SampleMass	SampleAmount
SamplemassUnit	SampleAmountUnit
-	Multiplier
-	Dilutor

Table 5 XML scheme

<Calibration>	**<Calibration>**
SampleType (Unknown, Blank, ControlSample, ControlSampleLevelI, Standard)	SampleType (Sample, Cal.Std.)
Level	Level
CalibrationMode (Add, ClearLevelOnly, ClearOldPoints)	CalibrationRuntype
<InternalStandardValues>	**<InternalStandard>**
InternalStandardItem /Item (ie: ISTD name) InternalStandardItem /Value -	- InternalStandardAmount InternalStandardAmountUnit
<Variables>	-
Variable/Identifier Variable/Value	Not Handled
*: mandatory in XML **: mandatory in the XML except if a default value is defined in the Configuration	*: mandatory in XML The list of mandatory parameters is defined in System Configuration/Command. **: default value defined in the Configuration

NOTE

It is possible to define tokens in the XML commands for Sample Scheduler for OpenLAB. The use of token is available for *Sample name, Result name,* and *Data file name* (OpenLAB CDS tokens (instrument :<I>, User:<U>, etc) and Scheduler tokens (Analysis variables:<A1>, Sample Custom Parameters <SCP1>).

XML mandatory parameters

In the case of Galaxie Scheduler, the parameters that must be assigned a value in a XML command are not configurable.

The minimal XML command (if all parameters defined in the configuration are assigned a default value, ex: Data File Name, Initial State Project, etc) must contain:

- ExperimentID
- MethodFullFileName (path/methodname)

In the case of Sample Scheduler for OpenLAB, the parameters that must be assigned a value in a XML command are configured in the System Configuration/ Command panel.

To know more on this feature, please refer to the *Sample Scheduler for OpenLAB Installation & Configuration User's guide*.

Priority rules between XML parameters and Configuration parameters

Some parameters can be assigned a value both in the XML and Scheduler configuration: Project, User, and State.

In the case of Galaxie Scheduler, some values can also be recovered from the method.

In both Schedulers, priority rules have been set to know which value is used for a given parameter.

In the case of Galaxie the priority rules are the following ones:

Table 6 Priority order

Parameter:	Priority Order for Galaxie Scheduler:
Data file name	Galaxie Method < XML command < SCHV2_Param.ini (= configuration)
User input variables	Galaxie Method < XML command < SCHV2_Param.ini
User/Group/Project	SCHV2_Param.ini < XML command
Initial State	SCHV2_Param.ini < XML command
Other parameters	XML command

In Sample Scheduler for OpenLAB, to have homogeneous priority rules management, *all the parameter values defined in the XML override the default values defined in the Scheduler Configuration.*

In both Galaxie Scheduler and Sample Scheduler for OpenLAB, the user can edit the values of acquisition parameters in the Client.

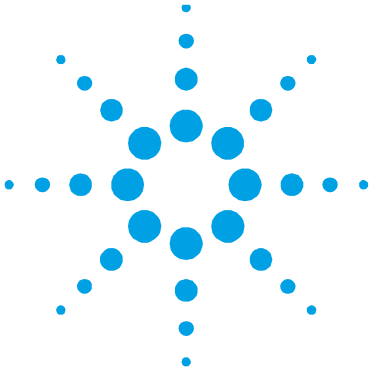
Cancel Command

The aim of the Galaxie Scheduler's Cancel commands is to remove programmatically an analysis that has not yet be performed by the Scheduler, from the database (Waiting and Scheduled analysis).

In Galaxie Scheduler, the user has to add the 'TypeCommand' tag in the XML, and define the ID of the analysis to remove from database in the 'Experiment ID' tag.

In Sample Scheduler for OpenLAB, another XML scheme is used to manage the 'Cancel' feature: SchedulerAction.xsd. The corresponding command looks like:

```
<SchedulerAction>
  <Identifier>SampleID of the experiment to cancel
  </Identifier>
  <Type>Delete</Type>
</SchedulerAction>
```



4. Scheduler Client Features

The Sample Scheduler Client interface has evolved relatively to the Galaxie Scheduler one, to accommodate the new features.

Table 7 Features

Galaxie Scheduler	Sample Scheduler for OpenLAB
Tool bar	Tool bar
Experiment queue grid: • List of analyses distributed over all instruments of the laboratory • No editing	Analysis table: • List of analyses distributed over all instruments of the laboratory • Edit all parameters
Experiment edition grid: • Edit acquisition parameters of an analysis in the Analysis queue grid	Sequence table: • Edit sequence lines

The Edition grid has been removed in the Sample Scheduler for OpenLAB. A sequence table has been added to allow the management of sequences inside the Scheduler.

Edit an Analysis

In Galaxie Scheduler, an analysis can be edited in the Edition grid, located under the Queue grid. Only acquisition parameter can be edited.

In Sample Scheduler for OpenLAB, edit the analysis directly in the Analysis Table. All the parameters defined in the command can be editable except the analysis Identifier.

Calibration

In Galaxie CDS, five calibration modes are proposed: Unknown, Standard, Blank, Control sample, Control sample of level i.

In Sample Scheduler for OpenLAB, all sample types and calibration modes are supported.

User variables

Galaxie Scheduler handles the Galaxie CDS Global user inputs variables. The user was able to define a value for each of these variables from the Scheduler Client and the XML command.

OpenLAB CDS variables are not handled by the Sample Scheduler for OpenLAB.

'Last modification user' parameter

In Galaxie Scheduler a *Last modification user* is associated to an analysis only when the analysis is Scheduled/Submitted/In progress or Ended (No *Last modification user* when analysis is in waiting state). When the analysis is scheduled manually by the user, or started from a Quick start, the *Last modification user* takes the name of the connected user until the analysis starts (submitted), then it takes the name of the user defined into the configuration file (SCHV2_param.ini). Indeed in Galaxie Scheduler, it is the *Run Manager* that manages all the acquisitions, and its associated name is the one defined in the configuration file. When opening the chromatogram audit trail, it is assigned to the user that started the analysis (Scheduled it).

In Sample Scheduler for OpenLAB, the management of the *Last modification by* has been improved.

- A *Last modification* by value is assigned to all analysis whatever their state.
- When a user edits an analysis, his name is assigned to the *Last modification by*.
- When the analysis is generated by the LIMS, *LIMS* value is assigned to the *Last modification by*.

Scheduler table parameters translation

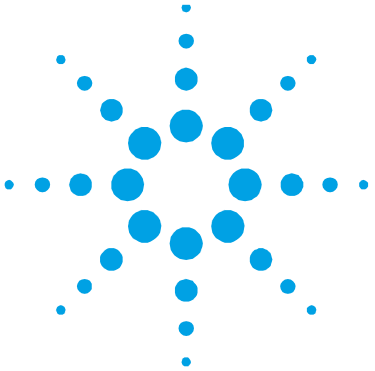
In Galaxie, it is possible to rename the title of all the columns of both the Experiment queue grid and the Experiment edition grid by user.

In Sample Scheduler for OpenLAB, it is not possible to rename the parameters.

Add an Analysis from Scheduler Client

In Galaxie Scheduler, the addition of an analysis from the Client is done by using the Quick Start feature.

In Sample Scheduler for OpenLAB, the mechanism of adding an analysis has been modified. *Quick start* has been replaced by *Add*. No dedicated screen is displayed; the new analysis is added directly in the Analysis Table in Edit mode to allow the user to define the desired parameters.



5. Sample Scheduler for OpenLAB Limitations

Method Acquisition & Processing Default Values

It is not possible to recover acquisition & processing parameter values (vial, injection volume, sample amount, etc.) from the OpenLAB CDS method, as it is the case with Galaxie CDS method.

Due to this limitation, the following Galaxie Scheduler features do not exist in Sample Scheduler for OpenLAB

- XML command completion with default method value (if no value defined in the command)
- Automatic completion of the analysis added by Quick Start with default method value

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In This Book

The manual describes the main differences between Galaxie Scheduler and Sample Scheduler for OpenLAB regarding:

- The deployment
- The Configuration
- The XML command structures
- The Features

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