# SRA Lab

## **User manual**



Dear user,

Thank you for choosing this SRA Instruments product.

This manual contains all the necessary information for the correct use of your software. Should you need further information or if you encounter any problems, please contact our After Sales Service:

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## **1. Presentation**

SRA Lab is an "addon" software package for chromatography software. Dedicated to a control function, SRA Lab enables a CDS, in just a few clicks, to start analyses which can then be imported from a LIMS.

The application supports as many instruments as the CDS can handle. It is designed to complete the sample sequence with default parameters (which can be modified) and launch the sequence after its validation.

With its own sequence (or task list), SRA Lab offers the operator the possibility of modifying it even while it is in use, without the need to pause it.

The results are visible in CDS or SRA Lab and can be sent to LIMS with the application of specific calculations.

### **1.1 The sequence**

SRA Lab uses a single sequence for each instrument. This sequence is initialized each time the application is launched and is specific to each instrument. It is updated each time an analysis is modified and can be reset at any time.

### **1.2 The status**

SRA Lab displays a sequence status for each instrument. This view shows the status of each analysis in the sequence, applying the "Lab at a Glance" concept of OpenLab CDS.

### 1.3 Results

SRA Lab uses analysis reports exported from CDS. These reports make all the analysis information available to SRA Lab so that it can perform specific calculations and present a customized results report to the operator for each analyser.

# 2. Configuration

### **2.1 Configuring AICs**

For a Client/Server configuration, the AICs must be configured before the client workstations.

For a Workstation configuration (OpenLab and SRA Lab on the same PC), this section is not necessary.

On the AICs, SRA Lab uses a Windows service called SIC (SRA Lab Instrument Controller), which must be configured after its installation (see document *SRA Lab Prerequisites and Installation guide*).

The role of the SIC is to communicate with all SRA Lab and OpenLab CDS clients on the AICs (connected to SRA Lab).

Once OpenLab CDS is installed and configured, and SRA Lab is also installed, go to the SRA Lab directory (on AICs using SRA Lab) and double-click on the Configuration shortcut:

Copy the OpenLab CDS connection string.
 The default string is net.tcp://OPENLABSERVERNAME:6577/Agilent/OpenLAB.





In the example below, the server's name is olsrv.

- Define the OpenLab CDS login to be used by the AIC.
- Set the SRA Lab TCP port used for dialog between SRA Lab clients, and the AICs SIC service. The default port is 8000. Please ensure that the network administrator does not block this port on the firewall.
- Specify the following folders:
  - $\circ$   $\;$  The directory where SRA Lab will store analysis results for the LIMS.
  - $\circ$   $\;$  The directory containing sequences created by the LIMS.
  - The directory that receives the CSV reports generated by OpenLab CDS.

SRALAB IC CONFIGURATION	¢   0   ×
OpenLab CDS	SRA Lab
Connection string net.pipe://localhost/Agilent/OpenLAB/	<sup>Port</sup> + -
Domain SRA	Conserver repository olsever sectory Conserver sectory Cons
User name labo	
Password ••••••	
× Cancel	√ Confirm

- Close the configuration utility.
- Restart the SIC to apply the configuration.
  - Display the Windows services manager (run " the services.msc" command in a command interpreter window).
  - Move the scrollbar to the SRA.SIC.ServiceSRALab service and click on it.
  - Click on "Restart". The SIC service should be started.

	0 🗟 🚺 🖬 🕨 🖬 🕪	×				
Services (local)	Services (local)					
	SRA.SIC.ServiceSRALab	Nom	Description	État	Type de démarrage	Ouvrir une session en tant que
		🏟 Service utilisateur du kit de	Service de c		Manuel	Système local
	Démarrer le service	🎑 Service utilisateur du Presse	Ce service ut	En co	Manuel	Système local
		🧟 Service Wi-Fi Direct Service	Gère les con		Manuel (Déclencher I	Service local
	Description :	🏟 Service Windows Insider	Offre la pris		Manuel (Déclencher I	Système local
	SRA Service SRALab	🤹 Service SSTP (Secure Socket	Prend en ch	En co	Manuel	Service local
		🥋 Services Bureau à distance	Autorise les	En co	Manuel	Service réseau
	Démarrer         le service         Service utilisateur du Presse         Ce service ut         En co         Manuel         Système local           Description :         Service Wi-Fi Direct Service         Gère les con         Manuel (Déclencher l         Service local           SRA Service SRALab         Service Strip (Secure Socket         Prend en ch         En co         Manuel         Service local           Sq. Service SRALab         Service Bureau à distance         Autorise les         En co         Manuel         Service réseau           Services de chiffrement         Fournit trois         En co         Maudel         Service réseau           Shared PC Acrount Manager         Manages pr         Déscritivé         Service réseau         Service réseau	Service réseau				
		🎇 Shared PC Account Manager	Manages pr		Type de démarrage     Ouvrir une session en tant que       Manuel     Système local       Manuel     Système local       Manuel (Déclencher I     Service local       Manuel (Déclencher I     Système local       Manuel (Déclencher I     Système local       Manuel     Service local       Manuel     Service réseau       Automatique     Système local       Manuel     Service réseau       Désactivé     Système local       Automatique     Système local       Automatique     Service réseau       Manuel     Service réseau	
		🥋 SMP de l'Espace de stockage	Service hôte	Manuel	Service réseau	
		Spouleur d'impression	Ce service m	En co	Automatique	Système local
		RASIC.ServiceSRALab	SRA Service		Automatique	Système local
		Station de travail	Crée et main	En co	Automatique	Service réseau
		🎑 Stockage des données utilis	Gère le stock		Manuel	Système local





### 2.2 Configuring SRA Lab Client

Launch the SRA Lab "Configuration" application (included in the software installation folder).

#### 2.2.1 Configuring Client/Server

Once you have logged in, click on "Configuration" to access the SRA Lab configuration.

If SRA Lab is installed as a Client/Server, the product must be installed on the client workstations and AICs (managed by SRA Lab). On a client workstation (Client/Server configuration), select "Client/Server". The view below appears.

🏠 SRA LAB	=x   4	
1 CDS configuration	2 Directories 3 Instruments	s list 🔳 Method
	♀ Mode Client/Server ▼	
0	Host name	Port
	AIC 1	<u>8000 + -</u>
	AIC 2	8000 + -
	× Cancel 🛛 🛩 Confirm	n

List all AICs to be managed by SRA Lab.

Click on the button 🕒 to add a line, type the name of the PC to be used as an AIC, then enter the TCP port used for the SRA Lab dialog (by default, this port is 8000).

You can remove an AIC by clicking on the red trash can 📋 in front of the line you want to delete.

Remember to save by clicking on "Confirm" at the bottom of the view.

#### 2.2.2 Workstation configuration

If SRA Lab is installed in a workstation configuration, select "Workstation" in the "CDS Configuration" tab.





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SRA LAB						<b>-   \$   @   6  </b>	- 0	×
1 CDS configuration	2 Directories	Instruments list	4 Method	5 Valves configu	uration	6 Events tables	7 Modbu	s
			♥ Mode Workstation ▼					
		Authenticatio	on CDS					
		Connection si e_ net.pipe://loc	tring alhost/Agilent/Open	LAB/				
			None -					
		× c	ancel 🛛 🛩 Co	nfirm				

In the "Connection string" field, keep the default "net.pipe://localhost/Agilent/OpenLAB/".

In the "Mode" list, select the identification mode configured in OpenLab CDS to use the software.

- If OpenLab CDS is configured without a user login, select "None". \_
- \_ If the CDS is configured to use a login created in OpenLab, select "Internal".
- -If OpenLab CDS is configured to use the PC's Windows login, select "Domain".

For "Internal" mode, enter the login and password to be used to communicate with OpenLab CDS. For "Domain" mode, enter the login, password and domain name to be used to communicate with OpenLab CDS.

Click on the "Confirm" button before continuing.

### 2.3 Software configuration

#### 2.3.1 Directories

To enable SRA Lab to interact with the LIMS, you must enter the storage folders for LIMS results and sequence files.

🏠 SRA LAB			=x   🔺   :	<b>\$</b>   @	0   -	×
1 CDS configuration	2 Directories 3 Instruments	iist 🛛 🕢 Metł	hod			
	Lims Results Directory     C:\CDSProjects\SRALab     Lims Sequences directory     C:\CDSProjects\SRALab     Methods directory     C:\CDSProjects\SRALab     C:\CDSProjects\SRALab     Log repository     C:\CDSProjects\SRALab	\Lims\Resultats   \Lims\Sequences   \Methods   Reports\				
	Replace file name with Events tables repository C:\CDSProjects\SRALab	user name (default \Events	error.log)			
	× Cancel	🛩 Confirm				





- <u>Lims results directory:</u> enter the directory where the final analysis reports for LIMS will be stored.
- <u>Lims sequence directory</u>: enter the directory of sequence files created by the LIMS.

If no LIMS is used, keep the first 2 fields blank. Click on the "Confirm" button before continuing.

- <u>Methods directory:</u> enter the directory containing the ".methods" files listing instrument methods.
- <u>Reports directory</u>: enter the directory that will contain the csv reports generated by OpenLab CDS Acquisition at the end of each analysis.
- <u>Log repository</u>: enter the directory where the AIC SRA Lab service logs and SRA Lab Client logs will be saved. By checking the "Replace file name..." box, the log file error.log will be replaced by a log file named the user's Windows account.
- <u>Event tables repository:</u> enter the directory where all event tables will be saved.

#### 2.3.2 Instruments list

🏠 SRA LAB	=x   4	.   ‡   ⊡   0	- 🗆 🗙
1 CDS configuration	2 Directories	Instruments list	4 Method
	Update instru	nents	
	Instrument name	Id Lims	
	sp101	0101	
	sp205	1201	
	SP503	1203	
	× Cancel 🖋	Confirm	

Click on the "Update instruments" button.

The application displays the list of instruments managed by the AICs selected by SRA Lab.

For each instrument, enter the number that identifies the instrument in the LIMS. The LIMS ID must contain 4 characters (2 for the instrument ID and 2 for the PC ID).

Click on the "Confirm" button before continuing. For instruments not linked to LIMS, set LIMS ID to 0000.

### 2.4 Methods configuration

#### 2.4.1 List of methods (Client/Server mode)

In the "Client/Server" version, SRA Lab cannot obtain the list of methods from OpenLab CDS. To be able to indicate which method to use to perform an analysis, the user must be able to choose a method from among all the analyser's acquisition and processing methods.

The list of methods is obtained by listing them in the "Configuration" section of SRA Lab; all the methods used in OpenLab CDS must be added, whether they are analysis or processing methods.





#### Before listing the methods, the configuration of the directories and instruments must be (i) operational.

Open the SRA Lab configuration, select the "Method" tab and then "List of methods".

By default, each instrument contains a method (default name "Method") and a tick to define whether the method is an acquisition and/or processing method.

To add a method to an instrument, click on the "+" button next to the instrument name. A method with default fields, to be adapted to your configuration, will be added.

1	SRA LAB					=x   🔺   🅸			×
10	CDS configuration	n 2 Directorie	s 3 Instruments list	4 Method					
		List of meth	ods			Method properti	es		
	⊕ sp205								
	Method name	Acquisition method	Processing method						
Î	M3	$\checkmark$							
Î	m4								
	m3								
	⊕ sp503								
	Method name	Acquisition method	Processing method						
Î	spg2302								
	m1								
	m2								
	m3								
	m4								
	m3 resolvedrequired	4 🔽							
								_	_
			×	Cancel 🤍 🛩 Co	nfirm				

To delete a method from an instrument, click on the delete button (red trash icon).

Once you have listed the methods, click on "Save".

#### 2.4.2 Method properties

Methods can be used with predefined parameters. For each method, you can predefine:

- \_ The injection source (front injector, rear injector, etc.)
- A multiplication factor -
- -The concentration to be sent to the LIMS (ISTD, Normalized, etc.)
- The injection volume

These parameters are specific to the methods and instruments entered. To customize these parameters, select the "Method" tab and then "Method properties".





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🧄 SRA LAB			=×	<u>▲   ‡   @   6   -</u>	
1 CDS configuration	2 Directories	<ol> <li>Instruments list</li> </ol>	4 Method		
Li	ist of methods			Method properties	
<ul> <li>Instrument name Meth</li> </ul>	nod name Calibration	n Injection			
■	m1 Estd •	External 👻			
sp101 -	m2 Estd •	External 👻			
sp101 -	m3 Estd •	External 👻			
■ sp205 ▼	m1 Estd •	External 👻			
<b>s</b> p205 ▼	m2 Estd •	External 👻			
<b>s</b> p205 ▼	m3 Estd •	External 👻			
SP503 ▼	m1 Estd •	External 👻			
SP503 ▼	m2 Estd •	External 👻			
SP503 ▼	m3 Estd •	External 👻			
		X c I - "	<i>c</i>		
sp205 ▼         sp205 ▼         sp205 ▼         SP503 ▼         SP503 ▼         SP503 ▼	m1     Estd ▼       m2     Estd ▼       m3     Estd ▼       m1     Estd ▼       m2     Estd ▼       m3     Estd ▼	External • External • External • External • External •	Confirm		

This utility generates the "MethodsParameters.json" file located in the methods directory (configured in chapter 2.3.1). This file contains all the information entered in the utility.

To add a method and its parameters, click on the "+" button: a new line containing the name of the instrument and the default parameters (which you can modify) will be added.

Enter the name of the method to be customized (in the "Method" column). Enter only the method name (without the extension).

<u>Please note</u>: Please respect upper and lower case.

If required, enter a multiplication factor to be applied to the analysis for this method. The default value of 1 has no effect on the results.

Select the type of concentration to be uploaded to the LIMS. Click on the cell in the "Calibration" column to display the list of possible choices and select the concentration to be uploaded.

Select the injection source. For each method entered, you can indicate the injection source (front or rear injector, valve, etc.). In this way, only the position of the vial will come from the LIMS, the injection source being defined by the properties of the method.

Finally, you can define the injection volume in the "Injection volume" column.

To delete a record, click on the line to be deleted and press the DEL key on the keyboard. Click "OK" to save and close the utility.





#### Please note:

Make sure you only enter (or select) data that already exists in the CDS. Only enter the name of a method that already exists in the CDS. Select an injection source configured in the CDS.

### 2.5 Hardware configuration (workstation only)

The instruments can be complemented by peripherals to add functionality to the analyses performed. Various peripherals can be configured via "Device configuration".

#### 2.5.1 Vici Valco Valve

Valves can be added to an instrument to select sampling channels during analysis.

General configuration:

🏠 SRA LAB					<b>.</b>   <b>\$</b>   <b>0</b>   <b>0</b>	- 🗆 ×
CDS configuration	2 Directories	Instruments list	4 Method	5 Valves configuration	6 Events tables	7 Modbus
General configuration	Streams configu	ration				
		Ge	eneral configura	ation 2		
		Attribution des vannes aux il sp205 Selection vannes • Vanne de selection Vanne 3 : 10 Voles Selection vannes • Vanne 5 : 10 Voles	vstruments Vanne 1 : 10 Voies Vanne 4 : 10 Voies	Vance 2 : 10 Voies		
		×c	ancel 🛛 🛩 Co	onfirm		

Select the PC serial port to which the valves are to be connected.



Assigning valves to instruments: Each instrument can be assigned from 0 to several valves.





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sp205		
Valve s	election 👻	
Vann	e de sélection Var	nne 1 : 10 Voies Vanne 2 : 10 Voies
Vanr	ne 3 : 10 Voies Var	nne 4 : 10 Voies
$\checkmark$	Selection valve	
$\checkmark$	Valve 1:10 Positions	
~	Valve 2:10 Positions	
~	Valve 3:10 Positions	
~	Valve 4:10 Positions	
-		

Simply click in an instrument and select the valves that will complement it.

#### **Streams configuration:**

Once all the valves to be used have been assigned to an instrument and the "Confirm" button has been pressed, the channels can be configured.

🍈 SRA LA	B						± † *	¢   💷   🛛   –	
1 CDS co	nfiguration	<ol> <li>Direct</li> </ol>	ories 🛛 🕄 In:	struments list	4 Method	S Valves configuration	6 Events tables	7 Modbus	
General co	onfiguration	Streams c	onfiguration						
sp205	sp503	sp504	sp508 sp	902					
Valve	Position	Name	Used ?	Purge activated					
1	1	Sample 1		0					
1	2	Sample 2	2 🔽	0					
1	3	Sample 3		0					
1	4	Sample 4		After seque	ence 👻				
1	5	Sample 5		0					
1	6	Sample 6	5 🔽	0					
1	7	Sample 7		0					
1	8	Sample 8	3 🔽	0					
1	9	Sample 9		0					~
				:	X Cancel	√ Confirm			

Valve: The valve on which the channel is located

**Position**: The position of the valve corresponding to the channel

Name: The stream name. It is possible to rename several channels at once by following these steps:

Name a channel with a name ending in a number -





- Right-click on this channel
- Click on " Increment for next " to rename all the following channels with the same name and the number incremented by 1 or " Increment for next " to do the same thing by decrementing the number.

**<u>Used?</u>**: Indicates whether the channel will be used and therefore displayed in SRA Lab.

**Purge**: The sample channel chosen as the purge channel will be automatically selected either at the end of each analysis or at the end of a sequence.

Use cases	How it works	Purge						
Single valve	Selectable sampling stream.	A single purge stream						
Several valves without	Selection of one sampling stream per valve.	One purge stream per valve						
selector valve								
Several valves with	Selection of a sampling stream for all valves.	A purge stream for the						
selector valve (selector	Example: The selection valve is on channel 2,	instrument						
valve has identifier 0)	each valve has 10 positions and valve 2 is on							
	channel 5 $\rightarrow$ the selected channel is channel							
	15							

#### **2.5.2 Event table configuration**

An event table is used to program events preceding an analysis. It can be configured for each instrument.

🧑 SR.	A LAB							🔺   🌣   🕮   🚯	- 0	×
1 CDS	5 configuration	2 Directories	Instruments list	4	Method	5 \	/alves configuration	6 Events tables	7 Modbu	s
sp101	sp205	SP503								
				o	Name					
				1	Event 1	Î				
				1	Events 2	Î				

To add a new event table, click on 🔂 To edit an existing event table, click on 🧪

To delete an event table (Warning: this action is irreversible), click on 📋

An event table is defined by:

- The event table name (2 event tables cannot have the same name for the same instrument)
- Adding an event: An event is defined by the time at which it should start a type and a command.

#### The different types of event

There are different types of events, and the command changes according to the type chosen:

1) Stream selection

If valves are configured for the selected instrument, the "Channel change" event is available. At the given time, the sampling channel chosen in the "Command" column will be selected.

2) Start analysis

This event is used to start the analysis while the event table is still running. This action pauses the event table until the injection has been completed.





#### Example of an event table:



For this example, as soon as the table is run, stream 1 will be selected, then after 10 seconds stream 2. After 20 seconds, execution pauses until injection takes place. Finally, 10 seconds after injection, stream 3 will be selected, followed by stream 4, 20 seconds later.

After clicking on the "Save" button, the event table is saved in the folder previously selected in the directory configuration.

### **2.6 Modbus configuration**

The Modbus protocol enables data to be exchanged between SRA Lab and other devices.

By configuring the Modbus part of SRA Lab, it will be possible to store analysis results as well as real-time status and other data in an address table.

The remote device can then access this data by targeting the correct address and can also send commands to SRA Lab by writing to specific addresses.

Access the Modbus configuration by clicking on

7 Modbus fr

from the SRA Lab configuration.

#### 2.6.1 Communication configuration

Different communications can be configured so that different devices can exchange data with SRA Lab.





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🥎 SRA LAB					<b>∔</b>   <b>\$</b>   <b>©</b>   <b>6</b>	- 🗆 🗙
1 CDS configuration	2 Directo	ories 3 Instrum	ients list 🛛 🕘 Met	hod <b>5</b> Valves configuration	on 6 Events table	es 7 Modbus
Communication	Registers					
	0	Slave identifiant	Communication	Configuration		
		1 +-	** TCP -	Port + -	··· 盲	
		2 + -	<sup>★</sup> Serial ▼	Port Tota transmission	<sup>n</sup> . 💮 🔳	
		× Can	cel all 🛛 🚿 Save a	Il modbus configuration		

Click on the button 🔮 to create a new communication.

To set up a Modbus communication correctly, you must specify the following fields:

- **Slave number**: Which can be between 1 and 255, this is the identifier that will have to be targeted from the remote device to synchronize with SRA Lab.
- **Communication Mode**: TCP or Serial
  - If TCP selected: TCP port to open for communication (default 502)
  - If Series selected:
    - PC serial port
    - Data transmission mode (RTU/ASCII)

By clicking on the button  $\odot$ , you will have access to the advanced settings, you will be able to set:

- The byte order for decimal values
- Byte order for short integer values

To save the changes, click on the "Save all Modbus configuration" button. To remove a communication, click on the button

Note: If a communication is deleted, it cannot be recovered by pressing "Cancel"

#### 2.6.2 Register configuration

Click on the "Registers" tab to access the registers configuration.

	1 TCP (Port : 502)													
🖾 🗬 😭	Value	Address	Format											
sp101				$\sim$	$\uparrow$									
1	Data ready	40001	Bit	Ē										
1	Top injection	40002	Bit	Î	$\downarrow$									





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Value to watch	Possible formats	Description
Year of analysis	Short integer	Year of last analysis of the selected instrument ended
Analysis Month	Short integer	Month of the last analysis of the selected instrument ended
Day of analysis	Short integer	The day of the last analysis of the selected instrument
Day of analysis	Short integer	ended
Hours of analysis	Short integer	Time of the last analysis of the selected instrument has
	0.0011.0080	ended
Minutes of the analysis	Short integer	Minute of the last analysis of the selected instrument has
····· · · · · · · · · · · · · · · · ·		ended
Seconds of the analysis	Short integer	Second of the last analysis of the selected instrument has
•	U	, ended
Data ready	Bit, Short integer	Set to 1 by SRA Lab when the results are ready, to be reset
		to 0 by the remote device
Concentration	Real, Short Integer	Concentration of the compound captured during the last
		analysis performed
Standardized	Real, Short Integer	Normalized concentration of the compound captured at the
concentration		time of the last analysis performed
Retention time	Real, Short Integer	Retention time of the compound captured in the last
		analysis performed
Surface	Real, Short Integer	Surface area of the compound captured during the last
		analysis performed
Type of analysis	Short integer	Type of last analysis performed
Top injection	Bit, Short integer	Set to 1 each time an injection is made during the time
		entered
Selected Path	Short integer	Selected stream if a compliant configuration is made for the
		instrument
Status instrument	Short integer	Status of the instrument:
		0: Not Connected
		1: Not ready
		2. Pie-luli 2: Injection
		4. Analysing 5: Collecting Results
		6: Post analysis
		7: Completed Analysis
		8: Analysis stopped
		9: Offline
		10: Ready
		11: Offline
Analysis state	Short integer	Scan progress status:
		0: Waiting to start
		1: Injection
		2: Analysing
		3: Post run
		4: Analysis completed
		5: Collecting Results
		6: Stopped
	-	7: Pre-run
Bit of Life	Short integer	This value is updated every second to verify data
<b>a a ·</b> ·		transmission (from 0 to 60)
Sequence Startup	Short integer	Set to 1 to start once the sequence is entered
		To be set to 2 to continuously start the sequence entered



Analysis	Short integer	Set to 1 to stop the sequence after the current analysis
		To be put at 2 to stop the sequence immediately

To add a register, click on one of the following buttons: 🔤 📽 😤

- **<u>Results</u>**: Records updated by SRA Lab for each analysis
- **<u>Status</u>**: Registers updated by SRA Lab with each state change
- **<u>Command</u>**: Register to be updated by the remote device

For each register, the "Instrument", "Format", "Address" and "Value" fields are mandatory. Depending on the selected value, fields can be added.

By default, the register type is "Holding"

#### 2.6.3 Usage

When starting an instrument from SRA Lab, if registers are configured for it, the corresponding connections will launch, and a notification will appear. The notification will display the connection type (TCP or serial) and slave number.

In addition, a Modbus connection information icon appears and when you hover the mouse over it, the status of the connections appears:

Communication established	Connection could not be established
	m  <b>1</b>  \$ @ 0 - 0 ×
Connection Slaves Communication	Connection Slaves Communication
TCP : 502 Slave 1	TCP : 502 Slave 1

If the connection is established, the icon is static, if any devices are communicating with SRA Lab, this icon flashes.

### 2.7 Configuring OpenLab CDS

All OpenLab CDS instruments and projects are added by default to the root of the Instruments pool (for instruments in the Instruments tab) and the Projects pool. You can organize instruments and projects by laboratory (or workgroup). This organization enables you to group users and give them access only to the instruments and projects they can use. In this way, users are not encumbered by resources (instruments, projects) they don't need. This organization is managed by the administrator.

#### **Configuration for exporting reports**

For OpenLab CDS to export analysis results to a text file, the CDS must grant the "Save Report to Disk" right. Saving csv reports at the end of each acquisition is authorized when the "Save Report to Disk" right is activated.

In the Control Panel, Administration tab:

- Click on "Roles", select "Chemist" then click on "Edit Role".
- List the privileges in the "Data" section, then tick the "Save reports to disk" box.





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Click OK to confirm. All user accounts required to export a csv report outside DataStore must be members of the "Chemist" group (configured as such).

Cp MANAGEMENT		Roles - Control Panel	
Create Role Role Roles			
Administration «	Roles		
P My Settings	Name	Edit Role	· ×
Local Configuration	Everything		
System Configuration	System Administrator	Name: Chemist	
Security Policy	Instrument Administrator	Description: Analytical chemist	
A Users	Project Administrator	Role type	
A Groups	Instrument User	Project Instrument Administrative	
🔁 Roles	Archivist	Role privileges Members	
System Activity Log	Content Management PDF Template Manager		
Licenses	Content Management Approver	Role privileges:	
Instrument Controllers	Content Management Contributor	Name	Description
E Diagnostics	Content Management Reader	Project Management	Project Privilege Group
🖆 Content Management	Technician	▷ E-Signature	E-Signature
জ্বি Instrument Options	Chemist	Sample Prep	Access to sample prep related functions
Administrative Reports	View project or project group	Acquisition Method	Access to method editing functions
	Manage project or project group	Processing Method	Access to processing method related function
	Edit content of project	Report Template	Access to report template designer
	Create and modify sample pren	Sequence Template	Access to sequence template related functi-
	Lise second second second second second	Sequence	Access to sequence related functions
	Use generic sample prep methods	Audit Trail	Access to audit trail related functions
	Create and modify acquisition method	Description Control	Access to instrument control related functic
	Use generic acquisition methods	Data Processing	Access to data processing related functions
	Create processing method	File and Folder Operations	Access to file and folder delete operations
	Save master method	Data	Access to data related functions
	Save result set method	Export data	OpenLab CDS OpenLab CDS
	Edit integration parameters	Save reports to disk	OpenLab CDS
	Edit identification parameters	Edit sample information	OpenLab CDS 👻
	Edit chromatogram extraction parameters		OK Save As Cancel
	Edit spectrum extraction parameters		
	Edit MS library search parameters		OpenLab CDS
	Edit calibration parameters		OpenLab CDS
In shown and a	Edit spectra parameters		OpenLab CDS
instruments	Edit system suitability parameters		OpenLab CDS
Projects	Edit custom calculation parameters		OpenLab CDS
Administration	Edit cisnal naramaters		Oneniah CDS





# **3. Using SRA Lab**

### 3.1 General presentation

When the application is launched, SRA Lab presents the list of available instruments.

sp101	Not connected	Ð
sp205	Not connected	Ð
SP503	Not connected	Ð
	ОК	

Click on the  $\oplus$  of the instrument you wish to use. If you want to select several instruments, click on the  $\oplus$ of the instrument, then wait until the instrument status is displayed before clicking on the  $\oplus$  of the next instrument, and so on.

Finally, click on "OK" to initiate instrument connection.

sp101	Not connected	O
sp205	Not connected	Ð
SP503	Not connected	Ð
	ОК	

This process takes some time to establish the connection, especially if there are several instruments to connect.

Note: SRA Lab does not require OpenLab to be started on client workstations to operate, but you can start the Acquisition module to view the continuous signal, for example.

SRA Lab's main window consists of a general commands panel on the left and a frame on the right displaying the data corresponding to the tab selected in the panel.





#### Banner tabs:



If you have clicked on Sequence in the control panel, the sequences of connected instruments are displayed.

🊺 SRA I	LAB	-	_		_	_	_		_		_	m † 2	•	<b>\$</b>   @		-		×
ø	🍘 sp101	×	🥌 SP503	×														
Status	Start									Loaded s	equence 💌	Save as	h	mport fre	) om Lim	15	Clear ta	: able
Sequence																		
				Ð	Sample Id	Lims Id	Method na	ame	Processing r	nethod	Injection	Events ta	able					
				+	PCP503	1583611	1	•	m1	*	External 🔻	Event 1 🗴 🗸	G	<b>\$</b>	Î			
Results				+	PCP603	1583620	m1	*	m1	•	External 🔻	None	•	\$	Ĩ			
I≱				+	PCP503	1583611	m1	•	m1	•	External	None	•	\$	Î			
selection				+	PCP603	1583620	m1	•	m1	-	External 👻	None	•	\$	Î			
				+	PCP503	1583611	m1	•	m1	*	External 🝷	Events 2 🔕 🕻	- •	<b>ə</b> 💠	Î			
				+	PCP603	1583620	m1	•	m1	*	External 🝷	None	•	\$	Î			
				+	PCP503	1583611	m1	*	m1	•	External 🔻	None	•	\$	Î			
				+	PCP603	1583620	m1	•	m1	•	External 🔻	None	•	\$	Î			
de				+	PCP503	1583611	m1	•	m1	•	External 🝷	None	•	\$	Î			
⊼ V				+	PCP603	1583620	m1	•	m1	•	External 🔻	None	•	\$	Î			
SRA																		
				Inst	rument state	: Ready						Run stat	te : W	/ait to sta	t			

Note: to display the sequence table of another instrument, click on the instrument name in the tab.







#### Commands in the top bar:

At the top right of the application, a series of commands are available:

- By clicking on you can enter the SRA Lab administrator login to access the software configuration.
- By clicking on **used** you display an application customization view.

You can:

- Change language.
- Switch to Dark (or Normal) mode.
   Dark mode features a dark background to reduce the bright surfaces and reduce eye fatigue.
   Light mode features the application's standard colour.
- Change the colour of the title bars by selecting the color in "Primary".
- Change the colour of the current tab selection in the "Accent" list.



Settings

<u>Note:</u> Customization is saved and applied automatically when the application is launched.

• By clicking on would be applied by the logs generated by SRA Lab. Il s'agit d'un fichier texte contenant tous les messages enregistrés par l'application. This is a text file containing all messages recorded by the application. You can save a copy of this file to communicate with our technical support (service@sra-instruments.com).

### 3.2 Status

SRA Lab constantly updates sequence and connection status with OpenLab CDS. By clicking on "Status" in the banner, you can display the status of the instrument sequence.

The sequence is reduced to sample name, LIMS ID and method name. You can see the % completed of the current acquisition and the status of all analyses.

	Sample Id	Lims Id	Method name	Events table
	PCP503	1583611	m1	Event 1 💿
10%	PCP603	1583620	m1	None
	PCP503	1583611	m1	None
	PCP603	1583620	m1	None
	PCP503	1583611	m1	Events 2 🔕 🛛 🧿
	PCP603	1583620	m1	None
	PCP503	1583611	m1	None
	PCP603	1583620	m1	None
	PCP503	1583611	m1	None
	PCP603	1583620	m1	None





In the title of each sequence, the duration is updated during the entire analysis:

sp101 (Running) (0.1/0.6 min)

In the sequence table view, at the bottom of the window, you can see the connection status:



<u>Note</u>: The analysis evolution time is also updated in the instrument name (sequence tab).

gc6890 (7.2/8.0 min)

#### Note:

When logging on to an instrument, SRA Lab displays the status "Not connected". The connection process takes some time, during which this status remains in this state. It is updated as soon as the connection is established. Until the connection is established, the sequence cannot be accessed.

If the status remains "Offline", check that the instrument is switched on and that the "Buffer Full" message is not displayed. In the latter case, restart the instrument.

Instrument state : Not connected

Run state : Wait to start

### **3.3 Sequence**

SRA Lab uses a sequence for each instrument. Each time the application is launched, SRA Lab initializes the sequence of the instruments. You can import a sequence from the LIMS, add, delete, insert, or edit an analysis.

The Sequence Editor is a table and a series of commands for each instrument.



🧑 SRA I	AB							_		m	<b>*</b>   <b>*</b>		- 🗆 🗙
Ø	🔵 sp101 (	(0.0/0.6 min)		🍘 SP50	3 X								
Status EX	C Stop								Loaded sequence 💌	Save as	Impo	ort from Lir	ns Clear table
Sequence				🕀 Sa	imple Id	Lims Id	Method name	Processing	method Injectio	n Events	table		
			~	P	CP503	1583611	m1	m1	External	Event 1	O	¢ 🔋	
Results			~	P	CP603	1583620	m1	m1	External	None		¢ 🔋	
]≱ Instrument			~	P	CP503	1583611	m1	m1	External	None		¢ 🔋	
selection			~	P	CP603	1583620	m1	m1	External	None		¢ 🔳	1
			~	P	CP503	1583611	m1	m1	External	Events 2	0	\$	
			~	P	CP603	1583620	m1	m1	External	None		\$	
			~	P	CP503	1583611	m1	m1	External	None		¢ 🖥	
			$\sim$	P	CP603	1583620	m1	m1	External	None		¢ 🔋	
ab			5%	P	CP503	1583611	m1	m1	External	None		\$	
A L				+ P	CP603	1583620	m1 •	m1	• External	• None	*	\$	_
SR													
			lr	nstrumen	t state : R	tunning				Runs	state : Run	ning	

In "Client/Server" configuration, the management of sequences between the client and AIC sessions requires particular attention. As every SRA Lab user has access to all instruments (managed by SRA Lab) at all times, the sequence of an instrument is stored on the AIC that drives the instrument. To access an instrument's sequence, it is necessary to import the sequence from the AIC, so that it can be subsequently modified. Once modifications have been completed, you can update the sequence to the AIC. Other operators using this same sequence receive a notification informing them that the sequence has just been modified and inviting them to update it (click on the "Retrieve sequence from AIC" button to get the updated sequence).

#### 3.3.1 The commands bar



an analysis), a message (see black banner above) prompts you to resend the sequence to the AIC. You can continue to make all the changes to the sequence before updating the AIC.

The sequence has been updated by another user	Download the sequence from AIC
If a user has edited the instrument sequence and updated it, the banr prompt you to retrieve the sequence that was just edited.	ner above will appear and

Once the sequence is ready, you can click "*Start*" to start the analysis cycle.





The sequence can be edited at any time without having to pause it. The status of the instrument in SRA Lab is updated on all devices connected to that instrument.

You can import the sequence recorded in the LIMS for this instrument. Click on *"Import from Lims*", the analyses of the LIMS sequence will be added to the sequence.



Check the contents and make sure that the processing method is the correct one (the names of the acquisition and processing methods may be different). Processing methods do not exist in LIMS; by default, SRA Lab uses the same method name for acquisition and processing. You can change the name as you wish.

<u>Note:</u> if the LIMS sequences folder is not specified in the SRA Lab configuration, this command will have no effect.

You can reset the table at any time by clicking on "*Delete table*". The application asks you whether you wish to reset the sequence or just delete the completed analyses. If the table is in use (acquisition), the analysis in progress remains displayed even if you reset the sequence.

	€	Sample I	d Lims Io	d Method name	Processing method	Injection	Vial		
40%		Smp1	1271332	m1	m1	Injecteur avant	1	۵	
	+	Smp2	1271333	m2 -	m2	<ul> <li>Injecteur avant</li> </ul>	2 +-	۵	Î
	+	Smp3	1271331	m3 -	m3	<ul> <li>Injecteur avant</li> </ul>	3 +-	۵	
	+	Smp4	1271232	m4 -	m4	<ul> <li>Injecteur avant</li> </ul>	4 +-	\$	

#### 3.3.2 Loading/Saving sequences

sp101 × SP503 sp205 = Ŧ Ē Loaded sequence Sequence 1 Start Import from Lims Clear table Save sequence Ð Sample Id Lims Id Method name Processing method Injection **Events table** PCP503 + 1583611 m1 m1 🝷 External 🝷 Event 1 🛽 🖉 0 ¢ PCP603 + 1583620 Ŧ External ¢ m1 m1 None Ŧ

The name of the currently loaded sequence is displayed in the select list.

By clicking on "Save As" and entering the name of the sequence in the window that appears, the sequence is saved in the SRA Lab installation directory.







This way, the created sequences are not lost.

Once a sequence has been loaded, the menu changes slightly and it is possible to overwrite the loaded sequence by clicking on "Save Sequence" or create a new save by clicking on "Save As".

Save seque	•	Impo	-+ 1
ssing metho		Save as	E

If changes have been made, the "Save Sequence" button will turn red and the button  $\bigcirc$  will reload the sequence before editing.

Loaded s	sequence se 1 🔹 🕻	5	Save seque	•	Impor	t f
Lims Id	Method name	Proces	ssing metho		Save as	E

#### 3.3.3 Add / Delete / Insert / Copy and paste

To <u>add</u> an analysis (at the end of the sequence), click on in the sequence header. This will add a new row to the sequence with default information to the analysis. Complete this information with your own settings.

To <u>delete</u> an analysis, click on the red trash 🔋

To insert (before) an analysis, click on the + of the analysis before which you want to add an analysis. The

app inserts a blank line that you will need to fill in. This line is identified as invalid <sup>99</sup> because parameters are missing. Fill in the missing data to clear this message.

To <u>copy and paste</u> an analysis, left click (without releasing the mouse button) on one of the fields of the analysis to be copied, then move the mouse to the desired position and release the mouse button to insert the analysis to be copied.

Ð	Sample Id	Lims Id	Method na	me Proce	essing m	ethod	Injection	Events table	
+	Analysis	n	m1	Ŧ	m2	*	External 💌	None 🔻	\$ Î
+	Analysis	6	Name <b>Analysis</b>	Method m1	name	Vial 1	Injection External	None 🔻	\$ Î
+	Analysis	U		•	mï	•	External 💌	None	\$ Î





Note : You can move an analysis by clicking on it, then holding down the left mouse button and moving the cursor to the desired position in the sequence.

#### 3.3.4 Sample information

The sequence table has the following components:

- Name and LIMS ID
- Acquisition and processing methods: OpenLab CDS has separated the acquisition of analyses from the reprocessing of results. This translates into an acquisition module and a processing module (Data Analysis). The acquisition parameters are stored in an acquisition method (.amx extension), the integration parameters, component table, and reports are stored in the processing method (.pmx extension). These methods (amx & pmx) may have different names, they are not linked in the analysis.
- The injection source: the element of the analyser that will physically start the acquisition. If you are performing a gas analysis, the injection source will be a GSV (Sampling Valve), if the start is sent by an external device, select the "External" injection source.
- The number of the bottle (if necessary): In the case of an automatic injector (front or back), the number of the bottle to be pricked must be indicated. Simply enter the vial number, SRA Lab will take care of converting this position to an OpenLab compatible position (101 / 201).

The other settings can be accessed in a separate view by clicking on . The following view is displayed, and you can change the desired information:

- Analysis Type: Categorizes each injection into an analytical sequence according to its specific role (blank, standard, sample, or quality control), thus determining the processing and interpretation of the resulting data.
- Username: Identifies the person who performed the analysis or who is responsible for it.
- **<u>Comment</u>**: Allows you to add specific notes or observations about the sample or analysis.
- Quantity: Represents the mass or volume of the sample being analysed.
- Dilution factor: Indicates whether the sample has been diluted and by what proportion prior to analysis.
- **Volume**: Corresponds to the volume of sample injected into the chromatographic system.
- <u>Multiplying factor</u>: Used to adjust results based on specific dilutions or concentrations.
- Internal Standard Quantity: Indicates the amount of internal standard added to the sample for quantification.

### 3.4 Results

#### 3.4.1 List of analysis results

If you display the list of results (click on "Results" in the command panel), you will see the list of results available per analyser.





🧄 SRA	LAB							m   🔺   🏟   🕮   🚳   🚽	ø ×
•	🌀 sp101	× 🥌 SP503 ×							
Status				-					1
		v =+ 👩 I	1	F					∠~
ଝ	Area	Add results Update Export to LIM	S Delet	e results					Trends
		Analysis name	Method nam	e Date p	eak@0.146min	peak@0.229min	n peak@0.313min peak	opeak@0.146min opeak@0.229min opeak@0.396mir	8
	1	AE_300524-164835 - Copie (6) - Copie	m1.amx	5/30/2024 4:48:49 PM	49.056	98.109	196.098	400	>
	±	AE_300524-165438 - Copie - Copie - Copie - Copie (2)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098	7.	s.
Results	±	AE_300524-165438 - Copie - Copie - Copie (3)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098	300 rend 0	end
	±	AE_300524-165438 - Copie - Copie (3) - Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098	200 .746	r=
」 Instrument	±	AE_300524-165438 - Copie - Copie (4)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098	0.220	
selection	±	AE_300524-165438 - Copie (3) - Copie - Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098	100 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	
	±	AE_300524-165438 - Copie (5) - Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098	0	
	±	AE_300524-165438 - Copie (5)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098		
	±	AE_300524-165438 - Copie (6) - Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098	5/29/2024 5:20 PM 6/5/2024 4:	:00 PM
	±	AM_040624-170042 - Copie (2)	m1.amx	6/4/2024 5:00:53 PM	49.056	98.109	196.098	●peak@0.313min ●peak@0.479min	8
	±	AM_040624-173555 - Copie (2)	m1.amx	6/4/2024 5:36:03 PM	49.056	98.109	196.098	900	
	±	AM_050624-090735 - Copie (2)	m1.amx	6/5/2024 9:07:42 AM	49.056	98.109	196.098		
	±	AM_300524-162244 - Copie - Copie - Copie - Copie (2)	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	600 17 en c	
	±	AM_300524-162244 - Copie - Copie - Copie (3)	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	2 500 0 2 T	
	±	AM_300524-162244 - Copie - Copie (3) - Copie	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	400 3	
	±	AM_300524-162244 - Copie - Copie (4)	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	200	
	±	AM_300524-162244 - Copie (3) - Copie - Copie	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	100	
	±	AM_300524-162244 - Copie (5) - Copie	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	L	
	±	AM_300524-162244 - Copie (5)	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	5/29/2024 5:20 PM 6/5/2024 4:	.00 PM
	±	AM_300524-162244 - Copie (6) - Copie	m1.amx	5/30/2024 4:22:56 PM	49.056	98.109	196.098	⊘peak@0.396min	8
	±	AM_300524-172315 - Copie - Copie - Copie - Copie (2)	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098	460	
	±	AM_300524-172315 - Copie - Copie - Copie (3)	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098	440	
	±	AM_300524-172315 - Copie - Copie (3) - Copie	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098	420 10	
	±	AM_300524-172315 - Copie - Copie (4)	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098		
_0	±	AM_300524-172315 - Copie (3) - Copie - Copie	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098	360 90 2	
a	±	AM_300524-172315 - Copie (5) - Copie	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098	340	
4	±	AM_300524-172315 - Copie (5)	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098	320	
N N	±	AM_300524-172315 - Copie (6) - Copie	m1.amx	5/30/2024 5:23:24 PM	49.056	98.109	196.098	500,	-00 PM
S			<.				4	5/2024 4:	UU PM
		Instrument state : Rea	dy					Run state : Wait to start	

The following items are displayed in this table:

- Analysis Name: The name assigned to the analysis.
- Method Name: The name of the analytical method.
- **<u>Processing method</u>**: Defined method for calculating chromatographic data.
- **<u>Sample Name</u>**: The specific designation of the sample being tested.
- **Unidentified peaks:** An indication of the number of chromatographic peaks detected but not attributed to known compounds.
- **Internal standard quantity**: The mass or concentration of the reference substance added to the sample for quantification.
- **Volume**: The amount of sample injected into the chromatographic system.
- **<u>Channel</u>**: A sampling channel used for data acquisition.
- File Path: The location of raw data and results in the computer system.
- **<u>Comment</u>**: Additional notes on the analysis or sample.
- Lims Id: A unique identifier referencing the LIMS.
- **Dilution Factor**: A factor indicating the dilution applied to the sample prior to analysis.
- **Type of analysis**: Categorization of the injection (blank, standard, sample, QC) determining its role in the sequence.
- **Event Table**: The name of the event table.
- **<u>Vial</u>**: Number or position of the sample in the autosampler.
- **Quantity**: The mass or volume of the sample prepared for analysis.
- **Multiplier factor:** Coefficient applied to the results to adjust concentrations.
- **Calibration level**: The position of the standard in the concentration series used for the calibration curve.

For each analyser, you can update this list (if new reports are generated in the meantime) by clicking on

Update

You can also suppress the results list to display only the results you want, by clicking on







#### 3.4.2 Trends

Trend lines provide a simplified graphical representation of results. They make it possible to quickly visualize if there is a drift in the retention time, variations of peak areas, concentration, ...

To configure trends, click on Trends , the next view will be visualized:

13:46:32	2 49.056	98.109	196.098	392.046	783.606
16:46: <mark>4</mark> (	0 49.056	98.109	196.098	392.046	783.606
16:46:	Trend 0.146 / 0.229 /0.396	× Trend 0.313	3 / 0.479 🗙	Trend 0.396	
16:46:					
16:46:					
16:46:	peak@0.146min 🛽		peak@0.	229min 🙁	
16:46:					
16:46:					
16:46:	peak@0.396min 🛛				
16:46:					
16:46:					<b></b> Q,
16:46:	Nom tendance				
16:46:	Trend 0.146 / 0.2	29 /0.396			
16:46:					
	Sauveo	arder		Annuler	
	Sauvey			Annalei	

- To add a trend, click on 🔛 . Each trend is defined by a "name". -
- To add a compound to the trend, click on  $(\mathbf{P}_{+})$ , and then add the desired compound. \_
- To remove a trend, click on the red cross on the tab.

Once the trends are set correctly, click on "Save".

Note: The maximum number of trends is 4.

### 3.5 Analyses reprocessing

When an analysis is complete, OpenLab processes the raw signal to generate results and reports. You can reprocess the results in OpenLab Data Analysis. Once the results have been validated, click on the "Processing" tab, then in "Print All", select "Print Selected Injections" to generate a new csv report.





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sf133714s - Connexio 💀	on Bureau à distance													
	Here	Dec es esia e	Audio II	ĉi m					gc6890 - Data J	Analysis				
File	Home	hod Close	Update Master Method	-Sign P Link Method	ک Reprocess Selected↓		Nequantify Selected	日 Show injection log 日 Show result set log	Save Selected Results	Save All Results	Print All	View PDF •	Launch CC Editor	Create New Result Set
	Methods						Pri	ocessing			L P P	rint All		
Data Proces	sing			« P	rocessi	ng Metł	nod	▲ Info Global				rint All Injo rint Select rint Seque	ections ed Injections nce Summary	Report(s)
↓ <b>F</b> by Sequence				- <b>I</b>	General		ð	Location	(206890	(Methods /m)	1 pray			
ג Single Sample ג AA_GAZ	s -11 - AA_GAZ-11_270	120-103441.dx	]	•	Properties Signals Integration	Events Chem	Station	Description	/50000	,	2.pmx			

Once you have reprocessed to the OpenLab Data analysis side, you will be able to return to SRA Lab and click on the "Update" button.

Note: You may not be able to access the "Print All" button or print the report. It is necessary to correct any errors reported by Data Analysis, save the results, save the method.

### 3.6 Sending analyses back to LIMS

You can send the results of an analysis back to the LIMS immediately without reprocessing. In the result row, click on 1 to export the result, i.e. generate the LIMS-compatible report and drop it in the appropriate folder.

In the list of results, the scan changes status and the icon *status* appears at the top of the line. This indicates that the analysis has been reported.

🧄 SRA	LAB							
Ø	🍘 sp101	× SP503 ×						
Status	Area	→ ➡ ♣ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥ ♥	<b>Export to LIMS</b>	Delete	results			
Sequence		Analysis name	N	lethod name	Date	peak@0.146min	peak@0.229min p	eak@0.313min peak
	±	AE_300524-164835 - Copie (6) -	Copie	m1.amx	5/30/2024 4:48:49 PM	49.056	98.109	196.098
Ē	±	AE_300524-165438 - Copie - Copie - Cop	ie - Copie (2)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
Results	~	AE_300524-165438 - Copie - Copie -	Copie (3)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
	±	AE_300524-165438 - Copie - Copie (	3) - Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
ĭ≱-	±	AE_300524-165438 - Copie - Cop	ie (4)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
Instrument	~	AE_300524-165438 - Copie (3) - Cop	ie - Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
selection	±	AE_300524-165438 - Copie (5) -	Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
	~	AE_300524-165438 - Copie (	5)	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
	±	AE_300524-165438 - Copie (6) -	Copie	m1.amx	5/30/2024 4:54:45 PM	49.056	98.109	196.098
	~	AM_040624-170042 - Copie (	2)	m1.amx	6/4/2024 5:00:53 PM	49.056	98.109	196.098
	±	AM_040624-173555 - Copie (	2)	m1.amx	6/4/2024 5:36:03 PM	49.056	98.109	196.098
	±	AM_050624-090735 - Copie	2)	m1.amx	6/5/2024 9:07:42 AM	49.056	98.109	196.098

In SRA Lab, in the "Results" tab, click on "Add Results" to select the new csv file. The new csv file has the same name as the original file, but it is incremented (\_0001 or 2 etc...)





sra 🚺	LAB							
Ø	🍘 sp101	×	🥌 SP503 🚿	×				
Status		~	_=+		6	1		ĪF
ন্থ	Area		Add res	sults	Update	Export to LIMS	S Delet	te re
Sequence				Ana	lysis name		Method nam	e
	<u>±</u>		AE_3005	24-164	835 - Copie (6) -	Copie	m1.amx	5,
	±	A	_300524-1654	38 - Co	pie - Copie - Co	pie - Copie (2)	m1.amx	5,
Results	<u>±</u>		AE_300524-1	65438	- Copie - Copie	- Copie (3)	m1.amx	5,
بال	<u>±</u>		AE_300524-1	65438	- Copie - Copie	(3) - Copie	m1.amx	5,
Ì\$ <mark>⊱</mark>	<u>±</u>		AE_3005	24-165	438 - Copie - Co	pie (4)	m1.amx	5,
selection	<u>±</u>		AE_300524-1	65438	- Copie (3) - Cop	pie - Copie	m1.amx	5,
	<u>±</u>		AE_3005	24-165	438 - Copie (5) -	Copie	m1.amx	5,

Select the file and click Open. The new results will be displayed in the updated results view. Then you can click on "Export to LIMS" to send the data to the LIMS.

				0	)uvrir Anı	nuler
mo	lu fichier : AA_GAZ-11_230420-110816_1_0001.csv	/	~	All file	es (*.*)	~
1	<					>
1	AA_GAZ-11_230420-110816_1.csv	23/04/2020 11:17	Fichier CSV Micro	2 Ko	23/04/2020 11:17	
L	🖬 AA_GAZ-02_230420-111722_1.csv	23/04/2020 11:26	Fichier CSV Micro	2 Ko	23/04/2020 11:26	
L	AA_GAZ-25_230420-112626_1.csv	23/04/2020 11:28	Fichier CSV Micro	2 Ko	23/04/2020 11:28	
L	AA_GAZ-11_230420-110816_1_0001.csv	13/04/2020 11:28	Fichier CSV Micro	2 Ko	23/04/2020 11:28	
	AA_GAZ-11_230420-112830_1.csv	23/04/2020 11:37	Fichier CSV Micro	2 Ko	23/04/2020 11:37	

### 3.7 Maintenance

#### 3.7.1 About us

The "About" menu provides information about the software.

To access this menu, please click on the "About" button:



A window similar to the following should appear:







Here are the available fields:

- Software Version
- Release date
- Commit
- Indication of license type: Permanent version or trial version
- The options:
  - Limit of use:
    - Number of instruments
    - Number of AIC
  - Mode of communication:
    - Client/Server
    - Workstation
  - Transmission:
    - Modbus
    - Lims
    - Analog output (coming soon)
  - $\circ$  Calculations:
    - Natural Gas Calculation (ISO 6976) (coming soon)
    - LPG calculation (ISO 8973) (coming soon)
    - Combustion calculations (coming soon)
  - Other:
    - MassHunter Coupling (coming soon)
    - Using Valco Vici Valves

#### 3.7.2 Failover mode

In "Client/Server" mode, the link between client workstations, AICs and the OpenLab server is permanent. To launch analyses or reprocess results, OpenLab must communicate with the OpenLab server. If this link is interrupted, the CDS can no longer operate normally in Client/Server mode. In this case, OpenLab CDS becomes unstable and closes (after a fairly long time) on client workstations and AICs.

Users must work directly on the AICs for the new analyses (Client workstations are no longer usable until the link with the server is re-established). Users must restart the OpenLab CDS Control Panel. A message





indicates whether they wish to switch to Failover mode: answer YES. Then start SRA Lab. Application initialization takes a longer time.

	gc6890 - (	Control Panel ? – 🗆	×			
Edit Delete Refresh Instrument Instrument All Instruments and Locations	Lock Create Configure Create Configure Create Configure Conner C	→     →       ose ection     Copy to Clipboard       Selected Row				
Instruments «	gc6890	Not Connected				
<ul> <li>▲ ⊕ Instruments</li> <li>▲ Ջ Controle</li> </ul>	Start Instrument					
🗖 gc6890	Project: gc6890	1 Launch & Launch Offline				
🙎 Recherche	▹ Status ▲ Details		î			
	Description:					
	Location:	Controle				
	Created by:					
	Creation date:	2020-06-01 09:33:26+02:00				
	Last configured by:	OlAdmin				
	Last configuration date/time:	2020-06-01 09:08:12+02:00				
Instruments	Last modified by:					
Projects	Last modified date/time:	2020-06-01 09:33:26+02:00				
Administration	Application:	OpenLab CDS	*			
Current user: SYSTEM		Failover mode	Ready			

The user must start OpenLab in Failover mode to launch new analyses and launch SRA Lab on AICs. When SRA Lab detects that OpenLab CDS is in Failover mode, it also switches to Failover mode (the initialization process is longer than in "Client/Server" mode). This mode works with OpenLab CDS locally, with a copy of the instrument methods managed by the AIC. The link with LIMS is maintained and csv files are always available.

SRA 🚺	LAB										m   2	•   \$		•	-	
o	🥌 sp101	C SP503														
Status	Start							Lo	aded s	sequence 🔻	Save as	Imp	ort from	m Lims	c	ilear table
Sequence			Ð	Sample Id	Lims Id	Method n	ame	Processing me	thod	Injection	Events t	able				
			+	PCP503	1583611	m1	Ŧ	m1	Ŧ	External 🔻	Event 1 🔕 🗸	0	\$	Î		
Results			+	PCP603	1583620	m1	•	m1	*	External 🔻	None	*	\$	•		
₹ĭ			+	PCP503	1583611	m1	Ŧ	m1	*	External	None	*	\$	•		
selection			+	PCP603	1583620	m1	Ŧ	m1	*	External 🖣	None	Ŧ	\$	•		
			+	PCP503	1583611	m1	*	m1	*	External	Events 2 🔕	•	\$	Î		
			+	PCP603	1583620	m1	*	m1	*	External 🔻	None	Ŧ	¢	1		
			+	PCP503	1583611	m1	*	m1	*	External	None	*	\$	•		
			+	PCP603	1583620	m1	*	m1	*	External	None	*	\$	•		
ab			+	PCP503	1583611	m1	*	m1	*	External	None	*	\$	Î		
A L			+	PCP603	1583620	m1	*	m1	*	External	None	*	\$	1		
SR																
			Inst	rument state	: Ready						Run stat	te : Wait	to start			Fail-over

Note: if the cause of the loss of connection with the OpenLab server is hardware, it is preferable to define the csv report folder elsewhere than on the OpenLab server.

As soon as the link with the OpenLab server is re-established, follow the procedure for transferring results to DataStore, then close OpenLab and SRA Lab on the AICs and work again on the client workstations.





#### 3.7.3 Logs

💷 in the SRA Lab completes a log file if an error is reported. This log file can be accessed by clicking on top right-hand corner of SRA Lab.

You can save a copy of the file and send it to our support team at service@sra-instruments.com to open a ticket (describing the problems encountered).

By default, the SRA Lab log file is called error.log. If you have activated the "Replace file name with username" option in SRA Lab configuration, SRA Lab (i.e. on the client side) will create a log file for each user connected to SRA Lab. If an error is detected in the SRALAB client, the user's log file will be completed.

AICs also generate logs. These are stored in the AICLogs folder defined in SRA Lab. Each log generated by the AICs bears the name of the AIC and the .log extension. If an error is detected in the SIC service, a record is added to the AIC log.

The SIC service also records the status of Openlab CDS services on the AIC in the file « AIC\_Name.diagnostic » (also in the log folder).





## 4. Appendix I: Analysis report template

SRA Lab uses the csv reports generated by OpenLab CDS to display the results of an analysis. For each analyser, the "Prochem.rdl" report template must be deposited in the DataStore "Report Template" repository.

The processing methods are configured to generate a csv report that follows the "prochem.rdl" template.

Processing Method							
m1 o <sup>o</sup>	General Scaling						
▲ General	+ Add Report	Report #1	2				
Properties	✓ Report #1	Report #1					
Signals		Report template	prochem.rdl		•		
Integration Events ChemStation	Report #2						
Standard		Report selected signals	All signals		•		
Advanced							
Manual Integration							
Compounds		Report for sample types	All sample types		•		
Identification							
Calibration		Report destination	None None	Printer	🔽 File 💙		
<ul> <li>System Suitability</li> </ul>			4				
Properties		Report file name	<dx></dx>		>		
Column			Example: demo file	name			
A Reports							
Injection Report		Eile fermat				Event werkbeek (* view)	
Tools		rifeformat					
Custom Calculation			Word document	(*.docx)		Plain text (*.txt)	
Post Processing Plugins		5	CSV (Comma del	imited) (*.csv)	6		
		Copy report to folder	○ None	) Storage	Windows file s	ystem 🚺	
		Destination folder	C:\CDSProjects\OLC	DSReports\ <i></i>	>		
			Example: C:\CDSProj Instrument	ects\OLCDSReports\Demo			

- 1. Click on "Injection report"
- 2. Select the template "prochem.rdl"
- 3. Check the "File" box
- 4. Select "DX" so that the csv file has the "Data filename"
- 5. Check the "CSV" box
- 6. Check « Windows File System »
- 7. Enter the name of the folder that will receive the csv files (don't forget to put the <I> field to have one folder per analyser)

#### Note:

<sup>(1)</sup> The reports directory is the folder you specified in the SRA Lab configuration:



<sup>(2)</sup> It is essential that the OpenLab account has "Save report to disk" privileges for the csv report to be saved in the specified folder. Without this "privilege", OpenLab will not deposit the csv file and this absence will not be notified in any log file.

<sup>(3)</sup> In Client/Server architecture, OpenLab CDS saves analyses directly (in its "DataStore" content manager, which is a database manager). The files are visible only on the DataStore web page, with the analyses accessible in OpenLab Data Analysis.





This model is created when installing SRA Lab, but it can be recreated in the "Intelligent Report" editor in DataAnalysis.

Cm Content Management » Conter 🗙	+	
(←) → ♂ @	0 🔏 🖬 s	<pre>srvcds/datastore/page/#filter=path %2Fgc6890%2FReport%2520Templates </pre>
📕 Office 365 \land OneDrive \land Redm	ine 🖨 Jira 🖨 S	AV AXONE 🌐 3CX HV 🌐 3CX Admin 💿 Synology 🔟 Ingram 🔟 Ingram Clo
CM Content Brows	er	
▼ Files	Select 🔻	+ Create • 1 Upload Selected Items •
I'm Editing	💼 Conte	nt > 🚞 gc6890 > 🚞 Report Templates
My Favorites  Repository		Acquisition_Method_Report_Letter.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:04 GMT+0100 99 KB
Content Archive		Acquisition_Method_Report.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:35 GMT+0100 99 KB
Demo gc6890 Methods		Audit_Trails_Report_Letter.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:05 GMT+0100 166 KB
Report Template;		Audit_Trails_Report.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:35 GMT+0100 166 KB
<ul> <li>Sequence Templates</li> <li>Sequences</li> </ul>		Calibration_Letter.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:05 GMT+0100 267 KB
GCMS177		Calibration.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:36 GMT+0100 267 KB
🖿 proj 🖿 virtualCtrl		ExtendedPerformance_Letter.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:06 GMT+0100 254 KB
		ExtendedPerformance.rdl Uploaded by Labo (Labo) on Fri 13 Mar 2020 10:53:37 GMT+0100 254 KB

In addition, the user's OpenLab CDS account configured in SRA Lab and used to log in to the CDS must have the "Save Reports to Disk" right. Assign this right to the "Chemist" role so that it can be used by all users with this role.

This "right" allows the OpenLab account to create and save reports outside of DataStore (on a disk, a network drive, etc.). Without this right, no csv report will be generated, and no logs will be filled.













## 5. Appendix II: DataStore

In "Client/Server" configuration, OpenLab CDS stores all data in its DataStore Enterprise Content Management (ECM). This one is installed during "Client/Server" installation and can be located on the OpenLab CDS server. DataStore uses a TOMCAT server (Alfrescot Tomcat) for data management (methods, analysis, configuration, reports, templates etc.). All data is automatically stored in DataStore and accessible in OpenLab CDS. No files can be accessed directly from the Windows Manager, but they can be accessed from the DataStore Web interface.

In the following example, DataStore is installed on the srvcds server. To display the Data Store web page, enter the following address: srvcds/datastore/page/



As a login, use an OpenLab account with DataStore access rights.

From DataStore, you can upload or archive files. To deposit files, you need an FTP client. For more details on how to use DataStore, please consult the DataStore user manual.







## 6. Appendix III: Report definition

To create a results report, SRA Lab uses the CSV report that OpenLab CDS can generate from a template (rdl extension). This template must be defined as follows and named prochem.rdl:

Instrument Name	sp102
Injection Data File Directory	/sp102/Results/AA_GAZ_11_150620-120850.sirrslt
Injection Data File Name	AA_GAZ_11_150620-120850.dx
Injection Acquired Date	2020-06-15 12 :10 :12+02:00
Injection Acq Method Name	m1.amx
Sample Name	AA_GAZ-11
Sample Lims IDs	976048
Sample Vial Number	101
Sample Description	\$m1/1\$Labo\$ISTD\$976048
Sample Amount	1.000
Injection DA Internal Standard Amounts	ISTD-1=2
Sample Dilution Factors	1 ;1 ;1 ;1
Sample Multipliers	1 ;1 ;1 ;1
Injection Volume	1.000
Sample Type	Sample
Sample Calibration Level	
Sample Acq Injection Source Info	Front

#### Signal : TST1A

Compound type	Group	Channel	Name	RT	Exp RT	Area	Concentration	Concentration Unit	Norm Concentration
1		TST1A	Peak1	0.250	0.250	989.669	20.003	%	15.625
1		TST1A	Majoritaire*	2.250	2.250	98.953	2.000	%	
1	Legers	TST1A	Leger1	5.250	5.250	98.953	2.000	%	1.562
3		TST1A	Inconnus	6.750	6.750	98.953	22.003	%	17.187

#### Table continued

Height	Compound Is Internal Standard	Compound Amount Unit	Concentration ppm
123.33	False		
12.333 12.333	False False		
12.333	False		

This template must be placed in the instruments' Report Template folder.

In the example below, we see the prochem.rdl file in the Report Templates folder of the gc6890 instrument in the DataStore web interface.







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💠 Tableau SL - Tableau Agile - Jira 🗙	Cu Content Management » Conte: X +
$\overleftarrow{\leftarrow}$ $\rightarrow$ $\overleftarrow{C}$	👽 🖋 srvcds2/datastore/page/ filter=path %2Fgc6890%2FReport%2520Templates &page=1
CM Content Brows	er
▼ Files	Select • + Create • 1 Upload Selected Items •
I'm Editing	Content > 💼 gc6890 > 💼 Report Templates
My Favorites	prochem.rdl
Repository	Uploaded by OlAdmin (OlAdmin) on Mon 15 Jun 2020 15:58:39 GMT+0200 190 KB
🗎 Content	1-1of1 << 1 >>
Archive	
🖿 gc6890	
Methods	
Report Templates	
Results	
Sequence Templates	
Sequences	





